

**Table A1.** Binding affinity and binding interactions of 112 compounds of *Piper sarmentosum* Roxb. docked with Nsp1

Compounds	Binding Affinity (kcal/mol)	Amino acid residues that formed interaction with the compounds
5-[(3aR-6R-6aR)-3-(1-3-benzodioxol-5-yl)-1-3-3a-4-6-6a-hexahydrofuro[3-4-c]furan-6-yl]-1-3-benzodioxole	-7.1	22,24,54,60,63
7-Methoxydichamanetin	-6.6	56,58,61,68,96,103
5-[3-(1-3-Benzodioxol-5-yl)-1-3-3a-4-6-6a-hexahydrofuro[3-4-c]furan-6-yl]-1-3-benzodioxole	-6.5	22,24,60
7-Methoxychamanetin	-6.5	22,24,54,55,57,60
Horsfieldin	-6.5	22,23,24,54,59,60,63
Sesamin	-6.5	22,23,24,60
Stigmasterol glucoside	-6.5	20,24,57,63,116
2-[[17-(5-ethyl-6-methylhept-3-en-2-yl)-10-13-dimethyl-2-3-4-7-8-9-11-12-14-15-16-17-dodecahydro-1H-cyclopenta[a]phenanthren-3-yl]oxy]-6-(hydroxymethyl)oxane-3-4-5-triol	-6.4	21, 23,55,57,58
5-7-Dihydroxy-6-[(2-hydroxyphenyl)methyl]-2-phenyl-2-3dihydrochromen-4-one	-6.3	56,70,104,105
5-7-Dihydroxyflavanone	-6.3	22,24,54,55,60,63
Isochamanetin	-6.3	56,56,70,104,105
Pinocembrin	-6.3	22,24,54,55,59,60,63
7-Methoxyisochamanetin	-6.0	22,23,24,54,55
Cepharadione A	-6.0	23,54,55,57,60
1-Phenylethanol-cinnamate	-5.9	22,23,24,55,116
Aristolactam All	-5.9	22,57,55,57,60,116
Piperolactam A	-5.9	22,55,60,116
Noraristolodione	-5.8	22,23,60,116
Alkene-29	-5.7	56,57,58,61,70,103
1-[3-(4-Methoxyphenyl)prop-2-enoyl]pyrrolidin-2-one	-5.6	22,23,24,116
6-hydroxy-4-4-7a-trimethyl-6-7dihydro-5H-1-benzofuran-2-one	-5.6	54,57,60
Piperlongumine	-5.6	22,23,24,55,57,63
Stigmast-5-en-3beta-ol	-5.6	20,23,54,55,116
1-(3-Phenylprop-2-enoyl)pyrrolidin-2-one	-5.5	20,23,24,116
1-[(E)-3-(4-Methoxyphenyl)propenoyl]pyrrolidine -2-one	-5.5	22,24
2'-4'-6'-Trihydroxydihydrochalcone	-5.5	58,63
3-Phenyl-1-(2-4-6-trihydroxyphenyl)prop-2-en-1-one	-5.5	22,55,57,60,116
Cepharadione B	-5.5	23,54,55,57,60
17-(5-ethyl-6-methylhept-3-en-2-yl)10-13-dimethyl-2-3-4-7-8-9-11-12-14-15-16-17-dodecahydro-1Hcyclopenta[a]phenanthren-3-ol	-5.4	56,61,102
3-(4-Methoxyphenyl)-1-(2-4-6trihydroxyphenyl)propan-1-one	-5.4	23,24,60
4-Methoxy-6-styryl-pyran-2-one	-5.4	20,22,23,24,54,55,116
Desmethoxyyangonin	-5.4	22,23,24,54,55,60,63
Sarmentosin	-5.4	21,22,23,24,55,58,63
1-Cinnamoylpyrrolidine-2-one	-5.3	22,26,60,116
Pinocembrin chalcone	-5.3	55,56,61,70,104,105
Sarmentosine	-5.3	22,23,24,55,63
1-(2-Methoxypyrrolidin-1-yl)-3phenylprop-2-en-1-one	-5.2	20,22,23,55,60
4-Hydroxy-3-5-5-trimethyl-4-(3-oxo-1-butenyl)-2-cyclohexen-1-one	-5.1	23,24,55,57,63
Dehydrovomifoliol	-5.1	22,23,24,55,63
1-(3-Phenylpropionyl)-3-pyrroline-2-one	-5.0	23,60,116
1-[(3S)-3alpha-4beta-Diacetoxypyrrolizino]-3-phenyl-2propene-1-one	-5.0	23,63,116
Loliolide	-5.0	22,23,54,55,57,60
Piperlotine A	-5.0	55,56,70,96,103
(E)-2-(hydroxymethyl)-4-[(2R-3R-4S-5S-6R)-3-4-5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxybut-2-enenitrile	-4.9	22,55,58,63
3-(4-Hydroxyphenyl)-1-pyrrol-1ylpropan-1-one	-4.8	21,22,54
4-(4-Hydroxy-2-2-6-trimethyl-7oxabicyclo[4-1-0]hept-1-yl)-3-buten-2-one	-4.8	22,23,24,57,60,63
4-(4-Hydroxy-2-2-6-trimethyl-7-oxabicyclo[4-1-0]hept-1-yl)-but-3-en-2-one	-4.8	22,23,24,57,60,63
Pipercollosidine	-4.8	22,23,54,55,57,60,116,117
Stigmast-5-en-3-ol	-4.8	22,23,57,60,116
1-[(2E-4E-8E)-9-(3-4methylenedioxyphenyl)-2-4-8nonatrienoyl]pyrrolidine	-4.7	58,61,62,66
1-[1-Oxo-3-(3-4-5-trimethoxyphenyl)prop-2-enyl]-2-3dihydropyridin-6-one	-4.7	22,23,57,60,116
1-Cinnamoylpyrrolidine	-4.7	20,23,55,60,116
3-Phenyl-1-(pyrrol-1-yl)propan-1-one	-4.7	55,56,61,70

4-Hydroxycinnamic-acid	-4.7	22,23,24
Stigmasterol	-4.7	95,96,99
(E)-1-Cinnamoylpyrrolidine	-4.6	23,22,23,54,60,116
3-(4-Methoxyphenyl)-1-pyrrolidin-1ylprop-2-en-1-one	-4.6	20,23,24,54,55,63
Piperlotine D	-4.6	22,23,24,57,60
1-Pyrrolizino-3-(2-4-5-trimethoxyphenyl)-2-propene-1-one	-4.5	22,23,63
3-Phenyl-1-(pyrrolidin-1-yl)prop-2-en-1-one	-4.5	61,70,103
Brachyamide B	-4.5	22,57,60
Vanillic acid	-4.5	21,22,23,54,60
Guineensine	-4.4	22,23,24,57,58,60
Methyl-piperate	-4.4	55,56
Moupinamide	-4.4	22,23,24,58,60,63
N-feruloyltyramine	-4.4	43,87,88,99,124,125
(Z)-1-(3-(3-4-5-Trimethoxyphenyl)acryloyl)-1Hpyrrol-2(5H)-one	-4.3	22,60
N-(2-Methylpropyl)octa-2-4dienimidic-acid	-4.3	22,24,54,55,60
1-(3-4-5-Trimethoxycinnamoyl)pyrrolidine	-4.2	56,61,103
1-Allyl-2-6-dimethoxy-3-4methylenedioxybenzene	-4.2	20,22,57
Methylparaben	-4.2	22,23,54
Nerolidol	-4.2	20,22,24,55,57
Pellitorin	-4.2	22,23,24,55,57
Sarisan	-4.2	23,24,57
1-Pyrrolidin-1-yl-3-(3-4-5trimethoxyphenyl)prop-2-en-1-one	-4.1	20,22,24,116
1-Pyrrolidin-1-yldeca-2-4-dien-1-one	-4.1	20,22,23,55,60,116
3-Phenylpropionic-acid	-4.1	22,23,55,60
(2E-4E)-N-isobutyllocta-2-4-dienamide	-4.0	56,61,70,103
(3S-6E)-Nerolidol	-4.0	20,23,54,55,57,60
1-2-4-Trimethoxy-5-propenylbenzene	-4.0	22,23,24,116
Brachystamide B	-4.0	56,61,70,103
gamma-Asarone	-4.0	23,24
(2E-4E-12E)-13-(1-3-benzodioxol-5yl)-N-[(2R)-butan-2-yl]trideca-2-4-12trienamide	-3.9	23,24,60,116
1-[9-(3-4-Methylenedioxyphenyl)-2-8nonadienoyl]pyrrolidine	-3.9	22,23,54,55,57,60
15-(1-3-benzodioxol-5-yl)-N-(2methylpropyl)pentadeca-2-4-14trienamide	-3.9	28,109,111
beta-Sitosterol	-3.9	95,96,99
Methyl-3-(4-hydroxyphenyl)propionate	-3.9	22,23,54,60
N-(2-methylbutyl)deca-2-4-dienamide	-3.9	55,56,61,70
Sarmentine	-3.9	23,24,55,60,63
(2E-4E)-N-(2-Methylbutyl)-2-4decadienamide	-3.8	35, 93,95,97
13-(1-3-benzodioxol-5-yl)-N-(2methylpropyl)trideca-2-4-12trienamide	-3.8	35,36,39,97
alpha Asarone	-3.8	23,54,60,63
Dodecadienoic-acid-isobutylamide	-3.8	20,22,23,54,55,60,116
Methyl-3-(4-methoxyphenyl)propanoate	-3.8	54,55,57,116
Pipercollosine	-3.8	58,61,62,66
(2E-4E)-N-[(2R)-2-methylbutyl]deca-2-4-dienamide	-3.7	56,61,70
(2E-4E)-N-[(2R)-butan-2-yl]deca-2-4dienamide	-3.7	22,23,55,60,116
(2E-4E)-N-Isobutyl-2-4hexadecadienamide	-3.7	22,23,24,55,57,60
2-4-Tetradecadienoic-acid-isobutylamide	-3.6	22,23,24,60,62,63
7-(1-3-benzodioxol-5-yl)-N-(2methylpropyl)hept-2-enamide	-3.6	14,122
Methyl-3-phenylpropionate	-3.6	22,55,60,116
Dodeca-2-4-dienamide	-3.5	21,22,23
N-(Butan-2-yl)deca-2-4-dienamide	-3.5	55,56
Pellitorine	-3.5	23,55,57,58,60
N-Isobutyl-(2E-4E)tetradecadienamide	-3.3	20,22,23,54,55,60,116
5-(Tetradec-1-EN-1-YL)-2H-1-3benzodioxole	-3.2	56,58,61,70,96,103
dodeca-2E-4E-dienoic acid isobutylamide	-3.2	20,22,23,54,55,60,116
5-[(E)-1-Tetradecenyl]-1-3benzodioxole	-3.0	58,61
Pipericine	-2.9	56,58,61,62,70,103
2-4-Dodecadienamide	-2.7	55,104,119
N-(2-Methylpropyl)octadeca-2-4dienamide	-2.6	43,87,125
Triaccontanoic acid	-2.1	14,79,122