

## Supporting Information

# (-) Arctigenin and (+) Pinoresinol are antagonists of the Human Thyroid Hormone Receptor $\beta$ .

*Ifedayo Victor Ogungbe\**, Rebecca A. Crouch, Teresa Demeritte.

Department of Chemistry and Biochemistry, Jackson State University, Jackson, MS 39217.

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\*[Ifedayo.v.ogungbe@jsums.edu](mailto:Ifedayo.v.ogungbe@jsums.edu).

**Table S1.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and phenolics.

<b>Phenolics</b>	<b>Scores</b>	<b>Phenolics</b>	<b>Scores</b>	<b>Phenolics</b>	<b>Scores</b>
5-Sinapoylquinic acid	-113.61	4,5-Dicaffeoylquinic acid	-125.52	Dihydro-p-coumaric acid	-75.93
1,2'-Disinapoyl-2-feruloylgentiobiose	No dock	4-Caffeoylquinic acid	-123.42	Dihydrocaffeic acid	-79.81
1,2,2'-Triferuloylgentiobiose	No dock	4-Feruloylquinic acid	-128.78	Ellagic Acid	-90.63
1,2,2'-Trisinapoylgentiobiose	No dock	4-Hydroxybenzoic acid	-70.857	Ellagic acid acetyl-arabioside	-95.00
1,2-Diferuloylgentiobiose	No dock	4-Hydroxybenzoic acid 4-O-glucoside	-106.43	Ellagic acid acetyl-xyloside	-114.45
1,2-Disinapoylgentiobiose	No dock	4-Hydroxyphenylacetic acid	-70.814	Ellagic acid arabioside	-128.81
1,3-Dicaffeoylquinic acid	-115.45	4-Sinapoylquinic acid	-130.89	Ellagic acid glucoside	-105.82
1,5-Dicaffeoylquinic acid	-153.82	4-p-Coumaroylquinic acid	-118.52	Ferulic acid	-87.17
1-Caffeoylquinic acid	-124.44	5,5'-Dehydrodiferulic acid	-103.70	Ferulic acid 4-O-glucoside	-103.22
1-Sinapoyl-2,2'-diferuloylgentiobiose	No dock	5,8'-Benzofuran dehydrodiferulic acid	-133.23	Feruloyl glucose	-130.25
1-Sinapoyl-2-feruloylgentiobiose	No dock	5,8'-Dehydrodiferulic acid	-115.29	Feruloyl tartaric acid	-120.11
2,3-Dihydroxybenzoic acid	-72.38	5-Caffeoylquinic acid	-128.60	Gallic acid	-75.40
2,4-Dihydroxybenzoic acid	-72.27	5-Feruloylquinic acid	-121.52	Gallic acid 3-O-gallate	-117.71
2,5-di-S-Glutathionyl caftaric acid	No dock	5-O-Galloylquinic acid	-124.15	Gallic acid 4-O-glucoside	-100.68
2,6-Dihydroxybenzoic acid	-72.04	5-p-Coumaroylquinic acid	-116.12	Gallic acid ethyl ester	-87.46
2-Hydroxybenzoic acid	-70.81	8-O-4'-Dehydrodiferulic acid	-139.59	Galloyl glucose	-108.69
2-S-Glutathionyl caftaric acid	-118.98	Avenanthramide 2c	-114.39	Gentisic acid	-76.76
2,4-Methylcholestanol ferulate	No dock	Avenanthramide 2f	-113.07	Homovanillic acid	-85.09
2,4-Methylcholesterol ferulate	No dock	Avenanthramide 2p	-113.47	Homoveratric acid	-86.48
2,4-Methylenecholestanol ferulate	No dock	Avenanthramide K	-107.58	Hydroxycaffeic acid	-89.29
2,4-Methylthosterol ferulate	No dock	Benzoic Acid	-67.16	Isoferulic acid	-82.13
3,4-Dicaffeoylquinic acid	-123.66	Caffeic acid	-81.20	Lambertianin C	No dock
3,4-Diferuloylquinic acid	-73.28	Caffeic acid 4-O-glucoside	-97.40	Methoxyphenylacetic acid	-72.21
3,4-Dihydroxyphenylacetic acid	-80.73	Caffeic acid ethyl ester	-94.55	Protocatechuic acid	-74.42
3,5-Dicaffeoylquinic acid	-88.47	Caffeoyl aspartic acid	-113.73	Protocatechuic acid 4-O-glucoside	-101.66
3,5-Diferuloylquinic acid	-91.16	Caffeoyl glucose	-117.73	Punicalagin	No dock
3,5-Dihydroxybenzoic acid	-75.46	Caffeoyl tartaric acid	-112.26	Rosmarinic acid	-141.06
3-Caffeoylquinic acid	-127.07	Campesterol ferulate	No dock	Sanguin H-6	No dock

**Table S1 Cont'd.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and phenolics.

<b>Phenolics</b>	<b>Scores</b>	<b>Phenolics</b>	<b>Scores</b>	<b>Phenolics</b>	<b>Scores</b>
3-Feruloylquinic acid	-127.30	Chicoric acid	-121.21	Schottenol ferulate	No dock
3-Hydroxybenzoic acid	-69.55	Cinnamic acid	-74.30	Sinapic acid	-94.22
3-Sinapoylquinic acid	-121.75	Cinnamoyl glucose	-95.86	Sinapine	-112.48
3-p-Coumaroylquinic acid	-111.40	Dicaffeoylquinic acid	-120.11	Sitostanyl ferulate	No dock
Sitosterol ferulate	No dock	m-Coumaric acid	-76.20	p-Coumaroyl glycolic acid	-101.77
Stigmastanol ferulate	No dock	o-Coumaric acid	-77.87	p-Coumaroyl malic acid	-109.41
Syringic acid	-85.58	p-Coumaric acid	-77.86	p-Coumaroyl tartaric acid	-111.66
Valoneic acid dilactone	-134.47	p-Coumaric acid 4-O-glucoside	-127.75	p-Coumaroyl tyrosine	-120.12
Vanillic acid	-79.70	p-Coumaric acid ethyl ester	-89.71	p-Coumaroylquinic acid	-112.44
Verbascoside	-43.75	p-Coumaroyl glucose	-112.21		

**Table S2.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and miscellaneous polyphenols.

Miscellaneous Polyphenols	Scores	Miscellaneous Polyphenols	Scores	Miscellaneous Polyphenols	Scores
1,4-Naphtoquinone	-65.96	Bisdemethoxycurcumin	-132.57	Protocatechuic aldehyde	-70.20
2,3-Dihydroxy-1-guaiacylpropanone	-91.69	Carnosic acid	-72.31	Psoralen	-84.02
2-Methoxy-5-prop-1-enylphenol	-72.70	Carnosol	-70.76	Pyrogallol	-63.35
3,4-DHPEA-AC	-90.02	Carvacrol	-71.41	Rosmadial	-73.66
3,4-DHPEA-EA	-125.32	Catechol	-56.72	Rosmanol	-81.13
3,4-DHPEA-EDA	-132.56	Coumarin	-72.26	Scopoletin	-79.16
3,4-Dihydroxyphenylglycol	-79.381	Curcumin	-144.68	Sinapaldehyde	-89.23
3-Methoxyacetophenone	-72.66	Demethoxycurcumin	-141.03	Syringaldehyde	-85.49
3-Methylcatechol	-62.92	Demethyloleuropein	-147.46	Thymol	-68.56
4-Ethylcatechol	-70.86	Epirosmanol	-85.56	Tyrosol	-71.33
4-Ethylguaiacol	-72.76	Esculetin	-80.13	Umbelliferone	-76.50
4-Ethylphenol	-64.81	Esculin	-118.84	Vanillin	-73.31
4-Hydroxybenzaldehyde	-63.66	Estragole	-71.07	Xanthotoxin	-93.28
4-Hydroxycoumarin	-72.80	Eugenol	-79.67	[6]-Gingerol	-117.70
4-Methylcatechol	-63.63	Ferulaldehyde	-84.04	p-Anisaldehyde	-69.49
4-Vinylguaiacol	-72.90	Gallic aldehyde	-66.69	p-HPEA-AC	-81.37
4-Vinylphenol	-64.45	Guaiacol	-63.43	p-HPEA-EDA	-81.27
4-Vinylsyringol	-97.99	Hydroxytyrosol	-75.94		
5-Heneicosylresorcinol	-138.94	Hydroxytyrosol 4-O-glucoside	-99.41		
5-Heptadecylresorcinol	-134.83	Isopimpinellin	-81.91		
5-Nonadecylresorcinol	-117.53	Juglone	-66.74		
5-Pentacosenylresorcinol	-103.49	Ligstroside	-140.52		
5-Pentacosylresorcinol	-106.99	Ligstroside-aglycone	-122.81		
5-Pentadecylresorcinol	-127.88	Mellein	-54.40		
5-Tricosenylresorcinol	-118.36	Oleoside 11-methylester	-103.57		
5-Tricosylresorcinol	-133.53	Oleoside dimethylester	-117.01		
Acetyl eugenol	-93.06	Oleuropein	-146.59		
Anethole	-69.41	Oleuropein-aglycone	-127.56		
Arbutin	-100.20	Phenol	-53.14		
Bergapten	-83.27	Phlorin	-103.18		

**Table S3.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and stilbenes.

Stilbenes	Scores	Stilbenes	Scores	Stilbenes	Scores
Pallidol	No dock	Pterostilbene	-104.26	Resveratrol 5-O-glucoside	-124.76
Piceatannol	-103.11	Resveratrol	-96.56	d-Viniferin	-75.79
Piceatannol 3-O-glucoside	-128.68	Resveratrol 3-O-glucoside	-134.08	e-Viniferin	-35.01
Pinosylvin	-89.18				

**Table S4.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and flavanols.

Flavanols	Score	Flavanols	Score	Flavanols	Score
(+)-Catechin	-102.16	(-)-Epigallocatechin 3-O-gallate	-71.40	Procyanidin trimer C2	no dock
(+)-Catechin 3-O-gallate	-79.90	Cinnamtannin A2	no dock	Procyanidin trimer EEC	no dock
(+)-Catechin 3-O-glucose	-96.18	Procyanidin dimer B1	no dock	Procyanidin trimer T2	no dock
(+)-Gallocatechin	-105.79	Procyanidin dimer B2	no dock	Prodelfinidin dimer B3	no dock
(+)-Gallocatechin 3-O-gallate	-100.41	Procyanidin dimer B3	no dock	Theaflavin	no dock
(-)-Epicatechin	-101.96	Procyanidin dimer B4	no dock	Theaflavin 3'-O-gallate	no dock
(-)-Epicatechin 3-O-gallate	-147.60	Procyanidin dimer B5	no dock	Theaflavin 3,3'-O-digallate	no dock
(-)-Epicatechin-(2a-7)(4a-8)-epicatechin 3-O-galactoside	no dock	Procyanidin dimer B7	no dock	Theaflavin 3-O-gallate	no dock
(-)-Epigallocatechin	-108.08	Procyanidin trimer C1	no dock		

**Table S5.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and flavanones.

Flavanones	Scores	Flavanones	Scores	Flavanones	Scores
6-Geranyl naringenin	-133.93	Hesperidin	-3.03	Narirutin 4'-O-glucoside	No dock
6-Prenyl naringenin	-128.56	Isoxanthohumol	-101.24	Neoeriocitrin	No dock
8-Prenyl naringenin	-106.38	Naringenin	-96.5	Neohesperidin	-44.51
Didymin	-65.95	Naringenin 7-O-glucoside	-112.5	Pinocembrin	-93.69
Eriocitrin	-84.44	Naringin	No dock	Poncirin	-0.15
Eriodictyol	-106.94	Naringin 4'-O-glucoside	-71.63	Sakuranetin	-90.01
Eriodictyol 7-O-glucoside	-125.86	Naringin 6'-malonate	No dock		
Hesperetin	-99.69	Narirutin	-76.95		

**Table S6.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and anthocyanins, chalcones and dihydrochalcones.

<b>Anthocyanins/chalcones/ dihydrochalcones</b>	<b>Score</b>	<b>Anthocyanins/chalcones/ dihydrochalcones</b>	<b>Score</b>	<b>Anthocyanins/chalcones/ dihydrochalcones</b>	<b>Score</b>
Cyanidin	-104.28	Delphinidin 3-O-sambubioside	-9.02	Petunidin 3-O-(6"-acetyl-galactoside)	-23.02
Cyanidin 35-O-diglucoside	-56.81	Delphinidin 3-O-xyloside	-83.61	Petunidin 3-O-(6"-acetyl-glucoside)	-36.85
Cyanidin 3-(6-p-caffeoyl)glucoside	-61.97	Malvidin 35-O-diglucoside	no dock	Petunidin 3-O-(6"-p-coumaroyl-glucoside)	-45.46
Cyanidin 3-O-(6"-acetyl-galactoside)	-83.90	Malvidin 3-O-(6"-acetyl-galactoside)	no dock	Petunidin 3-O-arabioside	-16.94
Cyanidin 3-O-(6"-acetyl-glucoside)	-84.75	Malvidin 3-O-(6"-acetyl-glucoside)	-82.42	Petunidin 3-O-galactoside	-92.43
Cyanidin 3-O-(6"-dioxalyl-glucoside)	-61.27	Malvidin 3-O-(6"-caffeoyl-glucoside)	-78.30	Petunidin 3-O-glucoside	-41.88
Cyanidin 3-O-(6"-malonyl-3"-glucosyl-glucoside)	no dock	Malvidin 3-O-(6"-p-coumaroyl-glucoside)	-52.40	Petunidin 3-O-rhamnoside	-79.47
Cyanidin 3-O-(6"-malonyl-glucoside)	-116.71	Malvidin 3-O-arabioside	-48.71	Petunidin 3-O-rutinoside	-99.16
Cyanidin 3-O-(6"-p-coumaroyl-glucoside)	-69.40	Malvidin 3-O-galactoside	-40.87	Pigment A	no dock
Cyanidin 3-O-(6"-succinyl-glucoside)	-105.01	Malvidin 3-O-glucoside	-56.67	Pinotin A	no dock
Cyanidin 3-O-arabioside	-102.61	Pelargonidin	-93.11	Vitisin A	no dock
Cyanidin 3-O-galactoside	-71.25	Pelargonidin 35-O-diglucoside	no dock	Butein	-108.11
Cyanidin 3-O-glucosyl-rutinoside	no dock	Pelargonidin 3-O-(6"-malonyl-glucoside)	-123.74	Xanthohumol	-128.90
Cyanidin 3-O-rhamnosylglucoside	-123.03	Pelargonidin 3-O-(6"-succinyl-glucoside)	-107.32	3-Hydroxyphloretin 2'-O-glucoside	-68.72
Cyanidin 3-O-sambubioside	-2.78	Pelargonidin 3-O-arabioside	-95.30	3-Hydroxyphloretin 2'-O-xylosyl-glucoside	-146.84
Cyanidin 3-O-sambubiosyl 5-O-glucoside	no dock	Pelargonidin 3-O-galactoside	-89.19	Phloretin	-104.95
Cyanidin 3-O-sophoroside	-29.53	Pelargonidin 3-O-glucoside	-108.56	Phloretin 2'-O-xylosyl-glucoside	-103.33
Cyanidin 3-O-xyloside	-98.18	Pelargonidin 3-O-glucosyl-rutinoside	no dock	Phloridzin	-133.84
Cyanidin 3-O-xylosyl-rutinoside	no dock	Pelargonidin 3-O-rutinoside	-122.62	Dihydromyricetin 3-O-rhamnoside	-63.15
Cyanidin-3-O-glucoside	-68.87	Pelargonidin 3-O-sambubioside	no dock	Dihydroquercetin	-102.46
Delphinidin 35-diglucoside	-42.26	Pelargonidin 3-O-sophoroside	-1.83	Dihydroquercetin 3-O-rhamnoside	-78.58
Delphinidin 3-O-(6"-acetyl-galactoside)	-72.88	Peonidin	-101.11		
Delphinidin 3-O-(6"-acetyl-glucoside)	-83.72	Peonidin 3-O-(6"-acetyl-galactoside)	-33.03		

**Table S6 Cont'd.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and anthocyanins, chalcones and dihydrochalcones.

<b>Anthocyanins/chalcones/ dihydrochalcones</b>	<b>Score</b>	<b>Anthocyanins/chalcones/ dihydrochalcones</b>	<b>Score</b>		
Delphinidin 3-O-(6"-malonyl-glucoside)	-53.54	Peonidin 3-O-(6"-acetyl-glucoside)	-44.09		
Delphinidin 3-O-(6"-p-coumaroyl-glucoside)	-9.977	Peonidin 3-O-(6"-malonyl-glucoside)	-46.77		
Delphinidin 3-O-arabinoside	-59.50	Peonidin 3-O-(6"-p-coumaroyl-glucoside)	-42.09		
Delphinidin 3-O-feruloyl-glucoside	-14.40	Peonidin 3-O-arabinoside	-86.99		
Delphinidin 3-O-galactoside	-90.99	Peonidin 3-O-galactoside	-56.12		
Delphinidin 3-O-glucoside	-54.74	Peonidin 3-O-glucoside	-104.69		
Delphinidin 3-O-glucosyl-glucoside	-131.99	Peonidin 3-O-rutinoside	-83.00		
Delphinidin 3-O-rutinoside	-119.84	Petunidin 35-O-diglucoside	no dock		

**Table S7.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and flavones.

<b>Flavones</b>	<b>Scores</b>	<b>Flavones</b>	<b>Scores</b>	<b>Flavones</b>	<b>Scores</b>
5,6-Dihydroxy-7,8,3'4'-tetramethoxyflavone	-119.77	Chrysoeriol 7-O-(6"-malonyl-glucoside)	-93.25	Luteolin 7-O-diglucuronide	No dock
6-Hydroxyluteolin	-112.86	Chrysoeriol 7-O-apiosyl-glucoside	-114.25	Luteolin 7-O-glucoside	-123.10
6-Hydroxyluteolin 7-O-rhamnoside	-98.88	Chrysoeriol 7-O-glucoside	-130.94	Luteolin 7-O-glucuronide	-111.02
7,3',4'-Trihydroxyflavone	-106.22	Cirsilineol	-110.78	Luteolin 7-O-malonyl-glucoside	-141.74
7,4'-Dihydroxyflavone	-95.86	Cirsimaritin	-93.83	Luteolin 7-O-rutinoside	No dock
Apigenin	-98.03	Diosmin	-51.10	Neodiosmin	No dock
Apigenin 6,8-di-C-glucoside	No dock	Eupatorin	-106.76	Nepetin	-117.42
Apigenin 6-C-glucoside	-123.53	Gardenin B	-111.72	Nobiletin	-120.13
Apigenin 7-O-(6"-malonyl-apiosyl-glucoside)	No dock	Geraldone	-108.33	Pebrellin	-111.68
Apigenin 7-O-apiosyl-glucoside	-5.47	Hispidulin	-105.54	Rhoifolin	No dock
Apigenin 7-O-diglucuronide	No dock	Isorhoifolin	-79.89	Rhoifolin 4'-O-glucoside	No dock
Apigenin 7-O-glucoside	-62.61	Jaceosidin	-119.20	Scutellarein	-100.41
Apigenin 7-O-glucuronide	-121.85	Luteolin	-107.82	Sinensetin	-108.32
Baicalein	-100.80	Luteolin 6-C-glucoside	-137.01	Tangeretin	-111.16
Chrysin	-90.33	Luteolin 7-O-(2-apiosyl-6-malonyl)-glucoside	No dock	Tetramethylscutellarein	-95.99
Chrysoeriol 7-O-(6"-malonyl-apiosyl-glucoside)	No dock	Luteolin 7-O-(2-apiosyl-glucoside)	No dock		

**Table S8.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and flavonols.

Flavonols	Scores	Flavonols	Scores	Flavonols	Scores
3,7-Dimethylquercetin	-96.45	Kaempferol 3-O-acetyl-glucoside	-57.91	Quercetin 3-O-(6-malonyl-glucoside)	-64.26
3-Methoxynobiletin	-104.63	Kaempferol 3-O-galactoside	-48.10	Quercetin 3-O-(6-malonyl-glucoside) 7-O-glucoside	No dock
3-Methoxysinensetin	-87.87	Kaempferol 3-O-galactoside 7-O-rhamnoside	No dock	Quercetin 3-O-acetyl-rhamnoside	-26.38
3-methylgalangin	-99.82	Kaempferol 3-O-glucoside	-96.38	Quercetin 3-O-arabinoside	-51.79
5,3'4'-Trihydroxy-3-methoxy-6,7-methylenedioxyflavone 4'-O-glucuronide	-102.09	Kaempferol 3-O-glucosyl-rhamnosyl-galactoside	No dock	Quercetin 3-O-galactoside 7-O-rhamnoside	No dock
5,4'-Dihydroxy-3,3'-dimethoxy-6,7-methylenedioxyflavone 4'-O-glucuronide	-48.25	Kaempferol 3-O-glucosyl-rhamnosyl-glucoside	No dock	Quercetin 3-O-glucosyl-rhamnosyl-galactoside	No dock
6,8-Dihydroxykaempferol	-102.89	Kaempferol 3-O-glucuronide	-92.00	Quercetin 3-O-glucosyl-rhamnosyl-glucoside	No dock
Galangin	-97.48	Kaempferol 3-O-rhamnoside	-105.61	Quercetin 3-O-glucosyl-xyloside	-102.06
Isorhamnetin	-94.99	Kaempferol 3-O-rhamnosyl-rhamnosyl-glucoside	No dock	Quercetin 3-O-glucuronide	-88.40
Isorhamnetin 3-O-galactoside	-14.55	Kaempferol 3-O-rutinoside	No dock	Quercetin 3-O-rhamnoside	-82.80
Isorhamnetin 3-O-glucoside	-84.08	Kaempferol 3-O-sophoroside	-44.60	Quercetin 3-O-rutinoside	-127.47
Isorhamnetin 3-O-glucoside 7-O-rhamnoside	No dock	Kaempferol 3-O-sophoroside 7-O-glucoside	No dock	Quercetin 3-O-sophoroside	-4.36
Isorhamnetin 3-O-glucuronide	-56.06	Kaempferol 3-O-xylosyl-glucoside	-95.69	Quercetin 3-O-xyloside	-76.13
Isorhamnetin 3-O-rutinoside	-93.22	Kaempferol 3-O-xylosyl-rutinoside	No dock	Quercetin 3-O-xylosyl-glucuronide	-49.20
Isorhamnetin 4'-O-glucoside	-130.14	Morin	-90.36	Quercetin 3-O-xylosyl-rutinoside	No dock
Isorhamnetin 7-O-rhamnoside	-109.14	Myricetin 3-O-arabinoside	-75.54	Quercetin 4'-O-glucoside	-129.45
Jaceidin 4'-O-glucuronide	-101.84	Myricetin 3-O-galactoside	-56.96	Quercetin 74'-O-diglucoside	No dock
Kaempferide	-93.55	Myricetin 3-O-glucoside	-112.59	Rhamnetin	-97.99
Kaempferol	-85.86	Myricetin 3-O-rhamnoside	No dock	Spinacetin 3-O-(2-feruloylglucosyl)(1-6)-[apiosyl(1-2)]-glucoside	No dock



**Table S8 Cont'd.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and flavonols.

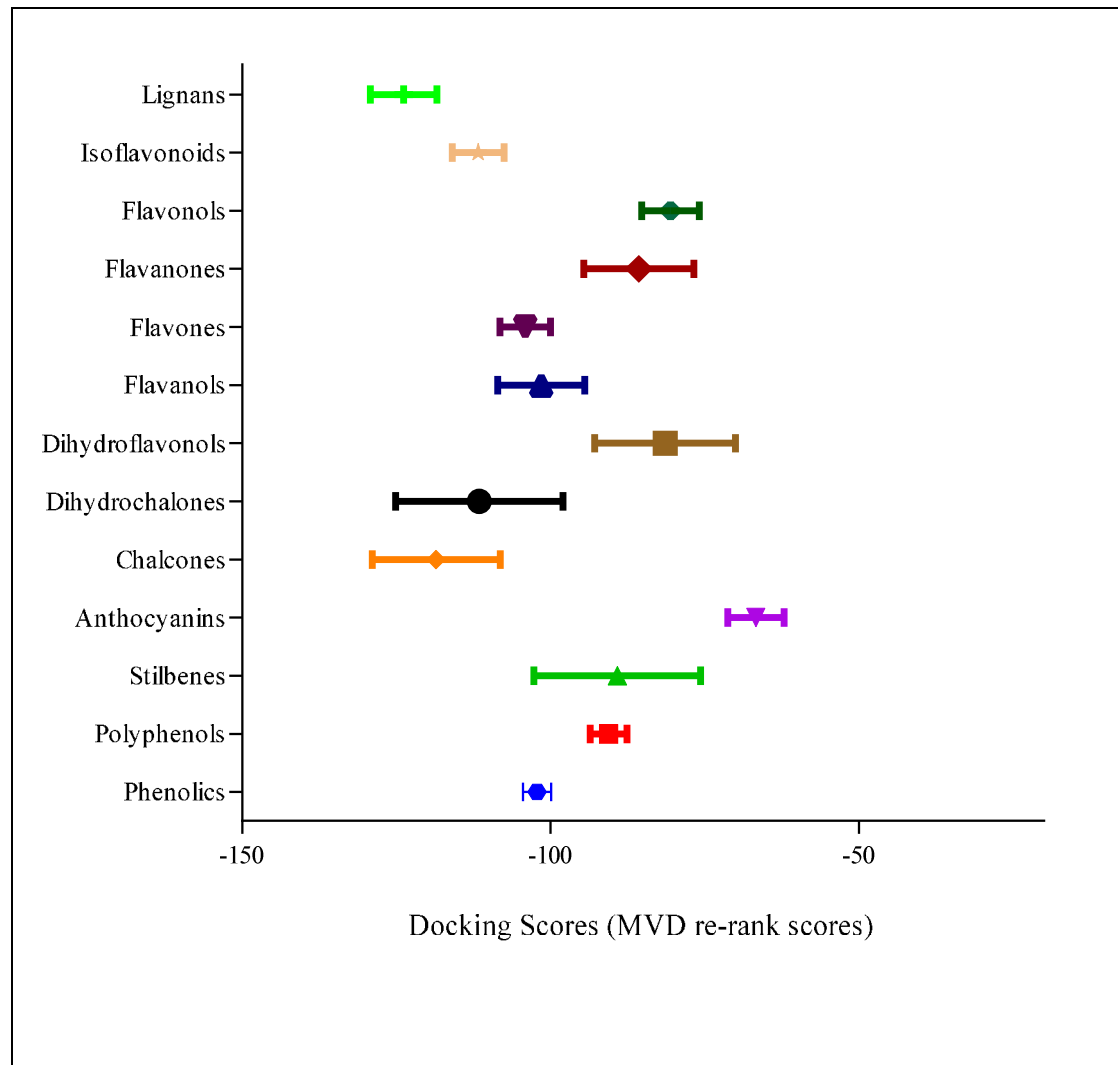
Kaempferol 3,7,4'-O-triglucoside	No dock	Myricetin 3-O-rutinoside	-28.75	Spinacetin 3-O-(2-p-coumaroylglucosyl)(1-6)-[apiosyl(1-2)]-glucoside	No dock
Kaempferol 3,7-O-diglucoside	No dock	Patuletin 3-O-(2"-feruloylglucosyl)(1-6)-[apiosyl(1-2)]-glucoside	No dock	Spinacetin 3-O-glucosyl-(1-6)-[apiosyl(1-2)]-glucoside	No dock
Kaempferol 3-O-(2"-rhamnosyl-6"-acetyl-galactoside)	No dock	Patuletin 3-O-glucosyl-(1-6)-[apiosyl(1-2)]-glucoside	No dock	Spinacetin 3-O-glucosyl-(1-6)-glucoside	No dock
Kaempferol 3-O-(2"-rhamnosyl-galactoside) 7-O-rhamnoside	No dock	Quercetin	-108.73	kaempferol 7-O-glucoside	-67.57
Kaempferol 3-O-(6"-acetyl-galactoside) 7-O-rhamnoside	0.99	Quercetin 3,4'-O-diglucoside	No dock	Myricetin	-115.28
Kaempferol 3-O-(6-malonyl-galactoside)	-86.42	Quercetin 3-O-(6"-acetyl-galactoside) 7-O-rhamnoside	No dock		

**Table S9.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and isoflavonoids.

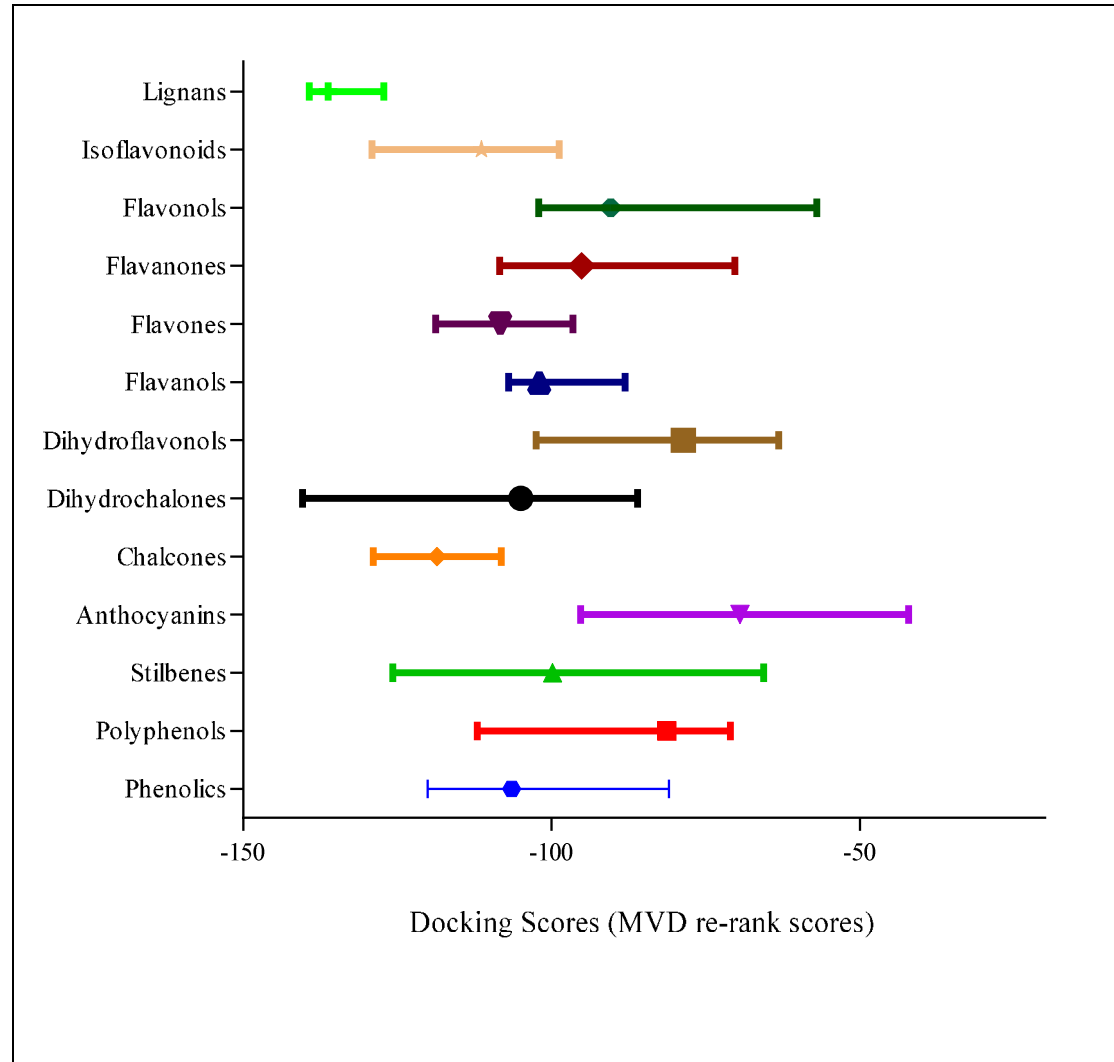
<b>Isoflavonoids</b>	<b>Scores</b>	<b>Isoflavonoids</b>	<b>Scores</b>	<b>Isoflavonoids</b>	<b>Scores</b>
6"-O-Acetyldaidzin	-120.41	6"-O-Malonylglucitin	-86.81	Formononetin	-99.38
6"-O-Acetylgenistin	-111.35	Biochanin A	-106.62	Genistein	-100.60
6"-O-Acetylglycitin	-121.46	Coumestrol	-86.79	Genistin	-134.90
6"-O-Malonyldaidzin	-130.52	Daidzein	-98.78	Glycitein	-96.36
6"-O-Malonylgenistin	-129.07	Daidzin	-129.23	Glycitin	-123.09

**Table S10.** Re-rank docking scores of human thyroid hormone receptor  $\beta$  and lignans.

<b>Lignans</b>	<b>Score</b>	<b>Lignans</b>	<b>Score</b>	<b>Lignans</b>	<b>Score</b>
1-Acetoxy-pinoreosinol	-57.03	Episesaminol	-130.75	Secoisolariciresinol-sesquilignan	-62.23
7-Hydroxymatairesinol	-136.28	Isohydroxymatairesinol	-140.07	Sesamin	-139.78
7-Hydroxysecoisolariciresinol	-134.65	Isolariciresinol	-45.78	Sesaminol	-125.54
7-Oxomatairesinol	-127.71	Lariciresinol	-136.14	Sesamolin	-137.84
Anhydro-secoisolariciresinol	-136.93	Lariciresinol-sesquilignan	-126.92	Sesamolol	-137.89
Arctigenin	-139.16	Matairesinol	-137.04	Syringaresinol	-139.36
Conidendrin	-91.08	Medioresinol	-143.02	Todolactol A	-139.25
Cyclolariciresinol	-73.67	Nortrachelogenin	-135.15	Trachelogenin	-144.24
Dimethylmatairesinol	-138.78	Pinoreosinol	-134.37		
Episesamin	-139.83	Secoisolariciresinol	-135.45		



**Figure S1.** Mean  $\pm$ SEM docking re-rank scores of polyphenolic compounds and human thyroid hormone receptor  $\beta$



**Figure S2.** Median docking scores with interquartile range of docking re-rank scores of polyphenolic compounds and human thyroid hormone receptor  $\beta$