Supplementary Data

This supplementary data is a part of a paper entitled "Screening of Potential Compounds in Tomato (*Solanum lycopersicum*) as Candidates for Anti Diabetes Mellitus Complications".

Table S1. Molinspiration screening result of the bioactive compound in tomato

CID	Compound	Canonical SMILES	miLogP	TPSA	MW	nON	nOHNH	nViolate	nrotb
932	Naringenin	C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC=C(C=C3)O	2.12	86.99	272.26	5	3	0	1
5280443	Apigenin	C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O	2.46	90.89	270.24	5	3	0	1
689043	Caffeic acid	C1=CC(=C(C=C1C=CC(=O)O)O)O	0.94	77.75	180.16	4	3	0	2
5281654	Isorhamnetin	COC1=C(C=CC(=C1)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O	1.99	120.36	316.26	7	4	0	2
5281708	Daidzein	C1=CC(=CC=C1C2=COC3=C(C2=O)C=CC(=C3)O)O	2.56	70.67	254.24	4	2	0	1
6441280	5-*p*-Coumaroylquinic acid	C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC=C(C=C2)O)O)O	0.04	144.52	338.31	8	5	0	5
8468	Vanillic acid	COC1=C(C=CC(=C1)C(=O)O)O	1.19	66.76	168.15	4	2	0	2
637542	*p*-coumaric acid	C1=CC(=CC=C1C=CC(=O)O)O	1.43	57.53	164.16	3	2	0	2
5280863	Kaempferol	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O	2.17	111.12	286.24	6	4	0	1
445858	Ferulic acid	COC1=C(C=CC(=C1)C=CC(=O)O)O	1.25	66.76	194.19	4	2	0	3
72276	Epicatechin	C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O	1.37	110.37	290.27	6	5	0	1
637775	Sinapinic acid	COC1=CC(=CC(=C1O)OC)C=CC(=O)O	1.26	76.00	224.21	5	2	0	4
4788	Phloretin	C1=CC(=CC=C1CCC(=O)C2=C(C=C(C=C2O)O)O)O	2.66	97.98	274.27	5	4	0	4
370	Gallic acid	C1=C(C=C(C(=C1O)O)O)C(=O)O	0.59	97.98	170.12	5	4	0	1
5280961	Genistein	C1=CC(=CC=C1C2=COC3=CC(=CC(=C3C2=O)O)O)O	2.27	90.89	270.24	5	3	0	1
9064	Catechin	C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O	1.37	110.37	290.27	6	5	0	1
10742	Syringic acid	COC1=CC(=CC(=C1O)OC)C(=O)O	1.20	76.00	198.17	5	2	0	3
5280343	Quercetin	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O	1.68	131.35	302.24	7	5	0	1
21676162	Quercetin 3'-*O*-sulfate	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)OS(=O)(=O)O)O	−0.75	174.73	382.30	10	5	0	3

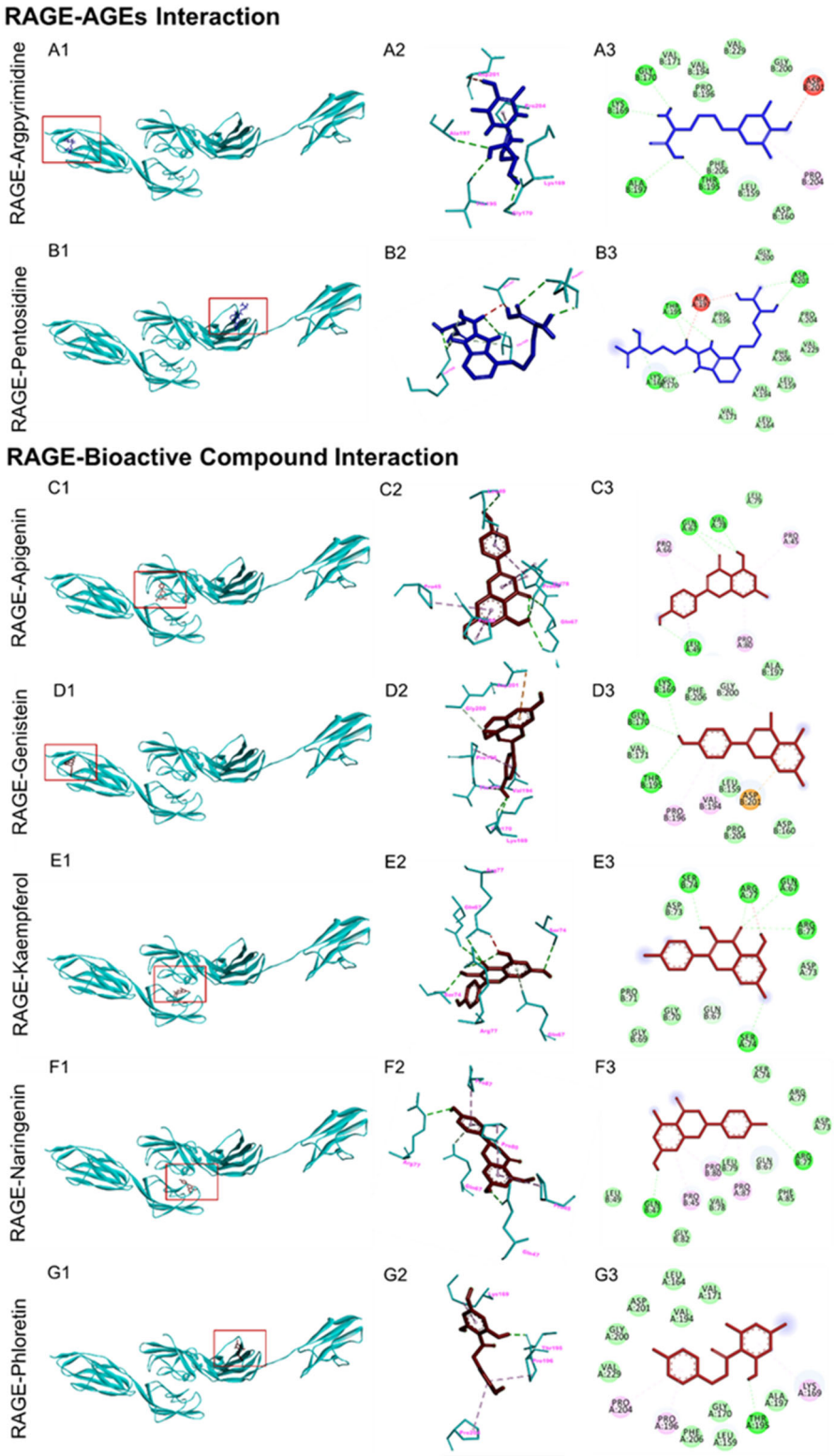

Fig S1. Comparation of binding poses and ligand interaction between RAGE-AGEs and RAGE-bioactive compound tomato fruit. Light blue represents RAGE, dark blue represents AGEs and red represents bioactive compounds tomato fruit

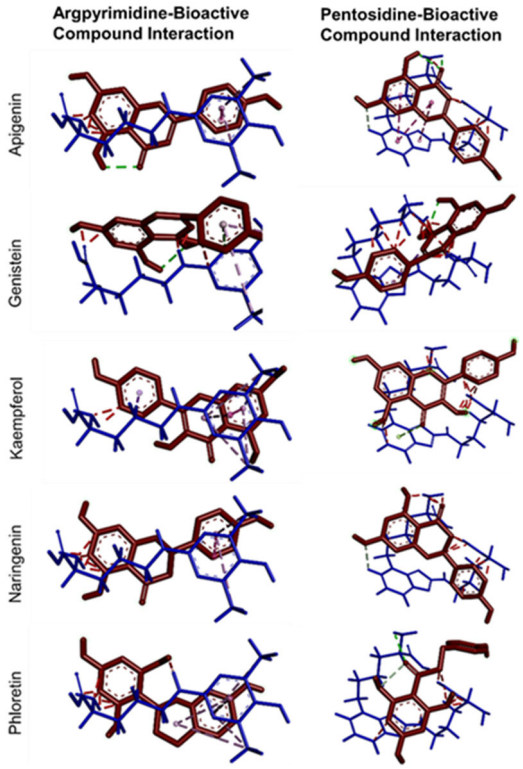

Fig S2. Comparation of binding poses and ligand interaction between AGEs with bioactive compound tomato fruit. Dark blue represents AGEs and red represents bioactive compounds tomato fruit

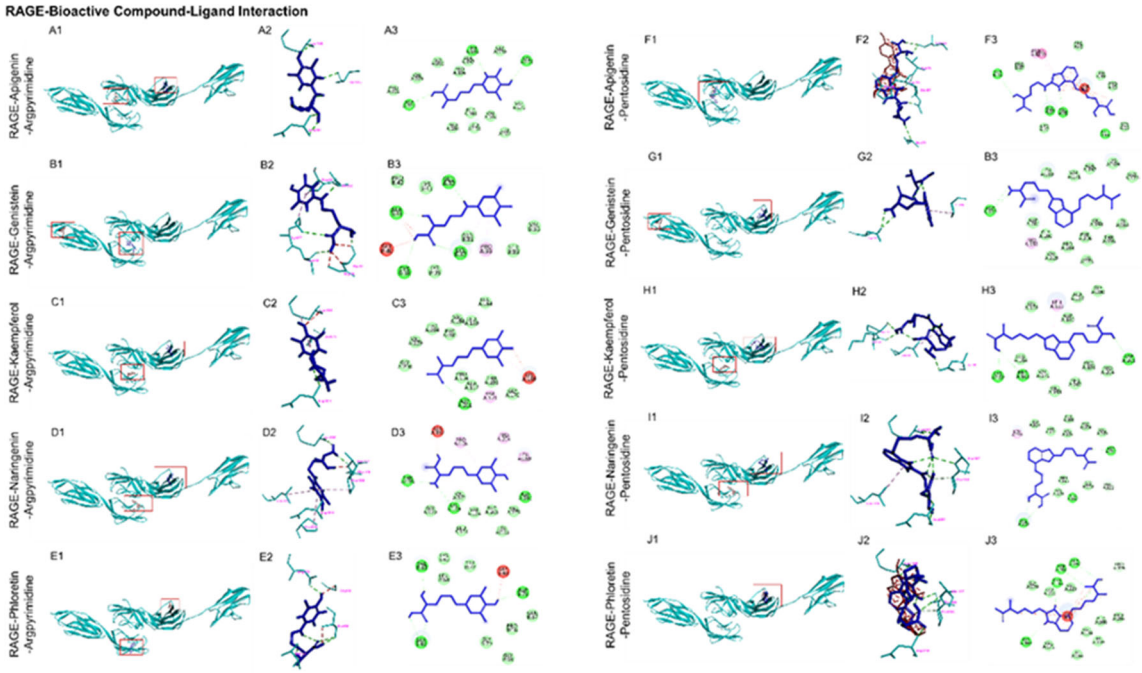

Fig S3. Comparation of binding poses and ligand interaction between complex RAGE-bioactive compound tomato fruit with AGEs. Light blue represents RAGE, dark blue represents AGEs and red represents bioactive compounds tomato fruit

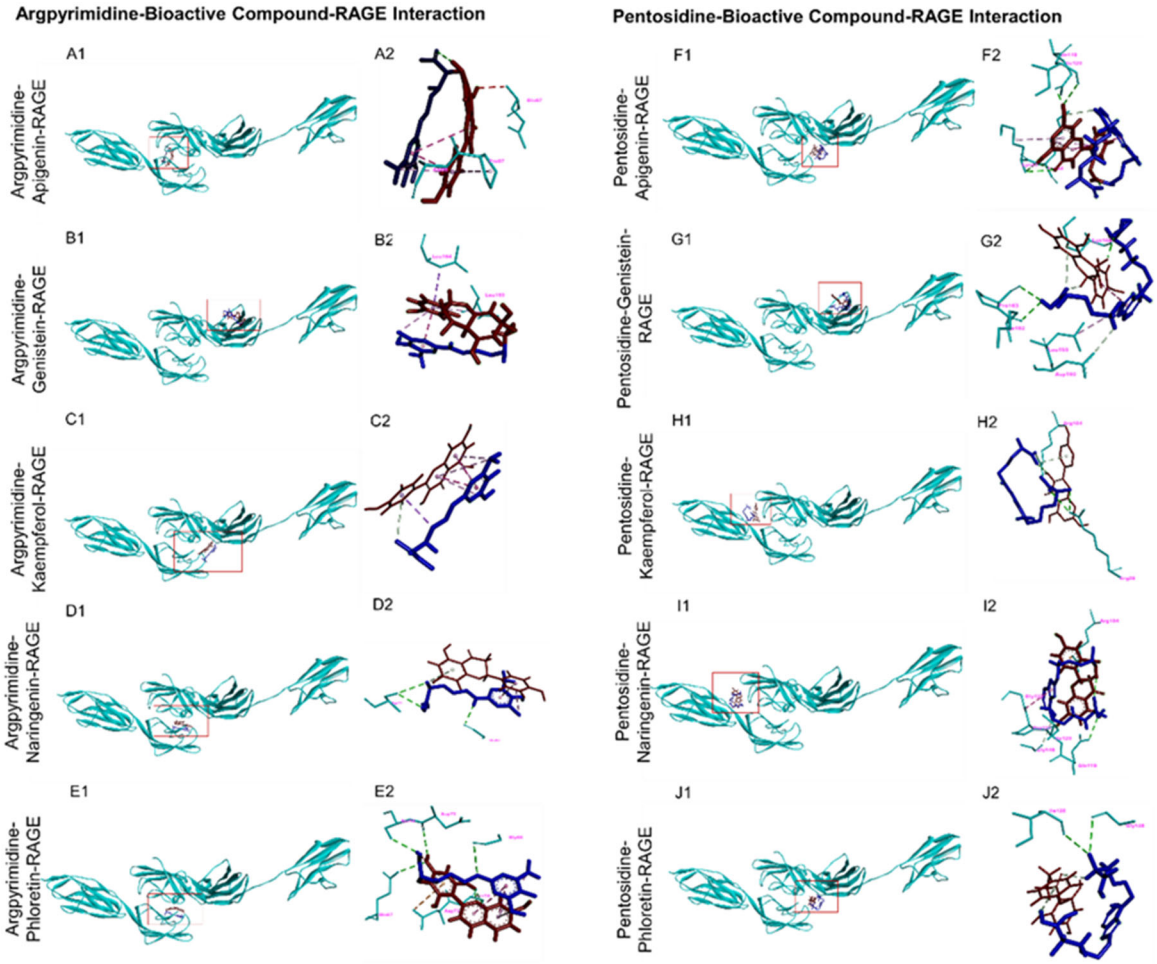

Fig S4. Comparation of binding poses and ligand interaction between complex AGEs-bioactive compound tomato fruit with RAGE. Dark blue represents AGEs and red represents bioactive compounds tomato fruit. Light blue represents RAGE, dark blue represents AGEs, and red represents bioactive compounds tomato fruit

Table S2. Interaction of RAGE with AGEs and RAGE with bioactive compound of tomato fruit

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
RAGE-Argpyrimidine			
N:UNK1:H - B:LYS169:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - B:GLY170:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - B:THR195:O	Hydrogen bond	Conventional hydrogen bond	−5.6
B:ALA197:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1 - B:PRO204	Hydrophobic	Pi-alkyl	
RAGE-Pentosidine			
N:UNK1:H - A:THR195:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:LYS169:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:ASP201:O	Hydrogen bond	Conventional hydrogen bond	−5.7
N:UNK1:HN - A:THR195:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:HN - A:LYS169:O	Hydrogen bond	Conventional hydrogen bond	

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
A:ASP201:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:C - A:LYS169:O	Hydrogen bond	Carbon hydrogen bond	
A:THR195:CB - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	
RAGE-Apigenin			
N:UNK1:H - A:LEU49:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:GLN67:OE1	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:VAL78:O	Hydrogen bond	Conventional hydrogen bond	
A:GLN67:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
A:LEU49:CD1 - N:UNK1	Hydrophobic	Pi-sigma	−6.6
N:UNK1 - A:PRO45	Hydrophobic	Pi-alkyl	
N:UNK1 - A:PRO66	Hydrophobic	Pi-alkyl	
N:UNK1 - A:VAL78	Hydrophobic	Pi-alkyl	
N:UNK1 - A:PRO80	Hydrophobic	Pi-alkyl	
N:UNK1 - A:PRO66	Hydrophobic	Pi-alkyl	
RAGE-Genistein			
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - B:LYS169:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - B:GLY170:O	Hydrogen bond	Conventional hydrogen bond	
B:THR195:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	−7.3
B:GLY200:CA - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	
B:ASP201:OD2 - N:UNK1	Electrostatic	Pi-anion	
N:UNK1 - B:VAL194	Hydrophobic	Pi-alkyl	
N:UNK1 - B:PRO196	Hydrophobic	Pi-alkyl	
RAGE-Kaempferol			
N:UNK1:H - B:SER74:OG	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
A:GLN67:NE2 - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
A:SER74:OG - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	−7.0
A:ARG77:NH1 - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
B:ARG77:NH1 - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
B:GLN67:NE2 - N:UNK1	Hydrogen bond	Pi-donor hydrogen bond	
RAGE-Naringenin			
N:UNK1:H - B:GLN47:OE1	Hydrogen bond	Conventional hydrogen bond	
B:ARG77:NE - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
B:GLN67:NE2 - N:UNK1	Hydrogen bond	Pi-donor hydrogen bond	
N:UNK1 - B:PRO45	Hydrophobic	Pi-alkyl	−6.9
N:UNK1 - B:PRO80	Hydrophobic	Pi-alkyl	
N:UNK1 - A:PRO87	Hydrophobic	Pi-alkyl	
N:UNK1 - B:PRO80	Hydrophobic	Pi-alkyl	
RAGE-Phloretin			
N:UNK1:H - A:THR195:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1 - A:LYS169	Hydrophobic	Pi-alkyl	−6.3
N:UNK1 - A:PRO196	Hydrophobic	Pi-alkyl	

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
N:UNK1 - A:PRO204	Hydrophobic	Pi-alkyl	

Table S3. Interaction of AGEs with bioactive compound of tomato fruit

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
Argpyrimidine-Apigenin			
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	20.1
N:UNK1 - :LIG1	Hydrophobic	Pi-pi stacked	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
Argpyrimidine-Genistein			
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	40.1
:LIG1:N - N:UNK1	Other	Pi-lone pair	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
Argpyrimidine-Kaempferol			
:LIG1:H - N:UNK1	Hydrophobic	Pi-sigma	10.2
N:UNK1 - :LIG1	Hydrophobic	Pi-pi stacked	
N:UNK1 - :LIG1	Hydrophobic	Pi-pi stacked	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
Argpyrimidine-Naringenin			
:LIG1:N - N:UNK1	Other	Pi-lone pair	29.3
N:UNK1 - :LIG1	Hydrophobic	Pi-pi stacked	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
Argpyrimidine-Phloretin			
:LIG1:N - N:UNK1	Other	Pi-lone pair	17.0
N:UNK1 - :LIG1	Hydrophobic	Pi-pi stacked	
:LIG1:C - N:UNK1	Hydrophobic	Alkyl	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - :LIG1:C	Hydrophobic	Pi-alkyl	
:LIG1 - N:UNK1	Hydrophobic	Pi-alkyl	
Pentosidine-Apigenin			
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	30.4
:LIG1:H1 - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
:LIG1:H - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	
N:UNK1 - :LIG1	Hydrophobic	Pi-pi T-shaped	
N:UNK1 - :LIG1	Hydrophobic	Pi-pi T-shaped	
:LIG1 - N:UNK1	Hydrophobic	Pi-pi T-shaped	
Pentosidine-Genistein			

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
:LIG1:H - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	50.0
N:UNK1:C - :LIG1	Hydrophobic	Pi-sigma	
Pentosidine-Kaempferol			
N:UNK1:O - :LIG1	Other	Pi-lone pair	32.8
Pentosidine-Naringenin			
:LIG1:H - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	36.1
Pentosidine-Phloretin			
:LIG1:H2 - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
:LIG1:HA - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	15.8
:LIG1:HA - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	

Table S4. Interaction of RAGE-bioactive compound of tomato fruit-AGEs

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
RAGE-Apigenin-Argpyrimidine			
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:ASP201:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:LYS169:O	Hydrogen bond	Conventional hydrogen bond	−5.4
N:UNK1:HN - A:THR195:O	Hydrogen bond	Conventional hydrogen bond	
A:ASP201:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
RAGE-Genistein-Argpyrimidine			
N:UNK1:H - A:GLU32:OE2	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - B:ALA41:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - B:CYS38:O	Hydrogen bond	Conventional hydrogen bond	−6.0
B:LYS37:NZ - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1 - A:PRO33	Hydrophobic	Pi-alkyl	
N:UNK1 - B:LYS37	Hydrophobic	Pi-alkyl	
RAGE-Kaempferol-Argpyrimidine			
A:ASP201:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1 - A:LYS169	Hydrophobic	Pi-alkyl	−5.5
N:UNK1 - A:VAL171	Hydrophobic	Pi-alkyl	
RAGE-Naringenin-Argpyrimidine			
N:UNK1:H - A:LYS169:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:THR195:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:ASP201:O	Hydrogen bond	Conventional hydrogen bond	−5.2
N:UNK1 - A:LEU159	Hydrophobic	Pi-alkyl	
N:UNK1 - A:PRO196	Hydrophobic	Pi-alkyl	
N:UNK1 - A:PRO204	Hydrophobic	Pi-alkyl	
RAGE-Phloretin-Argpyrimidine			
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - B:VAL63:O	Hydrogen bond	Conventional hydrogen bond	−5.1
N:UNK1:H - B:SER65:OG	Hydrogen bond	Conventional hydrogen bond	

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
N:UNK1:H - B:ASP73:OD1	Hydrogen bond	Conventional hydrogen bond	
B:SER65:OG - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
RAGE-Apigenin-Pentosidine			
N:UNK1:H - A:GLN67:OE1	Hydrogen bond	Conventional hydrogen bond	−5.8
N:UNK1:H - B:SER74:OG	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:LEU64:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:LEU64:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:HN - A:VAL78:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:C - A:VAL78:O	Hydrogen bond	Carbon hydrogen bond	
A:LEU79:C,O;PRO80:N - N:UNK1	Hydrophobic	Amide-pi stacked	
N:UNK1 - A:PRO80	Hydrophobic	Pi-alkyl	
RAGE-Genistein-Pentosidine			
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	−5.0
N:UNK1:H - A:ASP160:OD2	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:ASP160:OD2	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1 - A:PRO196	Hydrophobic	Pi-alkyl	
RAGE-Kaempferol-Pentosidine			
N:UNK1:H - A:LYS162:O	Hydrogen bond	Conventional hydrogen bond	−5.8
N:UNK1:H - A:PRO163:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:ASP201:OD2	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:HN - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1 - A:LEU159	Hydrophobic	Pi-alkyl	
RAGE-Naringenin-Pentosidine			
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	−5.3
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:ASP201:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:LYS169:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:LYS169:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:HN - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
A:ALA197:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
A:ASP201:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
A:PRO196:CA - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	
N:UNK1 - A:LEU159	Hydrophobic	Pi-alkyl	
RAGE-Phloretin-Pentosidine			
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	−5.0
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:HN - A:THR195:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:HN - A:LYS169:O	Hydrogen bond	Conventional hydrogen bond	
A:ALA197:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
A:ASP201:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:C - A:LYS169:O	Hydrogen bond	Carbon hydrogen bond	

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
N:UNK1:C - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	
A:PRO196:CA - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	

Table S5. Interaction of AGEs-bioactive compound of tomato fruit-RAGE

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
Argpyrimidine-Apigenin-RAGE			
N:UNK1:H - N:LIG1:O	Hydrogen bond	Conventional hydrogen bond	−8.2
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi stacked	
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi stacked	
N:LIG1:C - B:ALA88	Hydrophobic	Alkyl	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - B:PRO87	Hydrophobic	Pi-alkyl	
N:UNK1 - B:ALA88	Hydrophobic	Pi-alkyl	
Argpyrimidine-Genistein-RAGE			
A:LEU164:CB - N:UNK1	Hydrophobic	Pi-sigma	−8.4
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi stacked	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - A:LEU159	Hydrophobic	Pi-alkyl	
Argpyrimidine-Kaempferol-RAGE			
N:LIG1:N - N:UNK1	Hydrogen bond	Pi-donor hydrogen bond	−7.9
N:LIG1:C - N:UNK1	Hydrophobic	Pi-sigma	
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi stacked	
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi stacked	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
Argpyrimidine-Naringenin-RAGE			
N:LIG1:N - B:SER74:OG	Hydrogen bond	Conventional hydrogen bond	−9.3
N:LIG1:H - B:GLY68:O	Hydrogen bond	Conventional hydrogen bond	
B:SER74:OG - N:LIG1:O	Hydrogen bond	Conventional hydrogen bond	
N:LIG1:N - N:UNK1	Hydrogen bond	Pi-donor hydrogen bond	
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi stacked	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
Argpyrimidine-Phloretin-RAGE			
N:LIG1:N - B:GLY68:O	Hydrogen bond	Conventional hydrogen bond	−8.4
N:UNK1:H - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:SER74:OG	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - B:ASP73:O	Hydrogen bond	Conventional hydrogen bond	
A:GLN67:NE2 - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
A:SER74:OG - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
B:SER74:OG - N:LIG1:O	Hydrogen bond	Conventional hydrogen bond	
A:ASP73:OD2 - N:UNK1	Electrostatic	Pi-anion	
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi stacked	
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi stacked	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
N:UNK1 - N:LIG1:C	Hydrophobic	Pi-alkyl	
Pentosidine-Apigenin-RAGE			
N:LIG1:HO - N:LIG1:O	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:GLN119:OE1	Hydrogen bond	Conventional hydrogen bond	
N:UNK1:H - A:ILE120:O	Hydrogen bond	Conventional hydrogen bond	
B:LYS43:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
B:LYS43:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
B:LYS44:N - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	−8.5
N:LIG1:H - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi T-shaped	
N:UNK1 - B:LYS43	Hydrophobic	Pi-alkyl	
N:UNK1 - B:LYS44	Hydrophobic	Pi-alkyl	
N:UNK1 - B:LYS44	Hydrophobic	Pi-alkyl	
Pentosidine-Genistein-RAGE			
N:LIG1:N - A:LYS169:O	Hydrogen bond	Conventional hydrogen bond	
N:LIG1:HO - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
N:LIG1:HO - A:LYS162:O	Hydrogen bond	Conventional hydrogen bond	
N:LIG1:HO - A:PRO163:O	Hydrogen bond	Conventional hydrogen bond	
N:LIG1:H - A:ASP160:OD2	Hydrogen bond	Carbon hydrogen bond	−8.4
N:UNK1:H - N:LIG1:O	Hydrogen bond	Carbon hydrogen bond	
N:LIG1:O - N:UNK1	Hydrogen bond	Pi-donor hydrogen bond	
N:LIG1 - N:UNK1	Hydrophobic	Pi-pi stacked	
N:LIG1 - A:LEU159	Hydrophobic	Pi-alkyl	
Pentosidine-Kaempferol-RAGE			
N:LIG1:O - N:UNK1:O	Hydrogen bond	Conventional hydrogen bond	
A:ARG104:NH1 - N:LIG1:O	Hydrogen bond	Conventional hydrogen bond	
B:ARG29:NH2 - N:LIG1:N	Hydrogen bond	Conventional hydrogen bond	−8.6
B:ARG29:NH2 - N:LIG1:O	Hydrogen bond	Conventional hydrogen bond	
N:LIG1:O - N:UNK1	Hydrogen bond	Pi-donor hydrogen bond	
Pentosidine-Naringenin-RAGE			
N:LIG1:O - N:LIG1:O	Hydrogen bond	Conventional hydrogen bond	
B:GLN119:NE2 - N:LIG1:O	Hydrogen bond	Conventional hydrogen bond	
N:LIG1:C - B:ILE120:O	Hydrogen bond	Carbon hydrogen bond	
N:LIG1:C - B:GLY148:O	Hydrogen bond	Carbon hydrogen bond	−8.6
N:UNK1:H - N:LIG1:O	Hydrogen bond	Carbon hydrogen bond	
A:ARG104:NH1 - N:UNK1	Hydrogen bond; electrostatic	Pi-cation; pi-donor hydrogen bond	
B:PRO121:C,O;GLY122:N - N:LIG1	Hydrophobic	Amide-pi stacked	
Pentosidine-Phloretin-RAGE			
N:LIG1:N - A:ILE120:O	Hydrogen bond	Conventional hydrogen bond	−8.4

Point interaction	Chemistry bond	Type	Binding affinity (kcal/mol)
N:LIG1:N - A:GLY148:O	Hydrogen bond	Conventional hydrogen bond	
N:LIG1:H - N:UNK1:O	Hydrogen bond	Carbon hydrogen bond	
N:LIG1:HO - N:UNK1	Hydrogen bond	Pi-donor hydrogen bond	