

Supplementary Table S2. Peak areas from the full scan MS spectra for identified phenolics in French marigold flowers and leaves extracts obtained in water, methanol (MeOH) and dichloromethane (DCM)

		Flowers			Leaves		
		Water	MeOH	DCM	Water	MeOH	DCM
<i>Phenolic acids / glycosides</i>							
1	Galloylquinic acid I	2726763	5684281			1175310	
2	Gallic acid hexoside	353607			560503	3408919	
3	Gallic acid	17467976	3288340				
4	Galloylquinic acid II	7079504	12032618			3901552	
5	Dihydroxybenzoic acid hexoside	1639681	832143		21024399	18034291	
6	Caffeoylglucaric acid I	1874435					
7	Caffeoylglucaric acid II	2605216			223388		
8	Protocatechuic acid	30444008	7791086		4458420	2104843	
9	Digalloylquinic acid I	189880	219886			2680894	
10	3-O-Caffeoylquinic acid	3094608	625839		168874	224667	
11	Caffeic acid hexoside I				153964	551547	
12	Caffeoylglucaric acid III	2516540			219346		
13	Digalloyl-dihexoside	59036	5397848			411834	
14	Digalloylquinic acid II	2683052	6870984			4134116	
15	Hydroxybenzoic acid hexoside	489754	494786		1408275	3028240	
16	Syringoyl-galloyl hexoside I	977505	2437475			489190	
17	Caffeic acid hexoside II	382107	524731		342720	1602738	
18	Syringoyl-galloyl hexoside II	1464624	5096652			893096	
19	5-O-Caffeoylquinic acid	5500260	36174680		1756839	16229651	
20	Trigalloylquinic acid		160692			7401045	
21	Dicaffeoylmaltronic acid I	15697750					
22	Caffeic acid pentoside I				317579	1844521	
23	Ellagic acid hexoside		4967412			6598921	
24	Caffeic acid	43433276	1184675		608233	736138	

25	Syringoyl-methylgalloyl hexoside I	719315	1811086				
26	Caffeoyl-(iso)citric acid	905022	274949		25380759	16610842	92375
27	Caffeic acid pentoside II	595121	995968		2025565	17973326	125634
28	Syringoyl-methylgalloyl hexoside II	1608728	4334909		101729	137111	
29	Methyl chlorogenate	77044	880566		1756964	2190273	
30	Dicaffeoylaltraric acid II	4713779					
31	Coumaric acid hexoside	1320969	527512		2523052	756057	
32	Dicaffeoylaltraric acid III	4236650	144286				
33	Disyringoyl hexoside I	1540743	3031824				71269
34	Mehylellagic acid hexoside		2251357			7815412	
35	Disyringoyl hexoside II	2463099	6296924	177199	299008	340213	153758
36	Coumaroyl-(iso)citric acid	1629759	299576		43954373	16062630	
37	Feruloyl-(iso)citric acid	12525886	4508555		127066846	57148007	513137
38	Ellagic acid	1207313	11022261			1162901	
39	Vanillic acid	3133472	2571448		426515	488697	
40	Dicaffeoylquinic acid I	5720797	24025408	128982	102074	15703724	70072
41	Dicaffeoylquinic acid II			70239		3747503	
42	Tricaffeoylglucaric acid	11619014	7249802			158462	
43	Methylellagic acid	340985	3476514		142747	1194839	
44	Ferulic acid	257441	417898		4130087	2617146	
45	Dimethylellagic acid hexoside		1466942				
46	Dimethylellagic acid	2077834	97761721	2402785		1720916	84739
Flavonoids							
47	Quercetagenin	132480	29188850				
48	Luteolin ^a	3421116	81625041	185492		1379732	
49	6-Hydroxykaempferol	1224978	8529246	809880	315421	3034643	333329
50	8-Hydroxy-3-O-methylquercetagenin	1274384	28729475	313606		1930408	
51	Patuletin	40618617	337392962	15611804	528291	52811159	1363322
52	Apigenin ^a	144153	3604935			271657	

53	Kaempferol ^a	417270	2287967	657480	164870	1500441	261625
54	Chrysoeriol ^a		2785543				
55	6-Methoxykaempferol	360761	37796625	899009		2305050	237161
56	Axillarin		2353522			766458	242819
57	5,7-Dimethylquercetin					850982	174681
58	8-Hydroxyquercetagenin	3323127	22644123				
Flavonoid glycosides							
59	Quercetagenin 3,7-di-O-hexoside		502365			2289123	
60	Quercetagenin 3-O-pentoside-7-O-hexoside		167120			830331	
61	Quercetin 3,7-di-O-hexoside		1796508			4631457	
62	Patuletin 3,7-di-O-hexoside I		10166420			15362042	
63	Quercetin 3-O-pentoside-7-O-hexoside		694092			6839927	
64	Patuletin 3-O-pentoside-7-O-hexoside		1725930			9301886	
65	6-Methoxykaempferol 3-O-pentoside-7-O-hexoside					1885344	
66	Patuletin 3,7-di-O-hexoside II		3315580			123926	
67	Quercetin 3-O-hexoside-7-O-rhamnoside		21524649		425620	62476127	510893
68	Patuletin 3-O-(2"-hexosyl)hexoside	1358159	3011399				
69	Quercetin 3-O-rhamnoside-7-O-pentoside		9442613	61183	1704243	49634014	484744
70	Quercetin 3-O-(6"-hexosyl)hexoside	988151	8136907		5510269	19696048	119978
71	Quercetagenin 6-O-hexoside		58972571	147565		12179482	
72	Quercetin 3-O-(6"-galloyl)hexoside-7-O-hexoside		141399			4275669	
73	Patuletin 3-O-(6"-hexosyl)hexoside	1437344	18091487	206580	222044	3716661	
74	Quercetin 3-O-(6"-pentosyl)hexoside	1791935	3578742		177888	3345275	
75	Quercetin 3,7-di-O-rhamnoside		12307193	94847	6708679	54885163	527701
76	Kaempferol 3-O-pentoside-7-O-rhamnoside		255392		235238	9606619	78430
77	Kaempferol 3-O-hexoside-7-O-pentoside	76628	743223		2079529	19682381	205495
78	Kaempferol 3-O-(6"-hexosyl)hexoside		681257		1435699	20946406	77847

79	Quercetin 3-O-(6"-galloyl)hexoside	141746	1931768		26401271	103294
80	6-Methoxykaempferol 3-O-(6"-hexosyl)hexoside	225856	2175059	618228	2853561	
81	Patuletin 7-O-(6"-galloyl)hexoside	398307	2221821			
82	Kaempferol 3-O-rhamnoside-7-O-rhamnoside		174155	391095	11661628	149661
83	Quercetin 3-O-glucoside ^a	1001399	11129137	81054	2002753	83837241
84	Kaempferol 3-O-rhamnoside-7-O-pentoside			191295	5875294	766011
85	Kaempferol 7-O-(6"-galloyl)hexoside				3697732	
86	Patuletin 7-O-hexoside	1543862	167730168	2325685	28055167	142103
87	8-Hydroxy-3-O-methyl quercetagetin 6-O-hexoside		8104156		583970	
88	Quercetin 3-O-galloyl-rhamnoside-7-O-rhamnoside		220522		5351948	
89	Kaempferol 3-O-glucoside ^a	638089		1118234	4377422	
90	Quercetin 3-O-pentoside	2438489	7239489	5748534	46975440	174289
91	Patuletin 3-O-pentoside	432903	2028365	939071	4467177	
92	Quercetin 3-O-rhamnoside ^a	1125253	7040595	5617038	7953994	
93	Axillarin 7-O-(6"-rhamnosyl)hexoside			2547040	5696052	
94	Quercetin 3-O-(2"-galloyl)-pentoside	166544	2281634		25874199	107385
95	6-Methoxykaempferol 7-O-hexoside		17382518		2768290	
96	Kaempferol 3-O-galloyl-rhamnoside-7-O-rhamnoside				5514139	
97	Kaempferol 3-O-pentoside			562237	3032392	
98	Luteolin 7-O-glucoside ^a		10770488	178110	1113854	
99	Quercetagetin-7-methyl ether 6-O-hexoside	164016	22374573		556642	
100	5,7-Dimethylquercetin 3-O-rutinoside			1011260	3088918	
101	Axillarin 7-O-hexoside			100535	5006036	
102	Kaempferol 3-O-(2"-galloyl)-pentoside				2853731	
103	3,3'-Dimethylquercetin 7-O-hexoside		94477		3167728	

104	Trimethylquercetageretin rutinoside		643353	1867861
105	Patuletin 7- <i>O</i> -(6"-hydroxybenzoyl)hexoside		2006097	
106	Axillarin 7- <i>O</i> -(6"-caffeoyl)hexoside	65828	2701602	
107	Axillarin 7- <i>O</i> -pentoside			1079968
108	Patuletin 3- <i>O</i> -(6"- <i>p</i> -coumaroyl)hexoside		1403542	102815
109	Quercetin 3- <i>O</i> -(6"-vaniloyl)hexoside		101985	1412093
110	Quercetin 3- <i>O</i> -(2"-hydroxybenzoyl)-pentoside		231934	898591
111	Kaempferol 7- <i>O</i> -rhamnoside		136930	659536
112	Patuletin 7- <i>O</i> -(6"-benzoyl)hexoside		1173062	
113	Quercetin 3- <i>O</i> -(6"- <i>p</i> -coumaroyl)hexoside		226625	598889