# Supporting Information

# Chemical Constituents from Soft Coral *Clavularia* spp. Demonstrate Antiproliferative Effects on Oral Cancer Cells

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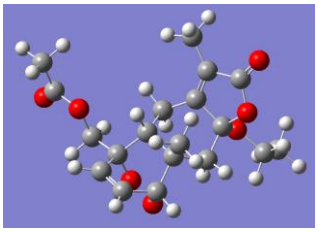
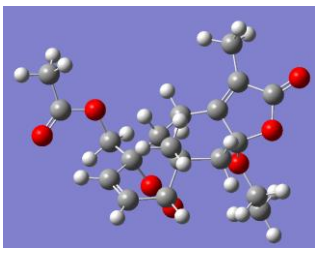
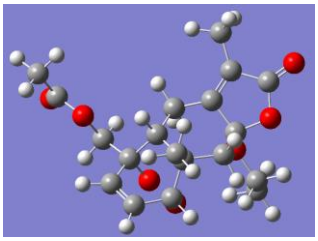
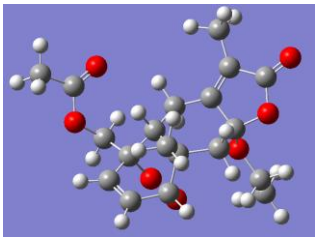
**Table S1** Energy analyses of 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (seven conformers)

| NO. | 3D conformers B3LYP/6-31G(d,p) | E (Hartree) | ΔE (KJ/mol) | Boltzmann distribution |
|---|---|---|---|---|
| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 1) |  | -1264.568384 | 2.31831548 | 27.52% |
| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 2) |  | -1264.563209 | 15.905272 | 0.11% |
| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 3) |  | -1264.563995 | 13.84162991 | 0.26% |
| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 4) |  | -1264.563230 | 15.85013653 | 0.12% |

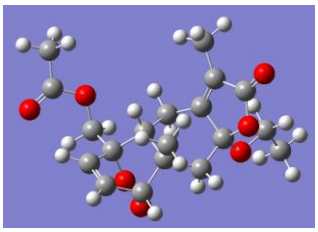
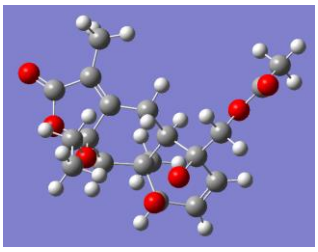
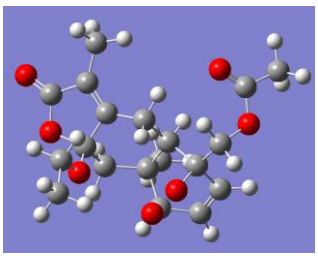
| | | | | |
|---|---|---|---|---|
| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 5) |  | -1264.569267 | 0 | 70.12% |
| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 6) |  | -1264.565610 | 9.601449275 | 1.46% |
| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 7) |  | -1264.564414 | 12.74154589 | 0.41% |

**Table S2** Cartesian coordinates of the low-energy re-optimized conformers of 1*R*,4*S*,5*R*,8*S*,10*S*-**5** calculated at B3LYP/6-31G(d,p) level of theory.

| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 1) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.729375 | -2.5384 | 1.124891 | H | 1.483165 | -1.928645 | -0.484878 |
| C | -2.571663 | -1.755794 | 1.124891 | H | 2.372164 | -1.813036 | 1.035669 |
| C | -1.929956 | -1.093283 | -0.072254 | H | -0.393706 | -0.615566 | 3.151261 |
| C | -0.744147 | -0.211507 | 0.414901 | H | 1.210964 | -1.375316 | 3.123082 |
| C | 0.299229 | -1.161384 | 1.147177 | H | 1.017151 | 0.300801 | 2.602778 |
| C | -0.362124 | -2.57292 | 1.169931 | H | 0.073187 | 3.641043 | 0.009474 |
| C | -0.125424 | 0.658086 | -0.718521 | H | 0.939344 | 3.846636 | 1.551095 |
| C | 1.205834 | 1.10365 | -0.227957 | H | 1.703988 | 4.343956 | 0.04919 |
| C | 2.255567 | 0.021529 | -0.12201 | H | -2.471358 | -0.032336 | -1.900929 |
| C | 1.650264 | -1.298367 | 0.391621 | H | -3.743433 | -1.076423 | -1.254364 |
| C | 1.661357 | 2.225443 | 0.343722 | H | 5.315012 | -1.572163 | -3.080365 |
| C | 2.983775 | 1.909758 | 0.956496 | H | 3.694491 | -1.142568 | -3.670774 |
| O | 3.244063 | 0.565941 | 0.776075 | H | 4.806185 | 0.130813 | -3.128611 |
| C | 0.544213 | -0.685435 | 2.590782 | H | 4.693712 | -0.760848 | -0.782807 |
| O | 3.719596 | 2.6354 | 1.576649 | H | 3.596792 | -2.050028 | -1.329505 |
| C | 1.052575 | 3.582019 | 0.493103 | H | -5.317629 | 2.157765 | 0.972736 |
| C | -2.937602 | -0.390301 | -0.980193 | H | -4.101985 | 3.228284 | 0.27355 |
| O | -1.388033 | -2.123791 | -0.945408 | H | -5.715316 | 3.109203 | -0.488944 |
| O | -0.521151 | -3.048866 | -0.189458 | | | | |
| O | 2.822346 | -0.111667 | -1.405195 | | | | |
| C | 4.467857 | -0.892328 | -2.937288 | | | | |
| C | 3.927588 | -1.019612 | -1.523121 | | | | |
| O | -3.467108 | 0.718365 | -0.230669 | | | | |
| O | -4.85172 | 1.16875 | -1.960908 | | | | |
| C | -4.447491 | 1.430508 | -0.852487 | | | | |
| C | -4.931236 | 2.556387 | 0.029004 | | | | |
| H | -1.989983 | -3.141636 | 2.66472 | | | | |
| H | -3.622836 | -1.610371 | 1.354641 | | | | |
| H | -1.145467 | 0.482678 | 1.159609 | | | | |
| H | 0.30744 | -3.320297 | 1.606886 | | | | |
| H | -0.002582 | 0.058611 | -1.628594 | | | | |
| H | -0.788697 | 1.498064 | -0.944715 | | | | |

| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 2) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.940982 | -2.250766 | 1.51976 | H | 2.02092 | -1.675424 | 1.53728 |
| C | -2.655418 | -1.459736 | 0.719216 | H | 1.998282 | -0.063443 | 2.205588 |
| C | -1.798167 | -0.716079 | -0.280429 | H | -1.376412 | -0.270153 | 3.087152 |
| C | -0.750076 | 0.202735 | 0.42927 | H | 0.189795 | -0.884569 | 3.649735 |
| C | 0.053576 | -0.697111 | 1.467914 | H | 0.050592 | 0.78084 | 3.068209 |
| C | -0.465577 | -2.14807 | 1.247506 | H | 0.990942 | 3.916651 | -0.620202 |
| C | 0.07681 | 0.977188 | -0.644212 | H | 2.30814 | 4.308641 | 0.51173 |
| C | 1.487856 | 1.198226 | -0.245466 | H | 2.662726 | 4.089729 | -1.195291 |
| C | 2.249411 | -0.048821 | 0.119599 | H | -1.992257 | 0.27421 | -2.207714 |
| C | 1.621101 | -0.668764 | 1.376586 | H | -3.413559 | -0.687391 | -1.72526 |
| C | 2.287508 | 2.266286 | -0.135019 | H | 3.652212 | -3.605638 | -2.326908 |
| C | 3.629406 | 1.782736 | 0.295722 | H | 2.133173 | -2.796542 | -2.772668 |
| O | 3.578436 | 0.414938 | 0.454991 | H | 3.682866 | -1.949488 | -2.974806 |
| C | -0.299059 | -0.244926 | 2.903435 | H | 3.99003 | -1.924199 | -0.480886 |
| O | 4.627574 | 2.425207 | 0.509554 | H | 2.446955 | -2.803701 | -0.296938 |
| C | 2.038339 | 3.720432 | -0.372998 | H | -6.023641 | 2.531563 | 0.17994 |
| C | -2.626328 | -0.020398 | -1.371215 | H | -4.365125 | 2.904503 | 0.740303 |
| O | -1.052906 | -1.711569 | -1.036487 | H | -4.827544 | 3.278276 | -0.920587 |
| O | -0.22374 | -2.531025 | -0.12975 | | | | |
| O | 2.290887 | -0.856617 | -1.016315 | | | | |
| C | 3.126214 | -2.644554 | -2.338318 | | | | |
| C | 3.003139 | -2.098472 | -0.92628 | | | | |
| O | -3.205769 | 1.196612 | -0.862338 | | | | |
| O | -5.235862 | 0.207311 | -0.606229 | | | | |
| C | -4.529224 | 1.187311 | -0.540902 | | | | |
| C | -4.971653 | 2.562551 | -0.104539 | | | | |
| H | -2.352244 | -2.932457 | 2.257818 | | | | |
| H | -3.738247 | -1.395356 | 0.688051 | | | | |
| H | -1.307293 | 0.945954 | 1.006954 | | | | |
| H | 0.132148 | -2.874778 | 1.805973 | | | | |
| H | 0.11963 | 0.361761 | -1.551455 | | | | |
| H | -0.432304 | 1.91356 | -0.891213 | | | | |

| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 3) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.602693 | -2.689494 | 1.493784 | H | 2.279612 | -1.750881 | 1.230385 |
| C | -2.454084 | -1.870525 | 0.877386 | H | 2.195207 | -0.245598 | 2.109507 |
| C | -1.768767 | -0.930365 | -0.086827 | H | -1.042589 | -0.880062 | 3.261268 |
| C | -0.734717 | -0.014609 | 0.646863 | H | 0.617594 | -1.414485 | 3.588018 |
| C | 0.242696 | -0.960875 | 1.474384 | H | 0.286296 | 0.291599 | 3.255611 |
| C | -0.175922 | -2.414054 | 1.103653 | H | 0.589916 | 3.951906 | -0.038942 |
| C | -0.088662 | 0.968489 | -0.378952 | H | 1.984893 | 4.314087 | 1.006439 |
| C | 1.335234 | 1.263973 | -0.087978 | H | 2.172639 | 4.34858 | -0.740387 |
| C | 2.226678 | 0.055812 | 0.030069 | H | -2.276242 | 0.389769 | -1.759513 |
| C | 1.784806 | -0.774142 | 1.244541 | H | -3.43849 | -0.907325 | -1.463133 |
| C | 2.055445 | 2.378113 | 0.091827 | H | 3.632285 | -3.01724 | -3.001442 |
| C | 3.469083 | 1.968826 | 0.324895 | H | 2.008623 | -2.312876 | -3.172152 |
| O | 3.54283 | 0.59298 | 0.29935 | H | 3.447076 | -1.299937 | -3.425683 |
| C | 0.00466 | -0.732439 | 2.984511 | H | 4.044094 | -1.547084 | -0.996648 |
| O | 4.430387 | 2.667476 | 0.530751 | H | 2.612703 | -2.589068 | -0.766772 |
| C | 1.669618 | 3.821774 | 0.079231 | H | -6.000044 | 2.840727 | -0.230176 |
| C | -2.768262 | -0.191951 | -0.978306 | H | -5.667468 | 1.653482 | 1.065686 |
| O | -1.028202 | -1.745485 | -1.036024 | H | -4.516957 | 2.956482 | 0.762861 |
| O | -0.044994 | -2.589983 | -0.328716 | | | | |
| O | 2.210939 | -0.593506 | -1.203673 | | | | |
| C | 3.029904 | -2.118165 | -2.830267 | | | | |
| C | 3.029683 | -1.761737 | -1.353774 | | | | |
| O | -3.519953 | 0.67951 | -0.113865 | | | | |
| O | -4.735903 | 1.332635 | -1.90491 | | | | |
| C | -4.501008 | 1.40222 | -0.721409 | | | | |
| C | -5.222 | 2.27211 | 0.279721 | | | | |
| H | -1.878629 | -3.489231 | 2.173994 | | | | |
| H | -3.535354 | -1.890229 | 0.973743 | | | | |
| H | -1.292624 | 0.587989 | 1.369272 | | | | |
| H | 0.532606 | -3.147202 | 1.500706 | | | | |
| H | -0.096782 | 0.488564 | -1.365571 | | | | |
| H | -0.689344 | 1.881241 | -0.440496 | | | | |

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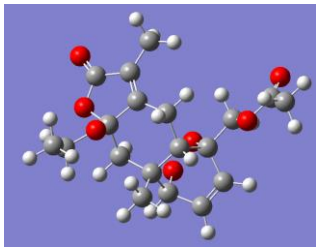
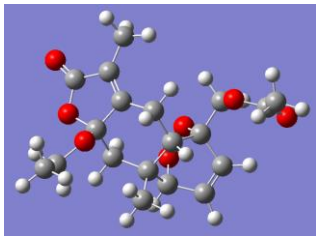
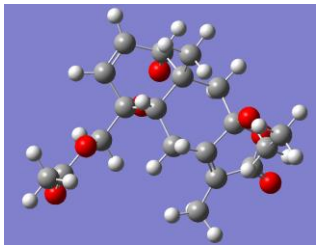
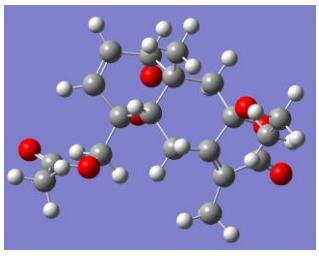
| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 4) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.783759 | -2.6785 | 1.332878 | H | 2.07927 | -1.645468 | 1.52729 |
| C | -2.590844 | -1.898829 | 0.61414 | H | 1.848206 | -0.064877 | 2.229555 |
| C | -1.837493 | -0.982855 | -0.324262 | H | -1.475557 | -0.777557 | 3.044133 |
| C | -0.87051 | -0.018225 | 0.441144 | H | 0.142484 | -1.262188 | 3.585558 |
| C | 0.013504 | -0.906765 | 1.424088 | H | -0.17415 | 0.420619 | 3.140302 |
| C | -0.333111 | -2.382914 | 1.069209 | H | 0.496836 | 3.878863 | -0.434452 |
| C | -0.115071 | 0.881137 | -0.588697 | H | 1.767111 | 4.359683 | 0.71774 |
| C | 1.267702 | 1.214651 | -0.170199 | H | 2.142492 | 4.244123 | -0.995016 |
| C | 2.148165 | 0.037838 | 0.155005 | H | -2.268685 | 0.429337 | -1.953502 |
| C | 1.567188 | -0.688909 | 1.37645 | H | -3.202566 | -1.090256 | -1.980231 |
| C | 1.954698 | 2.352616 | -0.007032 | H | 3.926775 | -3.267415 | -2.39818 |
| C | 3.333445 | 1.989914 | 0.424189 | H | 2.323592 | -2.618762 | -2.813061 |
| O | 3.41858 | 0.617595 | 0.531827 | H | 3.76923 | -1.602487 | -3.003863 |
| C | -0.405944 | -0.619617 | 2.884407 | H | 4.094862 | -1.60704 | -0.510629 |
| O | 4.260541 | 2.718396 | 0.678737 | H | 2.659064 | -2.65268 | -0.340986 |
| C | 1.558444 | 3.781897 | -0.190125 | H | -5.187654 | 3.173104 | 0.246354 |
| C | -2.776785 | -0.313254 | -1.340875 | H | -6.068302 | 1.779867 | -0.446349 |
| O | -1.010996 | -1.835019 | -1.166245 | H | -5.268862 | 1.610202 | 1.116967 |
| O | -0.061306 | -2.604459 | -0.337937 | | | | |
| O | 2.287582 | -0.715922 | -1.01032 | | | | |
| C | 3.298218 | -2.370056 | -2.381729 | | | | |
| C | 3.128925 | -1.874682 | -0.955822 | | | | |
| O | -3.889804 | 0.292604 | -0.655752 | | | | |
| O | -3.074338 | 2.386765 | -0.998089 | | | | |
| C | -3.930663 | 1.64901 | -0.564991 | | | | |
| C | -5.193324 | 2.088559 | 0.13534 | | | | |
| H | -2.106843 | -3.460459 | 2.013114 | | | | |
| H | -3.675093 | -1.939614 | 0.612231 | | | | |
| H | -1.483319 | 0.64183 | 1.06431 | | | | |
| H | 0.349877 | -3.084067 | 1.558135 | | | | |
| H | -0.018425 | 0.314881 | -1.523932 | | | | |
| H | -0.709144 | 1.774596 | -0.79195 | | | | |

| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 5) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -2.252963 | -2.189028 | 1.577042 | H | 1.306929 | -2.228109 | -0.246135 |
| C | -2.878686 | -1.339229 | 0.760699 | H | 1.99205 | -2.078771 | 1.370203 |
| C | -1.997245 | -0.855261 | -0.369223 | H | -0.838715 | -0.382068 | 2.996276 |
| C | -0.755751 | -0.127839 | 0.223068 | H | 0.619359 | -1.366123 | 3.235983 |
| C | 0.026168 | -1.163437 | 1.141149 | H | 0.756706 | 0.279448 | 2.610892 |
| C | -0.838383 | -2.460191 | 1.139447 | H | 0.635308 | 3.508674 | -0.210176 |
| C | 0.129451 | 0.54775 | -0.865581 | H | 1.290222 | 3.654553 | 1.438315 |
| C | 1.439333 | 0.834677 | -0.220755 | H | 2.32114 | 4.002814 | 0.0599 |
| C | 2.289502 | -0.382156 | 0.076117 | H | -2.13457 | 0.032012 | -2.342514 |
| C | 1.42905 | -1.545142 | 0.596605 | H | -3.68296 | -0.582378 | -1.703986 |
| C | 1.960638 | 1.915393 | 0.376147 | H | 5.239754 | -0.258158 | -3.399287 |
| C | 3.134853 | 1.456819 | 1.173246 | H | 4.963616 | -1.772653 | -2.510935 |
| O | 3.255292 | 0.08989 | 1.039344 | H | 3.698735 | -1.127776 | -3.575043 |
| C | 0.143878 | -0.626527 | 2.57979 | H | 3.44308 | 0.864714 | -2.059111 |
| O | 3.86509 | 2.107591 | 1.878858 | H | 4.710636 | 0.21577 | -0.996723 |
| C | 1.519474 | 3.343194 | 0.41223 | H | -5.432031 | 3.20591 | 0.144309 |
| C | -2.753404 | -0.071442 | -1.449773 | H | -3.687311 | 3.276592 | 0.537089 |
| O | -1.515604 | -2.010936 | -1.112674 | H | -4.224957 | 3.625477 | -1.106874 |
| O | -0.895432 | -2.996906 | -0.206035 | | | | |
| O | 2.956511 | -0.898333 | -1.053815 | | | | |
| C | 4.488809 | -0.853617 | -2.86849 | | | | |
| C | 3.91983 | -0.059712 | -1.704201 | | | | |
| O | -3.035508 | 1.269345 | -1.003301 | | | | |
| O | -5.186072 | 0.725382 | -0.509563 | | | | |
| C | -4.300286 | 1.546396 | -0.580032 | | | | |
| C | -4.42567 | 3.007848 | -0.225234 | | | | |
| H | -2.711884 | -2.699175 | 2.418265 | | | | |
| H | -3.922117 | -1.047883 | 0.823833 | | | | |
| H | -1.128668 | 0.675894 | 0.865905 | | | | |
| H | -0.349162 | -3.266069 | 1.695281 | | | | |
| H | 0.273941 | -0.142238 | -1.705837 | | | | |
| H | -0.364901 | 1.450318 | -1.235667 | | | | |

| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 6) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 1.820945 | -2.806476 | -1.252528 | H | -2.118416 | -2.16261 | -1.013716 |
| C | 2.599499 | -1.867662 | -0.715499 | H | -2.153578 | -0.821405 | -2.148821 |
| C | 1.834352 | -0.907211 | 0.165038 | H | 1.165386 | -1.184195 | -3.159469 |
| C | 0.725268 | -0.149165 | -0.636267 | H | -0.42795 | -1.900857 | -3.467727 |
| C | -0.154111 | -1.236615 | -1.394913 | H | -0.267691 | -0.149106 | -3.278368 |
| C | 0.373509 | -2.613139 | -0.888888 | H | -0.785873 | 3.730066 | -0.318684 |
| C | -0.021692 | 0.828546 | 0.321472 | H | -2.072693 | 3.90665 | -1.535781 |
| C | -1.441967 | 1.027351 | -0.058464 | H | -2.44643 | 4.137183 | 0.164837 |
| C | -2.274137 | -0.230656 | -0.131517 | H | 2.218252 | 0.593246 | 1.713645 |
| C | -1.713294 | -1.164343 | -1.208648 | H | 3.487625 | -0.621356 | 1.530891 |
| C | -2.180279 | 2.089468 | -0.407331 | H | -3.238746 | -0.798461 | 4.270193 |
| C | -3.555157 | 1.598181 | -0.708541 | H | -3.499141 | -2.129751 | 3.12123 |
| O | -3.588177 | 0.23407 | -0.530694 | H | -1.847574 | -1.636613 | 3.540523 |
| C | 0.102381 | -1.114795 | -2.914738 | H | -2.242044 | 0.596817 | 2.447469 |
| O | -4.516464 | 2.232868 | -1.067773 | H | -3.884164 | 0.08546 | 2.002899 |
| C | -1.842469 | 3.540122 | -0.528663 | H | 5.688775 | 3.248735 | -0.020856 |
| C | 2.762343 | -0.010752 | 0.985562 | H | 5.541773 | 1.892537 | -1.176686 |
| O | 1.163482 | -1.69845 | 1.182413 | H | 4.244425 | 3.082925 | -1.063952 |
| O | 0.243675 | -2.666335 | 0.552507 | | | | |
| O | -2.355664 | -0.955334 | 1.056936 | | | | |
| C | -2.862553 | -1.270997 | 3.356139 | | | | |
| C | -2.86927 | -0.274412 | 2.209872 | | | | |
| O | 3.443977 | 0.842398 | 0.04793 | | | | |
| O | 4.547243 | 1.78865 | 1.779995 | | | | |
| C | 4.336513 | 1.714522 | 0.592079 | | | | |
| C | 4.998473 | 2.542427 | -0.482693 | | | | |
| H | 2.165651 | -3.63902 | -1.857946 | | | | |
| H | 3.679347 | -1.807331 | -0.811034 | | | | |
| H | 1.2269 | 0.457099 | -1.396104 | | | | |
| H | -0.271968 | -3.433221 | -1.216401 | | | | |
| H | -0.01586 | 0.385103 | 1.325331 | | | | |
| H | 0.519295 | 1.7788 | 0.369176 | | | | |

| 1*R*,4*S*,5*R*,8*S*,10*S*-**5** (conformer 7) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.042624 | -2.661251 | -1.258445 | H | -1.885008 | -1.949299 | -1.593119 |
| C | 2.766755 | -1.793745 | -0.551542 | H | -1.731852 | -0.387314 | -2.382081 |
| C | 1.920116 | -0.928884 | 0.355537 | H | 1.675755 | -0.809383 | -2.987074 |
| C | 0.872722 | -0.073014 | -0.435099 | H | 0.140291 | -1.451254 | -3.598696 |
| C | 0.116794 | -1.044735 | -1.442511 | H | 0.277391 | 0.261331 | -3.177511 |
| C | 0.566407 | -2.480447 | -1.031605 | H | -0.738403 | 3.669221 | 0.372887 |
| C | -0.007414 | 0.718103 | 0.582666 | H | -1.915233 | 4.080194 | -0.898961 |
| C | -1.380185 | 0.970583 | 0.080113 | H | -2.441719 | 3.980141 | 0.773635 |
| C | -2.16838 | -0.249544 | -0.331417 | H | 2.187412 | 0.527804 | 1.979091 |
| C | -1.450188 | -0.949387 | -1.487349 | H | 3.288592 | -0.874626 | 2.01116 |
| C | -2.093594 | 2.080388 | -0.155756 | H | -3.651222 | -1.650543 | 3.724642 |
| C | -3.408802 | 1.656901 | -0.713635 | H | -3.767878 | -2.725351 | 2.31347 |
| O | -3.432325 | 0.283039 | -0.801787 | H | -2.17958 | -2.356431 | 3.012317 |
| C | 0.589755 | -0.747944 | -2.885563 | H | -2.451337 | 0.055821 | 2.343539 |
| O | -4.333165 | 2.347451 | -1.067576 | H | -4.024454 | -0.328458 | 1.613006 |
| C | -1.768972 | 3.52661 | 0.035741 | H | 4.766527 | 3.57918 | -0.239405 |
| C | 2.777143 | -0.153952 | 1.368595 | H | 5.803605 | 2.30232 | 0.461233 |
| O | 1.168397 | -1.841245 | 1.202622 | H | 5.03 | 2.031265 | -1.100671 |
| O | 0.281913 | -2.683442 | 0.375896 | | | | |
| O | -2.385583 | -1.191278 | 0.672678 | | | | |
| C | -3.166959 | -1.942006 | 2.786051 | | | | |
| C | -3.039943 | -0.740288 | 1.865666 | | | | |
| O | 3.814072 | 0.57259 | 0.681507 | | | | |
| O | 2.758127 | 2.558786 | 1.008751 | | | | |
| C | 3.695879 | 1.923255 | 0.581109 | | | | |
| C | 4.898767 | 2.503404 | -0.121911 | | | | |
| H | 2.444632 | -3.430453 | -1.910615 | | | | |
| H | 3.850445 | -1.740387 | -0.530892 | | | | |
| H | 1.42051 | 0.661449 | -1.035309 | | | | |
| H | -0.048129 | -3.247839 | -1.51087 | | | | |
| H | -0.098637 | 0.104862 | 1.488384 | | | | |
| H | 0.501658 | 1.646234 | 0.851248 | | | | |

**Table S3** Energy analyses of 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (eight conformers)

| NO. | 3D conformers B3LYP/6-31G(d,p) | E (Hartree) | ΔE (KJ/mol) | Boltzmann distribution |
|---|---|---|---|---|
| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 1) |  | -1264.567929 | 5.84173493 | 5.90% |
| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 2) |  | -1264.567006 | 8.265070363 | 2.22% |
| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 3) |  | -1264.570154 | 0 | 62.27% |
| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 4) |  | -1264.569214 | 2.467968914 | 23.01% |

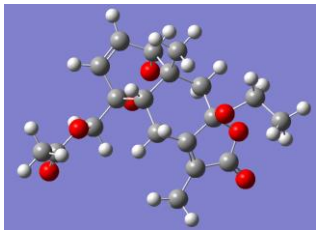
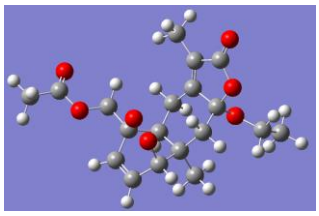
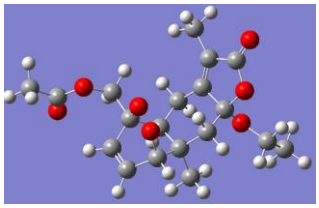
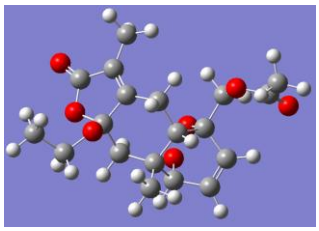
| | | | | |
|---|---|---|---|---|
| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 5) |  | -1264.566969 | 8.362213821 | 2.13% |
| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 6) |  | -1264.567201 | 7.753098088 | 2.73% |
| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 7) |  | -1264.566017 | 10.86168872 | 0.78% |
| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 8) |  | -1264.566217 | 10.33658895 | 0.96% |

**Table S4** Cartesian coordinates of the low-energy re-optimized conformers of 1*S*,4*R*,5*S*,8*S*,10*R*-**5** calculated at B3LYP/6-31G(d,p) level of theory.

| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 1) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 1.567642 | -3.102684 | -0.918507 | H | -2.537107 | -1.833471 | -0.740383 |
| C | 2.428696 | -2.123244 | -0.639176 | H | -1.522495 | -0.793163 | -1.726752 |
| C | 1.791175 | -0.750418 | -0.660481 | H | -1.268345 | -2.189642 | 1.873327 |
| C | 0.66088 | -0.762835 | 0.418622 | H | -1.581119 | -3.469604 | 0.689665 |
| C | -0.452933 | -1.767767 | -0.099698 | H | 0.037294 | -3.290672 | 1.393675 |
| C | 0.205922 | -2.56377 | -1.27386 | H | 0.446375 | 3.45792 | -0.240316 |
| C | 0.141716 | 0.625109 | 0.901536 | H | -0.401333 | 3.703877 | -1.784277 |
| C | -1.035 | 1.12373 | 0.145043 | H | -1.072729 | 4.376503 | -0.305061 |
| C | -2.194006 | 0.165047 | 0.032397 | H | 3.592767 | 0.240147 | -1.326629 |
| C | -1.72771 | -1.094844 | -0.698136 | H | 2.354145 | 1.355336 | -0.742605 |
| C | -1.3257 | 2.258902 | -0.502152 | H | -5.354778 | -1.183299 | 3.007925 |
| C | -2.692529 | 2.115302 | -1.073269 | H | -3.664946 | -1.112314 | 3.551582 |
| O | -3.169111 | 0.854625 | -0.766577 | H | -4.53624 | 0.386387 | 3.171539 |
| C | -0.836897 | -2.738872 | 1.030934 | H | -4.675986 | -0.29376 | 0.75878 |
| O | -3.330832 | 2.906957 | -1.719501 | H | -3.818382 | -1.80408 | 1.136501 |
| C | -0.538271 | 3.511007 | -0.713927 | H | 5.66958 | 1.825857 | 2.58383 |
| C | 2.814155 | 0.379054 | -0.571907 | H | 4.08661 | 1.201786 | 3.134585 |
| O | 1.189397 | -0.512124 | -1.965714 | H | 5.305265 | 0.075053 | 2.53571 |
| O | 0.400609 | -1.676903 | -2.402101 | | | | |
| O | -2.696075 | -0.052388 | 1.331323 | | | | |
| C | -4.40124 | -0.659493 | 2.878889 | | | | |
| C | -3.945103 | -0.753128 | 1.432573 | | | | |
| O | 3.389855 | 0.321784 | 0.7458 | | | | |
| O | 4.711702 | 2.072199 | 0.196219 | | | | |
| C | 4.35684 | 1.245613 | 1.003413 | | | | |
| C | 4.893738 | 1.081143 | 2.404533 | | | | |
| H | 1.815608 | -4.157564 | -0.982944 | | | | |
| H | 3.484959 | -2.250756 | -0.42209 | | | | |
| H | 1.120591 | -1.217483 | 1.300757 | | | | |
| H | -0.479613 | -3.317987 | -1.672541 | | | | |
| H | -0.185897 | 0.494287 | 1.941791 | | | | |
| H | 0.95318 | 1.35634 | 0.927379 | | | | |

| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 2) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 1.98683 | -2.515903 | -1.264098 | H | -2.264523 | -1.961677 | -0.962804 |
| C | 2.686202 | -1.452686 | -0.863447 | H | -1.444631 | -0.659118 | -1.808806 |
| C | 1.834204 | -0.208607 | -0.718358 | H | -0.921243 | -2.4151 | 1.600949 |
| C | 0.730699 | -0.529571 | 0.340597 | H | -1.040326 | -3.577315 | 0.269664 |
| C | -0.211718 | -1.63368 | -0.302468 | H | 0.537882 | -3.225352 | 0.998554 |
| C | 0.551853 | -2.166087 | -1.558436 | H | -0.183151 | 3.647625 | 0.195572 |
| C | -0.002609 | 0.689289 | 0.980375 | H | -1.068905 | 3.93244 | -1.321314 |
| C | -1.254458 | 1.07397 | 0.280337 | H | -1.832054 | 4.307781 | 0.217479 |
| C | -2.243211 | -0.040677 | 0.046381 | H | 3.496417 | 1.094388 | -1.183511 |
| C | -1.586243 | -1.111048 | -0.82549 | H | 2.028216 | 1.948308 | -0.642412 |
| C | -1.735549 | 2.21498 | -0.228379 | H | -5.102368 | -2.232079 | 2.818627 |
| C | -3.067431 | 1.91919 | -0.822094 | H | -3.439812 | -1.949801 | 3.377641 |
| O | -3.327915 | 0.570476 | -0.671945 | H | -4.549693 | -0.580035 | 3.173733 |
| C | -0.418792 | -2.782262 | 0.700821 | H | -4.608147 | -0.982409 | 0.696079 |
| O | -3.834197 | 2.667668 | -1.373538 | H | -3.509773 | -2.365392 | 0.896501 |
| C | -1.165723 | 3.595243 | -0.28267 | H | 5.803149 | 0.74392 | 2.739684 |
| C | 2.653939 | 1.066625 | -0.491485 | H | 4.642436 | 2.101642 | 2.817789 |
| O | 1.184244 | 0.085059 | -1.990684 | H | 4.092371 | 0.46756 | 3.190803 |
| O | 0.586699 | -1.1296 | -2.570697 | | | | |
| O | -2.687186 | -0.488995 | 1.306565 | | | | |
| C | -4.249248 | -1.547318 | 2.759173 | | | | |
| C | -3.803061 | -1.392295 | 1.315021 | | | | |
| O | 3.131106 | 1.139014 | 0.866189 | | | | |
| O | 5.206747 | 0.448892 | 0.249473 | | | | |
| C | 4.437143 | 0.832072 | 1.100755 | | | | |
| C | 4.771709 | 1.046009 | 2.556682 | | | | |
| H | 2.402724 | -3.498041 | -1.466631 | | | | |
| H | 3.756166 | -1.424518 | -0.684315 | | | | |
| H | 1.264596 | -1.006013 | 1.168216 | | | | |
| H | -0.008979 | -2.966946 | -2.050314 | | | | |
| H | -0.293251 | 0.383152 | 1.994578 | | | | |
| H | 0.679695 | 1.533404 | 1.102035 | | | | |

| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 4) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -2.194849 | 2.68452 | -0.592489 | H | 2.114612 | 2.438812 | -0.379856 |
| C | -2.791239 | 1.496813 | -0.476131 | H | 1.381202 | 1.37613 | -1.58611 |
| C | -1.832748 | 0.337314 | -0.653321 | H | 0.796802 | 2.141593 | 2.146675 |
| C | -0.737132 | 0.474163 | 0.452283 | H | 0.73398 | 3.600929 | 1.156033 |
| C | 0.090205 | 1.787383 | 0.118495 | H | -0.770297 | 2.905177 | 1.792018 |
| C | -0.741694 | 2.549446 | -0.96373 | H | 0.493025 | -3.411153 | -0.824291 |
| C | 0.114648 | -0.798737 | 0.75051 | H | 1.280507 | -3.141085 | -2.39654 |
| C | 1.372848 | -0.878749 | -0.036976 | H | 2.180527 | -3.900643 | -1.091913 |
| C | 2.260469 | 0.342785 | 0.029164 | H | -3.390312 | -0.943843 | -1.434277 |
| C | 1.495723 | 1.544022 | -0.513912 | H | -1.842859 | -1.775867 | -1.13516 |
| C | 1.909608 | -1.787759 | -0.86128 | H | 4.55736 | -0.451438 | 3.873674 |
| C | 3.191148 | -1.225718 | -1.373179 | H | 4.50977 | 1.182992 | 3.178006 |
| O | 3.37256 | 0.030425 | -0.832579 | H | 3.059863 | 0.502348 | 3.942841 |
| C | 0.215025 | 2.660658 | 1.379978 | H | 2.932633 | -1.245512 | 2.133413 |
| O | 3.978725 | -1.722612 | -2.139163 | H | 4.388657 | -0.565655 | 1.377779 |
| C | 1.431937 | -3.130389 | -1.31069 | H | -5.624867 | -1.828186 | 2.444315 |
| C | -2.536209 | -1.020456 | -0.760483 | H | -4.329396 | -3.03382 | 2.186851 |
| O | -1.187925 | 0.435098 | -1.957673 | H | -3.942344 | -1.49418 | 2.956461 |
| O | -0.708098 | 1.804891 | -2.206922 | | | | |
| O | 2.718237 | 0.664404 | 1.31825 | | | | |
| C | 3.933749 | 0.264368 | 3.327037 | | | | |
| C | 3.513381 | -0.322731 | 1.990492 | | | | |
| O | -2.971975 | -1.480038 | 0.534008 | | | | |
| O | -5.115063 | -0.849808 | 0.115347 | | | | |
| C | -4.294011 | -1.363146 | 0.840507 | | | | |
| C | -4.572369 | -1.966122 | 2.195695 | | | | |
| H | -2.697811 | 3.645022 | -0.537652 | | | | |
| H | -3.850603 | 1.32915 | -0.310716 | | | | |
| H | -1.290097 | 0.668133 | 1.376153 | | | | |
| H | -0.261711 | 3.494893 | -1.234501 | | | | |
| H | 0.400237 | -0.736451 | 1.810051 | | | | |
| H | -0.491524 | -1.702223 | 0.654798 | | | | |

| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 5) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.725006 | 3.133729 | -0.660228 | H | 2.42928 | 2.038375 | -0.483278 |
| C | -2.545173 | 2.097504 | -0.480554 | H | 1.485494 | 1.03908 | -1.580388 |
| C | -1.844477 | 0.760638 | -0.596435 | H | 1.09644 | 2.124218 | 2.114151 |
| C | -0.737688 | 0.736139 | 0.506522 | H | 1.375721 | 3.506221 | 1.043821 |
| C | 0.338613 | 1.828031 | 0.095749 | H | -0.247616 | 3.204043 | 1.693483 |
| C | -0.333153 | 2.686616 | -1.025737 | H | -0.307972 | -3.404607 | -0.479352 |
| C | -0.164526 | -0.661929 | 0.889518 | H | 0.587316 | -3.490987 | -2.013488 |
| C | 1.05143 | -1.043811 | 0.127161 | H | 1.254084 | -4.245419 | -0.572032 |
| C | 2.164059 | -0.025939 | 0.118618 | H | -3.584108 | -0.252149 | -1.382889 |
| C | 1.654224 | 1.263121 | -0.525549 | H | -2.307492 | -1.35459 | -0.859713 |
| C | 1.410836 | -2.109487 | -0.599212 | H | 5.882849 | 0.349331 | 2.298499 |
| C | 2.782553 | -1.860195 | -1.119252 | H | 4.626853 | -0.704202 | 2.98383 |
| O | 3.191272 | -0.606128 | -0.703425 | H | 5.142317 | -0.920088 | 1.296345 |
| C | 0.657033 | 2.720351 | 1.308783 | H | 4.185121 | 1.304056 | 0.700043 |
| O | 3.475166 | -2.570239 | -1.803372 | H | 3.710931 | 1.57558 | 2.386335 |
| C | 0.689216 | -3.37593 | -0.928155 | H | -5.666821 | -2.238426 | 2.336247 |
| C | -2.815643 | -0.416701 | -0.622948 | H | -4.127076 | -1.589429 | 2.973982 |
| O | -1.206051 | 0.655618 | -1.90188 | H | -5.384374 | -0.474751 | 2.435449 |
| O | -0.464792 | 1.886388 | -2.225768 | | | | |
| O | 2.62072 | 0.127498 | 1.441633 | | | | |
| C | 4.948081 | -0.180032 | 2.077617 | | | | |
| C | 3.879283 | 0.804343 | 1.624945 | | | | |
| O | -3.420495 | -0.491742 | 0.68072 | | | | |
| O | -4.648887 | -2.248444 | -0.03919 | | | | |
| C | -4.349457 | -1.474881 | 0.839847 | | | | |
| C | -4.923186 | -1.447484 | 2.235728 | | | | |
| H | -2.020244 | 4.178256 | -0.645774 | | | | |
| H | -3.6103 | 2.159905 | -0.278858 | | | | |
| H | -1.234955 | 1.097251 | 1.411225 | | | | |
| H | 0.324464 | 3.500454 | -1.3466 | | | | |
| H | 0.133474 | -0.601421 | 1.945084 | | | | |
| H | -0.940962 | -1.428817 | 0.835627 | | | | |

| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 6) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.522574 | -3.026358 | 0.644759 | H | 2.457982 | -1.561025 | 1.339854 |
| C | -2.292544 | -2.163065 | -0.019584 | H | 1.200799 | -0.428478 | 1.810671 |
| C | -1.699975 | -0.771124 | -0.080374 | H | 1.953916 | -2.435178 | -1.41315 |
| C | -0.316403 | -0.902317 | -0.800527 | H | 1.951931 | -3.470256 | 0.023728 |
| C | 0.628753 | -1.73333 | 0.165384 | H | 0.58221 | -3.516934 | -1.102001 |
| C | -0.314746 | -2.355537 | 1.24548 | H | -0.336165 | 3.373812 | -0.895046 |
| C | 0.302931 | 0.408629 | -1.378374 | H | 0.066705 | 3.939754 | 0.742311 |
| C | 1.223418 | 1.101517 | -0.44077 | H | 1.101591 | 4.376958 | -0.61006 |
| C | 2.318187 | 0.248654 | 0.149854 | H | -2.278716 | 1.278474 | -0.479958 |
| C | 1.683582 | -0.890824 | 0.947984 | H | -2.659589 | 0.144114 | -1.78773 |
| C | 1.31385 | 2.347559 | 0.039695 | H | 6.180477 | -1.411047 | -1.58024 |
| C | 2.474705 | 2.387949 | 0.97071 | H | 4.698127 | -1.54502 | -2.550201 |
| O | 3.030558 | 1.124335 | 1.038699 | H | 5.418446 | 0.048893 | -2.249907 |
| C | 1.317891 | -2.857099 | -0.629034 | H | 4.913057 | -0.172609 | 0.199886 |
| O | 2.903242 | 3.316801 | 1.607195 | H | 4.204026 | -1.775799 | -0.093261 |
| C | 0.485782 | 3.567984 | -0.199859 | H | -6.941707 | 1.426332 | -0.302978 |
| C | -2.6254 | 0.265748 | -0.699157 | H | -6.521692 | -0.300119 | -0.080526 |
| O | -1.474224 | -0.27906 | 1.273051 | H | -6.103984 | 0.86695 | 1.174515 |
| O | -0.81733 | -1.303398 | 2.103314 | | | | |
| O | 3.157295 | -0.160299 | -0.906029 | | | | |
| C | 5.221519 | -0.932765 | -1.807991 | | | | |
| C | 4.39488 | -0.790338 | -0.541145 | | | | |
| O | -3.941918 | 0.087347 | -0.155641 | | | | |
| O | -4.628562 | 1.864546 | -1.371535 | | | | |
| C | -4.86997 | 0.985995 | -0.574511 | | | | |
| C | -6.199792 | 0.73178 | 0.091993 | | | | |
| H | -1.76737 | -4.067323 | 0.831707 | | | | |
| H | -3.260002 | -2.385371 | -0.456713 | | | | |
| H | -0.514359 | -1.532819 | -1.674059 | | | | |
| H | 0.245718 | -2.990266 | 1.938815 | | | | |
| H | 0.903911 | 0.115373 | -2.249674 | | | | |
| H | -0.472369 | 1.081073 | -1.755601 | | | | |

| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 7) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -1.910473 | -2.517829 | 0.91124 | H | 2.254033 | -1.615454 | 1.466032 |
| C | -2.552472 | -1.602045 | 0.183944 | H | 1.188814 | -0.269849 | 1.838322 |
| C | -1.757313 | -0.324281 | 0.012012 | H | 1.576046 | -2.632954 | -1.205028 |
| C | -0.428045 | -0.730694 | -0.7105 | H | 1.447867 | -3.53249 | 0.314896 |
| C | 0.400353 | -1.611557 | 0.317081 | H | 0.064977 | -3.466882 | -0.793719 |
| C | -0.605515 | -1.995134 | 1.452662 | H | 0.216137 | 3.47083 | -1.218027 |
| C | 0.376708 | 0.408044 | -1.411114 | H | 0.688676 | 4.10173 | 0.376902 |
| C | 1.405131 | 1.036385 | -0.542976 | H | 1.784427 | 4.272061 | -0.987625 |
| C | 2.368127 | 0.08341 | 0.120523 | H | -1.977991 | 1.740731 | -0.576131 |
| C | 1.582503 | -0.873011 | 1.018464 | H | -2.682695 | 0.560032 | -1.726963 |
| C | 1.690838 | 2.291938 | -0.177769 | H | 5.912054 | -2.282689 | -1.462169 |
| C | 2.858145 | 2.238951 | 0.744314 | H | 4.416529 | -2.265513 | -2.420893 |
| O | 3.21721 | 0.917436 | 0.926478 | H | 5.374461 | -0.781481 | -2.248287 |
| C | 0.899572 | -2.887734 | -0.383528 | H | 4.866283 | -0.726612 | 0.209995 |
| O | 3.431566 | 3.14617 | 1.292022 | H | 3.919419 | -2.221935 | 0.045859 |
| C | 1.05374 | 3.597944 | -0.525726 | H | -7.030021 | 0.601109 | -0.420868 |
| C | -2.526828 | 0.802225 | -0.672566 | H | -6.09578 | 0.586485 | 1.107609 |
| O | -1.426819 | 0.230191 | 1.317772 | H | -6.206879 | 2.075891 | 0.171034 |
| O | -0.923878 | -0.815208 | 2.226165 | | | | |
| O | 3.120952 | -0.536742 | -0.896443 | | | | |
| C | 5.034867 | -1.683218 | -1.729367 | | | | |
| C | 4.252777 | -1.315995 | -0.479573 | | | | |
| O | -3.796538 | 1.038737 | -0.04172 | | | | |
| O | -4.891354 | -0.031828 | -1.717821 | | | | |
| C | -4.909468 | 0.593526 | -0.679627 | | | | |
| C | -6.146667 | 0.985711 | 0.089575 | | | | |
| H | -2.29869 | -3.499644 | 1.163883 | | | | |
| H | -3.527575 | -1.728765 | -0.273614 | | | | |
| H | -0.742661 | -1.395446 | -1.521869 | | | | |
| H | -0.134379 | -2.653153 | 2.189471 | | | | |
| H | 0.913997 | -0.056971 | -2.248607 | | | | |
| H | -0.292023 | 1.151106 | -1.854223 | | | | |

| 1*S*,4*R*,5*S*,8*S*,10*R*-**5** (conformer 8) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.087593 | -2.65243 | -0.882147 | H | -2.175008 | -2.178979 | -0.591628 |
| C | 2.758994 | -1.52318 | -0.649591 | H | -1.405581 | -0.991482 | -1.635747 |
| C | 1.871226 | -0.295928 | -0.670141 | H | -0.792268 | -2.221954 | 1.983079 |
| C | 0.791112 | -0.493535 | 0.441852 | H | -0.895265 | -3.564575 | 0.833897 |
| C | -0.125517 | -1.703313 | -0.022764 | H | 0.682088 | -3.073175 | 1.480515 |
| C | 0.639355 | -2.389412 | -1.200982 | H | -0.255152 | 3.595417 | -0.269125 |
| C | 0.029627 | 0.782407 | 0.915758 | H | -1.167002 | 3.638628 | -1.796572 |
| C | -1.242938 | 1.028428 | 0.191112 | H | -1.923645 | 4.20318 | -0.313312 |
| C | -2.198064 | -0.137021 | 0.131261 | H | 3.487484 | 0.973536 | -1.343649 |
| C | -1.520516 | -1.298569 | -0.594665 | H | 1.999723 | 1.853867 | -0.908656 |
| C | -1.766471 | 2.072317 | -0.463686 | H | -5.782045 | -1.178787 | 2.323003 |
| C | -3.097027 | 1.658786 | -0.985185 | H | -4.678009 | 0.001789 | 3.060913 |
| O | -3.31311 | 0.336487 | -0.644382 | H | -5.252781 | 0.244395 | 1.39637 |
| C | -0.289686 | -2.701236 | 1.13755 | H | -3.996645 | -1.775491 | 0.64838 |
| O | -3.896743 | 2.301395 | -1.617557 | H | -3.454215 | -2.079137 | 2.30842 |
| C | -1.241096 | 3.447597 | -0.719593 | H | 5.847636 | 1.262849 | 2.552718 |
| C | 2.654021 | 1.021733 | -0.641903 | H | 4.640996 | 2.578867 | 2.45592 |
| O | 1.196904 | -0.206474 | -1.960607 | H | 4.152723 | 0.997165 | 3.065596 |
| O | 0.631773 | -1.508791 | -2.352066 | | | | |
| O | -2.604535 | -0.431446 | 1.44667 | | | | |
| C | -4.938142 | -0.506467 | 2.126478 | | | | |
| C | -3.747611 | -1.294926 | 1.600041 | | | | |
| O | 3.143791 | 1.303393 | 0.683595 | | | | |
| O | 5.233 | 0.592447 | 0.140834 | | | | |
| C | 4.461143 | 1.071434 | 0.939956 | | | | |
| C | 4.80435 | 1.50172 | 2.345123 | | | | |
| H | 2.530752 | -3.641275 | -0.948195 | | | | |
| H | 3.82964 | -1.439105 | -0.49346 | | | | |
| H | 1.349303 | -0.832873 | 1.319456 | | | | |
| H | 0.097383 | -3.268294 | -1.563837 | | | | |
| H | -0.238366 | 0.61474 | 1.9679 | | | | |
| H | 0.687497 | 1.654158 | 0.905278 | | | | |

**Table S5** Experimental and calculated $^{1}$H NMR data for compound **5**.

| No. | **5**, exptl. $\delta_H$ [a] | 1*R*,4*S*,5*R*,8*S*,10*S*-**5**, calcd. $\delta_H$ [b] | 1*S*,4*R*,5*S*,8*S*,10*R*-**5**, calcd. $\delta_H$ [b] |
|---|---|---|---|
| 1 | 4.2 | 3.96 | 4.02 |
| 2 | 6.74 | 7.01 | 6.99 |
| 3 | 6.39 | 7.07 | 6.85 |
| 5 | 2.53 | 1.60 | 1.94 |
| 6 | 2.47 | 2.73 | 2.62 |
| | 2.61 | 2.86 | 2.82 |
| 9 | 1.4 | 2.16 | 2.23 |
| | 2.26 | 3.29 | 2.60 |
| 13 | 1.79 | 1.95 | 1.78 |
| 14 | 1.61 | 0.67 | 1.19 |
| 15 | 4.37 | 3.66 | 3.92 |
| | 4.43 | 4.88 | 4.50 |
| 4-OAc | 2.17 | 2.22 | 2.18 |
| 1′ | 3.15 | 3.37 | 3.03 |
| | 3.46 | 3.62 | 3.59 |
| 2′ | 1.21 | 1.28 | 1.23 |

[a] Recorded in $CDCl_3$ at 600 MHz.

[b] Calculated in $CDCl_3$

**Table S6** Experimental and calculated $^{13}C$ NMR data for compound **5**.

| No. | **5**, exptl. $\delta_C$ [a] | 1*R*,4*S*,5*R*,8*S*,10*S*-**5**, calcd. $\delta_C$ [b] | 1*S*,4*R*,5*S*,8*S*,10*R*-**5**, calcd. $\delta_C$ [b] |
|---|---|---|---|
| 1 | 79.5 | 76.06 | 74.25 |
| 2 | 135.8 | 135.54 | 134.13 |
| 3 | 129.2 | 137.27 | 135.89 |
| 4 | 79.8 | 75.79 | 75.45 |
| 5 | 42.5 | 44.36 | 43.80 |
| 6 | 22.8 | 18.67 | 17.55 |
| 7 | 155.8 | 163.69 | 156.63 |
| 8 | 105.3 | 103.90 | 100.25 |
| 9 | 43.8 | 39.23 | 38.05 |
| 10 | 38.7 | 33.46 | 35.02 |
| 11 | 124.2 | 126.51 | 121.86 |
| 12 | 171.1 | 172.11 | 168.83 |
| 13 | 8.3 | 5.42 | 4.83 |
| 14 | 29.2 | 24.27 | 23.57 |
| 15 | 62.8 | 58.50 | 58.99 |
| 4-OAc | 20.8 | 17.29 | 17.09 |
| | 170.7 | 172.53 | 170.57 |
| 1′ | 59.1 | 54.70 | 52.74 |
| 2′ | 15.1 | 10.92 | 10.81 |

[a] Recorded in $CDCl_3$ at 600 MHz.

[b] Calculated in $CDCl_3$

**Table S7** DP4+ analyses of calculated and experimental NMR chemical shifts of **5** (unscaled). Isomer 1: 1*R*,4*S*,5*R*,8*S*,10*S*-**5**; Isomer 2: 1*S*,4*R*,5*S*,8*S*,10*R*-**5**

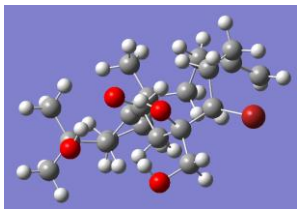
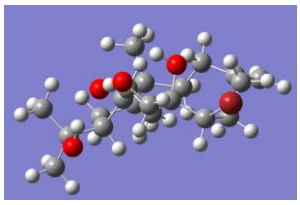
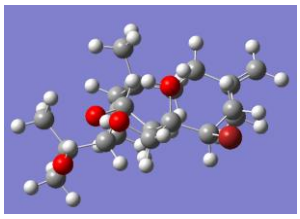
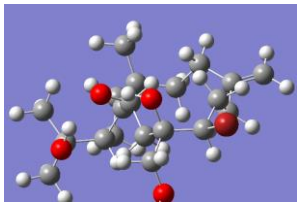
| Functional | Solvent? | Basis Set | Type of Data |
|---|---|---|---|
| mPW1PW91 | PCM | 6-311G(d,p) | Unscaled Shifts |

| | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 | Isomer 6 |
|---|---|---|---|---|---|---|
| sDP4+ (H data) | 0.02% | 99.98% | - | - | - | - |
| sDP4+ (C data) | 0.54% | 99.46% | - | - | - | - |
| sDP4+ (all data) | 0.00% | 100.00% | - | - | - | - |
| uDP4+ (H data) | 0.00% | 100.00% | - | - | - | - |
| uDP4+ (C data) | 100.00% | 0.00% | - | - | - | - |
| uDP4+ (all data) | 83.93% | 16.07% | - | - | - | - |
| DP4+ (H data) | 0.00% | 100.00% | - | - | - | - |
| DP4+ (C data) | 100.00% | 0.00% | - | - | - | - |
| DP4+ (all data) | 0.00% | 100.00% | - | - | - | - |

| Functional | Solvent? | Basis Set | Type of Data |
|---|---|---|---|
| mPW1PW91 | PCM | 6-311G(d,p) | Unscaled Shifts |

| | | DP4+ | 0.00% | 100.00% | - | - | - |
|---|---|---|---|---|---|---|---|
| Nuclei | sp2? | Experimental | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 |
| C | | 79.5 | 76.0622 | 74.2513 | | | |
| C | x | 135.8 | 135.5422 | 134.1323 | | | |
| C | x | 129.2 | 137.2658 | 135.8851 | | | |
| C | | 79.8 | 75.7858 | 75.4483 | | | |
| C | | 42.5 | 44.3624 | 43.8035 | | | |
| C | | 22.8 | 18.672 | 17.5512 | | | |
| C | x | 155.8 | 163.688 | 156.6318 | | | |
| C | | 105.3 | 103.9016 | 100.2476 | | | |
| C | | 43.8 | 39.2282 | 38.0503 | | | |
| C | | 38.7 | 33.4624 | 35.0231 | | | |
| C | x | 124.2 | 126.5138 | 121.8617 | | | |
| C | x | 171.1 | 172.1056 | 168.8265 | | | |
| C | | 8.3 | 5.415 | 4.8285 | | | |
| C | | 29.2 | 24.2716 | 23.5731 | | | |
| C | | 62.8 | 58.5036 | 58.9896 | | | |
| C | | 20.8 | 17.287 | 17.0932 | | | |
| C | x | 170.7 | 172.532 | 170.5733 | | | |
| C | | 59.1 | 54.7042 | 52.7385 | | | |
| C | | 15.1 | 10.9158 | 10.8119 | | | |
| H | | 4.2 | 3.9644 | 4.0166 | | | |
| H | x | 6.74 | 7.0112 | 6.9858 | | | |
| H | x | 6.39 | 7.07 | 6.8478 | | | |
| H | | 2.53 | 1.60 | 1.938 | | | |
| H | | 2.47 | 2.73 | 2.6221 | | | |
| H | | 2.61 | 2.86 | 2.8192 | | | |
| H | | 1.4 | 2.1576 | 2.2344 | | | |
| H | | 2.26 | 3.2894 | 2.6024 | | | |
| H | | 1.79 | 1.945733 | 1.78239962 | | | |
| H | | 1.61 | 0.674466 | 1.18653329 | | | |
| H | | 4.37 | 3.6628 | 3.9216 | | | |
| H | | 4.43 | 4.8826 | 4.4979 | | | |
| H | | 2.17 | 2.2174662 | 2.17953314 | | | |
| H | | 3.15 | 3.3732 | 3.0254 | | | |
| H | | 3.46 | 3.6174 | 3.5878 | | | |
| H | | 1.21 | 1.27806666 | 1.23139956 | | | |

**Table S8** Energy analyses of 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (six conformers)

| NO. | 3D conformers B3LYP/6-31G(d,p) | E (Hartree) | ΔE (KJ/mol) | Boltzmann distribution |
|---|---|---|---|---|
| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 1) |  | -3654.063991 | 5.243121193 | 9.99% |
| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 2) |  | -3654.016987 | 128.6520689 | 0.00% |
| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 3) |  | -3654.063212 | 7.288384793 | 4.38% |
| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 4) |  | -3654.060185 | 15.2357698 | 0.18% |

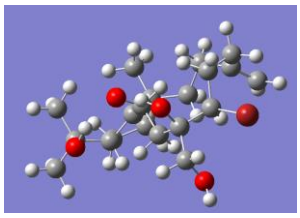
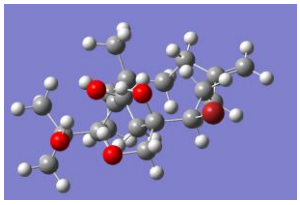
| | | | | |
|---|---|---|---|---|
| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 5) |  | -3654.065988 | 0 | 82.81% |
| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 6) |  | -3654.062738 | 8.532871245 | 2.65% |

**Table S9** Cartesian coordinates of the low-energy re-optimized conformers of 1*R*,7*R*,8*R*,10*S*,12*R*-**6** calculated at B3LYP/6-31G(d,p) level of theory

| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 1) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.119118 | 0.819963 | 1.209604 | H | -1.779646 | 3.858751 | -0.684575 |
| C | 2.324363 | 2.32985 | 0.937619 | H | 2.223916 | 0.46707 | -0.939718 |
| C | 1.302484 | 2.958018 | 0.000753 | H | 0.138285 | 0.969146 | -0.420426 |
| C | -0.131595 | 3.081214 | 0.523357 | H | -0.395416 | -2.03342 | -0.802196 |
| C | -1.27458 | 2.897543 | -0.526553 | H | 0.482626 | -0.967847 | -1.907779 |
| C | 2.382829 | -0.082604 | -0.011045 | H | -4.12088 | 2.646917 | -1.307613 |
| C | -2.383359 | 1.861369 | -0.191344 | H | -2.913804 | 1.827079 | -2.302317 |
| C | -1.912798 | 0.379138 | -0.167606 | H | -4.619893 | 0.107473 | -2.086865 |
| C | -0.479181 | 0.085908 | -0.335052 | H | -4.933655 | 0.527329 | -0.410948 |
| C | 0.225893 | -1.137586 | -0.853585 | H | -2.638102 | -1.060013 | -1.573805 |
| C | 1.547243 | -1.404724 | -0.060772 | H | 0.974002 | 3.883014 | -1.890391 |
| C | -3.429611 | 1.796904 | -1.332704 | H | 2.704016 | 3.344672 | -1.540958 |
| C | -4.141089 | 0.44191 | -1.161658 | H | -4.768272 | -3.447274 | 0.142737 |
| C | -3.039193 | -0.54569 | -0.691654 | H | -4.057301 | -2.979248 | -1.410526 |
| C | 1.672745 | 3.411775 | -1.203746 | H | -5.422105 | -2.052164 | -0.74242 |
| C | -3.509435 | -1.695235 | 0.253833 | H | -4.37085 | -2.090706 | 2.188046 |
| C | -4.504497 | -2.592853 | -0.488546 | H | -3.400614 | -0.610027 | 2.150433 |
| C | -4.115312 | -1.214788 | 1.583213 | H | -5.028483 | -0.626627 | 1.442259 |
| O | -2.388657 | -2.544135 | 0.544723 | H | -1.76005 | -1.98873 | 1.037367 |
| C | -3.06806 | 2.238956 | 1.138514 | H | -2.384669 | 2.133061 | 1.985847 |
| O | -1.104523 | -0.020226 | 0.983827 | H | -3.404695 | 3.281869 | 1.099007 |
| C | 2.281255 | -2.595915 | -0.708096 | H | -3.942312 | 1.616623 | 1.34627 |
| O | 1.240376 | -1.882372 | 1.256456 | H | 2.612228 | -2.340805 | -1.718889 |
| O | 1.431503 | -3.72259 | -0.816288 | H | 3.16906 | -2.819886 | -0.104663 |
| Br | 4.378164 | -0.366482 | -0.096317 | H | 0.512859 | -1.348754 | 1.614611 |
| H | 1.100705 | 0.664821 | 1.576118 | H | 1.097119 | -3.882862 | 0.082739 |
| H | 2.775682 | 0.503877 | 2.024522 | | | | |
| H | 3.333837 | 2.484692 | 0.540506 | | | | |
| H | 2.283375 | 2.845129 | 1.908192 | | | | |
| H | -0.228921 | 4.069079 | 0.994626 | | | | |
| H | -0.26628 | 2.368192 | 1.342011 | | | | |
| H | -0.840411 | 2.632096 | -1.497034 | | | | |

| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 2) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.659352 | 0.994019 | -1.216181 | H | -0.885992 | 3.655686 | -0.200797 |
| C | 2.951429 | 1.939896 | -0.006475 | H | 2.463075 | -1.038049 | -1.902749 |
| C | 1.883223 | 2.980733 | 0.282362 | H | -0.528714 | -0.077124 | 1.407973 |
| C | 0.565911 | 2.50069 | 0.890134 | H | -0.26872 | -1.270115 | -1.343165 |
| C | -0.616437 | 2.595816 | -0.103426 | H | 0.188053 | 0.401375 | -1.024506 |
| C | 2.567268 | -0.520168 | -0.94487 | H | -3.437003 | 3.355144 | -0.465996 |
| C | -1.958033 | 1.861033 | 0.198848 | H | -2.586517 | 2.52871 | -1.773056 |
| C | -2.045213 | 0.3462 | 0.036409 | H | -4.679619 | 1.308104 | -1.774205 |
| C | -1.04296 | -0.597425 | 0.575459 | H | -4.806758 | 1.365475 | -0.01973 |
| C | 0.080152 | -0.578718 | -0.569512 | H | -2.858625 | -0.276041 | -1.708489 |
| C | 1.4701 | -1.05288 | 0.013029 | H | 1.356684 | 5.040044 | 0.286128 |
| C | -3.041402 | 2.384923 | -0.783939 | H | 3.031057 | 4.63817 | -0.382133 |
| C | -4.096734 | 1.282325 | -0.850641 | H | -5.81029 | -2.381434 | -1.127553 |
| C | -3.282656 | -0.023618 | -0.714003 | H | -5.017269 | -1.368602 | -2.340537 |
| C | 2.098559 | 4.280171 | 0.047421 | H | -6.044603 | -0.622264 | -1.087804 |
| C | -4.094663 | -1.347628 | -0.364243 | H | -5.154999 | -2.231178 | 1.297819 |
| C | -5.319207 | -1.417131 | -1.288314 | H | -3.644356 | -1.42689 | 1.757336 |
| C | -4.526765 | -1.352984 | 1.115447 | H | -5.107463 | -0.461905 | 1.385777 |
| O | -3.313833 | -2.467849 | -0.672453 | H | -2.524184 | -2.425615 | -0.048274 |
| C | -2.411177 | 2.127934 | 1.670508 | H | -1.685652 | 1.738074 | 2.388301 |
| O | -1.415476 | -1.840982 | 0.926598 | H | -2.498528 | 3.211331 | 1.811891 |
| C | 1.48016 | -2.613122 | 0.139078 | H | -3.383675 | 1.678738 | 1.895656 |
| O | 1.681684 | -0.538265 | 1.310808 | H | 0.964718 | -3.065949 | -0.719363 |
| O | 0.897234 | -2.985191 | 1.369601 | H | 2.512458 | -2.967471 | 0.15416 |
| Br | 4.380223 | -1.099531 | -0.308892 | H | 1.486557 | -1.311932 | 1.893766 |
| H | 3.457452 | 1.116106 | -1.954843 | H | -0.07129 | -2.714999 | 1.300437 |
| H | 1.747888 | 1.311508 | -1.736123 | | | | |
| H | 3.894435 | 2.460536 | -0.200247 | | | | |
| H | 3.110745 | 1.329079 | 0.886727 | | | | |
| H | 0.332478 | 3.115272 | 1.768212 | | | | |
| H | 0.708359 | 1.483906 | 1.25525 | | | | |
| H | -0.289784 | 2.303799 | -1.107619 | | | | |

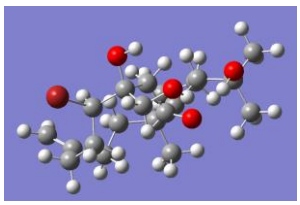
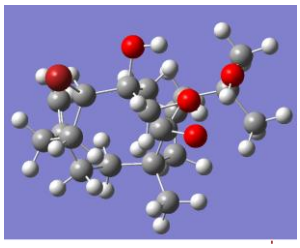
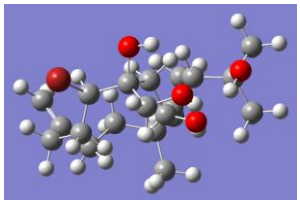
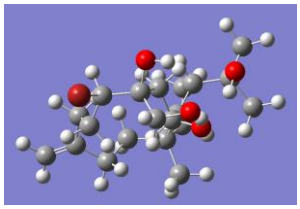
| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 3) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.301052 | 1.37567 | -0.137433 | H | -2.402785 | 3.570023 | -0.179323 |
| C | 1.284102 | 2.05842 | -1.090822 | H | 2.640455 | -0.196729 | -1.610377 |
| C | 0.712649 | 3.345712 | -0.525528 | H | 0.052068 | 0.589932 | 1.128676 |
| C | -0.388581 | 3.206484 | 0.509258 | H | -0.192869 | -2.039956 | -0.289747 |
| C | -1.739069 | 2.701385 | -0.089418 | H | 0.230476 | -0.73696 | -1.353865 |
| C | 2.64836 | -0.077806 | -0.523477 | H | -4.626319 | 1.008302 | 0.762689 |
| C | -2.53205 | 1.586258 | 0.669819 | H | -4.374412 | 2.487933 | -0.161419 |
| C | -1.948569 | 0.182171 | 0.32772 | H | -3.413686 | 1.237678 | -2.037484 |
| C | -0.529781 | -0.136863 | 0.57823 | H | -4.749576 | 0.215779 | -1.543949 |
| C | 0.289994 | -1.059725 | -0.306174 | H | -2.089586 | -0.646433 | -1.674895 |
| C | 1.788168 | -1.198352 | 0.11512 | H | 0.766496 | 5.466507 | -0.508434 |
| C | -3.951517 | 1.499871 | 0.052043 | H | 1.937968 | 4.640949 | -1.67638 |
| C | -3.796252 | 0.633193 | -1.2071 | H | -4.327369 | -3.492201 | -1.586979 |
| C | -2.763054 | -0.463793 | -0.829012 | H | -3.127706 | -2.59987 | -2.536671 |
| C | 1.159611 | 4.541315 | -0.923203 | H | -4.736881 | -1.89874 | -2.253172 |
| C | -3.402631 | -1.863781 | -0.51257 | H | -4.868304 | -2.81782 | 0.749991 |
| C | -3.935398 | -2.49348 | -1.804445 | H | -4.138416 | -1.385751 | 1.491555 |
| C | -4.513448 | -1.801616 | 0.550247 | H | -5.369645 | -1.201278 | 0.2247 |
| O | -2.388208 | -2.774317 | -0.056872 | H | -2.046694 | -2.366213 | 0.762849 |
| C | -2.594009 | 1.859361 | 2.177618 | H | -1.60872 | 1.829605 | 2.652345 |
| O | -1.562703 | -0.691263 | 1.429992 | H | -3.028007 | 2.849365 | 2.363976 |
| C | 2.269142 | -2.607701 | -0.31836 | H | -3.216077 | 1.114297 | 2.682798 |
| O | 1.915847 | -1.104348 | 1.524028 | H | 2.069586 | -2.777918 | -1.38579 |
| O | 1.658029 | -3.605849 | 0.498794 | H | 3.340506 | -2.698307 | -0.14196 |
| Br | 4.582684 | -0.36474 | -0.054195 | H | 1.716695 | -1.999142 | 1.858828 |
| H | 1.967209 | 1.392301 | 0.90392 | H | 0.76531 | -3.787046 | 0.164398 |
| H | 3.21596 | 1.971617 | -0.164193 | | | | |
| H | 0.459418 | 1.378171 | -1.326659 | | | | |
| H | 1.791148 | 2.263051 | -2.041622 | | | | |
| H | -0.549937 | 4.175754 | 0.992756 | | | | |
| H | -0.046176 | 2.540238 | 1.307221 | | | | |
| H | -1.570129 | 2.364647 | -1.119561 | | | | |

| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 4) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.288735 | 1.333555 | -0.126005 | H | -2.398753 | 3.503108 | -0.454375 |
| C | 1.306178 | 1.930251 | -1.168793 | H | 2.732142 | -0.355969 | -1.442904 |
| C | 0.719509 | 3.259928 | -0.73245 | H | 0.031291 | 0.661281 | 1.067196 |
| C | -0.396346 | 3.209185 | 0.294693 | H | -0.198659 | -2.108413 | -0.111152 |
| C | -1.736192 | 2.647453 | -0.276203 | H | 0.243208 | -0.896598 | -1.265601 |
| C | 2.654473 | -0.14097 | -0.376584 | H | -4.644103 | 1.063437 | 0.699013 |
| C | -2.541224 | 1.603234 | 0.567582 | H | -4.367241 | 2.454112 | -0.3472 |
| C | -1.968782 | 0.169394 | 0.340746 | H | -3.409556 | 1.03325 | -2.101188 |
| C | -0.546061 | -0.123184 | 0.596908 | H | -4.76777 | 0.080223 | -1.534562 |
| C | 0.27602 | -1.125693 | -0.195089 | H | -2.133481 | -0.8512 | -1.567824 |
| C | 1.762529 | -1.236597 | 0.264558 | H | 0.761603 | 5.374038 | -0.906831 |
| C | -3.959314 | 1.482406 | -0.0473 | H | 1.955453 | 4.453759 | -1.977433 |
| C | -3.809943 | 0.50878 | -1.225906 | H | -4.442322 | -3.615573 | -1.200787 |
| C | -2.800738 | -0.569411 | -0.74503 | H | -3.241701 | -2.837586 | -2.244366 |
| C | 1.166206 | 4.417693 | -1.229933 | H | -4.834825 | -2.082846 | -2.005136 |
| C | -3.471706 | -1.915737 | -0.292525 | H | -4.94438 | -2.712784 | 1.066287 |
| C | -4.036555 | -2.648631 | -1.51508 | H | -4.171845 | -1.238029 | 1.667161 |
| C | -4.568083 | -1.72799 | 0.771047 | H | -5.413917 | -1.138709 | 0.40084 |
| O | -2.474992 | -2.804127 | 0.230116 | H | -2.095531 | -2.329942 | 0.994182 |
| C | -2.606669 | 1.995805 | 2.048668 | H | -1.624075 | 1.993591 | 2.529811 |
| O | -1.565525 | -0.602651 | 1.51379 | H | -3.030785 | 3.001918 | 2.153822 |
| C | 2.271311 | -2.639383 | -0.121251 | H | -3.239571 | 1.299988 | 2.607924 |
| O | 1.865847 | -1.0891 | 1.679633 | H | 3.303944 | -2.754866 | 0.223281 |
| O | 2.160086 | -2.782223 | -1.533592 | H | 1.645614 | -3.380767 | 0.403794 |
| Br | 4.550767 | -0.384484 | 0.260913 | H | 1.184432 | -1.646173 | 2.089917 |
| H | 1.920244 | 1.439598 | 0.898541 | H | 2.644733 | -3.578424 | -1.79578 |
| H | 3.202995 | 1.929588 | -0.172224 | | | | |
| H | 0.489842 | 1.230896 | -1.376071 | | | | |
| H | 1.845749 | 2.054682 | -2.115266 | | | | |
| H | -0.567985 | 4.217141 | 0.68711 | | | | |
| H | -0.063886 | 2.619259 | 1.154835 | | | | |
| H | -1.551136 | 2.219242 | -1.268859 | | | | |

| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 5) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -2.018357 | 0.805505 | -1.284758 | H | 1.838992 | 3.756181 | 0.809724 |
| C | -2.216813 | 2.312392 | -0.99123 | H | -2.198128 | 0.408641 | 0.856125 |
| C | -1.221681 | 2.909697 | -0.006957 | H | -0.08583 | 0.887533 | 0.395643 |
| C | 0.229012 | 3.031084 | -0.479895 | H | 0.430597 | -2.126741 | 0.620317 |
| C | 1.334813 | 2.804301 | 0.600506 | H | -0.452567 | -1.133768 | 1.798121 |
| C | -2.324083 | -0.11625 | -0.09108 | H | 4.153083 | 2.503985 | 1.461769 |
| C | 2.447301 | 1.773804 | 0.262084 | H | 2.911051 | 1.653495 | 2.385378 |
| C | 1.96813 | 0.297194 | 0.166411 | H | 4.612455 | -0.06817 | 2.155605 |
| C | 0.52938 | 0.004971 | 0.286016 | H | 4.983646 | 0.416301 | 0.509267 |
| C | -0.19146 | -1.234524 | 0.737405 | H | 2.646171 | -1.20437 | 1.531196 |
| C | -1.521381 | -1.460291 | -0.05216 | H | -0.946781 | 3.783887 | 1.916222 |
| C | 3.456814 | 1.658175 | 1.431862 | H | -2.669393 | 3.271692 | 1.49793 |
| C | 4.16614 | 0.306277 | 1.229444 | H | 4.821005 | -3.524271 | -0.22181 |
| C | 3.075212 | -0.654595 | 0.684251 | H | 4.069487 | -3.117796 | 1.329823 |
| C | -1.627215 | 3.337236 | 1.195658 | H | 5.453855 | -2.16901 | 0.73759 |
| C | 3.569756 | -1.764693 | -0.294898 | H | 4.486024 | -2.081597 | -2.218496 |
| C | 4.542238 | -2.695531 | 0.436698 | H | 3.515518 | -0.602249 | -2.14693 |
| C | 4.213649 | -1.231098 | -1.58539 | H | 5.122526 | -0.650596 | -1.393821 |
| O | 2.456306 | -2.597772 | -0.651914 | H | 1.842776 | -2.022788 | -1.14177 |
| C | 3.175645 | 2.197593 | -1.030348 | H | 2.51889 | 2.127965 | -1.902175 |
| O | 1.187236 | -0.050969 | -1.019014 | H | 3.515657 | 3.236306 | -0.940482 |
| C | -2.278839 | -2.615686 | 0.63699 | H | 4.053172 | 1.578727 | -1.234362 |
| O | -1.265474 | -1.946495 | -1.366396 | H | -3.116422 | -2.909533 | -0.005765 |
| O | -2.697877 | -2.297126 | 1.95257 | H | -1.593106 | -3.464542 | 0.711573 |
| Br | -4.335055 | -0.387066 | -0.086847 | H | -0.543403 | -1.42306 | -1.748466 |
| H | -0.991055 | 0.64456 | -1.623781 | H | -3.517779 | -1.781168 | 1.863853 |
| H | -2.652227 | 0.510744 | -2.125366 | | | | |
| H | -3.237766 | 2.47122 | -0.625935 | | | | |
| H | -2.136908 | 2.845591 | -1.949559 | | | | |
| H | 0.35227 | 4.030327 | -0.920158 | | | | |
| H | 0.382695 | 2.338958 | -1.312971 | | | | |
| H | 0.867325 | 2.506394 | 1.545748 | | | | |

| 1*R*,7*R*,8*R*,10*S*,12*R*-**6** (conformer 6) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.29113 | 1.369772 | 0.147809 | H | -2.400185 | 3.560229 | -0.112455 |
| C | 1.258383 | 2.037489 | -1.092014 | H | 2.604335 | -0.219213 | -1.611614 |
| C | 0.699564 | 3.326553 | -0.520277 | H | 0.03472 | 0.525782 | 1.181673 |
| C | -0.37729 | 3.181427 | 0.537464 | H | -0.12828 | -2.119193 | -0.20335 |
| C | -1.737365 | 2.688698 | -0.045919 | H | 0.222594 | -0.827483 | -1.316444 |
| C | 2.641069 | -0.08253 | -0.528031 | H | -4.616221 | 0.984633 | 0.79972 |
| C | -2.522403 | 1.564271 | 0.705895 | H | -4.370971 | 2.493911 | -0.077797 |
| C | -1.953194 | 0.159559 | 0.334782 | H | -3.414801 | 1.301842 | -1.998017 |
| C | -0.54171 | -0.186924 | 0.605115 | H | -4.755082 | 0.272309 | -1.534424 |
| C | 0.296516 | -1.114865 | -0.259354 | H | -2.101975 | -0.610347 | -1.692386 |
| C | 1.807121 | -1.195555 | 0.153603 | H | 0.751762 | 5.447179 | -0.506224 |
| C | -3.947118 | 1.49908 | 0.100132 | H | 1.894661 | 4.621681 | -1.702474 |
| C | -3.79891 | 0.67331 | -1.186462 | H | -4.391492 | -3.416993 | -1.68987 |
| C | -2.773931 | -0.442634 | -0.842108 | H | -3.189071 | -2.508187 | -2.618889 |
| C | 1.135581 | 4.522056 | -0.92982 | H | -4.787543 | -1.796778 | -2.297481 |
| C | -3.434805 | -1.841416 | -0.567336 | H | -4.907407 | -2.815053 | 0.670393 |
| C | -3.989426 | -2.416097 | -1.876832 | H | -4.150867 | -1.421889 | 1.457438 |
| C | -4.538894 | -1.797503 | 0.50466 | H | -5.388661 | -1.173655 | 0.207174 |
| O | -2.437042 | -2.783802 | -0.159159 | H | -2.07347 | -2.424347 | 0.672175 |
| C | -2.565561 | 1.814668 | 2.2179 | H | -1.574756 | 1.772596 | 2.680606 |
| O | -1.601643 | -0.742093 | 1.423358 | H | -2.991202 | 2.804408 | 2.424405 |
| C | 2.308869 | -2.600003 | -0.241092 | H | -3.185761 | 1.065333 | 2.718761 |
| O | 1.956337 | -1.047226 | 1.557252 | H | 2.114303 | -2.79012 | -1.307578 |
| O | 1.587637 | -3.516822 | 0.58732 | H | 3.383371 | -2.672505 | -0.054592 |
| Br | 4.596668 | -0.342294 | -0.115053 | H | 1.688291 | -1.905156 | 1.93437 |
| H | 1.965936 | 1.388837 | 0.896017 | H | 2.049156 | -4.36748 | 0.575645 |
| H | 3.200827 | 1.972673 | -0.187344 | | | | |
| H | 0.431194 | 1.351638 | -1.303083 | | | | |
| H | 1.747052 | 2.234784 | -2.053976 | | | | |
| H | -0.525285 | 4.144748 | 1.03696 | | | | |
| H | -0.02237 | 2.501078 | 1.317831 | | | | |
| H | -1.584274 | 2.368463 | -1.083471 | | | | |

**Table S10** Energy analyses of 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (eight conformers)

| NO. | 3D conformers B3LYP/6-31G(d,p) | E (Hartree) | ΔE (KJ/mol) | Boltzmann distribution |
|---|---|---|---|---|
| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 1) |  | -3654.064038 | 0.270426381 | 45.59% |
| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 2) |  | -3654.059541 | 12.07729469 | 0.39% |
| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 3) |  | -3654.059542 | 12.07466919 | 0.39% |
| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 4) |  | -3654.061290 | 7.485297206 | 2.48% |

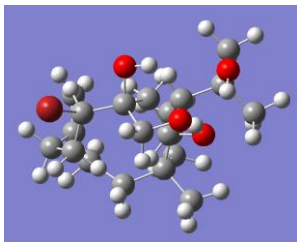
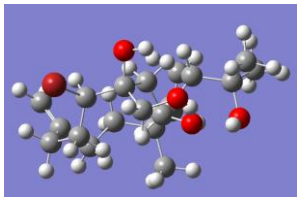
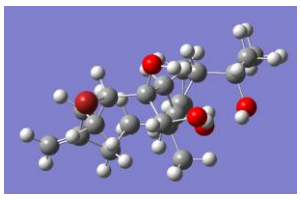
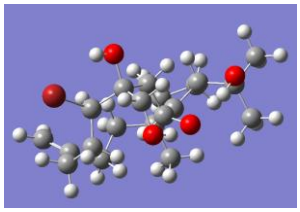
| | | | | |
|---|---|---|---|---|
| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 5) |  | -3654.059215 | 12.93320731 | 0.28% |
| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 6) |  | -3654.053768 | 27.23429952 | 0.00% |
| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 7) |  | -3654.056647 | 19.67548834 | 0.02% |
| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 8) |  | -3654.064141 | 0 | 50.85% |

**Table S11** Cartesian coordinates of the low-energy re-optimized conformers of 1*R*,7*R*,8*S*,10*S*,12*R*-**6** calculated at B3LYP/6-31G(d,p) level of theory.

| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 1) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.076147 | 0.801367 | 1.119422 | H | -1.993835 | 3.915337 | -0.421708 |
| C | 2.212506 | 2.338556 | 0.952384 | H | 2.403813 | 0.618035 | -1.038916 |
| C | 1.16328 | 3.019355 | 0.081804 | H | 0.10288 | 1.130389 | -0.446006 |
| C | -0.259492 | 3.114993 | 0.64822 | H | -0.375715 | -1.810226 | -1.143132 |
| C | -1.439728 | 2.969683 | -0.372164 | H | 0.463183 | -0.589661 | -2.099991 |
| C | 2.443417 | -0.011749 | -0.147433 | H | -4.306977 | 2.558944 | -1.119427 |
| C | -2.482542 | 1.851121 | -0.085736 | H | -3.069607 | 1.883487 | -2.183679 |
| C | -1.91044 | 0.414872 | -0.160537 | H | -4.647908 | 0.035025 | -2.012706 |
| C | -0.471737 | 0.217942 | -0.393236 | H | -4.929425 | 0.341829 | -0.306425 |
| C | 0.24147 | -0.911517 | -1.075162 | H | -2.55734 | -0.985701 | -1.636462 |
| C | 1.61663 | -1.298134 | -0.439171 | H | 0.787003 | 4.07047 | -1.732936 |
| C | -3.553741 | 1.767634 | -1.204364 | H | 2.525277 | 3.512761 | -1.465755 |
| C | -4.160948 | 0.352544 | -1.085583 | H | -4.249652 | -3.744995 | -0.023766 |
| C | -2.970295 | -0.570907 | -0.70823 | H | -3.51998 | -3.142523 | -1.522884 |
| C | 1.50338 | 3.555508 | -1.097543 | H | -5.048739 | -2.44758 | -0.937396 |
| C | -3.288438 | -1.818427 | 0.182658 | H | -4.140471 | -2.408221 | 2.0706 |
| C | -4.077684 | -2.848132 | -0.62748 | H | -3.455344 | -0.776709 | 2.09875 |
| C | -4.024658 | -1.487288 | 1.490719 | H | -5.022111 | -1.070377 | 1.316949 |
| O | -2.044388 | -2.466808 | 0.536665 | H | -1.547968 | -1.775003 | 1.018702 |
| C | -3.158059 | 2.104522 | 1.278337 | H | -2.448321 | 1.997345 | 2.103625 |
| O | -1.042159 | 0.006422 | 0.935347 | H | -3.564612 | 3.122514 | 1.307605 |
| C | 1.441149 | -2.197866 | 0.805678 | H | -3.984326 | 1.413736 | 1.467453 |
| O | 0.87575 | -3.452473 | 0.427783 | H | 0.845959 | -1.708683 | 1.584763 |
| O | 2.29917 | -2.063556 | -1.422093 | H | 2.433789 | -2.416303 | 1.210166 |
| Br | 4.396272 | -0.440501 | -0.030921 | H | -0.092483 | -3.355416 | 0.360765 |
| H | 1.0656 | 0.561442 | 1.45587 | H | 1.973267 | -2.974373 | -1.290289 |
| H | 2.738372 | 0.490171 | 1.932078 | | | | |
| H | 3.212281 | 2.555266 | 0.558324 | | | | |
| H | 2.17046 | 2.777852 | 1.959566 | | | | |
| H | -0.344312 | 4.084146 | 1.158559 | | | | |
| H | -0.365704 | 2.369101 | 1.441129 | | | | |
| H | -1.034842 | 2.812299 | -1.378299 | | | | |

| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 2) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.50924 | 1.511507 | 0.346047 | H | -2.505186 | 3.654086 | 0.607604 |
| C | 1.951762 | 2.665814 | -0.531629 | H | 2.723666 | 0.309601 | -1.471866 |
| C | 0.471306 | 2.657347 | -0.874842 | H | 0.037213 | 0.753108 | 1.018673 |
| C | -0.455874 | 3.144326 | 0.234768 | H | -0.09239 | -1.75299 | -0.710627 |
| C | -1.964046 | 2.814236 | 0.153146 | H | 0.399495 | -0.264033 | -1.477616 |
| C | 2.7505 | 0.167133 | -0.390291 | H | -4.571067 | 0.804067 | 1.143132 |
| C | -2.542183 | 1.538863 | 0.858164 | H | -4.523879 | 2.38201 | 0.356234 |
| C | -1.928383 | 0.216116 | 0.319133 | H | -3.731745 | 1.396892 | -1.742549 |
| C | -0.482984 | -0.008222 | 0.450207 | H | -4.922166 | 0.230968 | -1.2062 |
| C | 0.377392 | -0.786 | -0.515611 | H | -2.232726 | -0.395585 | -1.73403 |
| C | 1.848452 | -1.050855 | -0.071529 | H | -0.97898 | 2.373544 | -2.416012 |
| C | -4.020335 | 1.410109 | 0.414247 | H | 0.777979 | 2.106912 | -2.89413 |
| C | -3.964117 | 0.686367 | -0.941302 | H | -4.289129 | -3.380374 | -1.764397 |
| C | -2.822112 | -0.361633 | -0.810522 | H | -3.251724 | -2.306479 | -2.716132 |
| C | 0.064232 | 2.363462 | -2.115101 | H | -4.858314 | -1.753646 | -2.18883 |
| C | -3.344166 | -1.827585 | -0.601393 | H | -4.604652 | -3.01958 | 0.679285 |
| C | -3.980256 | -2.338972 | -1.89923 | H | -3.879573 | -1.636164 | 1.512383 |
| C | -4.332521 | -1.964825 | 0.570696 | H | -5.252761 | -1.39245 | 0.413028 |
| O | -2.238637 | -2.710232 | -0.372056 | H | -1.832693 | -2.385064 | 0.451456 |
| C | -2.410794 | 1.669107 | 2.381997 | H | -2.860915 | 0.812261 | 2.890712 |
| O | -1.400856 | -0.727583 | 1.321696 | H | -1.367334 | 1.728153 | 2.710625 |
| C | 1.931737 | -1.506337 | 1.399967 | H | -2.918725 | 2.578525 | 2.724322 |
| O | 1.17941 | -2.703988 | 1.58849 | H | 1.603601 | -0.72208 | 2.094291 |
| O | 2.328725 | -2.110603 | -0.89381 | H | 2.97089 | -1.751013 | 1.62754 |
| Br | 4.676319 | -0.354358 | -0.102752 | H | 0.249735 | -2.450115 | 1.706901 |
| H | 1.889456 | 1.364418 | 1.236044 | H | 1.958458 | -2.922402 | -0.501656 |
| H | 3.473001 | 1.853367 | 0.727953 | | | | |
| H | 2.541449 | 2.703884 | -1.455432 | | | | |
| H | 2.168904 | 3.599697 | 0.006988 | | | | |
| H | -0.358963 | 4.241297 | 0.240407 | | | | |
| H | -0.051936 | 2.842539 | 1.209824 | | | | |
| H | -2.27039 | 2.818683 | -0.897705 | | | | |

| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 3) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.509272 | 1.511517 | 0.34596 | H | -2.505227 | 3.654088 | 0.607421 |
| C | 1.951777 | 2.665854 | -0.531684 | H | 2.723873 | 0.309612 | -1.471914 |
| C | 0.471328 | 2.657489 | -0.874907 | H | 0.03721 | 0.753284 | 1.018332 |
| C | -0.455873 | 3.144344 | 0.234748 | H | -0.092349 | -1.752875 | -0.710963 |
| C | -1.964038 | 2.814202 | 0.153088 | H | 0.399523 | -0.263814 | -1.477798 |
| C | 2.75055 | 0.167143 | -0.390336 | H | -4.571016 | 0.804175 | 1.143476 |
| C | -2.542125 | 1.538889 | 0.858234 | H | -4.523872 | 2.38206 | 0.356474 |
| C | -1.928409 | 0.216119 | 0.319136 | H | -3.732181 | 1.396814 | -1.742367 |
| C | -0.482987 | -0.008157 | 0.450009 | H | -4.922402 | 0.23084 | -1.205706 |
| C | 0.377375 | -0.785885 | -0.515851 | H | -2.232944 | -0.395482 | -1.733986 |
| C | 1.848423 | -1.050816 | -0.071677 | H | -0.978945 | 2.374021 | -2.416147 |
| C | -4.02035 | 1.410147 | 0.414486 | H | 0.778008 | 2.107362 | -2.894276 |
| C | -3.964331 | 0.68632 | -0.941031 | H | -4.288958 | -3.38047 | -1.764432 |
| C | -2.822237 | -0.361608 | -0.810416 | H | -3.251868 | -2.306274 | -2.716162 |
| C | 0.064261 | 2.363826 | -2.115221 | H | -4.8585 | -1.753807 | -2.188585 |
| C | -3.344167 | -1.827652 | -0.601337 | H | -4.604497 | -3.019825 | 0.679345 |
| C | -3.98029 | -2.338991 | -1.899168 | H | -3.879467 | -1.636419 | 1.512489 |
| C | -4.332444 | -1.965044 | 0.570803 | H | -5.252739 | -1.392732 | 0.41323 |
| O | -2.238571 | -2.710213 | -0.372166 | H | -1.832538 | -2.385034 | 0.451303 |
| C | -2.410552 | 1.669153 | 2.382029 | H | -2.86078 | 0.812401 | 2.890814 |
| O | -1.400707 | -0.727595 | 1.32163 | H | -1.367054 | 1.728012 | 2.710572 |
| C | 1.931568 | -1.506301 | 1.399828 | H | -2.91829 | 2.578661 | 2.724404 |
| O | 1.179342 | -2.704054 | 1.588136 | H | 1.60318 | -0.722099 | 2.094077 |
| O | 2.328723 | -2.110566 | -0.893902 | H | 2.970728 | -1.750797 | 1.627585 |
| Br | 4.676296 | -0.354477 | -0.102566 | H | 0.24967 | -2.450302 | 1.706821 |
| H | 1.889523 | 1.364447 | 1.235986 | H | 1.958479 | -2.922361 | -0.501712 |
| H | 3.473042 | 1.853403 | 0.727827 | | | | |
| H | 2.541465 | 2.70395 | -1.455488 | | | | |
| H | 2.168981 | 3.599699 | 0.006977 | | | | |
| H | -0.35898 | 4.241314 | 0.240484 | | | | |
| H | -0.051924 | 2.84247 | 1.20977 | | | | |
| H | -2.27034 | 2.818496 | -0.897773 | | | | |

| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 4) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.380173 | 1.296101 | -0.125001 | H | -2.269689 | 3.586901 | -0.080662 |
| C | 1.400913 | 2.068097 | -1.051601 | H | 2.71992 | -0.189747 | -1.682571 |
| C | 0.844099 | 3.330797 | -0.418464 | H | 0.093049 | 0.57701 | 0.938905 |
| C | -0.267853 | 3.161944 | 0.602192 | H | -0.203235 | -2.039316 | -0.559001 |
| C | -1.625398 | 2.70181 | -0.019316 | H | 0.265713 | -0.687301 | -1.541953 |
| C | 2.68906 | -0.141346 | -0.591923 | H | -4.564825 | 1.090127 | 0.813786 |
| C | -2.448554 | 1.576244 | 0.696525 | H | -4.264171 | 2.592891 | -0.05533 |
| C | -1.924631 | 0.171615 | 0.260967 | H | -3.398694 | 1.377964 | -2.000655 |
| C | -0.498183 | -0.159459 | 0.409853 | H | -4.773765 | 0.401987 | -1.520078 |
| C | 0.291785 | -1.065954 | -0.513167 | H | -2.176008 | -0.597636 | -1.7492 |
| C | 1.781636 | -1.304154 | -0.115383 | H | 0.930826 | 5.446879 | -0.289015 |
| C | -3.883115 | 1.578875 | 0.10824 | H | 2.100125 | 4.665097 | -1.488559 |
| C | -3.795004 | 0.758969 | -1.187492 | H | -4.566408 | -3.315309 | -1.655767 |
| C | -2.811199 | -0.402155 | -0.877552 | H | -3.393691 | -2.430852 | -2.644037 |
| C | 1.313651 | 4.538478 | -0.74814 | H | -4.952621 | -1.680711 | -2.228809 |
| C | -3.509261 | -1.775376 | -0.577494 | H | -4.946011 | -2.706316 | 0.734003 |
| C | -4.148832 | -2.323992 | -1.858202 | H | -4.10287 | -1.343113 | 1.484942 |
| C | -4.551469 | -1.70159 | 0.551775 | H | -5.393169 | -1.04723 | 0.300631 |
| O | -2.517146 | -2.749557 | -0.227601 | H | -2.098747 | -2.401702 | 0.580479 |
| C | -2.471265 | 1.764412 | 2.218505 | H | -1.480596 | 1.666353 | 2.672345 |
| O | -1.475339 | -0.748743 | 1.312185 | H | -2.859236 | 2.75909 | 2.469379 |
| C | 1.903592 | -1.621262 | 1.391794 | H | -3.116769 | 1.018924 | 2.692962 |
| O | 1.124242 | -2.772256 | 1.714515 | H | 1.627001 | -0.764706 | 2.019904 |
| O | 2.224165 | -2.444613 | -0.84534 | H | 2.940337 | -1.880173 | 1.608808 |
| Br | 4.597503 | -0.550184 | -0.107713 | H | 0.202525 | -2.487923 | 1.825375 |
| H | 2.027779 | 1.287198 | 0.912063 | H | 1.866139 | -3.212061 | -0.363116 |
| H | 3.316409 | 1.858243 | -0.104422 | | | | |
| H | 0.569742 | 1.424025 | -1.355622 | | | | |
| H | 1.937038 | 2.321827 | -1.973593 | | | | |
| H | -0.418206 | 4.113469 | 1.123018 | | | | |
| H | 0.060622 | 2.463369 | 1.379079 | | | | |
| H | -1.459367 | 2.398195 | -1.060093 | | | | |

| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 5) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 1.898832 | 1.250355 | 0.845136 | H | -0.611983 | 2.050086 | 2.060167 |
| C | 1.632729 | 2.625016 | 0.198208 | H | 1.446372 | 0.237511 | -1.030529 |
| C | 0.316029 | 2.73604 | -0.55121 | H | -0.248315 | -0.318295 | 2.147126 |
| C | -0.9036 | 3.201721 | 0.227234 | H | 0.323434 | -2.64992 | 0.985533 |
| C | -1.445588 | 2.370632 | 1.424453 | H | 0.029881 | -1.849469 | -0.52604 |
| C | 2.09266 | 0.112799 | -0.161143 | H | -4.471512 | 0.986568 | 0.50609 |
| C | -2.43456 | 1.171411 | 1.233581 | H | -3.801485 | 2.589416 | 0.230376 |
| C | -1.808142 | -0.118428 | 0.613165 | H | -2.44434 | 1.785458 | -1.62706 |
| C | -0.615249 | -0.767519 | 1.221749 | H | -3.902145 | 0.840782 | -1.828612 |
| C | 0.373112 | -1.66634 | 0.493699 | H | -1.323348 | -0.230702 | -1.498235 |
| C | 1.892316 | -1.311749 | 0.401368 | H | -0.635239 | 2.667967 | -2.454522 |
| C | -3.556288 | 1.520825 | 0.225031 | H | 1.178173 | 2.319709 | -2.444511 |
| C | -3.068348 | 1.029044 | -1.14685 | H | -3.573817 | -2.609248 | -3.06651 |
| C | -2.226685 | -0.248541 | -0.878297 | H | -2.112011 | -1.629308 | -3.25968 |
| C | 0.280209 | 2.557829 | -1.878954 | H | -3.708257 | -0.845528 | -3.212986 |
| C | -2.980141 | -1.571259 | -1.27083 | H | -4.804627 | -2.661183 | -0.90242 |
| C | -3.104315 | -1.657758 | -2.797345 | H | -4.291203 | -1.680619 | 0.478951 |
| C | -4.366756 | -1.700267 | -0.613334 | H | -5.055444 | -0.90787 | -0.925334 |
| O | -2.193386 | -2.712746 | -0.915852 | H | -2.115351 | -2.673544 | 0.05503 |
| C | -3.025589 | 0.873099 | 2.62585 | H | -2.246428 | 0.6368 | 3.360117 |
| O | -1.926617 | -1.330399 | 1.424531 | H | -3.574367 | 1.748373 | 2.992464 |
| C | 2.641256 | -1.506329 | 1.740485 | H | -3.713892 | 0.025117 | 2.592992 |
| O | 2.763219 | -2.895864 | 2.053615 | H | 2.166357 | -0.958046 | 2.564246 |
| O | 2.433969 | -2.238099 | -0.528777 | H | 3.664539 | -1.141134 | 1.621143 |
| Br | 3.925825 | 0.321554 | -0.941473 | H | 1.921023 | -3.202282 | 2.424005 |
| H | 1.068049 | 1.005318 | 1.508461 | H | 2.69747 | -3.011267 | 0.00462 |
| H | 2.789242 | 1.324826 | 1.478527 | | | | |
| H | 2.463383 | 2.843143 | -0.481299 | | | | |
| H | 1.664611 | 3.383054 | 0.99217 | | | | |
| H | -1.719703 | 3.417509 | -0.469426 | | | | |
| H | -0.627864 | 4.17689 | 0.657553 | | | | |
| H | -2.00386 | 3.088865 | 2.039042 | | | | |

| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 6) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.56698 | 1.460846 | 0.42954 | H | -2.448596 | 3.63884 | 0.714879 |
| C | 2.036594 | 2.682825 | -0.373956 | H | 2.877127 | 0.383412 | -1.45169 |
| C | 0.565575 | 2.740111 | -0.755544 | H | 0.080477 | 0.802713 | 0.826778 |
| C | -0.392542 | 3.151733 | 0.360724 | H | -0.047599 | -1.643181 | -0.999929 |
| C | -1.899857 | 2.833339 | 0.210416 | H | 0.507907 | -0.107973 | -1.6357 |
| C | 2.817121 | 0.162466 | -0.384474 | H | -4.575314 | 0.801053 | 0.920673 |
| C | -2.519695 | 1.512537 | 0.789246 | H | -4.451127 | 2.420054 | 0.204919 |
| C | -1.891685 | 0.208904 | 0.202641 | H | -3.412032 | 1.455839 | -1.838713 |
| C | -0.435899 | 0.031705 | 0.272376 | H | -4.790151 | 0.42422 | -1.520976 |
| C | 0.427505 | -0.701105 | -0.719311 | H | -2.271685 | -0.605736 | -1.793792 |
| C | 1.862895 | -1.04686 | -0.220536 | H | -0.838328 | 2.640437 | -2.361202 |
| C | -3.974903 | 1.434275 | 0.259628 | H | 0.926695 | 2.36908 | -2.806713 |
| C | -3.836008 | 0.754728 | -1.10878 | H | -3.031568 | -3.875971 | -0.326469 |
| C | -2.830944 | -0.401576 | -0.872672 | H | -1.61147 | -2.848537 | -0.098148 |
| C | 0.193415 | 2.572479 | -2.02998 | H | -2.291443 | -3.064516 | -1.719585 |
| C | -3.496455 | -1.765179 | -0.429772 | H | -5.126276 | -3.068045 | -0.984289 |
| C | -2.542387 | -2.954069 | -0.657725 | H | -5.592785 | -1.37056 | -0.895006 |
| C | -4.792469 | -2.048651 | -1.201358 | H | -4.644136 | -1.956834 | -2.28303 |
| O | -3.895014 | -1.719134 | 0.947781 | H | -3.07606 | -1.68625 | 1.469383 |
| C | -2.467025 | 1.531803 | 2.323401 | H | -2.959934 | 0.649578 | 2.741096 |
| O | -1.291017 | -0.72449 | 1.165802 | H | -1.441453 | 1.547373 | 2.708757 |
| C | 1.832062 | -1.618378 | 1.212715 | H | -2.982012 | 2.422026 | 2.703519 |
| O | 0.971821 | -2.754797 | 1.271103 | H | 1.532586 | -0.861426 | 1.948516 |
| O | 2.359734 | -2.055478 | -1.097567 | H | 2.834959 | -1.964981 | 1.468905 |
| Br | 4.697927 | -0.450034 | 0.007173 | H | 0.064016 | -2.420978 | 1.375743 |
| H | 1.939306 | 1.259832 | 1.30337 | H | 1.956066 | -2.884747 | -0.783574 |
| H | 3.529238 | 1.77078 | 0.841324 | | | | |
| H | 2.648759 | 2.780336 | -1.278721 | | | | |
| H | 2.258057 | 3.569144 | 0.238429 | | | | |
| H | -0.296179 | 4.245594 | 0.443716 | | | | |
| H | -0.018455 | 2.783497 | 1.325153 | | | | |
| H | -2.1739 | 2.926718 | -0.845084 | | | | |

| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 7) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.475368 | 1.265338 | -0.046793 | H | -2.149141 | 3.606357 | -0.11043 |
| C | 1.562121 | 2.136691 | -0.955826 | H | 2.875103 | -0.121037 | -1.683017 |
| C | 0.969068 | 3.340639 | -0.24078 | H | 0.140278 | 0.650469 | 0.654407 |
| C | -0.211905 | 3.107171 | 0.689374 | H | -0.154853 | -1.976814 | -0.848815 |
| C | -1.528216 | 2.704767 | -0.05248 | H | 0.394143 | -0.586009 | -1.752442 |
| C | 2.769536 | -0.147386 | -0.596149 | H | -4.568026 | 1.164089 | 0.450504 |
| C | -2.428314 | 1.562689 | 0.533197 | H | -4.114524 | 2.637333 | -0.421724 |
| C | -1.888542 | 0.15246 | 0.107057 | H | -3.009498 | 1.277737 | -2.184525 |
| C | -0.445695 | -0.121494 | 0.17993 | H | -4.557631 | 0.491874 | -1.935585 |
| C | 0.349918 | -1.013484 | -0.74348 | H | -2.254348 | -0.923656 | -1.761471 |
| C | 1.802592 | -1.312341 | -0.259797 | H | 1.066469 | 5.435549 | 0.083409 |
| C | -3.80302 | 1.612739 | -0.191287 | H | 2.305226 | 4.74655 | -1.102899 |
| C | -3.6177 | 0.745139 | -1.441749 | H | -3.552666 | -3.774011 | 0.081808 |
| C | -2.833506 | -0.489148 | -0.937992 | H | -1.999402 | -2.927199 | 0.169607 |
| C | 1.470555 | 4.565955 | -0.429419 | H | -2.721348 | -3.287339 | -1.408948 |
| C | -3.712847 | -1.654325 | -0.334908 | H | -5.542598 | -2.731451 | -0.716354 |
| C | -2.943292 | -2.988667 | -0.377483 | H | -5.705829 | -0.986203 | -0.918934 |
| C | -5.036627 | -1.834278 | -1.086359 | H | -4.873419 | -1.948723 | -2.163628 |
| O | -4.097726 | -1.364488 | 1.018323 | H | -3.287848 | -1.407081 | 1.553045 |
| C | -2.596775 | 1.693698 | 2.052412 | H | -1.65394 | 1.566289 | 2.592916 |
| O | -1.34473 | -0.723397 | 1.145129 | H | -3.000833 | 2.682049 | 2.303148 |
| C | 1.79486 | -1.71179 | 1.233346 | H | -3.295722 | 0.938846 | 2.424422 |
| O | 0.909819 | -2.810766 | 1.442319 | H | 1.536103 | -0.865978 | 1.882638 |
| O | 2.268384 | -2.423601 | -1.021143 | H | 2.793746 | -2.055347 | 1.505281 |
| Br | 4.625359 | -0.654284 | -0.009843 | H | 0.011173 | -2.448649 | 1.527793 |
| H | 2.078005 | 1.195156 | 0.971482 | H | 1.869317 | -3.207039 | -0.601645 |
| H | 3.425588 | 1.794175 | 0.054765 | | | | |
| H | 0.75248 | 1.536883 | -1.383549 | | | | |
| H | 2.161524 | 2.476722 | -1.808248 | | | | |
| H | -0.392115 | 4.024305 | 1.260032 | | | | |
| H | 0.05807 | 2.359219 | 1.443673 | | | | |
| H | -1.292504 | 2.454647 | -1.094143 | | | | |

| 1*R*,7*R*,8*S*,10*S*,12*R*-**6** (conformer 8) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.166223 | 0.653562 | 1.118642 | H | -1.736007 | 3.854785 | -0.425067 |
| C | 2.378326 | 2.180235 | 0.974883 | H | 2.319392 | 0.507921 | -1.062077 |
| C | 1.335693 | 2.895588 | 0.129818 | H | 0.139239 | 0.921099 | -0.338989 |
| C | -0.0838 | 2.970115 | 0.699297 | H | -0.43272 | -2.025576 | -0.957504 |
| C | -1.245007 | 2.877007 | -0.340801 | H | 0.32164 | -0.866962 | -2.054301 |
| C | 2.417435 | -0.134295 | -0.184037 | H | -4.097244 | 2.741594 | -1.105592 |
| C | -2.367733 | 1.837436 | -0.070666 | H | -2.905052 | 1.996132 | -2.173546 |
| C | -1.923424 | 0.348392 | -0.165654 | H | -4.633537 | 0.290284 | -2.107676 |
| C | -0.491115 | 0.04397 | -0.331495 | H | -4.938667 | 0.563306 | -0.399916 |
| C | 0.182737 | -1.121724 | -0.996074 | H | -2.663029 | -0.941302 | -1.704963 |
| C | 1.616091 | -1.450076 | -0.459385 | H | 0.957758 | 3.990007 | -1.659248 |
| C | -3.418856 | 1.887108 | -1.2086 | H | 2.695046 | 3.422213 | -1.40817 |
| C | -4.148778 | 0.534189 | -1.157589 | H | -4.853551 | -3.439624 | -0.236837 |
| C | -3.061508 | -0.506926 | -0.779386 | H | -4.108495 | -2.849267 | -1.731639 |
| C | 1.673493 | 3.457557 | -1.038029 | H | -5.465511 | -1.957859 | -1.003102 |
| C | -3.563373 | -1.730712 | 0.048988 | H | -4.449559 | -2.287312 | 1.931917 |
| C | -4.563055 | -2.537934 | -0.785097 | H | -3.463028 | -0.820187 | 2.036204 |
| C | -4.17783 | -1.364087 | 1.410263 | H | -5.082642 | -0.754789 | 1.313479 |
| O | -2.461346 | -2.624725 | 0.274321 | H | -1.853904 | -2.139591 | 0.857483 |
| C | -3.035008 | 2.120701 | 1.290515 | H | -2.34428 | 1.941262 | 2.11936 |
| O | -1.135912 | -0.163426 | 0.95865 | H | -3.3586 | 3.167534 | 1.334757 |
| C | 1.589143 | -2.425309 | 0.74152 | H | -3.915423 | 1.494466 | 1.458983 |
| O | 1.005349 | -1.939968 | 1.939417 | H | 2.622056 | -2.681715 | 1.000522 |
| O | 2.183915 | -2.158322 | -1.559312 | H | 1.095639 | -3.343005 | 0.38819 |
| Br | 4.398434 | -0.557089 | -0.230203 | H | 0.118231 | -1.594433 | 1.74576 |
| H | 1.16248 | 0.453467 | 1.492101 | H | 3.132415 | -2.277918 | -1.371334 |
| H | 2.827531 | 0.268831 | 1.898211 | | | | |
| H | 3.377575 | 2.366745 | 0.563836 | | | | |
| H | 2.369861 | 2.606 | 1.988664 | | | | |
| H | -0.170517 | 3.913034 | 1.256774 | | | | |
| H | -0.19955 | 2.188515 | 1.45638 | | | | |
| H | -0.826715 | 2.673217 | -1.332851 | | | | |

**Table S12** Experimental and calculated $^{1}$H NMR data for compound **6**

| No. | **6**, exptl. $\delta_H$ [a] | 1*R*,7*R*,8*S*,10*R*,12*R*-**6**, calcd. $\delta_H$ [b] | 1*R*,7*R*,8*S*,10,12*R*-**6**, calcd. $\delta_H$ [b] |
|---|---|---|---|
| 2 | 1.25 | 1.38 | 1.28 |
| | 1.96 | 2.04 | 2.06 |
| 3 | 1.63 | 1.91 | 1.82 |
| | 2.11 | 2.10 | 2.08 |
| 5 | 2.28 | 2.32 | 2.26 |
| | 2.42 | 2.65 | 2.47 |
| 6 | 1.9 | 2.01 | 2.05 |
| | 2.11 | 2.59 | 2.81 |
| 7 | 4.04 | 4.53 | 4.61 |
| 9 | 2.25 | 1.94 | 1.81 |
| | 2.25 | 2.45 | 2.47 |
| 10 | 2.89 | 2.53 | 2.50 |
| 12 | 2.21 | 2.34 | 2.35 |
| 13 | 1.63 | 1.74 | 1.76 |
| | 1.9 | 1.85 | 1.82 |
| 14 | 1.76 | 1.51 | 1.50 |
| | 1.76 | 1.63 | 1.62 |
| 15 | 0.86 | 1.13 | 1.13 |
| 16 | 4.84 | 5.36 | 5.34 |
| | 5.03 | 5.54 | 5.52 |
| 17 | 3.65 | 3.34 | 3.61 |
| | 3.87 | 4.11 | 3.91 |
| 18 | 1.21 | 1.15 | 1.17 |
| 19 | 1.27 | 1.38 | 1.39 |

[a] Recorded in $CDCl_3$ at 600 MHz.

[b] Calculated in $CDCl_3$

**Table S13** Experimental and calculated $^{13}C$ NMR data for compound **6**

| No. | **6**, exptl. $\delta_C$ [a] | 1*R*,7*R*,8*S*,10*R*,12*R*-**6**, calcd. $\delta_H$ [b] | 1*R*,7*R*,8*S*,10,12*R*-**6**, calcd. $\delta_H$ [b] |
|---|---|---|---|
| 1 | 44.6 | 44.50 | 44.03 |
| 2 | 42.4 | 37.97 | 38.00 |
| 3 | 25.1 | 21.86 | 21.45 |
| 4 | 147.4 | 156.41 | 155.29 |
| 5 | 35.4 | 33.49 | 34.34 |
| 6 | 29.7 | 30.38 | 30.53 |
| 7 | 63 | 76.01 | 76.58 |
| 8 | 75 | 77.02 | 72.27 |
| 9 | 33.3 | 33.62 | 33.82 |
| 10 | 54.7 | 59.19 | 58.19 |
| 11 | 76.2 | 77.82 | 80.65 |
| 12 | 50.2 | 46.50 | 45.38 |
| 13 | 27.7 | 23.61 | 23.33 |
| 14 | 38.8 | 35.42 | 34.95 |
| 15 | 24.1 | 14.73 | 14.50 |
| 16 | 113.8 | 114.99 | 113.97 |
| 17 | 67 | 67.08 | 62.42 |
| 18 | 75.4 | 71.35 | 72.18 |
| 19 | 29.6 | 24.40 | 24.15 |
| 20 | 26 | 21.53 | 21.38 |

[a] Recorded in $CDCl_3$ at 600 MHz.

[b] Calculated in $CDCl_3$

**Table S 14** DP4+ analyses of calculated and experimental NMR chemical shifts of **6** (unscaled). Isomer 1: 1*R*,7*R*,8*S*,10*R*,12*R*-**6**; Isomer 2: 1*R*,7*R*,8*S*,10*S*,12*R*-**6**

| Functional | Solvent? | Basis Set | Type of Data |
|---|---|---|---|
| mPW1PW91 | PCM | 6-311G(d,p) | Unscaled Shifts |

| | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 | Isomer 6 |
|---|---|---|---|---|---|---|
| sDP4+ (H data) | 84.50% | 15.50% | - | - | - | - |
| sDP4+ (C data) | 99.99% | 0.01% | - | - | - | - |
| sDP4+ (all data) | 100.00% | 0.00% | - | - | - | - |
| uDP4+ (H data) | 0.80% | 99.20% | - | - | - | - |
| uDP4+ (C data) | 99.95% | 0.05% | - | - | - | - |
| uDP4+ (all data) | 94.52% | 5.48% | - | - | - | - |
| DP4+ (H data) | 4.23% | 95.77% | - | - | - | - |
| DP4+ (C data) | 100.00% | 0.00% | - | - | - | - |
| DP4+ (all data) | 100.00% | 0.00% | - | - | - | - |

| Functional | | Solvent? | Basis Set | | Type of Data | | |
|---|---|---|---|---|---|---|---|
| mPW1PW91 | | PCM | 6-311G(d,p) | | Unscaled Shifts | | |
| | | DP4+ | 100.00% | 0.00% | - | - | - |
| Nuclei | sp2? | Experimental | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 |
| C | | 44.6 | 44.4954 | 44.0338 | | | |
| C | | 42.4 | 37.9731 | 38.0005 | | | |
| C | | 25.1 | 21.8622 | 21.4497 | | | |
| C | x | 147.4 | 156.4149 | 155.2911 | | | |
| C | | 35.4 | 33.4935 | 34.344 | | | |
| C | | 29.7 | 30.3811 | 30.5338 | | | |
| C | | 63 | 76.0138 | 76.5803 | | | |
| C | | 75 | 77.0199 | 72.2694 | | | |
| C | | 33.3 | 33.6197 | 33.8159 | | | |
| C | | 54.7 | 59.1888 | 58.1856 | | | |
| C | | 76.2 | 77.8232 | 80.6474 | | | |
| C | | 50.2 | 46.5004 | 45.3765 | | | |
| C | | 27.7 | 23.614 | 23.3259 | | | |
| C | | 38.8 | 35.418 | 34.9465 | | | |
| C | | 24.1 | 14.7326 | 14.499 | | | |
| C | x | 113.8 | 114.992 | 113.9682 | | | |
| C | | 67 | 67.0767 | 62.417 | | | |
| C | | 75.4 | 71.3471 | 72.1775 | | | |
| C | | 29.6 | 24.3962 | 24.1539 | | | |
| C | | 26 | 21.5274 | 21.3832 | | | |
| H | | 1.25 | 1.3819 | 1.2792 | | | |
| H | | 1.96 | 2.0432 | 2.0601 | | | |
| H | | 1.63 | 1.9091 | 1.8248 | | | |
| H | | 2.11 | 2.1012 | 2.0765 | | | |
| H | | 2.28 | 2.3217 | 2.2561 | | | |
| H | | 2.42 | 2.6501 | 2.4668 | | | |
| H | | 1.9 | 2.0126 | 2.0459 | | | |
| H | | 2.11 | 2.5913 | 2.8141 | | | |
| H | | 4.04 | 4.5341 | 4.6118 | | | |
| H | | 2.25 | 1.9405 | 1.806 | | | |
| H | | 2.25 | 2.4485 | 2.4734 | | | |
| H | | 2.89 | 2.5307 | 2.4959 | | | |
| H | | 2.21 | 2.339 | 2.3474 | | | |
| H | | 1.63 | 1.7374 | 1.7576 | | | |
| H | | 1.9 | 1.847 | 1.8244 | | | |
| H | | 1.76 | 1.5056 | 1.5045 | | | |
| H | | 1.76 | 1.6255 | 1.6152 | | | |
| H | x | 0.86 | 1.13126601 | 1.129 | | | |
| H | x | 4.84 | 5.3612 | 5.3401 | | | |
| H | | 5.03 | 5.5369 | 5.5154 | | | |
| H | | 3.65 | 3.3435 | 3.608 | | | |
| H | | 3.87 | 4.1124 | 3.9077 | | | |
| H | | 1.21 | 1.14853272 | 1.16979934 | | | |
| H | | 1.27 | 1.37696631 | 1.39228302 | | | |

**Table S15** Energy analyses of 1*R*,7*R*,8*S*,10*R*-**8** (four conformers)

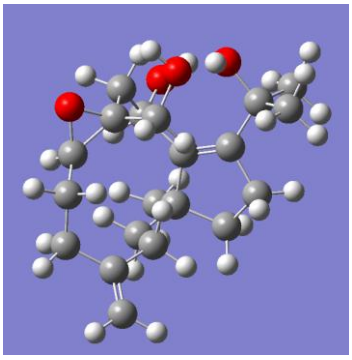
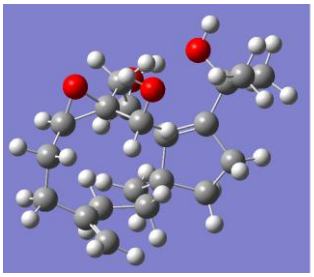
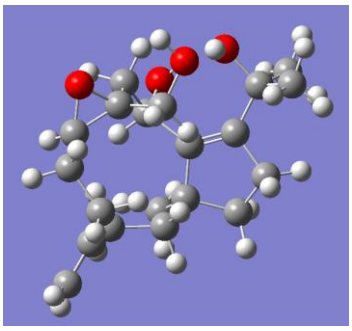
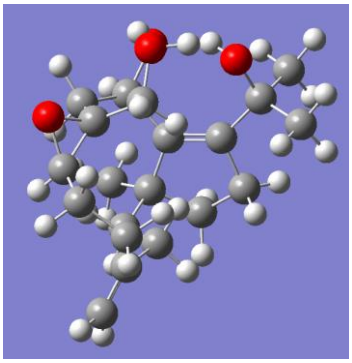
| NO. | 3D conformers B3LYP/6-31G(d,p) | E (Hartree) | ΔE (KJ/mol) | Boltzmann distribution |
|---|---|---|---|---|
| 1*R*,7*R*,8*S*,10*R*-**8** (conformer 1) |  | -1081.750344 | 0 | 96.27% |
| 1*R*,7*R*,8*S*,10*R*-**8** (conformer 2) |  | -1081.744634 | 14.9915984 | 0.23% |
| 1*R*,7*R*,8*S*,10*R*-**8** (conformer 3) |  | -1081.747207 | 8.236189876 | 3.47% |
| 1*R*,7*R*,8*S*,10*R*-**8** (conformer 4) |  | -1081.742677 | 20.12969964 | 0.03% |

**Table S16** Cartesian coordinates of the low-energy re-optimized conformers of 1*R*,7*R*,8*S*,10*R*-**8** calculated at B3LYP/6-31G(d,p) level of theory

| 1*R*,7*R*,8*S*,10*R*-**8** (conformer 1) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 3.450372 | 1.381008 | -0.146959 | H | 2.41802 | 1.379802 | 1.780163 |
| C | 4.023386 | -0.047126 | 0.045493 | H | -0.197979 | -0.088978 | 2.501219 |
| C | 3.411057 | -1.134861 | -0.818721 | H | 0.148255 | 2.145641 | 2.356366 |
| C | 1.917152 | -1.377861 | -0.742748 | H | -1.069566 | 2.408882 | 1.139014 |
| C | 1.415684 | -1.825124 | 0.642038 | H | -1.385868 | -3.682879 | 0.179699 |
| C | 2.267729 | 1.710303 | 0.746881 | H | 0.037481 | -3.528028 | -0.835285 |
| C | -0.118617 | -2.019818 | 0.790801 | H | -1.034455 | -1.824807 | -2.170189 |
| C | -0.939176 | -0.716773 | 0.627676 | H | -2.501536 | -2.538503 | -1.529623 |
| C | -0.840922 | 0.341665 | 1.729196 | H | 3.772089 | -2.649374 | -2.260955 |
| C | -0.2424 | 1.750671 | 1.412955 | H | 5.255515 | -1.693983 | -1.712143 |
| C | 0.851472 | 1.925197 | 0.368385 | H | -3.868365 | 1.013036 | -2.557632 |
| C | -0.726226 | -2.952437 | -0.301825 | H | -2.108994 | 0.859258 | -2.702856 |
| C | -1.562002 | -2.055717 | -1.232669 | H | -3.140289 | -0.572091 | -2.885868 |
| C | -1.783765 | -0.78494 | -0.42435 | H | -5.09906 | 0.140626 | -0.571087 |
| C | 4.183295 | -1.859631 | -1.636486 | H | -4.21668 | -0.614777 | 0.778649 |
| C | -2.944705 | 0.131501 | -0.813456 | H | -4.418159 | -1.492361 | -0.752043 |
| C | -3.015087 | 0.364584 | -2.334183 | H | -2.216243 | 1.966656 | -0.595436 |
| C | -4.254395 | -0.505214 | -0.309248 | H | 0.127704 | -2.098458 | 2.99171 |
| O | -2.894049 | 1.409534 | -0.157421 | H | -1.436218 | -2.689032 | 2.410288 |
| C | -0.365601 | -2.649773 | 2.183555 | H | 0.028491 | -3.67355 | 2.201921 |
| O | -2.092076 | 0.539672 | 2.3863 | H | -2.64995 | 0.973656 | 1.709195 |
| C | 0.414156 | 1.945005 | -1.086372 | H | 1.256472 | 2.215457 | -1.731432 |
| O | 1.73997 | 3.041777 | 0.671356 | H | 0.029369 | 0.972972 | -1.394495 |
| O | -0.674374 | 2.85399 | -1.301758 | H | -0.394531 | 3.729229 | -0.985322 |
| H | 3.222742 | 1.562004 | -1.202239 | | | | |
| H | 4.234179 | 2.101334 | 0.122575 | | | | |
| H | 5.098403 | -0.016409 | -0.161254 | | | | |
| H | 3.933288 | -0.316583 | 1.108766 | | | | |
| H | 1.649578 | -2.131826 | -1.491485 | | | | |
| H | 1.389135 | -0.463317 | -1.030186 | | | | |
| H | 1.743928 | -1.104307 | 1.402886 | | | | |
| H | 1.909019 | -2.773037 | 0.899495 | | | | |

| 1*R*,7*R*,8*S*,10*R*-**8** (conformer 2) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -3.88103 | -1.092555 | 0.07022 | H | -2.676699 | -1.256856 | 1.897441 |
| C | -4.253906 | 0.409359 | 0.13219 | H | -0.252134 | 0.381767 | 2.096014 |
| C | -3.261834 | 1.32315 | -0.564345 | H | -0.348656 | -2.029765 | 2.167433 |
| C | -2.055537 | 1.714282 | 0.26816 | H | 0.739214 | -2.18553 | 0.791631 |
| C | -0.805442 | 2.172428 | -0.498844 | H | 2.364937 | 3.303546 | 0.07083 |
| C | -2.627287 | -1.487134 | 0.827521 | H | 1.243391 | 3.554338 | -1.269316 |
| C | 0.540941 | 2.139684 | 0.289475 | H | 1.883271 | 1.414959 | -2.268639 |
| C | 1.111982 | 0.704165 | 0.492858 | H | 3.399349 | 1.875064 | -1.514072 |
| C | 0.544994 | -0.183896 | 1.608154 | H | -2.759563 | 2.370012 | -2.347521 |
| C | -0.053152 | -1.567357 | 1.219263 | H | -4.360047 | 1.451734 | -2.370532 |
| C | -1.255953 | -1.64392 | 0.284804 | H | 3.725931 | -2.229472 | -1.856977 |
| C | 1.644097 | 2.799111 | -0.584212 | H | 1.974781 | -1.918465 | -1.811126 |
| C | 2.351381 | 1.643977 | -1.298923 | H | 3.07634 | -0.780651 | -2.629907 |
| C | 2.16094 | 0.478961 | -0.333797 | H | 5.275899 | -1.038784 | -0.264558 |
| C | -3.465752 | 1.735371 | -1.820195 | H | 4.716029 | 0.39572 | 0.621277 |
| C | 3.143325 | -0.681284 | -0.443878 | H | 4.909996 | 0.443586 | -1.146984 |
| C | 2.960373 | -1.446077 | -1.768022 | H | 3.501829 | -2.354337 | 0.53221 |
| C | 4.596851 | -0.177419 | -0.303526 | H | -0.375485 | 2.513713 | 2.271791 |
| O | 2.912205 | -1.593244 | 0.652375 | H | 1.350997 | 2.864125 | 2.181331 |
| C | 0.411186 | 2.906832 | 1.62087 | H | 0.176473 | 3.961076 | 1.423721 |
| O | 1.501092 | -0.373273 | 2.652298 | H | 2.237764 | -0.856622 | 2.232785 |
| C | -0.970892 | -1.544199 | -1.205812 | H | -1.893771 | -1.391648 | -1.777285 |
| O | -2.105688 | -2.799027 | 0.567646 | H | -0.301702 | -0.706558 | -1.410885 |
| O | -0.289177 | -2.713327 | -1.653579 | H | -0.818519 | -3.464567 | -1.335867 |
| H | -3.802737 | -1.406304 | -0.974771 | | | | |
| H | -4.707707 | -1.67205 | 0.504698 | | | | |
| H | -5.244181 | 0.523605 | -0.323328 | | | | |
| H | -4.358713 | 0.709758 | 1.185317 | | | | |
| H | -1.806787 | 0.866643 | 0.908968 | | | | |
| H | -2.370282 | 2.505467 | 0.965568 | | | | |
| H | -0.965042 | 3.202258 | -0.845787 | | | | |
| H | -0.693351 | 1.564335 | -1.405143 | | | | |

| 1*R*,7*R*,8*S*,10*R*-**8** (conformer 3) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -3.490319 | -1.571645 | -0.465854 | H | -2.728224 | -1.312479 | 1.587622 |
| C | -3.468733 | -0.234556 | -1.248775 | H | -0.099996 | 0.577199 | 2.239713 |
| C | -3.583169 | 1.025171 | -0.40957 | H | -0.508253 | -1.654419 | 2.467893 |
| C | -2.360237 | 1.486774 | 0.362563 | H | 0.824732 | -2.15039 | 1.467266 |
| C | -1.201196 | 1.974166 | -0.534891 | H | 1.79261 | 3.569206 | -0.268226 |
| C | -2.435047 | -1.72199 | 0.618482 | H | 0.605183 | 3.501138 | -1.569221 |
| C | 0.185351 | 2.164555 | 0.153865 | H | 1.598506 | 1.450419 | -2.434551 |
| C | 0.951003 | 0.832988 | 0.421008 | H | 3.024805 | 2.151918 | -1.693458 |
| C | 0.615849 | -0.0092 | 1.659805 | H | -4.835304 | 2.609925 | 0.242793 |
| C | -0.005347 | -1.442489 | 1.518642 | H | -5.609575 | 1.401585 | -0.921967 |
| C | -0.974121 | -1.816444 | 0.40367 | H | 4.272604 | -1.526396 | -1.84868 |
| C | 1.144451 | 2.8912 | -0.836221 | H | 2.586656 | -1.304737 | -2.349338 |
| C | 2.009637 | 1.799011 | -1.474858 | H | 3.750082 | 0.022613 | -2.53922 |
| C | 1.980836 | 0.681237 | -0.44369 | H | 5.184927 | -0.41476 | 0.195909 |
| C | -4.730754 | 1.711285 | -0.360729 | H | 4.132665 | 0.595076 | 1.219028 |
| C | 3.121154 | -0.336457 | -0.461296 | H | 4.6826 | 1.198682 | -0.357519 |
| C | 3.448938 | -0.806499 | -1.891921 | H | 2.181674 | -2.038991 | -0.131155 |
| C | 4.36106 | 0.306669 | 0.188845 | H | -0.656922 | 2.601689 | 2.160726 |
| O | 2.84994 | -1.496779 | 0.340742 | H | 1.008572 | 3.138369 | 1.925078 |
| C | 0.039183 | 3.021899 | 1.42876 | H | -0.330901 | 4.021238 | 1.164933 |
| O | 1.743015 | -0.133391 | 2.527645 | H | 2.356418 | -0.72015 | 2.040401 |
| C | -0.403956 | -1.927746 | -0.997699 | H | -1.172902 | -2.266968 | -1.699464 |
| O | -1.772369 | -2.990475 | 0.744406 | H | -0.009379 | -0.969408 | -1.337024 |
| O | 0.71153 | -2.831362 | -1.031764 | H | 0.397474 | -3.683805 | -0.685251 |
| H | -3.376417 | -2.39689 | -1.177536 | | | | |
| H | -4.475659 | -1.695999 | 0.000165 | | | | |
| H | -2.548723 | -0.19805 | -1.846571 | | | | |
| H | -4.296789 | -0.261622 | -1.966406 | | | | |
| H | -2.00395 | 0.675501 | 1.003798 | | | | |
| H | -2.657751 | 2.298349 | 1.035149 | | | | |
| H | -1.504247 | 2.936788 | -0.967993 | | | | |
| H | -1.068947 | 1.293861 | -1.385947 | | | | |

| 1*R*,7*R*,8*S*,10*R*-**8** (conformer 4) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -3.514045 | -1.117597 | -0.901018 | H | -3.039236 | -0.44992 | 1.12501 |
| C | -3.18269 | 0.08072 | -1.831124 | H | 1.034845 | -0.208277 | 2.737555 |
| C | -2.893689 | 1.394776 | -1.119948 | H | -1.214446 | -0.544068 | 2.378215 |
| C | -1.432363 | 1.674506 | -0.780135 | H | -0.467746 | -2.113092 | 2.483692 |
| C | -1.137048 | 1.928 | 0.710837 | H | 1.988424 | 3.31421 | 0.986894 |
| C | -2.716032 | -1.188536 | 0.388563 | H | 0.594453 | 3.770927 | 0.008073 |
| C | 0.363079 | 1.880684 | 1.13677 | H | 1.23404 | 2.190775 | -1.730011 |
| C | 1.082375 | 0.540666 | 0.778802 | H | 2.824422 | 2.527508 | -1.076054 |
| C | 0.85969 | -0.631432 | 1.741365 | H | -3.678572 | 3.204861 | -0.328488 |
| C | -0.56846 | -1.237099 | 1.830744 | H | -4.906767 | 2.063879 | -1.102799 |
| C | -1.335313 | -1.700927 | 0.580804 | H | 3.337171 | -0.824277 | -3.058749 |
| C | 1.196983 | 2.917352 | 0.33944 | H | 1.640908 | -0.354134 | -2.843856 |
| C | 1.834904 | 2.136786 | -0.812151 | H | 2.902595 | 0.892749 | -2.942134 |
| C | 1.895191 | 0.700156 | -0.29663 | H | 5.014962 | -0.487795 | -1.212464 |
| C | -3.8712 | 2.262021 | -0.835278 | H | 4.48259 | 0.01849 | 0.405045 |
| C | 2.871251 | -0.218293 | -1.046144 | H | 4.560423 | 1.203346 | -0.912068 |
| C | 2.671942 | -0.10776 | -2.56698 | H | 2.714342 | -1.672059 | 0.225892 |
| C | 4.32227 | 0.162956 | -0.669055 | H | -0.226851 | 1.580531 | 3.249209 |
| O | 2.71422 | -1.611389 | -0.758239 | H | 1.444306 | 2.139267 | 3.028282 |
| C | 0.421994 | 2.221548 | 2.641307 | H | 0.090302 | 3.255182 | 2.798361 |
| O | 1.812006 | -1.707699 | 1.660246 | H | 1.331801 | -2.45345 | 1.231636 |
| C | -0.565529 | -2.220312 | -0.618843 | H | -1.264527 | -2.73265 | -1.288382 |
| O | -2.491575 | -2.482894 | 0.960763 | H | -0.13229 | -1.367282 | -1.154568 |
| O | 0.479043 | -3.125471 | -0.247157 | H | 1.272005 | -2.824643 | -0.741994 |
| H | -3.40334 | -2.054337 | -1.456652 | | | | |
| H | -4.570669 | -1.054448 | -0.609671 | | | | |
| H | -2.315933 | -0.181564 | -2.451155 | | | | |
| H | -4.026464 | 0.208774 | -2.518951 | | | | |
| H | -1.098065 | 2.540443 | -1.367016 | | | | |
| H | -0.823698 | 0.831681 | -1.119731 | | | | |
| H | -1.704098 | 1.212972 | 1.312158 | | | | |
| H | -1.524308 | 2.916729 | 0.991869 | | | | |

**Table S17** Energy analyses of 1*S*,7*S*,8*R*,10*S*-**8** (four conformers)

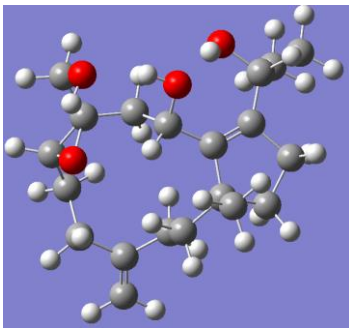
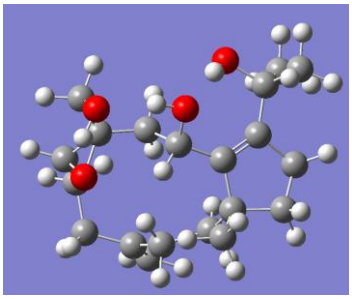
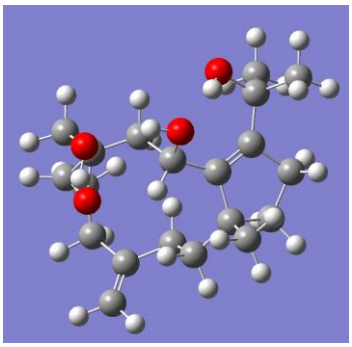
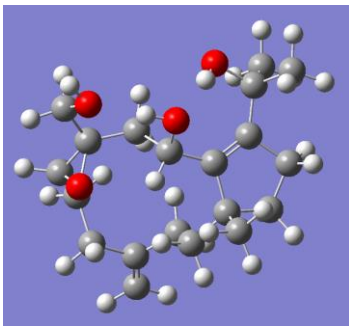
| NO. | 3D conformers B3LYP/6-31G(d,p) | E (Hartree) | ΔE (KJ/mol) | Boltzmann distribution |
|---|---|---|---|---|
| 1*S*,7*S*,8*R*,10*S*-**8** (conformer 1) |  | -1081.756891 | 0 | 88.45% |
| 1*S*,7*S*,8*R*,10*S*-**8** (conformer 2) |  | -1081.753153 | 9.814114681 | 1.69% |
| 1*S*,7*S*,8*R*,10*S*-**8** (conformer 3) |  | -1081.754016 | 7.548309178 | 4.21% |
| 1*S*,7*S*,8*R*,10*S*-**8** (conformer 4) |  | -1081.754294 | 6.8184205 | 5.65% |

**Table S18** Cartesian coordinates of the low-energy re-optimized conformers of 1*S*,7*S*,8*R*,10*S*-**8** calculated at B3LYP/6-31G(d,p) level of theory

| 1*S*,7*S*,8*R*,10*S*-**8** (conformer 1) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -3.314475 | 0.22175 | -1.25856 | H | -3.818856 | 2.332618 | -0.773084 |
| C | -3.598069 | -0.9237 | -0.239825 | H | -0.430773 | 0.548505 | 1.443159 |
| C | -2.921407 | -2.243562 | -0.566773 | H | 0.265565 | 1.80833 | -1.214293 |
| C | -1.404906 | -2.319463 | -0.471353 | H | -0.723218 | 0.37475 | -1.146043 |
| C | -0.851945 | -2.104919 | 0.957411 | H | 1.802852 | -3.682358 | 1.055156 |
| C | -3.041391 | 1.582819 | -0.610601 | H | 1.065672 | -3.236294 | -0.483819 |
| C | 0.663073 | -1.787231 | 1.097879 | H | 3.248772 | -2.456457 | -0.96942 |
| C | 1.135773 | -0.467643 | 0.441245 | H | 3.61261 | -2.100274 | 0.709931 |
| C | 0.324209 | 0.790061 | 0.685988 | H | -3.175788 | -4.271779 | -1.140013 |
| C | -0.436847 | 1.259928 | -0.579401 | H | -4.727413 | -3.279924 | -0.982083 |
| C | -1.678726 | 2.095776 | -0.298682 | H | 5.169809 | 1.29657 | -0.599216 |
| C | 1.569055 | -2.834259 | 0.401586 | H | 4.34001 | 0.892913 | 0.919089 |
| C | 2.815471 | -2.053696 | -0.046863 | H | 5.099555 | -0.391348 | -0.044681 |
| C | 2.319618 | -0.619684 | -0.189724 | H | 4.079585 | 0.764499 | -2.828088 |
| C | -3.64246 | -3.315763 | -0.91396 | H | 2.564566 | -0.155947 | -2.885726 |
| C | 3.216717 | 0.404913 | -0.885758 | H | 4.074705 | -0.955945 | -2.388374 |
| C | 4.541801 | 0.54998 | -0.102066 | H | 2.285156 | 1.946905 | -0.119549 |
| C | 3.502568 | -0.025157 | -2.336259 | H | 0.457843 | -0.887573 | 3.095826 |
| O | 2.616877 | 1.691092 | -1.009187 | H | 0.686897 | -2.643847 | 3.117895 |
| C | 0.985836 | -1.717523 | 2.611216 | H | 2.057908 | -1.566602 | 2.778316 |
| O | 1.160745 | 1.830432 | 1.229416 | H | 0.59695 | 2.631017 | 1.317891 |
| C | -1.472199 | 3.588375 | -0.104704 | H | -0.799867 | 4.003977 | -0.859462 |
| O | -2.554412 | 1.587548 | 0.744441 | H | -2.430529 | 4.121806 | -0.155414 |
| O | -0.847765 | 3.832593 | 1.164676 | H | -1.459626 | 3.469278 | 1.829147 |
| H | -4.171674 | 0.334435 | -1.930676 | | | | |
| H | -2.474911 | -0.053884 | -1.904544 | | | | |
| H | -3.273017 | -0.583926 | 0.748218 | | | | |
| H | -4.67897 | -1.084746 | -0.168994 | | | | |
| H | -0.951508 | -1.583501 | -1.148029 | | | | |
| H | -1.085767 | -3.297466 | -0.847329 | | | | |
| H | -1.065444 | -3.009059 | 1.543759 | | | | |
| H | -1.414827 | -1.304016 | 1.450896 | | | | |

| 1*S*,7*S*,8*R*,10*S*-**8** (conformer 2) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -3.395991 | 0.091977 | -1.476613 | H | -3.93233 | 2.111179 | -0.76574 |
| C | -3.833185 | -1.181798 | -0.680456 | H | -0.358688 | 0.553589 | 1.562739 |
| C | -2.728243 | -2.214302 | -0.520408 | H | 0.088701 | 1.627995 | -1.237166 |
| C | -1.721227 | -1.961749 | 0.590151 | H | -0.793748 | 0.140222 | -0.983933 |
| C | -0.28671 | -2.474015 | 0.333904 | H | 2.785408 | -2.466594 | 1.859793 |
| C | -3.149467 | 1.356986 | -0.656219 | H | 2.01688 | -3.630299 | 0.779288 |
| C | 0.85805 | -1.77129 | 1.134585 | H | 2.711905 | -2.355921 | -1.175754 |
| C | 1.237831 | -0.394769 | 0.528287 | H | 4.015416 | -1.913624 | -0.087246 |
| C | 0.325559 | 0.797811 | 0.742867 | H | -1.881973 | -4.019013 | -1.262264 |
| C | -0.539111 | 1.093637 | -0.517331 | H | -3.422366 | -3.445205 | -2.101125 |
| C | -1.817091 | 1.866983 | -0.23688 | H | 4.98554 | 1.751396 | -0.68378 |
| C | 2.18579 | -2.560612 | 0.946187 | H | 4.136097 | 1.390048 | 0.836531 |
| C | 2.926185 | -1.875091 | -0.209655 | H | 5.070699 | 0.120928 | 0.020012 |
| C | 2.373698 | -0.457029 | -0.199095 | H | 4.04205 | 0.956749 | -2.883108 |
| C | -2.671756 | -3.276203 | -1.332246 | H | 2.63195 | -0.117086 | -2.927491 |
| C | 3.148663 | 0.629298 | -0.949152 | H | 4.194186 | -0.724856 | -2.329127 |
| C | 4.41883 | 0.986644 | -0.141805 | H | 2.077704 | 2.125424 | -0.294104 |
| C | 3.530223 | 0.144147 | -2.357997 | H | -0.430732 | -1.178695 | 2.835943 |
| O | 2.403655 | 1.8242 | -1.171067 | H | 0.40789 | -2.716852 | 3.043337 |
| C | 0.508751 | -1.703117 | 2.634367 | H | 1.302452 | -1.192931 | 3.191722 |
| O | 1.094304 | 1.942218 | 1.156291 | H | 0.446632 | 2.649484 | 1.371839 |
| C | -1.688075 | 3.351415 | 0.069963 | H | -0.9922 | 3.840137 | -0.616941 |
| O | -2.720991 | 1.235107 | 0.71484 | H | -2.664617 | 3.846114 | -0.01232 |
| O | -1.157789 | 3.556016 | 1.387183 | H | -1.755476 | 3.077902 | 1.988804 |
| H | -4.187286 | 0.341808 | -2.192542 | | | | |
| H | -2.517518 | -0.152283 | -2.082684 | | | | |
| H | -4.2126 | -0.87929 | 0.30335 | | | | |
| H | -4.669724 | -1.644644 | -1.214429 | | | | |
| H | -2.112202 | -2.421817 | 1.510435 | | | | |
| H | -1.723091 | -0.892731 | 0.804202 | | | | |
| H | -0.057917 | -2.387828 | -0.735848 | | | | |
| H | -0.250817 | -3.547168 | 0.564899 | | | | |

| 1*S*,7*S*,8*R*,10*S*-**8** (conformer 3) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | 2.936646 | 0.224495 | 1.946072 | H | 3.89248 | 1.892359 | 0.866572 |
| C | 3.5474 | -1.154498 | 1.595589 | H | 0.474952 | 0.380992 | -1.41157 |
| C | 2.905305 | -1.928238 | 0.453999 | H | -0.246724 | 2.216793 | 0.841735 |
| C | 1.396325 | -2.140685 | 0.496699 | H | 0.392738 | 0.664874 | 1.290671 |
| C | 0.715638 | -2.194835 | -0.887556 | H | -1.94802 | -3.692051 | -0.617608 |
| C | 2.990207 | 1.274638 | 0.847087 | H | -1.139721 | -3.056988 | 0.819033 |
| C | -0.791823 | -1.835334 | -0.950336 | H | -3.312683 | -2.189926 | 1.270219 |
| C | -1.185392 | -0.441932 | -0.402383 | H | -3.715406 | -2.031349 | -0.430561 |
| C | -0.318637 | 0.750138 | -0.754358 | H | 3.262125 | -3.043699 | -1.321312 |
| C | 0.377827 | 1.394885 | 0.481874 | H | 4.749621 | -2.30525 | -0.518481 |
| C | 1.793472 | 1.871475 | 0.189834 | H | -5.178345 | 1.499989 | 0.528274 |
| C | -1.678676 | -2.769144 | -0.091135 | H | -4.459796 | 0.825563 | -0.949038 |
| C | -2.896733 | -1.912535 | 0.294363 | H | -5.154213 | -0.259638 | 0.27368 |
| C | -2.362486 | -0.48542 | 0.256213 | H | -3.972696 | 1.303313 | 2.745205 |
| C | 3.672338 | -2.452486 | -0.507596 | H | -2.431456 | 0.432211 | 2.854077 |
| C | -3.214683 | 0.643036 | 0.834685 | H | -3.944738 | -0.465785 | 2.588207 |
| C | -4.58997 | 0.668073 | 0.127849 | H | -2.290728 | 2.026298 | -0.217274 |
| C | -3.403588 | 0.455024 | 2.351089 | H | -0.722136 | -1.119696 | -3.026855 |
| O | -2.615237 | 1.928891 | 0.704744 | H | -0.95887 | -2.870483 | -2.879335 |
| C | -1.219358 | -1.899777 | -2.438203 | H | -2.299381 | -1.753301 | -2.546966 |
| O | -1.079847 | 1.719592 | -1.503643 | H | -0.445562 | 2.435565 | -1.722725 |
| C | 1.919612 | 3.240324 | -0.452491 | H | 1.385255 | 3.998546 | 0.12689 |
| O | 2.623373 | 0.894474 | -0.489437 | H | 2.974884 | 3.534826 | -0.524046 |
| O | 1.320537 | 3.250477 | -1.757405 | H | 1.824582 | 2.611355 | -2.289902 |
| H | 3.486588 | 0.628677 | 2.805601 | | | | |
| H | 1.910415 | 0.083496 | 2.29546 | | | | |
| H | 4.617346 | -1.03825 | 1.384322 | | | | |
| H | 3.48246 | -1.757755 | 2.514809 | | | | |
| H | 0.931612 | -1.34752 | 1.088307 | | | | |
| H | 1.187965 | -3.064648 | 1.056282 | | | | |
| H | 0.830969 | -3.200581 | -1.313646 | | | | |
| H | 1.265328 | -1.528632 | -1.561879 | | | | |

| 1*S*,7*S*,8*R*,10*S*-**8** (conformer 4) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Atomic | Standard Orientation (Å) | | | Atomic | Standard Orientation (Å) | | |
| Type | X | Y | Z | Type | X | Y | Z |
| C | -3.30308 | 0.331883 | -1.18387 | H | -3.779431 | 2.430847 | -0.637498 |
| C | -3.617829 | -0.829643 | -0.195306 | H | -0.470868 | 0.45883 | 1.463706 |
| C | -2.998457 | -2.161098 | -0.579652 | H | 0.330545 | 1.89636 | -1.066982 |
| C | -1.48436 | -2.285114 | -0.516197 | H | -0.692062 | 0.487395 | -1.147012 |
| C | -0.906104 | -2.169112 | 0.913642 | H | 1.71682 | -3.789173 | 0.896643 |
| C | -3.008643 | 1.668674 | -0.498423 | H | 0.969236 | -3.257972 | -0.610444 |
| C | 0.613632 | -1.877599 | 1.041687 | H | 3.164996 | -2.4948 | -1.084261 |
| C | 1.095056 | -0.538568 | 0.432797 | H | 3.54878 | -2.223405 | 0.606473 |
| C | 0.310434 | 0.723176 | 0.743086 | H | -3.33113 | -4.158017 | -1.218502 |
| C | -0.402702 | 1.315997 | -0.499765 | H | -4.845756 | -3.122792 | -0.991754 |
| C | -1.636762 | 2.158712 | -0.18353 | H | 5.191396 | 1.131475 | -0.612359 |
| C | 1.49112 | -2.907354 | 0.286205 | H | 4.430788 | 0.61603 | 0.907566 |
| C | 2.74603 | -2.128565 | -0.139597 | H | 5.075291 | -0.59806 | -0.217514 |
| C | 2.273545 | -0.681386 | -0.211249 | H | 3.980989 | 0.824459 | -2.817782 |
| C | -3.761375 | -3.196144 | -0.948949 | H | 2.402733 | 0.015677 | -2.868336 |
| C | 3.187237 | 0.354547 | -0.86682 | H | 3.874008 | -0.923409 | -2.521742 |
| C | 4.558649 | 0.365763 | -0.151838 | H | 2.323033 | 1.844631 | 0.066703 |
| C | 3.373133 | 0.035974 | -2.361922 | H | 0.461628 | -1.051036 | 3.074338 |
| O | 2.656727 | 1.676727 | -0.844071 | H | 0.651263 | -2.812326 | 3.026479 |
| C | 0.962696 | -1.873699 | 2.550724 | H | 2.040456 | -1.752693 | 2.705358 |
| O | 1.171055 | 1.689891 | 1.379712 | H | 0.656974 | 2.523964 | 1.434136 |
| C | -1.425158 | 3.654486 | -0.088819 | H | -1.058895 | 4.030078 | -1.054983 |
| O | -2.507309 | 1.64217 | 0.845723 | H | -2.37658 | 4.149263 | 0.145238 |
| O | -0.470231 | 3.918823 | 0.948924 | H | -0.104791 | 4.806666 | 0.822033 |
| H | -4.151366 | 0.478022 | -1.861107 | | | | |
| H | -2.463369 | 0.052529 | -1.828096 | | | | |
| H | -3.259092 | -0.533239 | 0.795332 | | | | |
| H | -4.703005 | -0.948593 | -0.106855 | | | | |
| H | -1.021287 | -1.519756 | -1.152639 | | | | |
| H | -1.196341 | -3.246564 | -0.954974 | | | | |
| H | -1.119292 | -3.106 | 1.446195 | | | | |
| H | -1.449986 | -1.394856 | 1.467124 | | | | |

**Table S19** Experimental and calculated $^{1}$H NMR data for compound **8**

| No. | **8**, exptl. $\delta_H$ [a] | 1*R*,7*R*,8*S*,10*R*-**8**, calcd. $\delta_H$ [b] | 1*S*,7*S*,8*R*,10*S*-**8**, calcd. $\delta_H$ [b] |
|---|---|---|---|
| 2 | 1.32 | 1.17 | 1.26 |
| | 1.74 | 1.68 | 1.73 |
| 3 | 1.79 | 1.79 | 2.03 |
| | 2.04 | 2.22 | 2.16 |
| 5 | 2.27 | 2.40 | 2.27 |
| | 2.46 | 2.45 | 2.66 |
| 6 | 1.49 | 1.18 | 1.44 |
| | 1.96 | 2.13 | 2.04 |
| 7 | 3.13 | 3.04 | 3.34 |
| 9 | 1.96 | 1.63 | 1.83 |
| | 2.58 | 2.83 | 3.01 |
| 10 | 4.37 | 4.18 | 4.44 |
| 13 | 2.2 | 2.29 | 2.32 |
| | 2.35 | 2.50 | 2.54 |
| 14 | 1.43 | 1.71 | 1.44 |
| | 1.74 | 1.98 | 1.89 |
| 15 | 1.05 | 1.22 | 1.11 |
| 16 | 4.67 | 5.02 | 5.00 |
| | 4.71 | 5.06 | 5.08 |
| 17 | 3.32 | 3.52 | 3.53 |
| | 3.98 | 4.52 | 4.00 |
| 19 | 1.35 | 1.42 | 1.35 |
| 20 | 1.38 | 1.41 | 1.38 |

[a] Recorded in $CDCl_3$ at 600 MHz.

[b] Calculated in $CDCl_3$

**Table S20** Experimental and calculated $^{13}C$ NMR data for compound **8**

| No. | **8**, exptl. $\delta_C$ [a] | 1*R*,7*R*,8*S*,10*R*-**8**, calcd. $\delta_C$ [b] | 1*S*,7*S*,8*R*,10*S*-**8**, calcd. $\delta_C$ [b] |
|---|---|---|---|
| 1 | 53.1 | 52.88 | 53.00 |
| 2 | 35.7 | 35.70 | 32.59 |
| 3 | 29.9 | 29.84 | 28.88 |
| 4 | 150.3 | 153.27 | 154.83 |
| 5 | 28.7 | 29.02 | 24.95 |
| 6 | 22.3 | 24.65 | 20.58 |
| 7 | 60.2 | 61.36 | 62.17 |
| 8 | 63.8 | 59.06 | 62.89 |
| 9 | 37.8 | 39.73 | 36.33 |
| 10 | 65 | 60.95 | 63.32 |
| 11 | 141.2 | 145.47 | 143.22 |
| 12 | 144.7 | 150.72 | 152.53 |
| 13 | 32.8 | 32.66 | 31.03 |
| 14 | 32.7 | 31.42 | 29.44 |
| 15 | 26.8 | 26.93 | 21.18 |
| 16 | 111.1 | 110.33 | 111.98 |
| 17 | 68.6 | 61.37 | 68.24 |
| 18 | 72.3 | 71.84 | 70.58 |
| 19 | 31 | 22.68 | 26.44 |
| 20 | 29.7 | 24.56 | 24.37 |

[a] Recorded in $CDCl_3$ at 600 MHz.

[b] Calculated in $CDCl_3$

**Table S21** DP4+ analyses of calculated and experimental NMR chemical shifts of **8** (unscaled). Isomer 1: 1*R*-7*R*-8*S*-10*R*-**8**; Isomer 2: 1*S*-7*S*-8*R*-10*S*-**8**

| Functional | Solvent? | Basis Set | Type of Data |
|---|---|---|---|
| mPW1PW91 | PCM | 6-311G(d,p) | Unscaled Shifts |

| | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 | Isomer 6 |
|---|---|---|---|---|---|---|
| sDP4+ (H data) | 0.00% | 100.00% | - | - | - | - |
| sDP4+ (C data) | 0.00% | 100.00% | - | - | - | - |
| sDP4+ (all data) | 0.00% | 100.00% | - | - | - | - |
| uDP4+ (H data) | 0.04% | 99.96% | - | - | - | - |
| uDP4+ (C data) | 99.97% | 0.03% | - | - | - | - |
| uDP4+ (all data) | 62.82% | 37.18% | - | - | - | - |
| DP4+ (H data) | 0.00% | 100.00% | - | - | - | - |
| DP4+ (C data) | 0.00% | 100.00% | - | - | - | - |
| DP4+ (all data) | 0.00% | 100.00% | - | - | - | - |

| Functional | Solvent? | Basis Set | Type of Data |
|---|---|---|---|
| mPW1PW91 | PCM | 6-311G(d,p) | Unscaled Shifts |

| | | DP4+ | 0.00% | 100.00% | - | - | - |
|---|---|---|---|---|---|---|---|
| Nuclei | sp2? | Experimental | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 |
| C | | 53.1 | 52.8765 | 52.998 | | | |
| C | | 35.7 | 35.7018 | 32.5932 | | | |
| C | | 29.9 | 29.8413 | 28.8842 | | | |
| C | x | 150.3 | 153.2658 | 154.8336 | | | |
| C | | 28.7 | 29.0241 | 24.9488 | | | |
| C | | 22.3 | 24.6492 | 20.5768 | | | |
| C | | 60.2 | 61.3587 | 62.1674 | | | |
| C | | 63.8 | 59.055 | 62.887 | | | |
| C | | 37.8 | 39.7287 | 36.3324 | | | |
| C | | 65 | 60.9468 | 63.3236 | | | |
| C | x | 141.2 | 145.4745 | 143.2214 | | | |
| C | x | 144.7 | 150.717 | 152.5332 | | | |
| C | | 32.8 | 32.664 | 31.0284 | | | |
| C | | 32.7 | 31.419 | 29.4386 | | | |
| C | | 26.8 | 26.9277 | 21.1754 | | | |
| C | x | 111.1 | 110.3292 | 111.9846 | | | |
| C | | 68.6 | 61.3713 | 68.2414 | | | |
| C | | 72.3 | 71.835 | 70.5804 | | | |
| C | | 31 | 22.6776 | 26.4434 | | | |
| C | | 29.7 | 24.5574 | 24.368 | | | |
| H | | 1.32 | 1.1742 | 1.2562 | | | |
| H | | 1.74 | 1.6818 | 1.7252 | | | |
| H | | 1.79 | 1.7907 | 2.0314 | | | |
| H | | 2.04 | 2.2218 | 2.1616 | | | |
| H | | 2.27 | 2.3967 | 2.2684 | | | |
| H | | 2.46 | 2.4456 | 2.6622 | | | |
| H | | 1.49 | 1.1787 | 1.4376 | | | |
| H | | 1.96 | 2.1279 | 2.0406 | | | |
| H | | 3.13 | 3.0423 | 3.3376 | | | |
| H | | 1.96 | 1.6332 | 1.833 | | | |
| H | | 2.58 | 2.8323 | 3.0124 | | | |
| H | | 4.37 | 4.1838 | 4.4444 | | | |
| H | | 2.2 | 2.2929 | 2.3236 | | | |
| H | | 2.35 | 2.4999 | 2.5426 | | | |
| H | | 1.43 | 1.7133 | 1.4384 | | | |
| H | | 1.74 | 1.9767 | 1.8928 | | | |
| H | | 1.05 | 1.2177 | 1.11466632 | | | |
| H | x | 4.67 | 5.0229 | 5.0036 | | | |
| H | x | 4.71 | 5.0631 | 5.0822 | | | |
| H | | 3.32 | 3.5232 | 3.5272 | | | |
| H | | 3.98 | 4.515 | 3.995 | | | |
| H | | 1.35 | 1.4159 | 1.34653326 | | | |
| H | | 1.38 | 1.412299 | 1.38059994 | | | |

**Table S22** Cytotoxicity of active compounds against Human Oral Cancer (Ca9-22)

| Compound/tumor cell | Ca9-22 (μM) | Compound/tumor cell | Ca9-22 (μM) |
|---|---|---|---|
| **1** | 212.64 ± 2.64 | **11** | 238.51 ± 9.24 |
| **3** | 239.09 ± 2.17 | **13** | 112.45 ± 1.4 |
| **4** | 231.02± 11.72 | **15** | 24.87 ± 3.0 |
| **5** | 87.39 ± 4.42 | **16** | 166.7 ± 2.97 |
| **6** | 31.51 ± 16.03 | **17** | 156.99 ± 20.47 |
| **7** | 15.65 ± 0.37 | **19** | 190.26 ± 13.59 |
| **8** | 118.72 ± 4.14 | **21** | 72.23 ± 12.74 |
| **10** | 194.62 ± 4.97 | **22** | 43.62 ± 5.79 |

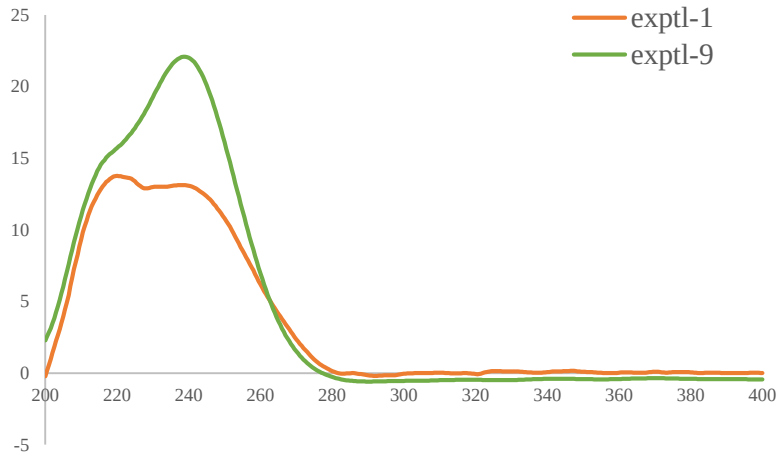



**Figure S1** Experimental ECD spectra of **1** and **9**

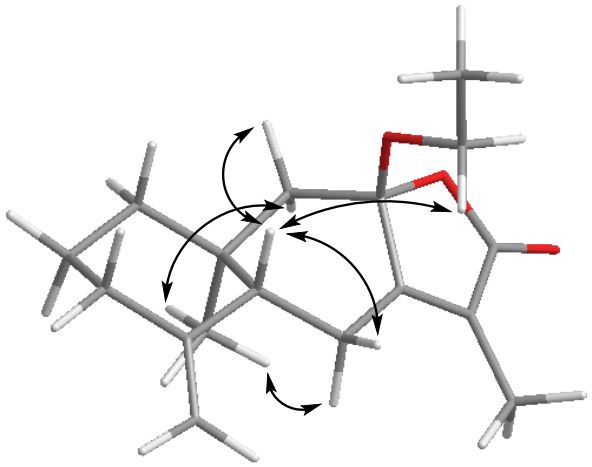


**Figure S2** NOESY (double arrow) correlations of **2**

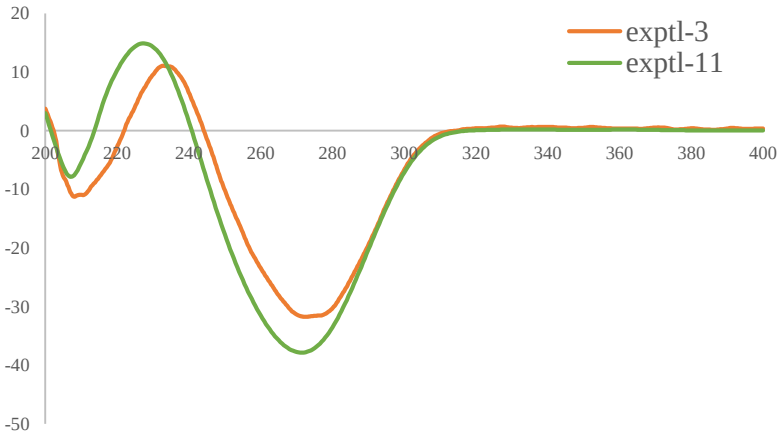



**Figure S3** Experimental ECD spectra of **3** and **11**

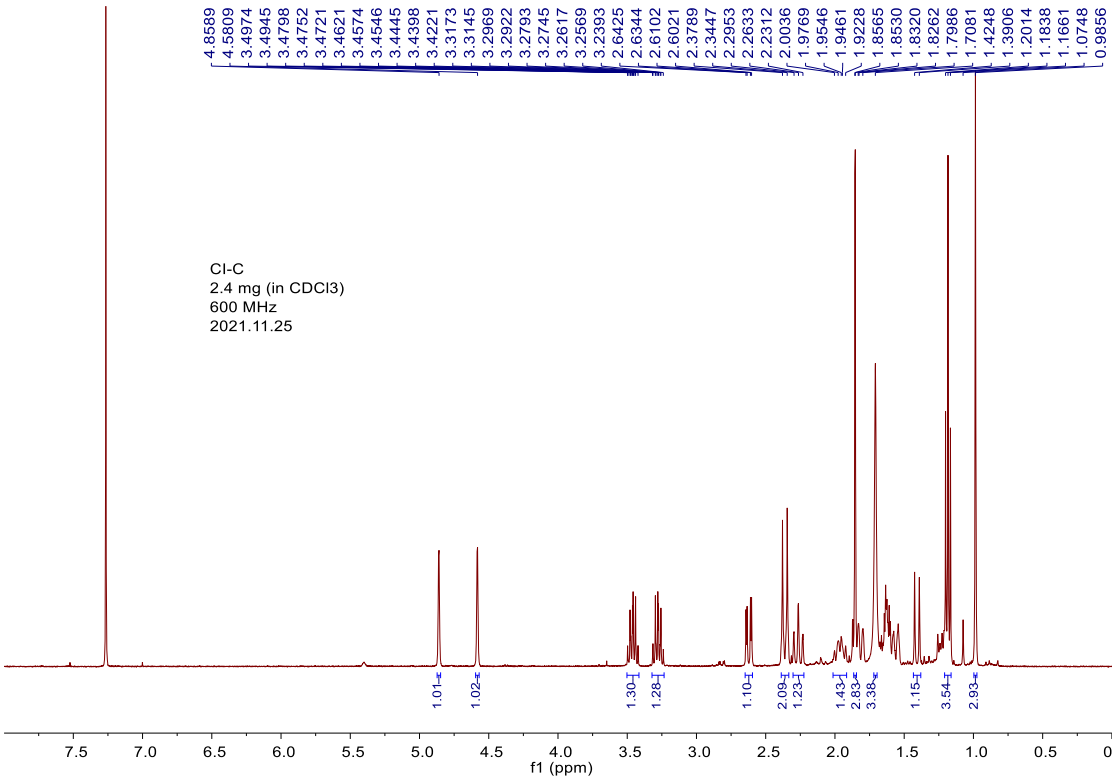



**Figure S4** $^{1}$H NMR spectrum of **1** (600 MHz, $CDCl_3$)

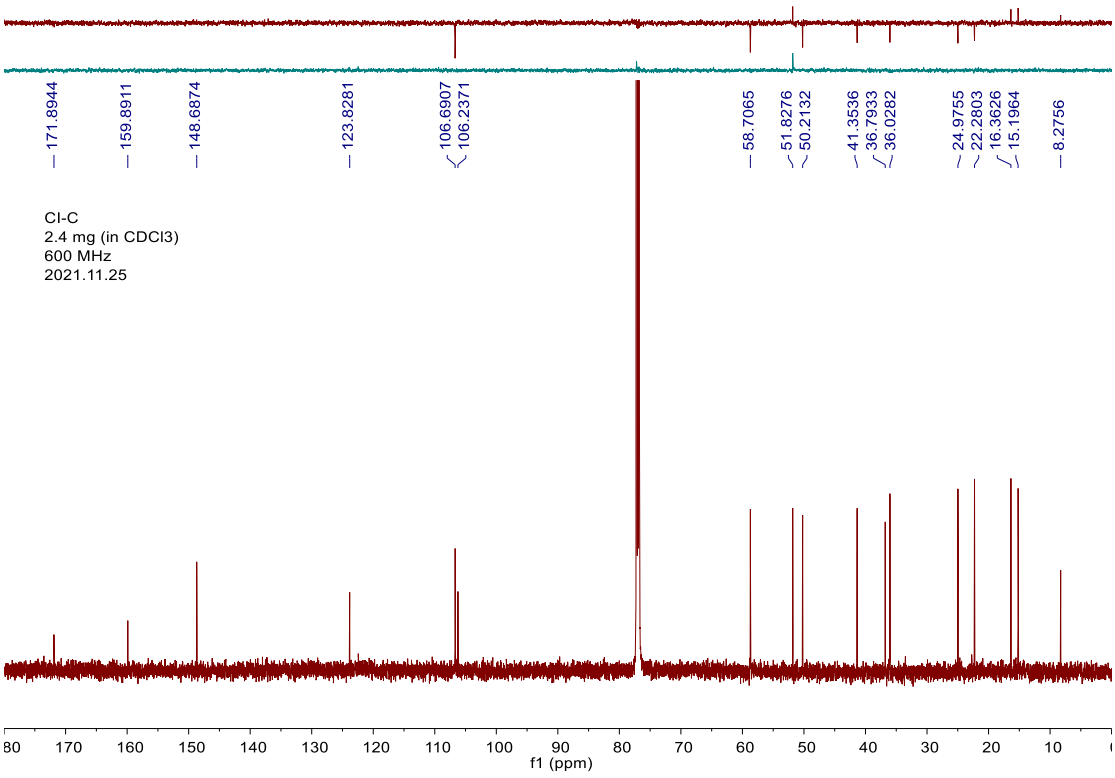



**Figure S5** $^{13}$C NMR spectrum of **1** (125 MHz, $CDCl_3$)

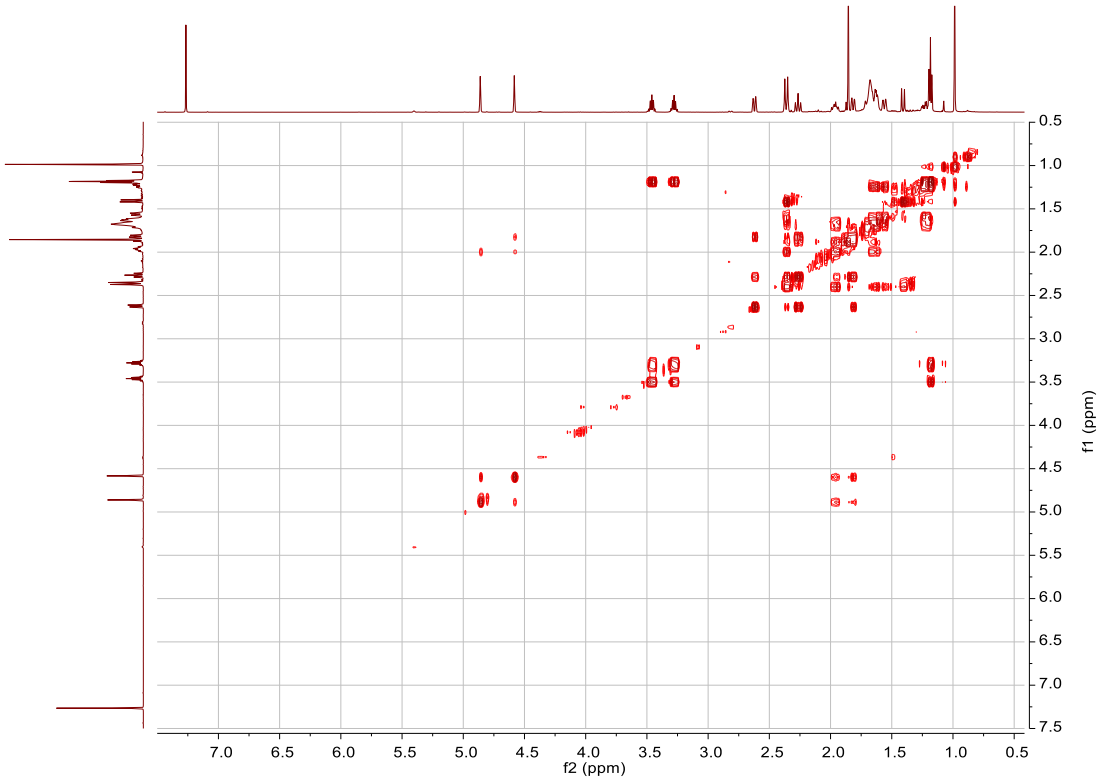



**Figure S6** COSY spectrum of **1**

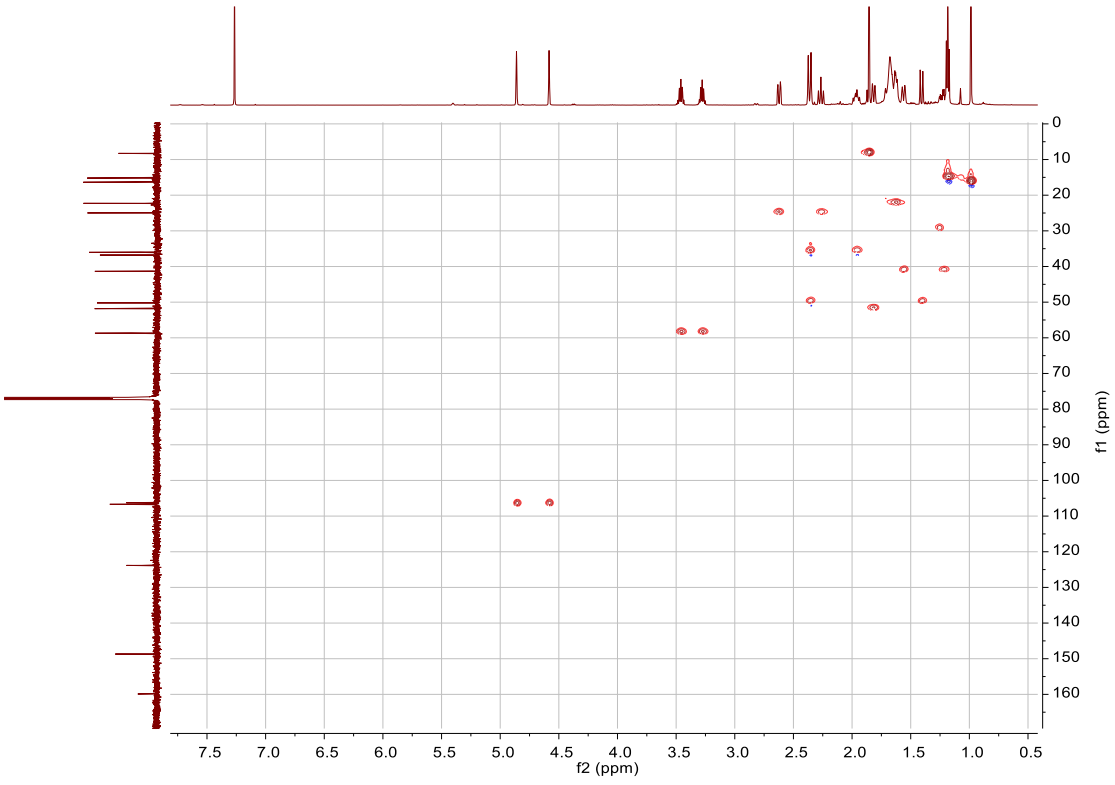



**Figure S7** HSQC spectrum of **1**

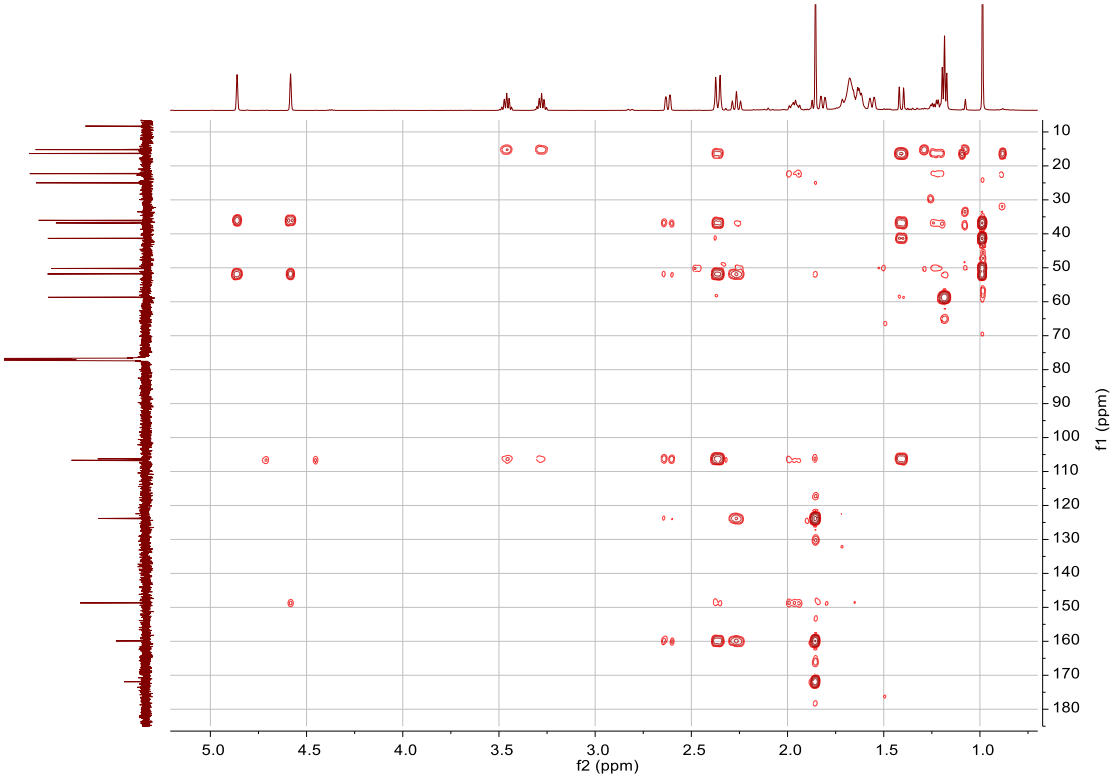



**Figure S8** HMBC spectrum of **1**

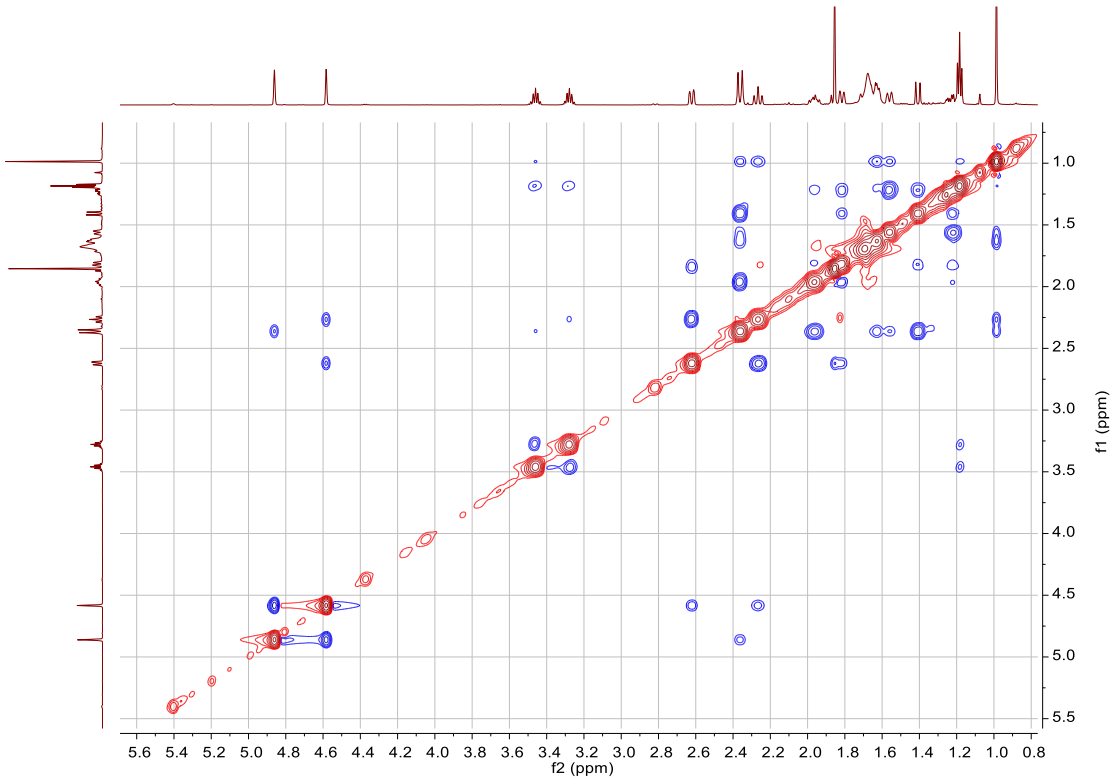
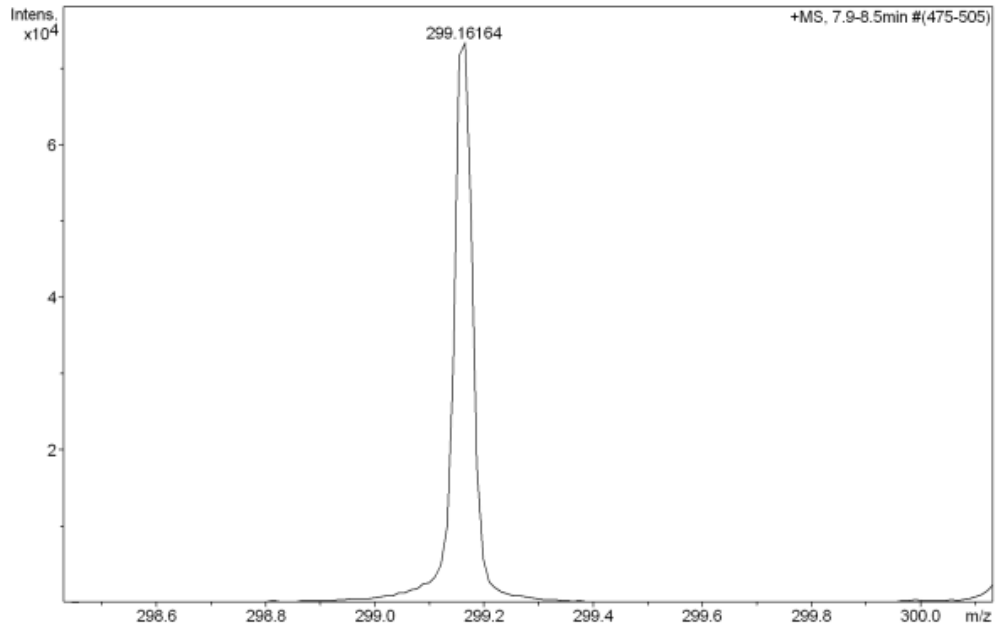



**Figure S9** NOESY spectrum of **1**

## Mass Spectrum SmartFormula Report

**Analysis Info**

| | | |
|---|---|---|
| Analysis Name | D:\QTOF\CICR.d | 12/23/2021 1:03:53 PM |
| Method | _tune_low_pos(50-1000)_20170502_Liao lab.m | Operator: YU HSIAO-CHING |
| Sample Name | CI-C | Instrument: BRUKER micrOTOF-Q |
| Comment | ESI Positive | |




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 299.16164 | 1 | C 17 H 24 Na O 3 | 100.00 | 299.16177 | 0.12 | 0.41 | 39.7 | 5.5 | even | ok |

**Figure S10** HRESIMS spectrum of **1**

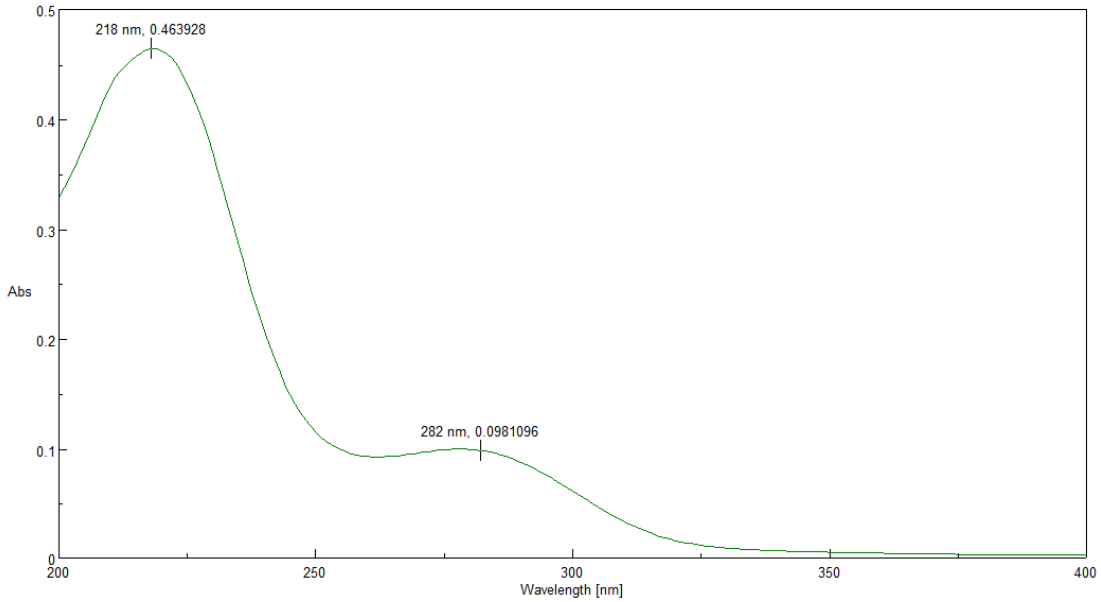



**Figure S11** UV spectrum of **1**

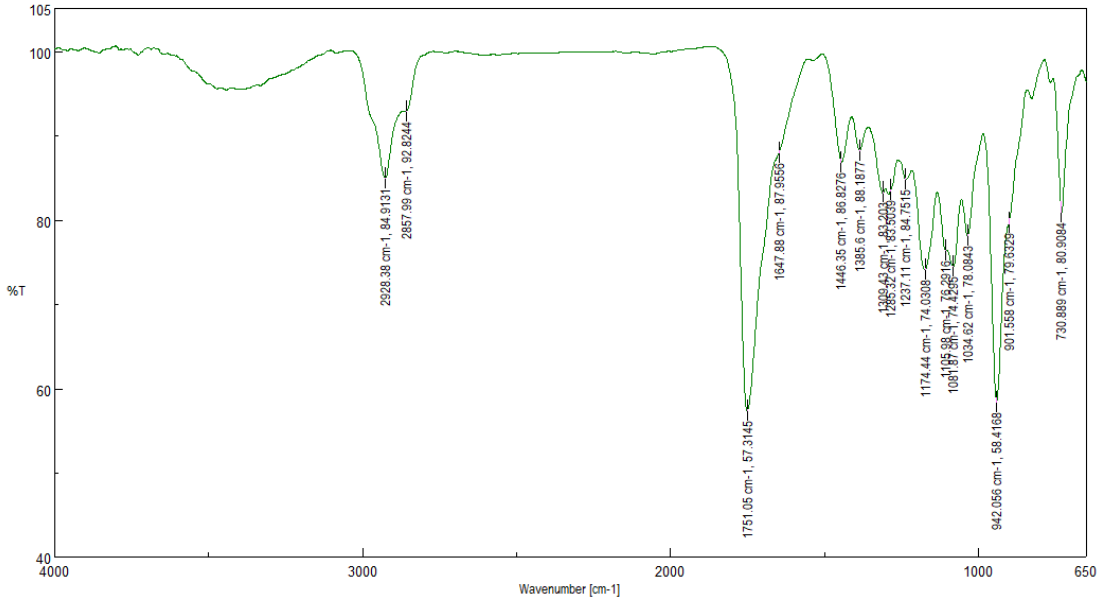



**Figure S12** IR spectrum of **1**

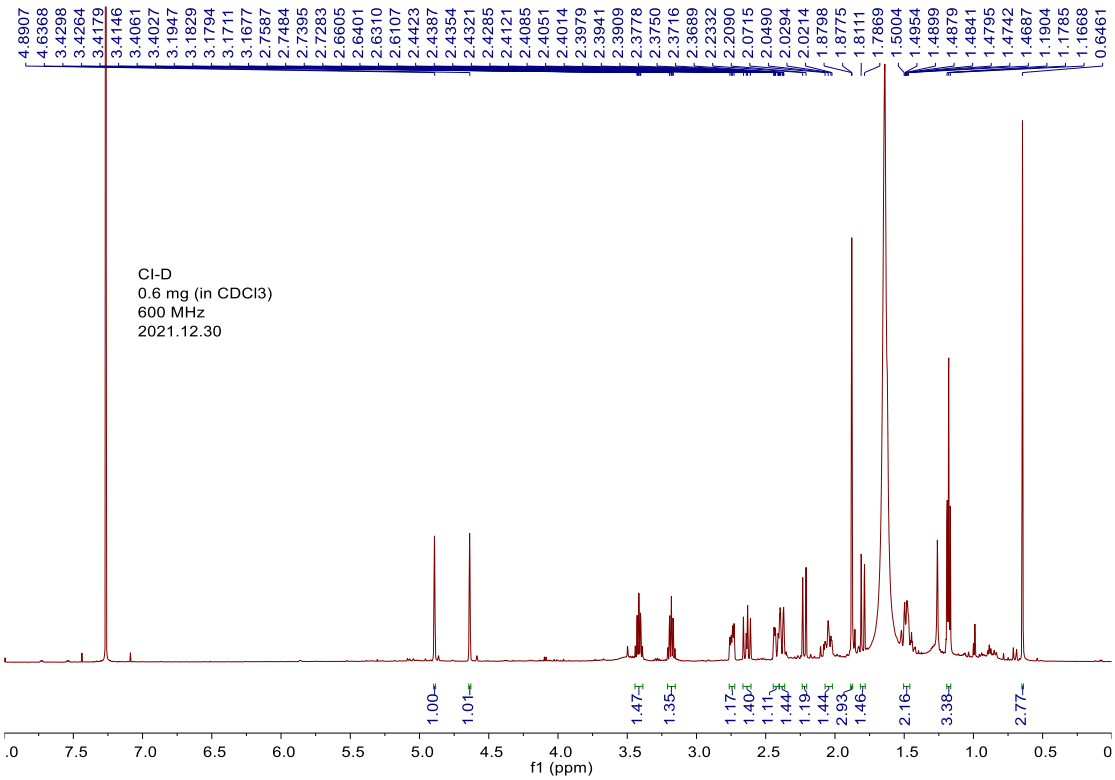



**Figure S13** $^{1}$H NMR spectrum of **2** (600 MHz, $CDCl_3$)

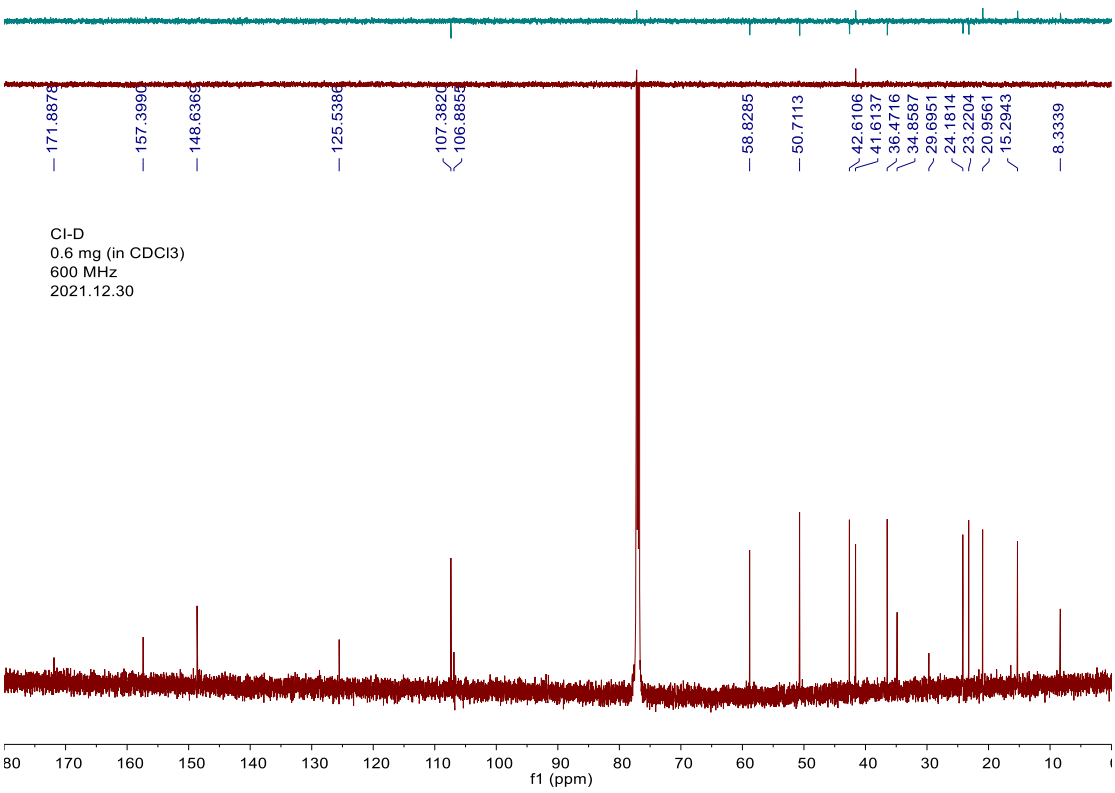



**Figure S14** $^{13}$C NMR spectrum of **2** (125 MHz, $CDCl_3$)

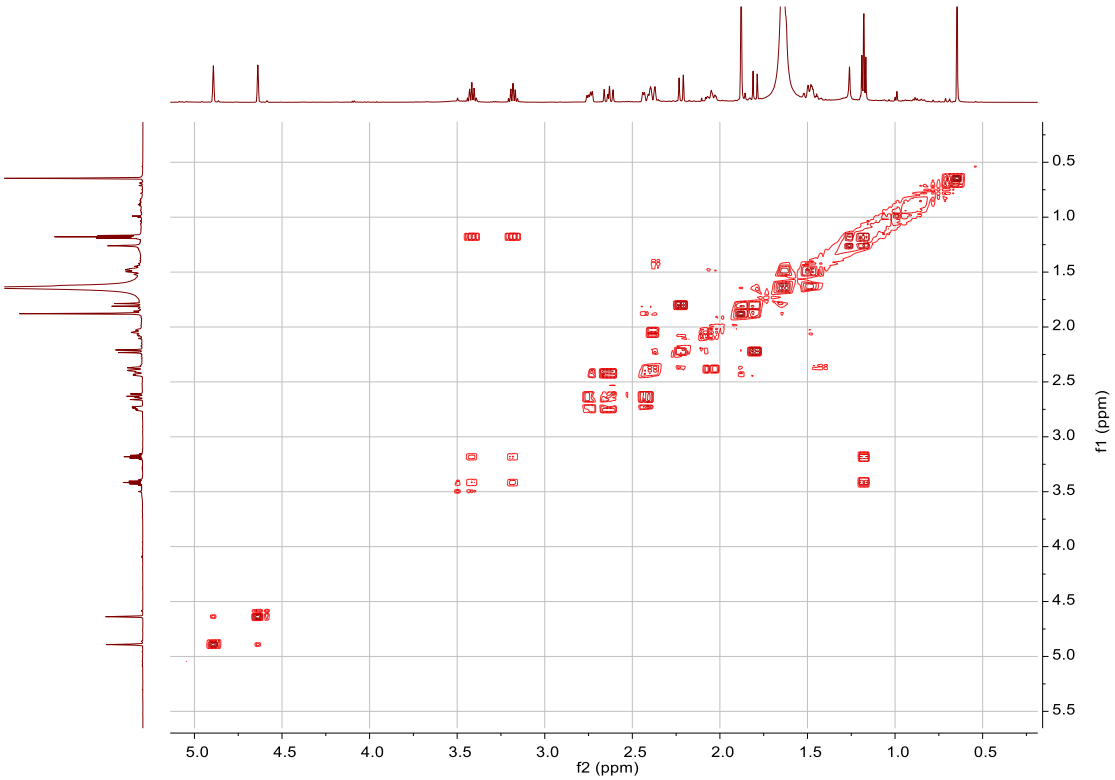



**Figure S15** COSY spectrum of **2**

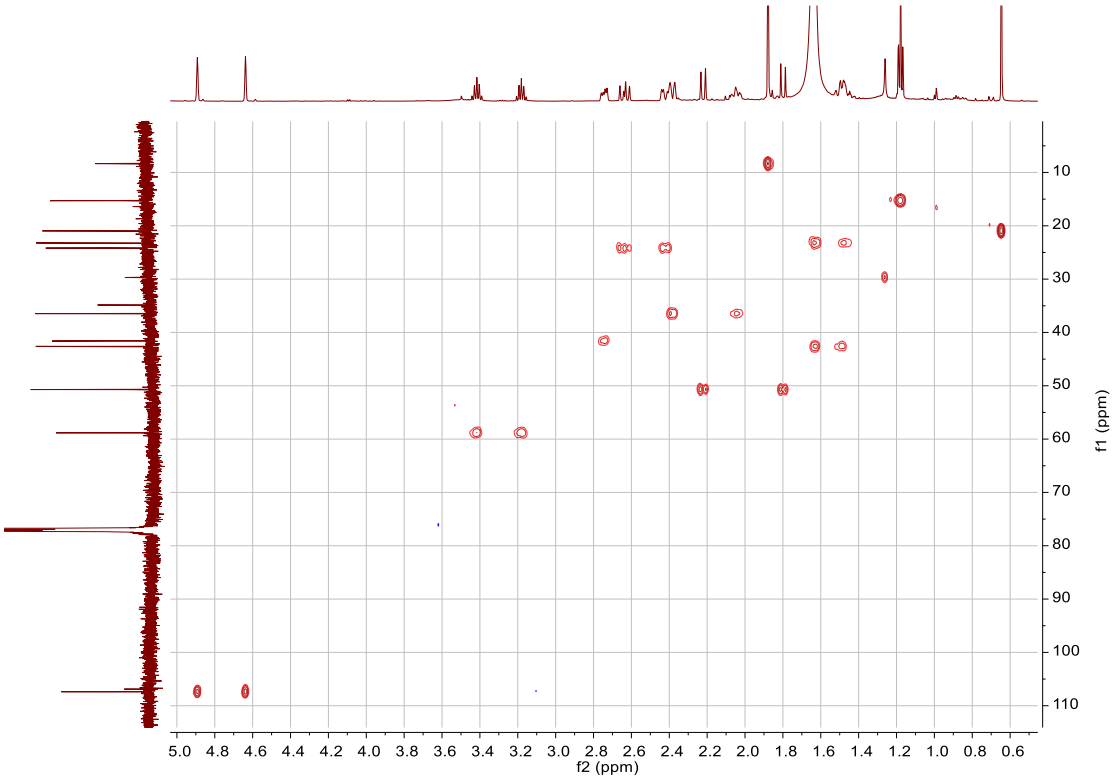



**Figure S16** HSQC spectrum of **2**

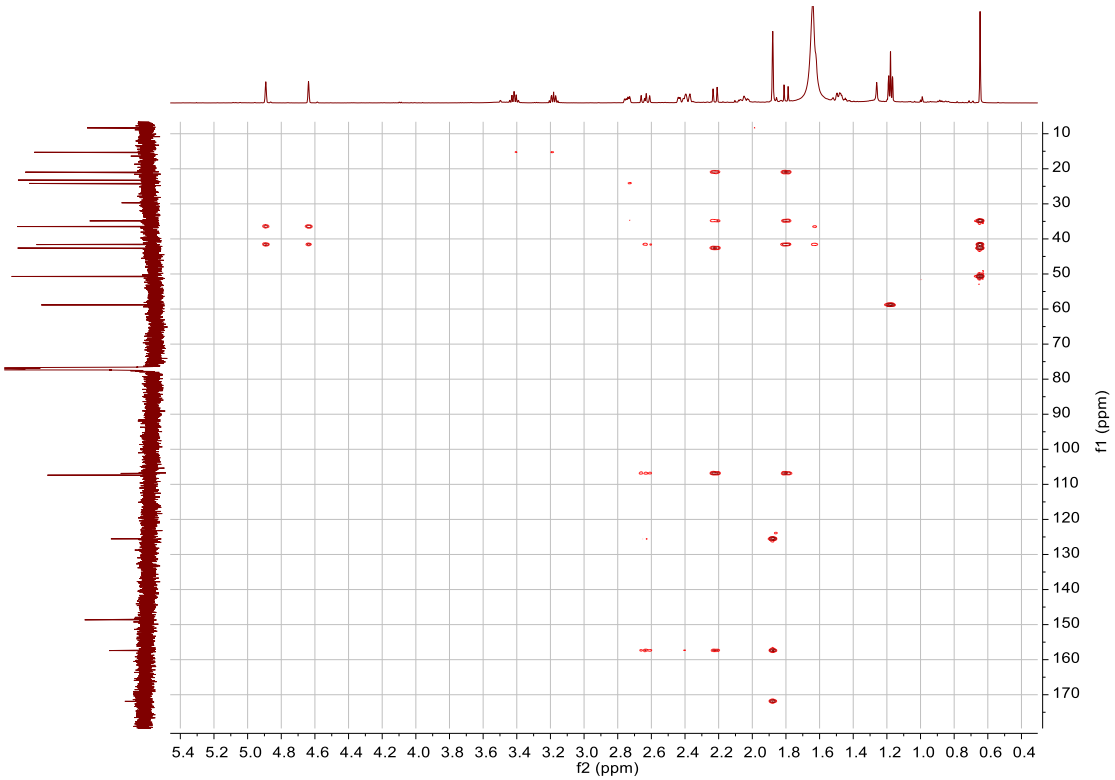



**Figure S17** HMBC spectrum of **2**

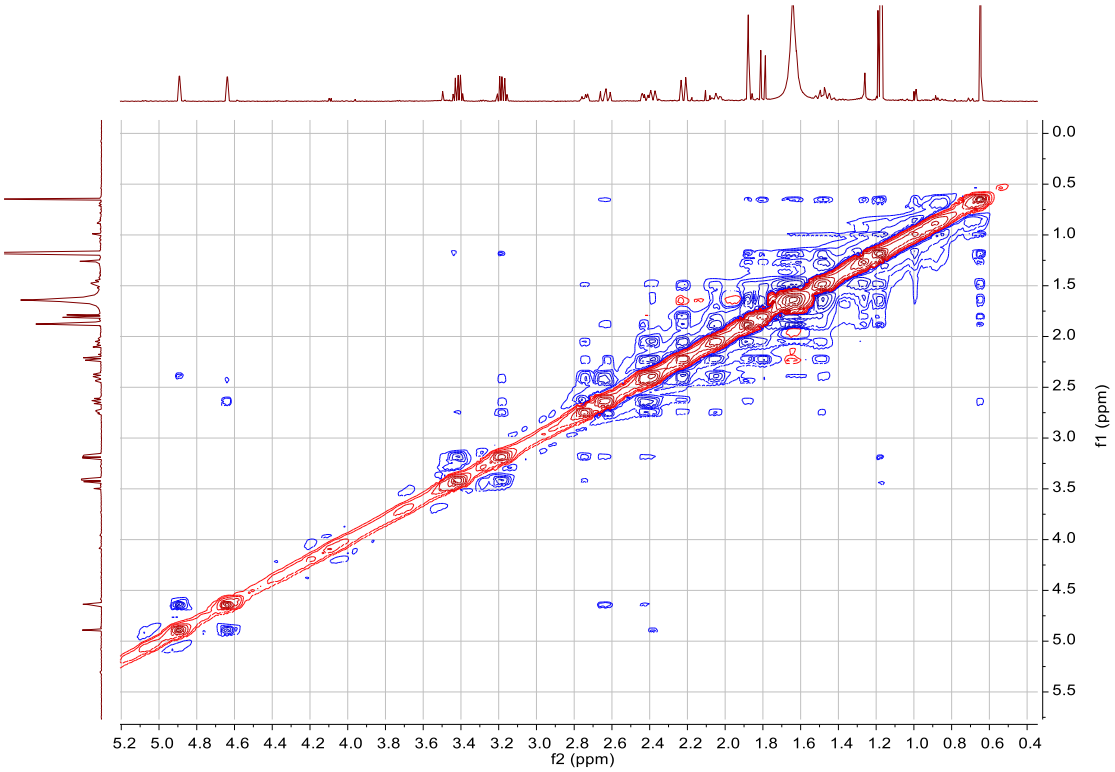
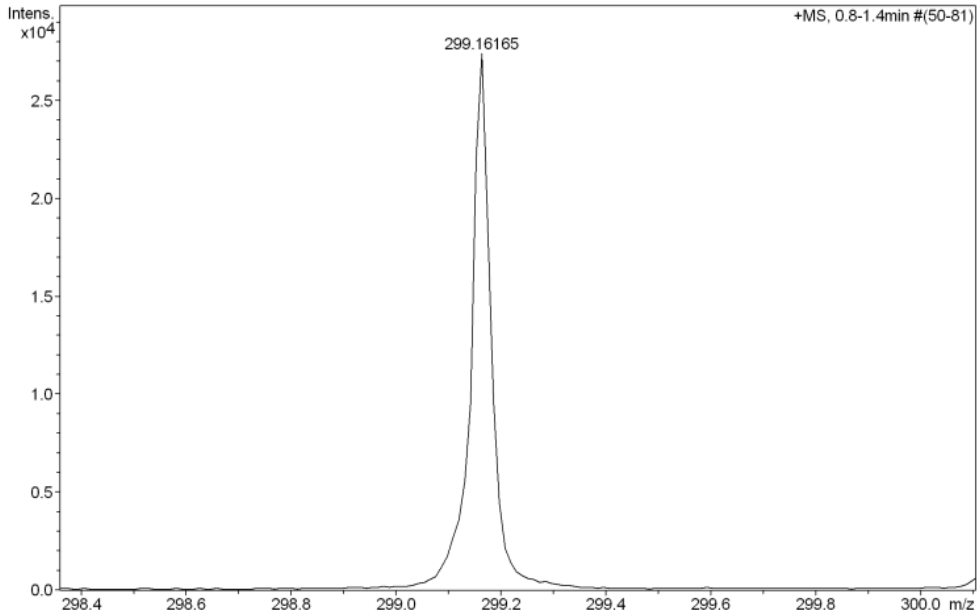



**Figure S18** NOESY spectrum of **2**

Mass Spectrum SmartFormula Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\1107\CIDR1.d | | 11/8/2022 2:41:15 PM |
| Method | tune_wide_pos_20220422.m | | Operator: YU HSIAO-CHING |
| Sample Name | CI-D | | Instrument: BRUKER micrOTOF-Q |
| Comment | ESI Positive | | |




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 299.16165 | 1 | C 17 H 24 Na O 3 | 100.00 | 299.16177 | 0.11 | 0.38 | 35.6 | 5.5 | even | ok |

**Figure S19** HRESIMS spectrum of **2**

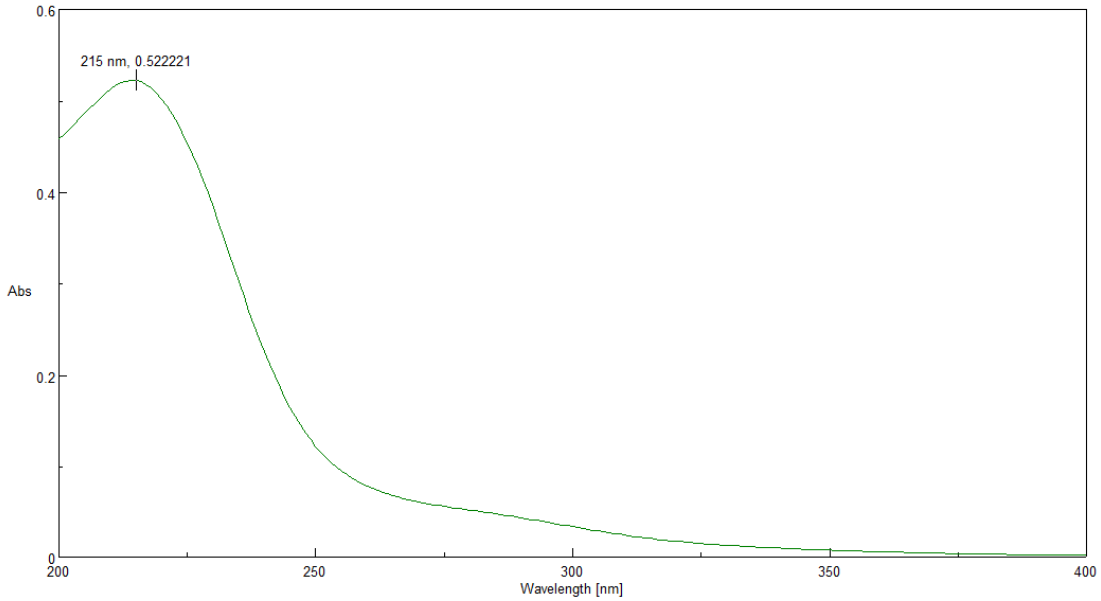



**Figure S20** UV spectrum of **2**

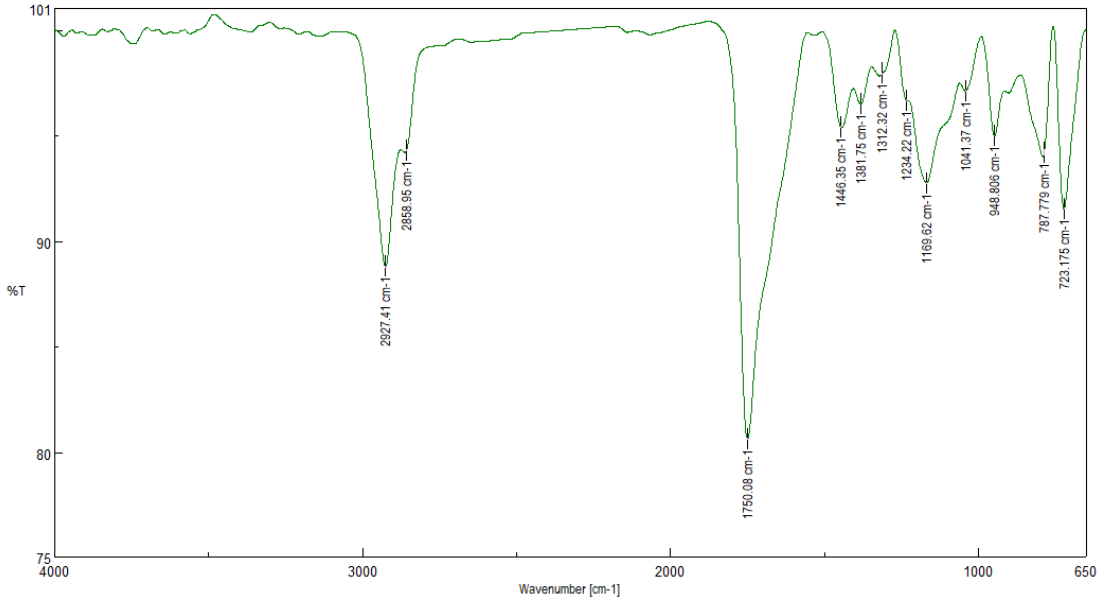



**Figure S21** IR spectrum of **2**

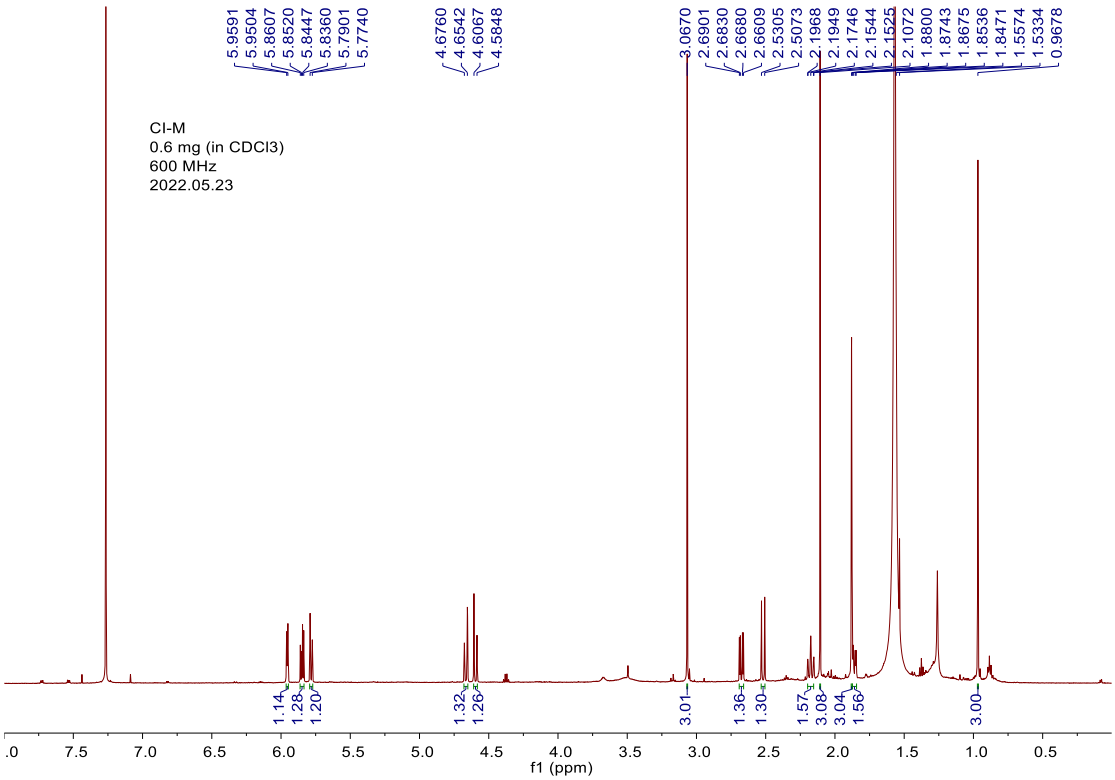



**Figure S22** $^{1}$H NMR spectrum of **3** (600 MHz, $CDCl_3$)

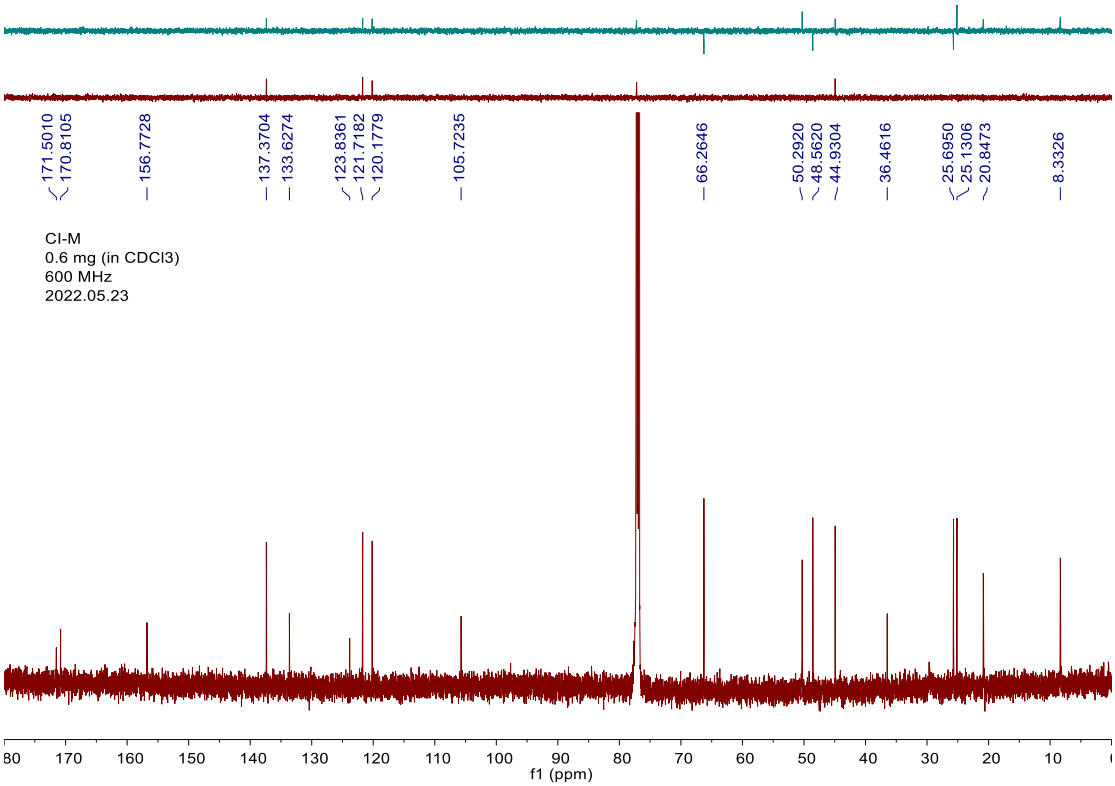



**Figure S23** $^{13}$C NMR spectrum of **3** (125 MHz, $CDCl_3$)

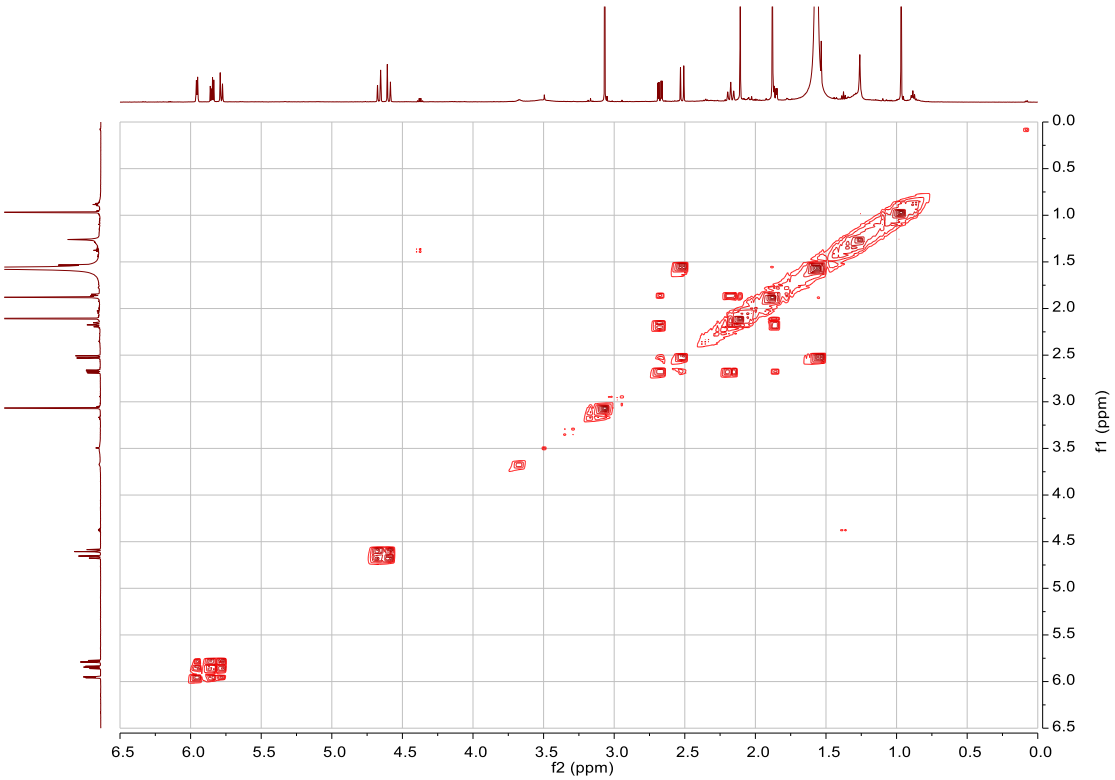



**Figure S24** COSY spectrum of **3**

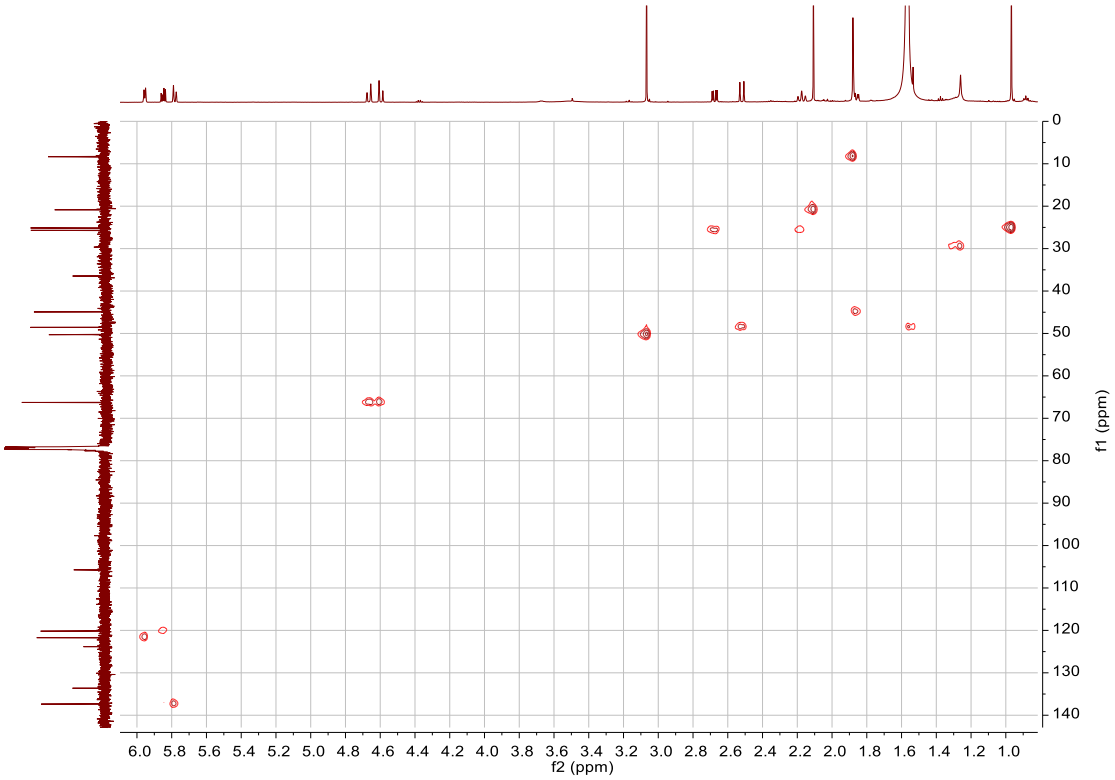



**Figure S25** HSQC spectrum of **3**

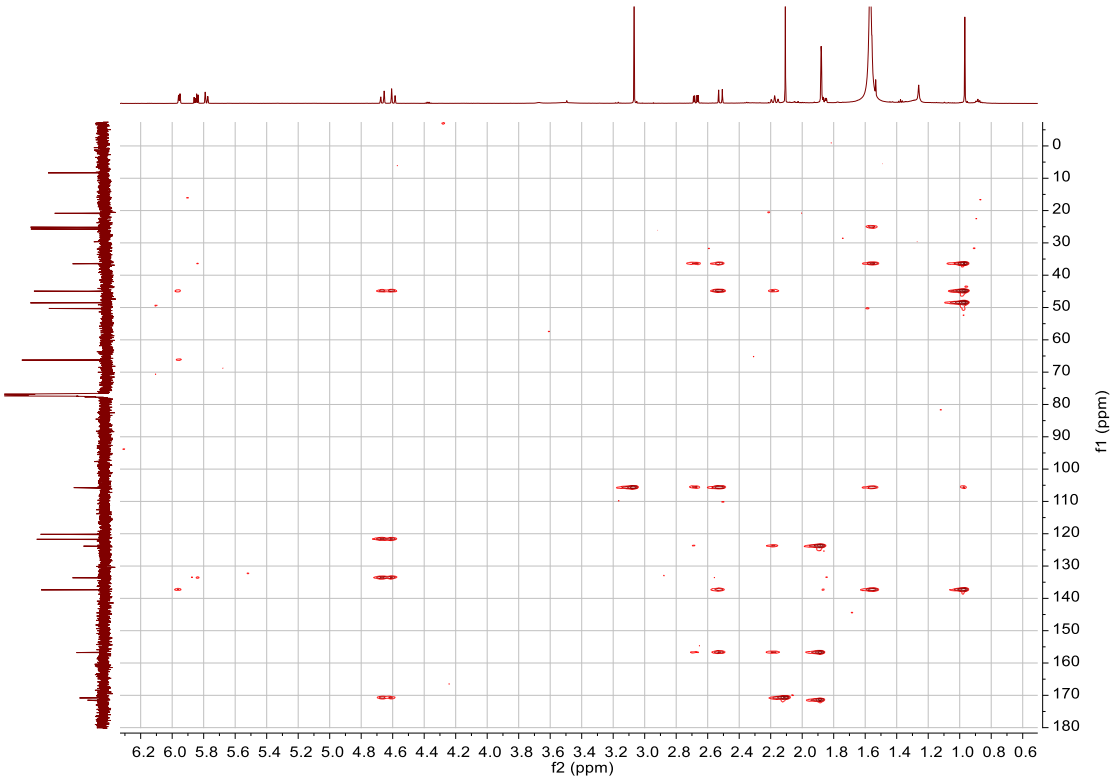



**Figure S26** HMBC spectrum of **3**

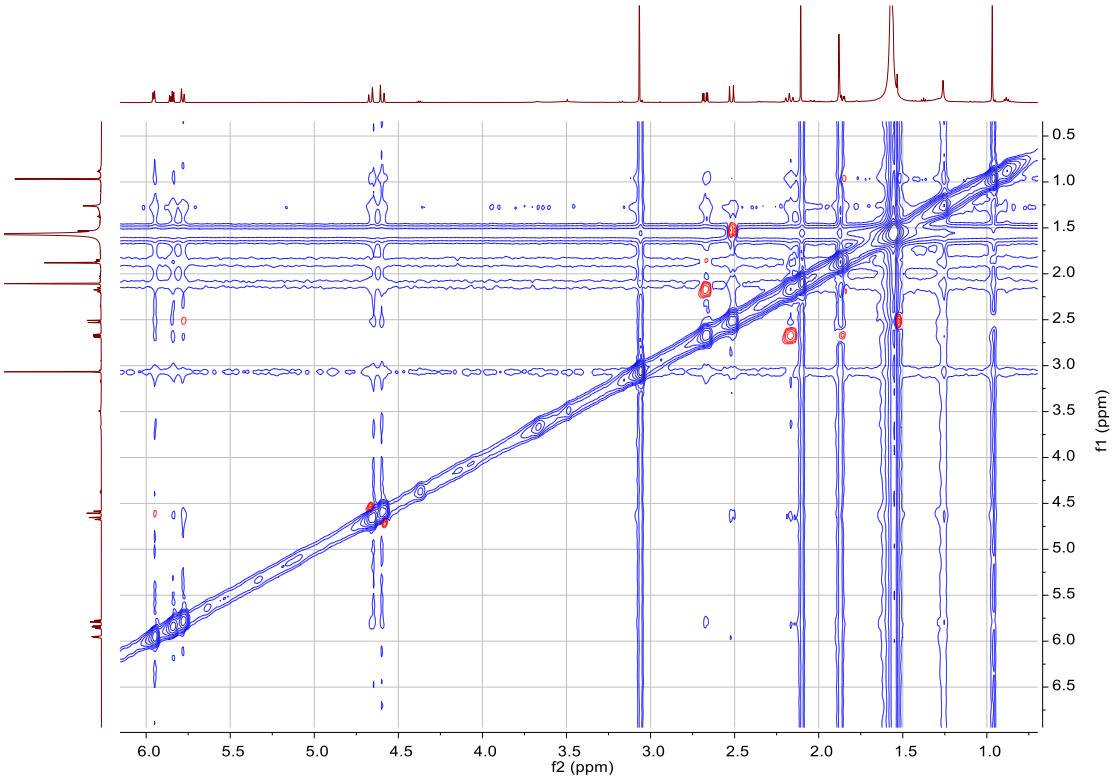
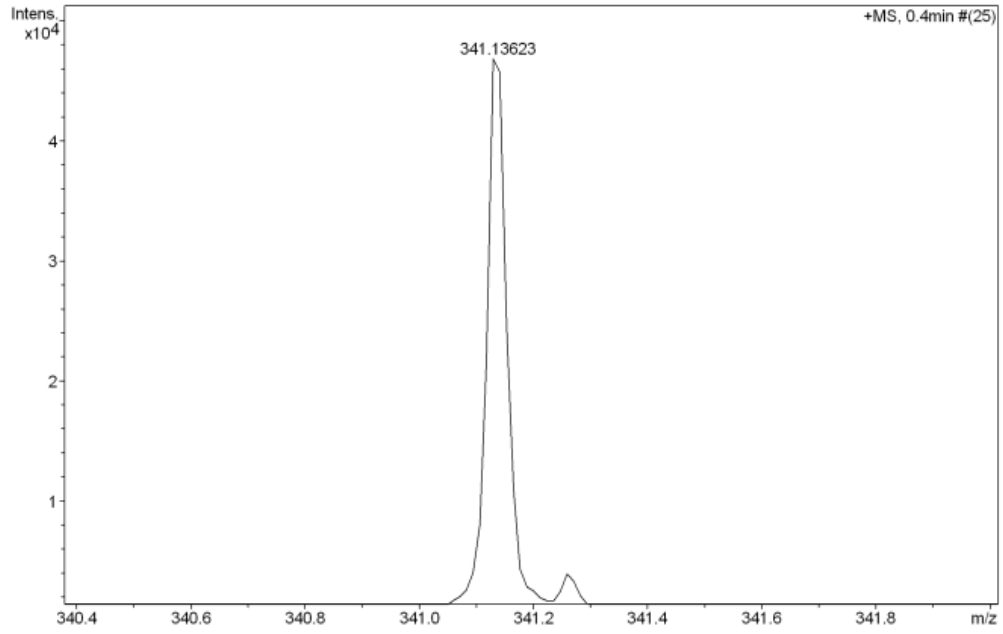



**Figure S27** NOESY spectrum of **3**

Mass Spectrum SmartFormula Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\0819\CIMR.d | | 8/23/2022 11:57:34 AM |
| Method | tune_wide_pos_20220422.m | | Operator: YU HSIAO-CHING |
| Sample Name | CI-M | | Instrument: BRUKER micrOTOF-Q |
| Comment | Positive | | |




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 341.13623 | 1 | C 18 H 22 Na O 5 | 100.00 | 341.13594 | -0.29 | -0.84 | 31.7 | 7.5 | even | ok |

**Figure S28** HRESIMS spectrum of **3**

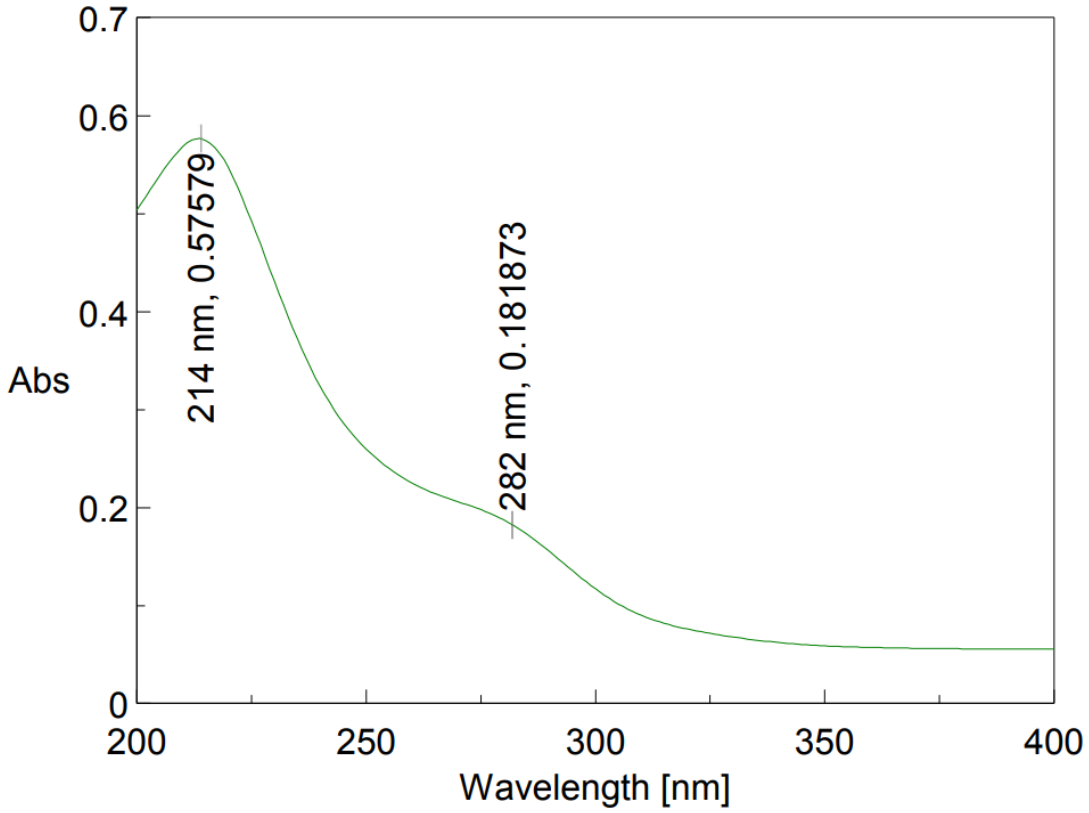



**Figure S29** UV spectrum of **3**

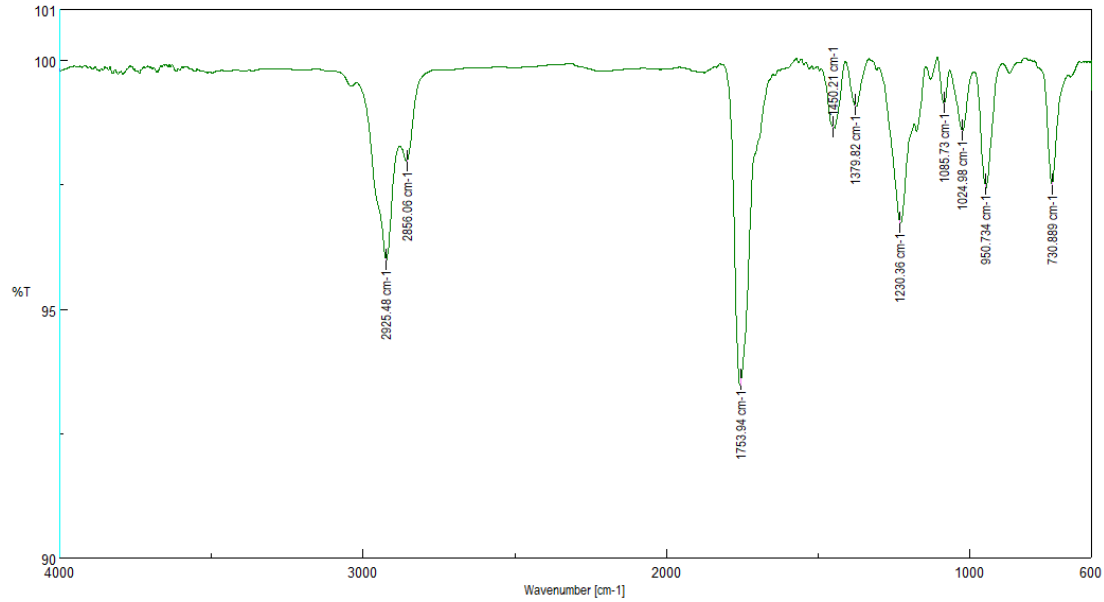



**Figure S30** IR spectrum of **3**

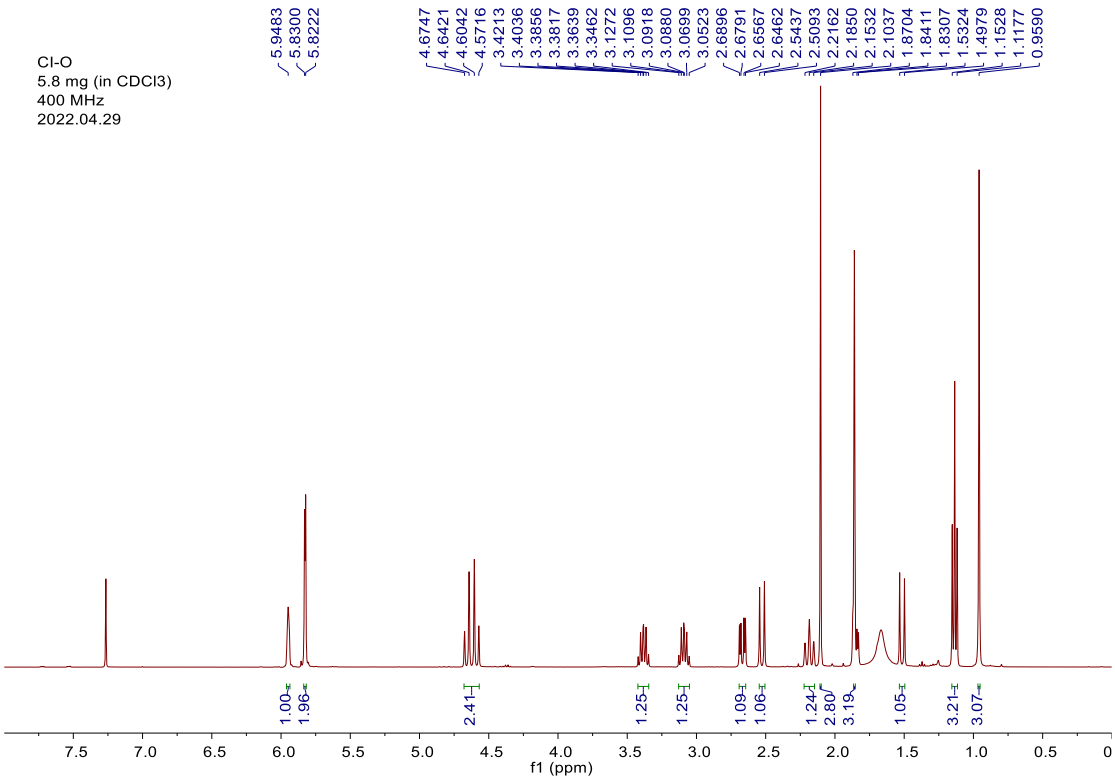



**Figure S31** $^{1}$H NMR spectrum of **4** (400 MHz, $CDCl_3$)

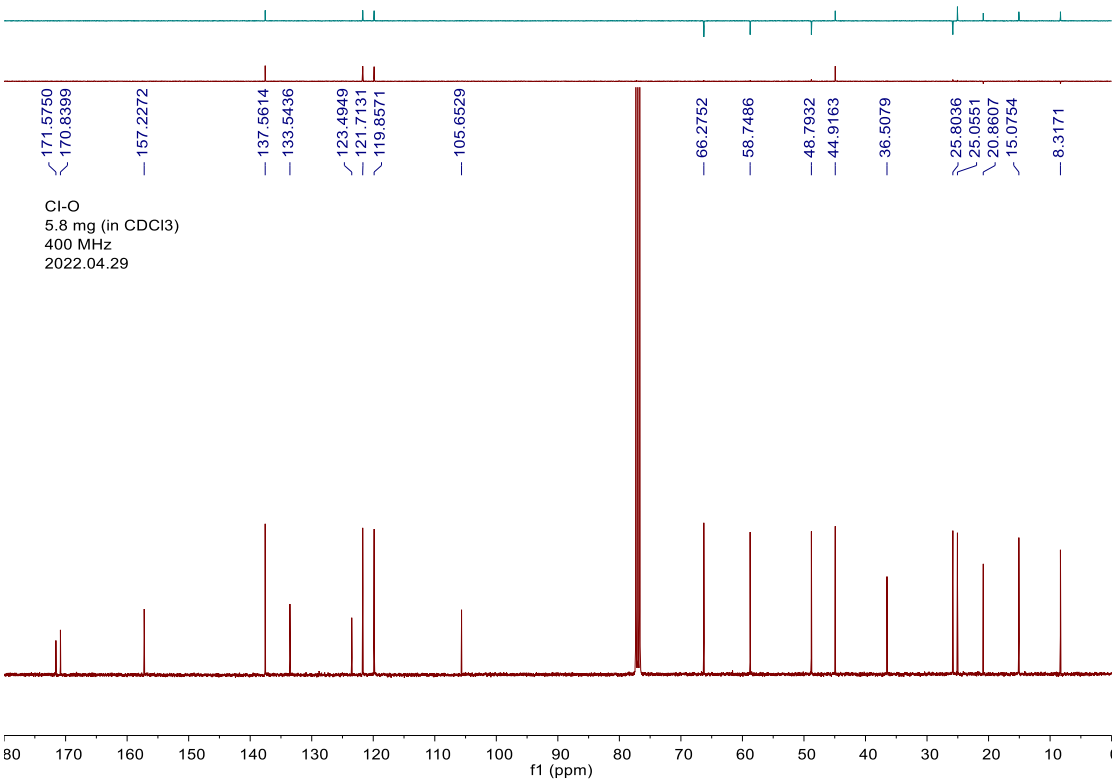



**Figure S32** $^{13}$C NMR spectrum of **4** (100 MHz, $CDCl_3$)

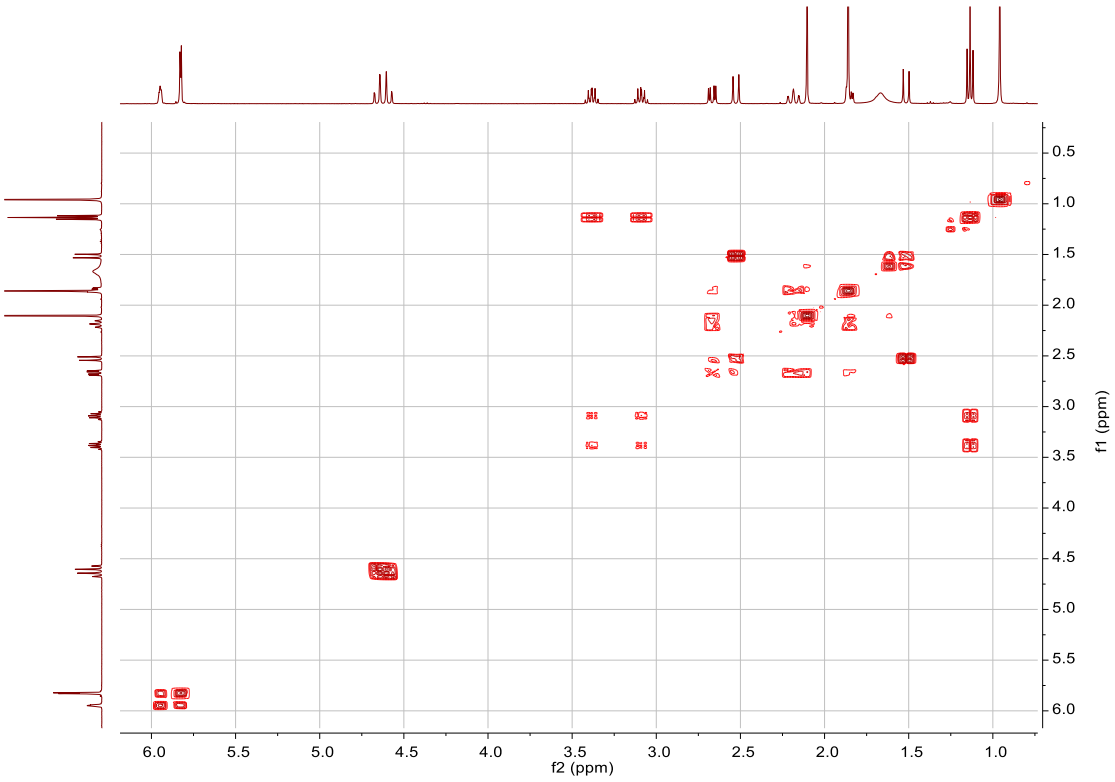



**Figure S33** COSY spectrum of **4**

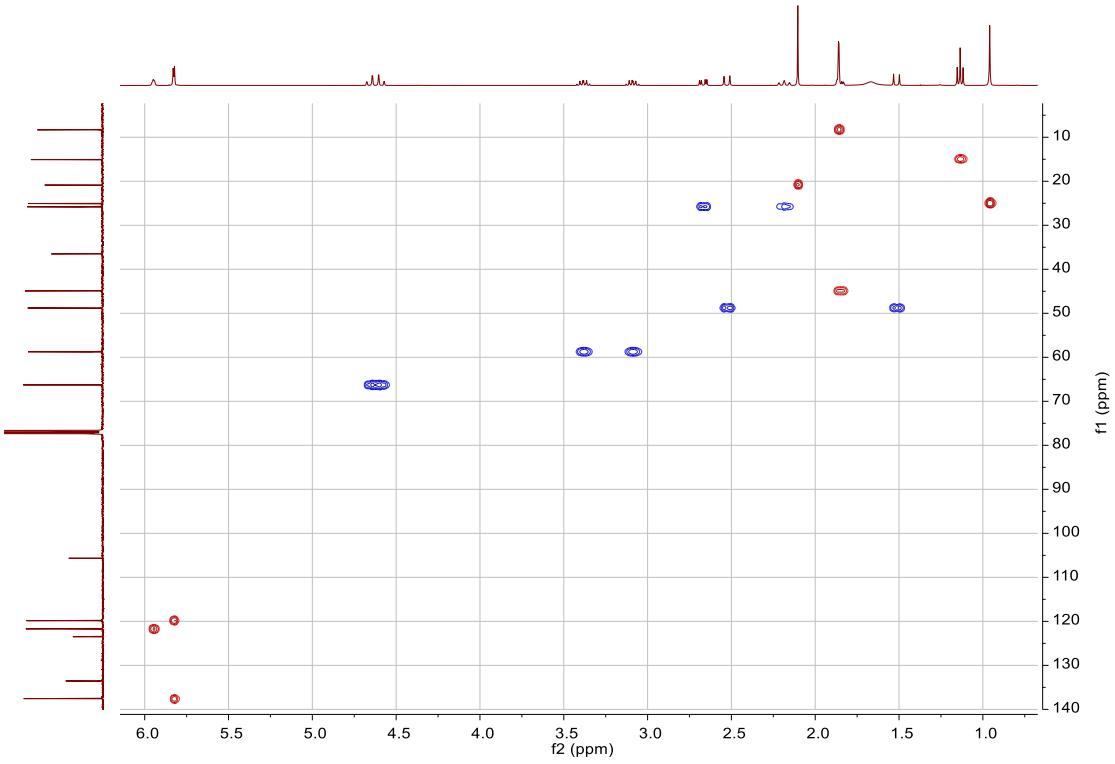



**Figure S34** HSQC spectrum of **4**

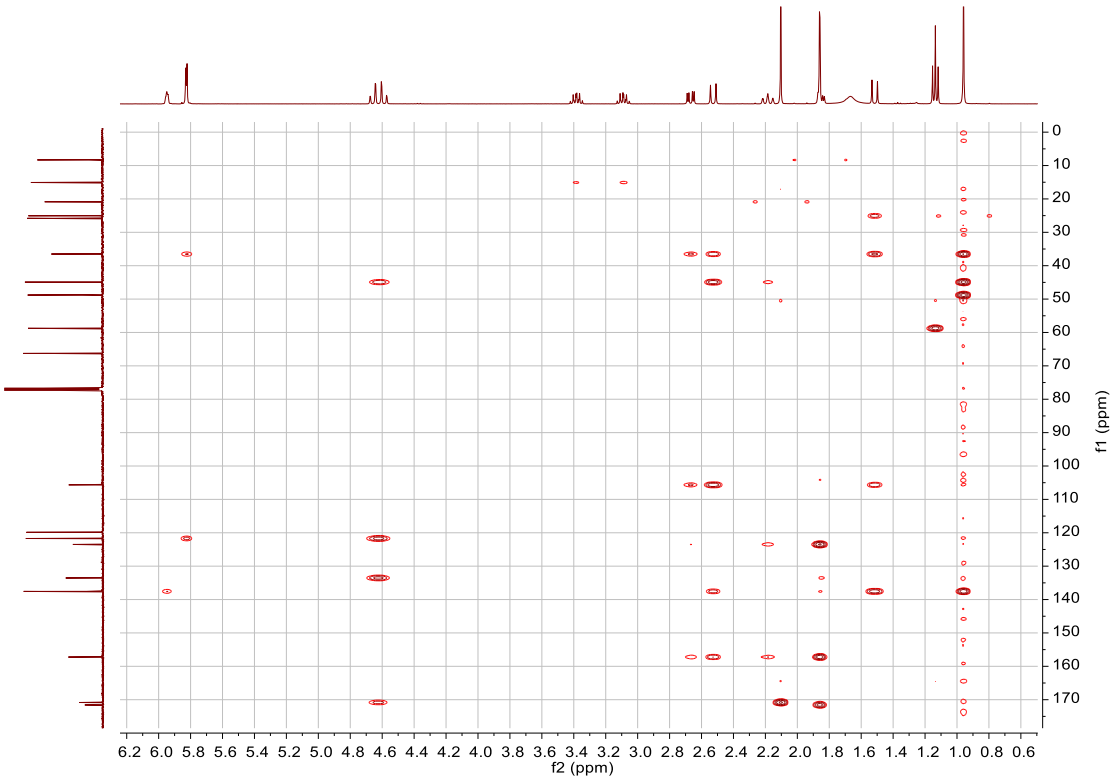



**Figure S35** HMBC spectrum of **4**

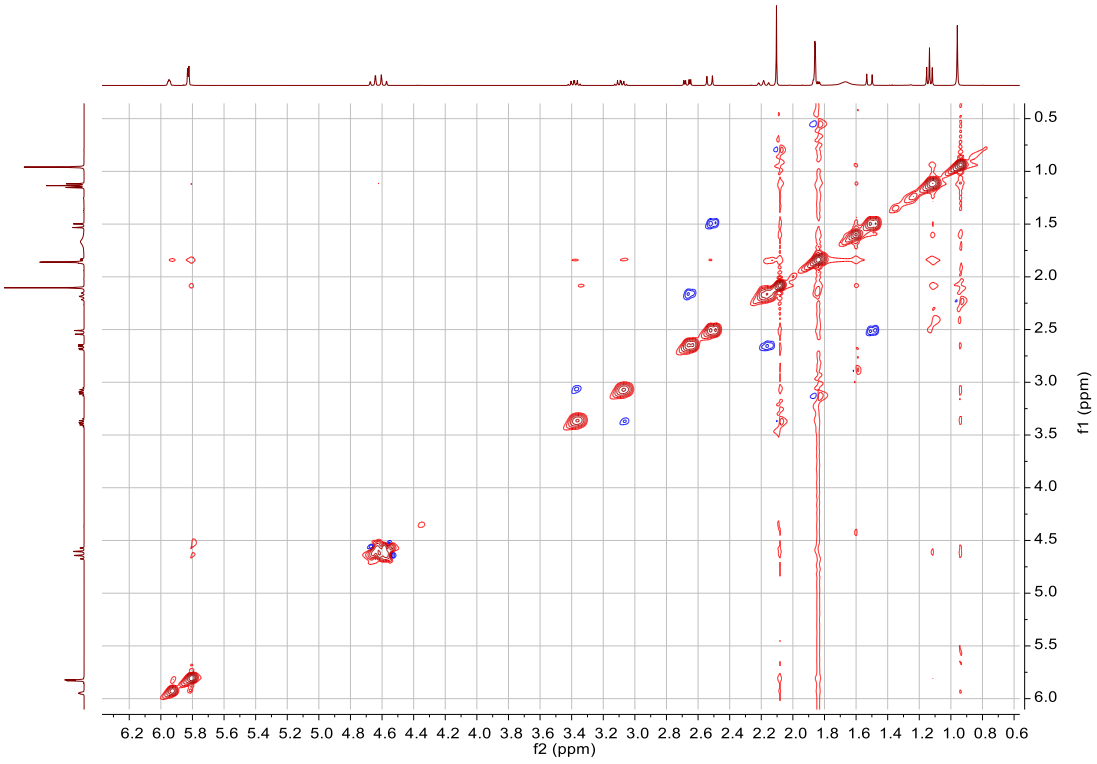
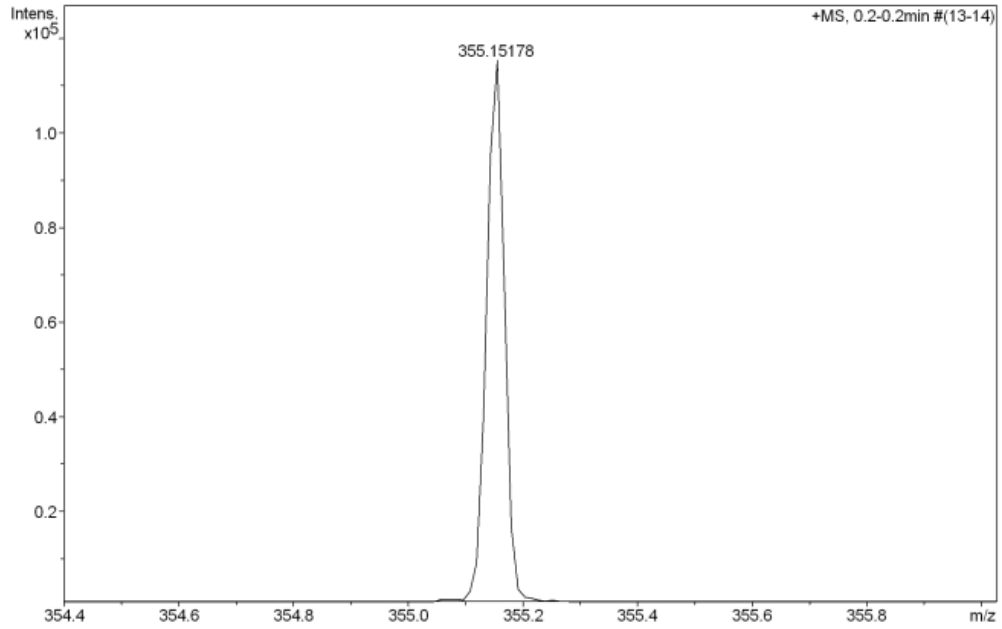



**Figure S36** NOESY spectrum of **4**

Mass Spectrum SmartFormula Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\0819\CIOR1.d | | 8/23/2022 11:59:58 AM |
| Method | tune_wide_pos_20220422.m | | Operator: YU HSIAO-CHING |
| Sample Name | CI-O | | Instrument: BRUKER micrOTOF-Q |
| Comment | Positive | | |




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 355.15178 | 1 | C 19 H 24 Na O 5 | 100.00 | 355.15159 | -0.19 | -0.52 | 25.5 | 7.5 | even | ok |

**Figure S37** HRESIMS spectrum of **4**

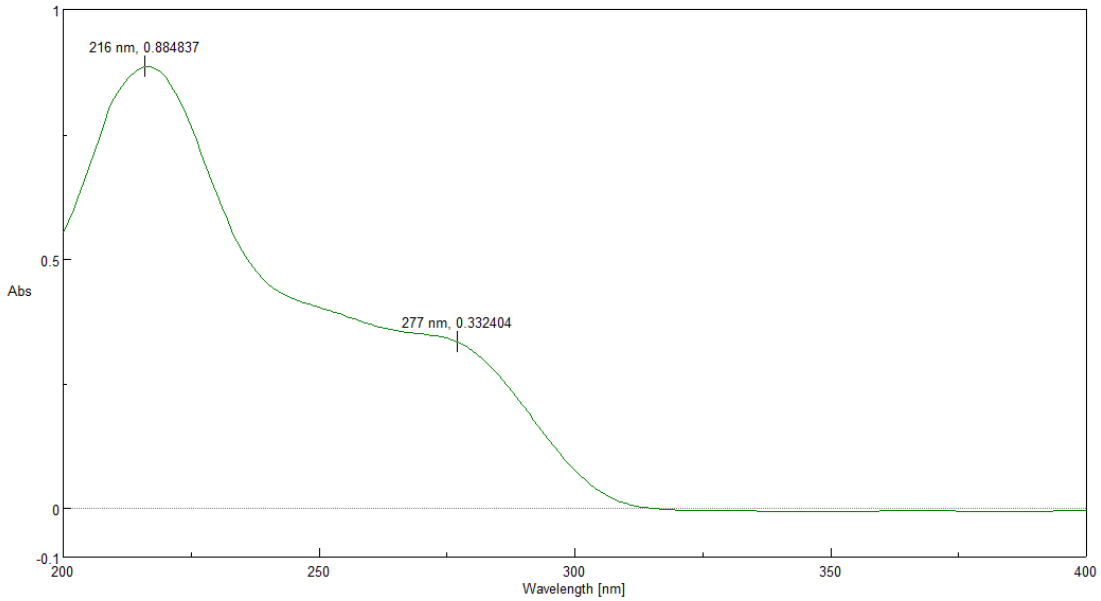



**Figure S38** UV spectrum of **4**

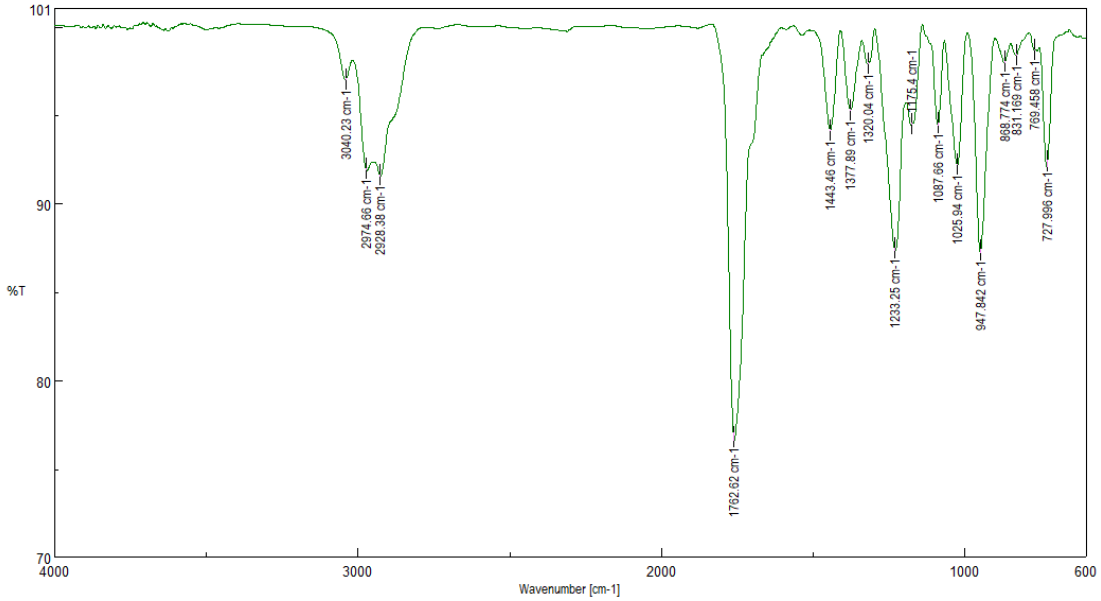



**Figure S39** IR spectrum of **4**

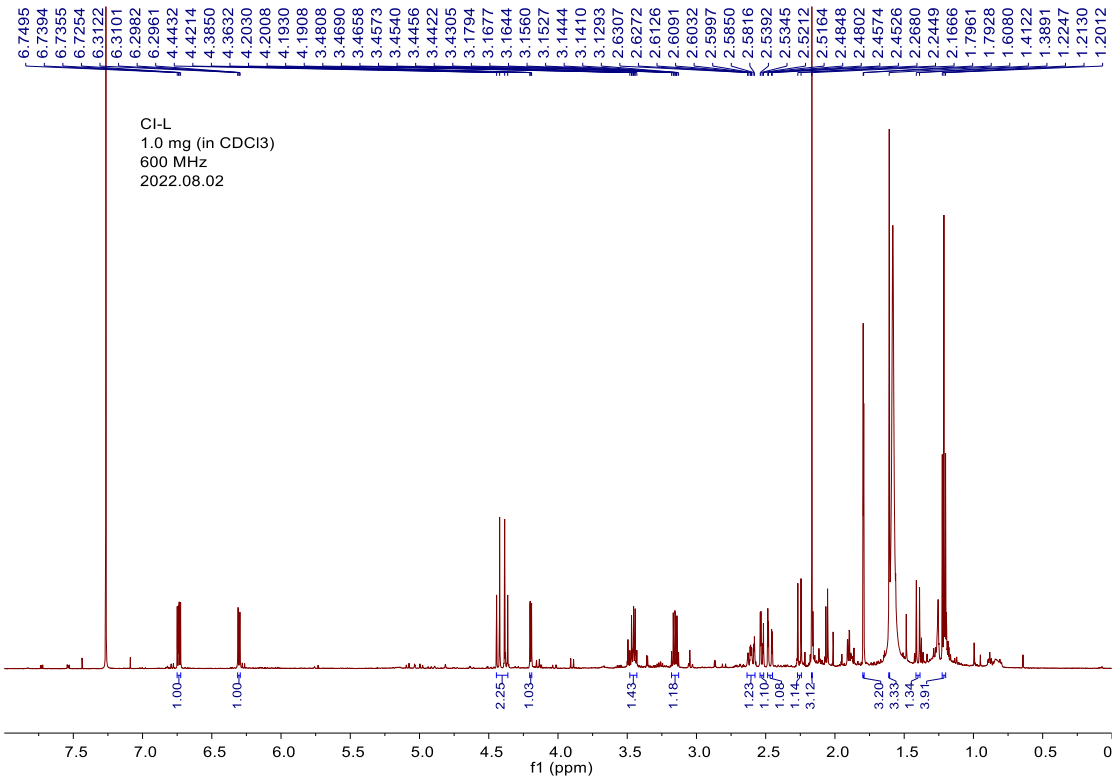



**Figure S40** $^{1}$H NMR spectrum of **5** (600 MHz, $CDCl_3$)

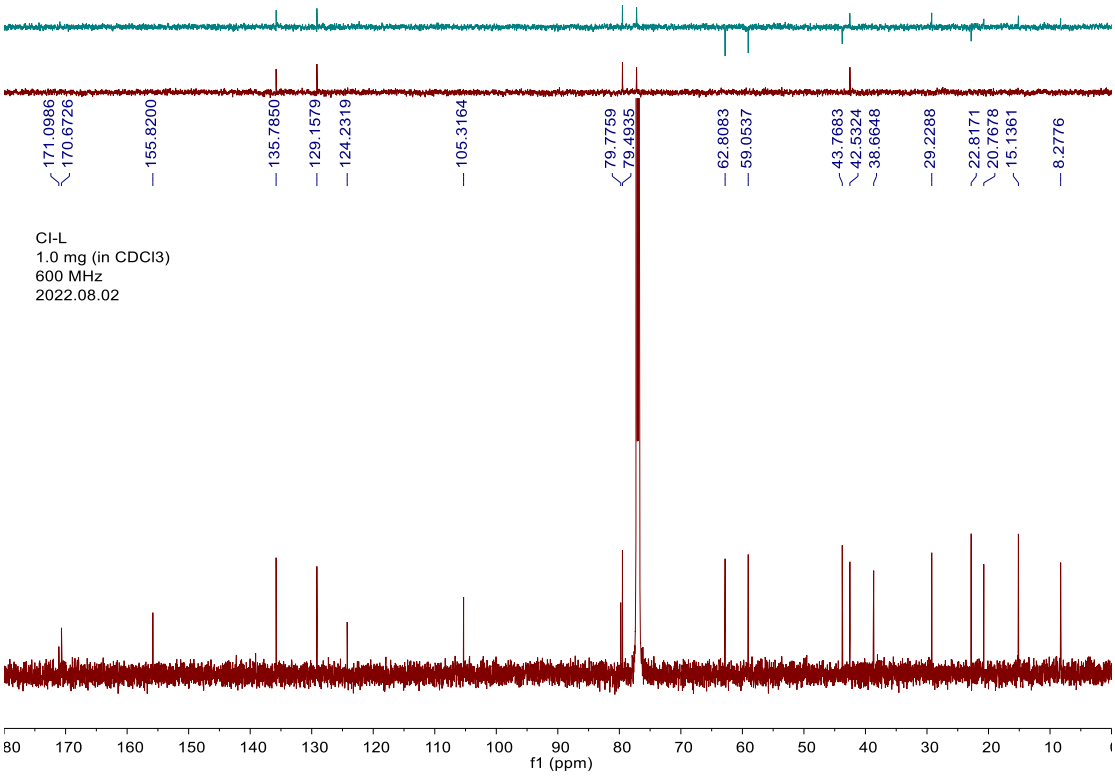



**Figure S41** $^{13}$C NMR spectrum of **5** (125 MHz, $CDCl_3$)

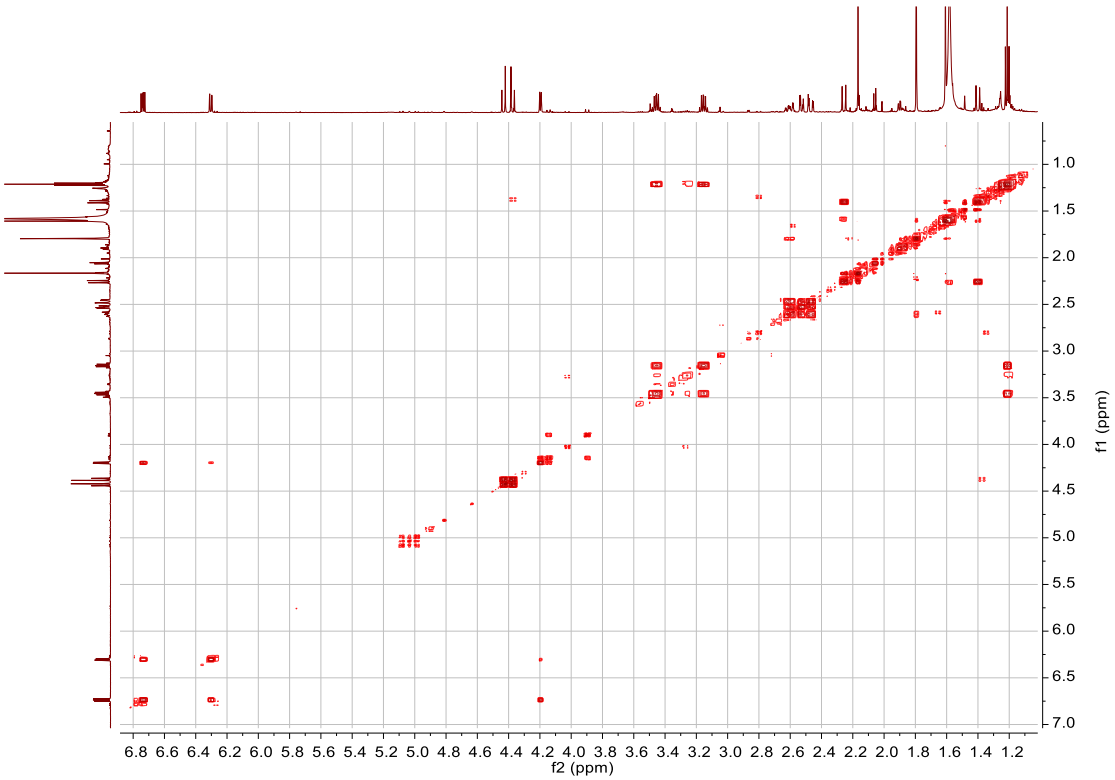



**Figure S42** COSY spectrum of **5**

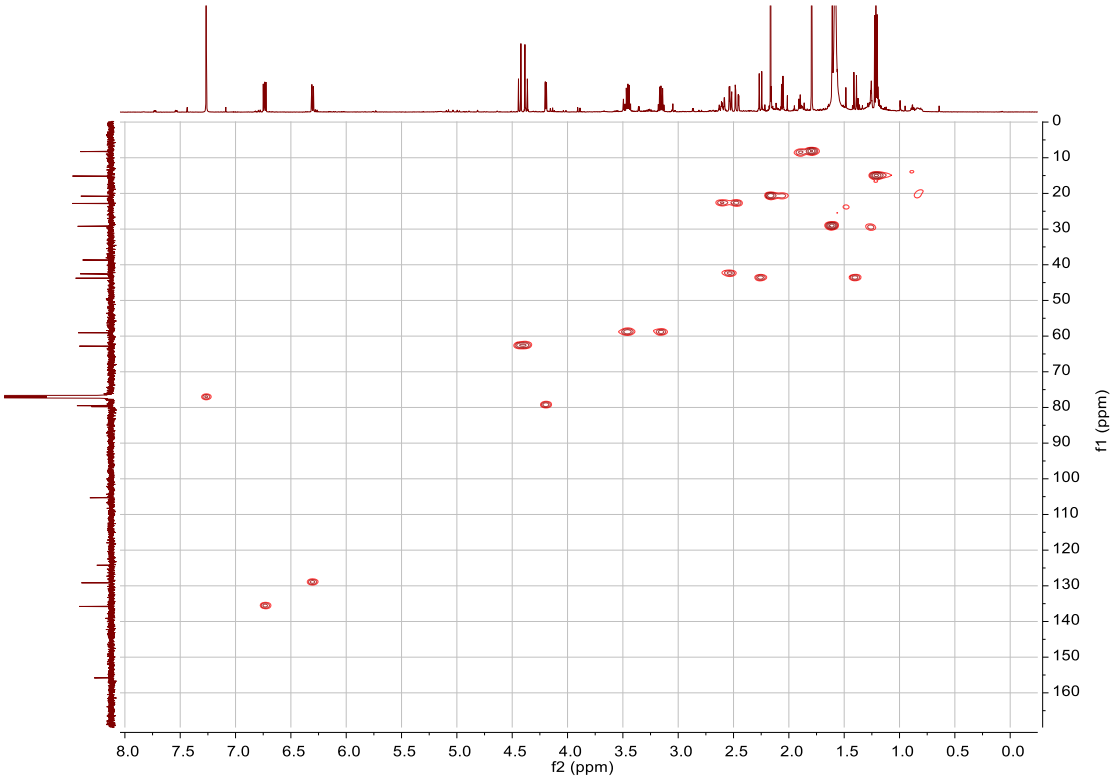



**Figure S43** HSQC spectrum of **5**

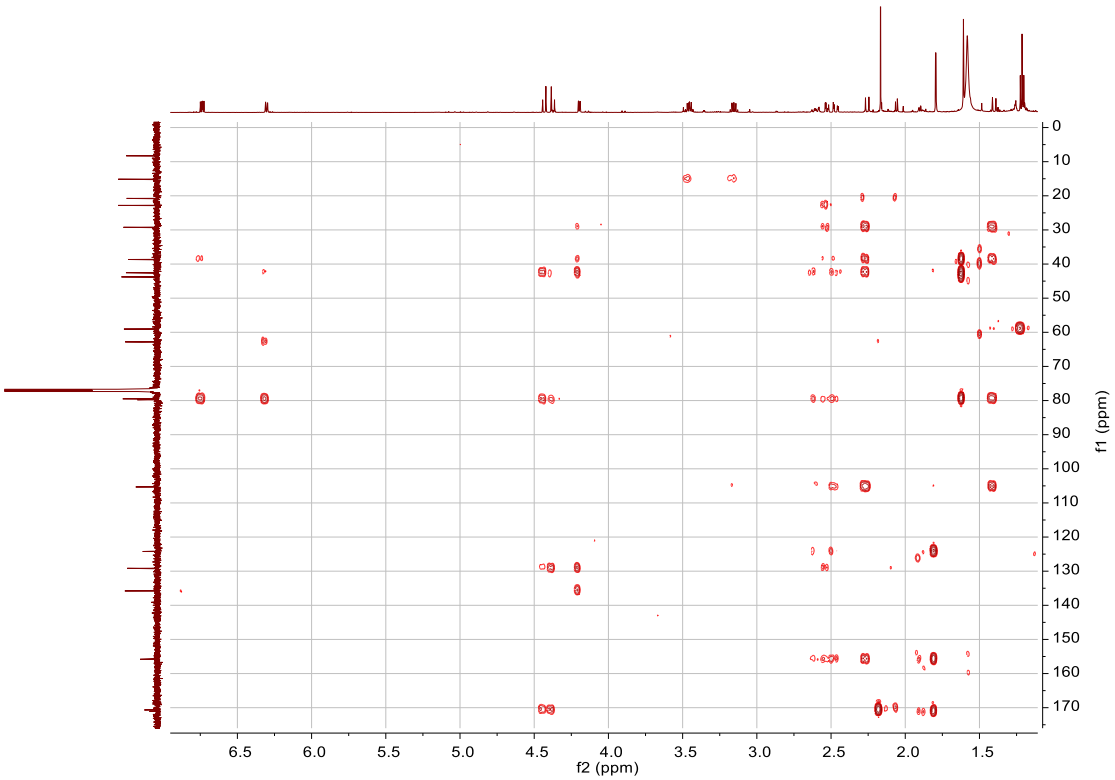



**Figure S44** HMBC spectrum of **5**

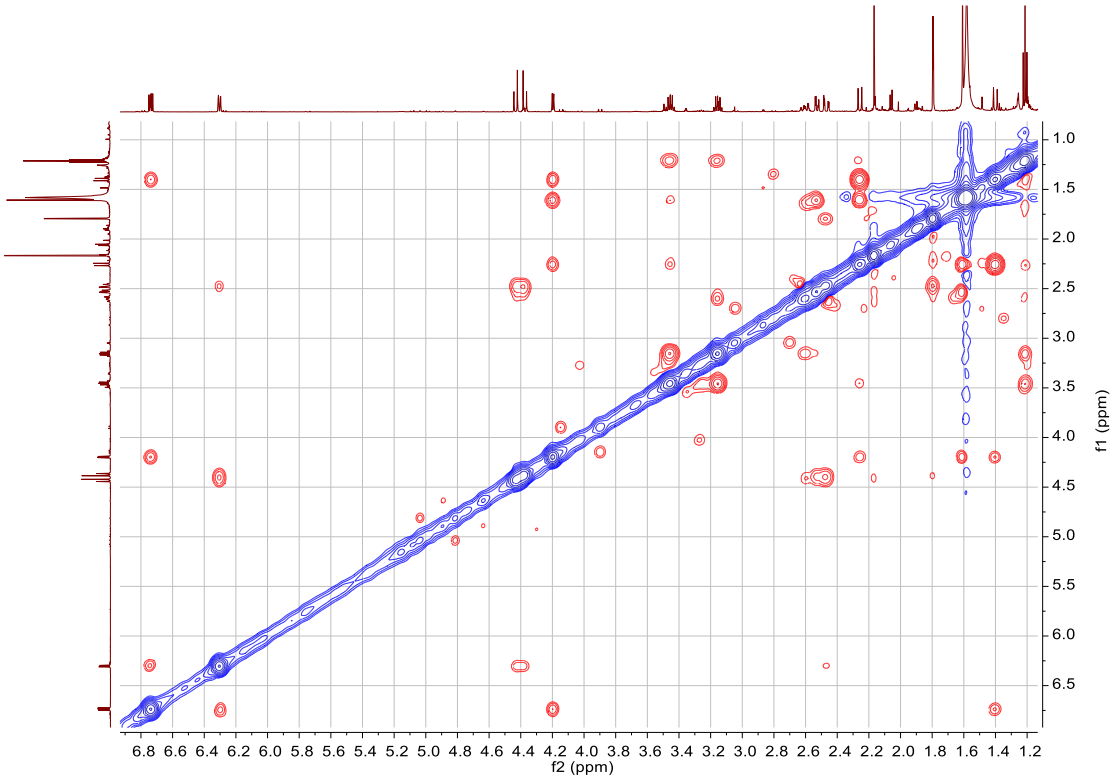
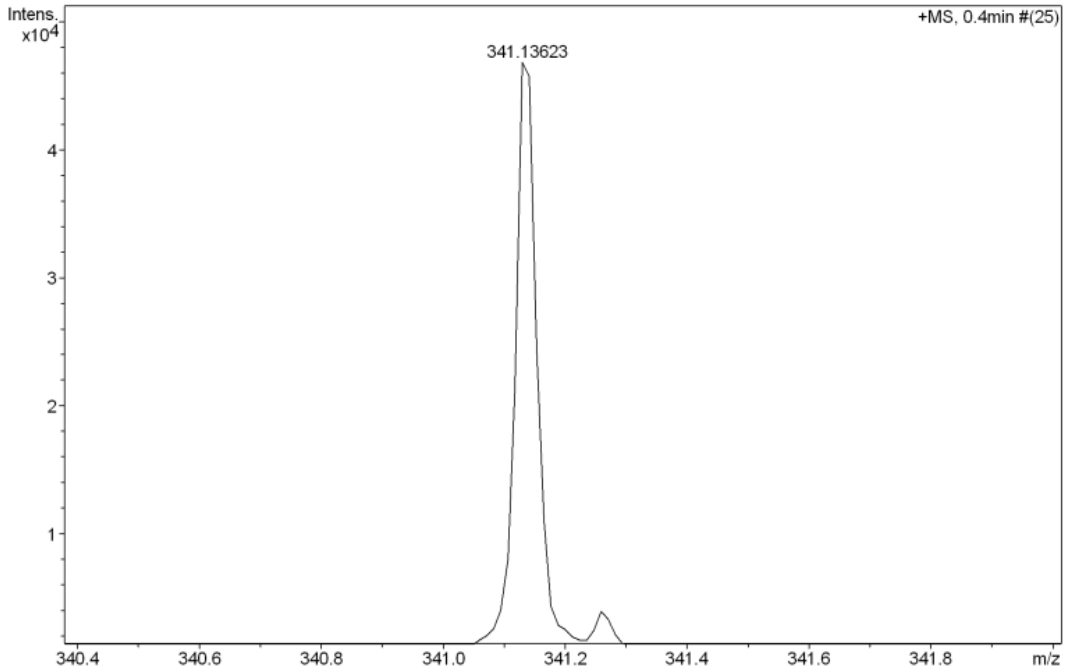



**Figure S45** NOESY spectrum of **5**

Mass Spectrum SmartFormula Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\0819\CIMR.d | | 8/23/2022 11:57:34 AM |
| Method | tune_wide_pos_20220422.m | | Operator: YU HSIAO-CHING |
| Sample Name | CI-M | | Instrument: BRUKER micrOTOF-Q |
| Comment | Positive | | |




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 341.13623 | 1 | C 18 H 22 Na O 5 | 100.00 | 341.13594 | -0.29 | -0.84 | 31.7 | 7.5 | even | ok |

**Figure S46** HRESIMS spectrum of **5**

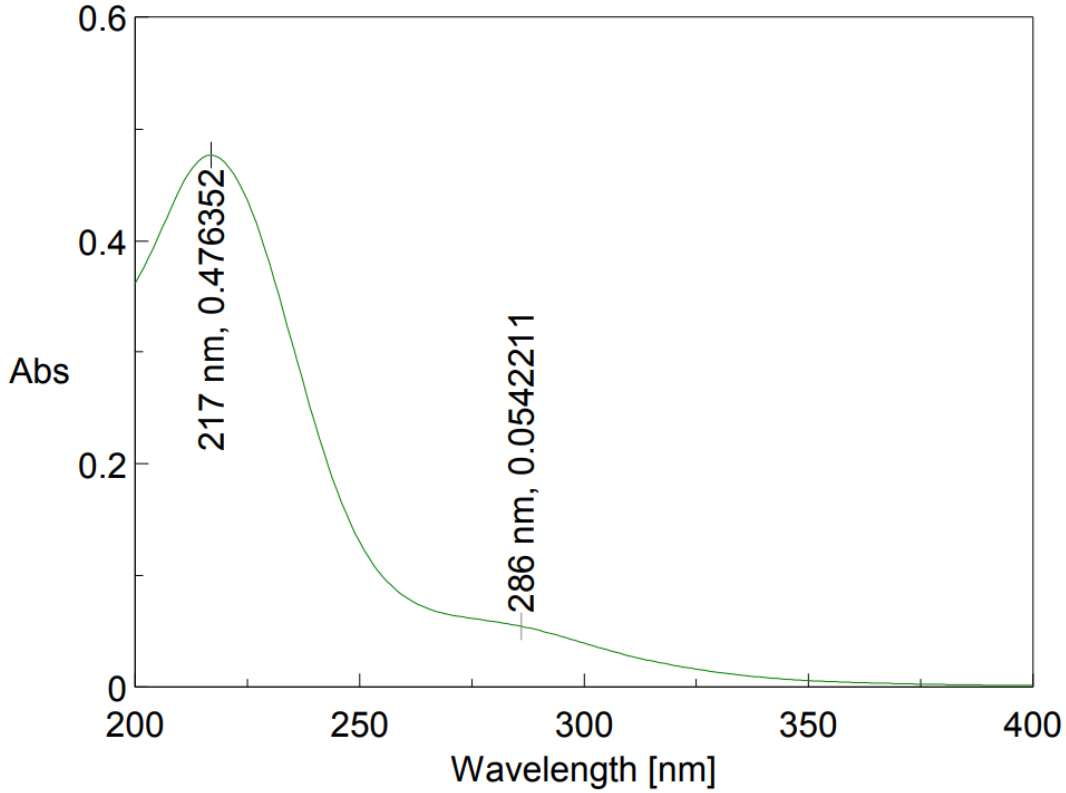



**Figure S47** UV spectrum of **5**

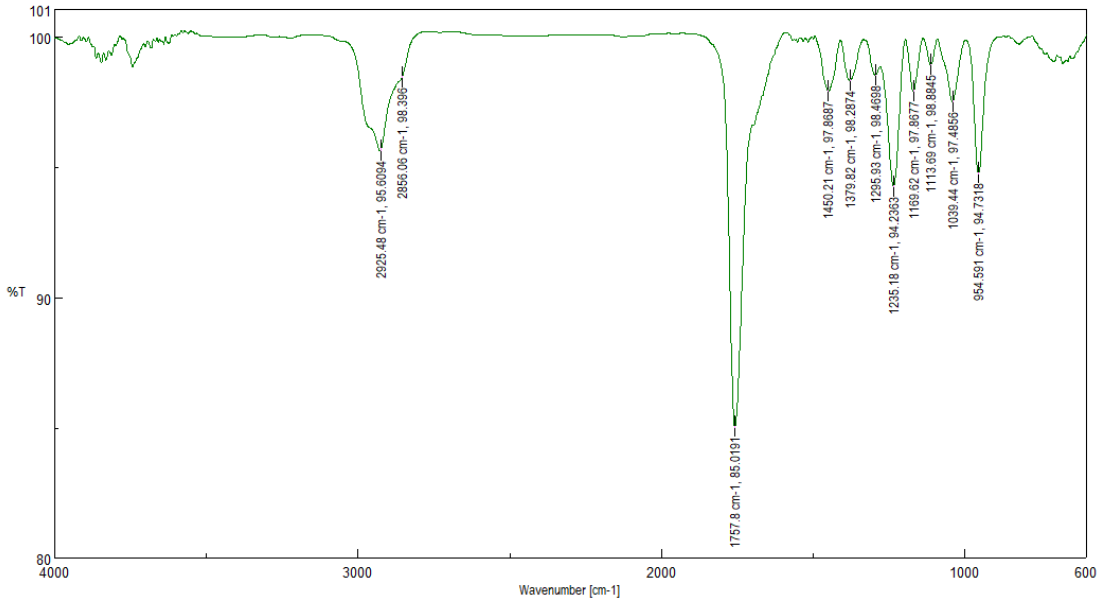



**Figure S48** IR spectrum of **5**

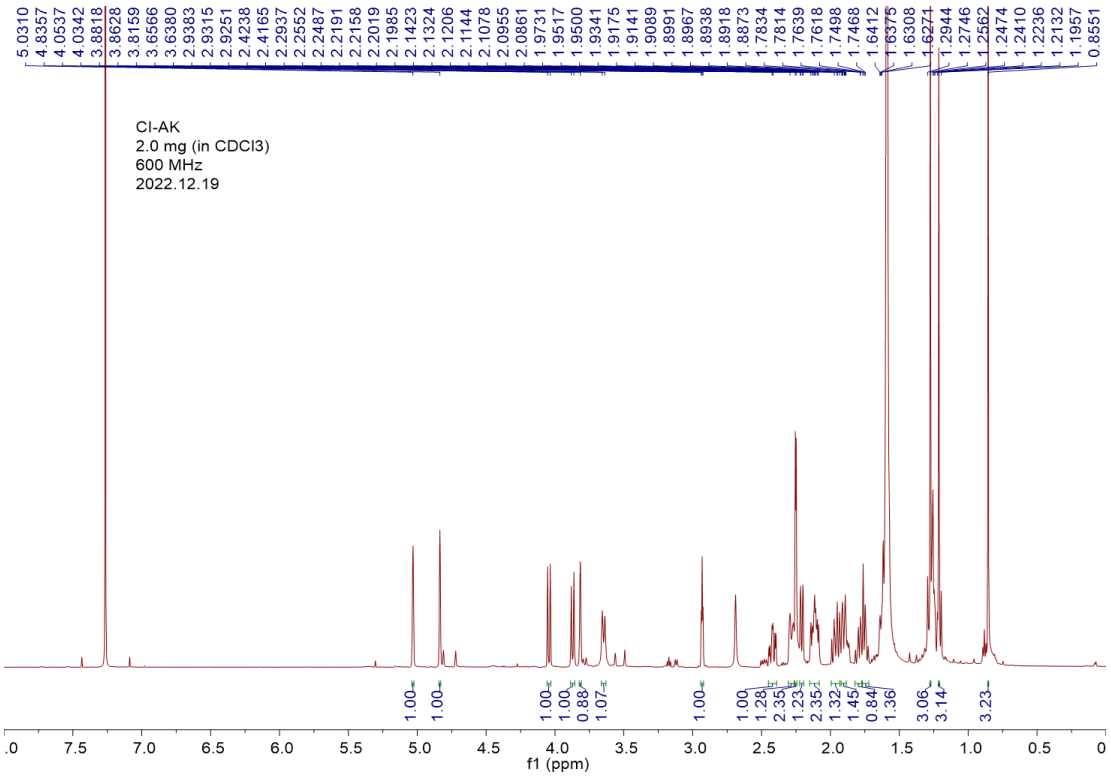



**Figure S49** $^{1}$H NMR spectrum of **6** (600 MHz, $CDCl_3$)

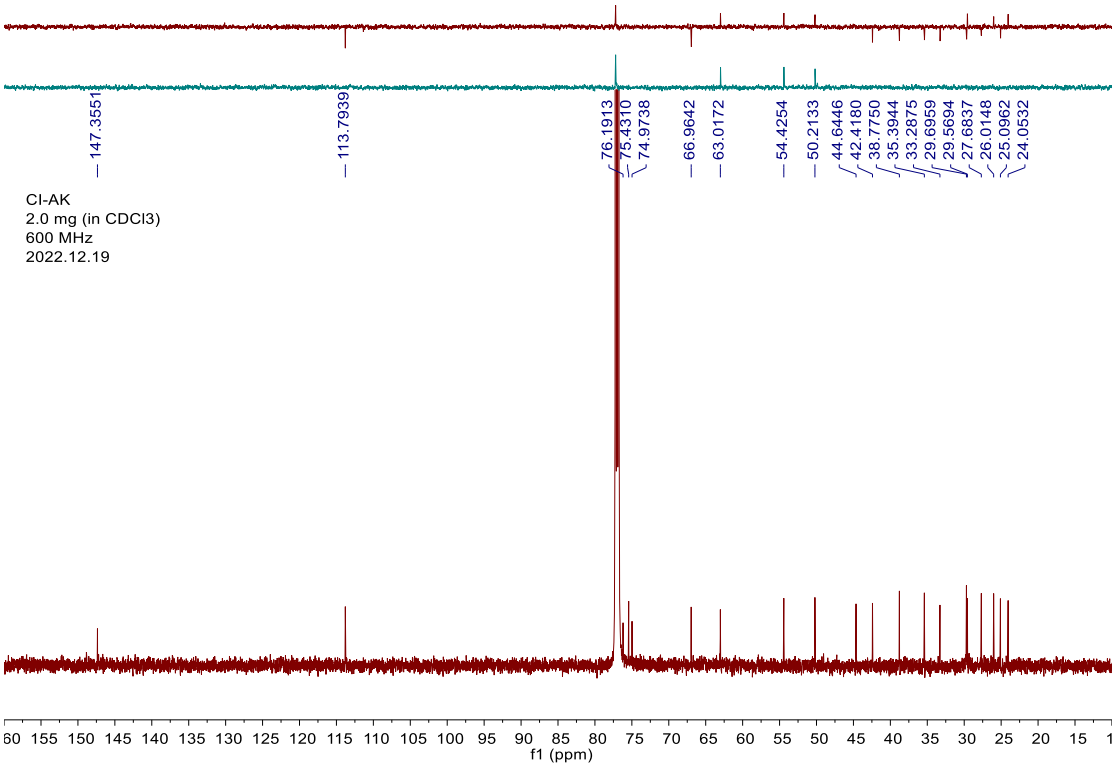



**Figure S50** $^{13}$C NMR spectrum of **6** (125 MHz, $CDCl_3$)

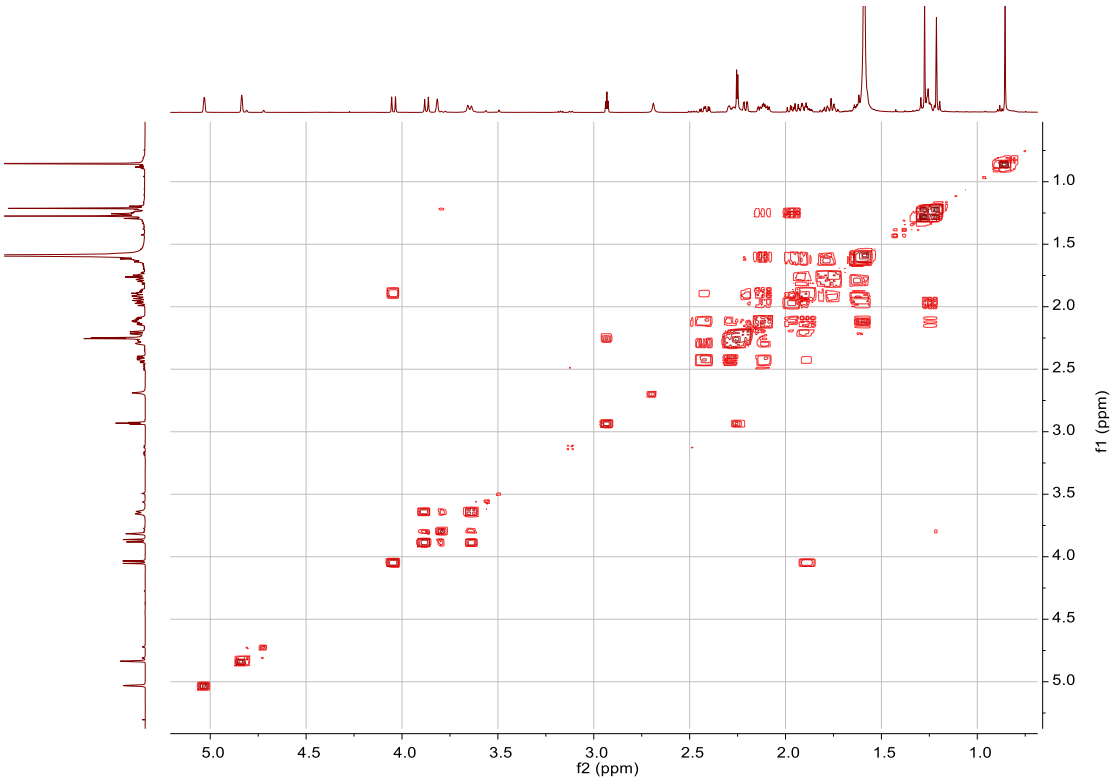



**Figure S51** COSY spectrum of **6**

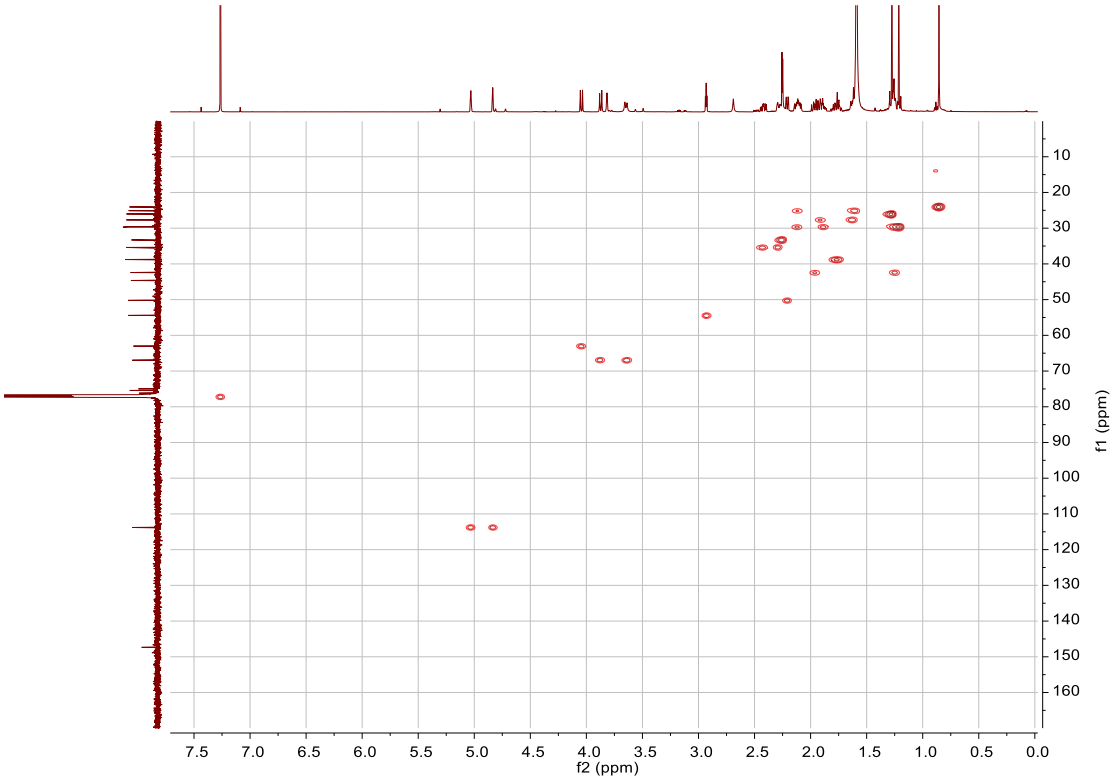



**Figure S52** HSQC spectrum of **6**

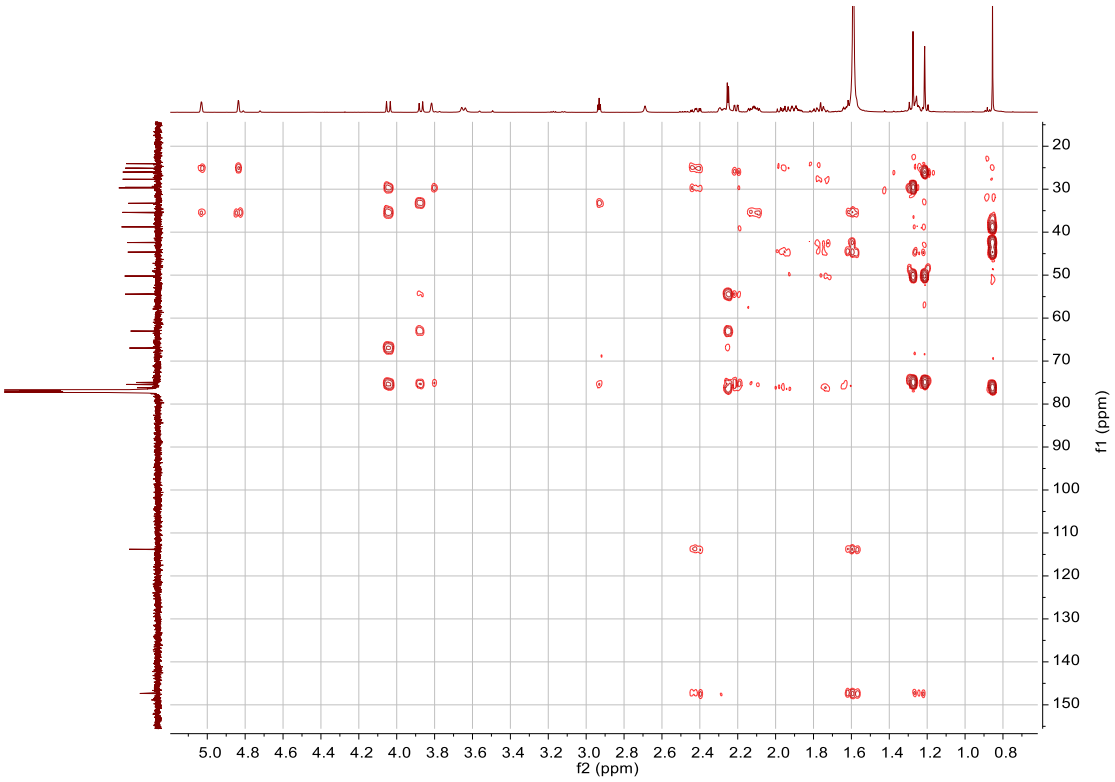



**Figure S53** HMBC spectrum of **6**

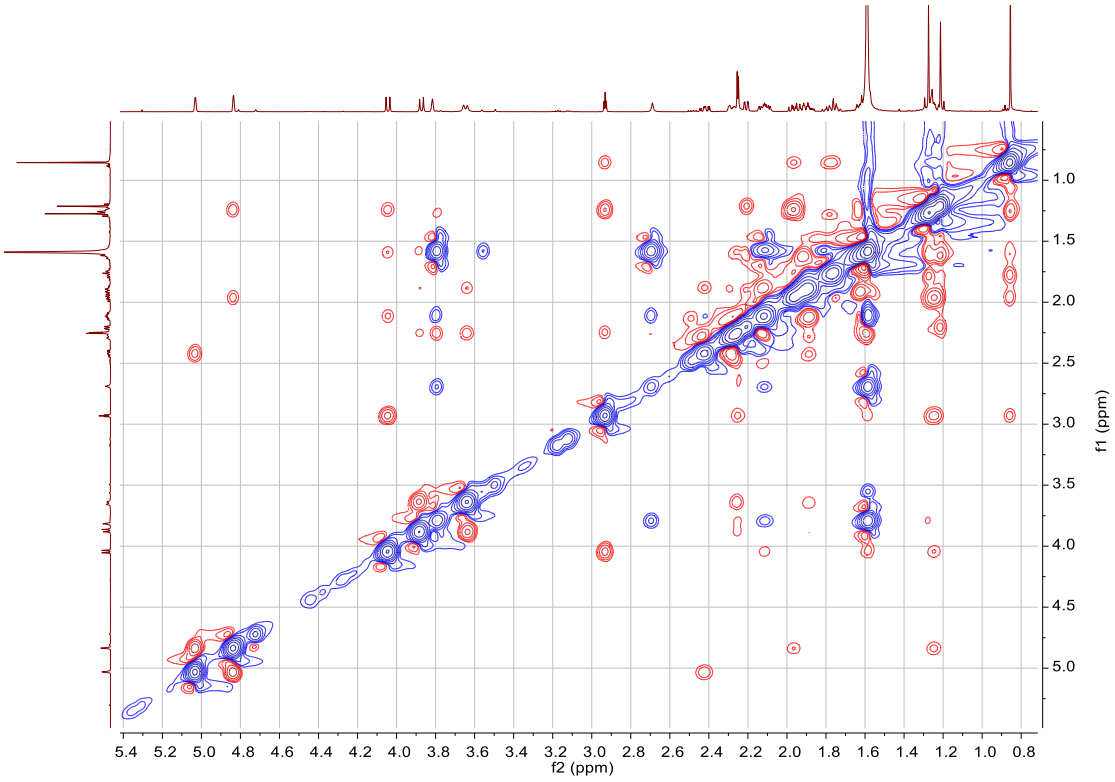
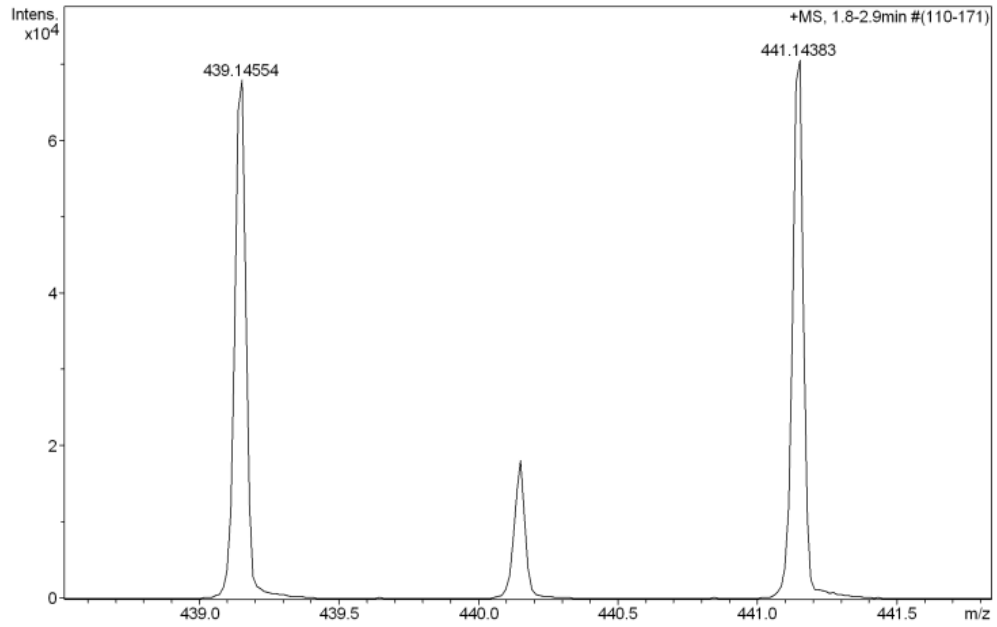



**Figure S54** NOESY spectrum of **6**

Mass Spectrum SmartFormula Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\1223\CIAKR.d | | 12/26/2022 11:30:15 AM |
| Method | tune_wide_pos_20220422.m | | Operator: YU HSIAO-CHING |
| Sample Name | CI-AK | | Instrument: BRUKER micrOTOF-Q |
| Comment | ESI Positive | | |




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 439.14554 | 1 | C 20 H 33 Br Na O 4 | 100.00 | 439.14544 | -0.10 | -0.22 | 23.8 | 3.5 | even | ok |

**Figure S55** HRESIMS spectrum of **6**

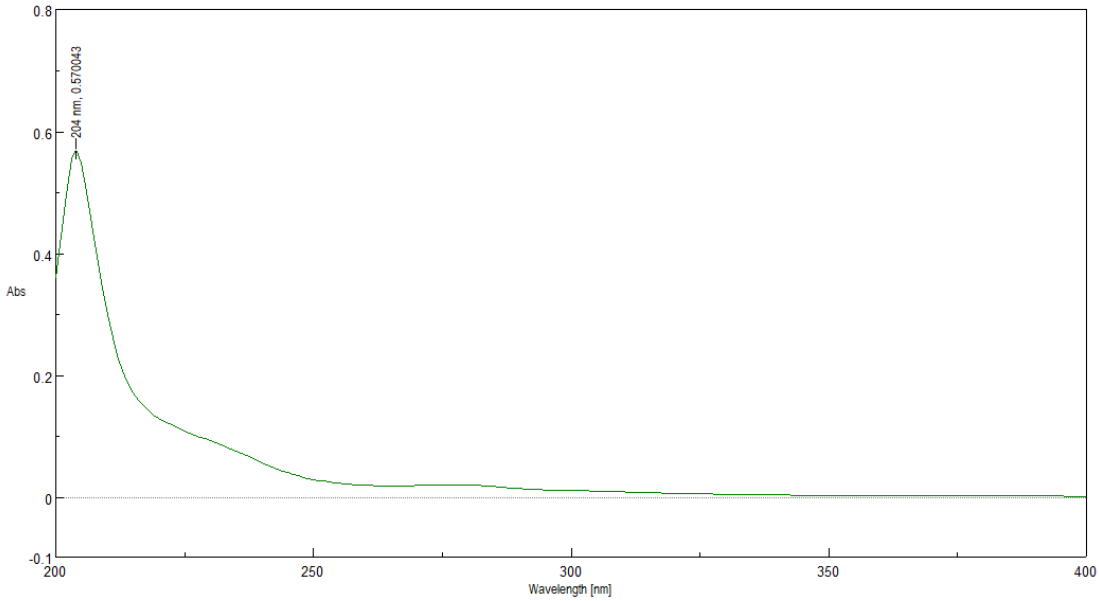



**Figure S56** UV spectrum of **6**

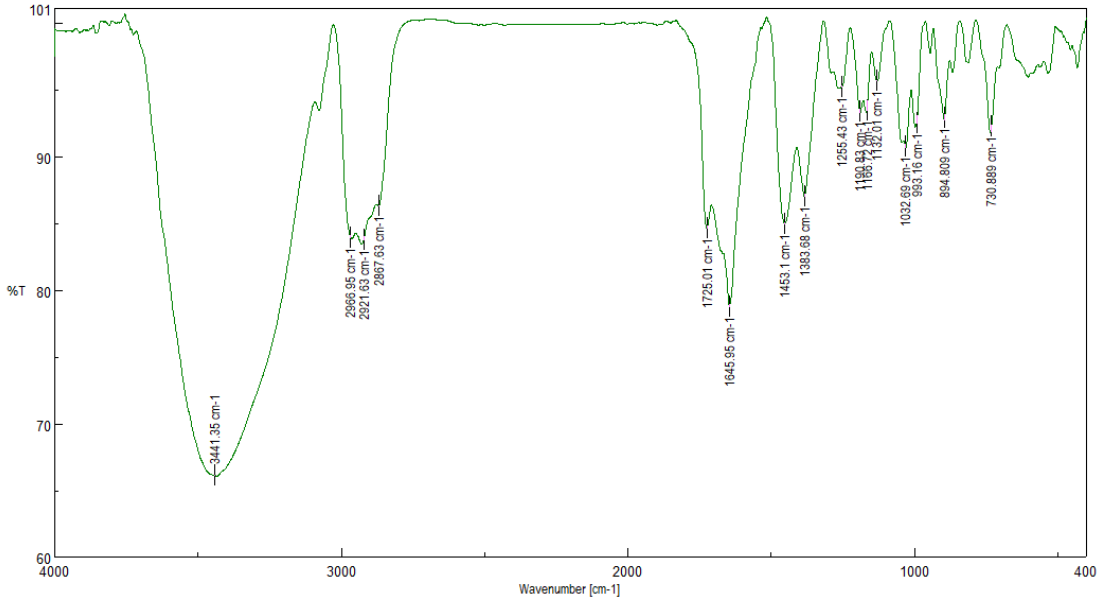



**Figure S57** IR spectrum of **6**

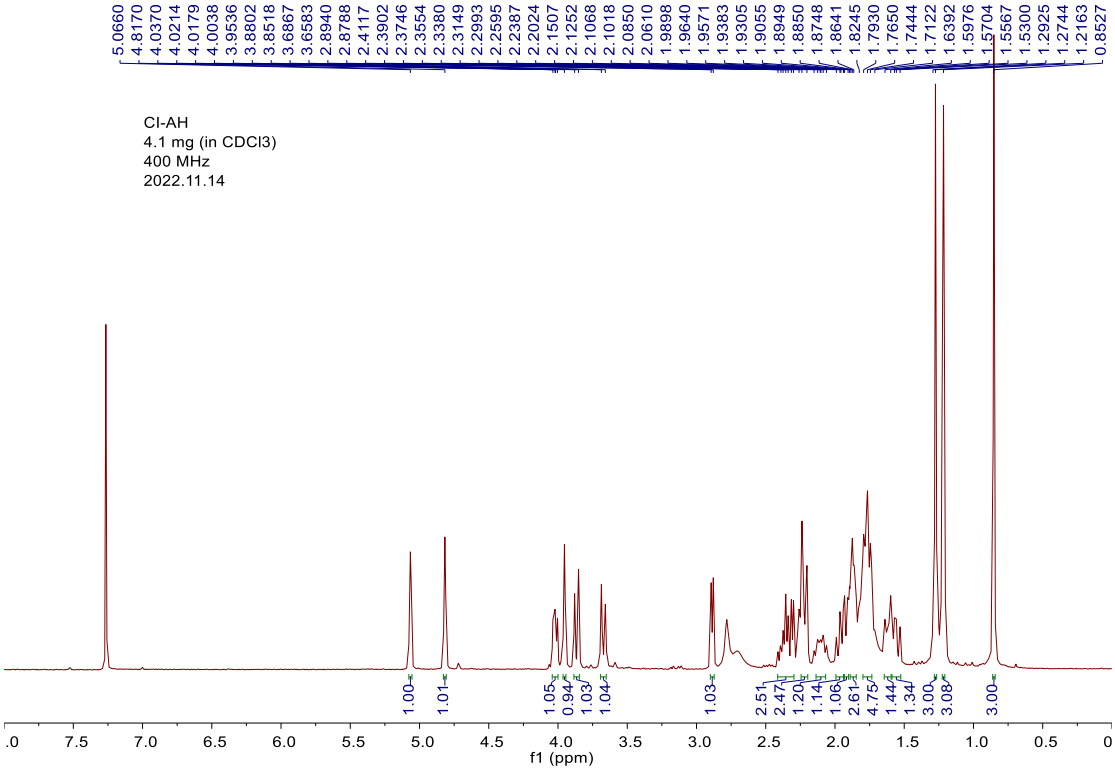



**Figure S58** $^{1}$H NMR spectrum of **7** (400 MHz, $CDCl_3$)

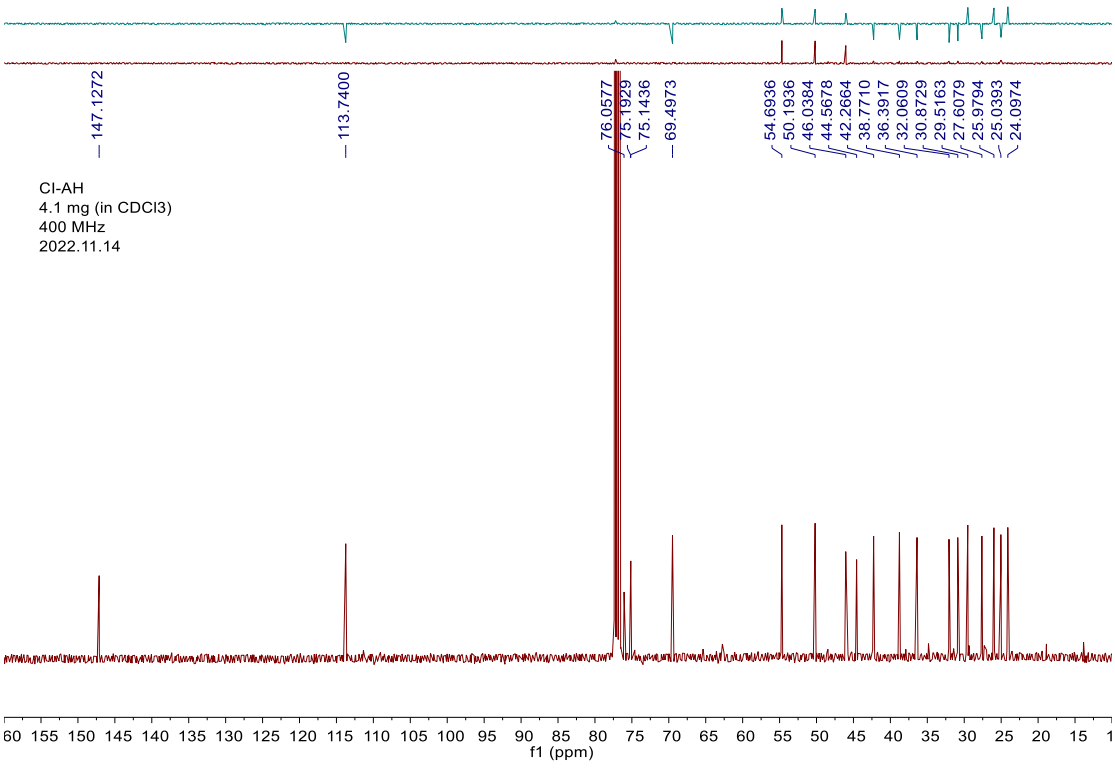



**Figure S59** $^{13}$C NMR spectrum of **7** (100 MHz, $CDCl_3$)

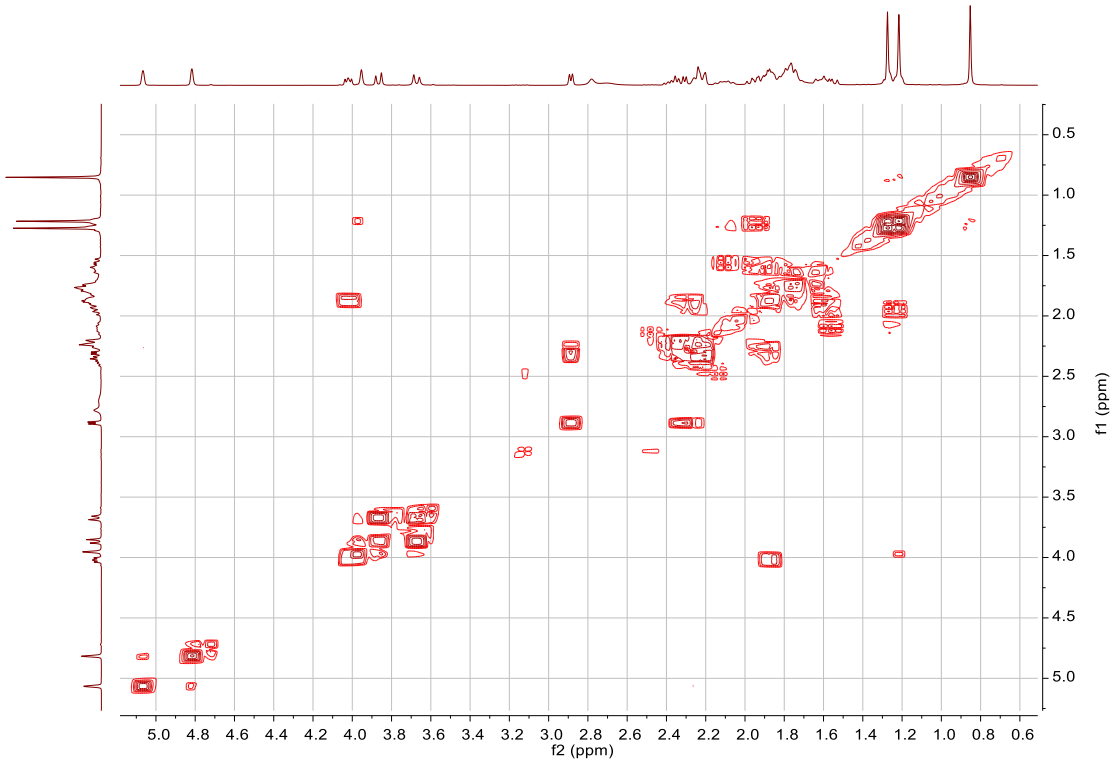



**Figure S60** COSY spectrum of **7**

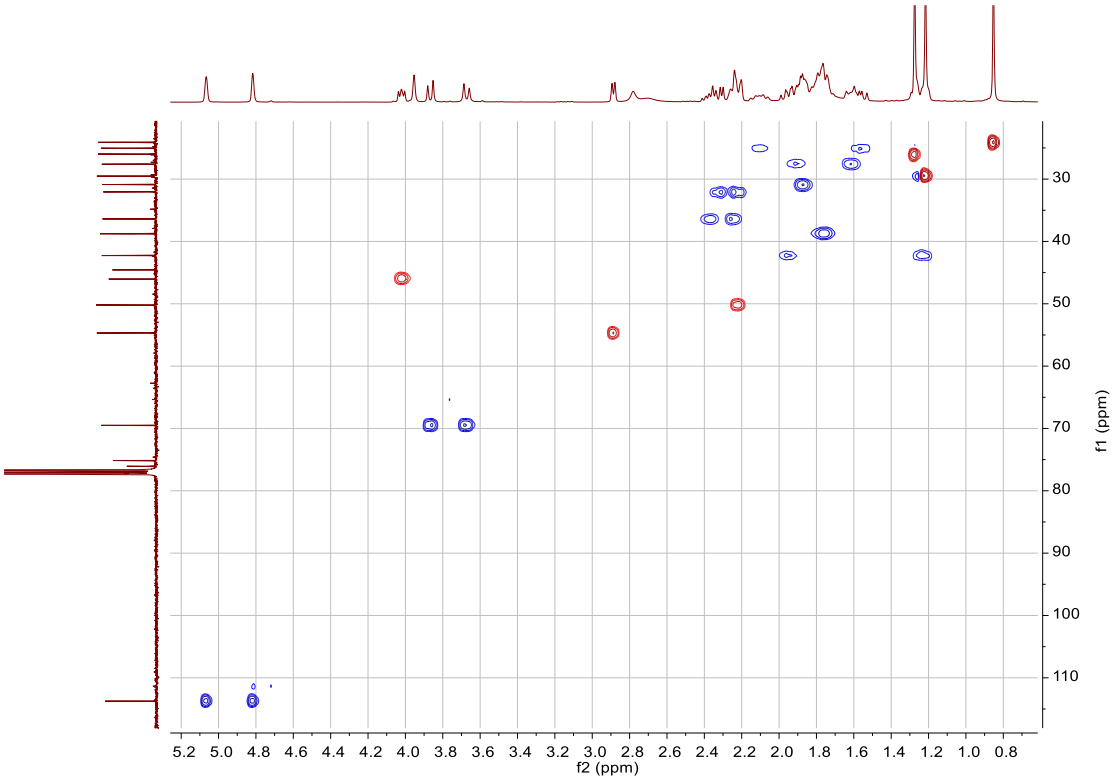



**Figure S61** HSQC spectrum of **7**

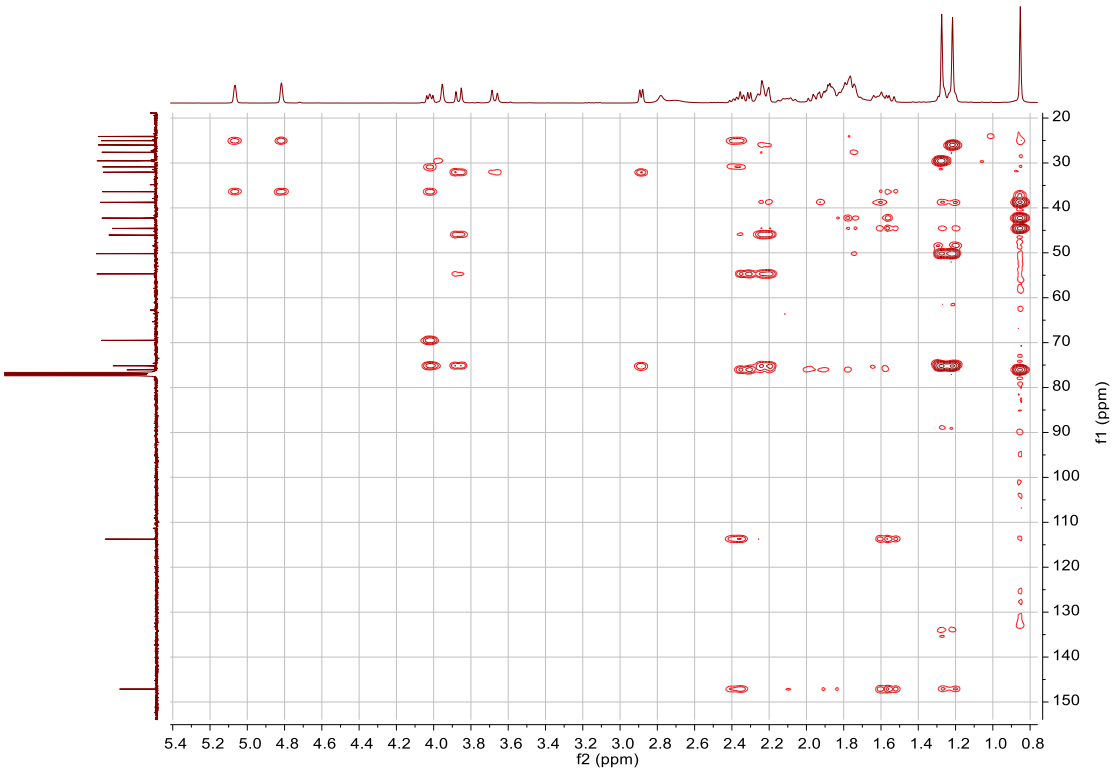



**Figure S62** HMBC spectrum of **7**

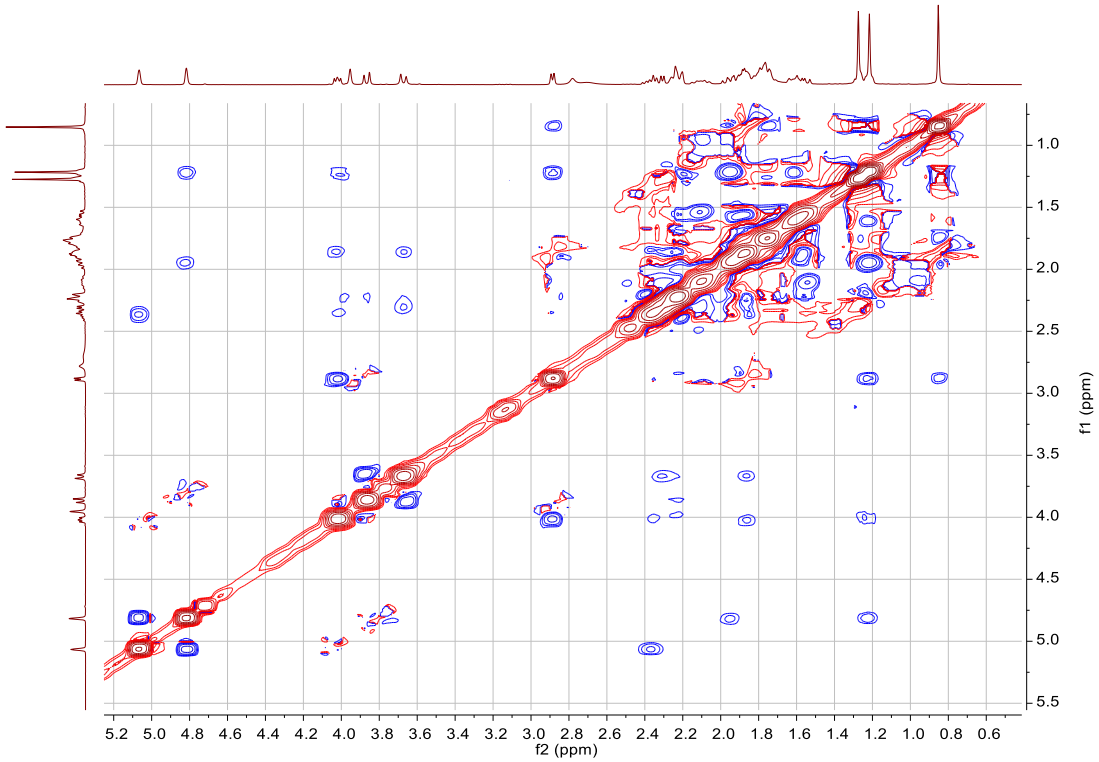
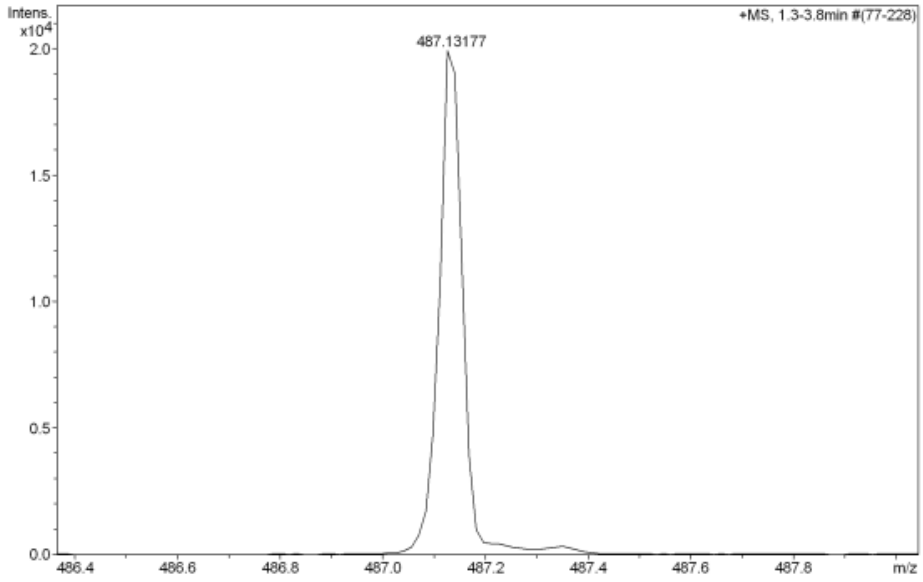



**Figure S63** NOESY spectrum of **7**

Mass Spectrum SmartFormula Report

**Analysis Info**

| | | |
|---|---|---|
| Analysis Name | D:\1219\CIAHR2.d | 12/20/2022 10:41:26 AM |
| Method | tune_wide_pos_20220422.m | Operator: YU HSIAO-CHING |
| Sample Name | CI-AH | Instrument: BRUKER micrOTOF-Q |
| Comment | ESI Positive | |




| Meas. m/z | # | Formula | Score | m/z | err [mDa] | err [ppm] | mSigma | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 487.13177 | 1 | C 20 H 33 I Na O 4 | 100.00 | 487.13157 | -0.20 | -0.41 | 27.7 | 3.5 | even | ok |

**Figure S64** HRESIMS spectrum of **7**

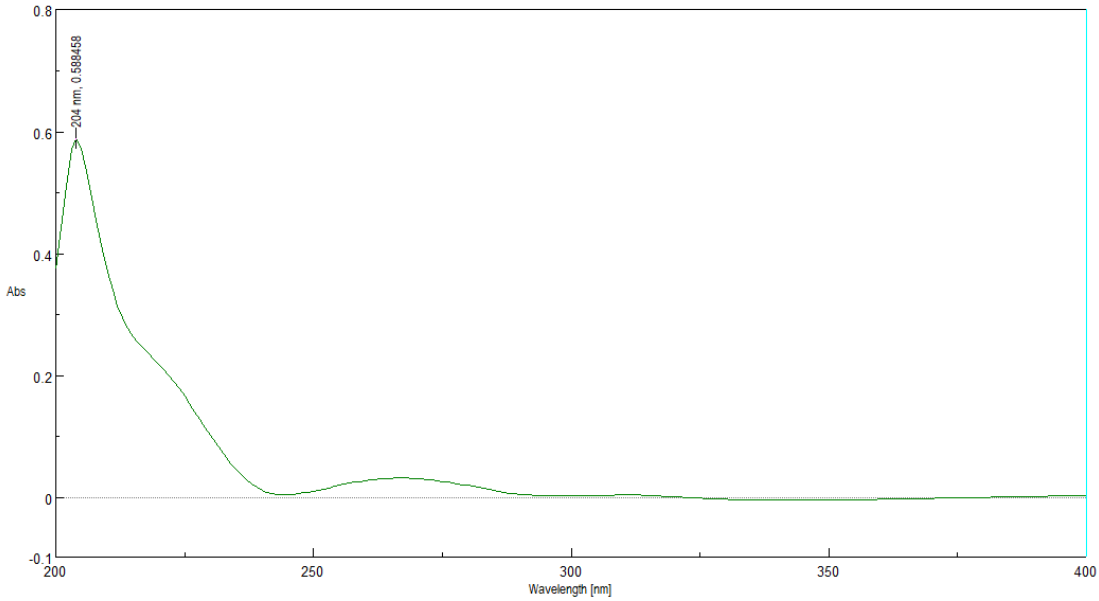



**Figure S65** UV spectrum of **7**

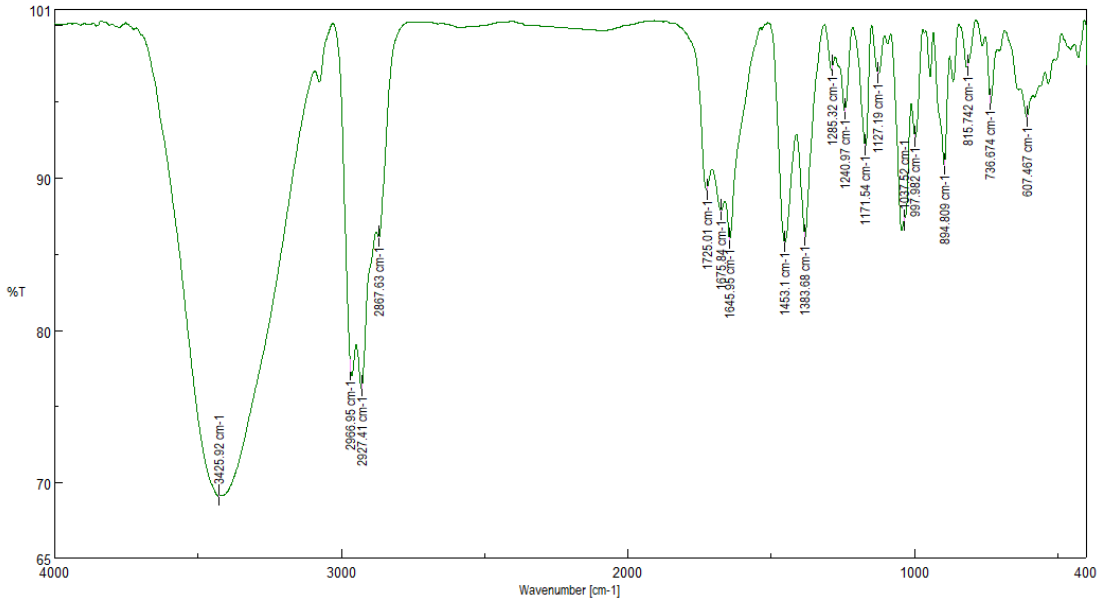



**Figure S66** IR spectrum of **7**

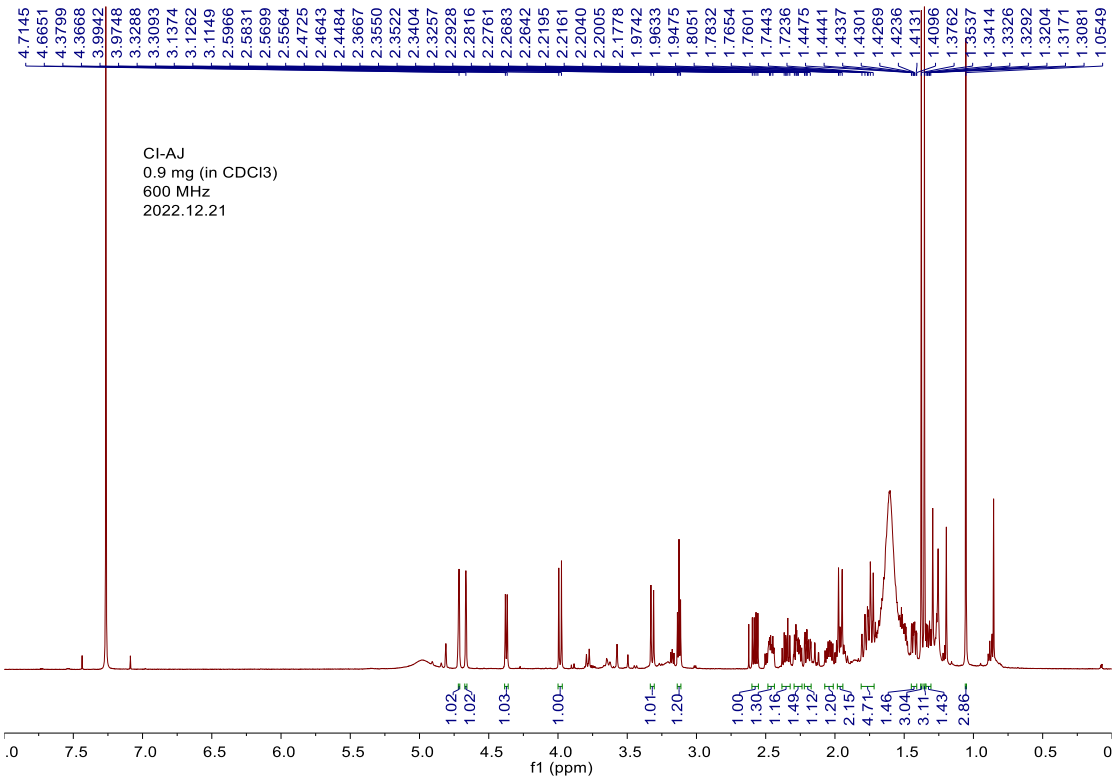



**Figure S67** $^{1}$H NMR spectrum of **8** (600 MHz, $CDCl_3$)

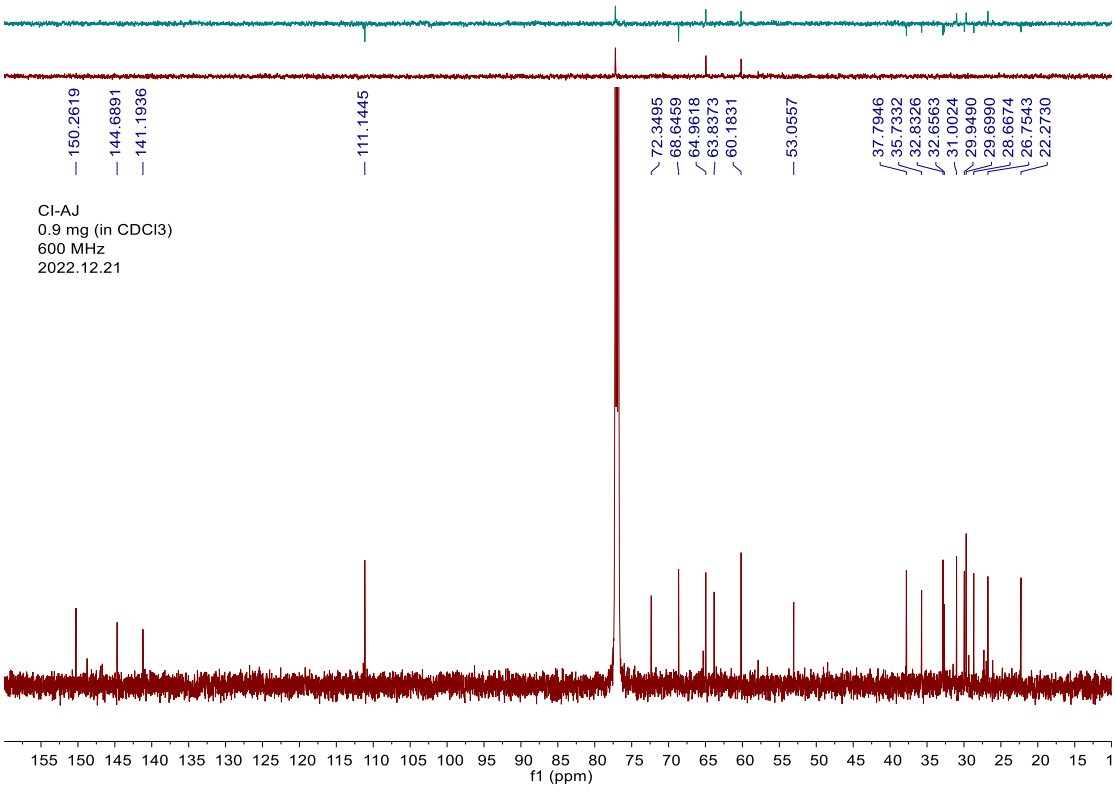



**Figure S68** $^{13}$C NMR spectrum of **8** (125 MHz, $CDCl_3$)


**Figure S69** COSY spectrum of **8**

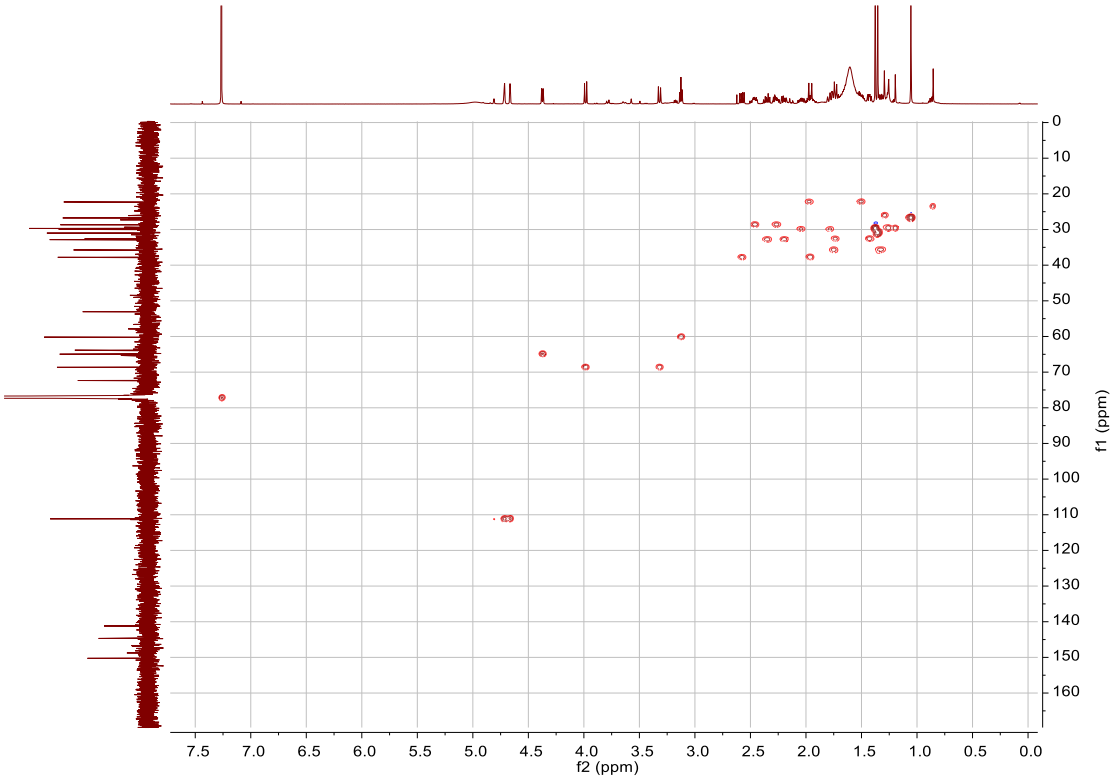



**Figure S70** HSQC spectrum of **8**

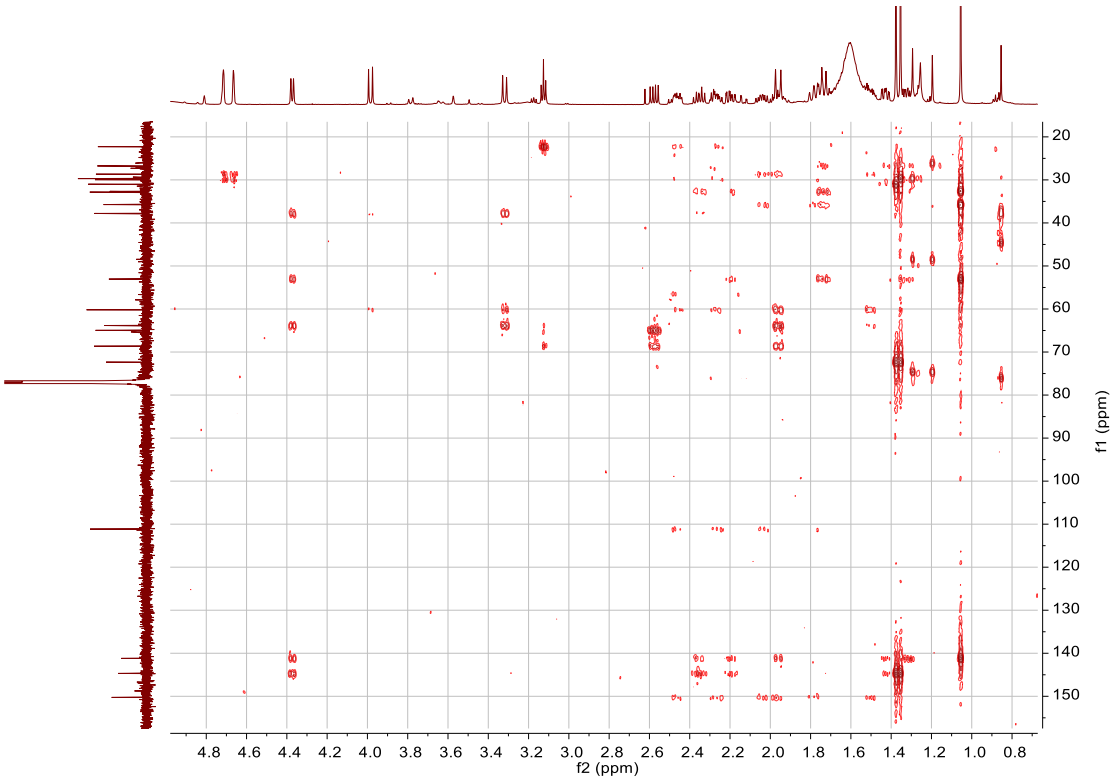



**Figure S71** HMBC spectrum of **8**

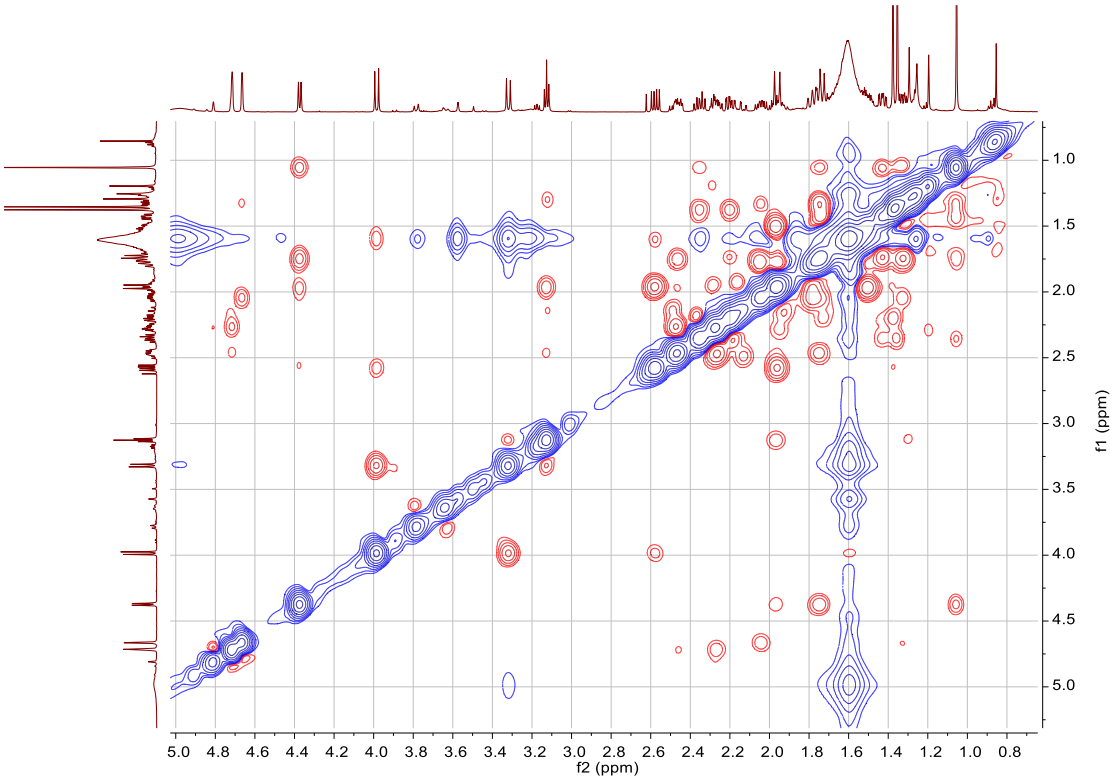
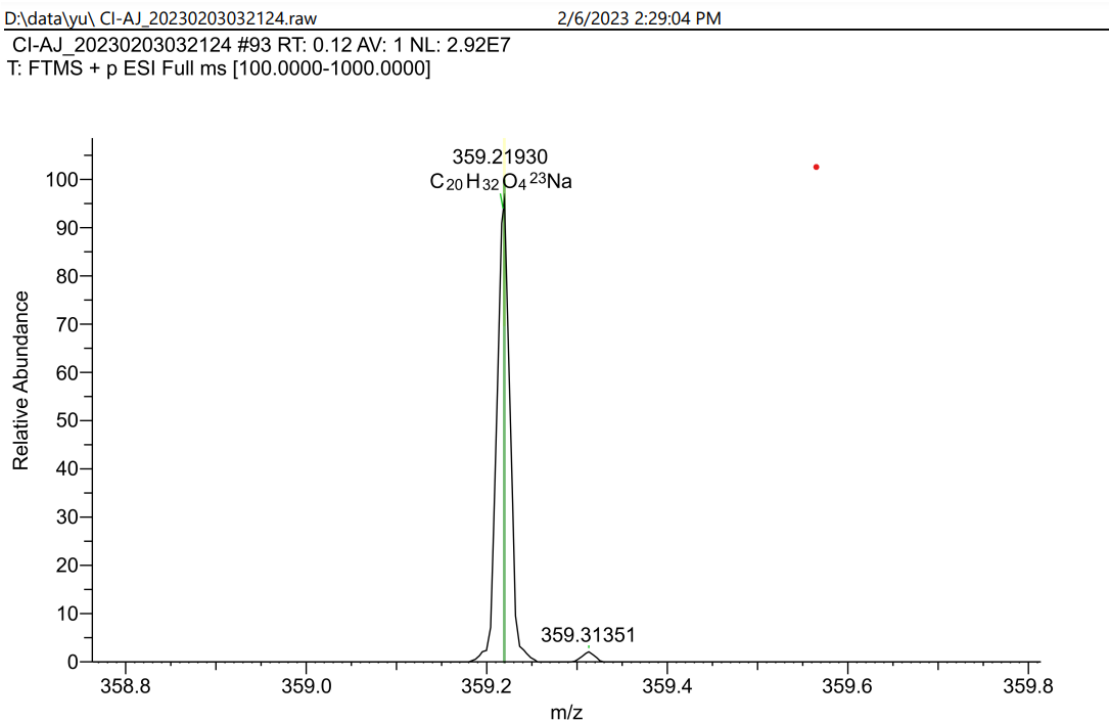



**Figure S72** NOESY spectrum of **8**




| Peak Mass | Display F... | S Fit | RDB | Delta [pp... | Theo. ma... | Rank | Combine... | # Match... | # Missed... | MS Cov.... | Pattern C... | MSMS M... |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 359.21930 | $C_{20}H_{32}O_4{}^{23}Na$ | 28.057822993545 7 | 4.50 | 0.05 | 359.21928 | 1 | 91.38 | 2 | 2 | 94.9 | 97.28 | (Collection) |

**Figure S73** HRESIMS spectrum of **8**

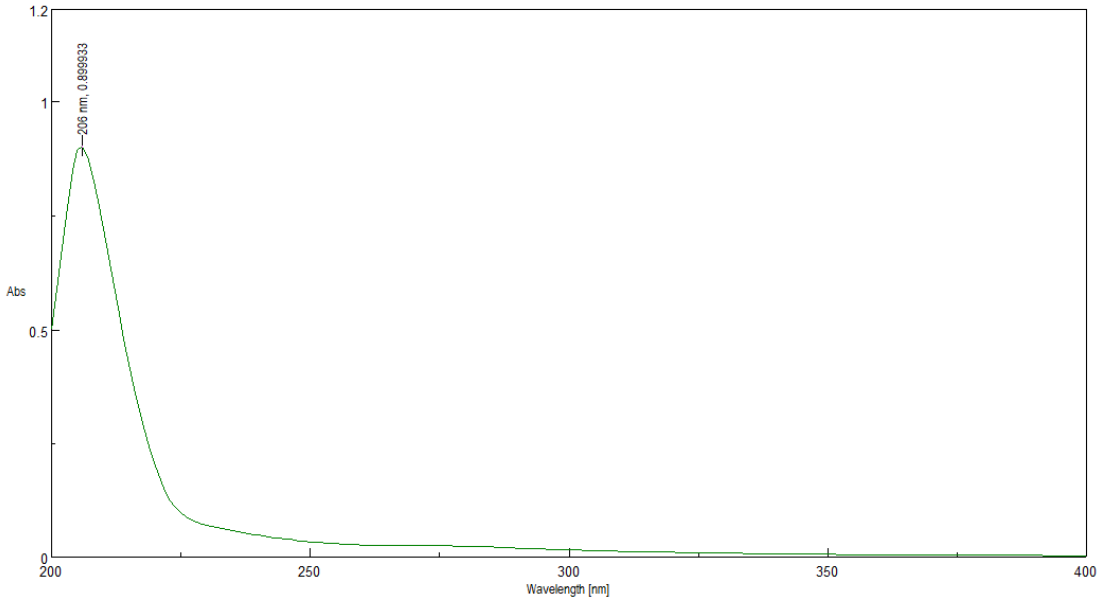



**Figure S74** UV spectrum of **8**

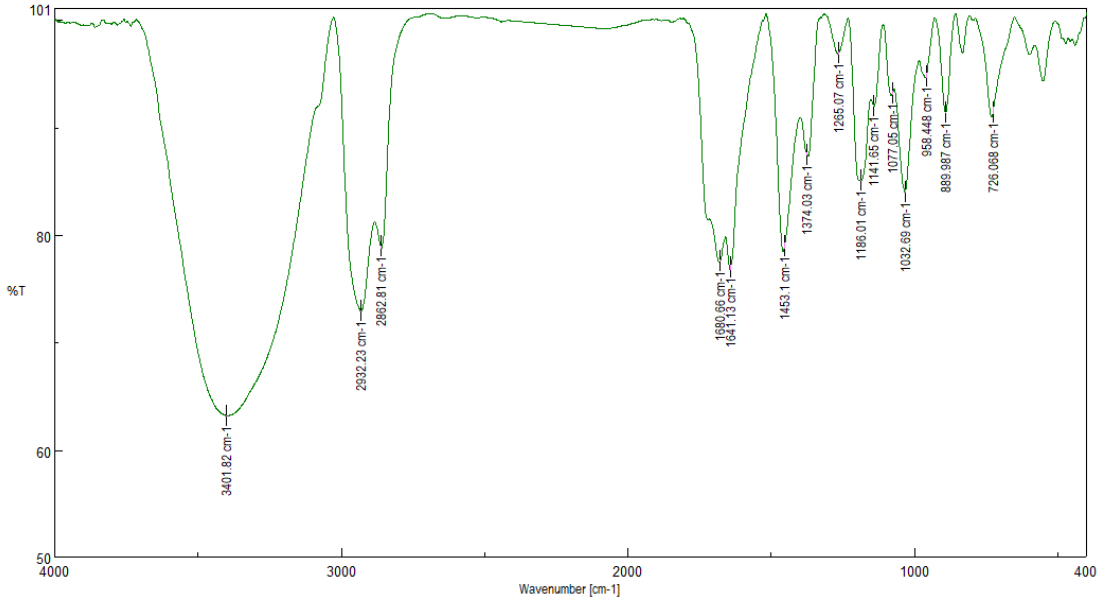



**Figure S75** IR spectrum of **8**