Supplementary 1 lists of *M. calabura* compounds used for docking

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| Code | CID | Name |
| 1 | 5272653 | (2S)-5'-hydroxy-7,3',4'- trimethoxyflavan |
| 2 | 23730738  | (2S)-7,8,3',4',5'-pentamethoxyflavan |
| 3 | 44567046   | (2S)-2'-hydroxy-7,8,3',4',5'-pentamethoxyflavan |
| 4 | 44567047  | (2S)-5'-hydroxy-7,8,3',4'-tetramethoxyflavan |
| 5 | 44567048   | (2S)-8-hydroxy-7,3',4',5'-tetramethoxyflavan |
| 6 | 44567055   | (2S)-8,2'-dihydroxy-7,3',4',5'-tetramethoxyflavan  |
| 7 | 44567056  | (2S)-8,5'-dihydroxy-7,3',4'-trimethoxyflavan  |
| 8 | 24750458   | 7,8,3',4',5'-pentamethoxyflavone |
| 10 | 9950661   | 5'-hydroxy-7,8,3',4'-tetramethoxyflavone |
| 12 | 44257590   | 8,5'-dihydroxy-7,3',4'-trimethoxyflavone |
| 13 | 639682   | (2R,3R)-7-methoxy-3,5,8-trihydroxyflavanone |
| 14 | 688857   | (2S)-7-hydroxyflavanone |
| 15 | 31013944  | (2S)-5,7-dihydroxyflavanone |
| 16 | 73202   | (2R,3R)-3,5,7-trihydroxyflavanone |
| 17 | 73201   | (2S)-5-hydroxy-7-methoxyflavanone |
| 18 | 5281894   | 7-hydroxyflavone |
| 19 | 5281607  | 5,7-dihydroxyflavone |
| 23 | 5378823  | 3,5-dihydroxy-7,4'-dimethoxyflavone  |
| 24 | 5491798 | 3,5-dihydroxy-7,8-dimethoxyflavone  |
| 25 | 21632881   | 5-hydroxy-3,7,8-trimethoxyflavone |
| 27 | - | 5-hydroxy-3,7,8,4'-tetramethoxyflavone |
| 28 | 6433293   | 2',4'-dihydroxychalcone |
| 29 | 77520393   | 4,2',4'-trihydroxychalcone |
| 30 | 5376891   | 7-hydroxyisoflavone  |
| 31 | 628528  | 7,3',4'-trimethoxyisoflavone  |
| 32 | 20977489  | 2',4'-dihydroxydihydrochalcone  |
| 33 | 370   | 3,4,5-trihydroxybenzoic acid  |
| 34 | 92158  | lupenone  |
| 35 | 73659   | 2α,3β-dihydroxy-olean-12-en-28-oic acid  |
| 36 | 129847689   | 8-hydroxy-7,3',4',5'-tetramethoxyflavone  |
| 37 | 102169932 | 8,4'-dihydroxy-7,3',5'-trimethoxyflavone |
| 39 | 88881   | 5,7-dimethoxyflavone |
| 40 | 13291608  | 3,5-dihydroxy-6,7-dimethoxyflavone |
| 41 | 60123241   | β-sitostenone |
| 43 | 521199   | β-sitosterol |
| 44 | 10742   | syringic acid |
| 45 | 8468   | vanillic acid |
| 50 | 129847697   | 2',4'-dihydroxy-3'-methoxydihydrochalcone  |
| 52 | 5272653 | (2S)-(-)-5'-hydroxy-7,3',4'-trimethoxyflavanone  |
| 54 | 5281954   | 5-hydroxy-7-methoxyflavone  |
| 55 | 5748697   | 3,7-dimethoxy-5-hydroxyflavone |
| 57 | 5318691 | 3,5-dihydroxy-7-methoxyflavone  |
| 58 | - | 8-methoxy-3,5,7-trihydroxyflavone  |
| 59 | 9972910   | 5,7-dihydroxy-3,8-dimethoxyflavone |
| 60 | 5281616   | galangin |
| 61 | 5281607  | chrysin  |
| 62 | 42607832   | 7-hydroxy-8-methoxyflavanone |
| 63 | 10265122   | 4'-hydroxy-7-methoxyflavanone  |
| 64 | 71935   | 2',4'-dihydroxy-3'-methoxychalcone |
| 65 | 145706584  | [2,3-dihydroxy-4,3',4',5'-tetramethoxydihydrochalcone |
| 66 | 21722167  | 4,2',4'-trihydroxy-3'-methoxydihydrochalcone |
| 67 | 145706492   | (2R,3R)-(-)-3,5-dihydroxy-6,7-dimethoxyflavanone |
| 68 | 5280794 | stigmasterol |
| 69 | 466268  | 7-methoxyflavone |
| 70 | 5281946  | 5,7-dihydroxy-3-methoxyflavone |
| 71 | 5320315   | 5,7-dihydroxy-6-methoxyflavone |
| 72 | 5318869   | 5,4'-dihydroxy-3,7-dimethoxyflavone |
| 73 | 23730738 | (2S)-7,8,3',4',5'-pentamethoxyflavan |
| 74 | 44567047   | (2S)-5'-hydroxy-7,8,3',4'-tetramethoxyflavan |
| 75 | - | methyl 4-hydrobenzoate |
| 76 | 12575 | isovanillic acid |
| 77 | 980  | p-nitrophenol  |
| 78 | 7428  | methyl gallate |
| 79 | 5319562   | trans-methyl p-coumarate |
| 80 | 12306160   | β-amyrenone |
| 81 | - | α-tocopherylquione |
| 85 | 145706471   | 5-hydroxy-3,8-dimethoxyflavone |
| 86 | 5378234   | 3,5,7-trihydroxy-8-methoxyflavone |
| 87 | 129848348   | 8-hydroxy-6-methoxyflavone |

Supplementary 2 lists of *A. lavenia* compounds used for docking

|  |  |  |
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| Code | CID | Name |
| 101 | 226486 | 4-Allyl-2,6-Dimethoxyphenol |
| 102 | 1549095 | coniferyl alcohol |
| 103 | 5280450 | linoleic acid |
| 104 | 575987 | 5h-1-Pyrindine |
| 105 | 6736 | 3-methylindole |
| 106 | 102527619 | 1-cyano-3-methylisoquinoline |
| 107 | 579053 | 6,7-Dihydro-3-Nitro-5h-Cyclopenta[B]Pyridin-2(1h)-One |
| 108 | 551125 | 5,10-Diethoxy-2,3,7,8-Tetrahydro-1h,6h-Dipyrrolo[1,2-A;1',2'-D] Pyrazine |
| 109 | 637542 | p-Coumaric acid |
| 110 | 5362796 | Z-Cycloundecene |
| 111 | 5362790 | E\_Cycloundecene |
| 112 | 572128 | 3,5-Heptadien-2-ol, 2,6-dimethyl- |
| 113 | 5365626 | (Z)6-Pentadecen-1-ol |
| 114 | 15304 | 3,6-Dimethylphenanthrene |
| 115 | 603766 | 1-Iodo-4-Phenylbicyclo(2 |
| 116 | 6660 | Corylon |
| 117 | 533622 | 2,5-Methano-2h-Furo[3,2-B] -8-One, Hexahydro- |
| 118 | 23415 | 2-Methyldecane |
| 119 | 9602952 | Carbazic Acid, 3-Pentylidene-, Ethyl Ester  |
| 120 | 445639 | Oleic Acid |
| 121 | 8183 | Adacene 12 |
| 122 | 5283361 | Trans-2-Dodecenal |
| 123 | 30874 | 1,12-Tridecadiene |
| 124 | 606063 | 1a,9b-Dihydro-1h-Cyclopropa[A]Anthracene |
| 125 | 9817754 | 9,12-Octadecadienoyl Chloride, |
| 126 | 8142 | 1-Chlorooctane |
| 127 | 9248 | Epoxycyclododecane |
| 128 | 5368351 | Cis-3-Undecene-1,5-Diyne  |
| 129 | 5282714 | 2-Octenoic Acid (Cas) |
| 130 | 5364492 | cis-9-Octadecenal |
| 131 | 5362688 | trans-Dodec-5-enal |
| 132 | 535532 | 6-Oxa-Bicyclo[3,1,0]Hexan-3-One |
| 133 | 83742 | 2-Imidazolidinone, 1,3-Diethenyl- |
| 134 | 713 | Methanamide |
| 135 | 6436740 | N-Phenyl-N'-Furaldehyde Hydrazone |
| 136 | 87568 | Pentadecanonitrile |
| 137 | 996 | Phenol (Cas) |
| 138 | 335 | O-Cresol |
| 139 | 460 | 460\_Guaiacol |
| 140 | 2879 | 2879\_P-Cresol |
| 141 | 6997 | O-Ethylphenol |
| 142 | 10364 | Carvacrol |
| 143 | 7041 | 2,6-Dimethoxyphenol |
| 144 | 12462 | 1,2,3-Trimethoxybenzene |
| 145 | 2724705 | 1,6-Anhydro-Beta-D-Glucopyranose; Levoglucosan |
| 146 | 17198 | Acetosyringone |
| 147 | 5374088 | 2,4-Hexadienedioic Acid, 3,4-Diethyl-, Dimethyl Este |
| 148 | 561602 | 5-beta,8-beta-Epoxy-3,5,8,8a-tetrahydro-1H-2-benzopyran |
| 149 | 43551 | Biphenyl, 3,4-Diethyl |
| 150 | 3033 | diclofenac |
| 151 | 444899  | arachidonic acid |
| 152 | - | ent-11α-hydroxy-15-oxo-kaur-16-en-19-oic acid |