

## SUPPLEMENTARY TABLES

**Supplementary Table 5. Molecular docking binding energy score.**

| <b>Protein name</b> | <b>PDB ID</b> | <b>Quercetin binding energy score (kcal/mol)</b> | <b>Kaempferol binding energy score (kcal/mol)</b> |
|---------------------|---------------|--|---|
| AKT1                | 4gv1          | -8.3   | -8.1  |
| STAT3               | 6njs          | -7.5   | -7.1  |
| JUN                 | 1a02          | -5.6   | -5.6  |
| MAPK3               | 4qtb          | -9.3   | -9.1  |
| TP53                | 4iby          | -6.8   | -6.3  |
| MAPK1               | 6slg          | -8.1   | -6.1  |
| TNF                 | 7jra          | -6.8   | -6.8  |
| RELA                | 6nv2          | -7.2   | -6.9  |
| MAPK14              | 3zs5          | -11  | -10.7   |
| IL6                 | 1alu          | -7.1   | -6.7  |

**Supplementary Table 6. Relevant coordinate of the docking box.**

| <b>Compounds-Protein</b> | <b>Grid size X, Y, Z</b> | <b>X, Y, Z coordinates</b> |
|--------------------------|--------------------------|----------------------------|
| Quercetin-AKT1           | 32, 44, 52               | -23.423, 5.856, 11.606     |
| Quercetin-STAT3          | 52, 90, 54               | 9.299, 54.795, 2.625       |
| Quercetin-MAPK14         | 42, 46, 56               | 22.544, 31.878, 17.449     |
| Quercetin-RELA/P65       | 40, 42, 64               | 27.293, 13.587, 2.039      |
| Quercetin-IL6            | 104, 118, 84             | 2.669, -19.932, 3.112      |
| Kaempferol-AKT1          | 32, 44, 52               | -23.423, 5.856, 11.606     |
| Kaempferol-STAT3         | 52, 90, 54               | 9.299, 54.795, 2.625       |
| Kaempferol-MAPK14        | 42, 46, 56               | 22.544, 31.878, 17.449     |
| Kaempferol-RELA/P65      | 40, 42, 64               | 27.293, 13.587, 2.039      |
| Kaempferol-IL6           | 104, 118, 84             | 2.669, -19.932, 3.112      |