Supplementary Material

Tabela S1: ΔGbind values obtained by the MM/GBSA method for all flavonoids used in this study.

|  |  |
| --- | --- |
| Ligands | MMGBSA (kcal/mol) |
| NuBBE\_867 | -51,5700 |
| NuBBE\_1884 | -50,1202 |
| NuBBE\_1310 | -49,5517 |
| NuBBE\_1890 | -48,2796 |
| NuBBE\_2328 | -47,0772 |
| NuBBE\_1880 | -45,9798 |
| NuBBE\_1870 | -44,8566 |
| NuBBE\_1878 | -44,1312 |
| NuBBE\_1879 | -43,7034 |
| NuBBE\_2007 | -42,6811 |
| NuBBE\_1333 | -42,5288 |
| NuBBE\_126 | -42,2776 |
| NuBBE\_1694 | -41,9867 |
| NuBBE\_1889 | -41,6262 |
| NuBBE\_128 | -41,6000 |
| NuBBE\_2172 | -41,3066 |
| NuBBE\_2003 | -40,9515 |
| NuBBE\_2417 | -40,7404 |
| NuBBE\_1444 | -40,7235 |
| NuBBE\_1888 | -40,6556 |
| NuBBE\_1219 | -40,5976 |
| NuBBE\_2001 | -40,0045 |
| NuBBE\_1308 | -39,9722 |
| NuBBE\_1864 | -39,8384 |
| NuBBE\_2174 | -39,6073 |
| NuBBE\_1871 | -39,6061 |
| NuBBE\_1886 | -39,2091 |
| NuBBE\_287 | -39,1142 |
| NuBBE\_1222 | -39,1089 |
| NuBBE\_1205 | -38,9831 |
| NuBBE\_1883 | -38,8293 |
| NuBBE\_1872 | -38,7946 |
| NuBBE\_1215 | -38,7667 |
| NuBBE\_2523 | -38,6801 |
| NuBBE\_1226 | -38,2976 |
| NuBBE\_2020 | -38,2747 |
| NuBBE\_1189 | -38,2024 |
| NuBBE\_1472 | -38,0646 |
| NuBBE\_1814 | -37,9741 |
| NuBBE\_1588 | -37,8712 |
| NuBBE\_2522 | -37,7396 |
| NuBBE\_2021 | -37,5849 |
| NuBBE\_1224 | -37,5840 |
| NuBBE\_2018 | -37,4563 |
| NuBBE\_2004 | -37,4385 |
| NuBBE\_1445 | -37,3497 |
| NuBBE\_1867 | -37,2255 |
| NuBBE\_1312 | -37,0784 |
| NuBBE\_1306 | -36,8273 |
| NuBBE\_1263 | -36,8071 |
| NuBBE\_1589 | -36,7372 |
| NuBBE\_2023 | -36,6255 |
| NuBBE\_1311 | -36,6206 |
| NuBBE\_1328 | -36,6186 |
| NuBBE\_1316 | -36,5996 |
| NuBBE\_1223 | -36,5458 |
| NuBBE\_1693 | -36,5311 |
| NuBBE\_1663 | -36,4961 |
| NuBBE\_1873 | -36,4915 |
| NuBBE\_1327 | -36,4608 |
| NuBBE\_1875 | -36,4367 |
| NuBBE\_1656 | -36,3525 |
| NuBBE\_1225 | -36,3444 |
| NuBBE\_2485 | -36,3140 |
| NuBBE\_2427 | -36,2966 |
| NuBBE\_2035 | -36,2510 |
| NuBBE\_1305 | -36,1845 |
| NuBBE\_2033 | -36,1613 |
| NuBBE\_1559 | -36,1094 |
| NuBBE\_1869 | -36,0911 |
| NuBBE\_2000 | -36,0216 |
| NuBBE\_1787 | -35,8936 |
| NuBBE\_2083 | -35,8806 |
| NuBBE\_1591 | -35,7800 |
| NuBBE\_2081 | -35,7247 |
| NuBBE\_1692 | -35,7010 |
| NuBBE\_1625 | -35,6850 |
| NuBBE\_178 | -35,6445 |
| NuBBE\_1580 | -35,6129 |
| NuBBE\_1221 | -35,5807 |
| NuBBE\_2275 | -35,5734 |
| NuBBE\_2434 | -35,5706 |
| NuBBE\_1894 | -35,3891 |
| NuBBE\_1893 | -35,0438 |
| NuBBE\_2486 | -35,0431 |
| NuBBE\_1586 | -34,7058 |
| NuBBE\_2225 | -34,6383 |
| NuBBE\_2175 | -34,5670 |
| NuBBE\_2082 | -34,5665 |
| NuBBE\_1318 | -34,5235 |
| NuBBE\_2399 | -34,4895 |
| NuBBE\_1868 | -34,4570 |
| NuBBE\_122 | -34,4333 |
| NuBBE\_1216 | -34,3931 |
| NuBBE\_1874 | -34,3652 |
| NuBBE\_1776 | -34,3132 |
| NuBBE\_2049 | -34,2696 |
| NuBBE\_1999 | -34,2229 |
| NuBBE\_1443 | -34,1949 |
| NuBBE\_1581 | -34,1847 |
| NuBBE\_1322 | -34,1598 |
| NuBBE\_2024 | -34,0285 |
| NuBBE\_1592 | -34,0272 |
| NuBBE\_2047 | -33,9968 |
| NuBBE\_68 | -33,9066 |
| NuBBE\_1865 | -33,9052 |
| NuBBE\_1321 | -33,8114 |
| NuBBE\_1590 | -33,7340 |
| NuBBE\_2222 | -33,6109 |
| NuBBE\_1895 | -33,6097 |
| NuBBE\_2432 | -33,4515 |
| NuBBE\_1777 | -33,2776 |
| NuBBE\_320 | -33,2295 |
| NuBBE\_2509 | -33,0321 |
| NuBBE\_563 | -32,9910 |
| NuBBE\_1073 | -32,8693 |
| NuBBE\_2048 | -32,7572 |
| NuBBE\_1558 | -32,6023 |
| NuBBE\_1307 | -32,5845 |
| NuBBE\_2526 | -32,5533 |
| NuBBE\_1768 | -32,5281 |
| NuBBE\_1309 | -32,5117 |
| NuBBE\_2415 | -32,3545 |
| NuBBE\_1220 | -32,3515 |
| NuBBE\_1217 | -32,2932 |
| NuBBE\_1218 | -32,2655 |
| NuBBE\_2005 | -32,2605 |
| NuBBE\_1695 | -31,9031 |
| NuBBE\_1662 | -31,7896 |
| NuBBE\_2524 | -31,7735 |
| NuBBE\_293 | -31,7655 |
| NuBBE\_2019 | -31,7438 |
| NuBBE\_1997 | -31,7179 |
| NuBBE\_1766 | -31,4219 |
| NuBBE\_1557 | -31,3978 |
| NuBBE\_2511 | -31,3426 |
| NuBBE\_1765 | -31,2925 |
| NuBBE\_1784 | -31,2613 |
| NuBBE\_426 | -31,2344 |
| NuBBE\_1815 | -31,2293 |
| NuBBE\_2452 | -31,1620 |
| NuBBE\_2431 | -31,0428 |
| NuBBE\_180 | -30,9939 |
| NuBBE\_139 | -30,9539 |
| NuBBE\_2034 | -30,9315 |
| NuBBE\_564 | -30,8886 |
| NuBBE\_2022 | -30,8486 |
| NuBBE\_67 | -30,6673 |
| NuBBE\_1593 | -30,6275 |
| NuBBE\_2450 | -30,4682 |
| NuBBE\_1995 | -30,4555 |
| NuBBE\_2508 | -30,3086 |
| NuBBE\_1582 | -30,2449 |
| NuBBE\_2006 | -30,0698 |
| NuBBE\_1844 | -29,9986 |
| NuBBE\_2416 | -29,9251 |
| NuBBE\_2443 | -29,8957 |
| NuBBE\_2413 | -29,7795 |
| NuBBE\_1769 | -29,7714 |
| NuBBE\_292 | -29,3012 |
| NuBBE\_1320 | -29,2594 |
| NuBBE\_562 | -29,1305 |
| NuBBE\_1188 | -29,0932 |
| NuBBE\_2224 | -29,0327 |
| NuBBE\_2046 | -29,0252 |
| NuBBE\_2080 | -28,9735 |
| NuBBE\_2386 | -28,9697 |
| NuBBE\_179 | -28,9201 |
| NuBBE\_866 | -28,9115 |
| NuBBE\_120 | -28,8815 |
| NuBBE\_1996 | -28,7719 |
| NuBBE\_1317 | -28,6687 |
| NuBBE\_1908 | -28,6615 |
| NuBBE\_355 | -28,6184 |
| NuBBE\_1892 | -28,6044 |
| NuBBE\_2173 | -28,0556 |
| NuBBE\_2402 | -27,9687 |
| NuBBE\_2025 | -27,9311 |
| NuBBE\_1314 | -27,8261 |
| NuBBE\_565 | -27,5631 |
| NuBBE\_2430 | -27,5170 |
| NuBBE\_2008 | -27,5055 |
| NuBBE\_1560 | -27,5019 |
| NuBBE\_1206 | -27,4505 |
| NuBBE\_2036 | -27,3368 |
| NuBBE\_2510 | -27,3228 |
| NuBBE\_141 | -27,0677 |
| NuBBE\_2282 | -27,0392 |
| NuBBE\_2401 | -26,9075 |
| NuBBE\_2279 | -26,8253 |
| NuBBE\_1046 | -26,7558 |
| NuBBE\_1562 | -26,2231 |
| NuBBE\_1313 | -25,5619 |
| NuBBE\_2280 | -25,0887 |
| NuBBE\_177 | -24,8832 |
| NuBBE\_2447 | -24,7817 |
| NuBBE\_567 | -24,6827 |
| NuBBE\_2448 | -24,0857 |
| NuBBE\_2449 | -23,1450 |
| NuBBE\_181 | -23,1124 |
| NuBBE\_363 | -22,8868 |
| NuBBE\_2451 | -20,4782 |
| NuBBE\_1045 | -20,3413 |
| NuBBE\_1866 | -11,8909 |