*File S1: The xyz coordinates of the three optimized structures of salicin.*

**xyz coordinates of salicin (gas)**

| | | | |
|---|---|---|---|
| O | 0.63341206 | 0.44755225 | -0.61642907 |
| O | -0.78611203 | -1.35403160 | -0.46576106 |
| O | 3.97547676 | -1.81188224 | 0.13644241 |
| O | 4.16621880 | 1.11287896 | 0.38840547 |
| O | 1.36282464 | -2.89426962 | 0.72533374 |
| O | 0.54425167 | 3.38862798 | -0.53371461 |
| O | -1.60925721 | 1.41189114 | -1.96007696 |
| C | 2.84727084 | -0.95742346 | 0.42658424 |
| C | 3.01812114 | 0.44356794 | -0.19896449 |
| C | 1.58440133 | -1.70452924 | -0.05593318 |
| C | 1.71036408 | 1.25565456 | -0.06415625 |
| C | 0.36761129 | -0.78233473 | 0.11258881 |
| C | 1.69921688 | 2.58704718 | -0.83057755 |
| C | -2.01820553 | -0.99976502 | 0.14248906 |
| C | -2.92482302 | -0.18353842 | -0.56346574 |
| C | -2.32526814 | -1.52533390 | 1.40233924 |
| C | -4.15176965 | 0.10622632 | 0.06036188 |
| C | -2.61287750 | 0.36101873 | -1.95028219 |
| C | -3.55363526 | -1.21646939 | 2.00031689 |
| C | -4.46905196 | -0.39663265 | 1.32830355 |
| H | 2.75576230 | -0.83360725 | 1.52360035 |
| H | 3.27235379 | 0.33503049 | -1.26139523 |
| H | 1.68586815 | -1.95013128 | -1.12534404 |
| H | 1.49725082 | 1.45997122 | 1.00190907 |
| H | 0.19529189 | -0.54570462 | 1.17548325 |
| H | 1.78069462 | 2.38000508 | -1.91045636 |
| H | 2.57257890 | 3.17522730 | -0.52761858 |
| H | 4.78017712 | -1.30517657 | 0.36797048 |
| H | 3.95757766 | 1.30893767 | 1.32453191 |
| H | 2.19675005 | -3.40459560 | 0.69683597 |
| H | -0.24658636 | 2.96629040 | -0.93105921 |
| H | -1.61052824 | -2.18460682 | 1.89244438 |
| H | -4.86714688 | 0.74069467 | -0.46334275 |
| H | -2.29323672 | -0.45921890 | -2.61149564 |
| H | -3.51889288 | 0.80810186 | -2.37377733 |
| H | -3.79523734 | -1.62560743 | 2.98037555 |
| H | -5.42670787 | -0.15305921 | 1.78632814 |
| H | -0.78397117 | 0.99820021 | -1.61981764 |

**xyz coordinates of salicin (aq)**

| | | | |
|---|---|---|---|
| O | 0.58928407 | 0.46180314 | -0.52617793 |
| O | -0.78347643 | -1.38942450 | -0.39352983 |
| O | 3.99723854 | -1.80260552 | -0.02497822 |
| O | 4.14446204 | 1.13413086 | 0.41336987 |
| O | 1.42025832 | -2.95464931 | 0.56532555 |
| O | 0.48980737 | 3.38917686 | -0.36367705 |
| O | -1.61210601 | 1.24259798 | -2.11195485 |
| C | 2.87402288 | -0.97562076 | 0.37071569 |
| C | 3.00490609 | 0.46323079 | -0.18136651 |
| C | 1.60273170 | -1.69581502 | -0.12322013 |
| C | 1.68835553 | 1.25128310 | 0.03212510 |
| C | 0.38555464 | -0.80427970 | 0.15678682 |
| C | 1.66885802 | 2.60448402 | -0.68387324 |
| C | -2.01228713 | -0.97487228 | 0.18799832 |
| C | -2.92053544 | -0.24762290 | -0.60625820 |
| C | -2.31632279 | -1.34957830 | 1.50071384 |
| C | -4.15469380 | 0.10287954 | -0.02769312 |
| C | -2.59000150 | 0.15205627 | -2.03306983 |
| C | -3.54887818 | -0.97954197 | 2.05582327 |
| C | -4.47076293 | -0.25191146 | 1.29036829 |
| H | 2.83178989 | -0.92466412 | 1.47134144 |
| H | 3.22884378 | 0.41565043 | -1.25448931 |
| H | 1.66876096 | -1.86126136 | -1.20975604 |
| H | 1.50688598 | 1.40077524 | 1.10886349 |
| H | 0.26072763 | -0.61838028 | 1.23371725 |
| H | 1.74626647 | 2.45026490 | -1.76992019 |
| H | 2.52780573 | 3.19459175 | -0.35207714 |
| H | 4.78804289 | -1.45765521 | 0.43722830 |
| H | 3.99379674 | 1.19685289 | 1.37993405 |
| H | 2.26783024 | -3.43947841 | 0.48373826 |
| H | -0.28612327 | 2.95362056 | -0.77269832 |
| H | -1.59991269 | -1.93187228 | 2.07766763 |
| H | -4.87289210 | 0.66426613 | -0.62519295 |
| H | -2.21356805 | -0.71072796 | -2.59929722 |
| H | -3.49128220 | 0.52552204 | -2.52777843 |
| H | -3.78753268 | -1.26940122 | 3.07809081 |
| H | -5.43140692 | 0.03431858 | 1.71593098 |
| H | -0.80125318 | 0.91790252 | -1.65323652 |

**xyz coordinates of salicin (EtOH)**

| | | | |
|---|---|---|---|
| O | 0.59608261 | 0.45887941 | -0.53423646 |
| O | -0.76899135 | -1.39426828 | -0.39786182 |
| O | 4.00844019 | -1.76947861 | 0.09408346 |
| O | 4.13778142 | 1.16815007 | 0.42608008 |
| O | 1.42585488 | -2.92791893 | 0.64407050 |
| O | 0.46558704 | 3.37949231 | -0.44264937 |
| O | -1.59206477 | 1.23449890 | -2.12675815 |
| C | 2.86953407 | -0.94115959 | 0.43432089 |
| C | 3.00382140 | 0.48019193 | -0.15895129 |
| C | 1.61499043 | -1.68446628 | -0.06908570 |
| C | 1.68256698 | 1.26711517 | 0.02038122 |
| C | 0.38576207 | -0.79589196 | 0.16672450 |
| C | 1.65973453 | 2.60461884 | -0.72452595 |
| C | -2.00935695 | -0.99070178 | 0.16688278 |
| C | -2.91200826 | -0.26323341 | -0.63383437 |
| C | -2.32851090 | -1.37846321 | 1.47247619 |
| C | -4.15640191 | 0.07255638 | -0.06789582 |
| C | -2.57079236 | 0.14600612 | -2.05609688 |
| C | -3.57115206 | -1.02332666 | 2.01435067 |
| C | -4.48733238 | -0.29482791 | 1.24301292 |
| H | 2.79851585 | -0.85585630 | 1.53193400 |
| H | 3.23701629 | 0.40190495 | -1.22829257 |
| H | 1.70445654 | -1.87343227 | -1.15039660 |
| H | 1.48676173 | 1.43930221 | 1.09152100 |
| H | 0.23669867 | -0.59333335 | 1.23819078 |
| H | 1.75939552 | 2.42826182 | -1.80564127 |
| H | 2.50547655 | 3.21239713 | -0.39013228 |
| H | 4.79504964 | -1.36221313 | 0.51137833 |
| H | 3.97320195 | 1.26997800 | 1.38712837 |
| H | 2.27273061 | -3.41621938 | 0.57942438 |
| H | -0.29976034 | 2.91856001 | -0.84459969 |
| H | -1.61532157 | -1.96230241 | 2.05188602 |
| H | -4.87208568 | 0.63301046 | -0.66949654 |
| H | -2.19391162 | -0.71537658 | -2.62471790 |
| H | -3.46903284 | 0.52237758 | -2.55452646 |
| H | -3.82205806 | -1.32527927 | 3.03018483 |
| H | -5.45615998 | -0.02001359 | 1.65740374 |
| H | -0.77792291 | 0.90049954 | -1.68204201 |