Supplementary Data

This supplementary data is a part of a paper entitled "On the Hypolipidemic Activity of Elicited Soybeans: Evidences Based on Computational Analysis".

Table S1. Toxicity profile of screened compounds from elicited soybeans

Name	CID	LD_{50} (mg/kg)	Class	Hepatotoxicity	Carcinogenicity	Immunotoxicity	Mutagenicity	Cytotoxicity
2-Amino-4-methylpyrimidine	7939	630	4	0.73	-0.72	-0.98	-0.87	-0.85
2-Hydroxyphenylalanine	91482	1460	4	-0.78	-0.7	-0.99	-0.69	-0.7
4-Piperidone	33721	338	4	-0.84	-0.74	-0.99	-0.83	-0.71
Choline	305	1391	4	-0.94	-0.78	-0.99	-0.91	-0.82
D-(+)-Maltose	439186	51	3	-0.91	-0.93	-0.97	-0.88	-0.79
D-(+)-Proline	8988	1000	4	-0.81	-0.66	-0.99	-0.74	-0.7
Daidzein	5281708	2430	5	-0.71	-0.58	-0.92	-0.85	-0.89
Daidzin	107971	3100	5	-0.82	-0.85	-0.59	-0.76	-0.69
DL-Alanine	602	2000	3	-0.84	-0.59	-0.99	-0.95	-0.66
DL-Arginine	232	7500	6	-0.96	-0.73	-0.99	-0.5	-0.7
DL-Carnitine	288	6690	6	-0.99	-0.62	-0.99	-0.9	-0.8
Genistein	5280961	2500	5	-0.69	-0.69	-0.97	-0.74	-0.91
Glycitein	5317750	2500	5	-0.72	-0.59	-0.52	-0.71	-0.89
Hexadecanamide	69421	1000	4	-0.82	-0.61	-0.99	-0.99	-0.72
Indole-3-acrylic acid	5375048	2500	5	0.65	0.67	-0.99	-0.86	-0.8
L-Aspartic acid	5960	923	4	-0.83	-0.79	-0.99	-0.94	-0.65
L-Glutamic acid	33032	4500	5	-0.84	-0.71	-0.99	-0.97	-0.64
L-Histidine	6274	15000	6	-0.66	-0.83	-0.99	-0.63	-0.74
L-Phenylalanine	6140	2400	5	-0.81	-0.82	-0.99	-0.87	-0.71
L-Pyroglutamic acid	7405	1000	4	-0.81	-0.72	-0.99	-0.85	-0.68
Oleoylethanolamide	5283454	10000	6	-0.76	0.51	-0.63	-0.93	-0.76
Pipecolic acid	849	5000	5	-0.73	-0.63	-0.99	-0.79	-0.73
Proline	145742	1000	4	-0.81	-0.66	-0.99	-0.74	-0.7
Trigonelline	5570	3720	5	-0.6	-0.66	-0.98	-0.94	-0.75
Valine	6287	12680	6	-0.82	-0.66	-0.99	-0.94	-0.64

Predicted by ProTox II

Table S2. Drug-likeness properties according to the Lipinski Rule of 5 from non-toxic compounds

Name	CID	miLogP	TPSA	MW	n H-acceptor	n H-donor	n Rotatable bond	n Violation
2-Hydroxyphenylalanine	91482	-1.29	83.55	181.19	4	4	3	0
4-Piperidone	33721	-0.68	29.1	99.13	2	1	0	0
Choline	305	-4.24	20.23	104.17	2	1	2	0
D-(+)-Proline	8988	-1.72	49.33	115.13	3	2	1	0
Daidzein	5281708	2.56	70.67	254.24	4	2	1	0
Daidzin	107971	0.77	149.82	416.38	9	5	4	0
DL-Arginine	232	-3.76	127.73	174.2	6	7	5	1
DL-Carnitine	288	-5.5	60.36	161.2	4	1	4	0
Genistein	5280961	2.27	90.89	270.24	5	3	1	0
Glycitein	5317750	2.38	79.9	284.27	5	2	2	0
Hexadecanamide	69421	6.54	43.09	255.45	2	2	14	2
Indole-3-acrylic acid	5375048	1.88	53.09	187.2	3	2	2	0
L-Aspartic acid	5960	-3.52	100.62	133.1	5	4	3	0
L-Glutamic acid	33032	-3.52	100.62	147.13	5	4	4	0
L-Histidine	6274	-3	92	155.16	5	4	3	0
L-Phenylalanine	6140	-1.23	63.32	165.19	3	3	3	0
L-Pyroglutamic acid	7405	-2.4	66.4	129.12	4	2	1	0
Oleoylethanolamide	5283454	6.81	49.33	325.54	3	2	17	2
Pipecolic acid	849	-1.22	49.33	129.16	3	2	1	0
Proline	145742	-1.72	49.33	115.13	3	2	1	0
Trigonelline	5570	-5.4	44.01	137.14	3	0	1	0
Valine	6287	-1.91	63.32	117.15	3	3	2	0

Table S3. Interaction of HMGCR's residues with the selected compounds

Compound	CID binding	Affinity	Residues	Distance	Category	Types	From	From chemistry	To	To chemistry
Daidzin	107971	-9.6	**A:LYS692:NZ -N:UNK1:O**	3.03427	**H-Bond**	**Convl. H-Bond**	A:LYS692:NZ	H-Donor	N:UNK1:O	H-Acceptor
			B:ASN755:ND2 - N:UNK1:O	3.29265	**H-Bond**	**Convl. H-Bond**	B:ASN755:ND2	H-Donor	N:UNK1:O	H-Acceptor
			B:ASN755:ND2 - N:UNK1:O	3.27517	**H-Bond**	**Convl. H-Bond**	B:ASN755:ND2	H-Donor	N:UNK1:O	H-Acceptor
			N:UNK1:H - A:SER684:OG	2.7973	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	A:SER684:OG	H-Acceptor
			N:UNK1:H - A:ASP690:O	2.37111	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	A:ASP690:O	H-Acceptor
			N:UNK1:H - A:ASP690:OD2	1.97389	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	A:ASP690:OD2	H-Acceptor
			B:LEU853:CD1 - N:UNK1	3.97328	Hydrophobic	Pi-Sigma	B:LEU853:CD1	C-H	N:UNK1	Pi-Orbitals
			B:LEU862:CD1 - N:UNK1	3.84722	Hydrophobic	Pi-Sigma	B:LEU862:CD1	C-H	N:UNK1	Pi-Orbitals
			N:UNK1 - B:LEU853	4.95043	Hydrophobic	Pi-Alkyl	N:UNK1	Pi-Orbitals	B:LEU853	Alkyl
			N:UNK1 - B:CYS561	4.95197	Hydrophobic	Pi-Alkyl	N:UNK1	Pi-Orbitals	B:CYS561	Alkyl
			N:UNK1 - B:LEU862	5.09967	Hydrophobic	Pi-Alkyl	N:UNK1	Pi-Orbitals	B:LEU862	Alkyl
			N:UNK1 - B:CYS561	4.34955	Hydrophobic	Pi-Alkyl	N:UNK1	Pi-Orbitals	B:CYS561	Alkyl
			N:UNK1 - B:ALA856	5.10395	Hydrophobic	Pi-Alkyl	N:UNK1	Pi-Orbitals	B:ALA856	Alkyl
Genistein	5280961	-8.6	**A:ARG590:NH2 - N:UNK1:O**	2.79121	**H-Bond**	**Convl. H-Bond**	A:ARG590:NH2	H-Donor	N:UNK1:O	H-Acceptor
			A:SER684:OG - N:UNK1:O	3.19659	**H-Bond**	**Convl. H-Bond**	A:SER684:OG	H-Donor	N:UNK1:O	H-Acceptor
			B:LYS735:NZ - N:UNK1:O	2.8359	**H-Bond**	**Convl. H-Bond**	B:LYS735:NZ	H-Donor	N:UNK1:O	H-Acceptor
			N:UNK1:H - B:ALA751:O	2.91581	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	B:ALA751:O	H-Acceptor
			N:UNK1:H - A:ASN658:OD1	1.96429	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	A:ASN658:OD1	H-Acceptor
			A:ARG590:NH1 - N:UNK1	4.26735	Electrostatic	Pi-Cation	A:ARG590:NH1	Positive	N:UNK1	Pi-Orbitals
			B:GLU559:OE2 - N:UNK1	4.00443	Electrostatic	Pi-Anion	B:GLU559:OE2	Negative	N:UNK1	Pi-Orbitals
			B:GLU559:OE2 - N:UNK1	3.94395	Electrostatic	Pi-Anion	B:GLU559:OE2	Negative	N:UNK1	Pi-Orbitals
			B:LEU853:CD2 - N:UNK1	3.50706	Hydrophobic	Pi-Sigma	B:LEU853:CD2	C-H	N:UNK1	Pi-Orbitals
			B:LEU862:CD1 - N:UNK1	3.72871	Hydrophobic	Pi-Sigma	B:LEU862:CD1	C-H	N:UNK1	Pi-Orbitals
			B:CYS561:SG - N:UNK1	5.54298	Other	Pi-Sulfur	B:CYS561:SG	Sulfur	N:UNK1	Pi-Orbitals
			N:UNK1 - B:LEU853	5.34734	Hydrophobic	Pi-Alkyl	N:UNK1	Pi-Orbitals	B:LEU853	Alkyl
			N:UNK1 - B:LEU862	5.25323	Hydrophobic	Pi-Alkyl	N:UNK1	Pi-Orbitals	B:LEU862	Alkyl
Daidzein	5281708	-8.5	**A:ARG590:NH2 - N:UNK1:O**	2.80075	**H-Bond**	**Convl. H-Bond**	A:ARG590:NH2	H-Donor	N:UNK1:O	H-Acceptor
			A:SER684:OG - N:UNK1:O	3.15974	**H-Bond**	**Convl. H-Bond**	A:SER684:OG	H-Donor	N:UNK1:O	H-Acceptor
			N:UNK1:H - A:ASN686:OD1	3.0307	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	A:ASN686:OD1	H-Acceptor
			N:UNK1:H - B:ALA751:O	2.80731	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	B:ALA751:O	H-Acceptor
			N:UNK1:H - B:GLY560:O	2.23544	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	B:GLY560:O	H-Acceptor
			A:ARG590:NH1 - N:UNK1	4.2511	Electrostatic	Pi-Cation	A:ARG590:NH1	Positive	N:UNK1	Pi-Orbitals
			B:GLU559:OE2 - N:UNK1	4.01366	Electrostatic	Pi-Anion	B:GLU559:OE2	Negative	N:UNK1	Pi-Orbitals
			B:GLU559:OE2 - N:UNK1	3.93646	Electrostatic	Pi-Anion	B:GLU559:OE2	Negative	N:UNK1	Pi-Orbitals
			B:LEU853:CD2 - N:UNK1	3.52474	Hydrophobic	Pi-Sigma	B:LEU853:CD2	C-H	N:UNK1	Pi-Orbitals
			B:LEU862:CD1 - N:UNK1	3.72139	Hydrophobic	Pi-Sigma	B:LEU862:CD1	C-H	N:UNK1	Pi-Orbitals
			B:CYS561:SG - N:UNK1	5.56651	Other	Pi-Sulfur	B:CYS561:SG	Sulfur	N:UNK1	Pi-Orbitals
			N:UNK1 - B:LEU853	5.33605	Hydrophobic	Pi-Alkyl	N:UNK1	Pi-Orbitals	B:LEU853	Alkyl
			N:UNK1 - B:LEU862	5.2419	Hydrophobic	Pi-Alkyl	N:UNK1	Pi-Orbitals	B:LEU862	Alkyl
Glycitein	5317750	-8.3	**A:ARG590:NH2 - N:UNK1:O**	2.82614	**H-Bond**	**Convl. H-Bond**	A:ARG590:NH2	H-Donor	N:UNK1:O	H-Acceptor
			A:SER684:OG - N:UNK1:O	3.10084	**H-Bond**	**Convl. H-Bond**	A:SER684:OG	H-Donor	N:UNK1:O	H-Acceptor
			N:UNK1:H - A:ASN686:OD1	2.8738	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	A:ASN686:OD1	H-Acceptor
			N:UNK1:H - B:ALA751:O	2.87066	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	B:ALA751:O	H-Acceptor
			N:UNK1:H - B:GLY560:O	1.95596	**H-Bond**	**Convl. H-Bond**	N:UNK1:H	H-Donor	B:GLY560:O	H-Acceptor
			N:UNK1:C - B:LEU862:O	3.41134	**H-Bond**	**Carbon H-Bond**	N:UNK1:C	H-Donor	B:LEU862:O	H-Acceptor
			A:ARG590:NH1 - N:UNK1	4.12612	**H-Bond; Electrostatic**	**Pi-Cation; Pi-Donor H-Bond**	A:ARG590:NH1	Positive; H-Donor	N:UNK1	Pi-Orbitals; Pi-Orbitals
			B:GLU559:OE2 - N:UNK1	3.98938	Electrostatic	Pi-Anion	B:GLU559:OE2	Negative	N:UNK1	Pi-Orbitals
			B:GLU559:OE2 - N:UNK1	3.88813	Electrostatic	Pi-Anion	B:GLU559:OE2	Negative	N:UNK1	Pi-Orbitals
			B:LEU853:CD2 - N:UNK1	3.67117	Hydrophobic	Pi-Sigma	B:LEU853:CD2	C-H	N:UNK1	Pi-Orbitals

Table S4. Interaction of PPAR-γ's residues with the selected compounds

Compound	CID binding	Affinity	Residues	Distance	Category	Types	From	From chemistry	To	To chemistry
Daidzin	107971	-9.4	N:LIG:H - A:PHE282:O	2.43755	**H-Bond**	**Convl. H-Bond**	N:LIG:H	H-Donor	A:PHE282:O	H-Acceptor
			N:LIG:H - A:TYR473:OH	2.26811	**H-Bond**	**Convl. H-Bond**	N:LIG:H	H-Donor	A:TYR473:OH	H-Acceptor
			A:ARG288:NH2 - N:LIG	3.74657	**Electrostatic**	Pi-Cation	A:ARG288:NH2	Positive	N:LIG	Pi-Orbitals
			N:LIG:H - N:LIG	2.86017	**H-Bond**	**Pi-Donor H-Bond**	N:LIG:H	H-Donor	N:LIG	Pi-Orbitals
			A:ILE326:CG2 - N:LIG	3.7403	Hydrophobic	Pi-Sigma	A:ILE326:CG2	C-H	N:LIG	Pi-Orbitals
			A:MET329:SD - N:LIG	5.67421	Other	Pi-Sulfur	A:MET329:SD	Sulfur	N:LIG	Pi-Orbitals
			A:MET329:C,O;LEU330:N - N:LIG	4.78194	Hydrophobic	Amide-Pi Stacked	A:MET329:C,O; LEU330:N	Amide	N:LIG	Pi-Orbitals
			N:LIG - A:CYS285	5.10379	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:CYS285	Alkyl
			N:LIG - A:ILE326	5.37822	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:ILE326	Alkyl
			N:LIG - A:ARG288	4.5586	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:ARG288	Alkyl
			N:LIG - A:ALA292	4.62351	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:ALA292	Alkyl
			N:LIG - A:LEU330	5.26033	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:LEU330	Alkyl
			N:LIG - A:ALA292	4.35872	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:ALA292	Alkyl
			N:LIG - A:ILE326	5.45466	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:ILE326	Alkyl
			N:LIG - A:LEU330	5.43682	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:LEU330	Alkyl
Genistein	5280961	-8.8	**A:TYR473:OH - N:LIG:O**	2.89748	**H-Bond**	**Convl. H-Bond**	A:TYR473:OH	H-Donor	N:LIG:O	H-Acceptor
			N:LIG:H - A:SER289:OG	2.50508	**H-Bond**	**Convl. H-Bond**	N:LIG:H	H-Donor	A:SER289:OG	H-Acceptor
			A:CYS285:SG - N:LIG	3.77324	**H-Bond; Other**	**Pi-Donor H-Bond; Pi-Sulfur**	A:CYS285:SG	H-Donor; Sulfur	N:LIG	Pi-Orbitals; Pi-Orbitals
			A:MET364:SD - N:LIG	5.44162	Other	Pi-Sulfur	A:MET364:SD	Sulfur	N:LIG	Pi-Orbitals
			A:PHE363 - N:LIG	4.78361	Hydrophobic	Pi-Pi Stacked	A:PHE363	Pi-Orbitals	N:LIG	Pi-Orbitals
			A:PHE363 - N:LIG	4.09096	Hydrophobic	Pi-Pi Stacked	A:PHE363	Pi-Orbitals	N:LIG	Pi-Orbitals
			A:PHE282 - N:LIG	5.56028	Hydrophobic	Pi-Pi T-shaped	A:PHE282	Pi-Orbitals	N:LIG	Pi-Orbitals
			A:HIS449 - N:LIG	4.63739	Hydrophobic	Pi-Pi T-shaped	A:HIS449	Pi-Orbitals	N:LIG	Pi-Orbitals
			N:LIG - A:CYS285	4.30893	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:CYS285	Alkyl
Daidzein	5281708	-8.2	A:ARG288:NE - N:LIG:O	3.22083	**H-Bond**	**Convl. H-Bond**	A:ARG288:NE	H-Donor	N:LIG:O	H-Acceptor
			N:LIG:C - A:ILE326:O	3.49014	**H-Bond**	**Carbon H-Bond**	N:LIG:C	H-Donor	A:ILE326:O	H-Acceptor
			A:ARG288:NH2 - N:LIG	3.78881	**Electrostatic**	Pi-Cation	A:ARG288:NH2	Positive	N:LIG	Pi-Orbitals
			A:ARG288:NH2 - N:LIG	3.35447	**H-Bond; Electrostatic**	**Pi-Cation; Pi-Donor H-Bond**	A:ARG288:NH2	Positive; H-Donor	N:LIG	Pi-Orbitals; Pi-Orbitals
			A:GLU295:OE1 - N:LIG	4.8574	**Electrostatic**	Pi-Anion	A:GLU295:OE1	Negative	N:LIG	Pi-Orbitals
			A:ILE326:CG2 - N:LIG	3.68906	Hydrophobic	Pi-Sigma	A:ILE326:CG2	C-H	N:LIG	Pi-Orbitals
			A:MET329:SD - N:LIG	5.80984	Other	Pi-Sulfur	A:MET329:SD	Sulfur	N:LIG	Pi-Orbitals
			A:MET329:SD - N:LIG	5.31762	Other	Pi-Sulfur	A:MET329:SD	Sulfur	N:LIG	Pi-Orbitals
			N:LIG - A:ALA292	4.2198	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:ALA292	Alkyl
			N:LIG - A:ILE326	5.27254	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:ILE326	Alkyl
			N:LIG - A:LEU330	5.37197	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:LEU330	Alkyl
			N:LIG - A:LEU333	4.77934	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:LEU333	Alkyl
			N:LIG - A:ARG288	4.89614	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:ARG288	Alkyl
			N:LIG - A:ALA292	5.16384	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:ALA292	Alkyl
			N:LIG - A:LEU330	4.84995	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:LEU330	Alkyl
Glycitein	5317750	-9	**A:SER289:OG - N:LIG:O**	3.07041	**H-Bond**	**Convl. H-Bond**	A:SER289:OG	H-Donor	N:LIG:O	H-Acceptor
			N:LIG:H - A:TYR473:OH	2.40194	**H-Bond**	**Convl. H-Bond**	N:LIG:H	H-Donor	A:TYR473:OH	H-Acceptor
			A:CYS285:SG - N:LIG	3.81406	**H-Bond; Other**	**Pi-Donor H-Bond; Pi-Sulfur**	A:CYS285:SG	H-Donor; Sulfur	N:LIG	Pi-Orbitals; Pi-Orbitals
			A:MET364:SD - N:LIG	5.48379	Other	Pi-Sulfur	A:MET364:SD	Sulfur	N:LIG	Pi-Orbitals
			A:PHE363 - N:LIG	4.68097	Hydrophobic	Pi-Pi Stacked	A:PHE363	Pi-Orbitals	N:LIG	Pi-Orbitals
			A:PHE363 - N:LIG	4.08115	Hydrophobic	Pi-Pi Stacked	A:PHE363	Pi-Orbitals	N:LIG	Pi-Orbitals
			A:PHE282 - N:LIG	5.50496	Hydrophobic	Pi-Pi T-shaped	A:PHE282	Pi-Orbitals	N:LIG	Pi-Orbitals
			A:HIS449 - N:LIG	5.25205	Hydrophobic	Pi-Pi T-shaped	A:HIS449	Pi-Orbitals	N:LIG	Pi-Orbitals
			A:HIS449 - N:LIG	4.74865	Hydrophobic	Pi-Pi T-shaped	A:HIS449	Pi-Orbitals	N:LIG	Pi-Orbitals
			N:LIG - A:CYS285	4.38482	Hydrophobic	Pi-Alkyl	N:LIG	Pi-Orbitals	A:CYS285	Alkyl