Supplementary Materials: HPLC–PDA and LC–MS/MS Analysis for the Simultaneous Quantification of the 14 Marker Components in Sojadodamgangki-Tang

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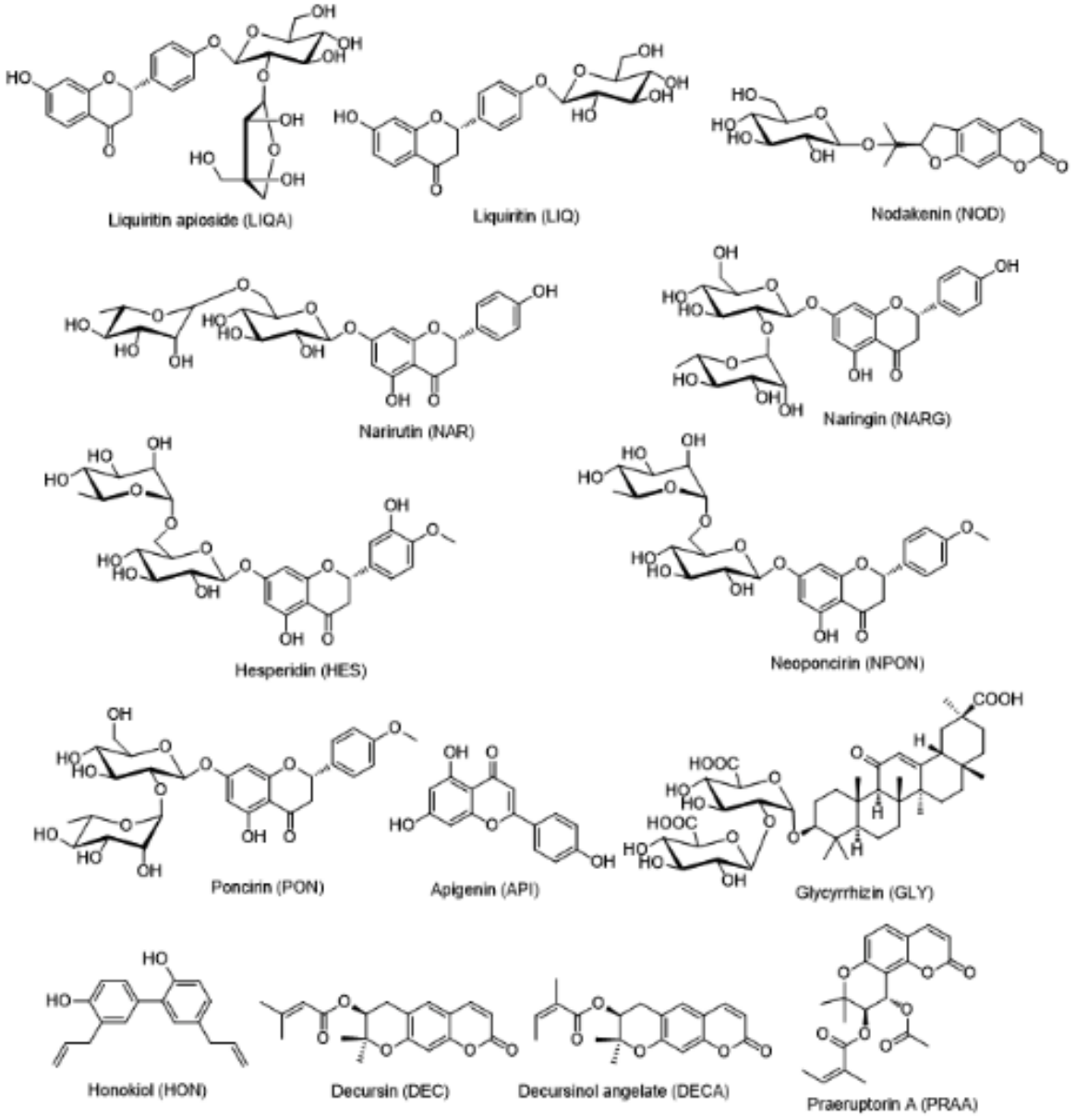
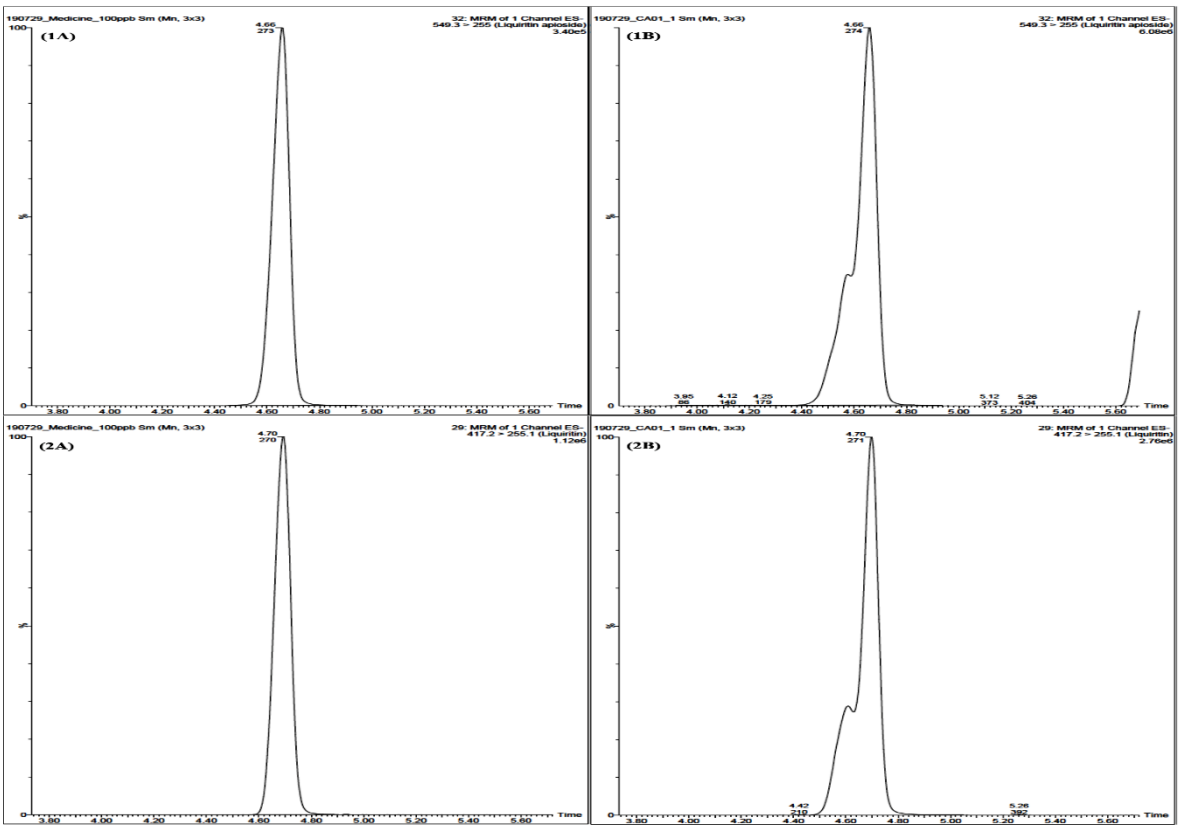
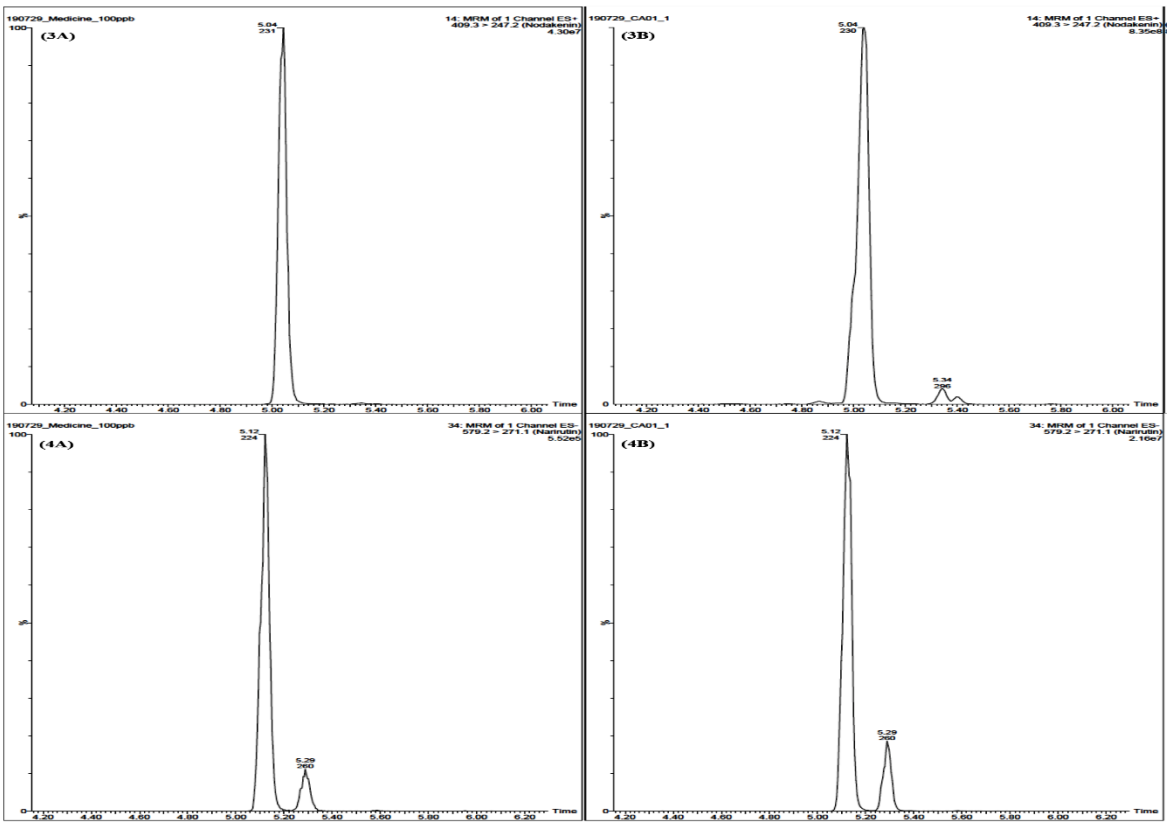
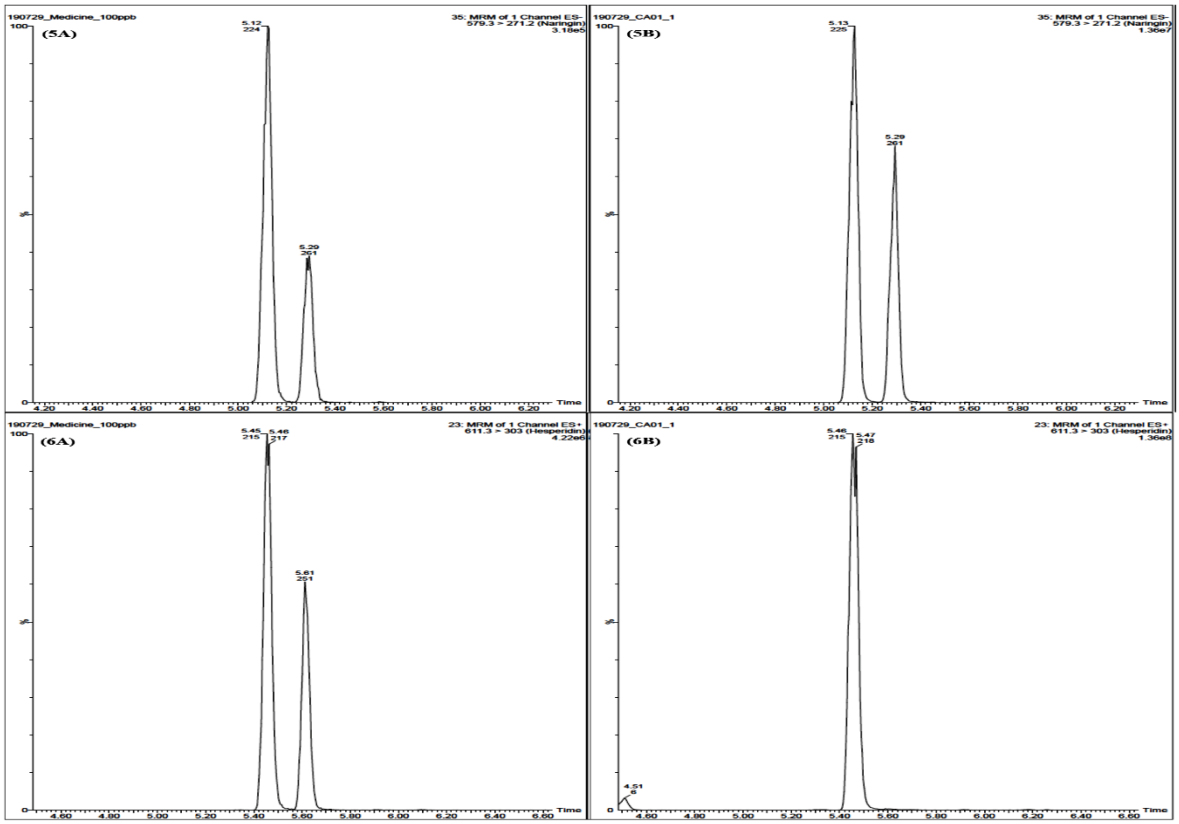
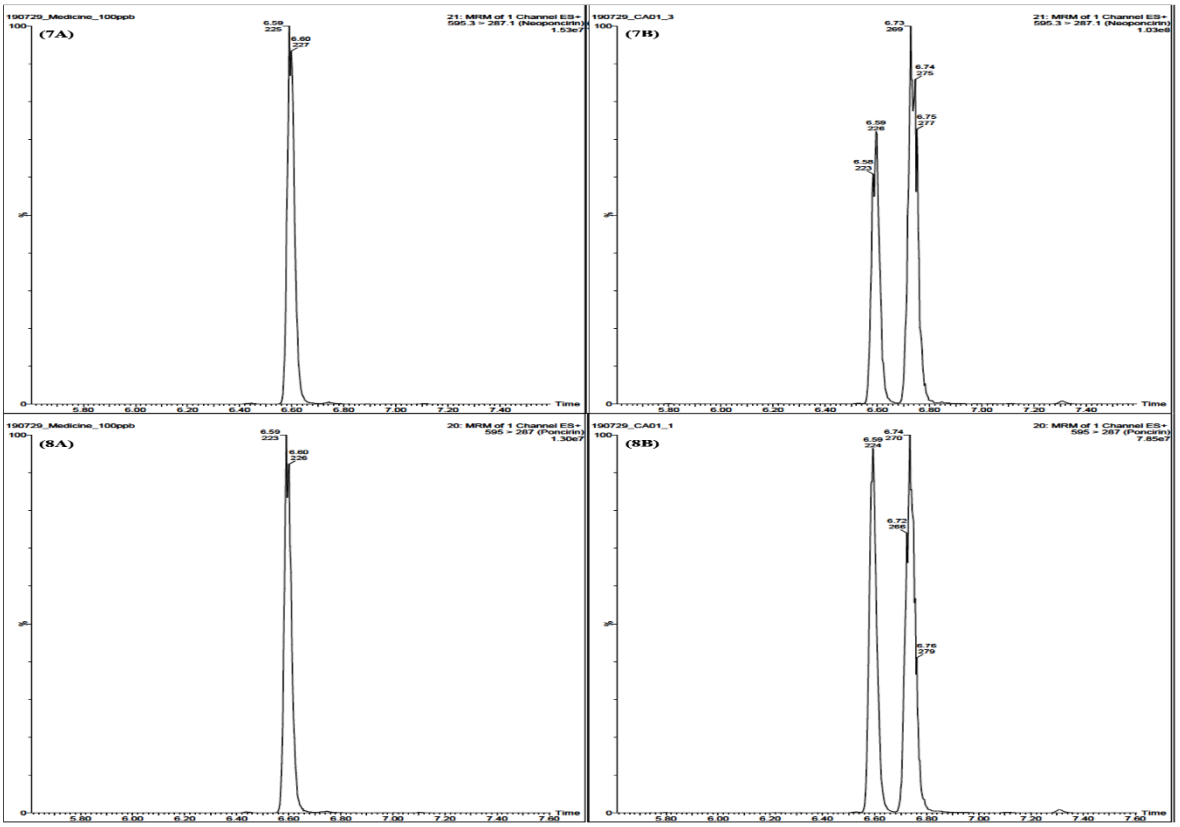


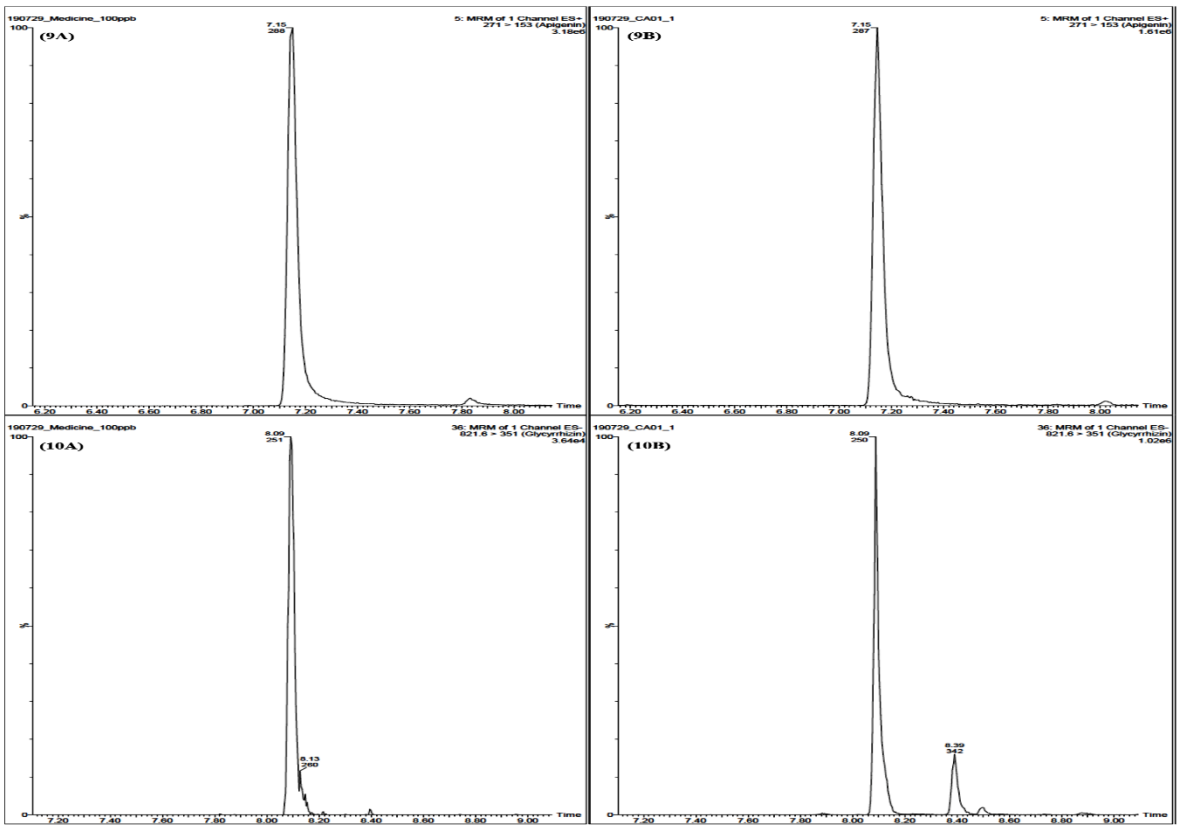
Figure S1. Chemical structures of the 14 marker components in Sojadodamgangki-tang (SDGT).

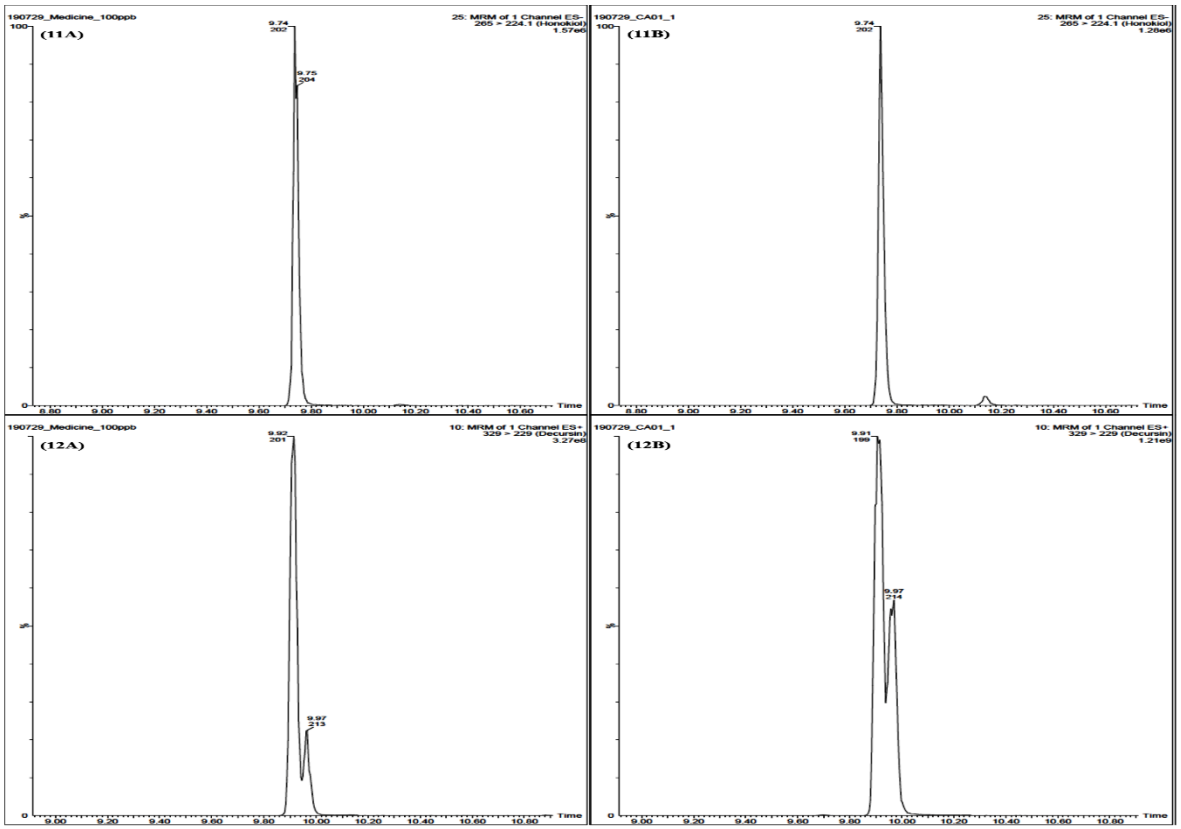

190729_Medicine_100ppb Sm (Mn, 3x3)
32: MRM of 1 Channel ES-
549.3 > 255 (Liquiritin apioside)
3.40e5
(1A)
4.66
273
190729_CA01_1 Sm (Mn, 3x3)
32: MRM of 1 Channel ES-
549.3 > 255 (Liquiritin apioside)
6.08e6
(1B)
4.66
274
3.85
4.12
4.25
5.12
5.26
190729_Medicine_100ppb Sm (Mn, 3x3)
29: MRM of 1 Channel ES-
417.2 > 255.1 (Liquiritin)
1.12e6
(2A)
4.70
270
190729_CA01_1 Sm (Mn, 3x3)
29: MRM of 1 Channel ES-
417.2 > 255.1 (Liquiritin)
2.76e6
(2B)
4.70
271
4.42
5.28
Time


190729_Medicine_100ppb
14: MRM of 1 Channel ES+
409.3 > 247.2 (Nodakenin)
4.30e7
(3A)
5.04
231
190729_CA01_1
14: MRM of 1 Channel ES+
409.3 > 247.2 (Nodakenin)
8.35e8
(3B)
5.04
230
5.34
190729_Medicine_100ppb
34: MRM of 1 Channel ES-
579.2 > 271.1 (Narirutin)
5.52e5
(4A)
5.12
224
5.29
190729_CA01_1
34: MRM of 1 Channel ES-
579.2 > 271.1 (Narirutin)
2.16e7
(4B)
5.12
224
5.29
Time


190729_Medicine_100ppb
35: MRM of 1 Channel ES-
579.3 > 271.2 (Naringin)
(5A)
5.12
224
5.29
261
190729_CA01_1
35: MRM of 1 Channel ES-
579.3 > 271.2 (Naringin)
(5B)
5.13
225
5.29
261
190729_Medicine_100ppb
23: MRM of 1 Channel ES+
611.3 > 303 (Hesperidin)
(6A)
5.45
215
5.46
217
5.61
251
190729_CA01_1
23: MRM of 1 Channel ES+
611.3 > 303 (Hesperidin)
(6B)
5.46
215
5.47
216
4.51
6
Time


190729_Medicine_100ppb
21: MRM of 1 Channel ES+
595.3 > 287.1 (Neoponcirin)
(7A)
6.59
225
6.60
227
190729_CA01_3
21: MRM of 1 Channel ES+
595.3 > 287.1 (Neoponcirin)
(7B)
6.73
269
6.74
275
6.75
277
6.59
226
6.58
223
190729_Medicine_100ppb
20: MRM of 1 Channel ES+
595 > 287 (Poncirin)
(8A)
6.59
223
6.60
226
190729_CA01_1
20: MRM of 1 Channel ES+
595 > 287 (Poncirin)
(8B)
6.74
270
6.59
224
6.72
268
6.75
275
Time


190729_Medicine_100ppb
5: MRM of 1 Channel ES+
271 > 153 (Apigenin)
3.18e6
(9A)
7.15
288
190729_CA01_1
5: MRM of 1 Channel ES+
271 > 153 (Apigenin)
1.61e6
(9B)
7.15
287
190729_Medicine_100ppb
36: MRM of 1 Channel ES-
821.6 > 351 (Glycyrrhizin)
3.64e4
(10A)
8.09
251
8.13
260
190729_CA01_1
36: MRM of 1 Channel ES-
821.6 > 351 (Glycyrrhizin)
1.02e6
(10B)
8.09
250
8.39
342
Time


190729_Medicine_100ppb
25: MRM of 1 Channel ES-
265 > 224.1 (Honokiol)
1.57e6
(11A)
9.74
202
9.75
204
190729_CA01_1
25: MRM of 1 Channel ES-
265 > 224.1 (Honokiol)
1.26e6
(11B)
9.74
202
190729_Medicine_100ppb
10: MRM of 1 Channel ES+
329 > 229 (Decursin)
3.27e6
(12A)
9.92
201
9.97
213
190729_CA01_1
10: MRM of 1 Channel ES+
329 > 229 (Decursin)
1.21e6
(12B)
9.91
199
9.97
214
Time

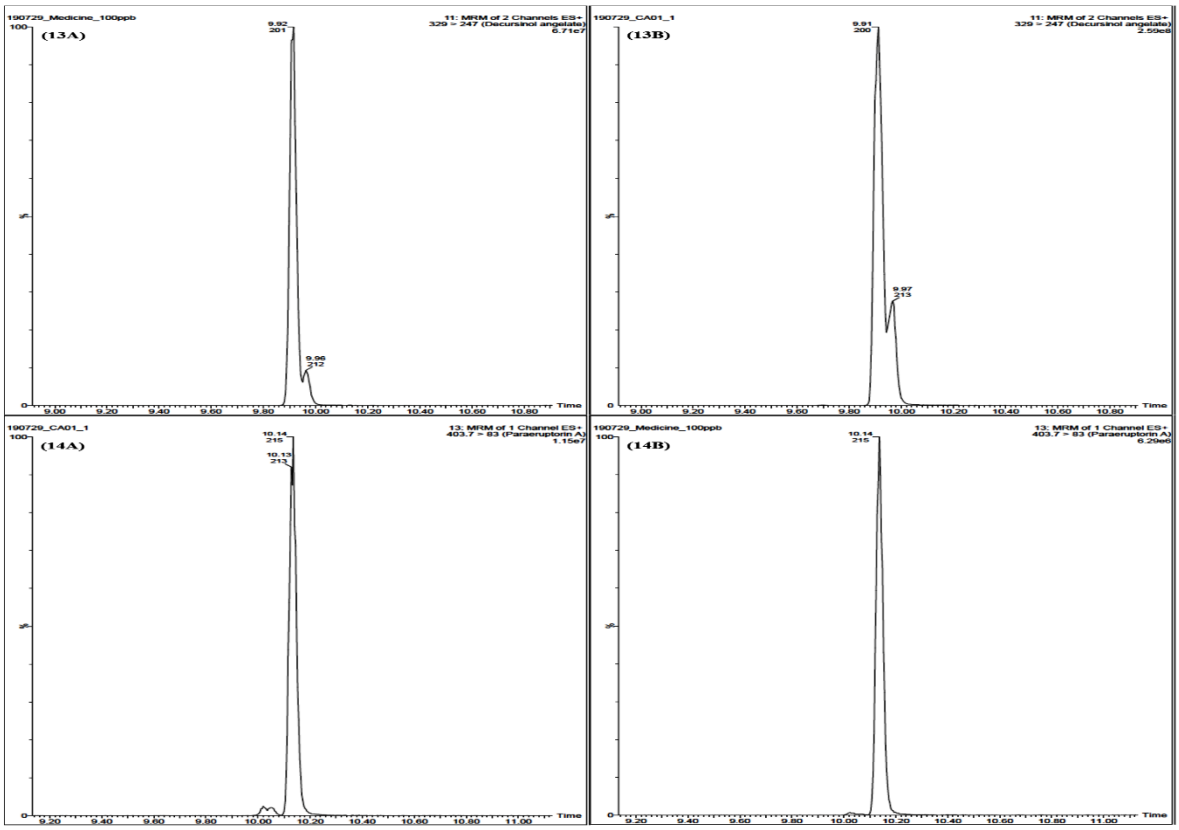


Figure S2. Extracted ion chromatograms of (A) the reference standard and (B) SDGT extract by LC–MS/MS MRM mode. (1) LIQA, (2) LIQ, (3) NOD, (4) NAR, (5) NARG, (6) HES, (7) NPON, (8) PON, (9) API, (10) GLY, (11) HON, (12) DEC, (13) DECA, and (14) PRAA.

Table S1. Composition of SDGT.

Herbal medicine	Scientific name	Family	Used part	Origin	Amount (g)
Perillae Fructus	*Perilla frutescens* (L.) Britt.	Labiatae	Fruit	China	890.21
Pinelliae Tuber	*Pinellia ternate* (Thunb.) Breit.	Araceae	Tuber	China	667.66
Angelicae Gigantis Radix	*Angelica gigas* Nakai	Umbelliferae	Root	Pyeongchang, Korea	667.66
Arisaematis Rhizoma	*Arisaema erubescens* Schott	Araceae	Rhizome	China	445.10
Citri Unshius Pericarpium	*Citrus unshiu* Markovich	Rutaceae	Peel	Jeju, Korea	445.10
Peucedani Radix	*Peucedamum praeruptorum* Dunn	Umbelliferae	Root	China	311.57
Magnoliae Cortex	*Magnolia officinalis* Rehd. et Wils.	Magnoliaceae	Bark	China	311.57
Ponciri Fructus Immaturus	*Poncirus trifoliata* Rafinesque	Rutaceae	Fruit	Bonghwa, Korea	311.57
Poria Sclerotium	*Poria cocos* Wolf	Polyporaceae	Sclerotium	Bonghwa, Korea	311.57
Glycyrrhizae Radix et Rhizoma	*Glycyrrhiza uralensis* Fischer	Leguminosae	Root and Rhizome	China	222.55
Zingiberis Rhizoma Recens	*Zingiber officinale* Roscoe	Zingiberaceae	Rhizome	Seosan, Korea	178.04
Zizyphi Fructus	*Zizyphus jujuba* Miller var. *hoonensis* T. B. Lee	Rhamnaceae	Fruit	Boeun, Korea	237.40
				Total (g)	5000.00

Table S2. MRM parameters for LC–MS/MS analysis of the 14 marker components in SDGT.

Compound	Mode	MW	Transition (*m*/*z*)	Collision energy (eV)	Cone voltage (V)
LIQA	Negative	550.17	549.4→255.0	30	45
LIQ	Negative	418.13	417.3→225.2	18	30
NOD	Positive	408.14	409.2→247.2	10	30
NAR	Negative	580.18	579.5→271.2	30	45
NARG	Negative	580.18	579.2→271.2	20	60
HES	Positive	610.19	611.4→303.2	20	20
NPON	Positive	594.19	595.1→287.1	20	20
PON	Positive	594.19	595.1→287.1	20	20
API	Positive	270.05	271.2→153.0	30	25
GLY	Negative	822.40	821.6→351.3	40	45
HON	Negative	266.13	265.1→224.2	20	45
DEC	Positive	328.13	329.2→229.1	20	35
DECA	Positive	328.13	329.2→229.1	20	35
PRAA	Positive	386.14	404.1→82.9	20	25

Table S3. System suitability for the 14 marker compounds using HPLC–PDA.

Compound	*k′*	*α*	*N*	*Rs*	*Tf*
LIQA	5.20	1.02	49766.94	2.17	1.21
LIQ	5.33	1.02	58800.19	2.17	1.09
NOD	5.62	1.01	119462.89	1.44	1.12
NAR	5.69	1.01	94495.22	1.44	1.05
NARG	5.92	1.02	70364.19	2.87	1.18
HES	6.07	1.02	60644.66	2.87	0.95
NPON	7.39	1.02	103346.18	2.64	1.08
PON	7.53	1.03	74148.42	2.64	1.06
API	7.73	1.03	66286.44	3.24	1.02
GLY	9.00	1.16	68400.65	18.58	1.06
HON	13.68	1.06	118879.64	6.23	1.05
DEC	14.11	1.01	359456.52	1.50	1.01
DECA	14.20	1.02	339568.43	1.50	1.09
PRAA	14.47	1.02	230652.83	4.09	1.31

Table 4. The linear range, regression equation, r^2, LOD, and LOQ of the analytes from SDGT using LC–MS/MS.

Compound	Retention time (min)	Linear range (ng/mL)	Regression equation [a]	r^2	LOD [b] (ng/mL)	LOQ [c] (ng/mL)
LIQA	4.65	10.00–1000.00	$y = 250.11x + 181.72$	0.9997	0.040	0.119
LIQ	4.70	10.00–1000.00	$y = 512.02x + 23806.79$	0.994	0.021	0.062
NOD	5.03	10.00–1000.00	$y = 13778.60x + 342858.23$	0.9905	0.004	0.012
NAR	5.12	10.00–1000.00	$y = 404.66x - 13673.67$	0.9929	0.501	1.502
NARG	5.27	10.00–1000.00	$y = 75.10x - 1828.87$	0.9977	0.192	0.577
HES	5.45	10.00–1000.00	$y = 1531.71x - 4.71$	0.9995	0.040	0.121
NPON+PON	6.58	20.00–2000.00	$y = 2422.38x + 19161.51$	0.9983	0.022	0.065
API	7.15	10.00–1000.00	$y = 1030.82x + 38351.35$	0.9936	0.024	0.071
GLY	8.09	10.00–1000.00	$y = 8.88x + 103.33$	0.9988	0.710	2.131
HON	9.74	10.00–1000.00	$y = 537.36x - 11400.81$	0.9958	0.020	0.059
DEC	9.91	10.00–500.00	$y = 70357.59x + 1982842.86$	0.9910	0.001	0.003
DECA	9.96	10.00–1000.00	$y = 15241.24x + 343092.33$	0.9968	0.001	0.003
PRAA	10.14	10.00–500.00	$y = 1227.24x + 39587.27$	0.9911	0.017	0.052

[a] Regression equation is expressed $y = ax + b$, where y and x are peak area and concentration of compound, respectively; [b] LOD = 3.3 × signal-to-noise ratio; [c] LOQ = 10 × signal-to-noise ratio.