

## **Supplementary Materials**

### **Network Pharmacology and Molecular Modeling to Elucidate the Potential Mechanism of Neem Oil against Acne Vulgaris**

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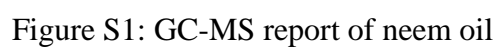


Table S1: Phytocompounds from neem oil based on GC-MS

Pk#	RT	Area%	Compound name
1	2.193	108.73	Cyclohexane
2	7.911	-0.10	(E)-2-bromobutyloxychalcone d-Threo-O-ethylthreonine Indolizine, 2-(4-methylphenyl)-
3	7.998	-0.22	Cyclopentasiloxane, decamethyl- Heptasiloxane,
4	9.793	-0.76	Cyclohexasiloxane, dodecamethyl-
5	10.901	-0.05	Hexahydropyridine, 1-methyl-4-[4,5 dihydroxyphenyl]- 4-(1H-[1,2,4]Triazole-3-carbonyl)- piperazine-1-carboxylic acid ethyl ester Oleic Acid
6	11.120	-0.69	Cycloheptasiloxane, tetradecamethyl- 3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetra siloxane 2-(2',4',4',6',6',8',8'-Heptamethyltetrasiloxan-2'-yloxy)-2,4,4,6,6,8,8,10,10-nonamethylcyclopentasiloxane
7	11.251	-0.09	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9, 11,11-dodecamethyl-Benzeneacetic acid, .alpha.-oxo trimethylsilyl ester 1-Propanone, 1,3-diphenyl-3-(trimethylsilyl)-
8	11.338	-0.02	1H-Benzo[4,5]furo[3,2-f]indole 2,3,5,6-Tetrafluorophenyl isothiocyanate N-Methyl-1-adamantaneacetamide
9	11.664	-0.14	1,4-Cyclohexanedimethanamine E-11-Tetradecenoic acid Chloroacetic acid, 2-tridecyl este
10	11.951	-0.28	Silane, trimethyl(4-phenylbutyl)- Acetamide, 2-[2,3-dihydro-2-methyl-5-(4-methylphenyl)-1,3,4-thiadiaz ol-2-yl]-N-phenyl- 2-Fluoro-5-(trifluoromethyl) benzamide
11	12.058	-0.04	Oleic Acid l-(+)-Ascorbic acid 2,6-dihexadecanoate D-Glucopyranose, 4,6-O-octylidene-
12	12.208	-0.35	N-(Trifluoroacetyl)-O,O',O''-tris(trimethylsilyl)epinephrine Cyclooctasiloxane, hexadecamethyl- N-(Trifluoroacetyl)-O,O',O''-tris(trimethylsilyl)norepinephrine
13	12.302	-0.07	

			Oleic Acid Trichloroacetic acid, 2-tetradecyl ester Methyl pentadecyl ether
14	12.383	-0.03	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester Cyclododecane Ethyl 9-hexadecenoate
15	12.646	-0.09	Oleic Acid 6-Octadecenoic acid 9-Octadecenoic acid, (E)-
16	12.815	-0.09	13-Octadecenal, (Z)- E-11-Hexadecenoic acid, ethyl este cis-11-Hexadecenal
17	13.109	-0.45	Morphinan, 7,8-didehydro-4,5-epoxy-17-methyl-3,6- bis[(trimethylsilyl)oxy]-, (5.alpha.,6.alpha.)- Cyclononasiloxane, octadecamethyl- Octasiloxane, 1,1,3,3,5,5,7,7,9,9, 11,11,13,13,15,15-hexadecamethyl-
18	13.346	-0.26	Oleic Acid Oleic Acid 6-Octadecenoic acid, (Z)-
19	13.396	-0.09	Oleic Acid 2-Trifluoroacetoxypentadecane 2-Tetradecanol
20	13.447	-0.13	Oleic Acid Z-10-Pentadecen-1-ol cis-1,2-Cyclododecanediol
21	13.490	-0.07	Oleic Acid Cyclopentadecanone, 2-hydroxy- 6-Octadecenoic acid, (Z)-
22	13.528	-0.09	Cyclopentadecanone, 2-hydroxy- 9-Octadecenal, (Z)- 13-Octadecenal, (Z)-
23	13.572	-0.11	13-Octadecenal, (Z)- Oleic Acid Butyl 9-octadecenoate or 9-18:1
24	13.753	-0.49	cis-11-Hexadecenal Cycloeicosane

			9-Hexadecenoic acid, methyl ester, (Z)-
25	13.797	-0.33	Cyclopropaneoctanal, 2-octyl- 9-Octadecenal, (Z)- 9-Tricosene, (Z)-
26	13.897	-0.30	Oleic Acid n-Propyl 9-octadecenoate 1,3-Dioxolane, 4-ethyl-5-octyl-2,2-bis(trifluoromethyl)-, trans-
27	14.041	-0.77	Oleic Acid 2-Methyl-Z, Z-3,13-octadecadienol 9-Octadecenoic acid (Z)-, methyl ester
28	14.078	-0.49	13-Octadecenal, (Z)- cis-11-Hexadecenal 1-Heptadecene
29	14.160	-0.26	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate cis-7,cis-11-Hexadecadien-1-yl acetate 2-Decen-1-ol, (E)-
30	14.216	-0.21	9-Hexadecenoic acid, methyl ester, (Z)- 12-Octadecenoic acid, methyl ester Ethyl 9-hexadecenoate
31	14.266	-0.10	Oleic Acid 3-Trifluoroacetoxypentadecane 2-Trifluoroacetoxypentadecane
32	14.285	-0.08	Oleic Acid E-11-Tetradecenoic acid Z-6-Pentadecen-1-ol acetate
33	14.341	-0.32	Oleic Acid l-(+)-Ascorbic acid 2,6-dihexadecanoate 9-Hexadecenoic acid, octadecyl ester
34	14.397	-0.43	Oleic Acid 5,14,23-Octadecatrien-14,15-diol Propanamide, N-(3-methoxyphenyl)-2,2-dimethyl-
35	14.591	-0.24	Oleic Acid Methyl pentadecyl ether Dodecane, 1-(methoxymethoxy)-

36	14.679	-0.23	n-Propyl 11-octadecenoate Methyl pentadecyl ether Oleic Acid
37	14.935	-0.05	Hexadecanoic acid, 2-hydroxy-, methyl ester Oleic Acid Methyl pentadecyl ether
38	15.004	-0.19	15-Tetracosenoic acid, methyl ester, (Z)- Oxacyclotetradecane-2,11-dione, 13-methyl- 6-Octadecenoic acid, (Z)-
39	15.092	-0.03	Oleic Acid 9-Hexadecenoic acid, octadecyl ester Oleic Acid