Table 1. Information of potential active compounds of the aqueous extract from Perilla stem (PSAE).

Number	Molecule name	Structure types	Molecular formula	Molecular weight	PubChem ID
S1	Luteolin-7-O-glucoside	flavonoid glycosides	$C_{21}H_{20}O_{11}$	448.377	5280637
S2	Luteolin-7-O-glucuronide	flavonoid glycosides	$C_{21}H_{18}O_{12}$	462.360	13607752
S3	Luteolin 7-O-diglucuronide	flavonoid glycosides	$C_{27}H_{26}O_{18}$	638.5	157009729
S4	Apigenin-7-glucuronide	flavonoid glycosides	$C_{21}H_{18}O_{11}$	446.361	5319484
S5	Apigenin-7-O-diglucuronide	flavonoid glycosides	$C_{27}H_{26}O_{17}$	622.5	126843388
S6	Gallic Acid	organic acids	$C_7H_6O_5$	170.12	370
S7	Caffeic Acid	organic acids	$C_9H_8O_4$	180.16	689043
S8	Methyl Caffeate	organic acids	$C_{10}H_{10}O_4$	194.184	689075
S9	Ethyl Caffeate	organic acids	$C_{11}H_{12}O_4$	208.21	5317238
S10	Rosmarinic Acid	organic acids	$C_{18}H_{16}O_8$	360.3	5281792
S11	Methyl Rosmarinate	organic acids	$C_{19}H_{18}O_8$	374.3	6479915
S12	3,3 '-ethoxy rosmarinic acid	organic acids	$C_{27}H_{22}O_{12}$	538.5	21582559
S13	Catechin	organic acids	$C_{15}H_{14}O_6$	290.27	9064
S14	Salvianic acid A	organic acids	$C_9H_{10}O_5$	198.17	11600642
S15	Protocatechuic Acid	organic acids	$C_7H_6O_4$	154.12	72
S16	Chlorogenic Acid	organic acids	$C_{16}H_{18}O_9$	354.309	1794427
S17	Citric Acid	organic acids	$C_6H_8O_7$	192.12	311
S18	Hydrocinnamic Acid	organic acids	$C_9H_{10}O_2$	150.17	107
S19	Hederagenin	triterpenes	$C_{30}H_{48}O_4$	472.70	73299
S20	Glochidone	triterpenes	$C_{30}H_{46}O$	422.69	13942832
S21	Jasmonic Acid	fatty acid	$C_{12}H_{18}O_3$	210.27	5281166
S22	6,7-Dihydroxycoumarin	coumarins	$C_9H_6O_4$	178.15	5281416
S23	Tyrosine	amino acids	$C_9H_{11}NO_3$	181.189	6057
S24	Adenosine	amino acids	$C_{10}H_{13}N_5O_4$	267.24	60961
S25	Pyroglutamic acid	amino acids	$C_5H_7NO_3$	129.114	7405
S26	Phenylalanine	amino acids	$C_9H_{11}NO_2$	165.19	6140
S27	Tryptophan	amino acids	$C_{11}H_{12}N_2O_2$	204.23	6305

Table 2. Basic information on the molecular docking of active ingredients and AR.

No.	Hydrogen bonds		Hydrophobic interactions		Binding energy (kcal/Mol)
	Residue	Distance	Residue	Distance	
S19	Arg-752	2.81	Leu-701; Met-780; Leu-704	5.41; 5.45; 3.99	-7.1
S20	Thr-877	3.0	Trp-741; Phe-764; Phe-891; Leu-880; Leu-701; Met-742; Met-895; Leu-704; Leu-707; Met-745; Met-749; Val-746; Met-787; Leu-873	5.34; 4.28,5.14,5.15,5.02,5.42; 4.38,5.20; 4.27,5.02; 3.74; 4.90,5.37; 5.31; 4.68,5.17,5.27; 4.52; 3.52,5.37; 4.01,4.73,2.84; 3.94,3.37; 4.18,4.47; 5.41,4.94	-1.8
S21	Arg-752	2.13	Phe-764; Phe-891; Phe-876; Met-749; Leu-704; Met-780; Leu-880; Val-889; Leu-701; Met-742; Met-745	4.97; 4.37,3.58; 5.21; 4.37; 5.38,5.15,2.82,5.20; 4.94; 4.28,4.07,3.81; 4.57; 3.80,4.59; 4.08,4.74; 4.74,4.15,3.91	-8.2

Table 3. Basic information on the molecular docking of active ingredients and AKT1.

No.	Hydrogen Bonds		Hydrophobic Interactions		Binding energy (kcal/Mol)
	Residue	Distance	Residue	Distance	
S1	Asp-292; Asp-274; Val-271	2.26; 2.33; 2.41	Trp-80; Leu-210; Leu-264; Val-270	4.95,4.72,4.90; 3.71; 5.38; 5.11,4.83	-10.9
S2	Val-271; Asn-54; Thr-82	2.12; 2.34; 2.97	Trp-80; Leu-210; Leu-264; Val-270	4.64,5.29,5.89; 3.63; 5.25; 4.47; 5.35	-11.3
S3	Gln-79; Tyr-326; Arg-273; Asn-54; Cys-296; Asp-274	2.45; 2.00; 2.57; 2.05,2.14; 3.08,3.69; 3.47	Trp-80; Gln-79; Leu-264; Val-270; Lys-268	4.13,4.54; 5.09,5.12; 5.50; 4.19,4.55; 5.10	-11.9
S4	Asn-54; Tyr-272; Thr-82; Asp-292; His-207	2.40,2.83; 2.22; 2.97; 2.20; 2.23	Trp-80; Leu-210; Leu-264; Val-270; Lys-268：	4.63,5.29,5.87; 3.61; 5.26; 2.20; 4.42,5.48; 5.28	-11.3
S5	Gln-79; Asp-292; Thr-82; Asp-274; Lys-297; Cys-310; Tyr-326; Cys-296;	2.24; 2.47; 2.70; 2.65; 1.86; 3.26; 3.06; 3.74	Cys-296; Cys-310	4.00,4.10; 5.08	-11.1
S7	Ile-290; Thr-211	2.47,2.91; 2.47	Trp-80; Leu-210; Leu-264	5.46; 4.05; 5.17	-6.7
S8	Trp-80; Thr-211; Ile-290	2.46; 2.29; 2.66	Leu-210; Leu-264	4.48; 5.43	-6.7
S9	Thr-211	2.35	Trp-80; Leu-210; Leu-264; Val-270	5.49; 4.04; 5.16; 3.80	-7.0
S10	Asp-292; Thr-211; Trp-80：	2.29; 3.67; 2.93	Trp-80; Tyr-272; Lys-268; Val-270	4.11; 5.26; 4.43; 4.58,5.31	-9.1
S11	Trp-80; Asp-292; Trp-80; Ser-205	2.43; 2.17; 3.72; 3.49	Trp-80; Tyr-272; Val-270; Trp-80; Lys-268; Val-270; Leu-264：	4.65; 5.57; 4.79; 6.01; 5.25; 5.35; 5.49	-8.6
S14	Trp-80; Thr-211; Ile-290	2.49; 2.70; 2.88	Lys-268; Trp-80	4.94;4.92	-6.7
S19	Cys-296	2.89	Trp-80; Tyr-272; Leu-210; Leu-264; Val-270; Ile-84：	4.86,5.36; 3.69; 4.08,4.83; 4.80,4.93; 4.70,4.75; 3.95,4.77	-10.5
S20	-	-	Lys-39; Pro-388; Lys-386; Lys-389	4.93,4.55; 4.93,5.12; 4.59; 4.69,5.34	-8.5
S22	Thr-211	2.19; 2.33	Trp-80; Leu-264; Leu-210：	5.05,5.41;3.73; 4.29,5.42	-7.0
S24	Asp-274; Gln-79; Asp-292	2.62; 2.39; 3.52	Thr-82	3.80,3.84	-7.1

Table 4. Basic information on the molecular docking of active ingredients and FoxO1.

No.	Hydrogen Bonds		Hydrophobic Interactions		Binding energy (kcal/Mol)
	Residue	Distance	Residue	Distance	
S1	Gly-208; Ser-205	3.63; 3.42	Trp-209	3.75	-8.3
S2	Tyr-165; Asn 204; Ser-206	2.62; 2.10,2.36; 3,57	Trp-209; Gly-208	3.66; 4.70	-8.8
S3	Tyr-165; Gly-208; Ser-212; Ser-205;	2.27; 3.95,3.11; 2.17; 3.35;	Trp-209; Gly-208	3.69; 4.61	-8.6
S4	Gly-208; Ser-205; Lys-200	2.28,2.17; 3.49; 3.49	Ala-207; Trp-209	3.74; 5.44	-8.7
S5	Arg-157; Asn-211; Asn-158; Ala-207; Ser-205; Gly-208; Ser-206	2.36; 2.27; 2.33; 2.52; 2.51; 3.52; 3.80	Trp-160; Gly-208; Ala-159	4.89; 3.97; 4.85	-8.8
S7	Gly-208; Ser-206; Tyr-165	2.18; 2.72; 2.61	Trp-209	3.60	-6.9
S8	Tyr-165; Gly-208; Ala-207	2.58,2.60; 1.93; 3.00	Trp-209	3.56	-6.8
S9	Gly-208; Ala-207	2.02; 3.03	Trp-209	3.62	-6.8
S10	Gly-208; Ser-212; Trp-209	2.57; 2.41; 3.50	Trp-160; Ala-159	4.76; 4.88	-7.6
S11	Asn-158; Ala-159; Tyr-165; Trp-209; Asn-204	1.90; 2.26; 2.43; 3.25; 3.69	Trp-160; Ala-159	4.69; 4.73	-7.2
S14	Gly-208; Tyr-165; Trp-209; Ser-205; Ala-207	2.41; 2.41,2.45; 2.81; 1.78; 3.55	Trp-209; Gly-208	3.76; 4.85	-7.0
S19	Trp-209	2.83	Tyr-165; Trp-160	5.39; 4.60	-7.9
S20	-	-	Trp-209; Phe-197; Tyr-196; Trp-160; Ala-159; Lys-200	5.09; 4.96; 4.98; 5.11,5.19; 4.17; 5.08	-8.0
S22	Trp-209; Gly-208; Tyr-165	3.04; 2.72; 2.62	Gly-208	3.75,3.84	-6.7
S24	Tyr-165	2.22	Trp-209	5.42,3.69	-6.5

Table 5. Basic information on the molecular docking of active glochidone and target proteins.

Targets	Hydrogen Bonds		Hydrophobic Interactions		Binding energy (kcal/Mol)
	Residue	Distance	Residue	Distance	
AR	-	-	Tyr-915; His-789; Lys-861; Pro-868	4.16,4.71; 5.14; 3.94,4.37; 3.99,4.31	-1.7
AKT1	-	-	Lys-39; Pro-388; Lys-386; Lys-389	4.93,4.55; 4.93,5.12; 4.59; 4.69,5.34	-8.5
Fox O1	-	-	Trp-209; Phe-197; Tyr-196; Trp-160; Ala-159; Lys-200	5.09; 4.96; 4.98; 5.11,5.19; 4.17; 5.08	-8.0
mTOR	-	-	Tyr-2105; Phe-2039; Tyr-2105; Trp-2101	3.83,5.20; 5.29,3.94,4.26,5.19; 4.73	-8.6
PPARγ	Lys-275	2.55	Arg-280; Ile-279; Phe-287; Tyr-473; His-466 :	4.80; 5.30; 4.90,5.21; 5.05; 4.99	-7.9