Electronic Supplementary Material (ESI) for Analytical Methods.

Supplemental information

A practical strategy for chemical profiling of herbal medicines using ultra-high performance liquid chromatography coupled with hybrid triple quadrupole-linear ion trap mass spectrometry: a case study of Mori Cortex

Wang-Hui Jing, Ru Yan*, Yi-Tao Wang*

State Key Laboratory of Quality Research in Chinese Medicine, Institute of Chinese Medical Sciences, University of Macau, Taipa, Macao, China

*To whom correspondence should be addressed

Prof. Yi-Tao Wang

Tel: 853-83974691

Fax: 853-28841358

Email: ytwang@umac.mo

Dr. Ru Yan

Tel: 853-83974876

Fax: 853-28841358

Email: ruyan@umac.mo

1.1 3.4. Characterization of the chemical constituents in MC extract

A pair of isomers (t_R: 9.8 min for **4** and 10.6 min for **5**) afforded the sodium adduct and pseudo-molecular ions at *m/z* 353 ($[M+Na]^+$) and 331 ($[M+H]^+$), indicating a molecular weight as 330 Da. The prominent product ions were observed at *m/z* 313, 289 and 153 (Table 1 and Fig. 9). However, the chemical structures of these two compounds couldn't be assigned.

Compound **6** exhibited sodium adduct and quasi-molecular ions at *m/z* 501 ($[M+Na]^+$), 479 ($[M+H]^+$) and 477 ($[M–H]^-$), suggesting a molecular weight as 478 Da. On the basis of our chemical reviews (Table S1), this component was tentatively characterized as Moracin W (Table 1).

Both compounds **28** (t_R: 22.2 min) and **92** (t_R: 43.3 min) showed sodium adduct and quasi-molecular ions at *m/z* 651 ($[M+Na]^+$), 629 ($[M+H]^+$) and 627 ($[M–H]^-$), and the positive product ions of compound **28** were observed at *m/z* 601 ($[M+H–CO]^+$), 570, 423, 395 and 367, while the deprotonated ion of compound **92** yielded diagnostic product ions at *m/z* 609, 517 and 407 (Table 1 and Fig. 9). Based on the mass spectral value, compounds **28** and **92** were tentatively identified as mulberrofuran K and yunanensin E. Similarly, the mass spectral values compounds **18** (t_R: 16.2 min), **19** (t_R: 16.4 min) and **23** (t_R: 21.9 min) included *m/z* 617 ($[M+Na]^+$), 595 ($[M+H]^+$), 567 ($[M+H–CO]^+$), 536, *et al*. (Table 1 and Fig. 9). Therefore, compounds **18**, **19** and **23** were provisionally characterized as the analogs of compound **28** with a molecular weight as 594 Da, thus these four compounds were characterized as kuwanon Z and its isomers.

The sodium adduct and protonated ions of compounds **30** (t_R: 23.7 min), **31** (t_R: 24.9 min) and **32** (t_R: 25.6 min) were exhibited at *m/z* 459 ($[M+Na]^+$) and 437 ($[M+H]^+$). The positive product ions were shown at *m/z* 419, 365, and 359, indicating the neutral losses of a H_2O group, a C_4H_8O (72 Da) group and a C_4H_8O group couple with a C_4H_8 group (56 Da) (Table 1 and Fig. 9). On the basis of our chemical reviews (Table S1), these three components were tentatively characterized as benzokuwanon E, sanggenon A and their isomer.

As one of major constituents in MC, kuwanon G (**73**) was detected at 38.1 min, and its mass spectral values were exhibited at *m/z* 715 ($[M+Na]^+$), 693 ($[M+H]^+$), 691 ($[M–H]^-$), 581 and 471, corresponding to the sodium adduct ion, protonated ion, deprotonated ion, the neutral loss of a $C_2H_6O_2$ (110 Da) group and the neutral loss of two $C_2H_6O_2$ groups (2 × 110 Da) (Fig. 5). Similar to this mass fragment pattern, the isomers of kuwanon G were observed at retention times of 26.1 min (**33**), 37.9 min (**72**), 39.4 min (**79**) and 40.5 min (**85**), sequentially (Table 1 and Fig. 9).

Compounds **37** and **39** were eluted at the retention times of 27.6 min and 28.4 min successively. The dominant product ions of the deprotonated ion (*m/z* 409 $[M–H]^-$) were yielded at *m/z* 391, 327, 309 and 209 (Table 1 and Fig. 9). Based on our summary on the chemical components of MC (Table S1), these two compounds were tentatively identified as wittifuran A and wittifuran U.

Morusin (**107**) was detected as the most abundant constituent in MC at the retention time of 48.0 min with the mass spectral values at *m/z* 443 ($[M+Na]^+$), 421 ($[M+H]^+$), 419 ($[M–H]^-$), 365 ($[M+H–C_4H_8]^+$), 337 ($[M+H–C_4H_8–H_2O]^+$) and 299. Meanwhile, its isomers were observed at 28.1 min (**38**), 33.7 min (**57**), 44.5 min (**97**), 46.1 min (**102**), 49.1 min (**110**), 49.5 min (**112**), 50.3 min (**115**) and 51.6 min (**121**) (Table 1 and Fig. 9).

Compound **40** was observed at 29.5 min, and the sodium adduct and quasi–molecular ions at *m/z* 353 ($[M+Na]^+$), 331 ($[M+H]^+$) and 329 ($[M–H]^-$), suggesting a molecular weight as 330 Da (Table 1 and Fig. 9). However, the chemical structure of this compound cannot be elucidated due to the insufficient structural information.

The sodium adduct and quasi-molecular ions of *m/z* 735 ($[M+Na]^+$), 713 ($[M+H]^+$) and 711 ($[M–H]^-$) were detected at retention times of 30.0 min (**41**), 30.2 min (**44**), 31.5 min (**48**), 32.6 min (**51**), 32.8 min (**53**) and 35.2 min (**63**) (Table 1 and Fig. 9). Meanwhile, the diagnostic product ions of the deprotonated ion were shown at *m/z* 601 and 491, suggesting the successively neutral losses of two resorcinol groups (2 × 110 Da). Above all, these compounds were tentatively identified as sanggenon T and its isomers.

Sodium adduct and pseudo-molecular ions of *m/z* 783 ($[M+Na]^+$), 761 ($[M+H]^+$) and 759 ($[M–H]^-$) were observed at 30.6 min (**45**), 36.7 min (**68**), 38.9 min (**77**), 42.6 min (**88**), 43.0 min (**90**). The characteristic product ions of the protonanted ion included *m/z* 705 ($[M+H–C_4H_8]^+$), 687 ($[M+H–C_4H_8–H_2O]^+$), 649 ($[M+H–C_4H_8–C_4H_8]^+$), 421, 365 and 355 (Table 1 and Fig. 9). Collectively, these five compounds were tentatively identified as kuwanon N, kuwanon H and their isomers.

Compound **46** was eluted at 31.1 min, and exhibited sodium adduct and quasi-molecular ions at *m/z* 615 ($[M+Na]^+$), 593 ($[M+H]^+$) and 591 ($[M–H]^-$). The negative MS^2 spectrum of the deprotonated ion gave diagnostic product ions at *m/z* 481 and 463, indicating the neutral loss of a resorcinol group and a H_2O group (Table 1 and Fig. 9), successively. Collectively, this component was tentatively characterized as mulberrofuran Q.

Compounds **47** (t_R: 31.4 min) and **49** (t_R: 32.3 min) showed sodium adduct ion, protonated ion and deprotonated ion at *m/z* 733 ($[M+Na]^+$), 711 ($[M+H]^+$) and 709 ($[M–H]^–$), respectively. In the negative MS^2 spectrum of the precursor ion at *m/z* 709 ($[M–H]^–$), the fragment ions were shown at *m/z* 599 $[M–H–C_6H_6O_2]^-$, 489 $[M–H–C_6H_6O_2–C_6H_6O_2]^-$, 437, 371 and 309 (Table 1 and Fig. 9). As a consequence, these two compounds were tentatively identified as moracenin D and its isomer.

Compound **50** was observed at 32.5 min, and exhibiting mass spectral values as *m/z* 587 ($[M+Na]^+$), 565 ($[M+H]^+$), 563 ($[M–H]^–$), 563 ($[M–H–H_2O]^–$) and 453 ($[M–H–C_6H_6O_2]^–$) (Table 1 and Fig. 9). Based on our phytochemical review (Table S1), this component was tentatively characterized as kuwanol A.

Sodium adduct ion and quasi-molecular ions of *m/z* 377 ($[M+Na]^+$), 355 ($[M+H]^+$) and 353 ($[M–H]^–$) were observed at 33.4 min (**55**), 34.8 min (**60**), 35.4 min (**65**) and 37.2 min (**69**), while the positive diagnostic fragment ions were given at *m/z* 337, 299 and 281, corresponding to the neutral losses of a H_2O group, a butene (C_4H_8, 56 Da) moiety, and a butene group plus H_2O molecule, respectively (Table 1 and Fig. 9). Consequently, these four compounds were characterized as glyasperin F, licoisofavanone, morachalcone C and their isomer.

The sodium adduct ion and quasi-molecular ions of *m/z* 631 ($[M+Na]^+$), 609 ($[M+H]^+$) and 607 ($[M–H]^–$), which were presupposed for guangsangon G and guangsangon I, were detected at 33.6 min (**56**) and 35.3 min (**64**). The MS^2 spectrum of the deprotonated ion showed diagnostic product ions at *m/z* 597 and 487, suggesting the successively neutral losses of two $C_6H_6O_2$ (110 Da) groups (Table 1 and Fig. 9). Thus, these two compounds were tentatively characterized as guangsangon G and guangsangon I.

Compound **59** was eluted at 33.9 min, and its sodium adduct ion and quasi-molecular ions were exhibited at *m/z* 649 ($[M+Na]^+$), 627 ($[M+H]^+$) and 625 ($[M–H]^–$), suggesting a molecular weight as 626 Da. The diagnostic product ions at *m/z* 499 and 389 corresponded to the sequentially neural losses of a $C_6H_6O_3$ (126 Da) group and a $C_6H_6O_2$ (110 Da) group (Table 1 and Fig. 9). Therefore, this compound was tentatively identified as kuwanon L or guangsangon K.

The sodium adduct ion and pseudo-molecular ions of *m/z* 585 ($[M+Na]^+$), 563 ($[M+H]^+$) and 561 ($[M–H]^–$) were detected at 34.9 min (**61**) and 35.5 min (**66**). The diagnostic product ion at *m/z* 451 under negative ionization suggested the neutral loss of a resorcinol ($C_6H_6O_2$, 110 Da) group

(Table 1 and Fig. 9). Hence, these two compounds were tentatively identified as mulberrofuran G, isomulberrofuran G, or kuwanol A.

The sodium adduct ion and quasi-molecular ions of *m/z* 717 ([M+Na]$^+$), 695 ([M+H]$^+$) and 693 ([M–H]$^-$) were presupposed for kuwanon O, and were observed at 35.2 min (**62**), 38.5 min (**75**), 39.1 min (**78**), 39.9 min (**83**), 41.4 min (**86**), 42.4 min (**87**) and 42.8 min (**89**). The diagnostic fragment ions for the protonated ion were detected at *m/z* 677 ([M+Na–H_2O]$^+$), 639 ([M+Na–C_4H_8]$^+$), 567 ([M+Na–C_4H_8O]$^+$), 519, 499, 341 and 323 (Table 1 and Fig. 9). Collectively, these components were tentatively identified as kuwanon O and its isomers.

The mass spectral values of compound **70** (37.5 min) included *m/z* 375 ([M+Na]$^+$), 353 ([M+H]$^+$), 323 and 295 (Table 1 and Fig. 9). Based on our summary on the chemical components of MC (Table S1), this compound was tentatively identified as cyclocommunol.

Oxidation is a common biosynthetic pathway in herb. The sodium adduct ion and pseudo-molecular ions of *m/z* 461 ([M+Na]$^+$), 439 ([M+H]$^+$) and 437 ([M–H]$^-$) were presupposed for the oxidation products of dihydromorusin and its isomers, and they were detected at 38.4 min (**74**), 39.6 min (**82**), 50.8 min (**117**), 51.0 min (**119**) and 51.2 min (**120**) (Table 1 and Fig. 9). However, the fragment patterns of these five components were categorized into two groups: compounds **74** and **82** yielded positive diagnostic product ions at *m/z* 421 ([M+H–H_2O]$^+$), 365 ([M+H–C_4H_8]$^+$), 347 ([M+H–H_2O–C_4H_8]$^+$) and 311, while compounds **117**, **119** and **120** afforded negative characteristic product ions at *m/z* 311 ([M–H–$C_6H_6O_3$]$^-$), 285 and 259, suggesting that the oxidation occurred on different positions for these two groups. Due to the observation of successively neutral losses of a H_2O group and a C_4H_8 group, the hydroxyl moiety was added onto the C_5 (isopentenyl) substituent of compounds **74** and **82**. At the meanwhile, the hydroxyl substituent was added onto the B-ring of the flavones skeleton for compounds **117**, **119** and **120**.

The sodium adduct ion and pseudo-molecular ions of *m/z* 447 ([M+Na]$^+$), 425 ([M+H]$^+$) and 423 ([M–H]$^-$) were detected at 38.9 min (**76**) (Table 1 and Fig. 9). Thus, the chemical structure of compound **76** was tentatively assigned as kuwanon E, cathayanon H, or lespedezaflavanone C. cannot be elucidated. At the meanwhile, compound **81** (t_R: 39.5 min) also could not be identified based on the mass spectral values, including: *m/z* 427 ([M–H]$^-$), 297, 257, 243 and 191 (Table 1 and Fig. 9).

Compound **91** exhibited sodium adduct and protonated ion at *m/z* 653 ([M+Na]$^+$), and 631

([M+H]$^+$), respectively, suggesting a molecular weight as 630 Da, while the fragment ions of the protonated ion were yielded at *m/z* 575 ([M+H–C_4H_8]$^+$), 521 ([M+H–C_6H_6O]$^+$), 509, 453 and 323 (Table 1 and Fig. 9). Based on our chemical review, this compound was tentatively characterized as mulberrofuran F or mongolicin A.

Compound **108** was eluted at 48.4 min and came out with the sodium adduct ion and quasi-molecular ions at *m/z* 429 ([M+Na]$^+$), 407 ([M+H]$^+$) and 405 ([M–H]$^-$), while the positive fragment ions were afforded at *m/z* 351 ([M+H–C_4H_8]$^+$), 339, 295 ([M+H–C_4H_8–C_4H_8]$^+$) and 283 (Table 1 and Fig. 9). Collectively, this compound was tentatively identified as kuwanon S or its isomer. At the meanwhile, the pseudo-molecular ions of *m/z* 427 ([M+Na]$^+$) and 405 ([M+H]$^+$) that were presupposed as the dehydrogenation product of kuwanon S, were detected at 51.0 min (**118**), 53.8 min (**127**) and 55.7 min (**131**). The positive diagnostic fragment ions were observed *m/z* 351 ([M+H–C_4H_8]$^+$), 321 and 283 (Table 1 and Fig. 9). Hence, compounds **118**, **127** and **131** were tentatively identified as dehydrogenation product of kuwanon S or its isomers, yet their structures could not be definitely identified.

Deprotonated ion at *m/z* 455 was detected at 56.4 min (**133**) and 57.1 min (**134**) (Table 1 and Fig. 9). Based on our summary on the chemical components of MC (Table S1), these two compounds were tentatively identified as mulberrofuran R and its isomer.

Table S1 The precursor ions (deprotonated, protonated and sodiated molecular ions) of potential chemical components in Mori Cortex adopted in the MIM-IDA-EPI

No.	[M–H]$^{-}$	[M+H]$^{+}$	[M+Na]$^{+}$	No.	[M–H]$^{-}$	[M+H]$^{+}$	[M+Na]$^{+}$	No.	[M-H]$^{-}$	[M+H]$^{+}$	[M+Na]$^{+}$
1	132	134	156	53	409	411	433	105	575	577	599
2	141	143	165	54	411	413	435	106	577	579	601
3	143	145	167	55	413	415	437	107	579	581	603
4	146	148	170	56	417	419	441	108	581	583	605
5	157	159	181	57	419	421	443	109	585	587	609
6	159	161	183	58	421	423	445	110	589	591	613
7	162	164	186	59	423	425	447	111	591	593	615
8	174	176	198	60	425	427	449	112	593	595	617
9	176	178	200	61	427	429	451	113	605	607	629
10	177	179	201	62	435	437	459	114	607	609	631
11	190	192	214	63	437	439	461	115	609	611	633
12	191	193	215	64	439	441	463	116	615	617	639
13	204	206	228	65	441	443	465	117	623	625	647
14	225	227	249	66	445	447	469	118	625	627	649
15	227	229	251	67	447	449	471	119	627	629	651
16	241	243	265	68	449	451	473	120	629	631	653
17	243	245	267	69	453	455	477	121	631	633	655
18	245	247	269	70	455	457	479	122	637	639	661
19	257	259	281	71	457	459	481	123	641	643	665
20	265	267	289	72	459	461	483	124	645	647	669
21	269	271	293	73	461	463	485	125	647	649	671
22	271	273	295	74	465	467	489	126	649	651	673
23	285	287	309	75	467	469	491	127	661	663	685
24	287	289	311	76	469	471	493	128	665	667	689
25	289	291	313	77	475	477	499	129	675	677	699
26	293	295	317	78	477	479	501	130	677	679	701

27	301	303	325	79	479	481	503	131	679	681	703
28	307	309	331	80	481	483	505	132	689	691	713
29	309	311	333	81	483	485	507	133	691	693	715
30	311	313	335	82	485	487	509	134	693	695	717
31	323	325	347	83	487	489	511	135	703	705	727
32	325	327	349	84	489	491	513	136	705	707	729
33	327	329	351	85	491	493	515	137	707	709	731
34	329	331	353	86	493	495	517	138	709	711	733
35	335	337	359	87	495	497	519	139	711	713	735
36	337	339	361	88	499	501	523	140	713	715	737
37	339	341	363	89	503	505	527	141	715	717	739
38	341	343	365	90	505	507	529	142	717	719	741
39	351	353	375	91	507	509	531	143	733	735	757
40	353	355	377	92	511	513	535	144	743	745	767
41	355	357	379	93	513	515	537	145	753	755	777
42	363	365	387	94	521	523	545	146	757	759	781
43	373	375	397	95	529	531	553	147	759	761	783
44	375	377	399	96	551	553	575	148	761	763	785
45	377	379	401	97	557	559	581	149	775	777	799
46	387	389	411	98	559	561	583	150	781	783	805
47	391	393	415	99	561	563	585	151	783	785	807
48	395	397	419	100	563	565	587	152	835	837	859
49	401	403	425	101	565	567	589	153	839	841	863
50	403	405	427	102	567	569	591	154	861	863	885
51	405	407	429	103	569	571	593	155	877	879	901
52	407	409	431	104	573	575	597				

Table S2 Chemical components from the genus *Morus* and their formula, molecular weight (M.W.), source and reference information

No.	Compound	Formula	M.W.	Source	Ref.
	DA type adducts				
1	Kuwanon N	$C_{45}H_{44}O_{11}$	760	*M. lhou*	1
2	Kuwanon O	$C_{40}H_{38}O_{11}$	694	*M. lhou*	1
3	Kuwanon K	$C_{40}H_{36}O_{11}$	692	*M. alba*	2
4	Guangsangon G	$C_{35}H_{28}O_{10}$	608	*M. macroura*	3
5	Guangsangon I	$C_{35}H_{28}O_{10}$	608	*M. macroura*	3
6	Kuwnon W	$C_{45}H_{42}O_{11}$	758	*M. lhou*	4
7	Kuwanon G	$C_{40}H_{36}O_{11}$	692	*M. alba*	5
8	Kuwanon H	$C_{45}H_{44}O_{11}$	760	*M. alba*	5
9	Mongolicin D	$C_{45}H_{44}O_{10}$	744	*M. mongolica*	6
10	Moracenin C	$C_{45}H_{44}O_{11}$	760	*M. sp.*	7
11	Multicaulisin	$C_{40}H_{36}O_{11}$	692	*M. multicaulis*	8
12	Moracenin D	$C_{40}H_{38}O_{12}$	710	*M. sp.*	9
13	Autralisine A	$C_{35}H_{26}O_{10}$	606	*M. australis*	10
14	Sanggenon C	$C_{40}H_{36}O_{12}$	708	*M. cathayana*	11
15	Sanggenon D	$C_{40}H_{36}O_{12}$	708	*M. cathayana*	11
16	Sanggenon E	$C_{45}H_{44}O_{12}$	776	*M. sp.*	12
17	Sanggenon P	$C_{45}H_{44}O_{12}$	776	*M. sp.*	12
18	Sanggenon O	$C_{40}H_{36}O_{12}$	708	*M. sp.*	13
19	Sangenol J	$C_{45}H_{44}O_{12}$	776	*M. cathayana*	11
20	Cathayanon A	$C_{40}H_{36}O_{12}$	708	*M. cathayana*	14
21	Cathayanon B	$C_{40}H_{36}O_{12}$	708	*M. cathayana*	14
22	Sanggenon Q	$C_{40}H_{36}O_{12}$	708	*M. mongolica*	15
23	Sanggenon T	$C_{40}H_{40}O_{12}$	712	*M. sp.*	16
24	Sanggenol M	$C_{45}H_{46}O_{11}$	762	*M. mongolica*	17
25	Kuwanon L	$C_{35}H_{30}O_{11}$	626	*M. alba*	18

26	Guangsangon F	$C_{40}H_{36}O_{10}$	676	*M. macroura*	3
27	Guangsangon D	$C_{35}H_{30}O_{10}$	610	*M. macroura*	17
28	Guangsangon H	$C_{40}H_{38}O_{10}$	678	*M. macroura*	3
29	Guangsangon K	$C_{35}H_{30}O_{11}$	626	*M. macroura*	19
30	Guangsangon M	$C_{35}H_{30}O_{10}$	610	*M. macroura*	19
31	Guangsangon N	$C_{35}H_{30}O_{10}$	610	*M. macroura*	19
32	Cathayanon E	$C_{40}H_{36}O_{12}$	708	*M. cathayana*	20
33	Kuwanon I	$C_{40}H_{38}O_{10}$	678	*M. alba*	21
34	Kuwanon J	$C_{40}H_{38}O_{10}$	678	*M. alba*	22
35	Kuwanon Q	$C_{40}H_{38}O_{9}$	662	*M. alba*	22
36	Kuwanon R	$C_{40}H_{38}O_{9}$	662	*M. alba*	22
37	Kuwanon V	$C_{40}H_{38}O_{8}$	646	*M. alba*	22
38	Mongolicin G	$C_{40}H_{40}O_{10}$	680	*M. mongolica*	23
39	Guangsangon C	$C_{35}H_{30}O_{10}$	610	*M. macroura*	17
40	Kuwanol E	$C_{39}H_{38}O_{9}$	650	*M. alba*	24
41	Kuwanon X	$C_{34}H_{30}O_{9}$	582	*M. lhou*	25
42	Kuwanon Y	$C_{34}H_{30}O_{9}$	582	*M. lhou*	26
43	Kuwanol A	$C_{34}H_{28}O_{8}$	564	*M. bombycis*	27
44	Kuwanol B	$C_{36}H_{26}O_{8}$	586	*M. bonbycis*	27
45	Kuwanon Z	$C_{34}H_{26}O_{10}$	594	*M. lhou*	26
46	Guangsangon B	$C_{34}H_{30}O_{8}$	566	*M. macroura*	17
47	Kuwanon P	$C_{34}H_{30}O_{9}$	582	*M. lhou*	25
48	Cathayanon C	$C_{34}H_{24}O_{8}$	560	*M. cathayana*	20
49	Cathayanon D	$C_{34}H_{24}O_{9}$	576	*M. cathayana*	20
50	Mulberrofuran C	$C_{34}H_{28}O_{9}$	580	*M. bombycis*	28
51	Mulberrofuran T	$C_{44}H_{44}O_{9}$	716	*M. alba*	24
52	Mulberrofuran U	$C_{39}H_{36}O_{9}$	648	*M. insignis*	29
53	Chalcomoracin	$C_{39}H_{36}O_{9}$	648	*M. alba*	30
54	Mulberrofuran O	$C_{39}H_{34}O_{9}$	646	*M. sp.*	31

55	Mulberrofuran E	$C_{39}H_{36}O_8$	632	*M. alba*	32
56	Mulberrofuran J	$C_{34}H_{28}O_9$	580	*M. lhou*	25
57	Mongolicin F	$C_{39}H_{36}O_9$	648	*M. mongolica*	6
58	Guangsangon A	$C_{39}H_{38}O_{10}$	666	*M. macroura*	17
59	Albafuran C	$C_{34}H_{28}O_9$	580	*M. alba*	17
60	Guangsangon E	$C_{39}H_{36}O_9$	648	*M. macroura*	17
61	Guangsangon J	$C_{39}H_{36}O_9$	648	*M. macroura*	14
62	Mulberrofuran F	$C_{39}H_{34}O_8$	630	*M. lhou*	33
63	Mulberrofuran G	$C_{36}H_{26}O_8$	586	*M. lhou*	33
64	Mongolicin A	$C_{39}H_{34}O_8$	630	*M. mongolica*	6
65	Mulberrofuran Q	$C_{39}H_{32}O_8$	628	*M. alba*	34
66	Mulberrofuran G	$C_{34}H_{25}O_8$	562	*M. alba*	35
67	Isomulberrofuran G	$C_{34}H_{25}O_8$	562	*M. alba*	35
68	Mongolicin A	$C_{39}H_{34}O_8$	630	*M. mongolica*	6
69	Mulberrofuran K	$C_{39}H_{32}O_8$	628	*M. sp.*	32
70	Albanol B	$C_{34}H_{22}O_8$	558	*M. alba*	24
71	Mulberrofuran P	$C_{34}H_{22}O_9$	574	*M. alba*	36
72	Mulberrofuran I	$C_{34}H_{24}O_8$	560	*M. alba*	37
73	Mulberrofuran S	$C_{34}H_{24}O_9$	576	*M. alba*	37
74	Mongolicin C	$C_{34}H_{26}O_9$	578	*M. mongolica*	6
75	Mulberrofuran Q	$C_{34}H_{24}O_{10}$	592	*M. alba*	34
76	Australisine B	$C_{39}H_{34}O_9$	646	*M. australis*	10
77	Australisine C	$C_{34}H_{28}O_9$	580	*M. australis*	10
78	Yunanensin A	$C_{39}H_{28}O_8$	624	*M. yunnanensis*	38
79	Yunanensin B	$C_{39}H_{34}O_9$	646	*M. yunnanensis*	38
80	Yunanensin C	$C_{39}H_{34}O_9$	646	*M. yunnanensis*	38
81	Yunanensin D	$C_{39}H_{30}O_9$	642	*M. yunnanensis*	38
82	Yunanensin E	$C_{39}H_{32}O_8$	628	*M. yunnanensis*	38
83	Kuwanon M	$C_{50}H_{48}O_{12}$	840	*M. lhou*	39

84	Mongolicin E	$C_{50}H_{48}O_{12}$	840	*M. mongolica*	6
85	Dimoracin	$C_{38}H_{32}O_8$	616	*M. alba*	40
86	Mulberrofuran H	$C_{27}H_{22}O_6$	442	*M. lhou*	41
87	Sanggenon R	$C_{20}H_{16}O_5$	336	*M. sp.*	16
88	Sanggenon B	$C_{33}H_{30}O_9$	570	*M. sp.*	42
89	Sanggenon S	$C_{40}H_{34}O_{12}$	706	*M. sp.*	16
90	Guangsangon L	$C_{27}H_{24}O_8$	476	*M. macroura*	19
91	Mongolicin B	$C_{28}H_{18}O_7$	466	*M. mongolica*	6
92	Mulberrofuran R	$C_{27}H_{20}O_7$	456	*M. lhou*	43
93	Mulberrofuran M	$C_{34}H_{22}O_{10}$	590	*M. alba*	44
94	Wittiorumin A	$C_{35}H_{28}O_{11}$	624	*M. wittiorum*	45
95	Wittiorumin B	$C_{40}H_{36}O_{12}$	708	*M. wittiorum*	45
96	Wittiorumin C	$C_{40}H_{36}O_{11}$	692	*M. wittiorum*	45
97	Wittiorumin D	$C_{35}H_{30}O_{10}$	610	*M. wittiorum*	45
98	Wittiorumin E	$C_{40}H_{38}O_{10}$	678	*M. wittiorum*	45
99	Wittiorumin F	$C_{39}H_{36}O_9$	648	*M. wittiorum*	45
100	Mulberrofuran F1	$C_{39}H_{34}O_9$	646	*M. alba*	46
101	Cathayanin A	$C_{25}H_{28}O_4$	392	*M. cathayana*	47
102	Cathayanin B	$C_{40}H_{34}O_{11}$	690	*M. cathayana*	47
103	Cathayanin C	$C_{40}H_{34}O_{11}$	690	*M. cathayana*	47
104	Morusyunnansin A	$C_{38}H_{32}O_8$	616	*M. yunnanensis*	48
105	Morusyunnansin B	$C_{38}H_{32}O_8$	616	*M. yunnanensis*	48
106	Morusyunnansin C	$C_{42}H_{48}O_8$	680	*M. yunnanensis*	48
107	Morusyunnansin D	$C_{42}H_{48}O_8$	680	*M. yunnanensis*	48
	Stilbenes and 2-arylbenzofuran				
108	Oxyresveratrol	$C_{14}H_{12}O_4$	244	*M. alba*	49
109	Resveratrol	$C_{14}H_{12}O_3$	228	*M. alba*	49
110	2,3,4′-trihydrox stilbene	$C_{14}H_{14}O_3$	230	*M. alba*	49
111	Mulberroside A	$C_{26}H_{32}O_{14}$	568	*M. alba*	49

112	*cis*-mulberroside A	$C_{26}H_{32}O_{14}$	568	*M. alba*	49
113	Andalasin A	$C_{28}H_{24}O_8$	488	*M. macroura*	50
114	4′-prenyloxyresveratrol	$C_{19}H_{20}O_4$	312	*M. alba*	51
115	Oxyresveratrol-2-glucoside	$C_{20}H_{22}O_9$	406	*M. alba*	49
116	Oxyresveratrol-3′-glucoside	$C_{20}H_{22}O_9$	406	*M. alba*	49
117	Resveratrol-4, 3′-diglucoside	$C_{26}H_{32}O_{13}$	552	*M. alba*	49
118	3′,5′,2,4-tetrahydroxy-4-(-3-methyl-1-butenyl)-2-benzylfuran	$C_{19}H_{20}O_4$	312	*M. alba*	49
119	2-(3,5-dihydroxyphenyl)-5,6-dihydroxybenzofuran	$C_{14}H_{10}O_5$	258	*M. wittiorum*	52
120	Moracin A	$C_{16}H_{14}O_5$	286	*M. alba*	53
121	Moracin B	$C_{16}H_{14}O_5$	294	*M. alba*	53
122	Moracin C	$C_{19}H_{18}O_4$	310	*M. alba*	54
123	Moracin D	$C_{19}H_{16}O_4$	308	*M. alba*	54
124	Moracin E	$C_{19}H_{16}O_4$	308	*M. alba*	55
125	Moracin F	$C_{16}H_{14}O_5$	294	*M. alba*	55
126	Moracin G	$C_{19}H_{16}O_4$	308	*M. alba*	55
127	Moracin H	$C_{20}H_{18}O_5$	338	*M. alba*	55
128	Moracin I	$C_{20}H_{20}O_4$	324	*M. alba*	56
129	Moracin J	$C_{20}H_{20}O_4$	324	*M. alba*	18
130	Moracin K	$C_{19}H_{16}O_5$	324	*M. mesozygia*	57
131	Moracin L	$C_{19}H_{16}O_5$	324	*M. alba*	18
132	Moracin M	$C_{14}H_{10}O_4$	242	*M. mesozygia*	57
133	Moracin N	$C_{19}H_{18}O_4$	310	*M. alba*	58
134	Moracin O	$C_{19}H_{18}O_5$	326	*M. alba*	58
135	Moracin P	$C_{19}H_{18}O_5$	326	*M. alba*	58
136	Moracin Q	$C_{21}H_{22}O_5$	354	*M. mesozygia*	57
137	Moracin R	$C_{19}H_{20}O_5$	328	*M. mesozygia*	57
138	Moracin S	$C_{19}H_{18}O_4$	310	*M. mesozygia*	57

139	Moracin T	$C_{20}H_{20}O_5$	340	*M. mesozygia*	57
140	Moracin U	$C_{19}H_{16}O_6$	340	*M. mesozygia*	57
141	Moracin V	$C_{19}H_{18}O_6$	342	*M. alba*	58
142	Moracin W	$C_{29}H_{34}O_6$	478	*M. alba*	58
143	Moracin X	$C_{16}H_{10}O_4$	266	*M. alba*	58
144	Moracin Y	$C_{15}H_{10}O_5$	270	*M. alba*	58
145	Moracin Z	$C_{19}H_{18}O_5$	326	*M. lhou*	59
146	Albafuran A	$C_{24}H_{26}O_4$	378	*M. nigra*	60
147	Albafuran B	$C_{24}H_{26}O_4$	378	*M. nigra*	60
148	Macrourin A	$C_{29}H_{32}O_5$	460	*M. macroura*	61
149	Macrourin B	$C_{28}H_{20}O_9$	500	*M. macroura*	61
150	Mulberroside C	$C_{24}H_{26}O_9$	458	*M. wittiorum*	52
151	Wittifuran A	$C_{24}H_{26}O_6$	410	*M. wittiorum*	60
152	Wittifuran B	$C_{24}H_{24}O_5$	392	*M. wittiorum*	60
153	Wittifuran C	$C_{29}H_{36}O_7$	496	*M. wittiorum*	60
154	Wittifuran D	$C_{19}H_{18}O_4$	310	*M. wittiorum*	52
155	Wittifuran E	$C_{14}H_{10}O_5$	258	*M. wittiorum*	52
156	Wittifuran F	$C_{29}H_{34}O_6$	478	*M. wittiorum*	60
157	Wittifuran G	$C_{29}H_{34}O_6$	478	*M. wittiorum*	60
158	Wittifuran H	$C_{29}H_{34}O_7$	494	*M. wittiorum*	62
160	Wittifuran I	$C_{29}H_{36}O_8$	512	*M. wittiorum*	62
161	Wittifuran J	$C_{29}H_{36}O_8$	512	*M. wittiorum*	63
162	Wittifuran K	$C_{29}H_{38}O_9$	530	*M. wittiorum*	63
163	Wittifuran L	$C_{29}H_{38}O_9$	530	*M. wittiorum*	63
164	Wittifuran M	$C_{29}H_{38}O_9$	530	*M. wittiorum*	63
165	Wittifuran N	$C_{29}H_{38}O_9$	530	*M. wittiorum*	63
166	Wittifuran O	$C_{29}H_{34}O_6$	478	*M. wittiorum*	63
167	Wittifuran P	$C_{19}H_{18}O_4$	310	*M. wittiorum*	63
168	Wittifuran Q	$C_{19}H_{18}O_5$	326	*M. wittiorum*	63

169	Wittifuran R	$C_{29}H_{34}O_6$	478	*M. wittiorum*	63
170	Wittifuran S	$C_{19}H_{18}O_5$	326	*M. wittiorum*	64
171	Wittifuran T	$C_{15}H_{12}O_5$	272	*M. wittiorum*	64
172	Wittifuran U	$C_{24}H_{26}O_6$	410	*M. wittiorum*	62
173	Wittifuran V	$C_{19}H_{18}O_5$	326	*M. wittiorum*	64
174	Wittifuran W	$C_{19}H_{18}O_5$	326	*M. wittiorum*	64
175	Wittifuran X	$C_{15}H_{12}O_5$	272	*M. wittiorum*	64
176	Macrourin D	$C_{28}H_{20}O_9$	500	*M. macroura*	65
177	Macrourin E	$C_{28}H_{20}O_9$	500	*M. alba*	66
178	Austrafuran B	$C_{28}H_{20}O_8$	484	*M. australis*	67
179	Mulferrofuran B	$C_{25}H_{28}O_4$	392	*M. alba*	66
180	Cathafuran A	$C_{34}H_{42}O_4$	514	*M. cathayana*	67
181	Cathafuran B	$C_{24}H_{26}O_4$	378	*M. cathayana*	67
182	Cathafuran C	$C_{24}H_{24}O_4$	376	*M. cathayana*	67
183	Cathafuran D	$C_{25}H_{28}O_5$	408	*M. cathayana*	67
184	3′,4,5′-trihydroxy-4′-gerarylstilbene	$C_{24}H_{28}O_3$	364	*M. cathayana*	68
185	Mulberrofuran V	$C_{24}H_{36}O_4$	388	*M. cathayana*	69
186	Artoindonesianin X	$C_{29}H_{34}O_4$	446	*M. cathayana*	68
187	Mulberrofuran B	$C_{25}H_{28}O_4$	392	*M. alba*	66
188	Mulberrofuran C	$C_{34}H_{28}O_9$	580	*M. alba*	70
189	Mulberrofuran N	$C_{25}H_{28}O_4$	392	*M. cathayana*	68
190	Mulberrofuran W	$C_{29}H_{34}O_4$	446	*M. mongolica*	71
191	Mulberrofuran X	$C_{29}H_{34}O_5$	462	*M. mongolica*	71
192	Mulberrofuran Y	$C_{25}H_{28}O_5$	408	*M. mongolica*	71
193	Mulberrofuran Z	$C_{30}H_{36}O_5$	476	*M. mongolica*	71
194	Demethylmoraccin I	$C_{19}H_{18}O_4$	310	*M. yunnanensis*	72
195	4′-(6,6-dimethyl-5-hydroxyl-2-methylenecyclohexylmethyl)-	$C_{24}H_{26}O_5$	396	*M. alba var. tatarica*	73

	3′,5′,6-trihydroxy-2-arylbenzofuran				
196	2′-(1,3,3-trimethyl-7-oxabicyclo[2.2.1]hept-2-ylmethyl)-3′-methoxy-5′,6-dihydroxy-2-arylbenzofuran	$C_{25}H_{28}O_5$	408	*M. alba var. tatarica*	73
197	2′-(6-hydroxy-3,7-dimethyl-2,7-octadien-1-yl)-3′-methoxy-5′,6-dihydroxy-2-arylbenzofuran	$C_{25}H_{28}O_5$	408	*M. alba var. tatarica*	73
198	4′-(6-hydroxy-3,7-di-methyl-2,7-octadien-1-yl)-3′,5′,6-trihydroxy-2-arylbenzofuan	$C_{24}H_{26}O_5$	396	*M. alba var. tatarica*	73
199	2′-(6,7-dihydroxy-3,7-dimethyl-2-octen-1-yl)-3′,5′,6-trihydroxy-2-arylbenzofuan	$C_{24}H_{28}O_6$	414	*M. alba var. tatarica*	73
200	4′-(6,7-dihydroxy-3,7-dimethyl-2-octen-1-yl)-3′,5′,6-trihydroxy-2-arylbenzofuan	$C_{24}H_{28}O_6$	414	*M. alba var. tatarica*	73
201	2′- (6,7-dihydroxy-3,7-dim ethyl-2-octen-1-yl)-3′-methoxy-5′,6-dihydroxy-2-arylbenzofuran	$C_{25}H_{30}O_6$	426	*M. alba var. tatarica*	73
202	2′-[(6S)-6-hydroxy-7-methoxy-3,7-dimethyl-2-octen- 1-yl]-3′-methoxy-5′,6-dihydroxy-2-arylbenzofuran.	$C_{26}H_{32}O_6$	440	*M. alba var. tatarica*	73
203	2′-[3-methyl-3-(4-methyl-3-penten-1-yl)-2-oxiranyl]methyl]-3′,5′,6-trihydroxy-2-arylbenzofuran	$C_{24}H_{26}O_5$	396	*M. alba var. tatarica*	73

204	Albafuran B	$C_{24}H_{26}O_4$	378	*M. alba*	60
	Flavnoids				
205	Yunanensol A	$C_{25}H_{28}O_7$	440	*M. yunnanensis*	63
206	Yunanensol B	$C_{20}H_{18}O_5$	338	*M. yunnanensis*	63
207	5′-(1″,1″-dimethyl)-8-(8″,8″-dimethyallyl)-2′,4′,5,7-tetrahydroylflavone	$C_{20}H_{18}O_6$	354	*M. mongolica*	23
208	Morunigrol A	$C_{25}H_{22}O_6$	418	*M. nigra*	60
209	Morunigrol B	$C_{25}H_{24}O_6$	420	*M. nigra*	60
210	Morunigrol E	$C_{25}H_{26}O_7$	438	*M. nigra*	74
211	Morunigrol G	$C_{25}H_{26}O_7$	438	*M. nigra*	74
212	Morunigrol H	$C_{25}H_{16}O_6$	412	*M. nigra*	74
213	Morachalcone B	$C_{20}H_{18}O_5$	338	*M. alba*	75
214	Morachalcone C	$C_{20}H_{18}O_6$	354	*M. alba*	75
215	Morachalcone A	$C_{20}H_{20}O_5$	340	*M. yunnanensis*	76
217	Isobacachalcone	$C_{20}H_{20}O_4$	324	*M. cathayana*	68
218	Morusin	$C_{25}H_{24}O_6$	420	*M. alba*	77
219	Cyclomorusin	$C_{25}H_{22}O_6$	418	*M. alba*	78
220	Kuwanon C	$C_{25}H_{26}O_6$	422	*M. alba*	77
221	3-(2″-hydroxyl-3″-methyl-3″-butenyl)-morusin	$C_{25}H_{24}O_7$	436	*M. cathayana*	68
222	6-geranylapigenin	$C_{25}H_{26}O_5$	406	*M. cathayana*	68
223	Licoisoflavanone	$C_{20}H_{18}O_6$	354	*M. cathayana*	68
224	Kamperfol-3-glucopyranoside	$C_{21}H_{20}O_{11}$	448	*M. cathayana*	68
225	Benzokuwanon E	$C_{25}H_{24}O_7$	436	*M. australia*	79
226	Hydroxymorusin	$C_{25}H_{26}O_7$	438	*M. australia*	79
227	Jisang	$C_{25}H_{26}O_6$	422	*M. australia*	79
228	Kuwanon E	$C_{25}H_{28}O_6$	424	*M. australia*	79
229	Kuwanon U	$C_{26}H_{30}O_6$	438	*M. australia*	79

230	Kuwanon S	$C_{25}H_{26}O_5$	406	*M. alba*	78
231	Morusignin L	$C_{25}H_{26}O_7$	438	*M. australia*	79
232	Morusinol	$C_{25}H_{26}O_7$	438	*M. australia*	79
233	Mulberranol	$C_{25}H_{26}O_7$	438	*M. australia*	79
234	Cathayanon F	$C_{25}H_{26}O_5$	406	*M. cathayana*	68
235	Cathayanon G	$C_{25}H_{26}O_6$	422	*M. cathayana*	68
236	Cathayanon H	$C_{25}H_{28}O_6$	424	*M. cathayana*	68
237	Cathayanon I	$C_{25}H_{28}O_7$	440	*M. cathayana*	68
238	Cathayanon J	$C_{30}H_{36}O_6$	492	*M. cathayana*	68
239	Sanggenol G	$C_{30}H_{34}O_7$	506	*M. cathayana*	68
240	sanggenol O	$C_{25}H_{24}O_6$	420	*M. atropurpurea*	80
241	Sanggenol P	$C_{30}H_{36}O_6$	492	*M. alba*	81
242	Sanggenol N	$C_{25}H_{26}O_6$	422	*M. alba*	81
243	Cyclomulberrin	$C_{25}H_{24}O_6$	420	*M. alba*	81
244	Cyclocommunol	$C_{20}H_{16}O_6$	352	*M. alba*	81
245	Sanggenol A	$C_{25}H_{24}O_7$	436	*M. cathayana*	68
246	Isolicoflavonol	$C_{20}H_{18}O_6$	354	*M. australis*	82
247	Quercetin	$C_{15}H_{10}O_7$	302	*M. australis*	82
248	Dihydromorin	$C_{15}H_{12}O_7$	304	*M. cathayana*	68
249	Glyasperin F	$C_{20}H_{18}O_6$	354	*M. cathayana*	68
250	Broussoflavonol F	$C_{25}H_{26}O_6$	422	*M. cathayana*	68
251	Lespedezaflavanone C	$C_{25}H_{28}O_6$	424	*M. cathayana*	68
252	Sanggenol B	$C_{30}H_{34}O_6$	490	*M. alba*	77
253	Sanggenol D	$C_{30}H_{36}O_6$	492	*M. alba*	77
254	Dihydrokaempferol	$C_{15}H_{12}O_6$	288	*M. nigra*	74
255	Norartocarpanone	$C_{15}H_{12}O_6$	288	*M. cathayana*	68
256	Nigrasin A	$C_{25}H_{26}O_8$	454	*M. nigra*	83
257	Nigrasin B	$C_{25}H_{26}O_8$	454	*M. nigra*	83
258	Nigrasin C	$C_{25}H_{26}O_8$	454	*M. nigra*	83

259	Nigrasin D	$C_{25}H_{26}O_8$	454	*M. nigra*	83
260	Nigrasin E	$C_{25}H_{26}O_7$	454	*M. nigra*	83
261	Nigrasin F	$C_{25}H_{24}O_7$	436	*M. nigra*	83
262	Nigrasin G	$C_{30}H_{34}O_8$	522	*M. nigra*	83
263	Nigrasin H	$C_{25}H_{26}O_6$	422	*M. nigra*	83
264	Nigrasin I	$C_{25}H_{26}O_6$	422	*M. nigra*	83
265	Nigrasin J	$C_{26}H_{28}O_8$	468	*M. nigra*	83
266	Sanggenol L	$C_{25}H_{26}O_6$	422	*M. mongolica*	71
267	Morusyunnansin E	$C_{21}H_{24}O_5$	356	*M. yunnanensis*	48
268	Morusyunnansin F	$C_{20}H_{22}O_4$	326	*M. yunnanensis*	48
269	Morusyunnansin G	$C_{21}H_{26}O_6$	374	*M. yunnanensis*	72
	Others				
270	1-deoxnojirimycin	$C_6H_{13}NO_4$	163	*M. alba*	84
271	N-methy-1-deoxynojirimycin	$C_7H_{15}NO_4$	177	*M. alba*	84
272	Fagomine	$C_6H_{13}NO_3$	147	*M. alba*	84
273	3-epi-fagomine	$C_6H_{13}NO_3$	147	*M. alba*	84
274	2-*O*-α-D-galaetopyranosyl-1-deoxynojirimycin	$C_{12}H_{23}NO_9$	325	*M. alba*	84
275	6-O-α-D-galactopyranosyl-1-deoxynojirimycin	$C_{12}H_{23}NO_9$	325	*M. alba*	84
276	2-O-α-D-glucopyranosyl-1-deoxynojirimycin	$C_{12}H_{23}NO_9$	325	*M. alba*	84
277	3-O-α-D-glucopyranosyl-1-deoxynojirimycin	$C_{12}H_{23}NO_9$	325	*M. alba*	84
278	3-O-α-D-glucopyranosyl-1-deoxynojirimycin	$C_{12}H_{23}NO_9$	325	*M. alba*	84
279	2-O-β-D-glucopyranosyl-1-deoxynojirimycin	$C_{12}H_{23}NO_9$	325	*M. alba*	84
280	3-O-β-D-glucopyranosyl-1-	$C_{12}H_{23}NO_9$	325	*M. alba*	85

	deoxynojirimycin				
281	4-O-β-D-glucopyranosyl-1-deoxynojirimycin	$C_{12}H_{23}NO_9$	325	*M. alba*	85
282	6-O-β-D-glucopyranosyl-1-deoxynojirimycin	$C_{12}H_{23}NO_9$	325	*M. alba*	85
283	1,4-dideoxy-1,4-imino-D-arabinitol	$C_5H_{11}NO_3$	133	*M. alba*	84
284	1,4-dideoxy-1,4-imino-D-ribitol	$C_5H_{11}NO_3$	133	*M. alba*	84
285	1,4-dideoxy-1,4-imino-(2-O-β-D-glucopyranosyl)-D-arabinitol	$C_{11}H_{21}NO_8$	295	*M. alba*	85
286	(2R,3R,4R)-2-hydroxymethyl-3,4-dihydroxypyrrolidine-N-propionamide	$C_8H_{16}N_2O_4$	205	*M. alba*	85
287	Calystegin B_2	$C_7H_{13}NO_4$	175	*M. alba*	84
288	Calystegin C_1	$C_7H_{13}NO_5$	191	*M. alba*	84
289	2α,3β-dihydroxynortropane	$C_7H_{14}NO_2$	144	*M. alba*	86
290	2β,3β-dihydroxynortropane	$C_7H_{14}NO_2$	144	*M. alba*	86
291	2α,3β,6exo-trihydroxynortropane	$C_7H_{12}NO_3$	158	*M. alba*	86
292	2α,3β,4α-trihydroxynortropane	$C_7H_{14}NO_3$	160	*M. alba*	86
293	3β,6exo-trihydroxynortropane	$C_7H_{12}NO_2$	142	*M. alba*	86
294	3β,6β-dihydroxynortropane	$C_7H_{14}NO_2$	144	*M. alba*	85

295	4-*O*-α-D-galactopyranosyl-calystegin	$C_{13}H_{23}NO_9$	337	*M. alba*	85

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