## **Electronic Supplementary Information** 1 2 On the use of a 2D-carbon microfiber fractionation system to 3 improve flow-injection QTOF-HRMS analysis in complex 4 matrices: the case of *Abelmoschus manihot* flower extracts 5 6 Chol-San Jon, <sup>a,\$</sup> Lei Yang, <sup>a,\$</sup> Zhao Wang, <sup>b</sup> Meiyu Cui, <sup>b</sup> Huaze Sun, <sup>b</sup> Liyuan Wang, <sup>b</sup> 7 Lu Liu, <sup>b</sup> Donatella Nardiello, <sup>c</sup> Maurizio Quinto, <sup>a,c</sup> Miao He, <sup>a,#</sup> Donghao Li\*a,<sup>b</sup> 8 9 10 <sup>a</sup> Interdisciplinary Program of Biological Functional Molecules, College of Integration Science, Yanbian University, Park Road 977, Yanji City, Jilin Province, 133002, PR 11 12 China. 13 <sup>b</sup> Department of Chemistry, Yanbian University, Park Road 977, Yanji City, Jilin 14 Province, 133002, PR China. 15 ° Department of Agriculture, Food, Natural resource, and Engineering (DAFNE), via 16 Napoli 25, I-71122 Foggia, Italy. \$: Chol-San Jon and Lei Yang contributed equally. 17 18 \*Corresponding author 19 E-mail: dhli@ybu.edu.cn 20 Tel.: +86-0433-2436456 21 Fax: +86-0433-2732456 22 \*#Co-Corresponding author 23 E-mail: hemiao@ybu.edu.cn 24 Tel.: +86-0433-2436456 25 26 Fax: +86-0433-2732456

Part1 Fig. S1-S6: 2DµCFs-QTOF-MS/MS spectra of the six predicted
compounds. (S3-S5)

30

31 Part2 Fig. S7-S13: Extracted ion chromatograms (EIC) of the seven
32 co-elution compounds by HPLC-MS. (S6-S8)

33

Part3 Table S1: List of investigated compounds obtained by the
2DµCFs-QTOF-MS/MS from *A. manihot* flower extracts. (S9-S10)

37 Part4 Table S2: Putative identification of chemical constituents of *A*.
38 *manihot* flower extracts by using HPLC-MS/MS in positive ion mode.
39 (S11-S12)

40

41 Part5 References: S13-S14

# 43 Part1: 2DµCFs-QTOF-MS/MS spectra of the six predicted



# 44 compounds. (Fig. S1-S6)





47 Fig. S2 Fragmentation results for m/z 130.0863 by 2DµCFs-QTOF-MS/MS in positive ion mode.



49 Fig. S3 Fragmentation results for m/z 138.0558 by 2DµCFs-QTOF-MS/MS in positive ion mode.



51 Fig. S4 Fragmentation results for m/z 144.1020 by 2DµCFs-QTOF-MS/MS in positive ion mode.



57 Fig. S5 Fragmentation results for m/z 180.0876 by 2DµCFs-QTOF-MS/MS in positive ion mode.



- 62
- 63
- 64

### 65 Part2: Extracted ion chromatograms (EIC) of the seven co-elution

## 66 compounds. (Fig. S7-S13)



67 Fig. S7 Extraction of ion chromatogram (EIC) of m/z 104.1 by HPLC-MS in positive ion mode.



69 Fig. S8 Extraction of ion chromatogram (EIC) of m/z 106.0 by HPLC-MS in positive ion mode.



71 Fig. S9 Extraction of ion chromatogram (EIC) of m/z 116.1 by HPLC-MS in positive ion mode.



72 Fig. S10 Extraction of ion chromatogram (EIC) of m/z 118.1 by HPLC-MS in positive ion mode.



74 Fig. S11 Extraction of ion chromatogram (EIC) of m/z 203.0 by HPLC-MS in positive ion mode.



76 Fig. S12 Extraction of ion chromatogram (EIC) of m/z 252.1 by HPLC-MS in positive ion mode.



77 Fig. S13 Extraction of ion chromatogram (EIC) of m/z 268.1 by HPLC-MS in positive ion mode.

# 78 **Part3**:

79	Table S1 List of	of investigated co	ompounds o	obtained by the	2DµCFs-Q	TOF-MS/MS	from A.	manihot flower extr	acts.
		U	1	2					

Peak	Fraction	Compound	Formula	Adduct	Calculated	Observed	Score	Err	Fragment ions (m/z)	Ref
NO.					mass (Da)	mass (Da)		[ppm]		
1	High-	γ-Aminobutyric acid	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	$[M+H]^+$	104.0706	104.0714	100	-7.7	87.0444; 86.0604	1
2	polar	Serine	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	$[M+H]^+$	106.0499	106.0506	100	-6.6	88.0398	1
3		Proline	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>	$[M+H]^+$	116.0706	116.0714	100	-6.8	70.0663	1
4		Valine	$C_5H_{11}NO_2$	$[M+H]^+$	118.0863	118.0871	100	-6.7	72.0809	1
7		Isoleucine/Leucine*	$C_6H_{13}NO_2$	$[M+H]^+$	132.1019	132.1027	100	-6.0	86.0965	1
8		Aspartic acid	C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>	$[M+H]^+$	134.0448	134.0459	100	-8.2	88.0394; 116.0341	1
9		Adenine	$C_5H_5N_5$	$[M+H]^+$	136.0627	136.0633	100	-4.4	119.0346	2
11		5-(hydroxymethyl)-2-furancarboxylic acid	$C_6H_6O_4$	$[M+H]^{+}$	143.0339	143.0345	100	-4.2		3
13		Glutamine	C5H10N2O3	$[M+H]^+$	147.0764	147.0773	100	-6.1	84.0445	4
14		Lysine	$C_6H_{14}N_2O_2$	$[M+H]^+$	147.1128	147.1131	100	-2.0	84.0820; 130.0875	1
15		Glutamate	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	$[M+H]^{+}$	148.0604	148.0613	100	-6.0	84.0446; 130.0501; 102.0548	1
16		Guanine	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O	$[M+H]^{+}$	152.0566	152.0572	100	-3.9	93.0092	2
17		Phenylalanine	$C_9H_{11}NO_2$	$[M+H]^{+}$	166.0863	166.0871	100	-4.8	120.0808	3
19		Tyrosine	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	$[M+H]^{+}$	182.0812	182.0820	100	-4.3	136.0762; 123.0445	1
20		Galactose/Glucose/Mannose*	$C_{6}H_{12}O_{6}$	$[M+Na]^+$	203.0526	203.0536	100	-4.9		5
21		Tryptophan	$C_{11}H_{12}N_2O_2$	$[M+H]^+$	205.0972	205.0986	100	-6.8	146.0610; 188.0715	1
22		Unknown H1	$C_{11}H_6O_5$	$[M+H]^+$	219.0288	219.0275	100	5.9	202.0710; 197.0286	
23		Cytidine	$C_9H_{13}N_3O_5$	$[M+H]^+$	244.0928	244.0927	100	0.4	112.0508	2
24		2'-Deoxyadenosine	$C_{10}H_{13}N_5O_3$	$[M+H]^+$	252.1091	252.1088	100	1.1	99.0443; 136.0624; 117.0545	2
25		Adenosine/2'-Deoxyguanosine*	$C_{10}H_{13}N_5O_4$	$[M+H]^+$	268.1040	268.1047	100	-2.6	136.0621; 117.0548	3
26		Unknown H2	$C_{12}H_{16}N_6O_4$	$[M+H]^+$	309.1306	309.1303	100	0.9	291.1189; 273.1083;	
									225.0872;	
									292.1030; 292.1217;	
									130.0862	
27		Unknown H3	$C_{17}H_{16}O_{10}$	$[M+H]^+$	381.0816	381.0804	100	3.1	203.0527; 364.1238;	
									290.0762;	

28         Medium         Uridine         C,BH <sub>12</sub> N <sub>2</sub> 0, C,BH <sub>10</sub> N <sub>2</sub> 0, Myricetin         M+H1' C,BH <sub>10</sub> O, C,BH <sub>10</sub> O, M,H1'         245.0768         245.0780         100         4.8         11.0346         6           29         polar         Quercetin         C,BH <sub>10</sub> O, Myricetin         M+H1' C,BH <sub>10</sub> O, BH <sub>10</sub> O, M+H1'         319.0448         119.0460         100         4.6         274.0437         7           30         Myricetin         C,BH <sub>10</sub> O, (BH <sub>10</sub> O, Boueretin 7-O-glucoside'Hyperin' Isoqueretin 3-O-glucoside' Myricetin 3-O-glucoside'         M+H1' C <sub>21</sub> H <sub>20</sub> O <sub>2</sub> M+H1' M+H1'         465.1023         465.1043         100         -3.2         30.0506, 85.0288, 91.0395, 97.0289, 127.0396         3           33         Myricetin 3-O-glucoside' Myricetin 3-O-glucosid											
28       Medium       Unindine       CHI260,0       [M+H]*       245,0760       100       -4.8       113,0346       6         29       polar       Quercetin       CHH0,0       [M+H]*       303,0499       303,01496       100       -4.6       274,0437       7         30       Myricetin       CraHn,0,       [M+H]*       319,0448       319,0460       100       -3.7       153,0178, 273,0397       8         31       Chlorogenic Acid       CraHn,0,       [M+H]*       355,1024       355,1037       100       -3.6       163,0396       80,288, 91,0395,       7         32       Quercetin 7-O-glucoside*Hyperin/       CraHn,0,0,       [M+H]*       481,0977       481,0980       100       -2.4       97,0289, 127,0396       3         33       Myricetin 3-O-glucoside*       CraHn,0,0,       [M+H]*       481,0977       481,0980       100       -0.4       120,0552,       120,0552,       120,0552,       120,0552,       120,0552,       120,0552,       120,0552,       120,0552,       147,0679, 85,0288       147,0679, 85,0288       147,0679, 83,0288,1       147,0679, 83,0288,1       147,0679, 83,0288,1       147,0679, 83,0288,1       147,0679, 83,0288,1       147,0679, 83,0288,1       147,0679, 83,0288,1       147,0679, 83,0288,1										219.0266; 201.0162; 274.0924	
29         polar         Quercetin         C <sub>H</sub> H <sub>0</sub> O <sub>7</sub> [M+H] <sup>+</sup> 303.04513         100         -4.6         274.0437         7           30         Myricetin         C <sub>H</sub> H <sub>0</sub> O <sub>7</sub> [M+H] <sup>+</sup> 319.0448         319.0446         100         -3.6         153.0178: 273.0377         8           31         Chlorogenic Acid         C <sub>H</sub> H <sub>0</sub> O <sub>7</sub> [M+H] <sup>+</sup> 355.1024         355.1037         100         -3.6         163.0395         3         3           32         Quercetin 7-O-glucoside/         C <sub>H</sub> H <sub>0</sub> O <sub>17</sub> [M+H] <sup>+</sup> 465.1024         465.1043         100         -3.6         163.0395         3         3           33         Myricetin 3-O-glucoside/         C <sub>H</sub> H <sub>1</sub> O <sub>17</sub> [M+H] <sup>+</sup> 481.0977         481.0989         100         -2.4         -2.4         3           34         Uaknown M1         C <sub>2</sub> H <sub>2</sub> O <sub>13</sub> [M+H] <sup>+</sup> 870.1133         507.1143         100         -0.4         -2.4         -2.5         129.0552:         129.0552:         129.0552:         147.0679:         85.0288         129.0552:         129.0552:         129.0552:         129.0552:         129.0552:         129.0552:         129.0552:         129.0552:         129.0552:         129.0552: <td>28</td> <td>Medium-</td> <td>Uridine</td> <td><math display="block">C_9H_{12}N_2O_6</math></td> <td><math>[M+H]^+</math></td> <td>245.0768</td> <td>245.0780</td> <td>100</td> <td>-4.8</td> <td>113.0346</td> <td>6</td>	28	Medium-	Uridine	$C_9H_{12}N_2O_6$	$[M+H]^+$	245.0768	245.0780	100	-4.8	113.0346	6
	29	polar	Quercetin	$C_{15}H_{10}O_7$	$[M+H]^+$	303.0499	303.0513	100	-4.6	274.0437	7
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	30		Myricetin	$C_{15}H_{10}O_8$	$[M+H]^+$	319.0448	319.0460	100	-3.7	153.0178; 273.0397	8
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	31		Chlorogenic Acid	$C_{16}H_{18}O_9$	$[M+H]^+$	355.1024	355.1037	100	-3.6	163.0395	3
33       Myricetin 3-O-glucoside/ Myricetin 3'-O-glucoside/ 2       C <sub>3</sub> H <sub>30</sub> O <sub>13</sub> [M+H] <sup>+</sup> 481.0977       481.0989       100       -2.4       3         34       Unknown M1       C <sub>30</sub> H <sub>40</sub> N <sub>10</sub> O <sub>6</sub> [M+H] <sup>+</sup> 487.0858       487.0860       100       -0.4       3         35       Quercetin 3-O-(6-acetylglucoside)       C <sub>21</sub> H <sub>22</sub> O <sub>13</sub> [M+H] <sup>+</sup> 507.1133       507.1143       100       -1.9       3         36       Quercetin 3-O-robinobioside/Rutin*       C <sub>21</sub> H <sub>20</sub> O <sub>16</sub> [M+H] <sup>+</sup> 611.1607       611.1632       100       -1.0       120.0552; 147.0679;       85.0288       120.0552; 147.0679;       85.0288       100       -1.6       120.0552; 147.0679;       85.0288       100       -1.6       120.0552; 147.0679;       85.0288;       48.086       100       -1.6       100       1.6       100       1.6       100       1.6       100       1.6       100       1.6       100       1.6       100       1.6       100       1.6       100       1.6       100       1.6       100       1.6       100       1.6       100       1.6       111.15       111.15       111.15       111.15       111.15       111.15       111.15       111.15       111.15       110.05<	32		Quercetin 7-O-glucoside/Hyperin/ Isoquercetin/Quercetin 3'-O-glucoside*	$C_{21}H_{20}O_{12}$	$[M+H]^{+}$	465.1028	465.1043	100	-3.2	303.0506; 85.0288; 91.0395; 97.0289; 127.0396	7
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	33		Myricetin 3-O-glucoside/ Myricetin 3'-O-glucoside*	$C_{21}H_{20}O_{13}$	$[M+H]^{+}$	481.0977	481.0989	100	-2.4		3
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	34		Unknown M1	C <sub>20</sub> H <sub>10</sub> N <sub>10</sub> O <sub>6</sub>	$[M+H]^+$	487.0858	487.0860	100	-0.4		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	35		Quercetin 3-O-(6-acetylglucoside)	C <sub>23</sub> H <sub>22</sub> O <sub>13</sub>	[M+H] <sup>+</sup>	507.1133	507.1143	100	-1.9		3
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	36		Quercetin 3-O-robinobioside/Rutin*	$C_{27}H_{30}O_{16}$	[M+H] <sup>+</sup>	611.1607	611.1632	100	-4.0	303.0506; 465.1040; 129.0552; 147.0679; 85.0288	8
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	37		Unknown M2	CuHaoOa	[M+H]+	951 1826	951 1810	100	16	147.0077; 05.0200	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	38	Weak-	L incleic acid	$C_{44}\Pi_{38}O_{24}$	$[M+H]^+$	281 2475	281 2480	100	-1.7	263 2368, 245 2266,	4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	50	polar		018113202	[141 - 11]	201.2475	201.2400	100	-1.7	83.0858; 07.1012 111.1159	-
35Ofele Acid $C_{18}H_{34}O_2$ $[M+H]^+$ $285.2652$ $285.2652$ $285.2653$ $100$ $-2.1$ $265.254^{\circ}$ $247.2418^{\circ}$ $153.1176$ $4$ 40Unknown W1 $C_{29}H_{48}O_2$ $[M+H]^+$ $429.3727$ $429.3735$ $100$ $-1.8$ $383.1036^{\circ}$ $249.0393^{\circ}$ 41Tocopherol $C_{29}H_{50}O_2$ $[M+H]^+$ $431.3884$ $431.3872$ $100$ $2.7$ $165.0919$ $9$ 42Hibifolin $C_{21}H_{18}O_{14}$ $[M+H]^+$ $495.0769$ $495.0785$ $100$ $-3.2$ $7$ 43Unknown W2 $C_{33}H_{45}NO_4$ $[M+H]^+$ $520.3421$ $520.3424$ $100$ $-0.5$ $130.0864^{\circ}$ $180.0870^{\circ}$ 44Unknown W3 $C_{29}H_{43}N_7O_2$ $[M+H]^+$ $522.3551$ $522.3556$ $100$ $-0.9$ $180.0868^{\circ}$ $104.070^{\circ}$ 45Lutein $C_{40}H_{56}O_2$ $[M+H]^+$ $569.4353$ $569.4364$ $100$ $-1.9$ $47.63653^{\circ}$ $175.1493$ $10$ 46Unknown W4 $C_{35}H_{36}N_4O_5$ $[M+H]^+$ $593.2758$ $593.2773^{\circ}$ $100$ $-2.5$ $252.1081^{\circ}$ $253.1114^{\circ}$ $234.0970^{\circ}$ $465.1023^{\circ}$ $415.0985^{\circ}$ $266.1238^{\circ}$ $266.1238^{\circ}$ $266.1238^{\circ}$	20			CUO	[]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]	282 2622	202 2620	100	2.1	97.1012; 111.1158	4
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	39 40		Unite over W1	$C_{18}\Pi_{34}O_2$	[M+11]+	203.2032	203.2030	100	-2.1	205.2524; 247.2418; 155.1170	4
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	40		Unknown w I	$C_{29}H_{48}O_2$	[M+H]	429.3727	429.3733	100	-1.8	249.0393; 219.0265;	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$										293.0720; 323.0828; 250.0470	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	41		Tocopherol	$C_{29}H_{50}O_2$	$[M+H]^{+}$	431.3884	431.3872	100	2.7	165.0919	9
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	42		Hibifolin	$C_{21}H_{18}O_{14}$	$[M+H]^+$	495.0769	495.0785	100	-3.2		7
44 Unknown W3 $C_{29}H_{43}N_7O_2$ $[M+H]^+$ 522.3551 522.3556 100 -0.9 $\begin{array}{cccccccccccccccccccccccccccccccccccc$	43		Unknown W2	C <sub>33</sub> H <sub>45</sub> NO <sub>4</sub>	$[M+H]^{+}$	520.3421	520.3424	100	-0.5	130.0864; 180.0870; 104.0706;	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$										252.1077; 268.1034; 184.0731	
45 Lutein $C_{40}H_{56}O_2$ $[M+H]^+$ 569.4353 569.4364 100 -1.9 476.3653; 175.1493 10 46 Unknown W4 $C_{35}H_{36}N_4O_5$ $[M+H]^+$ 593.2758 593.2773 100 -2.5 252.1081; 253.1114; 234.0970; 465.1023; 415.0985; 266.1238	44		Unknown W3	$C_{29}H_{43}N_7O_2$	$[M+H]^+$	522.3551	522.3556	100	-0.9	180.0868; 104.0707;	
45 Lutein $C_{40}H_{56}O_2$ $[M+H]^+$ 569.4353 569.4364 100 -1.9 476.3653; 175.1493 10 46 Unknown W4 $C_{35}H_{36}N_4O_5$ $[M+H]^+$ 593.2758 593.2773 100 -2.5 252.1081; 253.1114; 234.0970; 465.1023; 415.0985; 266.1238										184.0736;	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$										325.1127; 391.2841; 162.0765	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	45		Lutein	$C_{40}H_{56}O_2$	$[M+H]^+$	569.4353	569.4364	100	-1.9	476.3653; 175.1493	10
234.0970; 465.1023; 415.0985; 266.1238	46		Unknown W4	$C_{35}H_{36}N_4O_5$	$[M+H]^{+}$	593.2758	593.2773	100	-2.5	252.1081; 253.1114;	
465.1023; 415.0985; 266.1238										234.0970;	
										465.1023; 415.0985; 266.1238	

47	Unknown W5	C <sub>44</sub> H <sub>77</sub> N <sub>3</sub> O <sub>7</sub>	$[M+H]^{+}$	760.5816	760.5853	100	-4.8	104.0707; 130.0867; 184.0734;
								294.1550; 418.1551; 420.0900
49	Unknown W6	$C_{55}H_{74}N_4O_5$	$[M+H]^{+}$	871.5732	871.5731	100	0.1	

80 \*: Isobaric compounds

## 81 **Part4:**

## 82 Table S2 Putative identification of chemical constituents of *A. manihot* flower extracts

Peak NO.	Analyte	t <sub>R</sub> (min)	Formula	[M+H] <sup>+</sup> (m/z)	Fragment ions (m/z)	Ref
1	5-(hydroxymethyl)-2- furancarboxylic acid	2.70	$C_6H_6O_4$	143.0	99.0	3
2	Serine	3.20	$C_3H_7NO_3$	106.0	88.0,60	1,3
3	γ-Aminobutyric acid	3.22	$C_4H_9NO_2$	104.1	86.0,87.0	1
4	Adenosine	3.32	$C_{10}H_{13}N_5O_4$	268.1	136.1	3
5	2'-Deoxyadenosine	3.32	$C_{10}H_{13}N_5O_3$	252.1	99.0,136.1,117.1	2
6	Glucose	3.37	$C_6H_{12}O_6$	203.0		11
7	Valine	3.42	$C_5H_{11}NO_2$	118.1	72.1	1,3
8	Proline	3.61	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>	116.1	70.0	1,3
9	Unknown 1	3.87		260.0		
10	Phenylalanine	4.01	$C_9H_{11}NO_2$	166.1	120.1	1,3
11	Cytidine	4.08	$C_9H_{13}N_3O_5$	244.1	112.1	2
12	Unknown 2	5.30		130.0		
13	Unknown 3	5.78		348.0		
14	Unknown 4	6.42		238.1		
15	Leucine	9.06	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	132.1	86.1	1,3
16	Unknown 5	15.28		120.0		
17	Unknown 6	25.44		298.0		
18	Unknown 7	38.01		371.1		
19	Unknown 8	39.15		657.0		
20	Unknown 9	40.00		479.0		
21	Unknown 10	41.98		476.1		
22	Unknown 11	43.42		402.0		
23	Unknown 12	43.96		520.1		
24	Myricetin 3-O-glucoside	44.47	$C_{21}H_{20}O_{13}$	481.1	318.0	3
25	Lutein	45.80	$C_{40}H_{56}O_2$	569.4	175.1,476.3	10
26	Quercetin 3-O- robinobioside	47.23	$C_{27}H_{30}O_{16}$	611.0	303.0,465.0,129.1	3
27	Quercetin 7-O-glucoside	47.24	$C_{21}H_{20}O_{12}$	465.0	303.1,465.0	3
28	Rutin	47.63	$C_{27}H_{30}O_{16}$	611.0	85.0,129.1,147.1 303.1,465.1	3,7
29	Hyperin	48.85	$C_{21}H_{20}O_{12}$	465.0	303.0,273.1,257.0, 181.0,153.1	3,7
30	Isoquercetin	49.53	$C_{21}H_{20}O_{12}$	465.0	303.0,273.1,257.1 181.0,153.0	3,7
31	Myricetin 3'-O-glucoside	50.59	$C_{21}H_{20}O_{13}$	481.1	319.1	3
32	Unknown 13	52.28		551.0		
33	Hibifolin	54.79	$C_{21}H_{18}O_{14}$	495.1	319.0	3,7
34	Tocopherol	58.36	$C_{29}H_{50}O_2$	431.3	165.1	9
35	Myricetin	58.37	$C_{15}H_{10}O_8$	319.0	153.0,273.0,181.1	7
36	Quercetin 3'-O-glucoside	58.70	$C_{21}H_{20}O_{12}$	465.0	85.0,91.0,97.0,303.1, 127.0	3,7

83 by HPLC-MS/MS in positive ion mode.

37	Unknown 14	61.73		551.0		
38	Quercetin	64.84	$C_{15}H_{10}O_{7}$	303.0	274.0,153.1	7
39	Unknown 15	65.75		219.1		
40	Unknown 16	67.14		274.2		
41	Unknown 17	68.09		343.1		
42	Uridine	68.48	$C_9H_{12}N_2O_6$	245.1	113.0	6
43	Linoleic acid	69.09	$C_{18}H_{32}O_2$	281.2	83.1,97.1,111.1, 245.2,263.2	4
44	Oleic Acid	69.39	$C_{18}H_{34}O_2$	283.2	135.1,247.2,265.2	4

### 86 **Part5**:

#### 87 **References**

- 1 L. Y. Du, D. W. Qian, S. Jiang, J. M. Guo, S. L. Su and J. A. Duan, Anal. Methods,
- 89 2015, 7, 10280–10290.
- 90 2 L. Y. Du, D. W. Qian, S. Jiang, E. X. Shang, J. M. Guo, P. Liu, S. L. Su, J. A.
- Duan and M. Zhao, J. Chromatogr. B Anal. Technol. Biomed. Life Sci., 2015,
  1006, 130–137.
- 93 3 S. Yin, Y. Mei, L. Wei, L. Zou, Z. Cai, N. Wu, J. Yuan, X. Liu, H. Ge, D. Wang
  94 and D. Wang, *Molecules*, 2021, 26, 1864.
- 95 4 F. Luan, Q. Wu, Y. Yang, H. Lv, D. Liu, Z. Gan and N. Zeng, *Front. Pharmacol.*,
  96 2020, 11, 1068.
- 97 5 X. Wang, Y. Wang, M. Wu and X. Zhang, *Russ. J. Phys. Chem. A*, 2012, 86,
  98 1469–1472.
- 99 6 D. Zhou, J. Zeng, Q. Fu, D. Gao, K. Zhang, X. Ren, K. Zhou, Z. Xia and L. Wang,
  100 *J. Chromatogr. A*, 2018, **1571**, 165–175.
- J. Guo, C. Xue, J. A. Duan, D. Qian, Y. Tang and Y. You, *Phytomedicine*, 2011,
- **102 18**, 1250–1254.
- 103 8 J. Li, J. Zhang and M. Wang, *Molecules*, 2016, **21**, 810.
- 104 9 M. Taroreh, S. Raharjo, P. Hastuti and A. Murdiati, *Agric. Agric. Sci. Procedia*,
- **105** 2016, **9**, 271–278.
- 106 10 C. Puel, J. Mathey, S. Kati-Coulibaly, M. J. Davicco, P. Lebecque, B.
- 107 Chanteranne, M. N. Horcajada and V. Coxam, J. Ethnopharmacol., 2005, 99,

- 108 55–60.
- 109 11 X. X. Pan, J. H. Tao, S. Jiang, Y. Zhu, D. W. Qian and J. A. Duan, Int. J. Biol.
- 110 *Macromol.*, 2018, **107**, 9–16.