**Table S2.** Quantum Chemical local parametersfor saponin by B3LYP/LanL2DZ level with PCM model.

| $1_{prot}$ | Mulliken | $f_k^-$ | $f_k^+$ | %HOMO | %LUMO |
|---|---|---|---|---|---|
| C10 | -0.486 | 0.000 | 0.003 | 0.770 | 1.278 |
| C13 | -0.545 | -0.003 | 0.000 | 2.123 | 0.341 |
| C16 | -0.265 | -0.005 | 0.000 | 2.863 | 0.345 |
| C18 | 0.407 | 0.004 | 0.000 | 4.016 | 0.324 |
| C19 | -0.047 | 0.003 | 0.000 | 2.390 | 0.144 |
| C21 | -0.606 | 0.000 | 0.000 | 1.087 | 0.182 |
| C24 | -0.157 | -0.001 | 0.000 | 1.454 | 0.380 |
| C26 | 0.399 | 0.005 | 0.000 | 2.067 | 0.718 |
| C45 | -0.594 | 0.001 | 0.000 | 1.246 | 0.084 |
| C48 | -0.087 | 0.001 | 0.000 | 1.850 | 0.034 |
| C50 | -0.785 | 0.000 | 0.000 | 1.469 | 0.124 |
| C53 | -0.183 | -0.002 | 0.000 | 1.948 | 0.100 |
| C54 | 0.343 | -0.001 | 0.000 | 2.286 | 0.068 |
| C55 | -0.530 | 0.013 | 0.000 | 4.294 | 0.041 |
| C58 | 0.019 | -0.020 | 0.000 | 2.458 | 0.034 |
| O60 | -0.391 | 0.073 | 0.000 | 5.234 | 0.025 |
| C61 | -0.742 | 0.003 | 0.000 | 1.829 | 0.028 |
| O65 | -0.563 | 0.023 | 0.000 | 1.863 | 0.011 |
| C67 | -0.408 | 0.158 | 0.000 | 9.565 | 0.036 |
| C69 | 0.366 | 0.130 | 0.000 | 8.424 | 0.025 |
| C70 | -0.753 | -0.011 | 0.000 | 2.002 | 0.008 |
| C74 | -0.749 | -0.012 | 0.000 | 2.014 | 0.003 |
| O132 | -0.422 | 0.000 | 0.073 | 0.148 | 12.666 |
| S133 | 1.270 | 0.001 | 0.158 | 0.270 | 16.314 |
| O134 | -0.527 | -0.002 | 0.117 | 0.248 | 12.155 |
| O135 | -0.502 | 0.001 | 0.119 | 0.070 | 10.223 |
| O136 | -0.641 | 0.001 | 0.078 | 0.124 | 13.348 |
| O144 | -0.371 | 0.153 | 0.001 | 7.036 | 0.495 |