

Supplementary Materials for

Wound Healing Potential of an Oleoresin Essential Oil Chemotype from *Canarium schweinfurthii* Engl.

Michel Bonnard *, Enzo Martin and Isabelle Parrot *

* Correspondence: michel.bonnard@umontpellier.fr (M.B.); isabelle.parrot-smietana@umontpellier.fr (I.P.)

Table S1. Chemical composition of EO (% Area, non-polar phase) obtained from oleoresins of *C. schweinfurthii* collected in Gabon (Ntoum region, trees #1-#4).

No.	Compounds	Composition (% Area)			
		Tree #1	Tree #2	Tree #3	Tree #4
1	α -thujene	0.28	0.13	0.67	0.09
2	α -pinene	5.69	21.01	2.04	5.91
3	camphene	0.06	0.13	0.04	nd
4	sabinene	8.36	4.22	20.13	1.58
5	β -pinene	3.41	1.42	0.96	0.46
6	2-menthene	1.87	nd	nd	nd
7	α -phellandrene	19.04	20.49	4.71	3.20
8	δ^3 -carene	0.19	nd	nd	nd
9	α -terpinene	2.92	1.14	1.16	0.03
10	<i>p</i> -cymene	9.26	6.51	14.90	10.65
11	limonene	10.70	25.22	17.36	48.36
12	β -phellandrene	2.20	nd	nd	nd
13	eucalyptol	0.12	3.66	1.96	3.07
14	γ -terpinene	1.68	0.76	1.93	0.06
15	4-thujanol	0.09	nd	nd	nd
16	terpinolene	32.17	1.04	16.44	0.20
17	<i>p</i> -cymenene	0.25	nd	nd	nd
18	terpinen-4-ol	0.55	0.53	0.20	0.44
19	<i>p</i> -cymen-8-ol	0.92	nd	nd	nd
20	α -terpineol	0.26	9.09	4.71	24.31
21	<i>cis</i> -thujanol	nd	0.99	0.80	0.23
22	β -caryophyllene	nd	0.66	nd	nd
23	<i>trans</i> - β -ocimene	nd	0.21	0.14	0.25
24	α -dihydroterpineol	nd	0.21	nd	nd
25	<i>trans</i> -thujanol	nd	0.11	0.26	0.10
26	camphor	nd	0.09	nd	nd
27	<i>cis</i> -2-menthenol	nd	0.08	0.26	nd
28	humulene	nd	0.07	nd	nd
29	<i>trans</i> -2-menthenol	nd	0.06	0.04	nd
30	cyperene	nd	0.05	nd	nd
31	pipertone	nd	0.04	nd	0.06
32	2-(4-methylphenyl)propan-2-ol	nd	nd	2.92	nd

Tables S2. *In chemico* assessment of skin sensitization (raw data)

	Negative control		Positive control 1		Positive control 2		EO	
Cysteine peptide assays	(-)peptide	(+)peptide	(-)peptide	(+)peptide	(-)peptide	(+)peptide	(-)peptide	(+)peptide
FI ₁	2196	32857	1048	9535	2167	14238	2252	17223
FI ₂	2268	32878	1041	9755	2145	14224	2201	16943
FI ₃	2269	32742	1053	9637	2152	13763	2234	17005
Mean	2244	32826	1047	9642	2155	14075	2229	17057
St. Dev.	42	73	6	110	11	270	26	147
FI _{corr} = [FI ₍₊₎ – FI ₍₋₎]	FI _{corr}	30581	FI _{corr}	8595	FI _{corr}	11920	FI _{corr}	14828
Peptide depletion	PD _{Cyst.}	-	PD _{Cyst.}	71.9%	PD _{Cyst.}	61.0%	PD _{Cyst.}	51.5%

Calibration curve		
Cyst.	μM	FI
Std 0	0	2199
Std 1	6.25	3584
Std 2	12.5	4735
Std 3	25	6491
Std 4	50	10171
Std 5	100	17946
Std 6	200	32831

	Negative control		Positive control 1		Positive control 2		EO	
Lysine peptide assays	(-)peptide	(+)peptide	(-)peptide	(+)peptide	(-)peptide	(+)peptide	(-)peptide	(+)peptide
FI ₁	1684	30925	729	2972	1568	18024	1624	28819
FI ₂	1687	31465	718	3040	1587	17586	1581	28231
FI ₃	1673	31726	762	3003	1582	17834	1553	27930
Mean	1681	31372	736	3005	1579	17815	1586	28327
St. Dev.	7	409	23	34	10	220	36	452
FI _{corr} = [FI ₍₊₎ – FI ₍₋₎]	FI _{corr}	29691	FI _{corr}	2269	FI _{corr}	16236	FI _{corr}	26741
Peptide depletion	PD _{Lys.}	-	PD _{Lys.}	92.4%	PD _{Lys.}	45.3%	PD _{Lys.}	9.9%

Calibration curve		
Lys.	μM	FI
Std 0	0	1627.5
Std 1	3.125	2388.5
Std 2	6.25	3413
Std 3	12.5	5515.5
Std 4	25	9171
Std 5	50	16819
Std 6	100	31330.5

Tables S3. *In vitro* assessment of skin sensitization (raw data)

Cytotoxicity assay on THP1 cells – 24hrs treatment										
EO (mg/mL)	Control	0.00005	0.0001	0.0005	0.001	0.005	0.01	0.05	0.1	0.2
FI-1 _{corr}	40872	41024	40080	39830	39482	38235	37337	34986	27907	7315
FI-2 _{corr}	41096	40761	40382	39868	39139	38732	37069	34504	27541	7440
FI-3 _{corr}	40930	40818	40546	39874	39436	38591	37192	35108	28019	7338
Mean	40966	40868	40336	39858	39353	38520	37200	34866	27823	7365
St. Dev.	116	138	236	24	186	256	134	319	250	67
Viability (%)	100	100	98	97	96	94	91	85	68	18
Cytotoxicity (%)	-	0	2	3	4	6	9	15	32	82

Cytotoxicity assay on THP1 cells – 24hrs treatment										
EO (mg/mL)	Control	0.010	0.013	0.018	0.024	0.032	0.042	0.056	0.075	0.1
FI-1 _{corr}	40589	38788	38263	37665	37640	36710	35768	34033	31007	25738
FI-2 _{corr}	40554	38097	37858	37181	36290	35967	35671	34131	31412	25753
FI-3 _{corr}	40768	38302	37605	37697	37356	35681	35681	34210	31108	25539
FI-4 _{corr}	41098	37960	37963	37841	36966	36078	36078	33929	31238	25999
Mean	40752	38287	37922	37596	37063	36634	35799	34076	31191	25757
St. Dev.	249	363	272	287	585	518	191	122	175	188
Viability (%)	100	94	93	92	91	90	88	84	77	63
Cytotoxicity (%)	-	6	7	8	9	10	12	16	23	37

CD86 expression assay on THP1 cells – 24hrs treatment

	Control	Contr. _{EtOH}	PC	EO mg/mL					
CD86 assay	-	EtOH (0.2%)	DCNB 5µg/mL	0.036	0.043	0.052	0.063	0.075	0.090
OD _{mes.1}	0.226	0.236	0.761	0.358	0.417	0.543	0.598	0.614	0.627
OD _{mes.2}	0.210	0.233	0.743	0.340	0.440	0.558	0.587	0.608	0.643
OD _{mes.3}	0.225	0.239	0.792	0.343	0.410	0.567	0.608	0.632	0.625
Mean	0.220	0.236	0.766	0.347	0.422	0.556	0.598	0.618	0.632
St. Dev.	0.009	0.003	0.025	0.010	0.016	0.012	0.011	0.012	0.010
OD _{CD86}									
Mean	0.424	0.485	2.604	0.930	1.232	1.767	1.933	2.014	2.069
St. Dev.	0.036	0.013	0.100	0.038	0.062	0.049	0.042	0.049	0.039
Resazurin assay	-	EtOH (0.2%)	DNCB 5µg/mL	0.036	0.043	0.052	0.063	0.075	0.090
FI _{mes.1}	43401	43364	34974	38929	38050	36392	35889	34240	33455
FI _{mes.2}	43179	43152	35495	39383	37827	36915	34867	33926	32900
FI _{mes.3}	43417	42822	35043	39492	37610	36649	35223	34249	33432
Mean	43332	43113	35171	39268	37829	36652	35326	34138	33262
St. Dev.	133	273	283	299	220	262	519	184	314
Viability (% Control)									
Mean	100	100	80	90	87	84	81	78	75
St. Dev.	0.68	0.68	0.70	0.74	0.55	0.65	1.29	0.46	0.78
CD86 (%)									
Mean	100	100	770	212	292	434	494	534	565
St. Dev.	3.25	3.25	34.69	10.42	14.53	10.31	11.07	11.03	16.63

CD54 expression assay on THP1 cells – 24hrs treatment

	Control	Contr. _{EtOH}	PC	EO mg/mL					
CD54 assay	-	EtOH (0.2%)	DCNB 5µg/mL	0.036	0.043	0.052	0.063	0.075	0.090
OD _{mes.1}	0.279	0.252	0.794	0.552	0.567	0.590	0.671	0.700	0.712
OD _{mes.2}	0.262	0.280	0.819	0.540	0.585	0.637	0.701	0.707	0.711
OD _{mes.3}	0.268	0.264	0.793	0.538	0.582	0.597	0.681	0.711	0.702
Mean	0.270	0.265	0.802	0.543	0.578	0.608	0.684	0.706	0.708
St. Dev.	0.009	0.014	0.015	0.007	0.010	0.026	0.015	0.005	0.006
OD _{CD54}									
Mean	0.614	0.597	2.743	1.708	1.848	1.968	2.272	2.360	2.368
St. Dev.	0.036	0.057	0.060	0.030	0.039	0.102	0.062	0.022	0.023
Resazurin assay	-	EtOH (0.2%)	DNCB 5µg/mL	0.036	0.043	0.052	0.063	0.075	0.090
FI _{mes.1}	43401	43364	34974	38929	38050	36392	35889	34240	33455
FI _{mes.2}	43179	43152	35495	39383	37827	36915	34867	33926	32900
FI _{mes.3}	43417	42822	35043	39492	37610	36649	35223	34249	33432
Mean	43332	43113	35171	39268	37829	36652	35326	34138	33262
St. Dev.	133	273	283	299	220	262	519	184	314
Viability (% Control)									
Mean	100	100	80	90	87	84	81	78	75
St. Dev.	0.68	0.68	0.70	0.74	0.55	0.65	1.29	0.46	0.78
CD54 (%)									
Mean	100	100	560	316	356	392	471	509	525
St. Dev.	5.58	9.69	7.31	8.12	9.26	17.51	20.04	5.92	8.98

THP1 cell line reactivity control – CD86 expression assay on THP1 cells – 24hrs treatment

	Control	PC1	PC2
CD86 assay	-	DNCB	NiSO ₄
OD _{mes.1}	0.187	0.870	0.788
OD _{mes.2}	0.198	0.883	0.805
OD _{mes.3}	0.187	0.863	0.785
Mean	0.191	0.873	0.793
St. Dev.	0.006	0.010	0.011
OD _{CD86}			
Mean	0.320	3.045	2.729
St. Dev.	0.025	0.041	0.043
Resazurin assay	-	DNCB	NiSO ₄
FI _{mes.1}	42990	34704	36305
FI _{mes.2}	43385	34107	36812
FI _{mes.3}	42954	34143	36997
Mean	43113	34318	36705
St. Dev.	236	335	358
Viability (% Control)			
Mean	100	78	84
St. Dev.	0.59	0.83	0.89
CD86 (%)			
Mean	100	1219	1015
St. Dev.	7.33	22.80	18.24

	Control	NC1
CD86 assay	-	LA
OD _{mes.1}	0.187	0.210
OD _{mes.2}	0.198	0.241
OD _{mes.3}	0.187	0.209
Mean	0.191	0.220
St. Dev.	0.006	0.018
OD _{CD86}		
Mean	0.320	0.437
St. Dev.	0.025	0.072
XTT assay	-	LA
OD _{mes.1}	0.527	0.541
OD _{mes.2}	0.559	0.544
OD _{mes.3}	0.537	0.556
Mean	0.541	0.547
St. Dev.	0.016	0.008
Viability (% Control)		
Mean	100	102
St. Dev.	3.46	1.75
CD86 (%)		
Mean	100	135
St. Dev.	4.70	23.12

THP1 cell line reactivity control – CD54 expression assay on THP1 cells – 24hrs treatment

	Control	PC1	PC2
CD54 assay	-	DNCB	NiSO ₄
OD _{mes.1}	0.238	0.739	0.894
OD _{mes.2}	0.216	0.723	0.854
OD _{mes.3}	0.224	0.663	0.893
Mean	0.226	0.708	0.880
St. Dev.	0.011	0.040	0.023
OD _{CD54}			
Mean	0.471	2.401	3.088
St. Dev.	0.045	0.163	0.091
Resazurin assay	-	DNCB	NiSO ₄
FI _{mes.1}	42990	34704	36305
FI _{mes.2}	43385	34107	36812
FI _{mes.3}	42954	34143	36997
Mean	43113	34318	36705
St. Dev.	236	335	358
Viability (% Control)			
Mean	100	78	84
St. Dev.	0.59	0.83	0.89
CD54 (%)			
Mean	100	653	780
St. Dev.	9.94	40.08	26.74

	Control	NC1
CD54 assay	-	LA
OD _{mes.1}	0.238	0.182
OD _{mes.2}	0.216	0.174
OD _{mes.3}	0.224	0.223
Mean	0.226	0.193
St. Dev.	0.011	0.026

OD _{CD54}		
Mean	0.471	0.338
St. Dev.	0.045	0.105
XTT assay	-	LA
OD _{mes.1}	0.527	0.541
OD _{mes.2}	0.559	0.544
OD _{mes.3}	0.537	0.556
Mean	0.541	0.547
St. Dev.	0.016	0.008
Viability (% Control)		
Mean	100	102
St. Dev.	3.46	1.75
CD54 (%)		
Mean	100	70
St. Dev.	12.78	20.50