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Article

Exploring the Therapeutic Potential of Ammodaucus leucotrichus Seed Extracts: A Multi-Faceted Analysis of Phytochemical Composition, Anti-Inflammatory Efficacy, Predictive Anti-Arthritic Properties, and Molecular Docking Insights

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Supplementary information

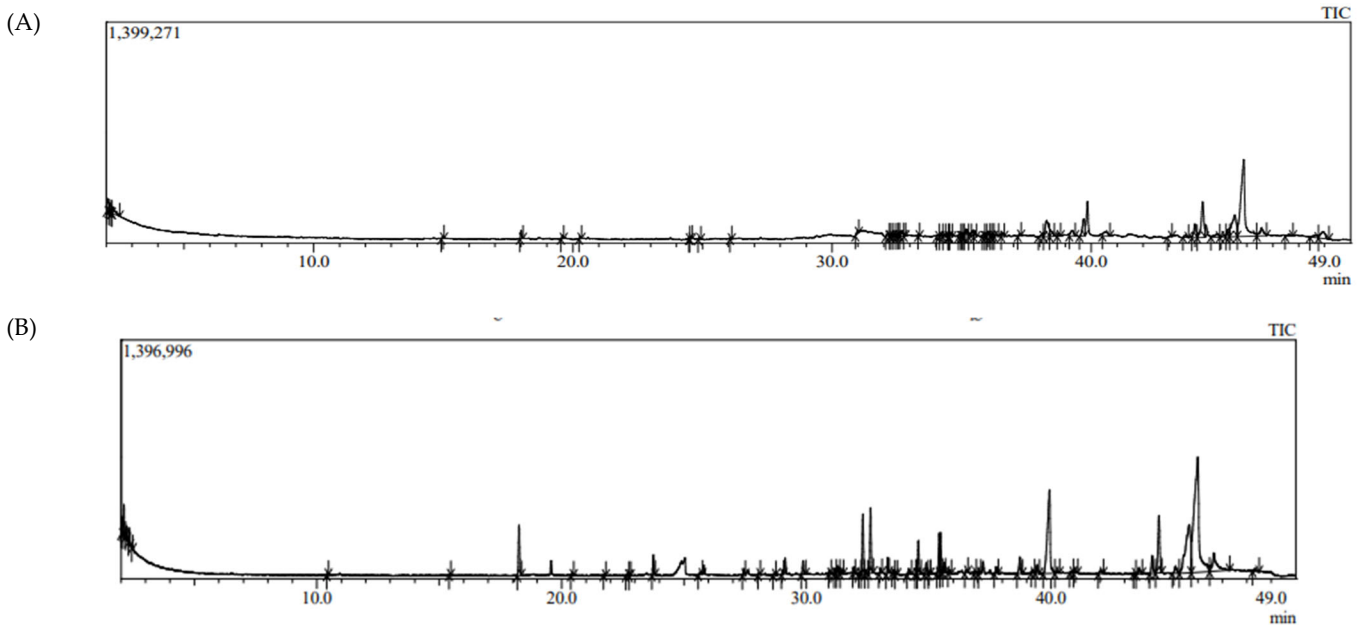
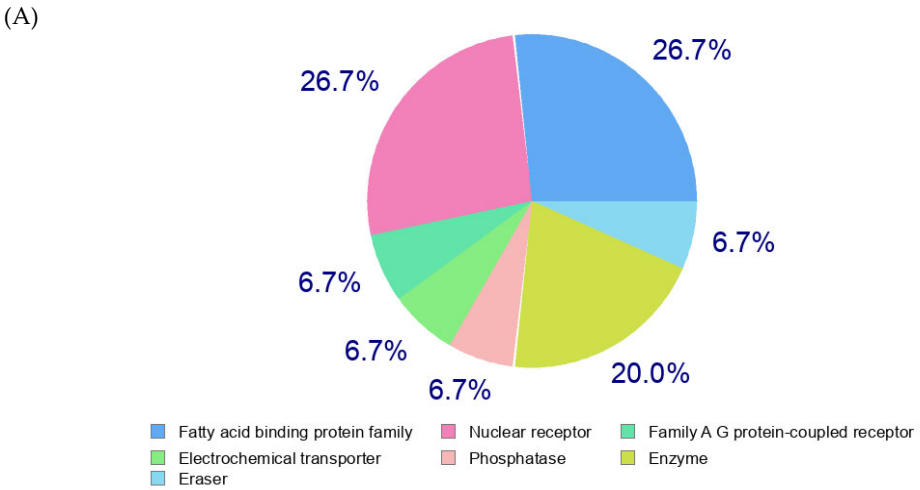


Figure S1. Gas chromatography-mass spectrometry analysis of (A) the methanol and (B) n-hexane extracts of *Ammodaucus leucotrichus* seeds. The chromatograms show the abundance of the different compounds in relation to their retention time (in minutes).



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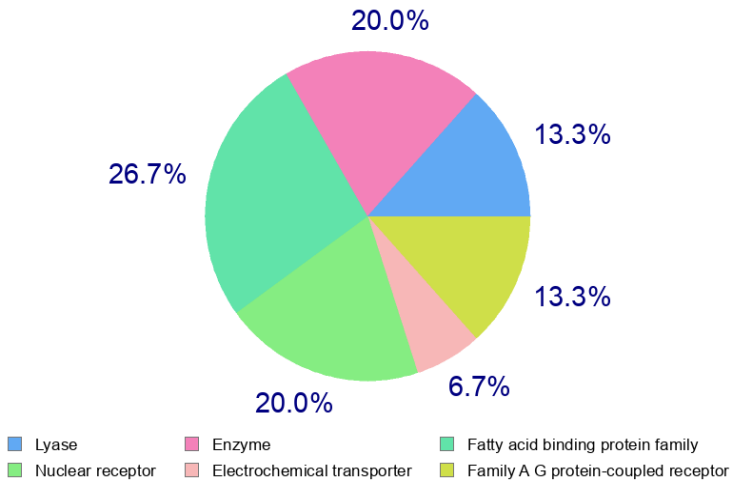
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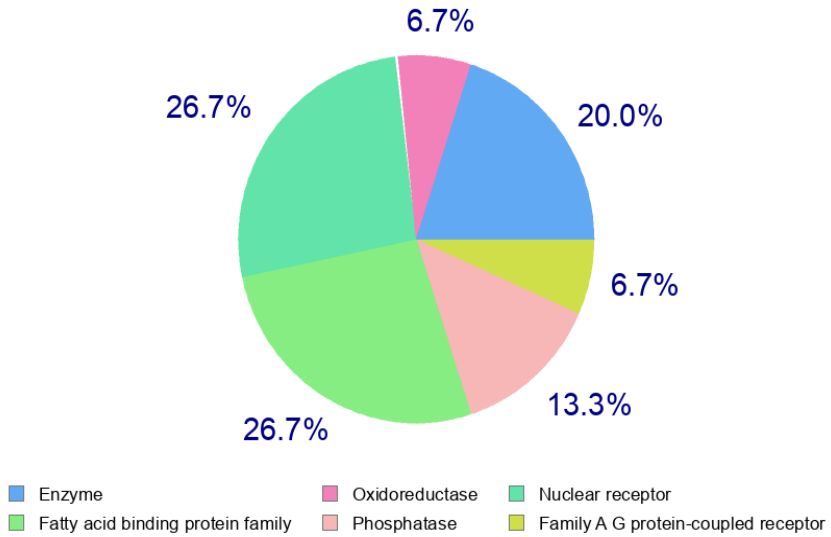
13.3%
26.7%
13.3%
6.7%
20.0%
Lyase
Enzyme
Fatty acid binding protein family
Nuclear receptor
Electrochemical transporter
Family A G protein-coupled receptor

(C)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26.7%
20.0%
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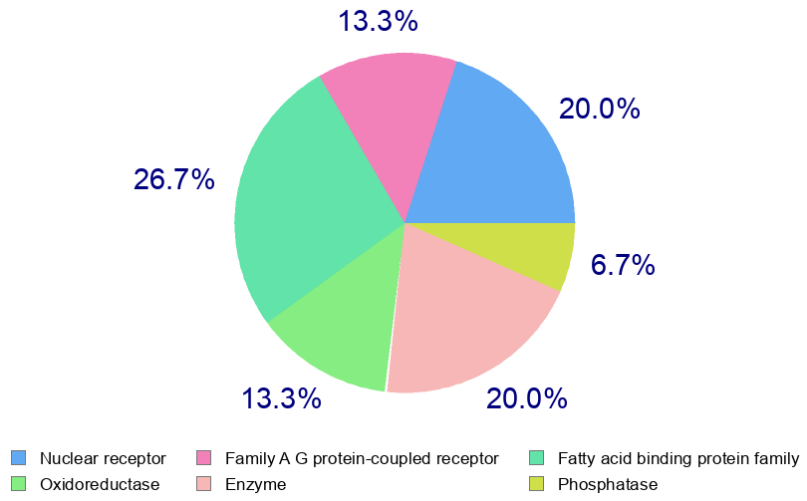
Enzyme
Oxidoreductase
Nuclear receptor
Fatty acid binding protein family
Phosphatase
Family A G protein-coupled receptor

(D)


13.3%
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Nuclear receptor
Family A G protein-coupled receptor
Fatty acid binding protein family
Oxidoreductase
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Phosphatase

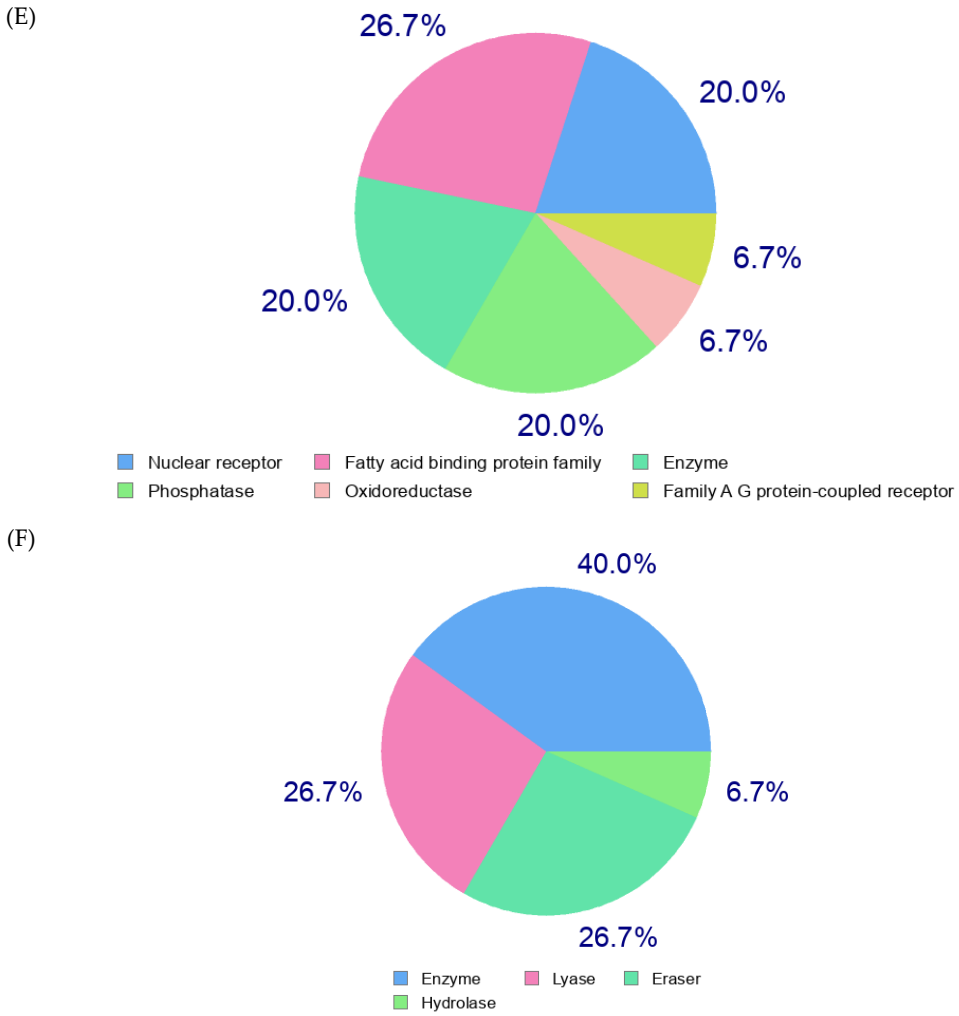

Figure S2. Data on the predicted target of the selected compounds identified in the Ammodaucus leucotrichus methanol extract. The selected compounds, namely (A) n-hexadecanoic acid, (B) hexadecanoic acid methyl ester, (C) 9-octadecenoic acid methyl ester (E)-, (D) (9Z, 12Z)-Octadeca-9,12-dienoic acid, (E) 9-octadecenoic acid, and (F) 2-hydroxyacetohydrazide, exhibit interactions with probable targets, including enzymes, the fatty acid binding protein family, G-protein-coupled receptors, and nuclear receptors.

Table S1. Comprehensive list of the phytochemicals identified in the methanol extract by gas chromatography-mass spectrometry. The table includes compound name, molecular formula, molecular weight, retention time, peak area, and PubChem Compound Identifier (CID).

N°	*Compound*	Classification	*Chemical formula*	*Molecular weight (g/mol)*	*Retention time (min)*	*Peak area (%)*	PubChem CID
S1	9-Octadecenoic acid	Fatty Acid	C18H34O2	282.5	45.880	29.69	637517
S2	Methyl(9Z,12Z)-octadeca-9,12-dienoate	Fatty Acid Ester	C19H36O2	296.5	44.296	8.87	5280590
S3	Octadeca-9,12-dienoic acid	Fatty Acid	C18H32O2	280.4	45.537	8.77	5280450
S4	Methyl hexadecanoate	Fatty Acid Ester	C17H34O2	270.5	38.275	4.87	8181

S5	n-Hexadecanoic acid	Fatty Acid	C16H32O2	256.42	39.713	3.86	985
S6	Methyl (9Z,12Z)-octadeca-9,12-dienoate	Fatty Acid Ester	C19H34O2	294.5	43.994	2.89	5284421
S7	Trichothec-9-ene-3,4,8,15-tetrol, 12,13-epoxy-, 15-acetate 8-(3-methylbutanoate), (3.alpha.,4.beta.,8.alpha.)-	Trichothecene	C22H32O8	424.5	48.948	2.89	520286
S8	Octadecanoic acid	Fatty Acid	C18H36O2	284.5	46.557	2.76	5281
S9	(6Z,9Z,12Z,15Z)-neophytadiene	Sesquiterpene	C20H38	278.5	35.173	1.82	10446
S10	Methyl-5,9,13-trimethyltetradecanoate	Fatty Acid Ester	C18H36O2	284.5	45.295	1.75	554056
S11	Cis-7,8-Epoxy-2-methyloctadecane	Pheromone	C19H38O	282.5	40.551	1.61	205983
S12	3-Isopropyl-6,7-dimethyltricyclo[4.4.0.0(2,8)]decane-9,10-diol	Tricyclic Alcohol	C15H26	238.366	38.410	1.57	491383
S13	2-hydroxyacetohydrazide	Hydrazide	C2H6N2O2	90.08	2.240	1.53	350536
S14	Phthalic acid, butyl hept-4-yl ester	Phthalate Ester	C19H28O4	320.4	38.269	1.45	91720764
S15	Kauren-19-yl-acetate	Diterpene Ester	C22H34O2	330	44.870	1.31	537596
S16	4,4-Dimethyl-2-pentanone	Ketone	C7H14O	114.19	2.134	1.36	11546
S17	trans-(R,R)-chrysanthemyl (R)-2-methylbutanoate	Ester	C15H26O2	238.37	48.635	1.17	91693481
S18	3-Isopropyl-6,7-dimethyltricyclo[4.4.0.0(2,8)]decane-9,10-diol	Tricyclic Alcohol	C15H26O2	238.37	32.642	0.97	565273
S19	Phthalic acid, tetradecyl trans-dec-3-enyl ester	Phthalate Ester	C32H52O4	500.8	36.002	0.97	91719824
S20	5-Hydroxymethylfurfural	Furfural Derivative	C6H6O3	126.11	18.004	0.87	237332
S21	(1S,2R,4aS,8aS)-1,2,4a,5,8,8a-hexahydro-1,4a-dimethyl-7-(1-methylethyl)-1-naphthalenol	Sesquiterpene Alcohol	C15H24O	220.35	35.490	0.76	102303030
S22	8-Isopropyl-1,5-dimethyltricyclo[4.4.0.02,7]dec-4-en-3-one	Tricyclic Ketone	C15H22O	218.33	35.345	0.75	12313013
S23	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	Sesquiterpene Alcohol	C20H40O	296.5	36.591	0.68	5366244
S24	1-Tetracontane	Saturated Hydrocarbon	C40H82	563.1	47.624	0.68	20149

S25	5-nitrobenzofuran-2(3H)-one	Nitrobenzofuran	C8H3NO5	193.11	36.288	0.64	230976
S26	6-(3-Hydroxyprop-1-en-2-yl)-4,8α-dimethyl-2,4α,5,6,7,8-hexahydro-1H-naphthalen-2-ol	Naphthalene Derivative	C15H24O2	236.35	43.610	0.64	535256
S27	(1R,3R,4S,7S)-3,7-dimethyl-1-(propan-2-yl)bicyclo[4.4.0]dec-3-ene-2,6-diol	Sesquiterpene Alcohol	C15H24O	220.35	32.184	0.63	102303030
S28	(2R,5S)-5-[(1R)-1,5-dimethylhex-4-en-1-yl]-2-methylcyclohex-2-en-1-one	Sesquiterpene Aldehyde	C15H24O	220.35	34.931	0.60	565584
S29	1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1ar-(1a.alpha.,4a.alpha.,7.beta.,7a.beta.,7b.alpha.)]-	Sesquiterpene Alcohol	C15H24O	220.35	34.590	0.59	6432640
S30	2,4,7,14-Tetramethyl-4-vinyl-tricyclo[5.4.3.0(1,8)]tetradecan-6-ol	Sesquiterpene Alcohol	C20H34O	290.5	35.872	0.59	590916
S31	2-(trans-2,6,6-Trimethylbicyclo[3.3.1]heptan-3-yl)buta-1,3-diene	Terpene	C14H22	190	45.116	0.58	13895
S32	2-aminopropan-1-ol	Amino Alcohol	C3H9NO	75.11	2.205	0.57	5126
S33	(1R,4R,6R,10S)-4,12,12-Trimethyl-9-methylene-5 oxatricyclo[8.2.0.04,6]dodecane	Tricyclic Terpene	C15H24O	220.35	30.995	0.55	1742210
S34	Octahydro-2-benzothiophene	Polycyclic Aromatic Hydrocarbon (PAH)	C20H20O	276.4	35.940	0.54	155017
S35	n-tetradecanoic acid	Fatty Acid	C14H28O2	228.37	34.215	0.49	11005
S36	Methyl 16-R/S-hydroxy-cleroda-3,13(14)-Z-dien-15,16-olide	Diterpene	C22H32O4	360.5	35.014	0.47	16042541
S37	3beta-Trimethylsiloxy-5alpha,6alpha-epoxycholestane	Steroid	C30H54O2Si	474.8	32.394	0.43	16082384
S38	Methyl hexadecanoate	Fatty Acid Ester	C17H34O2	270.5	38.736	0.41	8181
S39	1-dodecyltrichlorosilane	Organosilicon Compound	C12H25Cl3Si	303.8	32.610	0.38	20568
S40	4-Isopropyl-1,7,11-trimethyl-2,7,11-cyclotetradecatrien-1-ol	Not available	C20H34O	290.5	32.330	0.39	5363523

S41	3-Hydroxy-3-methyl-butyric acid, hydrazide	Hydrazide	C5H12N2O2	132.16	35.075	0.38	299142
S42	4-Prop-1-en-2-ylcyclohexene-1-carboxylic acid	Carboxylic Acid	C10H14O	150.22	19.592	0.35	16441
S43	2-Ethylidene-1,7,7-trimethylbicyclo[2.2.1]heptane	Terpene	C12H20	164.29	34.099	0.33	143908
S44	octadecamethyl-1,2,3,4,5,6,7,8,9-nonasiloxane	Siloxane	C18H54O9Si9	667.4	36.130	0.33	11172
S45	Spiro[5.6]dodecan-7-one	Ketone	C12H20O	180.29	32.535	0.30	282264
S46	1-(1,5-Dimethylhexyl)-10-hydroxy-3a,6,6,9a,11a-pentamethylhexadecahydrocyclopenta[7,8]- phenanthro[8a,9-b]oxiren-7-yl acetate	Terpene Ester	C32H54O4	502.8	34.350	0.31	541562
S47	(2R,5S)-5-[(1R)-1,5-dimethylhex-4-en-1-yl]-2-methylcyclohex-2-en-1-one	Sesquiterpene Aldehyde	C15H24	220.350	37.249	0.30	103883460
S48	Heptadecanoic acid	Fatty Acid	C17H34O2	270.5	43.056	0.29	10465
S49	4-Prop-1-en-2-ylcyclohexene-1-carboxylic acid	Carboxylic Acid	C10H14O2	166.22	24.881	0.28	1256
S50	1,2,3,4,5-Penta-O-acetyl-D-xylitol	Xylitol Derivative	C15H22O10	362.33	36.225	0.27	219891
S51	2-isopropyl-5-methylphenol	Phenol Derivative	C10H14O	150.22	20.286	0.25	6989
S52	4'-Hydroxybutyrophenone oxime	Phenolic Oxime	C10H13NO2	179.22	32.775	0.22	135822598
S53	3,5-Dihydroxy-6-methyl-2,3-dihydropyran-4-one	Phenol Derivative	C6H8O4	144.12	14.971	0.20	119838
S54	Formic acid, undecyl ester	Formate Ester	C12H24O2	200.32	26.082	0.20	229382
S55	Cyclopentanol	Cycloalkanol	C5H10O	86.13	24.533	0.19	7298
S56	2,2-bis(oxidanylidene)-1,5-dihydroimidazo[4,5-c][1,2,6]thiadiazin-4-one	Imidazothiadiazinone	C4H4N4O3S	188.17	32.245	0.19	12413165
S57	Spiro[5.5]undeca-1,7-diene	Diene	C11H16	148.24	33.340	0.15	590470
S58	[(Z)-4-Methylsulfonyloxybut-2-enyl] 2-(tert-butoxycarbonylamino)acetate	Ester	C12H21NO7S	323.36	24.495	0.13	5365168
S59	2H-Quinolizine-1-methanol, octahydro-	Quinolizine Derivative	C10H19NO	169.26	34.510	0.13	297272
S60	Fumaric acid, 3,5-dimethylphenyl cyclohexylmethyl ester	Fumarate Ester	C19H24O4	316.4	34.485	0.09	91711292

Table S2. Comprehensive list of the phytochemicals identified in the n-hexane extract by gas chromatography-mass spectrometry. The table includes compound name, molecular formula, molecular weight, retention time, peak area, and PubChem Compound Identifier (CID).

N°	*Compound*	Classification	*Chemical formula*	*Molecular weight (g/mol)*	*Retention time (min)*	*Peak area (%)*	PubChem CID
S1	*9-Octadecenoic acid*	*Fatty Acid*	*C18H34O2*	*282.5*	*45.998*	*29.17*	637517
S2	*Octadeca-9,12-dienoic acid*	*Fatty Acid*	*C18H32O2*	*280.4*	*45.652*	*12.49*	5280450
S3	*n-Hexadecanoic acid*	*Fatty Acid*	*C16H32O2*	*256.42*	*39.938*	*11.81*	985
S4	*Methyl(9Z,12Z)-octadeca-9,12-dienoate*	*Ester*	*C19H36O2*	*296.5*	*44.412*	*5.36*	5280590
S5	*Octadecanoic acid*	*Fatty Acid*	*C18H36O2*	*284.5*	*46.660*	*4.17*	5281
S6	*3-Isopropyl-6,7-dimethyltricyclo[4.4.0.(2,8)]decane-9,10-diol*	*Terpenoid*	*C15H26O2*	*238.37*	*32.416*	*3.96*	565273
S7	*Cyclohexanol, 3-ethenyl-3-methyl-2-(1-methylethenyl)-6-(1-methylethyl)-, (1R,2S,3S,6S)-*	*Alcohol*	*C15H26O*	*222.37*	*32.190*	*3.63*	101316861
S8	*4-Prop-1-en-2-ylcyclohexene-1-carbaldehyde*	*Aldehyde*	*C10H14O*	*150.22*	*15.435*	*3.02*	16441
S9	*Citronellyl tiglate*	*Ester*	*C15H26O2*	*238.37*	*35.032*	*2.53*	6386037
S10	*Isospathulenol*	*Alcohol*	*C15H24O*	*220.35*	*35.430*	*2.34*	14038848
S11	*Spathulenol*	*Alcohol*	*C15H24O*	*220.35*	*34.504*	*2.02*	92231
S12	*Methyl (9Z,12Z)-octadeca-9,12-dienoate*	*Ester*	*C19H34O2*	*294.5*	*44.135*	*1.63*	5284421
S13	*Methyl hexadecanoate*	*Ester*	*C17H34O2*	*270.5*	*38.723*	*1.27*	8181
S14	*3-Methylheptane*	*Hydrocarbon*	*C8H18*	*114.23*	*2.024*	*1.22*	11519
S15	*5,5-diethyl-4-methyl-6-spiro[2.3]hexan*	*Hydrocarbon*	*C11H18O*	*166.26*	*22.783*	*1.05*	550247
S16	*6-Methyl-1,2,3,5,8,8a-hexahydronaphthalene*	*Hydrocarbon*	*C11H16*	*148.24*	*33.025*	*0.88*	562093
S17	*2,6-Dimethoxy-4-(prop-2-en-1-yl)phenol*	*Phenol*	*C11H14O3*	*194.23*	*29.040*	*0.79*	226486
S18	*(3,7,7-Trimethyl-bicyclo[2.2.1]hept-2-yl)-methanol*	*Alcohol*	*C11H20O*	*168.28*	*34.191*	*0.75*	558050
S19	*Stigmastan-6,22-dien, 3,5-dedihydro-*	*Sterol*	*C29H46*	*394.7*	*45.088*	*0.74*	5364573
S20	*1,4-Dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,5,6,7,8-octahydroazulene*	*Terpenoid*	*C15H24*	*204.35*	*31.183*	*0.71*	5317844
S21	*2(3H)-Benzofuranone, 6-ethenylhexahydro-3,6-dimethyl-5-(1-methylethenyl)-*	*Lactone*	*C15H22O2*	*234.33*	*34.577*	*0.65*	14038380

S22	*3-Isopropyl-6,7-dimethyltricyclo[4.4.0.(2,8)]decane-9,10-diol*	*Terpenoid*	*C15H26O2*	*238.37*	*39.430*	*0.62*	565273
S23	*Cholest-5-en-3-ol (3.beta.)-, propanoate*	*Steroid*	*C30H50O2*	*442.7*	*43.595*	*0.59*	12451
S24	*2(3H)-Benzofuranone, 6-ethenylhexahydro-3,6-dimethyl-5-(1-methylethenyl)-*	*Lactone*	*C15H22O2*	*234.33*	*35.483*	*0.58*	14038380
S25	*Myristic acid*	*Fatty Acid*	*C14H28O2*	*228.37*	*33.676*	*0.44*	11005
S26	*2-Isopropyl-4a-methyl-8-methylenedecalin-1,5-diol*	*Terpenoid*	*C15H26O2*	*238.37*	*37.755*	*0.42*	14137570
S27	*Cyclohexanol, 3-ethenyl-3-methyl-2-(1-methylethenyl)*	*Alcohol*	*C15H26O*	*222.37*	*25.630*	*0.36*	101316861
S28	*2,2-Dimethylhexane*	*Hydrocarbon*	*C8H18*	*114.23*	*2.204*	*0.34*	11551
S29	*Gamma-dodecalactone*	*Lactone*	*C12H22O2*	*198.3*	*31.423*	*0.34*	16821
S30	*1H-cycloprop(e)azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-(1AR,4AR,7S,7AR,7BR)-*	*Terpenoid*	*C15H24O*	*220.35*	*28.699*	*0.32*	92231
S31	*1,3,5-Trimethyl-2,6-di(cyclopentyl)benzene*	*Hydrocarbon*	*C19H28*	*256.399*	*42.018*	*0.30*	620628
S32	*1,1,4,7tetramethyldecahydro-1H-cyclopropa(e)azulen-4-ol*	*Terpenoid*	*C15H26O*	*222.37*	*32.623*	*0.27*	11996452
S33	*2(3H)-Furanone, 5-hexyldihydro-*	*Lactone*	*C10H18O2*	*170.25*	*23.746*	*0.26*	12813
S34	*2-(Tricyclo[3.3.1.13,7]dec-1-yl)propanoic acid*	*Carboxylic Acid*	*C13H18O2*	*206.28*	*32.311*	*0.26*	609874
S35	*2-Naphthalenemethanol, decahydro-.al*	*Alcohol*	*C15H26O*	*222.37*	*30.962*	*0.25*	91457
S36	*Juniper camphor (1,4a-dimethyl-7-propan-2-ylidene-3,4,5,6,8,8a-hexahydro-2H-naphthalen-1-ol)*	*Terpenoid*	*C15H26O*	*222.37*	*31.297*	*0.24*	521214
S37	*Taylorione (4-[(1S,3R)-2,2-dimethyl-3-(5-methylidenecyclopenten-1-yl)cyclopropyl]butan-2-one)*	*Terpenoid*	*C15H22O*	*218.33*	*40.235*	*0.24*	12152394
S38	*Sinulariolide ((8Z)-12-hydroxy-5,9,13-trimethyl-16-methylidene-4,14-dioxatricyclo[11.3.2.03,5]octadec-8-en-15-one)*	*Macrolide*	*C20H30O4*	*334.4*	*39.252*	*0.22*	5358848
S39	*1-((1S,3aR,4R,7S,7aS)-4-Hydroxy-7-isopropyl-4-methyloctahydro-1H-inden-1-yl)ethan-1-one*	*Ketone*	*C15H26O2*	*238.37*	*33.324*	*0.21*	10466745
S40	*1,1,4,7-Tetramethyldecahydro-1H-cyclopropa[e]azulen-7-ol*	*Terpenoid*	*C15H26O*	*222.37*	*35.633*	*0.21*	11996452

S41	*4-Isobenzofuranol, octahydro-3a,7a-dimethyl-*	*Alcohol*	*C10H18O2*	*170.25*	*36.541*	*0.21*	41057
S42	*(1S,3aS,4S,5S,7aR,8R)-5-Isopropyl-1,7a-dimethyloctahydro-1H-1,4-methanoinden-8-ol*	*Terpenoid*	*C15H26O*	*222.37*	*29.866*	*0.20*	12303891
S43	*2-Oxabicyclo[4.2.0]oct-4-en-3-one, rel*	*Ketone*	*C28H22F2O6*	*492.5*	*48.336*	*0.20*	5377136
S44	*Platambin (4a-methyl-8-methylidene-2-propan-2-yl-1,2,3,4,5,6,7,8a-octahydronaphthalene-1,5-diol)*	*Terpenoid*	*C15H26O2*	*238.37*	*37.086*	*0.19*	613194
S45	*(1R,7S,E)-7-Isopropyl-4,10-dimethylenecyclodec-5-enol*	*Terpenoid*	*C15H24O*	*220.35*	*31.944*	*0.15*	13304974
S46	*(E)-Valerenyl isovalerate*	*Ester*	*C20H32O2*	*304.5*	*40.978*	*0.15*	91730081
S47	*Dodecanoic acid*	*Fatty Acid*	*C12H24O2*	*200.32*	*28.066*	*0.14*	3893
S48	*1-Nonadecene*	*Alkene*	*C19H38*	*266.5*	*40.815*	*0.11*	29075
S49	*(S)-(-)-(4-Isopropenyl-1-cyclohexenyl)methanol*	*Alcohol*	*C10H16O*	*152.23*	*18.261*	*0.11*	369312
S50	*4-(1-Methylvinyl)cyclohex-1-ene-1-ethyl formate*	*Ester*	*C12H18O2*	*194.27*	*21.755*	*0.10*	3023295
S51	*Spathulenol ((1aR,4aR,7S,7aR,7bR)-1,1,7-trimethyl-4-methylidene-1a,2,3,4a,5,6,7a,7b-octahydrocyclopropa[h]azulen-7-ol)*	*Alcohol*	*C15H24O*	*220.35*	*33.549*	*0.10*	92231
S52	*1-Naphthalenepropanol, .alpha.-ethenyldecahydro-2-hydroxy-alpha, 2,5,5,8a-pentamethyl*	*Terpenoid*	*C20H36O2*	*308.5*	*36.901*	*0.10*	163263
S53	*1,2-Cyclohexanediol, 1-methyl-4-(1-methylethenyl)*	*Alcohol*	*C10H18O2*	*170.25*	*20.427*	*0.09*	441246
S54	*3-Methylhexane*	*Hydrocarbon*	*C7H16*	*100.2*	*2.119*	*0.08*	11507
S55	*(3E)-6-Methyl-3,5-heptadien-2-one*	*Ketone*	*C8H12O*	*124.18*	*22.650*	*0.08*	5370101
S56	*Tricyclo[4.4.0.0(2,7)]dec-8-ene-3-methanol*	*Terpenoid*	*C15H24O*	*220.35*	*27.448*	*0.08*	521030
S57	*1-Nonadecene*	*Alkene*	*C19H38*	*266.5*	*34.896*	*0.08*	29075
S58	*(Z)-Dodec-5-en-4-olide*	*Lactone*	*C12H20O2*	*196.29*	*43.401*	*0.08*	67469926
S59	*3-Cyclohexene-1-carboxaldehyde*	*Aldehyde*	*C7H10O*	*110.15*	*2.459*	*0.05*	7508
S60	*4-Isopropenylcyclohexanone*	*Ketone*	*C9H14O*	*138.21*	*10.440*	*0.05*	549291
S61	*Heptane*	*Hydrocarbon*	*C7H16*	*100.2*	*2.329*	*0.04*	8900

Table S3. Comparison of the key phytocomponents (with their peak area) present in the methanol and n-hexane extracts, identified by gas chromatography/mass spectrometry.

N°	Methanol extraction		n-Hexane extraction	
	Compounds (IUPAC Name)	*Peak area (%)*	Compounds (IUPAC Name)	*Peak area (%)*
1	9-Octadecenoic acid	29.69	9-Octadecenoic acid	29.17
2	Methyl(9Z,12Z)-octadeca-9,12-dienoate	8.87	Octadeca-9,12-dienoic acid	12.49
3	Octadeca-9,12-dienoic acid	8.77	n-Hexadecanoic acid	11.81
4	Methyl hexadecanoate	4.87	Methyl(9Z,12Z)-octadeca-9,12-dienoate	5.36
5	n-Hexadecanoic acid	3.86	Octadecanoic acid	4.17
6	Methyl (9Z,12Z)-octadeca-9,12-dienoate	2.89	3-Isopropyl-6,7-dimethyltricyclo [4.4.0.(2,8)]decane-9,10-diol	3.96
7	Trichothec-9-ene-3,4,8,15-tetrol, 12,13-epoxy-, 15-acetate 8-(3-methylbutanoate), (3.alpha.,4.beta.,8.alpha.)-	2.89	Cyclohexanol, 3-ethenyl-3-methyl-2-(1-methylethenyl)-6-(1-methylethyl)-, (1R,2S,3S,6S)-	3.63
8	Octadecanoic acid	2.76	4-Prop-1-en-2-ylcyclohexene-1-carbaldehyde	3.02
9	Neophytadiene	1.82	Citronellyl tiglate	2.53
10	Methyl-5,9,13-trimethyltetradecanoate	1.75	Isospathulenol	2.34
11	Disparlure	1.61	Spathulenol	2.02
12	3-Isopropyl-6,7-dimethyltricyclo [4.4.0.0(2,8)]decane-9,10-diol	1.57	Methyl (9Z,12Z)-octadeca-9,12-dienoate	1.63
13	2-hydroxyacetohydrazide	1.53	Methyl hexadecanoate	1.27
14	Phthalic acid, butyl hept-4-yl ester	1.45	3-Methylheptane	1.22
15	2-Pentanone, 4,4-dimethyl-	1.36	5,5-diethyl-4-methyl-6-spiro[2.3]hexan	1.05
	Sum	76.10	Sum	85.67

Table S4: Impact of different concentrations of the methanol and n-hexane extracts from *Ammodaucus leucotrichus* seeds on BSA denaturation. Comparison with diclofenac (reference anti-inflammatory drug) in a BSA denaturation assay and IC_{50} values (µg/ml) for BSA denaturation inhibition. Data are the mean ± standard error of the mean.

Active ingredients	Concentration (µg/mL)	Log concentration (µg/mL)	Inhibition (%)	IC_{50} (µg/mL)
Methanol extract	3.00	0.59	5.67 ±0.50	5408.00
	7.81	0.89	13.67 ±0.50	
	15.62	1.19	14.67 ±0.50	
	31.20	1.49	17.67 ±0.50	
	62.50	1.79	22.00 ±0.00	
	125.00	2.09	24.67 ±0.50	
	250.00	2.39	26.00 ±0.00	
n-hexane extract	3.00	0.59	8.30 ±0.45	14.30
	7.81	0.89	20.93 ±0.32	

	15.62	1.19	56.14 ±0.05	
	31.20	1.49	84.05 ±0.45	
	62.50	1.79	90.36 ±0.57	
	125.00	2.09	91.33 ±0.57	
	250.00	2.39	94.00 ±0.00	
Diclofenac	3.00	0.59	10.67 ±0.15	42.30
	7.81	0.89	24.67 ±0.50	
	15.62	1.19	30.00 ±0.00	
	31.20	1.49	34.10 ±0.49	
	62.50	1.79	51.36 ±0.90	
	125.00	2.09	76.85 ±0.57	
	250.00	2.39	99.22 ±0.41	

Table S5: Trypsin inhibition by the methanol and n-hexane extracts from *Ammodaucus leucotrichus* seeds compared with Diclofenac (reference drug) at different concentrations, and IC_{50} values (µg/ml) for trypsin inhibition. Data are the mean ± standard error of the mean.

Active ingredients	Concentration (µg/mL)	Log concentration (µg/mL)	Inhibition (%)	IC_{50} (µg/mL)
Methanol extract	31.20	1.49	3.00 ±0.00	82.97
	62.50	1.79	23.00±0.00	
	125.00	2.09	85.00±0.57	
	250.00	2.39	100.00±0.01	
	500.00	2.69	100.00 ±0.01	
n-Hexane extract	31.20	1.49	6.00±0.00	202.70
	62.50	1.79	10.33±0.57	
	125.00	2.09	30.00±0.00	
	250.00	2.39	51.00±0.48	
	500.00	2.69	100.00±0.00	
Diclofenac	31.20	1.49	6.00±0.00	97.04
	62.50	1.79	23.00±0.00	
	125.00	2.09	64.67±0.57	
	250.00	2.39	100.00±0.00	
	500.00	2.69	100.00±0.00	

Table S6: Binding energies (in kJ/mol) of the 59 key compounds identified in the methanol extract from *Ammodaucus leucotrichus* seeds and of diclofenac during their interactions with trypsin. The different binding energy values reflect variations in the inhibitory potential of the compounds against trypsin.

N°	Compound	Classification	PubChem CID	Binding energy (KJ/mol)
S1	2-hydroxyacetohydrazide	Hydrazide	350536	-17.13

S2	3-Hydroxy-3-methyl-butyric acid, hydrazide	Hydrazide	299142	-14.44
S3	2,2-bis(oxidanylidene)-1,5-dihydroimidazo[4,5-c][1,2,6]thiadiazin-4-one	Imidazo Thiadiazinone	12413165	-14.39
S4	4'-Hydroxybutyrophenone oxime	Oxime	135822598	-13.45
S5	Diclofenac (2-[(2,6-dichlorophenyl)amino]benzeneacetic acid)		3033	-13.01
S6	3,5-Dihydroxy-6-methyl-2,3-dihydropyran-4-one	Pyranone	119838	-12.41
S7	6-(3-Hydroxyprop-1-en-2-yl)-4,8α-dimethyl-2,4α,5,6,7,8-hexahydro-1H-naphthalen-2-ol	Alcohol	535256	-11.44
S8	5-Hydroxymethylfurfural	Furfural	237332	-11.21
S9	5-nitrobenzofuran-2(3H)-one	Benzofuranone	230976	-9.89
S10	1-Propanol, 2-amino-, (.+/-.)-	Amino Alcohol	5126	-8.28
S11	(7S)-1,1,7-Trimethyl-4-methylidene-1α,2,3,4α,5,6,7α,7β-octahydrocyclopropa[h]azulen-7-ol	Sesquiterpene Alcohol	6432640	-8.01
S12	Spiro[5.6]dodecan-7-one	Ketone	282264	-7.27
S13	(1R,4R,6R,10S)-4,12,12-Trimethyl-9-methylene-5-oxatricyclo[8.2.0.04,6]dodecane	Triterpene	1742210	-5.99
S14	Cyclopentanol	Alcohol	7298	-5.83
S15	Thymol (2-isopropyl-5-methylphenol.)	Phenol	6989	-5.51
S16	Isospathulenol ((1R,4R,6R)-1,4,7,7-tetramethylbicyclo[4.1.0]heptan-2-ol)	Sesquiterpene Alcohol	102303030	-5.17
S17	Fumaric acid (3,5-dimethylphenyl cyclohexylmethyl ester)	Fumarate Ester	91711292	-4.87
S18	4-Prop-1-en-2-ylcyclohexene-1-carboxylic acid	Carboxylic Acid	1256	-4.82
S19	2H-Quinolizine-1-methanol, octahydro-	Quinolizine Alcohol	297272	-4.67
S20	8-Isopropyl-1,5-dimethyltricyclo[4.4.0.02,7]dec-4-en-3-one	Ketone	12313013	-4.74
S21	Formic acid undecyl ester (Undecyl methanoate)	Carboxylic Acid Ester	229382	-4.19
S22	[(Z)-4-Methylsulfonyloxybut-2-enyl] 2-(tert-butoxycarbonylamino)acetate	Ester	5365168	-4.17
S23	Phthalic acid, butyl hept-4-yl ester	Phthalate Ester	91720764	-3.19
S24	trans-(R,R)-chrysanthemyl (R)-2-methylbutanoate	Terpenoid Ester	91693481	-2.10
S25	4,4-dimethylpentan-2-one	Ketone	11546	-2.00
S26	2-Ethylidene-1,7,7-trimethylbicyclo[2.2.1]heptane	Bicyclic Hydrocarbon	143908	-1.51
S27	Thunbergol (4-Isopropyl-1,7,11-trimethyl-2,7,11-cyclotetradecatrien-1-ol)	Terpenoid	5363523	-1.39

S28	Methyl 16-R/S-hydroxy-cleroda-3,13(14)-Z-dien-15,16-olide	Diterpenoid Lactone	16042541	-0.56
S29	3beta-Trimethylsiloxy-5alpha,6alpha-epoxycholestane	Steroid	16082384	0
S30	Trichloro(dodecyl)silane	Organosilane	20568	0
S31	3-Isopropyl-6,7-dimethyltricyclo[4.4.0.0(2,8)]decane-9,10-diol	Sesquiterpene Alcohol	565273	0
S32	Spiro[5.5]undeca-1,7-diene (1,1,7,7-tetracyclo[6.4.0.0^{2,6}.0^{7,11}]dodeca-2,4,6,8,10-pentaene)	Hydrocarbon	590470	0
S33	n-tetradecanoic acid	Fatty Acid	11005	0
S34	1-(1,5-Dimethylhexyl)-10-hydroxy-3a,6,6,9a,11a-pentamethylhexadecahydrocyclopenta[7,8]-phenanthro[8a,9-b]oxiren-7-yl acetate	Sesquiterpene Ester	541562	0
S35	Longifolenaldehyde (2R,5S)-5-[(1R)-1,5-dimethylhex-4-en-1-yl]-2-methylcyclohex-2-en-1-one)	Aldehyde	565584	0
S36	Neophytadiene ((6Z,9Z,12Z,15Z)-neophytadiene)	Sesquiterpene	10446	0
S37	2,4,7,14-Tetramethyl-4-vinyl-tricyclo[5.4.3.0(1,8)]tetradecan-6-ol	Terpenoid Alcohol	590916	0
S38	Benzo - octahydro -acephenanthrylene	Hydrocarbon	155017	0
S39	Phthalic acid, tetradecyl trans-dec-3-enyl ester	Phthalate Ester	91719824	0
S40	Octadecamethyl-cyclononasiloxane	Siloxane	11172	0
S41	1,2,3,4,5-Penta-O-acetyl-D-xylitol	Xylitol Ester	219891	0
S42	4-Prop-1-en-2-ylcyclohexene-1-carbaldehyde	Aldehyde	16441	0
S43	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	Terpenoid Alcohol	5366244	0
S44	Longifolenaldehyde ((2R,5S)-5-[(1R)-1,5-dimethylhex-4-en-1-yl]-2-methylcyclohex-2-en-1-one)	Aldehyde	103883460	0
S45	Cyclopropanebutanoic acid, Methyl-4-[2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-cyclopropyl]butanoate	Cyclopropane Carboxylic Acid Ester	554084	0
S46	Methyl hexadecanoate	Fatty Acid Ester	8181	0
S47	n-Hexadecanoic acid	Fatty Acid	985	0
S48	Disparlure (cis-7,8-epoxy-2-methyloctadecane)	Pheromone	205983	0
S49	Heptadecanoic acid	Fatty Acid	10465	0
S50	Methyl (9Z,12Z)-octadeca-9,12-dienoate	Fatty Acid Ester	5284421	0
S51	Methyl(9Z,12Z)-octadeca-9,12-dienoate	Fatty Acid Ester	5280590	0
S52	Kauren-19-yl-acetate	Diterpene Ester	5284421	0
S53	2-(trans-2,6,6-Trimethylbicyclo[3.3.1]heptan-3-yl)buta-1,3-diene	Terpenoid Diene	5280590	0
S54	Methyl-5,9,13-trimethyltetradecanoate	Fatty Acid Ester	554056	0
S55	Octadeca-9,12-dienoic acid	Fatty Acid	5280450	0

S56	9-Octadecenoic acid	Fatty Acid	637517	0
S57	Octadecanoic acid	Fatty Acid	5281	0
S58	Tetracontane	Hydrocarbon	20149	0
S59	Trichothec-9-ene-3,4,8,15-tetrol, 12,13-epoxy-, 15-acetate 8-(3-methylbutanoate), (3.alpha.,4.beta.,8.alpha.)-	Trichothecene Mycotoxin	520286	0

Table S7. PASS prediction of the bioactivities of the 59 phytochemicals identified in the methanol extract from *Ammodaucus leucotrichus* seeds.

N°	Compound	Anti-inflammatory effects		RA therapeutic target
		Pa	Pi	
S1	Tetradecanoic acid	0.935	0.003	Sphinganine kinase inhibitor
S2	Octadecanoic acid	0.935	0.003	
S3	Heptadecanoic acid	0.935	0.003	
S4	n-Hexadecanoic acid	0.935	0.003	
S5	Tetracontane	0.915	0.004	
S6	Methyl(9Z,12Z)-octadeca-9,12-dienoate	0.905	0.004	
S7	9-Octadecenoic acid	0.905	0.002	
S8	Octadeca-9,12-dienoic acid	0.873	0.005	
S9	2-Pentanone, 4,4-dimethyl-	0.867	0.004	
S10	Phthalic acid, tetradecyl trans-dec-3-enyl ester	0.866	0.007	
S11	Methyl hexadecanoate	0.845	0.009	
S12	Formic acid, undecyl ester	0.819	0.012	
S13	Trichloro(dodecyl)silane	0.814	0.012	
S14	1,2,3,4,5-Penta-O-acetyl-D-xylitol	0.819	0.012	
S15	Disparlure	0.818	0.012	
S16	Phthalic acid, butyl hept-4-yl ester	0.754	0.018	
S17	Methyl (9Z,12Z)-octadeca-9,12-dienoate	0.648	0.029	
S18	Cyclopentanol	0.860	0.004	JAK2 expression inhibitor
S19	Thymol	0.737	0.014	
S20	3,5-Dihydroxy-6-methyl-2,3-dihydropyran-4-one	0.730	0.014	
S21	2-Ethylidene-1,7,7-trimethylbicyclo[2.2.1]heptane	0.724	0.015	
S22	Octahydro-2-benzothiophene	0.715	0.016	
S23	Spiro[5.5]undeca-1,7-diene	0.707	0.017	
S24	Spiro[5.6]dodecan-7-one	0.684	0.019	
S25	3-Isopropyl-6,7-dimethyltricyclo[4.4.0.0(2,8)]decane-9,10-diol	0.571	0.037	

S26	2-(trans-2,6,6-Trimethylbicyclo[3.3.1]heptan-3-yl)buta-1,3-diene	0.868	0.002	Transcription factor NF kappa B stimulant
S27	8-Isopropyl-1,5-dimethyltricyclo[4.4.0.02,7]dec-4-en-3-one	0.735	0.004	
S28	4-Prop-1-en-2-ylcyclohexene-1-carboxylic acid	0.733	0.004	
S29	thunbergol ((2E,7E,11E)-1,7,11-trimethyl-4-propan-2-ylcyclotetradeca-2,7,11-trien-1-ol)	0.730	0.004	
S30	Neophytadiene (7,11,15-trimethyl-3-methylidenehexadec-1-ene)	0.620	0.008	
S31	2,4,7,14-Tetramethyl-4-vinyl-tricyclo[5.4.3.0(1,8)]tetradecan-6-ol	0.563	0.013	
S32	Cyclopropanebutanoic acid, Methyl-4-[2-[[2-[[2-[(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-cyclopropyl]butanoate	0.388	0.057	
S33	1-amino-propan-2-ol racemate.	0.926	0.003	G-protein-coupled receptor kinase inhibitor
S34	5-Hydroxymethylfurfural	0.749	0.018	
S35	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	0.694	0.023	
S36	2H-Quinolizine-1-methanol, octahydro-	0.680	0.025	
S37	3-Hydroxy-3-methyl-butyric acid, hydrazide	0.656	0.027	
S38	Isospathulenol ((1R,4R,6R)-1,4,7,7-tetramethylbicyclo[4.1.0]heptan-2-ol)	0.729	0.005	MMP9 expression inhibitor
S39	2,2-bis(oxidanylidene)-1,5-dihydroimidazo[4,5-c][1,2,6]thiadiazin-4-one	0.675	0.032	Methylenetetrahydrofolate reductase (NADPH) inhibitor
S40	5-nitrobenzofuran-2(3H)-one	0.878	0.004	Glutathione S-transferase
S41	[(Z)-4-Methylsulfonyloxybut-2-enyl] 2-(tert-butoxycarbonylamino)acetate	0.840	0.006	
S42	Methyl-5,9,13-trimethyltetradecanoate	0.641	0.032	
S43	Octadecamethyl-cyclononasiloxane	0.852	0.004	Complement factor D inhibitor
S44	4'-Hydroxybutyrophenone oxime	0.619	0.034	
S45	Trichothec-9-ene-3,4,8,15-tetrol, 12,13-epoxy-, 15-acetate 8-(3-methylbutanoate), (3.alpha.,4.beta.,8.alpha.)-	0.858	0.002	Immunosuppressant
S46	1-(1,5-Dimethylhexyl)-10-hydroxy-3a,6,6,9a,11a-pentamethylhexadecahydrocyclopenta[7,8]- phenanthro[8a,9-b]oxiren-7-yl acetate	0.795	0.005	
S47	6-(3-Hydroxyprop-1-en-2-yl)-4,8α-dimethyl-2,4α,5,6,7,8-hexahydro-1H-naphthalen-2-ol	0.759	0.010	
S48	(1R,4R,6R,10S)-4,12,12-Trimethyl-9-methylene-5-oxatricyclo[8.2.0.04,6]dodecane	0.758	0.010	
S49	3beta-Trimethylsiloxy-5alpha,6alpha-epoxycholestane	0.727	0.014	
S50	4-Prop-1-en-2-ylcyclohexene-1-carbaldehyde	0.722	0.014	
S51	(7S)-1,1,7-Trimethyl-4-methylidene-1α,2,3,4α,5,6,7α,7β-octahydrocyclopropa[h]azulen-7-ol	0.713	0.015	

S52	Longifolenaldehyde ((2R,5S)-5-[(1R)-1,5-dimethylhex-4-en-1-yl]-2-methylcyclohex-2-en-1-one)	0.713	0.015	
S53	Methyl 16-R/S-hydroxy-cleroda-3,13(14)-Z-dien-15,16-olide	0.675	0.020	
S54	Isospathulenol ((1R,4R,6R)-1,4,7,7-tetramethylbicyclo[4.1.0]heptan-2-ol)	0.658	0.022	
S55	Thunbergol (4-Isopropyl-1,7,11-trimethyl-2,7,11-cyclotetradecatrien-1-ol)	0.613	0.027	
S56	Kauren-19-yl-acetate	0.613	0.027	
S57	trans-(R,R)-chrysanthemyl (R)-2-methylbutanoate	0.473	0.048	
S58	Fumaric acid, 3,5-dimethylphenyl cyclohexylmethyl ester	0.402	0.065	
S59	2-hydroxyacetohydrazide			Carbons 1 < 3