Table SI. LC-HRMS analysis of *Citrus sinensis* peel extract.

No.	Compound name	PubChem CID	Formula	RT (min)	Area (max.)
1	Stachydrine	115244	$C_7H_{13}NO_2$	1,043	198.089.512,10
2	Choline	305	$C_5H_{14}NO^+$	1,11	46.516.618,69
3	Nobiletin	72344	$C_{21}H_{22}O_8$	1,022	34.888.603,55
4	Tangeretin	68077	$C_{20}H_{20}O_7$	1,021	32.204.065,85
5	Proline	145742	$C_5H_9NO_2$	1,053	31.118.178,97
6	Pipecolic acid	849	$C_6H_{11}NO_2$	1,047	15.583.296,54
7	Triethanolamine	7618	$C_6H_{15}NO_3$	26,42	5.317.829,83
8	Cetrimonium	2681	$C_{19}H_{42}N^+$	20,789	5.227.685,44
9	Hesperidin	10621	$C_{28}H_{34}O_{15}$	8,205	4.991.984,77
10	Scoparone	8417	$C_{11}H_{10}O_4$	8,78	2.480.670,15
11	Alminoprofen	2097	$C_{13}H_{17}NO_2$	13,919	1.361.444,86
12	Limonin	179651	$C_{26}H_{30}O_8$	0,91	864.458,82
13	Naringin	442428	$C_{27}H_{32}O_{14}$	7,83	578.282,28
14	Linoleic acid	5280934	$C_{18}H_{30}O_2$	20,431	522.473,58
15	Nootkatone	1268142	$C_{15}H_{22}O$	16,921	515.800,60
16	Chanoclavine	5281381	$C_{16}H_{20}N_2O$	12,883	378.926,05

LC/HRMS, liquid chromatography/high resolution mass spectrometry; RT, retention time.

Table SII. Toxicity analysis of chosen compounds in *Citrus sinensis* peels extract.

Compounds	**Mutagenic**	**Tumorigenic**	**Irritant**	**Reproductive effect**
Stachydrine	1	1	1	1
Choline	-	-	-	-
Nobiletin	0.6	0.6	1	1
Tangeretin	0.6	0.6	1	1
Proline	0.6	1	1	1
Pipecolic acid	0.6	1	1	1
Triethanolamine	0.6	0.6	0.6	1
Cetrimonium	-	-	-	-
Hesperidin	1	1	1	1
Scoparone	1	1	1	0.8
Alminoprofen	1	1	1	0.8
Limonin	1	1	1	1
Naringin	1	1	1	1
α-linolenic acid	1	1	1	1
Nootkatone	1	1	1	1
Chanoclavine	1	1	1	0.8

In the table 1 indicates no risk, 0.8 indicates medium risk, and 0.6 indicates high risk.