## Cartesian coordinates of the optimized geometries

The Cartesian coordinates of optimized geometries are given below in the standard XYZ format, and units are in Å.

==========

Compound 30

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| | | | |
|---|---|---|---|
| C | -7.561280251 | 1.221169949 | 2.331205845 |
| C | -8.468633652 | 0.041181866 | 2.689749718 |
| C | -9.262335777 | -0.455722272 | 1.475544930 |
| N | -8.310274124 | -0.750833809 | 0.420226097 |
| C | -7.608533382 | 0.460259110 | -0.014876123 |
| C | -6.683869839 | 0.900196850 | 1.108543873 |
| C | -8.673611641 | -1.627013683 | -0.690361142 |
| C | -9.203442574 | -0.817685604 | -1.898062468 |
| C | -8.077070236 | 0.106185354 | -2.417808533 |
| C | -6.961562634 | 0.114103429 | -1.367630363 |
| C | -6.372217178 | -1.269430876 | -1.315680623 |
| C | -7.382843494 | -2.358057499 | -1.102494955 |
| O | -9.586345673 | -1.659242630 | -2.969389677 |
| O | -5.890869617 | 0.976473510 | -1.688395739 |
| C | -4.725549221 | 0.245525807 | -1.771551013 |
| C | -5.062400341 | -1.183805108 | -1.543868303 |
| O | -3.669066429 | 0.759676933 | -2.003974676 |
| H | -8.320640564 | 1.289417028 | -0.194244161 |
| O | -8.430041313 | 2.313880444 | 2.078987837 |
| C | -7.780072689 | 3.554571867 | 1.948198438 |
| H | -6.917972565 | 1.466521740 | 3.192136526 |
| H | -7.847432137 | -0.781564176 | 3.057971239 |
| H | -9.145627022 | 0.354813397 | 3.489753485 |
| H | -10.002193451 | 0.308576465 | 1.179187536 |
| H | -9.804668427 | -1.371425390 | 1.733593345 |
| H | -5.992260933 | 0.086161442 | 1.353926301 |
| H | -6.091170311 | 1.768856525 | 0.808529794 |
| H | -9.436841965 | -2.336413622 | -0.350713730 |
| H | -10.055818558 | -0.213007808 | -1.554653168 |
| H | -8.432574272 | 1.126105666 | -2.586651087 |
| H | -7.703216076 | -0.293837756 | -3.365023375 |
| H | -7.062979221 | -3.049566031 | -0.319424063 |
| H | -7.534038067 | -2.920949459 | -2.030877829 |
| H | -10.369703293 | -2.154039860 | -2.704346895 |
| H | -4.313162804 | -1.960758567 | -1.600995779 |
| H | -8.554141998 | 4.324270725 | 1.948447824 |
| H | -7.096518040 | 3.736605883 | 2.790250778 |
| H | -7.209468365 | 3.634215832 | 1.014071226 |

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Compound 42

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| | | | |
|---|---|---|---|
| C | -9.526927948 | 1.946158409 | 0.941412449 |
| C | -10.563442230 | 0.873967052 | 1.310192227 |
| C | -9.905400276 | -0.471140712 | 1.640130401 |
| N | -9.052383423 | -0.840858757 | 0.528880179 |
| C | -7.975303173 | 0.134207591 | 0.342651814 |
| C | -8.573796272 | 1.445196033 | -0.143465444 |
| C | -8.614712715 | -2.226151705 | 0.365126640 |
| C | -8.494735718 | -2.412918806 | -1.165285587 |
| C | -7.612031937 | -1.272293448 | -1.719953060 |
| C | -6.933039188 | -0.560222626 | -0.545996308 |
| C | -6.274012566 | -1.586105943 | 0.339431345 |
| C | -7.240895748 | -2.521492243 | 1.004414082 |
| O | -7.870195389 | -3.636548281 | -1.506086826 |
| O | -5.899629116 | 0.307557762 | -0.957470179 |
| C | -4.696247578 | -0.137908295 | -0.452553928 |
| C | -4.965247154 | -1.344846368 | 0.374711841 |
| O | -3.663218021 | 0.423716158 | -0.677526176 |
| H | -7.467552662 | 0.346502155 | 1.307159424 |
| O | -10.134855270 | 3.123769760 | 0.458750039 |
| C | -10.707962036 | 3.925271273 | 1.460728884 |
| H | -8.928610802 | 2.185103416 | 1.840632558 |
| H | -11.224780083 | 0.741758049 | 0.446951330 |
| H | -11.171756744 | 1.202984333 | 2.159001589 |
| H | -9.342782021 | -0.393497944 | 2.590952635 |
| H | -10.674646378 | -1.238559127 | 1.774223685 |
| H | -7.793984413 | 2.189686537 | -0.325257123 |
| H | -9.137421608 | 1.288928270 | -1.069573760 |
| H | -9.385534286 | -2.887274265 | 0.776357234 |
| H | -9.501411438 | -2.348730326 | -1.595959544 |
| H | -8.195379257 | -0.553639710 | -2.300040245 |
| H | -6.846915245 | -1.705783248 | -2.369004726 |
| H | -7.268237591 | -2.332747459 | 2.084199667 |

| | | | |
|---|---|---|---|
| H | -6.953309059 | -3.564429998 | 0.852504253 |
| H | -8.456509590 | -4.359376431 | -1.254794836 |
| H | -4.176668644 | -1.854642272 | 0.910331488 |
| H | -11.089181900 | 4.824599743 | 0.974280655 |
| H | -11.541290283 | 3.426733971 | 1.973729849 |
| H | -9.961462021 | 4.216859341 | 2.214213133 |

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Compound 50

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| | | | |
|---|---|---|---|
| C | -9.443593025 | 2.285618544 | 1.182548404 |
| C | -10.594126701 | 1.317284465 | 1.467658401 |
| C | -10.093309402 | -0.118571453 | 1.664778709 |
| N | -9.308746338 | -0.483826131 | 0.497618645 |
| C | -8.123691559 | 0.371946543 | 0.372483045 |
| C | -8.577883720 | 1.778380156 | 0.015311085 |
| C | -9.027518272 | -1.890945673 | 0.217013448 |
| C | -8.950262070 | -1.966699839 | -1.325254321 |
| C | -7.957563400 | -0.886406720 | -1.809635758 |
| C | -7.184497833 | -0.354233265 | -0.599598229 |
| C | -6.629512787 | -1.516511440 | 0.181062192 |
| C | -7.685193539 | -2.385764122 | 0.798827291 |
| O | -8.466524124 | -3.218274117 | -1.777239561 |
| O | -6.066749573 | 0.426790267 | -0.965831339 |
| C | -4.913302898 | -0.192282438 | -0.533167064 |
| C | -5.301421642 | -1.427133679 | 0.198325291 |
| O | -3.828283548 | 0.270143688 | -0.739388227 |
| H | -7.587049007 | 0.447173923 | 1.337736845 |
| O | -8.706107140 | 2.372176647 | 2.390072584 |
| C | -7.675957203 | 3.330478668 | 2.378446817 |
| H | -9.847071648 | 3.281600237 | 0.936674178 |
| H | -11.286377907 | 1.331717134 | 0.619603753 |
| H | -11.125734329 | 1.661401033 | 2.359599590 |
| H | -9.510664940 | -0.182190582 | 2.600296736 |
| H | -10.945474625 | -0.801171124 | 1.748407483 |
| H | -7.716934681 | 2.430283070 | -0.157844529 |
| H | -9.181389809 | 1.760333538 | -0.898437560 |
| H | -9.860106468 | -2.495943785 | 0.592893422 |
| H | -9.950250626 | -1.760756969 | -1.726290584 |
| H | -8.469446182 | -0.063224539 | -2.313647509 |
| H | -7.257515907 | -1.344069839 | -2.513193846 |
| H | -7.673210621 | -2.275362968 | 1.889530063 |

| | | | |
|---|---|---|---|
| H | -7.519401550 | -3.439719439 | 0.564641178 |
| H | -9.116762161 | -3.894528627 | -1.555380464 |
| H | -4.565994263 | -2.064407110 | 0.668869555 |
| H | -7.338122368 | 3.450697422 | 3.409348965 |
| H | -6.820553303 | 3.019142389 | 1.764859915 |
| H | -8.037581444 | 4.300179005 | 2.006463766 |

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Compound 51

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| | | | |
|---|---|---|---|
| C | -7.491712570 | 0.924648166 | 2.582974434 |
| C | -8.445995331 | -0.254891753 | 2.776980639 |
| C | -9.270983696 | -0.547770321 | 1.520342112 |
| N | -8.347790718 | -0.712576330 | 0.416413426 |
| C | -7.602260113 | 0.517103314 | 0.154566735 |
| C | -6.645147324 | 0.767427742 | 1.311256289 |
| C | -8.741203308 | -1.420215726 | -0.798584282 |
| C | -9.254372597 | -0.438897282 | -1.879302740 |
| C | -8.105916977 | 0.520712733 | -2.271126986 |
| C | -6.981362820 | 0.348198771 | -1.244915009 |
| C | -6.433617592 | -1.046244860 | -1.391765714 |
| C | -7.474183559 | -2.124608994 | -1.317102551 |
| O | -9.659701347 | -1.113519669 | -3.054377079 |
| O | -5.889202118 | 1.214799285 | -1.456363916 |
| C | -4.746465206 | 0.468349308 | -1.653845310 |
| C | -5.124124527 | -0.967798054 | -1.621354699 |
| O | -3.677559853 | 0.978465319 | -1.827120304 |
| H | -8.286946297 | 1.390405774 | 0.096431285 |
| O | -6.719064713 | 1.005825043 | 3.759494066 |
| C | -5.937421322 | 2.171544075 | 3.853930473 |
| H | -8.087153435 | 1.851921439 | 2.474910736 |
| H | -9.092688560 | -0.048274226 | 3.634959698 |
| H | -7.840659618 | -1.136078954 | 3.013505697 |
| H | -9.841117859 | -1.472605944 | 1.653915882 |
| H | -9.996800423 | 0.269593000 | 1.343301296 |
| H | -5.966625690 | -0.086001262 | 1.424683332 |
| H | -6.054157257 | 1.667040944 | 1.114997149 |
| H | -9.522213936 | -2.147504807 | -0.549891531 |
| H | -10.091516495 | 0.132108018 | -1.450916886 |
| H | -8.433139801 | 1.563679695 | -2.289319515 |
| H | -7.749253750 | 0.251112282 | -3.269486189 |
| H | -7.170941353 | -2.923532248 | -0.636508286 |

| | | | |
|---|---|---|---|
| H | -7.646640301 | -2.553203821 | -2.310716629 |
| H | -10.449458122 | -1.628679872 | -2.854905367 |
| H | -4.398623943 | -1.750409007 | -1.793145537 |
| H | -6.546515942 | 3.074899197 | 3.700979471 |
| H | -5.515861988 | 2.195104122 | 4.860302448 |
| H | -5.113376141 | 2.182166815 | 3.129281998 |

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Secu'amamine E (13)

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| | | | |
|---|---|---|---|
| C | -7.494416714 | 0.923014283 | 2.585191965 |
| C | -8.444312096 | -0.266031414 | 2.784416676 |
| C | -9.267708778 | -0.549069047 | 1.523202777 |
| N | -8.344943047 | -0.708647668 | 0.417795420 |
| C | -7.601076603 | 0.522757947 | 0.152413905 |
| C | -6.649172783 | 0.775812805 | 1.311668873 |
| C | -8.740546227 | -1.416700482 | -0.796157897 |
| C | -9.253718376 | -0.435480654 | -1.876974463 |
| C | -8.104072571 | 0.520321310 | -2.273441315 |
| C | -6.980288506 | 0.347926974 | -1.246175528 |
| C | -6.434334278 | -1.047263026 | -1.393424153 |
| C | -7.476044178 | -2.124293804 | -1.316211462 |
| O | -9.665636063 | -1.110354424 | -3.050018311 |
| O | -5.886038303 | 1.211978793 | -1.459719896 |
| C | -4.744706631 | 0.464438438 | -1.658457279 |
| C | -5.124882221 | -0.971157372 | -1.624566436 |
| O | -3.675299883 | 0.972736835 | -1.834328651 |
| H | -8.288201332 | 1.394364595 | 0.094051033 |
| H | -8.087059975 | 1.842813015 | 2.503358126 |
| H | -9.109856606 | -0.080445439 | 3.633872747 |
| H | -7.858543396 | -1.164085627 | 3.009732485 |
| H | -9.842542648 | -1.473042130 | 1.644952536 |
| H | -9.988934517 | 0.274485052 | 1.351992607 |
| H | -5.959911346 | -0.072796091 | 1.397054315 |
| H | -6.061465263 | 1.679565668 | 1.128340006 |
| H | -9.523073196 | -2.141775131 | -0.546379507 |
| H | -10.087223053 | 0.138509631 | -1.445813656 |
| H | -8.429538727 | 1.563622475 | -2.294404507 |
| H | -7.748292923 | 0.247580126 | -3.271154165 |
| H | -7.173241615 | -2.923290968 | -0.635344863 |
| H | -7.650967121 | -2.553103924 | -2.309192657 |
| H | -10.456656456 | -1.622016549 | -2.846478939 |
| H | -4.402814865 | -1.756965399 | -1.796191931 |
| H | -6.852071285 | 1.041084766 | 3.463216782 |

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*ent*-Virosine B (44)

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| | | | |
|---|---|---|---|
| C | -9.538094521 | 1.942815542 | 0.939228594 |
| C | -10.570762634 | 0.867969036 | 1.305903792 |
| C | -9.904086113 | -0.470132887 | 1.642237902 |
| N | -9.048774719 | -0.838709176 | 0.531380773 |
| C | -7.972554207 | 0.136226565 | 0.341981232 |
| C | -8.569241524 | 1.449367285 | -0.144602194 |
| C | -8.612509727 | -2.223914385 | 0.366630226 |
| C | -8.495825768 | -2.411490440 | -1.163406014 |
| C | -7.609086037 | -1.275101900 | -1.720220327 |
| C | -6.932077408 | -0.561112285 | -0.546427727 |
| C | -6.271913052 | -1.585642099 | 0.339147627 |
| C | -7.237569332 | -2.522362947 | 1.003365159 |
| O | -7.878634930 | -3.638845444 | -1.505821228 |
| O | -5.897955418 | 0.306287885 | -0.959058642 |
| C | -4.695909500 | -0.138058394 | -0.451873064 |
| C | -4.963483810 | -1.342926145 | 0.374774694 |
| O | -3.663723707 | 0.425353527 | -0.676741302 |
| H | -7.464497089 | 0.352828681 | 1.305685759 |
| H | -8.956037521 | 2.201304197 | 1.832685232 |
| H | -11.240645409 | 0.703516960 | 0.454493761 |
| H | -11.181871414 | 1.202722669 | 2.150223017 |
| H | -9.338745117 | -0.381114423 | 2.590842247 |
| H | -10.663317680 | -1.246893525 | 1.780880570 |
| H | -7.773563862 | 2.178257704 | -0.323757470 |
| H | -9.103738785 | 1.281534672 | -1.086693525 |
| H | -9.383385658 | -2.884486437 | 0.778207719 |
| H | -9.503287315 | -2.342199802 | -1.590987444 |
| H | -8.189163208 | -0.558268905 | -2.305945158 |
| H | -6.842768669 | -1.711299181 | -2.365529776 |
| H | -7.262440681 | -2.337035656 | 2.083358288 |
| H | -6.950370312 | -3.564683676 | 0.846064806 |
| H | -8.470138550 | -4.357612133 | -1.255301237 |
| H | -4.175865650 | -1.852967143 | 0.911145270 |
| H | -10.044687271 | 2.858004808 | 0.617828906 |

# Vibrational frequencies (in $cm^{-1}$) of the optimized structures.

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Compound 30

==========

46.62 63.14 68.48 92.57 134.13 156.23
184.45 215.12 247.97 263.58 277.54 302.39
316.99 344.64 354.71 382.23 385.26 406.89
429.27 454.16 492.32 503.62 527.72 569.85
585.66 600.78 666.90 672.71 716.37 758.72
776.08 805.04 824.94 859.75 863.77 880.98
898.94 922.22 947.00 960.41 975.48 978.60
999.60 1037.02 1080.87 1085.04 1091.82 1108.43
1122.70 1131.68 1154.45 1164.81 1174.55 1184.27
1187.04 1192.46 1197.48 1206.64 1226.18 1229.30
1237.89 1268.82 1280.01 1286.24 1290.32 1300.65
1316.69 1343.86 1347.47 1349.26 1368.71 1374.15
1383.91 1393.72 1399.33 1402.32 1420.61 1442.67
1443.96 1462.02 1475.54 1487.85 1495.94 1503.99
1512.51 1517.52 1530.22 1760.72 1935.91 2961.22
2995.97 3015.97 3031.75 3038.75 3090.21 3090.87
3093.29 3097.62 3098.89 3102.94 3112.81 3150.37
3152.63 3152.97 3161.33 3164.54 3293.43 3886.55

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Compound 42

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45.32 66.77 75.65 107.87 121.15 165.84
172.33 195.48 221.52 268.08 271.63 294.88
303.07 328.65 344.09 384.66 394.21 417.79
438.63 458.38 482.58 509.50 524.48 541.76
586.60 591.93 617.03 624.81 726.12 749.82
785.04 811.84 835.66 859.02 874.04 881.94
905.92 938.84 940.83 951.64 972.97 993.31
1012.58 1040.98 1075.36 1086.19 1096.39 1117.42
1133.57 1144.83 1160.35 1166.77 1173.69 1186.50
1190.47 1198.11 1204.02 1216.16 1225.81 1234.96
1256.65 1264.07 1275.32 1284.45 1285.95 1304.16
1307.06 1336.56 1345.38 1350.44 1355.41 1366.55
1380.60 1392.69 1402.71 1416.41 1421.39 1432.76
1453.70 1460.27 1485.39 1492.33 1495.54 1503.22
1509.93 1515.05 1527.81 1764.04 1937.56 2922.15
2957.37 2978.28 3027.82 3073.51 3081.51 3086.28
3089.02 3095.75 3101.77 3113.41 3114.63 3140.73
3153.23 3159.42 3168.71 3172.24 3291.94 3880.63

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Compound 50

==========

48.51 60.83 87.03 97.75 137.29 169.75
179.03 194.79 247.44 258.69 295.12 312.97
329.96 341.21 352.38 387.15 392.98 415.95
436.15 456.45 490.40 511.15 532.34 579.06
586.36 591.63 618.19 684.72 737.01 749.42
785.01 813.49 833.73 858.24 861.15 883.08
907.47 922.92 940.55 948.48 972.25 973.74
985.90 1027.38 1060.84 1083.62 1086.50 1116.36
1122.62 1137.17 1149.28 1165.96 1172.35 1187.20
1189.32 1191.85 1200.30 1211.92 1224.37 1234.22
1242.48 1262.59 1276.03 1282.50 1292.17 1305.39
1319.25 1343.83 1349.69 1355.77 1367.61 1372.58
1381.71 1392.07 1394.75 1401.52 1420.31 1432.32
1453.12 1459.56 1476.21 1487.15 1493.26 1495.93
1513.59 1516.54 1530.85 1764.25 1937.32 2968.77
3000.11 3015.65 3030.58 3071.80 3087.98 3090.44
3092.55 3099.71 3101.29 3112.69 3113.63 3150.34
3153.51 3154.69 3165.72 3170.62 3292.81 3880.78

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Compound 51

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52.22 60.69 82.16 108.67 128.73 164.63
179.64 199.83 237.92 249.35 274.07 288.55
310.18 321.10 338.71 376.01 396.95 405.17
439.51 460.94 487.15 499.10 517.64 530.81
567.07 586.59 625.61 671.01 695.10 755.98
774.28 805.69 827.81 852.01 874.24 883.89
906.10 928.64 954.57 967.26 986.81 996.08
1005.82 1054.38 1082.89 1086.09 1106.46 1106.90
1134.27 1140.59 1156.58 1169.15 1174.80 1181.22
1188.04 1197.04 1205.16 1217.55 1223.30 1233.36
1248.94 1268.60 1282.09 1284.21 1286.32 1299.95
1304.02 1337.68 1344.29 1345.60 1352.04 1369.40
1382.83 1398.14 1405.41 1416.41 1420.44 1439.85
1442.57 1461.94 1486.60 1493.48 1501.84 1503.59
1511.35 1514.79 1529.29 1762.65 1939.96 2913.37
2957.59 2966.78 3028.76 3036.58 3086.12 3092.88
3093.85 3094.32 3100.83 3104.03 3116.38 3148.73
3150.47 3154.93 3162.08 3167.30 3293.58 3885.48

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Secu'amamine E (13)

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67.90 89.61 114.73 144.21 194.66 227.19
266.00 278.93 308.39 312.81 324.49 358.02
382.57 398.07 411.87 460.92 474.38 506.46
516.74 565.94 586.50 611.25 665.76 695.70
756.62 772.69 797.80 822.20 847.43 864.74
870.62 884.52 909.57 927.72 954.85 968.08
975.59 987.56 1033.37 1074.59 1083.23 1086.17

1108.21 1109.80 1140.24 1160.86 1161.89 1172.31

1175.67 1195.35 1205.29 1224.27 1230.11 1262.38

1272.04 1285.96 1288.42 1292.23 1300.93 1338.45

1344.07 1347.65 1349.03 1370.59 1375.19 1390.62

1394.83 1399.76 1417.64 1439.62 1442.56 1461.62

1488.23 1494.18 1503.66 1505.26 1514.55 1762.48

1939.60 2912.93 2952.11 3037.65 3069.61 3080.25

3083.28 3094.00 3101.22 3104.96 3111.90 3125.25

3134.39 3147.99 3154.26 3163.05 3293.27 3884.80

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*ent*-Virosine B (44)

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68.43 93.67 115.78 147.94 194.32 208.75

261.39 290.47 315.65 319.09 338.73 351.83

386.67 398.56 435.79 458.02 486.64 508.73

519.13 578.95 586.60 605.75 616.34 726.44

748.07 784.40 805.45 832.85 852.82 864.39

876.34 884.36 908.14 941.04 941.45 951.07

972.52 978.25 1019.89 1063.92 1077.06 1086.95

1098.74 1118.19 1146.86 1154.78 1167.36 1172.58

1188.04 1194.60 1205.00 1225.91 1234.29 1258.52

1269.54 1277.39 1291.32 1294.71 1307.34 1335.55

1345.79 1353.63 1357.49 1364.59 1375.25 1385.76

1393.95 1397.73 1418.31 1432.60 1449.08 1459.56

1487.12 1491.44 1495.45 1505.87 1515.69 1764.47

1938.70 2920.64 2954.87 3070.51 3074.63 3080.45

3084.94 3089.43 3102.77 3111.75 3115.34 3125.86

3134.89 3147.08 3153.40 3172.58 3293.69 3881.64