

# Supporting Information

## Antibacterial activity and untargeted metabolomics profiling of *Acalypha arvensis* Poepp

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## 1. Photograph of *Acalypha arvensis* Poepp. Individual



**Figure S1:** Photograph of a *Acalypha arvensis* Poepp (taken by Josia Richardson)

## 2. Figures untargeted analysis of GC × GC-TOFMS metabolite profiles of the methanol: chloroform extract (50:50), F6

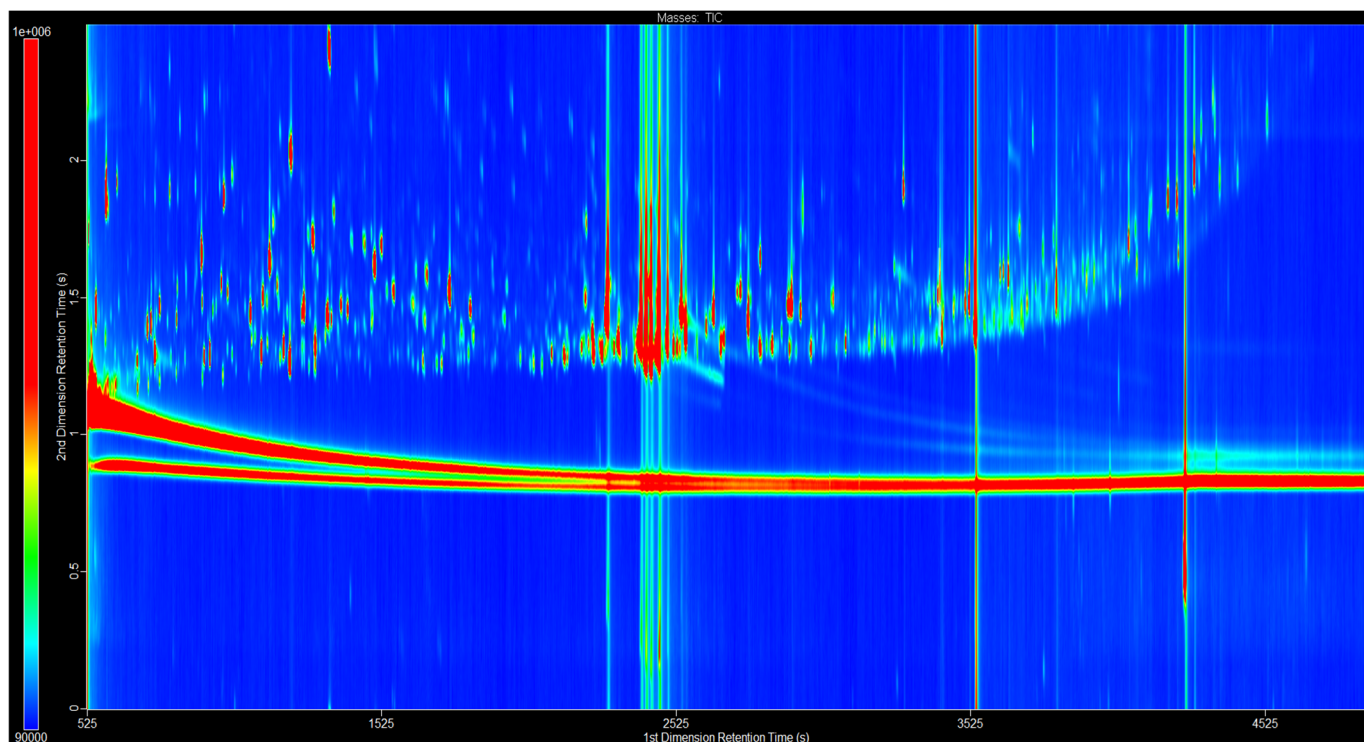


Figure S2: GC×GC total ion chromatogram *A. arvensis* extract F6 derivatized

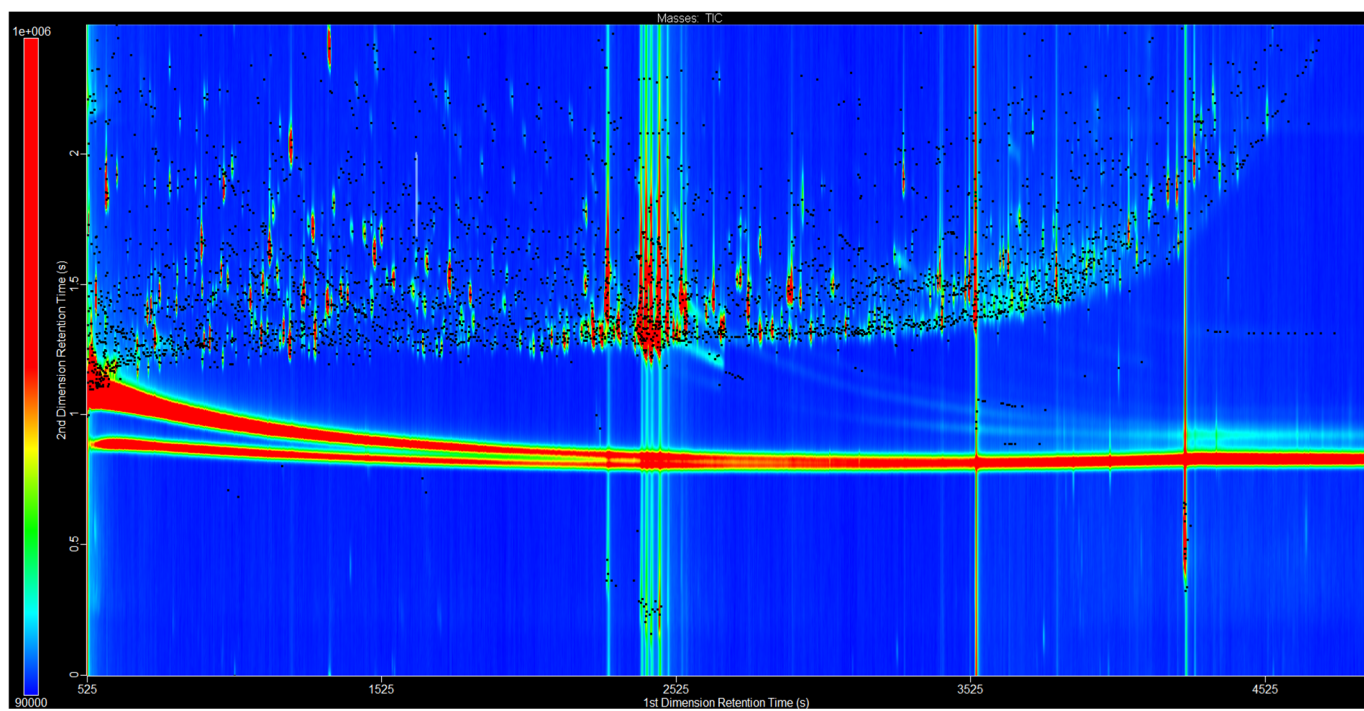
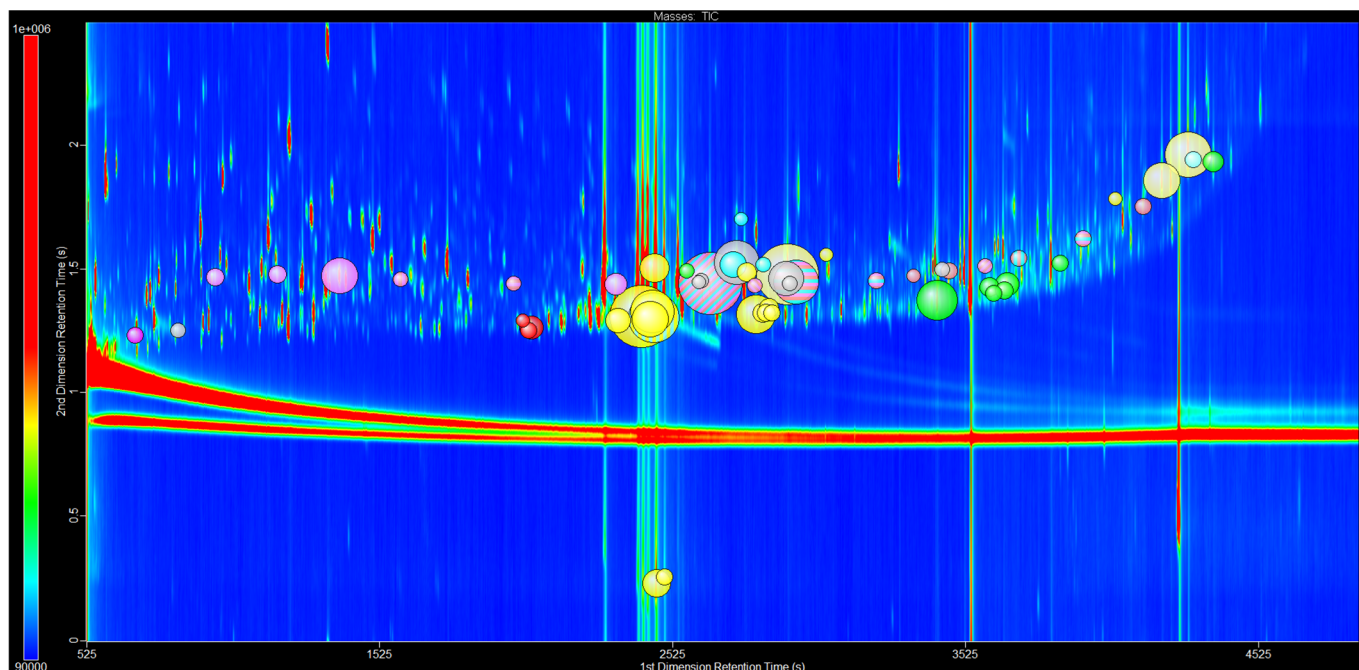
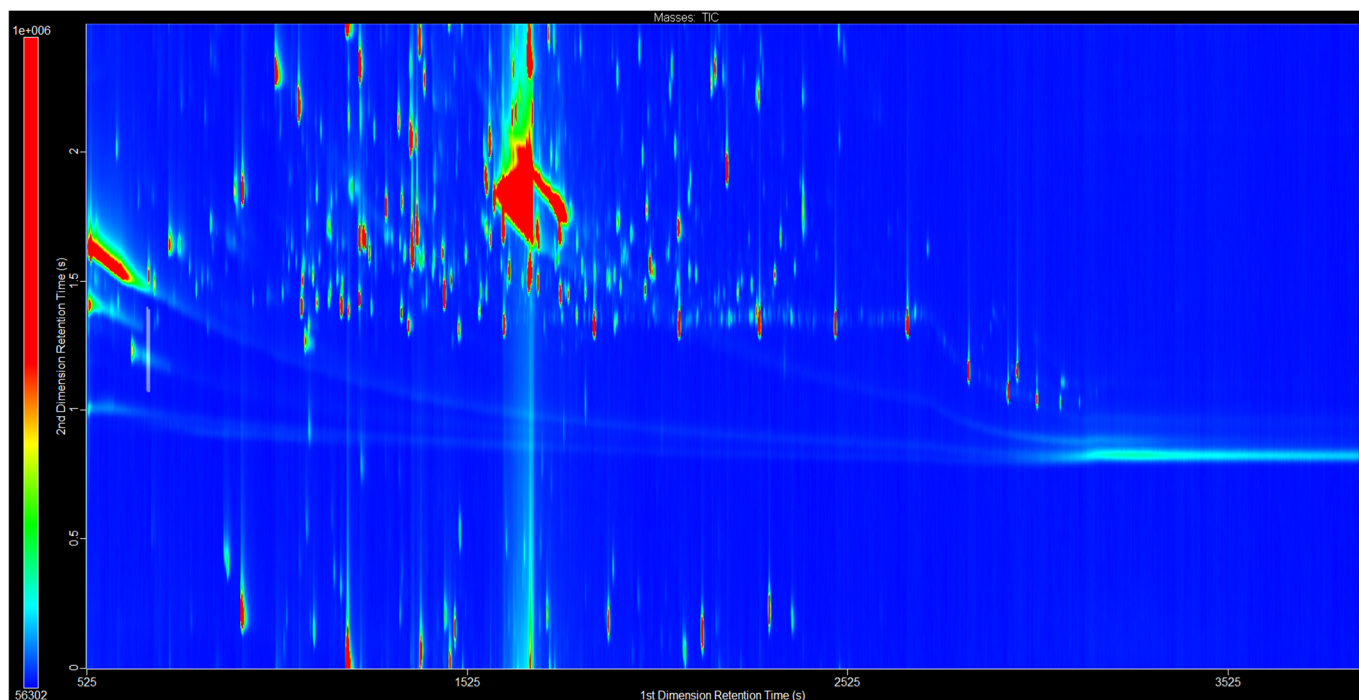


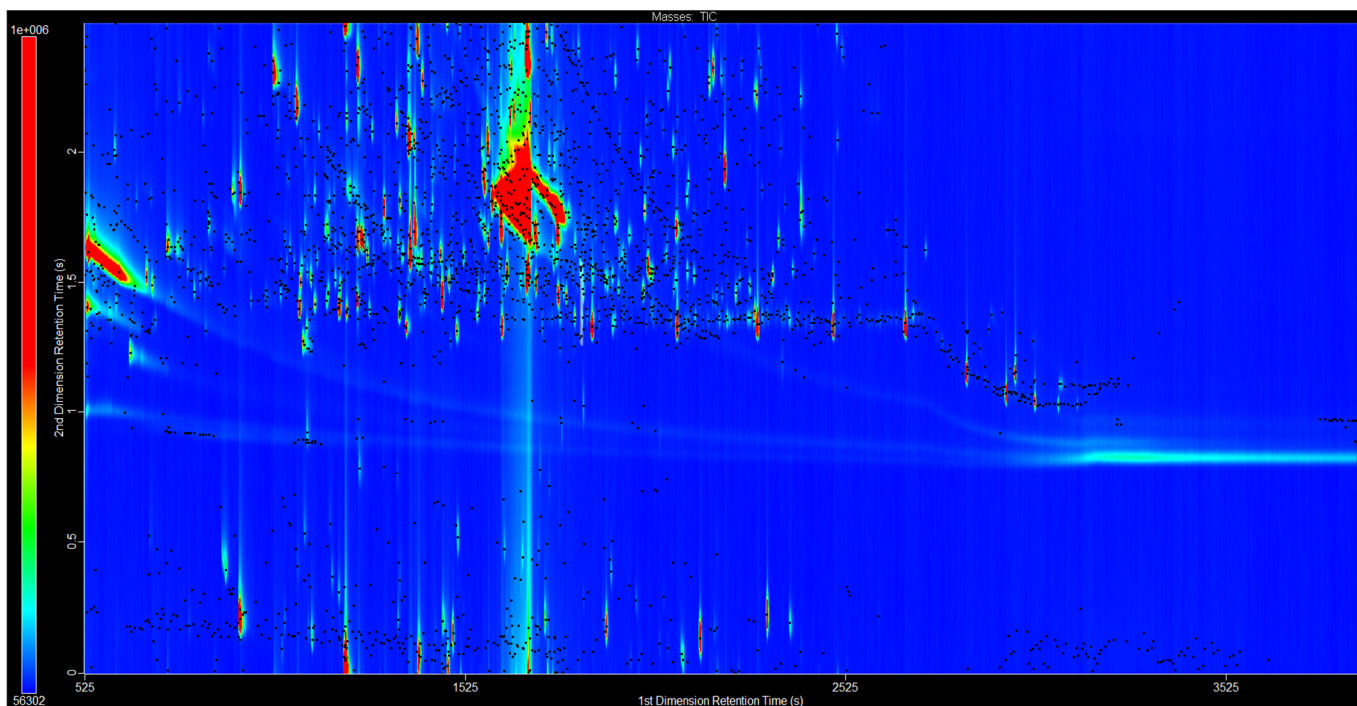
Figure S3: GC×GC total ion chromatogram *A. arvensis* extract F6 derivatized (with peak markers)



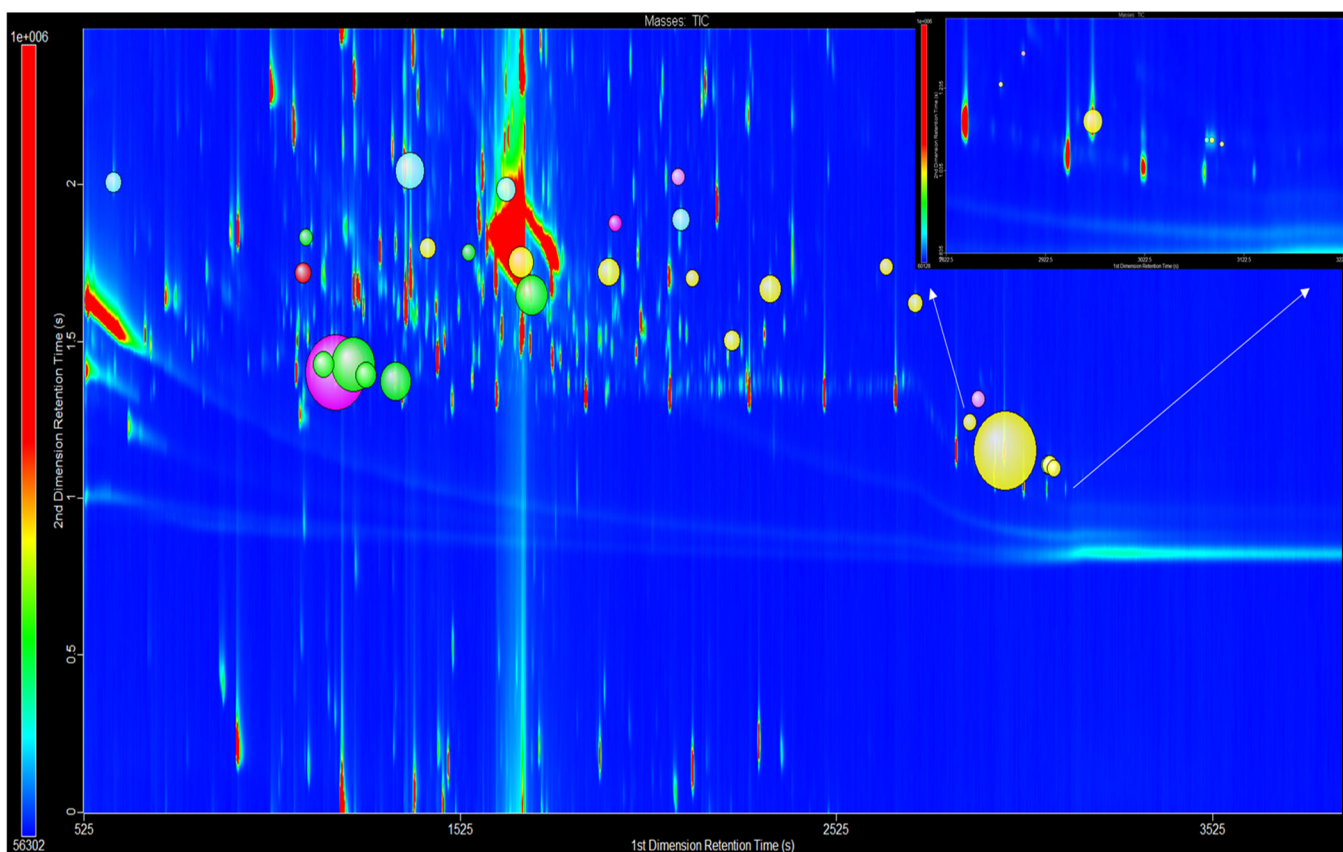
**Figure S4:** GC×GC total ion chromatogram *A. arvensis* extract F6 derivatized with Scripts



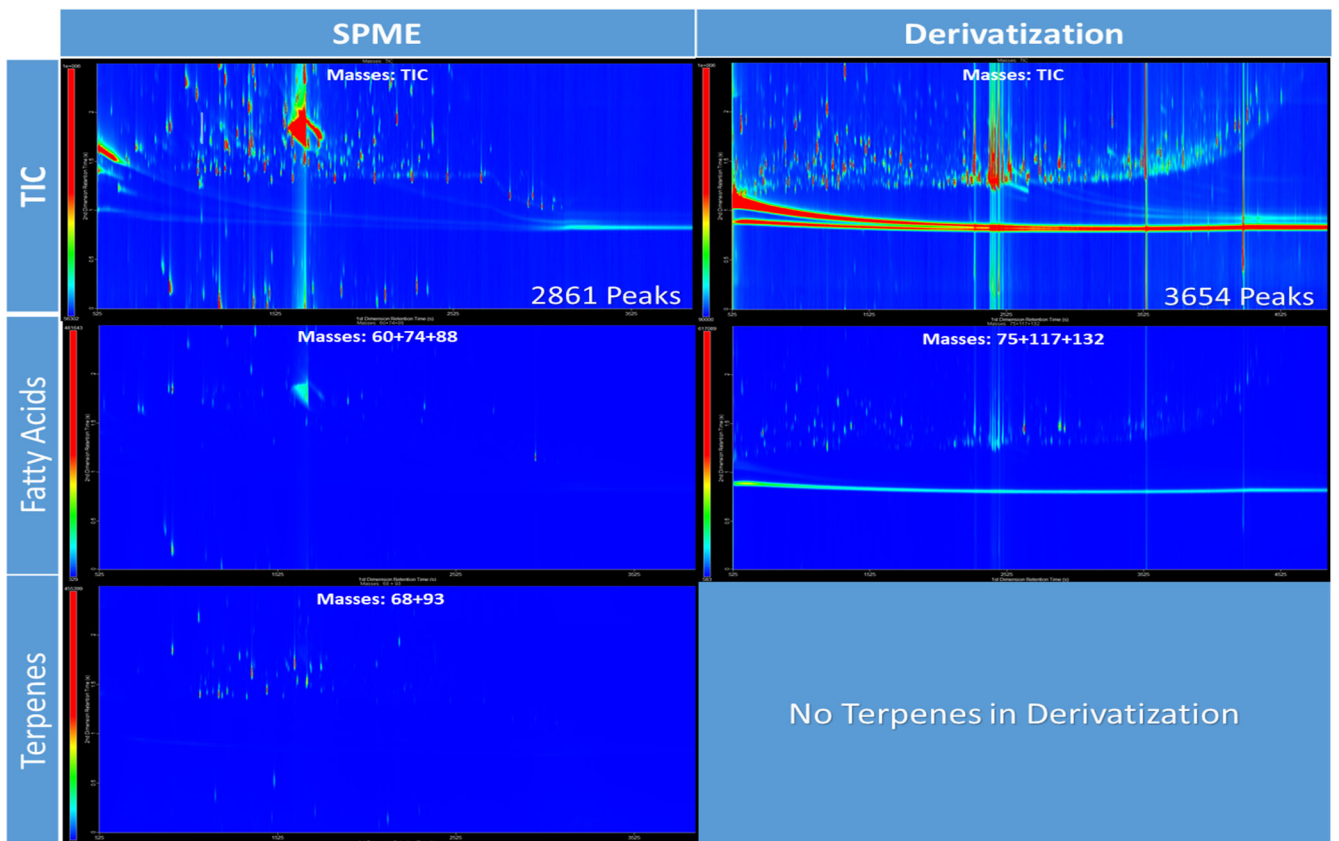
**Figure S5 :** GC×GC total ion chromatogram *A. arvensis* extract F6 SPME



**Figure S6:** GCxGC total ion chromatogram *A. arvensis* extract F6 SPME (with peak markers)



**Figure S7:** GCxGC total ion chromatogram *A. arvensis* extract F6 SPME with Scripts



**Figure S8 : GC×GC Methods Comparison**

### 3. Tables untargeted analysis of GC × GC-TOFMS metabolite profiles

**Table S1. Fifty-eight compounds identified by derivatization peaks that were detected by derivatization. <sup>1</sup>tR, <sup>2</sup>tR represent primary and secondary retention times, respectively.**

Peak #	Name	Similarity	Classifications	<sup>1</sup> tR, <sup>2</sup> tR (s)	UniqueMass	Quant S/N	Area
417	Limonene	936	monoterpene	687.5 , 1.235	68	1707	283112
647	Tris(trimethylsilyl)hydroxylamine	680	cysteine_TMS	835 , 1.255	146	410.06	37014
841	Heptanoic acid, trimethylsilyl ester	899	SatFA_TMS	962.5 , 1.470	75	1758.6	821644
1200	Octanoic acid, trimethylsilyl ester	974	SatFA_TMS	1175 , 1.480	117	1731.2	442217
1511	Nonanoic acid, trimethylsilyl ester	988	SatFA_TMS	1387.5 , 1.475	117	9015.7	2393950
1808	Decanoic acid, trimethylsilyl ester	967	SatFA_TMS	1595 , 1.460	117	764.66	184704
2327	Dodecanoic acid, trimethylsilyl ester	929	SatFA_TMS	1980 , 1.445	117	1002	232718
2364	Ribitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-	803	sugars_4TMS	2012.5 , 1.295	103	432.23	126318
2386	Ribitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-	824	sugars_4TMS	2030 , 1.255	103	1652	426671
2397	Ribitol, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-	831	sugars_4TMS	2040 , 1.265	103	5129.1	1670019
2772	Myristic acid, TMS derivative	807	SatFA_TMS	2330 , 1.440	285	509.48	83166
2775	3-Keto-glucose, bis(O-methyloxime), tetrakis-O-(trimethylsilyl)-	867	sugars_5TMS	2335 , 1.295	73	4663	1.2E+07
2914	D-Fructose, 1,3,4,5,6-pentakis-O-(trimethylsilyl)-, O-methyloxime	905	sugars_5TMS	2417.5 , 1.310	173	1584.1	1708356
2993	d-Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxime, (1Z)-	925	sugars_5TMS	2445 , 1.300	73	8343.5	2.7E+07
3008	d-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxime, (1E)-	888	sugars_5TMS	2452.5 , 1.330	87	535.32	139884
3015	d-Glucose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxime, (1E)-	949	sugars_5TMS	2457.5 , 1.305	160	9738.5	1.2E+07
3027	Hexadecanoic acid, methyl ester	965	Linear_saturated_FAMES	2460 , 1.505	87	9592.1	3836100
3043	d-Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxime, (1Z)-	938	sugars_5TMS	2467.5 , 0.235	205	1836.1	1537107
3099	d-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxime, (1Z)-	917	sugars_5TMS	2495 , 0.260	160	189.3	108498
3221	Ethyl pentadecanoate	909	FAEE	2570 , 1.495	88	1026.6	244166
3259	Palmitoleic acid 1TMS	822	MonoenoicFA_TMS	2612.5 , 1.450	117	169.84	53967
3266	15-Tetracosenoic acid, (Z)-, TMS derivative	869	MonoenoicFA_TMS	2620 , 1.455	117	342.54	132307
3293	Hexadecanoic acid, trimethylsilyl ester	970	SatFA_TMS	2650 , 1.445	132	15244	5192772
3362	9,12-Octadecadienoic acid, methyl ester	924	Linear_dienoicFAME	2730 , 1.520	67	4485.3	1692296



3371	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-	939	Linear_trienoicFAME	2742.5 , 1.530	67	8735.7	3463550
3406	Octadecanoic acid, methyl ester	910	Linear_saturated_FAMES	2775 , 1.490	74	3421.7	1523706
3428	Heptadecanoic acid, TMS derivative	951	SatFA_TMS	2802.5 , 1.435	132	351.57	78943
3431	d-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxyme, (1Z)-	896	sugars_5TMS	2807.5 , 1.320	73	10112	1.6E+07
3446	d-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxyme, (1Z)-	908	sugars_5TMS	2830 , 1.325	103	1603.1	585452
3449	9,12-Octadecadienoic acid, methyl ester, (E,E)-	873	Linear_dienoicFAME	2832.5 , 1.520	67	447.44	161532
3456	d-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxyme, (1Z)-	828	sugars_5TMS	2842.5 , 1.325	73	2108.3	2132816
3460	d-Galactose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxyme, (1Z)-	814	sugars_5TMS	2850 , 1.345	147	713.49	235777
3464	d-Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, o-methyloxyme, (1Z)-	838	sugars_5TMS	2860 , 1.325	147	452.94	320633
3500	trans-9-Octadecenoic acid, trimethylsilyl ester	892	MonoenoicFA_TMS	2910 , 1.465	117	5742.2	944596
3503	$\alpha$ -Linolenic acid, trimethylsilyl ester	928	multienoicFA_TMS	2915 , 1.480	108	5737.4	1968665
3512	15-Tetracosenoic acid, (Z)-, TMS derivative	839	MonoenoicFA_TMS	2922.5 , 1.445	117	344.54	261762
3529	Octadecanoic acid, trimethylsilyl ester	988	SatFA_TMS	2945 , 1.450	117	13573	4039101
3620	Methyl (6E,9E,12E)-6,9,12-octadecatrienoate	623	FA	3047.5 , 1.560	91	98.991	31688
3780	Eicosanoic acid, trimethylsilyl ester	967	SatFA_TMS	3217.5 , 1.455	117	1436.2	310003
3900	Heneicosanoic acid, TMS derivative	814	SatFA_TMS	3345 , 1.475	132	103.32	15384
3964	Maltose 8TMS	833	sugars_8TMS	3425 , 1.375	204	10751	4491939
3982	15-Tetracosenoic acid, (Z)-, TMS derivative	825	MonoenoicFA_TMS	3442.5 , 1.500	117	225.79	94233
4012	Docosanoic acid, trimethylsilyl ester	880	SatFA_TMS	3467.5 , 1.495	132	487.28	55957
4159	Tricosanoic acid, trimethylsilyl ester	926	SatFA_TMS	3587.5 , 1.515	132	251.87	46322
4176	Maltose, octakis(trimethylsilyl)-	794	sugars_8TMS	3602.5 , 1.430	204	1589.4	771335
4193	D-Turanose, heptakis(trimethylsilyl)-	758	sugars_8TMS	3617.5 , 1.405	179	323.58	74146
4239	Maltose, octakis(trimethylsilyl)-	777	sugars_8TMS	3655 , 1.415	361	559.56	503216
4254	D-Turanose, heptakis(trimethylsilyl)-	840	sugars_8TMS	3665 , 1.440	73	3494.9	5710906
4300	Tetracosanoic acid, trimethylsilyl ester	965	SatFA_TMS	3702.5 , 1.545	117	1423.7	397263
4485	Maltose, octakis(trimethylsilyl)-	802	sugars_8TMS	3845 , 1.525	204	891.22	467784
4589	Docosanoic acid, trimethylsilyl ester	894	SatFA_TMS	3922.5 , 1.625	117	1394.4	447380
4718	3-Bromocholest-5-ene	770	FA	4032.5 , 1.785	105	90.826	22843
4810	Tetracosanoic acid, trimethylsilyl ester	804	SatFA_TMS	4127.5 , 1.755	117	1486.5	478749

4858	Campesterol tms	884	cholesterol_TMS	4192.5 , 1.860	129	4915.7	2095533
4965	$\beta$ -Sitosterol trimethylsilyl ether	831	cholesterol_TMS	4282.5 , 1.965	129	8160.9	5024644
4981	Pregn-5-en-20-one, 3,16-bis[(trimethylsilyl)oxy]-, (3 $\beta$ ,16 $\alpha$ )-	742	sterol_TMS	4297.5 , 1.945	55	657.92	407467
5051	D-Turanose, heptakis(trimethylsilyl)-	848	sugars_8TMS	4367.5 , 1.935	73	2562.1	4776193

Fatty acid (FA); Fatty acid ethyl esters (FAEE); FAMES (fatty acid methyl esters); TMS (trimethylsilyl ether); SatFA\_TMS (Saturated Fatty acid\_trimethylsilyl ether).

**Table S2. Twenty-nine compounds identified by SPME peaks that were detected by derivatization. <sup>1</sup>tR, <sup>2</sup>tR represent primary and secondary retention times, respectively.**

Peak #	Name	Similarity	Classifications	1tR, 2tR (s)	UniqueMass	Quant S/N	Area
86	Hexanal	935	linear_aldehyde	602.5 , 2.010	41	1760.5	1278565
474	Hexanoic acid	951	linear_FA	1105 , 1.720	60	4149.4	2447456
486	Hexanoic acid, ethyl ester	932	FAEE	1112.5 , 1.835	88	805.48	154325
533	1-Isopropyl-4-methyl-1,4-cyclohexadiene	888	terpenes1	1160 , 1.430	93	4078.9	902565
586	4-Isopropenyl-1-methyl-1-cyclohexene	960	terpenes2	1192.5 , 1.405	68	34613	6260079
675	1,3,6-Octatriene, 3,7-dimethyl-1-Isopropyl-4-methyl-1,4-cyclohexadiene	941	terpenes1	1240 , 1.430	93	18121	3095421
742	1-Methyl-4-(1-methylethylidene)-1-cyclohexene	908	terpenes1	1272.5 , 1.395	93	5272.3	727499
847	1-cyclohexene	924	terpenes1	1352.5 , 1.375	93	10476	1795404
929	Nonanal	940	linear_aldehyde	1390 , 2.045	57	7715.1	1433560
1014	Octanoic acid, methyl ester	973	Linear_saturated_FAMES	1437.5 , 1.800	74	4037.3	1141873
1221	5,7-Octadien-2-ol, 2,6-dimethyl-	882	terpenes1	1545 , 1.785	93	357.1	74961
1455	Decanal	936	linear_aldehyde	1645 , 1.985	57	1976.9	496294
1566	Nonanoic acid, methyl ester	906	Linear_saturated_FAMES	1685 , 1.755	87	7480.9	1046417
1642	Bicyclo[2.2.1]hept-2-ene, 1,7,7-trimethyl-	839	terpenes1	1712.5 , 1.650	93	10292	1814198
2077	Decanoic acid, methyl ester	979	Linear_saturated_FAMES	1917.5 , 1.725	74	9841.9	2323317
2104	(1R,2S,4R)-2,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol	733	terpenes2	1935 , 1.880	85	128.06	30844
2362	6-Dodecanone	855	ketones	2102.5 , 2.025	43	464.5	210649
2373	Dodecanal	945	linear_aldehyde	2110 , 1.890	41	1729.5	628829
2408	Undecanoic acid, methyl ester	935	Linear_saturated_FAMES	2140 , 1.705	74	505.85	122333
2535	Naphthalene, 1,2,3,5,6,7,8,8a-octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1 $\alpha$ ,7 $\beta$ ,8 $\alpha$ )]-	840	terpenes3	2245 , 1.505	91	717.6	134886
2631	Dodecanoic acid, methyl ester	944	Linear_saturated_FAMES	2347.5 , 1.670	74	10186	1875553
2802	Patchouli alcohol	850	terpenes3	2655 , 1.740	41	132.78	42116
2835	Tetradecanoic acid, methyl ester	969	Linear_saturated_FAMES	2732.5 , 1.625	74	2363.3	643488

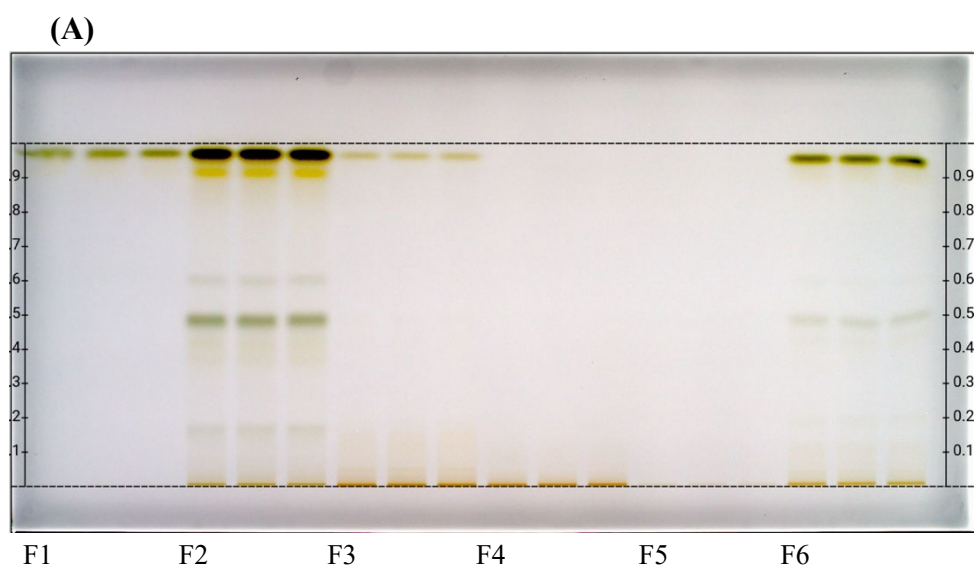
2890	Pentadecanoic acid, methyl ester	960	Linear_saturated_FAMES	2877.5 , 1.245	74	587.4	83335
2904	2-Undecanone, 6,10-dimethyl-	868	ketones	2900 , 1.320	43	651.19	145010
2941	Hexadecanoic acid, methyl ester	990	Linear_saturated_FAMES	2970 , 1.155	74	48039	6751820
3022	9,12-Octadecadienoic acid, methyl ester, (E,E)-	912	Linear_dienoicFAME	3085 , 1.110	67	1066.3	142572
3025	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-	908	terpenes3	3090 , 1.110	79	858.09	184721
3032	Tetradecanoic acid, methyl ester	889	Linear_saturated_FAMES	3100 , 1.100	74	621	94072

Fatty acid (FA); Fatty acid ethyl esters (FAEE); FAMES (fatty acid methyl esters).

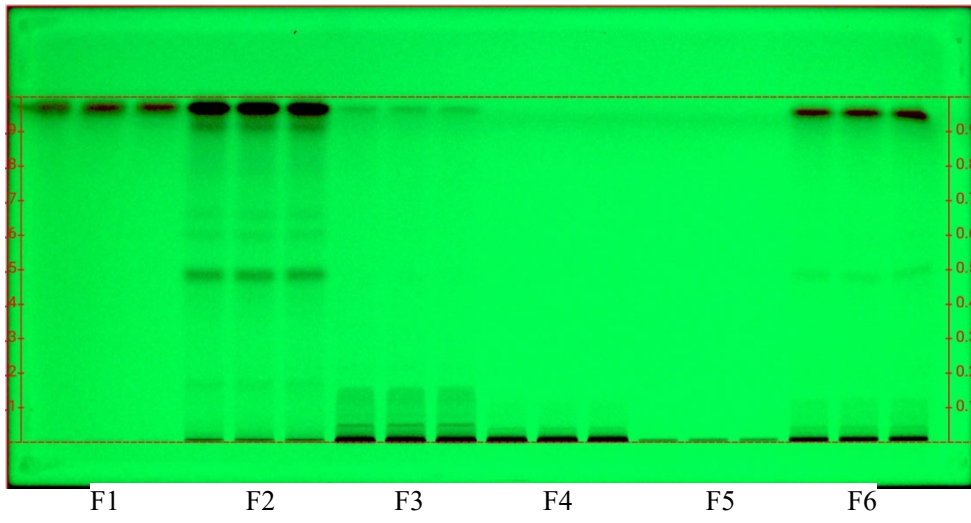
#### 4. TLC plate of all fraction of *Acalypha arvensis* Poepp

Figure S9. TLC plate of all fraction of *Acalypha arvensis* Poepp

HPTLC plates of the six fractions obtained from *A. arvensis*. Fractions were prepared at a concentration of 5mg/mL and deposited on a silica gel 60 F254 20 × 10 cm HPTLC plate (Merck) using the CAMAG Automatic TLC Sampler 4 (ATS 4) depositor (CAMAG, Muttenz, Switzerland). A deposit of 5  $\mu$ L was thus carried out in three replicates for each fraction. The migration was performed with the eluent system ethyl acetate/methanol (90/10) over a distance of 70 mm with the CAMAG Automatic Developing Chamber 2 (ADC 2). The developed TLC plates were visualized under Visible light (A), UV 254 (B) and 366 nm (C) using the CAMAG TLC Visualizer.



**(B)**



**(C)**

