

Supplementary Table S1. Chemical dataset of phytoconstituents from Djiboutian medicinal plants

Plant	Cocmpound	No	Smiles	Extract	Part of the Plant and Collection Zone
Tagetes minuta L.	D-Limonene	1	<chem>CC1=CC[C@@H](CC1)C(=C)C</chem>	stems, leaves and flowers	Day (North Djibouti) (11°45.180 N; 42°37.730
	Camphor	2	<chem>CC1(C2CCC1(C(=O)C2)C)C</chem>		
	Estragole	3	<chem>COC1=CC=C(C=C1)CC=C</chem>		
	Verbenone	4	<chem>CC1=CC(=O)[C@@H]2C[C@H]1C2(C)C</chem>		
	(Z)-Tagetenone	5	<chem>CC(=CC(=O)/C=C(/C)\C=C)C</chem>		
	Piperitone	6	<chem>CC1=CC(=O)C(CC1)C(C)C</chem>		
	2-Undecanone	7	<chem>CCCCCCCCC(=O)C</chem>		
	Benzene, 2-tert-butyl-1,4-dimethoxy-	8	<chem>CC(C)(C)C1=C(C=CC(=C1)OC)OC</chem>		
	(-)-Spathulenol	9	<chem>C[C@@]1(CC[C@@H]2[C@@H]1[C@H]3[C@H](C3(C)C)CCC2=C)O</chem>		
	Cubenol	10	<chem>C[C@@H]1CC[C@H]([C@H]2[C@]1(CCC(=C2)C)O)C(C)C</chem>		
	τ-Cadinol	11	<chem>CC1=C[C@H]2[C@@H](CC[C@]([C@@H]2CC1)(C)O)C(C)C</chem>		
	Dihydrotagetone	12	<chem>CC(C)CC(=O)CC(C)C=C</chem>		

	Artemisia	13	<chem>CC(=CC(=O)C(C)(C)C=C)C</chem>		
<i>Lavandula coronopifolia</i> L.	α -Pinene	14	<chem>CC1=CCC2CC1C2(C)C</chem>	stems, leaves and flowers	Day (North Djibouti) (11°45.180 N; 42°37.730
	Linalol	15	<chem>CC(=CCCC(C)(C=C)O)C</chem>		
	Isopinocarveol	16	<chem>CC1([C@@H]2C[C@H]1C(=C)[C@@H](C2)O)C</chem>		
	Verbenol	17	<chem>CC1=CC(C2CC1C2(C)C)O</chem>		
	Myrtenol	18	<chem>CC1(C2CC=C(C1C2)CO)C</chem>		
	D-Verbenone	19	<chem>CC1=CC(=O)[C@@H]2C[C@H]1C2(C)C</chem>		
	Bornyl Acetate	20	<chem>CC(=O)O[C@@H]1C[C@@H]2CC[C@]1(C2(C)C)C</chem>		
	α -Terpineol Acetate	21	<chem>CC1=CC(CCC1)C(C)(C)OC(=O)C</chem>		
	Copaene	22	<chem>CC1=CC[C@H]2[C@H]3[C@@H]1[C@@]2(CC[C@H]3C(C)C)C</chem>		
	Cubenene	23	<chem>C12C3C4C1=C5C2C3=C45</chem>		
	Zingiberene	24	<chem>CC1=CC[C@@H](C=C1)[C@@H](C)CCC=C(C)C</chem>		
	Cis-Caryophyllene	25	<chem>C/C/1=C/CCC(=C)[C@H]2CC([C@@H]2CC1)(C)C</chem>		
	α -Bergamotene	26	<chem>CC1=CCC2CC1C2(C)CCC=C(C)C</chem>		
	β -Sesquiphellandrene	27	<chem>C[C@@H](CCC=C(C)C)[C@H]1CCC(=C)C=C1</chem>		
	Humulene	28	<chem>C/C/1=C\CC(/C=C/C/C(=C/CC1)/C)(C)C</chem>		
	Aromadendrene	29	<chem>C[C@@H]1CC[C@@H]2[C@@H]1[C@H]3[C@H](C3(C)C)CCC2=C</chem>		

	Germacrene D	30	<chem>C/C/1=C\CCC(=C)/C=C/[C@@H](CC1)C(C)C</chem>		
	β-Eudesmene	31	<chem>CC(=C)[C@@H]1CC[C@]2(CCCC(=C)[C@@H]2C1)C</chem>		
	Methyl (2E)-2-nonenolate	32	<chem>CCCCC/C=C/C(=O)OC</chem>		
	Bisabolene	33	<chem>CC1=CCC(=C(C)CCC=C(C)C)CC1</chem>		
	τ-Cadinene	34	<chem>CC1=C[C@H]2[C@H](CC1)C(=C)CC[C@@H]2C(C)C</chem>		
	δ-Cadinene	35	<chem>CC1=C[C@H]2[C@@H](CCC(=C2CC1)C)C(C)C</chem>		
	α-Panasinsen	36	<chem>CC1=CCCC2(C13CC(C3CC2)(C)C)C</chem>		
	α-Caryophyllene	37	<chem>C/C/1=C\CC(/C=C/C/C(=C/CC1)/C)(C)C</chem>		
	β- Elemol	38	<chem>CC([C@@H]1C[C@H](C(C)(O)C)CC[C@]1(C=C)C)=C</chem>		
	Epiglobulol	39	<chem>C[C@@H]1CC[C@@H]2[C@@H]1[C@H]3[C@@H](CC[C@@]2(O)C)C3(C)C</chem>		
	Dehydronerolidol	40	<chem>CC(C)=CCC/C(C)=C/CC[C@@](C#C)(O)C</chem>		
	Farnesyl acetone	41	<chem>CC(=CCC/C(=C/CC/C(=C/CCC(=O)C)/C)/C)C</chem>		
	Caryophyllene Oxide	42	<chem>C[C@@]12CC[C@@H]3[C@H](CC3(C)C)C(=C)CC[C@H]1O2</chem>		
	12-Heptadecyn-1-ol	43	<chem>CCCCC#CCCCCCCCCCCCCO</chem>		
	Longipinane	44	<chem>CC1CCC2C3C1C2(CCCC3(C)C)C</chem>		
	Humulene Epoxide	45	<chem>C/C/1=C\CC(/C=C/C[C@@]2([C@H](O2)CC1)C)(C)C</chem>		
	α-Cadinol	46	<chem>CC1=C[C@H]2[C@@H](CC[C@@]([C@@H]2CC1)(C)O)C(C)C</chem>		

	10-epi-β-eudesmol	47	<chem>C[C@H]1C[C@@H]([C@H]([C@]2([C@H]1C[C@@H](CC2)C(=C)C)C)O)O</chem>		
	Viridiflorol	48	<chem>C[C@@H]1CC[C@H]2[C@@H]1[C@H]3[C@H](C3(C)C)CC[C@]2(C)O</chem>		
	α-Bisabolol	49	<chem>CC1=CC[C@H](CC1)[C@](C)(CCC=C(C)C)O</chem>		
	Isolongifolanone	50	<chem>CC1(CCC(=O)C2[C@@]13CC[C@@H](C3)C2(C)C)C</chem>		
	Trans-Farnesol	51	<chem>CC(=CCC/C(=C/CC/C(=C/CO)/C)/C)C</chem>		
R. chalepensis L.	2-nonanone	52	<chem>CCCCCCCCC(=O)C</chem>	Aerial parts	Foret de Day National Park of the Republic of Djibouti (11°45'03.600 N 42°41'13.200 E)
	Cyclohexene, 3,4- diethenyl-3-methyl-	53	<chem>CC1(C=CCCC1C=C)C=C</chem>		
	2-decanone	54	<chem>CCCCCCCCC(=O)C</chem>		
	Octyl acetate	55	<chem>CCCCCCCCOC(=O)C</chem>		
	Chloromethyl octyl ether	56	<chem>CCCCCCCCOCCl</chem>		
	2-undecanol	57	<chem>CCCCCCCCC(C)O</chem>		
	Stearic acid	58	<chem>CCCCCCCCCCCCCCCCC(=O)O</chem>		
	2-acetoxytridecane	59	<chem>CCCCCCCCCCCC(C)OC(=O)C</chem>		
	2-dodecanone	60	<chem>CCCCCCCCC(=O)C</chem>		
	1-Methyl-2-decalone	61	<chem>CC1C2CCCC2CCC1=O</chem>		
	2-acetoxytetradecane	62	<chem>CCCCCCCCCCCC(C)OC(=O)C</chem>		

	Bicyclosquiphellandrene	63	<chem>C[C@@H]1CC[C@H](C2=CC(=C)CC[C@H]12)C(C)C</chem>		
	5-ketobornyl acetate	64	<chem>CC(=O)OC1CC2C(=O)CC1(C2(C)C)C</chem>		
	Germacrene D	65	<chem>C/C/1=C\CCC(=C)/C=C/[C@@H](CC1)C(C)C</chem>		
	2-tridecanone	66	<chem>CCCCCCCCCCCCC(=O)C</chem>		
	B- elemol	67	<chem>CC(=C)[C@@H]1C[C@@H](CC[C@@]1(C)C=C)C(C)(C)O</chem>		
	Nerolidol	68	<chem>CC(=CCC/C(=C/CCC(C)(C=C)O)/C)C</chem>		
	T-cadinol	69	<chem>CC1=C[C@H]2[C@@H](CC[C@]([C@@H]2CC1)(C)O)C(C)C</chem>		
	3-Heptenoic acid, 7-phenyl-, ethyl ester,	70	<chem>CCOC(=O)C/C=C/CCCC1=CC=CC=C1</chem>		
	Dihydrosafrol	71	<chem>CCCC1=CC2=C(C=C1)OCO2</chem>		
	Piperonyl acetone	72	<chem>CC(=O)/C=C/C1=CC2=C(C=C1)OCO2</chem>		
	3-Methyl-2-butenic acid, cyclobutyl ester	73	<chem>CC(=CC(=O)OC1CCC1)C</chem>		
<i>Ocimum basilicum</i> L.	Linalol	15	<chem>CC(=CCCC(C)(C=C)O)C</chem>	Aerial parts	Ambouli (11°33'29.3" N 43°08'47.7" E)
	Estragole	3	<chem>COC1=CC=C(C=C1)CC=C</chem>		
	α-bergamotene	26	<chem>CC1=CCC2CC1C2(C)CCC=C(C)C</chem>		
	τ-cadinol	11	<chem>CC1=C[C@H]2[C@@H](CC[C@]([C@@H]2CC1)(C)O)C(C)C</chem>		
	δ-cadinene	35	<chem>CC1=C[C@H]2[C@@H](CCC(=C2CC1)C)C(C)C</chem>		

	Cis-caryophyllene	25	<chem>C/C/1=C/CCC(=C)[C@H]2CC([C@@H]2CC1)(C)C</chem>		
	Bornyl acetate	20	<chem>CC(=O)O[C@@H]1C[C@@H]2CC[C@]1(C2(C)C)C</chem>		
	Elemene	74	<chem>CC(C)C1=C[C@@H]([C@@](CC1)(C)C=C)C(=C)C</chem>		
	Camphor	2	<chem>CC1(C2CCC1(C(=O)C2)C)C</chem>		
	Epiglobulol	39	<chem>C[C@@H]1CC[C@@H]2[C@@H]1[C@H]3[C@@H](CC[C@@]2(O)C)C3(C)C</chem>		
	Viridiflorol	48	<chem>C[C@@H]1CC[C@H]2[C@@H]1[C@H]3[C@H](C3(C)C)CC[C@]2(C)O</chem>		
	10-epi- β -eudesmol	47	<chem>C[C@H]1C[C@@H]([C@H]([C@]2([C@H]1C[C@@H](CC2)C(=C)C)C)O)O</chem>		
	Caryophyllene oxide	42	<chem>C[C@@]12CC[C@@H]3[C@H](CC3(C)C)C(=C)CC[C@H]1O2</chem>		
	Humulene	28	<chem>C/C/1=C\CC(/C=C/C/C/C(=C/CC1)/C)(C)C</chem>		
	Cadinol	75	<chem>CC1=CC2[C@@H](CC[C@@](C2CC1)(C)O)C(C)C</chem>		
	(-)-Spathulenol	76	<chem>C[C@]1(CC[C@H]2[C@H]1[C@@H]3[C@@H](C3(C)C)CCC2=C)O</chem>		
	Linalol oxide	77	<chem>CC1(C(O1)CCC(C)(C=C)O)C</chem>		
	α -bulnesene	78	<chem>C[C@H]1CCC2=C(CC[C@H](C[C@@H]12)C(=C)C)C</chem>		
	Epoxide farnesene	79	<chem>CC(=CCC/C(=C/CCC(=C)C1CO1)/C)C</chem>		
	β -elemol	38	<chem>CC([C@@H]1C[C@H](C(C)(O)C)CC[C@]1(C=C)C)=C</chem>		
	Jasmone	80	<chem>CC1=C(C/C=C\CC)C(CC1)=O</chem>		
	β -sesquiphellandrene	27	<chem>C[C@@H](CCC=C(C)C)[C@H]1CCC(=C)C=C1</chem>		

	Nerolidol	68	<chem>CC(=CCC/C(=C/CCC(C)(C=C)O)/C)C</chem>		
	Humulene epoxide	45	<chem>C/C/1=C\CC(/C=C/C[C@@]2([C@H](O2)CC1)C)(C)C</chem>		
	Octyl acetate	55	<chem>CCCCCCCCOC(=O)C</chem>		
	Bisabolene	33	<chem>CC1=CCC(=C(C)CCC=C(C)C)CC1</chem>		
	α -farnesene	81	<chem>C=C/C(C)=C/C/C=C(CC/C=C(C)/C)\C</chem>		
	Cis-carveol	82	<chem>C=C(C)[C@@H]1C[C@H](O)C(C)=CC1</chem>		
	Cyclopentanone, 3-[3,5-decadienyl]-,	83	<chem>O=C1CC(CC/C=C/C=C/CCCC)CC1</chem>		
	Isolongifolanone	50	<chem>CC1(CCC(=O)C2[C@@]13CC[C@@H](C3)C2(C)C)C</chem>		
	Cis-3-hexenyl isobutyrate	84	<chem>CC(C)C(OCC/C=C\CC)=O</chem>		
	Copaene	22	<chem>CC1=CC[C@H]2[C@H]3[C@@H]1[C@@]2(CC[C@H]3C(C)C)C</chem>		
	Methyl isoeugenol	85	<chem>COC1=CC(C=CC)=CC=C1OC</chem>		
	Bergamotene trans	86	<chem>CC(=CCC[C@@]1([C@H]2CCC(=C)[C@@H]1C2)C)C</chem>		
	β -eudesmene	31	<chem>CC(=C)[C@@H]1CC[C@]2(CCCC(=C)[C@@H]2C1)C</chem>		
	Spiro [4.5]decane, 6-methylene-	87	<chem>C=C(CCCC1)C21CCCC2</chem>		
	Carvotanacetol	88	<chem>CC1=CC[C@@H](C[C@@H]1O)C(C)C</chem>	Aerial parts	Day (11°45'07.1"
	Estragole	3	<chem>COC1=CC=C(C=C1)CC=C</chem>		

<i>Ocimum americanum</i> L.	α -bergamotene	26	<chem>CC1=CCC2CC1C2(C)CCC=C(C)C</chem>		N 42°41'50.1" E)
	τ -cadinol	11	<chem>CC1=C[C@H]2[C@@H](CC[C@]([C@@H]2CC1)(C)O)C(C)C</chem>		
	δ -cadinene	35	<chem>CC1=C[C@H]2[C@@H](CCC(=C2CC1)C)C(C)C</chem>		
	Elemene	74	<chem>CC(C)C1=C[C@@H]([C@@](CC1)(C)C=C)C(=C)C</chem>		
	Germacrene D	30	<chem>C/C/1=C\CCC(=C)/C=C/[C@@H](CC1)C(C)C</chem>		
	β -elemol	38	<chem>CC([C@@H]1C[C@H](C(C)(O)C)CC[C@]1(C=C)C)=C</chem>		
	10-epi- β -eudesmol	47	<chem>C[C@H]1C[C@@H]([C@H]([C@]2([C@H]1C[C@@H](CC2)C(=C)C)C)O)O</chem>		
	Bornyl acetate	20	<chem>CC(=O)O[C@@H]1C[C@@H]2CC[C@]1(C2(C)C)C</chem>		
	Camphor	2	<chem>CC1(C2CCC1(C(=O)C2)C)C</chem>		
	Cadinol	75	<chem>CC1=CC2[C@@H](CC[C@](C2CC1)(C)O)C(C)C</chem>		
	Trans-4-methoxycinnamaldehyde	89	<chem>O=C/C=C/C1=CC=C(OC)C=C1</chem>		
	α -bulnesene	78	<chem>C[C@H]1CCC2=C(CC[C@H](C[C@@H]12)C(=C)C)C</chem>		
	β -cedrene	90	<chem>C[C@@H]1CC[C@@H]2[C@]13CCC(=C)[C@H](C3)C2(C)C</chem>		
	Humulene	28	<chem>C/C/1=C\CC(/C=C/C/C(=C/CC1)/C)(C)C</chem>		
	Linalol oxide	77	<chem>CC1(C(O1)CCC(C)(C=C)O)C</chem>		
	Jasmone	80	<chem>CC1=C(C/C=C\CC)C(CC1)=O</chem>		

	Nerolidol	68	<chem>CC(=CCC/C(=C/CCC(C)(C=C)O)/C)C</chem>		
	3,7-octadiene-2,6-diol, 2,6-dimethyl-	91	<chem>CC(O)(C)C=CCC(O)(C)C=C</chem>		
	Piperitone	6	<chem>CC1=CC(=O)C(CC1)C(C)C</chem>		
	Caryophyllene oxide	42	<chem>C[C@@]12CC[C@@H]3[C@H](CC3(C)C)C(=C)CC[C@H]1O2</chem>		
	Octyl acetate	55	<chem>CCCCCCCCOC(=O)C</chem>		
	β-eudesmene	31	<chem>CC(=C)[C@@H]1CC[C@]2(CCCC(=C)[C@@H]2C1)C</chem>		
	Oxirane, 2-(hexyn-1-yl)-3- methoxymethylene-	92	<chem>COC=C1C(C#CCCC)O1</chem>		
	1,5,9-trimethyl cyclododecatriene	93	<chem>CC1CC/C=C(C)\C=C\C=C(C)/CCC1</chem>		
	Beta-bourbonene	94	<chem>CC(C)[C@@H]1CC[C@@]2([C@H]1[C@@H]3[C@H]2CCC3=C)C</chem>		
	Bicyclosesquiphellandrene	63	<chem>C[C@@H]1CC[C@H](C2=CC(=C)CC[C@H]12)C(C)C</chem>		
	α-caryophyllene	37	<chem>C/C/1=C\CC(/C=C/C/C(=C/CC1)/C)(C)C</chem>		
	Methyl crotonate	95	<chem>C/C=C/C(OC)=O</chem>		
	Cis-caryophyllene	25	<chem>C/C/1=C/CCC(=C)[C@H]2CC([C@@H]2CC1)(C)C</chem>		
	Bisabolene	33	<chem>CC1=CCC(=C(C)CCC=C(C)C)CC1</chem>		
	Isolongifolanone	50	<chem>CC1(CCC(=O)C2[C@@]13CC[C@@H](C3)C2(C)C)C</chem>		

	Copaene	22	<chem>CC1=CC[C@H]2[C@H]3[C@@H]1[C@@]2(CC[C@H]3C(C)C)C</chem>		
	Methyl isoeugenol	85	<chem>COC1=CC(C=CC)=CC=C1OC</chem>		
	Octen-1-ol, acetate	96	<chem>CCCCCCC=COC(C)=O</chem>		
	Bergamol	97	<chem>C/C(C)=C\CCC(C)(C=C)OC(C)=O</chem>		
	γ -eudesmol	98	<chem>CC1=C2C[C@@H](CC[C@]2(CCC1)C)C(C)(C)O</chem>		
	Eudesma-4,11-dien-2-ol	99	<chem>CC(CC(O)C[C@@](C)1CC2)=C1C[C@@H]2C(C)=C</chem>		
	Longipinocarveol	100	<chem>CC1(CCCC2(C3C1C2C(=C)C(C3)O)C)C</chem>		
	(-)-Spathulenol	76	<chem>C[C@]1(CC[C@H]2[C@H]1[C@@@H]3[C@@H](C3(C)C)CCC2=C)O</chem>		
	β -sesquiphellandrene	27	<chem>C[C@@H](CCC=C(C)C)[C@H]1CCC(=C)C=C1</chem>		
	Cyclopentanone, 3-[3,5-decadienyl]-,	83	<chem>O=C1CC(CC/C=C/C=C/CCCC)CC1</chem>		
	Bergamotene trans	86	<chem>CC(=CCC[C@@]1([C@H]2CCC(=C)[C@@H]1C2)C)C</chem>		
<i>Cymbopogon schoenanthus</i> (L.) Spreng.	3-Isopropenyl-5-methyl-1-cyclohexene	101	<chem>CC1CC(C(C)=C)C=CC1</chem>	Plant materials	Mouloud region (south-west of Djibouti; 11°10'18.3" N 42°30'01.4" E)
	D-Limonene	1	<chem>CC1=CC[C@@H](CC1)C(=C)C</chem>		
	α -Terpineol	102	<chem>CC(O)(C1CCC(C)=CC1)C</chem>		
	β - elemol	38	<chem>CC([C@@H]1C[C@H](C(C)(O)C)CC[C@]1(C=C)C)=C</chem>		
	2-p-Menthen-1-ol	103	<chem>CC1(O)CCC(C(C)C)C=C1</chem>		

	Geraniol acetate	104	<chem>C/C(CC/C=C(C)\C)=C\COC(C)=O</chem>		
	Terpineol, cis-,beta,-	105	<chem>CC(=C)C1CCC(CC1)(C)O</chem>		
	10-epi-β-eudesmol	47	<chem>C[C@H]1C[C@@H]([C@H]([C@]2([C@H]1C[C@@H](CC2)C(=C)C)C)O)O</chem>		
	4-Nonanone	106	<chem>CCCC(CCCCC)=O</chem>		
	cis-Piperitol	107	<chem>CC1=C[C@@H]([C@@H](CC1)C(C)C)O</chem>		
	β-trans-Ocimene	108	<chem>C=C/C(C)=C/C/C=C(C)/C</chem>		
	trans-Piperitol	109	<chem>CC1=C[C@@H]([C@H](CC1)C(C)C)O</chem>		
	Eudesm-7(11)-en-4-ol	110	<chem>C[C@]([C@](C/1)2[H])(O)CCC[C@]2(C)CCC1=C(C)\C</chem>		
	Caryophyllene oxide	42	<chem>C[C@@]12CC[C@@H]3[C@H](CC3(C)C)C(=C)CC[C@H]1O2</chem>		
	Ocimene	111	<chem>C=CC(C)=CC/C=C(C)/C</chem>		
	Cyclohexene, 3-acetoxy-4-(1-hydroxy-1-methylethyl)-1-methyl-	112	<chem>CC1=CC(OC(C)=O)C(C(C)(O)C)CC1</chem>		
	Elemene	74	<chem>CC(C)C1=C[C@@H]([C@@](CC1)(C)C=C)C(=C)C</chem>		
	Cis-caryophyllene	25	<chem>C/C/1=C/CCC(=C)[C@H]2CC([C@@H]2CC1)(C)C</chem>		
	Anethofuran	113	<chem>CC(CC1)=C[C@@]2([H])[C@]1([H])[C@H](C)CO2</chem>		
	α-Phellandren-8-ol	114	<chem>CC1=CCC(C=C1)C(C)(C)O</chem>		
	γ-eudesmol	98	<chem>CC1=C2C[C@@H](CC[C@]2(CCC1)C)C(C)(C)O</chem>		

	Viridiflorol	48	<chem>C[C@@H]1CC[C@H]2[C@@H]1[C@H]3[C@H](C3(C)C)CC[C@]2(C)O</chem>		
	Isogeraniol	115	<chem>C/C(C)=C/C/C=C(C)CCO</chem>		
	δ-cadinene	35	<chem>CC1=C[C@H]2[C@@H](CCC(=C2CC1)C)C(C)C</chem>		
	τ-cadinol	11	<chem>CC1=C[C@H]2[C@@H](CC[C@]([C@@H]2CC1)(C)O)C(C)C</chem>		
	β-Phellandrene	116	<chem>CC(C)C1CCC(=C)C=C1</chem>		
	L-Fenchone	117	<chem>C[C@@]12CC[C@@H](C1)C(C2=O)(C)C</chem>		
	Neryl acetate	118	<chem>CC(OC/C=C(CC/C=C(C)/C)/C)=O</chem>		
	cis-Geraniol	119	<chem>C/C(CC/C=C(C)/C)=C/CO</chem>		
	2-Acetoxy-1,8-cineole	120	<chem>CC(OC1CC2CCC1(C)OC2(C)C)=O</chem>		
	Eudesm-5-en-11-ol	121	<chem>C[C@H]1CCC[C@]2(C1=C[C@@H](CC2)C(C)(C)O)C</chem>		
	4-Undecanone	122	<chem>CCCCCCCCC(=O)CCC</chem>		
	2-Caren-10-al	123	<chem>CC1(C2C1C=C(CC2)C=O)C</chem>		
	1-Tetradecyne	124	<chem>C#CCCCCCCCCCCCC</chem>		
	4-Dodecanone, 11-methyl-	125	<chem>CCCC(CCCCCC(C)C)=O</chem>		
	Germacrene D	30	<chem>C/C/1=C\CCC(=C)/C=C/[C@@H](CC1)C(C)C</chem>		
	τ-cadinene	34	<chem>CC1=C[C@H]2[C@H](CC1)C(=C)CC[C@@H]2C(C)C</chem>		
	Eudesma-4,11-dien-2-ol	99	<chem>CC(CC(O)C[C@@](C)1CC2)=C1C[C@@H]2C(C)=C</chem>		

	longipinocarveol	100	<chem>CC1(CCCC2(C3C1C2C(=C)C(C3)O)C)C</chem>		
	α -Phellandrene	126	<chem>CC1=CCC(C=C1)C(C)C</chem>		
	cis-p-menth-2-en-1-ol	127	<chem>CC(C)[C@H]1CC[C@](C=C1)(C)O</chem>		
	Cyclohexene, 2-ethenyl-1,3,3-trimethyl-	128	<chem>CC1=C(C(CCC1)(C)C)C=C</chem>		
	α -Bergamotene	26	<chem>CC1=CCC2CC1C2(C)CCC=C(C)C</chem>		
	β -eudesmene	31	<chem>CC(=C)[C@@H]1CC[C@]2(CCCC(=C)[C@@H]2C1)C</chem>		
	Methyl (2E)-2-nonenoate	32	<chem>CCCCC/C=C/C(=O)OC</chem>		
	Cis-carveol	82	<chem>C=C(C)[C@@H]1C[C@H](O)C(C)=CC1</chem>		
	Trans-2-Hydroxy-1,8-cineole	129	<chem>CC1(C2CCC(O1)(C(C2)O)C)C</chem>		
<i>Nepeta azurea</i> R.Br. <i>ex Benth</i>	Methyl (2E)-2-nonenoate	32	<chem>CCCCC/C=C/C(=O)OC</chem>	Plant materials	Day region (north of Djibouti; 11°44'46.6" N 42°41'03.5" E)
	Phellandral	130	<chem>CC(C)C1CCC(=CC1)C=O</chem>		
	1-Methyl-2-decalone	61	<chem>CC1C2CCCCC2CCC1=O</chem>		
	Cis-caryophyllene	25	<chem>C/C1=C/CCC(=C)[C@H]2CC([C@@H]2CC1)(C)C</chem>		
	Cyclohexanol, acetate	131	<chem>CC(=O)OC1CCCCC1</chem>		
	Boschnialactone	132	<chem>C[C@@H]1CC[C@H]2[C@@H]1COC(=O)C2</chem>		
	Caryophyllene oxide	42	<chem>C[C@@]12CC[C@@H]3[C@H](CC3(C)C)C(=C)CC[C@H]1O2</chem>		

	L-calamenene	133	<chem>C[C@H]1CC[C@H](C2=C1C=CC(=C2)C)C(C)C</chem>		
	Oplopanone	134	<chem>CC(C)[C@@H]1CC[C@@]([C@H]2[C@H]1[C@H](CC2)C(=O)C)(C)O</chem>		
	piperitone	6	<chem>CC1=CC(=O)C(CC1)C(C)C</chem>		
	Isogeraniol	115	<chem>C/C(C)=C/C/C=C(C)CCO</chem>		
	Cubenol	10	<chem>C[C@@H]1CC[C@H]([C@H]2[C@]1(CCC(=C2)C)O)C(C)C</chem>		
	Viridiflorol	48	<chem>C[C@@H]1CC[C@H]2[C@@H]1[C@H]3[C@H](C3(C)C)CC[C@]2(C)O</chem>		
	Limonene oxide	135	<chem>CC(=C)C1CCC2(C(C1)O2)C</chem>		
	2-Undecanone	7	<chem>CCCCCCCCC(=O)C</chem>		
	1-Tetradecyne	124	<chem>C#CCCCCCCCCCCCC</chem>		
	β-Bourbonene	136	<chem>CC(C)[C@@H]1CC[C@@]2([C@H]1[C@@H]3[C@H]2CCC3=C)C</chem>		
	Elemene	74	<chem>CC(C)C1=C[C@@H]([C@@](CC1)(C)C=C)C(=C)C</chem>		
	Linalol	15	<chem>CC(=CCCC(C)(C=C)O)C</chem>		

ID	SMILES
A1	<chem>OC(CCCCCCCCCCCCCCCCCC)=O</chem>
A2	<chem>C~~Si~~(C)O~~Si~~(C)C</chem>
A3	<chem>OC(CCCCCCCCCCCCCCCCCC)=O</chem>
A4	<chem>O=C(CCCCCC/C=C\C(CCCCCC)O</chem>
A5	<chem>O=C/C(CCCCC)=C\C1=CC=CC=C1</chem>
A6	<chem>O=C1CCCCC1</chem>

A7	<chem>OC@@HC@HCC</chem>
A8	<chem>C/C(CC/C=C(C)/CCC=C(C)C)=C\CC/C=C(C)/CC/C=C(C)/CCC=C(C)C</chem>
A9	<chem>BrC@HCCCCCCCCCCCC</chem>
A10	<chem>ClC@@(C(Cl)=C2Cl)C@H[C@H]3[C@@]12Cl</chem>
A11	<chem>ClC@((C(Cl)=C2Cl)C@@H[C@@H]4[C@]12Cl</chem>
B1	<chem>CSi(C)OSi(C)C</chem>
B2	<chem>FC1=CC=C(C=C1)C2=CC=CC=C2</chem>
B3	<chem>ClC(C(OCC(OC)=O)=C1)=CC(Cl)=C1Cl</chem>
B4	<chem>C(C1=CC=CC=C1)(C=C2)=CC=C2OC3=CC=CC=C3</chem>
B5	<chem>ClC(C=C1)=C(C=C1Cl)N+=O</chem>
B6	<chem>CSi(C)C(C=C1Si(C)C)=C(C=C1)Si(C)C</chem>
B7	<chem>OC1=CC=C(C=C1)SC(C=C2)=CC=C2O</chem>
B8	<chem>OC(CCCCCC/C=C\CCCCCCCC)=O</chem>
B9	<chem>CSi(C)C</chem>
B10	<chem>O=C(CCCCCCCCCCCCCC)OCCCCCCCC</chem>
B11	<chem>ClC1=CC(C(C2=CC=CC=C2)=NC3)=C(C=C1)N(C)C3=O</chem>
C1	<chem>O=C(CCCCCC/C=C\CCCCCCCC)OCCCC</chem>
C2	<chem>OC@@(C)CCCC(C)C</chem>
C4	<chem>O=C/C(CCCCC)=C/C1=CC=CC=C1</chem>
C5	<chem>OC@HCCCCCCCCCCCC</chem>
C6	<chem>ClC@@(C(Cl)=C2Cl)[C@H]3C@@H[C@@H]4[C@H]5O[C@H]5[C@H]3C4</chem>
C7	<chem>ClC@@(C(Cl)=C2Cl)[C@H]3C@@H[C@H]4[C@@H]5O[C@@H]5[C@@H]3C4</chem>
C8	<chem>ClC@@(C(Cl)=C2Cl)C@@HC@@H[C@@]12Cl</chem>
C9	<chem>O=C(CCCCCCCCC=C)OCCCC</chem>
C10	<chem>ClC1=C(C=CC(Cl)=C1)OC(C=C2)=CC(C(OC)=O)=C2N+=O</chem>
D1	<chem>C[Si]1(C)OSi(C)OSi(C)OSi(C)O1</chem>
D2	<chem>O=C(CCCCC)OC1CCCCC1</chem>
D3	<chem>OCCC#CCCCC</chem>
D5	<chem>C=CCCCCCCCCCCC=C</chem>

D6	[O-] N ⁺ =O
D8	O=C(CC)CCCCCCCCCCCC
D9	O=C(CCCCCCCCCCCCCCCCCC)OCCCC
D10	CC @H NC
E1	ClC1=CC=CC(N ⁺ =O)=C1
E2	OCCOCCOCC
E3	ClC(C=C(C=C1)NC(OC)=O)=C1Cl
E4	OC(CCCCCCCCC#C)=O
E5	C=CCOC1=NC(OCC=C)=NC(OCC=C)=N1
E6	ClC1=CC=C(C=O)S1
E7	C/C(CC=C)=C\CC
E8	ClC1=C(C=CC(Cl)=C1)O P @ @ (OCC)=S
E9	BrC1CCCC1
F1	CC(C)=CCCC=C
F2	OC(CCCCCCCCC)=O
F3	O=C(C)/C=C/C1=C(C)CCCC1(C)C
F5	ClC(Cl)(C[C @ @]1(C2=CC(Cl)=CC(Cl)=C2)OC1)Cl
F6	CC Sn (CC)CC
F7	ClCCCCCCCCCCCCCCCCCCCC
G1	S=C=NC
G2	VC/C=C/C(C=C1)=CC=C1OC
G3	ClC1=C(C(Cl)=O)C=CC(Cl)=C1
G4	Cl C @ (C(Cl)=C2Cl) C @ @H [C @ @H]3[C @]12Cl
G6	OC @H C(C)(C)C
G7	OC/C=C(C)/CC/C=C(C)/CCC=C(C)C
H1	OC(CC(OCCCCC)=O)(C(OCCCCC)=O)CC(OCCCCC)=O
H2	OC(CCC1CCCCC1)=O
H3	OC1(CN ⁺ =O)CCCCC1
H4	C1(C2=CSN=C2)=CC=CC=C1
H5	BrC(C(C(C)C)=CC(C(C)C)=C1)=C1C(C)C
H6	CCCCCCCCCCCCCCCCC=C

I1	<chem>ClC1=CC(Cl)=CC=C1</chem>
I2	<chem>OC(CCCC)=O</chem>
I3	<chem>OC@HCCCCCCCC</chem>
I4	<chem>[O-][N+]=O</chem>
I5	<chem>CCCCCCCCCCCCCCCCCCCCCCCCCCCC</chem>
I6	<chem>OCC1CCCCCCC1</chem>
I7	<chem>OC@HCCC</chem>
J1	<chem>O=C(C)CCCCCCCCCCC</chem>
J2	<chem>OC@@(C=C)CC/C=C(C)/CCC=C(C)C</chem>
J3	<chem>C[C@]1(C[C@@H]2C3)C[C@]3(C)CC@@HC1</chem>
J4	<chem>CC1=C2N3C(SC2=CC=C1)=NN=C3</chem>
J5	<chem>O=C1C(C(C)C)=CC(C(C)=C1)=O</chem>
J6	<chem>BrC1([C@H]2[C@H]1CCCCC2)Br</chem>
J7	<chem>C12=CC=CC=C1NCCC2</chem>
J8	<chem>C#CCCCCCCC#C</chem>
J9	<chem>O=C(CCCCCCCCCCCCCC(OC)=O)OC</chem>
J10	<chem>OC(C1CCCC1)=O</chem>
J11	<chem>BrCCCCCCCCCCCC(O)=O</chem>