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Research Article

Revealing metabolite diversity in seeds of species belonging to *Orchis* and *Anacamptis* genus

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Abstract: This study aims to compare the chemical compositions of methanol extracts from seeds of 10 different species belonging to the *Anacamptis* and *Orchis* genera, highlighting significant differences among these species. Seeds collected from various locations in Samsun, Muğla, and İzmir during 2022 and 2023 were analyzed using GC-MS. The results revealed various secondary metabolites in seeds of both *Anacamptis* and *Orchis* species. *A. palustris* seeds, hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester was found at a rate of 16.21%, while methyl stearate was found at 11.14%. In contrast, *O. purpurea* seeds contained hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester at 34.94% and methyl stearate at 8.69%. These findings indicate significant variability in the distribution of compounds among species. The rare compound tricyclo [20.8.0.0(7,16)] triacontane, found in *O. provincialis*, contains tricyclic structures with a 1(22),7(16)-diepoxy group, highlighting its potential role in the chemical profile of this species. Additionally, other rare compounds like tricyclo [20.8.0.0(7,16)] triacontane in *O. provincialis* emphasize their potential roles in chemical profiles across different species. This study is considered a significant step towards understanding the similarities and differences in biochemical components of seeds from *Anacamptis* and *Orchis*, thereby contributing to the understanding of their roles in plant physiological adaptations and ecosystem dynamics. The findings provide valuable insights for plant conservation strategies and biological applications.

1. INTRODUCTION

They are distributed globally and can thrive in almost every type of habitat, except deserts, and are found on every continent except Antarctica (Parkins *et al.*,2023). Epiphytic orchids, which make up about a quarter of all described terrestrial orchids, are typically found in tropical and subtropical regions. The abundance, species diversity, and distribution of orchids vary significantly among continents and regions (Baishnab *et al.*, 2024).

Seed morphology offers valuable insights into orchid evolution and adaptations, serving as a key resource for comparative studies due to its genetic conservation. Previous research has employed seed morphology to explore taxonomic, phylogenetic, and phytogeographic relationships among orchid species (Diantina *et al.*, 2020). Monographic studies focus on the

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detailed examination and classification of specific plant groups. Molecular findings by Kretzschmar *et al.* (2007) supported Bateman *et al.* (2003), leading to the identification of the genera Anacamptis, Neotinea, and Orchis (including Aceras) through novel morphological traits such as lip structure, tooth filaments, and stigmatic cavity. Researchers identified 11 species of *Anacamptis* (including 20 subspecies), 21 species of *Orchis* (including 16 subspecies), and 4 species of *Neotinea* (including 2 subspecies). They also noted natural hybrids within the same genus but did not observe hybrids spanning across three genera. Hybridization within *Orchis* was confined to taxa within each subgenus, excluding inter-subgeneric hybrids.

Tyteca *et al.* (2008) proposed a new taxonomic classification of Orchis sensu *lato*, delineating various species into the genera *Herorchis*, *Androrchis*, and *Odontorchis*. They reinstated the previous monotypic status of *Neotinea* and *Anacamptis* genus. While the *Androrchis* genus encompassed all species of the *Orchis* genus, excluding groups with anthropomorphic labels. Subsequently, Tyteca and Klein (2009) embraced the expanded genus of *Anacamptis* and *Neotinea* but reaffirmed the distinct classification of the *Androrchis* genus (Tyteca *et al.*, 2008). Delforge (2009) introduced a new classification of *Orchis* sensu lato. In this proposal, while acknowledging the taxonomic position of the *Orchis* and *Neotinea* genus, they did not support the expanded *Anacamptis* genus, considering it monotypic. Delforge allocated the remaining species to the genera *Herorchis*, *Vermeulenia*, *Anteriorchis*, and the new *Paludorchis*. Researchers have predominantly focused on morphological and molecular classifications. However, distinctions made through biochemical studies could complement phylogenetic research (Delforge, 2006).

Orchid seeds are notably small and lightweight compared to those of other botanical families, with the potential to produce up to a million seeds per capsule (Lee and Yeung, 2023). A distinctive feature of orchid seeds is the presence of a membranous testa with an 'air cavity' surrounding a small spherical embryo, rather than endosperm. The volume of this air cavity varies among specie (Gamarra *et al.*, 2012). Previous investigations have emphasized the diagnostic and phylogenetic significance of specific quantitative and qualitative seed attributes, highlighting a strong correlation between seed micromorphology and molecular phylogeny (Arditti *et al.*, 1979; Clifford & Smith, 1969; Gamarra *et al.*, 2007, 2008).

Preserving orchid seeds is critical for their biochemical processes, which are essential for healthy development and reproductive success. Orchid seeds are distinguished by their unique structures, including air cavities and absence of endosperm, which require specific biochemical processes for proper germination and growth. This includes the presence of suitable microorganisms for seed germination, breakdown of seed coat compounds, and nutrient release for embryo nourishment (Chen *et al.*, 2022; Gao *et al.*, 2022). Additionally, natural antioxidants and protective compounds are crucial for withstanding environmental stresses. Biochemical processes play a significant role in the ecological role of orchid seeds and the sustainability of their populations (Namrata *et al.*, 2022). Therefore, understanding these processes and preserving their natural habitats are essential for the conservation and sustainability of orchid species.

In this context, this study aims to elucidate the similarities and differences in seed chemistry structures of the *Anacamptis* and *Orchis* genus within the orchid family.

2. MATERIAL and METHODS

2.1. Collection of Seed

The seeds of *Orchis* and *Anacamptis* species were harvested upon maturation of the capsules during the years 2022 and 2023. *Anacamptis papilionacea*, *Anacamptis pyramidalis*, *Orchis purpurea*, *Orchis provincialis*, *Orchis mascula*, and *Anacamptis palustris* were collected in 2023 from Samsun in the Central Black Sea region, while *Anacamptis morio* and *Orchis italica* were gathered in 2022 from Muğla, and *Anacamptis sancta* was obtained in 2022 from İzmir. *Orchis punctulate* was procured in 2022 from Antalya. During collection, the seeds were

extracted from the capsules and left to air-dry naturally between cellulose material (or paper) to eliminate moisture. Subsequently, they were preserved in brown bottles at +4°C in the laboratory.

2.2. GC-MS Analysis of Seeds

For gas chromatography-mass spectrometry (GC-MS) analysis, 1 gram of seeds from each *Orchis* and *Anacamptis* species underwent pulverization within a sterile environment. Subsequently, 20 milliliters of 100% methanol were introduced for extraction using the maceration technique at 30°C for 24 hours, following the methodology outlined by Aytar (2024). Following this, the samples underwent centrifugation at 3500 revolutions per minute for 10 minutes, and the resulting supernatant was utilized for GC-MS analysis. The GC-MS analysis was conducted in accordance with the protocol provided by Aytar (2024), utilizing the NIST Standard Reference Database for the analysis.

3. FINDINGS

The GC-MS analyses of the seeds identified various secondary metabolites across different species. The number of bioactive components detected in each species is as follows: 16 in *Anacamptis palustris*, 12 in *Anacamptis morio*, 16 in *Orchis provincialis*, 15 in *Orchis purpurea*, 24 in *Anacamptis papilionacea*, 13 in *Orchis italica*, 16 in *Anacamptis sancta*, 14 in *Orchis punctulata*, 14 in *Anacamptis pyramidalis*, and 12 in *Orchis mascula*.

The GC-MS results for the methanol extract of *Anacamptis palustris* are detailed in Table S1. The major compounds identified in this extract include hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester (16.21%), methyl stearate (11.14%), 2-propenoic acid, 3-(2-hydroxyphenyl)-, (E)- (7.79%), and tetracosamethyl-cyclododecasiloxane (6.79%). The GC-MS results for the methanol extract of *Anacamptis morio* are presented in Table S2. The major compounds identified in this extract include hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester (43.79%), hexadecanoic acid, methyl ester (9.32%), and methyl stearate (7.48%).

The GC-MS results of the methanol extract of *A. papilionacea* are presented in Table S3. According to these results, the major compounds identified were hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester (28.86%), methyl stearate (10.54%), and hexatriacontane (3.98%). The GC-MS results of the methanol extract of *O. provincialis* are presented in Table S4. According to these results, the major compounds identified were hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester (16.21%), methyl stearate (11.14%), 2-propenoic acid, 3-(2-hydroxyphenyl)-, (E)- (7.79%), and tetracosamethyl-cyclododecasiloxane (6.79%).

The GC-MS results of the methanol extract of *A. pyramidalis* are presented in Table S5. According to these results, the major compounds identified were 2,2-dimethoxybutane (27.21%), hydroxyacetic acid, hydrazide (20.56%), 1,3-Dioxolane-4-methanol, 2-ethyl- (9.05%), and Silane, dimethoxymethyl (7.92%). The GC-MS results of the methanol extract of *O. purpurea* are presented in Table S6. According to these results, the major compounds identified were hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester (34.94%), Methyl stearate (8.69%), hexadecanoic acid, methyl ester (7.51%), 2-propenoic acid, 3-(2-hydroxyphenyl)-, (E)- (4.00%), and cyclononasiloxane, octadecamethyl- (3.97%).

The GC-MS results of the methanol extract of *O. italica* are presented in Table S7. According to these results, the major compounds identified were 2,2-dimethoxybutane (33.26%), Di-sec-butyl ether (13.81%), silane, dimethoxymethyl- (10.20%), decane (7.83%), 9,12-octadecadienoic acid (Z,Z)-, methyl ester (5.55%), and hydroxyacetic acid, hydrazide (5.46%).

The GC-MS results of the methanol extract of *O. sancta* are presented in Table S8. According to these results, the major compounds identified were 2,2-dimethoxybutane (29.13%), hydroxyacetic acid, hydrazide (19.88%), 1,3-Dioxolane-4-methanol, 2-ethyl- (8.45%), Propanoic acid, 2-methyl- (6.70%), and 3,5-Dithiahexanol 5,5-dioxide (6.49%). The GC-MS results of the methanol extract of *O. puntlata* are presented in Table S9. According to these

results, the major compounds identified were 2,2-dimethoxybutane (38.62%), 1-pentanol, 5-cyclopropylidene- (13.92%), silane, dimethoxymethyl- (7.00%), and butyl 2-(2-(2-butoxyethoxy) ethoxy) acetate (6.93%). The GC-MS results of the methanol extract of *O. mascula* are presented in Table S10. According to these results, the major compounds identified were 2,2-dimethoxybutane (30.53%), hydrazinecarbothioamide (12.39%), 1,3-dioxolane-4-methanol, 2-ethyl- (11.40%), and propane, 1,1-dimethoxy- (7.15%).

It is observed that both genera have various proportions of major compounds. However, certain species contain specific secondary metabolites exclusively. The distinct secondary metabolites present in species belonging to the *Anacamptis* and *Orchis* genus are illustrated in Figure 1 and Figure 2.

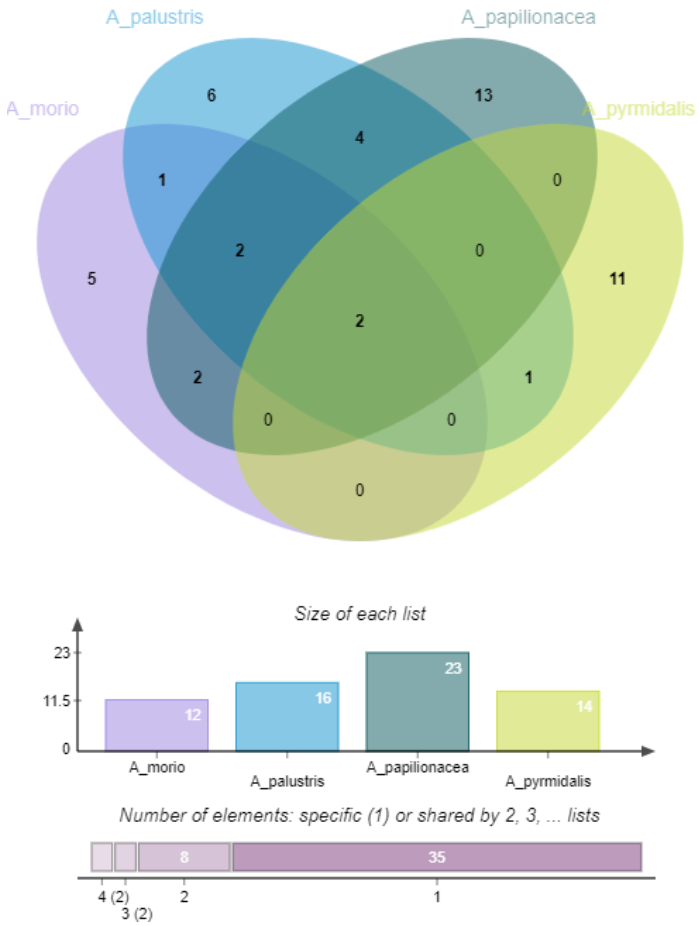

Figure 1. The Venn diagram of species belonging to the *Anacamptis* genus.

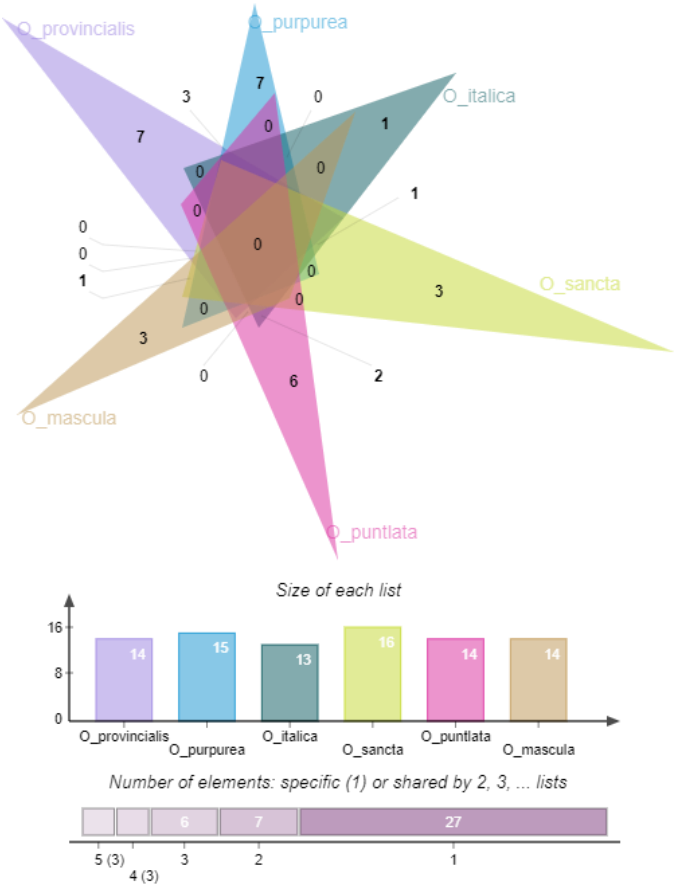

Figure 2. The Venn diagram of species belonging to the *Orchis* genus.

4. DISCUSSION and CONCLUSION

Differences in the percentage composition of major compounds can be attributed to the species and environmental conditions in which plants grow. Variations in chemical composition among plants may be associated with genetic differences, climatic conditions of their habitats, soil properties, and other environmental factors influencing the plants.

2,2-dimethoxybutane, a prominent component in the methanol extracts of plant species such as *O. puntlata*, *O. italica*, *O. sancta*, and *O. mascula*, holds significant percentage proportions. This compound reaches its highest percentage in the methanol extract of *O. puntlata* (38.62%). Similarly, *O. italica*, *O. sancta*, and *O. mascula* exhibit high percentages of 2,2-dimethoxybutane (33.26%, 29.13%, 30.53% respectively). This compound occupies a notable position in the chemical profiles of these plant species, potentially serving as a crucial element in understanding their biological properties and potential pharmacological effects.

Hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester, identified as a significant component in the methanol extracts of plant species such as *A. papilionacea*, *O. purpurea*, *O. provincialis*, and *O. mascula*. This compound attains its highest percentage in the methanol extract of *O. purpurea* (34.94%). Similarly, *A. papilionacea*, *O. provincialis*, and *O. mascula* exhibit high percentages of this compound (28.86%, 16.21%, 11.40% respectively). Methyl stearate, another important component detected in the methanol extracts of plant species such as *O. provincialis*, *A. papilionacea*, *O. purpurea*, and *O. mascula*. This compound reaches its highest percentage in the methanol extract of *O. provincialis* (11.14%). Similarly, *A. papilionacea*, *O. purpurea*, and *O. mascula* show high percentages of methyl stearate (10.54%, 8.69%, 12.39% respectively).

In a study by Aytar *et al.* (2023), hydroxyacetic acid hydrazide was detected at 12.42% in *Anacamptis coriophora* seeds, while it was found to be 5.46% in *O. italica*, 19.88% in *O. sancta*, and 5.59% in *O. mascula* through GC-MS analysis. Additionally, another common

compound, 2,2-dimethoxybutane, was found at a rate of 27.91%, whereas it was 33.26% in *O. italica*, 29.13% in *O. sancta*, 38.62% in *O. puntlata*, and 30.53% in *O. mascula*. In the same study, *A. coriophora* was reported to contain cyclohexasiloxane, dodecamethyl at 1.01%, while it was found to be 1.89% in *O. provincialis* and 1.01% in *O. purpurea*. Furthermore, the compound 9,12-octadecadienoic acid (Z, Z)-, methyl ester was detected in all species except *O. puntlata* and *O. provincialis*.

The rare compound Tricyclo [20.8.0.0(7,16)] triacontane, 1(22),7(16)-diepoxy-found in *O. provincialis* contains tricyclic structures with a diepoxy group, potentially contributing to the chemical profile of the species. Meanwhile, 2-tert-butyl-1,4-dimethoxybenzene present in *O. provincialis* includes a 2-tertiary butyl group and a 1,4-dimethoxybenzene ring, whereas triarachine in *O. purpurea* comprises the special structure of triarachidin. Conversely, 6,6-Diethylhoctadecane, a rare compound in *O. provincialis*, encompasses diethyl groups and hoctadecane structures. Methyl 18-methylnonadecanoate found in *A. papilionacea* includes methyl and methyl nonadecanoate groups, while ethanone, 1-[3-[2-methyl-2-(5-methyl-2-furanyl) propyl]oxiranyl] has a complex structure contributing to understanding the species' metabolic processes and lipid metabolism. Isopropyl palmitate in *A. papilionacea* contains isopropyl and palmitate groups, whereas octadecanal comprises an 18-carbon aliphatic chain. 2,3-Bis[(trimethylsilyl)oxy] propyl icosanoate, a rare silil ester compound found in *A. papilionacea*, includes two trimethylsilyloxypropyl and one icosanoate group. Lastly, Hexatriacontane in *A. papilionacea* constitutes long aliphatic hydrocarbon chains, serving as a significant component of the species' lipid structure. Further exploration of the role of these compounds in determining interspecies differences is warranted. Additionally, studies on the biological activities and effects of these compounds could deepen our understanding of the species' physiology and environmental adaptations.

Previous studies have reported the presence of the tricyclo [20.8.0.0(7,16)] triacontane, 1(22),7(16)-diepoxy compound in various plants. This compound has been observed in white rice at a rate of 0.76% (Kuswaha *et al.* 2021), in *C. corymbosus* root extract at 0.129% (Pauldasan *et al.* 2020), and in *Momordica cymbalaria* at 1.90% (Gopu et al. 2021). 2-tert-Butyl-1,4-dimethoxybenzene is a naturally occurring product found in *Valeriana officinalis*, with available data on its presence in this plant. Additionally, it has been found in *Moringa oleifera* volatile oil at a rate of 0.39%. However, no study has reported the presence of this compound in *Chlorophytum borivilianum*, where it is present at a rate of 4.81% (Chuhang *et al.* 2007). Hexatriacontane, octadecanal, and isopropyl palmitate are natural compounds found in *Camellia sinensis*, *Solanum tuberosum*, and other organisms with available data. In the methanol extract of *Gypsophila pilulifera*, the compound 2,3-Bis[(trimethylsilyl)oxy] propyl icosanoate has been determined to be present in the leaves at a rate of 0.6%. These findings come from a study investigating the chemical composition of endemic and endangered *G. pilulifera* produced by in vitro micropropagation (Ustuner *et al.* 2024).

In conclusion, a comprehensive investigation of these rare chemical compounds could significantly contribute to understanding interspecies differences and physiological adaptations. This study represents an important step toward comprehending the complexity of natural life and developing conservation strategies. Future research into the biological activities and potential applications of these compounds is recommended.

Declaration of Conflicting Interests and Ethics

The author declares no conflict of interest. This research study complies with research and publishing ethics. The scientific and legal responsibility for manuscripts published in IJSM belongs to the author.

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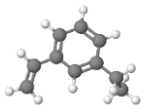
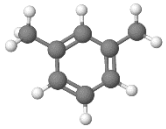
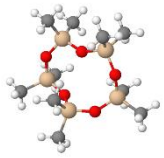
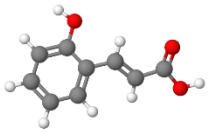
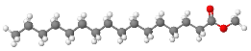
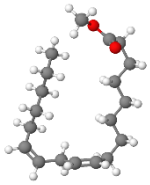
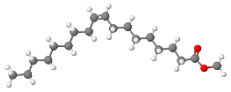
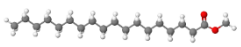
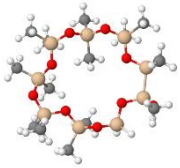
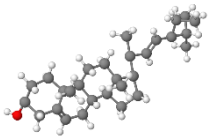
APPENDIX

Supplementary Material

Table S1. The GC-MS analysis results of *A.palustris* seeds.

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Area (%)	3D Chemical Structure
1	9.569	Benzene, 1-ethenyl-3-ethyl-	$C_{10}H_{12}$	132.20	3.06	
2	11.370	Benzene, 1,3-dimethyl-	C_8H_{10}	106.16	1.59	
3	14.937	Cyclopentasiloxane, decamethyl-	$C_{10}H_{30}O_5Si_5$	370.76	1.20	
4	28.618	2-Propenoic acid, 3-(2-hydroxyphenyl)-, (E)-	$C_9H_8O_3$	164.15	7.79	
5	47.371	Hexadecanoic acid, methyl ester	$C_7H_{14}O_2$	270.45	3.95	
6	49.735	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	2.34	
7	49.812	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	296.48	1.18	
8	50.132	Methyl stearate	$C_{19}H_{38}O_2$	298.50	11.14	
9	50.672	Cyclononasiloxane, octadecamethyl-	$C_{18}H_{14}O_9Si_9$	667.40	5.91	
10	51.881	Stigmasterol	$C_{29}H_{48}O$	412.70	2.74	

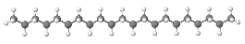
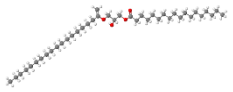
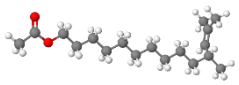
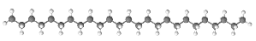
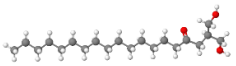
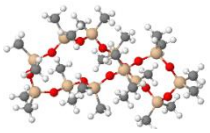
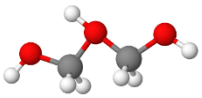
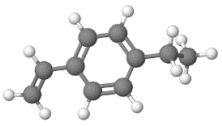
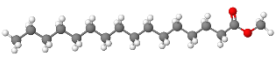
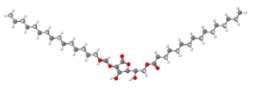
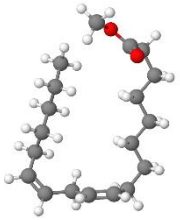
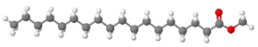
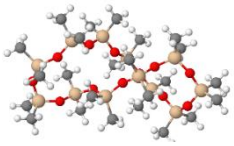
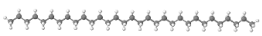
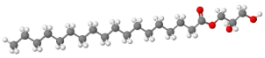
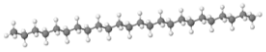
11	51.957	Heneicosane	$C_{21}H_{44}$	296.60	4.22	
12	52.569	1,3-Distearin	$C_{39}H_{76}O_5$	625.02	1.32	
13	53.768	11,13-Dimethyl-12-tetradecen-1-ol acetate	$C_{18}H_{34}O_2$	282.50	1.03	
14	54.392	Pentacosane	$C_{25}H_{52}$	296.48	1.76	
15	54.582	Hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester	$C_{19}H_{38}O_4$	330.50	16.21	
16	55.226	Tetracosamethyl-cyclododecasiloxane	$C_{24}H_{72}O_{12}Si_{12}$	889.80	6.79	

Table S2. The GC-MS analysis results of *A. morio* seeds.

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	No	Retention Time (minutes)
1	5.087	Glycerin	$C_3H_8O_3$	92.09	1.56	
2	9.515	Benzene, 1-ethenyl-4-ethyl-	$C_{10}H_{12}$	132.20	1.78	
3	47.382	Hexadecanoic acid, methyl ester	$C_7H_{14}O_2$	270.45	9.32	
4	47.988	l-(+)-Ascorbic acid 2,6-dihexadecanoate	$C_{38}H_{68}O_8$	652.90	1.00	
5	49.738	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	2.01	
6	50.134	Methyl stearate	$C_{19}H_{38}O_2$	298.50	7.48	
7	50.634	Tetracosamethyl-cyclododecasiloxane	$C_{24}H_{72}O_{12}Si_{12}$	889.80	3.35	
8	51.956	Heptacosane	$C_{27}H_{56}$	380.70	1.92	
9	52.575	Octadecanoic acid, 2,3-dihydroxypropyl ester	$C_{21}H_{42}O_4$	358.55	1.15	
10	53.073	Tetracosane	$C_{24}H_{50}$	338.70	1.26	

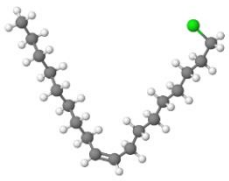
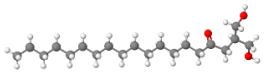
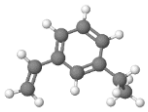
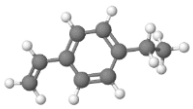
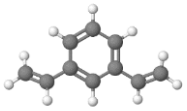
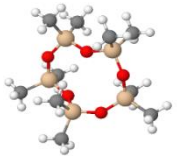
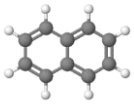
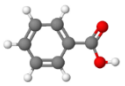
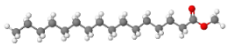
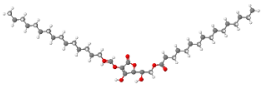
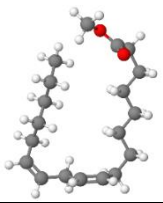
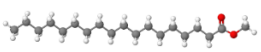
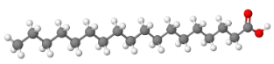
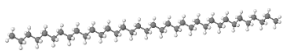
11	53.655	cis-1-Chloro-9-octadecene	$C_{18}H_{35}Cl$	286.92	1.35	
12	54.632	Hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester	$C_{19}H_{38}O_4$	330.50	43.79	

Table S3. The GC-MS analysis results of *A. papilionacea* seeds.

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Area (%)	3D Chemical Structure
1	1.383	Benzene, 1-ethenyl-3-ethyl-	$C_{10}H_{12}$	132.20	1.60	
2	10.014	Benzene, 1-ethenyl-4-ethyl-	$C_{10}H_{12}$	132.20	1.27	
3	11.383	Benzene, 1,3-diethenyl-	$C_{10}H_{10}$	130.18	1.59	
4	14.942	Cyclopentasiloxane, decamethyl-	$C_{10}H_{30}O_5Si_5$	370.76	1.08	
5	15.353	Naphthalene	$C_{10}H_8$	128.17	1.28	
6	15.842	Benzoic acid	$C_7H_6O_2$	122.12	1.14	
7	47.378	Hexadecanoic acid, methyl ester	$C_7H_{14}O_2$	270.45	3.64	
8	47.989	l-(+)-Ascorbic acid 2,6-dihexadecanoate	$C_{38}H_{68}O_8$	652.90	1.19	
9	49.742	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	2.83	
10	50.135	Methyl stearate	$C_{19}H_{38}O_2$	298.50	10.54	
11	50.551	Octadecanoic acid	$C_{27}H_{56}$	380.70	1.04	
12	51.520	Hexatriacontane	$C_{36}H_{74}$	507.00	3.98	

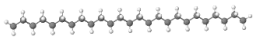
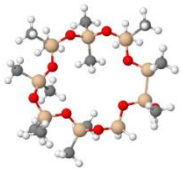
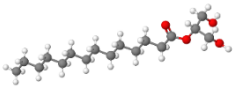
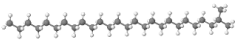
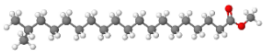
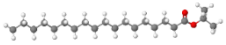
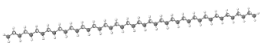
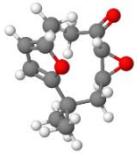
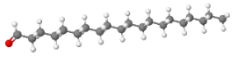
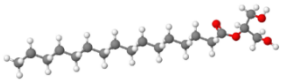
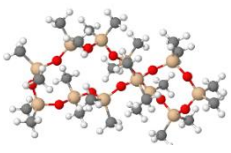
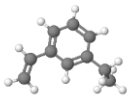
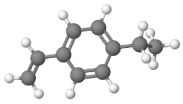
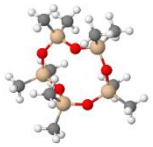
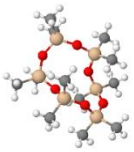
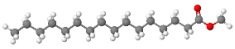
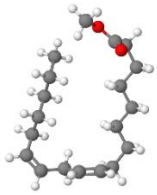
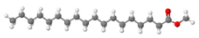
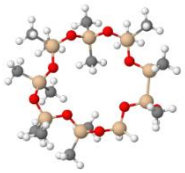
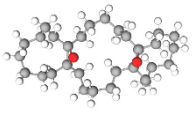
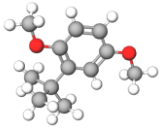
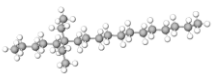
13	54.402	Heneicosane	$C_{21}H_{44}$	296.60	1.23	
14	51.848	Cyclononasiloxane, octadecamethyl-	$C_{18}H_{14}O_9Si_9$	667.40	1.66	
15	51.996	Tetradecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	$C_{17}H_{34}O_4$	302.44	1.92	
16	52.155	2-methylhexacosane	$C_{27}H_{56}$	380.70	1.00	
17	52.273	Methyl 18-methylnonadecanoate	$C_{21}H_{42}O_2$	326.60	1.66	
18	52.578	Isopropyl palmitate	$C_{19}H_{38}O_2$	298.50	1.94	
19	52.846	Hexacontane	$C_{60}H_{122}$	843.60	1.07	
20	53.221	Ethanone, 1-[3-[2-methyl-2-(5-methyl-2-furanyl)propyl]oxiranyl]-	$C_{13}H_{18}O_3$	222.28	1.07	
21	53.459	Octadecanal	$C_{18}H_{36}O$	268.50	1.94	
22	54.137	2,3-Bis[(trimethylsilyl)oxy]propyl icosanoate	$C_{29}H_{62}O_4S_2$	531.00	2.11	
23	54.603	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	$C_{19}H_{38}O_4$	330.50	25.86	
24	55.226	Tetracosamethyl-cyclododecasiloxane	$C_{24}H_{72}O_{12}Si_{12}$	889.80	2.58	

Table S4. The GC-MS analysis results of *O. provincialis* seeds.

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight(g/mol)	Area (%)	3D Chemical Structure
1	9.569	Benzene, 1-ethenyl-3-ethyl-	$C_{10}H_{12}$	132.20	1.38	
2	9.969	Benzene, 1-ethenyl-4-ethyl-	$C_{10}H_{12}$	132.20	1.69	
3	14.941	Cyclopentasiloxane, decamethyl-	$C_{10}H_{30}O_5Si_5$	370.76	1.70	
4	24.479	Cyclohexasiloxane, dodecamethyl-	$C_{12}H_{36}O_6Si_6$	444.92	1.89	
5	47.373	Hexadecanoic acid, methyl ester	$C_7H_{14}O_2$	270.45	4.33	
6	49.265	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	2.09	
8	50.133	Methyl stearate	$C_{19}H_{38}O_2$	298.50	12.37	
9	50.677	Cyclononasiloxane, octadecamethyl-	$C_{18}H_{14}O_9Si_9$	667.40	8.78	
10	51.717	Tricyclo[20.8.0.0(7,16)]triacontane, 1(22),7(16)-diepoxy-	$C_{30}H_{52}O_2$	444.70	1.36	
11	52.056	2-tert-Butyl-1,4-dimethoxybenzene	$C_{12}H_{18}O_2$	194.27	2.26	
12	52.569	6,6-Diethylhoctadecane	$C_{22}H_{46}$	310.60	2.06	

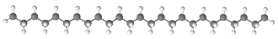
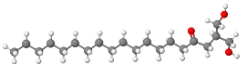
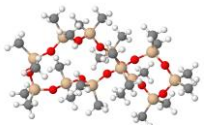
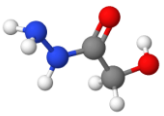
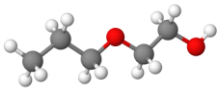
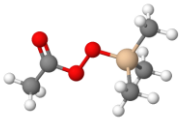
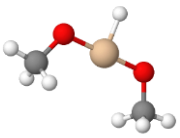
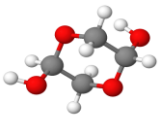
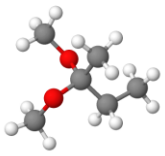
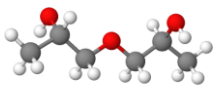
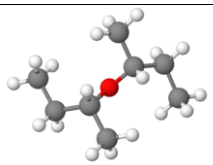
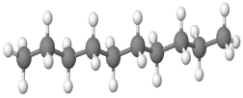
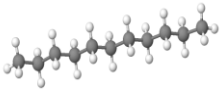
14	54.395	Pentacosane	$C_{25}H_{52}$	296.48	1.41	
15	54.587	Hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester	$C_{19}H_{38}O_4$	330.50	16.91	
16	55.222	Tetracosamethyl-cyclododecasiloxane	$C_{24}H_{72}O_{12}Si_{12}$	889.80	4.87	

Table S5. The GC-MS analysis results of *A. pyramidalis* seeds

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Area (%)	3D Chemical Structure
1	3.055	Hydroxyacetic acid, hydrazide	$C_2H_6N_2O_2$	90.08	20.56	
2	3.274	Ethanol, 2-propoxy-	$C_5H_{12}O_2$	104.14	6.65	
3	3.433	Trimethylsilyl ethaneperoxoate	CH_5N_3S	148.23	3.54	
4	3.474	Silane, dimethoxymethyl-	$C_3H_{10}O_2Si$	106.20	7.92	
5	3.695	Glycolaldehyde dimer	$C_4H_8O_4$	120.10	2.49	
6	5.029	2,2-dimethoxybutane	$C_6H_{14}O_2$	118.17	27.21	
7	7.114	2-Propanol, 1,1'-oxybis-	$C_6H_{14}O_3$	134.17	4.82	
8	7.314	1,3-Dioxolane-4-methanol, 2-ethyl-	$C_6H_{12}O_3$	132.16	9.05	
9	10.504	Decane	$C_{19}H_{36}O_2$	296.48	4.33	
10	12.385	Undecane	$C_{11}H_{24}$	156.31	1.64	

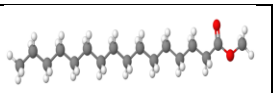
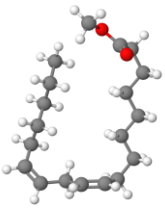
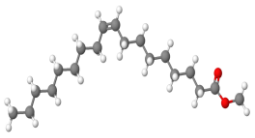
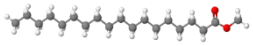
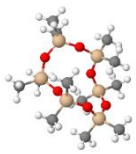
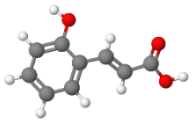
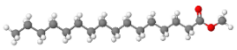
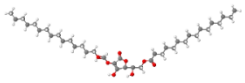
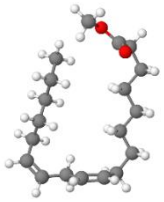
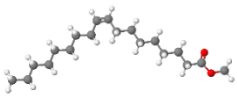
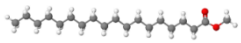
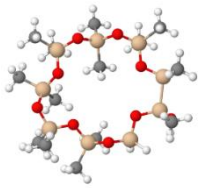
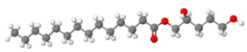
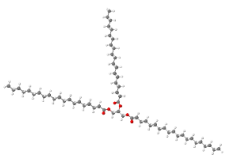
11	34.968	Hexadecanoic acid, methyl ester	$C_7H_{14}O_2$	270.45	1.17	
12	42.423	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	4.01	
13	42.706	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	296.48	1.75	
14	43.880	Methyl stearate	$C_{19}H_{38}O_2$	298.50	1.89	

Table S6. The GC-MS analysis results of *O. purpurea* seeds.

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Area (%)	3D Chemical Structure
1	24.481	Cyclohexasiloxane, dodecamethyl-	$C_{12}H_{36}O_6Si_6$	444.92	1.01	
2	28.623	2-Propenoic acid, 3-(2-hydroxyphenyl)-, (E)-	$C_9H_8O_3$	164.15	4.00	
3	47.380	Hexadecanoic acid, methyl ester	$C_7H_{14}O_2$	270.45	7.51	
4	47.991	l-(+)-Ascorbic acid 2,6-dihexadecanoate	$C_{38}H_{68}O_8$	652.90	1.00	
5	49.738	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	2.11	
6	49.816	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	296.48	1.27	
7	50.134	Methyl stearate	$C_{19}H_{38}O_2$	298.50	8.69	
8	50.684	Cyclononasiloxane, octadecamethyl-	$C_{18}H_{14}O_9Si_9$	667.40	3.97	
9	51.998	Tetradecanoic acid, 2,3-dihydroxypropyl ester	$C_{17}H_{34}O_4$	302.44	1.86	
10	52.573	Triarachine	$C_{63}H_{122}O_6$	975.63	1.08	

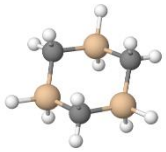
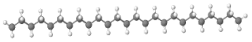
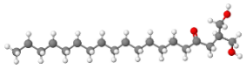
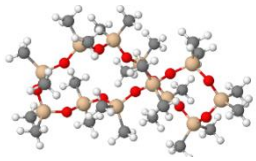
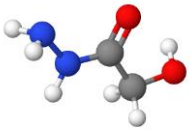
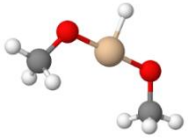
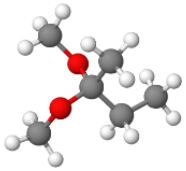
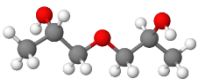
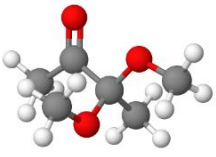
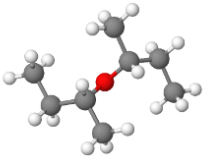
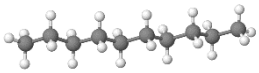
11	53.072	2-methylhexacosane	$C_{27}H_{56}$	380.70	1.67	
12	54.131	1,3,5-Trisilacyclohexane	$C_3H_6Si_3$	126.33	1.01	
13	54.402	Heneicosane	$C_{21}H_{44}$	296.60	1.23	
14	54.632	Hexadecanoic acid 2-hydroxy-1-(hydroxymethyl) ethyl ester	$C_{19}H_{38}O_4$	330.50	34.94	
15	55.232	Tetracosamethyl-cyclododecasiloxane	$C_{24}H_{72}O_{12}Si_{12}$	889.80	1.80	

Table S7. The GC-MS analysis results of *O. italica* seeds.

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Area (%)	3D Chemical Structure
1	3.041	Hydroxyacetic acid, hydrazide	$C_2H_6N_2O_2$	90.08	5.46	
2	3.470	Silane, dimethoxymethyl-	$C_3H_{10}O_2Si$	106.20	10.20	
3	4.890	2,2-dimethoxybutane	$C_6H_{14}O_2$	118.17	33.26	
4	7.114	2-Propanol, 1,1'-oxybis-	$C_6H_{14}O_3$	134.17	3.52	
5	7.154	3,3-Dimethoxy-2-butanone	$C_6H_{12}O_3$	132.16	4.88	
6	7.255	Di-sec-Butyl ether	$C_8H_{18}O$	130.22	13.81	
7	10.491	Decane	$C_{19}H_{36}O_2$	296.48	7.83	

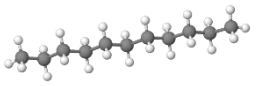
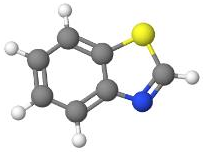
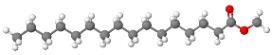
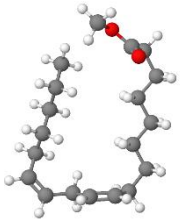
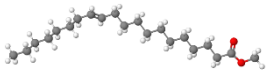
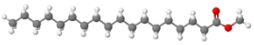
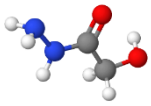
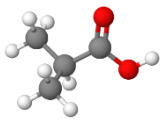
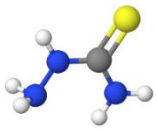
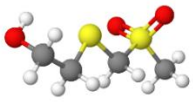
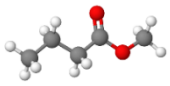
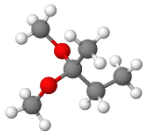
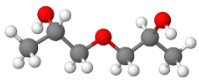
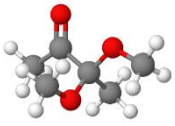
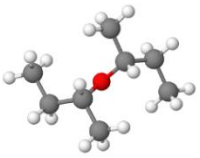
8	12.367	Undecane	$C_{11}H_{24}$	156.31	3.30	
9	14.656	Benzothiazole	C_7H_5NS	135.19	1.99	
10	34.950	Hexadecanoic acid, methyl ester	$C_7H_{14}O_2$	270.45	4.67	
11	42.392	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	5.55	
12	42.686	10-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	296.48	1.58	
13	43.870	Methyl stearate	$C_{19}H_{38}O_2$	298.50	2.30	

Table S8. The GC-MS analysis results of *O. sancta* seeds.

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Area (%)	3D Chemical Structure
1	3.037	Hydroxyacetic acid, hydrazide	$C_2H_6N_2O_2$	90.08	19.88	
2	3.270	Propanoic acid, 2-methyl-	$C_4H_8O_2$	88.10	6.70	
3	3.443	Hydrazinecarbothioamide	CH_5N_3S	91.13	5.71	
4	3.477	3,5-Dithiahexanol 5,5-dioxide	$C_4H_{10}O_3S_2$	170.25	6.49	
5	4.193	Butanoic acid, methyl ester	$C_5H_{10}O_2$	102.13	1.24	
6	4.890	2,2-dimethoxybutane	$C_6H_{14}O_2$	118.17	29.13	
7	7.120	2-Propanol, 1,1'-oxybis-	$C_6H_{14}O_3$	134.17	1.87	
8	7.169	3,3-Dimethoxy-2-butanone	$C_6H_{12}O_3$	132.16	3.72	
9	7.265	1,3-Dioxolane-4-methanol, 2-ethyl-	$C_6H_{12}O_3$	132.16	8.45	

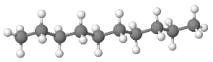
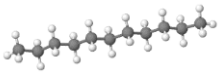
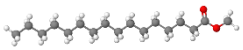
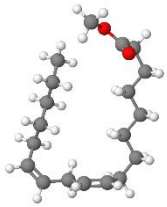
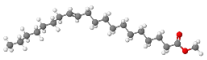
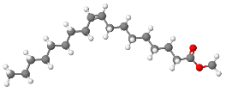
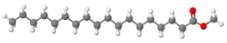
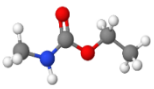
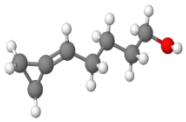
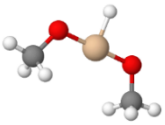
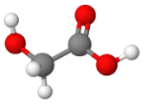
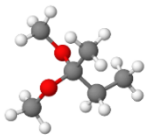
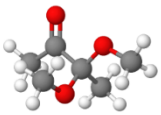
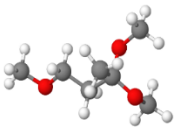
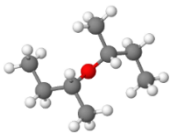
10	10.504	Decane	$C_{19}H_{36}O_2$	296.48	4.39	
11	12.384	Undecane	$C_{11}H_{24}$	156.31	1.82	
12	34.975	Hexadecanoic acid, methyl ester	$C_7H_{14}O_2$	270.45	1.63	
13	42.695	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	2.99	
14	42.686	10-Octadecenoic acid, methyl ester	$C_{19}H_{36}O_2$	296.48	1.58	
15	42.695	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	296.48	1.26	
16	43.870	Methyl stearate	$C_{19}H_{38}O_2$	298.50	1.91	

Table S9. The GC-MS analysis results of *O. punctulata* seeds

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Area (%)	3D Chemical Structure
1	3.049	Ethyl N-methylcarbamate	$C_4H_9NO_2$	103.12	5.97	
2	3.125	1-Pentanol, 5-cyclopropylidene-	$C_4H_8O_2$	88.10	13.92	
3	3.453	Silane, dimethoxymethyl-	$C_3H_{10}O_2Si$	106.20	7.00	
4	3.570	Acetic acid, hydroxy-	$C_2H_4O_3$	76.05	1.66	
5	4.890	2,2-dimethoxybutane	$C_6H_{14}O_2$	118.17	38.62	
6	7.120	3,3-Dimethoxy-2-butanone	$C_6H_{12}O_3$	132.16	3.03	
7	7.160	1,3,3-Trimethoxybutane	$C_7H_{16}O_3$	148.20	3.42	
8	7.263	1,3-Dioxolane-4-methanol, 2-ethyl-	$C_6H_{12}O_3$	132.16	4.02	

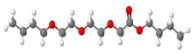
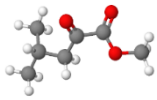
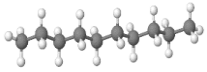
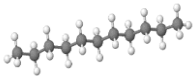
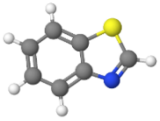
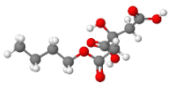
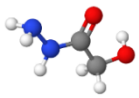
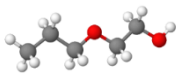
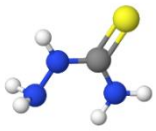
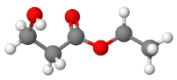
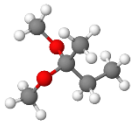
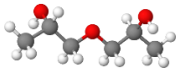
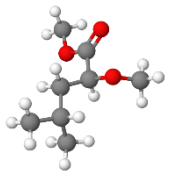
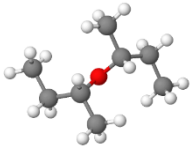
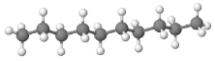
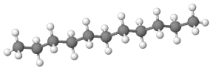
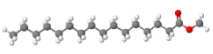
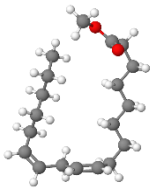
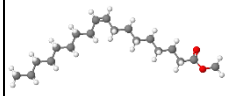
9	7.302	Butyl 2-(2-(2-butoxyethoxy)ethoxy)acetate	$C_{10}H_{20}O_4$	204.26	6.93	
10	9.974	Pentanoic acid, 4-methyl-2-oxo-, methyl ester	$C_6H_{10}O_3$	130.14	1.00	
11	10.500	Decane	$C_{19}H_{36}O_2$	296.48	5.44	
12	12.382	Undecane	$C_{11}H_{24}$	156.31	2.26	
13	14.673	Benzothiazole	C_7H_5NS	135.19	1.30	
14	46.756	Butyl citrate	$C_{18}H_{32}O_7$	360.40	1.57	

Table S10. The GC-MS analysis results of *O. mascula* seeds.

No	Retention Time (minutes)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Area (%)	3D Chemical Structure
1	3.050	Hydroxyacetic acid, hydrazide	$C_2H_6N_2O_2$	90.08	5.59	
2	3.295	Propane, 1,1-dimethoxy-	$C_5H_{12}O_2$	104.14	7.15	
3	3.463	Hydrazinecarbothioamide	CH_5N_3S	91.13	12.39	
4	3.474	Acetic acid, hydroxy-, ethyl ester	$C_4H_8O_3$	104.10	2.15	
5	5.580	2,2-dimethoxybutane	$C_6H_{14}O_2$	118.17	30.53	
6	7.128	2-Propanol, 1,1'-oxybis-	$C_6H_{14}O_3$	134.17	2.54	
7	7.164	2-Hydroxyisocaproic acid, methyl ether, methyl ester	$C_8H_{16}O_3$	160.21	3.17	
8	7.314	1,3-Dioxolane-4-methanol, 2-ethyl-	$C_6H_{12}O_3$	132.16	11.40	
9	10.503	Decane	$C_{19}H_{36}O_2$	296.48	5.14	
10	12.383	Undecane	$C_{11}H_{24}$	156.31	1.98	
11	34.972	Hexadecanoic acid, methyl ester	$C_7H_{14}O_2$	270.45	5.64	

12	42.418	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294.47	5.88	
13	42.704	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	296.48	1.35	
14	43.876	Methyl stearate	$C_{19}H_{38}O_2$	298.50	2.96