Supplementary Materials: The Blood-Brain Barrier Permeability of Lignans and Malabaricones from the Seeds of *Myristica fragrans* in the MDCK-pHaMDR Cell Monolayer Model

Ni Wu, Wei Xu, Gui-Yun Cao, Yan-Fang Yang, Xin-Bao Yang and Xiu-Wei Yang *

Table S1. The mobile phase, retention time, detection wavelength of HPLC method and linear equation, correlation coefficient (r^2), linear range, LOQ and LOD for the test compounds.

Compound	Mobile Phase (*v*/*v*)	Retention Time (min)	Detection Wavelength (nm)	Linear Equation (*y* Peak Area; *x* Concentration, μM)	r^2	Linear Range (μM)	LOQ (μM)	LOD (μM)
1	MeOH–H_2O 78:22	12.3	270	$y = 0.0195x - 0.1096$	0.9994	0.25–200.00	0.049	0.015
2	MeOH–H_2O 90:10	4.8	274	$y = 0.0468x - 1.5821$	0.9992	0.25–200.00	0.058	0.018
3	MeOH–H_2O 90:10	7.9	274	$y = 0.0258x - 1.8230$	0.9990	0.125–200.00	0.122	0.037
4	MeOH–H_2O 90:10	7.3	274	$y = 0.0332x - 2.4962$	0.9990	0.125–200.00	0.121	0.036
5	MeOH–H_2O 83:17	7.4	274	$y = 0.2535x - 2.3293$	0.9991	5.00–200.00	4.429	1.329
6	MeOH–H_2O 90:10	4.2	274	$y = 0.1940x - 2.4585$	0.9990	0.25–200.00	0.040	0.012
7	MeOH–H_2O 77:23	5.9	272	$y = 0.0998x + 0.1368$	0.9996	0.50–200.00	0.450	0.135
8	MeOH–H_2O 87:13	3.6	274	$y = 0.0922x - 0.4613$	0.9993	0.25–200.00	0.025	0.008
9	MeOH–H_2O 87:13	3.7	274	$y = 0.0942x - 0.3602$	0.9996	0.25–200.00	0.019	0.006
10	MeOH–H_2O 85:15	5.7	274	$y = 0.4497x - 1.6266$	0.9993	0.50–200.00	0.484	0.145
11	MeOH–H_2O 85:15	6.1	274	$y = 0.0787x - 0.3489$	0.9991	0.25–200.00	0.254	0.076
12	MeOH–H_2O 85:15	8.2	274	$y = 0.0904x + 1.3975$	0.9992	0.25–200.00	0.241	0.072
13	MeOH–H_2O (with 0.4% acetic acid) 89:11	12.6	272	$y = 0.0374x - 0.3967$	0.9991	0.125–200.00	0.125	0.038
14	MeOH–H_2O (with 0.4% acetic acid) 83:17	9.2	272	$y = 0.0324x - 0.0880$	0.9995	0.125–200.00	0.124	0.037
15	MeOH–H_2O (with 0.4% acetic acid) 85:15	5.7	272	$y = 0.0393x + 0.0085$	0.9994	0.125–200.00	0.089	0.027
caffeine	MeOH-H_2O 40:60	5.0	272	$y = 0.0551x + 0.0154$	0.9995	5.00-25.00	4.743	1.423
atenolol	CH_3CN–H_2O (with 0.2% phosphoric acid) 8:92	6.2	204	$y = 0.0723x + 2.8512$	0.9993	4.00-200.00	3.996	1.199
rhodamine 123	MeOH–H_2O 40:60	4.8	210	$y = 0.0017x + 0.0018$	0.9993	0.20-10.00	0.183	0.055

Table S2. The precision, accuracy and recovery for the test compounds (n = 3)

Compound	Concentration (μM)	Precision (RSD, %)		Accuracy (%)		Recovery (%)	
		Intra-day	Inter-day	Intra-day	Inter-day	Mean	RSD
1	10	2.17	3.74	98.51	100.37	95.36	2.43
	50	2.64	2.85	95.26	96.75	93.95	3.37
	100	1.58	3.02	100.49	99.58	98.84	2.81
2	10	3.36	4.73	97.39	99.26	97.59	1.79
	50	2.11	4.11	102.56	105.68	99.86	0.92
	100	2.04	3.98	103.61	101.96	98.50	2.63
3	10	1.96	2.74	99.41	101.63	101.55	2.97
	50	3.41	3.92	97.58	98.21	99.61	3.23
	100	2.88	2.98	98.82	101.38	97.95	1.59
4	10	2.61	3.49	95.63	99.05	100.35	2.07
	50	1.40	4.07	100.74	103.86	104.38	4.21
	100	1.37	3.28	99.58	96.45	96.59	3.63
5	10	3.53	5.01	96.79	99.30	103.25	2.40
	50	2.95	3.37	97.38	96.49	99.57	2.93
	100	3.73	3.62	95.41	97.73	100.28	1.67
6	10	4.49	4.71	103.43	105.29	101.96	2.95
	50	1.02	2.39	99.73	97.48	98.26	3.26
	100	3.14	3.53	98.40	102.35	99.58	2.74
7	10	3.68	3.94	96.77	97.93	96.05	2.84
	50	2.37	2.69	98.59	95.47	96.37	1.79
	100	1.72	3.08	98.71	100.83	99.25	2.41
8	10	2.39	4.21	102.37	100.59	104.81	3.04
	50	2.31	3.49	101.79	103.33	102.47	2.53
	100	1.88	3.00	99.85	102.87	101.26	2.66
9	10	3.49	2.99	97.37	99.21	98.53	2.75
	50	4.03	3.58	98.52	100.03	100.39	1.93
	100	3.84	3.75	97.73	98.39	99.02	4.22

Table S2. *Cont.*

Compound	Concentration (μM)	Precision (RSD, %)		Accuracy (%)		Recovery (%)	
		Intra-day	Inter-day	Intra-day	Inter-day	Mean	RSD
10	10	4.56	3.22	98.59	100.54	99.13	2.09
	50	1.99	2.00	96.49	98.17	101.68	2.85
	100	2.06	2.48	102.97	103.27	99.89	1.56
11	10	5.01	4.79	94.28	94.97	95.85	2.48
	50	3.37	3.44	96.71	99.93	96.95	3.02
	100	2.15	4.20	95.49	97.36	98.01	3.87
12	10	3.23	3.01	96.37	97.29	101.76	3.69
	50	1.62	1.76	98.66	100.07	99.74	2.16
	100	2.08	2.27	96.11	96.04	98.92	0.92
13	10	3.67	4.57	99.20	103.44	100.73	0.99
	50	2.18	3.98	103.64	100.39	103.21	2.53
	100	3.02	3.38	102.73	103.56	105.26	1.68
14	10	4.28	5.24	96.32	98.49	100.03	2.42
	50	3.44	3.81	99.68	95.35	99.46	3.33
	100	3.26	4.49	97.13	99.30	95.96	2.05
15	10	3.29	3.22	98.83	103.15	101.39	2.73
	50	1.03	3.07	104.72	100.35	100.29	1.79
	100	3.16	4.10	99.43	102.42	96.98	2.06
caffeine	5	1.76	2.63	99.37	102.46	101.43	3.36
	10	2.48	4.01	100.64	99.76	98.26	2.94
	20	2.51	3.15	98.58	101.23	97.30	2.35
atenolol	10	3.17	3.02	96.65	97.53	95.68	2.77
	50	2.46	4.79	97.29	99.41	99.87	1.82
	100	2.98	3.75	96.82	97.35	96.24	2.20
rhodamine 123	1	4.23	4.73	97.25	105.00	98.75	2.39
	5	2.59	1.87	100.30	101.80	101.10	2.71
	10	1.08	1.79	98.13	101.15	99.88	1.77