

**Table S2** The prediction of blood-brain barrier (BBB) permeability of compounds in maca.

Name	ADMET_BBB_Level	ADMET_AlogP98	ADMET_PSA_2D
N-benzyl-9-oxo-12Z,15Z-octadecadienamide	0	6.155	47.411
5-Oxo-6E,8E-octadecadienoic acid	1	5.414	55.417
N-benzyl-9,16-dioxo-10E,12E,14E-octadecatrienamide	1	5.130	64.712
N-benzyl-16(S)-hydroxy-9-oxo-10E,12E,14E-octadecatrienamide	1	5.030	68.227
N-benzyl-9Z,12Z,15Z-octadecatrienamide	1	3.905	30.111
N-(3-methoxybenzyl)-9Z,12Z,15Z-octadecatrienamide	1	3.888	39.041
Macapyrrolin A	1	2.645	31.579
Macapyrrolin B	2	2.403	52.394
Macapyrrolin C	2	2.237	43.464
1,2-Dihydro-N-hydroxypyridine derivative (macaridine)	2	1.715	41.468
1R,3S-1-methyltetrahydro-β-carboline-3-carboxylic acid	3	1.915	65.981
N-(3,4-dimethoxybenzyl)-hexadecanamide	4	7.522	47.971
N-benzyl-9-oxo-12Z-octadecenamide	4	6.599	47.411
N-benzyl-5-oxo-6E,8E-octadecadienamide	4	6.576	47.411
N-benzyl-9-oxo-10E,12E-octadecadienamide	4	6.576	47.411
N-benzyl-9-oxo-10E,12Z-octadecadienamide	4	6.576	47.411
N-benzyl-13-oxo-9E,11E-octadecadienamide	4	6.576	47.411
N-(3-methoxybenzyl)-octadecanamide	4	8.450	39.041
N-(3-methoxybenzyl)-9Z-octadecenamide	4	8.006	39.041
N-(3-methoxybenzyl)-hexadecanamide	4	7.538	39.041
N-(3-methoxybenzyl)-9Z,12Z-octadecadienamide	4	7.117	39.041
N-benzyl-tetracosanamide	4	11.204	30.111
N-benzyl-15Z-tetracosenamide	4	10.759	30.111
N-benzyl-octadecanamide	4	8.467	30.111

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N-benzyl-9Z-octadecenamide	4	8.444	30.111
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Table S2 (continued)

Name	ADMET_BBB_Level	ADMET_AlogP98	ADMET_PSA_2D
N-benzyl-heptadecanamide	4	8.011	30.111
N-benzyl-hexadecanamide	4	7.554	30.111
N-benzyl-9Z,12Z-octadecadienamide	4	7.133	30.111
N-benzyl-pentadecanamide	4	7.098	30.111
$\beta$ -Sitosterol	4	8.084	20.815
Stigmasterol	4	7.639	20.815
Campesterol	4	7.627	20.815
Brassicasterol	4	7.431	20.815
Ergosteryl	4	7.183	20.815
Tricin 4'-O-[threo- $\beta$ -guaiacyl-(7''-O-methyl)-glyceryl] ether	4	3.315	154.143
Tricin 4'-O-(erythro- $\beta$ -guaiacyl-glyceryl) ether	4	2.907	166.028
Glucobrassicin	4	-0.613	179.402
4-Methoxyglucobrassicin	4	-0.629	188.333
Glucotropaeolin	4	-0.906	164.347
p-Methoxybenzyl glucosinolate	4	-0.923	173.277
Glucolimnanthin	4	-0.923	173.277
Glucobrassicinapin	4	-0.961	164.347
m-Hydroxybenzyl glucosinolate	4	-1.148	185.163
Glucosinalbin	4	-1.148	185.163
Glucoalyssin	4	-2.210	181.648