

Supplementary Data

This supplementary data is a part of paper entitled “Potential *Adenostemma lavenia* and *Muntingia calabura* Extracts to Inhibit Cyclooxygenase-2 Activity as a Therapeutic Strategy for Anti-inflammation: Experimental and Theoretical Studies”.

Suppl. 1. Lists of *M. calabura* compounds used for docking

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	2 α ,3 β -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

Suppl. 1. Lists of *M. calabura* compounds used for docking (Continued)

Code	CID	Name
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	stigmaterol
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

Suppl. 2. Lists of *A. lavenia* compounds used for docking

Code	CID	Name
101	226486	4-Allyl-2,6-Dimethoxyphenol
102	1549095	coniferyl alcohol
103	5280450	linoleic acid
104	575987	5h-1-Pyridine
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	Carbamic 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

Suppl. 2. Lists of *A. lavenia* compounds used for docking (*Continued*)

Code	CID	Name
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-11 α -hydroxy-15-oxo-kaur-16-en-19-oic acid