

Supplementary file

Phenolic Constituents from *Wendlandia tinctoria* var. *grandis* (Roxb.) DC. Stem Deciphering Pharmacological Potentials Against Oxidation, Hyperglycemia and Diarrhea: Phyto-Pharmacological and Computational Approaches

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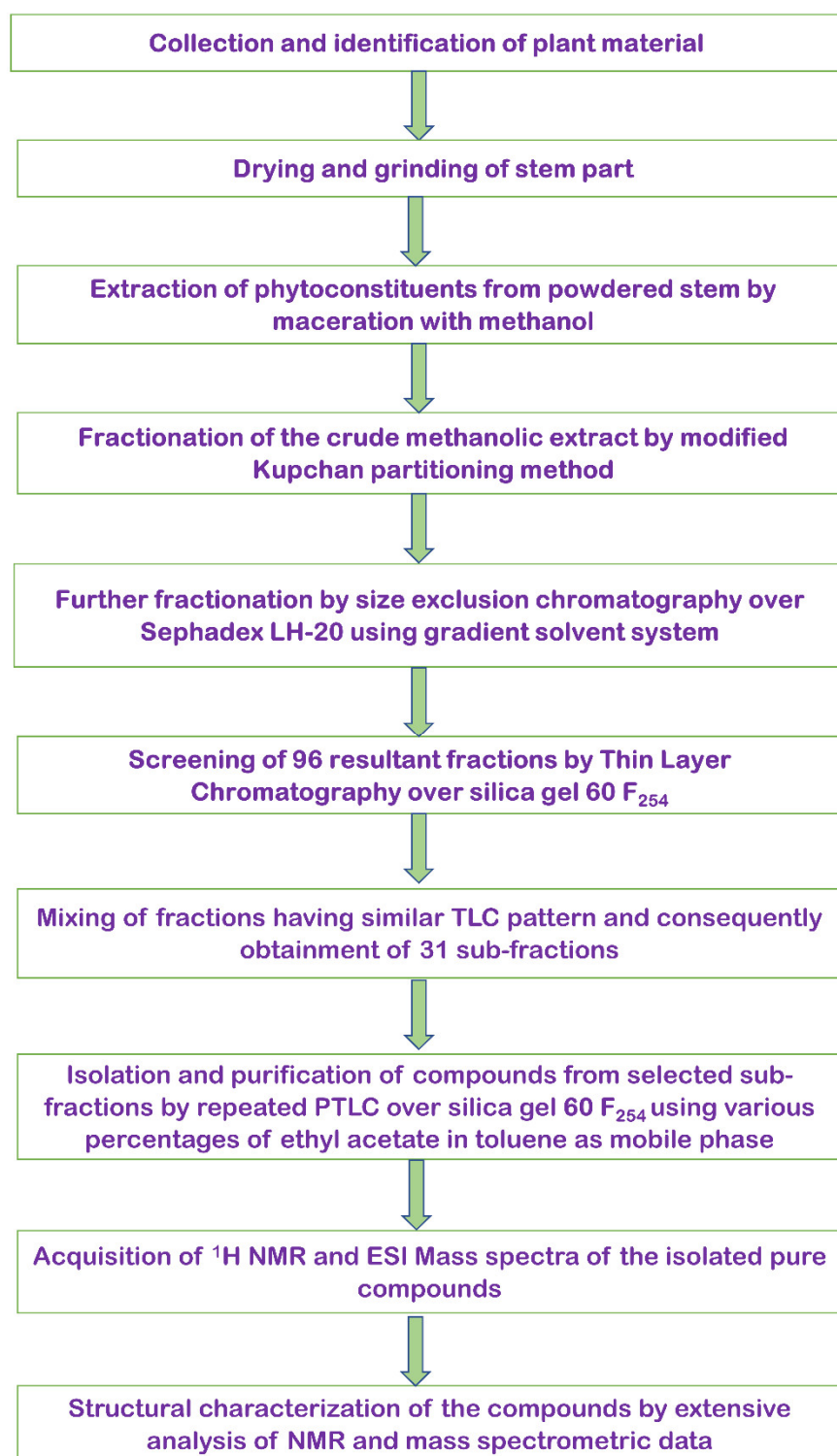


Figure S1: The schematic diagram of whole phytochemical isolations.

Table S1. Gradient solvent system used in size exclusion chromatographic technique.

Solvent System	Fraction Numbers*	Total Volume Collected (mL)
Hexane : DCM : Methanol (2 : 5 : 1)	1-17	51
10% Methanol in DCM (10 : 90 = 1 : 9)	18-35	54
20% Methanol in DCM (20 : 80 = 1 : 4)	36-53	54
50% Methanol in DCM (50 : 50 = 1 : 1)	54-71	54
80% Methanol in DCM (80 : 20 = 4 : 1)	72-89	54
100% Methanol	90-96	21

*Fractions were collected in test tubes. 3 mL of eluate had been collected in each test tube.

Table S2. Mixing of fractions based on similar TLC pattern.

Fraction Numbers	Sub-fraction
1-5	F-1
6-9	F-2
10-13	F-3
14-17	F-4
18-20	F-5
21-23	F-6
24-26	F-7
27-29	F-8
30-31	F-9
32-33	F-10
34-35	F-11
36-39	F-12
40-43	F-13
44-47	F-14
48-50	F-15
51-53	F-16
54-56	F-17
57-60	F-18
61-63	F-19
64-65	F-20
66-68	F-21
69-71	F-22
72-74	F-23
75-77	F-24
78-79	F-25
80-81	F-26
82-83	F-27
84-85	F-28
86-87	F-29
88-89	F-30
90-96	F-31

Table S3. Isolation of compounds by PTLC technique from different sub-fractions.

Sub-fraction	Solvent System of Preparative TLC Technique	Isolated Compounds	Amount of Pure Compounds (mg)
F-23	50 % Ethyl Acetate in Toluene	Compound 6 (Ferulic acid)	4.0
F-24	55% Ethyl Acetate in Toluene	Compound 5 (Glabridin)	4.3
F-25	55% Ethyl Acetate in Toluene	Compound 1 (Liquiritigenin)	4.5
F-26	50 % Ethyl Acetate in Toluene	Compound 2 (Naringenin)	4.1
F-27	55% Ethyl Acetate in Toluene	Compound 3 (Apigenin)	4.2
F-28	50 % Ethyl Acetate in Toluene	Compound 8 (4-Hydroxybenzaldehyde)	3.8
F-29	55% Ethyl Acetate in Toluene	Compound 7 (4-Hydroxybenzoic acid)	3.9
F-30	60 % Ethyl Acetate in Toluene	Compound 4 (Kaempferol)	4.6

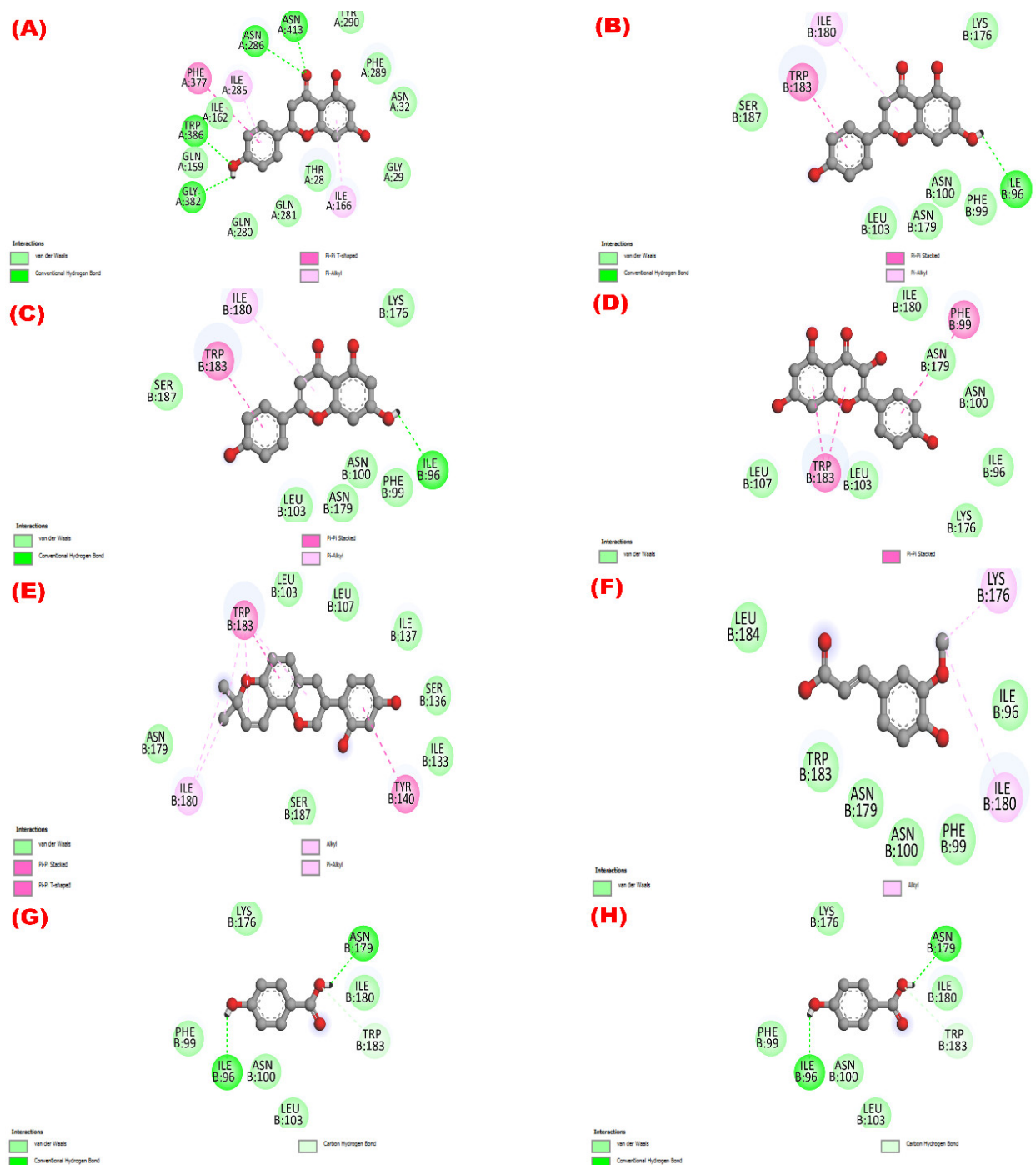


Figure S3. The isolated phytochemicals' potential as antidiarrheal agents showing their 2D molecular interactions with the kappa opioid receptor (PDB ID: 6VI4). (The 2D visual images of the molecular docking of the molecules (1 to 8) liquiritigenin, naringenin, apigenin, kaempferol, glabridin, ferulic acid, 4-hydroxybenzoic acid, and 4-hydroxybenzaldehyde are shown in A, B, C, D, E, F, G, and H, respectively).

Table S4: Interactions of amino acids of the glutathione reductase enzyme (PDB ID: 3GRS) with the isolated compounds (**1** to **8**) from *Wendlandia tinctoria* (Roxb.) DC. and the standard drug Butylated Hydroxy toluene (BHT) during molecular docking.

Compound	Bond (AA and Ligand)	Bond length	Bond type	Bond nature
Liquiritigenin (1)	A:SER51:HN - N:UNK1:O	2.75893	Hydrogen Bond	Conventional Hydrogen Bond
	A:GLU50:CA - N:UNK1:O	3.53249	Hydrogen Bond	Carbon Hydrogen Bond
	A:GLU50:OE2 - N:UNK1	4.4349	Electrostatic	Pi-Anion
	A:THR156:CG2 - N:UNK1	3.44276	Hydrophobic	Pi-Sigma
	N:UNK1 - A:LEU298	5.44018	Hydrophobic	Pi-Alkyl
Naringenin (2)	A:SER51:HN - N:UNK1:O	2.53482	Hydrogen Bond	Conventional Hydrogen Bond
	A:GLU50:OE2 - N:UNK1	4.48616	Electrostatic	Pi-Anion
	A:THR156:CG2 - N:UNK1	3.49392	Hydrophobic	Pi-Sigma
	A:HIS129 - N:UNK1	4.7889	Hydrophobic	Pi-Pi Stacked
	N:UNK1 - A:LEU298	5.43351	Hydrophobic	Pi-Alkyl
Apigenin (3)	N:UNK1:H - A:GLU50:OE1	2.13242	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASP331:OD1 - N:UNK1	4.20119	Electrostatic	Pi-Anion
	N:UNK1 - A:ALA342	5.01057	Hydrophobic	Pi-Alkyl
Kaempferol (4)	A:SER51:HN - N:UNK1:O	3.08093	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:THR57:OG1	2.1136	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - N:UNK1:O	2.2186	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:ASN294:OD1	2.91263	Hydrogen Bond	Conventional Hydrogen Bond
	A:GLU50:OE2 - N:UNK1	4.33452	Electrostatic	Pi-Anion
	A:THR156:CG2 - N:UNK1	3.49098	Hydrophobic	Pi-Sigma
	A:HIS129 - N:UNK1	4.71522	Hydrophobic	Pi-Pi Stacked
	N:UNK1 - A:LEU298	4.93945	Hydrophobic	Pi-Alkyl
Glabridin (5)	A:ASN294:HD21 - N:UNK1:O	2.6422	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1 - A:MET159	5.40639	Hydrophobic	Alkyl
	N:UNK1:C - A:VAL61	4.0771	Hydrophobic	Alkyl
	N:UNK1:C - A:VAL61	5.21401	Hydrophobic	Alkyl
	N:UNK1:C - A:PRO160	5.09846	Hydrophobic	Alkyl
	A:HIS52 - N:UNK1	5.34463	Hydrophobic	Pi-Alkyl
Ferulic acid (6)	A:GLY31:HN - N:UNK1:O	2.29547	Hydrogen Bond	Conventional Hydrogen Bond
	A:THR339:HN - N:UNK1:O	2.75951	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:ASP331:OD2	2.33705	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:ALA155:O	2.18953	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:C - A:VAL329:O	3.44338	Hydrogen Bond	Carbon Hydrogen Bond
	A:GLY29:C,O;SER30:N - N:UNK1	4.73456	Hydrophobic	Amide-Pi Stacked
	A:ALA155 - N:UNK1:C	3.33905	Hydrophobic	Alkyl
	A:ALA342 - N:UNK1:C	4.18634	Hydrophobic	Alkyl
	N:UNK1:C - A:VAL329	5.35381	Hydrophobic	Alkyl
	N:UNK1 - A:ALA342	5.27267	Hydrophobic	Pi-Alkyl
4-Hydroxybenzoic acid	A:SER51:HN - N:UNK1:O	3.08093	Hydrogen Bond	Conventional Hydrogen Bond

(7)	N:UNK1:H - A:THR57:OG1	2.1136	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - N:UNK1:O	2.2186	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:ASN294:OD1	2.91263	Hydrogen Bond	Conventional Hydrogen Bond
	A:GLU50:OE2 - N:UNK1	4.33452	Electrostatic	Pi-Anion
	A:THR156:CG2 - N:UNK1	3.49098	Hydrophobic	Pi-Sigma
	A:HIS129 - N:UNK1	4.71522	Hydrophobic	Pi-Pi Stacked
4-Hydroxybenzaldehyde (8)	N:UNK1 - A:LEU298	4.93945	Hydrophobic	Pi-Alkyl
	A:SER30:HN - N:UNK1:O	2.2803	Hydrogen Bond	Conventional Hydrogen Bond
	A:THR57:HN - N:UNK1:O	2.62161	Hydrogen Bond	Conventional Hydrogen Bond
	A:CYS58:HN - N:UNK1:O	2.19969	Hydrogen Bond	Conventional Hydrogen Bond
	A:GLY157:HN - N:UNK1:O	2.9589	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:VAL329:O	2.59624	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1 - A:ALA342	4.76081	Hydrophobic	Pi-Alkyl
Butylated Hydroxy Toluene (BHT)	N:UNK1:H - A:GLY158:O	2.63579	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:C - A:LYS53	4.38415	Hydrophobic	Alkyl
	N:UNK1:C - A:VAL61	4.80028	Hydrophobic	Alkyl

Table S5: Interactions of amino acids of the urase oxidase enzyme (PDB ID: 1R4U) with the isolated compounds (**1** to **8**) from *Wendlandia tinctoria* (Roxb.) DC. and the standard drug Butylated Hydroxy toluene (BHT) during molecular docking.

Compound	Bond (AA and Ligand)	Bond length	Bond type	Bond nature
Liquiritigenin (1)	A:PRO76:CD - N:UNK1:O	3.64553	Hydrogen Bond	Carbon Hydrogen Bond
	A:MET32:SD - N:UNK1	5.5761	Other	Pi-Sulfur
	A:CYS103:SG - N:UNK1	3.64542	Other	Pi-Sulfur
	A:TYR30 - N:UNK1	5.02944	Hydrophobic	Pi-Pi T-shaped
	N:UNK1 - A:PRO76	5.24592	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ARG105	4.43966	Hydrophobic	Pi-Alkyl
Naringenin (2)	N:UNK1:H - A:VAL73:O	2.67752	Hydrogen Bond	Conventional Hydrogen Bond
	A:PRO76:CD - N:UNK1:O	3.69628	Hydrogen Bond	Carbon Hydrogen Bond
	A:PRO76:CD - N:UNK1:O	3.21635	Hydrogen Bond	Carbon Hydrogen Bond
	A:MET32:SD - N:UNK1	5.42942	Other	Pi-Sulfur
	A:CYS103:SG - N:UNK1	3.64118	Other	Pi-Sulfur
	A:TYR30 - N:UNK1	5.03267	Hydrophobic	Pi-Pi T-shaped
	N:UNK1 - A:PRO76	5.41381	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ARG105	4.42633	Hydrophobic	Pi-Alkyl
Apigenin (3)	N:UNK1:H - A:VAL73:O	2.38223	Hydrogen Bond	Conventional Hydrogen Bond
	A:PRO76:CD - N:UNK1:O	3.23331	Hydrogen Bond	Carbon Hydrogen Bond
	A:MET32:SD - N:UNK1	5.44523	Other	Pi-Sulfur
	A:CYS103:SG - N:UNK1	3.66988	Other	Pi-Sulfur
	A:TYR30 - N:UNK1	5.68215	Hydrophobic	Pi-Pi T-shaped
	A:TYR30 - N:UNK1	5.00672	Hydrophobic	Pi-Pi T-shaped
	N:UNK1 - A:PRO76	5.43513	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:CYS103	4.40463	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ARG105	4.29356	Hydrophobic	Pi-Alkyl
Kaempferol (4)	A:TRP106:HN - N:UNK1:O	2.09023	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:VAL73:O	1.68644	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:VAL29:O	2.20195	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:THR107:OG1	2.36105	Hydrogen Bond	Conventional Hydrogen Bond
	A:MET32:SD - N:UNK1	5.20113	Other	Pi-Sulfur
	A:CYS103:SG - N:UNK1	3.60193	Other	Pi-Sulfur
	A:TYR30 - N:UNK1	5.0092	Hydrophobic	Pi-Pi T-shaped
	N:UNK1 - A:ARG105	4.06825	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:PRO76	5.27194	Hydrophobic	Pi-Alkyl
Glabridin (5)	N:UNK1:H - A:GLU31:O	2.46697	Hydrogen Bond	Conventional Hydrogen Bond
	A:MET32:SD - N:UNK1	5.55821	Other	Pi-Sulfur
	A:CYS103:SG - N:UNK1	3.80112	Other	Pi-Sulfur
	A:TYR30 - N:UNK1	4.84733	Hydrophobic	Pi-Pi T-shaped
	A:TRP208 - N:UNK1	5.21519	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:PRO76	5.27332	Hydrophobic	Pi-Alkyl

Ferulic acid (6)	A:ARG128:HH11 - N:UNK1:O	2.65297	Hydrogen Bond	Conventional Hydrogen Bond
	A:ARG128:HH12 - N:UNK1:O	2.7048	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:ASP205:OD2	2.63582	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:C - A:VAL29:O	3.63376	Hydrogen Bond	Carbon Hydrogen Bond
	A:MET32:SD - N:UNK1	5.55891	Other	Pi-Sulfur
	A:CYS103:SG - N:UNK1	3.73779	Other	Pi-Sulfur
	A:TYR30 - N:UNK1	4.9124	Hydrophobic	Pi-Pi T-shaped
	A:TYR30 - N:UNK1:C	5.23047	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:PRO76	5.17868	Hydrophobic	Pi-Alkyl
4-Hydroxybenzoic acid (7)	A:PRO76:CD - N:UNK1:O	3.48004	Hydrogen Bond	Carbon Hydrogen Bond
	A:MET32:SD - N:UNK1	5.80393	Other	Pi-Sulfur
	A:CYS103:SG - N:UNK1	3.80232	Other	Pi-Sulfur
	A:TYR30 - N:UNK1	4.92498	Hydrophobic	Pi-Pi T-shaped
	N:UNK1 - A:PRO76	5.24399	Hydrophobic	Pi-Alkyl
4-Hydroxybenzaldehyde (8)	A:PRO76:CD - N:UNK1:O	3.48004	Hydrogen Bond	Carbon Hydrogen Bond
	A:MET32:SD - N:UNK1	5.80393	Other	Pi-Sulfur
	A:CYS103:SG - N:UNK1	3.80232	Other	Pi-Sulfur
	A:TYR30 - N:UNK1	4.92498	Hydrophobic	Pi-Pi T-shaped
	N:UNK1 - A:PRO76	5.24399	Hydrophobic	Pi-Alkyl
Butylated Hydroxy Toluene (BHT)	N:UNK1:C - A:TRP208	3.90117	Hydrophobic	Pi-Sigma
	N:UNK1:C - A:CYS103	4.42683	Hydrophobic	Alkyl
	N:UNK1:C - A:ARG105	4.80501	Hydrophobic	Alkyl
	N:UNK1:C - A:ARG128	4.8105	Hydrophobic	Alkyl
	A:TYR30 - N:UNK1:C	5.16445	Hydrophobic	Pi-Alkyl

Table S6: Interactions of amino acids of the glucose transporter 3 (GLUT 3) (PDB ID: 4ZWB) with the isolated compounds (**1** to **8**) from *Wendlandia tinctoria* (Roxb.) DC. and the standard drug glibenclamide during molecular docking.

Compound	Bond (AA and Ligand)	Bond length	Bond type	Bond nature
Liquiritigenin (1)	A:ASN315:HD21 - N:UNK1:O	2.42169	Hydrogen Bond	Conventional Hydrogen Bond
	A:PHE289 - N:UNK1	5.00603	Hydrophobic	Pi-Pi Stacked
	N:UNK1 - A:ILE285	2.69255	Hydrogen Bond	Conventional Hydrogen Bond
Naringenin (2)	A:ASN286:HD22 - N:UNK1:O	2.51237	Hydrogen Bond	Conventional Hydrogen Bond
	A:TRP386:HE1 - N:UNK1:O	2.13081	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN413:HD21 - N:UNK1:O	2.92491	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:GLY382:O	5.21554	Hydrophobic	Pi-Pi T-shaped
	A:PHE377 - N:UNK1	5.25385	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ILE166	4.96032	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ILE285	2.74792	Hydrogen Bond	Conventional Hydrogen Bond
Apigenin (3)	A:ASN286:HD22 - N:UNK1:O	2.74792	Hydrogen Bond	Conventional Hydrogen Bond
	A:TRP386:HE1 - N:UNK1:O	2.50964	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN413:HD21 - N:UNK1:O	2.09824	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:GLY382:O	2.83774	Hydrogen Bond	Conventional Hydrogen Bond
	A:PHE289 - N:UNK1	5.08793	Hydrophobic	Pi-Pi Stacked
	N:UNK1 - A:ILE166	5.27196	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ILE285	5.21415	Hydrophobic	Pi-Alkyl
Kaempferol (4)	A:ASN286:HD22 - N:UNK1:O	2.81097	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN413:HD21 - N:UNK1:O	2.0868	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN413:HD21 - N:UNK1:O	2.24774	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:GLY382:O	3.06051	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:GLN281:OE1	2.78735	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1 - A:ILE166	5.17702	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ILE285	5.32515	Hydrophobic	Pi-Alkyl
Glabridin (5)	N:UNK1:H - A:GLN281:OE1	2.79923	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:GLN159:OE1	1.99103	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:GLY382:O	2.91833	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:C - A:VAL67	4.67268	Hydrophobic	Alkyl
	N:UNK1:C - A:ILE31	5.38653	Hydrophobic	Alkyl
	N:UNK1:C - A:VAL67	4.45202	Hydrophobic	Alkyl
	A:PHE24 - N:UNK1	5.13569	Hydrophobic	Pi-Alkyl
	A:PHE70 - N:UNK1:C	5.06367	Hydrophobic	Pi-Alkyl
Ferulic acid (6)	A:GLN159:HE21 - N:UNK1:O	2.15033	Hydrogen Bond	Conventional Hydrogen Bond
	A:GLN159:HE21 - N:UNK1:O	2.74877	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN286:HD22 - N:UNK1:O	2.62438	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN413:HD21 - N:UNK1:O	1.87569	Hydrogen Bond	Conventional Hydrogen Bond
	A:PHE289 - N:UNK1	5.01893	Hydrophobic	Pi-Pi T-shaped
	A:PHE377 - N:UNK1	5.43843	Hydrophobic	Pi-Pi T-shaped

	A:PHE377 - N:UNK1:C	4.93806	Hydrophobic	Pi-Alkyl
	A:TRP386 - N:UNK1:C	5.25696	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ILE166	5.30112	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ILE285	4.40702	Hydrophobic	Pi-Alkyl
4-Hydroxybenzoic acid (7)	A:GLN159:HE21 - N:UNK1:O	2.42414	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:ASN315:OD1	2.26254	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:GLU378:OE2	2.12521	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1 - A:ILE285	4.03797	Hydrophobic	Pi-Alkyl
4-Hydroxybenzaldehyde (8)	A:ASN315:HD21 - N:UNK1:O	2.10624	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN413:HD21 - N:UNK1:O	2.70796	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN413:HD22 - N:UNK1:O	2.94407	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:ASN315:OD1	2.88038	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:GLU378:OE2	2.02856	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1 - A:ILE285	4.09051	Hydrophobic	Pi-Alkyl
Glibenclamide	A:ASN32:HD21 - N:UNK1:O	2.19182	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN286:HD21 - N:UNK1:O	2.44125	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN286:CA - N:UNK1:O	3.67123	Hydrogen Bond	Carbon Hydrogen Bond
	N:UNK1:C - A:ASN286:OD1	3.53833	Hydrogen Bond	Carbon Hydrogen Bond
	A:GLY417:C,O;LEU418:N - N:UNK1	4.06449	Hydrophobic	Amide-Pi Stacked
	A:ALA68 - N:UNK1:CI	3.7508	Hydrophobic	Alkyl
	A:ILE285 - N:UNK1	5.2546	Hydrophobic	Alkyl
	N:UNK1:CI - A:LEU418	3.9955	Hydrophobic	Alkyl
	A:TYR290 - N:UNK1:C	4.22531	Hydrophobic	Pi-Alkyl
	A:PHE414 - N:UNK1:CI	4.03962	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:VAL67	5.31698	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ALA68	4.51755	Hydrophobic	Pi-Alkyl

Table S7: Interactions of amino acids of the kappa opioid receptor (PDB ID: 6VI4) with the isolated compounds (**1** to **8**) from *Wendlandia tinctoria* (Roxb.) DC. and the standard drug loperamide during molecular docking.

Compound	Bond (AA and Ligand)	Bond length	Bond type	Bond nature
Liquiritigenin (1)	A:ASN286:HD22 - N:UNK1:O	2.69255	Hydrogen Bond	Conventional Hydrogen Bond
	A:TRP386:HE1 - N:UNK1:O	2.51237	Hydrogen Bond	Conventional Hydrogen Bond
	A:ASN413:HD21 - N:UNK1:O	2.13081	Hydrogen Bond	Conventional Hydrogen Bond
	N:UNK1:H - A:GLY382:O	2.92491	Hydrogen Bond	Conventional Hydrogen Bond
	A:PHE377 - N:UNK1	5.21554	Hydrophobic	Pi-Pi T-shaped
	N:UNK1 - A:ILE166	5.25385	Hydrophobic	Pi-Alkyl
	N:UNK1 - A:ILE285	4.96032	Hydrophobic	Pi-Alkyl
Naringenin (2)	N:UNK1:H - B:ILE96:O	2.53534	Hydrogen Bond	Conventional Hydrogen Bond
	B:TRP183 - N:UNK1	3.74398	Hydrophobic	Pi-Pi Stacked
	B:TRP183 - N:UNK1	4.20626	Hydrophobic	Pi-Pi Stacked
	N:UNK1 - B:ILE180	5.4624	Hydrophobic	Pi-Alkyl
Apigenin (3)	N:UNK1:H - B:ILE96:O	2.53534	Hydrogen Bond	Conventional Hydrogen Bond
	B:TRP183 - N:UNK1	3.74398	Hydrophobic	Pi-Pi Stacked
	B:TRP183 - N:UNK1	4.20626	Hydrophobic	Pi-Pi Stacked
	N:UNK1 - B:ILE180	5.4624	Hydrophobic	Pi-Alkyl
Kaempferol (4)	B:PHE99 - N:UNK1	5.40779	Hydrophobic	Pi-Pi Stacked
	B:TRP183 - N:UNK1	3.74362	Hydrophobic	Pi-Pi Stacked
	B:TRP183 - N:UNK1	3.95697	Hydrophobic	Pi-Pi Stacked
	B:TRP183 - N:UNK1	4.87118	Hydrophobic	Pi-Pi Stacked
	B:TRP183 - N:UNK1	3.90906	Hydrophobic	Pi-Pi Stacked
	B:TRP183 - N:UNK1	3.84787	Hydrophobic	Pi-Pi Stacked
Glabridin (5)	B:TRP183 - N:UNK1	3.94883	Hydrophobic	Pi-Pi Stacked
	B:TYR140 - N:UNK1	4.75559	Hydrophobic	Pi-Pi T-shaped
	N:UNK1:C - B:ILE180	3.94788	Hydrophobic	Alkyl
	N:UNK1:C - B:ILE180	4.57153	Hydrophobic	Alkyl
	B:TRP183 - N:UNK1	5.25665	Hydrophobic	Pi-Alkyl
	B:TRP183 - N:UNK1	4.82862	Hydrophobic	Pi-Alkyl
	B:TRP183 - N:UNK1:C	4.58348	Hydrophobic	Pi-Alkyl
	B:TRP183 - N:UNK1	4.33359	Hydrophobic	Pi-Alkyl
	N:UNK1:C - B:LYS176	3.89225	Hydrophobic	Alkyl
Ferulic Acid (6)	N:UNK1:C - B:ILE180	4.87741	Hydrophobic	Alkyl
	N:UNK1:H - B:ASN179:O	2.26424	Hydrogen Bond	Conventional Hydrogen Bond
4-Hydroxybenzoic acid (7)	N:UNK1:H - B:ILE96:O	2.0668	Hydrogen Bond	Conventional Hydrogen Bond
	B:TRP183:CD1 - N:UNK1:O	3.3447	Hydrogen Bond	Carbon Hydrogen Bond
	B:ILE180:CA - N:UNK1:O	3.42981	Hydrogen Bond	Carbon Hydrogen Bond
4-Hydroxybenzaldehyde (8)	B:TRP183:CD1 - N:UNK1:O	3.57398	Hydrogen Bond	Carbon Hydrogen Bond
Loperamide	N:UNK1:C - B:TRP183	3.8229	Hydrophobic	Pi-Sigma

	B:TRP183 - N:UNK1	5.13627	Hydrophobic	Pi-Pi Stacked
	N:UNK1:CI - B:ILE96	4.88724	Hydrophobic	Alkyl
	B:PHE99 - N:UNK1:CI	5.38651	Hydrophobic	Pi-Alkyl
	B:TRP183 - N:UNK1	5.04811	Hydrophobic	Pi-Alkyl
	N:UNK1 - B:LEU107	5.2433	Hydrophobic	Pi-Alkyl