

Phytochemical Composition of *Commiphora* Oleogum Resins and their Cytotoxicity against Skin Cancer Cells

Judith Ulrich ^{1,†}, Svenja Stiltz ^{1,†}, Alexis St-Gelais ², Menna El Gaafary ^{1,3}, Thomas Simmet ¹, Tatiana Syrovets ¹ and Michael Schmiech ^{1,*}

¹ Institute of Pharmacology of Natural Products and Clinical Pharmacology, Ulm University, 89081 Ulm, Germany; judith.ulrich@uni-ulm.de (J.U.), svenja.stiltz@winsie.de (S.S.), mennat_elgaafary@yahoo.com (M.E.), thomas.simmet@uni-ulm.de (Th.S.), tatiana.syrovets@uni-ulm.de (Ta.S.)

² Laboratoire PhytoChemia, Saguenay, QC G7J 1H4, Canada; a.st-gelais@phytochemia.com (A.S.-G.)

³ Department of Pharmacognosy, College of Pharmacy, Cairo University, Cairo 11562, Egypt

* Correspondence: michael.schmiech@uni-ulm.de (M.S.); Tel.: +49-731-500-65622

[†] These authors contributed equally to this work

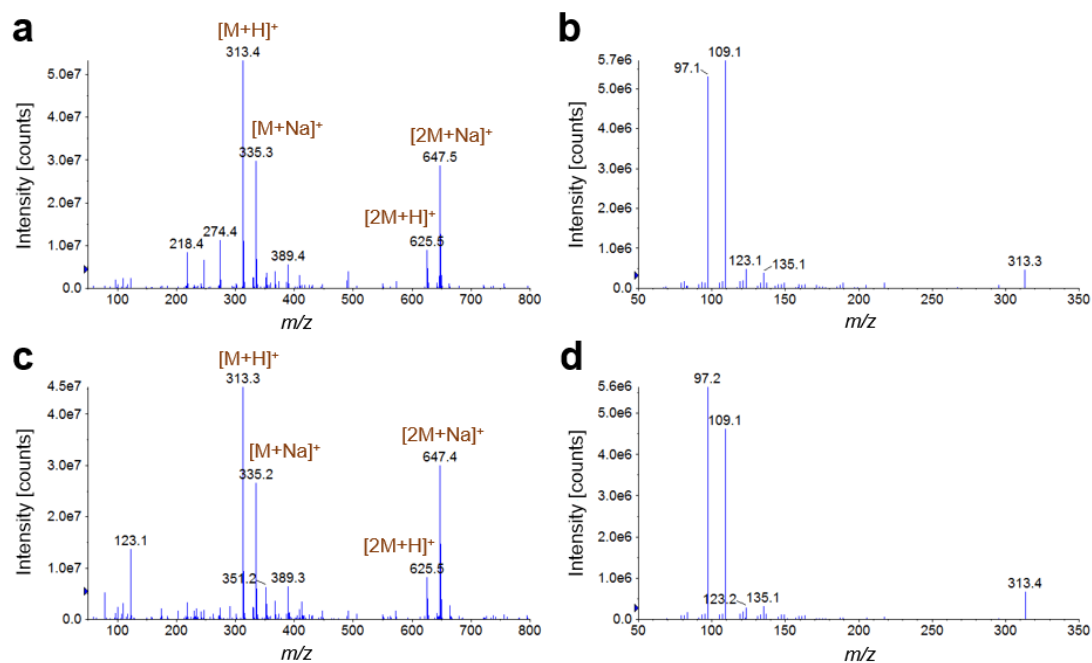


Figure S1. Mass spectra of (*E*)-guggulsterone and (*Z*)-guggulsterone with positive ionization mode (centroided). (a) Mass spectrum of (*E*)-guggulsterone. (b) Product ion mass spectrum of (*E*)-guggulsterone with m/z 313 as precursor ion. (c) Mass spectrum of (*Z*)-guggulsterone. (d) Product ion mass spectrum of (*Z*)-guggulsterone with m/z 313 as precursor ion.

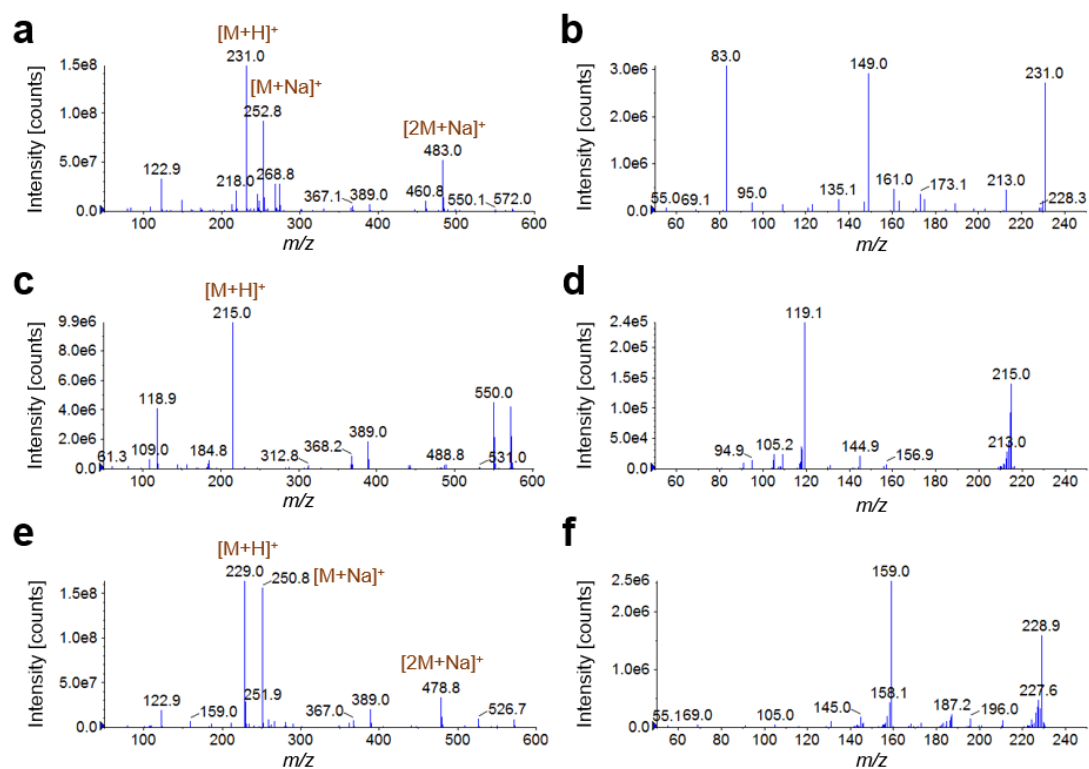


Figure S2. Mass spectra of curzerenone, furanoeudesma-1,3-diene, and myrrhone with positive ionization mode (centroided). (a) Mass spectrum of curzerenone. (b) Product ion mass spectrum of curzerenone with m/z 231 as precursor ion. (c) Mass spectrum of furanoeudesma-1,3-diene. (d) Product ion mass spectrum of furanoeudesma-1,3-diene with m/z 215 as precursor ion. (e) Mass spectrum of myrrhone. (f) Product ion mass spectrum of myrrhone with m/z 229 as precursor ion.

Table S1. Design of Experiments (DoE) for optimization of chromatographic parameters for selective and rapid guggulsterone analysis. Level conditions for three independent variables: Variable A (starting concentrations of eluent B), variable B (slope of gradient), and variable C (flow rate of eluent). As response, two dependent variables were investigated: chromatographic resolution (R) and averaged retention time (\bar{t}_R) of (*E*)-guggulsterone and (*Z*)-guggulsterone. $\alpha = 1.682$.

Exp.	Independent variables, uncoded (coded)			Dependent variables	
	A [%]	B [%/min]	C [mL/min]	R	\bar{t}_R [min]
1	32.0 (-1)	2.00 (-1)	0.400 (-1)	3.78	23.8
2	68.0 (1)	2.00 (-1)	0.400 (-1)	1.99	7.3
3	32.0 (-1)	4.00 (1)	0.400 (-1)	2.90	15.9
4	68.0 (1)	4.00 (1)	0.400 (-1)	1.77	6.7
5	32.0 (-1)	2.00 (-1)	0.600 (1)	4.33	20.5
6	68.0 (1)	2.00 (-1)	0.600 (1)	1.99	5.2
7	32.0 (-1)	4.00 (1)	0.600 (1)	3.34	13.5
8	68.0 (1)	4.00 (1)	0.600 (1)	1.93	4.8
9	19.7 ($-\alpha$)	3.00 (0)	0.500 (0)	4.40	21.3
10	80.3 (α)	3.00 (0)	0.500 (0)	1.27	3.2
11	50.0 (0)	1.32 ($-\alpha$)	0.500 (0)	3.59	15.5
12	50.0 (0)	4.68 (α)	0.500 (0)	2.43	9.4
13	50.0 (0)	3.00 (0)	0.332 ($-\alpha$)	2.87	14.1
14	50.0 (0)	3.00 (0)	0.668 (α)	3.28	9.6
15	50.0 (0)	3.00 (0)	0.500 (0)	2.94	11.3

Table S2. Quantification of (*E*)-guggulsterone, (*Z*)-guggulsterone, curzerenone, furanoeudesma-1,3-diene, and myrrhone in *Commiphora* oleogum resin extracts and botanical drugs. Analysis by HPLC-MS/MS, in duplicates. Contents below limit of quantification or detection (<LOQ/<LOD) are indicated as “-”.

Species (origin)	Contents of guggulsterones and furanosesquiterpenoids in <i>Commiphora</i> extracts or botanical drugs [$\mu\text{g}/\text{mg}$]				
	(<i>E</i>)-Guggulsterone	(<i>Z</i>)-Guggulsterone	Curzerenone	Furanoeudesma-1,3-diene	Myrrhone
<i>C. myrrha</i> (Somalia)	–	–	0.099	328.500	0.004
<i>C. erythraea</i> (Somalia)	–	–	2.180	–	0.755
<i>C. mukul</i> (Nepal)	3.555	8.290	–	–	–
<i>C. kataf</i> (Kenya)	–	–	2.710	–	4.110
<i>C. holtziana</i> (Kenya)	–	–	14.950	102.000	0.557
<i>C. confusa</i> (Kenya)	–	–	0.006	–	–
<i>C. kua</i> (Socotra, Yemen)	–	–	–	–	–
<i>C. from Tarraxo</i> (Somalia)	–	–	54.700	–	0.174
<i>C. from Ogaden</i> (Ethiopia)	0.956	0.610	7.740	–	3.045
Myrrhinil-Intest®	–	–	0.016	0.456	0.007
Gugulipid®	7.410	12.100	–	–	–

Table S3. Analysis of essential oils in *Commiphora* oleogum resins. Relative quantification by gas chromatography and flame ionization detection (GC-FID) using internal normalization, areas in uncorrected %. List of components with area >0.2% in at least one sample. Retention indices (RI) using DB-5 or DB-Wax columns. Hydrodistillation of *Commiphora* oleogum resin from Tarraxo (Somalia) yielded no essential oil. Traces tr <0.05%. Main ions of unknown compounds and substance groups are shown in the footnote.

Compound	Retention indices (RI)		Content [%]							
	DB-5	DB-Wax	<i>C. myrrha</i> (Somalia)	<i>C. erythraea</i> (Somalia)	<i>C. mukul</i> (Nepal)	<i>C. kataf</i> (Kenya)	<i>C. holtziana</i> (Kenya)	<i>C. confusa</i> (Kenya)	<i>C. kua</i> (Socotra, Yemen)	<i>C. from</i> Ogaden (Ethiopia)
Toluene	761	1004	–	–	tr	–	–	0.2	–	–
α -Thujene	926	1000	–	tr	0.2	0.2	0.1	9.0	–	tr
α -Pinene	930	994	–	0.5	8.5	5.8	0.8	39.5	tr	0.5
Camphene	943	1027	–	tr	0.5	0.2	tr	0.7	–	tr
Unknown I	943	1095	–	–	–	tr	–	1.0	–	–
Thuja-2,4(10)-diene	949	1086	–	tr	0.1	0.1	tr	0.9	–	–
3,7,7-Trimethyl- cyclohepta-1,3,5- triene	965	1135	–	–	2.2	–	–	tr	–	–
β -Pinene	971	1066	–	0.1	2.0	3.5	0.1	8.9	–	0.1
Sabinene	971	1086	–	tr	0.2	0.3	tr	1.1	–	tr
Menthatriene unidentified isomer	999	1176	–	–	tr	tr	–	0.3	–	–
Δ^3 -Carene	1007	1111	–	tr	29.8	tr	–	–	–	tr
<i>ortho</i> - Methylanisole	1007	1363	–	0.1	–	–	–	0.5	–	tr
α -Terpinene	1014	1140	–	–	0.3	0.1	–	0.3	–	–
<i>meta</i> -Cymene	1019	1229	–	–	0.4	–	–	0.1	–	–
<i>para</i> -Cymene	1021	1228	–	0.1	2.1	0.2	0.1	10.0	–	0.1
Sylvestrene	1023	1156	–	–	0.8	–	–	–	–	–
Limonene	1026	1158	0.1	0.1	1.2	0.2	0.1	1.1	0.1	0.1
β -Phellandrene	1026	1165	–	–	0.1	–	–	0.2	–	–
γ -Terpinene	1056	1206	–	–	0.4	0.1	tr	0.5	–	tr
Unknown II	1067	1279	–	–	0.1	–	–	0.2	–	–
<i>meta</i> -Cymenene	1079	1381	–	–	0.6	–	–	–	–	–
Terpinolene	1086	1241	–	–	0.7	tr	–	0.2	–	tr
<i>para</i> -Cymenene	1086	1388	–	–	0.8	tr	–	0.6	–	–
<i>endo</i> -Fenchol	1109	1542	–	–	0.3	tr	–	0.2	–	–
β -Thujone	1111	1387	–	–	–	–	tr	1.0	–	–
α -Campholenal	1121	1437	–	–	0.1	0.1	–	0.4	–	–
Nopinone	1129	1512	–	–	–	–	–	0.2	–	–
<i>trans</i> -Pinocarveol	1132	1605	–	–	0.3	0.3	0.1	2.0	tr	tr
<i>trans</i> -Verbenol	1141	1633	–	–	0.1	0.1	–	0.5	tr	tr
<i>meta</i> -Mentha-4,6- dien-8-ol	1146	1615	–	–	0.1	0.1	–	0.6	–	–
Pinocamphone	1156	1454	–	–	0.1	tr	–	0.3	–	–
Pinocarvone	1157	1509	–	–	0.3	tr	–	0.5	–	–
Phellandrenol isomer	1157	1674	–	–	0.4	–	–	–	–	–
Borneol	1161	1653	–	–	0.1	tr	–	0.2	–	–
α -Phellandren- 8-ol	1164	1683	–	tr	0.3	0.2	–	1.6	–	tr

Table S3. *Cont.*

Umbellulone	1167	1581	–	–	–	–	–	0.3	–	–
<i>cis</i> -Sabinol	1168	1743	–	–	–	–	–	0.3	–	–
Terpinen-4-ol	1173	1557	–	tr	1.0	0.1	tr	4.5	tr	tr
<i>meta</i> -Cymen-8-ol	1180	1798	–	–	1.2	–	–	–	–	–
<i>para</i> -Cymen-8-ol	1183	1801	–	–	0.7	tr	–	0.7	–	–
Unknown III	1186	1651	–	–	2.8	–	–	–	–	–
Myrtenal	1188	1564	–	–	0.2	0.3	–	0.9	–	–
α -Terpineol	1188	1651	–	tr	1.3	0.1	–	1.0	–	tr
Myrtenol	1193	1743	–	–	0.2	0.2	–	1.0	tr	–
Verbenone	1202	1636	–	tr	1.3	0.1	tr	1.6	tr	tr
Octyl acetate	1217	1444	–	–	–	–	0.3	–	–	–
<i>trans</i> -Carveol	1217	1788	–	–	0.1	tr	–	0.3	–	–
Cuminal	1234	1714	–	–	0.1	–	–	0.3	–	tr
3,5-Dimethoxy- toluene	1265	1782	–	–	–	0.1	–	0.3	–	–
Bornyl acetate	1285	1529	–	–	0.2	0.1	–	0.1	–	–
4-Vinylguaicol	1307	2129	–	–	0.7	–	–	–	–	–
δ -Elemene isomer	1332	1427	0.1	0.1	–	0.5	0.1	–	tr	0.1
δ -Elemene	1335	1432	2.0	1.1	–	25.1	1.8	–	0.9	1.8
Bicycloelemene	1335	1436	0.1	–	–	0.9	0.1	–	tr	–
Unknown IV	1338	1631	–	–	0.3	–	–	–	–	–
α -Longipinene	1343	1416	–	–	0.7	–	–	–	–	0.5
α -Cubebene	1346	1418	0.1	0.6	–	0.5	0.2	–	0.6	0.4
α -Terpinyl acetate	1347	1645	–	–	1.1	–	–	0.1	–	–
Cyclosativene I	1358	1436	–	tr	0.2	0.3	–	–	–	–
Longicyclene	1361	1440	–	–	1.0	–	–	–	–	–
α -Ylangene	1366	1436	0.1	0.3	0.1	0.3	0.1	–	0.1	0.1
α -Copaene	1371	1444	0.4	1.3	0.1	1.4	2.2	tr	1.5	0.6
β -Bourbonene	1378	1469	1.2	5.2	–	3.7	1.3	–	0.9	2.1
1,5- <i>diepi</i> - β - Bourbonene	1381	1461	0.1	0.5	–	0.4	0.1	–	0.1	0.2
<i>cis</i> - β -Elemene	1381	1533	0.3	0.2	–	–	0.2	–	–	0.3
Sativene	1383	1471	–	–	0.6	–	–	–	–	–
β -Cubebene	1386	1491	0.1	0.1	–	0.3	0.1	–	0.2	0.2
β -Elemene	1389	1544	9.1	11.1	0.1	4.7	9.6	tr	0.9	12.8
Longifolene	1397	1509	–	–	24.3	–	–	–	–	–
α -Gurjunene	1403	1479	0.1	tr	–	0.1	0.1	–	0.9	0.1
β -Ylangene	1412	1520	0.2	0.9	–	0.6	0.2	–	0.2	0.6
<i>cis</i> - α - Bergamotene	1412	1526	0.2	–	–	1.2	0.5	–	–	0.1
β -Caryophyllene	1412	1540	0.7	1.1	0.7	1.2	0.9	–	7.7	1.0
Cascarilladiene	1416	1520	0.2	–	–	0.3	0.2	–	–	0.5
β -Copaene	1422	1536	0.4	1.1	–	1.0	0.4	–	0.3	0.7
γ -Elemene	1430	1590	2.7	1.1	–	0.5	1.8	–	0.2	3.8
<i>trans</i> - α - Bergamotene	1433	1540	0.1	1.8	–	–	0.3	–	0.4	0.9
α -Guaiene	1433	1543	–	–	–	0.4	–	–	–	–
6,9-Guaiadiene	1437	1557	tr	tr	–	0.3	tr	–	0.1	0.1
Isogermacrene D	1437	1586	0.2	0.8	–	0.5	0.2	–	–	0.4
Unknown V	1442	1569	–	–	–	0.7	0.2	–	0.2	–

Table S3. *Cont.*

Unknown VI	1444	1574	–	–	–	0.4	–	–	0.2	–
α -Humulene	1445	1608	0.5	0.7	0.1	1.0	0.5	–	3.9	0.7
<i>allo</i> - Aromadendrene	1453	1586	0.1	0.3	–	0.3	0.2	–	3.8	0.2
<i>cis</i> -Cadina-1(6),4- diene	1456	1586	–	0.1	–	0.1	–	–	1.7	0.2
<i>cis</i> -Muurolo- 4(15),5-diene	1459	1615	–	0.3	–	0.3	–	–	0.2	0.2
Unknown VII	1466	1615	0.1	0.1	–	0.7	0.1	–	–	0.1
<i>trans</i> -Cadina- 1(6),4-diene	1468	1605	0.1	0.3	–	0.6	0.1	–	0.3	0.1
Selina-4,11-diene	1470	1620	0.3	0.2	–	–	0.4	–	0.4	0.2
γ -Muurolene	1472	1633	0.2	1.7	–	1.6	0.6	–	2.0	1.0
Germacrene D	1474	1649	3.3	1.2	–	13.7	1.8	–	1.5	8.3
β -Selinene	1478	1656	1.1	1.9	–	2.1	1.8	–	1.2	1.1
<i>allo</i> -Aromadendr- 9-ene	1481	1629	–	–	–	–	–	–	0.3	–
<i>trans</i> - β - Bergamotene	1481	1633	–	0.5	–	–	–	–	–	–
δ -Selinene	1482	1639	0.2	–	–	0.5	–	–	–	0.2
Unknown VIII	1482	1649	0.3	–	–	–	2.8	–	–	–
Unknown IX	1482	1650	–	–	–	0.7	–	–	–	–
<i>trans</i> -Muurolo- 4(15),5-diene	1484	1656	–	0.2	–	–	–	–	0.2	0.2
Viridiflorene	1488	1638	–	–	–	–	–	–	0.8	–
Valencene	1488	1659	–	–	–	0.4	–	–	0.4	–
α -Selinene	1488	1662	1.2	2.2	–	0.9	1.8	–	1.8	1.3
<i>epi</i> -Cubebol	1488	1836	–	–	–	–	–	–	0.3	0.1
Unknown X	1493	1662	–	–	–	0.4	1.4	–	–	–
Isorotundene	1494	1658	–	–	–	–	–	–	0.3	–
Curzerene	1494	1813	29.7	37.8	–	–	18.7	–	tr	32.6
α -Muurolene	1497	1669	–	0.5	–	0.4	0.3	–	1.0	0.4
Germacrene A	1497	1697	0.4	–	–	0.2	0.2	–	–	0.1
δ -Amorphene	1502	1669	0.1	–	–	0.5	0.1	–	0.2	0.1
(Z)- α -Bisabolene	1502	1683	–	4.8	–	–	–	–	–	0.2
β -Bisabolene	1507	1679	–	1.2	0.1	–	–	–	–	0.1
γ -Cadinene	1508	1697	0.1	0.9	–	1.2	0.4	–	24.0	2.0
(Z)- γ -Bisabolene	1510	1680	–	–	–	–	–	–	0.3	–
Cubebol	1510	1887	–	–	–	–	–	–	0.4	tr
Unknown XI	1516	1701	–	–	–	0.3	–	–	–	–
δ -Cadinene	1519	1701	0.4	2.3	tr	1.7	0.9	–	8.9	1.4
<i>cis</i> -Calamenene	1519	1767	–	–	–	0.1	–	–	0.6	–
Unknown XII	1520		–	–	–	0.5	–	–	–	–
Selina-4(15),7(11)- diene	1527	1713	0.2	0.4	–	0.1	0.3	–	–	0.1
α -Cadinene	1532	1732	–	0.2	–	0.2	–	–	1.9	0.1
Selina-3,7(11)- diene	1533	1713	0.2	0.4	–	tr	0.3	–	–	0.3
α -Calacorene	1535	1848	0.1	0.4	–	0.2	0.1	–	0.2	0.1
α -Elemol	1544	2026	0.2	1.1	–	0.5	0.4	–	0.1	1.1

Table S3. *Cont.*

Longicamph-enilone	1547	1947	–	–	0.3	–	–	–	–	–
Germacrene B	1548	1760	4.6	1.3	–	0.7	2.6	–	0.3	4.9
1,5-Epoxy-salvial-4(14)-ene	1557		0.1	0.1	–	0.3	0.1	–	–	0.1
Furanoeudesma-1,4-diene	1570	1977	0.8	–	–	–	0.4	–	–	–
Caryophyllene oxide	1572	1905	0.1	0.2	0.2	0.2	0.1	–	0.4	0.1
Viridiflorol	1582	2019	–	–	–	–	–	–	0.5	tr
Gleenol	1587	1982	–	–	–	–	–	–	0.2	–
β -Elemenone	1597	2019	0.1	–	–	–	–	–	–	0.5
Curzerenone	1597	2140	0.6	0.3	–	2.6	2.2	–	0.1	2.7
10- <i>epi</i> -Cubenol	1603	1998	–	0.1	–	0.3	–	–	3.3	0.2
Junenol	1607	1982	–	0.3	–	0.2	–	–	–	–
Unknown XIII	1613	2036	–	–	–	–	–	–	–	0.3
Furanoeudesma-1,3-diene	1619	2047	17.4	–	–	–	23.9	–	tr	–
1- <i>epi</i> -Cubenol	1620	1998	–	–	–	–	–	–	0.2	0.1
Alismol	1620	2191	–	0.1	–	0.7	–	–	0.1	tr
Lindestrene	1625	2051	8.7	–	–	–	6.5	–	tr	–
τ -Cadinol	1633	2107	0.2	0.2	–	0.6	0.2	–	16.9	0.6
τ -Muurolol	1633	2123	–	0.1	–	0.1	–	–	0.3	–
β -Eudesmol	1640	2157	0.1	0.2	–	0.2	0.1	–	0.6	0.1
Valerianol	1643	2146	–	–	–	–	–	–	–	0.4
Unknown XIV	1645	2026	–	0.3	–	–	–	–	–	–
Atractylone	1645	2040	0.1	0.5	–	–	0.3	–	–	0.1
α -Eudesmol	1645	2150	0.1	0.2	–	tr	0.1	–	0.2	0.1
Furanodiene	1651	2040	0.4	1.1	–	–	0.4	–	–	–
α -Cadinol	1651	2165	–	0.1	–	0.1	–	–	0.3	0.1
Longibornyl acetate	1672	1953	–	–	0.5	–	–	–	–	–
α -Elemyl acetate	1674	1977	0.8	–	–	–	0.7	–	–	–
2-Methoxy-isofurano-germacrene (?)	1682	2102	0.3	–	–	–	–	–	–	–
Unknown XV	1682	2107	1.7	1.7	–	–	0.9	–	–	1.3
Germacrene	1684	2142	0.4	0.3	–	0.2	0.3	–	–	1.8
2-Methoxy-furanodiene	1714	2168	1.1	–	–	–	0.4	–	–	–
Unknown XVI	1731	2364	–	–	–	0.6	0.2	–	–	–
Unknown XVII	1732	2277	–	–	–	–	–	–	–	0.8
Cembrene	1919		–	–	0.2	–	0.1	–	–	–
(3 <i>E</i>)-Cembrene A	1949	2171	–	–	0.3	–	0.1	–	–	–
Dolabella-6,10,15-triene (?)	1955	2209	–	–	–	–	–	–	0.4	–
Unknown XVIII		1197	–	–	0.3	–	–	–	–	–
TOTAL			94.9	95.0	94.1	93.8	95.0	94.2	96.0	94.8

Main ions of unknown compounds [*m/z* (relative intensity); molecular ion bolded out if known]: Unknown I : 91 (100), 92 (47), 65 (11)... 134 (1); Unknown II : 79 (100), 93 (60), 43 (40)... 152 (18); Unknown III : 93 (100), 59 (85), 81 (36), 92 (35); Unknown IV : 93 (100), 43 (50), 121 (50), 136 (35); Unknown V : 91 (100), 161 (92), 105 (85)... 204 (46); Unknown VI : 161 (100), 105 (70), 91 (51)... 204 (45); Unknown VII : 121 (100), 93 (86), 161 (61)... 204 (19); Unknown

VIII : 79 (100), 107 (99), 91 (88)... 204 (12); Unknown IX : 161 (100), 189 (96), 91 (74), 204 (73); Unknown X : 93 (100), 81 (96), 80 (80), 147 (68); Unknown XI : 121 (100), 93 (78), 136 (56)... 204 (13); Unknown XII : 122 (100), 107 (38), 105 (26)... 204 (5); Unknown XIII : 91 (100), 133 (100), 105 (91)... 218 (33); Unknown XIV : 216 (100), 145 (76), 201 (61), 159 (36); Unknown XV : 108 (100), 216 (29), 93 (26), 109 (21); Unknown XVI : 159 (100), 145 (37), 160 (28)... 230 (11); Unknown XVII : 175 (100), 232 (52), 161 (39), 162 (32); Unknown XVIII : 93 (100), 79 (93), 137 (76)... 152 (9).

Aliphatic ester: Octyl acetate.

Diterpenes: Cembrene, (3*E*)-Cembrene A, Dolabella-6,10,15-triene.

Monoterpenes: α -Thujene, α -Pinene, Camphene, Unknown I, Thuja-2,4(10)-diene, *meta*-Cymene, β -Pinene, Sabinene, Menthatriene isomer, Δ^3 -Carene, α -Terpinene, *ortho*-Cymene, *para*-Cymene, Sylvestrene, Limonene, β -Phellandrene, γ -Terpinene, *meta*-Cymenene, Terpinolene, *para*-Cymenene.

Monoterpenic alcohols: *endo*-Fenchol, *trans*-Pinocarveol, *trans*-Verbenol, *meta*-Mentha-4,6-dien-8-ol, Phellandrenol isomer, Borneol, α -Phellandren-8-ol, *cis*-Sabinol, Terpinen-4-ol, *meta*-Cymen-8-ol, *para*-Cymen-8-ol, α -Terpineol, Myrtenol, *trans*-Carveol.

Monoterpenic aldehydes: α -Campholenal, Myrtenal, Cuminal.

Monoterpenic esters: Bornyl acetate, Unknown IV, α -Terpinyl acetate.

Monoterpenic ketones: β -Thujone, Pinocamphone, Pinocarvone, Umbellulone, Verbenone.

Normonoterpenic ketone: Nopinone.

Norsesquiterpenic ketone: Longicamphenilone.

Oxygenated monoterpenes: Unknown II, Unknown III, Unknown XVIII.

Oxygenated sesquiterpenes: Unknown XIII, Unknown XIV, Unknown XV, Unknown XVII.

Sesquiterpenes: δ -Elemene isomer, δ -Elemene, Bicycloelemene, α -Longipinene, α -Cubebene, Cyclosativene I, Longicyclene, α -Ylangene, α -Copaene, β -Bourbonene, 1,5-*diepi*- β -Bourbonene, *cis*- β -Elemene, Sativene, β -Cubebene, β -Elemene, Longifolene, α -Gurjunene, β -Ylangene, *cis*- α -Bergamotene, β -Caryophyllene, Cascarilladiene, β -Copaene, γ -Elemene, *trans*- α -Bergamotene, α -Guaiane, 6,9-Guaiadiene, Isogermacrene D, Unknown V, Unknown VI, α -Humulene, *allo*-Aromadendrene, *cis*-Cadina-1(6),4-diene, *cis*-Muurola-4(15),5-diene, Unknown VII, *trans*-Cadina-1(6),4-diene, Selina-4,11-diene, γ -Muurolene, Germacrene D, β -Selinene, *allo*-Aromadendr-9-ene, *trans*- β -Bergamotene, δ -Selinene, Unknown VIII, Unknown IX, *trans*-Muurola-4(15),5-diene, Viridiflorene, Valencene, α -Selinene, Isorotundene, α -Muurolene, Germacrene A, δ -Amorphene, (*Z*)- α -Bisabolene, β -Bisabolene, γ -Cadinene, (*Z*)- γ -Bisabolene, Unknown XI, δ -Cadinene, *cis*-Calamenene, Unknown XII, Selina-4(15),7(11)-diene, α -Cadinene, Selina-3,7(11)-diene, α -Calacorene, Germacrene B.

Sesquiterpenic alcohols: *epi*-Cubebol, Cubebol, α -Elemol, Viridiflorol, Gleenol, 10-*epi*-Cubenol, Junenol, 1-*epi*-Cubenol, Alismol, τ -Cadinol, τ -Muurolol, β -Eudesmol, Valerianol, α -Eudesmol, α -Cadinol.

Sesquiterpenic esters: Longibornyl acetate, α -Elemyl acetate, Curzerene, 1,5-Epoxyisoval-4(14)-ene, Furanoesdesma-1,4-diene, Caryophyllene oxide, Furanoesdesma-1,3-diene, Lindestrene, Atractylone, Furanodiene, 2-Methoxyisofuranogermacrene, 2-Methoxyfuranodiene.

Sesquiterpenic ketones: β -Elemenone, Curzerenone, Germacrone.

Simple phenolic: Toluene, *ortho*-Methylanisole, 3,5-Dimethoxytoluene, 4-Vinylguaiacol.

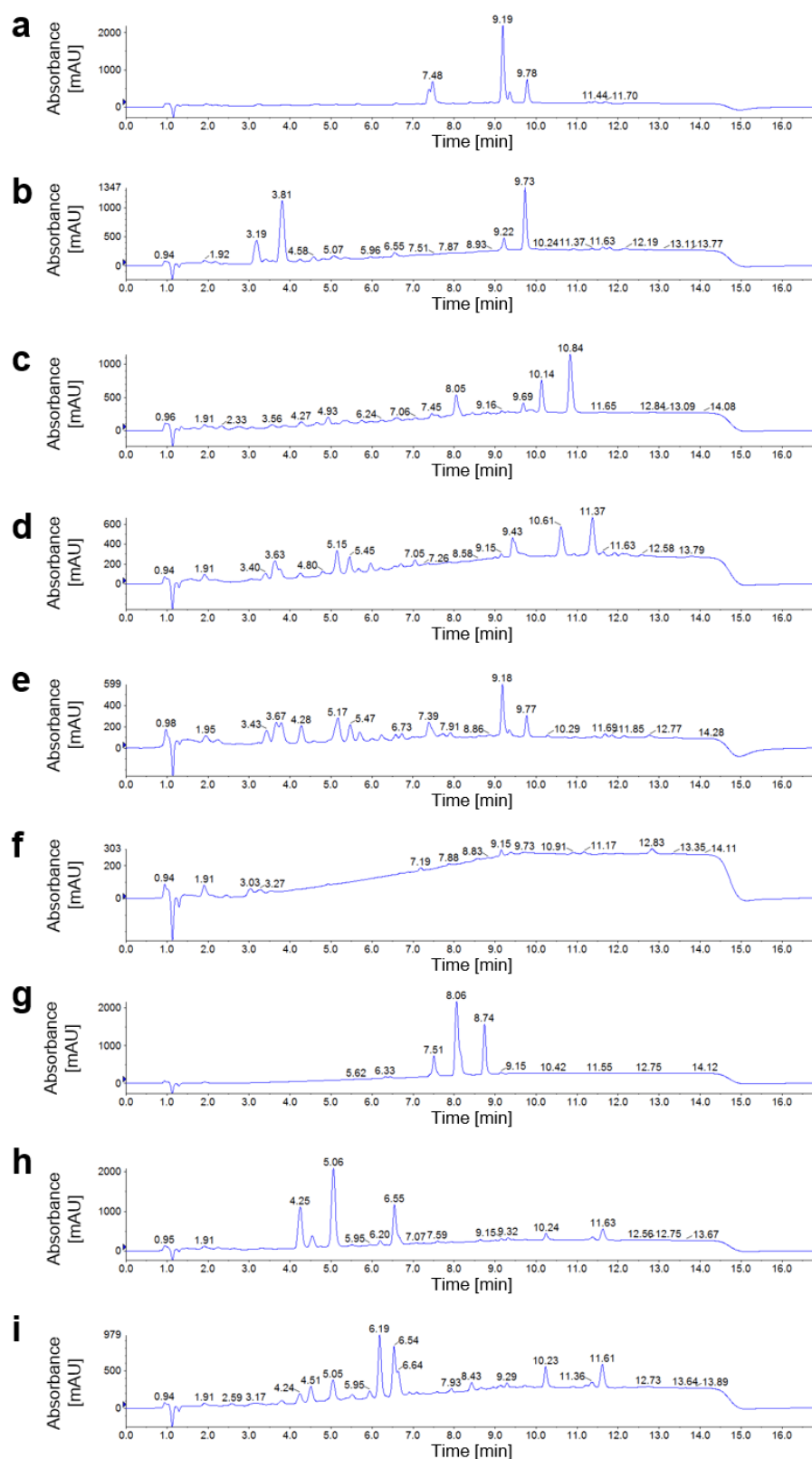


Figure S3. Total wavelength chromatograms (TWC) of *Commiphora* oleogum resin extracts with detection at 210 nm, 254 nm, and 280 nm. (a) *C. myrrha*. (b) *C. erythraea*. (c) *C. mukul*. (d) *C. kataf*. (e) *C. holtziana*. (f) *C. confusa*. (g) *C. kua*. (h) *Commiphora* oleogum resin from Tarraxo (Somalia). (i) *Commiphora* oleogum resin from Ogaden (Ethiopia). $t_R((E)\text{-Guggulsterone}) = 4.3$ min, $t_R((Z)\text{-Guggulsterone}) = 4.9$ min, $t_R(\text{Curzerenone}) = 4.3$ min, $t_R(\text{Myrrhone}) = 6.0$ min, and $t_R(\text{Furanoedesma-1,3-diene -}) = 9.2$ min.

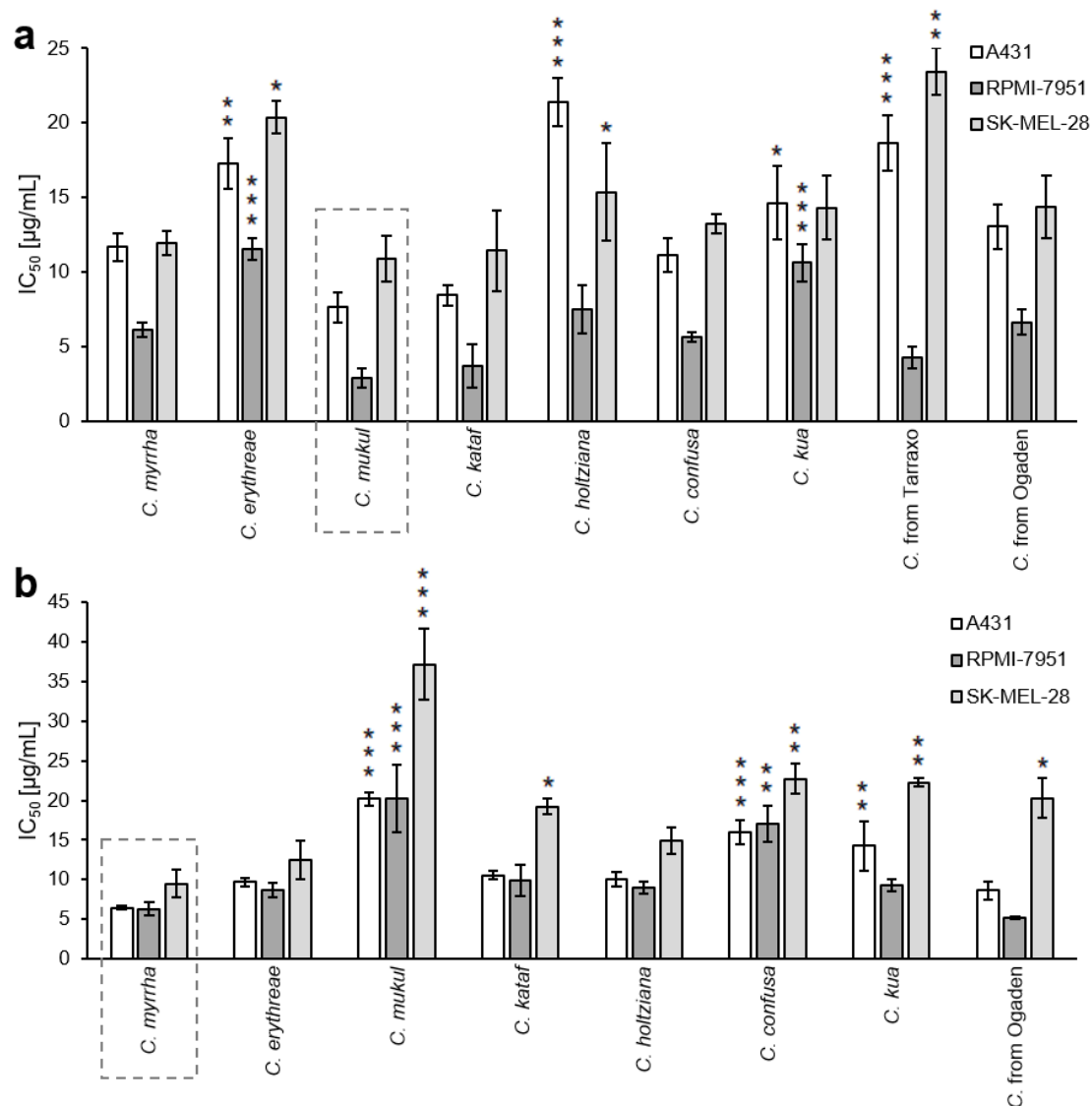


Figure S4. Cytotoxicity of *Commiphora* extracts and essential oils against the epidermoid carcinoma cell line A431 and the malignant melanoma cell lines RPMI-7951 and SK-MEL-28. (a) Cytotoxicity of *Commiphora* extracts: The extract obtained from *C. mukul* exhibited the highest cytotoxic efficacies against all investigated skin cancer cell lines. (b) Cytotoxicity of *Commiphora* essential oils: Comparison of the individual samples revealed that the essential oil from *C. myrrha* exhibited the highest cytotoxicity against A431 and SK-MEL-28 cell lines and high cytotoxicity against RPMI-7951 cells. XTT assay, 72 h, $n = 3$ (and each experiment additionally performed in triplicates). All data are mean \pm standard error of mean (SEM). Statistical evaluation by ANOVA and *post hoc* Dunnett's test with * $p < 0.05$, ** $p < 0.01$, and *** $p < 0.001$. Comparison of the individual samples with (a) *C. mukul* extract or (b) *C. myrrha* essential oil.