

## Supplementary Materials

# Chemical Profiling and Biological Activity of *Psydrax dicoccos* Gaertn

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**Table S1.** Qualitative phytochemical screening of *P. dicoccos* leaf powder extracts.

Test	Aqueous	Methanol	Ethanol	Acetone	Chloroform	Hexane
Triterpenoid	+	+	+	+	-	+
Sugar	+	+	-	+	-	-
Flavonoid	-	+	+	-	+	-
Catachin	-	-	-	-	-	-
Saponin	+	-	+	-	-	-
Tannin	+	+	+	+	-	+
Anthraquinone	-	-	-	-	-	-
Amino acid	+	+	+	+	+	+
Sterol	+	+	-	-	+	+
Carbohydrate	+	+	+	+	+	-

**Table S2.** Quantitative analysis of methanolic *P. dicoccos* leaf extract.

Test	Amount of compounds present (mg/g)
Chlorophyll a	8.07 ± 0.2
Chlorophyll b	10.45 ± 0.1
Total chlorophyll	14.48 ± 0.4
Total carotenoids	2.18 ± 2.4
Total sugar	257 ± 0.2
Total protein	1.2 ± 1.1
Total lipids	182 ± 2.0
Total free amino acids	0.9 ± 0.1
Total phenolics	81.11 ± 1.1
Total tannin	51.09 ± 2.2
Total flavonoids	159 ± 2.8

**Table S3.** Anti-bacterial activity profiling of methanolic *P. dicoccos* leaf extract.

Antibiotic (µg/disc)	Zones represented as radius (mm)						
	Leaf extract conc. (mg/mL)	<i>E. coli</i>	<i>P. aeruginosa</i>	<i>S. aureus</i>	<i>S. flexneri</i>	<i>K. pneumoniae</i>	<i>S. typhimurium</i>
-	6	1.2±0.609	0.3±0.795	-	0.4±0.410	0.4±0.193	-
-	7	0.7±0.552	0.3±0.728	-	0.3±0.447	0.6±0.217	-
-	8	1.2±0.453	0.7±0.704	0.0±0.332	1.2±0.456	0.3±0.234	-
-	9	1.1±0.537	0.4±0.757	0.9±0.270	0.7±0.297	0.3±0.259	-
-	10	1.9±0.611	2.3±0.757	0.4±0.038	0.6±0.225	0.6±0.287	-
Amikacin (10 µg)	-	12±2.1	13±1.3	10±1.2	11±0.8	12±1.8	13±1.5
Chlorampheni col (10 µg)	-	11±2.1	6±1.3	3±1.0	4±1.8	5±1.8	8±0.8
Bacitracin (10 µg)	-	NE	NE	NE	NE	NE	NE
Penicillin G (30 µg)	-	NE	NE	NE	NE	NE	NE
Methicillin (5 µg)	-	NE	NE	NE	NE	NE	NE

NE – not effective. *Escherichia coli* (*E. coli*); *Pseudomonas aeruginosa* (*P. aeruginosa*); *Staphylococcus aureus* (*S. aureus*); *Shigella flexneri* (*S. flexneri*); *Klebsiella pneumoniae* (*K. pneumoniae*); *Salmonella typhimurium* (*S. typhimurium*).

**Table S4.** GC-MS study of methanolic *P. dicoccos* leaf extract.

Peak	Retention time	Name	Area	Retention Index	Molecular formula	Molecular weight	Docking results
1	11.603	Benzenecarboxylic acid	38374943	0	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	122	-
2	12.049	2,3-Dihydro-Benzofuran	712375	1036	C <sub>8</sub> H <sub>8</sub> O	120	+
3	14.13	2-Methoxy-4-Vinylphenol	804363	0	C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>	150	-
4	19.952	4-Methyloxy-6-methylcoumarin	939973	0	C <sub>11</sub> H <sub>10</sub> O <sub>3</sub>	190	-
5	20.078	Cyclopenta[C]Pyran-4-Carboxylic Acid, 7-Methyl-, Methyl Ester	13844412	1402	C <sub>11</sub> H <sub>10</sub> O <sub>3</sub>	190	-
6	20.71	Megastigmatrienone	1655818	1454	C <sub>13</sub> H <sub>18</sub> O	190	+
7	21.09-21.464	1,3,4,5-Tetrahydrocyclohexanecarboxylic Acid	8979051	0	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub>	192	-
10	21.954	3,4-Dihydrocoumarin, 7,8-dimethyl-	4580894	1618	C <sub>11</sub> H <sub>12</sub> O <sub>2</sub>	176	-
11	22.075	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol	2247222	0	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	194	-
12	22.41	1H,3H-Pyrano[3,4-c]pyran-1-one, 5-ethenyl-6-(.beta.-D-glucopyranosyloxy)-5,6-dihydro-, (5R-trans)-	9452624	3042	C <sub>16</sub> H <sub>20</sub> O <sub>9</sub>	356	-
13	22.603	Mome Inositol	9435268	1647	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub>	194	-
14	22.81	(E)-4-(3-Hydroxyprop-1-en-1-yl)-2-methoxyphenol	4232584	1653	C <sub>10</sub> H <sub>12</sub> O <sub>3</sub>	180	-
15	23.202	Tetradecanoic Acid	772831	1769	C <sub>14</sub> H <sub>28</sub> O <sub>2</sub>	228	-
16	24.533	Neophytadiene	1078998	0	C <sub>20</sub> H <sub>38</sub>	278	-
17	24.95-25.265	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	290870	2045	C <sub>20</sub> H <sub>40</sub> O	296	-
19	26.029	Methyl palmitate	1002064	1878	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	270	-
20	26.298	17-Pentatriacontene	467597	3508	C <sub>35</sub> H <sub>70</sub>	490	-
21	26.67	n-Hexadecanoic acid	7886533	1968	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	256	-
22	28.698	Linoleic acid	489690	2093	C <sub>19</sub> H <sub>34</sub> O <sub>2</sub>	294	-
23	28.79	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-	1458002	2101	C <sub>19</sub> H <sub>32</sub> O <sub>2</sub>	292	-
24	28.964	Phytol	753451	2045	C <sub>20</sub> H <sub>40</sub> O	269	-
25	29.321	9,12-Octadecadienoic acid (Z,Z)-	2128485	2183	C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>	280	-
26	29.431	Dichloroacetic acid	9177045	2042	C <sub>15</sub> H <sub>24</sub> Cl <sub>2</sub> O <sub>2</sub>	306	-
27	29.773	Octadecanoic acid	2242046	2167	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>	284	-
28	31.012	2-Oxa-3-azabicyclo[2.2.2]oct-5-ene, 3-benzoyl-	1262046	1755	C <sub>13</sub> H <sub>13</sub> NO <sub>2</sub>	215	-
29	31.861	2-Octyl benzoate	955456	1692	C <sub>15</sub> H <sub>22</sub> O <sub>2</sub>	234	+
30	34.602	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	1836502	2498	C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>	330	-

31	34.881	Oxirane, hexadecyl-	399182	1901	C <sub>18</sub> H <sub>36</sub> O	268	-
32	36.923	Linolenic acid	1773973	2721	C <sub>21</sub> H <sub>36</sub> O <sub>4</sub>	352	-
33	37.203	Stearic acid	888524	2681	C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>	358	-
34	38.32	Squalene	4467855	2914	C <sub>30</sub> H <sub>50</sub>	410	-
35	39.984	delta-Tocopherol	992557	2923	C <sub>27</sub> H <sub>46</sub> O <sub>2</sub>	402	-

**Table S5.** LC-MS study of methanolic *P. dicoccos* leaf extract.

M/Z ratio	Compounds	Retention Time	Retention Index	Docking studies
160.9	Caffeoyl-O-hexoside	16.93	58	–
162.9	5-O-p-coumaroylshikimic acid (5-p-CoSA)	21.13	45	–
169	Quercetin	35.84	62	–
191.1	(E)Catechin–(E)Gallocatechin a	27.56	41	–
195.8	Rhamnosylhexosyl luteolin	24.21	54	–
197.8	Kaempferol	26.65	32	+
199	4-O-p-coumaroylshikimic acid (3-p-CoSA)	22.92	86	–
274.3	5-O-p-coumaroylshikimic acid (5-p-CoSA)	21.13	42	–
377.2	Quercetin rutinoside	28.9	59	+
593.3	Rhamnosylhexosyl methyl quercetin	24.67	76	–
696.4	(E)Catechin–(E)Catechin– (E)Catechin–(E)Catechina	30.54	59	–
717.3	4-O-p-coumaroylshikimic acid (3-p-CoSA)	22.92	70	–
740.4	(E)Catechin–(E)Catechin– (E)Catechin–(E)Catechina	30.54	83	–

761.4	(E)-3-(3,4-diacetoxy-5-methoxyphenyl)acryl-4-O-p-coumaroyl-5-O-caffeoylquinic acid	37.5	74	-
849.4	(E)Catechin-(E)Catechin-(E)Catechin a	21.42	48	-

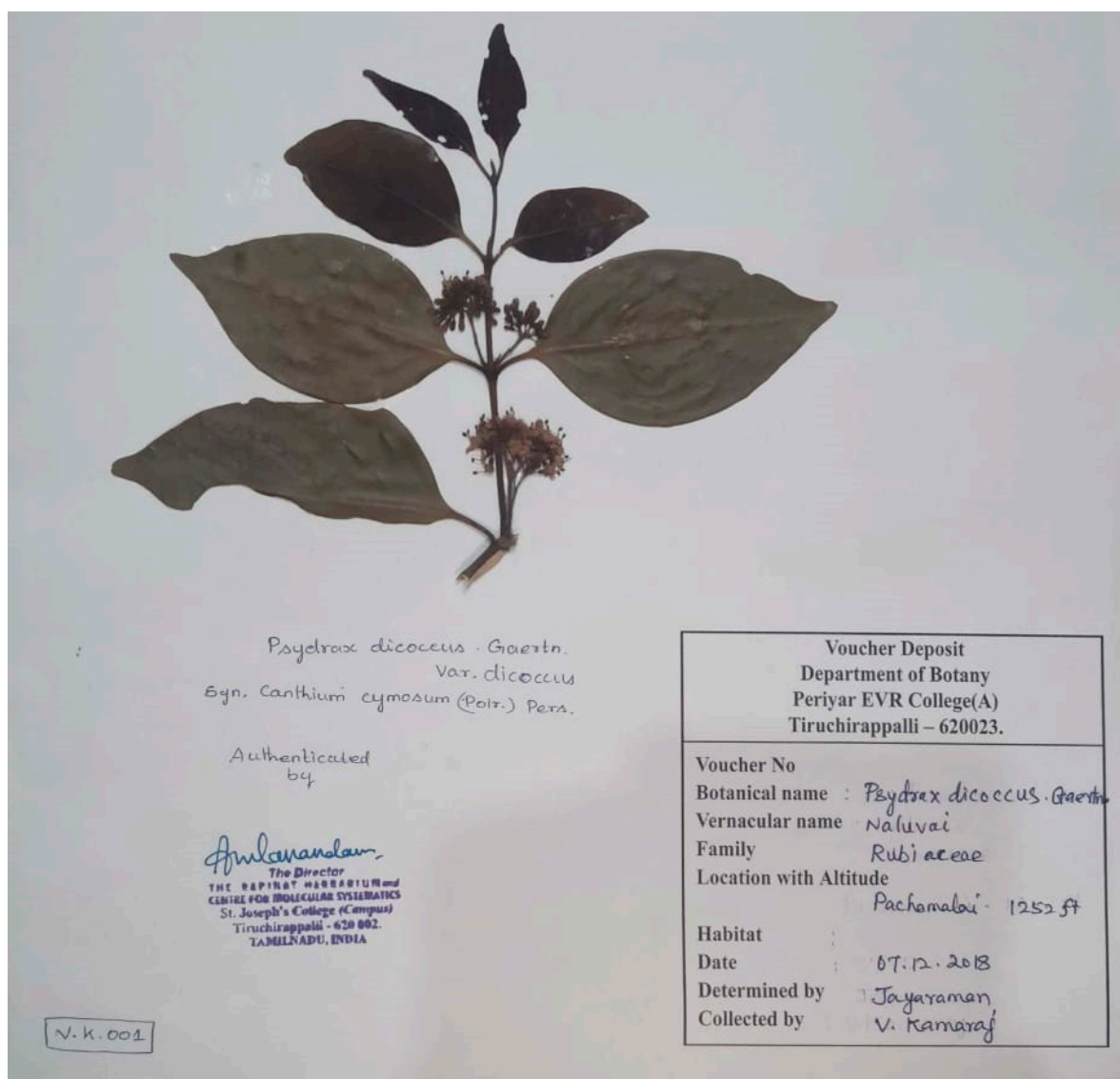


Figure S1. *P. dicoccus* botanical sample (Specimen #VK001).