Supplementary Data

This supplementary data is a part of a paper entitled "Study of Potential α-Glucosidase Inhibitor from *Tithonia diversifolia*: *In Vitro*, Pharmacokinetics, Toxicology, and Molecular Docking".

Table S1. Characterization of metabolites compound from stem *T. diversifolia* extracts by LC-HRMS/MS

Name compound	Formula	Exact mass	Calculated mass	Error (ppm)	RT (min)	Area (Max.)	Group compound
Eupatoriochromene	$C_{13}H_{14}O_3$	218.09371	218.09430	-2.68	11.357	35263424135	Polyketides
1-(2,2-Dimethyl-*2H*-chromen-6-Yl)ethanone	$C_{13}H_{14}O_2$	202.09888	202.09938	-2.47	10.561	32199847475	Polyketides
6-Acetyl-2,2-dimethylchromene	$C_{13}H_{14}O_3$	218.09371	218.09430	-2.68	8.656	21471800222	Polyketides
5-Acetyl-6-hydroxy-2-isopropenyl-2,3-dihydrobenzofuran	$C_{13}H_{14}O_3$	218.09371	218.09430	-2.68	12.041	14667329620	Polyketides
1-(2-(Hydroxymethyl)-2-methyl-*2H*-chromen-6-yl)ethanone	$C14H_{16}O_3$	232.10932	232.10995	-2.69	11.047	6893816950	Polyketides
1-(7-Hydroxy-2-(hydroxymethyl)-2-methyl-*2H*-chromen-6-yl)ethanone	$C_{13}H_{14}O_4$	234.08869	234.08921	-2.22	8.150	3953132775	Polyketides
4,4-Dimethyl-5a-cholesta-8,14,24-trien-3beta-ol	$C_{29}H_{46}O$	410.35352	410.35487	-3.27	18.654	1019085067	Steroid
Gingerdione	$C_{13}H_{14}O$	186.10407	186.10447	-2.12	9.361	904641641.1	Phenolic
2-Phenyl-4-pentenal	$C_{17}H_{24}O_4$	292.16689	292.16746	-1.95	11.75	867689348.5	Aromatic
Encecalin	$C_{13}H_{16}O_5$	252.09941	252.09978	-1.44	7.200	822596825.8	Polyketides
Sitostenone	$C_{29}H_{48}O$	412.36895	412.37052	-3.79	18.888	654434886.2	Steroid
7-Acetyl-3.6-dihydroxy-8-methyl-tetralone	$C_{13}H_{14}O_4$	234.08874	234.08921	-2.00	9.276	650095590.3	Polyketides
1-[4-Hydroxy-3-(3-methylbut-2-en-1-yl)phenyl]ethan-1-one	$C_{13}H_{16}O_2$	204.1146	204.11503	-2.10	9.991	594552218	Polyketides
Precocene II	$C_{13}H_{16}O_3$	220.10907	220.10995	-3.97	7.220	553963236.4	Polyketides
Myristicin	$C_{11}H_{12}O_3$	192.07822	192.07865	-2.21	6.885	498789790.8	Phenylpropane
Tremetone	$C_{13}H_{14}O_2$	202.09889	202.09938	-2.42	9.807	472621724.8	Polyketides
6-Acetyl-2.2-dimethylchromene-8-*O*-*D*-glucoside	$C_{15}H_{20}N_6O_6$	380.14606	380.14712	-2.78	6.506	458032414.9	Polyketides
p-Cymene	$C_{10}H_{14}$	134.10933	134.10955	-1.64	5.560	456447718.3	Terpene
p-Cresol	C_7H_8O	108.05754	108.05752	-0.23	8.070	434269129.6	Terpene
2-Hydroxy-7-methoxy-5-methyl-1-naphthoic acid	$C_{13}H_{12}O_4$	232.07312	232.07356	-1.89	7.614	420652366.9	Polyketides
4-Coumaric acid	$C_9H_8O_3$	164.04718	164.04735	-1.00	5.176	409950388.6	Phenylpropane
trans-Anethole	$C_{10}H_{12}O$	148.08862	148.08882	-1.31	5.103	407350390.2	Phenylpropane
Thymol	$C_{10}H_{14}O$	150.10422	150.10447	-1.63	5.143	372256315.3	Terpene
Zingerol	$C_{11}H_{16}O_3$	196.10958	196.10995	-1.86	5.939	356619248.1	Phenolic
Octinoxate	$C_{18}H_{26}O_3$	290.18762	290.18820	-1.98	10.038	351880948.2	Phenylpropane
7-Hydroxy-6-methoxy-*2H*-chromen-2-one	$C_{10}H_8O_4$	192.04196	192.04226	-1.56	5.603	264849474.4	Polyketides
(*E*)-*p*-Coumaric acid	$C_9H_8O_3$	164.04704	164.04735	-1.85	6.615	243903129.3	Phenylpropane
Sinensal	$C_{15}H_{22}O$	218.16643	218.16707	-2.91	8.238	237360711	Terpene
Ethyl palmitoleate	$C_{18}H_{34}O_2$	282.25527	282.25588	-2.16	13.166	233125754.7	Fatty acid
Sorbic acid	$C_6H_8O_2$	112.05257	112.05243	-1.24	2.522	220484341.6	Fatty acid
Indole	C_8H_7N	117.05782	117.05785	-0.24	5.563	214131007.8	Alkaloid
Cinnamic acid	$C_9H_8O_2$	148.05225	148.05243	-1.21	9.991	183260711.5	Phenylpropane
Estriol	$C_{18}H_{24}O_3$	288.17223	288.17255	-1.09	10.447	180702693.5	Steroid
4-Indolecarbaldehyde	C_9H_7NO	145.05264	145.05276	-0.85	6.111	163631295	Alkaloid
Vanillin	$C_8H_8O_3$	152.04714	152.04735	-1.34	4.975	152874947	Phenolic
3,5-Dimethoxybenzoic acid	$C_9H_{10}O_4$	182.05763	182.05791	-1.53	5.404	149036017.9	Phenolic

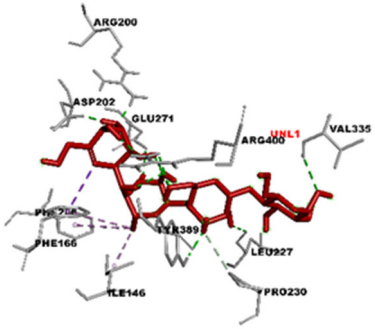
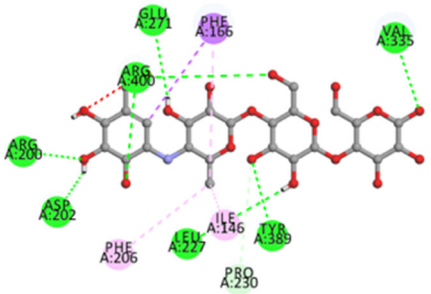
Name compound	Formula	Exact mass	Calculated mass	Error (ppm)	RT (min)	Area (Max.)	Group compound
5-Hydroxy-4-methoxy-6-(2-phenylethyl)-5,6-dihydro-*2H*-pyran-2-one	$C_{14}H_{16}O_4$	248.10451	248.10486	-1.41	9.705	142599781.4	Aromatic
Cumene	C_9H_{12}	120.09381	120.09390	-0.74	5.100	123170407.7	Aromatic
Ricinoleic acid	$C_{18}H_{34}O_3$	298.25014	298.25080	-2.19	11.599	122479537.3	Fatty acid
Citral	$C_{10}H_{16}O$	152.11988	152.12012	-1.54	5.895	122462279.6	Terpene
Carvone	$C_{10}H_{14}O$	150.1042	150.10447	-1.76	8.069	120243881.3	Terpene
13-apo-beta-Carotenone	$C_{18}H_{26}O$	258.19783	258.19837	-2.07	12.849	118243680.5	Terpene
(24*R*)-Ergost-4-en-3-one	$C_{28}H_{46}O$	398.35393	398.35487	-2.34	18.474	114976412.6	Steroid
Ulipristal	$C_{28}H_{35}NO_3$	433.26084	433.26169	-1.97	9.880	110355069.7	Other compounds
8-Hydroxyquinoline	C_9H_7NO	145.05264	145.05276	-0.85	3.057	102400965	Alkaloid
Senkyunolide A	$C_{12}H_{16}O_2$	192.11458	192.11503	-2.34	12.24	101836599.6	Other compounds
Aurin	$C_{19}H_{14}O_3$	290.09357	290.09430	-2.49	8.972	101743754.2	Phenolic
Methyl isonicotinate	$C_7H_7NO_2$	137.04738	137.04768	-2.18	0.814	93702606.73	Alkaloid
Salicylic acid	$C_7H_6O_3$	138.03147	138.03170	-1.63	6.106	93487333.82	Phenolic
Hymecromone	$C_{10}H_8O_3$	176.0472	176.04735	-0.82	9.632	81101160.22	Polyketides
Ecgonine methyl ester	$C_{10}H_{17}NO_3$	199.12048	199.12084	-1.82	1.136	71601924.15	Alkaloid
4-Hydroxybenzaldehyde	$C_7H_6O_2$	122.03672	122.03678	-0.49	4.186	70590957.22	Phenolic
Methyl palmitate	$C_{17}H_{34}O_2$	270.25533	270.25588	-2.03	16.852	70108475.32	Fatty acid
Stigmasterol	$C_{29}H_{48}O$	412.36967	412.37052	-2.04	16.198	69946172.12	Steroid
Scopoletin acetate	$C_{12}H_{10}O_5$	234.05324	234.05282	-1.77	8.444	68854560.69	Phenylpropane
6-Methoxymellein	$C_{11}H_{12}O_4$	208.07303	208.07356	-2.54	8.557	65630351.77	Phenylpropane
Erucic acid	$C_{22}H_{42}O_2$	338.31767	338.31848	-2.39	15.163	61074210.51	Fatty acid
Vanylglycol	$C_9H_{12}O_4$	184.07334	184.07356	-1.19	6.429	60293274.77	Phenylpropane
4-Methylumbelliferone hydrate	$C_{10}H_8O_3$	176.0472	176.04735	-0.82	7.400	58466951.44	Phenylpropane
6-(2-Hydroxy-4-methylphenyl)-2-Methyl-2-hepten-4-one	$C_{15}H_{20}O_2$	232.14549	232.14633	-3.61	11.952	58163424.95	Phenolic
Methyl cinnamate	$C_{10}H_{10}O_2$	162.06783	162.06808	-1.54	9.702	56098013.27	Phenylpropane
Citrinin	$C_{13}H_{14}O_5$	250.08386	250.08413	-1.05	7.126	55955150.64	Polyketides
Nepodin	$C_{13}H_{12}O_3$	216.07825	216.07865	-1.82	8.149	54153771.85	Polyketides
Ethyl 1-methylpyrrolo[1,2-a]pyrazine-7-carboxylate	$C_{11}H_{12}N_2O_2$	204.08971	204.08988	-0.82	1.713	53582035.29	Alkaloid
3,4,5-Trimethoxyphenyl acetate	$C_{11}H_{14}O_5$	226.0838	226.08413	-1.43	4.518	52025587.94	Phenolic
(8*E*)-10-Hydroxy-8-decenoic acid	$C_{10}H_{18}O_3$	186.1253	186.12560	-1.58	5.051	44923839.81	Fatty acid
Shinpterocarpin	$C_{20}H_{18}O_4$	322.11977	322.12051	-2.29	10.893	43948699.38	Flavonoid
Graminiliatrin	$C_{22}H_{26}O_9$	434.15676	434.15769	-2.13	6.932	41397970.11	Other compounds
6-Methylquinoline	$C_{10}H_9N$	143.07335	143.07350	-1.04	3.297	39753267.48	Alkaloid
Pipecolic acid	$C_6H_{11}NO_2$	129.07877	129.07898	-1.61	0.804	39280695.99	Alkaloid
Eugenol	$C_{10}H_{12}O_2$	164.08357	164.08373	-0.97	6.090	38640539.02	Phenylpropane
Menadione	$C_{11}H_8O_2$	172.0520	172.05243	-2.49	7.858	37321422.37	Polyketides
7-Dechlorogriseofulvin	$C_{17}H_{18}O_6$	318.10988	318.11034	-1.44	6.010	36591379.53	Polyketides
Geranyl glucoside	$C_{16}H_{28}O_6$	316.18804	316.18859	-1.73	7.617	34747127.24	Terpene
Equisetin	$C_{22}H_{31}NO_4$	373.22441	373.22531	-2.40	9.097	33616769.72	Terpene
Phenylglyoxylic acid	$C_8H_6O_3$	150.03154	150.03170	-1.03	4.105	33357230.16	Aromatic
3,4-Dimethoxyphenethylamine	$C_{10}H_{15}NO_2$	181.11008	181.11028	-1.09	5.262	33250606.03	Aromatic
2-Methoxy-phloroglucinol	$C_7H_8O_4$	156.04209	156.04226	-1.08	1.948	33159143.77	Polyketides
6-Hydroxymelatonin	$C_{13}H_{16}N_2O_3$	248.11595	248.11609	-0.57	1.559	31839509.23	Alkaloid
Nicotinic acid	$C_6H_5NO_2$	123.03191	123.03203	-0.96	0.985	27850792.73	Alkaloid
Naringenin	$C_{15}H_{12}O_5$	272.06801	272.06848	-1.70	8.334	27335762.84	Flavonoid
Anataline	$C_{15}H_{17}N_3$	239.1418	239.14225	-1.86	5.513	27107189.68	Alkaloid
19-Norandrostenedione	$C_{18}H_{24}O_2$	272.1772	272.17763	-1.57	9.866	24411106.57	Steroid
Azafrin	$C_{27}H_{38}O_4$	426.27626	426.27701	-1.75	12.411	23755987.92	Terpene
Nicotinamide	$C_6H_6N_2O$	122.04791	122.04801	-0.84	1.005	22768517.79	Alkaloid
5a-Ergosta-7,22-diene-3b,5-diol	$C_{28}H_{46}O_2$	414.34886	414.34978	-2.22	16.045	21176892.82	Steroid
epi-Tulipinolide	$C_{17}H_{22}O_4$	290.15083	290.15181	-3.37	11.313	17379593.73	Terpene

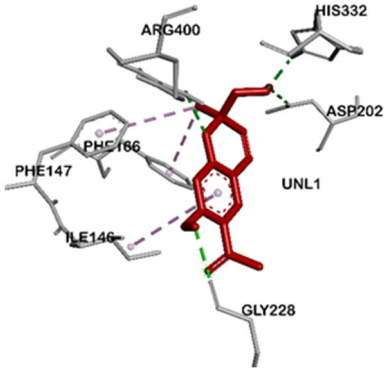
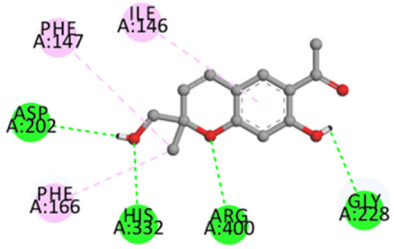
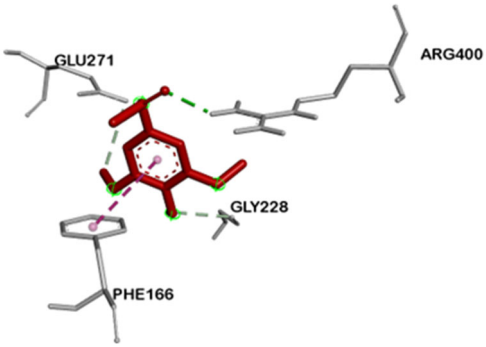
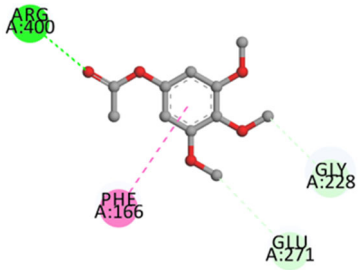
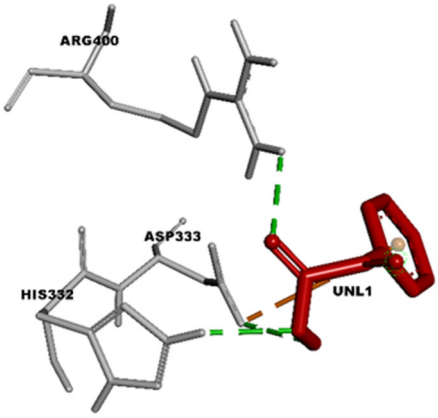
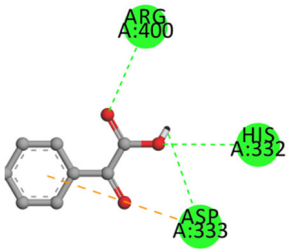
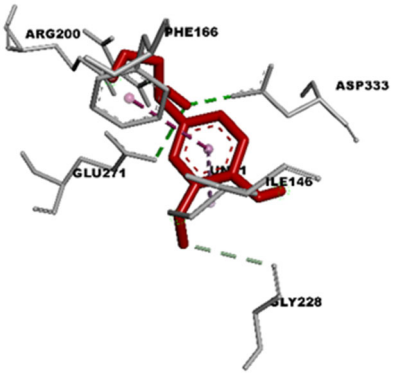
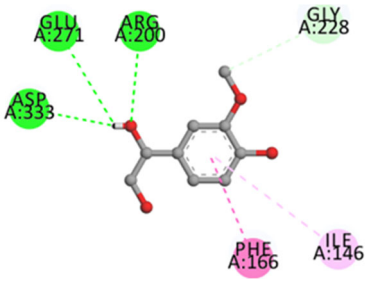
Name compound	Formula	Exact mass	Calculated mass	Error (ppm)	RT (min)	Area (Max.)	Group compound
Verrucarol	$C_{15}H_{22}O_4$	266.15157	266.15181	-0.90	9.965	16417936.36	Terpene
7,8,3',4'-Tetrahydroxyflavone	$C_{14}H_{22}N_6O_6$	370.15984	370.16008	-0.65	4.907	14015403.41	Flavonoid
Lacinilene C 7-methyl ether	$C_{16}H_{20}O_3$	260.14034	260.14125	-3.47	17.246	13799679.93	Aromatic
Soyasapogenol A	$C_{30}H_{50}O_4$	474.36962	474.37091	-2.71	18.586	13568057.22	Terpene
6-(a-D-Glucosaminyl)-*1D*-myo-inositol	$C_{12}H_{23}NO_{10}$	341.13124	341.13220	-2.81	0.700	13242568.74	Other compounds
N-Stearoylglycine	$C_{20}H_{39}NO_3$	341.2918	341.29299	-3.49	11.179	7392323.81	Other compounds
3-Phenylpropanoic acid	$C_9H_{10}O_2$	150.0678	150.06808	-1.86	7.246	6193243.365	Phenylpropane

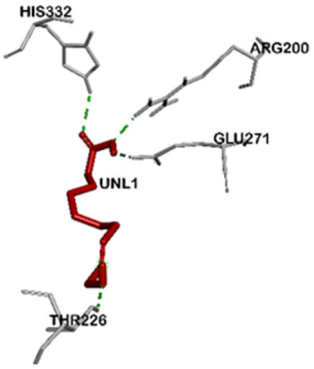
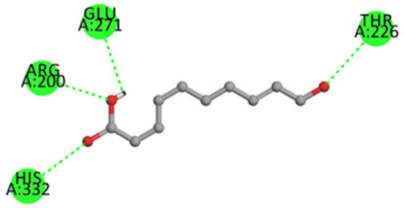
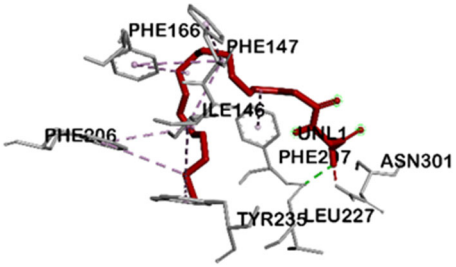
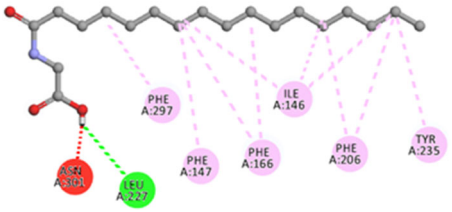
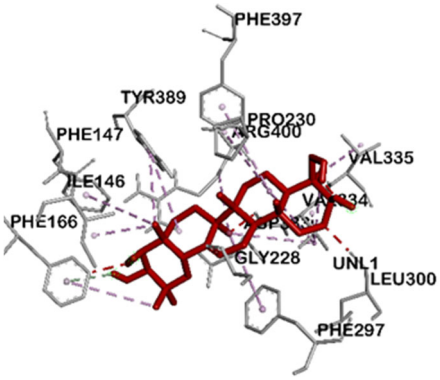
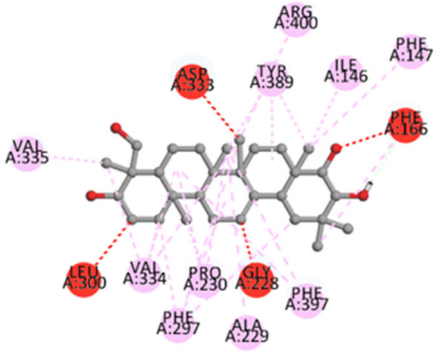
Table S2. Prediction results of compounds on antidiabetic activity from PASS Online

Name	Antidiabetic activity p.a. value	
	α-Glucosidase (Pa)	Antidiabetic
1-(7-Hydroxy-2-(hydroxymethyl)-2-methyl-*2H*-chromen-6-yl) ethanone	0.102	0.402
Sorbic acid	0.086	0.305
3,5-Dimethoxybenzoic acid	0.114	0.388
Carvone	-	0.317
Senkyunolide A	0.124	0.42
Methyl palmitate	0.131	0.332
6-Methoxymellein	0.121	0.345
Erucic acid	0.146	0.416
Vanylglycol	0.118	0.302
Nepodin	0.111	0.336
3,4,5-Trimethoxyphenyl acetate	0.079	0.335
(8*E*)-10-Hydroxy-8-decenoic acid	0.132	0.334
Graminiliatrin	-	0.316
Geranyl glucoside	-	0.598
Phenylglyoxylic acid	0.102	0.535
Nicotinic acid	0.089	0.334
Naringenin	0.321	0.301
Azafrin	-	0.466
Verrucarol	0.182	0.652
Soyasapogenol A	0.546	0.372
6-(a-*D*-glucosaminyl)-*1D*-myo-inositol	0.772	0.636
N-Stearoylglycine	0.102	0.318
3-Phenylpropanoic acid	0.099	0.518

Table S3. Visualization of the docking results of compounds with the α-glucosidase enzyme receptor

Compound	3D	2D
Acarbose (positive control)		

Compound	3D	2D
1-(7-Hydroxy-2-(hydroxymethyl)-2-methyl-*2H*-chromen-6-yl)ethenone (**1**)		
3,4,5-Trimethoxyphenylacetate (**2**)		
Phenylglyoxylicacid (**3**)		
Vanylglycol (**4**)		

Compound	3D	2D
(8*E*)-10-Hydroxy-8-decenoicacid (**5**)		
N-Stearoylglycine (**6**)		
SoyasapogenolA (**7**)		
Geranylglucoside (**8**)