Supplementary Materials: Metabolism of 20(*S*)-Ginsenoside Rg$_2$ by Rat Liver Microsomes: Bioactivation to Metabolites of Activating SIRT1

Li-Yuan Ma, Qi-Le Zhou, Xin-Bao Yang, Hong-Ping Wang and Xiu-Wei Yang

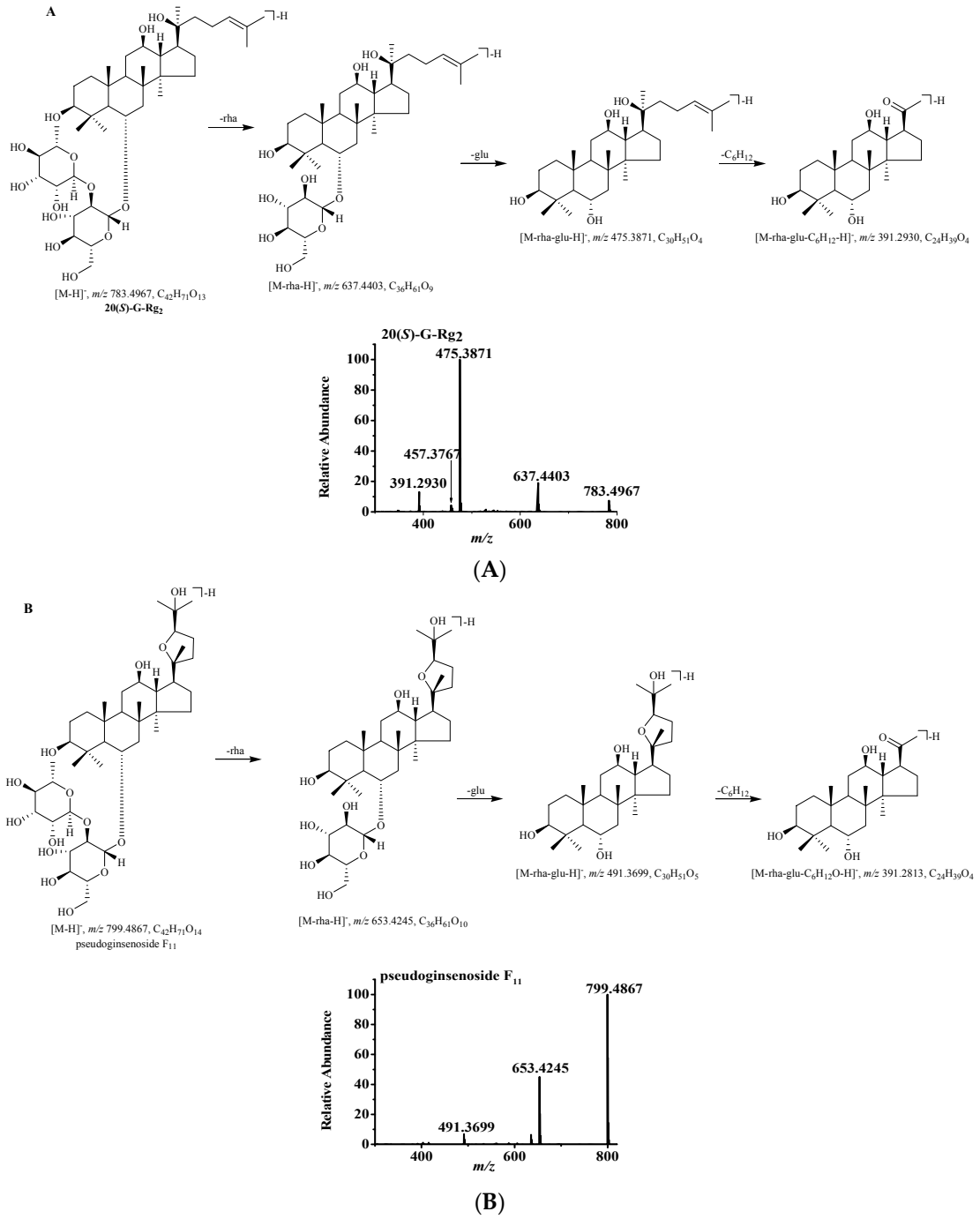

Figure S1. The typical mass spectra and possible fragmentations of 20(*S*)-G-Rg2 (**A**) and pseudoginsenoside F11 (**B**).

Table S1. ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data in pyridine-d_5 (δ_{ppm}) of **1** and **M3** [a].

No.	20(*S*)-Ginsenoside-Rg$_2$ (1)		Pseudoginsenoside F$_{11}$ (M3)	
	^{1}H (*J* in Hz)	^{13}C	^{1}H (*J* in Hz)	^{13}C
1α	0.96 (1H, m)	39.7t	0.96 (1H, m)	39.7t
1β	1.60 (1H, m)		1.62 (1H, m)	
2α	1.85 (1H, m)	28.0t	1.86 (1H, m)	27.8t
2β	1.77 (1H, m)		1.77 (1H, m)	
3β	3.46 (1H, dd, 11.1, 4.3)	78.9d	3.48 (1H, dd, 11.4, 4.8)	78.5d
4	–	40.2s	–	40.2s
5α	1.40 (1H, d, 11.1)	61.1d	1.41 (1H, d, 10.7)	61.0d
6β	4.66 (1H, br dd, 11.1, 3.0)	74.7d	4.72 (1H, br dd, 10.7, 3.1)	74.4d
7α	1.98 (1H, t, 10.6)	46.3t	1.93 (1H, t, 12.6)	46.1t
7β	2.27 (1H, dd, 10.6, 3.0)		2.27 (1H, dd, 12.6, 3.1)	
8	–	39.9s	–	41.2s
9α	1.48 (1H, br d, 12.0)	50.0d	1.48 (1H, dd, 12.6, 2.4)	50.2d
10	–	41.4s	–	39.6s
11α	2.12 (1H, m)	32.3t	2.06 (1H, m)	32.6t
11β	1.81 (1H, m)		1.27 (1H, m)	
12α	3.93 (1H, m)	71.3d	3.71 (1H, td, 9.9, 4.3)	71.3d
13	2.00 (1H, t, 10.3)	48.5d	2.17 (1H, t, 9.9)	48.4d
14	–	51.9s	–	52.3s
15α	1.54 (1H, m)	31.6t	1.42 (1H, m)	32.9t
15β	1.45 (1H, m)		0.89 (1H, m)	
16α	1.84 (1H, m)	27.1t	2.14 (1H, m)	25.6t
16β	1.55 (1H, m)		1.87 (1H, m)	
17α	2.30 (1H, m)	54.9d	1.78 (1H, m)	49.6d
18β	1.38 (3H, s)	17.2q	1.21 (3H, s)	17.0q
19β	0.95 (3H, s)	18.0q	0.95 (3H, s)	18.0q
20	–	73.3s	–	86.8s
21α	1.38 (3H, s)	27.3q	1.25 (3H, s)	27.1q
22a	2.01 (1H, m)	36.1t	1.79 (1H, dd, 12.5, 3.7)	31.8t
22b	1.64 (1H, m)		1.58 (1H, dt, 12.5, 3.9)	
23a	2.57 (1H, m)	23.2t	1.85 (1H, m)	28.9t
23b	2.27 (1H, m)		1.30 (1H, dt, 10.1, 7.9)	
24	5.32 (1H, t, 6.6)	126.6d	3.94 (1H, t, 7.8)	85.8d
25	–	131.0s	–	70.5s
26	1.67 (3H, s)	26.1q	1.26 (3H, s)	27.1q
27	1.62 (3H, s)	17.9q	1.46 (3H, s)	27.3q
28β	2.07 (3H, s)	32.4q	2.11 (3H, s)	32.3q
29α	1.33 (3H, s)	17.9q	1.34 (3H, s)	17.7q
30α	0.90 (3H, s)	17.4q	0.91 (3H, s)	18.3q
		6-Glc		
1′	5.22 (1H, d, 6.8)	102.14d	5.26 (1H, d, 6.9)	102.1d
2′	4.35 (1H, dd, 8.9, 6.8)	79.6d	4.38 (1H, dd, 9.0, 6.9)	79.6d
3′	4.33 (1H, dd, 8.9, 8.4)	78.7d	4.36 (1H, dd, 9.0, 8.4)	78.7d
4′	4.18 (1H, dd, 8.9, 8.4)	72.9d	4.21 (1H, dd, 9.2, 8.4)	72.8d
5′	3.93 (1H, br dd, 8.4, 5.0)	78.6d	3.96 (1H, br dd, 8.4, 5.6)	78.6d
6′a	4.34 (1H, dd, 11.2, 5.3)	63.4t	4.38 (1H, dd, 11.5, 5.6)	63.3t
6′b	4.49 (1H, dd, 11.2, 2.3)		4.54 (1H, dd, 11.5, 2.3)	
		Rha		
1″	6.43 (1H, brs)	102.05d	6.49 (1H, brs)	101.9d
2″	4.76 (1H, br d, 3.6)	72.5d	4.80 (1H, br d, 3.7)	72.4d
3″	4.66 (1H, dd, 9.8, 3.6)	72.6d	4.67 (1H, dd, 9.5, 3.7)	72.6d
4″	4.32 (1H, dd, 9.8, 2.1)	74.4d	4.33 (1H, dd, 9.5, 2.1)	74.3d
5″	4.96 (1H, dd, 9.8, 5.6)	69.7d	4.96 (1H, dd, 9.5, 6.1)	69.6d
6″	1.75 (1H, d, 5.6)	19.0q	1.79 (1H, d, 6.2)	18.9t