

**Supplementary Table 1 Results of molecular docking**

<b>Protein name/ID in PDB</b>	<b>Ligand</b>	<b>Vina score</b>	<b>Cavity volume (Å<sup>3</sup>)</b>	<b>Center (x, y, z)</b>
<b>MMP9/ 1ITV</b>	Quercetin	-7.92	350	1, 48, 23
	Glepidotin A	-4.72	155	10, 36, 21
	7-Acetoxy-2-methylisoflavone	-7.89	350	1, 48, 23
	Gancaonin G	-6.05	44	15, 49, 19
	Licoagrocarpin	-7.22	463	-5, 46, 1
	Dehydroglyasperins C	-6.12	187	-11, 48, 20
<b>Mmp2/ 1QIB</b>	Quercetin	-3.33	89	3, 7, 65
	Glepidotin A	-3.88	123	1, 38, 61
	7-Acetoxy-2-methylisoflavone	-4.66	145	11, 12, 72
	Gancaonin G	-3.56	138	9, 45, 68
	Licoagrocarpin	-3.98	91	5, 18, 61
	Dehydroglyasperins C	-3.27	89	3, 7, 65
<b>IL-6/ 2L3Y</b>	Quercetin	-4.36	612	-7, 138, 0
	Glepidotin A	-5.52	1551	-1, 134, 12
	7-Acetoxy-2-methylisoflavone	-5.59	1551	-1, 134, 12
	Gancaonin G	-3.88	669	-1, 151, -5
	Licoagrocarpin	-5.72	582	7, 134, -18
	Dehydroglyasperins C	-3.76	1662	-3, 113, -7
<b>PTGS2/ 5F19</b>	Quercetin	-3.38	4431	14, 49, 65
	Glepidotin A	-3.67	26146	22, 39, 36
	7-Acetoxy-2-methylisoflavone	-5.52	1167	31, 42, 38
	Gancaonin G	-4.33	1233	28, 28, 59
	Licoagrocarpin	-4.54	1234	32, 37, 18
	Dehydroglyasperins C	-3.62	26146	22, 39, 36
<b>HMOX1/ 1OZE</b>	Quercetin	-4.15	3920	7, -12, -1
	Glepidotin A	-4.18	3716	7, -9, 38
	7-Acetoxy-2-methylisoflavone	-5.54	620	18, -10, 19
	Gancaonin G	-4.73	103	32, -5, 39
	Licoagrocarpin	-5.56	107	32, -16, -2
	Dehydroglyasperins C	-4.69	103	32, -5, 39
<b>CCL2/ 4USP</b>	Quercetin	-5.12	60	19, 51, 36
	Glepidotin A	-5.24	201	0, 47, 46
	7-Acetoxy-2-methylisoflavone	-6.06	75	32, 45, 35

	Gancaonin G	-5.34	186	29, 47, 19
	Licoagrocarpin	-6.65	52	37, 55, 25
	Dehydroglyasperins C	-4.97	60	19, 51, 36