# Supporting Information

## Neoantimycins A and B, two unusual benzamido nine-membered dilactones from marine-derived *Streptomyces antibioticus* H12-15

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# Contents

**Table S1.** 1D and 2D NMR data of **1** ($\delta$ in ppm) in $CDCl_3$.

| No. | $\delta$c | $\delta_H$ (*J* in Hz) | $^1$H-$^1$H COSY | HMBC | NOE |
|---|---|---|---|---|---|
| 2 | 170.8 | - | - | - | - |
| 3 | 54.2 | 5.34, t, 7.8 | H-4, 7'-NH | C-2, 4, 11 | H-4, H-8 |
| 4 | 71.5 | 5.75, p, 6.7 | H-3, H-11 | C-2, 3, 6, 11 | H-3, H-8 |
| 6 | 173.2 | - | - | - | - |
| 7 | 50.3 | 2.50, m | H-8, H-1‴ | C-6, 8, 1", 2" | H-9 |
| 8 | 75.6 | 5.09, t, 9.9 | H-7, H-9 | C-7, 9, 10, 1", 1"' | H-3, H-4 |
| 9 | 74.6 | 4.99, m | H-8, H-10 | C-7, 8, 11 | H-7 |
| 10 | 18.0 | 1.28, d, 6.1 | H-9 | C-2, 8, 9 | - |
| 11 | 15.2 | 1.32, d, 6.7 | H-4 | 2-2, 3 | - |
| 1' | 133.4 | - | - | - | - |
| 2' | 127.3 | 7.82, d, 7.7 | H-3' | C-1', 3', 4', 7' | - |
| 3' | 128.9 | 7.47, t, 7.7 | H-2', H-4' | C-1', 2', 4', 5' | - |
| 4' | 132.3 | 7.55, t, 7.4 | H-3', H-5' | C-2', 3', 5', 6' | - |
| 5' | 128.9 | 7.47, t, 7.7 | H-4', H-6' | C-1', 3', 4', 6' | - |
| 6' | 127.3 | 7.82, d, 7.7 | H-5' | C-1', 4', 5', 7' | - |
| 7' | 167.0 | - | - | - | - |
| 1" | 28.6 | 1.67, m<br>1.25, m | H-7, H-2" | C-6, 8 | -<br>- |
| 2" | 22.6 | 1.25, m | H-1", H-3" | - | - |
| 3" | 27.1 | 1.25, m | H-2", H-4" | - | - |
| 4" | 31.6 | 1.25, m | H-3", H-5" | - | - |
| 5" | 29.1 | 1.25, m | H-4", H-6" | - | - |
| 6" | 14.2 | 0.85, t, 6.6 | H-5" | C-4", 5" | - |
| 1"' | 175.4 | - | - | - | - |
| 2"' | 41.4 | 2.41, dt, 10.6, 5.3 | H-3"', H-5"' | C-1"', 3"', 4"', 5"' | - |
| 3"' | 26.6 | 1.71, m<br>1.49, m | H-2"', H-4"' | C-1"', 2"', 4"', 5"' | -<br>- |
| 4"' | 11.9 | 0.94, t, 7.4 | H-3"' | C-2"', 3"' | - |
| 5"' | 16.9 | 1.18, d, 7.0 | H-2"' | C-1"', 2"', 3"' | - |
| 7'-NH | - | 6.86, d, 7.8 | H-2 | C-2, 7' | - |

**Table S2.** 1D and 2D NMR data of **2** ($\delta$ in ppm) in $CDCl_3$.

| No. | $\delta$c | $\delta_H$ (*J* in Hz) | $^1$H-$^1$H COSY | HMBC | NOE |
|---|---|---|---|---|---|
| 2 | 170.8 | - | - | - | - |
| 3 | 54.2 | 5.34, t, 7.8 | H-4, 7'-NH | C-2, 4, 11 | H-4, H-8 |
| 4 | 71.5 | 5.75, p, 6.8 | H-3, H-11 | C-2, 3, 6, 11 | H-3, H-8 |
| 6 | 173.2 | - | - | - | - |
| 7 | 50.3 | 2.52, m | H-8, H-1‴ | C-6, 8, 1", 2" | H-9 |
| 8 | 75.6 | 5.08, t, 9.9 | H-7, H-9 | C-7, 9, 10, 1", 1"' | H-3, H-4 |
| 9 | 74.6 | 5.00, m | H-8, H-10 | C-7, 8, 11 | H-7 |
| 10 | 18.0 | 1.28, d, 6.5 | H-9 | C-2, 8, 9 | - |
| 11 | 15.2 | 1.32, d, 6.7 | H-4 | C-2, 3 | - |
| 1' | 133.4 | - | - | - | - |
| 2' | 127.3 | 7.82, d, 7.4 | H-3' | C-1', 3', 4', 7' | - |
| 3' | 128.9 | 7.47, t, 7.7 | H-2', H-4' | C-1', 2', 4', 5' | - |
| 4' | 132.3 | 7.55, t, 7.4 | H-3', H-5' | C-2', 3', 5', 6' | - |
| 5' | 128.9 | 7.47, t, 7.7 | H-4', H-6' | C-1', 3', 4', 6' | - |
| 6' | 127.3 | 7.82, d, 7.4 | H-5' | C-1', 4', 5', 7' | - |
| 7' | 167.0 | - | - | - | - |
| 1" | 28.6 | 1.66, m<br>1.25, m | H-7, H-2" | C-6, 8 | -<br>- |
| 2" | 22.6 | 1.25, m | H-1", H-3" | - | - |
| 3" | 27.1 | 1.25, m | H-2", H-4" | - | - |
| 4" | 31.6 | 1.25, m | H-3", H-5" | - | - |
| 5" | 29.1 | 1.25, m | H-4", H-6" | - | - |
| 6" | 14.2 | 0.86, t, 6.8 | H-5" | C-4", 5" | - |
| 1"' | 175.7 | - | - | - | - |
| 2"' | 34.3 | 2.61, t, 7.0 | H-3"', H-5"' | C-1"', 3"', 4"' | - |
| 3"' | 19.1 | 1.22, d, 2.5 | H-2"', H-4"' | C-1"', 2"', 4"' | -<br>- |
| 4"' | 19.1 | 1.21, d, 2.5 | H-2"', H-3"' | C-2"', 3"' | - |
| 7'-NH | - | 6.86, d, 7.8 | H-2 | C-2, 7' | - |

**Table S3.** B3LYP-Calculated relative energies (kcal $mol^{-1}$) and conformational population (%) for the most stable conformers of (3*R*,4*S*,7*R*,8*R*,9*S*,2'''*S*)-**1**.

| Conformers | Rel. E | Percent (%) |
|---|---|---|
| **1-a** | 0 | 58.46% |
| **1-b** | 0.239705 | 39.00% |
| **1-c** | 2.579025 | 0.75% |
| **1-d** | 2.582163 | 0.75% |
| **1-e** | 2.756607 | 0.56% |
| **1-f** | 2.826260 | 0.49% |
| **1-g** | 3.123695 | 0.30% |
| **1-h** | 3.177660 | 0.27% |
| **1-i** | 3.202760 | 0.26% |
| **1-j** | 3.371557 | 0.20% |
| **1-k** | 3.384735 | 0.19% |
| **1-l** | 3.519020 | 0.15% |
| **1-m** | 3.567965 | 0.14% |
| **1-n** | 3.763745 | 0.10% |
| **1-o** | 3.935052 | 0.08% |

**Table S4.** Coordinates of computations ((3*R*,4*S*,7*R*,8*R*,9*S*,2'''*S*)-**1**)

**Conformer 1-a**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.366453 | 0.356599 | -0.229171 |
| 2 | 6 | 0 | -7.379725 | 0.693531 | -1.139236 |
| 3 | 6 | 0 | -8.721485 | 0.531648 | -0.795832 |
| 4 | 6 | 0 | -9.068459 | 0.041184 | 0.467093 |
| 5 | 6 | 0 | -8.066109 | -0.284736 | 1.384750 |
| 6 | 6 | 0 | -6.721988 | -0.129672 | 1.038944 |
| 7 | 6 | 0 | -4.946535 | 0.562165 | -0.679845 |
| 8 | 7 | 0 | -3.964676 | -0.042257 | 0.054049 |
| 9 | 8 | 0 | -4.671567 | 1.248826 | -1.665850 |
| 10 | 6 | 0 | -2.572343 | 0.033430 | -0.337409 |
| 11 | 6 | 0 | -1.849128 | 1.377274 | 0.106034 |
| 12 | 8 | 0 | -0.503679 | 1.046848 | 0.550592 |
| 13 | 6 | 0 | 0.460416 | 0.856082 | -0.389945 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 6 | 0 | 1.664009 | 0.124689 | 0.203588 |
| 15 | 6 | 0 | 1.627526 | -1.370666 | -0.224370 |
| 16 | 8 | 0 | 0.365988 | 1.215382 | -1.542361 |
| 17 | 6 | 0 | 0.361662 | -2.145820 | 0.206875 |
| 18 | 8 | 0 | -0.737481 | -1.438186 | -0.433480 |
| 19 | 6 | 0 | -1.840059 | -1.152499 | 0.279639 |
| 20 | 8 | 0 | -2.184760 | -1.722162 | 1.295026 |
| 21 | 6 | 0 | 0.336632 | -3.603030 | -0.233804 |
| 22 | 8 | 0 | 2.742846 | -2.018335 | 0.433449 |
| 23 | 6 | 0 | 3.641880 | -2.715499 | -0.320999 |
| 24 | 6 | 0 | 4.724487 | -3.335167 | 0.552423 |
| 25 | 6 | 0 | 6.089963 | -3.322094 | -0.158377 |
| 26 | 8 | 0 | 3.552435 | -2.843397 | -1.523007 |
| 27 | 6 | 0 | 6.652362 | -1.918646 | -0.411713 |
| 28 | 6 | 0 | 4.295189 | -4.770804 | 0.927521 |
| 29 | 6 | 0 | 2.970388 | 0.814963 | -0.237727 |
| 30 | 6 | 0 | 3.105311 | 2.252443 | 0.286055 |
| 31 | 6 | 0 | 4.432976 | 2.912484 | -0.112663 |
| 32 | 6 | 0 | 4.562888 | 4.360934 | 0.377414 |
| 33 | 6 | 0 | 5.890560 | 5.025619 | -0.012203 |
| 34 | 6 | 0 | 6.005811 | 6.476299 | 0.470837 |
| 35 | 6 | 0 | -2.512580 | 2.094122 | 1.269112 |
| 36 | 1 | 0 | -7.092083 | 1.082583 | -2.110697 |
| 37 | 1 | 0 | -9.496909 | 0.790331 | -1.512152 |
| 38 | 1 | 0 | -10.114198 | -0.081625 | 0.737140 |
| 39 | 1 | 0 | -8.328437 | -0.654885 | 2.372341 |
| 40 | 1 | 0 | -5.964640 | -0.369655 | 1.780817 |
| 41 | 1 | 0 | -4.181996 | -0.670296 | 0.817542 |
| 42 | 1 | 0 | -2.504526 | -0.030959 | -1.426257 |
| 43 | 1 | 0 | -1.775691 | 2.026800 | -0.767178 |
| 44 | 1 | 0 | 1.579068 | 0.160367 | 1.296525 |
| 45 | 1 | 0 | 1.757323 | -1.452875 | -1.306896 |
| 46 | 1 | 0 | 0.227082 | -2.069041 | 1.290149 |
| 47 | 1 | 0 | 0.442551 | -3.684429 | -1.320509 |
| 48 | 1 | 0 | -0.610654 | -4.060139 | 0.067784 |
| 49 | 1 | 0 | 1.148873 | -4.162675 | 0.238744 |
| 50 | 1 | 0 | 4.784939 | -2.742549 | 1.473688 |
| 51 | 1 | 0 | 5.998843 | -3.863029 | -1.108144 |
| 52 | 1 | 0 | 6.793265 | -3.889900 | 0.465428 |
| 53 | 1 | 0 | 6.003560 | -1.340259 | -1.079505 |
| 54 | 1 | 0 | 7.640132 | -1.975939 | -0.883480 |
| 55 | 1 | 0 | 6.764462 | -1.357873 | 0.525439 |
| 56 | 1 | 0 | 4.195667 | -5.394360 | 0.031700 |
| 57 | 1 | 0 | 3.340744 | -4.780053 | 1.465434 |

| | | | | | |
|---|---|---|---|---|---|
| 58 | 1 | 0 | 5.050947 | -5.225344 | 1.577814 |
| 59 | 1 | 0 | 3.816162 | 0.220997 | 0.126267 |
| 60 | 1 | 0 | 3.017872 | 0.814667 | -1.333854 |
| 61 | 1 | 0 | 2.275394 | 2.864223 | -0.094048 |
| 62 | 1 | 0 | 3.015414 | 2.251908 | 1.383027 |
| 63 | 1 | 0 | 5.269853 | 2.317480 | 0.283773 |
| 64 | 1 | 0 | 4.532880 | 2.890126 | -1.208122 |
| 65 | 1 | 0 | 4.453610 | 4.386361 | 1.472698 |
| 66 | 1 | 0 | 3.728995 | 4.955215 | -0.026108 |
| 67 | 1 | 0 | 6.002795 | 4.994769 | -1.105817 |
| 68 | 1 | 0 | 6.724463 | 4.436422 | 0.396928 |
| 69 | 1 | 0 | 5.931379 | 6.537948 | 1.564381 |
| 70 | 1 | 0 | 5.206168 | 7.098876 | 0.049177 |
| 71 | 1 | 0 | 6.964136 | 6.921129 | 0.176735 |
| 72 | 1 | 0 | -2.600786 | 1.443056 | 2.145473 |
| 73 | 1 | 0 | -1.908386 | 2.965285 | 1.542709 |
| 74 | 1 | 0 | -3.508972 | 2.442327 | 0.985815 |

**Conformer 1-b**

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.332634 | 0.362910 | -0.313724 |
| 2 | 6 | 0 | -6.781908 | -0.824866 | 0.281115 |
| 3 | 6 | 0 | -8.136128 | -1.000456 | 0.565103 |
| 4 | 6 | 0 | -9.051982 | 0.007742 | 0.258702 |
| 5 | 6 | 0 | -8.611827 | 1.188890 | -0.344174 |
| 6 | 6 | 0 | -7.260815 | 1.362820 | -0.633834 |
| 7 | 6 | 0 | -4.894653 | 0.627521 | -0.655049 |
| 8 | 7 | 0 | -3.961128 | -0.135941 | -0.009694 |
| 9 | 8 | 0 | -4.561963 | 1.491540 | -1.464828 |
| 10 | 6 | 0 | -2.551019 | -0.009506 | -0.304815 |
| 11 | 6 | 0 | -1.877928 | 1.310183 | 0.260158 |
| 12 | 8 | 0 | -0.521434 | 0.988855 | 0.673125 |
| 13 | 6 | 0 | 0.425564 | 0.855908 | -0.292925 |
| 14 | 6 | 0 | 1.661709 | 0.144755 | 0.257106 |
| 15 | 6 | 0 | 1.637683 | -1.351369 | -0.165886 |
| 16 | 8 | 0 | 0.295790 | 1.241464 | -1.431820 |
| 17 | 6 | 0 | 0.388880 | -2.139294 | 0.287836 |
| 18 | 8 | 0 | -0.713144 | -1.476740 | -0.389663 |
| 19 | 6 | 0 | -1.832753 | -1.205628 | 0.305564 |
| 20 | 8 | 0 | -2.194017 | -1.785306 | 1.307201 |

| | | | | | |
|---|---|---|---|---|---|
| 21 | 6 | 0 | 0.398903 | -3.613317 | -0.092177 |
| 22 | 8 | 0 | 2.782054 | -1.973324 | 0.461181 |
| 23 | 6 | 0 | 3.640793 | -2.688310 | -0.323152 |
| 24 | 6 | 0 | 4.789976 | -3.246465 | 0.505729 |
| 25 | 6 | 0 | 6.064542 | -3.384728 | -0.343360 |
| 26 | 8 | 0 | 3.475290 | -2.872673 | -1.507925 |
| 27 | 6 | 0 | 6.637312 | -2.049207 | -0.828563 |
| 28 | 6 | 0 | 4.352548 | -4.598593 | 1.108316 |
| 29 | 6 | 0 | 2.937389 | 0.854506 | -0.235503 |
| 30 | 6 | 0 | 3.083199 | 2.282886 | 0.306938 |
| 31 | 6 | 0 | 4.378904 | 2.968255 | -0.146683 |
| 32 | 6 | 0 | 4.526927 | 4.398207 | 0.388055 |
| 33 | 6 | 0 | 5.820773 | 5.090855 | -0.059074 |
| 34 | 6 | 0 | 5.958468 | 6.518517 | 0.479408 |
| 35 | 6 | 0 | -2.560017 | 1.879574 | 1.492120 |
| 36 | 1 | 0 | -6.088173 | -1.633449 | 0.495367 |
| 37 | 1 | 0 | -8.476066 | -1.927529 | 1.018401 |
| 38 | 1 | 0 | -10.106516 | -0.129939 | 0.482256 |
| 39 | 1 | 0 | -9.323092 | 1.972514 | -0.590544 |
| 40 | 1 | 0 | -6.897937 | 2.266253 | -1.112719 |
| 41 | 1 | 0 | -4.202664 | -0.715530 | 0.783125 |
| 42 | 1 | 0 | -2.407523 | -0.013650 | -1.387125 |
| 43 | 1 | 0 | -1.836391 | 2.041830 | -0.547054 |
| 44 | 1 | 0 | 1.616229 | 0.179908 | 1.351958 |
| 45 | 1 | 0 | 1.739490 | -1.434521 | -1.251083 |
| 46 | 1 | 0 | 0.241517 | -2.025326 | 1.366119 |
| 47 | 1 | 0 | 0.531749 | -3.738773 | -1.170989 |
| 48 | 1 | 0 | -0.548269 | -4.070251 | 0.208196 |
| 49 | 1 | 0 | 1.208479 | -4.137685 | 0.422863 |
| 50 | 1 | 0 | 4.969793 | -2.546522 | 1.331082 |
| 51 | 1 | 0 | 5.842689 | -4.026064 | -1.204293 |
| 52 | 1 | 0 | 6.815753 | -3.909768 | 0.260917 |
| 53 | 1 | 0 | 5.927507 | -1.526889 | -1.478883 |
| 54 | 1 | 0 | 7.557048 | -2.205543 | -1.402745 |
| 55 | 1 | 0 | 6.880167 | -1.388627 | 0.013274 |
| 56 | 1 | 0 | 4.122047 | -5.320568 | 0.316869 |
| 57 | 1 | 0 | 3.467848 | -4.485597 | 1.743558 |
| 58 | 1 | 0 | 5.159231 | -5.012958 | 1.722276 |
| 59 | 1 | 0 | 3.806628 | 0.262202 | 0.071059 |
| 60 | 1 | 0 | 2.924087 | 0.874970 | -1.331947 |
| 61 | 1 | 0 | 2.226024 | 2.888674 | -0.017269 |
| 62 | 1 | 0 | 3.050011 | 2.260821 | 1.406433 |
| 63 | 1 | 0 | 5.241944 | 2.367128 | 0.176587 |
| 64 | 1 | 0 | 4.414050 | 2.985193 | -1.245691 |

| | | | | | |
|---|---|---|---|---|---|
| 65 | 1 | 0 | 4.486814 | 4.381506 | 1.487665 |
| 66 | 1 | 0 | 3.664006 | 4.997965 | 0.062551 |
| 67 | 1 | 0 | 5.860516 | 5.108437 | -1.157457 |
| 68 | 1 | 0 | 6.683350 | 4.491733 | 0.266230 |
| 69 | 1 | 0 | 5.957636 | 6.530585 | 1.576454 |
| 70 | 1 | 0 | 5.128060 | 7.150953 | 0.142005 |
| 71 | 1 | 0 | 6.890822 | 6.985581 | 0.142114 |
| 72 | 1 | 0 | -2.639636 | 1.129155 | 2.285659 |
| 73 | 1 | 0 | -1.972195 | 2.721762 | 1.869586 |
| 74 | 1 | 0 | -3.559199 | 2.242340 | 1.241516 |

**Table S5.** B3LYP-Calculated relative energies (kcal $mol^{-1}$) and conformational population (%) for the most stable conformers of (3*R*,4*S*,7*R*,8*R*,9*S*,2'''*R*)-**1**.

| Conformers | Rel. E | Percent (%) |
|---|---|---|
| **1-a** | 0 | 81.17 |
| **1-b** | 1.714957 | 4.48 |
| **1-c** | 1.736292 | 4.32 |
| **1-d** | 1.787747 | 3.96 |
| **1-e** | 1.910110 | 3.22 |
| **1-f** | 1.986665 | 2.83 |
| **1-g** | 1.988547 | 2.82 |
| **1-h** | 2.262137 | 1.78 |
| **1-i** | 2.423405 | 1.35 |
| **1-j** | 2.956152 | 0.55 |

**Table S6.** Coordinates of computations ((3*R*,4*S*,7*R*,8*R*,9*S*,2'''*R*)-**1**)

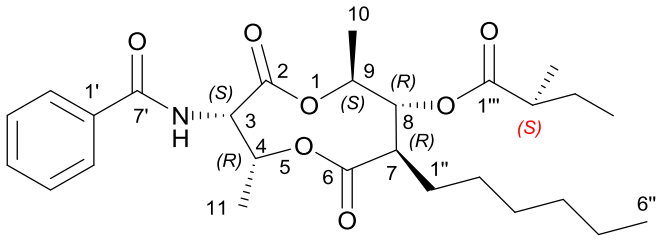
**Conformer 2-a**

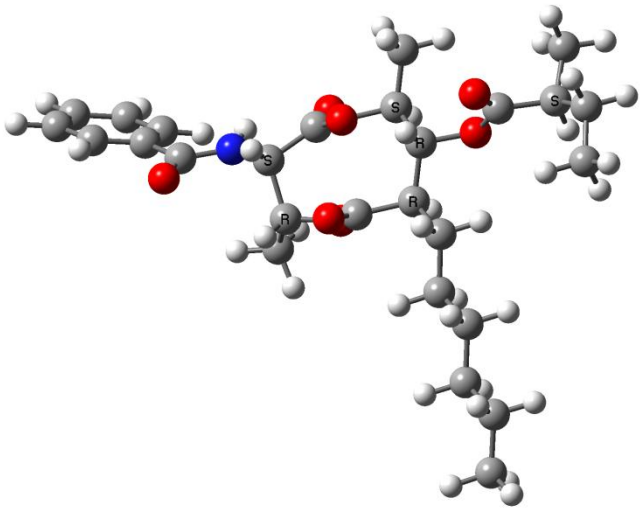
| Standard orientation: | | | | | |
|---|---|---|---|---|---|
| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
| Number | Number | Type | X | Y | Z |
| 1 | 6 | 0 | -6.146977 | -0.128755 | -0.310721 |
| 2 | 6 | 0 | -7.160333 | 0.800115 | -0.583149 |
| 3 | 6 | 0 | -8.494287 | 0.477633 | -0.346802 |
| 4 | 6 | 0 | -8.831407 | -0.782142 | 0.154678 |
| 5 | 6 | 0 | -7.829282 | -1.719272 | 0.413043 |
| 6 | 6 | 0 | -6.492486 | -1.395497 | 0.181791 |
| 7 | 6 | 0 | -4.734579 | 0.297492 | -0.590297 |
| 8 | 7 | 0 | -3.744004 | -0.429124 | 0.011583 |
| 9 | 8 | 0 | -4.471475 | 1.255606 | -1.315166 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | 6 | 0 | -2.347304 | -0.145348 | -0.233631 |
| 11 | 6 | 0 | -1.815572 | 1.171510 | 0.470002 |
| 12 | 8 | 0 | -0.426302 | 0.960964 | 0.845573 |
| 13 | 6 | 0 | 0.512391 | 1.011564 | -0.136172 |
| 14 | 6 | 0 | 1.830985 | 0.401166 | 0.340309 |
| 15 | 6 | 0 | 1.946327 | -1.068072 | -0.157711 |
| 16 | 8 | 0 | 0.318762 | 1.470805 | -1.238226 |
| 17 | 6 | 0 | 0.783098 | -1.997800 | 0.252108 |
| 18 | 8 | 0 | -0.377005 | -1.420158 | -0.405069 |
| 19 | 6 | 0 | -1.526286 | -1.316338 | 0.287111 |
| 20 | 8 | 0 | -1.840005 | -2.007383 | 1.232669 |
| 21 | 6 | 0 | 0.950589 | -3.445014 | -0.188632 |
| 22 | 8 | 0 | 3.140514 | -1.624135 | 0.438384 |
| 23 | 6 | 0 | 4.099277 | -2.136046 | -0.388426 |
| 24 | 6 | 0 | 5.301965 | -2.621641 | 0.409495 |
| 25 | 6 | 0 | 5.930083 | -3.863669 | -0.245847 |
| 26 | 8 | 0 | 4.004033 | -2.164585 | -1.594650 |
| 27 | 6 | 0 | 5.019531 | -5.095510 | -0.251269 |
| 28 | 6 | 0 | 6.318541 | -1.465461 | 0.521356 |
| 29 | 6 | 0 | 3.010577 | 1.257273 | -0.157737 |
| 30 | 6 | 0 | 3.054580 | 2.659712 | 0.464993 |
| 31 | 6 | 0 | 4.240355 | 3.491278 | -0.044040 |
| 32 | 6 | 0 | 4.389681 | 4.867493 | 0.628278 |
| 33 | 6 | 0 | 3.223182 | 5.849633 | 0.418336 |
| 34 | 6 | 0 | 2.982446 | 6.242759 | -1.043993 |
| 35 | 6 | 0 | -2.540949 | 1.523031 | 1.757224 |
| 36 | 1 | 0 | -6.875710 | 1.767625 | -0.983256 |
| 37 | 1 | 0 | -9.272282 | 1.206822 | -0.555751 |
| 38 | 1 | 0 | -9.872335 | -1.035766 | 0.336680 |
| 39 | 1 | 0 | -8.087925 | -2.706000 | 0.787190 |
| 40 | 1 | 0 | -5.729261 | -2.149196 | 0.356283 |
| 41 | 1 | 0 | -3.943605 | -1.095415 | 0.745754 |
| 42 | 1 | 0 | -2.184227 | -0.033065 | -1.307109 |
| 43 | 1 | 0 | -1.865760 | 1.985347 | -0.253822 |
| 44 | 1 | 0 | 1.819217 | 0.377445 | 1.436374 |
| 45 | 1 | 0 | 2.052606 | -1.084325 | -1.245516 |
| 46 | 1 | 0 | 0.620334 | -1.946849 | 1.333031 |
| 47 | 1 | 0 | 0.057151 | -4.012833 | 0.085625 |
| 48 | 1 | 0 | 1.811226 | -3.899323 | 0.310057 |
| 49 | 1 | 0 | 1.096124 | -3.509804 | -1.271624 |
| 50 | 1 | 0 | 4.951530 | -2.872388 | 1.418068 |
| 51 | 1 | 0 | 6.857861 | -4.094600 | 0.293429 |
| 52 | 1 | 0 | 6.213501 | -3.608980 | -1.273721 |
| 53 | 1 | 0 | 4.112587 | -4.915152 | -0.838707 |

| | | | | | |
|---|---|---|---|---|---|
| 54 | 1 | 0 | 4.718442 | -5.375476 | 0.766124 |
| 55 | 1 | 0 | 5.531406 | -5.956991 | -0.693834 |
| 56 | 1 | 0 | 6.660447 | -1.153809 | -0.471617 |
| 57 | 1 | 0 | 5.885097 | -0.596039 | 1.026562 |
| 58 | 1 | 0 | 7.191639 | -1.790777 | 1.097155 |
| 59 | 1 | 0 | 3.945735 | 0.734408 | 0.070728 |
| 60 | 1 | 0 | 2.942400 | 1.339536 | -1.249020 |
| 61 | 1 | 0 | 2.115504 | 3.183339 | 0.245659 |
| 62 | 1 | 0 | 3.114417 | 2.572111 | 1.560423 |
| 63 | 1 | 0 | 5.167937 | 2.924314 | 0.120463 |
| 64 | 1 | 0 | 4.153720 | 3.613605 | -1.132255 |
| 65 | 1 | 0 | 5.313326 | 5.336229 | 0.259566 |
| 66 | 1 | 0 | 4.534916 | 4.718404 | 1.708102 |
| 67 | 1 | 0 | 3.431118 | 6.756306 | 1.002473 |
| 68 | 1 | 0 | 2.300269 | 5.429043 | 0.839724 |
| 69 | 1 | 0 | 3.889838 | 6.665252 | -1.494031 |
| 70 | 1 | 0 | 2.190476 | 6.996153 | -1.122984 |
| 71 | 1 | 0 | 2.678569 | 5.384934 | -1.654255 |
| 72 | 1 | 0 | -2.049230 | 2.381474 | 2.224795 |
| 73 | 1 | 0 | -3.578646 | 1.792575 | 1.548927 |
| 74 | 1 | 0 | -2.523419 | 0.686251 | 2.463336 |

**Table S7.** 2D Structure of compound **1**.

| Label | Structure |
|---|---|
| **1** |  |

| Label | Conformer | Boltzmann weighting factors |
|---|---|---|
| **1-a** |  | **58.46%** |

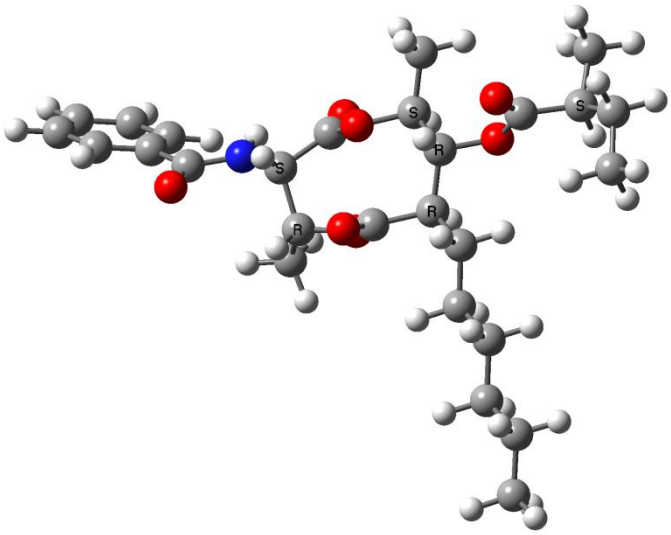
| | | |
|---|---|---|
| **1-b** |  | **39.00%** |

**Figure S1.** B3LYP/6-31 G optimized lowest energy 3D conformer of **1**.

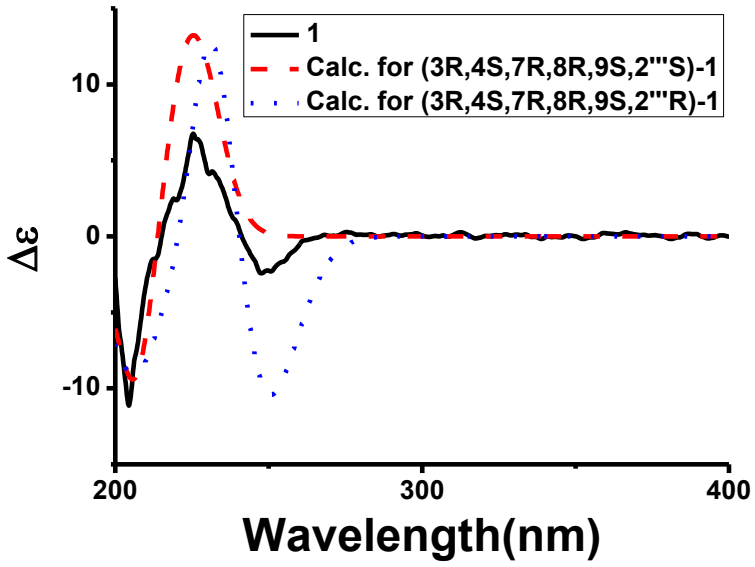



**Figure S2.** Experimental ECD spectra of **1** and calculated ECD spectra for (3*R*,4*S*,7*R*,8*R*,9*S*,2'''*S*)-**1** and (3*R*,4*S*,7*R*,8*R*,9*S*,2'''*R*)-**1**.

**The spectra of neoantimycin A (1)**

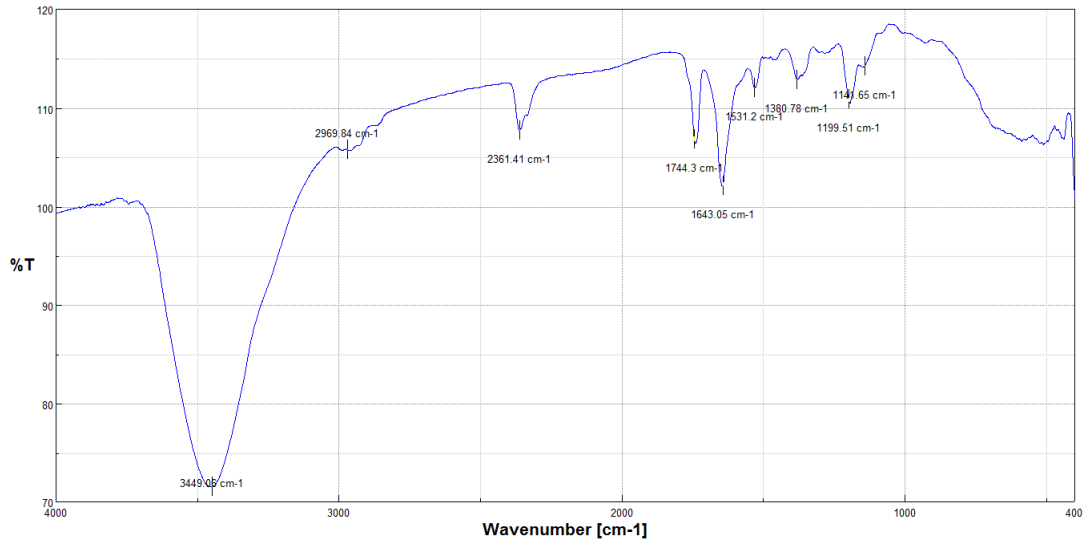



**Figure S3.** IR spectrum of compound 1.

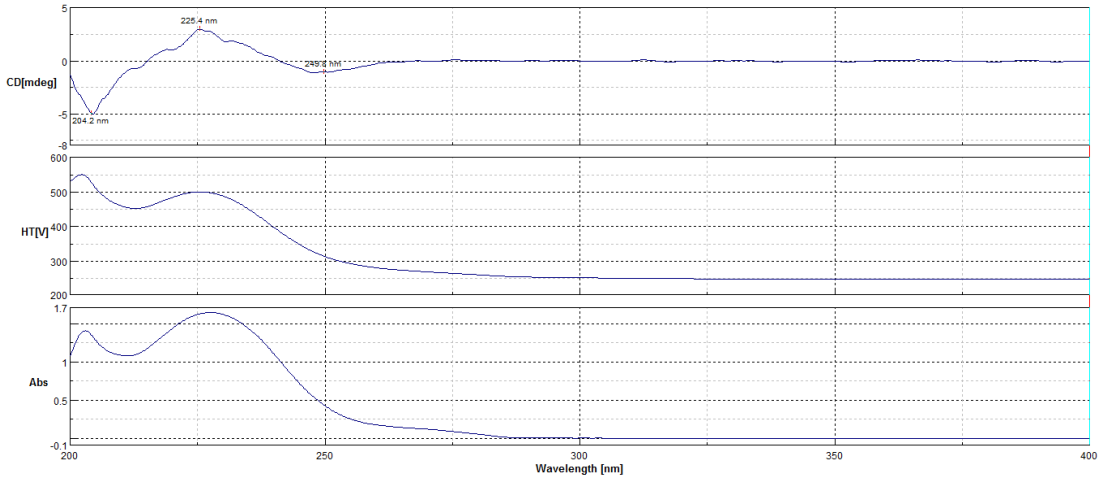



**Figure S4.** CD spectrum and UV spectrum of compound **1** in MeOH.

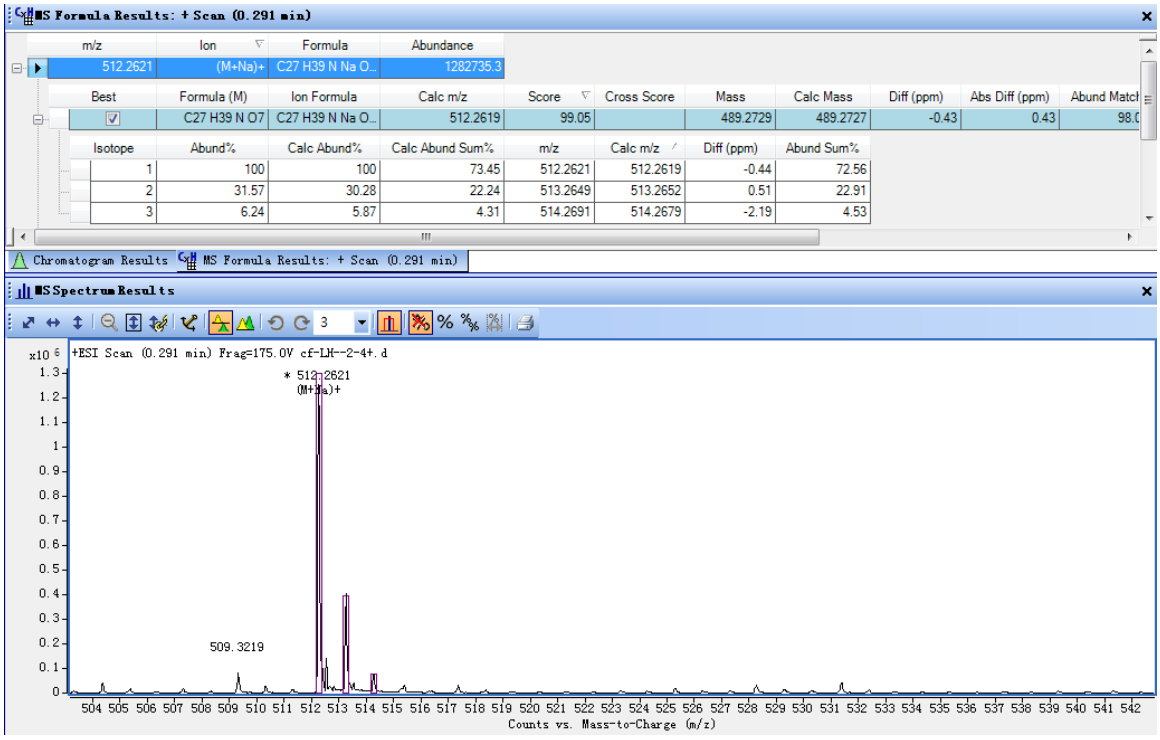



**Figure S5.** HR-TOF-MS of compound **1**.

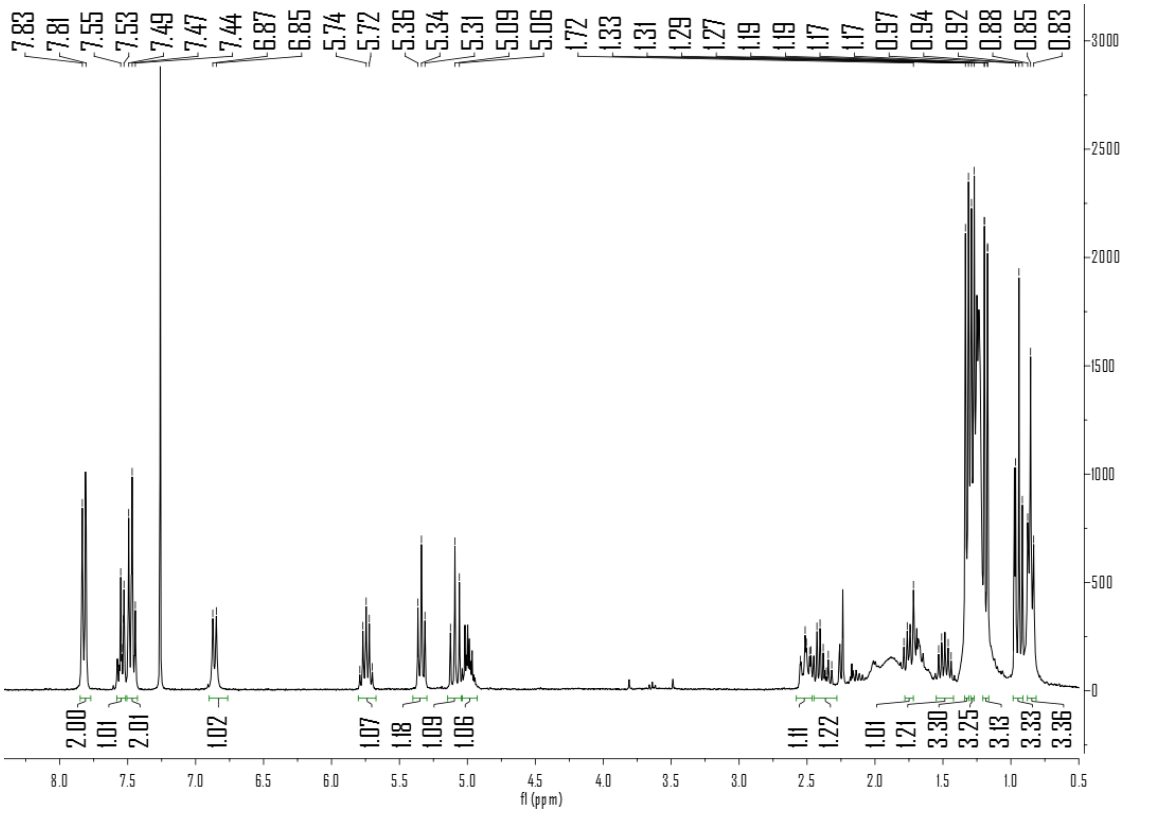



**Figure S6.** The $^{1}$H-NMR spectrum of compound **1**.

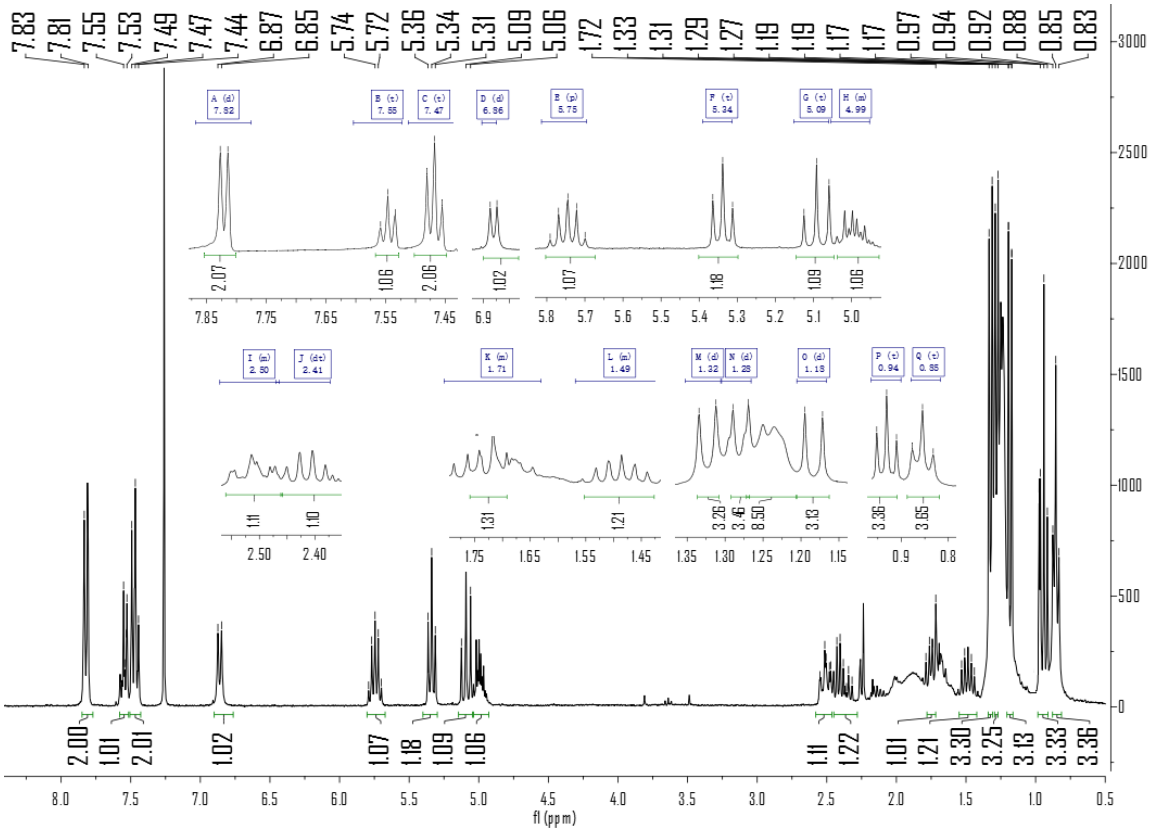


**Figure S7.** The $^{1}$H-NMR spectrum of compound **1**.

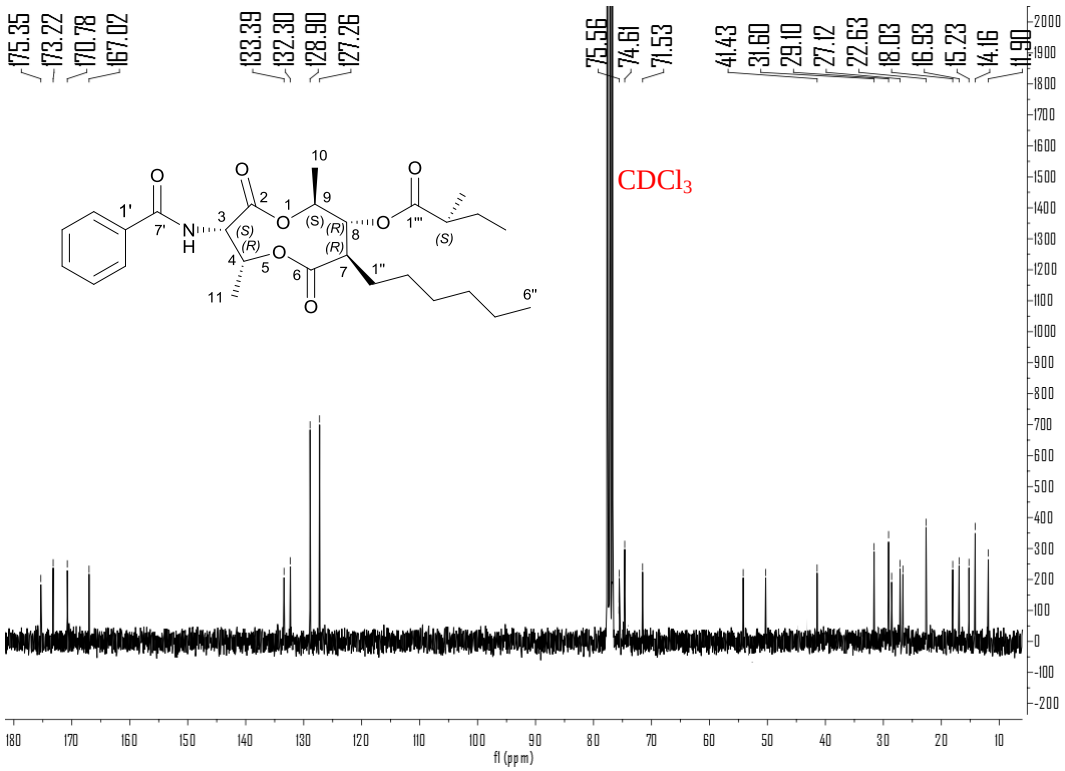



**Figure S8.** The $^{13}$C-NMR spectrum of compound **1**.

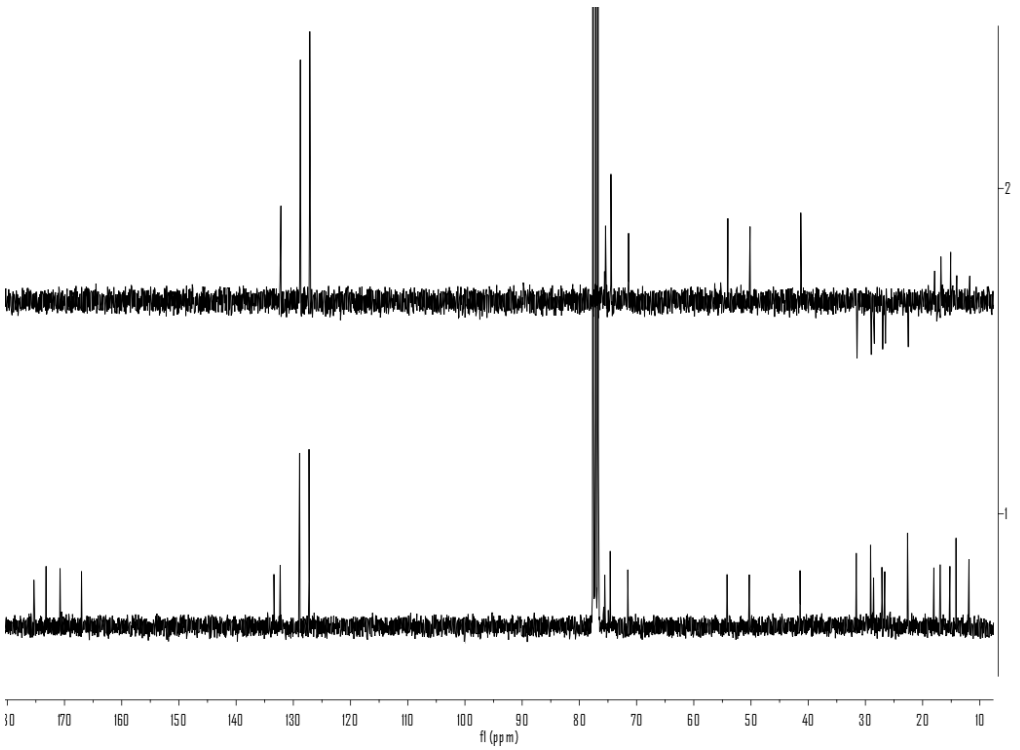



**Figure S9.** The $^{13}$C-NMR and DEPT spectra of compound **1**.

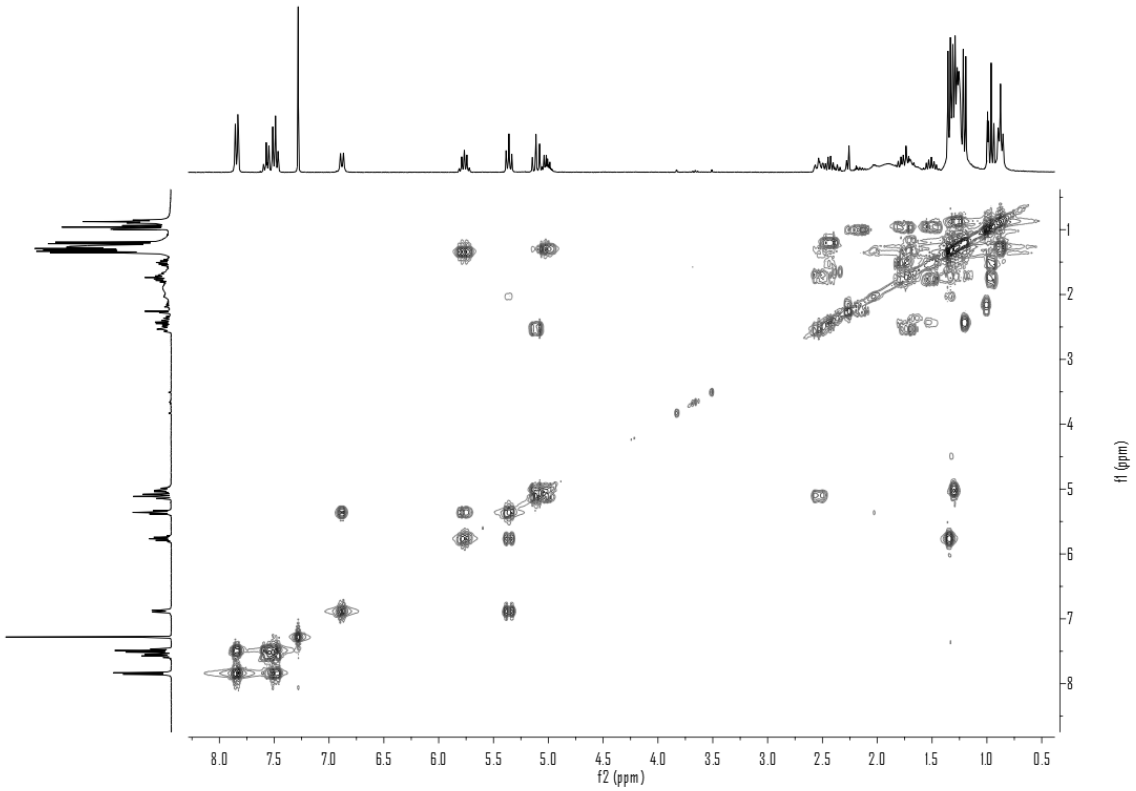



**Figure S10.** The $^{1}$H-$^{1}$H COSY spectrum of compound **1**.

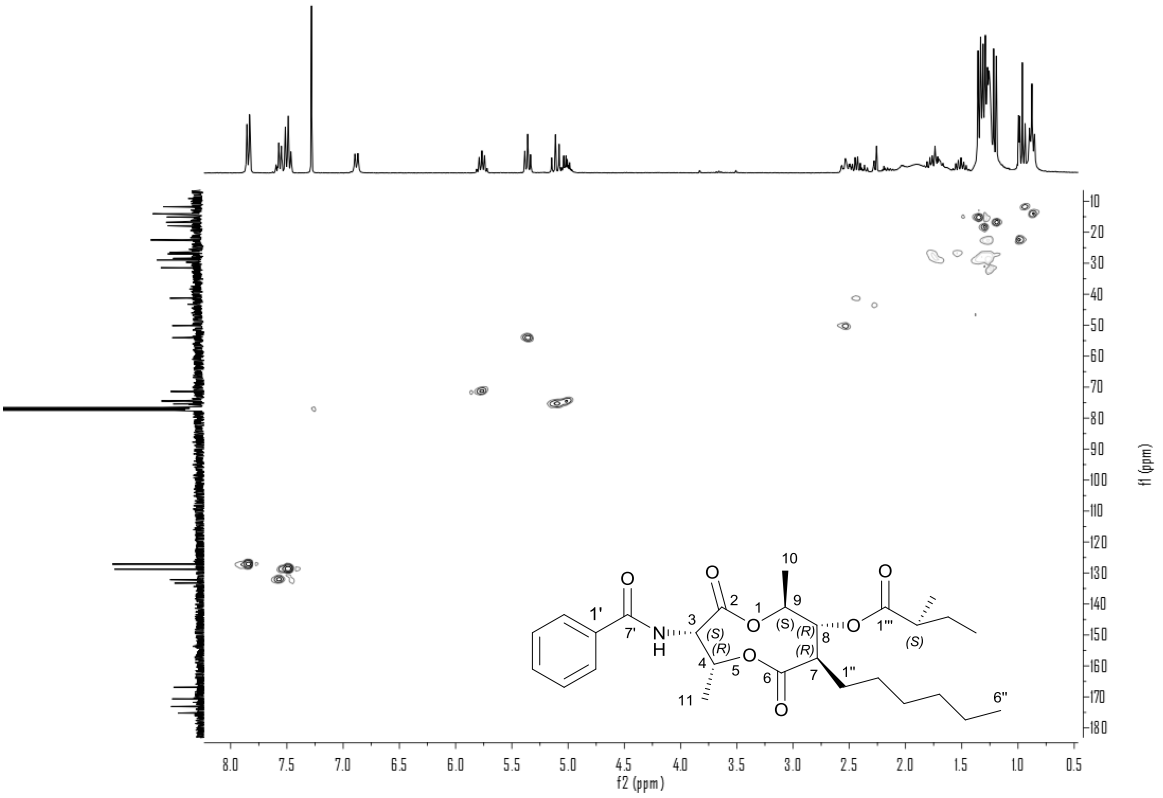



**Figure S11.** The HSQC spectrum of compound **1**.

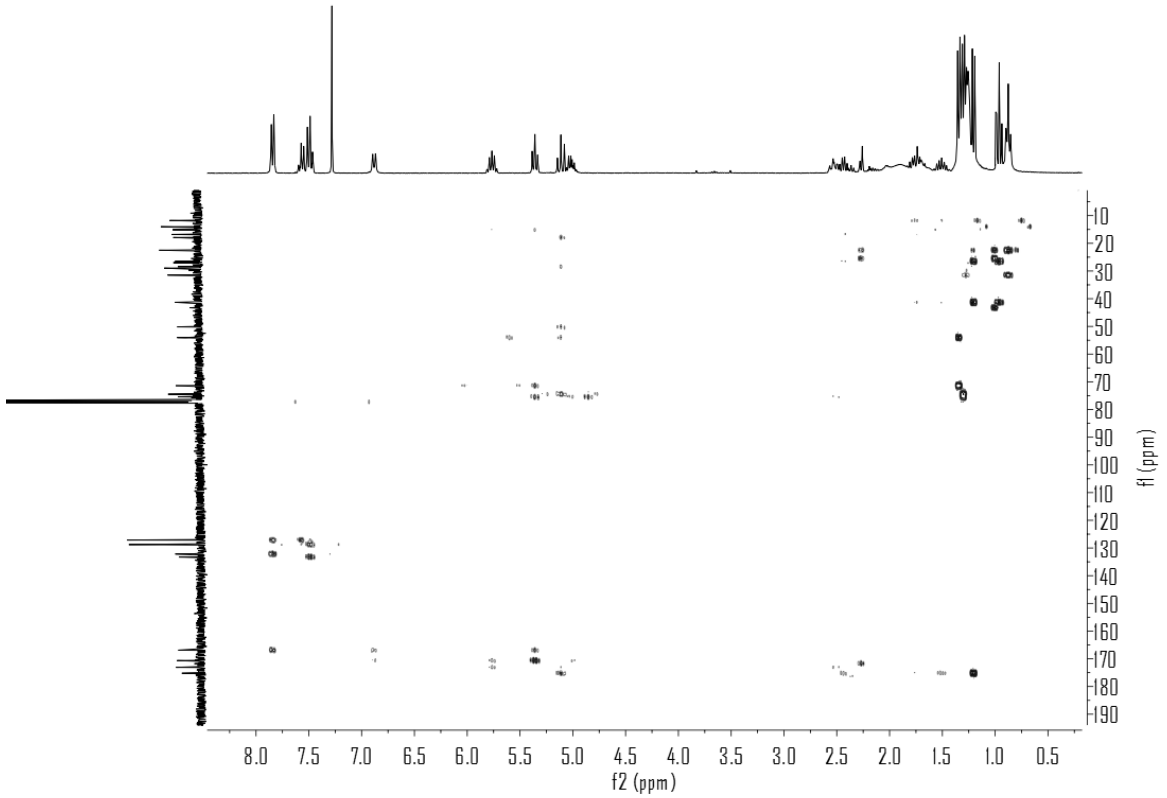



**Figure S12.** The HMBC spectrum of compound **1.**

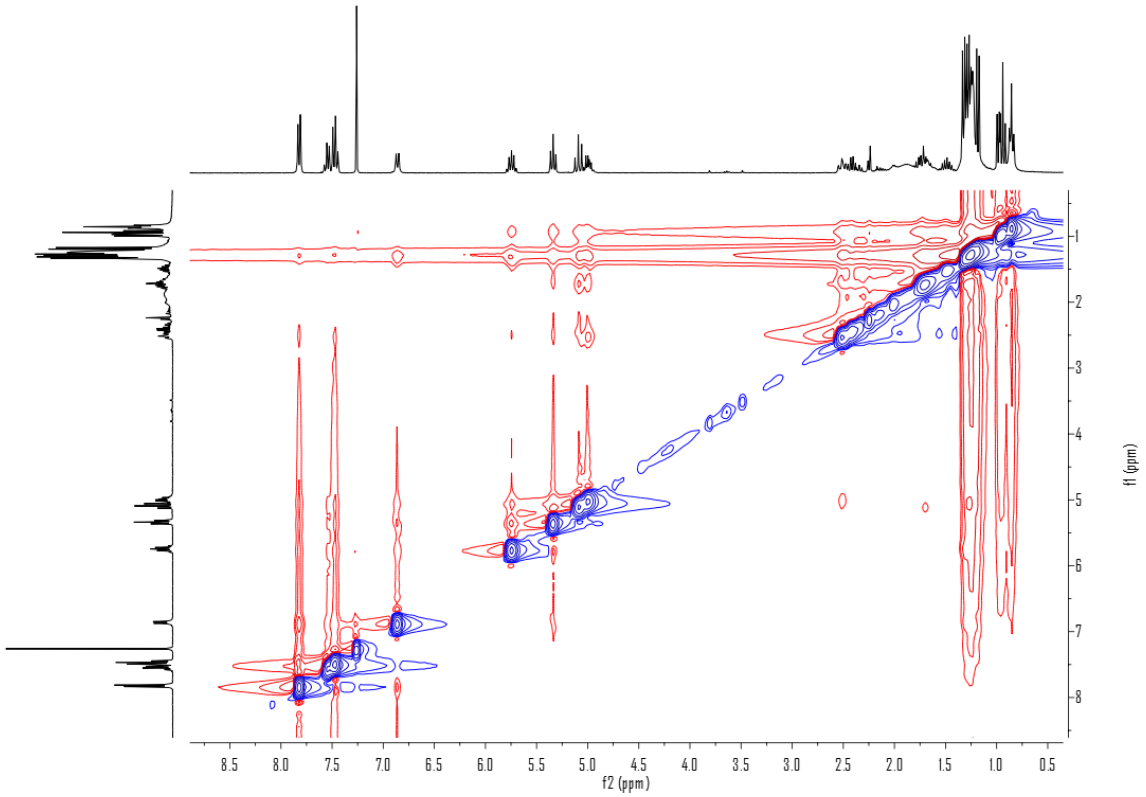



**Figure S13.** The NOESY spectrum of compound **1.**

**The spectra of neoantimycin B (2)**

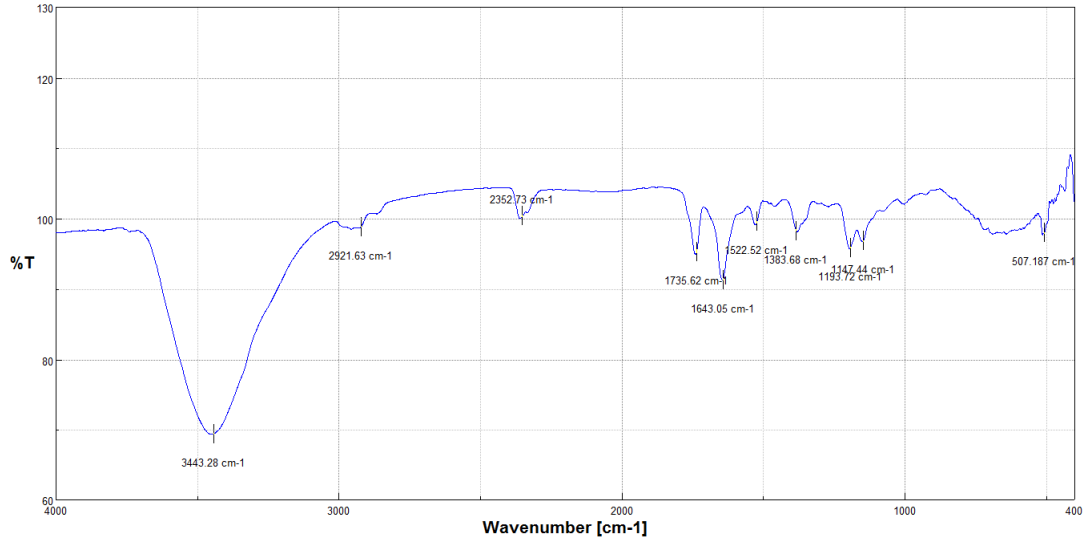



**Figure S14.** IR spectrum of compound **2.**

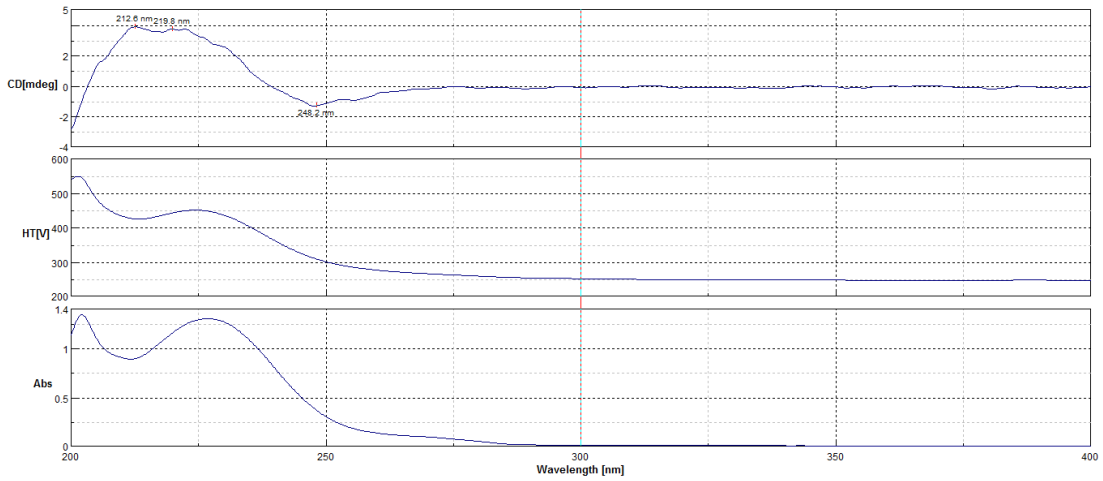



**Figure S15.** CD spectrum and UV spectrum of compound **2** in MeOH.

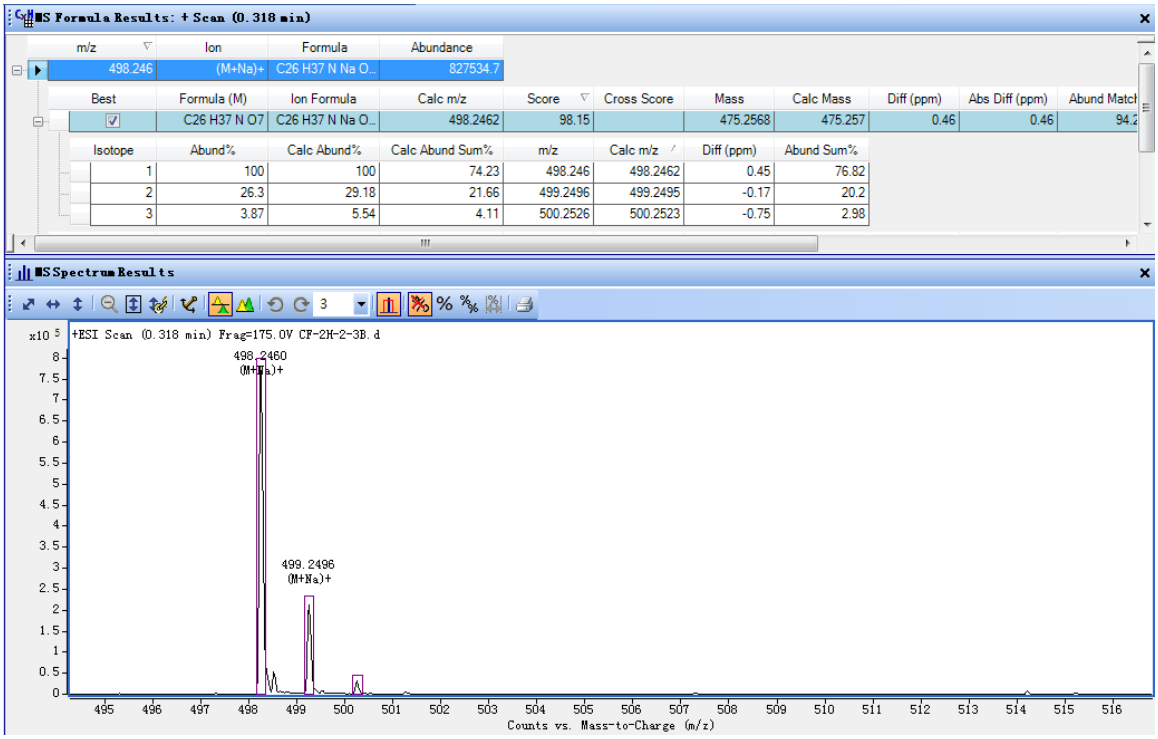



**Figure S16.** HR-TOF-MS of compound **2**.

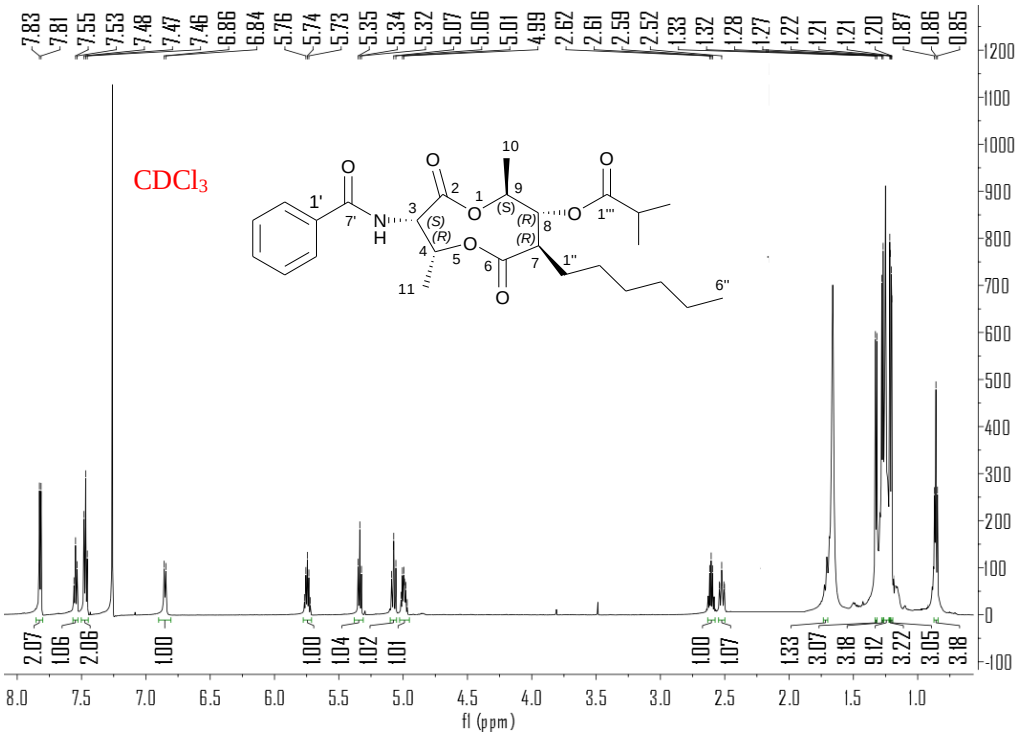



**Figure S17.** The $^{1}$H-NMR spectrum of compound **2**.

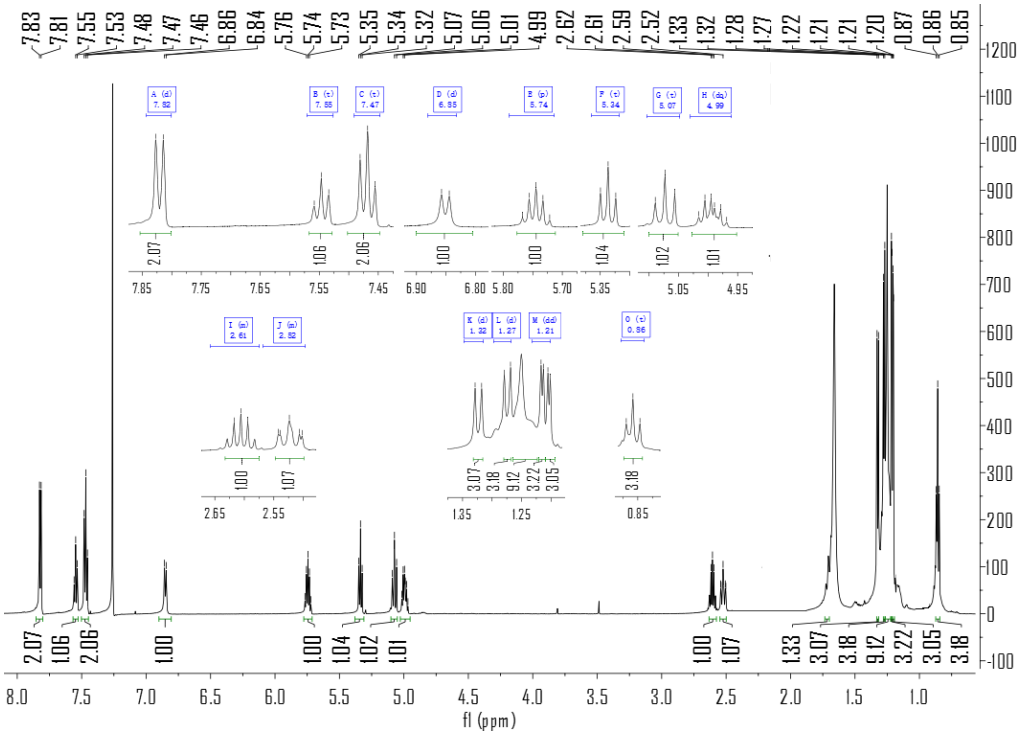



**Figure S18.** The $^{1}$H-NMR spectrum of compound **2.**

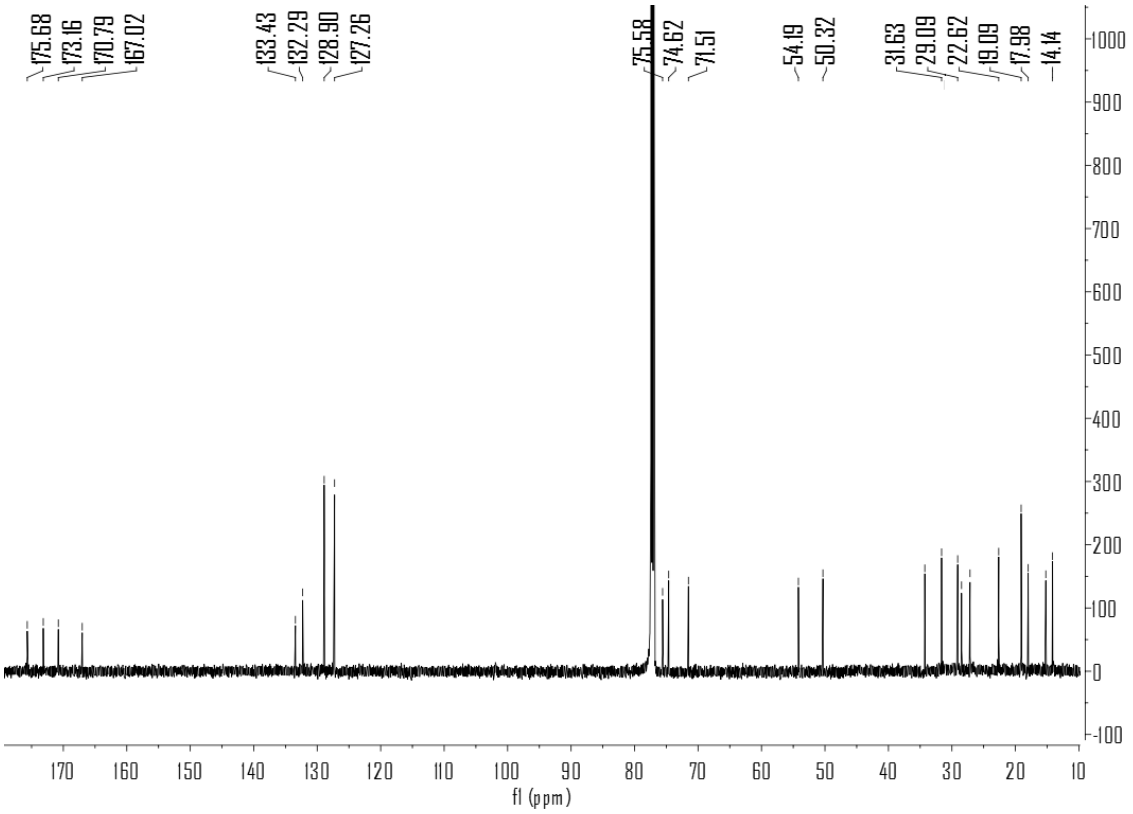



**Figure S19.** The $^{13}$C-NMR spectrum of compound **2**.

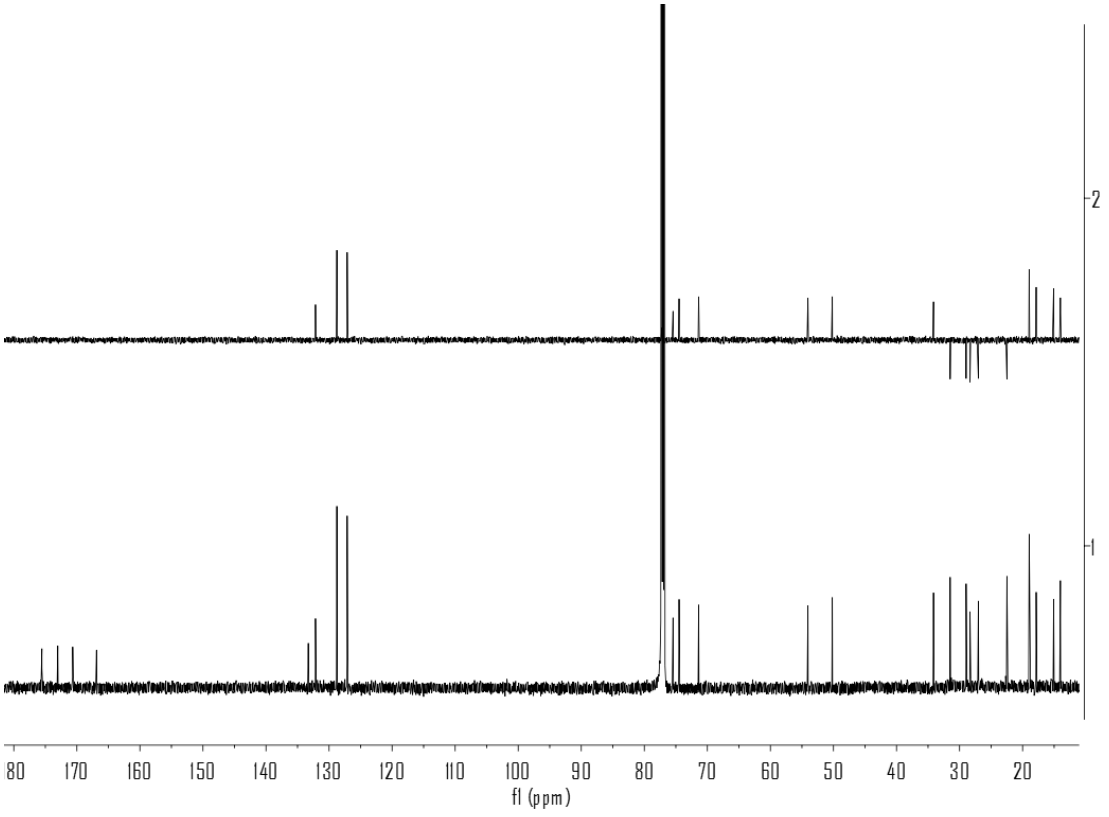



**Figure S20.** The $^{13}$C-NMR and DEPT spectra of compound **2**.

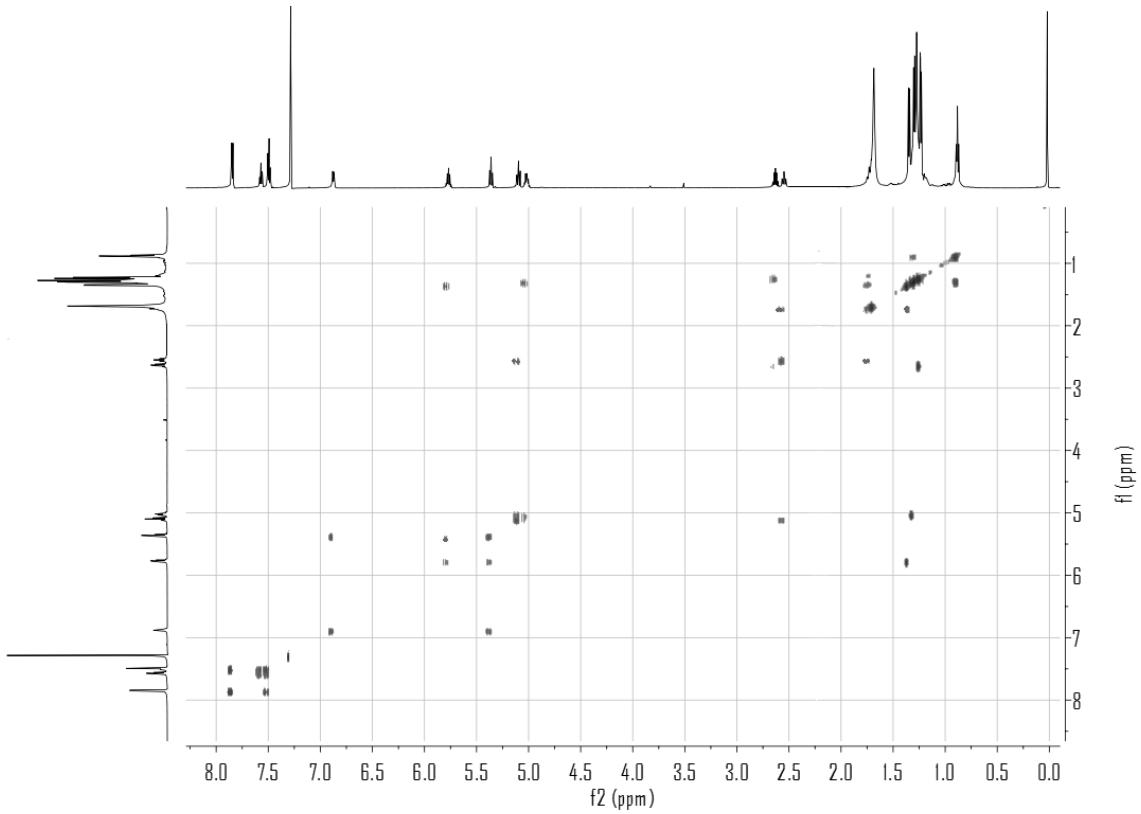



**Figure S21.** The $^{1}$H-$^{1}$H COSY spectrum of compound **2**.

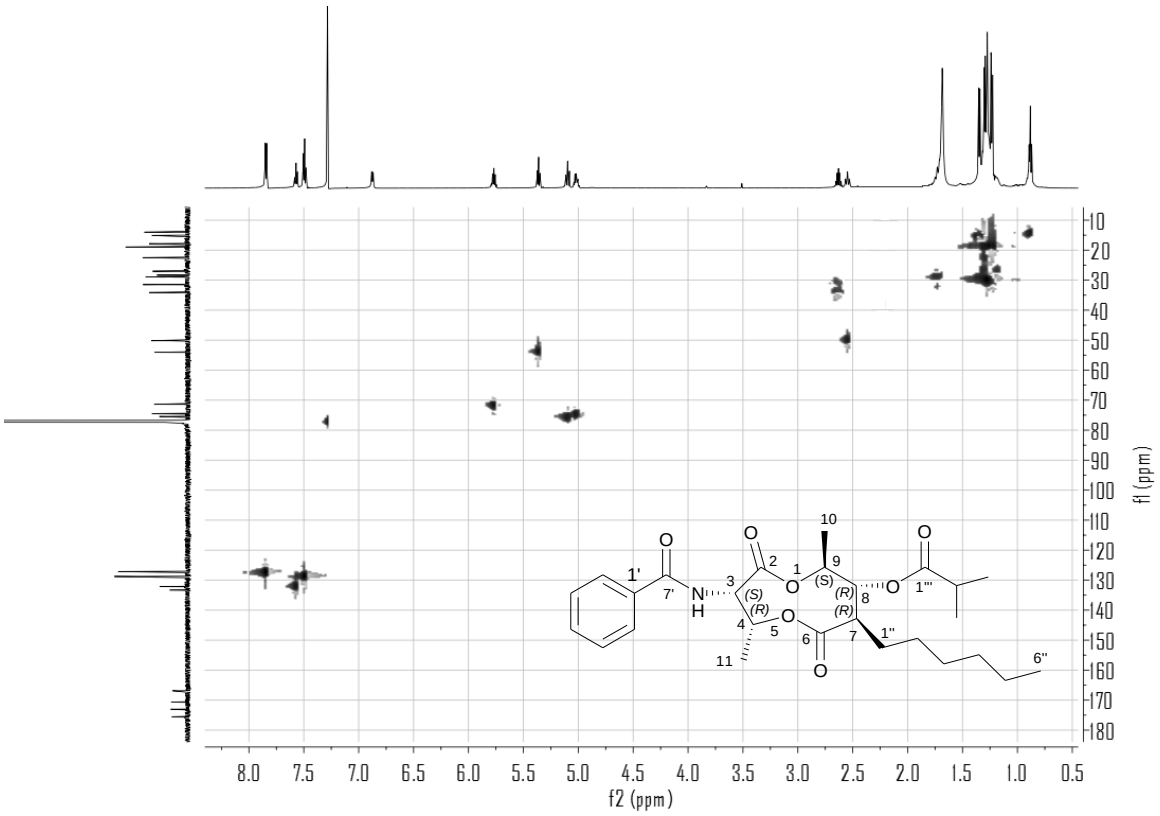



**Figure S22.** The HSQC spectrum of compound **2**.

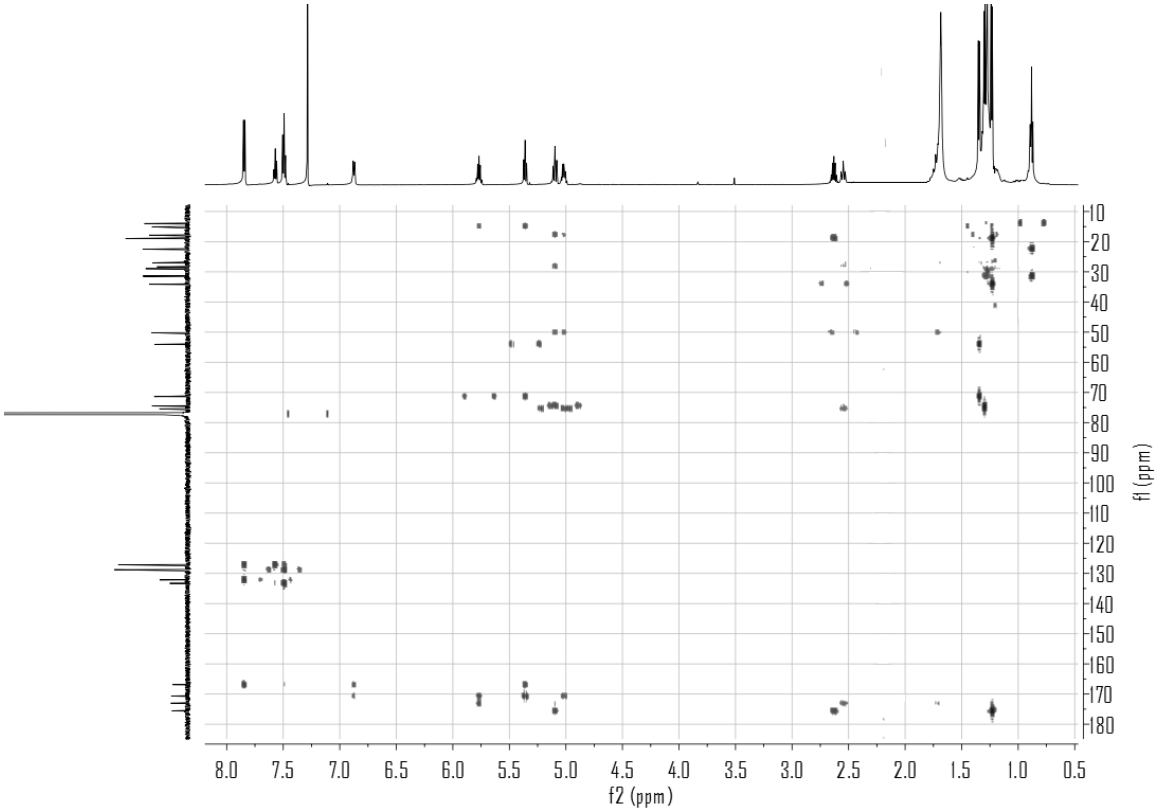



**Figure S23.** The HMBC spectrum of compound **2**.

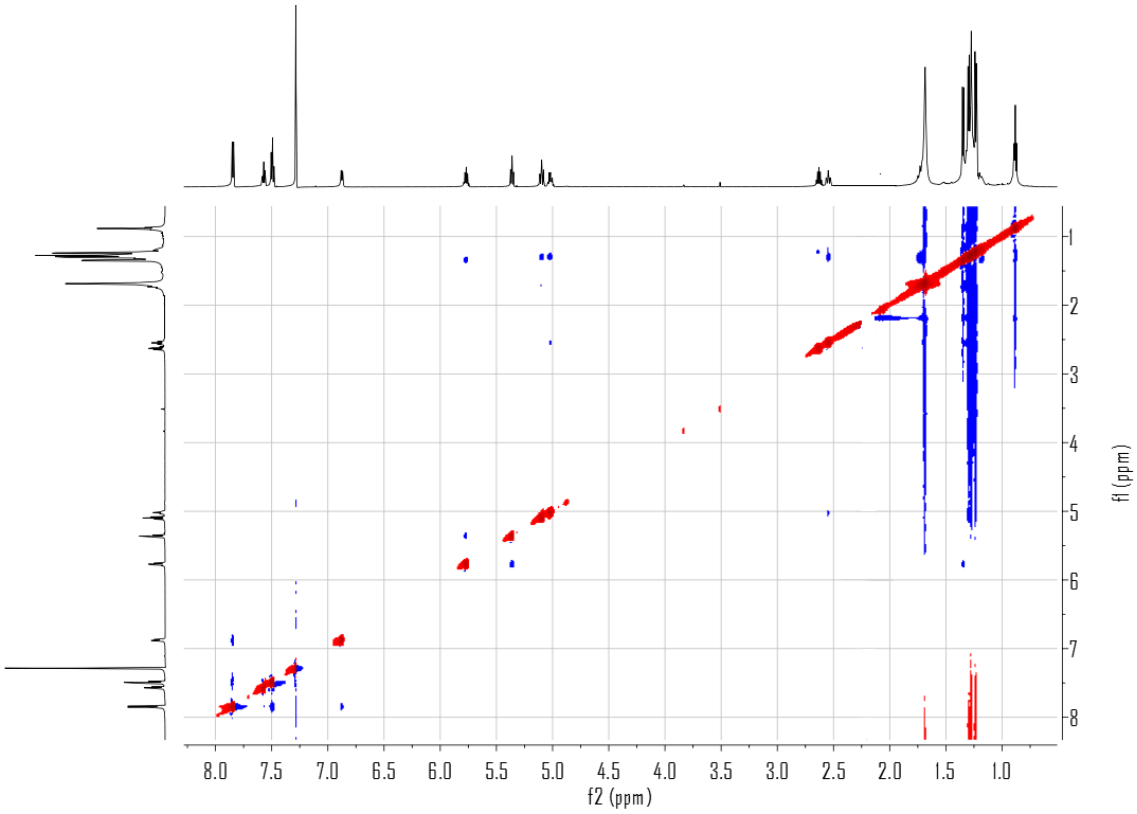



**Figure S24.** The NOESY spectrum of compound **2**.

**Table S5.** $^{1}$H (300 MHz) and $^{13}$C (75 MHz) NMR data of **3-5** ($\delta$ in ppm $J$ in Hz).

| No. | 3 | | 4 | | 5 | |
|---|---|---|---|---|---|---|
| | $\delta_C$ | $\delta_H$ | $\delta_C$ | $\delta_H$ | $\delta_C$ | $\delta_H$ |
| **2** | 170.1 | | 170.1 | | 170.1 | |
| **3** | 53.7 | 5.32 (1H, t, 7.7) | 53.6 | 5.32 (1H, t, 7.7 ) | 53.6 | 5.32 (1H, t, 7.7 ) |
| **4** | 70.9 | 5.75 (1H, p, 7.0) | 70.9 | 5.75 (1H, p, 7.0) | 70.9 | 5.75 (1H, p,7.0) |
| **6** | 172.9 | | 172.9 | | 172.9 | |
| **7** | 50.2 | 2.52 (1H, m) | 50.1 | 2.52 (1H, m) | 50.1 | 2.52 (1H, m) |
| **8** | 75.4 | 5.11 (1H, t, 9.9) | 75.4 | 5.11 (1H, t, 9.9) | 75.4 | 5.11 (1H, t, 9.9) |
| **9** | 74.7 | 4.97 (1H, m) | 74.9 | 4.97 (1H, m) | 74.9 | 4.97 (1H, m) |
| **10** | 17.8 | 1.28 (3H, d, 6.3) | 17.8 | 1.28 (3H, d, 6.3) | 17.8 | 1.28 (3H, d, 6.3) |
| **11** | 14.9 | 1.30 (3H, d, 6.7) | 15 | 1.30 (3H, d, 6.7) | 15 | 1.30 (3H, d, 6.7) |
| **1′** | 112.6 | | 112.5 | | 112.5 | |
| **2′** | 150.6 | | 150.6 | | 150.6 | |
| **3′** | 127.5 | | 127.4 | | 127.4 | |
| **4′** | 124.8 | 8.54 (1H, d, 8.1） | 124.8 | 8.54 (1H, d, 8.1） | 124.8 | 8.54 (1H, d, 8.1） |
| **5′** | 118.9 | 6.89 (1H, t, 8.1） | 119 | 6.89 (1H, t, 8.1） | 119 | 6.89 (1H, t, 8.1） |
| **6′** | 120.1 | 7.23 (1H, d, 8.3） | 120.1 | 7.23 (1H, d, 8.3） | 120.1 | 7.23 (1H, d, 8.3） |
| **7′** | 169.4 | | 169.3 | | 169.3 | |
| **8′** | 159.1 | 8.50 (1H, d, 1.7) | 159.1 | 8.50 (1H, d, 1.7) | 159.1 | 8.50 (1H, d, 1.7) |
| **1″** | 28.6 | 1.68 (1H, m) | 28.3 | 1.68 (1H, m) | 28.3 | 1.68 (1H, m) |
| **2″** | 22.6 | 1.23 (2H, m) | 22.5 | 1.23 (2H, m) | 22.5 | 1.23 (2H, m) |
| **3″** | 27.2 | 1.23 (2H, m) | 27 | 1.23 (2H, m) | 27 | 1.23 (2H, m) |
| **4″** | 31.4 | 1.23 (2H, m) | 31.5 | 1.23 (2H, m) | 31.5 | 1.23 (2H, m) |
| **5″** | 29.2 | 1.23 (2H, m) | 28.9 | 1.23 (2H, m) | 28.9 | 1.23 (2H, m) |
| **6″** | 14.2 | 0.85 (3H, t, 7.1) | 14 | 0.85 (3H, t, 7.1) | 14 | 0.85 (3H, t, 7.1) |
| **7′-NH** | | 8.43 (1H, d, 8.1) | | 8.43 (1H, d, 8.1) | | 8.43 (1H, d, 8.1) |
| **8′-NH** | | 9.20 (1H, br.s) | | 9.20 (1H, br.s) | | 9.20 (1H, br.s) |
| **a** | | | | | | |
| **1‴** | 175.2 | | 175.6 | | 175.6 | |
| **2‴** | 41.3 | 2.41 (1H, m) | 34.1 | 2.61 (1H, t, 7.0) | 34.1 | 2.61 (1H, t, 7.0) |
| **3‴** | 26.5 | 1.74 (1H, m), 1.50 (1H, m) | 18.9 | 1.22 (3H, d, 2.5) | 18.9 | 1.22 (3H, d, 2.5) |
| **4‴** | 11.7 | 0.94 (3H, t, 7.4) | 18.9 | 1.21, (3H, d, 2.5) | 18.9 | 1.21, (3H, d, 2.5) |
| **5‴** | 16.7 | 1.18 (3H, d, 7.0) | | | | |
| **b** | | | | | | |
| **1‴** | 171.7 | | | | | |
| **2‴** | 43.2 | 2.24 (2H, d, 6.8) | | | | |
| **3‴** | 25.5 | 2.13 (1H, m) | | | | |
| **4‴** | 22.4 | 0.98 (3H, d, 6.6) | | | | |
| **5‴** | 22.4 | 0.98 (3H, d, 6.6) | | | | |

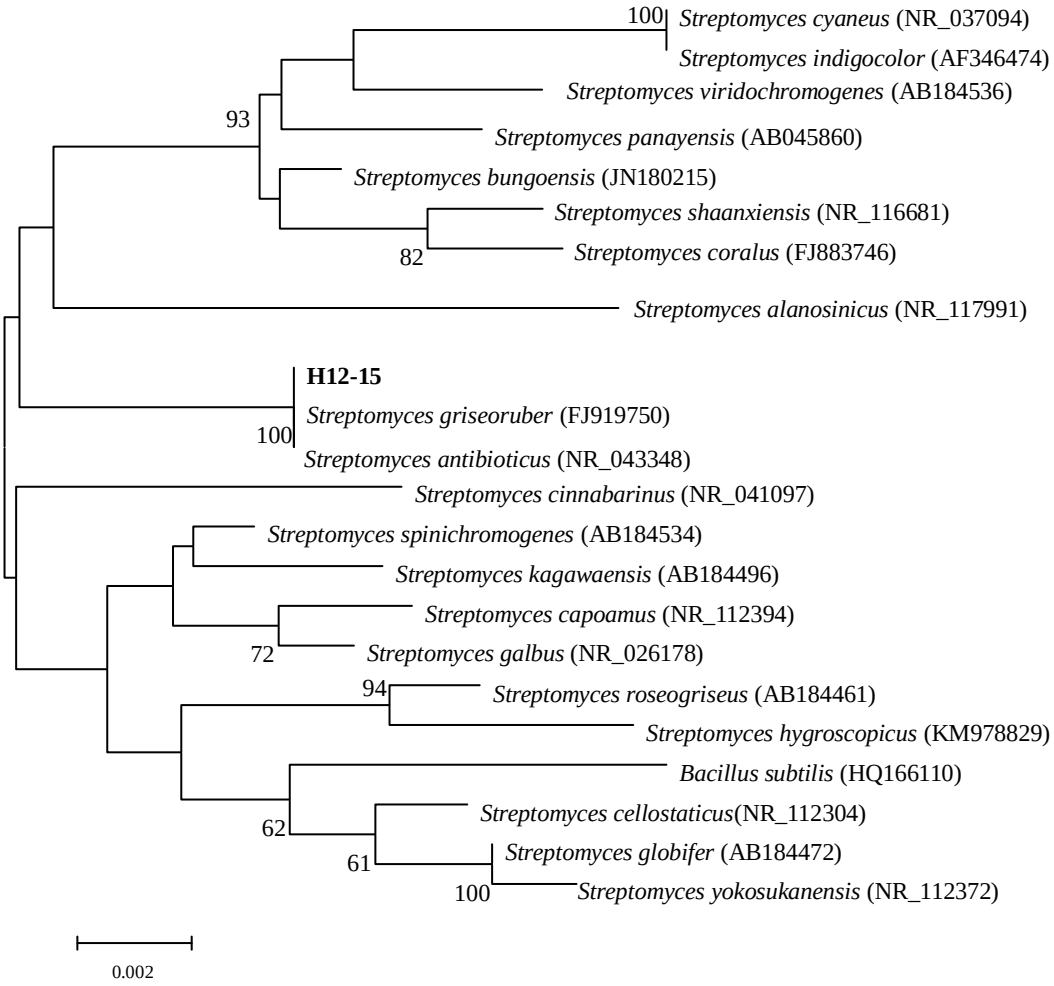



**Figure S25.** Phylogenetic tree of H12-15.

1CGGCTTGCCGCGTGCTACCATGCAAGTCGAACGATGAAGCCCTTCGGGGTGGATTAG
58TGGCGAACGGGTGAGTAACACGTGGGCAATCTGCCCTGCACTCTGGGACAAGCCCT
114GGAAACGGGGTCTAATACCGGATATCACTCTTGCAGGCATCTGTGAGGGTCGAAAG
170CTCCGGCGGTGCAGGATGAGCCCGCGGCCTATCAGCTTGTTGGTGAGGTAATGGCT
226CACCAAGGCGACGACGGGTAGCCGGCCTGAGAGGGCGACCGGCCACACTGGGAC
280TGAGACACGGCCCAGACTCCTACGGGAGGCAGCAGTGGGGAATATTGCACAATGG
335GCGAAAGCCTGATGCAGCGACGCCGCGTGAGGGATGACGGCCTTCGGGTTGTAAA
390CCTCTTTCAGCAGGGAAGAAGCGAAAGTGACGGTACCTGCAGAAGAAGCGCCGG
444CTAACTACGTGCCAGCAGCCGCGGTAATACGTAGGGCGCAAGCGTTGTCCGGAATT
500ATTGGGCGTAAAGAGCTCGTAGGCGGCTTGTCACGTCGGGTGTGAAAGCCCGGGG
555CTTAACCCCGGGTCTGCATTCGATACGGGCTAGCTAGAGTGTGGTAGGGGAGATCG
621GAATTCCTGGTGTAGCGGTGAAATGCGCAGATATCAGGAGGAACACCGGTGGCGA
676AGGCGGATCTCTGGGCCATTACTGACGCTGAGGAGCGAAAGCGTGGGGAGCGAAC
731AGGATTAGATACCCTGGTAGTCCACGCCGTAAACGGTGGGAACTAGGTGTTGGCGA
787CATTCCACGTCGTCGGTGCCGCAGCTAACGCATTAAGTTCCCCGCCTGGGGAGTAC
843GGCCGCAAGGCTAAAACTCAAAGGAATTGACGGGGGCCCGCACAAGCAGCGGAG

897CATGTGGCTTAATTCGACGCAACGCGAAGAACCTTACCAAGGCTTGACATACACCG
953GAAACGGCCAGAGATGGTCGCCCCCTTGTGGTCGGTGTACAGGTGGTGCATGGCT
1008GTCGTCAGCTCGTGTCGTGAGATGTTGGGTTAAGTCCCGCAACGAGCGCAACCCT
1063TGTTCTGTGTTGCCAGCATGTCCTTCGGGATGATGGGGACTCACAGGAGACCGCC
1118GGGGTCAACTCGGAGGAAGGTGGGGACGACGTCAAGTCATCATGCCCCTTATGTC
1173TTGGGCTGCACACGTGCTACAATGGCCGGTACAAAGAGCAGCGATACCGTGAGGT
1228GGAGCGAATCTCAAAAAGCCGGTCTCAGTTCGGATTGGGGTCTGCAACTCGACCC
1283CATGAAGTCGGAGTTGCTAGTAATCGCAGATCAGCATTGCTGCGGTGAATACGTTC
1349CCGGGCCTTGTACACACCGCCCGTCACGTCACGAAAGTCGGTAACACCCGAAGC
1403CGGTGGCCCAACCCCTTGTGGGAGGGAGCTTCGAAGTGAACCGAACTT

**Figure S26.** 16S rDNA gene sequence of H12-15.

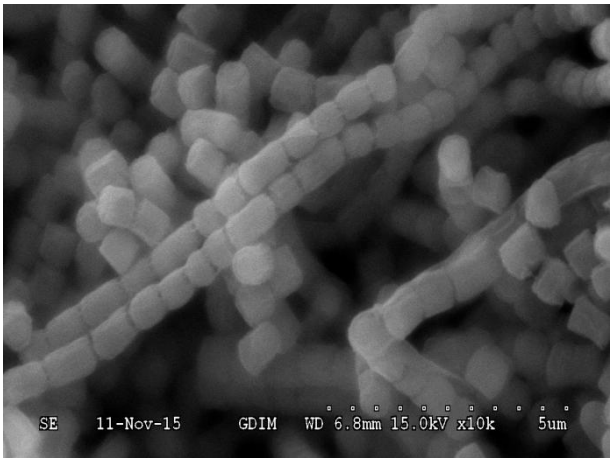



**Figure** S27. **Scaning electron micrographs of strain H12-15 on Gauze No.1 medium**