

Influence of the CH/ π hydrogen bond on the enhancement of circular dichroism (CD) amplitude of 5,7-diene steroids: ergosterol, lumisterol, pirocarciferol, isopirocarciferol and structurally related cyclohexadienes

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Supplementary materials

Optimized Cartesian coordinates of model molecules.

(a) **1'**

| | | | |
|---|----------|----------|----------|
| C | -2.88783 | -0.3435 | 4.020874 |
| H | -3.84228 | -0.29792 | 4.557626 |
| H | -2.48458 | -1.34677 | 4.180168 |
| C | -3.1743 | -0.12912 | 2.536276 |
| H | -2.26449 | -0.27399 | 1.946266 |
| H | -3.8895 | -0.88178 | 2.195908 |
| C | -3.71285 | 1.275574 | 2.294424 |
| H | -4.6333 | 1.41707 | 2.868679 |
| C | -2.66942 | 2.299439 | 2.734351 |
| H | -3.03674 | 3.321031 | 2.609085 |
| H | -1.80128 | 2.198175 | 2.070635 |
| C | -2.2325 | 2.099187 | 4.161192 |
| C | -1.89631 | 3.152235 | 4.944295 |
| H | -2.02002 | 4.160733 | 4.561788 |
| C | -1.35209 | 2.97914 | 6.275918 |
| H | -0.95588 | 3.844644 | 6.794908 |
| C | -1.40486 | 1.778283 | 6.899797 |
| C | -2.10881 | 0.63181 | 6.193697 |
| H | -3.18459 | 0.813079 | 6.3679 |

| | | | |
|---|----------|----------|----------|
| C | -1.93065 | 0.689938 | 4.650469 |
| C | -1.78711 | -0.77237 | 6.756036 |
| H | -0.91216 | -1.177 | 6.247158 |
| H | -2.61288 | -1.44468 | 6.514617 |
| C | -1.52372 | -0.8266 | 8.266476 |
| H | -1.18826 | -1.8334 | 8.535992 |
| H | -2.4523 | -0.64183 | 8.817761 |
| C | -0.49903 | 0.221799 | 8.67876 |
| C | -1.09317 | 1.598545 | 8.35019 |
| H | -2.05998 | 1.617746 | 8.881008 |
| C | -0.17401 | 2.587034 | 9.069733 |
| H | -0.67219 | 3.530869 | 9.293692 |
| H | 0.687923 | 2.820405 | 8.44179 |
| C | 0.253083 | 1.824113 | 10.35282 |
| H | -0.167 | 2.283357 | 11.24786 |
| H | 1.336706 | 1.84629 | 10.47172 |
| C | -0.25802 | 0.369991 | 10.18435 |
| H | -1.20494 | 0.237533 | 10.71501 |
| C | -0.47877 | 0.40348 | 4.221074 |
| H | -0.36966 | 0.546699 | 3.1459 |
| H | -0.17441 | -0.6194 | 4.445051 |
| H | 0.200831 | 1.092513 | 4.723007 |
| C | 0.835757 | 0.000463 | 7.96264 |
| H | 0.757778 | 0.178747 | 6.891133 |
| H | 1.175789 | -1.02623 | 8.115427 |
| H | 1.609253 | 0.663461 | 8.350173 |
| H | 0.441916 | -0.37163 | 10.57505 |
| H | -3.96323 | 1.421728 | 1.241182 |

(b) 2'

| | | | |
|---|----------|----------|----------|
| C | 7.817078 | 7.211964 | 0.294526 |
| C | 8.490179 | 7.408224 | 1.668677 |
| C | 10.59101 | 8.482764 | 0.575467 |
| C | 11.41765 | 9.777631 | 0.439786 |
| C | 11.62139 | 10.50729 | 1.784684 |
| C | 11.38139 | 9.527881 | 2.953673 |

| | | | |
|---|----------|----------|----------|
| C | 11.92464 | 10.25927 | 4.181288 |
| C | 13.10458 | 11.10466 | 3.629726 |
| C | 13.05566 | 10.95842 | 2.089991 |
| C | 10.67885 | 11.71156 | 1.881386 |
| C | 9.243034 | 6.132949 | 2.083046 |
| C | 6.54594 | 6.365752 | 0.319135 |
| C | 5.531891 | 6.952061 | 1.29304 |
| C | 6.133348 | 6.973528 | 2.696391 |
| C | 7.451284 | 7.698867 | 2.74713 |
| C | 7.789876 | 8.454864 | 3.820841 |
| C | 9.127135 | 8.995788 | 3.988861 |
| C | 9.976121 | 9.028129 | 2.937772 |
| C | 9.438876 | 8.626341 | 1.577104 |
| H | 7.558443 | 8.199198 | -0.10501 |
| H | 8.795318 | 9.454326 | 1.234043 |
| H | 11.24488 | 7.67103 | 0.902459 |
| H | 10.2145 | 8.198006 | -0.4083 |
| H | 12.38569 | 9.5295 | -0.00524 |
| H | 10.92055 | 10.44915 | -0.26582 |
| H | 12.0497 | 8.673799 | 2.763437 |
| H | 12.23396 | 9.569036 | 4.966824 |
| H | 11.15209 | 10.90142 | 4.607287 |
| H | 14.06188 | 10.76357 | 4.024389 |
| H | 13.00026 | 12.1486 | 3.926668 |
| H | 8.539654 | 6.771247 | -0.39691 |
| H | 13.75014 | 10.17944 | 1.764222 |
| H | 10.80392 | 12.25524 | 2.817731 |
| H | 10.89083 | 12.40466 | 1.065069 |
| H | 9.63396 | 11.41217 | 1.808146 |
| H | 9.965682 | 5.83546 | 1.321687 |
| H | 9.77193 | 6.299295 | 3.022157 |
| H | 8.549916 | 5.303792 | 2.225704 |
| H | 6.128893 | 6.314219 | -0.6895 |
| H | 6.777824 | 5.33799 | 0.613848 |
| H | 4.605755 | 6.372638 | 1.28832 |
| H | 6.28161 | 5.933194 | 3.012874 |

| | | | |
|---|----------|----------|----------|
| H | 5.445079 | 7.421502 | 3.417396 |
| H | 7.064714 | 8.599065 | 4.615841 |
| H | 9.441355 | 9.328414 | 4.971681 |
| H | 13.33013 | 11.87829 | 1.56898 |
| H | 5.278138 | 7.971073 | 0.986067 |

(c) 3'

| | | | |
|---|----------|----------|----------|
| C | 4.193176 | -4.32977 | 3.42223 |
| C | 3.177618 | -5.36004 | 2.895037 |
| C | 1.410823 | -4.07595 | 4.4039 |
| C | 0.234377 | -4.31679 | 5.366841 |
| C | -0.90788 | -5.09378 | 4.716231 |
| C | -0.33942 | -6.41429 | 4.130014 |
| C | -1.58875 | -7.20465 | 3.75044 |
| C | -2.5973 | -6.84458 | 4.876289 |
| C | -1.97461 | -5.65893 | 5.660823 |
| C | -1.5872 | -4.23713 | 3.644558 |
| C | 3.800746 | -6.76988 | 2.919005 |
| C | 5.361157 | -4.06525 | 2.474968 |
| C | 4.82865 | -3.55849 | 1.13881 |
| C | 3.912837 | -4.60949 | 0.514943 |
| C | 2.821097 | -5.07413 | 1.44515 |
| C | 1.615246 | -5.45763 | 0.964707 |
| C | 0.599004 | -6.05465 | 1.811731 |
| C | 0.740285 | -6.08617 | 3.156965 |
| C | 1.92408 | -5.40791 | 3.812653 |
| H | 4.549917 | -4.65556 | 4.405033 |
| H | 3.687948 | -3.37313 | 3.569512 |
| H | 2.204853 | -3.57689 | 4.961522 |
| H | 1.119026 | -3.4044 | 3.59141 |
| H | 0.603527 | -4.88911 | 6.225932 |
| H | -0.12639 | -3.35961 | 5.756767 |
| H | 0.122117 | -6.93265 | 4.983849 |
| H | -1.96781 | -6.88969 | 2.777392 |
| H | -1.39374 | -8.27545 | 3.687823 |
| H | -3.56605 | -6.57184 | 4.456854 |

| | | | |
|---|----------|----------|----------|
| H | -2.77201 | -7.69505 | 5.535597 |
| H | -1.49328 | -6.0187 | 6.574295 |
| H | -0.91875 | -4.00762 | 2.816713 |
| H | -1.91733 | -3.29734 | 4.091521 |
| H | -2.46781 | -4.72939 | 3.232113 |
| H | 3.054752 | -7.5061 | 2.618171 |
| H | 4.65066 | -6.84894 | 2.24205 |
| H | 4.143267 | -7.01307 | 3.927924 |
| H | 6.031434 | -3.32875 | 2.924523 |
| H | 5.952454 | -4.97111 | 2.316207 |
| H | 5.647024 | -3.32303 | 0.454537 |
| H | 4.534627 | -5.4702 | 0.238058 |
| H | 3.466228 | -4.24243 | -0.41254 |
| H | 1.400066 | -5.33589 | -0.09239 |
| H | -0.29278 | -6.45997 | 1.347124 |
| H | 2.218088 | -6.01842 | 4.679983 |
| H | 4.269347 | -2.63251 | 1.302883 |
| H | -2.71672 | -4.91348 | 5.954257 |

(d) 4'

| | | | |
|---|----------|----------|----------|
| C | -2.92823 | -2.64919 | 6.222406 |
| C | -3.26873 | -1.44589 | 7.129261 |
| C | -4.24918 | -3.0283 | 8.947387 |
| C | -5.29562 | -3.13939 | 10.07417 |
| C | -6.69473 | -2.65081 | 9.641925 |
| C | -6.79341 | -2.65696 | 8.102235 |
| C | -8.28468 | -2.47999 | 7.815621 |
| C | -8.98608 | -3.19822 | 9.000131 |
| C | -7.86555 | -3.57643 | 9.998633 |
| C | -6.97072 | -1.25167 | 10.20298 |
| C | -2.04099 | -1.03095 | 7.954445 |
| C | -1.86524 | -2.30233 | 5.172071 |
| C | -2.21894 | -1.06169 | 4.347912 |
| C | -2.5966 | 0.137862 | 5.236413 |
| C | -3.66893 | -0.33408 | 6.174378 |
| C | -4.97282 | -0.05743 | 5.926546 |

| | | | |
|---|----------|----------|----------|
| C | -6.05163 | -0.83151 | 6.514439 |
| C | -5.79708 | -1.72543 | 7.4943 |
| C | -4.41839 | -1.74118 | 8.128315 |
| H | -3.85006 | -2.96649 | 5.722772 |
| H | -4.34628 | -3.88584 | 8.277601 |
| H | -3.25018 | -3.09063 | 9.382125 |
| H | -5.34554 | -4.1809 | 10.40511 |
| H | -4.95726 | -2.55957 | 10.93752 |
| H | -6.52805 | -3.68106 | 7.797286 |
| H | -8.53893 | -1.41894 | 7.79709 |
| H | -8.56917 | -2.89294 | 6.847256 |
| H | -9.7207 | -2.54134 | 9.466672 |
| H | -9.52806 | -4.08392 | 8.667979 |
| H | -7.55875 | -4.61417 | 9.843877 |
| H | -6.24612 | -0.52084 | 9.846236 |
| H | -6.91447 | -1.28008 | 11.2928 |
| H | -7.96388 | -0.89294 | 9.932941 |
| H | -1.17156 | -0.81906 | 7.337301 |
| H | -1.75921 | -1.82198 | 8.649563 |
| H | -2.26662 | -0.13287 | 8.531456 |
| H | -1.72737 | -3.15598 | 4.50363 |
| H | -3.08235 | -1.28824 | 3.715931 |
| H | -2.96981 | 0.956776 | 4.617064 |
| H | -1.71283 | 0.507858 | 5.761746 |
| H | -2.5792 | -3.49241 | 6.825466 |
| H | -0.90223 | -2.14727 | 5.664467 |
| H | -5.21718 | 0.679989 | 5.168117 |
| H | -7.04402 | -0.74758 | 6.086039 |
| H | -4.39388 | -0.89573 | 8.834784 |
| H | -1.38984 | -0.80357 | 3.683625 |
| H | -8.1782 | -3.48109 | 11.04078 |

(e) 5'

| | | | |
|---|----------|----------|----------|
| C | -4.20048 | -0.92622 | 0.166541 |
| C | -4.12151 | -1.8956 | 1.101977 |
| C | -1.73886 | -0.34903 | 0.51842 |

| | | | |
|---|----------|----------|----------|
| C | -2.93455 | -0.40603 | -0.45733 |
| C | -0.39124 | -1.98631 | 2.021798 |
| C | 0.806409 | -1.86493 | 1.080407 |
| C | 0.860481 | -0.46514 | 0.470237 |
| C | -0.43656 | -0.18042 | -0.31988 |
| C | -1.94367 | 0.806173 | 1.518478 |
| C | -2.81767 | -2.33851 | 1.582871 |
| C | -1.68412 | -1.63413 | 1.337151 |
| C | 2.043159 | -0.31861 | -0.48095 |
| C | 2.143564 | 1.065758 | -1.14374 |
| C | 0.871782 | 1.300523 | -1.95419 |
| C | 2.35221 | 2.193603 | -0.12273 |
| C | 3.461705 | -0.58109 | 0.043231 |
| C | 4.382682 | 0.11279 | -1.00413 |
| C | -0.37423 | 1.168719 | -1.06276 |
| C | 3.434485 | 0.893183 | -1.95583 |
| H | -5.16286 | -0.57733 | -0.2001 |
| H | -5.0196 | -2.33695 | 1.52695 |
| H | -2.66171 | -1.07434 | -1.29227 |
| H | -3.10599 | 0.58756 | -0.88536 |
| H | -0.2306 | -1.29645 | 2.864909 |
| H | -0.46429 | -2.99549 | 2.445405 |
| H | 0.721312 | -2.60409 | 0.270266 |
| H | 1.734985 | -2.07726 | 1.624719 |
| H | 0.965554 | 0.262435 | 1.290393 |
| H | -0.4789 | -0.97023 | -1.09191 |
| H | -1.09072 | 0.902938 | 2.198198 |
| H | -2.08187 | 1.760721 | 0.999675 |
| H | -2.8399 | 0.612664 | 2.11786 |
| H | -2.76559 | -3.21523 | 2.226699 |
| H | 1.866495 | -1.03071 | -1.30768 |
| H | 0.887294 | 2.290863 | -2.43057 |
| H | 0.823159 | 0.552023 | -2.75863 |
| H | 2.408093 | 3.15292 | -0.65161 |
| H | 3.287549 | 2.067209 | 0.431573 |
| H | 1.54178 | 2.261135 | 0.607759 |

| | | | |
|---|----------|----------|----------|
| H | 3.677515 | -1.64958 | 0.135792 |
| H | 3.587264 | -0.13584 | 1.037529 |
| H | 5.088191 | 0.790663 | -0.51406 |
| H | 4.978216 | -0.61876 | -1.55821 |
| H | -0.38563 | 1.990165 | -0.33799 |
| H | -1.26781 | 1.288623 | -1.68565 |
| H | 3.218042 | 0.294181 | -2.84981 |
| H | 3.859429 | 1.848273 | -2.28633 |

(f) 6'

| | | | |
|---|----------|----------|----------|
| C | 0.33398 | 0.087336 | -0.07162 |
| H | 0.375466 | 0.449129 | 0.948519 |
| C | 1.068469 | -0.97245 | -0.45824 |
| H | 1.738705 | -1.46849 | 0.233306 |
| C | -0.56898 | 0.737754 | -1.01248 |
| H | -1.05288 | 1.662142 | -0.71485 |
| C | 1.057352 | -1.40125 | -1.89746 |
| H | 1.328719 | -2.45411 | -1.9755 |
| C | -0.28231 | -1.15016 | -2.61212 |
| C | -0.8919 | 0.17634 | -2.20012 |
| C | -1.99576 | 0.736204 | -3.05146 |
| C | -0.094 | -1.25221 | -4.1423 |
| C | -1.68997 | 0.644076 | -4.54359 |
| H | -2.54974 | 0.99187 | -5.12165 |
| H | -0.84602 | 1.295405 | -4.7955 |
| C | -1.34174 | -0.79258 | -4.92136 |
| H | -2.19172 | -1.42745 | -4.63467 |
| H | -2.91017 | 0.158959 | -2.86209 |
| H | -2.20833 | 1.765443 | -2.75114 |
| H | 1.836098 | -0.83949 | -2.43301 |
| C | 0.373907 | -2.65486 | -4.56184 |
| H | -0.33746 | -3.39292 | -4.17793 |
| H | 1.331462 | -2.87952 | -4.08853 |
| C | -1.0797 | -0.95831 | -6.41083 |
| H | -0.18051 | -0.36413 | -6.63733 |
| C | -0.73427 | -2.40019 | -6.81833 |

| | | | |
|---|----------|----------|----------|
| C | 0.532815 | -2.81542 | -6.07957 |
| H | 0.805756 | -3.84839 | -6.31838 |
| H | 1.359706 | -2.18207 | -6.41969 |
| C | -2.15582 | -0.53818 | -7.41641 |
| H | -2.19628 | 0.542742 | -7.55228 |
| H | -3.14339 | -0.85235 | -7.07041 |
| C | -0.59983 | -2.23366 | -8.33638 |
| H | -0.63885 | -3.18388 | -8.87344 |
| H | 0.364476 | -1.76979 | -8.56167 |
| C | -1.7574 | -1.2791 | -8.72179 |
| H | -1.44631 | -0.58008 | -9.49833 |
| H | -2.60364 | -1.83565 | -9.12572 |
| H | -0.99661 | -1.93816 | -2.31834 |
| H | 0.70499 | -0.54335 | -4.4094 |
| C | -1.87159 | -3.38621 | -6.5296 |
| H | -2.78245 | -3.12105 | -7.06591 |
| H | -1.57509 | -4.38418 | -6.85894 |
| H | -2.11913 | -3.44782 | -5.47147 |

(g) 7'd

| | | | |
|---|----------|----------|----------|
| C | 4.572667 | 6.86043 | 5.124753 |
| C | 3.48601 | 6.966249 | 4.040028 |
| C | 1.873022 | 8.317605 | 5.644884 |
| C | 1.371476 | 9.559989 | 4.964142 |
| C | 0.589954 | 9.463631 | 3.871365 |
| C | 0.343555 | 8.167649 | 3.249507 |
| C | 3.778294 | 8.162758 | 3.129441 |
| C | 5.950668 | 6.498364 | 4.567429 |
| C | 5.9051 | 5.20168 | 3.763887 |
| C | 4.833878 | 5.262633 | 2.677616 |
| C | 3.467545 | 5.620177 | 3.265401 |
| C | 2.353542 | 5.538449 | 2.220779 |
| C | 0.975537 | 5.776236 | 2.854863 |
| C | 1.024338 | 7.060078 | 3.62317 |
| C | 2.080728 | 7.116679 | 4.701826 |
| H | 4.645275 | 7.80122 | 5.675639 |

| | | | |
|---|----------|----------|----------|
| H | 0.195875 | 5.80861 | 2.089889 |
| H | 0.746538 | 4.939485 | 3.524409 |
| H | 1.969746 | 6.214086 | 5.318122 |
| H | 2.783593 | 8.526309 | 6.208035 |
| H | 1.566306 | 10.52234 | 5.422554 |
| H | -0.36505 | 8.106052 | 2.430018 |
| H | 4.269301 | 6.092597 | 5.846839 |
| H | 3.906278 | 9.065096 | 3.728765 |
| H | 2.960445 | 8.343882 | 2.43444 |
| H | 4.688924 | 8.020776 | 2.549616 |
| H | 6.318652 | 7.308769 | 3.933293 |
| H | 6.662579 | 6.40572 | 5.391441 |
| H | 6.883553 | 4.988201 | 3.326886 |
| H | 5.673545 | 4.371964 | 4.43965 |
| H | 3.246374 | 4.850882 | 4.021688 |
| H | 2.522785 | 6.280675 | 1.435507 |
| H | 2.382844 | 4.556089 | 1.739469 |
| H | 1.123745 | 8.025872 | 6.391447 |
| H | 4.759692 | 4.296735 | 2.169681 |
| H | 0.169402 | 10.35074 | 3.413483 |
| H | 5.116096 | 5.991511 | 1.912444 |

(h) 8'

| | | | |
|---|----------|----------|----------|
| C | 0.405588 | 0.139695 | -0.16439 |
| H | 0.464524 | 0.535015 | 0.842466 |
| C | 1.161893 | -0.90892 | -0.54362 |
| H | 1.86769 | -1.3663 | 0.139198 |
| C | -0.53583 | 0.732849 | -1.10238 |
| H | -1.02382 | 1.663727 | -0.83246 |
| C | 1.112781 | -1.36524 | -1.97263 |
| H | 1.461465 | -2.39655 | -2.05308 |
| C | -0.28485 | -1.23964 | -2.61201 |
| C | -0.88349 | 0.115937 | -2.25716 |
| C | -2.00073 | 0.644487 | -3.1105 |
| C | -0.12289 | -1.39302 | -4.15289 |
| H | 0.719371 | -0.7412 | -4.43134 |

| | | | |
|---|----------|----------|----------|
| C | -1.67175 | 0.544822 | -4.59499 |
| H | -2.51422 | 0.896618 | -5.19768 |
| H | -0.81853 | 1.191227 | -4.82696 |
| C | -1.32212 | -0.89005 | -4.97238 |
| H | -2.1892 | -1.52702 | -4.747 |
| C | -1.21967 | -2.30881 | -2.01909 |
| H | -0.81092 | -3.31063 | -2.15359 |
| H | -1.33883 | -2.13243 | -0.94994 |
| H | -2.20571 | -2.27767 | -2.48339 |
| H | -2.90983 | 0.059871 | -2.92249 |
| H | -2.22741 | 1.674002 | -2.8219 |
| H | 1.813772 | -0.7502 | -2.55435 |
| C | 0.246142 | -2.81946 | -4.58238 |
| H | -0.59119 | -3.48936 | -4.36597 |
| H | 1.101214 | -3.18576 | -4.01076 |
| C | -1.03463 | -0.99971 | -6.4726 |
| H | -1.91086 | -0.66269 | -7.03377 |
| H | -0.22013 | -0.30863 | -6.71811 |
| C | -0.63805 | -2.4103 | -6.89548 |
| H | -1.48352 | -3.0872 | -6.73668 |
| H | -0.40891 | -2.43597 | -7.96345 |
| C | 0.552768 | -2.89769 | -6.07681 |
| H | 0.813721 | -3.92223 | -6.35264 |
| H | 1.425867 | -2.27675 | -6.30123 |