Supplementary Data

**Table S1**

Biological source and docking energy value for constituents from *Goniothalamus sp*.

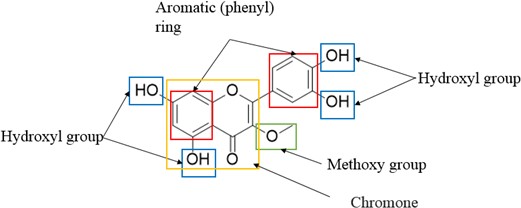
|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **NO** | **NAME & STRUCTURE** | **BIOLOGICAL SOURCE** | **DOCKING ENERGY**  **(-Kcal/mol)** | | | | **REFRENCES** |
| Envelope protein (1OKE) | NS3/NS2B (2FOM) | NS5  methyltransferase (1R6A) | NS5 RdRp (3VWS) |
| 1 | 6S,7S,8S,6S,7S,8S-(+)-gonioanceolatin\_A | *G. lanceolatus*  bark- DCM crude extract | 7.8 | 16.6 | 12.7 | 19.4 | **27** |
| 2 | 6S,7S,8R,6S,7S,8S-(+)-goniolanceolatin\_B | 13.5 | 14.9 | 8.4 | 13.1 |
| 3 | 6S,7S,8S,6S,7S,8S-(-)-goniolanceolatin\_C | 12.6 | 8.9 | 0.5 | 13.1 |
| 4 | 6S,7S,8S,6S,7S,8R-(+)-goniolanceolatin\_D | 12.9 | -2.1 | 5.8 | 20.7 |
| 5 | 6S,7S,8S,1S,5S,7S,8R-(+)-  goniolanceolatin\_F | 8.7 | 9.0 | 6.5 | 15.3 |
| 6 | 6S,7S,8S,1S,5S,7S,8R-(+)-  goniolanceolatin\_H | 8.2 | -15.5 | 9.7 | 18.4 |
| 7 | 6S-(-)-Goniothalamin | 4.8 | 7.3 | -7.8 | 4.7 | **28 & 41** |
| 8 | 6S,7S,8S-(-)-Goniodiol | *G. lanceolatus*  Barks/ leaves & roots- DCM crude extract | 14.4 | 12.2 | 2.2 | 5.6 | **27** |
| 9 | 6S,7S,8R-(-)-8-Chlorogoniodiol | 14.2 | 11.8 | 9.6 | 6.7 | **28** |
| 10 | 6S,7S,8S-(-)-Goniodiol-7-Monoacetate | 18.9 | 19.1 | 14.3 | 14.4 |
| 11 | 6S,7S,8S-(-)-Goniodiol-8-monoacetate | 25.9 | 24.5 | 17.3 | 14.7 |
| 12 | 6S,7R,8R-(-)-ent-Goniothalamin\_Oxide | 10.6 | 11.6 | 3.2 | 5.7 |
| 13 | 1S,5S,7R,8R-(-)-9-Deoxygoniopypyrone (Parvistone D) | 10.7 | 5.9 | 1.7 | 3.3 |
| 14 | 1S,5S,7R,8S-(-)-8-epi-9-  Deoxygoniopypyrone | 20.0 | 22.2 | 12.1 | 16.6 |
| 15 | 1S,5S,7S,8S-(-)-Goniopypyrone\_B | 5.4 | 6.1 | -0.9 | 0.1 |
| 16 | 2-acetyl-3-amino-1\_4-naphthoquinone | 18.2 | 21.7 | 11.3 | 12.0 |
| 17 | 2-acetyl-3-amino-5-hydroxy-1\_4-  naphthoquinone | 21.4 | 23.6 | 14.3 | 17.0 |
| 18 | 5R,6R-5-acetylgoniothalamin | 10.9 | 16.6 | 3.7 | 7.5 |
| 19 | (-)-goniolanceolactam | *G. lanceolatus*  Barks & roots- DCM crude extract | -23.2 | -24.9 | -41.4 | -25.0 |
| 20 | 5R,6R-5-hydroxygoniothalamin | *G. lanceolatus*  Barks/ leaves & roots- DCM crude extract | 8.3 | 8.3 | 0.4 | 7.6 |
| 21 | 5R,6R-5-hydroxy-6-styrltetrahydropyrane-2- one | 13.6 | 11.8 | 8.8 | 7.6 |
| 22 | Cleistopholine | 14.6 | 18.7 | 13.1 | 14.6 |
| 23 | Goniolanceolatin\_E | 23.0 | 21.9 | 17.3 | 23.8 |
| 24 | Lirodenine | *G. lanceolatus*  Barks & roots- DCM crude extract | -18.2 | -21.0 | -27.3 | -18.4 |
| 25 | Etharvendiol | *G. arvensis*-stem bark | 17.4 | 14.3 | 8.2 | 11.3 | **29** |
| 26 | (R)-Goniothalamin | *G. andersonii*-Whole plant  *G. fulvus, G. giganteus*- Stem bark | 4.2 | 6.5 | -2.7 | 4.3 | **12 & 30** |
| 27 | 5-acetoxygoniothalamin | *G. uvaroides* | 13.0 | 16.5 | 10.0 | 14.8 | **31** |
| 28 | Dehydrogoniothalamin | *G. dolichocarpus*- Stem bark | 14.4 | 17.2 | 4.5 | 13.8 | **32** |
| 29 | 5-Acetoxyisogoniothalamin oxide | *G. ridleyi* - stem bark, stem, roots,  and fruit | 20.1 | 24.3 | 6.4 | 19.0 | **33** |
| 30 | Cheliensisin A | *G. cheliensis Hu,* | 18.2 | 21.1 | 7.8 | 18.0 | **34** |
| 31 | Howiinin A | *G. laoticus -* Flower | 20.2 | 19.6 | 10.7 | 16.4 | **35** |
| 32 | 7-epi-goniodiol | 16.9 | 13.4 | 9.9 | 10.6 |
| 33 | 7-Acetylgoniodiol | *G. amuyon*-Leaf, *G. sesquipedalis,*  *G. grifithii* | 22.6 | 20.5 | 14.9 | 17.8 | **36** |
| 34 | 8-Acetylgoniodiol | *G. amuyon*-Leaf  *G. giganteus*- Stem bark | 25.9 | 24.5 | 14.3 | 16.3 | **36** |
| 35 | Goniodiol diacetate | *G. grifithii*  *G. sesquipedalis* | 27.8 | 33.1 | 18.5 | 26.0 | **36** |
| 36 | 8-Methoxygoniodiol | 17.3 | 16.2 | 5.2 | 12.0 |
| 37 | Leiocarpin C | 24.1 | 21.8 | 15.12 | 18.0 |
| 38 | Goniotriol | *G. amuyon*  *G. arvensis*-stem bark | 18.2 | 12.6 | 6.8 | 9.2 | **37** |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | *G. giganteus*- Stem bark  *G. sesquipedalis* |  |  |  |  |  |
| 39 | 8-Acetylgoniotriol | *G. giganteus* | 23.0 | 17.9 | 12.9 | 22.3 | **38** |
| 40 | Garvensintriol | *G. arvensis*-stem bark | 23.6 | 20.3 | 12.7 | 14.9 | **29** |
| 41 | (+)-goniothalamin epoxide | 10.7 | 11.7 | 4.9 | 5.6 |
| 42 | Goniomicin A | *G. howii* | 13.7 | 16.4 | 4.6 | 13.4 | **30** |
| 43 | Goniomicin B | 12.9 | 17.2 | 4.5 | 8.6 |
| 44 | Goniomicin C | 14.3 | 16.4 | 5.5 | 9.1 |
| 45 | Goniomicin D | 11.9 | 13.5 | 5.5 | -0.1 |
| 46 | Howiinol | 25.6 | 23.3 | 18.0 | 24.0 |
| 47 | Altholactone | *G. arvensis*-stem bark  *G. giganteus* | 4.1 | 1.2 | -3.0 | -3.9 | **39 & 41** |
| 48 | Goniofupyrone | *G. giganteus*- Stem bark | 11.7 | 5.1 | 4.5 | 19.2 | **38** |
| 49 | Goniotharversin | *G. arvensis*-stem bark | 4.1 | 1.2 | -12.5 | -3.9 | **39** |
| 50 | Etharvensin | -8.5 | -8.6 | -17.6 | -9.7 | **40** |
| 51 | (+)-goniothalenol | 3.8 | 1.2 | -1.6 | -2.3 |
| 52 | (+)-3-Acetylaltholactone | *G. laoticus* -Flower | -2.3 | -2.0 | -3.9 | -5.5 | **35** |
| 53 | Cardiopetalolactone | *G. giganteus* | -71.2 | -80.4 | -72.3 | -69.1 | **12** |
| 54 | Goniofufurone | *G. arvensis*  *G. borneensis*- Bark  *G. giganteus*- Stem bark | 9.4 | 7.3 | -10.8 | 2.3 | **13, 29 & 38** |
| 55 | Arvensin | *G. arvensis*-stem bark | 2.4 | 0.9 | -11.5 | -2.5 | **40** |
| 56 | 8-Acetylgoniofufurone | 12.9 | 11.0 | -5.1 | 9.7 |
| 57 | Diacetylgoniofufurone | *G. griffithii* | 21.2 | 22.1 | 9.8 | 20.3 | **42** |
| 58 | Goniopypyrone | *G. giganteus*- Stem bark | 11.0 | 7.2 | -5.1 | 5.0 | **43** |
| 59 | Leiocarpin-A | *G. leiocarpus* | 12.4 | 11.8 | 15.1 | 8.3 | **44** |
| 60 | 9-Deoxyisogoniopypyrone | 8.8 | 4.9 | -5.7 | 3.9 |
| 61 | 8-Acetylgoniopypyrone | *G. giganteus*- Stem bark | 15.5 | 13.0 | 15.2 | 17.8 | **45** |
| 62 | Goniobutenolide A | *G. borneensis*- Bark  *G. giganteus*- Stem bark | 2.5 | -1.2 | -17.5 | -2.7 | **46** |
| 63 | Goniobutenolide B | 1.3 | -1.8 | -4.6 | -6.6 |
| 64 | Gonioheptolides A | *G. giganteus*- Stem bark | 11.7 | 4.3 | 1.2 | 6.3 | **47** |
| 65 | Gonioheptolides B | 13.6 | 8.0 | -3.7 | 7.8 |
| 66 | Almuheptolides A | *G. arvensis*-stem bark | 14.6 | 5.8 | 9.1 | 12.1 | **40** |
| 67 | Almuheptolides B | 17.1 | 7.1 | 4.4 | 10.1 |
| 68 | Cardiobutanolide | 19.7 | 16.3 | 7.3 | 13.5 |
| 69 | Donhepocin | 29.4 | 16.3 | - | 27.5 |
| 70 | Donhexocin | 24.2 | 14.2 | - | 17.8 |
| 71 | Donbutocin | 24.5 | 20.6 | - | 24.7 |
| 72 | Gigantransenins A | 8.1 | - | - | 5.9 |
| 73 | Gigantransenins C | -2.5 | -6.6 | - | 5.9 |
| 74 | Howiicin A | 10.3 | 8.6 | - | 21.5 |
| 75 | Howiicin C | 14.3 | 0.9 | - | 20.0 |
| 76 | Goniothalamicin | 11.3 | -1.0 | - | 15.0 |
| 77 | Donnaienin A | 16.6 | - | -1.2 | 14.1 | **48** |
| 78 | Donnaienin B | 23.5 | 16.2 | 6.2 | 20.2 |
| 79 | Isoannonacin | - | 3.4 | -39.5 | 39.1 |
| 80 | Gardnerinin | 18.6 | 7.8 | -6.3 | 23.8 | **30** |
| 81 | Howiicin F | 20.37 | - | - | 11.84 |
| 82 | Howiicin G | 10.1 | 4.8 | -27.9 | 13.2 |
| 83 | Howiicin D | *G. amuyon* (Stem, leaves,  Seeds) | -6.3 | -12.7 | -12.9 | -8.7 |
| 84 | Goniodonin | *G. donnaiensis* | 12.7 | 13.3 | -3.6 | 15.4 |
| 85 | Goniotrionin | *G. giganteus* | 17.0 | - | - | 12.7 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |  |
| 86 | Howiicin B | 6.9 | -979.9 | - | 22.0 |
| 87 | Howiicin E | 21.2 | -612.0 | 2.4 | 12.8 |
| 88 | Longifolicin | 21.8 | - | - | 21.1 |
| 89 | 4-Deoxyannomontacin | 14.6 | - | -21.3 | 19.9 |
| 90 | Giganenin | 5.4 | - | -61.6 | 8.2 |
| 91 | 4-Acetylgigantrocin A | 6.6 | - | - | 27.3 |
| 92 | cis-gigantrionenin | 4.6 | -9.5 | -57.8 | 6.0 |
| 93 | Goniotetracin | 6.0 | - | -54.0 | 19.8 | **12** |
| 94 | Annomontacin | 40.0 | - | - | 51.5 |
| 95 | Gigantetrocinone | 42.9 | - | - | 54.8 |
| 96 | Gonioneninone | 46.1 | - | 41.0 | 59.0 |
| 97 | Xylomaticinone | 48.4 | - | - | 52.0 |
| 98 | (2\_4-cis\_and\_trans)-Gonioneninone | 25.3 | -3.4 | 4.8 | 30.8 |
| 99 | Pyranicin | 24.5 | - | - | 32.0 |
| 100 | Annomontacinone | 43.0 | 47.1 | 12.9 | 49.6 |
| 101 | Pyragonicin | - | - | - | 28.4 |
| 102 | Gardnerilin A | *G. gardneri* | 15.5 | 23.2 | - | 27.1 |
| 103 | Gardnerilin B | 26.1 | 31.5 | - | 32.8 |
| 104 | Goniodenin | -2.4 | -13.9 | -24.3 | -8.8 |
| 105 | Asimilobin | 7.6 | -0.9 | -14.1 | 5.1 |
| 106 | Longimicin | 16.5 | -0.3 | -18.0 | 3.0 |
| 107 | Squamocin | 5.0 | -17.2 | -24.1 | 8.7 |
| 108 | Goniotriocin | 10.9 | - | -11.0 | 10.4 |
| 109 | Gigantecin | -3.1 | - | -32.1 | 4.3 |
| 110 | 4-deoxygigantecin | - | - | - | 7.2 |
| 111 | Goniocin | -8.7 | -23.0 | - | -6.5 |
| 112 | Friedelin | -35.1 | -137.1 | -46.0 | -34.2 |
| 113 | Friedelinol | -44.1 | -52.6 | -48.6 | -40.0 |
| 114 | Betullinic acid | -73.2 | -76.0 | -73.1 | -58.6 |
| 115 | Crytomeridiol | 5.0 | -6.2 | -13.3 | 0.7 |
| 116 | Griffithazanone A | 13.0 | 16.8 | -1.5 | 11.8 |
| 117 | Griffithazanone B | 13.6 | 15.2 | 8.0 | 11.3 |
| 118 | Velutinam | *G. velutinus* (Airy Shaw) | -43.1 | -42.3 | -50.6 | -41.8 | **49** |
| 119 | Cepharanone B | -40.0 | -40.4 | -46.2 | -372 |
| 120 | Griffithdione | -7.2 | -10.3 | -10.1 | -4.4 |
| 121 | Nordicentrine | *G. laoticus -*Flower | -9.2 | -7.2 | -16.5 | -10.0 | **35** |
| 122 | Scorazanone | 13.0 | 15.1 | 23.0 | 24.6 |
| 123 | Marcanine A | 8.57 | 12.80 | 4.76 | 6.33 |
| 124 | Marcanine B | 2.62 | 6.31 | -0.46 | 1.97 |
| 125 | Marcanine C | 4.02 | 6.00 | -0.04 | 2.69 |
| 126 | Marcanine D | 5.49 | 10.94 | 2.16 | 4.39 |
| 127 | Marcanine E | 2.71 | 7.55 | 5.02 | 1.92 |
| 128 | Dielsiquinone | 4.99 | 9.58 | 1.77 | 2.74 |
| 129 | Taliscanine | -45.3 | -50.0 | -51.7 | -43.0 |
| 130 | Aristolactam A-II | -38.6 | -38.4 | -44.2 | -37.3 |
| 131 | Griffithinam | -39.0 | -41.1 | -41.9 | -38.8 |
| 132 | Goniothalactam | -36.9 | -38.1 | -45.9 | -37.2 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 133 | 2'-hydroxy-4,4',6'-  trimethoxydihydrochalcone |  | 26.4 | 24.7 | 9.2 | 21.1 |  |
| 134 | 2',4'-dihydroxy-4,6'-  dimethoxydihydrochalcone | 27.4 | 31.1 | 19.1 | 22.3 |
| 135 | 4,2',4'-trihydroxy-6'-  methoxydihydrochalcone | - | 33.9 | 14.0 | 21.8 |
| 136 | Flavokawain A | 18.8 | 25.5 | 15.3 | 15.5 |
| 137 | 2',4'-dihydroxy-4,6- Dimethoxydihydrochalcone | 21.3 | 26.6 | 12.9 | 17.8 |
| 138 | Aristolactam I | -35.2 | -37.7 | -41.5 | -36.6 | **49** |
| 139 | Aristolactam BII | -18.2 | -13.6 | -27.2 | -19.8 |
| 140 | Ouregidione | -8.9 | 0.2 | -13.2 | -7.8 | **38** |
| 141 | dihydrochrysine | 25.2 | 26.5 | 14.3 | 23.7 | **35** |
| 142 | Tapisoidin | -8.9 | -13.2 | -26.5 | -9.1 | **12** |
| 143 | Naringenin trimethyl ether | 19.8 | 17.3 | 8.0 | 15.2 |
| 144 | Kumatakenin | 21.3 | 20.3 | 4.8 | 15.6 |
| 145 | Mearnsitrin | 32.6 | 9.3 | 26.1 | 28.6 |
| 146 | Annulatin | 43.1 | 35.1 | 28.6 | 44.5 |
| 147 | Retusin | *G. cheliensis* | 15.5 | 14.4 | 10.9 | 11.6 |
| 148 | 3,5,7,3',4'-pentamethoxyflavone | *G. tenuifolius* | 11.9 | 10.5 | 4.6 | 8.6 | **21** |
| 149 | 5,7,3',4'-tetrahydroxy-3-methoxyflavone | *G. tenuifolius* | 45.9 | 36.9 | 53.6 | 56.8 |
| 150 | Pachypodol | *G. cheliensis* | 22.4 | 19.4 | 10.8 | 15.9 | **12** |
| 151 | 4'-hydroxy-3,5,7,3'-tetramethoxyflavone | 13.1 | 14.4 | 4.2 | 12.1 | **21** |
| 152 | 3'-hydroxy-3,5,7,4'-tetramethoxyflavone | 14.6 | 20.0 | 7.0 | 11.7 |
| 153 | Goniolactone B | 22.5 | 21.8 | -13.9 | 24.1 | **50** |
| 154 | Giganin | 33.4 | 31.2 | - | 35.5 |
| 155 | Donnaienin | 32.4 | 42.1 | - | 47.8 |
| 156 | Goniothalamusin | 23.0 | 20.1 | -20.7 | 19.2 |
| 157 | Cinammic acid | 22.8 | 21.7 | 23.8 | 27.5 |
| 158 | Pterodondiol | 1.7 | -7.9 | -8.6 | -3.3 |
| 159 | 2-Acetyl-3-amino-5,6-dihydroxy-1,4-  naphthoquinone; 6-Me ether (Goniothalaminone B) | *G. scortechinii*- roots | 21.81 | 23.32 | 25.77 | 18.73 |
| 160 | Almuheptolide A; 3-Deethoxy | *G. arvensis* | 14.5 | 13.4 | 11.7 | 11.0 |
| 161 | Altholactone; 6,7-Dihydro | 1.9 | 1.2 | 2.8 | 0.9 |
| 162 | Altholactone; 7a-Epimer, 6,7-dihydro, 7β-  hydroxy | 1.0 | 1.24 | 2.76 | 2.55 |
| 163 | 3-Amino-2,5-dihydroxy-1,4-naphthoquinone;  (Goniothalaminone A) | *G. scortechinii*- roots | 15.8 | 19.2 | 17.4 | 13.5 |
| 164 | 3-Amino-4,5-dihydroxy-7-phenyl-6- heptenoic acid (Goniotamiric acid) | *G. tamirensis*- leaves | 18.6 | 25.3 | 21.3 | 14.2 |
| 165 | 1,2-Bis(4-hydroxyphenyl)-3,4-bis(2,4,6- trihydroxybenzoyl)cyclobutane; (1α,2β,3α,4β)-form, 2''',2'''',4',4''-Tetra-Me  ether | *G. gardneri* | -379.9 | - | 20.0 | 34.5 |
| 166 | Cheliensisamine | *G. cheliensis*- bark | -104.4 | -103.8 | -102.7 | -110.8 |
| 167 | Cheliensisaminone | 11.6 | 12.5 | 8.4 | 7.5 |
| 168 | Cheliensisine | *G. cheliensis* | 23.3 | 24.6 | 24.0 | 26.1 |
| 169 | Cycloart-23-ene-16,25-diol; (Griffithine A) | *G. griffithii* | -37.2 | -46.0 | -39.3 | -35.7 |
| 170 | 5-Deoxy-7-epigoniopypyrone | *G. dolichocarpus* | 12.4 | 11.7 | 15.3 | 9.5 |
| 171 | 5-Deoxygoniopypyrone; (4R,6R,7R,8S)-  form, Ac | *G. scortechinii*- leaves | 17.7 | 16.7 | 16.8 | 15.9 |
| 172 | 5-Deoxygoniopypyrone; (4R,6R,7S,8S)-  form | *G. giganteusand* and *G. tamirensis* | 17.7 | 22.4 | 22.2 | 17.5 |
| 173 | Parvistone E | *G. tamirensis* and *Polyalthia*  *parviflora* | 13.1 | 11.6 | 11.2 | 8.6 |
| 174 | (-)-Medioresinol | *Dirca occidentalis G. dumontetii*  and *Dendrobium loddigesii* | -14.0 | -19.2 | -15.6 | -16.1 |
| 175 | Longimicin C | *Annona longifoliaand G. giganteus* | 0.0 | - | 2.2 | 3.7 |
| 176 | Digoniodiol | *G. amuyon*- aerial parts | 15.5 | -6.6 | 15.0 | 15.7 |
| 177 | Digoniodiol; Mono-Ac | *G. cheliensis*- roots | 12.5 | 3.4 | 24.6 | 28.5 |
| 178 | 1,3-Dihydro-3-hydroxy-4,9-dimethoxy-3- methyl-2H-benz[f]indol-2-one; (S)-form | *G. cheliensis*- roots | -11.5 | -12.6 | -8.5 | -12.3 |
| 179 | Tapsoidine | *G. tapisoides*- stem bark | -6.0 | -8.4 | -4.9 | -5.8 |
| 180 | 1,3-Dihydroxydibenz[cd,f]indol-4(5H)-one; Di-Me ether | *G. griffithii*- bark | -21.6 | -16.4 | -15.5 | -18.3 |
| 181 | Gonioquinone | *G. cheliensis*- roots | 22.6 | 28.3 | 25.8 | 18.6 |
| 182 | Goniodiol 7-acetate | *Goniothalamus spp.* | 22.4 | 23.5 | 17.0 | 21.3 |
| 183 | Goniodiol 8-acetate | *G. amuyon* | 26.0 | 24.5 | 19.0 | 19.5 |
| 184 | Howiinol A | *G. howii* | 24.2 | 24.2 | 18.6 | 24.0 |
| 185 | 8-*O*-Methylgoniodiol | *G. amuyon*- leaves and stems | 20.1 | 16.1 | 15.7 | 14.5 |
| 186 | Donnaienin D | *G. donnaiensis*- roots | 20.7 | 26.2 | 34.6 | 28.3 |
| 187 | Epidonnaienin D | *G. donnaiensis* | 41.4 | 22.5 | 42.6 | 30.8 |
| 188 | Gigantetrocin A | *G. giganteus, Annona muricata* and  other *Annonaceae* | 12.9 | -1.8 | 16.3 | 16.8 |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 189 | Gigantetrocin B | *Annona muricata, Asimina*  *longifoliaand G.howii* | 14.6 | 17.7 | 15.5 | 14.9 |  |
| 190 | 4-Acetylgigantetrocin A | *G. giganteus* | 26.5 | - | 17.0 | 26.3 |
| 191 | Muricatetrocin A | *Annona muricata, Asimina longifolia* and *G. howii* | 16.6 | -12.2 | 11.0 | 17.5 |
| 192 | Cheliensisin C | *G. cheliensis* | 11.6 | - | 0.1 | 11.2 |
| 193 | Cheliensisin B | 25.7 | -22.9 | 11.6 | 18.1 |
| 194 | Gigantecinone | *G. giganteus* | 28.9 | 15.8 | 18.7 | 33.1 |
| 195 | 7-Ac 7-Acetylgoniofufurone | *G. griffithii*- rhizomes | -1.3 | -9.1 | -9.4 | -9.5 |
| 196 | Goniofufurone acetonide | *G. cheliensis*- roots | -12.2 | -20.0 | -15.6 | -16.0 |
| 197 | Hexahydro-3,7-dihydroxy-2-phenyl-5*H*-  furo[3,2-*b*]pyran-5-one | *G. giganteus*- stem bark | 4.0 | 3.9 | 2.7 | -0.9 |
| 198 | Goniofupyrone A | *G. amuyon* | 7.9 | 6.8 | 5.3 | 2.5 |
| 199 | Acetylgoniofupyrone A | *G. cheliensis*- roots | 12.9 | 13.7 | 8.8 | 8.8 |
| 200 | Gonioheptenolactone | *G. cheliensis*- leaves | 5.7 | -1.9 | 1.1 | -1.2 |
| 201 | Goniothalesacetate | *G. amuyon*- stems | 24.9 | 23.4 | 21.6 | 19.1 |
| 202 | Goniolactone I | *G. cheliensis*- roots and bark | -3.1 | -1.0 | 1.4 | 0.8 |
| 203 | Goniolactone D | *G. cheliensis*- roots | 22.8 | 17.2 | 23.2 | 23.1 |
| 204 | Goniolactone C | 19.6 | 25.0 | 26.6 | 26.3 |
| 205 | Goniolactone E | -10.3 | -7.0 | -2.5 | -6.9 |
| 206 | Goniolactone F | -4.1 | -5.5 | 2.2 | 3.4 |
| 207 | Goniolactone G | *G. cheliensis*- roots and bark | 10.1 | -19.3 | 14.2 | 15. |
| 208 | Goniolactone H | -17.2 | -13.1 | -13.5 | -9.5 |
| 209 | Goniolandrene A | *G. macrophyllus* | -52.9 | -55.7 | -59.1 | -56.4 |
| 210 | Goniolandrene B | *G. macrophyllus*- roots | -30.8 | -34.6 | -35.5 | -34.3 |
| 211 | 5-Acetylgoniopypyrone | *G. griffithii*- rhizomes | 15.6 | 10.5 | 16.6 | 16.5 |
| 212 | 7-Ac 7-Acetylgoniopypyrone | 14.0 | 20.7 | 22.0 | 14.9 |
| 213 | 5,7-Dideoxy-3-hydroxygoniopypyrone | *G. wightii*- leaves | 8.9 | 9.2 | 11.3 | 5.8 |
| 214 | Goniothalesdiol | *G. borneensis* | 13.2 | 13.9 | 12.8 | 7.3 |
| 215 | Goniothalesdiol A | *G. amuyon*- stems | 21.9 | 25.6 | 25.0 | 18.0 |
| 216 | Goniothaline A | *G. australis* | -1.5 | 1.1 | 2.4 | -0.3 |
| 217 | Goniothaline B | 7.1 | 6.1 | 9.3 | 8.4 |
| 219 | Griffinine | *G. griffithii*- stems | -6.2 | -9.8 | -3.3 | -5.4 |
| 220 | Laoticuzanone A | *G. laoticus*- stems | 15.8 | 16.4 | 17.2 | 12.5 |
| 221 | 5-Hydroxyheptadecanoic acid; (β)-form,  Lactone | *Goniothalamus wightii*- leaves | 35.5 | 36.1 | 34.7 | 26.6 |
| 222 | Dihydroflavokawain A | *G. gardneri* | 26.2 | 25.7 | 22.3 | 19.2 |
| 223 | Goniotamirine | *G. tamirensis*- leaves | -0.7 | -3.3 | 2.4 | 1.0 |
| 224 | Leiocarpin B | *G. leiocarpus*- stem bark | 21.0 | 18.1 | 25.8 | 24.5 |
| 225 | Leiocarpin E | 7.5 | 4.4 | 8.4 | 12.3 |
| 226 | Griffiazanone B | *Annona glabra, G. griffithii, G. marcanii, Polyalthia plagioneura*  and *Saprosma hainanense* | 10.7 | 15.2 | 13.1 | 11.0 |
| 227 | 3-Methyl-1H-benz[f]indole-4,9-dione | *G. scortechinii* and *G. tapis* | 18.4 | 21.2 | 17.3 | 12.0 |
| 228 | Nonadecyl alcohol | *G. wightii* | 43.9 | 40.5 | 39.4 | 33.5 |
| 229 | 8-Chloro-8-deoxygoniodiol | *G. amuyon*- leaves and stems | 17.2 | 10.4 | 10.4 | 10.5 |
| 230 | 6-(2-Phenylethenyl)-2H-pyran-2-one; (E)- form | *Aniba parviflora* and *G.umbrosus* | 10.4 | 17.2 | 6.1 | 5.2 |
| 231 | Piperolide | *G. tamirensis*- leaves | 3.4 | 5.8 | 1.8 | 0.0 |
| 232 | Squamoxinone A; 22-Epimer, 11-deoxy,  10R-hydroxy | *G. giganteus* | 35.9 | - | 32.7 | 43.6 |
| 233 | Goniopetaline (incorr.) | *Dasymaschalon trichphorum, G. sesquipedalis* and *Pararistolochia*  *flos-avis* | -20.4 | -21.6 | -15.4 | -20.1 |
| 234 | Uvarilactam, Gonioffithine | *G. griffithii*- roots and *Uvaria*  *macrocarpa*- stems | -15.6 | -11.4 | -12.4 | -14.3 |



**Fig. S1**. Functional groups of ligand **149**