# Supporting Information

## Meroterpenoids and steroids from the marine-derived fungus *Trametes* sp. ZYX-Z-16

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# Content

ITS1 gene sequences of *Trametes* sp. ZYX-Z-16

GGCCTACGAGTGCGGGACTCGCGGTCACCTCCCACCCGTGTCTCTCTCTAC
CTGTTGCTTTGGCGGGCCCACCGGGGCCACCCGGTCGCCGGGGGACGTCG
TCCCCGGGCCCGCGCCCGCCGAAGCGCTCTGTGAACCCTGATGAAGATGG
GCTGTCTGAGTCGAATGAAAATTGTCAAAACTTTCAACAATGGATCTCTTG
GTTCCGGCATCGATGAAGAACGCAGCGAAATGCGATAAGTAATGTGAATTG
CAGAATTCCGTGAATCATCGAATCTTTGAACGCACATTGCGCCCCCTGGCAT
TCCGGGGGGCATGCCTGTCCGAGCGTCATTTCTGCCCTCAAGCCCGGCTTG
TGTGTTGGGCGTGGTCCCCCCGGGGACCTGCCCGAAAGGCAGCGGCGACG
TCCGTCTGGTCCTCGAGCGTATGGGGCTCTGTCACTCGCTCGGGACGGATC
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GTAGGAGTTACCCGCTGAACTTAAGCATATCAAAG

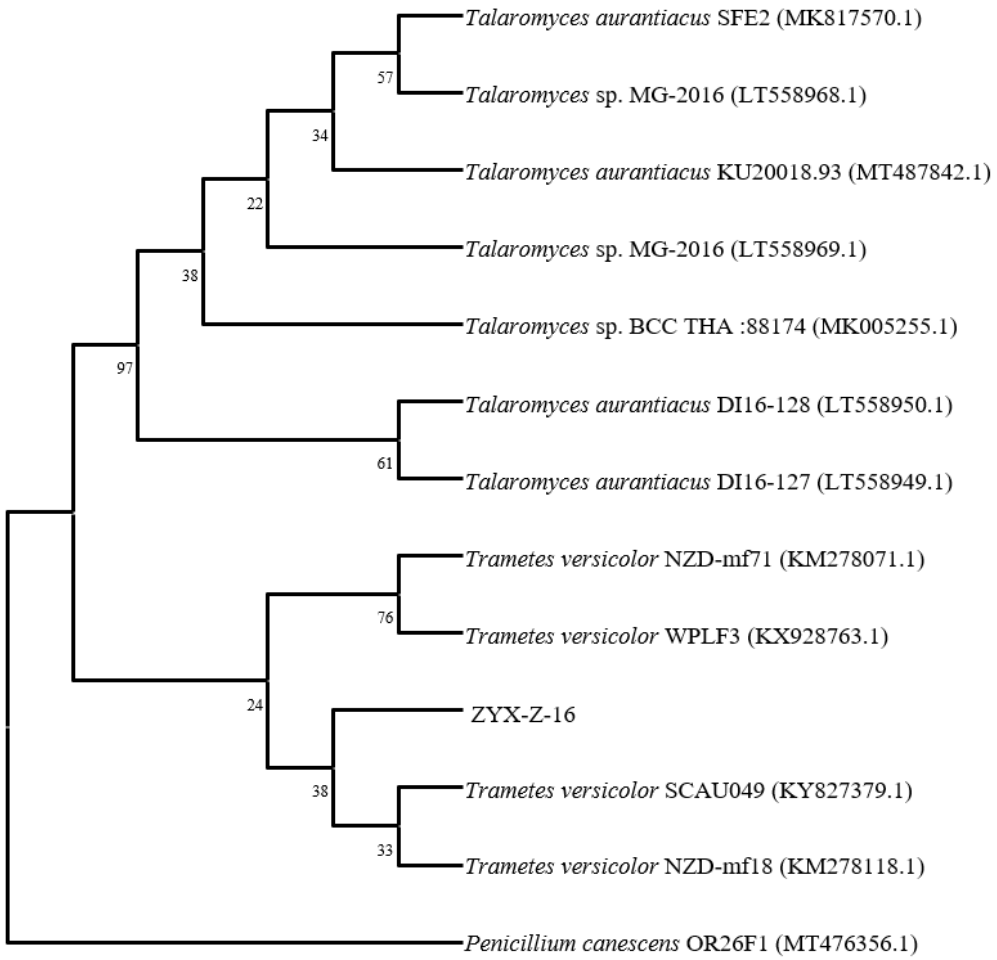



**Figure S1.** Original tree of *Trametes* sp. ZYX-Z-16

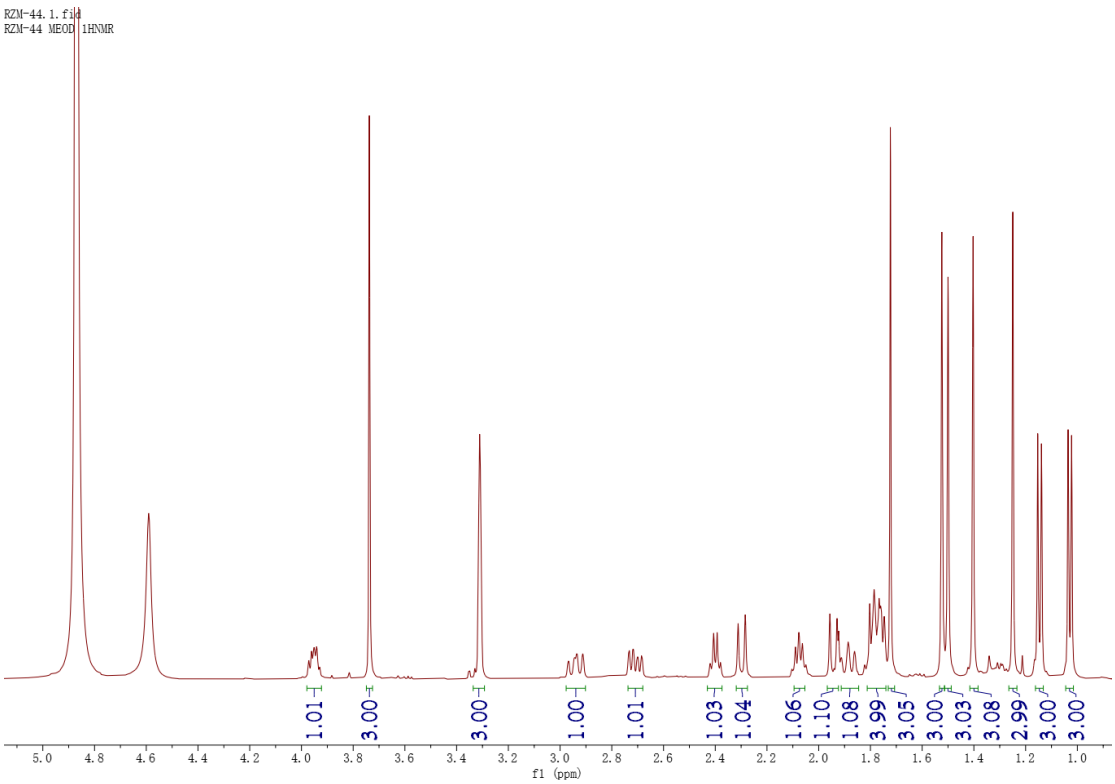



**Figure S2.** $^{1}$H-NMR spectrum of compound **1** (500 MHz, $CD_3OD$)

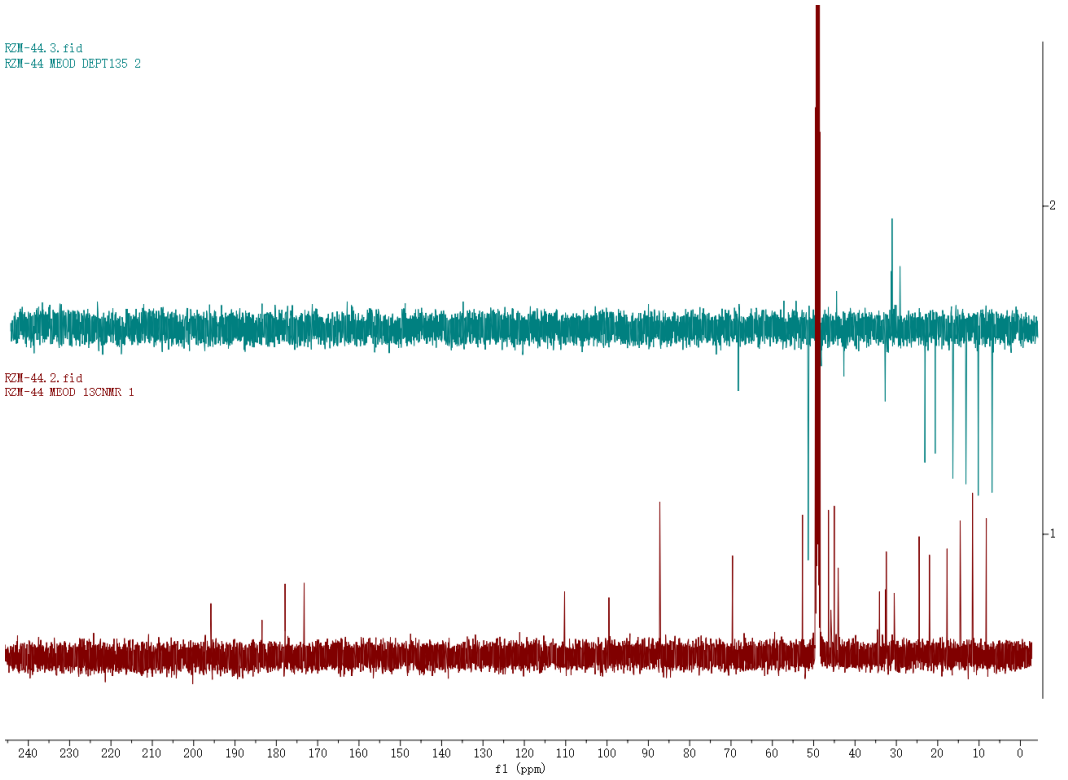



**Figure S3.** $^{13}$C-NMR and DEPT spectra of compound **1** (125 MHz, $CD_3OD$)

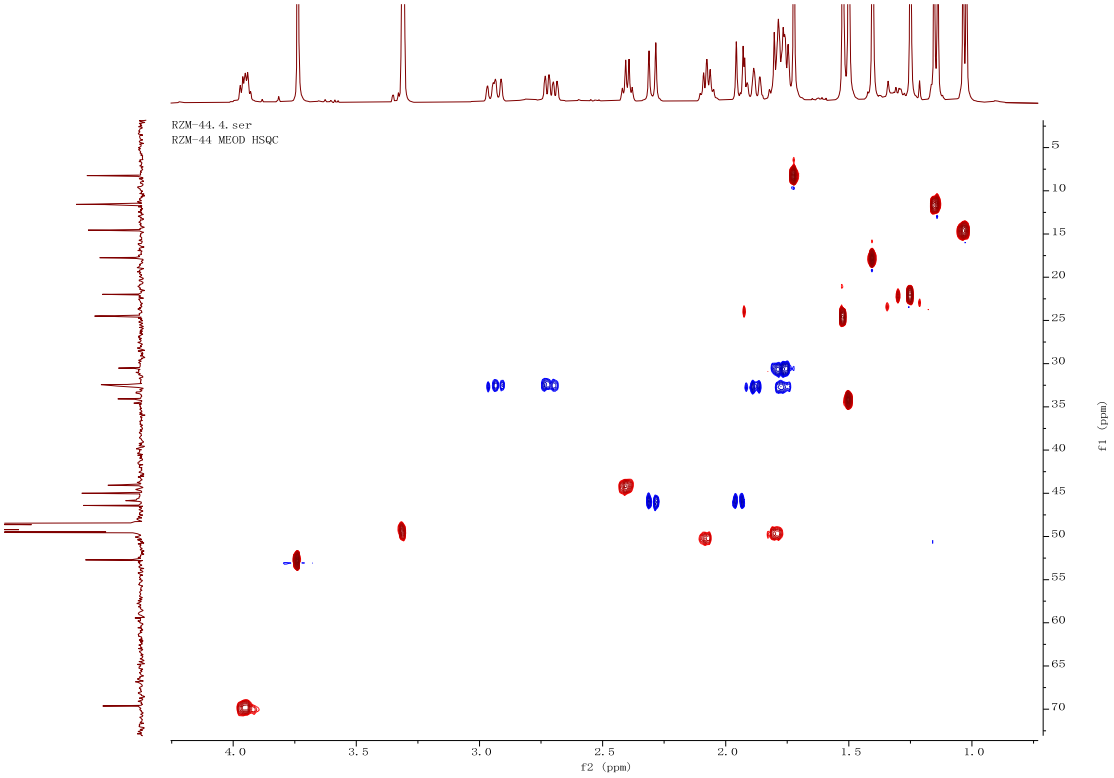



**Figure S4.** HSQC spectrum of compound **1** (125 MHz, $CD_3OD$)

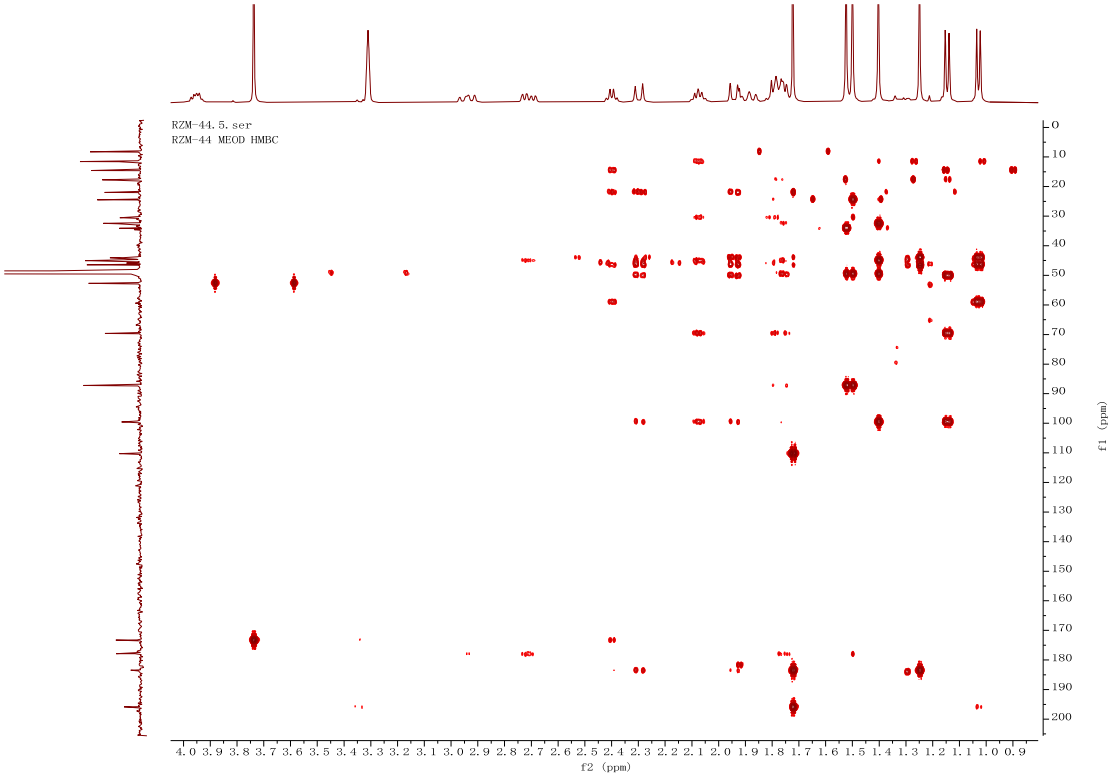



**Figure S5.** HMBC spectrum of compound **1** (125 MHz, $CD_3OD$)

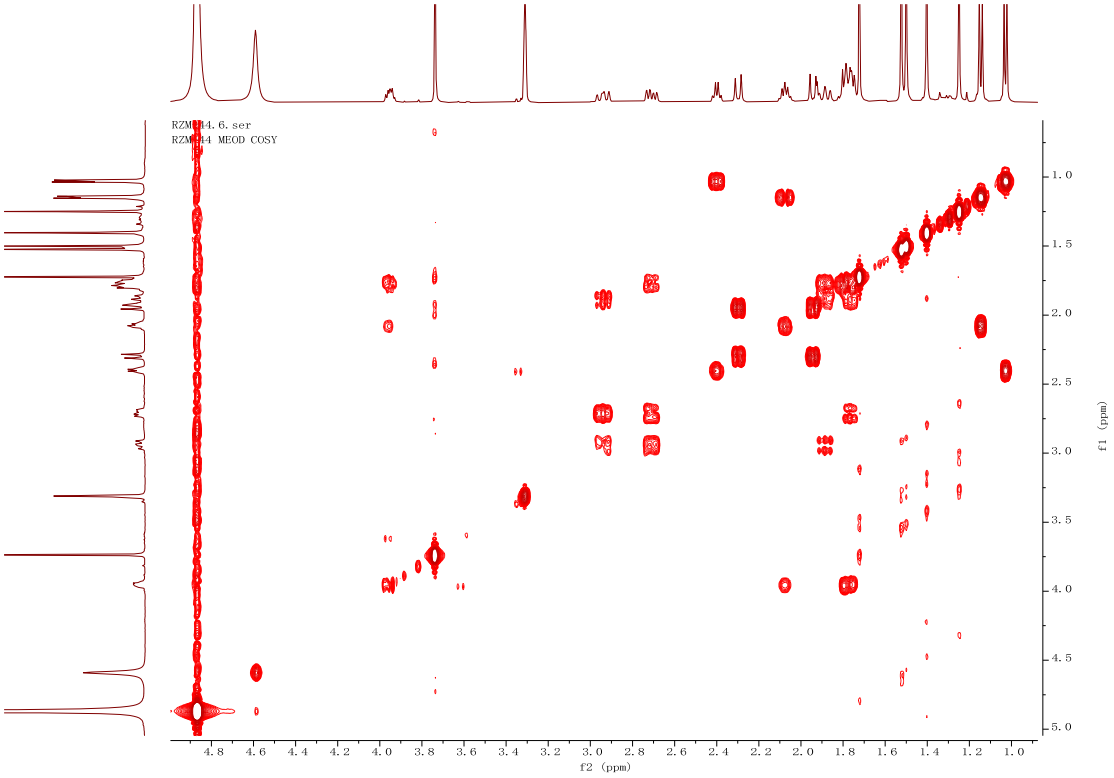



**Figure S6.** $^{1}$H-$^{1}$H COSY spectrum of compound **1** (125MHz, $CD_3OD$)

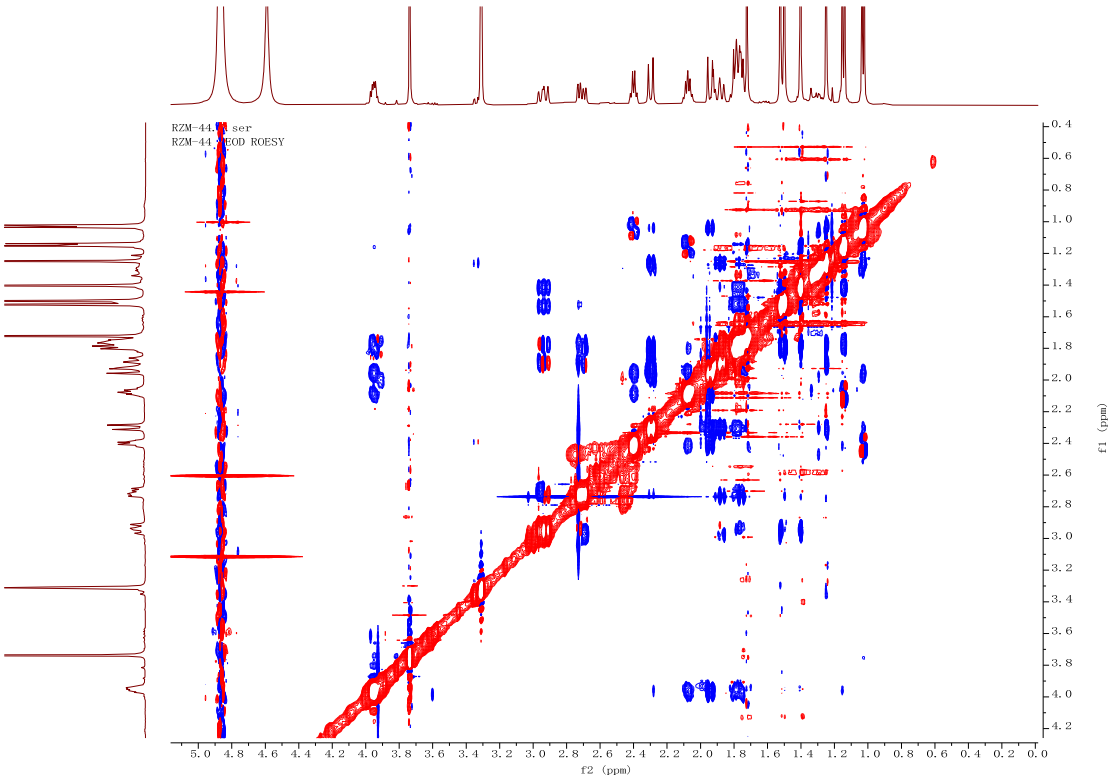
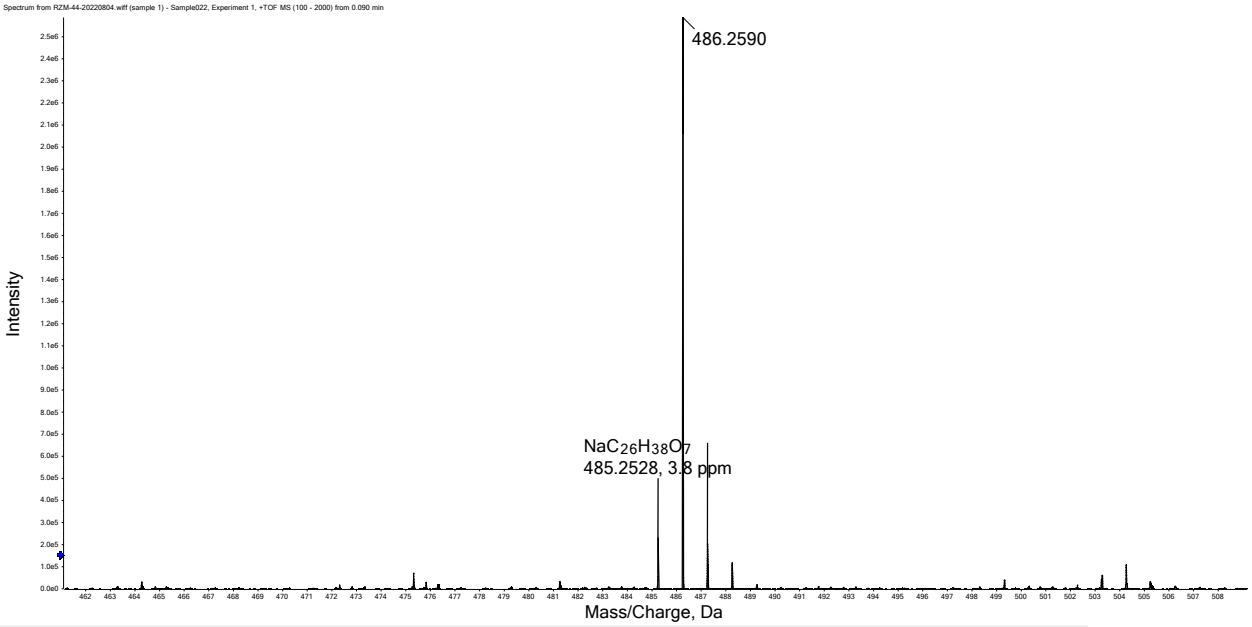



**Figure S7.** ROESY spectrum of compound **1** (125 MHz, $CD_3OD$)




| Hit | Formula | m/z | RDB | ppm | MS Rank | MSMS ppm | MSMS Rank | Found |
|---|---|---|---|---|---|---|---|---|
| 1 | C26H38O7 | 485.2510 | 8.0 | 3.8 | 1 | | | NA/NA |

**Figure S8.** HRESIMS of compound **1** (MeOH)

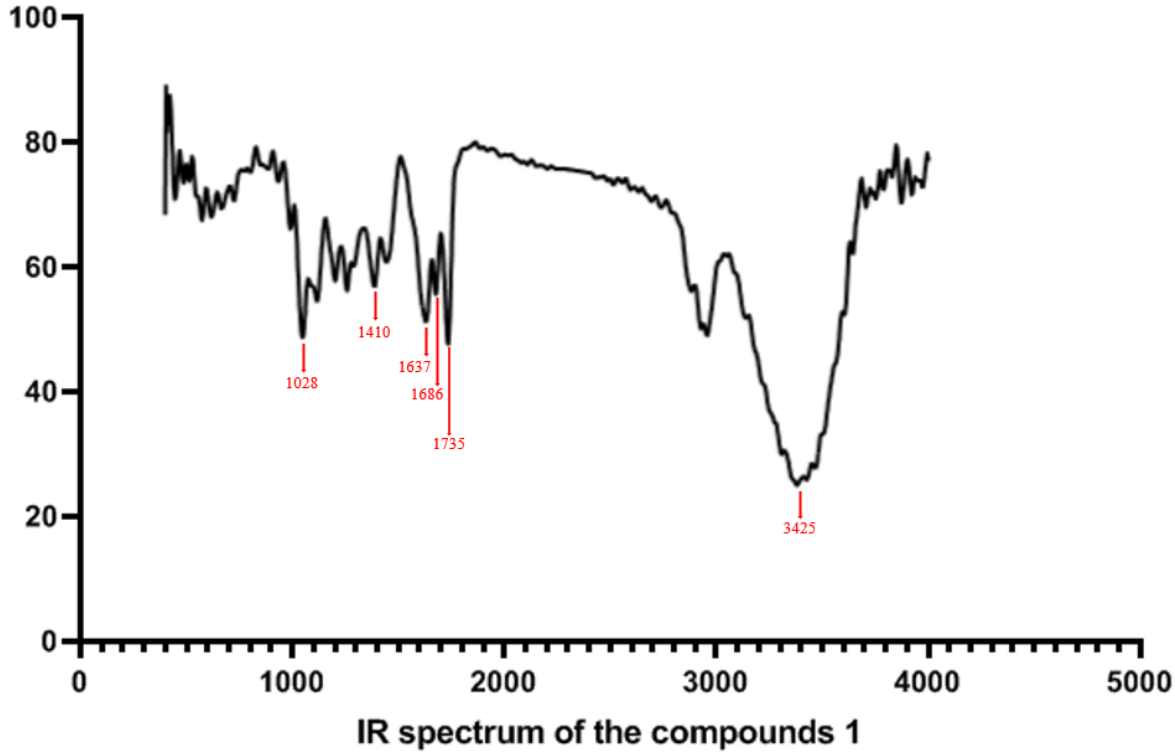



**Figure S9.** IR spectrum of the compound **1**

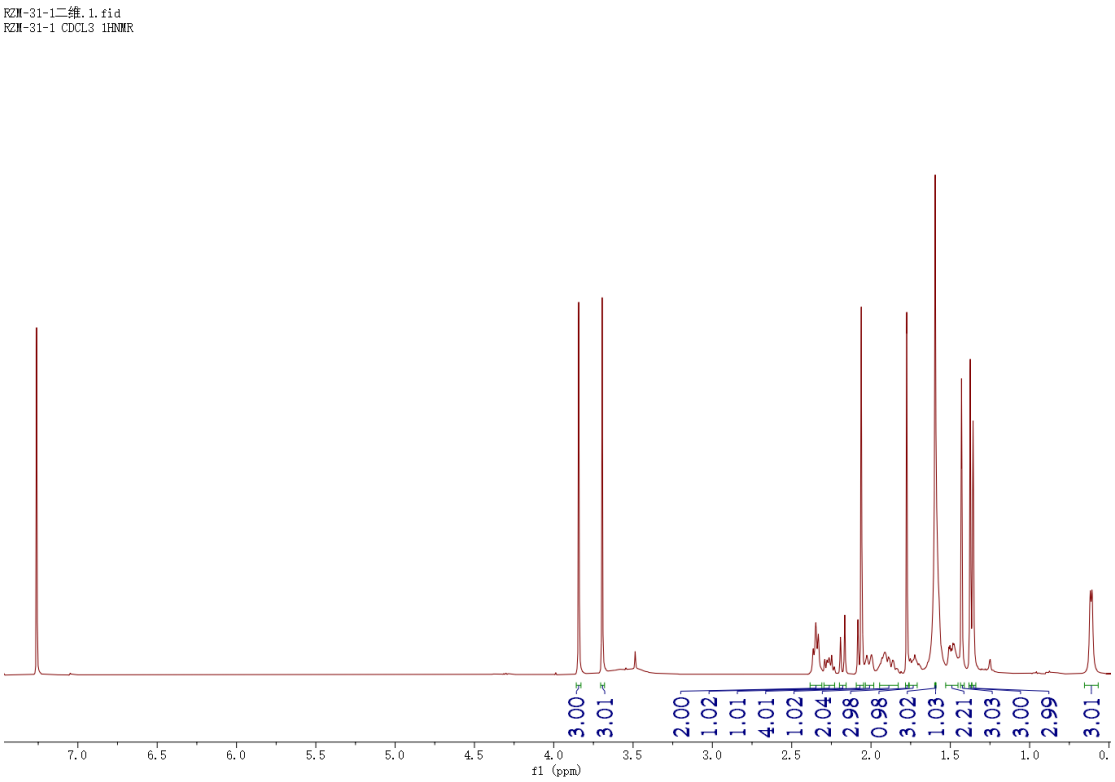



**Figure S10.** $^{1}$H-NMR spectrum of compound **2** (500 MHz, $CDCl_3$)

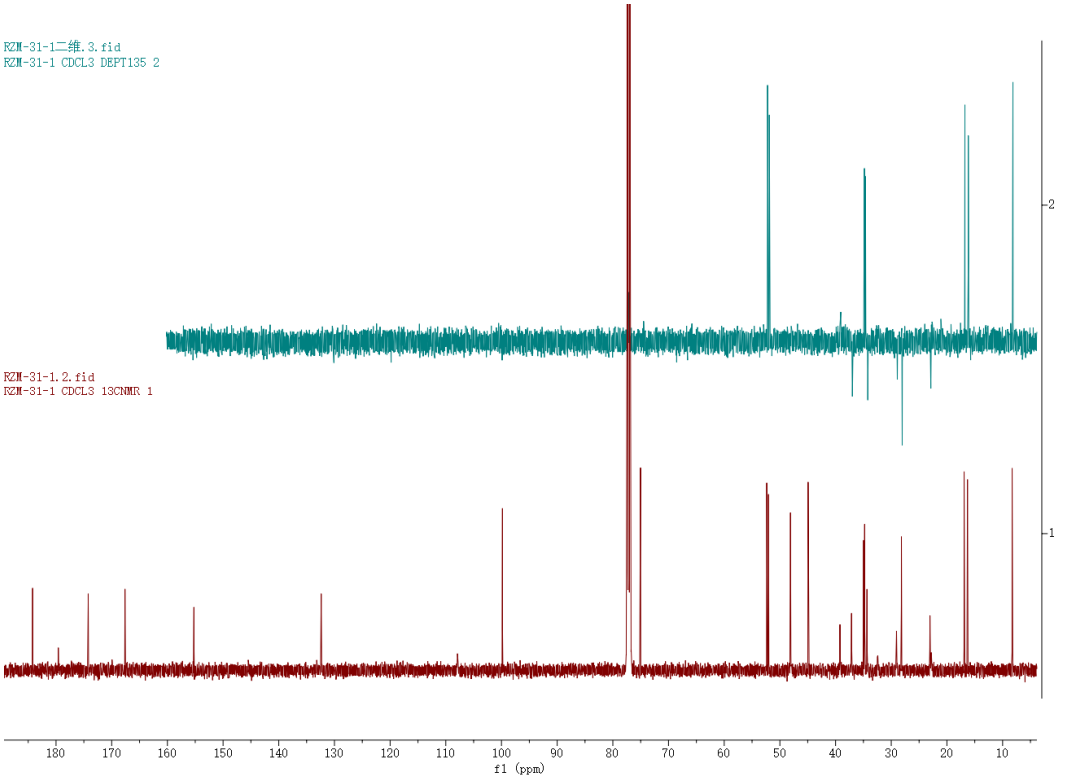



**Figure S11.** $^{13}$C-NMR and DEPT spectra of compound **2** (125 MHz, $CDCl_3$)

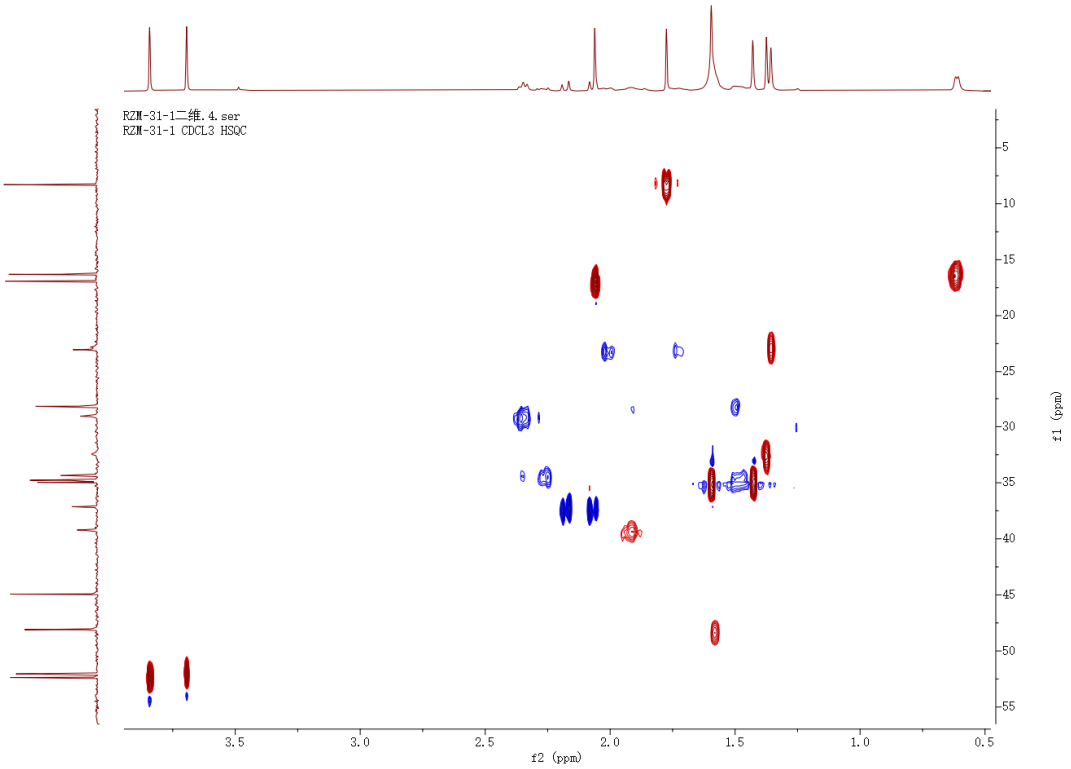



**Figure S12.** HSQC spectrum of compound **2** (125 MHz, $CDCl_3$)

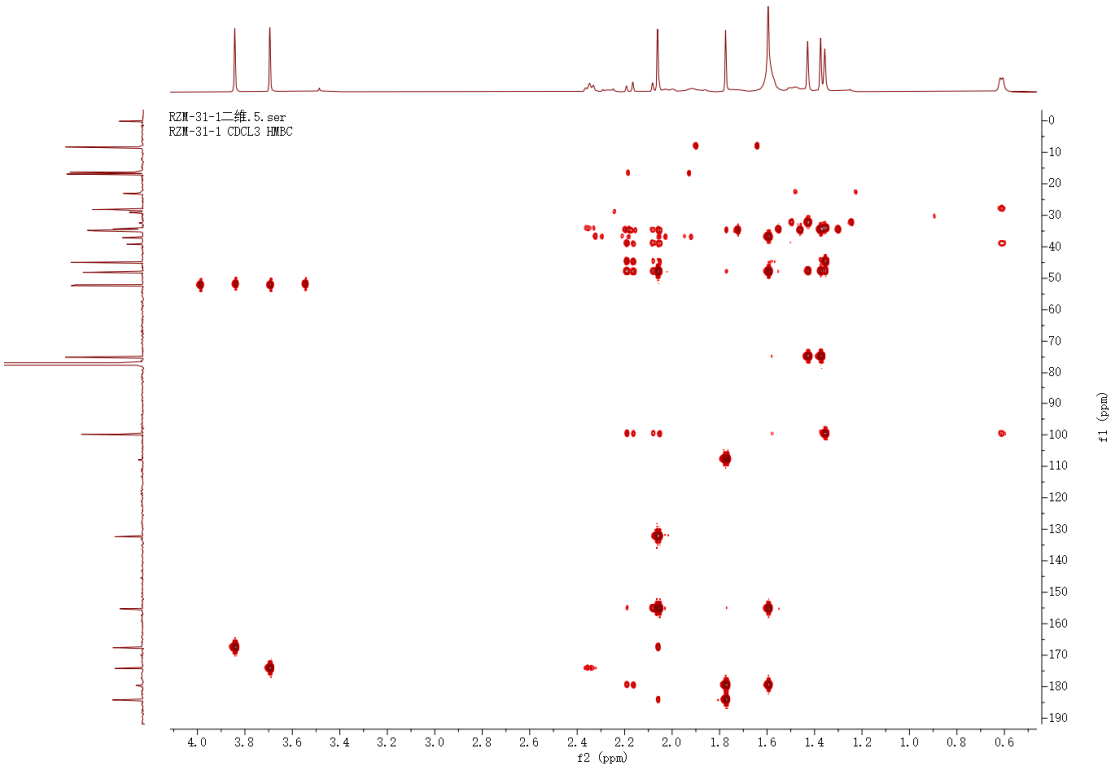



**Figure S13.** HMBC spectrum of compound **2** (125 MHz, $CDCl_3$)

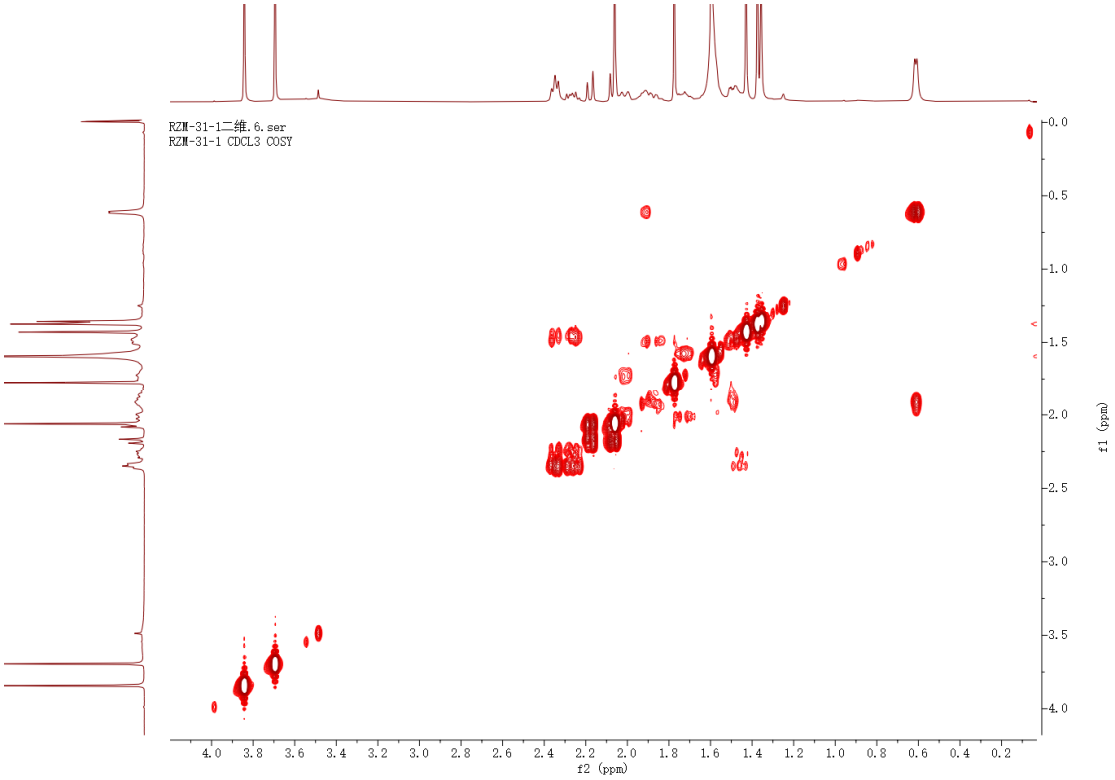



**Figure S14**. $^{1}$H-$^{1}$H COSY spectrum of compound **2** (125MHz, $CDCl_3$)

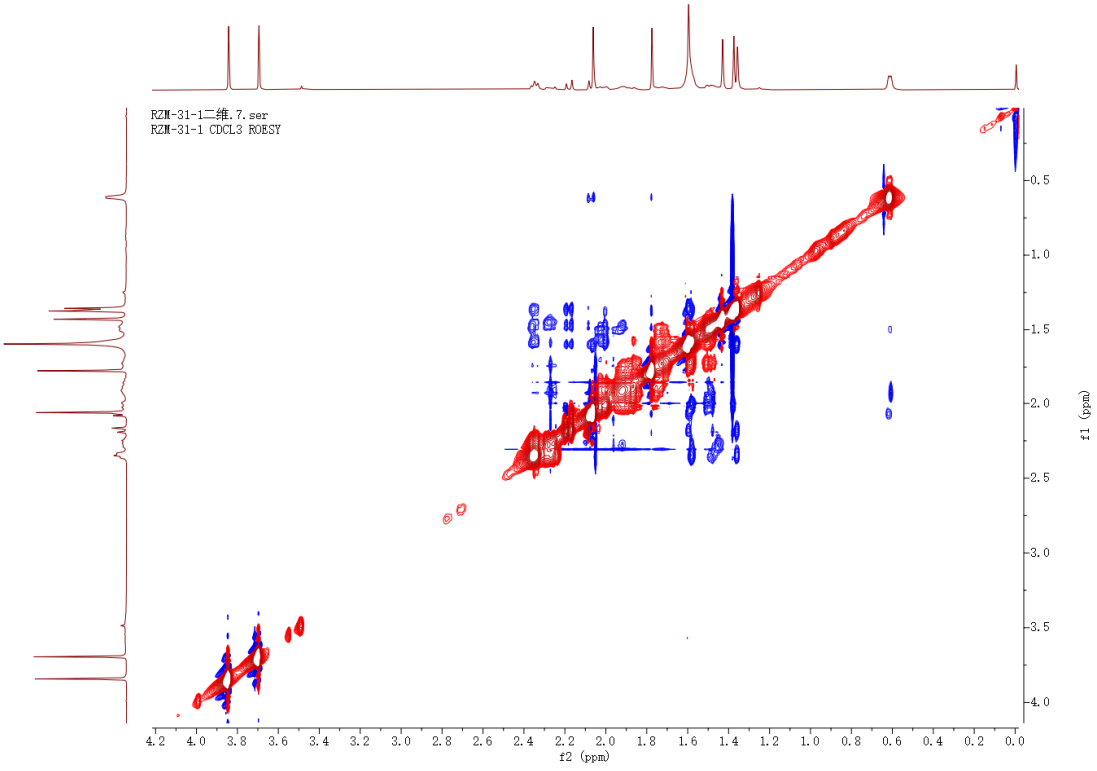
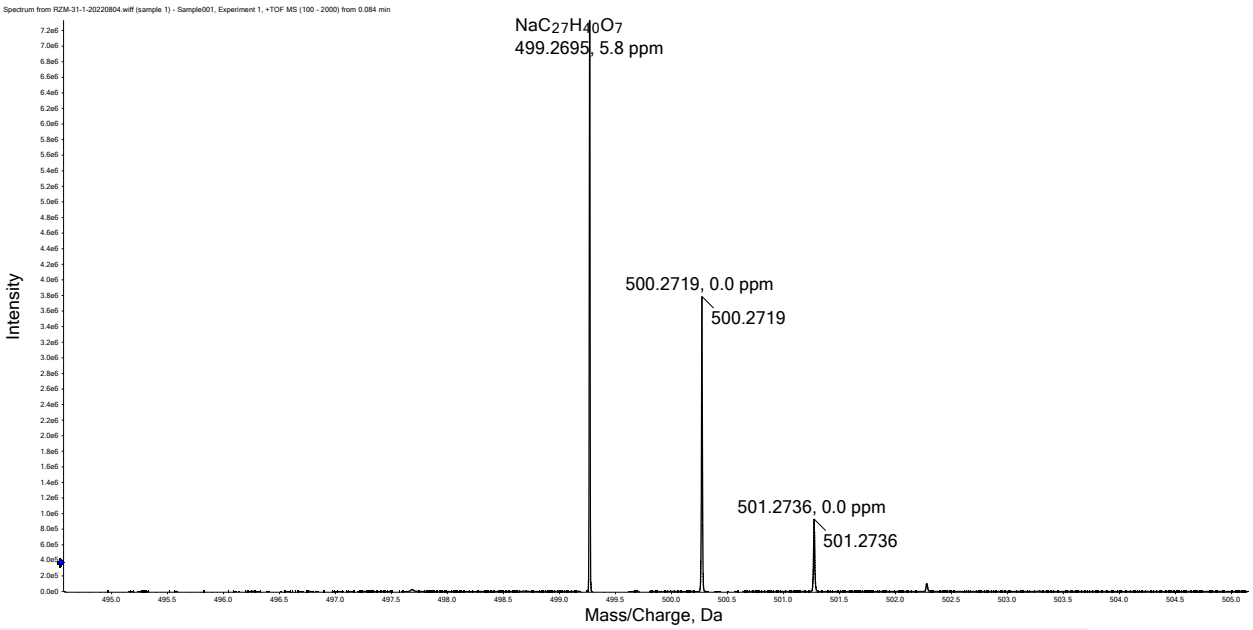



**Figure S15.** ROESY spectrum of compound **2** (125 MHz, $CDCl_3$)




| Hit | Formula | m/z | RDB | ppm | MS Rank | MSMS ppm | MSMS Rank | Found |
|---|---|---|---|---|---|---|---|---|
| 1 | C27H40O7 | 499.2666 | 8.0 | 5.8 | 1 | | | NA/NA |

**Figure S16.** HRESIMS of compound **2** (MeOH)

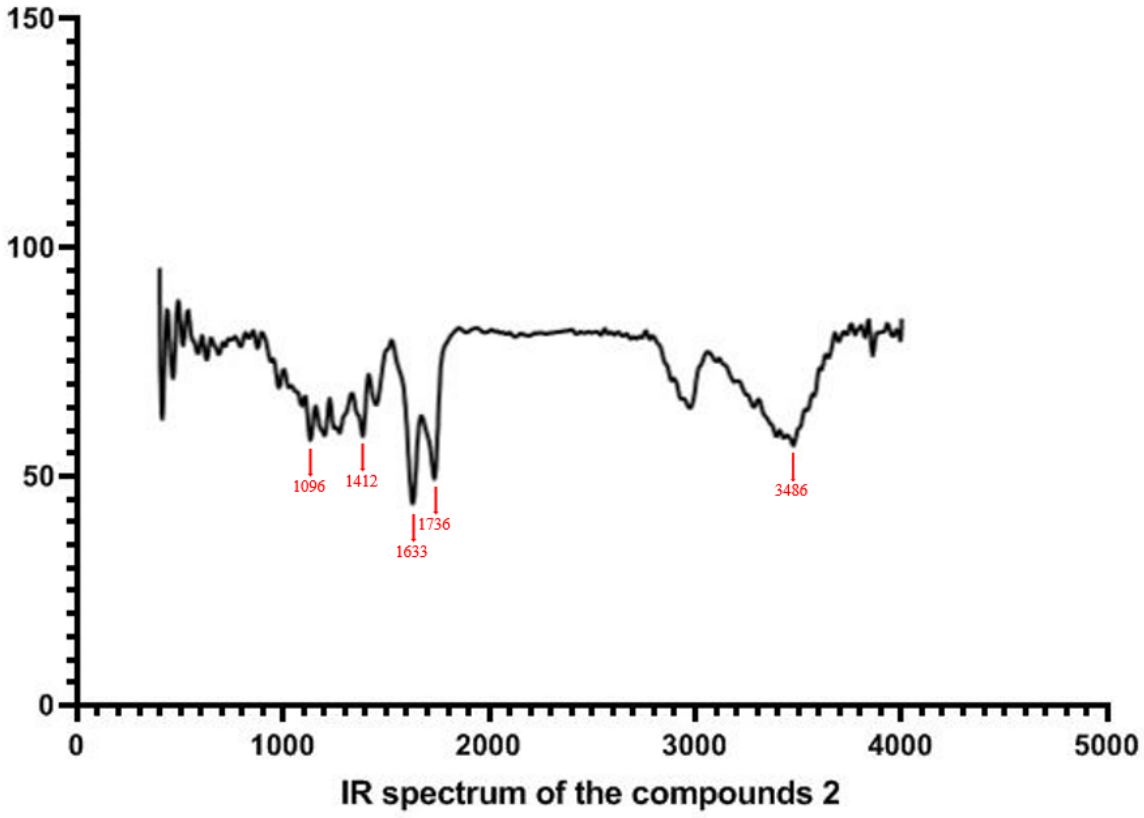



**Figure S17.** IR spectrum of the compound **2**

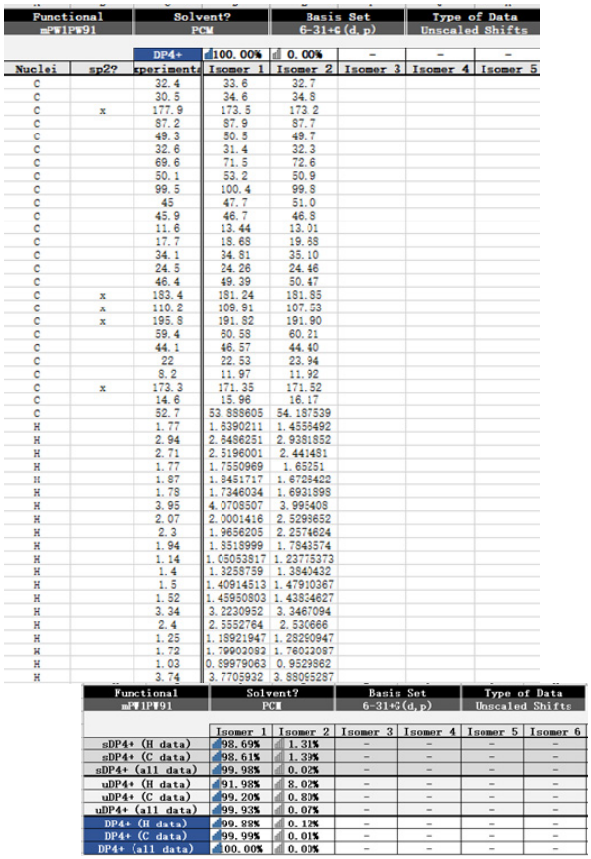
**Table S1.** Experimental and calculated $^{13}C$ NMR chemical shifts of **1.**

| No. | Experimental ($\delta_C$, ppm) | Calculated ($\delta_C$, ppm) | | Corrected ($\delta_C$, ppm) | |
|---|---|---|---|---|---|
| | | (5*R*,7*S*,8*S*,9*S*,*10S*, 1′*R*,5′*S*,6′*S*)-**1** | (5*R*,7*S*,8*S*,9*S*,10*S*, 1′*S*,5′*R*,6′*R*)-**1** | (5*R*,7*S*,8*S*,9*S*,10*S*, 1′*R*,5′*S*,6′*S*)-**1** | (5*R*,7*S*,8S,9S,10*S*, 1′*S*,5′*R*,6′*R*)-**1** |
| 1 | 32.6 | 33.6 | 32.7 | 31.8 | 30.9 |
| 2 | 32.4 | 34.6 | 34.8 | 32.9 | 33.0 |
| 3 | 177.9 | 173.5 | 173.2 | 175.9 | 175.9 |
| 4 | 87.2 | 87.9 | 87.7 | 87.8 | 87.6 |
| 5 | 49.3 | 50.5 | 49.7 | 49.2 | 48.4 |
| 6 | 30.5 | 31.4 | 32.3 | 29.6 | 30.4 |
| 7 | 69.6 | 71.5 | 72.6 | 70.9 | 72.0 |
| 8 | 50.1 | 53.2 | 50.9 | 52.0 | 49.7 |
| 9 | 99.5 | 100.4 | 99.8 | 100.6 | 100.1 |
| 10 | 45 | 47.7 | 51.0 | 46.4 | 49.7 |
| 11 | 45.9 | 46.7 | 46.8 | 45.4 | 45.4 |
| 12 | 11.6 | 13.4 | 13.0 | 11.1 | 10.5 |
| 13 | 17.7 | 18.7 | 19.7 | 16.5 | 17.4 |
| 14 | 34.1 | 34.8 | 35.1 | 33.1 | 33.3 |
| 15 | 24.5 | 24.3 | 24.5 | 22.2 | 22.3 |
| 1' | 46.4 | 49.4 | 50.5 | 48.1 | 49.2 |
| 2' | 183.4 | 181.2 | 181.9 | 183.9 | 184.8 |
| 3' | 110.2 | 109.9 | 107.5 | 110.5 | 108.1 |
| 4' | 195.8 | 191.8 | 191.9 | 194.8 | 195.2 |
| 5' | 59.4 | 60.6 | 60.2 | 59.7 | 59.2 |
| 6' | 44.1 | 46.6 | 44.4 | 45.2 | 42.9 |
| 7' | 22 | 22.5 | 23.9 | 20.5 | 21.8 |
| 8' | 8.2 | 12.0 | 11.9 | 9.6 | 9.4 |
| 9' | 173.3 | 171.3 | 171.5 | 173.7 | 174.1 |
| 10' | 14.6 | 16.0 | 16.2 | 13.7 | 13.8 |
| 11' | 52.7 | 53.9 | 54.2 | 52.8 | 53.0 |
| **$R^2$** | | **0.9996** | **0.9992** | | |
| **MAE** | | **1.75** | **1.89** | | |
| **CMAE** | | | | **0.97** | **1.17** |

**Table S2.** Experimental and calculated $^{1}H$ NMR chemical shifts of **1.**

| No. | Experimental ($\delta_H$, ppm) | Calculated ($\delta_H$, ppm) | | Corrected ($\delta_H$, ppm) | |
|---|---|---|---|---|---|
| | | (5*R*,7*S*,8*S*,9*S*,*10S*, 1′*R*,5′*S*,6′*S*)-**1** | (5*R*,7*S*,8*S*,9*S*,10*S*, 1′*S*,5′*R*,6′*R*)-**1** | (5*R*,7*S*,8*S*,9*S*,10*S*, 1′*R*,5′*S*,6′*S*)-**1** | (5*R*,7*S*,8S,9S,10*S*, 1′*S*,5′*R*,6′*R*)-**1** |
| 1a | 1.87 | 1.67 | 1.38 | 1.75 | 1.44 |

| | | | | | |
|---|---|---|---|---|---|
| 1b | 1.77 | 1.60 | 1.53 | 1.68 | 1.58 |
| 2a | 2.94 | 2.65 | 2.94 | 2.71 | 2.94 |
| 2b | 2.71 | 2.52 | 2.44 | 2.58 | 2.46 |
| 5 | 1.8 | 1.76 | 1.65 | 1.83 | 1.70 |
| 6 | 1.77 | 1.79 | 1.68 | 1.86 | 1.73 |
| 7 | 3.95 | 4.07 | 4.00 | 4.10 | 3.96 |
| 8 | 2.07 | 2.00 | 2.53 | 2.07 | 2.55 |
| 11a | 2.3 | 1.97 | 2.26 | 2.04 | 2.28 |
| 11b | 1.94 | 1.85 | 1.78 | 1.93 | 1.83 |
| 12 | 1.14 | 1.05 | 1.24 | 1.14 | 1.30 |
| 13 | 1.4 | 1.33 | 1.38 | 1.41 | 1.44 |
| 14 | 1.5 | 1.41 | 1.48 | 1.49 | 1.53 |
| 15 | 1.52 | 1.46 | 1.44 | 1.54 | 1.49 |
| 5' | 3.34 | 3.22 | 3.35 | 3.27 | 3.34 |
| 6' | 2.4 | 2.56 | 2.53 | 2.61 | 2.55 |
| 7' | 1.25 | 1.19 | 1.28 | 1.28 | 1.34 |
| 8' | 1.72 | 1.80 | 1.76 | 1.87 | 1.81 |
| 10' | 1.03 | 0.90 | 0.95 | 0.99 | 1.03 |
| 11' | 3.74 | 3.77 | 3.88 | 3.81 | 3.85 |
| **$R^2$** | | **0.9798** | **0.9561** | | |
| **MAE** | | **0.11** | **0.13** | | |
| **CMAE** | | | | **0.09** | **0.12** |



| Functional | Solvent? | Basis Set | Type of Data |
|---|---|---|---|
| mPW1PW91 | PCM | 6-31+G(d,p) | Unscaled Shifts |

| Nuclei | sp2? | DP4+ Experiments | 100.00% Isomer 1 | 0.00% Isomer 2 | – Isomer 3 | – Isomer 4 | – Isomer 5 |
|---|---|---|---|---|---|---|---|
| C | | 32.4 | 33.6 | 32.7 | | | |
| C | | 30.5 | 34.6 | 34.8 | | | |
| C | x | 177.9 | 173.5 | 173.2 | | | |
| C | | 87.2 | 87.9 | 87.7 | | | |
| C | | 49.3 | 50.5 | 49.7 | | | |
| C | | 32.6 | 31.4 | 32.3 | | | |
| C | | 69.6 | 71.5 | 72.6 | | | |
| C | | 50.1 | 53.2 | 50.9 | | | |
| C | | 99.5 | 100.4 | 99.8 | | | |
| C | | 45 | 47.7 | 51.0 | | | |
| C | | 45.9 | 46.7 | 46.8 | | | |
| C | | 11.6 | 13.44 | 13.01 | | | |
| C | | 17.7 | 18.68 | 19.88 | | | |
| C | | 34.1 | 34.81 | 35.10 | | | |
| C | | 24.5 | 24.26 | 24.46 | | | |
| C | | 46.4 | 49.39 | 50.47 | | | |
| C | x | 183.4 | 181.24 | 181.85 | | | |
| C | x | 110.2 | 109.91 | 107.53 | | | |
| C | x | 195.8 | 191.82 | 191.90 | | | |
| C | | 59.4 | 60.58 | 60.21 | | | |
| C | | 44.1 | 46.57 | 44.40 | | | |
| C | | 22 | 22.53 | 23.94 | | | |
| C | | 8.2 | 11.97 | 11.92 | | | |
| C | x | 173.3 | 171.35 | 171.52 | | | |
| C | | 14.6 | 15.96 | 16.17 | | | |
| C | | 52.7 | 53.888605 | 54.187539 | | | |
| H | | 1.77 | 1.5390211 | 1.4556492 | | | |
| H | | 2.94 | 2.8486251 | 2.9381852 | | | |
| H | | 2.71 | 2.5196001 | 2.441481 | | | |
| H | | 1.77 | 1.7550969 | 1.65251 | | | |
| H | | 1.87 | 1.8451717 | 1.6728422 | | | |
| H | | 1.78 | 1.7346034 | 1.6931898 | | | |
| H | | 3.95 | 4.0708507 | 3.995408 | | | |
| H | | 2.07 | 2.0001416 | 2.5299652 | | | |
| H | | 2.3 | 1.9656205 | 2.2574624 | | | |
| H | | 1.94 | 1.8518999 | 1.7843574 | | | |
| H | | 1.14 | 1.05053817 | 1.23775373 | | | |
| H | | 1.4 | 1.3258759 | 1.3840432 | | | |
| H | | 1.5 | 1.40914513 | 1.47910367 | | | |
| H | | 1.52 | 1.45950803 | 1.43834627 | | | |
| H | | 3.34 | 3.2230952 | 3.3467094 | | | |
| H | | 2.4 | 2.3552764 | 2.530666 | | | |
| H | | 1.25 | 1.18921947 | 1.28250947 | | | |
| H | | 1.72 | 1.79602092 | 1.76012097 | | | |
| H | | 1.03 | 0.89979063 | 0.9529862 | | | |
| H | | 3.74 | 3.7705932 | 3.88065287 | | | |

| Functional | Solvent? | Basis Set | Type of Data |
|---|---|---|---|
| mPW1PW91 | PCM | 6-31+G(d,p) | Unscaled Shifts |

| | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 | Isomer 6 |
|---|---|---|---|---|---|---|
| sDP4+ (H data) | 98.69% | 1.31% | – | – | – | – |
| sDP4+ (C data) | 98.61% | 1.39% | – | – | – | – |
| sDP4+ (all data) | 99.98% | 0.02% | – | – | – | – |
| uDP4+ (H data) | 91.98% | 8.02% | – | – | – | – |
| uDP4+ (C data) | 99.20% | 0.80% | – | – | – | – |
| uDP4+ (all data) | 99.93% | 0.07% | – | – | – | – |
| DP4+ (H data) | 99.88% | 0.12% | – | – | – | – |
| DP4+ (C data) | 99.99% | 0.01% | – | – | – | – |
| DP4+ (all data) | 100.00% | 0.00% | – | – | – | – |

**Figure S18.** DP4+ analyses of calculated and experimental NMR chemical shifts of 20*R*-**1** and 20*S*-**1.**

**Table S3.** Conformational analysis of the optimized isomers of **1** in methanol.

| Conformations | *G* (hartree) | *ΔG* (kcal/mol) | Boltzmann distributions (%) |
|---|---|---|---|
| (5*R*,7*S*,8*S*,9*S*,*10S*,1′*R*,5′*S*,6′*S*)-**1-1** | -1540.278906 | 0 | 47.9 |
| (5*R*,7*S*,8*S*,9*S*,*10S*,1′*R*,5′*S*,6′*S*)-**1-2** | -1540.278754 | 0.095695 | 40.7 |
| (5*R*,7*S*,8*S*,9*S*,*10S*,1′*R*,5′*S*,6′*S*)-**1-3** | -1540.277548 | 0.852103 | 11.4 |
| (5*R*,7*S*,8*S*,9*S*,10*S*,1′*S*,5′*R*,6′*R*)-**1-1** | -1540.280724 | 0 | 34.1 |

| | | | |
|---|---|---|---|
| (5*R*,7*S*,8*S*,9*S*,10*S*,1′*S*,5′*R*,6′*R*)-**1-2** | -1540.280635 | 0.056413149 | 31.1 |
| (5*R*,7*S*,8*S*,9*S*,10*S*,1′*S*,5′*R*,6′*R*)-**1-3** | -1540.2804 | 0.203752497 | 24.2 |
| (5*R*,7*S*,8*S*,9*S*,10*S*,1′*S*,5′*R*,6′*R*)-**1-4** | -1540.279625 | 0.690072747 | 10.6 |

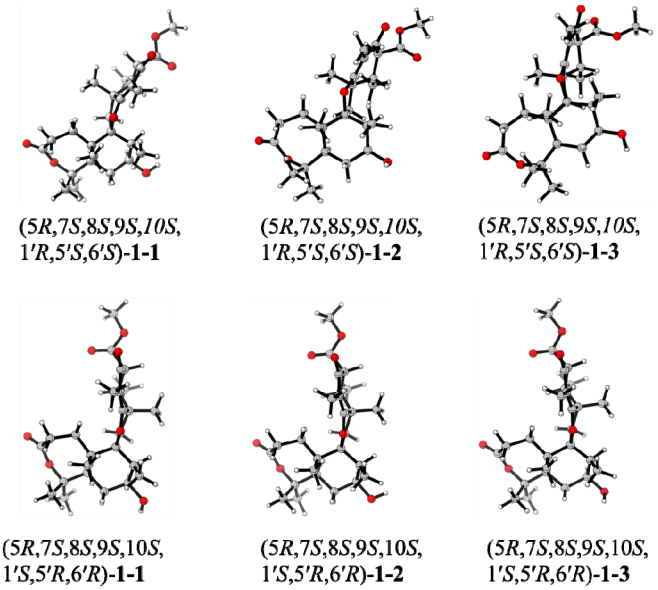



**Figure S19.** Optimized conformers of compound **1**

**Table S4.** Optimized cartesian coordinates of conformers of (5*R*,7*S*,8*S*,9*S*,*10S*,1′*R*,5′*S*,6′*S*)-**1** at B3LYP/6-311G(d) level in methanol**.**

| | (5*R*,7*S*,8*S*,9*S*,*10S*,1′*R*,5′*S*,6′*S*)-**1-1** | | | (5*R*,7*S*,8*S*,9*S*,*10S*,1′*R*,5′*S*,6′*S*)-**1-2** | | | (5*R*,7*S*,8*S*,9*S*,*10S*,1′*R*,5′*S*,6′*S*)-**1-3** | | |
|---|---|---|---|---|---|---|---|---|---|
| C | 0.68799 | 0.52586 | 0.29894 | 0.68767 | 0.52835 | 0.29475 | 0.61818 | 0.43499 | 0.36721 |
| C | 2.15318 | 0.06146 | 0.63761 | 2.15302 | 0.06672 | 0.63648 | 2.10634 | 0.00625 | 0.65445 |
| C | 3.02152 | 0.4483 | -0.6079 | 3.02012 | 0.44133 | -0.61339 | 2.95766 | 0.60449 | -0.51682 |
| C | 2.92854 | 1.96497 | -0.87491 | 2.92798 | 1.95677 | -0.89287 | 2.77968 | 2.13673 | -0.57145 |
| C | 1.50008 | 2.40333 | -1.1499 | 1.49473 | 2.40154 | -1.1664 | 1.32299 | 2.52824 | -0.80244 |
| C | 0.5435 | 2.044 | 0.00004 | 0.53886 | 2.04306 | -0.01644 | 0.38985 | 1.96995 | 0.27405 |
| C | 2.11028 | -1.46217 | 0.89164 | 2.10971 | -1.45441 | 0.90475 | 2.14338 | -1.53772 | 0.69854 |
| C | 3.43078 | -2.17377 | 1.20664 | 3.43006 | -2.16383 | 1.2251 | 3.50017 | -2.21549 | 0.92059 |
| C | 4.2514 | -2.48272 | -0.0196 | 4.24889 | -2.48575 | 0.00096 | 4.33082 | -2.3115 | -0.33331 |
| O | 4.55282 | -1.50065 | -0.88979 | 4.54722 | -1.51301 | -0.8811 | 4.59285 | -1.20279 | -1.05073 |
| C | 4.49884 | -0.03703 | -0.68275 | 4.49628 | -0.04744 | -0.68825 | 4.45918 | 0.21305 | -0.64247 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| O | 4.60497 | -3.60643 | -0.29973 | 4.60323 | -3.61199 | -0.26726 | 4.72938 | -3.36783 | -0.77092 |
| C | 2.61342 | 0.73383 | 1.95404 | 2.6144 | 0.75103 | 1.94603 | 2.52668 | 0.51523 | 2.05484 |
| C | 5.42132 | 0.36687 | 0.46585 | 5.42295 | 0.366 | 0.45355 | 5.3549 | 0.50246 | 0.56075 |
| C | 5.14375 | 0.43373 | -1.99507 | 5.13727 | 0.40962 | -2.00732 | 5.08219 | 0.8945 | -1.87021 |
| C | -0.02674 | -0.25689 | -0.84649 | 0.02615 | -0.26227 | -0.84549 | 0.05239 | -0.22492 | -0.87845 |
| C | -1.37336 | -0.12382 | 1.10441 | 1.37358 | -0.11593 | 1.10437 | 1.40524 | -0.42748 | 1.06155 |
| O | -0.1436 | 0.2525 | 1.48568 | 0.14354 | 0.26279 | 1.48349 | 0.19853 | -0.03737 | 1.49935 |
| C | -1.33818 | -0.81121 | -0.23412 | 1.3381 | -0.81193 | -0.22968 | 1.32908 | -0.93132 | -0.35537 |
| C | -2.60628 | -0.42333 | -1.02275 | 2.60608 | -0.42921 | -1.0211 | 2.61777 | -0.51445 | -1.09584 |
| C | -3.85259 | -0.72411 | -0.16956 | 3.85251 | -0.72435 | -0.16605 | 3.8427 | -1.00591 | -0.29593 |
| C | -3.77544 | -0.21958 | 1.28797 | 3.77557 | -0.21053 | 1.28817 | 3.79747 | -0.68363 | 1.21101 |
| C | -2.47542 | 0.10062 | 1.85625 | 2.47553 | 0.11331 | 1.85461 | 2.51914 | -0.36183 | 1.82618 |
| C | -2.43202 | 0.72695 | 3.22144 | 2.43274 | 0.74849 | 3.21572 | 2.51444 | 0.08861 | 3.25949 |
| O | -4.81759 | -0.06216 | 1.91708 | 4.81759 | -0.04932 | 1.9164 | 4.84736 | -0.67408 | 1.84708 |
| C | -5.09227 | -0.10882 | -0.7924 | 5.09215 | -0.11306 | -0.79299 | 5.14511 | -0.46883 | -0.85885 |
| O | -6.10288 | -0.98364 | -0.85905 | 6.10232 | -0.98885 | -0.85546 | 5.14968 | 0.87309 | -0.87258 |
| O | -5.16266 | 1.03347 | -1.18432 | 5.16294 | 1.02697 | -1.19116 | 6.06181 | -1.14716 | -1.2574 |
| C | -7.34279 | -0.4782 | -1.39577 | 7.342 | -0.487 | -1.39613 | 6.34772 | 1.50021 | -1.36942 |
| C | -2.69642 | -1.08508 | -2.3982 | 2.69615 | -1.10051 | -2.39192 | 2.67036 | -0.98606 | -2.54887 |
| C | -1.23569 | -2.33686 | -0.01219 | 1.23592 | -2.33612 | 0.00245 | 1.13826 | -2.46407 | -0.33565 |
| C | 0.65544 | 3.00921 | 1.18531 | 0.64682 | 3.01547 | 1.16451 | 0.44474 | 2.7687 | 1.58147 |
| O | 1.53759 | 3.80777 | -1.40713 | 1.42976 | 3.78654 | -1.50694 | 1.15747 | 3.94648 | -0.8341 |
| H | 1.44283 | -1.626 | 1.73948 | 1.44281 | -1.61006 | 1.75452 | 1.48736 | -1.8498 | 1.51298 |
| H | 1.6614 | -1.98071 | 0.04497 | 1.65972 | -1.98021 | 0.06319 | 1.72078 | -1.95914 | -0.21298 |
| H | 2.55724 | -0.05027 | -1.46687 | 2.55257 | -0.06192 | -1.46779 | 2.52323 | 0.20569 | -1.44127 |
| H | 1.16517 | 1.89055 | -2.06016 | 1.15902 | 1.89747 | -2.07577 | 1.02261 | 2.11887 | -1.77532 |
| H | -0.48065 | 2.15623 | -0.37914 | 0.48135 | 2.1571 | -0.40072 | 0.63496 | 2.08286 | -0.09936 |
| H | 0.57975 | -1.05554 | -1.26375 | 0.58009 | -1.06446 | -1.25624 | 0.59842 | -0.92288 | -1.39728 |
| H | -0.25389 | 0.41668 | -1.67003 | 0.25283 | 0.40533 | -1.67416 | 0.3197 | 0.54102 | -1.60349 |
| H | -4.01531 | -1.80379 | -0.11418 | 4.01537 | -1.80364 | -0.10369 | 3.92181 | -2.09304 | -0.38083 |
| H | -2.57328 | 0.66207 | -1.16266 | 2.57303 | 0.65516 | -1.16847 | 2.64344 | 0.57941 | -1.08611 |
| H | 3.33536 | 2.5425 | -0.04207 | 3.34658 | 2.53344 | -0.06308 | 3.14885 | 2.61709 | 0.33676 |
| H | 3.51118 | 2.23949 | -1.7511 | 3.50759 | 2.22413 | -1.77327 | 3.35651 | 2.55502 | -1.39525 |
| H | 3.21456 | -3.13912 | 1.66325 | 3.21362 | -3.12442 | 1.69153 | 3.33609 | -3.24365 | 1.24147 |
| H | 4.03285 | -1.62672 | 1.93248 | 4.03362 | -1.61035 | 1.9448 | 4.0747 | -1.73985 | 1.71545 |
| H | 3.06649 | 1.70959 | 1.80722 | 3.35593 | 0.15293 | 2.46955 | 2.93019 | 1.52326 | 2.04676 |
| H | 1.77142 | 0.85327 | 2.63222 | 3.05857 | 1.72988 | 1.79188 | 1.67704 | 0.4992 | 2.73372 |
| H | 3.3467 | 0.12569 | 2.47782 | 1.77483 | 0.86678 | 2.62797 | 3.28797 | -0.1214 | 2.49911 |
| H | 6.43778 | 0.03613 | 0.24469 | 6.43792 | 0.03049 | 0.23284 | 5.30992 | 1.56452 | 0.80716 |
| H | 5.13711 | -0.0431 | 1.42862 | 5.1406 | -0.03351 | 1.42126 | 6.38872 | 0.26177 | 0.30629 |
| H | 5.43719 | 1.45361 | 0.56218 | 5.44224 | 1.45363 | 0.53903 | 5.09168 | -0.05203 | 1.45473 |
| H | 6.05188 | -0.14592 | -2.16074 | 5.41498 | 1.46216 | -1.97873 | 5.30458 | 1.94356 | -1.68118 |
| H | 4.4758 | 0.27533 | -2.84425 | 6.04421 | -0.17258 | -2.17035 | 6.01933 | 0.39038 | -2.10618 |
| H | 5.42018 | 1.4862 | -1.955 | 4.46629 | 0.24352 | -2.85262 | 4.42564 | 0.82237 | -2.73979 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| H | -3.07389 | 1.61026 | 3.26764 | 3.06474 | 1.63942 | 3.25236 | 1.51613 | 0.39043 | 3.57345 |
| H | -2.79824 | 0.03067 | 3.98151 | 2.81134 | 0.0615 | 3.97806 | 3.19713 | 0.92927 | 3.40707 |
| H | -1.41676 | 1.01828 | 3.48738 | 1.41587 | 1.03028 | 3.48576 | 2.85381 | -0.71345 | 3.92128 |
| H | -7.19652 | -0.12315 | -2.41537 | 7.7153 | 0.33043 | -0.77994 | 6.16289 | 2.56877 | -1.30731 |
| H | -8.03017 | -1.31894 | -1.37763 | 7.19503 | -0.1379 | -2.41767 | 6.53094 | 1.20174 | -2.40124 |
| H | -7.71529 | 0.33572 | -0.77446 | 8.02908 | -1.32788 | -1.3736 | 7.20063 | 1.22188 | -0.75092 |
| H | -3.53034 | -0.67218 | -2.97015 | 1.78724 | -0.93578 | -2.97501 | 2.75915 | -2.07244 | -2.61926 |
| H | -1.78757 | -0.91609 | -2.98018 | 2.85047 | -2.17843 | -2.30554 | 3.52913 | -0.5514 | -3.06592 |
| H | -2.85044 | -2.16361 | -2.31935 | 3.52985 | -0.69132 | -2.96683 | 1.77436 | -0.68397 | -3.09574 |
| H | -0.42211 | -2.57686 | 0.67083 | 2.15083 | -2.7441 | 0.43237 | 2.02659 | -2.98065 | 0.02784 |
| H | -2.15035 | -2.74807 | 0.4152 | 1.0386 | -2.85115 | -0.93942 | 0.9125 | -2.83131 | -1.33838 |
| H | -1.03843 | -2.84548 | -0.95757 | 0.42264 | -2.57176 | 0.68736 | 0.31194 | -2.74481 | 0.31552 |
| H | 1.67977 | 3.19653 | 1.50004 | 1.66971 | 3.21657 | 1.48063 | 0.01569 | 3.74193 | 1.41308 |
| H | 0.09553 | 2.63644 | 2.04227 | 0.09951 | 2.64099 | 2.02818 | 1.45494 | 2.94929 | 1.94235 |
| H | 0.22882 | 3.97111 | 0.89947 | 0.196 | 3.96842 | 0.88171 | 0.11321 | 2.26031 | 2.36705 |
| H | 0.65802 | 4.08913 | -1.68579 | 1.81297 | 4.2986 | -0.78452 | 1.66433 | 4.28725 | -1.58029 |

**Table S5.** Optimized cartesian coordinates of conformers of (5*R*,7*S*,8*S*,9*S*,10*S*,1′*S*,5′*R*,6′*R*)-**1** at B3LYP/6-311G(d) level in methanol**.**

| | (5*R*,7*S*,8*S*,9*S*,10*S*,1′*S*,5′*R*,6′*R*)-**1-1** | | | (5*R*,7*S*,8*S*,9*S*,10*S*,1′*S*,5′*R*,6′*R*)-**1-2** | | | (5*R*,7*S*,8*S*,9*S*,10*S*,1′*S*,5′*R*,6′*R*)-**1-3** | | | (5*R*,7*S*,8*S*,9*S*,10*S*,1′*S*,5′*R*,6′*R*)-**1-4** | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -0.98591 | -1.18765 | 0.08144 | -0.98574 | -1.18668 | 0.08447 | -0.95854 | -1.21887 | 0.0872 | -0.98678 | -1.18692 | 0.07967 |
| C | -1.86779 | 0.0062 | 0.63659 | -1.86899 | 0.00679 | 0.6367 | -1.78257 | 0.01045 | 0.65208 | -1.87019 | 0.00453 | 0.63563 |
| C | -2.93023 | 0.29938 | -0.47551 | -2.92819 | 0.29874 | -0.47903 | -2.85255 | 0.33906 | -0.4429 | -2.92484 | 0.30443 | -0.48209 |
| C | -3.76269 | -0.97192 | -0.74944 | -3.76309 | -0.96888 | -0.75767 | -3.74412 | -0.89641 | -0.69359 | -3.76167 | -0.96126 | -0.76857 |
| C | -2.89112 | -2.13253 | -1.22157 | -2.89833 | -2.12772 | -1.22479 | -2.93705 | -2.10047 | -1.1693 | -2.89812 | -2.12953 | -1.23463 |
| C | -1.77299 | -2.48151 | -0.23497 | -1.77495 | -2.47857 | -0.23211 | -1.80017 | -2.48258 | -0.20453 | -1.77236 | -2.47856 | -0.24491 |
| C | -0.91477 | 1.19433 | 0.91736 | -0.917 | 1.19523 | 0.91952 | -0.77933 | 1.16187 | 0.90933 | -0.91745 | 1.18989 | 0.92863 |
| C | -1.53897 | 2.51446 | 1.38343 | -1.54282 | 2.51528 | 1.38353 | -1.34328 | 2.50766 | 1.37882 | -1.54275 | 2.50868 | 1.39681 |
| C | -2.12808 | 3.32856 | 0.26046 | -2.12955 | 3.32868 | 0.25882 | -1.91745 | 3.33912 | 0.26089 | -2.12277 | 3.32943 | 0.27393 |
| O | -3.06089 | 2.78699 | -0.54483 | -3.0595 | 2.78605 | -0.54899 | -2.88104 | 2.82921 | -0.52875 | -3.04907 | 2.79241 | -0.54212 |
| C | -3.84735 | 1.5502 | -0.34563 | -3.84632 | 1.54935 | -0.35158 | -3.71501 | 1.62772 | -0.30823 | -3.84006 | 1.55704 | -0.35375 |
| O | -1.75384 | 4.45164 | 0.00539 | -1.75544 | 4.45198 | 0.00449 | -1.50433 | 4.44582 | -0.00525 | -1.74612 | 4.45367 | 0.02808 |
| C | -2.48814 | -0.39398 | 1.99667 | -2.49285 | -0.39326 | 1.99517 | -2.39248 | -0.3595 | 2.02516 | -2.4989 | -0.40257 | 1.98952 |
| C | -4.69876 | 1.65886 | 0.91812 | -4.70109 | 1.65811 | 0.9099 | -4.54159 | 1.78045 | 0.9674 | -4.70036 | 1.66281 | 0.90424 |
| C | -4.78705 | 1.64455 | -1.55724 | -4.78306 | 1.6431 | -1.56555 | -4.66839 | 1.75205 | -1.50639 | -4.77058 | 1.65796 | -1.57192 |
| C | -0.09898 | -0.80621 | -1.14177 | -0.09853 | -0.80644 | -1.13891 | -0.08783 | -0.87875 | -1.15936 | -0.09931 | -0.80178 | -1.14159 |
| C | 1.23426 | -1.19436 | 0.77231 | 1.2346 | -1.19223 | 0.77577 | 1.27561 | -1.30015 | 0.72683 | 1.23332 | -1.19612 | 0.77175 |
| O | -0.01455 | -1.50886 | 1.14176 | -0.01421 | -1.50602 | 1.14596 | 0.02517 | -1.56862 | 1.12756 | -0.01606 | -1.51011 | 1.14086 |
| C | 1.35527 | -1.12917 | -0.72355 | 1.35552 | -1.12987 | -0.72033 | 1.36336 | -1.25187 | -0.77286 | 1.35431 | -1.12885 | -0.72418 |
| C | 2.37373 | -0.03566 | -1.10028 | 2.37439 | -0.03753 | -1.09939 | 2.40918 | -0.19522 | -1.18055 | 2.374 | -0.03594 | -1.09948 |
| C | 3.69126 | -0.28097 | -0.3425 | 3.69189 | -0.28143 | -0.34113 | 3.7366 | -0.4893 | -0.4521 | 3.69127 | -0.28299 | -0.34183 |
| C | 3.51814 | -0.53212 | 1.17109 | 3.51873 | -0.52943 | 1.17298 | 3.58998 | -0.71605 | 1.06567 | 3.5177 | -0.53581 | 1.17132 |
| C | 2.22471 | -0.97075 | 1.66716 | 2.22519 | -0.9668 | 1.66998 | 2.29308 | -1.10148 | 1.59676 | 2.22381 | -0.97427 | 1.66679 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C | 2.03642 | -1.09692 | 3.15254 | 2.03701 | -1.08947 | 3.15568 | 2.13535 | -1.20644 | 3.08726 | 2.03565 | -1.10174 | 3.15207 |
| O | 4.46905 | -0.32833 | 1.92072 | 4.46957 | -0.32414 | 1.92223 | 4.56696 | -0.54461 | 1.78949 | 4.46842 | -0.3335 | 1.92147 |
| C | 4.632 | 0.89927 | -0.49872 | 4.63255 | 0.89862 | -0.4997 | 4.765 | 0.60353 | -0.6737 | 4.63218 | 0.89737 | -0.49656 |
| O | 5.86949 | 0.5097 | -0.82794 | 5.87018 | 0.50851 | -0.82777 | 4.29283 | 1.79775 | -0.28382 | 5.8693 | 0.50833 | -0.82782 |
| O | 4.30702 | 2.05455 | -0.34696 | 4.30734 | 2.05417 | -0.35056 | 5.86358 | 0.4384 | -1.14803 | 4.30745 | 2.05238 | -0.34226 |
| C | 6.85039 | 1.55966 | -0.95544 | 6.85091 | 1.55841 | -0.95739 | 5.18997 | 2.91545 | -0.42845 | 6.8499 | 1.55866 | -0.95515 |
| C | 2.60048 | 0.09143 | -2.60685 | 2.60113 | 0.08619 | -2.60625 | 2.60459 | -0.07867 | -2.69184 | 2.60096 | 0.09265 | -2.6059 |
| C | 1.76333 | -2.52518 | -1.24806 | 1.76305 | -2.52695 | -1.24233 | 1.70901 | -2.66448 | -1.29613 | 1.7606 | -2.5244 | -1.25106 |
| C | -2.26147 | -3.30778 | 0.96087 | -2.26804 | -3.30483 | 0.96106 | -2.28916 | -3.28603 | 1.00707 | -2.2608 | -3.31229 | 0.94623 |
| O | -3.66324 | -3.31407 | -1.43916 | -3.77489 | -3.23028 | -1.46047 | -3.78052 | -3.21311 | -1.46692 | -3.69218 | -3.26957 | -1.5634 |
| H | -0.22358 | 0.8773 | 1.69979 | -0.22778 | 0.87865 | 1.70387 | -0.08712 | 0.82203 | 1.6811 | -0.23215 | 0.86799 | 1.71415 |
| H | -0.29709 | 1.42338 | 0.04885 | -0.29711 | 1.4241 | 0.05248 | -0.16902 | 1.36201 | 0.02844 | -0.29349 | 1.42176 | 0.06534 |
| H | -2.36541 | 0.50721 | -1.39174 | -2.36063 | 0.50776 | -1.39309 | -2.29673 | 0.51617 | -1.37076 | -2.3541 | 0.514 | -1.39398 |
| H | -2.43358 | -1.8329 | -2.17317 | -2.44036 | -1.83522 | -2.17813 | -2.50048 | -1.84292 | -2.13736 | -2.4475 | -1.84645 | -2.18903 |
| H | -1.07109 | -3.12457 | -0.77466 | -1.06745 | -3.12095 | -0.76813 | -1.13753 | -3.15492 | -0.75735 | -1.07111 | -3.1198 | -0.78692 |
| H | -0.19688 | 0.24107 | -1.41429 | -0.19573 | 0.24095 | -1.41121 | -0.1534 | 0.16992 | -1.43617 | -0.19457 | 0.24722 | -1.40834 |
| H | -0.38223 | -1.37963 | -2.0211 | -0.38203 | -1.37939 | -2.01854 | -0.41225 | -1.4463 | -2.02852 | -0.3831 | -1.3699 | -2.02437 |
| H | 4.1978 | -1.16148 | -0.74715 | 4.19854 | -1.16269 | -0.74397 | 4.18729 | -1.39679 | -0.86337 | 4.19762 | -1.16312 | -0.74751 |
| H | 1.97251 | 0.91376 | -0.73124 | 1.97344 | 0.9128 | -0.7324 | 2.04572 | 0.76607 | -0.80528 | 1.97367 | 0.91345 | -0.7294 |
| H | -4.3327 | -1.27664 | 0.13024 | -4.33633 | -1.27057 | 0.1214 | -4.31213 | -1.1567 | 0.20382 | -4.34218 | -1.25262 | 0.11112 |
| H | -4.49203 | -0.78291 | -1.53633 | -4.48821 | -0.78709 | -1.54752 | -4.47793 | -0.69287 | -1.47 | -4.48252 | -0.77698 | -1.56175 |
| H | -0.75975 | 3.13868 | 1.81932 | -0.76494 | 3.13997 | 1.82114 | -0.53321 | 3.10249 | 1.79928 | -0.76546 | 3.12938 | 1.84105 |
| H | -2.28038 | 2.36392 | 2.16793 | -2.28614 | 2.36472 | 2.16624 | -2.0773 | 2.38996 | 2.17573 | -2.28961 | 2.35568 | 2.17568 |
| H | -2.67523 | 0.47749 | 2.61957 | -1.80628 | -1.02689 | 2.55223 | -2.5441 | 0.52203 | 2.64346 | -2.69684 | 0.46602 | 2.61293 |
| H | -3.43313 | -0.92098 | 1.90722 | -2.68097 | 0.4782 | 2.61779 | -3.35429 | -0.85888 | 1.95667 | -3.44017 | -0.93508 | 1.89228 |
| H | -1.79981 | -1.02716 | 2.552 | -3.43802 | -0.91953 | 1.90326 | -1.71381 | -1.00785 | 2.57508 | -1.81068 | -1.0324 | 2.54898 |
| H | -4.12667 | 1.74978 | 1.83473 | -5.33426 | 0.77421 | 1.00245 | -5.21356 | 0.92739 | 1.07491 | -5.33757 | 0.78109 | 0.98992 |
| H | -5.33172 | 0.77497 | 1.01231 | -5.35333 | 2.52964 | 0.82922 | -5.1543 | 2.68078 | 0.89398 | -5.34897 | 2.5371 | 0.82457 |
| H | -5.35106 | 2.53052 | 0.83941 | -4.13155 | 1.74926 | 1.82809 | -3.95267 | 1.84844 | 1.8753 | -4.13486 | 1.74765 | 1.82552 |
| H | -5.61851 | 0.94561 | -1.47979 | -5.19499 | 2.6515 | -1.60663 | -5.04011 | 2.77593 | -1.54716 | -5.18076 | 2.66715 | -1.61038 |
| H | -5.1993 | 2.65286 | -1.59677 | -4.24507 | 1.4541 | -2.49682 | -4.15476 | 1.53586 | -2.44544 | -4.22821 | 1.47246 | -2.50132 |
| H | -4.25125 | 1.45646 | -2.48999 | -5.61453 | 0.94411 | -1.48974 | -5.52595 | 1.08771 | -1.41184 | -5.60357 | 0.95996 | -1.50362 |
| H | 2.35165 | -0.18388 | 3.66351 | 0.99511 | -1.28791 | 3.40429 | 2.72307 | -2.03818 | 3.48693 | 2.64697 | -1.91347 | 3.55735 |
| H | 0.9942 | -1.29422 | 3.40069 | 2.64584 | -1.90195 | 3.56328 | 2.49486 | -0.30023 | 3.58089 | 2.34629 | -0.18728 | 3.66338 |
| H | 2.64376 | -1.91161 | 3.55798 | 2.35055 | -0.17451 | 3.66428 | 1.09301 | -1.36402 | 3.36194 | 0.99434 | -1.30404 | 3.39996 |
| H | 6.96348 | 2.08349 | -0.00672 | 7.77591 | 1.0585 | -1.22973 | 6.08387 | 2.75904 | 0.17483 | 7.77429 | 1.05974 | -1.23133 |
| H | 7.77515 | 1.06019 | -1.22941 | 6.55121 | 2.26183 | -1.73358 | 5.4711 | 3.0421 | -1.47355 | 6.54871 | 2.2652 | -1.72791 |
| H | 6.55053 | 2.26505 | -1.72978 | 6.96345 | 2.08458 | -0.00989 | 4.63586 | 3.77983 | -0.07394 | 6.96437 | 2.08102 | -0.00579 |
| H | 1.6541 | 0.20756 | -3.14012 | 3.21101 | 0.96329 | -2.83286 | 1.65052 | 0.06958 | -3.20284 | 3.21148 | 0.97008 | -2.82948 |
| H | 3.11313 | -0.78244 | -3.01527 | 1.6548 | 0.20147 | -3.1398 | 3.07764 | -0.96993 | -3.11013 | 1.65476 | 0.2104 | -3.13911 |
| H | 3.21009 | 0.96922 | -2.83153 | 3.11353 | -0.78874 | -3.01275 | 3.23975 | 0.77645 | -2.93441 | 3.11274 | -0.78127 | -3.01528 |
| H | 1.09194 | -3.2931 | -0.86227 | 2.77546 | -2.79572 | -0.93988 | 1.63446 | -2.69551 | -2.38428 | 2.77283 | -2.79485 | -0.94947 |
| H | 1.70953 | -2.55262 | -2.33751 | 1.09307 | -3.29452 | -0.8533 | 2.71485 | -2.97188 | -1.009 | 1.09004 | -3.29285 | -0.86492 |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H | 2.77505 | -2.79519 | -0.94442 | 1.70743 | -2.55703 | -2.33162 | 1.0162 | -3.40425 | -0.89359 | 1.70501 | -2.55062 | -2.34043 |
| H | -2.5105 | -4.31024 | 0.61402 | -1.48864 | -3.38964 | 1.71822 | -2.55918 | -4.29204 | 0.68107 | -3.15635 | -2.91979 | 1.42597 |
| H | -3.15061 | -2.90277 | 1.43885 | -2.51316 | -4.31074 | 0.61906 | -3.15826 | -2.85669 | 1.50368 | -1.48381 | -3.39199 | 1.7057 |
| H | -1.47684 | -3.39385 | 1.71248 | -3.16188 | -2.90164 | 1.43152 | -1.49737 | -3.3861 | 1.74862 | -2.48661 | -4.32359 | 0.60341 |
| H | -4.30202 | -3.12645 | -2.13653 | -3.26274 | -3.94748 | -1.85269 | -4.27722 | -3.44312 | -0.67229 | -4.20334 | -3.52275 | -0.7851 |

**Table S6.** Conformational analysis of the optimized isomers of **2** in chloroform

| Conformations | *G* (hartree) | *ΔG* (kcal/mol) | Boltzmann distributions (%) |
|---|---|---|---|
| **2-1** | -1579.501745 | 0 | 79.8 |
| **2-2** | -1579.499694 | 1.287021779 | 9.1 |
| **2-3** | -1579.498935 | 1.763301414 | 4.1 |
| **2-4** | -1579.498698 | 1.912021142 | 3.2 |
| **2-5** | -1579.498324 | 2.146709657 | 2.1 |
| **2-6** | -1579.498156 | 2.252131237 | 1.7 |

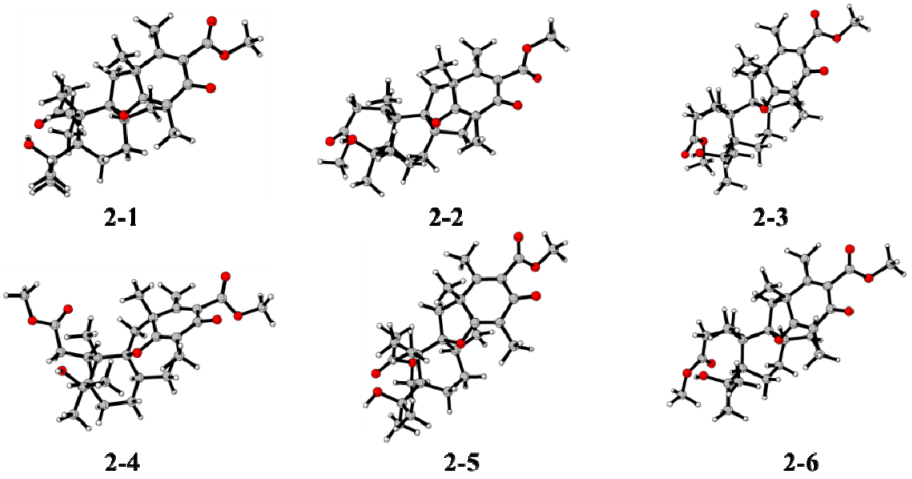



**Figure S20.** Optimized conformers of compound **2**

**Table S7.** Optimized cartesian coordinates of conformers of **2** at B3LYP/6-311G(d) level in chloroform**.**

| | **2-1** | | | **2-2** | | | **2-3** | | |
|---|---|---|---|---|---|---|---|---|---|
| C | -2.4531 | 0.67803 | 1.73141 | -2.45328 | -1.79266 | -0.30502 | -2.46501 | -1.76469 | -0.40323 |
| C | -2.62636 | 2.09034 | 1.15729 | -3.77853 | -2.03837 | -1.0599 | -3.83275 | -1.94836 | -1.0973 |
| C | -4.16583 | -3.0149 | 0.08247 | -2.26283 | 2.89103 | -1.12741 | -2.27839 | 2.96692 | -0.8817 |
| C | -4.2622 | -1.49621 | -0.06957 | -3.31256 | 1.89724 | -0.63639 | -3.30969 | 1.94537 | -0.4089 |
| C | -2.89413 | -0.78278 | -0.36096 | -2.74305 | 0.70314 | 0.20319 | -2.70742 | 0.68736 | 0.30525 |
| C | -1.91214 | -0.4793 | 0.83813 | -1.80235 | -0.39037 | -0.49131 | -1.81505 | -0.35446 | -0.52002 |
| C | -2.13347 | -1.47617 | -1.50246 | -2.19056 | 1.18811 | 1.55685 | -2.08008 | 1.06355 | 1.66103 |
| C | -1.13506 | -0.50478 | -2.14241 | -1.70203 | 0.01541 | 2.39612 | -1.55479 | -0.17228 | 2.37896 |
| C | -0.58569 | 0.5277 | -1.1388 | -0.51275 | -0.71559 | 1.74207 | -0.40728 | -0.85288 | 1.60687 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C | -0.48078 | -0.12079 | 0.26144 | -0.40661 | -0.44561 | 0.21633 | -0.38284 | -0.4666 | 0.10295 |
| C | 0.446 | 0.66085 | 1.22796 | 0.63613 | -1.42602 | -0.39993 | 0.61836 | -1.3985 | -0.6431 |
| C | 1.79569 | -0.1039 | 1.23117 | 1.86014 | -0.55819 | -0.78646 | 1.82648 | -0.50716 | -1.0259 |
| C | 1.57045 | -1.1751 | 0.20554 | 1.52634 | 0.77016 | -0.17017 | 1.53321 | 0.77128 | -0.29407 |
| O | 0.26109 | -1.39905 | 0.04376 | 0.20558 | 0.89249 | 0.02083 | 0.22547 | 0.88111 | -0.02296 |
| C | 3.06747 | 0.67168 | 0.98848 | 3.22767 | -1.05172 | -0.37434 | 3.21058 | -1.03561 | -0.72364 |
| C | 4.04689 | 0.06687 | 0.29299 | 4.13557 | -0.13976 | 0.01081 | 4.14577 | -0.1563 | -0.32311 |
| C | 3.89742 | -1.27942 | -0.33511 | 3.83192 | 1.3111 | 0.16803 | 3.85754 | 1.28547 | -0.06222 |
| C | 2.55099 | -1.83192 | -0.44726 | 2.43086 | 1.7169 | 0.15472 | 2.45984 | 1.68978 | 0.04636 |
| C | 2.31449 | -2.98434 | -1.3782 | 2.0687 | 3.07942 | 0.66809 | 2.13734 | 3.01497 | 0.67164 |
| O | 4.88173 | -1.83756 | -0.82652 | 4.74698 | 2.10118 | 0.41744 | 4.7885 | 2.06557 | 0.15393 |
| C | 5.39319 | 0.6946 | 0.10153 | 5.54281 | -0.51385 | 0.3636 | 5.57706 | -0.55009 | -0.12416 |
| O | 5.56919 | 1.07662 | -1.17044 | 6.32278 | -0.58059 | -0.72522 | 5.90425 | -0.53773 | 1.17478 |
| O | 6.22085 | 0.84698 | 0.97092 | 5.93243 | -0.72857 | 1.48711 | 6.34691 | -0.84632 | -1.00947 |
| C | -5.23481 | -1.17555 | -1.21934 | -4.35819 | 2.65974 | 0.19981 | -4.29939 | 2.64862 | 0.53973 |
| O | -4.87189 | -1.02789 | 1.14871 | -3.99742 | 1.42202 | -1.81428 | -4.06361 | 1.56475 | -1.57908 |
| C | -3.82155 | 2.25791 | 0.25342 | -5.00919 | -1.49436 | -0.37808 | -5.01781 | -1.44755 | -0.30964 |
| O | -3.55025 | 3.03029 | -0.80262 | -5.22494 | -2.08923 | 0.79945 | -5.1687 | -2.11903 | 0.83648 |
| O | -4.92207 | 1.78045 | 0.45878 | -5.74055 | -0.62619 | -0.81932 | -5.7671 | -0.54917 | -0.6482 |
| C | -4.64091 | 3.28769 | -1.71443 | -6.35364 | -1.61713 | 1.56525 | -6.24493 | -1.69272 | 1.69865 |
| C | 0.69754 | 1.15873 | -1.68915 | 0.78842 | -0.40562 | 2.49275 | 0.9347 | -0.60381 | 2.30687 |
| C | 1.97785 | -0.81847 | 2.6077 | 1.93664 | -0.36836 | -2.33388 | 1.82372 | -0.20068 | -2.55635 |
| C | 3.19079 | 2.0254 | 1.61718 | 3.52291 | -2.51339 | -0.52355 | 3.47339 | -2.4872 | -0.98456 |
| C | 6.86097 | 1.63074 | -1.49198 | 7.70846 | -0.90963 | -0.49004 | 7.28192 | -0.83081 | 1.48348 |
| C | -1.76708 | -1.67449 | 1.79404 | -1.57554 | -0.17633 | -1.9992 | -1.67079 | -0.02886 | -2.018 |
| H | -1.81015 | 0.76763 | 2.60675 | -2.6224 | -2.00342 | 0.75098 | -2.57605 | -2.05487 | 0.64153 |
| H | -3.40985 | 0.34851 | 2.12485 | -1.74923 | -2.54988 | -0.65647 | -1.78757 | -2.49516 | -0.85066 |
| H | -1.73595 | 2.47269 | 0.66212 | -3.92046 | -3.11977 | -1.13637 | -3.98895 | -3.02079 | -1.24222 |
| H | -2.81229 | 2.76424 | 2.00169 | -3.74958 | -1.64106 | -2.07211 | -3.85734 | -1.48009 | -2.07888 |
| H | -3.77151 | -3.48039 | -0.82142 | -2.76092 | 3.70915 | -1.65357 | -2.79603 | 3.82897 | -1.30975 |
| H | -5.16742 | -3.41403 | 0.25768 | -1.55088 | 2.4351 | -1.80966 | -1.61465 | 2.56124 | -1.64008 |
| H | -3.53799 | -3.30918 | 0.91973 | -1.7058 | 3.31481 | -0.29131 | -1.66679 | 3.31714 | -0.04974 |
| H | -3.18401 | 0.1919 | -0.76296 | -3.6435 | 0.15382 | 0.48541 | -3.59692 | 0.12302 | 0.59207 |
| H | -1.61128 | -2.35237 | -1.11711 | -1.38416 | 1.90842 | 1.41669 | -1.27768 | 1.79088 | 1.53452 |
| H | -2.82332 | -1.83852 | -2.2652 | -2.98373 | 1.69872 | 2.10314 | -2.83955 | 1.53144 | 2.28755 |
| H | -1.61439 | 0.04185 | -2.96082 | -2.53558 | -0.67788 | 2.55044 | -2.38332 | -0.8735 | 2.52395 |
| H | -0.30346 | -1.0607 | -2.58324 | -1.41415 | 0.36523 | 3.39112 | -1.21156 | 0.09832 | 3.38108 |
| H | -1.31906 | 1.33213 | -1.04795 | -0.68212 | -1.79341 | 1.82268 | -0.57828 | -1.93345 | 1.61408 |
| H | 0.55063 | 1.6945 | 0.91003 | 0.90153 | -2.18698 | 0.33052 | 0.9162 | -2.21474 | 0.01087 |
| H | 0.05079 | 0.68474 | 2.23795 | 0.25121 | -1.94882 | -1.27043 | 0.18401 | -1.85095 | -1.52958 |
| H | 1.24969 | -3.19752 | -1.47111 | 0.98877 | 3.22465 | 0.66385 | 1.05997 | 3.16008 | 0.74682 |
| H | 2.71701 | -2.77538 | -2.37329 | 2.43529 | 3.2278 | 1.68836 | 2.56957 | 3.09515 | 1.67369 |
| H | 2.81468 | -3.88851 | -1.01898 | 2.52336 | 3.8612 | 0.05339 | 2.55497 | 3.83588 | 0.08222 |
| H | -6.19762 | -1.65095 | -1.01958 | -5.08888 | 1.97184 | 0.63573 | -5.01144 | 1.93388 | 0.96318 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| H | -4.87735 | -1.53094 | -2.18707 | -4.89219 | 3.34384 | -0.4624 | -4.86276 | 3.38414 | -0.03764 |
| H | -5.39795 | -0.09804 | -1.29106 | -3.91595 | 3.24729 | 1.00515 | -3.80675 | 3.17073 | 1.36076 |
| H | -5.07104 | -0.08538 | 1.02977 | -4.70205 | 0.81364 | -1.53761 | -4.75734 | 0.94071 | -1.3102 |
| H | -4.96321 | 2.35805 | -2.18189 | -6.36478 | -2.22499 | 2.46499 | -6.21451 | -2.36561 | 2.55038 |
| H | -5.47589 | 3.7428 | -1.18425 | -6.22182 | -0.56475 | 1.81472 | -6.08245 | -0.66344 | 2.01738 |
| H | -4.2383 | 3.96906 | -2.45784 | -7.2747 | -1.74837 | 0.99941 | -7.19851 | -1.77067 | 1.17885 |
| H | 1.50667 | 0.43259 | -1.78115 | 0.70831 | -0.77037 | 3.51917 | 1.12799 | 0.46411 | 2.4218 |
| H | 1.05774 | 1.9947 | -1.08726 | 0.97305 | 0.66916 | 2.53566 | 1.78699 | -1.04198 | 1.78225 |
| H | 0.49897 | 1.55031 | -2.69023 | 1.66879 | -0.87767 | 2.05061 | 0.90836 | -1.04634 | 3.30513 |
| H | 1.12539 | -1.46737 | 2.80959 | 2.76242 | 0.29333 | -2.59421 | 1.94728 | -1.12677 | -3.12083 |
| H | 2.88544 | -1.4215 | 2.61182 | 2.09223 | -1.33373 | -2.81918 | 0.88368 | 0.25474 | -2.85853 |
| H | 2.04033 | -0.07852 | 3.40782 | 1.01291 | 0.05659 | -2.71894 | 2.63881 | 0.47684 | -2.80953 |
| H | 2.60556 | 2.75951 | 1.05395 | 3.10065 | -3.07419 | 0.31647 | 3.01656 | -2.80784 | -1.92416 |
| H | 2.79387 | 2.02474 | 2.6354 | 3.07129 | -2.91957 | -1.43151 | 4.53701 | -2.71269 | -1.02909 |
| H | 4.22189 | 2.37143 | 1.6535 | 4.59275 | -2.71748 | -0.55622 | 3.02751 | -3.10093 | -0.19541 |
| H | 7.0443 | 2.53103 | -0.90609 | 8.17301 | -0.92182 | -1.47172 | 7.93598 | -0.10056 | 1.00751 |
| H | 7.64286 | 0.89852 | -1.29178 | 8.17041 | -0.15398 | 0.14461 | 7.35658 | -0.76334 | 2.565 |
| H | 6.81926 | 1.86573 | -2.55163 | 7.78914 | -1.88656 | -0.01435 | 7.54256 | -1.83238 | 1.1425 |
| H | -2.71409 | -1.85829 | 2.29782 | -1.17731 | -1.08029 | -2.46384 | -2.61532 | 0.28149 | -2.44687 |
| H | -1.4557 | -2.58134 | 1.28063 | -2.49616 | 0.09003 | -2.50316 | -0.96778 | 0.78342 | -2.17749 |
| H | -1.0222 | -1.46097 | 2.5636 | -0.8705 | 0.62978 | -2.17966 | -1.31038 | -0.89791 | -2.57161 |

| | **2-4** | | | **2-5** | | | **2-6** | | |
|---|---|---|---|---|---|---|---|---|---|
| C | 2.67694 | 0.84113 | 1.49073 | -2.49873 | 0.66424 | 1.75879 | -2.40944 | -1.88601 | -0.11739 |
| C | 4.0359 | 1.47295 | 1.16878 | -2.54102 | 2.12807 | 1.27461 | -3.81075 | -2.1227 | -0.71628 |
| C | 1.94671 | -2.94887 | -1.42452 | -4.12651 | -3.04819 | -0.15405 | -2.30558 | 2.75548 | -1.12098 |
| C | 3.17179 | -2.41695 | -0.68016 | -4.27563 | -1.52322 | -0.05441 | -3.31008 | 1.79578 | -0.48861 |
| C | 2.93041 | -1.47561 | 0.54834 | -2.95974 | -0.72797 | -0.34421 | -2.68405 | 0.62365 | 0.33827 |
| C | 2.10408 | -0.12846 | 0.40115 | -1.95029 | -0.4724 | 0.83998 | -1.7875 | -0.4846 | -0.38985 |
| C | 2.51156 | -2.23129 | 1.82895 | -2.23451 | -1.31947 | -1.56236 | -2.04774 | 1.13986 | 1.64267 |
| C | 1.00865 | -2.40226 | 1.99827 | -1.24203 | -0.3121 | -2.15142 | -1.48581 | -0.01 | 2.46742 |
| C | 0.28341 | -1.05666 | 2.00643 | -0.63788 | 0.63002 | -1.09252 | -0.33174 | -0.73483 | 1.74769 |
| C | 0.56934 | -0.27536 | 0.70256 | -0.52789 | -0.10406 | 0.26134 | -0.34303 | -0.50483 | 0.21144 |
| C | 0.21424 | 1.07153 | 0.67982 | 0.41584 | 0.60323 | 1.26792 | 0.66421 | -1.48905 | -0.45544 |
| C | 1.35558 | 0.87541 | -0.34902 | 1.74886 | -0.18831 | 1.22814 | 1.84331 | -0.61787 | -0.95733 |
| C | 1.2774 | -0.59271 | -0.64736 | 1.50627 | -1.18849 | 0.1361 | 1.5371 | 0.72325 | -0.35402 |
| O | 0.04951 | -1.06272 | -0.3884 | 0.19461 | -1.37755 | -0.04392 | 0.23324 | 0.83439 | -0.06485 |
| C | 2.74559 | 1.31465 | 0.04421 | 3.03483 | 0.5785 | 1.03542 | 3.24576 | -1.08344 | -0.63589 |
| C | 3.78296 | 0.56431 | -0.36732 | 4.0053 | 0.00112 | 0.30488 | 4.1691 | -0.14788 | -0.35288 |
| C | 3.62217 | -0.72572 | -1.10073 | 3.83347 | -1.30203 | -0.40387 | 3.85356 | 1.30661 | -0.23458 |
| C | 2.29707 | -1.33646 | -1.12234 | 2.47791 | -1.82079 | -0.55405 | 2.4498 | 1.69046 | -0.13098 |
| C | 2.17087 | -2.77683 | -1.52241 | 2.22429 | -2.90767 | -1.55667 | 2.11052 | 3.06579 | 0.3633 |
| O | 4.61289 | -1.28448 | -1.57918 | 4.80979 | -1.84841 | -0.92394 | 4.77096 | 2.12407 | -0.124 |
| C | 5.20466 | 0.97953 | -0.14484 | 5.36183 | 0.61689 | 0.15232 | 5.61419 | -0.48737 | -0.15289 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| O | 5.79969 | 0.19714 | 0.76544 | 5.55352 | 1.05376 | -1.09958 | 5.96968 | -0.34529 | 1.13092 |
| O | 5.75572 | 1.90068 | -0.70344 | 6.18496 | 0.71813 | 1.03362 | 6.37157 | -0.84651 | -1.02548 |
| C | 4.04506 | -3.61573 | -0.2646 | -5.35385 | -1.04674 | -1.03919 | -4.25924 | 2.61231 | 0.40921 |
| O | 3.97413 | -1.62515 | -1.58941 | -4.732 | -1.19751 | 1.27601 | -4.11114 | 1.27764 | -1.57457 |
| C | 3.93482 | 2.7094 | 0.30513 | -3.65115 | 2.42755 | 0.29485 | -4.93497 | -1.71662 | 0.20598 |
| O | 5.00025 | 2.83499 | -0.5029 | -3.18106 | 2.91306 | -0.87117 | -5.79881 | -0.85458 | -0.38291 |
| O | 3.03189 | 3.51587 | 0.34265 | -4.83038 | 2.27135 | 0.51617 | -5.07881 | -2.11181 | 1.33838 |
| C | 5.02426 | 4.00502 | -1.34432 | -4.16413 | 3.21161 | -1.88138 | -6.94 | -0.45683 | 0.41016 |
| C | 1.20586 | -1.2737 | 2.30282 | 0.65723 | 1.25003 | -1.62797 | 1.0139 | -0.37805 | 2.3916 |
| C | 1.02405 | 1.63477 | -1.67267 | 1.91749 | -0.98949 | 2.55754 | 1.80132 | -0.47281 | -2.51089 |
| C | 2.8819 | 2.60907 | 0.78596 | 3.17882 | 1.88923 | 1.74597 | 3.53753 | -2.54841 | -0.75111 |
| C | 7.19598 | 0.46097 | 1.01007 | 6.85525 | 1.60353 | -1.3858 | 7.36118 | -0.5748 | 1.43159 |
| C | 2.28143 | 0.51917 | -0.98106 | -1.79474 | -1.70016 | 1.75435 | -1.67954 | -0.31586 | -1.91699 |
| H | 2.76693 | 0.31402 | 2.43847 | -1.92893 | 0.6592 | 2.68953 | -2.4673 | -2.08858 | 0.95244 |
| H | 1.98223 | 1.66016 | 1.67375 | -3.51138 | 0.3755 | 2.0281 | -1.74378 | -2.64433 | -0.53414 |
| H | 4.73783 | 0.77351 | 0.71492 | -1.59046 | 2.47831 | 0.87833 | -3.93949 | -3.19824 | -0.86879 |
| H | 4.50042 | 1.80201 | 2.10521 | -2.75751 | 2.74169 | 2.15449 | -3.93096 | -1.64848 | -1.68755 |
| H | 1.35327 | -2.15018 | -1.85646 | -3.87496 | -3.36964 | -1.16561 | -2.84312 | 3.58354 | -1.5896 |
| H | 1.29928 | -3.5298 | -0.76693 | -5.07881 | -3.51883 | 0.10887 | -1.69867 | 2.27508 | -1.88248 |
| H | 2.27678 | -3.61371 | -2.23019 | -3.36748 | -3.42896 | 0.52644 | -1.63684 | 3.16894 | -0.36581 |
| H | 3.95341 | -1.13471 | 0.73238 | -3.30412 | 0.26009 | -0.65698 | -3.56606 | 0.08132 | 0.68695 |
| H | 3.00444 | -3.20041 | 1.87804 | -1.71111 | -2.22992 | -1.26846 | -1.26331 | 1.86824 | 1.43377 |
| H | 2.88947 | -1.68303 | 2.69664 | -2.95121 | -1.60902 | -2.33286 | -2.80861 | 1.65061 | 2.23287 |
| H | 0.80378 | -2.92421 | 2.93841 | -1.73822 | 0.30584 | -2.90679 | -2.29637 | -0.71177 | 2.68904 |
| H | 0.59028 | -3.02509 | 1.20285 | -0.43836 | -0.84607 | -2.66572 | -1.13756 | 0.36242 | 3.4345 |
| H | 0.69753 | -0.44623 | 2.81756 | -1.34056 | 1.44853 | -0.94056 | -0.47159 | -1.81298 | 1.86952 |
| H | 0.59375 | 1.29822 | 1.67339 | 0.54776 | 1.64834 | 1.00318 | 0.99454 | -2.22532 | 0.27367 |
| H | 0.41244 | 1.90881 | 0.38879 | 0.01454 | 0.58548 | 2.27639 | 0.22192 | -2.04158 | -1.2791 |
| H | 1.16461 | -3.14751 | -1.33018 | 2.6442 | -2.64861 | -2.53262 | 2.61134 | 3.27872 | 1.31214 |
| H | 2.88497 | -3.3997 | -0.97663 | 2.69732 | -3.84492 | -1.24878 | 2.44139 | 3.82977 | -0.34611 |
| H | 2.38553 | -2.9102 | -2.5869 | 1.15569 | -3.08737 | -1.67395 | 1.03564 | 3.17526 | 0.50532 |
| H | 4.88936 | -3.29599 | 0.35091 | -5.05905 | -1.19276 | -2.08031 | -4.93844 | 1.96285 | 0.96964 |
| H | 4.44732 | -4.0859 | -1.16642 | -5.55485 | 0.01343 | -0.87704 | -4.86158 | 3.25981 | -0.23048 |
| H | 3.48724 | -4.38285 | 0.27476 | -6.28407 | -1.60146 | -0.88065 | -3.72837 | 3.24298 | 1.12326 |
| H | 4.12871 | -2.15731 | -2.37926 | -5.59666 | -1.60916 | 1.39424 | -4.78041 | 0.68378 | -1.20422 |
| H | 4.17143 | 3.99783 | -2.02286 | -4.88807 | 3.93321 | -1.50506 | -7.54856 | -1.32785 | 0.64751 |
| H | 5.00016 | 4.90991 | -0.73782 | -3.60585 | 3.6271 | -2.71536 | -6.6108 | 0.02277 | 1.33092 |
| H | 5.95481 | 3.94266 | -1.90132 | -4.67966 | 2.30024 | -2.18412 | -7.49374 | 0.24122 | -0.2106 |
| H | 1.79828 | -0.35729 | 2.27653 | 1.06249 | 2.02856 | -0.97921 | 1.1779 | 0.70091 | 2.39182 |
| H | 1.31402 | -1.69589 | 3.30474 | 0.45308 | 1.71784 | -2.59478 | 1.86961 | -0.84474 | 1.89817 |
| H | 1.65298 | -1.97867 | 1.60034 | 1.4362 | 0.50284 | -1.78869 | 1.01738 | -0.71532 | 3.43048 |
| H | 0.07675 | 1.29032 | -2.08269 | 2.81651 | -1.60445 | 2.52487 | 0.84677 | -0.06726 | -2.83735 |
| H | 1.80653 | 1.46825 | -2.41276 | 1.98947 | -0.3014 | 3.40194 | 2.59763 | 0.18812 | -2.85229 |
| H | 0.94256 | 2.70591 | -1.47873 | 1.05607 | -1.63742 | 2.71835 | 1.93017 | -1.45073 | -2.97852 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| H | 2.58715 | 2.47985 | 1.8323 | 2.61551 | 2.66819 | 1.22173 | 3.05969 | -2.97764 | -1.63518 |
| H | 2.22155 | 3.37312 | 0.36832 | 2.76987 | 1.83611 | 2.758 | 4.60485 | -2.75323 | -0.80807 |
| H | 3.90054 | 2.99149 | 0.76592 | 4.21639 | 2.21012 | 1.81357 | 3.13378 | -3.08435 | 0.11379 |
| H | 7.33043 | 1.47495 | 1.38576 | 7.62567 | 0.8529 | -1.21088 | 7.98473 | 0.12474 | 0.87527 |
| H | 7.76815 | 0.33252 | 0.09151 | 6.82629 | 1.88465 | -2.43461 | 7.45765 | -0.40651 | 2.50032 |
| H | 7.50154 | -0.2671 | 1.75599 | 7.04514 | 2.4752 | -0.76004 | 7.64106 | -1.59669 | 1.1771 |
| H | 3.33225 | 0.59436 | -1.24237 | -2.7429 | -1.9219 | 2.23735 | -2.63602 | -0.06153 | -2.35689 |
| H | 1.8117 | -0.07107 | -1.7626 | -1.45963 | -2.57869 | 1.20708 | -0.98858 | 0.48042 | -2.17629 |
| H | 1.85428 | 1.52051 | -1.00277 | -1.0595 | -1.50295 | 2.53717 | -1.32138 | -1.23493 | -2.38425 |

**Table S8.** $\alpha$-Glucosidase and acetylcholinesterase inhibitory activities of all compounds ($IC_{50}$, $\mu$M)

| Compounds | α-glucosidase | acetylcholinesterase |
|---|---|---|
| **1** | >200 | >200 |
| **2** | >200 | >200 |
| **3** | >200 | >200 |
| **4** | >200 | >200 |
| **5** | >200 | >200 |
| **6** | >200 | >200 |
| **7** | >200 | >200 |
| **8** | >200 | >200 |
| **9** | 104.1 | >200 |
| **10** | 111.3 | >200 |
| **11** | >200 | >200 |
| **12** | >200 | >200 |
| **13** | >200 | >200 |
| **14** | >200 | >200 |
| **15** | >200 | >200 |
| **16** | >200 | >200 |
| **17** | >200 | >200 |
| **18** | >200 | >200 |
| **Acarbose** | 304.6 | |
| **Genistein** | 19.95 | |
| **Tacrine** | | Undetermined |

**Table S9.** Antibacterial activities of all compounds MIC ($\mu$g/mL)

| Compounds | *Staphylococcus aureus* | *Bacillus subtilis* | *Escherichia coli* | *Listeria monocytogenes* |
|---|---|---|---|---|
| **1** | >128 | >128 | >128 | >128 |
| **2** | >128 | >128 | >128 | >128 |
| **3** | >128 | >128 | >128 | >128 |
| **4** | >128 | >128 | >128 | >128 |
| **5** | 128 | >128 | >128 | >128 |
| **6** | >128 | >128 | >128 | >128 |
| **7** | >128 | >128 | >128 | >128 |
| **8** | >128 | >128 | >128 | >128 |
| **9** | >128 | >128 | >128 | >128 |
| **10** | >128 | >128 | >128 | >128 |
| **11** | >128 | >128 | >128 | >128 |
| **12** | 32 | 16 | >128 | >128 |
| **13** | >128 | >128 | >128 | >128 |
| **14** | >128 | >128 | >128 | >128 |

| | | | | |
|---|---|---|---|---|
| **15** | >128 | >128 | >128 | >128 |
| **16** | >128 | >128 | >128 | >128 |
| **17** | >128 | >128 | >128 | >128 |
| **18** | >128 | >128 | >128 | >128 |
| **Ampicillin** | <1 | <1 | <1 | <1 |

**Table S10.** Antifungal activities of all compounds MIC ($\mu$g/mL)

| Compounds | Fusarium oxysporum f. sp. cubense | *Fusarium spp.* | *Peronophythora litchii* | *Colletotrichum gloeosporioides* | *Hylocereus undatus* |
|---|---|---|---|---|---|
| **1** | >128 | >128 | >128 | >128 | >128 |
| **2** | >128 | >128 | >128 | >128 | >128 |
| **3** | >128 | >128 | >128 | >128 | >128 |
| **4** | >128 | >128 | >128 | >128 | >128 |
| **5** | >128 | >128 | >128 | >128 | >128 |
| **6** | >128 | >128 | >128 | >128 | >128 |
| **7** | >128 | >128 | >128 | >128 | >128 |
| **8** | >128 | >128 | >128 | >128 | >128 |
| **9** | >128 | >128 | >128 | >128 | >128 |
| **10** | >128 | >128 | >128 | >128 | >128 |
| **11** | >128 | >128 | >128 | >128 | >128 |
| **12** | >128 | >128 | >128 | >128 | >128 |
| **13** | >128 | >128 | >128 | >128 | >128 |
| **14** | >128 | >128 | >128 | >128 | >128 |
| **15** | >128 | >128 | >128 | >128 | >128 |
| **16** | >128 | >128 | >128 | >128 | >128 |
| **17** | >128 | >128 | >128 | >128 | >128 |
| **18** | >128 | >128 | >128 | >128 | >128 |
| **Carbendazim** | <1 | <1 | <1 | <1 | <1 |