Supplementary Table 1: Details of the interaction of Q (see **Figure 4A**) and Q3GA (see **Figure 4B**) docked to the human PPARα.

Ligand name	Protein target (receptor)	Cluster RMSD	Cluster number	Binding energy for the best docked compound of the cluster (ΔG, kcal/mol)	Dissoc. constant for the best docked compound of the cluster [μM]	Members	Amino acid residues at the binding cavity	**Number of hydrogen bonds**, and amino acid residues/chain responsible for H bond formation	**Number of hydrophobic interactions** and amino acid residues/chain implicated in the interaction
quercetin (Q)	PPARα	0	1	-11.44	0.0041	3.50%	Tyr214, Phe218, Met220, Asn221, Lys222, Thr279, Glu282, Thr283, Glu286, Met320, Ser323, Val324, Val332, Ala333, Tyr334, Gly335, Asp372, Ile375	**9**, (Tyr214/A, Tyr214/A, Lys22/A, Thr283/A, Glu286/A, Ser323/A, Tyr334/A, Tyr334/A, Asp372/A)	**4**, (Phe281/A, Thr279/A, Met320/A, Val324/A)
quercetin (Q)	PPARα	0	2	-10.33	0.0265	4.80%	Phe218, Asn219, Met220, Cys275, Cys278, Thr279, Glu282, Thr283, Glu286, Leu331, Val332, Ala333, Tyr334	**9**, (Asn219/A, Met220/A, Thr279/A, Glu282/A, Glu282/A, Glu286/A, Glu286/A, Ala333/A, Tyr334/A)	**5**, (Asn219/A, Met220/A, Thr279/A, Glu282/A, Tyr334/A)
quercetin (Q)	PPARα	0	3	-10.30	0.0279	1.10%	Tyr214, Phe218, Met220, Asn221, Lys222, Thr279, Thr283, Glu286, Met320, Leu321, Ser323, Val324, Met330, Leu331, Val332, Ala333, Tyr334, Gly335, Asp372, Ile375	**6**, (Tyr214/A, Lys222/A, Thr283/A, Ser323/A, Leu331/A, Leu331/A)	**4**, (Tyr214/A, Thr279/A, Leu321/A, Val324/A)
quercetin-3-O-glucuronide (Q3GA)	PPARα	0	1	-11.56	0.0033	4.80%	Ile272, Phe273, Cys275, Cys276, Thr279, Ser280, Thr283, Tyr314, Ile317, Leu321, Met330, Val332, Ile339, Leu344, Ile354, Met355, His440, Val444, Leu460, Tyr464	**5**, (Thr279/A, Thr283/A, Thr283/A, His440/A, Tyr464/A)	**5**, (Phe273/A, Thr279/A, Tyr314/A, Ile317/A, Leu321/A)

quercetin-3-O-glucuronide (Q3GA)	PPARα	0	2	-11.41	0.0043	5.20%	Val227, Ile228, Leu229, Ser230, Gly231, Lys232, Ala233, Ser234, Asn236, Pro237, Pro238, Val240, Leu331, Phe338	**6**, (Thr279/A, Glu282/A, Glu282/A, Leu331/A, Leu331/A, Ala333/A)	**4**, (Thr279/A, Glu282/A, Val332/A, Tyr334/A)
quercetin-3-O-glucuronide (Q3GA)	PPARα	0	3	-11.33	0.0049	6.10%	Met220, Val255, Ile272, Cys275, Cys276, Cys278, Thr279, Glu282, Val324, Met330, Leu331, Val332, Ala333, Tyr334, Ile339	**8**, (Asn219/A, Met220/A, Ser280/A, Thr283/A, Glu286/A, Leu331/A, Ala333/A, Tyr334/A)	**3**, (Thr283/A, Ile317/A, Met320/A)
quercetin-3-O-glucuronide (Q3GA)	PPARα	0	4	-11.19	0.0062	3.10%	Phe218, Asn219, Met220, Asn221, Cys276, Thr279, Ser280, Thr283, Glu286, Tyr314, Ile317, Met320, Leu321, Ser323, Val324, Met330, Leu331, Val332, Ala333, Tyr334, Gly335	**4**, (Thr279/A, Thr283/A, Ala333/A, Tyr334/A)	**2**, (Glu282/A, Tyr334/A)
quercetin-3-O-glucuronide (Q3GA)	PPARα	0	5	-10.83	0.0114	4.70%	Met220, Val255, Ile272, His274, Cys275, Cys276, Cys278, Thr279, Glu282, Thr283, Glu286, Met330, Leu331, Val332, Ala333, Tyr334	4, (Ser280/A, Leu331/A, Ala333/A, Tyr334A)	4, (Ile272/A, Thr279/A, Ile317/A, Val332/A)

Supplementary Table 2: Details of the interaction of Q (see **Figure 4C**) and Q3GA (see **Figure 4D**) docked to the human FASN.

Ligand name	Protein target (receptor)	Cluster RMSD	Cluster number	Binding energy for the best docked compound of the cluster (ΔG, kcal/mol)	Dissoc. constant for the best docked compound of the cluster [μM]	Members	Amino acid residues at the binding cavity	**Number of hydrogen bonds**, and amino acid residues/chain responsible for H bond formation	**Number of hydrophobic interactions** and amino acid residues/chain implicated in the interaction
quercetin (Q)	FASN	0	1	-11.28	0.0053	7.17%	Glu115, Phe117, Lys210, Asp214, Val217, Glu218, Leu244, Leu245, Pro247, His248, Leu251, Asn438, Met483, Phe494, Arg495, His496, Gly651, Arg652, Gly653	**11**, (Glu115/A, Lys210/A, Leu244/A, His248A, Phe494/A, Arg495/A, Arg495/A, His496/A, His496/A, Arg652/A, Arg652/A)	**1**, (His248/A)
quercetin (Q)	FASN	0	2	-10.97	0.009	5.75%	Phe117, Lys210, Asp214, Val217, Glu218, Met220, Pro221, Leu223, Leu245, His248, Asn438, Arg441, Arg442, Val482, Met483, Arg495, His496, Arg652	**12**, (Asp214/A, Glu218/A, Glu218/A, Met220/A, Arg441/A, Arg441/A, Arg442/A, Arg442/A, Arg495/A, His496/A, His496/A, Arg652/A)	**3**, (Asp214/A, Glu218/A, Glu218/A)
quercetin (Q)	FASN	0	3	-10.46	0.0213	7.07%	Gly517, Gly520, Gly521, Phe522, Gly523, Leu597, Lys621, Phe645, Ser646, Ser647, Val648, Trp686, Gly687, Ala688, Ile689, Gly693, Ile694, Leu695	**9**, (Gly517/A, Gly521/A, Phe522/A, Gly523/A, Phe645/A Ser646/A, Trp686/A, Gly687/A, Ile689/A)	**3**, (Phe522/A, Leu597/A, Trp686/A)

quercetin (Q)	FASN	0	4	-10.00	0.0463	1.51%	Val217, Glu218, Asn219, Met220, Leu223, His248, Pro249, Leu250, Asn438, Arg441, Arg442, Val482, Arg652, Gly653, Asn654, Ala655, Ser707	**7**, (Glu218/A, Met220/A, His248/A, Arg441/A, Arg441/A, Arg442/A, Asn654/A)	**4**, (Leu223/A, Leu250/A, Arg441/A, Arg442/A)
quercetin (Q)	FASN	0	5	-9.85	0.0596	2.62%	Gly517, Gly520, Gly521, Phe522, Gly523, Leu597, Val599, Phe645, Ala688, Ile689, Val692, Gly693, Ile694, Leu695, Val696	**7**, (Leu597/A, Ile689, Ile689, Ile689, Ile694/A, Leu695/A, Val696/A)	**2**, (Ile689/A, Ile694/A)
quercetin (Q)	FASN	0	6	-9.80	0.0649	2.42%	Gly517, Leu519, Gly520, Gly521, Ser542, Arg543, Ser544, Asn571, Ile572, Ser573, Leu597, Ala598, Val599, Val600, Lys619, Pro620	**9**, (Ser542/A, Arg543/A, Arg543/A, Asn571/A, Asn571/A, Asn571/A, Ile572/A, Leu597/A, Val599/A)	**5**, (Arg543/A, Ala598/A, Val599/A, Val600/A, Pro620/A)
quercetin (Q)	FASN	0	7	-9.74	0.0718	3.64%	Ile113, Glu115, Lys210, Pro247, His248, Pro249, Val648, Arg652, Gly687, Ala688, Val706, Ser707, Thr709, Phe735	**6**, (Glu115/A, His248/A, Arg652/A, Ala688/A, thr709/A, Thr709/A)	**7**, (Pro249/A, Val648/A, Thr709/A, Phe735/A, Phe735/A, Phe735/A, Phe735/A)
quercetin (Q)	FASN	0	8	-9.61	0.0894	2.22%	Gly517, Leu519, Gly520, Thr541, Ser542, Arg543, Ser544, Gly545, Gln551, Ser570, Asn571, Ile572, Ser573, Ala598, Val599, Val600, Lys619, Pro620	**9**, (Gly517/A, Thr541/A, Ser542/A, Arg543/A, Gln551/A, Ser570/A, Ile572/A, Val599/A, Val599/A)	**3**, (Arg543/A, Ile572/A, Ala598/A)

quercetin-3-O-glucuronide (Q3GA)	FASN	0	1	-13.67	0.0001	1.01%	Phe117, Lys210, Asp214, Val217, Glu218, Asn219, Met220, Leu223, His248, Pro249, Leu250, Asn438, Arg441, Arg442, Val482, Met483, Phe494, Arg495, His496, Gly651, Arg652, Gly653, Ser707	**14**, (Asp214/A, Glu218/A, Glu218/A, Asn438/A, Asn438/A, Arg441/A, Arg441/A, Arg442/A, Phe494/A, Arg495/A, His496/A, His496/A, Arg652/A, Arg652/A)	**5**, (Leu223/A, Pro249/A, Leu250/A, Arg441/A, Arg652/A)
quercetin-3-O-glucuronide (Q3GA)	FASN	0	2	-13.18	0.00	1.21%	Gly517, Gly520, Gly521, Phe522, Gly523, Leu597, Ala598, Val599, Lys621, Phe645, Ser646, Ser647, Val648, Tyr660, Asn664, Trp686, Gly687, Ala688, Ile689, Val692, Gly693, Ile694, Leu695, Val696	**10**, (Leu597/A, Lys621/A, Ser646/A, Tyr660/A, Tyr660/A, Trp686/A, Ile689/A, Ile689/A, Ile694/A, Leu695A)	**1**, (Ile694/A)
quercetin-3-O-glucuronide (Q3GA)	FASN	0	3	-12.68	0.0005	1.82%	Ala516, Gly517, Gly518, Leu519, Gly520, Thr541, Ser542, Arg543, Ser544, Gly545, Arg547, Gln551, Asn571, Ile572, Ser573, Leu597, Ala598, Val599, Val600, Lys619, Pro620, Ile694	**18**, (Gly517/A, Leu519/A, Leu519/A, Gly520/A, Thr541/A, Thr541/A, Thr541/A, Ser542/A, Arg543/A, Arg543/A, Ser544/A, Gly545/A, Gln551/A, Asn571/A, Asn571/A, Ile572/A, Ser 573/A, Val599/A)	**4**, (Ile572/A, Ala598/A, Val599/A, Pro620/A)

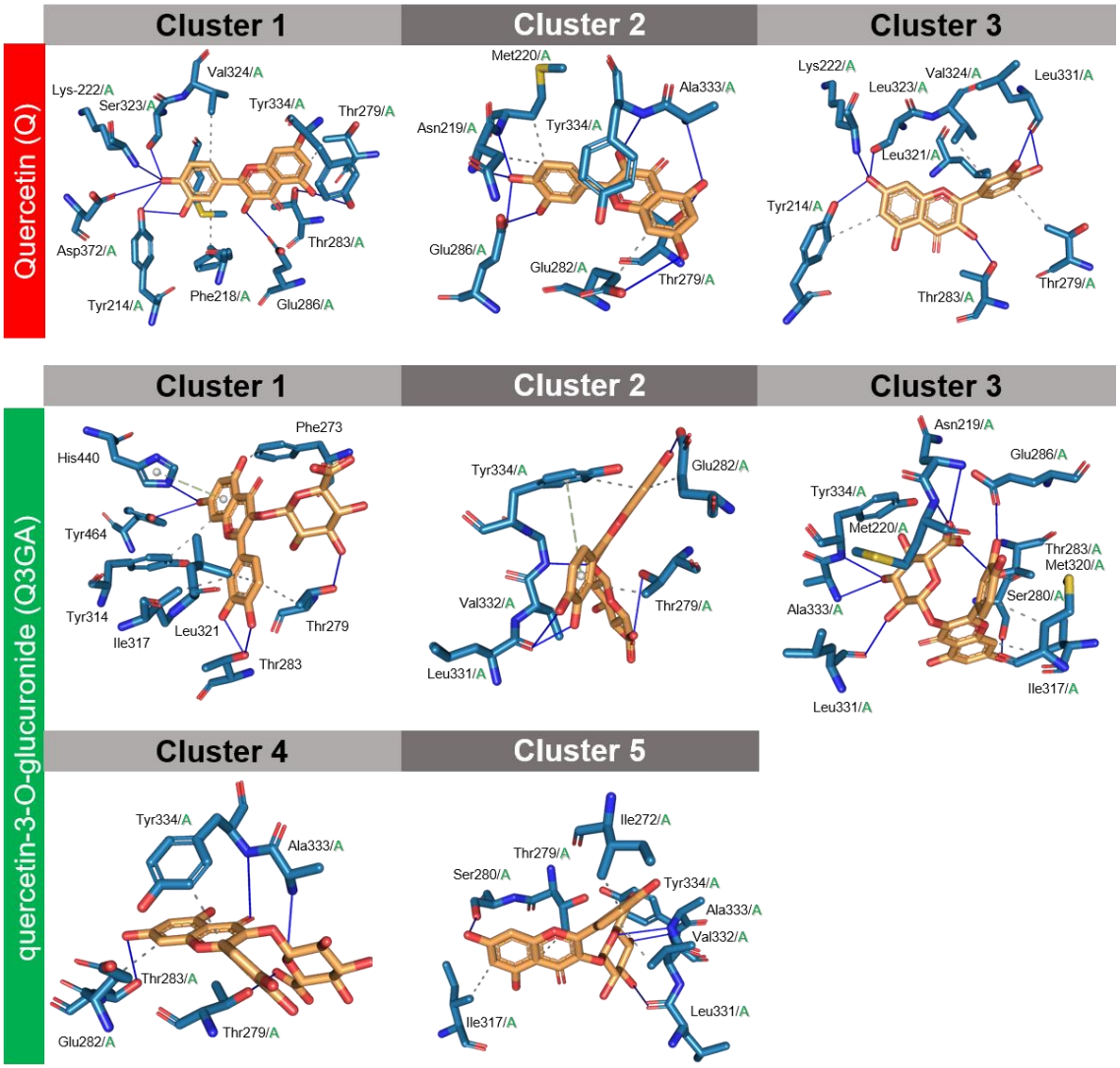
Supplementary Table 3: Details of the interaction of Q (see **Figure 4E**) and Q3GA (see **Figure 4F**) docked to the human AMPK.

Ligand name	Protein target (receptor)	Cluster RMSD	Cluster number	Binding energy for the best docked compound of the cluster (ΔG, kcal/mol)	Dissoc. constant for the best docked compound of the cluster [μM]	Members	Amino acid residues at the binding cavity	**Number of hydrogen bonds**, and amino acid residues/chain responsible for H bond formation	**Number of hydrophobic interactions** and amino acid residues/chain implicated in the interaction
quercetin (Q)	AMPK	0	1	-9.42	0.1233	4.50%	Pro365, His366, Pro367 (chain A) and Ile240, Asp245, Arg269, Tyr272, Phe273, Gly275, Val276, Leu277, Val297, His298, Arg299, Leu300, Val301 (chain E)	**5**, (Arg269/E, Leu277/E, Leu277/E, Arg299/E, Pro365/A)	**5**, (Ile240/E, Tyr272/E, Phe273/E, Leu277/E, Val279/E)
quercetin (Q)	AMPK	0	2	-9.36	0.1364	3.90%	Val11, Leu18, Lys29, Lys31, Ile46, Asn48, Asp88, Phe90 (chain A) and Val81, Arg83, Thr106, Arg107, Ser108, Asn111, Val113, Ile115 (chain B)	**3**, (Lys29/A, Lys31/A, Asn111/B)	**8**, (Val11/A, Val11/A, Leu18/A, Lys29/A, Lys31/A, Ile46/A, Ile46/A, Val113/B)
quercetin (Q)	AMPK	0	3	-9.29	0.1536	6.10%	Arg70, Met85, Thr87, Thr89, Asp90, Arg118, Tyr121, Leu122, Lys127, Ile150, His151, Arg152, Ser226, Lys243 (chain E)	**8**, (Arg70/E, Thr87/E, Thr89/E, Lys127/E, His151/E, Arg152/E, Arg152/E, Arg152/E)	**1**, (Thr87/E)

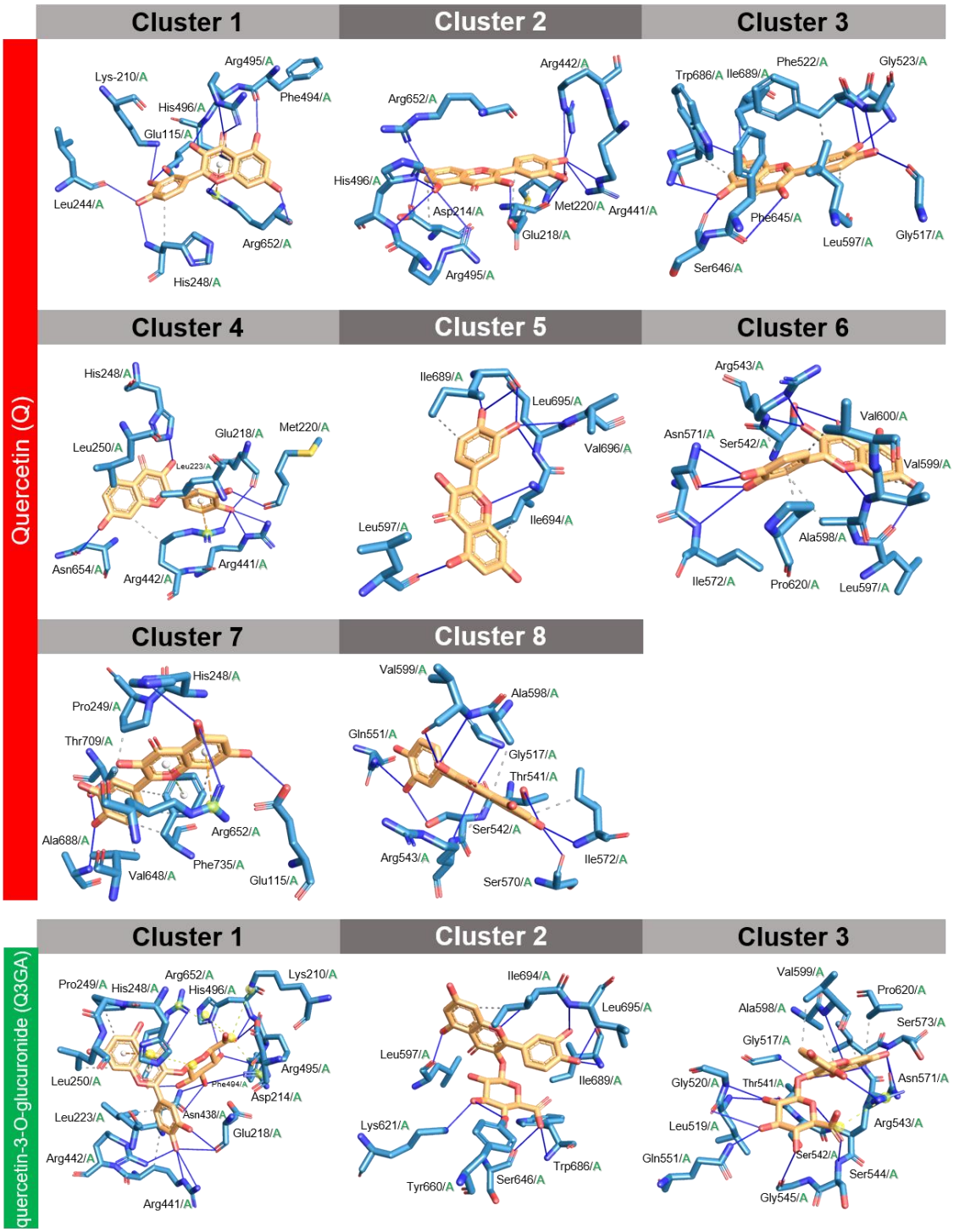
quercetin (Q)	AMPK	0	4	-8.86	0.3174	4.80%	Lys398, Lys399, Ala400, Trp402 (chain A) and Leu215, Leu242, Asp246, Val248, Val250, Leu265, Tyr267 (chain B) and Leu55, Lys59, Phe62, Ala63, Thr66, Asn67 (chain E)	**6**, (Lys59/E, Thr66/E, Asn67/E, Tyr267/B, Ala400/A, Trp402/A)	**2**, (Val248/B, Ala400/A)
quercetin-3-O-glucuronide (Q3GA)	AMPK	0	1	-10.36	0.0252	3.90%	Pro365, His366, Pro367, Arg369, (chain A) and Ala227, Ile240, Ser242, Phe244, Asp245, His268, Arg269, Tyr272, Phe273, Glu274, Gly275, Val276, Leu277, Ala295, Val297, His298, Arg299 (chain E)	**6**, /Ser242/E, Arg269/E, Leu277/E, Ala295/E, Arg299/E, Arg369/A)	**2**, (Glu247/E, Pro367/A)
quercetin-3-O-glucuronide (Q3GA)	AMPK	0	2	-9.64	0.085	2.60%	Arg70, Gly84, Met85, Thr87, Ile88, Thr89, Asp90, Tyr121, Lys127, Val130, Lys149, Ile150, His151, Arg152, Arg224, Ser226, Lys243 (chain E)	**10**, (Arg70/E, Arg70/E, Met85/E, Thr87/E, Thr89/E, Tyr121/E, Lys127/E, Arg152/E, Arg152/E, Lys243/E)	**3**, (Thr87/E, Ile150/E, Lys243/E)
quercetin-3-O-glucuronide (Q3GA)	AMPK	0	3	-9.25	0.1643	4.60%	Leu373, Ala375, Asp376, Val397, Lys398, Lys399, Ala400, Trp402 (chain A) and Leu242, Lys245, Asp246, Val248, Tyr267 (chain B) and Lys59, Phe62, Ala63, Thr66, Asn67, Lys253 (chain E)	**10**, (Thr66/E, Asp264/B, Lys253/E, Tyr267/B, Ala375//A, Asp376/A, Lys398/A, Ala400/A)	**2**, (Thr66/E, Tyr267/B)

quercetin-3-O-glucuronide (Q3GA)	AMPK	0	4	-9.11	0.2081	5.10%	Asp128, His131, Arg132, Met164, Ala191, Pro193, Glu194, Ile197, Pro253, Leu254, Arg256, Ala257, Thr258, Ile259, Lys260, Arg263 (chain A) and His209, Glu230, Pro231, Asn232, His233, Val234, Tyr261 (chain B)	**9**, (Asp128/A, Asp128/A, Glu230/B, Asn232/B, Asn232/B , Asn232/B, His233/B, Arg256/A, Tyr261/B)	**2**, (Glu194/A, Thr258/A)
quercetin-3-O-glucuronide (Q3GA)	AMPK	0	5	-9.02	0.2423	2.40%	Arg369, Met370, Pro371, Pro372, Leu373, Val397, Lys399, Ala400, Trp402 (chain A) and Leu215, Asn216, Asp218, Thr219, Ile221 (chain B) and Lys47, Val65, Thr66, Asn67 (chain E)	**10**, (Lys47/E, Val65/E, Thr66/E, Thr219/B, Thr219/B, Arg369/A, Leu373/A, Ala400/A, Ala400/A, Trp402/A)	**1**, (Asp218/B)
quercetin-3-O-glucuronide (Q3GA)	AMPK	0	6	-8.40	0.69	3.90%	Glu279, Glu291, Arg331, Met334, Asn335, Ser338, Tyr341, Leu342 (chain A) and Lys259, Lys260 (chain B) and Tyr39, Asp40, Thr44 (chain E)	**8**, (Tyr39/E, Asp40/E, Thr44/E, Thr44/E, Lys259/B, Lys260/B, Glu279/A, Glu291/A)	

Supplementary Figure 1: Each inset shows the detailed interactions of the best docked compound (Q or Q3GA) of each cluster to PPARα human protein. The participating amino acids involved in the interaction and the type of interaction (hydrogen bonds, hydrophilic interactions, salt bridges, π-stacking, etc.) are indicated. Blue lines indicate H bonds interactions and grey dashed lines show hydrophobic interactions. These pictures have been created from the data included in **Supplementary Table 1** using PyMol v2.3.0.



Supplementary Figure 2: Each inset shows the detailed interactions of the best docked compound (Q or Q3GA) of each cluster to FASN human protein. The participating amino acids involved in the interaction and the type of interaction (hydrogen bonds, hydrophilic interactions, salt bridges, π-stacking, etc.) are indicated. Blue lines indicate H bonds interactions and grey dashed lines show hydrophobic interactions. These pictures have been created from the data included in **Supplementary Table 2** using PyMol v2.3.0.



Supplementary Figure 3: Each inset shows the detailed interactions of the best docked compound (Q or Q3GA) of each cluster to AMPK human protein. The participating amino acids involved in the interaction and the type of interaction (hydrogen bonds, hydrophilic interactions, salt bridges, π-stacking, etc.) are indicated. Blue lines indicate H bonds interactions and grey dashed lines show hydrophobic interactions. These pictures have been created from the data included in **Supplementary Table 3** using PyMol v2.3.0.