Supporting Information

Isolation and Identification of Twelve Metabolites of Isocorynoxeine in Rat Urine and their Neuroprotective Activities in HT22 Cell Assay

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Fig. 1S ESI-QTOF-MS spectra of 5-oxoisocorynoxeinic acid-22-*O*-*β*-D-glucuronide (M-3) and 10-hydroxyisocorynoxeine (M-4), (**A**); corynoxeine (M-6), (**B**); 17-O-demethyl-16,17-dihydro-5-oxoisocorynoxeine (M-7), (**C**); isocorynoxeine-*N*-oxide (M-8), (**D**).

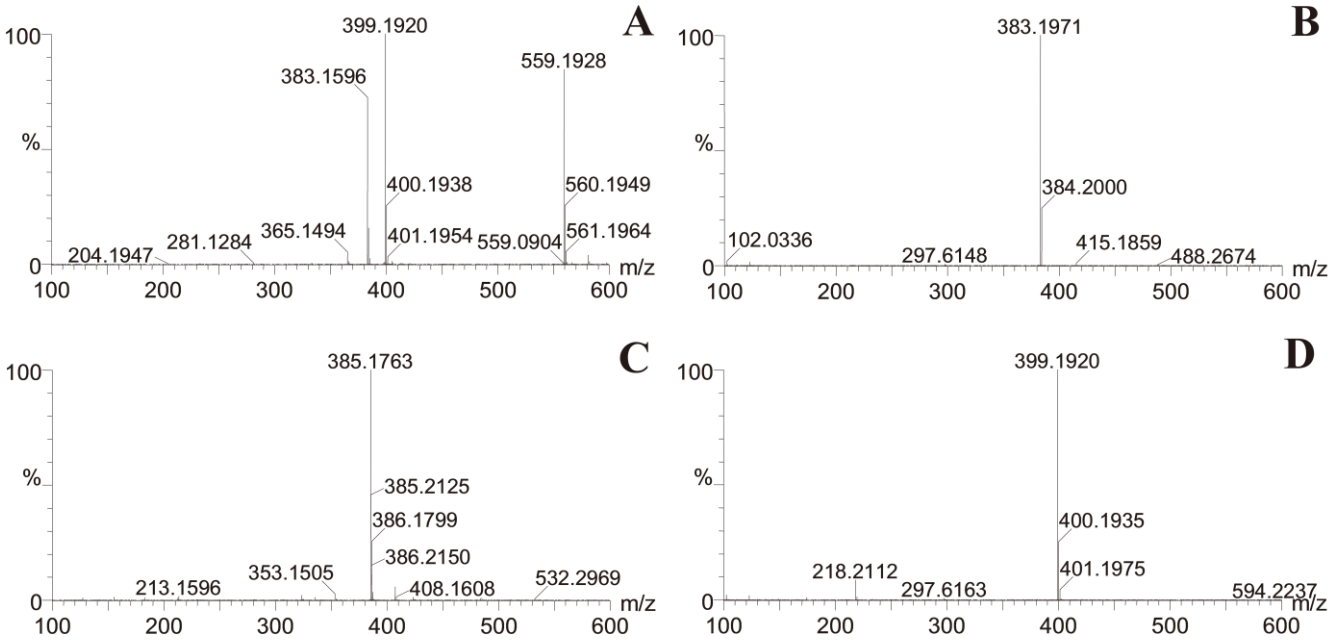

Table 1S ^{1}H NMR data of ICN (M-0) and its metabolites M-1, M-5, M-6, M-8, and M-9.

No.	M-0[a]	M-1[a]	M-5[a]	M-6[a]	M-8[b]	M-9[a]
3	3.31, m	2.89 br, s	2.36 br, s	3.39, t (8.0)	3.92, m	4.45 br, s
5	2.53-3.17, m	2.54 br, s α	2.47 br, t α (7.8)	2.41-2.55, m	3.80, m	4.28 br, s β
		3.63 br, s β	3.41 br, s β		3.07, m	4.50 br, s α
6	1.96-2.09, m	2.28, m α	2.03, dd α (11.8, 7.3)	1.98-2.05, m	2.46, m	2.46 m α
		2.35 br, s β	2.53, dd β (19.9, 7.7)		2.51, m	2.85 br, s β
9	7.46, d (6.6)	7.27, s	7.23, d (7.0)	7.22, d (7.5)	8.13, d (7.2)	7.60 br, s
10	7.06, t (7.1)	6.44 br, s	7.05, dd (7.3, 7.2)	7.04, t (7.5)	7.05, t (7.6)	7.03 t (7.8)
11	7.16, m	7.02 br, s	7.18, dd (7.6, 7.6)	7.18, t (7.5)	7.20, td (8.0, 0.8)	7.20 t (7.8)
12	6.86, d (7.4)	6.86 br, s	6.88, d (7.6)	6.85, d (7.4)	6.92, d (8.0)	7.10 d (7.2)
14	1.49, d α (11.9)	2.20, m α	2.22, m α	1.86, m	0.81, m	1.33 t (7.2) α

	1.07, d β (11.2)	1.18 br, d β (9.9)	1.15 br, d β (9.7)	1.24, t (10.9)	2.95, m	2.67 dd β (6.6, 12.0)
15	3.20, d (7.8)	2.64 br, d (11.9)	2.42, dd (13.3, 10.2)	3.27, d (10.7)	2.78 d (10.4)	2.80 td (11.4, 3.6)
17	7.27, s	7.27 s	7.32, s	7.23, s	7.27, s	7.30 s
18	4.94, m	5.00 d (18.0)	5.03, d (17.0)	3.17-4.97, m	5.01, d (10.4)	5.07 d (17.4)
		4.99 d (10.4)	4.93, d (10.3)		5.04, d (17.2)	5.04 dd (11.4, 1.2)
19	5.52, m	5.51 m	5.50, m	5.51, m	5.48, m	5.47 m
20	2.83, m	3.49 br, s	3.12, m	3.00, m	3.64, m	3.64 m
21	2.53-3.17, m	2.25 m α	1.93 br, t α (10.2)	2.30, d (9.7)	4.10, m	3.64 m α
	3.27, d β (12.5)	3.31 br, s β	3.29 br, d β (7.8)	2.55, m	2.67, m	3.94 d β (7.8)
17-OCH_3	3.69, s	3.72 s	3.74, s	3.73, s	3.73, s	3.76 s
22-OCH_3	3.58, s			3.61, s	3.62, s	3.61 s
NH	8.07, s	8.55 br, s		7.94, s	10.0, s	8.70 s

[a] Measured separately at 600 MHz in $CDCl_3$. [b] Measured separately at 400 MHz in $CDCl_3$.