

Table SI. GC-MS analysis of PNEO extracted by MAE.

No.	CAS	Compound	Molecular formula	Rt/min	Similarity	Relative peak area (%)
Aldehydes (2.488%)						
1	100-52-7	Benzaldehyde	C ₇ H ₆ O	5.31	94.12	0.152
2	-	(1R,4aR,4bS,7S,10aR)-1,4a,7-Trimethyl-7-vinyl-1,2,3,4,4a,4b,5,6,7,8,10,10a-dodecahydrophenanthrene-1-carbaldehyde	C ₂₀ H ₃₀ O	44.87	88.92	0.945
3	19898-57-8	(1R,4aR,4bS,10aR)-1,4a-dimethyl-7-propan-2-ylidene-3,4,4b,5,6,9,10,10a-octahydro-2H-phenanthrene-1-carbaldehyde	C ₂₀ H ₃₀ O	50.96	88.47	0.157
4	13601-88-2	1-Phenanthrenecarboxaldehyd	C ₂₀ H ₂₈ O	46.98	82.52	1.054
5	25152-83-4	(E,Z)-2,4-Decadienal	C ₁₀ H ₁₆ O	11.58	81.50	0.180
Hydrocarbons (9.175%)						
1	500-00-5	Cyclohexene, 4-methyl-1-(1-methylethyl)-	C ₁₀ H ₁₈	5.71	85.62	0.104
2	1124-20-5	Benzene, 1-methyl-3-(1-methylethenyl)-	C ₁₀ H ₁₂	7.57	93.18	0.284
3	765-46-8	<u>Spiro[2.4]hepta-4,6-diene</u>	C ₇ H ₈	7.99	87.19	0.044
4	3479-89-8	1,3,5-Cycloheptatriene, 3,7,7-trimethyl-	C ₁₀ H ₁₄	8.76	86.84	0.027
5	24703-35-3	(1S,2E,6E,10R)-3,7,11,11-Tetramethyl-bicyclo[8.1.0]undeca-2,6-diene	C ₁₅ H ₂₄	11.89	89.99	0.902
6	267665-20-3	(1S,4S,4aS)-1-Isopropyl-4,7-dimethyl-1,2,3,4,4a,5-hexahydronaphthalene	C ₁₅ H ₂₄	12.33	89.12	0.732
7	39029-41-9	(R)- γ -cadinene	C ₁₅ H ₂₄	14.48	89.02	0.131
8	489-28-1	α -maalinene	C ₁₅ H ₂₄	14.54	87.81	0.150
9	1898-13-1	Cembrene	C ₂₀ H ₃₂	39.17	87.02	1.139
10	-	Naphthalene, 1,2,3,5,6,7,8,8a- octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1. α ., 7. β ., 8a. α .)]-	C ₁₅ H ₂₄	14.73	89.66	0.498
11	64363-64-0	(1E,3E,7E,11E)-4-Isopropyl-1,7,11-trimethylcyclotetradeca-1,3,7,11-tetraene	C ₂₀ H ₃₂	36.22	90.93	1.048
12	630-04-6	<u>Hentriacontane</u>	C ₃₁ H ₆₄	72.88	88.48	2.189
13	108-88-3	Toluene	C ₇ H ₈	6.74	83.76	0.018
14	-	4b,8-Dimethyl-2-isopropylphenanthrene, 4b,5,6,7,8,8a,9,10-octahydro-	C ₁₉ H ₂₈	36.49	81.96	0.104
15	629-94-7	Heneicosane	C ₂₁ H ₄₄	44.68	81.69	0.082
16	274-09-9	1,3-Benzodioxole	C ₇ H ₆ O ₂	6.75	81.61	0.017
17	1758-88-9	Benzene, 2-ethyl-1,4-dimethyl-	C ₁₀ H ₁₄	7.98	81.13	0.022
18	13943-77-6	Naphthalene,1,2,3,4,4a,5,6,7-octahydro-4a-methyl-	C ₁₁ H ₁₈	11.29	81.04	0.328

19	-	3,4-dimethylfuran	C ₆ H ₈ O	5.38	80.92	0.009
20	515-17-3	γ-selinene	C ₁₅ H ₂₄	18.51	80.84	1.196
21	547-60-4	Bicyclo[3.1.1]heptan-3-one,2,6,6-trimethyl-, (1.α.,2.α.,5.α.)-	C ₁₀ H ₁₆ O	8.90	80.72	0.151
22	18127-14-5	Bicyclo[2.2.1]heptane,2-(2-methylpropyl)-	C ₁₁ H ₂₀	29.85	80.05	0.154
Terpenes (8.886%)						
1	99-83-2	α-Phellandrene	C ₁₀ H ₁₆	6.06	89.46	0.045
2	99-86-5	α-Terpinene	C ₁₀ H ₁₆	6.27	92.71	0.825
3	4889-83-2	3,6,6-Trimethyl-bicyclo(3.1.1)hept-2-ene	C ₁₀ H ₁₆	6.59	86.80	0.020
4	13466-78-9	carene	C ₁₀ H ₁₆	6.78	85.81	0.465
5	99-85-4	γ-terpinene	C ₁₀ H ₁₆	7.01	93.59	0.077
6	1879-07-8	cis-1-methyl-4-(1-methylethenyl)-Cyclohexane	C ₁₀ H ₁₈	6.08	84.90	0.029
7	3387-41-5	4-methylene-1-(1-methylethyl)-Bicyclo[3.1.0]hexane	C ₁₀ H ₁₆	11.49	84.69	0.163
8	-	1-ethenyl-1-methyl-2-(1-methylethenyl)-4-(1-methylethylidene)-Cyclohexane	C ₁₅ H ₂₄	29.26	84.32	0.940
9	20230-48-2	(5β,8α,9β,10α,12α)-Atis-16-ene	C ₂₀ H ₃₂	37.22	83.68	0.046
10	73209-42-4	trans-Calamenene	C ₁₅ H ₂₂	17.20	83.28	0.159
11	5256-65-5	Cyclohexene,3-methyl-6-(1-methylethyl)-	C ₁₀ H ₁₈	6.37	83.23	0.003
12	5989-27-5	D-Limonene	C ₁₀ H ₁₆	5.27	83.06	0.020
13	471-84-1	α-fenchene	C ₁₀ H ₁₆	5.78	82.84	0.488
14	24406-05-1	α-cadinene	C ₁₅ H ₂₄	17.52	82.51	1.534
15	504-96-1	Neophytadiene	C ₂₀ H ₃₈	45.55	82.51	1.306
16	29837-12-5	Cubenene	C ₁₅ H ₂₄	17.36	82.24	0.567
17	-	Cadala-1(10),3,8-triene	C ₁₅ H ₂₂	28.17	82.27	0.297
18	3310-2-9	Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, (1.α.,3.α.,5.α.)-	C ₁₀ H ₁₆ O	8.51	82.16	0.279
19	18479-64-6	Shisool	C ₁₀ H ₁₈ O	10.36	82.10	0.170
20	81968-62-9	4(15),5,10(14)-Germacatrien-1-ol	C ₁₅ H ₂₄ O	26.15	81.22	0.473
21	-	((8R,8aS)-8-Isopropyl-5-methyl-3,4,6,7,8,8a-hexahydronaphthalen-2-yl)methanol	C ₁₅ H ₂₄ O	27.50	81.20	0.509
22	73809-82-2	Salvial-4(14)-en-1-one	C ₁₅ H ₂₄ O	32.14	80.07	0.471
Alcohols (11.346%)						
1	78-70-6	Linalool	C ₁₀ H ₁₈ O	7.71	85.03	0.460
2	1908-44-7	Labda-8(17),14-diene-13,19-diol	C ₂₀ H ₃₄ O ₂	45.30	89.03	0.651
3	29803-82-5	cis-4-(Isopropyl)-1-methylcyclohex-2-en-1-ol	C ₁₀ H ₁₈ O	8.16	87.28	0.213
4	-	1,7,7-Trimethylbicyclo[2.2.1]hept-5-en-2-ol	C ₁₀ H ₁₆ O	8.25	87.87	0.093
5	25269-17-4	Thunbergol	C ₂₀ H ₃₄ O	42.63	87.59	3.938

6	19894-97-4	(-)-myrteno	C ₁₀ H ₁₆ O	9.53	86.01	0.393
7	536-50-5	1-(4-Methylphenyl)ethanol	C ₉ H ₁₂ O	9.65	86.30	0.150
8	3772-55-2	Dehydroabietadienol	C ₂₀ H ₃₂ O	50.72	86.81	0.059
9	374925-73-2	cis-3,14-Clerodadien-13-ol	C ₂₀ H ₃₄ O	37.59	87.21	0.265
10	514-99-8	6,6-dimethylbicyclo[3.1.1]heptane-2-methanol	C ₁₀ H ₁₈ O	10.69	85.39	0.149
11	36653-82-4	1-Hexadecanol	C ₁₆ H ₃₄ O	48.21	83.23	0.287
12	70000-19-0	Verticillol	C ₂₀ H ₃₄ O	36.40	86.75	3.597
13	586-82-3	4-(isopropyl)-1-methylcyclohex-3-en-1-ol	C ₁₀ H ₁₈ O	8.38	83.07	0.042
14	1686-20-0	p-Mentha-1,5-dien-8-ol	C ₁₀ H ₁₆ O	8.67	81.97	0.019
15	-	2-((2R,4aR,8aS)-4a-Methyl-8-methylenedecahydronaphthalen-2-yl)prop-2-en-1-ol	C ₁₅ H ₂₄ O	24.10	81.58	0.720
16	1632-73-1	Fenchol	C ₁₀ H ₁₈ O	8.03	81,23	0.071
17	7220-78-2	(2E,6E,11Z)-3,7,13-Trimethyl-10-propan-2-ylcyclohexadeca-2,6,11-triene-1,13-diol	C ₂₀ H ₃₄ O ₂	49.45	85.19	0.239
Esters (8.052%)						
1	78277-23-3	Cinnamoin	C ₁₆ H ₁₄ O ₂	39.76	86.40	0.043
2	1686-54-0	Isopimara-8(14),15-dien-19-saeure-methylester	C ₂₁ H ₃₂ O ₂	46.40	92.70	1.517
3	1235-74-1	Methyl dehydroabietate	C ₂₁ H ₃₀ O ₂	50.00	90.84	1.842
4	-	(6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl ethyl carbonate	C ₁₃ H ₂₀ O ₃	11.80	87.70	0.108
5	-	Phthalic acid, di(oct-3-yl) ester	C ₂₄ H ₃₈ O ₄	58.31	85.52	0.011
6	80-26-2	α-Terpinyl acetate	C ₁₂ H ₂₀ O ₂	12.27	85.23	1.901
7	84-74-2	dibutyl phthalate	C ₁₆ H ₂₂ O ₄	34.39	89.48	0.126
8	1000373-80-3	Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate	C ₁₃ H ₂₂ O ₄	7.26	83.61	0.101
9	-	(2E,6E,10E)-3,7,11,15-Tetramethylhexadeca-2,6,10,14-tetraen-1-yl formate	C ₂₁ H ₃₄ O ₂	37.44	83.32	0.272
10	1079-01-2	Myrtenyl acetate	C ₁₂ H ₁₈ O ₂	11.34	82.92	0.361
11	7042-36-6	t-Butyl cinnamate	C ₁₃ H ₁₆ O ₂	31.08	81.98	0.466
12	78-35-3	Linalyl isobutyrate	C ₁₄ H ₂₄ O ₂	10.49	81.89	0.762
13	-	Butyl 6,9,12-hexadecatrienoate	C ₂₀ H ₃₄ O ₂	40.45	81.59	0.542
Phenols (1.364%)						
1	93-15-2	Methyleugenol	C ₁₁ H ₁₄ O ₂	13.58	94.44	0.513
2	119-47-1	2,2-Methylenebis(6-Tert-Butyl-4-Methylphenol)	C ₂₃ H ₃₂ O ₂	53.24	93.68	0.851
Ketones (1.057%)						
1	2426-02-0	3,4,5,6-Tetrahydrophthalic anhydride	C ₈ H ₈ O ₃	5.94	85.48	0.004

2	464-48-2	(-)-Camphor	C ₁₀ H ₁₆ O	8.62	92.99	0.423
3	473-08-5	α-Cyperone	C ₁₅ H ₂₂ O	25.37	83.43	0.542
4	1196-01-6	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-, (1S)-	C ₁₀ H ₁₄ O	9.78	81.98	0.088
Others (5.017%)						
1	21195-59-5	1,5,8-p-Menthatriene	C ₁₀ H ₁₄	8.43	89.59	0.058
2	31574-44-4	2-isopropyl-4-methyl anisole	C ₁₁ H ₁₆ O	10.15	85.27	0.466
3	540-97-6	Cyclohexasiloxane, dodecamethyl-	C ₁₂ H ₃₆ O ₆ Si ₆	10.30	86.53	0.074
4	556-67-2	Octamethylcyclotetrasiloxane	C ₈ H ₂₄ O ₄ Si ₄	5.82	90.44	0.002
5	242794-76-9	Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	C ₁₅ H ₂₄	13.77	84.75	0.751
6	66575-55-1	Hexacosane, 1-iodo-	C ₂₆ H ₅₃ I	68.71	84.62	0.042
7	934-74-7	Benzene, 1-ethyl-3,5-dimethyl-	C ₁₀ H ₁₄	6.41	84.20	0.310
8	1686-62-0	Isopimaric acid methyl ester	C ₂₁ H ₃₂ O ₂	48.10	83.91	0.445
9	-	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,4a-dimethyl-7-(1-methylethylidene)-, methyl ester, [1R-(1.α,4a.β,10a.α.)]-	C ₂₁ H ₃₂ O ₂	53.79	83.84	0.520
10	483-78-3	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-	C ₁₅ H ₁₈	22.52	83.40	0.388
11	18772-36-6	Cyclodecasiloxane, eicosamethyl-	C ₂₀ H ₆₀ O ₁₀ Si ₁₀	54.36	83.17	0.032
12	63180-33-6	Muurol-5-en-4-one <cis-14-nor->	C ₁₄ H ₂₂ O	24.53	83.15	1.126
13	106-49-0	p-Aminotoluene	C ₇ H ₉ N	19.13	83.15	0.505
14	-	5-(4-Hexyloxybenzoyloxy)-2-(4-nitrophenyl)pyrimidine	C ₂₃ H ₂₃ N ₃ O ₅	47.79	82.57	0.101
15	618-47-3	m-Toluamide	C ₈ H ₉ NO	12.16	81.39	0.123
16	1918-11-2	terbucarb	C ₁₇ H ₂₅ NO ₂	15.80	80.65	0.054
17	78134-83-5	Isoparvifuran	C ₁₆ H ₁₄ O ₃	36.62	80.52	0.007
18	17978-55-1	Phenyl-1,2-diamine, N,4,5-trimethyl-	C ₉ H ₁₄ N ₂	9.45	80.26	0.013

"-" Indicates that the component is not queried in the database.