Data Article

Computational data of phytoconstituents from *Hibiscus rosa-sinensis* on various anti-obesity targets

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**Abstract**

Molecular docking analysis of twenty two phytoconstituents from *Hibiscus rosa-sinensis*, against seven targets of obesity like pancreatic lipase, fat and obesity protein (FTO protein), cannabinoïd receptor, hormones as ghrelin, leptin and protein as SCH1 and MCH1 is detailed in this data article. Chemical structures of phytoconstituents were downloaded from PubChem and protein structures were retrieved from RCSB protein databank. Docking was performed using FlexX software Lead IT version 2.3.2; BioSolved IT. Visualization and analysis was done by Schrodinger maestro software. The docking score and interactions with important amino acids were analyzed and compared with marketed drug, orlistat. The findings suggest exploitation of best ligands experimentally to develop novel anti-obesity agent.

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This dataset contains docking analysis of phytoconstituents of *Hibiscus rosa-sinensis* on different targets of obesity. Different secondary metabolites present in *Hibiscus rosa-sinensis* were selected. Chemical structures of selected phytoconstituents were taken from database and were subjected to energy minimization. Seven receptor structures were selected as potential targets of obesity [1–8]. Protein structures available in database were downloaded from RCSB protein databank. Table 1 gives details of the selected receptors. Two receptors model were prepared using I-TASSER server online. Table 2 summarizes FASTA sequence of Ghrelin and MCH1 receptor subjected to model preparation. Phytoconstituents were docked on the above targets to understand binding interactions. Tables 3–9 summarizes the dock score, bond distance and interacting amino acid residue of all phytoconstituents on seven different targets. Fig. 1–14 gives docked images of phytoconstituents with lowest dock score and standard drug orlistat with seven receptor proteins.

2. Experimental design, materials, and methods

2.1. Ligand preparation

Twenty two phytoconstituents present in *Hibiscus rosa-sinensis* were selected. Structures of all phytoconstituents were downloaded from PubChem database. Orlistat (PubChem CID 3034010) only available synthetic drug was used as reference standard.

2.2. Energy minimization

All structures were subjected to energy minimization using Avogadro software where universal force field (UFF) and first order steepest descent algorithm were used. This gave energetically stable
conformations for the structures. Avogadro is free open source molecular builder software used for molecular modeling. It calculates the lowest energy conformation from the bond lengths and bond angles with smallest steric energy. Energy minimization helps in attaining structure conformation with lower delta G values which is considered close to biological system.

2.3. Retrieval of protein structure and preparation

Seven targets which play important role in maintaining energy balance of body and thus address obesity were selected. Protein structures of ligands were downloaded from the RCSB Protein Data Bank, database for 3D structures of large biological molecules, including proteins and nucleic acids. Downloaded protein structures were prepared X ray crystal structure of PDB ID 1LPB, 3LFM, 3TGZ, 1AX8, 4XWX for pancreatic lipase [2], FTO protein [3], cannabinoid receptor [4], hormones leptin [5] and protein SCH1 [6] respectively were selected. Data summarized in Table 1.

X- Ray crystal structure for Ghrelin [7] and MCH1 [8] receptor is not available in PDB databank so model protein structure was created using I-TASSER server online. FASTA sequence was taken from Uniprot ID of protein and submitted for model preparation. Table 2 summarizes FASTA sequence of Ghrelin and MCH1. Model was evaluated for C-score, TM score and RMSD. Model with C-score between −5 and 2, TM score greater than 0.5 were selected. Finalized model were validated on PROSA, Saves v5.0, Ramachandran plot and ProQ and then were used as receptors.

2.4. Molecular docking studies

Molecular docking techniques dock small molecules into the protein binding site. In order to understand how these ligands bind to the enzyme, docking analysis were performed using FlexX

### Table 1
Table summarizing details of targets selected.

| Target                  | PDB ID | Description                                                                 | Resolution | R value free | R value work |
|-------------------------|--------|------------------------------------------------------------------------------|------------|--------------|--------------|
| Pancreatic Lipase       | 1LPB   | The 2.46 Å resolution structure of the pancreatic lipase colipase complex inhibited by a c11 alkyl phosphonate | 2.46 Å     | 0.285        | 0.183        |
| Fat And Obesity Protein | 3LFM   | Crystal structure of the fat mass and obesity associated (FTO) protein reveals basis for its substrate specificity | 2.5 Å      | 0.285        | 0.239        |
| Cannabinoid Receptor    | 5TGZ   | Crystal structure analysis of w35f/h207w mutant of human cl1                 | 2.3 Å      | 0.306        | 0.240        |
| Leptin                  | 1AX8   | Human obesity protein, leptin                                                | 2.4 Å      | 0.283        | 0.185        |
| SCH1 Protein            | 4XWX   | Crystal structure of the PTB domain of SHC                                  | 1.87 Å     | 0.191        | 0.168        |

### Table 2
Uniprot ID and FASTA sequence of ghrelin and MCH1 receptor.

| Target                | UniProt ID | FASTA sequence                                                                 |
|-----------------------|------------|--------------------------------------------------------------------------------|
| Ghrelin receptor      | Q9UBU3     | MPSPTVCSSLLLGMGLWLDLAMAGSSFLSPEHQRVQQRKESK KPPAKLQPRALAGWLPEDGGQAEQAGAEDEVFNFAPFD VGIKLSGYQQHSQALCKFLQDLWEEAKEAPADK |
| MCH1 receptor         | Q99705     | MSGVAMKKKGVGRAVGLGGSGGQATEDLPNGCAGACPGQGGRR WLPQPAVVVEGSSALREWQATGWMDEASLPTG PNASNSTDGPSDLTASGSPPTGSIYINIMPSVFGTICLGLGINSTVFIAV VIKSKLHWCNINPVDFIINLSDVLDLFLGMPFIHMQLMNGVWHFGETMCT-LITAMADNSQFTSTYLTAMAIERYLATVHPISSTKFRKPSVATLVCIL WALSFSITPPYWLYARLPPFGAVGCGLGPLPNDLDLYWFLYYQFLAFALP FVVTIAAYRILQRMSTSSVAPASQRILRRTKRTVTAIAICLVFFVCWVAPYVLQLT QLSISRPTLTFVYLYNANASILGYANSLNPFPVFYVLCCETFRKKLVLSVKPAAQQLRAVS NAQTADEERTESKGT |
## Table 3
Summary of docking analysis with pancreatic lipase (PDB ID 1LPB).

| Sr. No | Posename                                      | Score   | Interacting Residues | Bond Type               | Bond Distance |
|--------|----------------------------------------------|---------|----------------------|-------------------------|---------------|
| 1      | Niacin                                       | -27.2868| SER 333, ARG 265     | HB, Pi-Pi Stacking      | 2.01, 5.21    |
|        |                                              |         | LYS 239, Salt bridge | Salt bridge             | 3.08          |
| 2      | Quercetin 3, 7 diglucoside                   | -21.223 | LYS 239, ARG 265     | HB, Salt bridge         | 1.93, 2.73    |
|        |                                              |         | ASP 247, ASP 257,    | HB, Salt bridge         | 1.93, 1.71    |
|        |                                              |         | THR 271, LYS 268     | HB, Pi cation           | 2.70, 1.48    |
| 3      | Ascorbic acid                                | -20.6315| SER 333, ASP 247,    | HB, Salt bridge         | 2.32, 2.06    |
|        |                                              |         | ARG 265, ASP 257,    | HB, Salt bridge         | 2.18          |
|        |                                              |         | THR 271, LYS 268     | HB, Pi cation           | 2.70, 1.48    |
| 4      | Quercetin 3, 3’ diglucoside                  | -20.3198| SER 333, ASP 247,    | HB, Pi-Pi Stacking      | 2.01, 5.21    |
|        |                                              |         | ARG 265, ASP 257,    | HB, Pi-Pi Stacking      | 2.18          |
|        |                                              |         | THR 271, LYS 268     | HB, Pi cation           | 2.70, 1.48    |
| 5      | Quercetin 3,4’ diglucoside                   | -18.4448| ARG 265, SER 333,    | HB, Salt bridge         | 2.34          |
|        |                                              |         | PHE 335, LYS 239     | Salt Bridge             | 2.04          |
| 6      | 8 nonynoic acid                              | -17.7764| LYS 239, ARG 265     | HB, Salt bridge         | 2.04          |
|        |                                              |         | ASP 249, SER 333     | Salt Bridge             | 3.91          |
| 7      | 9 Decynoic acid                              | -17.4676| ARG 265, LYS 239     | HB, Salt bridge         | 4.67          |
| 8      | Cyanidine 3, 5 diglucoside                   | -15.6327| ARG 265, ASP 247,    | HB, Salt Bridge         | 4.92          |
|        |                                              |         | ASP 257, ASP 249     | Salt Bridge             | 4.60          |
|        |                                              |         | GLU 253, SER 333     | HB, Salt Bridge         | 2.29, 2.39    |
| 9      | Riboflavin                                   | -15.3182| ARG 249, SER 333,    | HB, Salt bridge         | 1.36          |
|        |                                              |         | GLU 253, LYS 268     | Salt Bridge             | 2.16, 1.71    |
| 10     | Thiamine                                     | -14.7694| ASP 249, ARG 265     | HB, Salt Bridge         | 1.97          |
|        |                                              |         | LYS 268, ASP 247     | Salt Bridge             | 4.85          |
| 11     | Beta rosasterol                              | -9.4736 | LYS 239, ARG 265     | HB, Salt Bridge         | 2.16, 2.16    |
| 12     | Cyanidin 3-sophoroside-5-glucoside           | -8.2017 | ASP 249, ASP 272     | HB, Salt Bridge         | 1.46, 2.02, 1.91 |
|        |                                              |         | GLU 253, LYS 239     | Salt Bridge             | 1.82, 1.81    |
| 13     | Methyl non-8-ynoate                          | -7.2264 | LYS 239, ARG 265     | HB, Salt Bridge         | 2.16, 2.16    |
Table 3 (continued)

| Sr. No | Posename | Score  | Interacting Residues | Bond Type | Bond Distance |
|--------|----------|--------|-----------------------|-----------|---------------|
| 14     | Methyl Dec-9-ynoate | -5.9149 | ARG 265, LYS 239, ARG 265 | HB, HB | 1.94, 2.05 |
| 15     | Methyl (E)-11-methoxy-9-oxononadec-10-enoate | -4.9341 | SER 333, ARG 265, TRY 267, LYS 268 | HB, HB | 2.14, 2.14 |
| 16     | Methyl malvalate | -3.6439 | ARG 265, LYS 239, ARG 265 | HB, HB | 1.94, 2.05 |
| 17     | Methyl 8-oxooctadec-9-ynoate | -2.8512 | SER 333, LYS 239, ARG 265 | HB, HB, HB | 2.10, 1.89, 2.02 |
| 18     | Methyl Sterculate | -1.1816 | ARG 265, LYS 239 | HB, HB | 1.98, 2.06 |
| 19     | Campesterol | 1.5909 | GLU 253 | HB | 2.28 |
| 20     | Stigmasterol | 2.651 | ASP 249, GLU 253 | HB, HB | 1.90, 2.12 |
| 21     | Beta sitosterol | 3.2084 | No interaction | | |
| 22     | Orlistat | 0.1075 | ASP 249, SER 333, TYR 267 | HB, HB | 1.68, 1.94, 2.23 |

Orlistat, as only standard drug used in market is used as standard reference for docking studies. Hence the docking result of orlistat in all tables is bold for ease of comparison.

Table 4
Summary of docking analysis with fat and obesity protein (PDB ID 3LFM).

| Sr. No | Ligand | Score  | Interacting Residues | Bond Type | Bond Distance |
|--------|--------|--------|-----------------------|-----------|---------------|
| 1      | Riboflavin | -27.3248 | ARG 96, SER 229, GLU 234 | HB, HB, HB | 1.62, 2.07, 2.01 |
| 2      | Niacin | -21.5279 | ARG 322, GLU 234, ARG 96 | HB, HB, HB | 1.93, 1.84, 4.26 |
| 3      | Thiamine | -19.313 | TRY 108, HIP 231, SER 229 | Pi-Pi Stacking, Pi-Cation | 4.26, 6.38, 4.42 |
| 4      | Ascorbic acid | -16.8546 | ASP 233, ARG 322, ARG 96 | HB, HB, HB | 1.99, 2.45, 1.99 |
| 5      | Cyanidine 3, 5 diglucoside | -14.6454 | ARG 322, GLU 234 | Pi-Cation | 5.23, 1.90 |
| 6      | Quercetin 3,4’ diglucoside | -12.747 | ARG 322, TRY 106, HIP 231 | Pi-Cation, Pi-Pi Stacking | 5.23, 4.81 |

(continued on next page)
| Sr. No. | Ligand                                | Score  | Interacting Residues | Bond Type | Bond Distance |
|---------|---------------------------------------|--------|----------------------|-----------|---------------|
| 7       | 8 nonynoic acid                       | -12.149| ASN 205              | HB        | 1.96          |
|         |                                       |        | ARG 322              | HB        | 2.05          |
|         |                                       |        | Salt bridge          |           | 3.78          |
| 8       | 9 Decynoic acid                       | -11.8069| ARG 96               | HB        | 1.78          |
|         |                                       |        | GLU 234              | HB        | 1.97          |
| 9       | Quercetin 3,3' diglucoside            | -11.2637| TYR 108             | Pi-Pi Stacking | 4.55     |
|         |                                       |        | ARG 96               | HB        | 2.66          |
|         |                                       |        | VAL 94               | HB        | 1.79          |
|         |                                       |        | ALA 227              | HB        | 2.24          |
|         |                                       |        | GLU 234              | HB        | 1.62          |
| 10      | Quercetin 3,7 diglucoside             | -7.7494| GLU 234              | HB        | 2.04          |
|         |                                       |        | TYR 108             | Pi-Pi Stacking | 4.94 |
|         |                                       |        | ARG 322              | HB        | 2.15          |
|         |                                       |        | MET 103              | HB        | 2.06          |

| Sr. No. | Ligand                                | Score  | Interacting Residues | Bond Type | Bond Distance |
|---------|---------------------------------------|--------|----------------------|-----------|---------------|
| 11      | Methyl 8-oxooctadec-9-ynoate          | -6.5642| HIP 232              | HB        | 1.93          |
|         |                                       |        | ARG 96               | HB        | 1.92          |
| 12      | Methyl Dec-9-ynoate                   | -4.8041| ARG 96               | HB        | 2.15          |
| 13      | Methyl non-8-ynoate                   | -4.4543| ARG 96               | HB        | 2.15          |
| 14      | (9) Methyl (E)-11-methoxy-9-oxononadec-10-enoate | -2.4721| ARG 96               | HB        | 2.15          |
| 15      | Beta roasterol                        | -1.029 | VAL 94               | HB        | 1.78          |
| 16      | Methyl Sterculate                     | 0.5157 | ARG 96               | HB        | 1.84          |
| 17      | Methyl malvalate                      | 0.7329 | ARG 96               | HB        | 1.88          |
| 18      | Beta sitosterol                       | 1.2521 | ALA 227              | HB        | 2.2           |
| 19      | Campesterol                           | 1.447  | ALA 227              | HB        | 2.21          |
| 20      | Orlistat                              | -7.2466| ARG 322              | HB        | 2.20          |
|         |                                       |        | GLU 234              | HB        | 2.04          |
|         |                                       |        | HIP 232              | HB        | 1.66          |

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| Sr. No. | Ligand                                | Score  | Interacting Residues | Bond Type | Bond Distance |
|---------|---------------------------------------|--------|----------------------|-----------|---------------|
| 1       | Niacin                                | -14.7132| MET 103             | HB        | 1.84          |
|         |                                       |        | ASP 104             | HB        | 2.07          |
| 2       | Thiamine                              | -13.5476| PHE 102            | Pi-Pi Stacking | 4.52 |
|         |                                       |        | SER 383             | HB        | 1.81          |
|         |                                       |        | SER 123             | HB        | 1.69          |
| 3       | Ascorbic acid                         | -11.9942| ASP 163            | HB        | 2.30          |
|         |                                       |        | TRP 356             | HB        | 1.70          |
|         |                                       |        | CYS 386             | HB        | 1.86          |
|         |                                       |        | SER 199             | HB        | 2.44          |
|         |                                       |        | ALA 162             | HB        | 2.12          |
| 4       | Riboflavin                            | -9.4202| PHE 170             | Pi-Pi Stacking | 5.43 |
|         |                                       |        | MET 103             | HB        | 1.96          |
|         |                                       |        | SER 383             | HB        | 2.06          |
| 5       | 8 nonynoic acid                       | -4.3902| ASP 104             | HB        | 1.84          |
| 6       | 9 Decynoic acid                       | -3.8828| ASP 104             | HB        | 1.95          |
|         |                                       |        | MET 103             | HB        | 1.83          |
| 7       | Methyl 8-oxooctadec-9-ynoate          | -3.0906| ASN 389             | HB        | 2.66          |
|         |                                       |        | TRP 356             | HB        | 1.86          |
| 8       | Methyl non-8-ynoate                   | -2.5398| TRP 356             | HB        | 1.95          |
| 9       | Methyl Dec-9-ynoate                   | -2.4934| TRP 356             | HB        | 1.95          |
| 10      | (9) Methyl (E)-11-methoxy-9-oxononadec-10-enoate | -2.1673| TRP 356             | HB        | 1.95          |

Table 4 (continued)

Table 5
Summary of docking analysis with cannabinoid receptor (PDB ID 3TGZ).

| Sr. No. | Ligand                                | Score  | Interacting Residues | Bond Type | Bond Distance |
|---------|---------------------------------------|--------|----------------------|-----------|---------------|
| 1       | Niacin                                | -14.7132| MET 103             | HB        | 1.84          |
|         |                                       |        | ASP 104             | HB        | 2.07          |
| 2       | Thiamine                              | -13.5476| PHE 102            | Pi-Pi Stacking | 4.52 |
|         |                                       |        | SER 383             | HB        | 1.81          |
|         |                                       |        | SER 123             | HB        | 1.69          |
| 3       | Ascorbic acid                         | -11.9942| ASP 163            | HB        | 2.30          |
|         |                                       |        | TRP 356             | HB        | 1.70          |
|         |                                       |        | CYS 386             | HB        | 1.86          |
|         |                                       |        | SER 199             | HB        | 2.44          |
|         |                                       |        | ALA 162             | HB        | 2.12          |
| 4       | Riboflavin                            | -9.4202| PHE 170             | Pi-Pi Stacking | 5.43 |
|         |                                       |        | MET 103             | HB        | 1.96          |
|         |                                       |        | SER 383             | HB        | 2.06          |
| 5       | 8 nonynoic acid                       | -4.3902| ASP 104             | HB        | 1.84          |
| 6       | 9 Decynoic acid                       | -3.8828| ASP 104             | HB        | 1.95          |
|         |                                       |        | MET 103             | HB        | 1.83          |
| 7       | Methyl 8-oxooctadec-9-ynoate          | -3.0906| ASN 389             | HB        | 2.66          |
|         |                                       |        | TRP 356             | HB        | 1.86          |
| 8       | Methyl non-8-ynoate                   | -2.5398| TRP 356             | HB        | 1.95          |
| 9       | Methyl Dec-9-ynoate                   | -2.4934| TRP 356             | HB        | 1.95          |
| 10      | (9) Methyl (E)-11-methoxy-9-oxononadec-10-enoate | -2.1673| TRP 356             | HB        | 1.95          |
Table 5 (continued)

| Sr. No. | Ligand               | Score  | Interacting Residues | Bond Type | Bond Distance |
|---------|----------------------|--------|----------------------|-----------|---------------|
| 11      | Quercetin 3,3’ diglucoside | -1.505 | SER 383 | HB          | 2.61          |
|         |                      |        | TRP 356 | HB          | 2.51          |
|         |                      |        | SER 390 | HB          | 1.50          |
| 12      | Methyl malvalate     | -0.5677| No Interaction      |           |               |
| 13      | Methyl Stercule       | -0.2554| ASN 389 | HB          | 2.50          |
|         |                      |        | TRP 356 | HB          | 1.85          |
| 14      | Quercetin 3,4’ diglucoside | -0.201 | PHE 174 | Pi-Pi Stacking | 5.44        |
|         |                      |        | ASP 104 | HB          | 2.14          |
| 15      | Campesterol          | 3.5794 | No Interaction      |           |               |
| 16      | Beta rosasterol      | 6.6198 | MET 103 | HB          | 1.82          |
| 17      | Beta sitosterol       | 6.6198 | ASP 104 | HB          | 2.09          |
| 18      | Orlistat             | -1.7877| SER 383 | HB          | 1.65          |

Orlistat, as only standard drug used in market is used as standard reference for docking studies. Hence the docking result of orlistat in all tables is bold for ease of comparison.

Table 6
Summary of docking analysis with leptin (PDB ID 1AX8).

| Sr. No. | Ligand               | Dock Score | Interacting residues | Bond Type | Bond distance |
|---------|----------------------|------------|----------------------|-----------|---------------|
| 1       | Riboflavin           | -18.4869   | GLN 134 | HB          | 2.22          |
|         |                      |            | GLN 130 | HB          | 1.91          |
|         |                      |            | ASP 40  | HB          | 2.12          |
|         |                      |            | GLN 134 | HB          | 1.72          |
|         |                      |            | ASP 40  | HB          | 2.08          |
|         |                      |            | ILE 21   | HB          | 1.58          |
| 2       | Cyanidine 3, 5 diglucoside | -13.4683 | ASP 40  | HB          | 2.40          |
|         |                      |            | GLN 130 | HB          | 1.75          |
|         |                      |            | ASP 40  | HB          | 1.68          |
|         |                      |            | GLN 134 | HB          | 1.87          |
|         |                      |            | ILE 42   | HB          | 1.83          |
|         |                      |            | GLN 134 | HB          | 2.41          |
|         |                      |            | ILE 21   | HB          | 1.86          |
| 3       | Thiamine             | -11.3807   | GLN 134 | HB          | 2.21          |
|         |                      |            | ASP 40  | HB          | 2.15          |
|         |                      |            | ILE 42   | HB          | 1.84          |
| 4       | Ascorbic acid        | -11.1364   | GLY 44  | HB          | 1.94          |
|         |                      |            | GLN 134 | HB          | 1.98          |
|         |                      |            | ILE 42   | HB          | 2.20          |
| 5       | Quercetin 3,4’ diglucoside | -10.9657 | GLY 44  | HB          | 2.57          |
|         |                      |            | ASP 40  | HB          | 2.27          |
|         |                      |            | ASP 40  | HB          | 2.15          |
|         |                      |            | ASP 40  | HB          | 1.90          |
|         |                      |            | ASP 40  | HB          | 2.05          |
|         |                      |            | LEU 39  | HB          | 1.84          |
| 6       | Quercetin 3,3’ diglucoside | -10.3108 | ASP 40  | HB          | 2.29          |
|         |                      |            | SER 127 | HB          | 1.60          |
| 7       | Quercetin 3,7 diglucoside | -10.2723 | PHE 41  | Pi-Pi Stacking | 5.04       |
|         |                      |            | GLN 130 | HB          | 1.97          |
|         |                      |            | ASP 40  | HB          | 2.07          |
|         |                      |            | GLY 131 | HB          | 1.56          |
|         |                      |            | GLY 44  | HB          | 1.64          |
|         |                      |            | ASP 135 | HB          | 1.56          |

(continued on next page)
Table 6 (continued)

| Sr. No. | Ligand                                      | Dock Score | Interacting residues | Bond Type | Bond distance |
|---------|---------------------------------------------|------------|----------------------|-----------|---------------|
| 8       | Niacin                                      | –9.3776    | ASP 40               | HB        | 1.84          |
| 9       | Beta rosasterol                             | –6.3064    | GLY 44               | HB        | 1.82          |
| 10      | Cyanidin 3-sophoroside-5-glucoside          | –5.2426    | GLN 134              | HB        | 1.84          |
|         |                                             |            | ASP 135              | HB        | 2.07          |
|         |                                             |            |                      | HB        | 2.54          |
|         |                                             |            | LEU 39               | HB        | 1.84          |
|         |                                             |            | GLN 130              | HB        | 1.99          |
|         |                                             |            | PHE 41               | HB        | 1.84          |
|         |                                             |            |                       | HB        | 1.91          |
| 11      | Campesterol                                 | –3.5982    | No interaction       |           |               |
| 12      | Stigmasterol                                | –2.8915    | ASP 135              | HB        | 2.22          |
| 13      | 8 nonynoic acid                             | 0.1127     | OHE 41               | HB        | 2.01          |
| 14      | Beta sitosterol                             | 0.4685     | ASP 135              | HB        | 1.97          |
| 15      | 9 Decynoic acid                             | 1.1976     | ASP 40               | HB        | 1.88          |
| 16      | Methyl non-8-ynoate                         | 2.0473     | PHE 41               | HB        | 1.89          |
| 17      | Methyl Dec-9-ynoate                         | 2.8153     | PHE 41               | HB        | 1.95          |
| 18      | Methyl 8-oxooctadec-9-ynoate                | 5.4298     | PHE 41               | HB        | 1.87          |
| 19      | (9) Methyl (E)-11-methoxy-9-oxononadec-10-enoate | 6.5759    | PHE 41               | HB        | 1.83          |
| 20      | Methyl Sterculate                           | 6.9274     | PHE 41               | HB        | 1.87          |
| 21      | Methyl malvalate                            | 8.0895     | PHE 41               | HB        | 1.87          |
| 22      | **Orlistat**                                | **8.3009** | **ASP 40**           | **HB**    | **1.71**      |
|         |                                             |            | GLU 134              | HB        | 1.80          |
|         |                                             |            | GLY 44               | HB        | 1.99          |

Orlistat, as only standard drug used in market is used as standard reference for docking studies. Hence the docking result of orlistat in all tables is bold for ease of comparison.

Table 7
Summary of docking analysis with SCH1 protein (PDB ID 4XWX).

| Sr. No. | Ligand                              | Dock score | Interacting residues | Bond type            | Bond angle |
|---------|-------------------------------------|------------|----------------------|----------------------|------------|
| 1       | Riboflavin                          | –13.553    | ARG 74               | Pi cation            | 5.25       |
|         |                                     |            |                      | Pi-Pi stacking       | 4.72       |
|         |                                     |            | ILE 150              | HB                   | 1.68       |
|         |                                     |            | ALA 153              | HB                   | 1.84       |
|         |                                     |            | SER 151              | HB                   | 1.95       |
|         |                                     |            |                      | HB                   | 2.19       |
| 2       | Niacin                              | –11.0861   | PHE 198              | Pi-Pi Stacking       | 4.93       |
|         |                                     |            | ALA 153              | HB                   | 2.20       |
|         |                                     |            | SER 151              | HB                   | 1.58       |
|         |                                     |            |                      | HB                   | 1.88       |
| 3       | Ascorbic acid                       | –8.3129    | ALA 153              | HB                   | 2.20       |
|         |                                     |            | SER 151              | HB                   | 1.58       |
|         |                                     |            |                      | HB                   | 1.88       |
| 4       | Thiamine                            | –8.2065    | ALA 153              | HB                   | 1.53       |
|         |                                     |            | PHE 198              | Pi-Pi Stacking       | 4.09       |
|         |                                     |            | ILE 150              | HB                   | 1.73       |
|         |                                     |            |                      | HB                   | 2.49       |
| 5       | Quercetin 3,3' diglucoside          | –6.2583    | GLY 195              | HB                   | 1.94       |
|         |                                     |            | ALA 153              | HB                   | 1.58       |
|         |                                     |            | ILE 191              | HB                   | 2.10       |
|         |                                     |            |                      | HB                   | 2.49       |
|         |                                     |            | PHE 198              | Pi – Pi Stacking     | 5.06       |
|         |                                     |            | SER 151              | HB                   | 2.24       |
|         |                                     |            | ILE 150              | HB                   | 1.61       |
|         |                                     |            |                      | HB                   | 1.75       |
| 6       | Cyanidine 3, 5' diglucoside         | –4.9771    | GLU 199              | Salt Bridge          | 2.92       |
|         |                                     |            | PHE 198              | Pi Pi Stacking       | 4.73       |
|         |                                     |            | ALA 153              | HB                   | 2.15       |
|         |                                     |            | SER 151              | HB                   | 1.84       |
|         |                                     |            | WATER                | HB                   | 2.43       |
|         |                                     |            | ILE 150              | HB                   | 1.81       |
|         |                                     |            |                      | HB                   | 1.77       |
| Sr. No. | Ligand                          | Dock score | Interacting residues | Bond type | Bond angle |
|--------|--------------------------------|------------|----------------------|-----------|------------|
| 7      | Campesterol                    | -4.5453    | ALA 153              | HB        | 1.92       |
| 8      | Beta sitosterol                | -1.7076    | ILE 191              | HB        | 1.95       |
| 9      | 9 Decynoic acid                | -1.6636    | ARG 74               | Salt Bridge | 4.96     |
| 10     | 8 nonynoic acid                | -1.5286    | ARG 74               | Salt Bridge | 4.96     |
| 11     | Stigmasterol                   | -1.0801    | No interaction       |           |            |
| 12     | Quercetin 3,4’ diglucoside     | 0.3325     | WATER                | HB        | 2.43       |
|        |                                 |            | ALA 153              |           |            |
|        |                                 |            | ILE 191              |           |            |
|        |                                 |            | GLY 153              |           |            |
|        |                                 |            | GLU 36               |           |            |
|        |                                 |            | PRO 49               |           |            |
|        |                                 |            | ASN 76               |           |            |
|        |                                 |            | GLN 36               |           |            |
|        |                                 |            | HIE 32               |           |            |
| 13     | Beta rosasterol                | 0.3474     | No interaction       |           |            |
| 14     | Methyl non-8-ynoate            | 0.477      |                      |           |            |
| 15     | Methyl Dec-9-ynoate            | 1.0452     |                      |           |            |
| 16     | Quercetin 3,7 diglucoside      | 2.2611     | WATER                | HB        | 1.14       |
|        |                                 |            | GLN 36               |           |            |
|        |                                 |            | ALA 77               |           |            |
|        |                                 |            | ASN 76               |           |            |
|        |                                 |            | GLN 36               |           |            |
|        |                                 |            | GLU 36               |           |            |
|        |                                 |            | PRO 49               |           |            |
|        |                                 |            | ASN 76               |           |            |
|        |                                 |            | HIE 32               |           |            |
| 17     | Methyl 8-oxooctadec-9-ynoate   | 3.4243     |                      |           |            |
| 18     | Methyl malvalate               | 5.8575     |                      |           |            |
| 19     | Methyl Sterculate              | 6.8808     |                      |           |            |
| 20     | (9) Methyl (E)-11-methoxy-9-oxononadec-10-enoate | 7.7443 |                      |           |            |
| 21     | Cyanidin 3-sophoroside-5-glucoside | 8.5222 |                      |           |            |
| 22     | Orlistat                       | 10.3508    | ALA 153              | HB        | 1.86       |

*Orlistat, as only standard drug used in market is used as standard reference for docking studies. Hence the docking result of orlistat in all tables is bold for ease of comparison.

**Table 8**

Summary of docking analysis with ghrelin.

| Sr. No. | Ligand                          | Dock score | Interacting residues | Bond type | Bond angle |
|--------|--------------------------------|------------|----------------------|-----------|------------|
| 1      | Niacin                          | -11.1374   | ALA 53               | HB        | 2.36       |
| 2      | Ascorbic acid                   | -7.2393    | PRO 49               | HB        | 2.15       |
|        |                                 |            | ASN 76               |           | 1.85       |
|        |                                 |            | GLN 36               |           | 1.77       |
|        |                                 |            | ALA 77               |           | 2.18       |
| 3      | Riboflavin                      | -7.0131    | ALA 77               | HB        | 2.40       |
|        |                                 |            | GLN 36               |           | 1.68       |
|        |                                 |            | ASN 76               |           | 1.62       |
|        |                                 |            | GLN 36               |           | 1.77       |
|        |                                 |            | ALA 77               |           | 2.13       |
|        |                                 |            | HIE 32               |           | 5.33       |
| 4      | Thiamine                        | -4.7344    | GLN 36               | HB        | 2.20       |
|        |                                 |            | ASN 76               |           | 1.84       |
|        |                                 |            | ALA 77               |           | 2.13       |
|        |                                 |            | HIE 32               |           | 5.33       |
| 5      | 8 nonynoic acid                 | 1.9189     | GLU 36               | HB        | 2.20       |
| 6      | 9 Decynoic acid                 | 2.7981     | GLU 36               | HB        | 1.92       |
| 7      | Methyl non-8-ynoate             | 2.9037     | ALA 77               | HB        | 2.18       |
| 8      | Methyl Dec-9-ynoate             | 4.0035     |                      |           |            |
| 9      | Campesterol                     | 6.9115     |                      |           |            |
| 10     | Methyl 8-oxooctadec-9-ynoate    | 8.7284     | GLU 36               | HB        | 2.20       |
|        |                                 |            | ASN 76               |           | 1.84       |
|        |                                 |            | ALA 77               |           | 2.13       |
| 11     | Methyl malvalate                | 11.8293    | ALA 77               | HB        | 2.18       |
| 12     | Methyl Sterculate               | 12.0917    |                      |           |            |
| 13     | Beta sitosterol                 | 12.2015    |                      |           |            |
| 14     | (9) Methyl (E)-11-methoxy-9-oxononadec-10-enoate | 13.2915 |                      |           |            |
| 15     | Orlistat                        | 15.8166    | ASN 76               | HB        | 1.65       |
|        |                                 |            | ALA 77               |           | 2.20       |
| Sr. No. | Ligand                          | Dock score | Interacting residues | Bond type | Bond angle |
|--------|---------------------------------|------------|----------------------|-----------|------------|
|        |                                 |            | GLY 80               | HB        | 1.76       |
| 1      | Quercetin 3,3’ diglucoside      | –13.7266   | GLY 18               | HB        | 2.00       |
|        |                                 |            | SER 57               | HB        | 1.73       |
|        |                                 |            | GLY 80               | HB        | 1.76       |
| 2      | Riboflavin                      | –12.9742   | GLY 18               | HB        | 2.19       |
|        |                                 |            | SER 87               | HB        | 2.36       |
|        |                                 |            | SER 57               | HB        | 1.55       |
| 3      | Thiamine                        | –9.527     | LEU 16               | HB        | 1.82       |
|        |                                 |            | GLU 54               | Salt Bridge | 4.99     |
|        |                                 |            | GLU 54               | HB        | 1.90       |
| 4      | Quercetin 3,7 diglucoside       | –8.7967    | VAL 3                | HB        | 2.02       |
|        |                                 |            | LEU 76               | HB        | 1.63       |
|        |                                 |            | ACE 0                | HB        | 2.10       |
|        |                                 |            | GLU 80               | HB        | 2.24       |
|        |                                 |            | ASP 91               | HB        | 2.35       |
| 5      | Cyanidine 3, 5’ diglucoside     | –8.3388    | LEU 76               | HB        | 1.68       |
|        |                                 |            | ACE 0                | HB        | 1.63       |
|        |                                 |            | VAL 3                | HB        | 2.31       |
|        |                                 |            | ASP 91               | HB        | 1.55       |
|        |                                 |            | GLU 54               | HB        | 1.76       |
|        |                                 |            | SER 87               | HB        | 1.76       |
|        |                                 |            | GLY 18               | HB        | 2.31       |
| 6      | Ascorbic acid                   | –7.7733    | SER 57               | HB        | 2.19       |
|        |                                 |            | GLU 54               | HB        | 1.80       |
|        |                                 |            | GLU 54               | HB        | 1.76       |
|        |                                 |            | GLU 54               | HB        | 1.65       |
| 7      | Cyanidin 3-sophoroside-5-glucoside | –5.7144     | LEU 76               | HB        | 1.70       |
|        |                                 |            | ASP 91               | HB        | 1.62       |
|        |                                 |            | VAL 3                | HB        | 2.35       |
|        |                                 |            | SER 87               | HB        | 1.74       |
|        |                                 |            | SER 57               | HB        | 2.20       |
|        |                                 |            | ASP 91               | HB        | 1.56       |
| 8      | Quercetin 3,4’ diglucoside      | –5.236     | GLY 15               | HB        | 2.09       |
|        |                                 |            | VAL 14               | HB        | 2.35       |
|        |                                 |            | SER 87               | HB        | 1.74       |
|        | Niacin                          | –5.127     | VAL 3                | HB        | 1.84       |
| 9      |                                 |            | GLU 54               | HB        | 2.16       |
| 10     | Campesterol                     | –0.843     | GLU 54               | HB        | 1.93       |
| 11     | Stigmasterol                    | –0.787     | GLU 54               | HB        | 2.00       |
| 12     | Beta sitosterol                 | 1.849      | GLU 54               | HB        | 2.00       |
| 13     | Beta rosasterol                 | 2.848      | No interaction       |           |            |
| 14     | 8 nonynic acid                  | 3.749      | VAL 3                | HB        | 1.84       |
| 15     | 9 Decynic acid                  | 4.120      | VAL 3                | HB        | 1.84       |
| 16     | Methyl Dec-9-ynoate             | 5.030      | VAL 3                | HB        | 1.89       |
| 17     | Methyl non-8-ynoate             | 5.193      | VAL 3                | HB        | 1.89       |
| 18     | (9) Methyl (E)-11-methoxy-9-oxononadec-10-enoate | 8.373 | TRP 61               | HB        | 1.75       |
| 19     | Methyl 8-oxo-octadec-9-ynoate   | 8.384      | SER 2                | HB        | 2.03       |
| 20     | Methyl malvalate                | 11.003     | VAL 3                | HB        | 1.89       |
| 21     | Methyl Sterculate               | 11.447     | VAL 3                | HB        | 1.89       |
| 22     | Orlistat                        | 11.712     | Glu 54               | HB        | 2.09       |

Orlistat, as only standard drug used in market is used as standard reference for docking studies. Hence the docking result of orlistat in all tables is bold for ease of comparison.
Fig. 1. 1LPB interaction with Niacin.

Fig. 2. 1LPB interaction with Orlistat.

Fig. 3. 3LFM interaction with Riboflavin.
Fig. 4. 3LFM interaction with Orlistat.

Fig. 5. 3TGZ interaction with Niacin.

Fig. 6. 3TGZ interaction with Orlistat.
Fig. 7. 1AX8 interaction with Riboflavin.

Fig. 8. 1AX8 interaction with Orlistat.

Fig. 9. 4XWX interaction with Riboflavin.
**Fig. 10.** 4XWX interaction with Orlistat.

**Fig. 11.** Ghrelin interaction with Niacin.

**Fig. 12.** Ghrelin interaction with Orlistat.
software. The receptor ligand interactions were done using Maestro software. Interacting amino acid residue, bond type and bond distance were noted. Data summarized in Tables 3–9 and Fig. 1–14.

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