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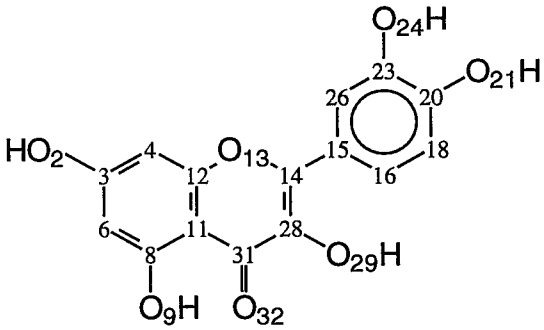
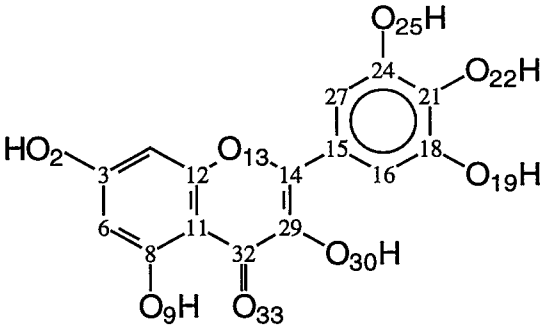
## Atom Nomenclature and Atomic Charges for the Flavonoid Inhibitors




**quercetin**




**myricetin**

| atom no. | atom type | charge | atom no. | atom type | charge |
|---|---|---|---|---|---|
| H1 | HO | 0.3474 | H1 | HO | 0.3455 |
| O2 | OH | -0.4863 | O2 | OH | -0.4849 |
| C3 | C | 0.5641 | C3 | C | 0.5658 |
| C4 | CA | -0.5526 | C4 | CA | -0.5436 |
| H5 | HC | 0.1805 | H5 | HC | 0.1816 |
| C6 | CA | -0.6014 | C6 | CA | -0.6007 |
| H7 | HC | 0.1946 | H7 | HC | 0.1948 |
| C8 | C | 0.6532 | C8 | C | 0.6453 |
| O9 | OH | -0.4640 | O9 | OH | -0.4673 |
| H10 | HO | 0.3367 | H10 | HO | 0.3398 |
| C11 | CB | -0.7315 | C11 | CB | -0.7029 |
| C12 | CB | 0.5539 | C12 | CB | 0.5293 |
| O13 | OX | -0.3098 | O13 | OX | -0.3061 |
| C14 | CX | 0.1949 | C14 | CX | 0.2044 |
| C15 | CA | -0.0372 | C15 | CX | 0.0048 |
| C16 | CA | -0.0855 | C16 | CA | -0.2501 |
| H17 | HC | 0.1325 | H17 | HC | 0.1582 |
| C18 | CA | -0.2300 | C18 | C | 0.2103 |
| H19 | HC | 0.1311 | O19 | OH | -0.4700 |
| C20 | C | 0.2141 | H20 | HO | 0.3434 |
| O21 | OH | -0.0855 | C21 | C | 0.0685 |
| H22 | HO | 0.1325 | O22 | OH | -0.4477 |
| C23 | C | -0.2300 | H23 | HO | 0.3482 |
| O24 | OH | 0.1311 | C24 | C | 0.2424 |
| H25 | HO | 0.2141 | O25 | OH | -0.4557 |
| C26 | CA | -0.4908 | H26 | HO | 0.3465 |
| H27 | HC | 0.3476 | C27 | CA | -0.2229 |
| C28 | CX | 0.1913 | H28 | HC | 0.1583 |
| O29 | OH | -0.4617 | C29 | CX | -0.1018 |
| H30 | HO | 0.3474 | O30 | OH | -0.4116 |
| C31 | C | 0.7507 | H31 | HO | 0.3358 |
| O32 | O | -0.4945 | C32 | C | 0.7323 |
| | | | O33 | O | -0.4899 |

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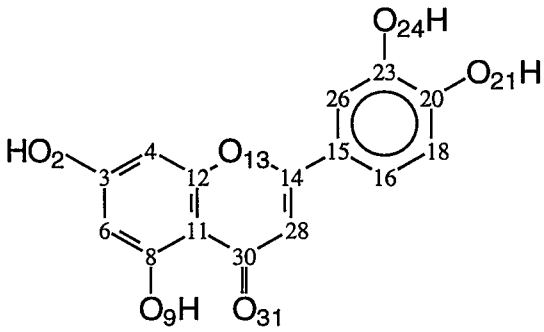
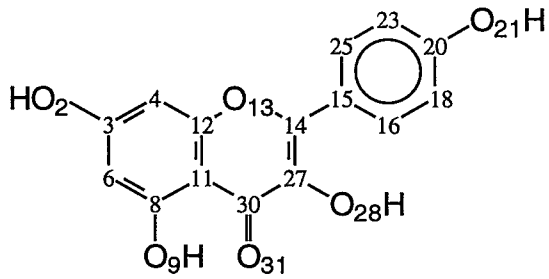


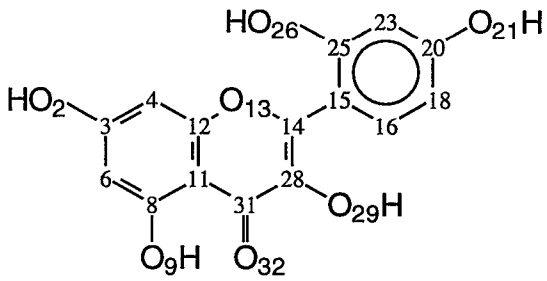

**luteolin**



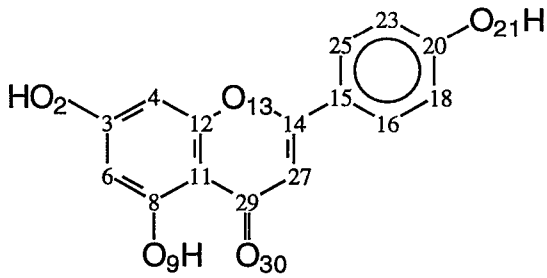

**kaempferol**

| atom no. | atom type | charge | atom no. | atom type | Charge |
|---|---|---|---|---|---|
| H1 | HO | 0.3449 | H1 | HO | 0.3453 |
| O2 | OH | -0.4875 | O2 | OH | -0.4874 |
| C3 | C | 0.5405 | C3 | C | 0.5740 |
| C4 | CA | -0.5443 | C4 | CA | -0.5682 |
| H5 | HC | 0.1840 | H5 | HC | 0.1841 |
| C6 | CA | -0.5647 | C6 | CA | -0.6044 |
| H7 | HC | 0.1889 | H7 | HC | 0.1935 |
| C8 | C | 0.5868 | C8 | C | 0.6510 |
| O9 | OH | -0.4427 | O9 | OH | -0.4657 |
| H10 | HO | 0.3311 | H10 | HO | 0.3378 |
| C11 | CB | -0.6603 | C11 | CB | -0.7218 |
| C12 | CB | 0.5309 | C12 | CB | 0.5623 |
| O13 | OX | -0.3512 | O13 | OX | -0.3134 |
| C14 | CX | 0.4248 | C14 | CX | 0.1727 |
| C15 | CA | -0.1349 | C15 | CA | -0.0881 |
| C16 | CA | -0.0736 | C16 | CA | -0.0058 |
| H17 | HC | 0.1213 | H17 | HC | 0.1202 |
| C18 | CA | -0.2288 | C18 | CA | -0.2880 |
| H19 | HC | 0.1305 | H19 | HC | 0.1244 |
| C20 | C | 0.2229 | C20 | C | 0.3816 |
| O21 | OH | -0.4911 | O21 | OH | -0.4945 |
| H22 | HO | 0.3492 | H22 | HO | 0.3411 |
| C23 | C | 0.1906 | C23 | CA | -0.2739 |
| O24 | OH | -0.4628 | H24 | HC | 0.1446 |
| H25 | HO | 0.3526 | C25 | CA | 0.0001 |
| C26 | CA | -0.1275 | H26 | HC | 0.1061 |
| H27 | HC | 0.1462 | C27 | CX | -0.0967 |
| C28 | CX | -0.5493 | O28 | OH | -0.4133 |
| H29 | HC | 0.1827 | H29 | HO | 0.3323 |
| C30 | C | 0.7937 | C30 | C | 0.7417 |
| O31 | O | -0.5029 | O31 | O | -0.4934 |

## Atom Nomenclature and Atomic Charges for the Flavonoid Inhibitors



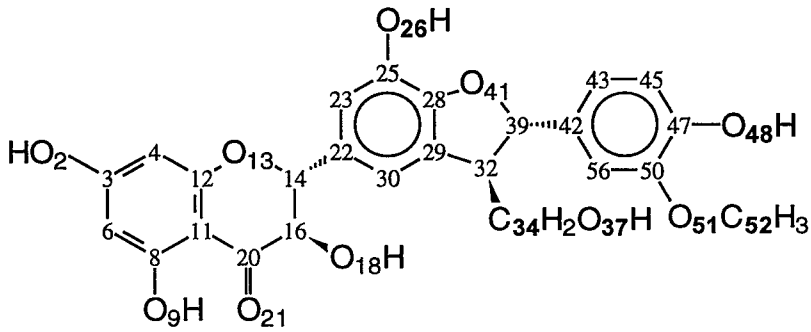

**morin**




**apigenin**

| atom no. | atom type | charge | atom no. | atom type | charge |
|---|---|---|---|---|---|
| H1 | HO | 0.3438 | H1 | HO | 0.3456 |
| O2 | OH | -0.4842 | O2 | OH | -0.4887 |
| C3 | C | 0.5548 | C3 | C | 0.5484 |
| C4 | CA | -0.5488 | C4 | CA | -0.5641 |
| H5 | HC | 0.1841 | H5 | HC | 0.1852 |
| C6 | CA | -0.6017 | C6 | CA | -0.5689 |
| H7 | HC | 0.1919 | H7 | HC | 0.1880 |
| C8 | C | 0.6566 | C8 | C | 0.5930 |
| O9 | OH | -0.4692 | O9 | OH | -0.4477 |
| H10 | HO | 0.3374 | H10 | HO | 0.3333 |
| C11 | CB | -0.7330 | C11 | CB | -0.6637 |
| C12 | CB | 0.5590 | C12 | CB | 0.5521 |
| O13 | OX | -0.3130 | O13 | OX | -0.3544 |
| C14 | CX | 0.2789 | C14 | CX | 0.3967 |
| C15 | CA | -0.2724 | C15 | CA | -0.1923 |
| C16 | CA | 0.0639 | C16 | CA | 0.0148 |
| H17 | HC | 0.1192 | H17 | HC | 0.1097 |
| C18 | CA | -0.3630 | C18 | CA | -0.3027 |
| H19 | HC | 0.1371 | H19 | HC | 0.1262 |
| C20 | C | 0.4483 | C20 | C | 0.4105 |
| O21 | OH | -0.4890 | O21 | OH | -0.4989 |
| H22 | HO | 0.3408 | H22 | HO | 0.3442 |
| C23 | CA | -0.4650 | C23 | CA | -0.2839 |
| H24 | HC | 0.1733 | H24 | HC | 0.1473 |
| C25 | C | 0.4470 | C25 | CA | 0.0395 |
| O26 | OH | -0.4667 | H26 | HC | 0.1028 |
| H27 | HO | 0.3360 | C27 | CX | -0.5330 |
| C28 | CX | -0.1468 | H28 | HC | 0.1752 |
| O29 | OH | -0.4054 | C29 | C | 0.7864 |
| H30 | HO | 0.3320 | O30 | O | -0.5007 |
| C31 | C | 0.7523 | | | |
| O32 | O | -0.4980 | | | |

## Atom Nomenclature and Atomic Charges for the Flavonoid Inhibitors




**silychristin**

| atom no. | atom type | charge | atom no. | atom type | charge |
|---|---|---|---|---|---|
| H1 | HO | 0.3405 | C29 | CB | -0.0336 |
| O2 | OH | -0.4773 | C30 | CA | -0.1601 |
| C3 | C | 0.5528 | H31 | HC | 0.1386 |
| C4 | CA | -0.5150 | C32 | CT | -0.1050 |
| H5 | HC | 0.1767 | H33 | HC | 0.0808 |
| C6 | CA | -0.5755 | C34 | CT | 0.2516 |
| H7 | HC | -0.2072 | H35 | HC | -0.0016 |
| C8 | C | 0.6915 | H36 | HC | 0.0366 |
| O9 | OH | 0.6915 | O37 | OH | 0.5400 |
| H10 | HO | 0.3902 | H38 | HO | 0.3149 |
| C11 | CB | -0.7968 | C39 | CY | 0.1778 |
| C12 | CB | 0.5166 | H40 | HC | 0.0595 |
| O13 | OX | -0.4105 | O41 | OS | -0.3390 |
| C14 | CY | 0.2768 | C42 | CA | -0.0706 |
| H15 | HC | 0.0487 | C43 | CA | -0.0726 |
| C16 | CY | -0.0066 | H44 | HC | 0.1269 |
| H17 | HC | 0.1007 | C45 | CA | -0.2050 |
| O18 | OH | -0.4990 | H46 | HC | 0.1446 |
| H19 | HO | 0.3200 | C47 | C | 0.2190 |
| C20 | C | 0.7331 | O48 | OH | -0.4532 |
| O21 | O | -0.5330 | H49 | HO | 0.3388 |
| C22 | CA | -0.0477 | C50 | C | 0.1909 |
| C23 | CA | -0.1758 | O51 | OS | -0.3657 |
| H24 | HC | 0.1495 | C52 | CT | 0.0949 |
| C25 | C | 0.2472 | H53 | HC | 0.0607 |
| O26 | OH | -0.4765 | H54 | HC | 0.0412 |
| H27 | HO | 0.3536 | H55 | HC | 0.0315 |
| C28 | CB | 0.0696 | C56 | CA | -0.2427 |
| | | | H57 | HC | 0.1450 |

## Additional AMBER Force Field Parameters

| van der Waals | R* (Å) | ε (kcal mol$^{-1}$) |
|---|---|---|
| CX | 1.85 | 0.12 |
| CY | 1.75 | 0.16 |
| OX | 1.85 | 0.12 |

| bond | *Kr* (kcal mol$^{-1}$ Å$^2$) | $r_{eq}$ (Å) |
|---|---|---|
| CX-CX | 549. | 1.35 |
| CY-CY | 317. | 1.52 |
| C - C | 460. | 1.41 |
| CX-CA | 387. | 1.46 |
| CY-CA | 327. | 1.50 |
| CX-C | 372. | 1.47 |
| CX-HC | 330. | 1.12 |
| CB-OX | 315. | 1.38 |
| OX-CX | 315. | 1.39 |
| OX-CY | 320. | 1.44 |
| CX-OH | 315. | 1.38 |
| CY-OH | 315. | 1.42 |
| CY-C | 317. | 1.51 |
| CY-HC | 330. | 1.12 |
| CB-CT | 388. | 1.46 |
| CA-OS | 300. | 1.40 |
| C-OS | 300. | 1.40 |
| CB-CT | 310. | 1.50 |
| CB-OS | 320. | 1.41 |
| CT-CY | 317. | 1.52 |
| CY-OS | 320. | 1.41 |

| dihedral angle | *idivf* | $V_n/2$ (kcal mol$^{-1}$) | γ (deg) |
|---|---|---|---|
| X-CB-OX-CX | 2 | 1.8 | 180. |
| X-CB-OX-CY | 2 | 1.8 | 180. |
| X-CY-C-X | 6 | 0. | 180. |
| CB-OX-CY-X | 3 | 0.5 | 0. |
| CB-OX-CX-X | 2 | 1.8 | 180. |
| X-CY-CY-X | 9 | 1.3 | 0. |
| X-C-C-X | 4 | 5.3 | 180. |
| X-CX-CX-X | 4 | 5.3 | 180. |
| X-CX-OH-HO | 2 | 1.8 | 180. |
| X-CB-CT-X | 6 | 0. | 0. |
| X-CT-CY-X | 9 | 1.3 | 0. |
| X-OS-CY-X | 3 | 1.8 | 180. |
| X-CA-CY-X | 6 | 0.0 | 0. |
| X-CA-CX-X | 4 | 2.05 | 180. |

## Additional AMBER Force Field Parameters (contd.)

| angle | $K_\phi$ (kcal mol$^{-1}$ rad$^{-2}$) | $\phi_{eq}$ (deg) | angle | $K_\phi$ (kcal mol$^{-1}$ rad$^{-2}$) | $\phi_{eq}$ (deg) |
|---|---|---|---|---|---|
| C -CA-C | 85. | 118.8 | HC-CY-HC | 35. | 108. |
| C -CA-CB | 85. | 118.0 | HC-CY-CY | 35. | 109.5 |
| CA-CB-OX | 70. | 114.6 | CY-CY-OH | 35. | 107.9 |
| CA-C -CB | 85. | 121.6 | HC-CY-CA | 35. | 110.1 |
| CA-CB-C | 85. | 121.5 | HC-CY-C | 35. | 108.5 |
| C-CB-C | 85. | 122.6 | HC-CX-C | 35. | 116.5 |
| OH-C -CB | 70. | 116.9 | OX-CX-CA | 80. | 111.1 |
| CB-CB-OX | 80. | 123.2 | OX-CY-HC | 35. | 101.4 |
| CB-C -CX | 85. | 114.0 | OH-CY-HC | 35. | 109.5 |
| CB-C -CY | 85. | 114.3 | OH-CY-C | 85. | 110.9 |
| CB-OX-CY | 85. | 117.0 | CA-CA-CT | 85. | 131.4 |
| CB-OX-CX | 85. | 117.5 | CT-CY-OS | 80. | 107.7 |
| OX-CY-CY | 80. | 113.5 | HC-CY-OX | 35. | 104.8 |
| OX-CX-CX | 80. | 123.2 | OX-CY-CA | 80. | 109.4 |
| CX-CX-CA | 85. | 125.5 | C -C -OS | 85. | 114.9 |
| CX-OH-HO | 35. | 107.1 | CA-OS-CT | 46.5 | 113. |
| CY-OH-HO | 35. | 107.1 | C -OS-CT | 46.5 | 113. |
| CX-CX-OH | 70. | 119.5 | CA-CA-OS | 70. | 120. |
| CX-CX-C | 85. | 122.6 | OS-CT-HC | 35. | 110. |
| CY-CY-C | 63. | 112.7 | OS-C -CA | 80. | 124.7 |
| CX-CA-C | 85. | 121.7 | CA-CT-OS | 54. | 111. |
| CA-C -C | 85. | 120.1 | CA-C -O | 80. | 119.7 |
| CA-CY-CY | 63. | 113.3 | OH-CT-C | 85. | 110.9 |
| C -C -OH | 85. | 122.8 | CA-C -CT | 85. | 114.3 |
| C -C -C | 85. | 119.3 | C -CA-OS | 70. | 114.6 |
| CX-C -O | 80. | 122.2 | CB-OS-CY | 60. | 107.3 |
| CY-C -O | 80. | 121. | C -CB-OS | 80. | 124.7 |
| OH-CX-C | 85. | 117.6 | CB-CB-CT | 70. | 106.2 |
| CY-CA-CA | 85. | 120. | CB-CT-HC | 35. | 109.5 |
| CX-CA-CA | 85. | 119.9 | CB-CT-CT | 63. | 114. |
| CX-CX-HC | 35. | 121.1 | CB-CT-CY | 35. | 103. |
| CT-CY-CA | 63. | 113.3 | CB-CB-OS | 70. | 113.5 |
| HC-CT-CY | 35. | 109.5 | CT-CY-HC | 35. | 109.5 |
| CT-CT-CY | 40. | 109.5 | HC-CT-HC | 35. | 108. |
| HC-CY-OS | 35. | 104.8 | CA-CB-CT | 70. | 130. |
| OS-CY-CA | 80. | 109.4 | | | |