基于天然精油分离气味分子的香氛创作

Fragrance creation based on the isolation of odor molecules from natural essential oils

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Yunnan enjoys the reputation of “plant kingdom”, “medicine kingdom”, “natural gardens”, “hometown of fragrance” and “tourism kingdom”. It has over 400 known natural fragrance, ranking first in China in terms of quantity. The fragrant plant species are diverse, widely distributed and have many unique varieties. The abundance of natural fragrance resources is also extremely rare in the world.













Our Team

Brief Introduction

Established in 2012

We are contemporary alchemists, we extract 'liquid gold' from plants - natural fragrances (or essential oils). Our plants come from mountains, plains, and the earth, behind us are fragrance farmers composed of families. We are passionate about this and enjoy in it. All of what we do can give hope to mountain farmers, give us a sense of achievement simultaneously, and also in favour of you the quality natural fragrances.

久逾12年来，作为云南天然香料研究的尖兵，尹开云和他的团队始终坚持从遍布全省的香料种植园中，选取有特色的天然植物，作为开发天然香氛的原料。云南是全球众多香料种植区域中最具有特色和物种最为丰富的地区。

For a long time in over 12 years, as a vanguard in the field of natural fragrance research in Yunnan, Kaiyun Yin and his team have always insisted on selecting unique natural plants from fragrance plantations throughout the province as raw materials for developing natural fragrance. Yunnan is the most distinctive and diverse region among many fragrance planting areas in the world.

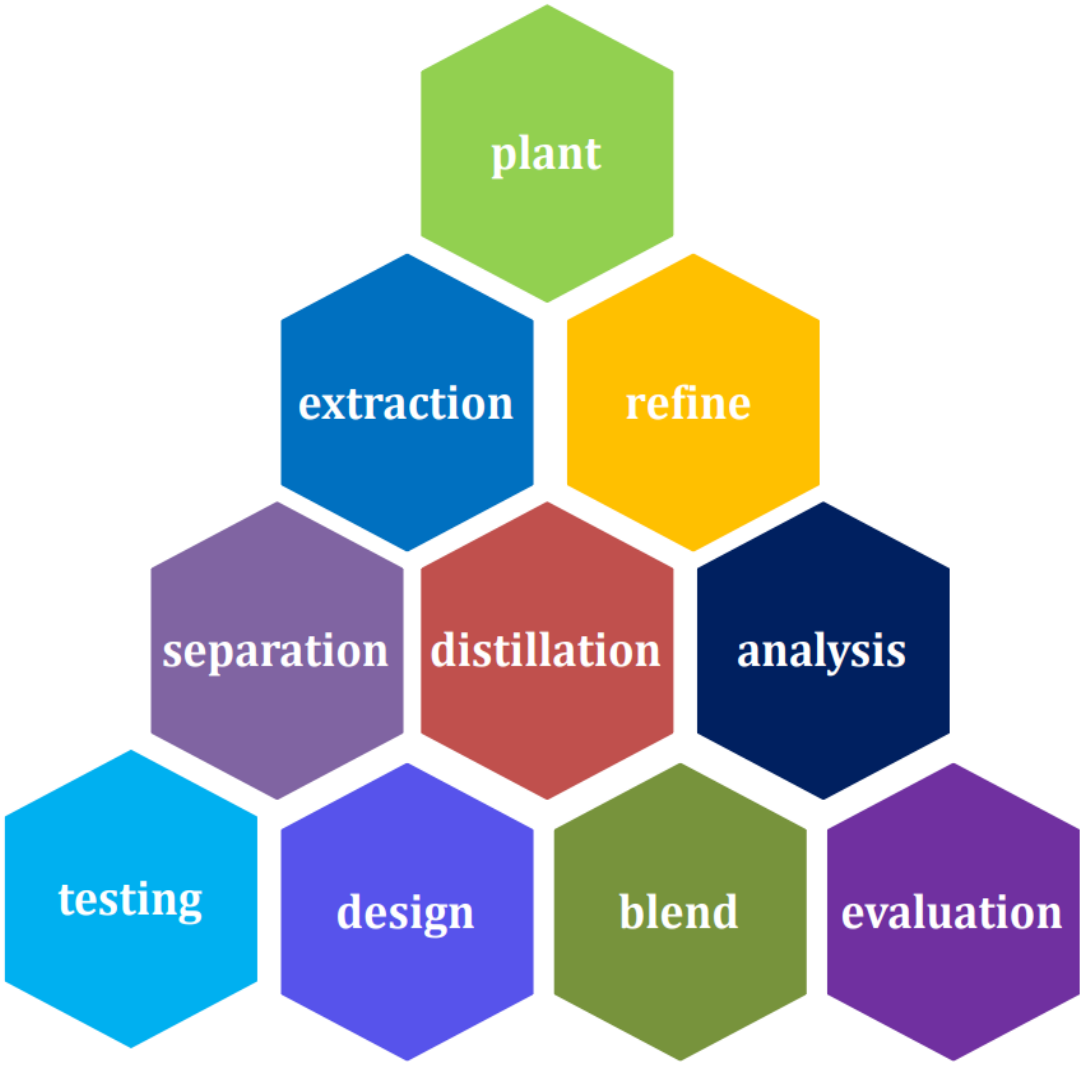
homo sapiens vs primitive machines



Our Work

What can we do?

We do everything related to natural fragrance. We focus on botany, chemistry, biology, art, product incubation and brand communication. In the field of natural fragrances, we engage in the cultivation, harvesting, distillation, and purification of fragrance plants. Our fragrance are widely used in food, medicine, health products, cosmetics, and other industrial products. We research and developing aromatic plants, designing products formulas, analyzing and testing all these products, providing technical support and services to numerous clients, conducting scientific and technological training, and promoting your brands.



Our Work

What have we done?

We have supported a large number of brands in the past twelve years.

云南白药 YUNNAN BAIYAO

SMOORE 思摩尔

HANGSEN

真味生物 ZINWI BIO-TECH

MUJI 無印良品

广汽集团 GAC GROUP

红塔集团 HONGTA GROUP

红云红河集团 HONGYUNHONGHE GROUP

Our Work

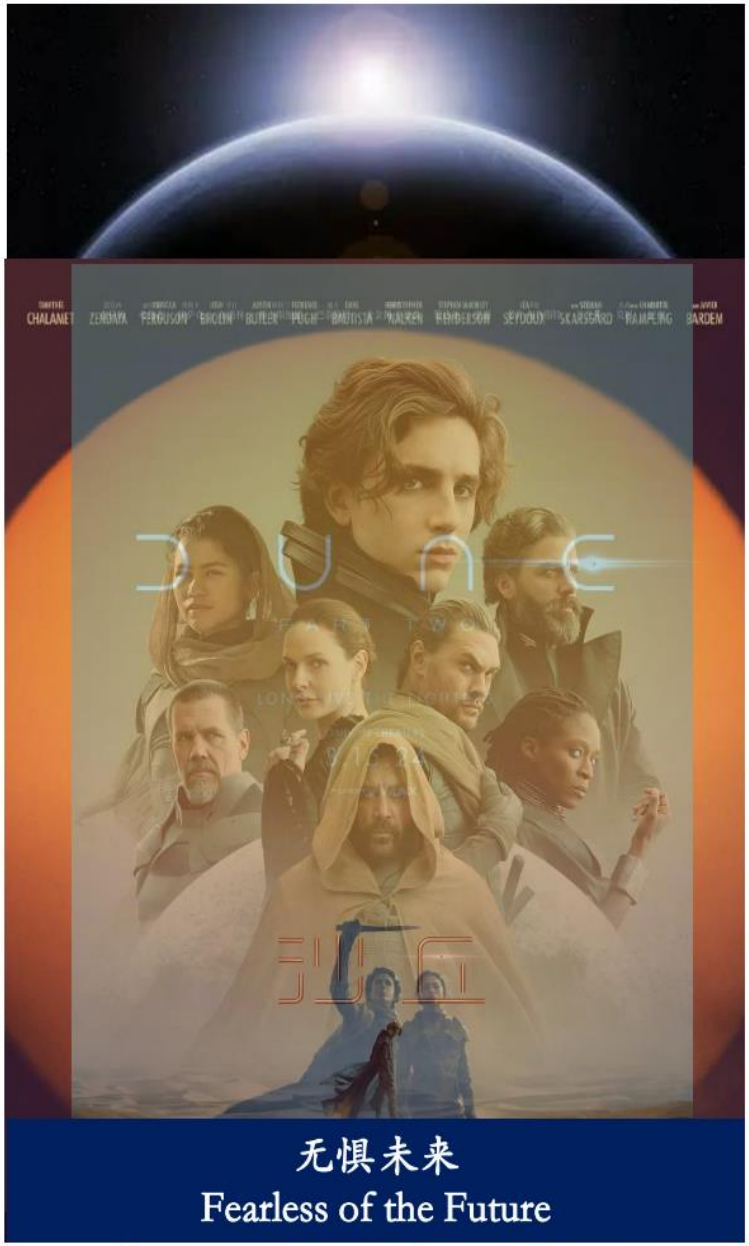
What are we going to do?

Our journey is the stars and the sea of fragrance empire.

我们的征程是香料帝国的星辰大海！



In 2021, the global perfume market will reach 46.5 billion US dollars, and the retail sales of China's perfume market will reach 10.9 billion yuan, which is expected to reach 30 billion yuan by 2025.



Theory

Philosophical thinking on fragrance

Principles:

1. Less is more.

Our purpose of this trip is to assist perfumers in performing mathematical subtraction.

2. Find the right fragrance.

We must put quality before quantity; we should rather go without than have something shoddy.

3. Use quality fragrance boldly.

Quantitative changes induce qualitative changes, boldly using good ingredients will bring unexpected effects.

4. Learn to wait.

All good things are friends of time. Trust your intuition, learn to wait, and wait for miracles to happen.

5. Ameliorate cognition and self-reflection.

Ignorance and blind confidence not only fail to make good products, but also ruin an excellent perfumer. Self reflection real-time, learning and inspiring, as well as ameliorate cognition, are very necessary.





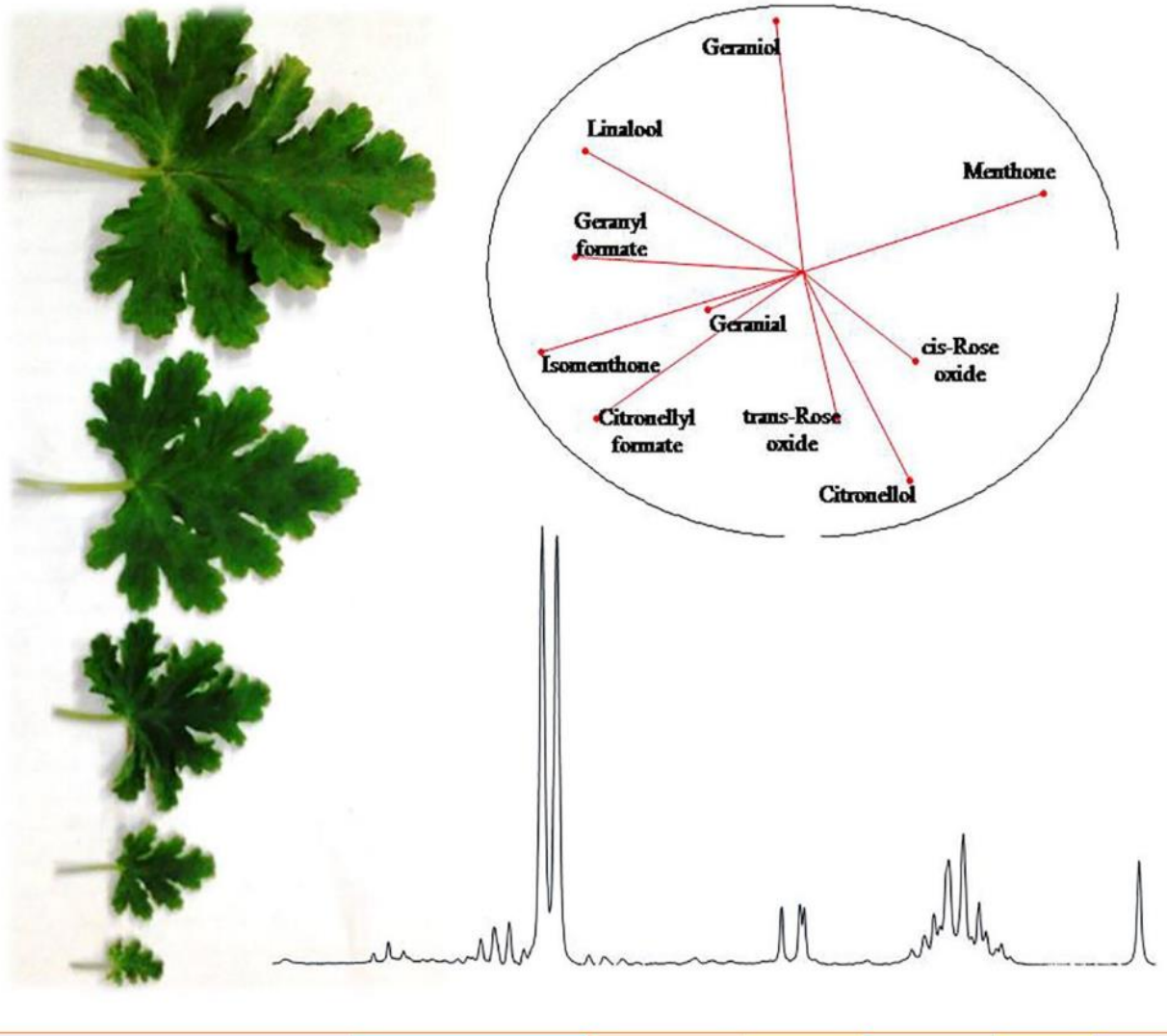




Methodology

Isolation method of geranium oil

It is important to studying the chemical composition of essential oil before starting isolation the odor molecules from it. An image to illustrating the main components of geranium oil. A set of data of GC-MS analysis of the geranium essential oil, prepared by hydro-distillation from *Pelargonium graveolens*, showed the presence of iso-menthone (15.71%), *epi-α*-cadinol (15.49%), *iso*-menthol (6.46%), geranyl formate (6.22%), geraniol (6.16%) and citronellol (5.53%)[7] .



Implementation Method

Isolation by molecular distillation

Fractional Distilation



Geranium Essential Oil
香叶天竺葵精油
Pelargonium graveolens

Primary Distillation 一级分馏

- Fragrant Segment 1 芳香片段1
- Fragrant Segment 2 芳香片段2
- Fragrant Segment 3 芳香片段3

Secondary Distillation 二级分馏

- Keynotes 11
- Keynotes 12
- Keynotes 13
- Keynotes 21
- Keynotes 22
- Keynotes 23
- Keynotes 31
- Keynotes 32
- Keynotes 33

Third Distillation 三级分馏

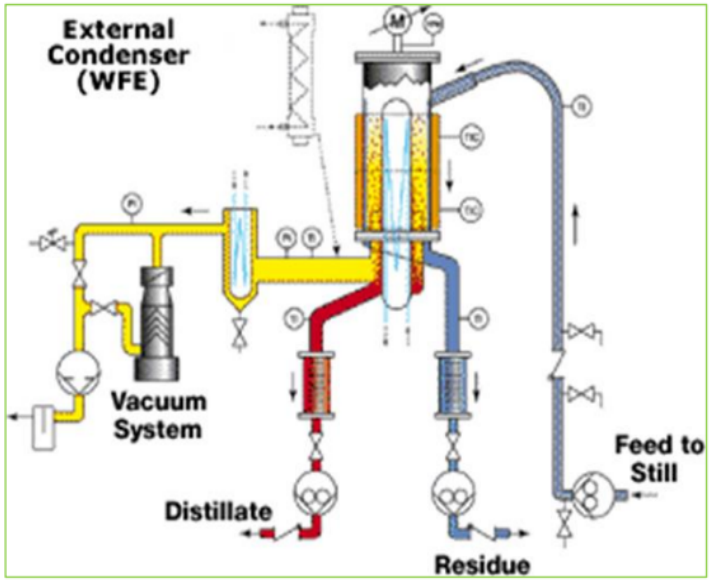
Keynotes 111, Keynotes 112, Keynotes 113, Keynotes 121, Keynotes 122, Keynotes 123, Keynotes 131, Keynotes 132, Keynotes 133, Keynotes 211, Keynotes 212, Keynotes 213, Keynotes 221, Keynotes 222, Keynotes 223, Keynotes 231, Keynotes 232, Keynotes 233, Keynotes 331, Keynotes 332, Keynotes 333, Keynotes 321, Keynotes 322, Keynotes 323, Keynotes 331, Keynotes 332, Keynotes 333

Note: The geranium oil is separated into three fragrant segments at the first(or primary) distillation, nine fragrant segments at the second distillation, and 27 fragrant segments after the third distillation. Theoretically, we can cut it *n* times to obtain n^3 fragments.

Technologies

Process and Equipment Parameters

蒸发器主体(main equipment/evaporator)：
蒸发器材质(Evaporator material)：S304
蒸发面积(Evaporator area)：0.05 m^2
内置冷凝器材质(material of built-in condenser)：S304
冷凝面积(Condensation area)：0.1 m^2
冷却介质(Cooling medium)：实验室自来水(tap-water)
加热形式(Heating form)：导热油(Thermal oil)
处理量(Processing capacity)（单位：KG/h）：5～10
真空度(Vacuum degree)（单位：Pa）：≤500（空载绝压）
轮式刮膜(Wheel scraping film)：聚四氟乙烯(teflon)
真空机组(Vacuum unit)：
罗茨旋片真空机组(Rotary vane Roots vacuum pump)
极限真空(Ultimate Pressure)20Pa
前级泵(the booster pump)：二级旋片真空泵
抽气速率(Pumping speed)：5L/S
电机功率(Motor power)：1.5KW
型号(Type)：2X-15
主泵(Main pump)：罗茨真空泵(Roots vacuum pump)
抽气速率(Pumping speed)：20L/S
功率(Power)：2.2KW

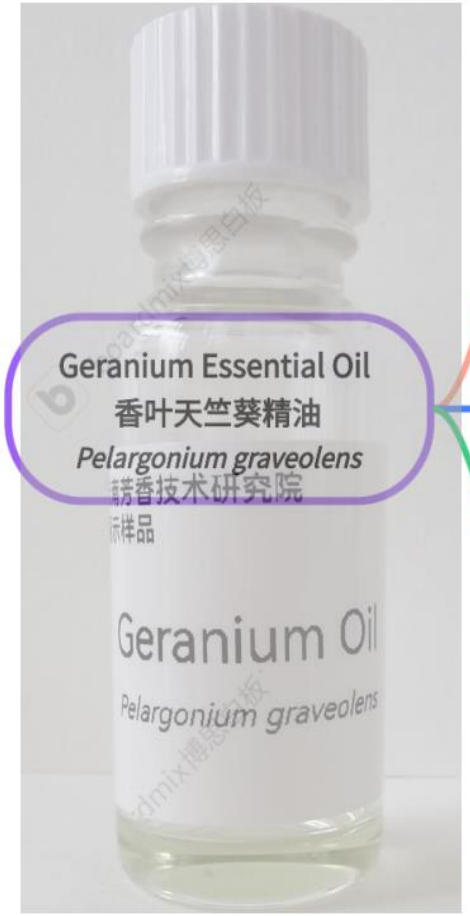


The basic working process of molecular distillation: The feed liquid enters the distiller under vacuum, and is rapidly unfolded into a thin film on the inner wall by the rotation of the scraper. It moves downward and fully contacts the evaporation surface. The heating wall (orange red part) and high vacuum (yellow part) drive the more volatile components (distillate) to gather on the surface of the built-in condenser at a close distance, while the non-volatile components (residue) continue to move downward along the inner wall of the distillation column and are collected. The separated distillate flows out through a separate discharge port.

Experiments

Isolation by molecular distillation

Fractional Distilation

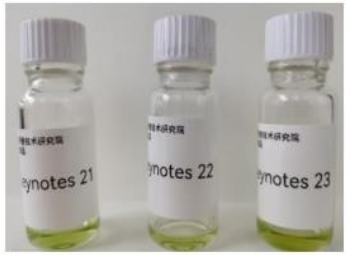


Primary Distillation
一级分馏

Secondary Distillation
二级分馏

- Fragrant Segment 1 芳香片段1
  - Keynotes 11
  - Keynotes 12
  - Keynotes 13
- Fragrant Segment 2 芳香片段2
  - Keynotes 21
  - Keynotes 22
  - Keynotes 23
- Fragrant Segment 3 芳香片段3
  - Keynotes 31
  - Keynotes 32
  - Keynotes 33





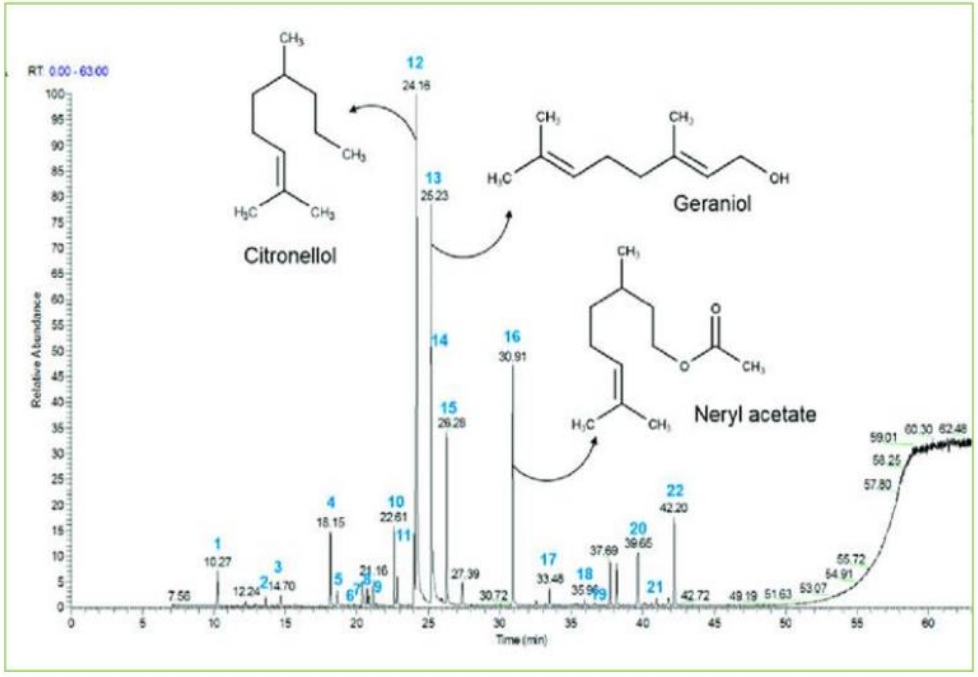


Testing & Verification

Chemical Components Analysis

GC-MS Analysis Data

Gas chromatography-mass spectrometry: glass capillary column (30m × 0.25mm × 0.25 μ m) with a pre column pressure of 68.95kPa; Program heating conditions: The initial temperature is 180 ℃ and kept constant for 2 minutes, then raised to 230 ℃ at a rate of 20 ℃/min and kept constant for 2 minutes, and then raised to 270 ℃ at a rate of 25 ℃/min and kept constant for 15 minutes; Injection port temperature: 280 ℃; Carrier gas: high-purity helium gas with a pre column pressure of 71kPa and a flow rate of 1mL/min, with a split ratio of 50:1; Interface temperature: 280 ℃; Ionization method: EI; Electron energy: 70eV ion source temperature 230 ℃ quadrupole temperature 150 ℃; Tuning method: standard tuning; Quality scanning method: SCAN; Solvent delay: 3 minutes; Scanning range: 10-550 amu; Electron multiplier voltage: 1635V. Micro sampler: 5 μ L; Injection volume: 4 μ L.



TESTING REPORT 测试报告

NAME:GERANIUM OIL(*Pelargonium graveolens*) 香叶天竺葵精油
CODE:T005#
BATCH:2022/1
DATE:2022/12/20
TESTED BY:AROMATIQUE INSTITUTE OF YUNNAN

检测样品名称 Test ample	中文名称：香叶天竺葵精油 英文名称：GERANIUM ESSENTIAL OIL 植物学名：Pelargonium graveolens L'Herit.
产地 Origin	YUNNAN 云南
蒸馏年份 Distillation Year	2022
生产工艺 Production Technology	Hydro-distillation, molecular distillation水蒸气蒸馏-分子蒸馏
产品编号 Code of Products	T005#
外观 Appearance	浅绿色透明液体 Light green colour transparent clear liquid
香气描述 Description	似玫瑰甜香 Characteristic aroma & sweet of rose flower
FEMA号	2508
CAS 登录号	8000-46-2
INCI Name	Pelargonium Graveolens Steam Leaf Oil
国际化妆品原料名称	
EINECS 登录号	290-140-0
理化指标PHYSICO-CHEMICAL PROPERTIES	
密度 Density(d20/20)	0.8870 g/mL at 25 °C
折光指数 Refractive Index n20/D	n20/D 1.4630
旋光度(20℃) Optical Rotation	aD25 -11°
酸值 Acid Value	<10
挥发成分含量 Volatiles Content	99.9
沸点 Boiling Point	197 °C
闪点 Flash Point	64 °C
乙醇中的溶混度（25℃）	1体积试样溶于20体积95%乙醇溶于中
CONTENT OF MAIN COMPOUNDS (BY GC-MS) 气相色谱检测主要成分	
	香叶醇、香茅醇、芳樟醇、异薄荷酮、薄荷酮、甲酸香叶酯、甲酸香茅酯、橙花醇、香叶醛、丁香酚、异戊醇等。Geraniol, citronellol, linalool, isomenthone, menthone, geranyl formate, citronell formate, nerol, geranyl aldehyde, eugenol, isoamyl alcohol, etc.
货架期及保存条件 Shelf & Storage	在干燥和阴凉的储存条件下，24个月。 Dark,Dry,Cool,24Months.
安全法规 Legislation & Law	遵守英国ISCSH，符合美国FDA-GRAS(一般认为安全的标准)及欧盟EEC(JECFA)食品添加剂法规。GB 2760—96规定为允许使用的食用香料。
免责申明 Disclaimer	

Testing & Verification

GERANIUM ESSENTIAL OIL

Chemical Components Analysis

The open published papers show geranium (Pelargonium graveolens)have seventy-nine components representing 95.1% of the total oil were identified [1]. Other papers show that thirty compounds accounting for 99.1% of the oil were identified[2] [3] [4] [5] [6]. The main components identified were citronellol (33.6%), geraniol(26.8%), linalool(10.5%), citronellyl formate (9.7%) and *p*-menthone (6.0%). In this discussion, we only listed 15 main representative components.

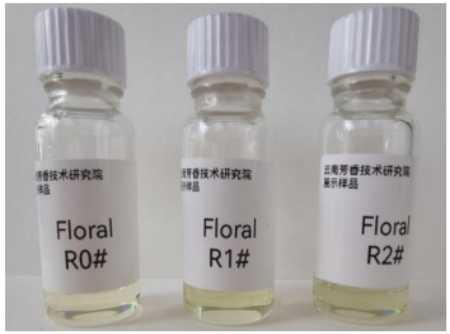
ITEM 项目	KEY CONSTITUENTS 主要成分	CAS 化学文摘编号	CONTENT (%) 含量	FORMULA 分子式	MOLECULAR WEIGHT 分子量	BOILING POINT 沸点
1	d-CITRONELLOL d-香茅醇/香草醇 l-CITRONELLOL(RHODINOL) l-香茅醇（玫瑰醇）	106-22-9	29.5	$C_{10}H_{20}O$	156.27	225℃
2	GERANIOL香叶醇（*trans-*） NEROL橙花醇*(cis-)*	106-24-1	13.2	$C_{10}H_{18}O$	154.25	229-230℃
3	CITRONELLYL FORMATE 甲酸香茅酯	105-85-1	12.6	$C_{11}H_{20}O_2$	184.28	235℃
4	LINALOOL芳樟醇	78-70-6	3.1	$C_{10}H_{18}O$	154.25	194-197℃
5	ISOMENTHONE异薄荷酮	491-07-6	7.1	$C_{10}H_{18}O$	154.25	217.64℃
6	GUAIADIENE古芸烯	489-40-7	6.3	$C_{15}H_{24}$	204.35	76-77℃
7	GERANYL FORMATE 甲酸香叶酯	105-86-2	4.5	$C_{11}H_{18}O_2$	182.26	216℃
8	GERANYL TIGLATE 惕各酸香叶酯	7785-33-3	1.5	$C_{15}H_{24}O_2$	236.35	149-151℃
9	β-CARYOPHYLLENE β-石竹烯	87-44-5	1.1	$C_{15}H_{24}$	204.35	129-130℃
10	GERANYL PROPIONATE 丙酸香叶酯	105-90-8	1.1	$C_{13}H_{22}O_2$	210.31	252℃
11	GERANYL BUTYRATE 丁酸香叶酯	106-29-6	1.0	$C_{14}H_{24}O_2$	224.34	151-153℃
12	cis-ROSE OXIDE 左旋玫瑰醚	3033-23-6	0.92	$C_{10}H_{18}O$	154.25	196.7℃
13	Alpha-PINENE α-蒎烯	80-56-8	0.75	$C_{10}H_{16}$	136.23	155-156℃
14	CITRONELLYL ACETATE乙酸香茅酯	150-84-5	0.4	$C_{12}H_{22}O_2$	198.30	240℃
15	GERANIUM ACETATE 乙酸香叶酯	105-87-3	0.21	$C_{12}H_{20}O_2$	196.29	138℃

Testing & Verification

FRAGRANCE CREATION 香氛创作配方演示

Recipe Verification of Keynotes

Demonstration Formula 0808# (part of floral)



	English Name	Chinese Name	R0#(%)	R1#(%)	R2#(%)	Remarks
Floral	Acalea Tt	甲位戊基桂醛TT	1.20	1.20	1.20	
	Benzyl Acetate	乙酸苄酯	4.30	4.30	4.30	
	Citronellol Coeur	香草醇 优级	0.70	-	-	replacement
	Geranium Keynotes 22	香叶油分离香气片段Keynotes 22	-	0.70	-	
	Citronellyl Acetate	乙酸香草酯	2.30	-	-	replacement
	Geranium Keynotes 32	香叶油分离香气片段Keynotes 32	-	2.30	-	
	Floralozone	清风醛	0.20	0.20	0.20	
	Geraniol Coeur	香叶醇 优级	3.60	-	-	replacement
	Geranium Keynotes 23	香叶油分离香气片段Keynotes 23	-	3.60	-	
	Hexyl Cinnamic Aldehyde	甲位己基桂醛	8.00	8.00	8.00	
	Kharismal®	高顺式二氢茉莉酮酸甲酯	5.00	5.00	5.00	
	Peomosa	邻甲基苯乙醇	4.70	4.70	4.70	
	Phenyl Ethyl Alcohol	苯乙醇	0.10	0.10	0.10	
	Rosetone	玫瑰酮	0.30	0.30	0.30	
	Geranium Oil Chinese	香叶天竺葵精油（云南）	-	-	6.6	replacement

Testing & Verification

FRAGRANCE CREATION 样品品鉴与评估

Appreciation and Evaluation

We choose the floral-block of a perfume formula for teaching to verify whether this geranium keynotes is more advantageous than synthetic compounds or direct use of geranium essential oil.

Items	Ranking of Aroma	Cost	General Description
Sample R0#	No.2	Low	This is an ordinary floral building of flavoring, a classic and old formula. All raw materials are chemically synthesized, and the cost is very low.
Sample R1#	No.1	High (acceptable)	We replaced the three main floral ingredients in Formula R0 # with aroma fragments separated from geranium oil, namely replacing Citronello Coeur with Geranium Keynotes 22, replacing Citronelly Acetate with Geranium Keynotes 32, and replacing Geraniol Coeur with Geranium Keynotes 23. This floral building of flavoring has a natural and harmonious floral note and sense of beauty, and its aroma quality has been greatly improved.
Sample R2#	No.3	Medium	We replaced all three important ingredients(Citronello Coeur , Citronelly Acetate, Geraniol Coeur) in formula R0# with geranium oil, and obtained formula R2#, this floral building of flavoring has a strong smell of geranium oil. The harmony and balance of this flavor have been destroyed.

Discussion

1. Molecular distillation is a powerful and effective technique, which support us to cut(or separate) an essential oil *n* times to obtain novel fragrant segments abundantly. Actually, the amount of new products we can obtain can be calculated by a mathematical formula:

Σ (total fragrant segments）$=3^1+3^2+3^3+\cdots+3^n$

(Example: 3+9+27=39, We acquired 39 fragrant segments after 3 times separation and distillation.)

Splitting a natural fragrance into 39 new ingredients with different odor will greatly enrich the perfumer's ammunition storehouse.

2. The key outstanding advantages of this process are: short retention time of the feed liquid and optimal material and heat conduction. The result of this efficient thermal separation technology is minimal product degradation and the highest product quality.

3. The economic value of this technology lies in the use of a low-cost essential oil to separate and obtain a low-cost "rose notes" that is closer to the aroma of roses rather than the aroma of geranium oil.

Conclusion

This technology can be widely applied to the field of natural fragrance, especially in obtaining a large amount of new raw materials from numerous natural essential oils. These raw materials are 100% originated from plants, are sustainable, have good scent and quality, and the production process is environmentally friendly. Used for the creation of fragrance products, it is indispensable and difficult to imitate and replace, which can greatly enrich the raw material library of perfumers. The development and application of these new raw materials will greatly promote the widespread use of natural essential oils in the field of fragrances.

Acknowledgements

We appreciate the organizer **Notes Shanghai**. 感谢“气味上海”！
Thanks to **Ms. Leeney Zhou**, for helping and facilitating this speech! 感谢周凌祎女士的帮助和支持！

References

一个民族的文明程度反映在他们使用香料的水平上。
The degree of civilization of a nation is reflected in the level of their use of fragrance.

1. Farukh S. Sharopov, Hanjing Zhang and William N. Setzer. Composition of geranium (Pelargonium graveolens) essential oil from Tajikistan. American Journal of Essential Oils and Natural Products 2014; 2 (2): 13-16
2. XU Yu-Sheng, GUO Shi-Yin, SHEN Ke, LIU Heng, JIANG Zhi-Lin. Chemical Composition Analysis of Antibacterial and Anti-inflammatory Functions of Volatile Oils from Pelargonium graveolens L'Herit.[J]. Chinese Journal of Biochemistry and Molecular Biology, 2021, 37(11):1502-1509.
3. Virendra S. Rana , Jitendra P. Juyal, M. Amparo Blazquez. Chemical constituents of essential oil of Pelargonium graveolens leaves. International Journal of Aromatherapy, Volume 12, Issue 4, December 2002, Pages 216-218.
4. Miroslava Kaˇcániová 1,2,* , Milena Vukic 1,3 , Nenad L. Vukovic 3 , Natália Cmikov ˇ á 1 , Andrea Verešová 1 , Marianna Schwarzová 1 , Mária Babošová 4 , Jana Ivaniˇc Porhajašová 4 , Maciej Kluz 2 , Bozena Waszkiewicz-Robak ˙ 2 , Anis Ben Hsouna 5,6 , Rania Ben Saad 5 and Stefania Garzoli. An In-Depth Study on the Chemical Composition and Biological Effects of Pelargonium graveolens Essential Oil. Foods 2024, 13, 33.
5. Zakya M’hamdi, Aziz Bouymajane, Ouassima Riffi, Fouzia Rhazi Filali, Mostafa Ettarchouch, Mohammed Elhourri, Ali Amechrouq. Chemical composition and antibacterial activity of essential oil of *Pelargonium graveolens* and its fractions. Arabian Journal of Chemistry, Volume 17, Issue 1, January 2024, 105375
6. Ana M. Dzamic, Marina D. Sokovic, Mihailo S. Ristic, Slavica M. Grujic, Ksenija S. Mileski, Petar D. Marin. Chemical composition, antifungal and antioxidant activity of Pelargonium graveolens essential oil. Journal of Applied Pharmaceutical Science 4 (03); 2014: 001-005.
7. Fekri N, El Amir D, Owis A, AbouZid S. Studies on essential oil from rose-scented geranium, *Pelargonium graveolens* L'Hérit. (Geraniaceae). Nat Prod Res. 2021 Aug;35(15):2593-2597.

Thanks for attention

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