**Supplementary material JKSUS\_2016\_807**

**Table 1:** Following parameters were employed during ESI-MS analysis;

Instrument : Waters, Micromass Q-TOF micro  
Separation module : Waters Alliance 2795  
Ionization : Electro spray Positive (ES+)  
Acquisition : MRM, unit resolution  
Injection volume : 20 µl  
Flow rate : 0.4 ml/min  
Desolvation  gas : 500 Lts/Hr  
Cone gas : 45 Lts/Hr  
Desolvation  temperature : 250 °C  
Source temperature : 120 °C  
Capillary voltage : 3000 V  
Cone voltage : 30 V  
Mobile phase used : MeOH  
Nebulization gas : N2

Collision gas : Argon

**Table 2.** Lipid inhibitory molecules which were examined in *insilico* analysis.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Lipase inhibitor/ fat loss molecule** | **Molecular formula** | **Molecular weight** | **Aromatic carbons** | **Rotatable bonds** | **TORSDOF\*** |
| Akuammine | C22H26N2O4 | 382.452 | 6 | 3 | 3 |
| Apigenin | C15H10O5 | 270.236 | 15 | 4 | 4 |
| Asperglaucide | C27H28N2O4 | 444.522 | 21 | 10 | 9 |
| Biochanin A | C16H12O5 | 284.263 | 15 | 4 | 4 |
| Butein | C15H12O5 | 272.252 | 12 | 8 | 8 |
| Caffeine | C8H10N4O2 | 194.190 | 5 | 0 | 0 |
| Carnosic acid | C20H28O4 | 332.433 | 17 | 3 | 3 |
| Caulerpenyne | C21H26O6 | 374.427 | - | 16 | 16 |
| Cerulenin | C12H17NO3 | 223.268 | 2 | 10 | 9 |
| Chiisanoside | C48H74O19 | 955.089 | 42 | 17 | 17 |
| Chisetsusaponin V | C48H76O19 | 957.105 | 42 | 15 | 15 |
| Crocin | C44H64O24 | 976.964 | 20 | 41 | 41 |
| Curcumin | C21H20O6 | 368.379 | 12 | 12 | 12 |
| Cyclocarioside A | C43H72O13 | 797.023 | 35 | 12 | 12 |
| Dioscin | C45H72O16 | 869.043 | 41 | 9 | 9 |
| Diosmetin | C16H12O6 | 300.262 | 15 | 5 | 5 |
| Ebelactone A | C20H34O4 | 338.481 | 3 | 11 | 11 |
| Ebelactone B | C21H36O4 | 352.508 | 3 | 12 | 12 |
| Elaidic acid | C18H34O2 | 282.461 | - | 18 | 18 |
| Epipervilline | C22H22O5 | 366.407 | 17 | 3 | 3 |
| Escin 1A | C55H86O24 | 1131.256 | 46 | 23 | 23 |
| Escin 1B | C55H86O24 | 1131.256 | 45 | 18 | 18 |
| Esterastin | C28H46N2O6 | 506.674 | 10 | 18 | 17 |
| Fisetin | C15H10O6 | 286.236 | 15 | 5 | 5 |
| Fucoxanthinol | C40H56O5 | 616.869 | 18 | 19 | 19 |
| Gallic acid | C7H6O5 | 170.119 | 6 | 5 | 5 |
| Glycitein | C16H12O5 | 284.263 | 15 | 4 | 4 |
| 9-Hexadecenoic acid | C16H30O2 | 254.408 | - | 15 | 15 |
| Licochalcone A | C21H22O4 | 338.396 | 15 | 7 | 7 |
| Majoridine | C23H28N2O3 | 380.480 | 18 | 5 | 5 |
| Okanin | C15H12O6 | 288.252 | 12 | 9 | 9 |
| Orlistat | C29H53NO5 | 495.734 | 8 | 20 | 20 |
| D-Penicillamine | C5H11NO2S | 149.211 | 3 | 4 | 4 |
| Pentadecenoic acid | C22H39NO3 | 365.549 | - | 14 | 14 |
| Phenylboronic acid | C6H7BO2 | 121.929 | 6 | 3 | 3 |
| Piperanine | C17H21NO3 | 287.353 | 12 | 6 | 5 |
| Platycodin D | C57H92O28 | 1225.323 | 52 | 20 | 20 |
| Prosapogenin | C42H66O17 | 842.963 | 36 | 12 | 12 |
| Rhamnazin | C17H14O7 | 330.288 | 15 | 6 | 6 |
| Rimonabant | C22H21Cl3N4O | 463.787 | 20 | 3 | 2 |
| Sessiloside | C48H76O18 | 941.106 | 35 | 19 | 19 |
| Shogaol | C17H24O3 | 276.370 | 6 | 11 | 11 |
| Sibutramine | C17H26ClN | 279.848 | 12 | 2 | 2 |
| Tangeretin | C20H20O7 | 372.368 | 15 | 6 | 6 |
| Tricetin | C15H10O7 | 302.235 | 15 | 6 | 6 |
| Tricin | C17H14O7 | 330.288 | 15 | 6 | 6 |
| Triclosan | C12H7Cl3O2 | 289.541 | 12 | 3 | 3 |
| Valilactone | C22H39NO5 | 397.548 | 3 | 17 | 17 |
| Vibralactone | C12H20O4 | 228.284 | 7 | 6 | 6 |

**\***Torsional degree of freedom



**Figure 1.**FT-IR spectrum of B821 fraction. Absorption frequencies (cm-1) denotes following functional classes. 3346.67: O-H stretch phenol; 2959, 2934, 2873.66: C-H stretches aromatic; 1648.81: -C=C- stretch; 1463.76: C-C stretch (in ring) aromatics; 1379.77, 1214.81: C-N stretches tertiary amine (aromatic); 1071.71, 1043.72: C-O stretches ester ether and 953.79: C-O stretch phenol.

**Table 3.** Binding affinities (kcal/mol) of lipid inhibitory molecules with fat metabolism proteins.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Lipid inhibitory molecule** | **1ETH** | **1HLG** | **1LPB** | **3LFM** |
| Akuammine | -9.0 | -7.6 | -8.3 | -7.1 |
| Apigenin | -8.2 | -10.3 | -9.7 | -8.5 |
| Asperglaucide | -8.9 | -10.6 | -8.4 | -8.5 |
| Biochanin A | -8.4 | -10.1 | -8.1 | -7.9 |
| Butein | -7.8 | -9.7 | -6.7 | -8.0 |
| Caffeine | -6.6 | -7.0 | -5.9 | -5.9 |
| Carnosic acid | -10.2 | -11.8 | -9.9 | -10.5 |
| Caulerpenyne | -6.1 | -7.2 | -5.9 | -6.6 |
| Cerulenin | -6.1 | -6.4 | -5.4 | -6.0 |
| Chiisanoside | -15.3 | -13.3 | -13.0 | -11.6 |
| Chisetsusaponin V | -14.5 | -12.8 | -13.1 | -13.4 |
| Crocin | -8.7 | -7.0 | -8.0 | -7.3 |
| Curcumin | -8.1 | -7.8 | -7.3 | -7.2 |
| Cyclocarioside A | -12.3 | -11.5 | -12.2 | -12.8 |
| Dioscin | -16.4 | -15.2 | -14.4 | -17.1 |
| Diosmetin | -8.5 | -10.4 | -9.0 | -8.7 |
| Ebelactone A | -7.1 | -7.5 | -5.9 | -8.6 |
| Ebelactone B | -6.8 | -6.1 | -6.3 | -6.1 |
| Elaidic acid | -5.8 | -6.0 | -5.8 | -5.8 |
| Epipervilline | -9.6 | -9.7 | -9.0 | -9.6 |
| Escin 1A | -13.5 | -11.8 | -11.7 | -12.2 |
| Escin 1B | -15.3 | -12.7 | -12.9 | -12.1 |
| Esterastin | -7.3 | -8.2 | -7.7 | -7.3 |
| Fisetin | -8.7 | -10.6 | -8.0 | -9.0 |
| Fucoxanthinol | -8.1 | -11.6 | -8.1 | -8.3 |
| Gallic acid | -6.0 | -7.0 | -6.0 | -7.0 |
| Glycitein | -8.3 | -10.2 | -7.6 | -8.1 |
| 9-Hexadecenoic acid | -5.4 | -5.9 | -4.4 | -4.7 |
| Licochalcone A | -8.3 | -9.4 | -8.3 | -8.6 |
| Majoridine | -9.8 | -10.3 | -9.2 | -9.3 |
| Okanin | -8.0 | -9.8 | -7.1 | -7.8 |
| Orlistat | -6.8 | -6.7 | -7.1 | -6.2 |
| D-Penicillamine | -5.0 | -5.5 | -4.8 | -6.1 |
| Pentadecenoic acid | -5.2 | -4.9 | -4.4 | -4.7 |
| Phenylboronic acid | -5.4 | -6.1 | -5.9 | -5.6 |
| Piperanine | -7.7 | -8.9 | -7.6 | -7.9 |
| Platycodin D | -15.2 | -12.6 | -13.7 | -12.6 |
| Prosapogenin | -13.9 | -13.0 | -13.2 | -13.9 |
| Rhamnazin | -8.7 | -9.2 | -8.0 | -8.5 |
| Rimonabant | -10.8 | -11.9 | -9.7 | -11.5 |
| Sessiloside | -13.8 | -13.0 | -11.8 | -13.2 |
| Shogaol | -6.4 | -6.9 | -5.9 | -7.0 |
| Sibutramine | -8.4 | -8.3 | -6.9 | -8.1 |
| Tangeretin | -8.3 | -7.7 | -8.0 | -7.5 |
| Tricetin | -8.8 | -10.7 | -8.3 | -9.7 |
| Tricin | -8.2 | -8.5 | -8.8 | -8.5 |
| Triclosan | -7.4 | -9.0 | -8.6 | -6.3 |
| Valilactone | -6.0 | -6.9 | -6.3 | -5.8 |
| Vibralactone | -6.7 | -7.8 | -6.4 | -6.6 |