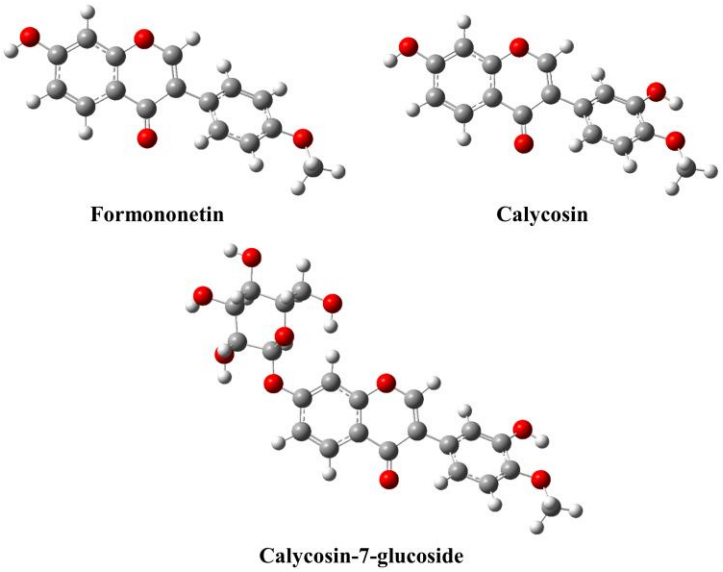


**Figure S1** Optimized structures of the formononetin, calycosin, and calycosin-7-glucoside at M06-2X/6-311+G(d,p) level in the gas phase.

**Table S1** Calculated natural bond orbital (NBO) charges on the hydrogen atoms of phenolic hydroxyls for formononetin, calycosin, and calycosin-7-glucoside.

| Reactions | Formononetin | Calycosin | Calycosin-7-glucoside |
|---|---|---|---|
| 3′-OH | | 0.494 | 0.494 |
| 7-OH | 0.478 | 0.478 | |

**Table S2** Optimized coordinates (x, y, z) of formononetin, calycosin, and calycosin-7-glucoside at M06-2X level.

**Formononetin**

| | | | |
|---|---|---|---|
| O | 1.84472700 | -1.77071800 | 0.39298200 |
| O | 0.31503100 | 1.93376200 | -0.35323400 |
| O | -5.71419200 | -0.24474600 | -0.21185600 |
| O | 6.26778000 | -0.28085900 | 0.08010600 |
| C | -0.08269000 | -0.37411200 | 0.06341900 |
| C | 2.20962700 | 0.55230500 | -0.08927900 |
| C | -1.55722300 | -0.29682800 | -0.01764500 |
| C | 0.76075900 | 0.82085100 | -0.14690000 |
| C | 2.69143200 | -0.72953400 | 0.17416100 |
| C | 0.51626200 | -1.55041000 | 0.33363200 |
| C | 3.14154400 | 1.57601400 | -0.30170600 |
| C | 4.05225800 | -1.01163800 | 0.23314100 |
| C | -2.25634700 | 0.76803400 | 0.54756700 |
| C | -2.29164000 | -1.30662600 | -0.65359500 |
| C | 4.94822400 | 0.02095200 | 0.01831100 |
| C | 4.49445000 | 1.32368700 | -0.25148500 |
| C | -3.64665600 | 0.82090200 | 0.50680900 |
| C | -3.67307100 | -1.26835100 | -0.69881400 |
| C | -4.36082300 | -0.20259400 | -0.11446400 |
| C | -6.44688600 | 0.82749800 | 0.34303200 |
| H | -0.03400400 | -2.45908900 | 0.54211500 |
| H | 2.75966300 | 2.56898400 | -0.50692200 |
| H | -1.71021900 | 1.57256000 | 1.02182200 |
| H | -1.76882600 | -2.12188000 | -1.14205300 |
| H | 4.40031900 | -2.01436400 | 0.44165500 |
| H | 5.21198400 | 2.12022100 | -0.41772700 |
| H | -4.15346500 | 1.66289300 | 0.95808800 |
| H | -4.24456600 | -2.04217800 | -1.19604300 |
| H | 6.79424200 | 0.50662800 | -0.08272400 |
| H | -6.28019000 | 0.90381600 | 1.42197400 |
| H | -7.49469700 | 0.60627000 | 0.15365100 |
| H | -6.18233500 | 1.77572500 | -0.13493000 |

**Calycosin**

| | | | |
|---|---|---|---|
| O | 2.01938500 | 1.67375100 | -0.59476000 |
| O | 0.64588800 | -2.00279700 | 0.50891300 |
| O | -5.47120500 | -0.07057300 | 0.03193200 |
| O | -4.21958100 | 2.08373400 | 0.90988700 |
| O | 6.49822800 | 0.43495900 | -0.05815000 |
| C | 0.15113300 | 0.22956600 | -0.15142300 |
| C | 2.47915900 | -0.56677500 | 0.13265200 |
| C | -1.32151400 | 0.09426600 | -0.09291000 |
| C | 1.04279300 | -0.89676700 | 0.19481600 |
| C | 2.90795700 | 0.70193700 | -0.25548200 |
| C | 0.70191700 | 1.39915500 | -0.53159600 |
| C | -2.10009100 | 1.14733500 | 0.40517200 |
| C | -1.95469700 | -1.05921700 | -0.54856400 |
| C | 3.45185700 | -1.51766100 | 0.46597400 |
| C | 4.25543500 | 1.04061800 | -0.32210300 |
| C | -3.47888300 | 1.05730800 | 0.42167000 |
| C | -4.10830100 | -0.10375200 | -0.05010100 |
| C | -3.34517400 | -1.15756300 | -0.52946500 |
| C | 5.19262900 | 0.07934000 | 0.01373200 |
| C | 4.79275900 | -1.20820600 | 0.41123100 |
| C | -6.17860300 | -1.22050600 | -0.38854100 |
| H | 0.11517200 | 2.25519800 | -0.83960700 |
| H | -1.64300200 | 2.04104000 | 0.81395900 |
| H | -1.36557800 | -1.88935900 | -0.91167900 |
| H | 3.11120000 | -2.50077400 | 0.76822300 |
| H | 4.56166800 | 2.03175800 | -0.62857500 |
| H | -3.81879400 | -2.06188200 | -0.88802600 |
| H | 5.54199500 | -1.94824400 | 0.67192100 |
| H | -5.14877700 | 1.82919300 | 0.86189400 |
| H | 7.05603400 | -0.30578700 | 0.19471700 |
| H | -5.99623000 | -1.42358500 | -1.44772500 |
| H | -7.23288500 | -1.00267300 | -0.23546200 |
| H | -5.89278700 | -2.09194600 | 0.20741600 |

**Calycosin-7-glucoside**

| | | | |
|---|---|---|---|
| C | -4.76877000 | -1.57273200 | -0.34509700 |
| C | -6.23566100 | -1.20060300 | -0.15708200 |
| C | -6.34650000 | -0.07383400 | 0.85758200 |
| C | -5.46822600 | 1.09724600 | 0.45259100 |
| C | -4.04802100 | 0.59044200 | 0.24525200 |
| H | -6.63708000 | -0.84392800 | -1.11678800 |
| H | -4.36390900 | -1.95825600 | 0.60244800 |
| H | -5.82186900 | 1.51303800 | -0.49941600 |
| H | -3.63770800 | 0.20353800 | 1.19217200 |
| H | -6.00006100 | -0.44753800 | 1.83284100 |
| O | 0.74906900 | -0.82713000 | 0.22862500 |
| O | 2.99773700 | 2.46654700 | -0.60679600 |
| O | 8.46479100 | -0.81168000 | 0.26663800 |
| O | 6.82843100 | -1.87309000 | 2.04788500 |
| O | -3.28350800 | 1.66887400 | -0.19922300 |
| C | 2.92426600 | 0.15993400 | -0.02283600 |
| C | 0.86463200 | 1.50810000 | -0.30302600 |
| C | 4.38935900 | -0.04141600 | 0.03412200 |
| C | 2.34008200 | 1.47935800 | -0.33967500 |
| C | 0.13573900 | 0.35996200 | -0.01745100 |
| C | 2.09570300 | -0.87666600 | 0.21192000 |
| C | 4.94430900 | -0.85104700 | 1.03393300 |
| C | 5.23063900 | 0.54315100 | -0.90897900 |
| C | 0.15686600 | 2.69321200 | -0.55774000 |
| C | -1.26078500 | 0.34852800 | 0.01998200 |
| C | 6.30472200 | -1.08973500 | 1.07220900 |
| C | 7.14302400 | -0.50633200 | 0.11086100 |
| C | 6.60451700 | 0.30954500 | -0.87234900 |
| C | -1.92364200 | 1.53810200 | -0.22521700 |
| C | -1.21627100 | 2.71639400 | -0.52025200 |
| C | 9.37999000 | -0.23585900 | -0.64482500 |
| H | 2.44641500 | -1.88171300 | 0.40849900 |
| H | 4.32884800 | -1.28446800 | 1.81374400 |
| H | 4.81936700 | 1.18993900 | -1.67090700 |
| H | 0.73177500 | 3.58412100 | -0.78021900 |
| H | -1.77010300 | -0.58637700 | 0.21015800 |
| H | 7.24216600 | 0.77184600 | -1.61418600 |

| | | | |
|---|---|---|---|
| H | -1.77772100 | 3.62172800 | -0.71154800 |
| H | 7.78468200 | -1.90315900 | 1.92432300 |
| H | 9.16493300 | -0.55846600 | -1.66754700 |
| H | 10.36556200 | -0.58878000 | -0.35084400 |
| H | 9.34863100 | 0.85599400 | -0.58924000 |
| O | -4.03770600 | -0.41078600 | -0.73811400 |
| O | -5.54298400 | 2.04908800 | 1.48989700 |
| H | -5.03365300 | 2.82423200 | 1.23403200 |
| O | -7.70750400 | 0.29114500 | 0.93465500 |
| H | -7.78684000 | 1.02301100 | 1.55541000 |
| O | -6.92552800 | -2.34744600 | 0.28003900 |
| H | -7.81461000 | -2.07312800 | 0.52996100 |
| C | -4.54493200 | -2.60139900 | -1.43557900 |
| H | -5.04466800 | -3.52978300 | -1.16143500 |
| H | -4.98202400 | -2.22870700 | -2.37077500 |
| O | -3.17191700 | -2.88184500 | -1.58758500 |
| H | -2.73541000 | -2.05866200 | -1.82889000 |