Supplementary Materials

Table S1 Metabolite identification in extracts from different parts of *G. xanthochymus.*

No.	RT	Type of ion	Mass	Formular	Score	Identification	Class	Extract parts
1	1.497	[M-H] $^-$	243.94	$C_8H_5BrO_4$	67.62	4-Bromoisophthalic acid	Other	BH
2	1.634	[M-H] $^-$	311.94	$C_8H_4F_3IN_2$	83.24	3-(Trifluoromethyl)-3-(3-iodophenyl) diazirine	Other	BH
3	1.739	[M+H] +	163.08	$C_6H_{13}NO_4$	77.97	4-Amino-4,6-dideoxy-D-mannose	Flavonoid	LA
4	1.806	[M+H] +	706.26	$C_{38}H_{42}O_{13}$	67.78	unknow	Flavonoid	BH, TH, TM
5	1.892	[M-H] $^-$	194.00	$C_7H_2F_4O_2$	59.54	2,3,4,5-Tetrafluorobenzoic acid	Other	BH
6	2.469	[M-H] $^-$	192.03	$C_6H_8O_7$	95.53	Citric acid	Flavonoid	TH
7	6.151	[M+H] +	230.16	$C_{11}H_{22}N_2O_3$	81.27	D-Leucyl-D-valine	Flavonoid	LM
8	7.161	[M-H] $^-$	112.02	$C_5H_4O_3$	86.45	Pyromeconic acid	Other	BH
9	7.998	[M+H] +	394.15	$C_{16}H_{26}O_{11}$	92.78	3-Methylbut-2-enoyl-1-O-β-D-glucopyranosyl-β-D-apiofuranoside	Other	BM
10	8.024	[M+H] +	432.11	$C_{21}H_{20}O_{10}$	86.56	Vitexin	Flavonoid	BM
11	8.809	[M+H] +	168.04	$C_8H_8O_4$	45.62	4-Methoxysalicylic acid	Flavonoid	LA
12	10.624	[M-H] $^-$	166.03	$C_8H_6O_4$	99.66	Terephthalic acid	Benzophenone	TH
13	10.663	[M-H] $^-$	122.04	$C_7H_6O_2$	86.76	2-Hydroxybenzaldehyde	Flavonoid	BD
14	10.669	[M-H] $^-$	166.03	$C_8H_6O_4$	92.85	Terephthalic acid	Flavonoid	BD
15	11.321	[M-H] $^-$	154.03	$C_7H_6O_4$	88.23	Gentisic acid	Flavonoid	BD
16	11.616	[M+H] +	420.16	$C_{25}H_{24}O_6$	64.82	Pomiferin	Flavonoid	LH, LD
17	12.059	[M+H] +	652.25	$C_{35}H_{40}O_{12}$	91.84	Triptofordin F4	Flavonoid	BH
18	12.114	[M-H] $^-$	178.03	$C_9H_6O_4$	85.11	3,5-Dihydroxybenzoic acid	Phloroglucinol	BD
19	12.431	[M+H] +	414.24	$C_{14}H_{34}N_6O_8$	91.98	2,2'-Azobis[n-(2-carboxyethyl)-2-methylpropionamidine]	Flavonoid	LA
20	12.947	[M-H] $^-$	198.05	$C_9H_{10}O_5$	80.55	Syringic acid	Flavonoid	BD
21	13.604	[M-H] $^-$	166.06	$C_9H_{10}O_3$	83.83	Tropic acid	Other	TD
22	13.604	[M-H] $^-$	182.06	$C_9H_{10}O_4$	80.00	Hydroxy tropic acid	Other	TD
23	13.606	[M+H] +	508.21	$C_{29}H_{32}O_8$	75.22	Gomisin G	Flavonoid	BD
24	14.451	[M+H] +	596.42	$C_{41}H_{56}O_3$	94.12	Bacteriorubixanthinal	Carotenoid	LM
25	14.494	[M+H] +	596.42	$C_{41}H_{56}O_3$	91.09	Bacteriorubixanthinal	Polyphenol	BD

No.	RT	Type of ion	Mass	Formular	Score	Identification	Class	Extract parts
26	16.147	[M+H] +	252.12	$C_{11}H_{16}N_4O_3$	85.90	Histidylproline	Flavonoid	LD
27	16.329	[M+H] +	602.36	$C_{38}H_{50}O_6$	94.79	(-)-Guttiferone E	Xanthone	BD, LM, TH, TA, TM
28	16.341	[M+H] +	602.36	$C_{38}H_{50}O_6$	85.00	Guttiferone F	Xanthone	TA
29	16.713	[M-H] $^-$	286.10	$C_{20}H_{14}O_2$	61.31	1,2-Dibenzoylbenzene	Benzophenone	TH
30	16.718	[M+H] +	740.47	$C_{40}H_{68}O_{12}$	69.17	Gypenoside LXXVII	Flavonoid	LD
31	17.108	[M-H] $^-$	374.10	$C_{19}H_{18}O_8$	99.43	1,5,8-Trihydroxy-3-methyl-6-prenylxanthone	Xanthone	BM, LH, LM
32	17.181	[M-H] $^-$	718.15	$C_{36}H_{30}O_{16}$	78.81	Fukugiside	Flavonoid	TA
33	17.221	[M+H] +	354.11	$C_{20}H_{18}O_6$	80.95	Curcumin derivative	Flavonoid	LD
34	17.556	[M+H] +	288.06	$C_{15}H_{12}O_6$	72.35	3',4',5,7-Tetrahydroxyisoflavanone	Flavonoid	TA
35	17.601	[M-H] $^-$	704.17	$C_{36}H_{32}O_{15}$	67.47	Occidentoside	Flavonoid	TA
36	18.221	[M+H] +	532.30	$C_{30}H_{44}O_8$	43.07	Ganoderic acid	Flavonoid	TH
37	18.247	[M-H] $^-$	556.10	$C_{30}H_{20}O_{11}$	81.04	Morelloflavone	Flavonoid	TM
38	18.248	[M+H] +	556.10	$C_{30}H_{20}O_{11}$	77.02	Ephedrannin A	Other	TA, TD
39	18.552	[M-H] $^-$	358.07	$C_{18}H_{14}O_8$	80.75	Psoromic acid	Xanthone	BH, LD, LA, TD
40	18.581	[M-H] $^-$	540.11	$C_{30}H_{20}O_{10}$	73.51	Volkensiflavone	Flavonoid	TM
41	18.590	[M+H] +	518.12	$C_{28}H_{22}O_{10}$	71.78	Xanosporolactone	Other	TA, TD
42	18.595	[M-H] $^-$	402.10	$C_{20}H_{18}O_9$	96.88	4-O-Demethyl-13-dihydroadriamycinone	Flavonoid	BH
43	18.600	[M-H] $^-$	224.10	$C_{12}H_{16}O_4$	70.95	Aspidinol	Other	BH
44	18.618	[M-H] $^-$	542.12	$C_{30}H_{22}O_{10}$	97.39	Neochamaejasmin A	Flavonoid	TM
45	18.808	[M-H] $^-$	396.16	C_{23} H_{24} O_6	94.48	4-(1,1-Dimethyl-2-propenyl)-1,3,5,6 tetrahydroxy-7-prenylxanthone	Xanthone	BH
46	18.811	[M+H] +	396.16	$C_{23}H_{24}O_6$	77.26	4-(1,1-Dimethyl-2-propenyl)-1,3,5,6-tetrahydroxy-7-prenylxanthone	Xanthone	BH
47	18.887	[M-H] $^-$	478.05	$C_{24}H_{14}O_{11}$	55.55	Fucofuroeckol B	Flavonoid	TM
48	19.273	[M-H] $^-$	372.08	$C_{19}H_{16}O_8$	87.36	7-Hydroxy-3,5,8-trimethoxy-3',4'-methylenedioxyflavone	Flavonoid	BM, LH, LD, LA, LM, TM
49	19.375	[M+H] +	394.14	C_{23} H_{22} O_6	79.87	Garcinone B	Xanthone	BH
50	19.538	[M-H] $^-$	320.05	C_{15} H_{12} O_8	76.20	2,7-Dimethoxy-1,3,6,8 tetrahydroxyxanthone	Xanthone	BH
51	19.708	[M-H] $^-$	326.08	C_{18} H_{14} O_6	68.17	O-Demethylforbexanthone	Xanthone	BH
52	19.712	[M-H] $^-$	594.14	$C_{30}H_{26}O_{13}$	79.58	Tiliroside	Flavonoid	TM
53	20.480	[M-H] $^-$	326.08	C_{18} H_{14} O_6	80.76	Globulixanthone C	Xanthone	BH

No.	RT	Type of ion	Mass	Formular	Score	Identification	Class	Extract parts
54	20.619	[M-H] $^-$	566.12	$C_{32}H_{22}O_{10}$	74.23	Podocarpusflavone B	Flavonoid	BM, LD
55	20.672	[M-H] $^-$	412.15	C_{23} H_{24} O_7	76.78	1,3,8-Trihydroxy-2-(3-methyl-2 butenyl)-4-(3-hydroxy-3 methylbutanoyl)-xanthone	Xanthone	BH
56	20.845	[M-H] $^-$	342.11	$C_{19}H_{18}O_6$	99.02	1,5,8-Trihydroxy-3-methyl-2-prenylxanthone	Xanthone	BM, LH, LA, LM
57	20.848	[M-H] $^-$	342.11	C_{19} H_{18} O_6	83.17	1,5,8-Trihydroxy-3-methyl-2 prenylxanthone	Xanthone	BH
58	20.848	[M-H] $^-$	342.11	C_{19} H_{18} O_6	83.17	Dulxanthone D	Xanthone	BH
59	20.958	[M-H] $^-$	396.16	C_{23} H_{24} O_6	82.71	Formoxanthone C	Xanthone	BH
60	20.964	[M+H] +	396.16	$C_{23}H_{24}O_6$	77.54	Formoxanthone C	Xanthone	BH
61	21.225	[M-H] $^-$	394.14	C_{23} H_{22} O_6	81.93	Formoxanthone A	Xanthone	BH
62	21.693	[M-H] $^-$	380.16	C_{23} H_{24} O_5	71.89	7-Geranyloxy-1,3 dihydroxyxanthone	Xanthone	BH
63	21.712	[M-H] $^-$	396.16	C_{23} H_{24} O_6	81.99	Isoalvaxanthone	Xanthone	BH
64	21.950	[M+H] +	394.14	C_{23} H_{22} O_6	73.15	Formoxanthone A	Xanthone	BH
65	22.315	[M-H] $^-$	438.20	C_{26} H_{30} O_6	53.05	Hydroxy-8-(2-hydroxy-3 methylbut-3-enyl)-3,6,7 trimethoxy-2-(3-methylbut-2 enyl)-xanthone	Xanthone	BH
66	22.756	[M-H] $^-$	464.22	C_{28} H_{32} O_6	51.58	1,3,5,6-Tetrahydroxy-4,7,8-tri (3 methyl-2-butenyl) xanthone	Xanthone	BH
67	23.345	[M-H] $^-$	378.15	C_{23} H_{22} O_5	88.03	Blancoxanthone	Xanthone	BH
68	23.651	[M-H] $^-$	394.18	C_{24} H_{26} O_5	47.43	1,3,8-Trihydroxy-4-methyl-2,7 diprenylxanthone	Xanthone	BH
69	24.003	[M-H] $^-$	408.16	C_{24} H_{24} O_6	87.15	6,8-Dihydroxy-1,7 diprenylxanthone-2-carboxylic acid	Xanthone	BH
70	24.395	[M-H] $^-$	408.19	C_{25} H_{28} O_5	79.20	1-Hydroxy-3,5-dimethoxy-2,4 diprenylxanthone	Xanthone	BH
71	24.856	[M-H] $^-$	462.20	C_{28} H_{30} O_6	97.33	Virgataxanthone B	Xanthone	BH
72	24.866	[M+H] +	462.20	C_{28} H_{30} O_6	92.63	Virgataxanthone B	Xanthone	BH
73	25.336	[M+H] +	328.17	C_{20} H_{24} O_4	93.68	7-Geranyloxy-5-methoxycoumarin	Coumarin	BH

B: Bark, L: Leave, T: Twig, H: Hexanes, D: Dichloromethane, A: Acetone, M: Methanol

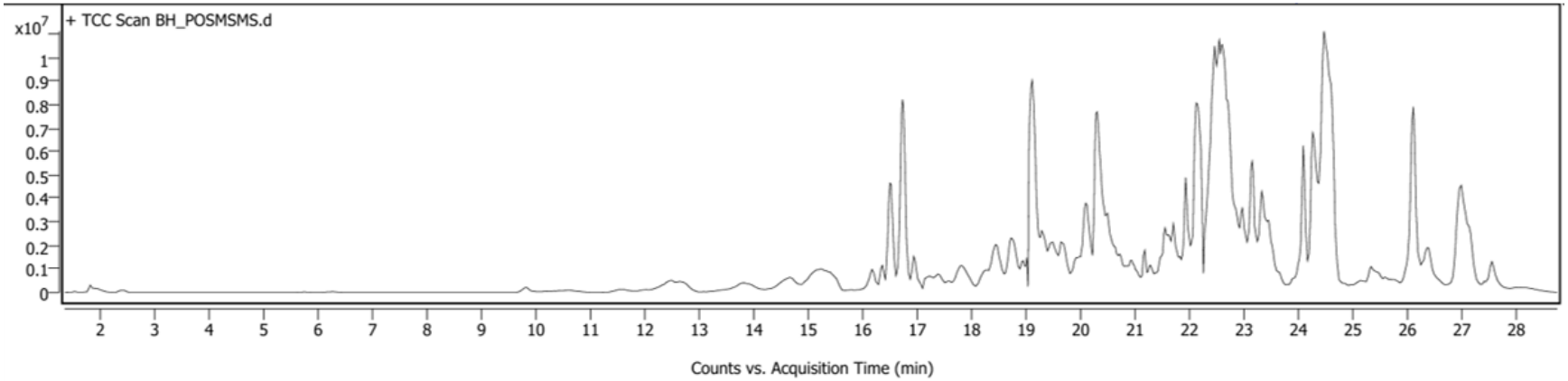


Figure S1 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* bark extract with hexanes (Positive).

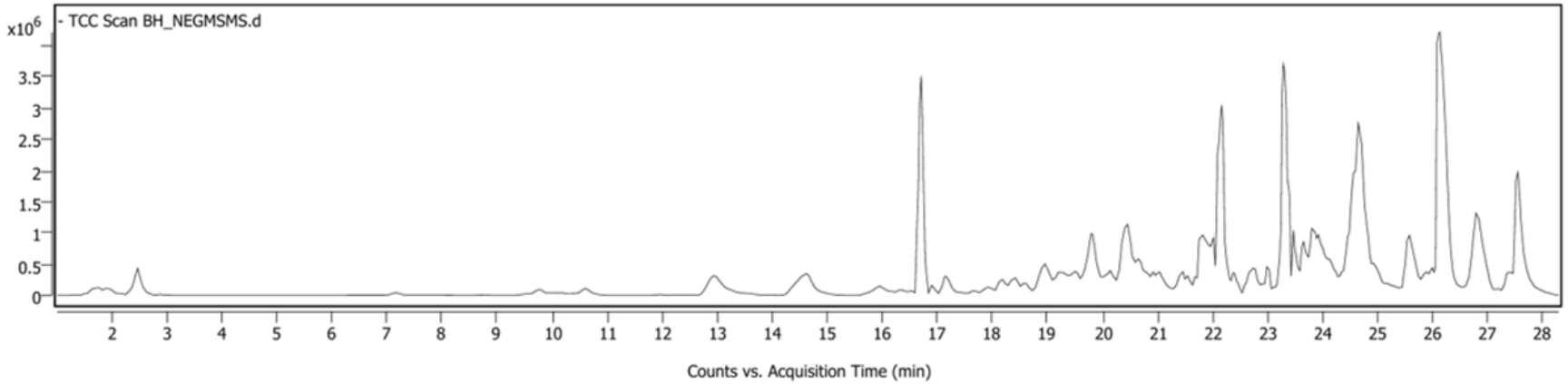
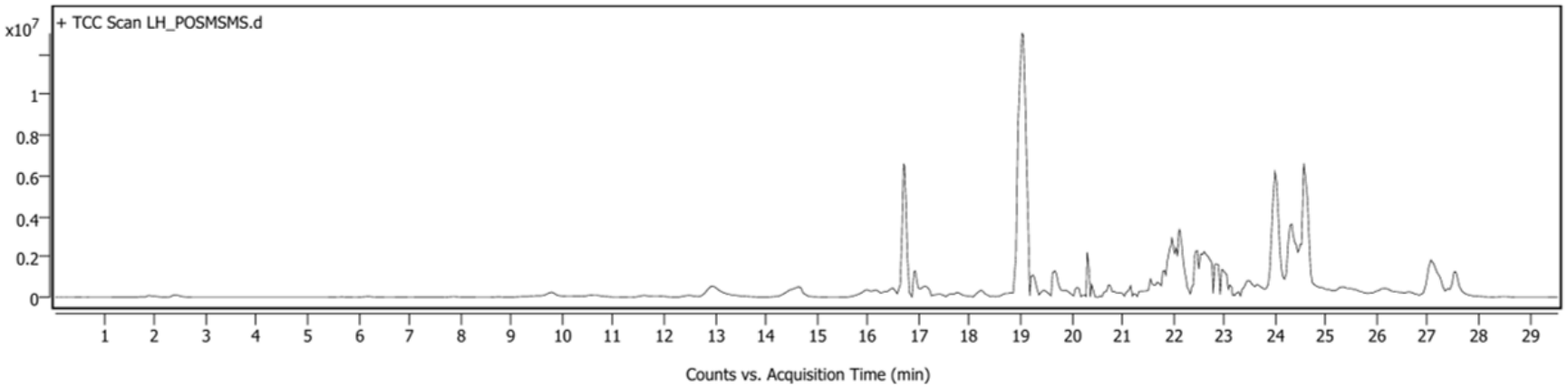
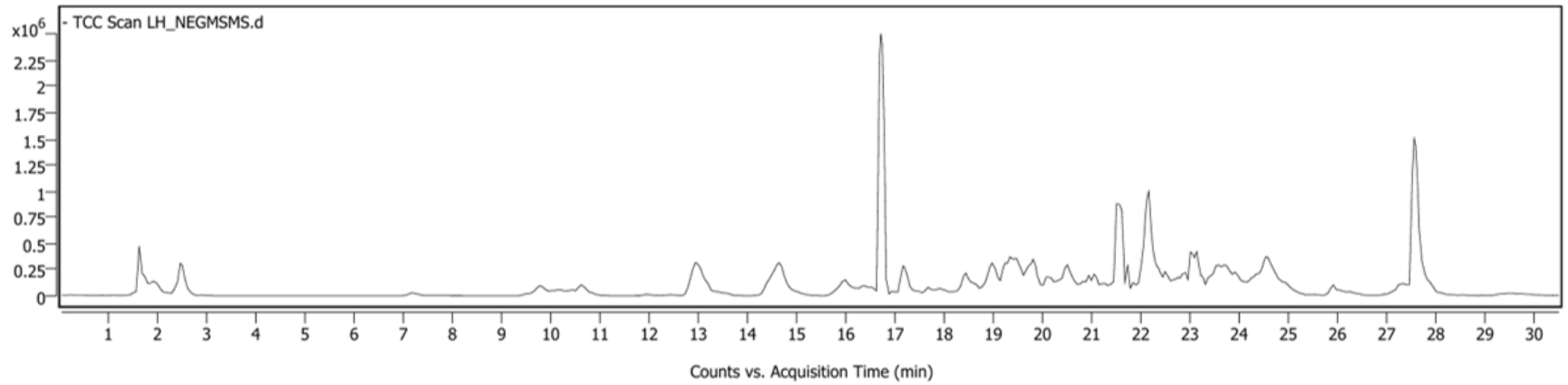


Figure S2 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* bark extract with hexanes (Negative).


+ TCC Scan LH_POSMSMS.d
x10^7
1
0.8
0.6
0.4
0.2
0
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29
Counts vs. Acquisition Time (min)


- TCC Scan LH_NEGMSMS.d
x10^6
2.25
2
1.75
1.5
1.25
1
0.75
0.5
0.25
0
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30
Counts vs. Acquisition Time (min)

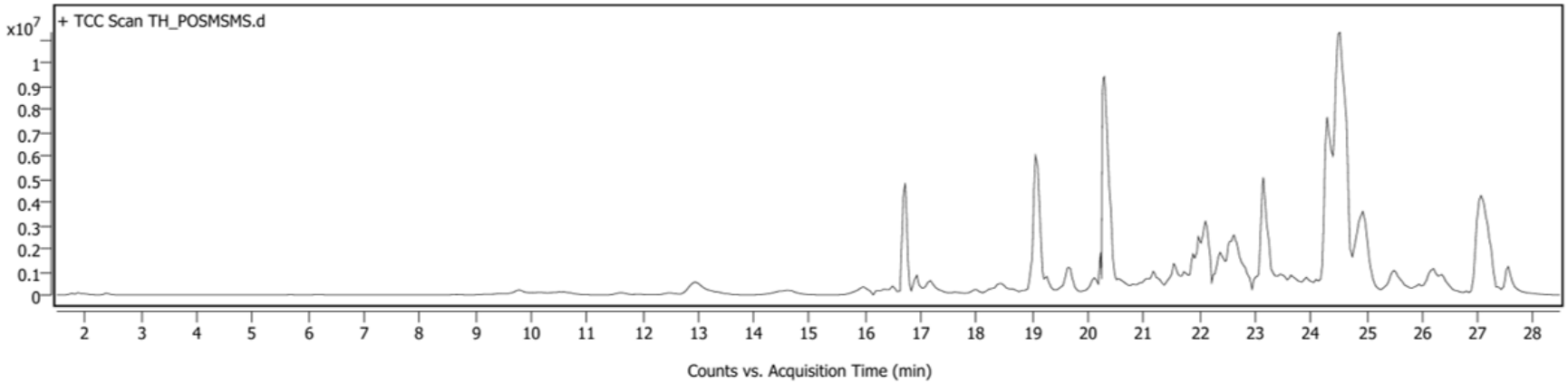


Figure S5 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* twig extract with hexanes (Positive).

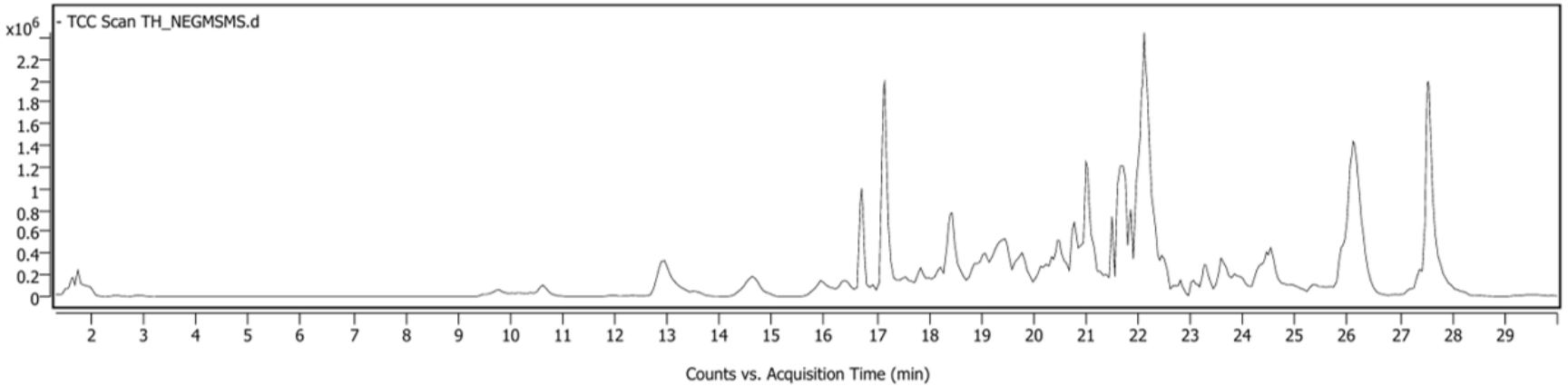


Figure S6 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* twig extract with hexanes (Negative).

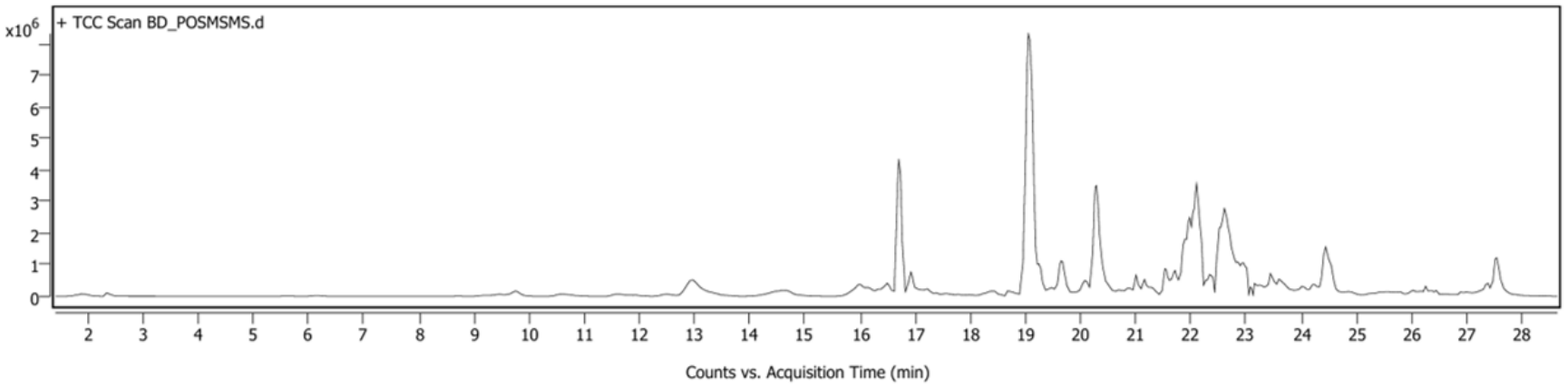


Figure S7 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* bark extract with dichloromethane (Positive).

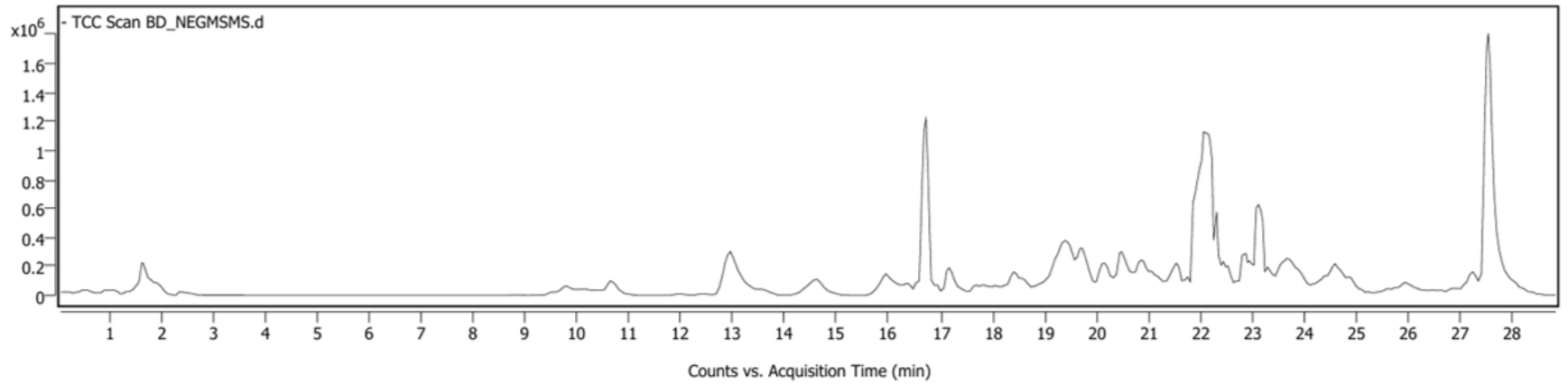


Figure S8 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* bark extract with dichloromethane (Negative).

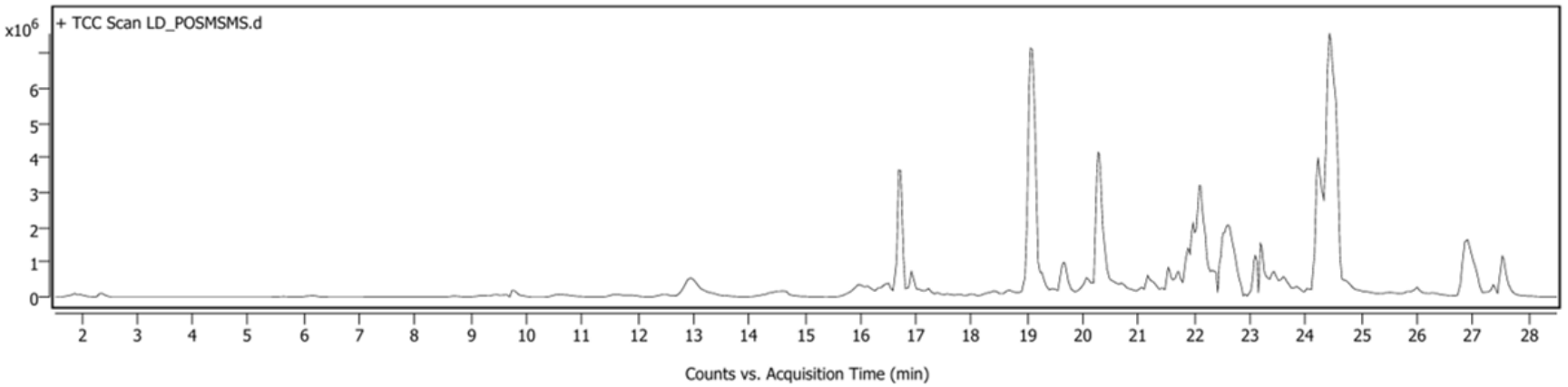
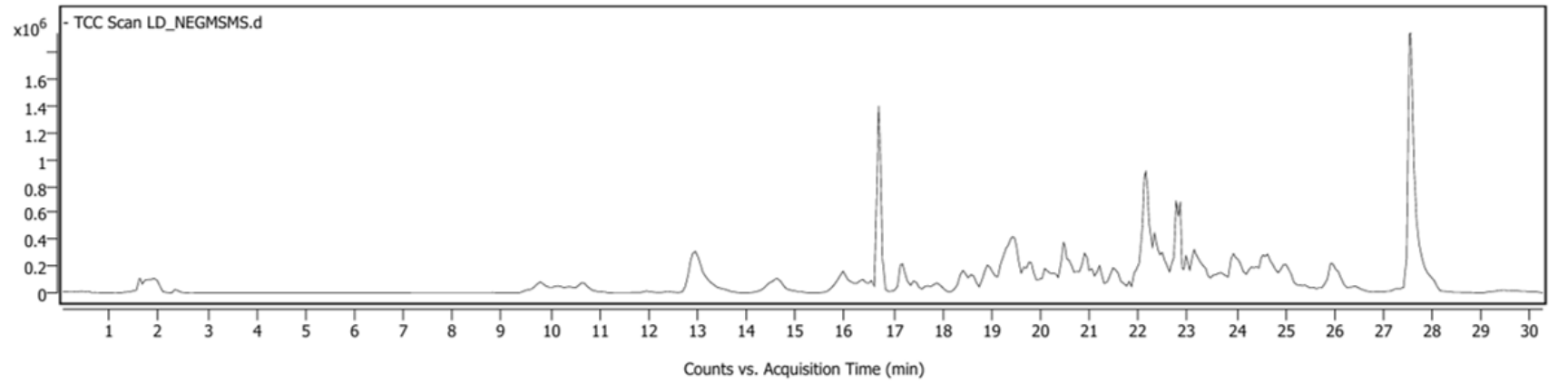
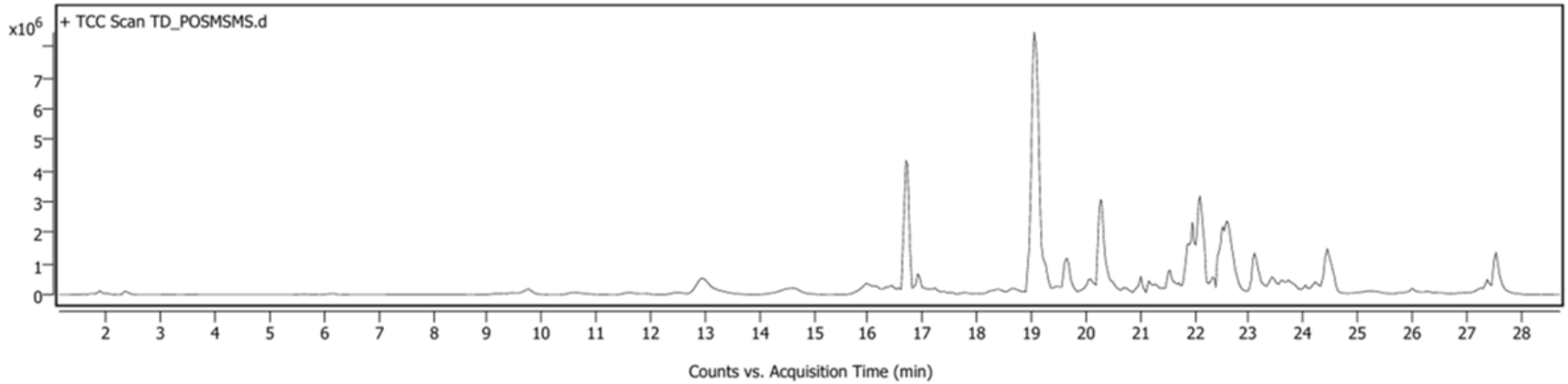
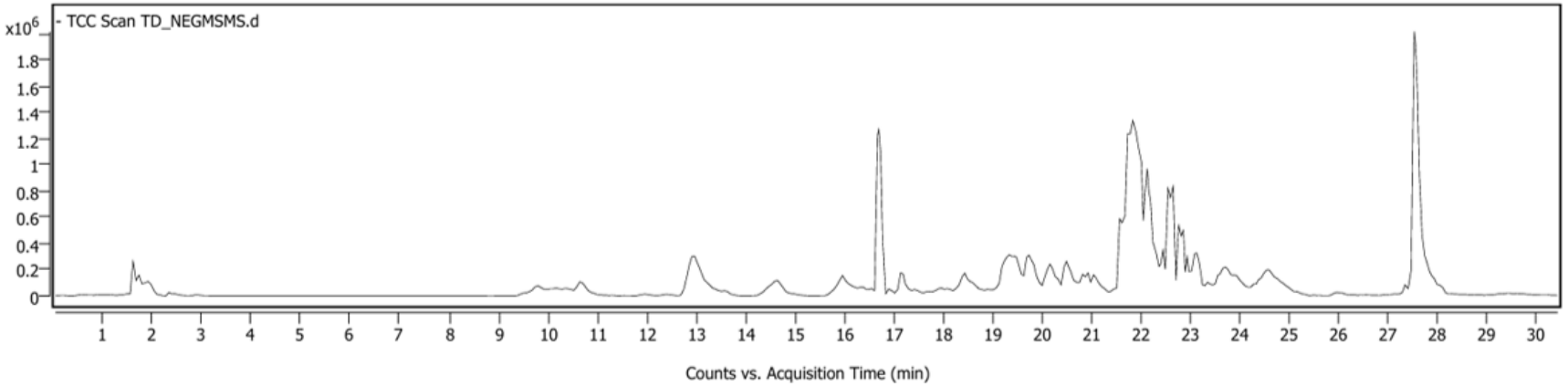


Figure S9 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* leave extract with dichloromethane (Positive).




x10^6
+ TCC Scan TD_POSMSMS.d
7
6
5
4
3
2
1
0
2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28
Counts vs. Acquisition Time (min)


x10^6
- TCC Scan TD_NEGMSMS.d
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30
Counts vs. Acquisition Time (min)

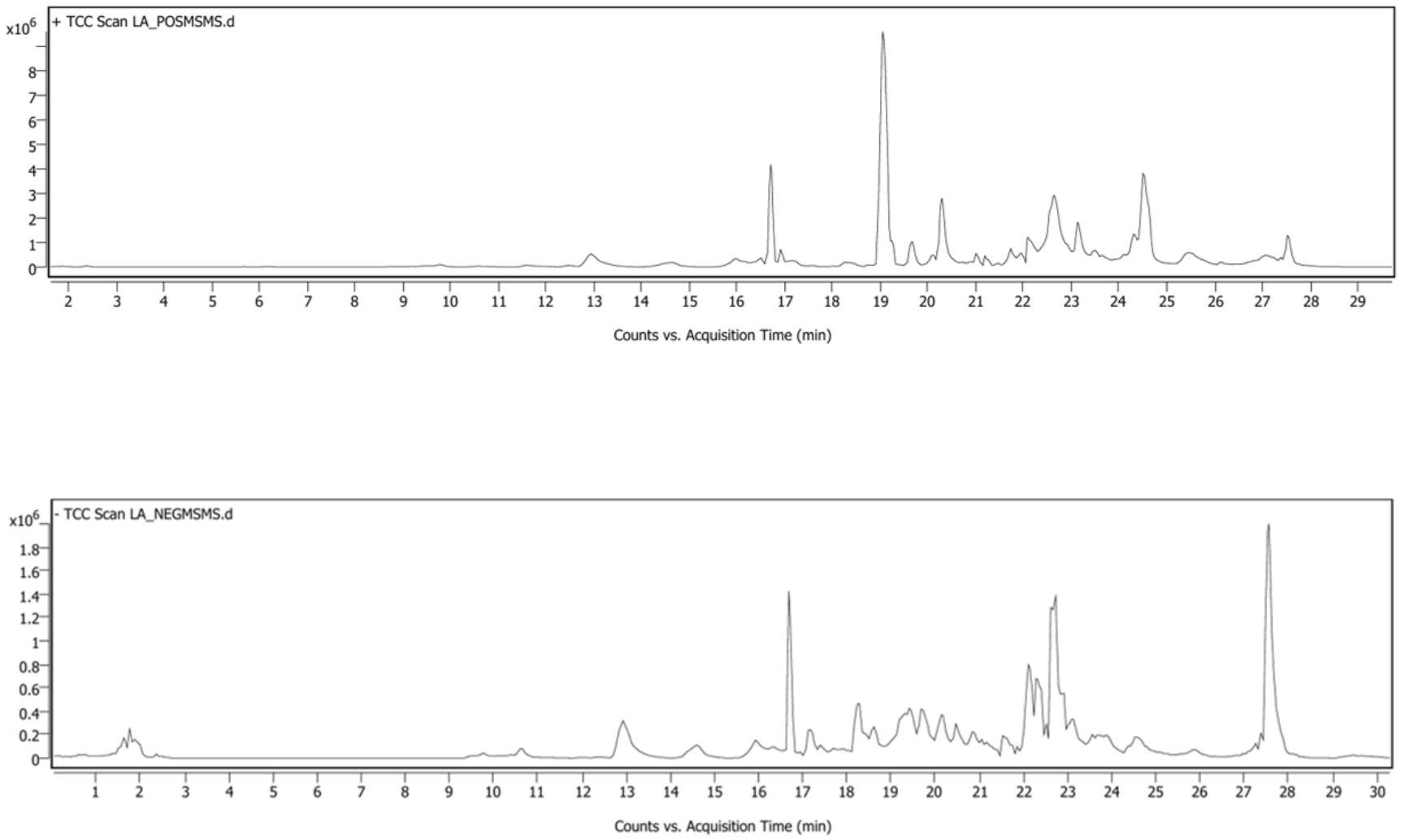


Figure S14 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* leave extract with acetone (Negative).

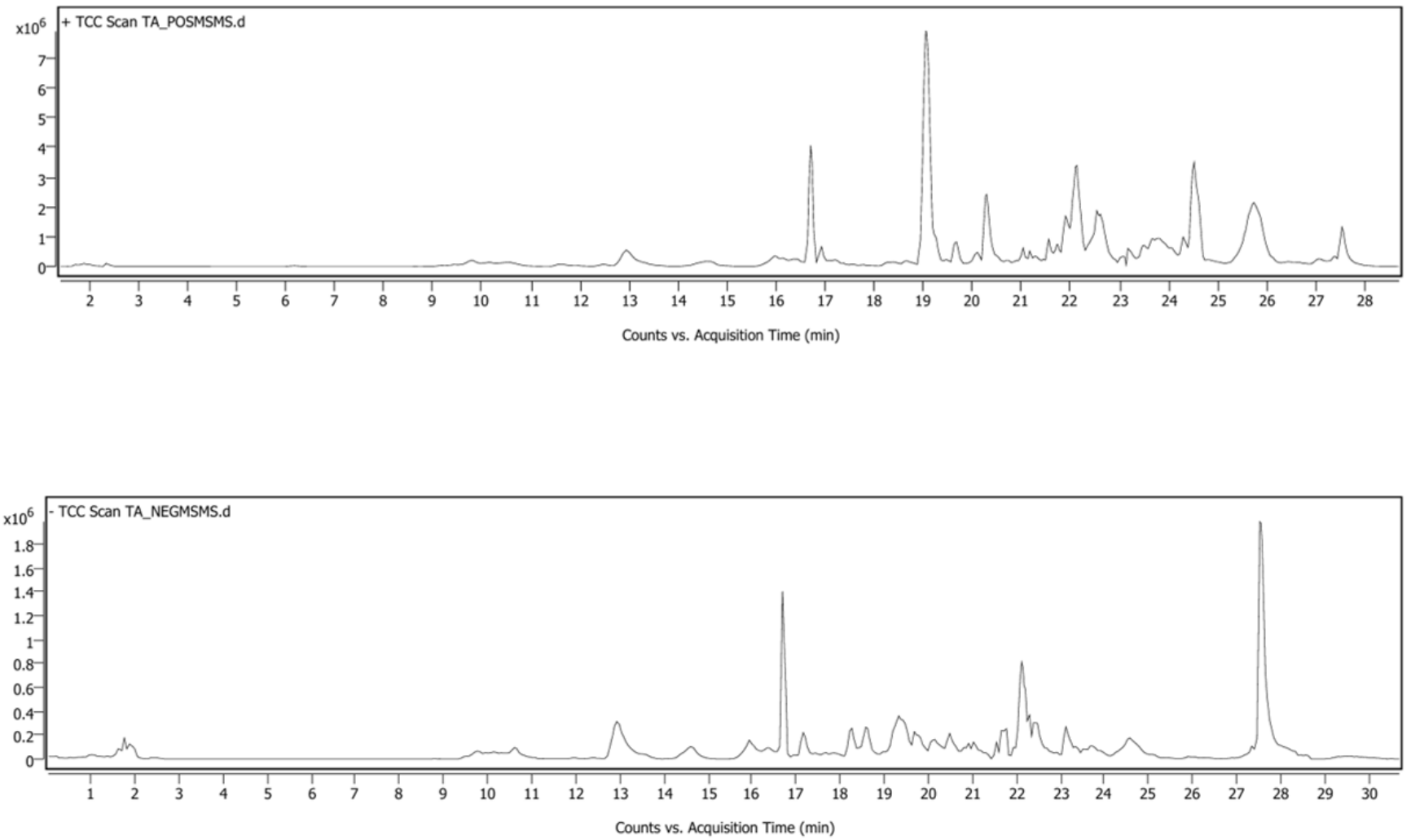


Figure S16 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* twig extract with acetone (Negative).

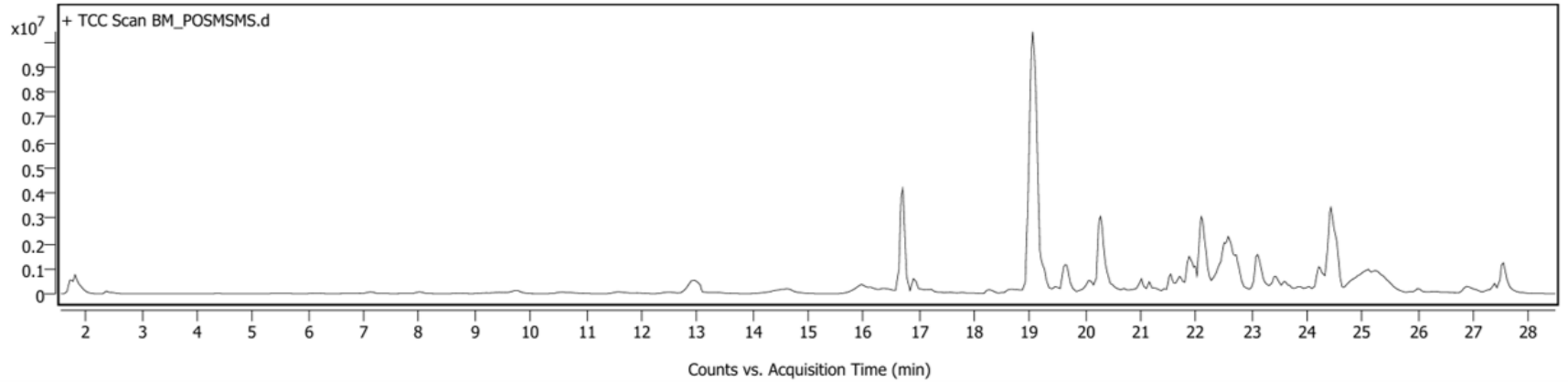


Figure S17 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* bark extract with methanol (Positive).

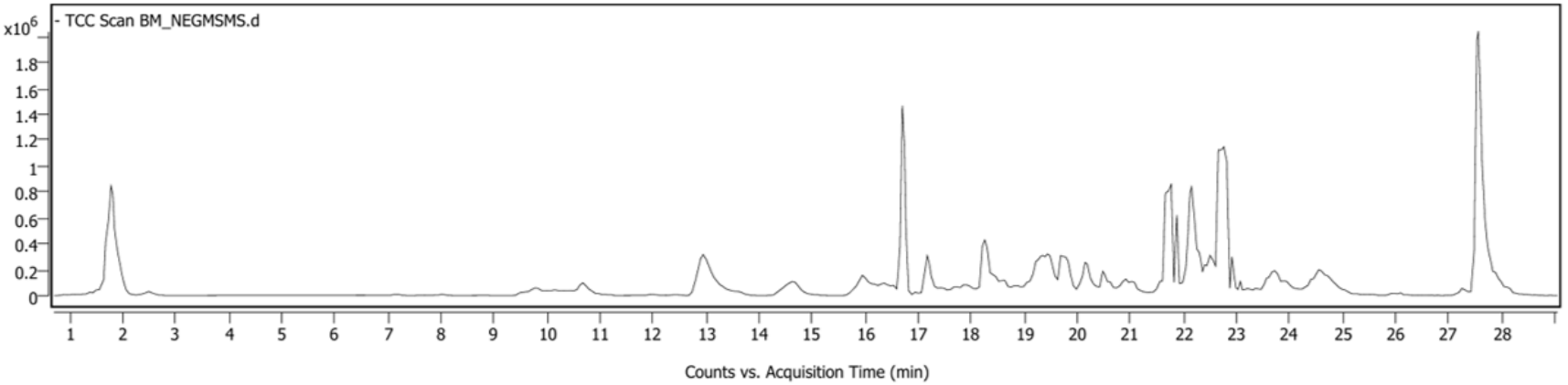


Figure S18 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* bark extract with methanol (Negative).

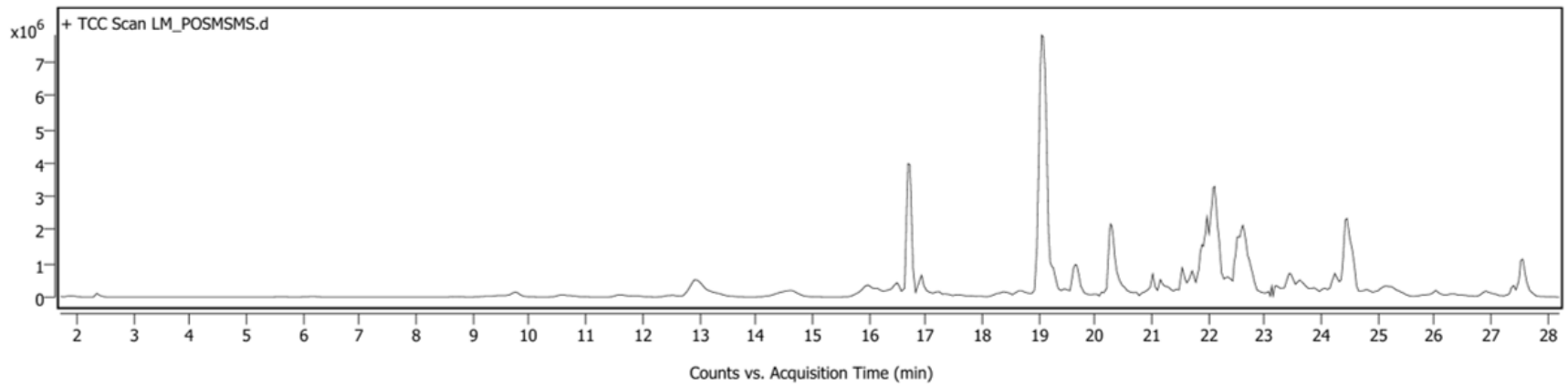


Figure S19 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* leave extract with methanol (Positive).

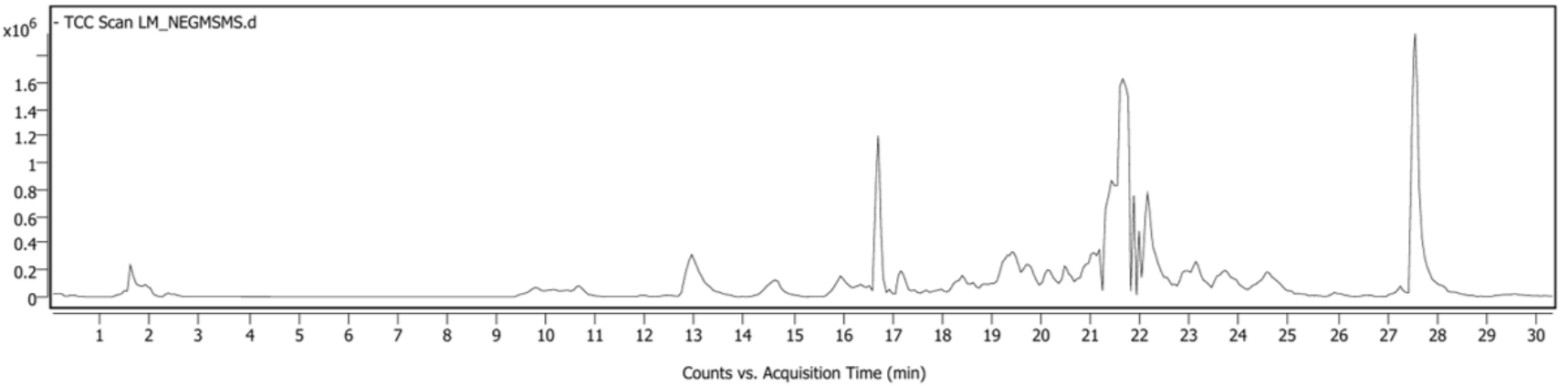
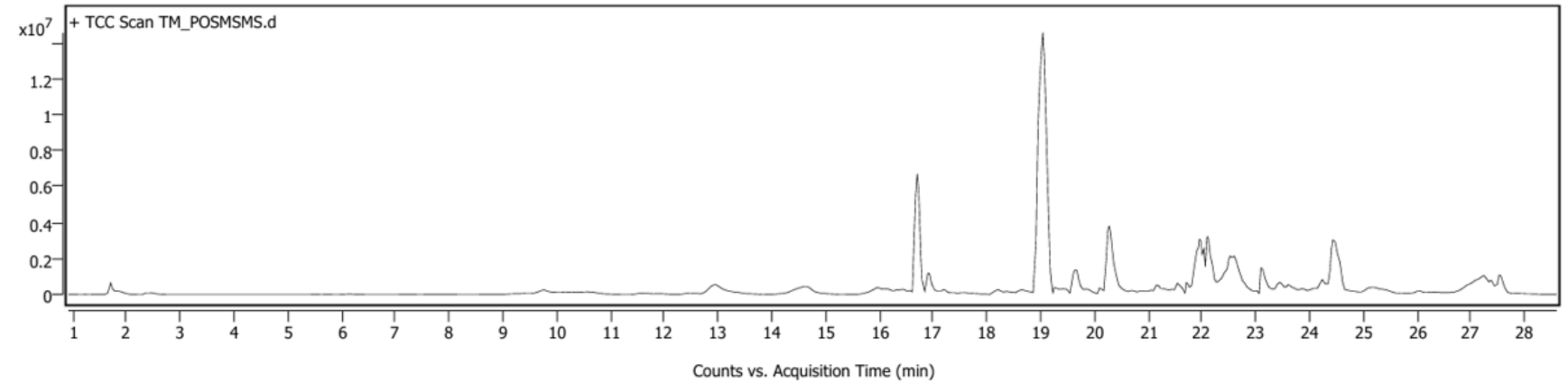
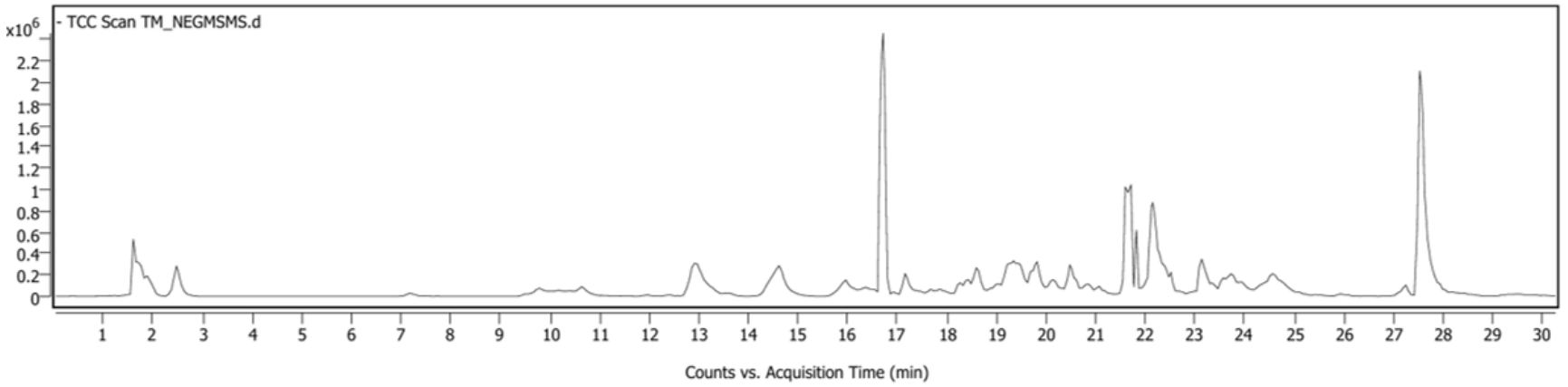


Figure S20 Total compound chromatogram (TCC) of UHPLC-QTOF analysis of *G. xanthochymus* leave extract with methanol (Negative).


x10^7
+ TCC Scan TM_POSMSMS.d
1.2
1
0.8
0.6
0.4
0.2
0
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28
Counts vs. Acquisition Time (min)


x10^6
- TCC Scan TM_NEGMSMS.d
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30
Counts vs. Acquisition Time (min)