# Colletotrikalactones A and B, Unusual Tricyclic Polyketides from Mangrove Associated Fungus *Colletotrichum* sp. J065

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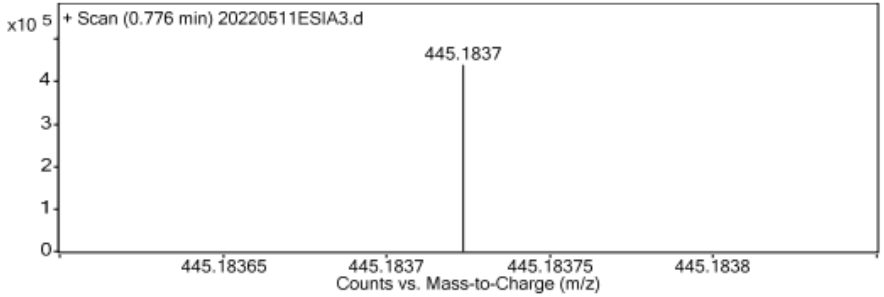
# List of Supporting Information

**Figure S1.** HRESIMS spectrum of compound **1**

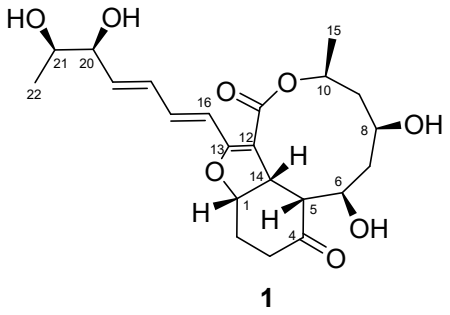
**User Spectra**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 250 | 0 | ESI |




**Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 274.2737 | 1 | 80487.79 | | |
| 445.1837 | 1 | 438057.66 | C22 H30 Na O8 | M+ |
| 446.1864 | 1 | 96446.55 | C22 H30 Na O8 | M+ |
| 461.1579 | 1 | 141662.89 | | |
| 653.2728 | 2 | 100096.79 | | |
| 653.7742 | 2 | 73834.44 | | |
| 867.3771 | 1 | 297287.19 | | |
| 868.38 | 1 | 138769.64 | | |
| 922.0098 | 1 | 246440.88 | | |
| 1289.57 | 1 | 88526.82 | | |




**1**

**Formula Calculator Element Limits**

| Element | Min | Max |
|---|---|---|
| C | 0 | 200 |
| H | 0 | 400 |
| O | 0 | 10 |
| Na | 1 | 1 |

**Formula Calculator Results**

| Formula | CalculatedMass | Mz | Diff.(mDa) | Diff. (ppm) | DBE |
|---|---|---|---|---|---|
| C22 H30 Na O8 | 445.1838 | 445.1837 | 0.1 | 0.3 | 7.5 |

**Figure S2.** IR spectrum of compound **1**

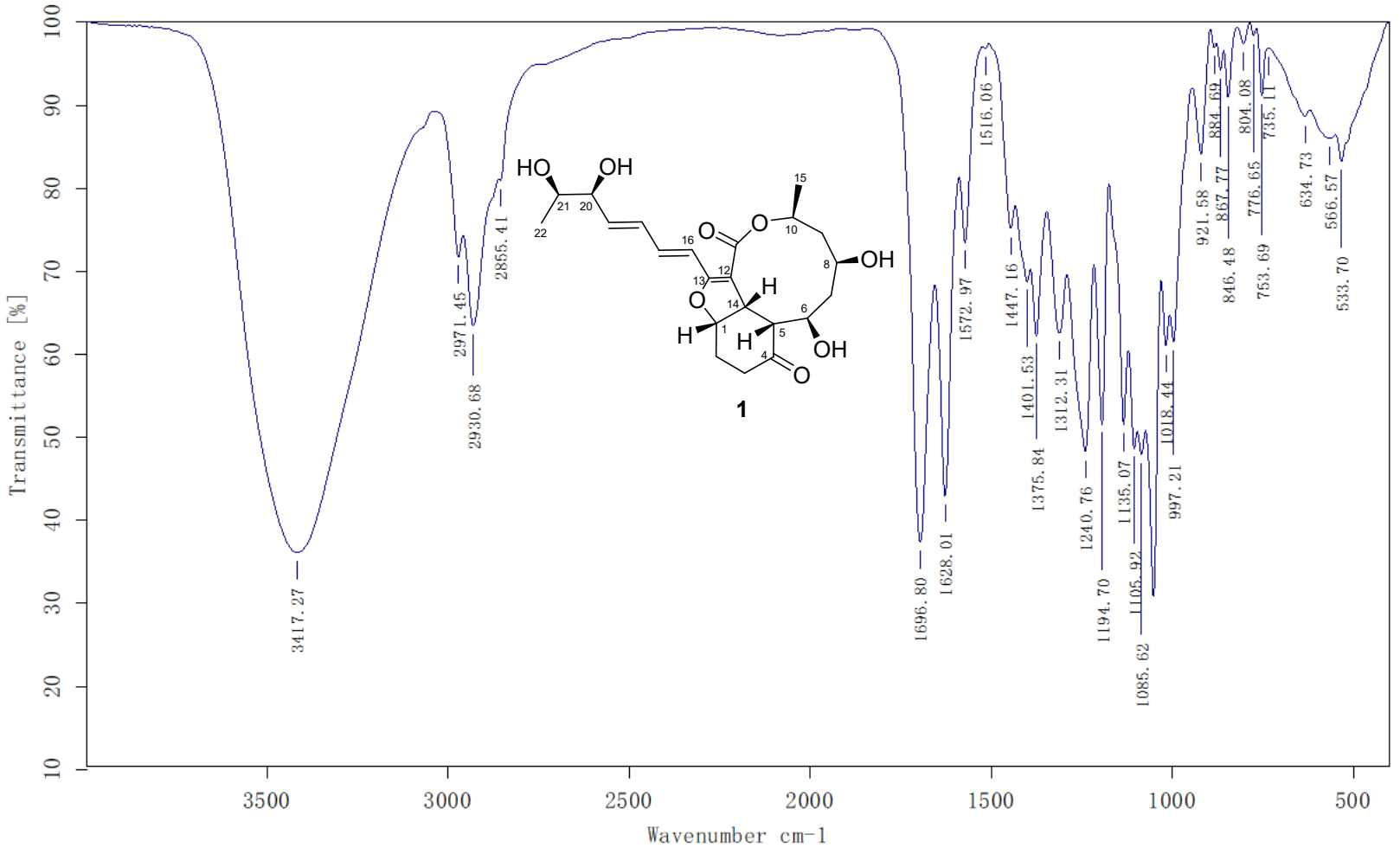
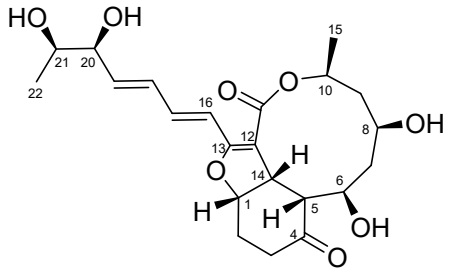


**Figure S3.** Optical rotation spectrum of compound **1**




**1**

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 18-AUG-2022

Set Temperature : 25.0

Time Delay : Disabled

Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | 184.80 | 0.45 | 0.24 | 185.00 | 184.00 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 6A-C-19 | 02:11:31 PM | 185.00 | SR | 0.185 | 589 | 100.00 | 0.100 | 24.9 |
| 2 | 6A-C-19 | 02:11:37 PM | 185.00 | SR | 0.185 | 589 | 100.00 | 0.100 | 24.9 |
| 3 | 6A-C-19 | 02:11:43 PM | 185.00 | SR | 0.185 | 589 | 100.00 | 0.100 | 25.0 |
| 4 | 6A-C-19 | 02:11:49 PM | 185.00 | SR | 0.185 | 589 | 100.00 | 0.100 | 25.0 |
| 5 | 6A-C-19 | 02:11:56 PM | 184.00 | SR | 0.184 | 589 | 100.00 | 0.100 | 25.0 |

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**Figure S4.** $^{1}$H NMR spectrum of compound **1** in DMSO-$d_6$ (600 MHz)

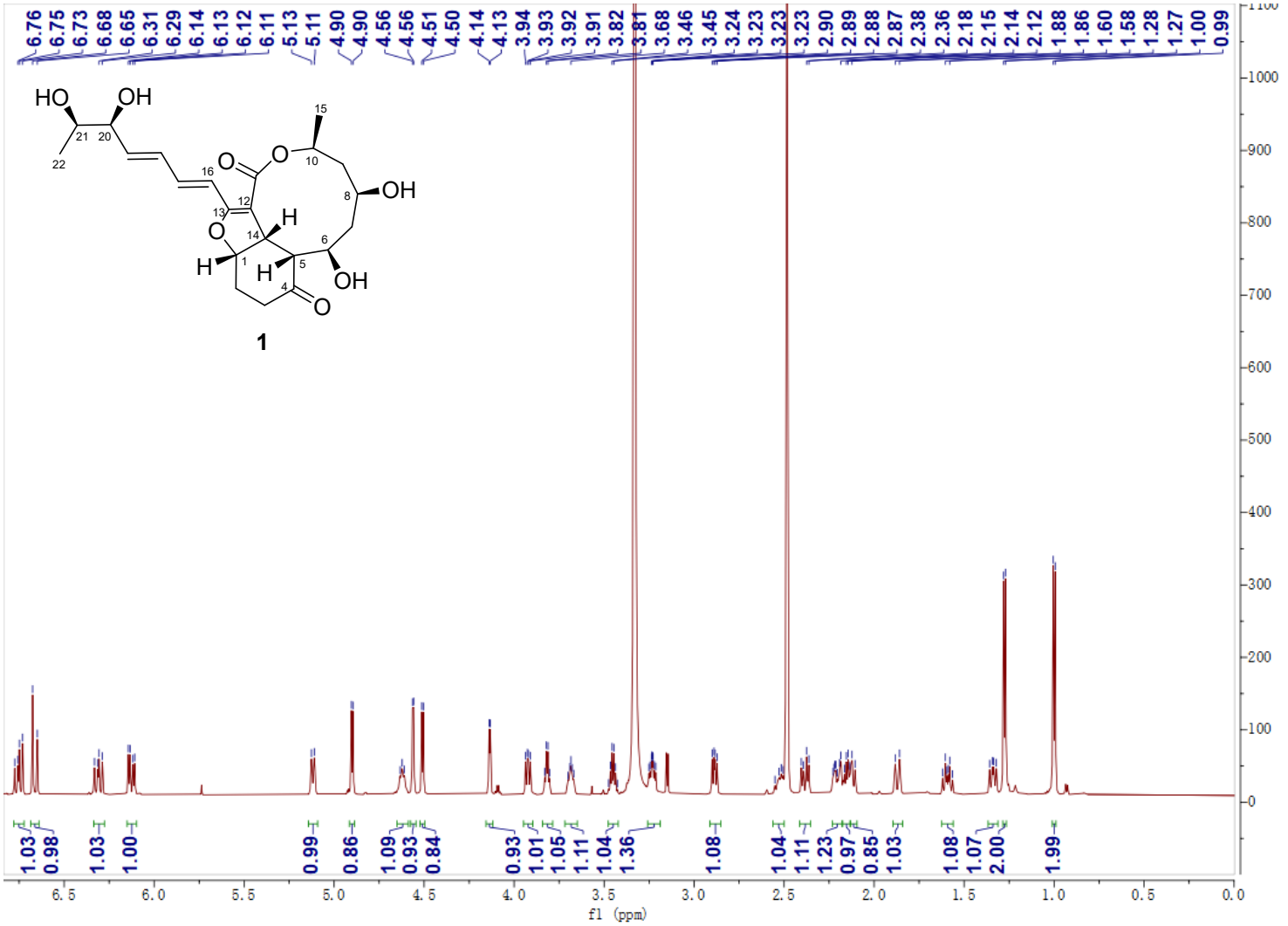


**Figure S5.** $^{13}C$ NMR spectrum of compound **1** in DMSO-$d_6$ (150 MHz)

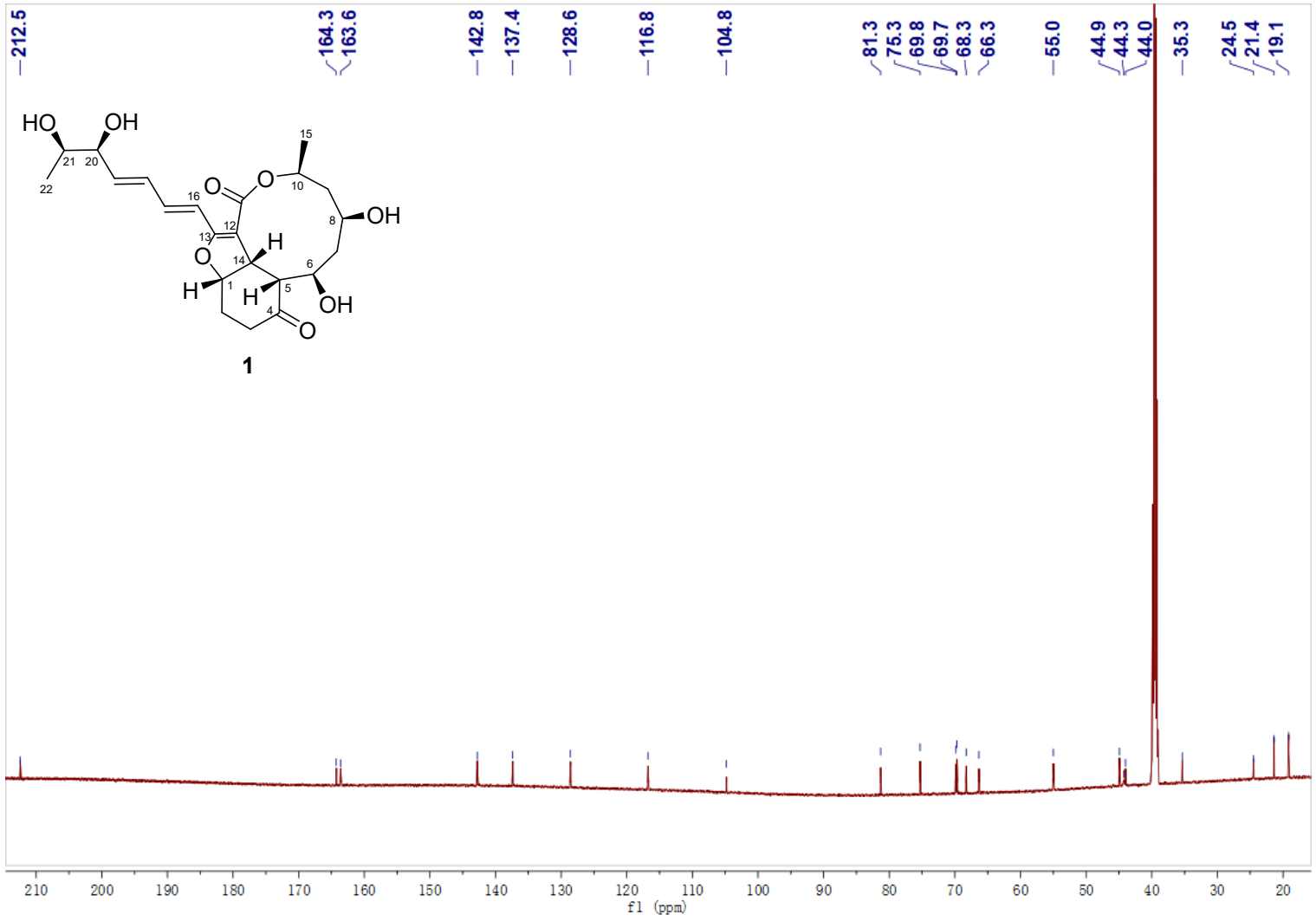


**Figure S6.** DEPT 135 spectrum of compound **1** in DMSO-$d_6$ (150 MHz)

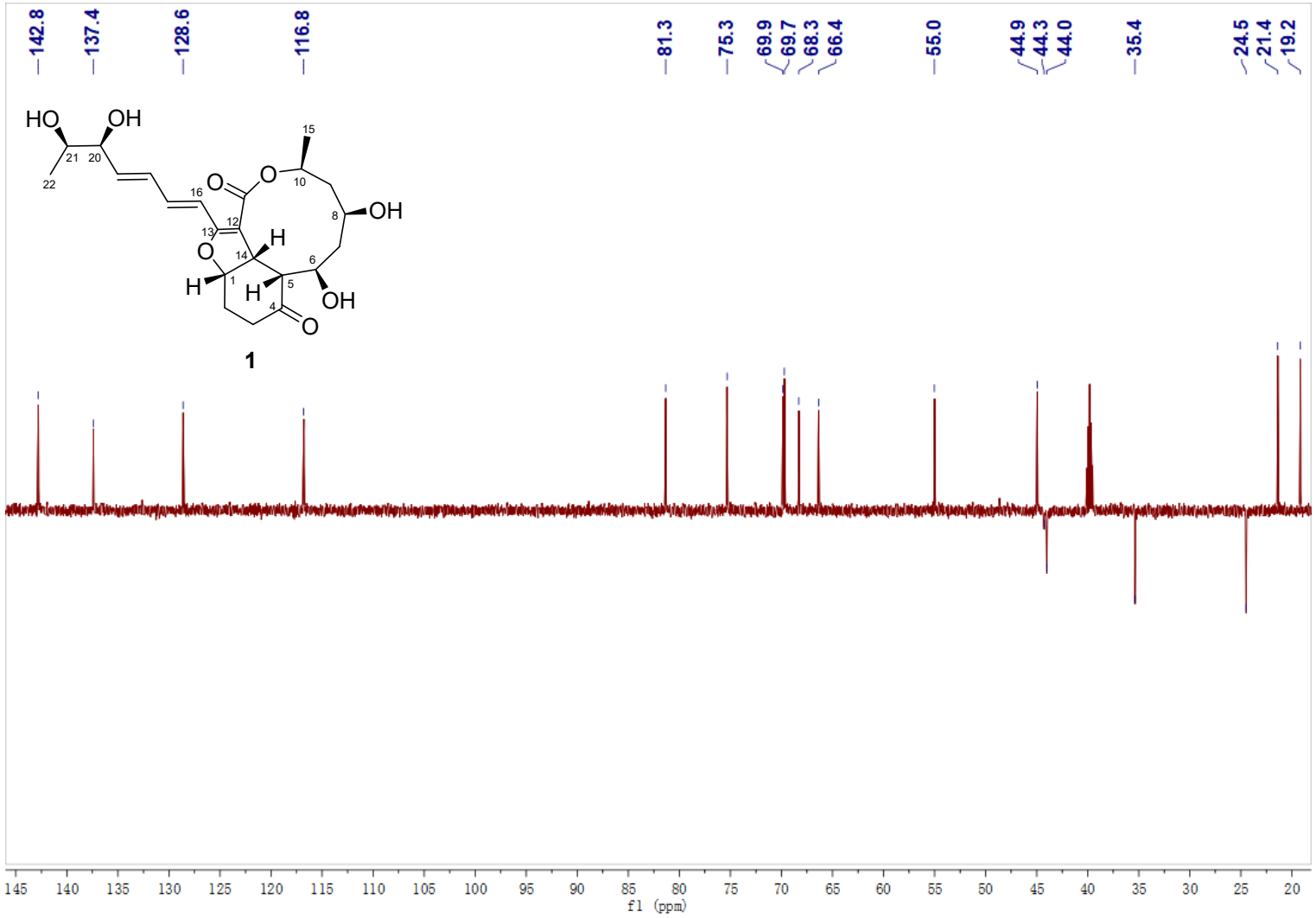


**Figure S7.** HSQC spectrum of compound **1** in DMSO-$d_6$ (600 MHz)

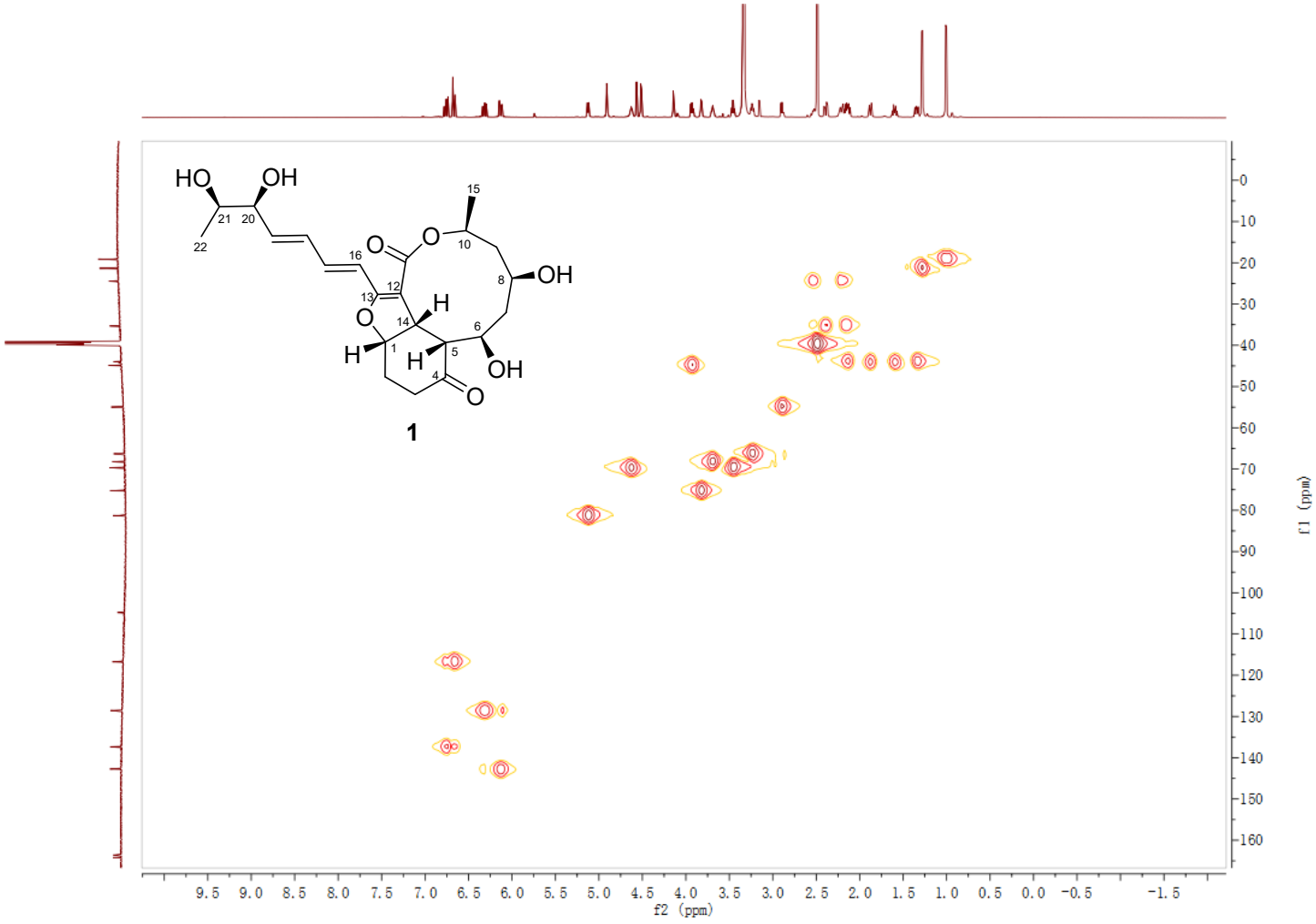


**Figure S8.** $^{1}$H-$^{1}$H COSY spectrum of compound **1** in DMSO-$d_6$ (600 MHz)

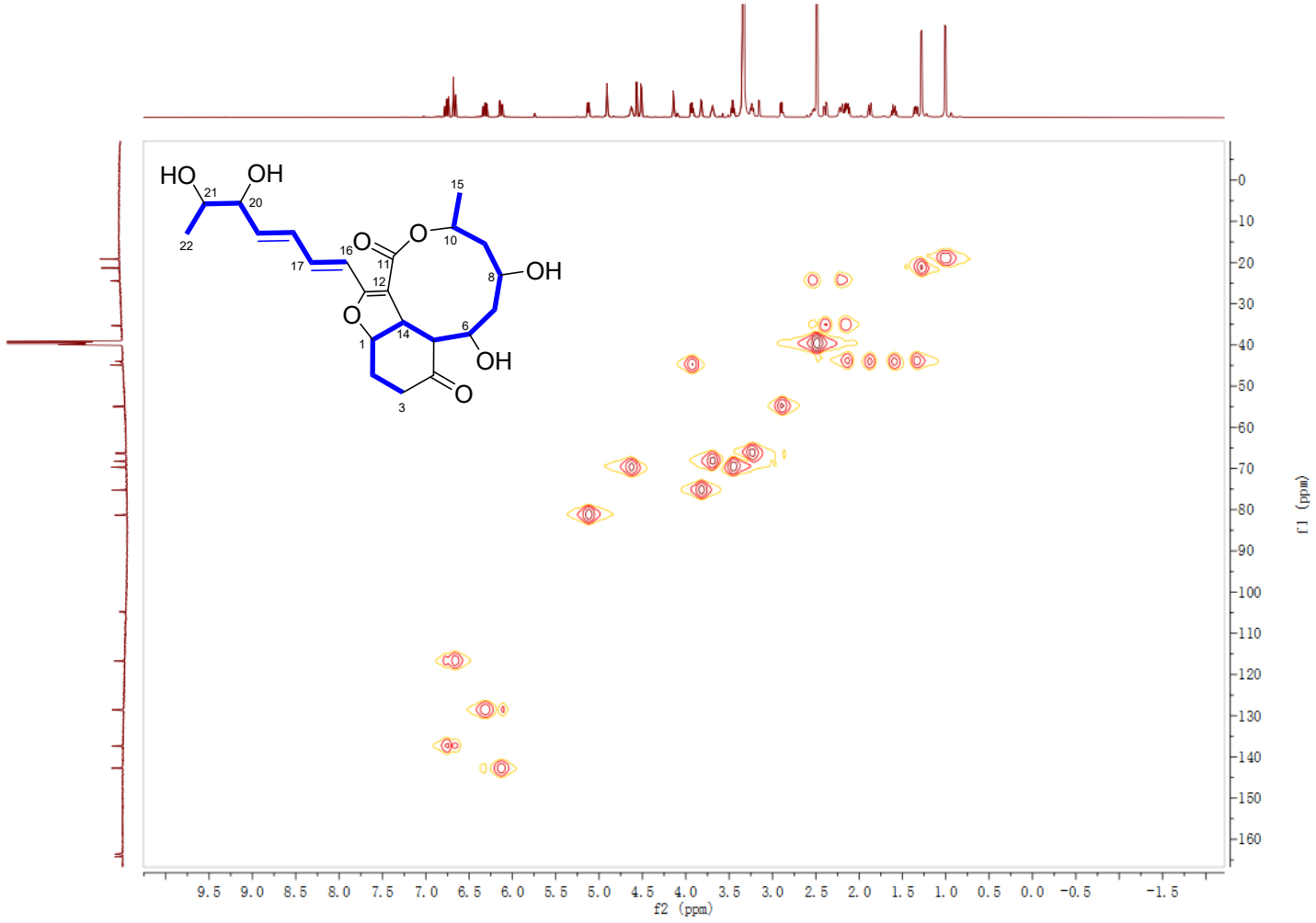


**Figure S9.** HMBC spectrum of compound **1** in DMSO-$d_6$ (600 MHz)

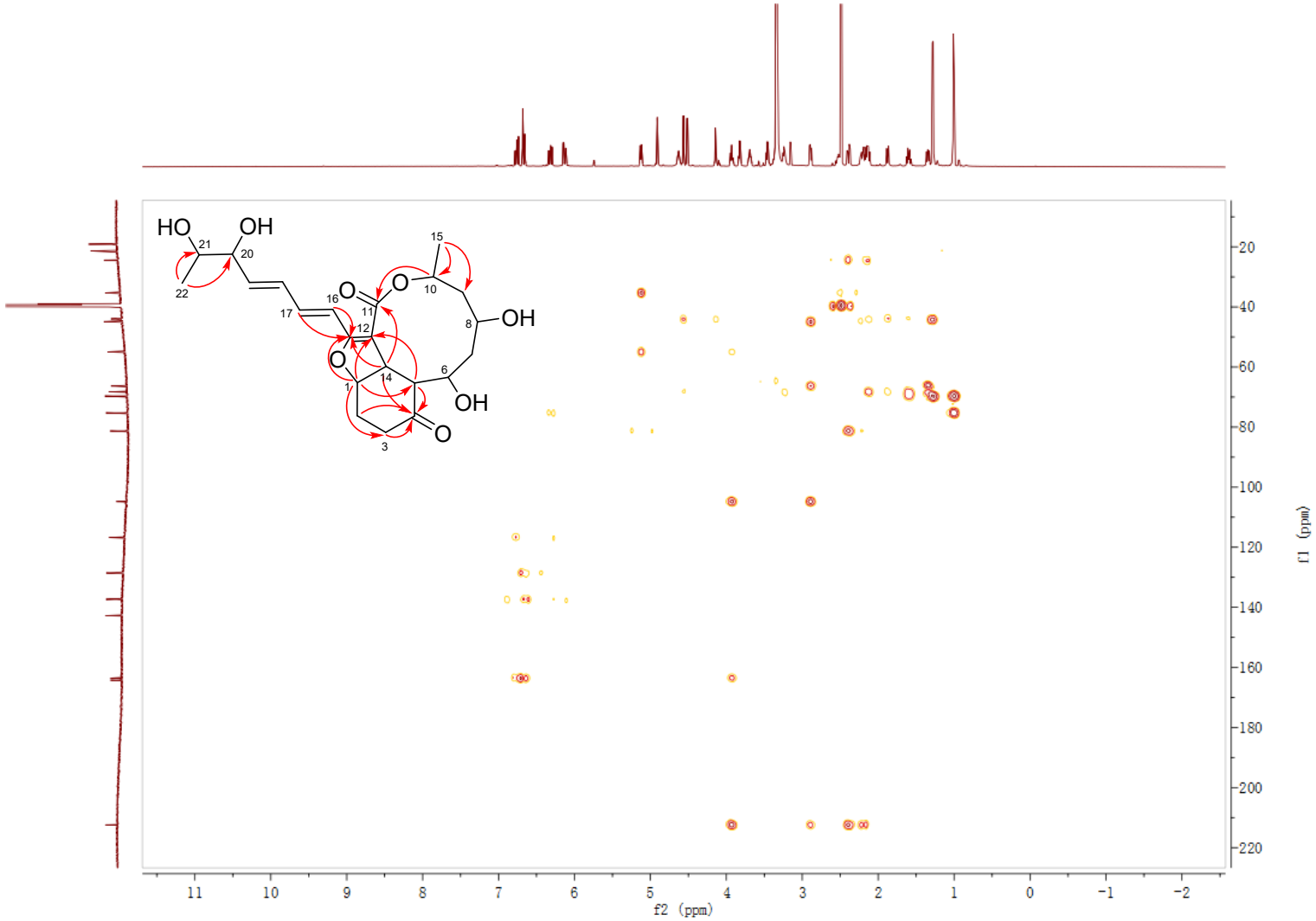


**Figure S10.** ROESY spectrum of compound **1** in DMSO-$d_6$ (600 MHz)

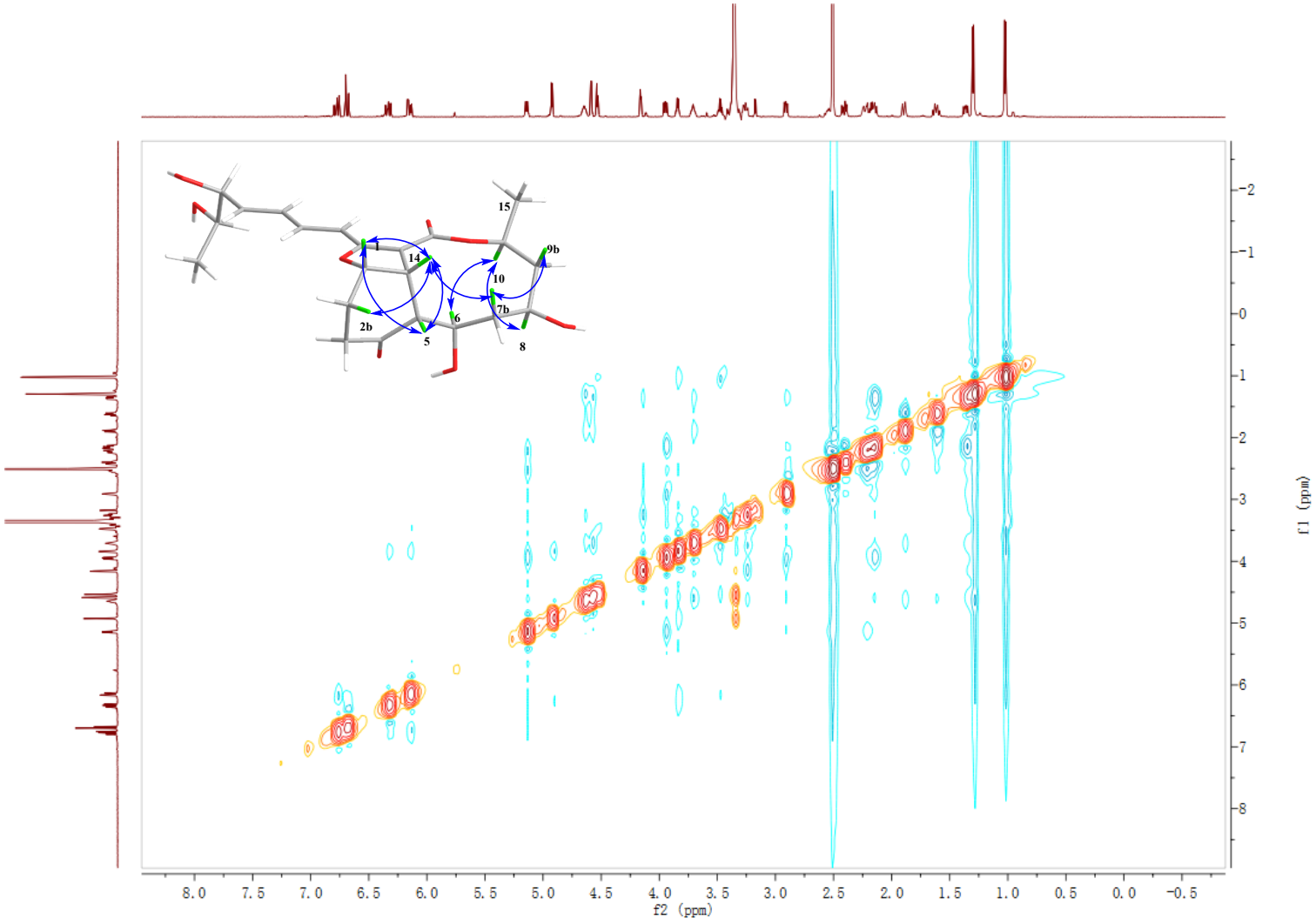
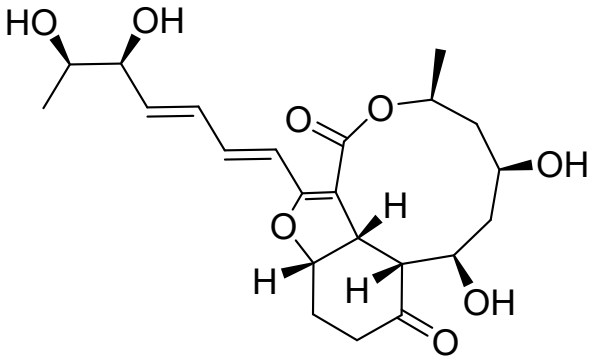
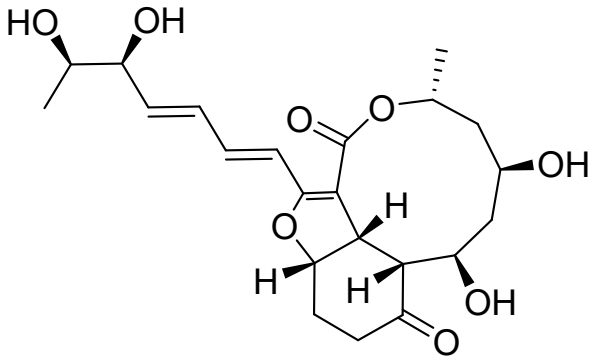


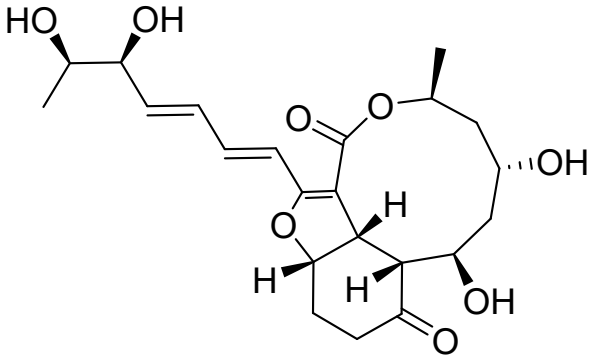
**Figure S11.** Possible isomers of **1** (four types of relative configuration)



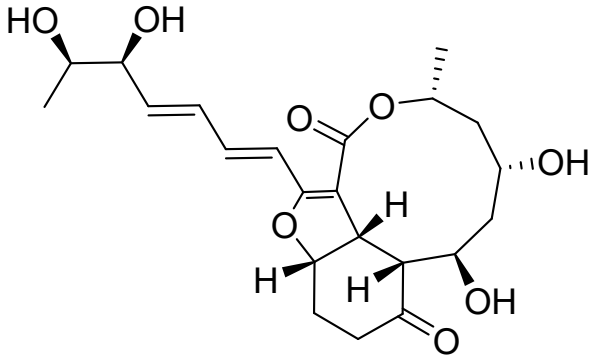
Isomer **1-1**



Isomer **1-2**



Isomer **1-3**



Isomer **1-4**

‘

**Figure S12.** Detailed results of the DP4+ probability analysis of **1**

| Functional | Solvent? | | Basis Set | | Type of Data | |
|---|---|---|---|---|---|---|
| mPW1PW91 | PCM | | 6-311+G(d,p) | | Shielding Tensors | |
| | Isomer 1 | Isomer 2 | Isomer 3 | Isomer 4 | Isomer 5 | Isomer 6 |
| sDP4+ (H data) | 16.59% | 0.00% | 26.29% | 57.12% | – | – |
| sDP4+ (C data) | 99.78% | 0.00% | 0.22% | 0.00% | – | – |
| sDP4+ (all data) | 99.65% | 0.00% | 0.35% | 0.00% | – | – |
| uDP4+ (H data) | 0.88% | 0.00% | 3.06% | 96.05% | – | – |
| uDP4+ (C data) | 99.99% | 0.00% | 0.01% | 0.00% | – | – |
| uDP4+ (all data) | 99.97% | 0.00% | 0.03% | 0.00% | – | – |
| DP4+ (H data) | 0.26% | 0.00% | 1.44% | 98.30% | – | – |
| DP4+ (C data) | 100.00% | 0.00% | 0.00% | 0.00% | – | – |
| DP4+ (all data) | 100.00% | 0.00% | 0.00% | 0.00% | – | – |

**Figure S13.** ECD curve of compound **1**

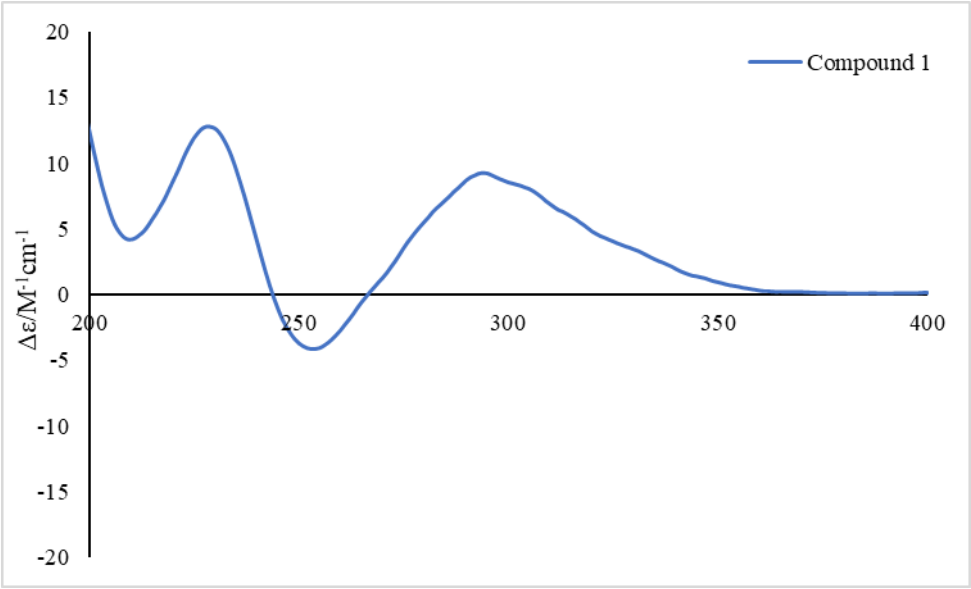


**Figure S14.** Optimized geometries of predominant conformers for compound **1a** at the B3LYP/6-31G(d,p) level in the gas phase

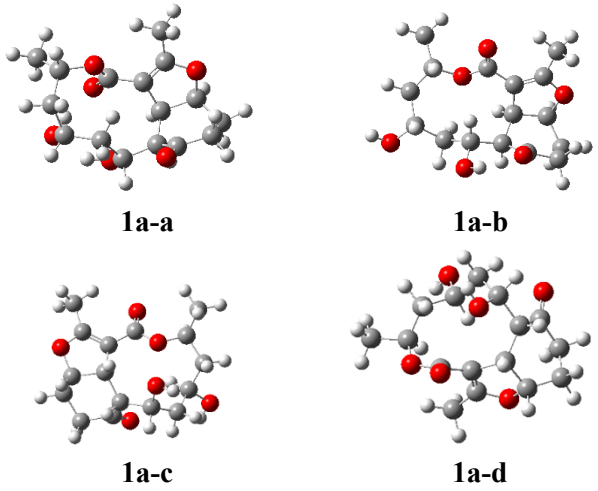


**Table S1.** Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **1a** at B3LYP/6-31G(d,p) level in the gas phase

| Conformations | E+ZPE | G | % |
|---|---|---|---|
| **1-a** | -1073.928249 | -1073.974389 | 0 |
| **1-b** | -1073.951592 | -1073.999351 | 100 |
| **1-c** | -1073.920997 | -1073.969248 | 0 |
| **1-d** | -1073.908469 | -1073.956760 | 0 |

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors

**Table S2.** Optimized *Z*-matrixes of compound **1a** in the gas phase (Å) at B3LYP/6-31G(d,p) l**evel**

| **1-a** | | | | **1-b** | | | |
|---|---|---|---|---|---|---|---|
| C | -0.894848 | -1.525329 | 0.823345 | C | -1.738395 | -1.633011 | -0.592594 |
| C | 0.088294 | -2.151411 | -0.22024 | C | -0.593166 | -1.527989 | 0.42404 |
| C | -2.438777 | -1.52716 | 0.562049 | C | -3.109741 | -1.223256 | -0.027403 |
| C | -3.121452 | -0.352627 | 1.309739 | C | -3.552322 | 0.213004 | -0.37645 |
| C | -3.026284 | 1.102687 | 0.774686 | C | -2.730201 | 1.379379 | 0.173092 |
| O | -1.635245 | 1.499017 | 0.517461 | O | -1.394558 | 1.22431 | -0.376427 |
| C | -0.980456 | 1.06183 | -0.581132 | C | -0.35115 | 1.769634 | 0.304941 |
| C | 0.478421 | 1.109356 | -0.466607 | C | 0.911292 | 1.21958 | -0.189306 |
| C | 1.362 | 0.030607 | -1.083945 | C | 1.066022 | -0.05025 | -1.017228 |
| C | 1.415848 | -1.367148 | -0.352294 | C | 0.797762 | -1.395615 | -0.24257 |
| C | 2.741109 | 0.753647 | -1.056534 | C | 2.550073 | 0.084179 | -1.475968 |
| C | 3.907992 | -0.084186 | -0.551789 | C | 3.389402 | -1.17598 | -1.314831 |
| C | 3.603016 | -0.662981 | 0.833734 | C | 3.339309 | -1.672892 | 0.135878 |
| C | 2.230546 | -1.330035 | 0.931892 | C | 1.940826 | -1.6222 | 0.742132 |
| O | 2.579256 | 1.890579 | -0.141345 | O | 3.13566 | 1.126723 | -0.630319 |
| C | 1.250787 | 2.0758 | 0.076239 | C | 2.13103 | 1.776415 | 0.009103 |
| O | 1.857696 | -1.831763 | 1.977593 | O | 1.781431 | -1.753835 | 1.945759 |
| O | -2.856928 | -1.613778 | -0.804029 | O | -4.056506 | -2.135751 | -0.596764 |
| C | -4.010023 | 1.469869 | -0.3398 | C | -3.306106 | 2.738037 | -0.21638 |
| O | -1.537687 | 0.593975 | -1.566829 | O | -0.492179 | 2.593971 | 1.194453 |
| H | 2.968755 | 1.188014 | -2.036843 | H | 2.603635 | 0.460967 | -2.503472 |
| H | 1.047995 | -0.180418 | -2.10788 | H | 0.40818 | -0.038215 | -1.889818 |
| H | 2.025381 | -1.981929 | -1.036083 | H | 0.881649 | -2.204089 | -0.986278 |
| O | -0.39542 | -2.289031 | -1.547602 | O | -0.664059 | -2.715988 | 1.206334 |
| C | 0.913438 | 3.316709 | 0.827669 | C | 2.551955 | 2.970077 | 0.790445 |
| H | -0.57097 | -0.51434 | 1.058509 | H | -1.526695 | -1.064231 | -1.501028 |
| H | -0.736485 | -2.066272 | 1.759903 | H | -1.808677 | -2.68956 | -0.869391 |
| H | 0.366226 | -3.145673 | 0.162626 | H | -0.736962 | -0.658446 | 1.077601 |
| H | -2.845553 | -2.441765 | 1.006786 | H | -3.083878 | -1.349571 | 1.066842 |
| H | -2.731532 | -0.360762 | 2.334554 | H | -4.579305 | 0.350314 | -0.009403 |
| H | -4.193952 | -0.569114 | 1.38221 | H | -3.600417 | 0.292311 | -1.46984 |
| H | -3.259099 | 1.749406 | 1.625413 | H | -2.644122 | 1.320699 | 1.264397 |
| H | 4.811805 | 0.53273 | -0.519509 | H | 3.005216 | -1.93614 | -2.005156 |
| H | 4.099254 | -0.883163 | -1.277998 | H | 4.421956 | -0.972371 | -1.615027 |
| H | 4.353799 | -1.401779 | 1.135922 | H | 3.994579 | -1.080643 | 0.781079 |

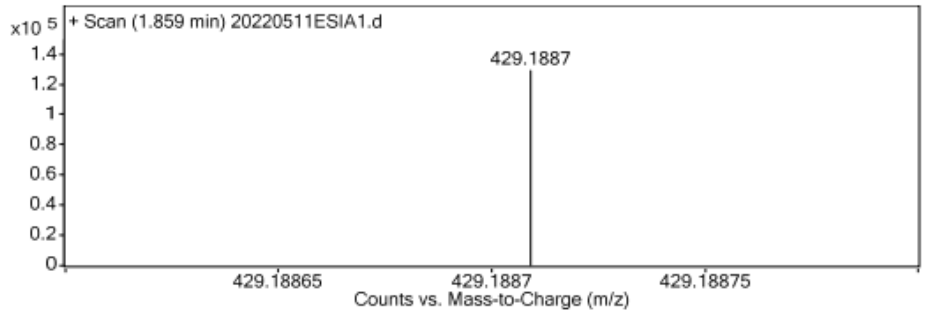
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 3.630973 | 0.12749 | 1.591444 | H | 3.689731 | -2.709984 | 0.209004 |
| H | -2.532213 | -0.809099 | -1.25751 | H | -4.920508 | -1.949269 | -0.20575 |
| H | -3.802282 | 2.478893 | -0.706815 | H | -2.684585 | 3.538679 | 0.187457 |
| H | -5.019444 | 1.469275 | 0.085527 | H | -3.3535 | 2.835679 | -1.3058 |
| H | -3.993317 | 0.782 | -1.181364 | H | -4.319459 | 2.849114 | 0.183056 |
| H | -1.363453 | -2.379596 | -1.496538 | H | -0.022353 | -2.591698 | 1.92389 |
| H | 1.295798 | 4.194832 | 0.296669 | H | 3.26711 | 2.667696 | 1.563553 |
| H | -0.162505 | 3.406565 | 0.967773 | H | 1.686707 | 3.433708 | 1.261005 |
| H | 1.399789 | 3.29495 | 1.809147 | H | 3.063863 | 3.684931 | 0.137374 |
| **1-c** | | | | **1-d** | | | |
| C | 2.149814 | -1.846565 | 0.372449 | C | -0.215439 | 2.602982 | 0.15316 |
| C | 0.928284 | -1.698764 | 1.308642 | C | 0.673447 | 1.932474 | 1.221991 |
| C | 2.607196 | -0.777735 | -0.633494 | C | -1.067791 | 1.714804 | -0.748215 |
| C | 3.223045 | 0.487497 | -0.003432 | C | -2.33992 | 1.1755 | -0.06072 |
| C | 2.346493 | 1.716671 | -0.212155 | C | -2.782676 | -0.226247 | -0.5263 |
| O | 1.037817 | 1.306327 | 0.257602 | O | -2.540566 | -1.216569 | 0.510674 |
| C | -0.051524 | 1.770243 | -0.386365 | C | -1.340399 | -1.260422 | 1.174191 |
| C | -1.243176 | 1.041879 | 0.050046 | C | -0.081288 | -1.211411 | 0.392984 |
| C | -1.335152 | -0.220781 | 0.917233 | C | 1.229313 | -0.698196 | 0.984248 |
| C | -0.531779 | -1.564734 | 0.751158 | C | 1.66926 | 0.810773 | 0.797605 |
| C | -2.846294 | -0.521817 | 0.721216 | C | 2.227781 | -1.688425 | 0.324876 |
| C | -3.173798 | -1.332924 | -0.547207 | C | 3.562845 | -1.118563 | -0.119028 |
| C | -2.293955 | -2.578303 | -0.756771 | C | 3.344669 | 0.064366 | -1.060875 |
| C | -0.82562 | -2.208008 | -0.602079 | C | 2.456499 | 1.152136 | -0.472203 |
| O | -3.455216 | 0.784149 | 0.527848 | O | 1.53672 | -2.196264 | -0.86399 |
| C | -2.491353 | 1.572135 | -0.027973 | C | 0.199781 | -2.036889 | -0.642597 |
| O | -0.011744 | -2.406401 | -1.485451 | O | 2.469795 | 2.27242 | -0.950314 |
| O | 3.635483 | -1.352751 | -1.45456 | O | -1.409646 | 2.52203 | -1.883947 |
| C | 2.805877 | 2.957804 | 0.540154 | C | -4.274269 | -0.330959 | -0.816853 |
| O | -0.016754 | 2.671996 | -1.211118 | O | -1.341838 | -1.452883 | 2.368774 |
| H | -3.301819 | -0.963003 | 1.611933 | H | 2.373319 | -2.55588 | 0.980483 |
| H | -1.15166 | 0.073434 | 1.956947 | H | 1.19594 | -0.861625 | 2.062378 |
| H | -1.102299 | -2.195717 | 1.449506 | H | 2.473664 | 0.885942 | 1.550434 |
| O | 1.076052 | -0.702807 | 2.317625 | O | -0.06957 | 1.374701 | 2.309311 |
| C | -2.988298 | 2.864236 | -0.572371 | C | -0.669766 | -2.856855 | -1.53412 |
| H | 3.007578 | -2.059713 | 1.029349 | H | 0.439134 | 3.185651 | -0.495112 |
| H | 1.978778 | -2.764899 | -0.196626 | H | -0.866578 | 3.320056 | 0.674758 |
| H | 0.907516 | -2.684369 | 1.805978 | H | 1.305999 | 2.750437 | 1.598449 |
| H | 1.755877 | -0.499226 | -1.265312 | H | -0.452428 | 0.867779 | -1.082429 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | 4.197409 | 0.658808 | -0.471338 | H | -2.199306 | 1.140838 | 1.022614 |
| H | 3.39425 | 0.347244 | 1.069732 | H | -3.132891 | 1.908194 | -0.249821 |
| H | 2.256406 | 1.944558 | -1.279248 | H | -2.220261 | -0.513634 | -1.426089 |
| H | -4.23353 | -1.606243 | -0.536591 | H | 4.130339 | -0.81547 | 0.769686 |
| H | -3.026849 | -0.667189 | -1.403661 | H | 4.146048 | -1.902214 | -0.613256 |
| H | -2.451466 | -3.004378 | -1.750403 | H | 4.281907 | 0.534893 | -1.371667 |
| H | -2.535023 | -3.350383 | -0.013326 | H | 2.853092 | -0.289051 | -1.975792 |
| H | 3.221983 | -2.058049 | -1.971125 | H | -1.87116 | 1.959971 | -2.520282 |
| H | 2.135535 | 3.795449 | 0.333531 | H | -4.546729 | -1.352951 | -1.09446 |
| H | 2.817892 | 2.77176 | 1.618801 | H | -4.853912 | -0.049678 | 0.067092 |
| H | 3.816495 | 3.238677 | 0.225769 | H | -4.546482 | 0.338993 | -1.638752 |
| H | 1.898813 | -0.888992 | 2.788238 | H | -0.58483 | 2.083342 | 2.716189 |
| H | -3.662299 | 2.67699 | -1.416123 | H | -0.325071 | -3.895617 | -1.531567 |
| H | -2.157286 | 3.479718 | -0.911003 | H | -0.602559 | -2.497841 | -2.568014 |
| H | -3.569966 | 3.386414 | 0.195093 | H | -1.708674 | -2.820022 | -1.207781 |

**Figure S15.** HRESIMS spectrum of compound **2**

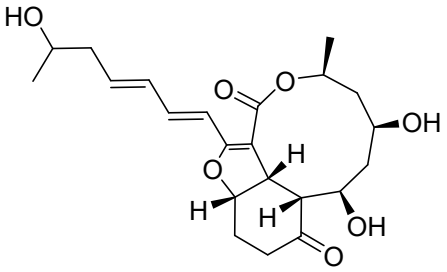
**User Spectra**

| Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|
| 400 | 0 | ESI |




**Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 105.0432 | 1 | 45039.14 | | |
| 429.1887 | 1 | 129073.71 | C22 H30 Na O7 | M+ |
| 430.1921 | 1 | 34491.77 | C22 H30 Na O7 | M+ |
| 445.1629 | 1 | 46338.15 | | |
| 446.1668 | 1 | 13698.38 | | |
| 835.3862 | 1 | 41398.34 | | |
| 836.3898 | 1 | 23891.83 | | |
| 851.3602 | 1 | 14316.07 | | |
| 922.0098 | 1 | 139643.47 | | |
| 923.013 | 1 | 24163.64 | | |




**2**

**Formula Calculator Element Limits**

| Element | Min | Max |
|---|---|---|
| C | 0 | 200 |
| H | 0 | 400 |
| O | 0 | 10 |
| Na | 1 | 1 |

**Formula Calculator Results**

| Formula | CalculatedMass | Mz | Diff.(mDa) | Diff. (ppm) | DBE |
|---|---|---|---|---|---|
| C22 H30 Na O7 | 429.1889 | 429.1887 | 0.2 | 0.5 | 7.5 |

**Figure S16.** IR spectrum of compound **2**

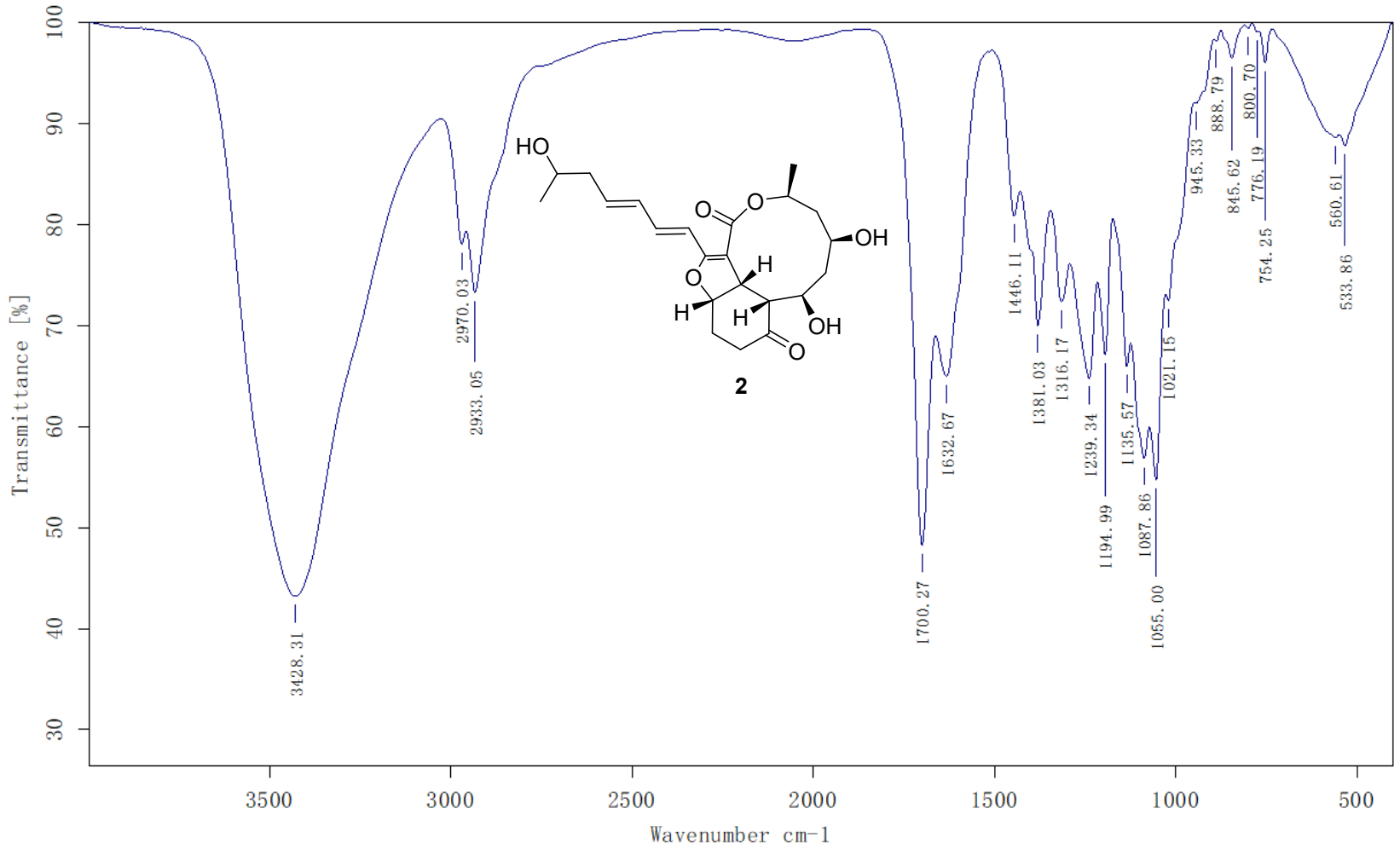
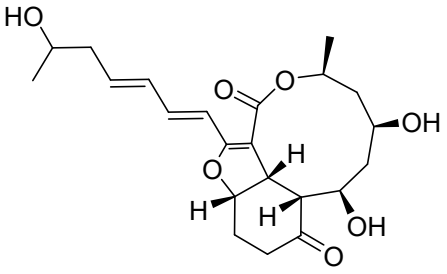


**Figure S17.** Optical rotation spectrum of compound **2**




**2**

**Rudolph Research Analytical**

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 18-AUG-2022

Set Temperature : 25.0

Time Delay : Disabled

Delay between Measurement : Disabled

| n | Average | Std.Dev. | % RSD | Maximum | Minimum |
|---|---|---|---|---|---|
| 5 | 96.80 | 0.45 | 0.46 | 97.00 | 96.00 |

| S.No | Sample ID | Time | Result | Scale | OR °Arc | WLG.nm | Lg.mm | Conc.g/100ml | Temp. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 6A-C-16 | 02:03:59 PM | 97.00 | SR | 0.097 | 589 | 100.00 | 0.100 | 25.0 |
| 2 | 6A-C-16 | 02:04:05 PM | 96.00 | SR | 0.096 | 589 | 100.00 | 0.100 | 25.1 |
| 3 | 6A-C-16 | 02:04:12 PM | 97.00 | SR | 0.097 | 589 | 100.00 | 0.100 | 25.1 |
| 4 | 6A-C-16 | 02:04:18 PM | 97.00 | SR | 0.097 | 589 | 100.00 | 0.100 | 25.1 |
| 5 | 6A-C-16 | 02:04:24 PM | 97.00 | SR | 0.097 | 589 | 100.00 | 0.100 | 25.1 |

**Figure S18.** $^{1}$H NMR spectrum of compound **2** in DMSO-$d_6$ (600 MHz)

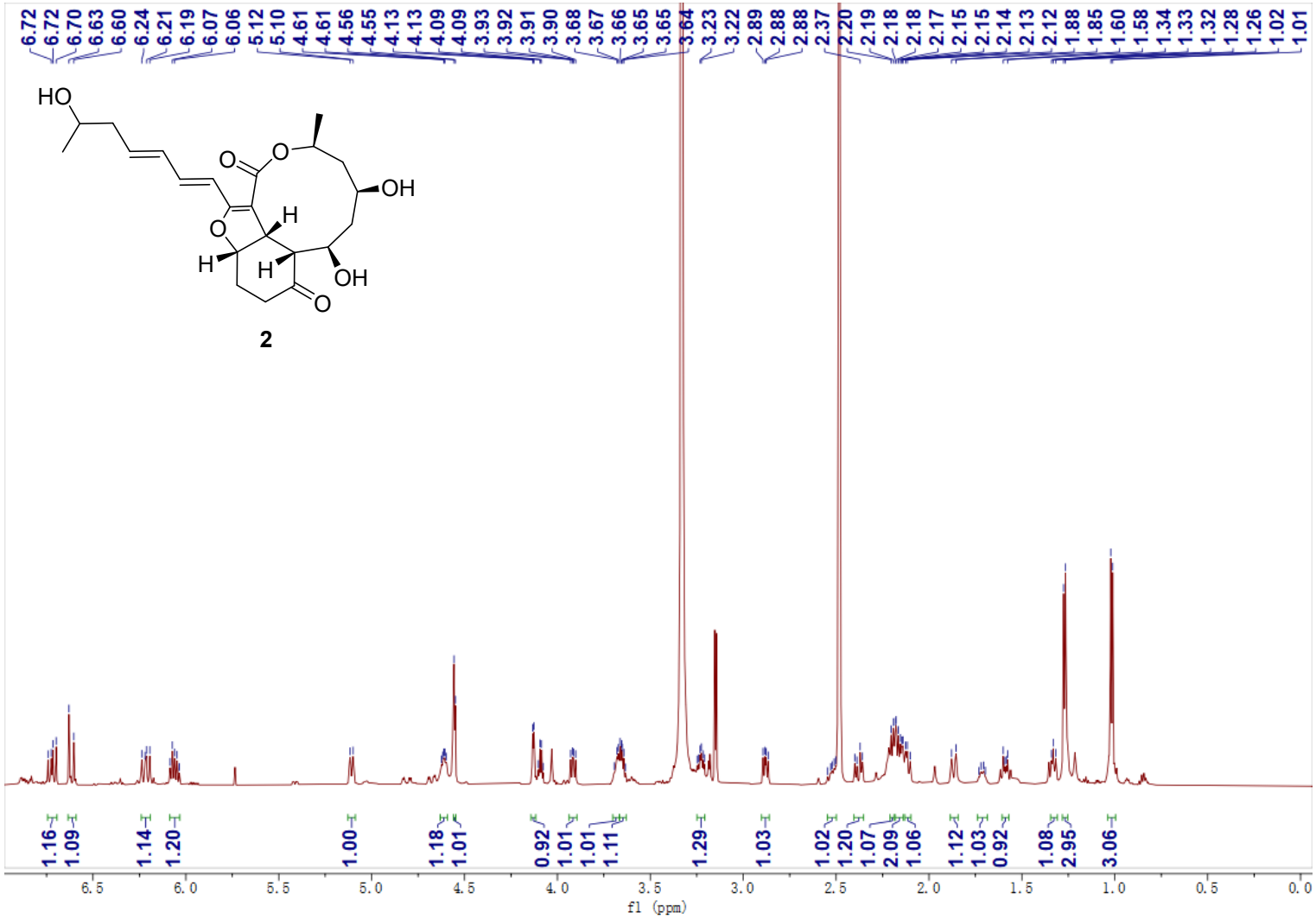


**Figure S19.** $^{13}C$ NMR spectrum of compound **2** in DMSO-$d_6$ (150 MHz)

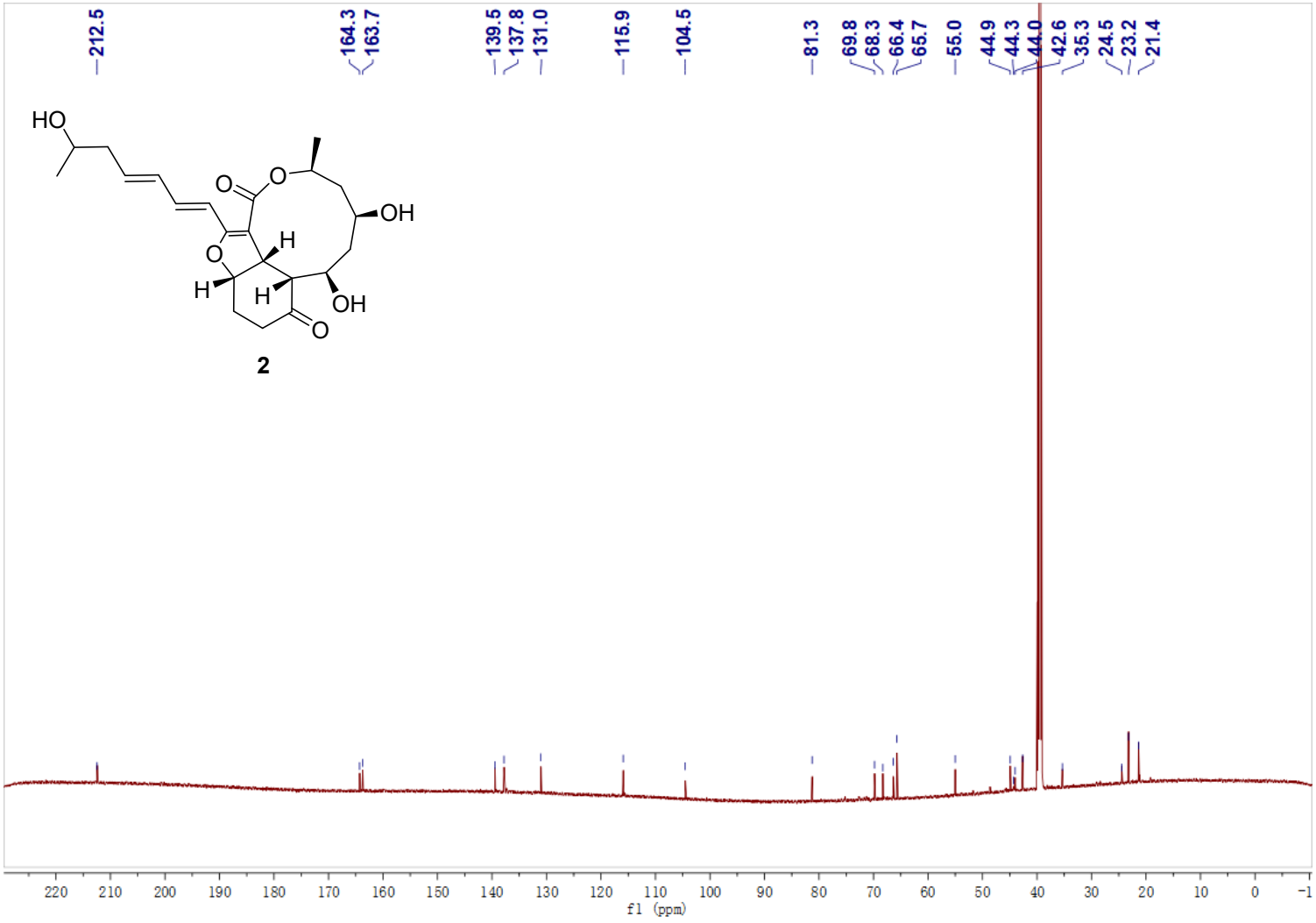


**Figure S20.** DEPT spectrum of compound **2** in DMSO-$d_6$ (150 MHz)

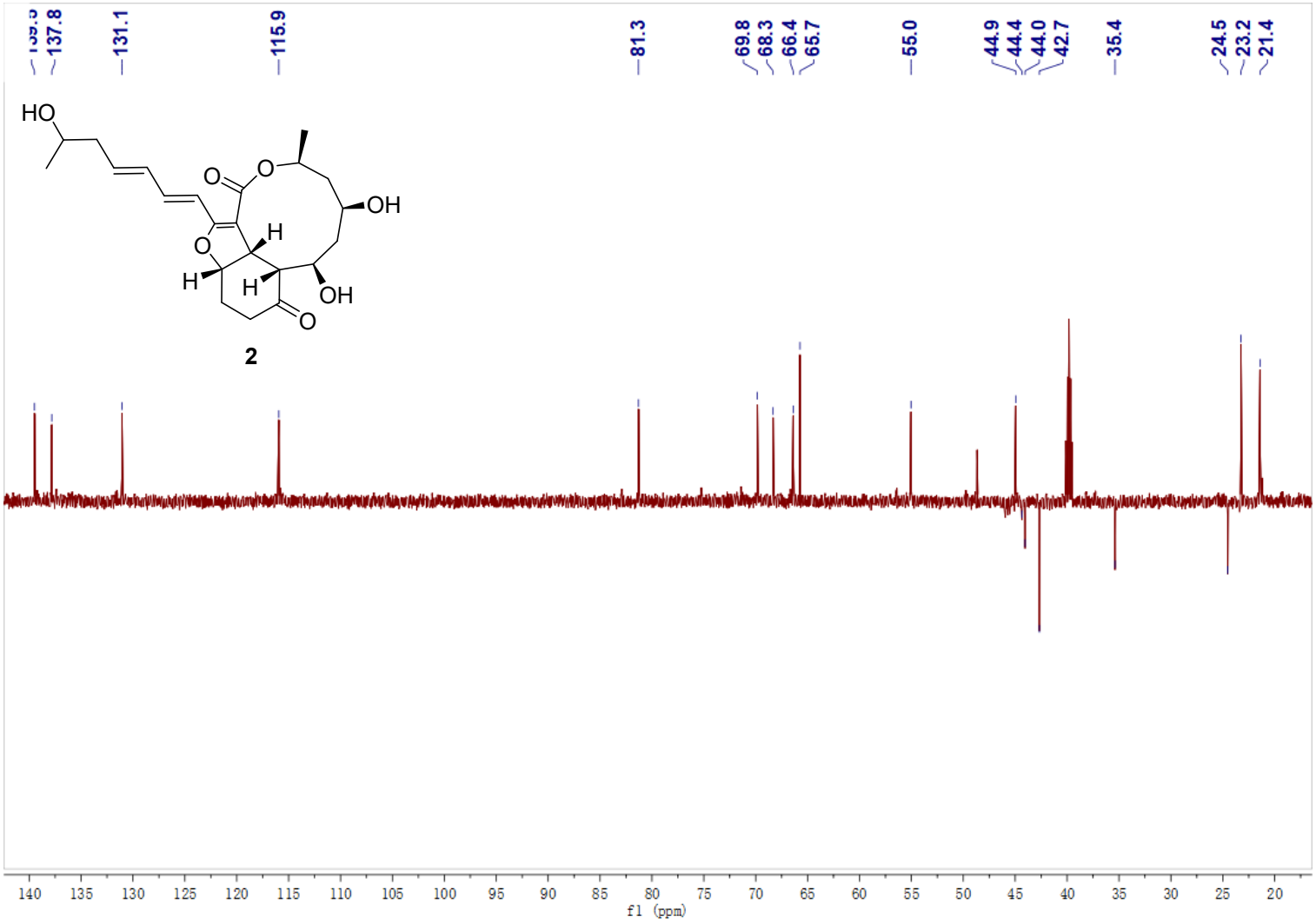


**Figure S21.** (a) Key HMBC (arrow) and $^{1}$H–$^{1}$H COSY (bold) correlations of **2**; (b) Key ROESY correlations of **2**.

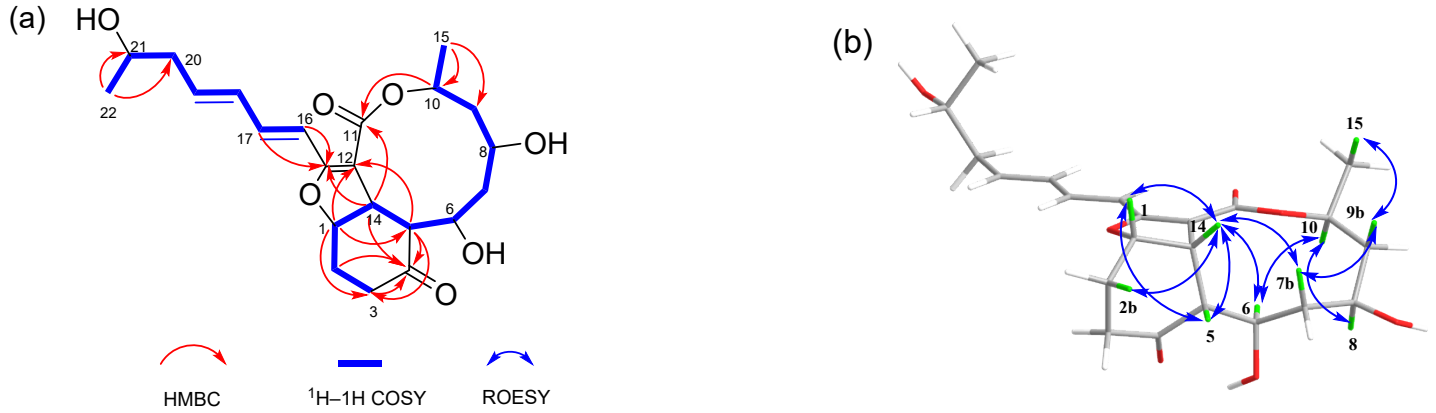


**Figure S22.** HSQC spectrum of compound **2** in DMSO-$d_6$ (600 MHz)

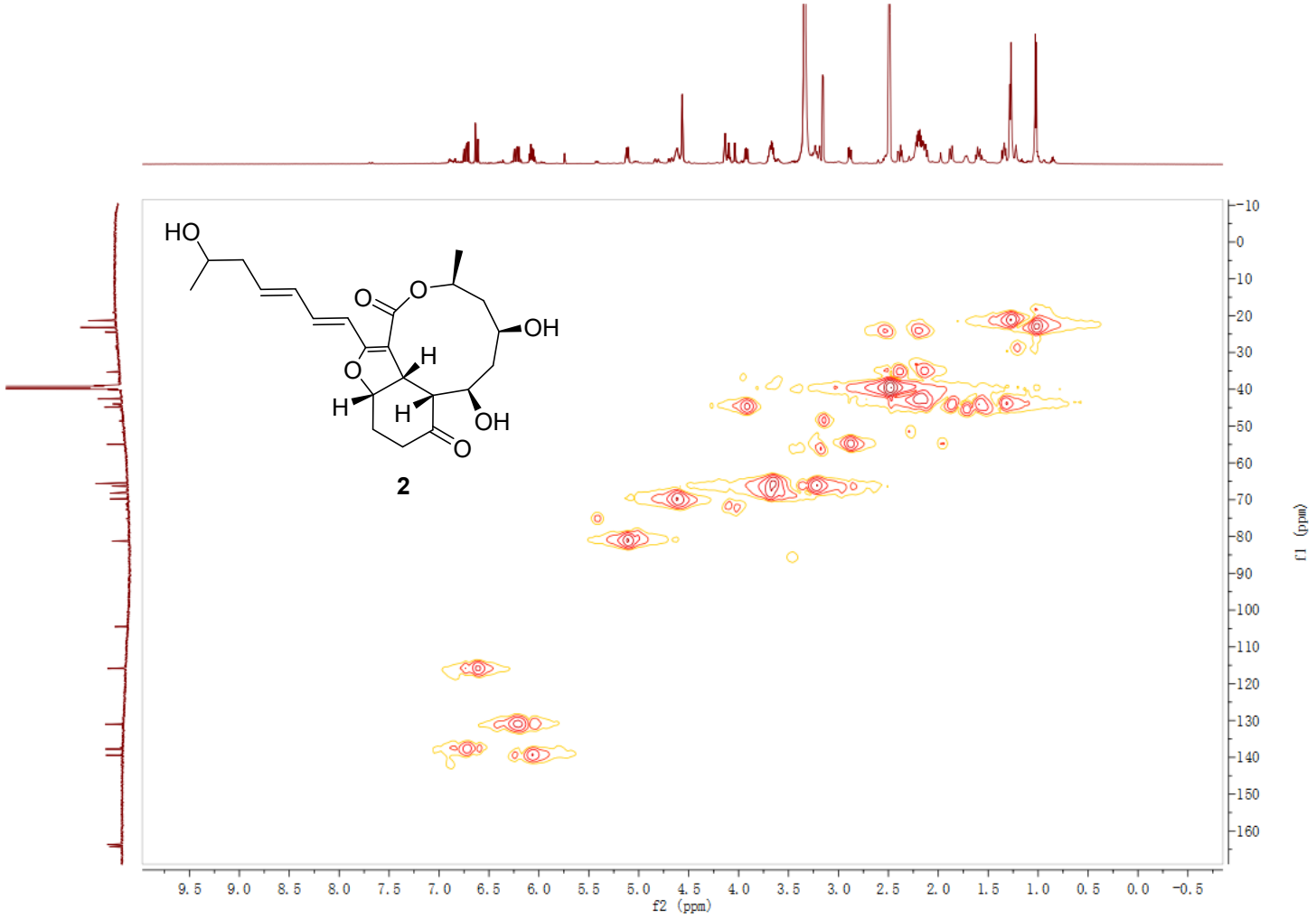


**Figure S23.** $^{1}$H-$^{1}$H COSY spectrum of compound **2** in DMSO-$d_6$ (600 MHz)

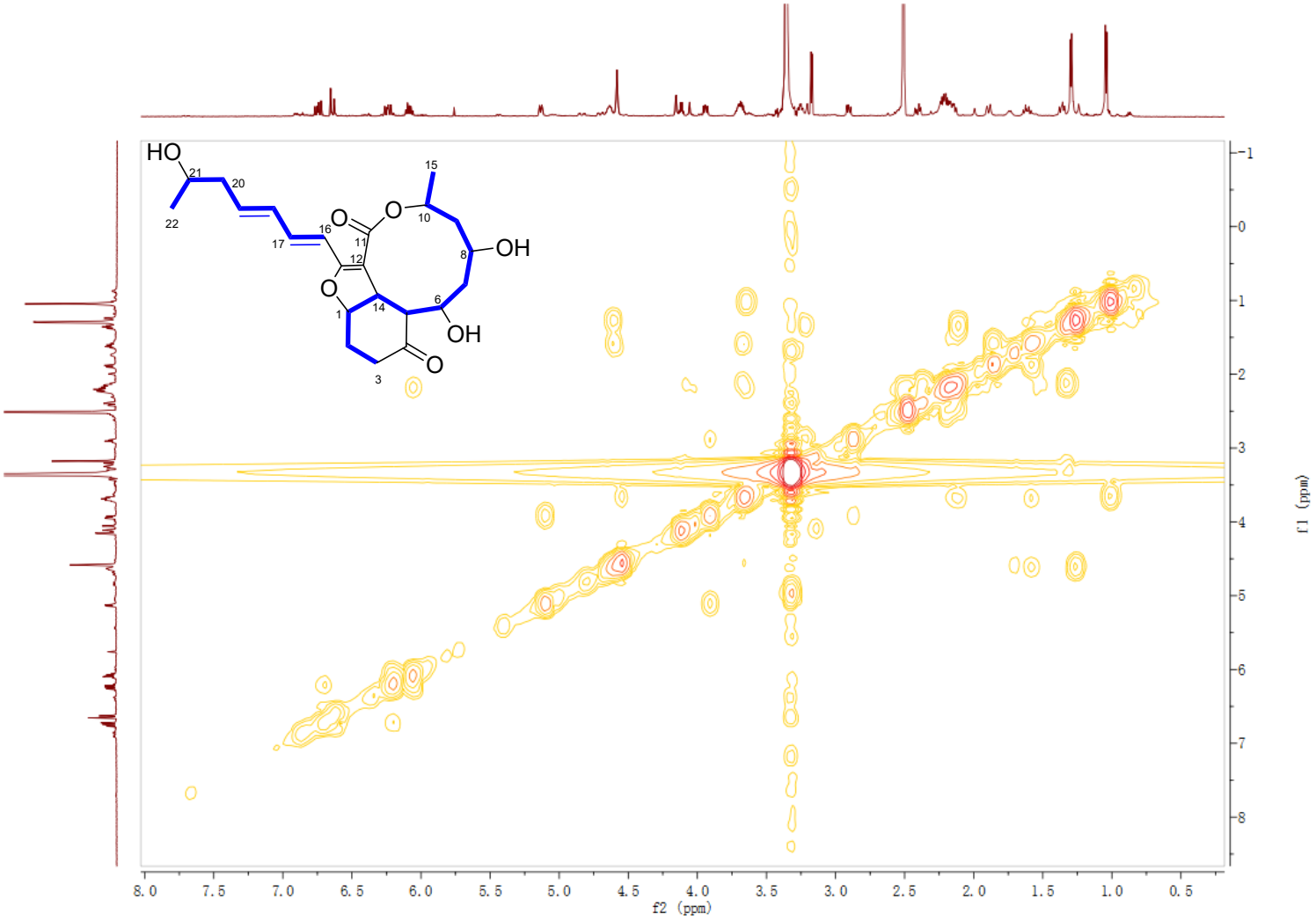


**Figure S24.** HMBC spectrum of compound **2** in DMSO-$d_6$ (600 MHz)

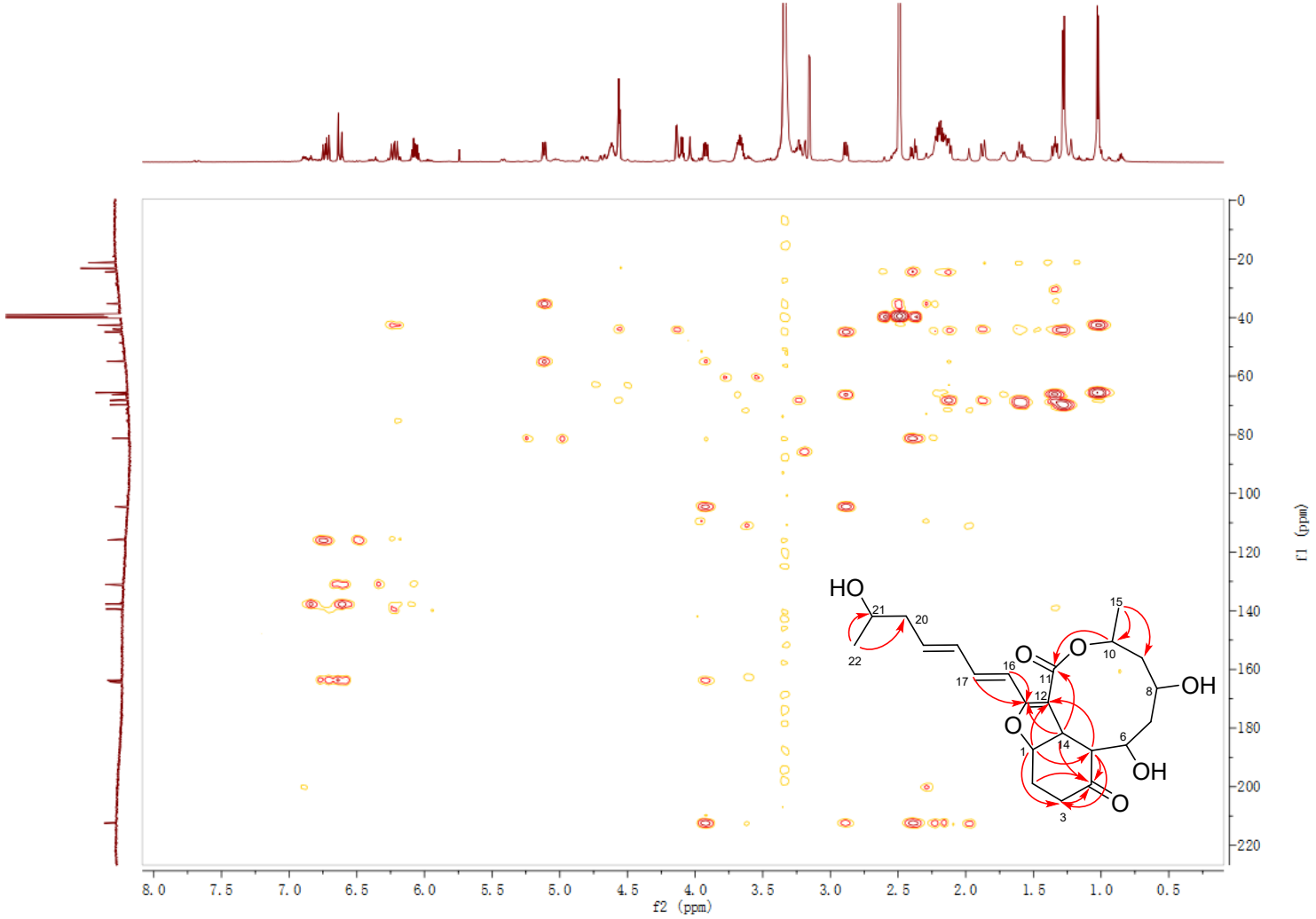


**Figure S25.** ROESY spectrum of compound **2** in DMSO-$d_6$ (600 MHz)

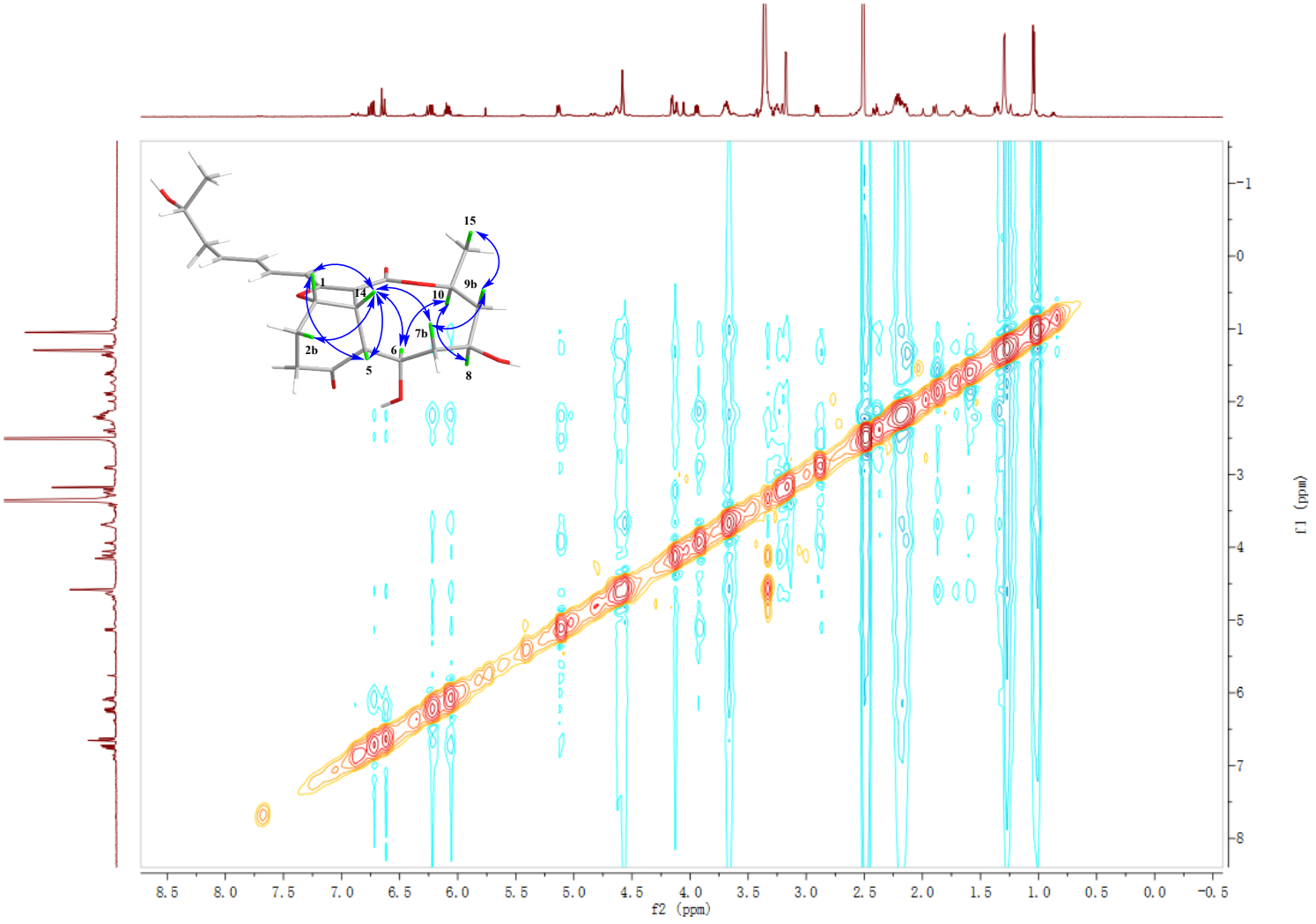


**Figure S26.** ECD curve of compound **2**

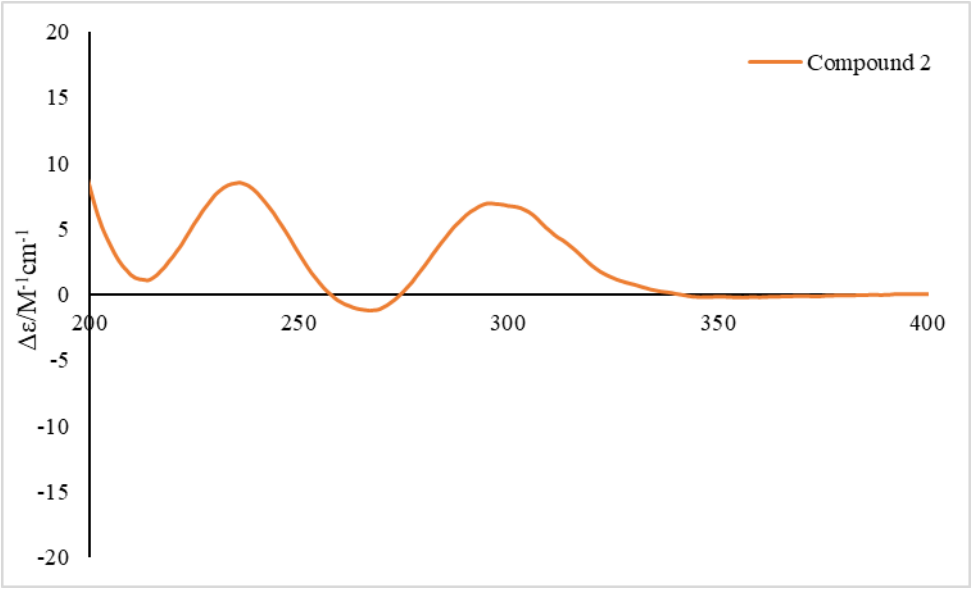


**Figure S27.** $^{1}$H NMR spectrum of compound **3** in methanol-$d_4$ (600 MHz)

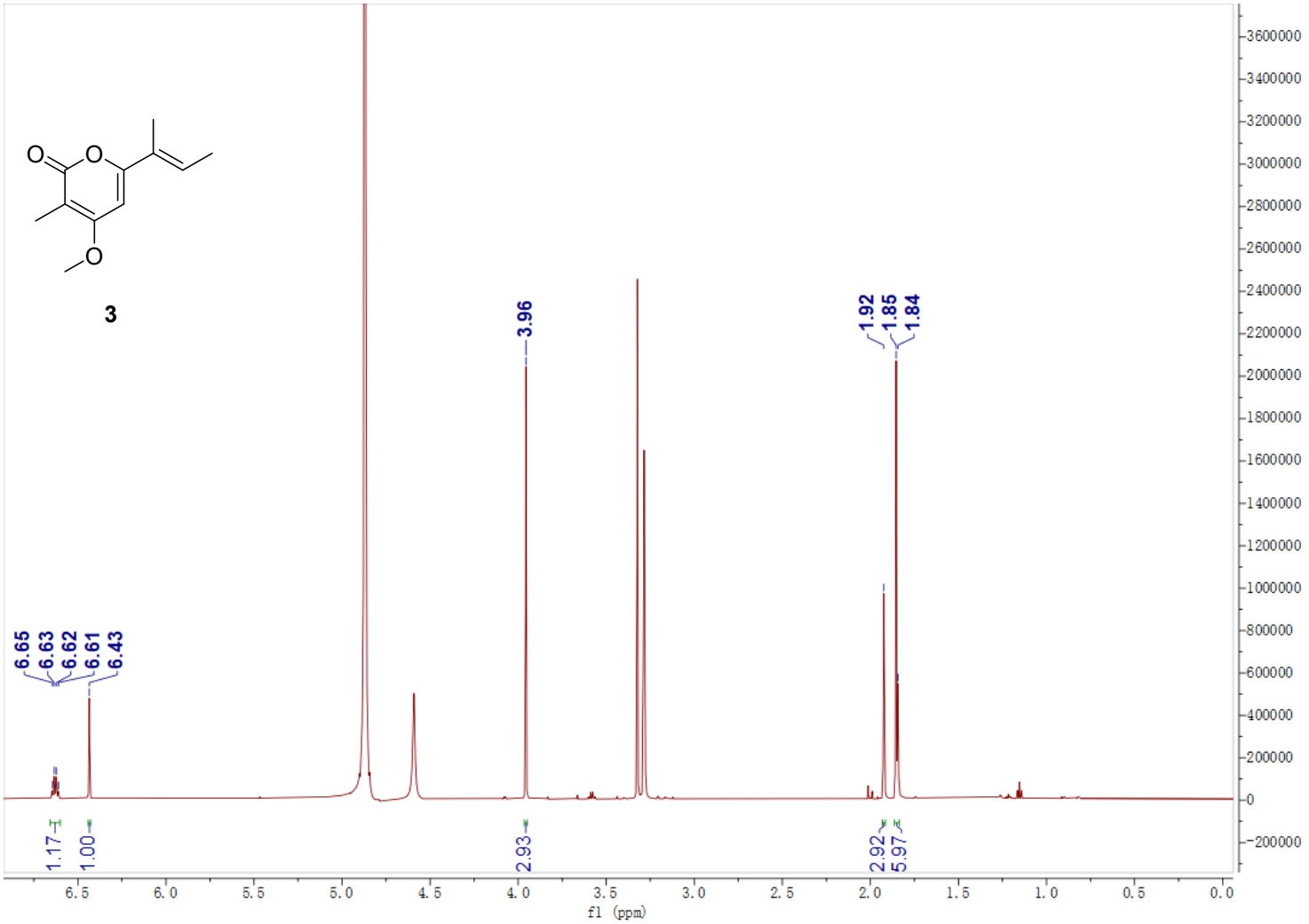


**Figure S28.** $^{13}C$ NMR spectrum of compound **3** in methanol-$d_4$ (125 MHz)

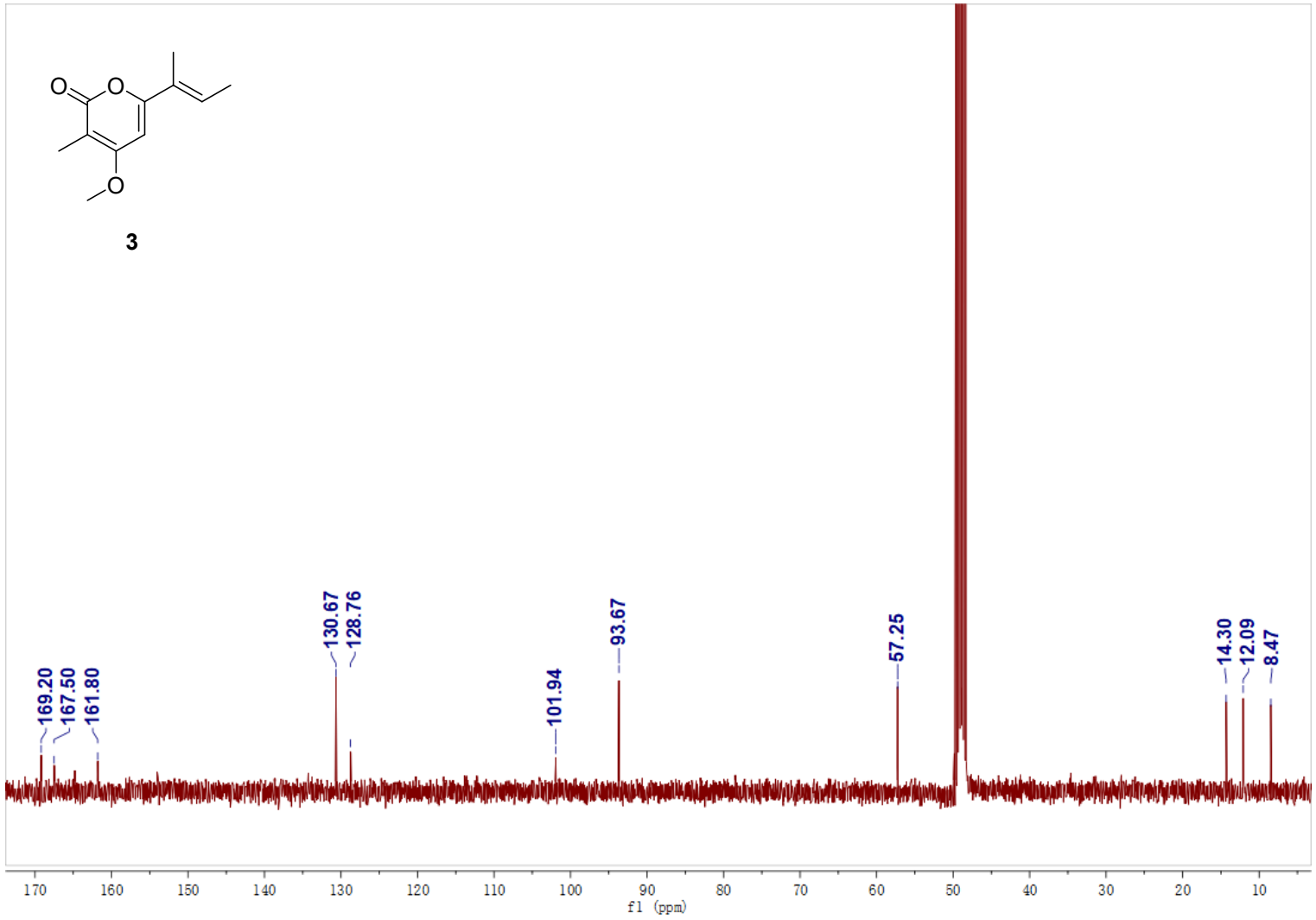


**Figure S29.** $^{1}$H NMR spectrum of compound **4** in methanol-$d_4$ (600 MHz)

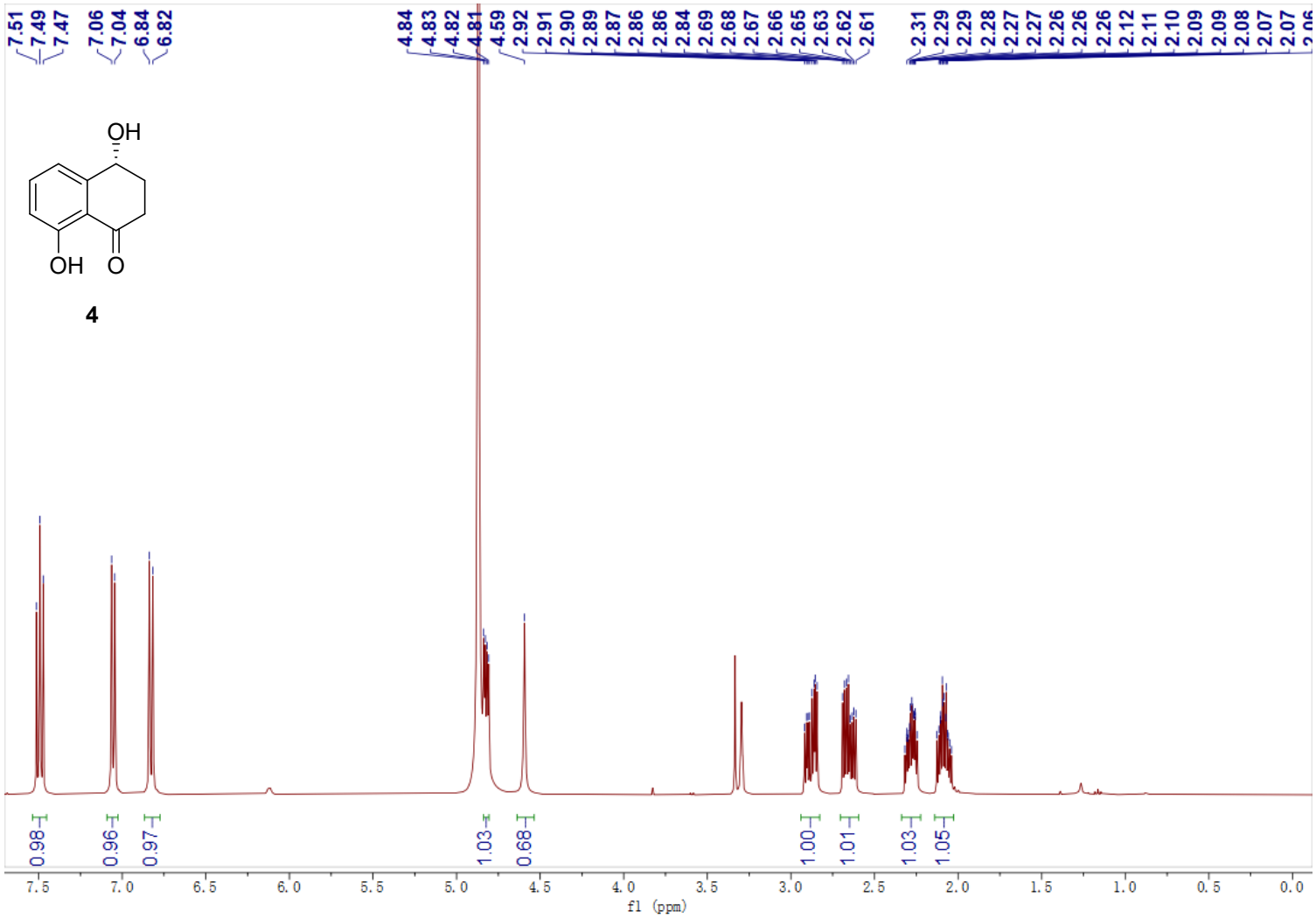


**Figure S30.** $^{13}C$ NMR spectrum of compound **4** in methanol-$d_4$ (125 MHz)

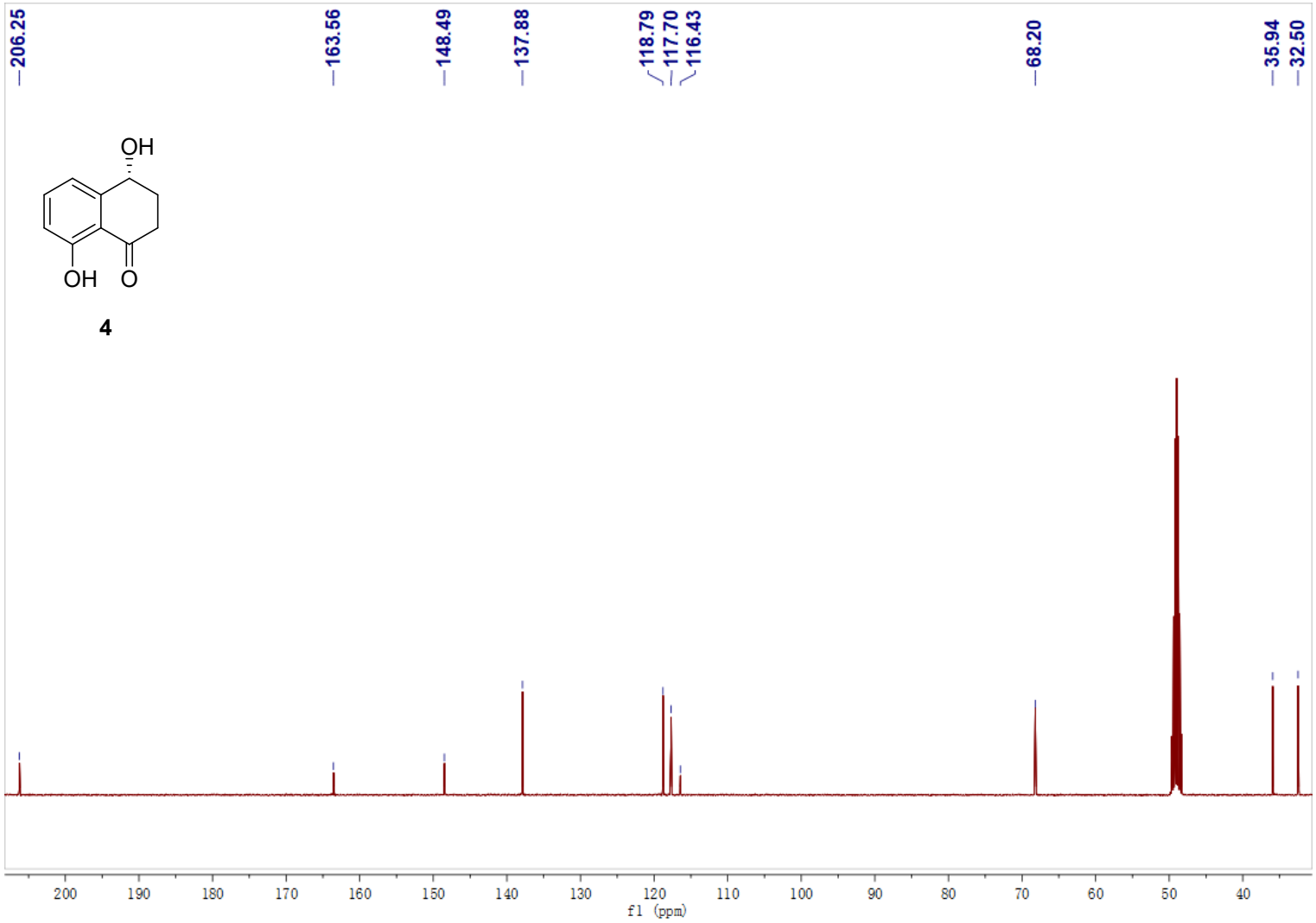


**Figure S31.** [1]H NMR spectrum of compound **5** in methanol-$d_4$ (600 MHz)

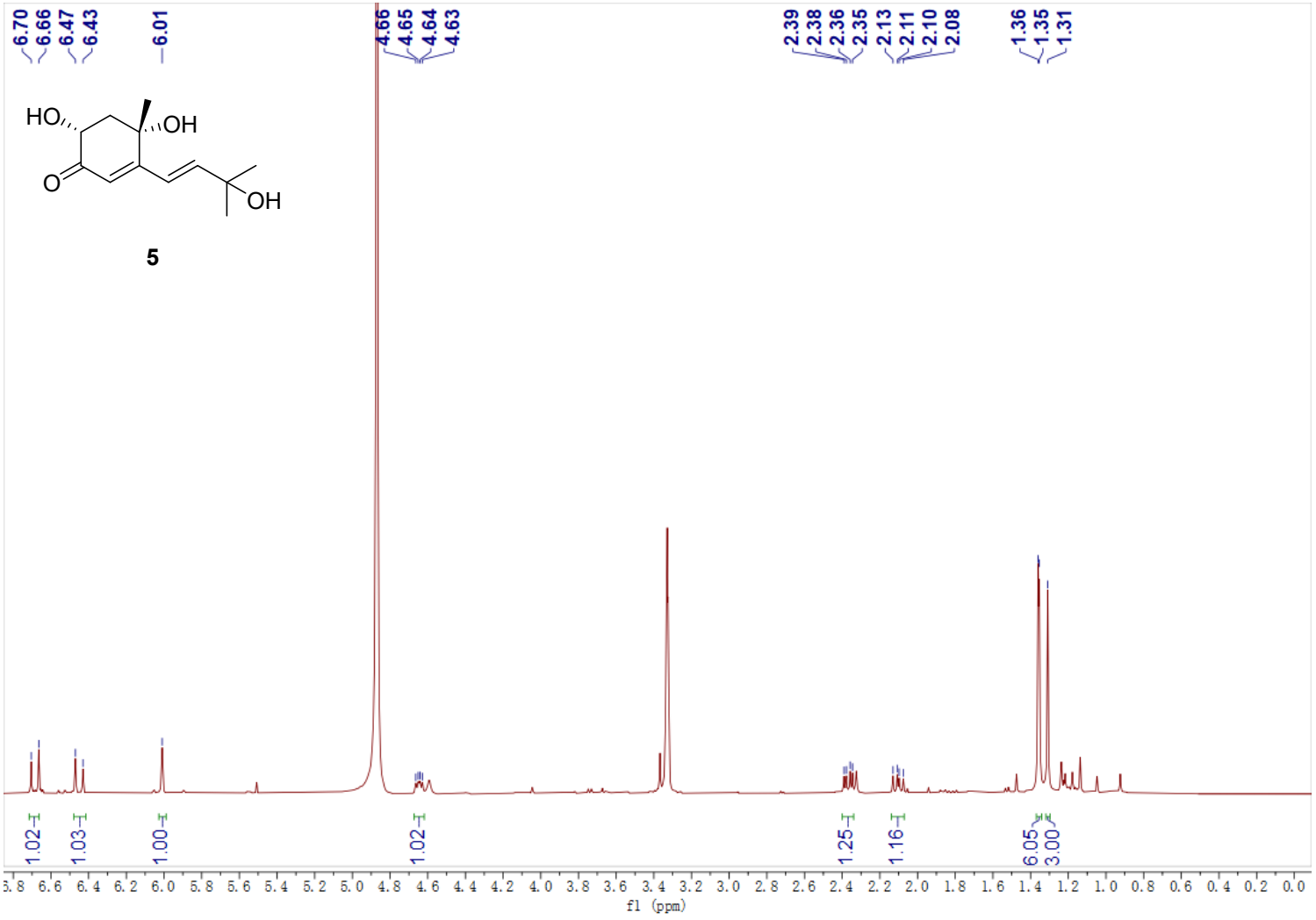


**Figure S32.** $^{13}C$ NMR spectrum of compound **5** in methanol-$d_4$ (125 MHz)

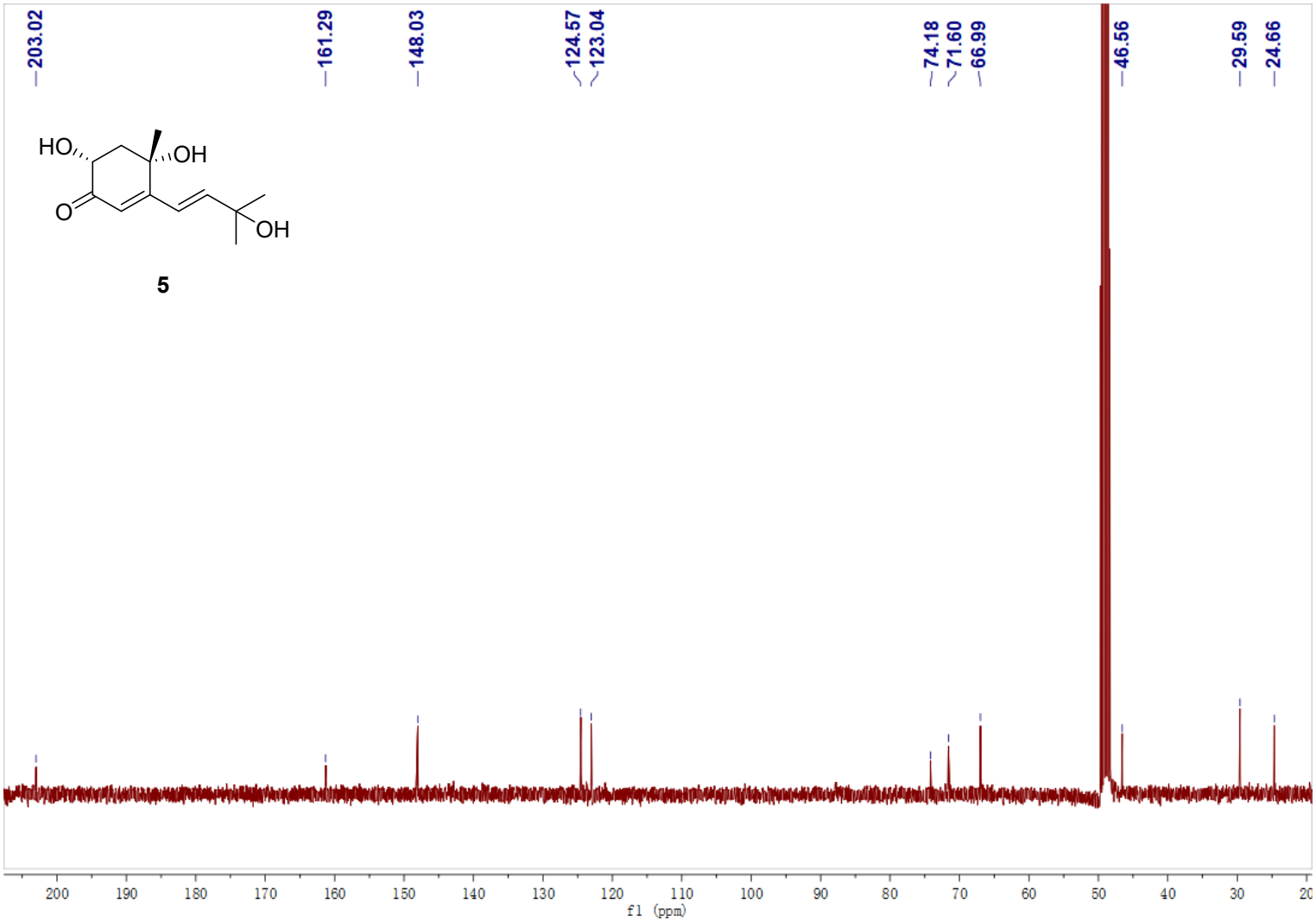


**Figure S33.** $^{1}$H NMR spectrum of compound **6** in methanol-$d_4$ (600 MHz)

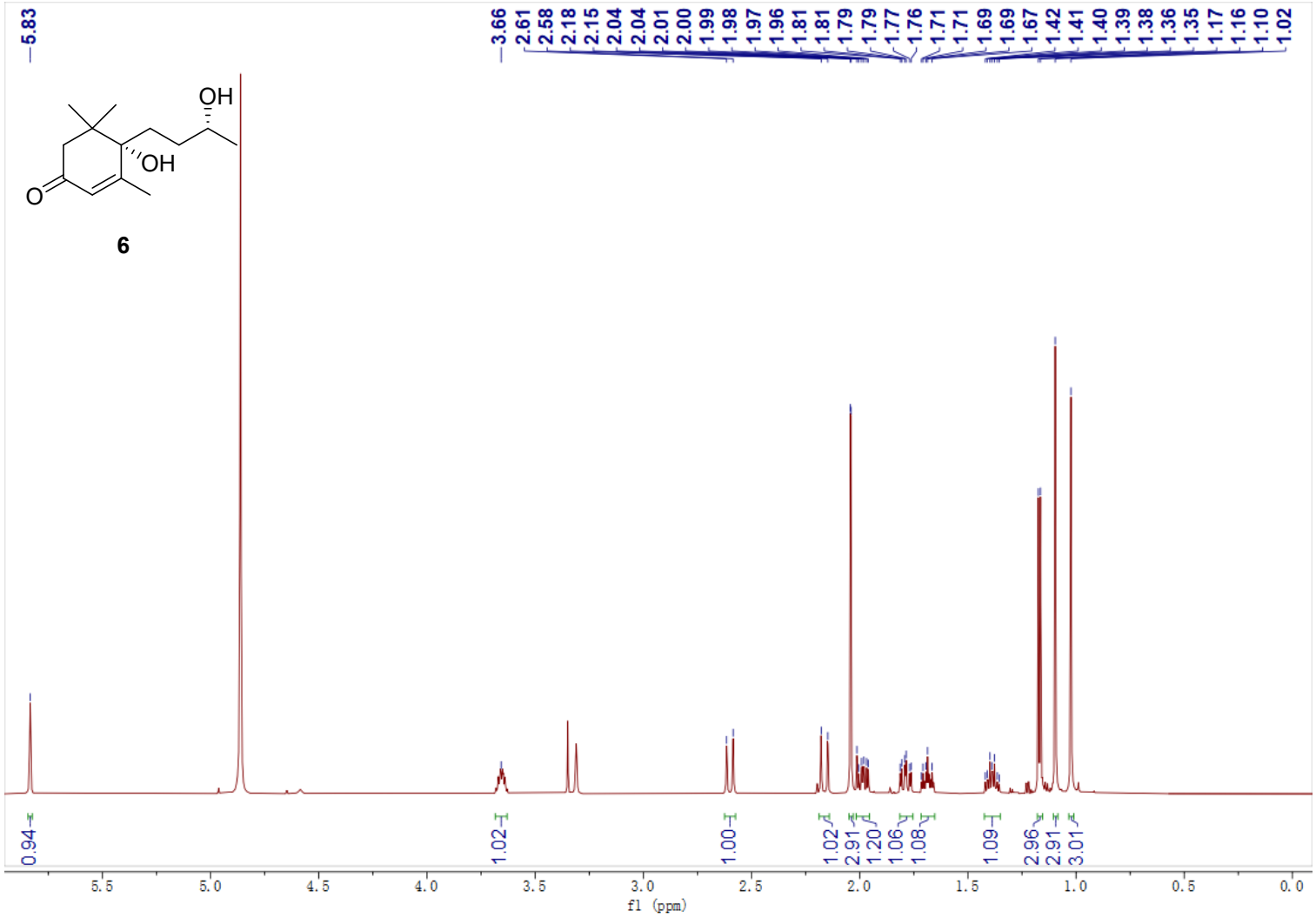


**Figure S34.** $^{13}C$ NMR spectrum of compound **6** in methanol-$d_4$ (125 MHz)

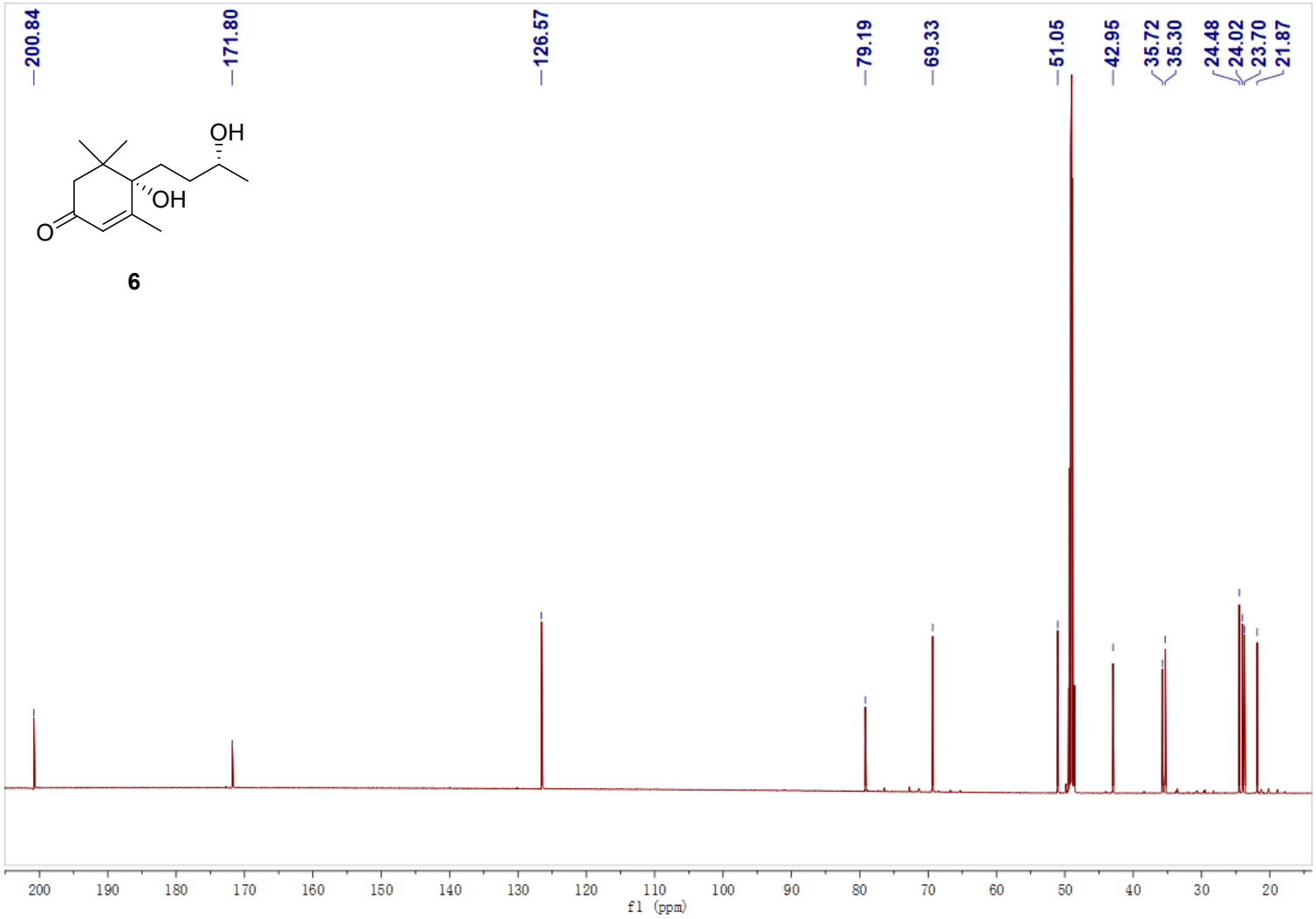


**Figure S35.** $^{1}$H NMR spectrum of compound **7** in methanol-$d_4$ (600 MHz)

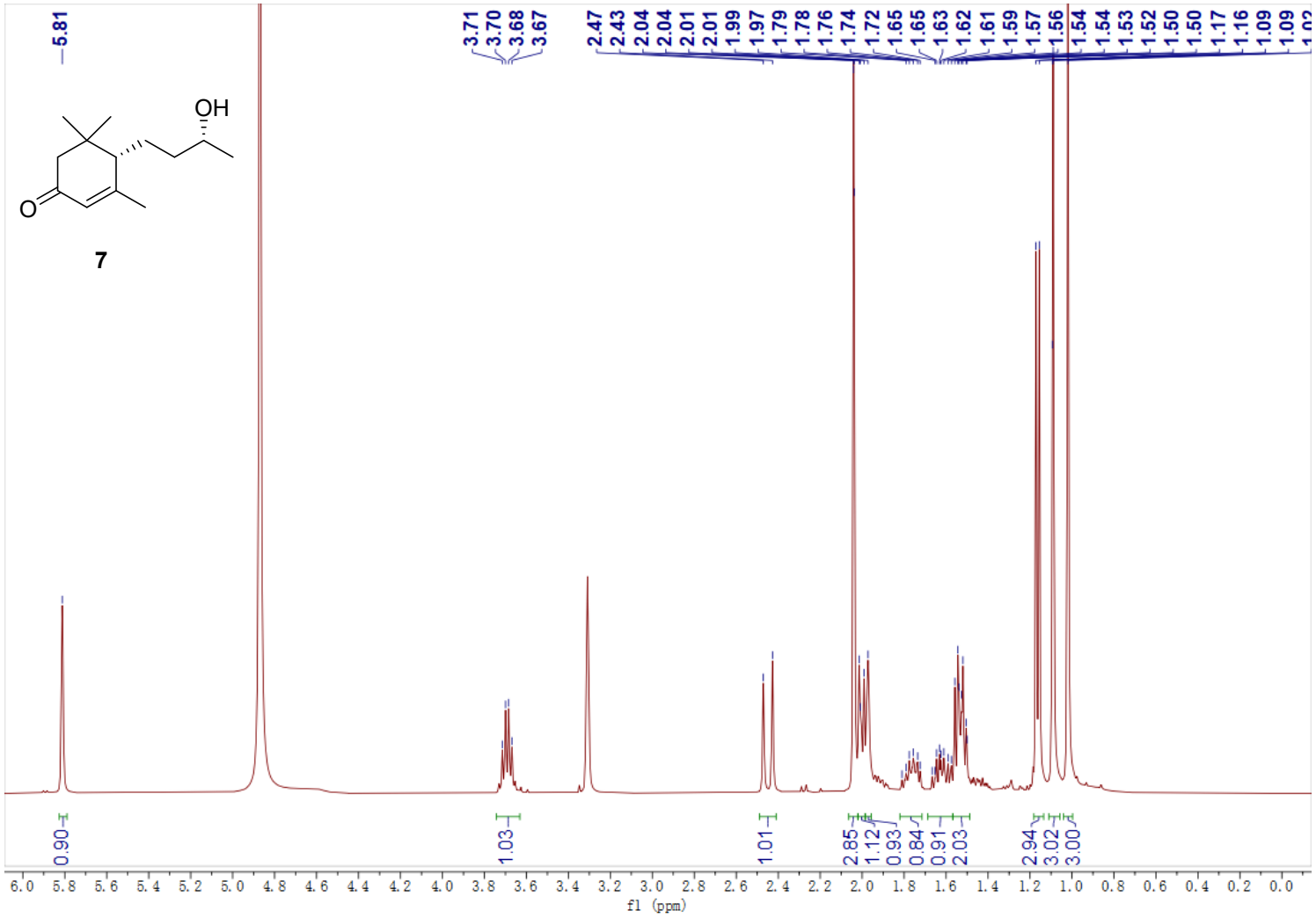


**Figure S36.** $^{13}C$ NMR spectrum of compound **7** in methanol-$d_4$ (125 MHz)

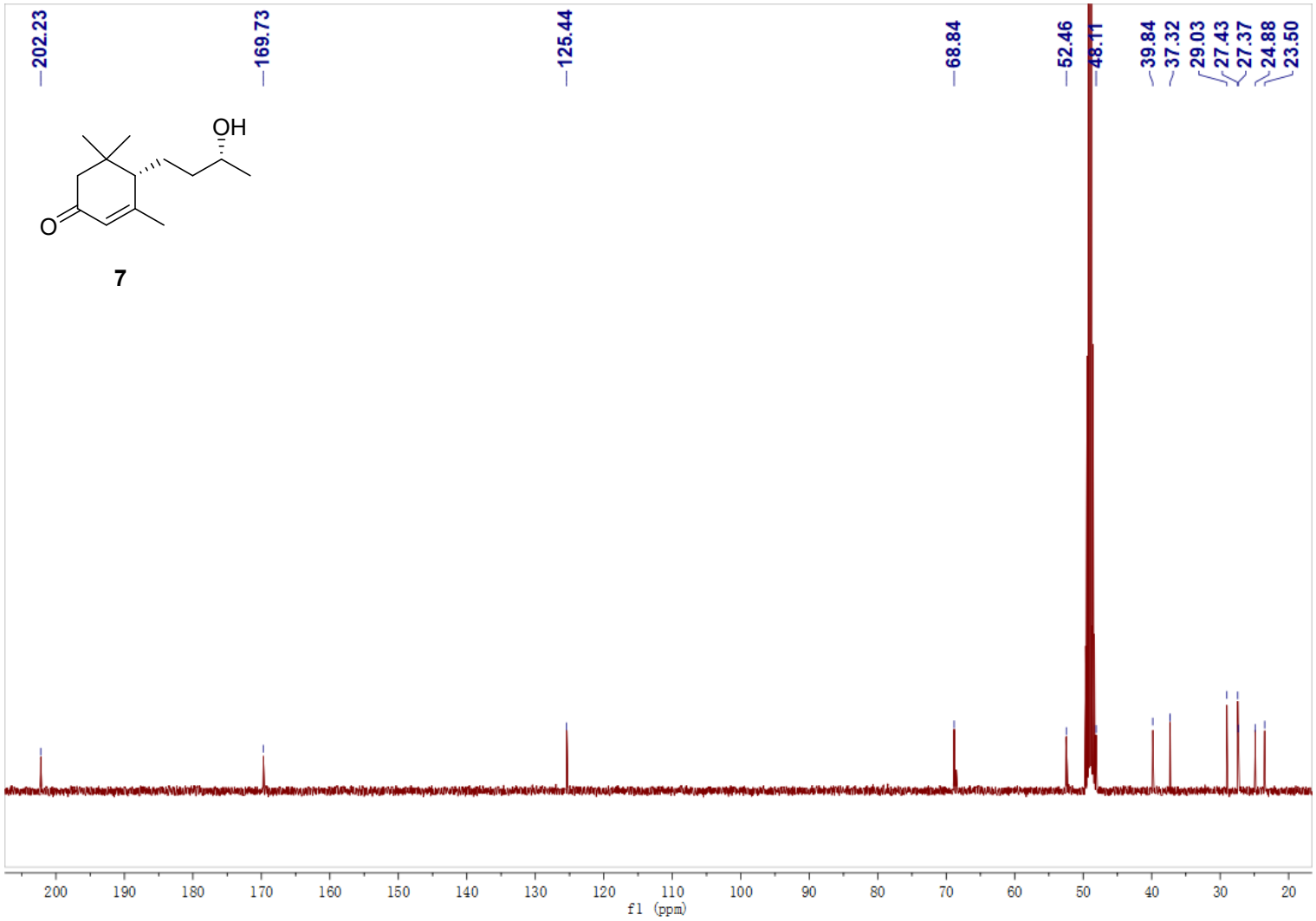


**Figure S37.** $^{1}$H NMR spectrum of compound **8** in methanol-$d_4$ (600 MHz)

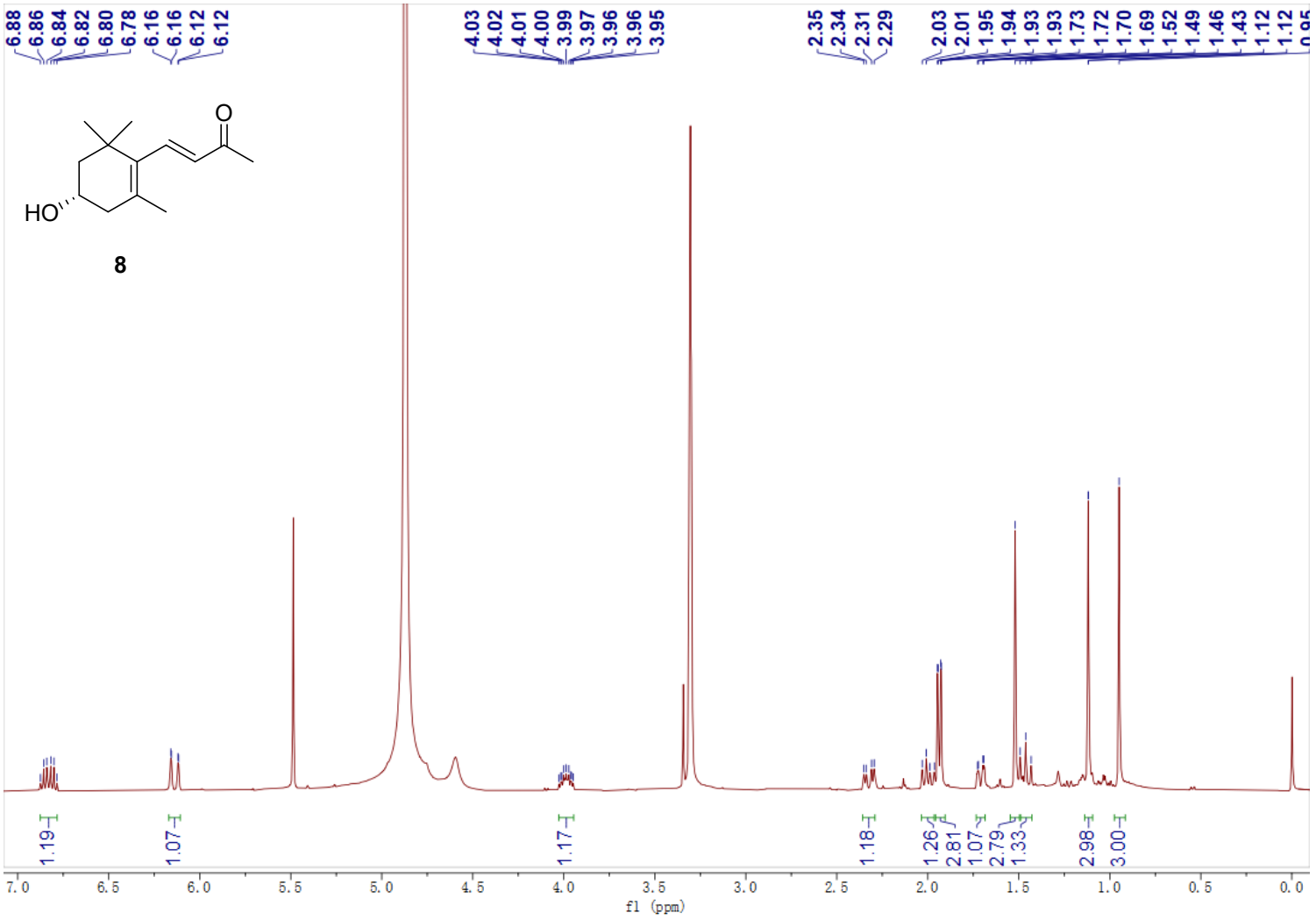


**Figure S38.** $^{13}C$ NMR spectrum of compound **8** in methanol-$d_4$ (125 MHz)

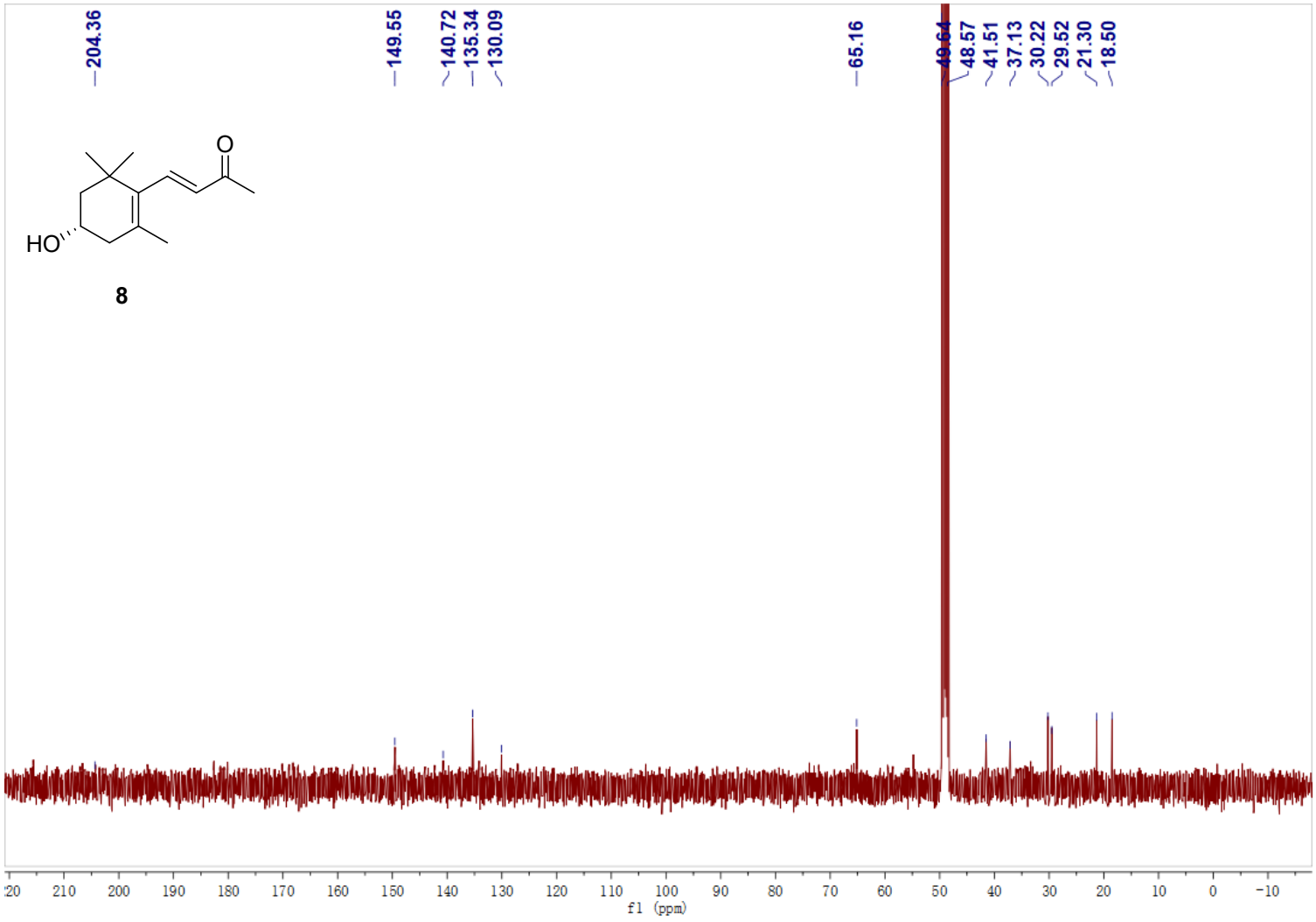


**Figure S39.** $^{1}$H NMR spectrum of compound **9** in methanol-$d_4$ (600 MHz)

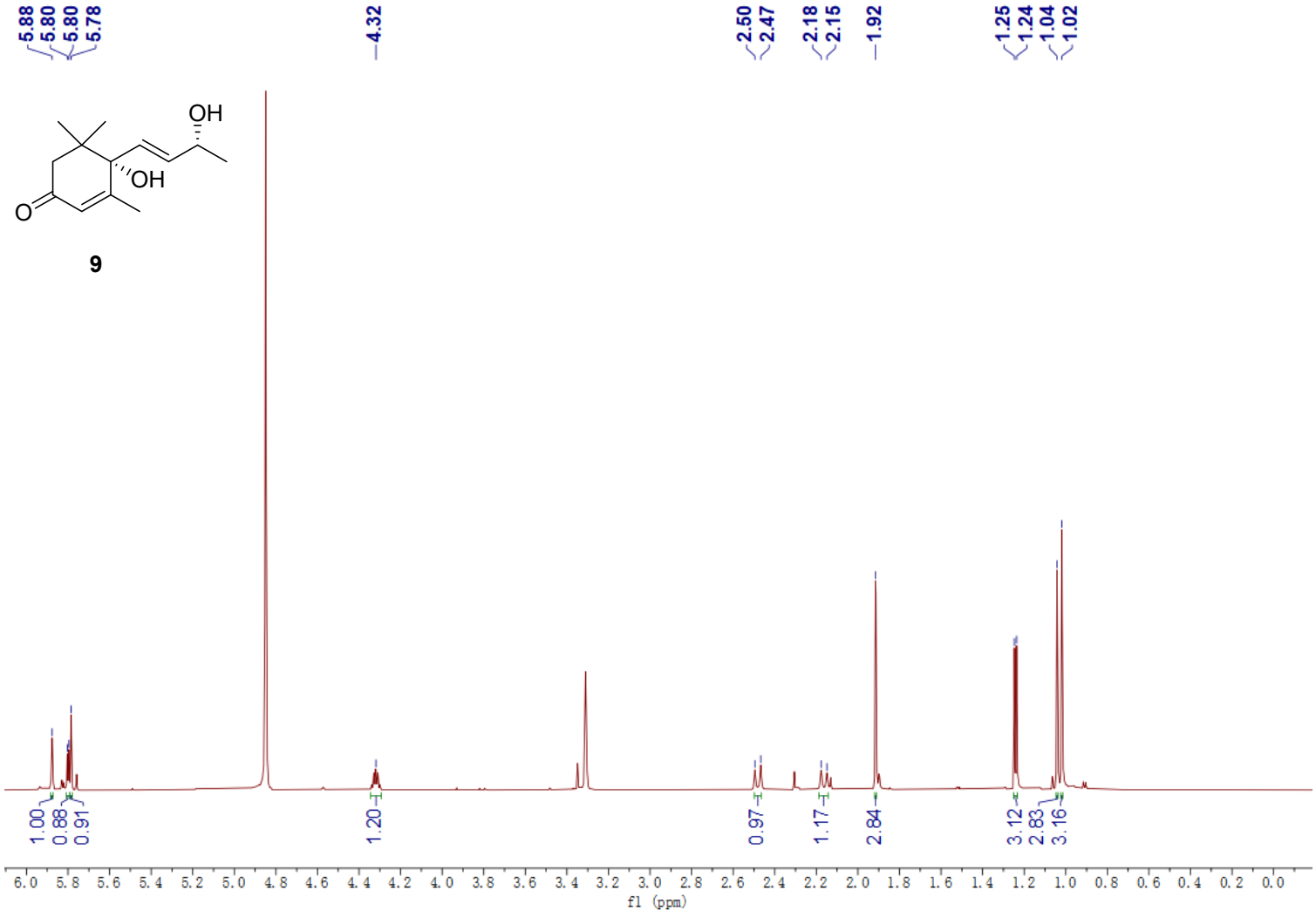


**Figure S40.** $^{13}C$ NMR spectrum of compound **9** in methanol-$d_4$ (125 MHz)

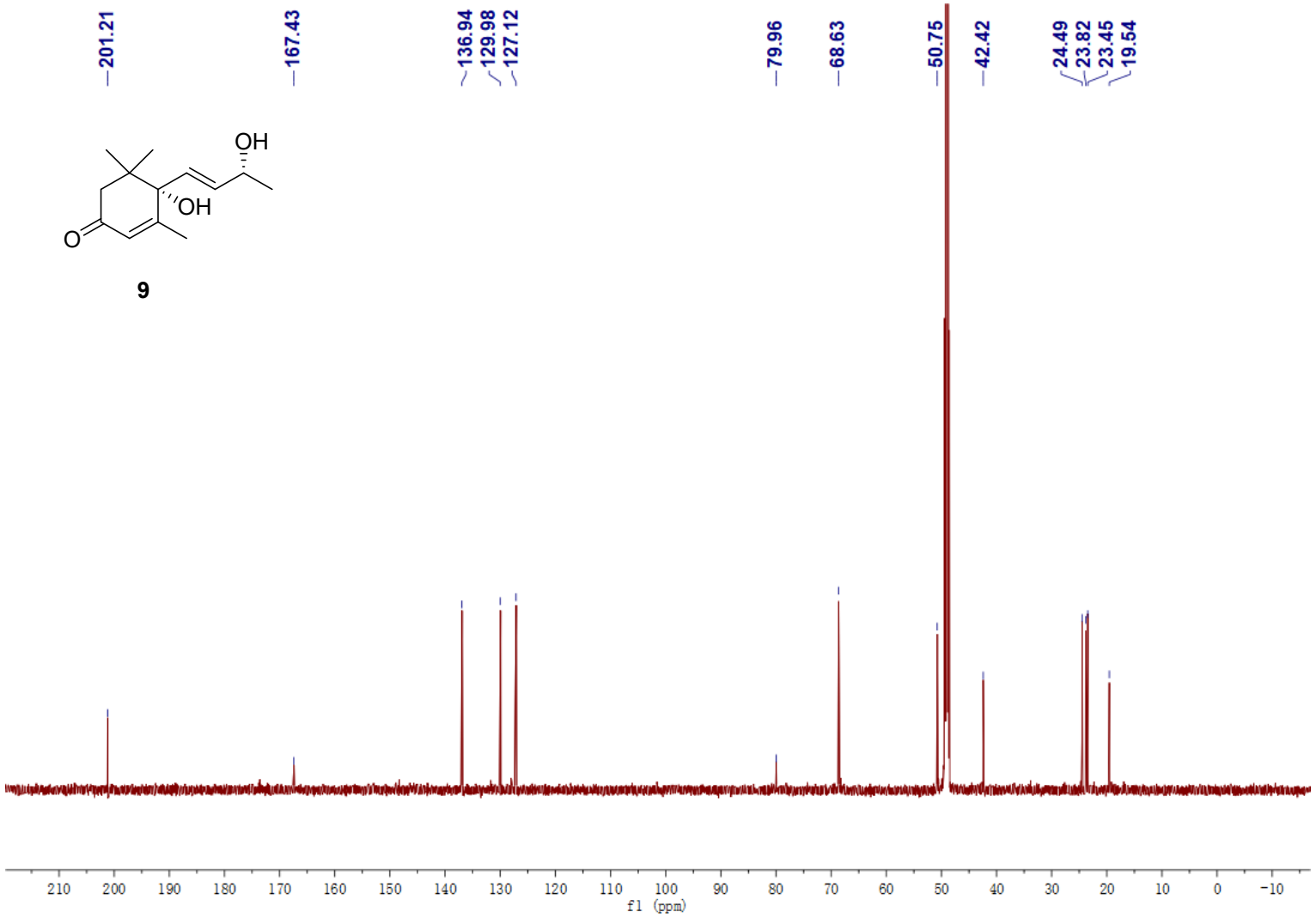


**Figure S41.** $^{1}$H NMR spectrum of compound **10** in methanol-$d_4$ (600 MHz)

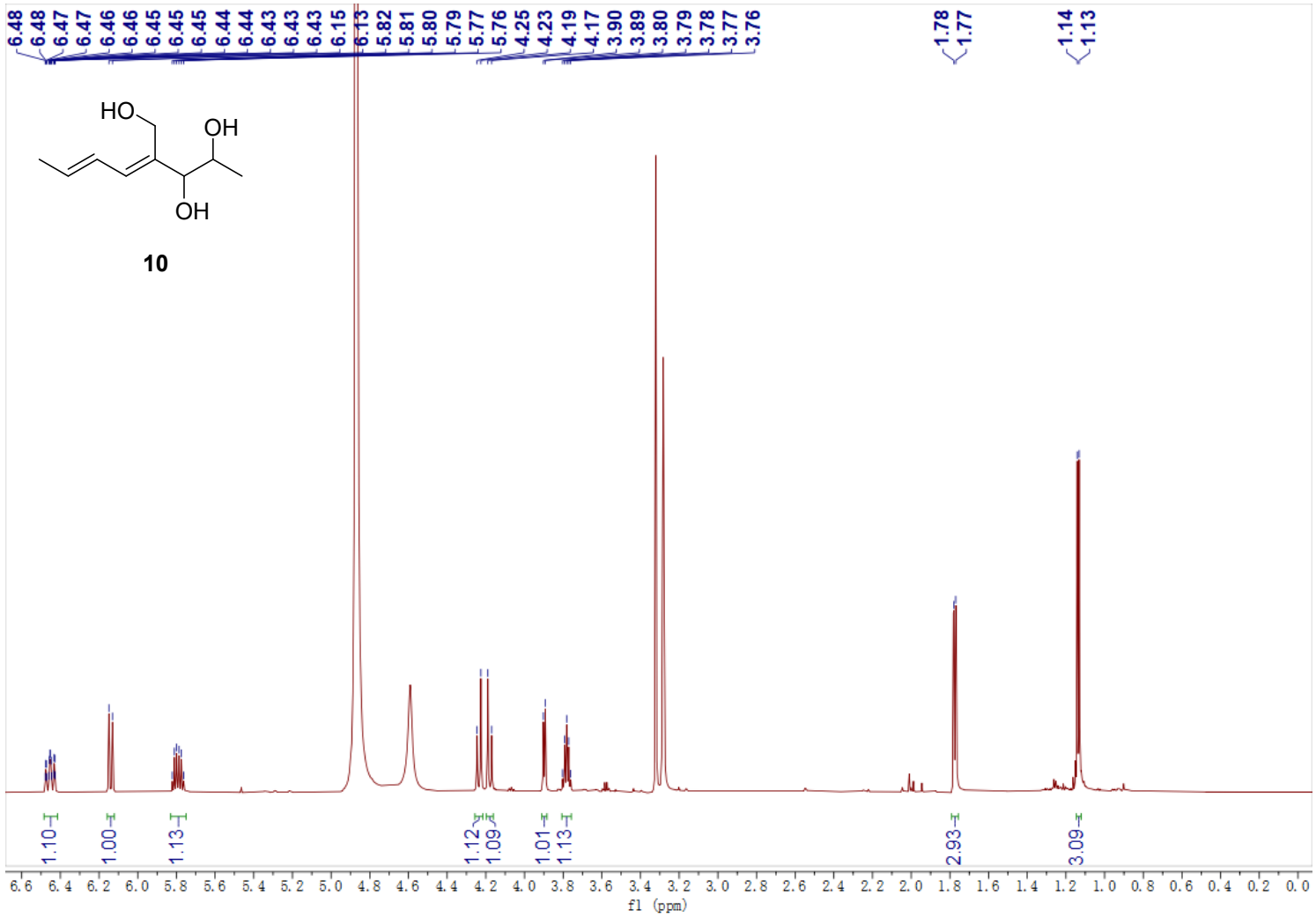


**Figure S42.** $^{13}$C NMR spectrum of compound **10** in methanol-$d_4$ (125 MHz)

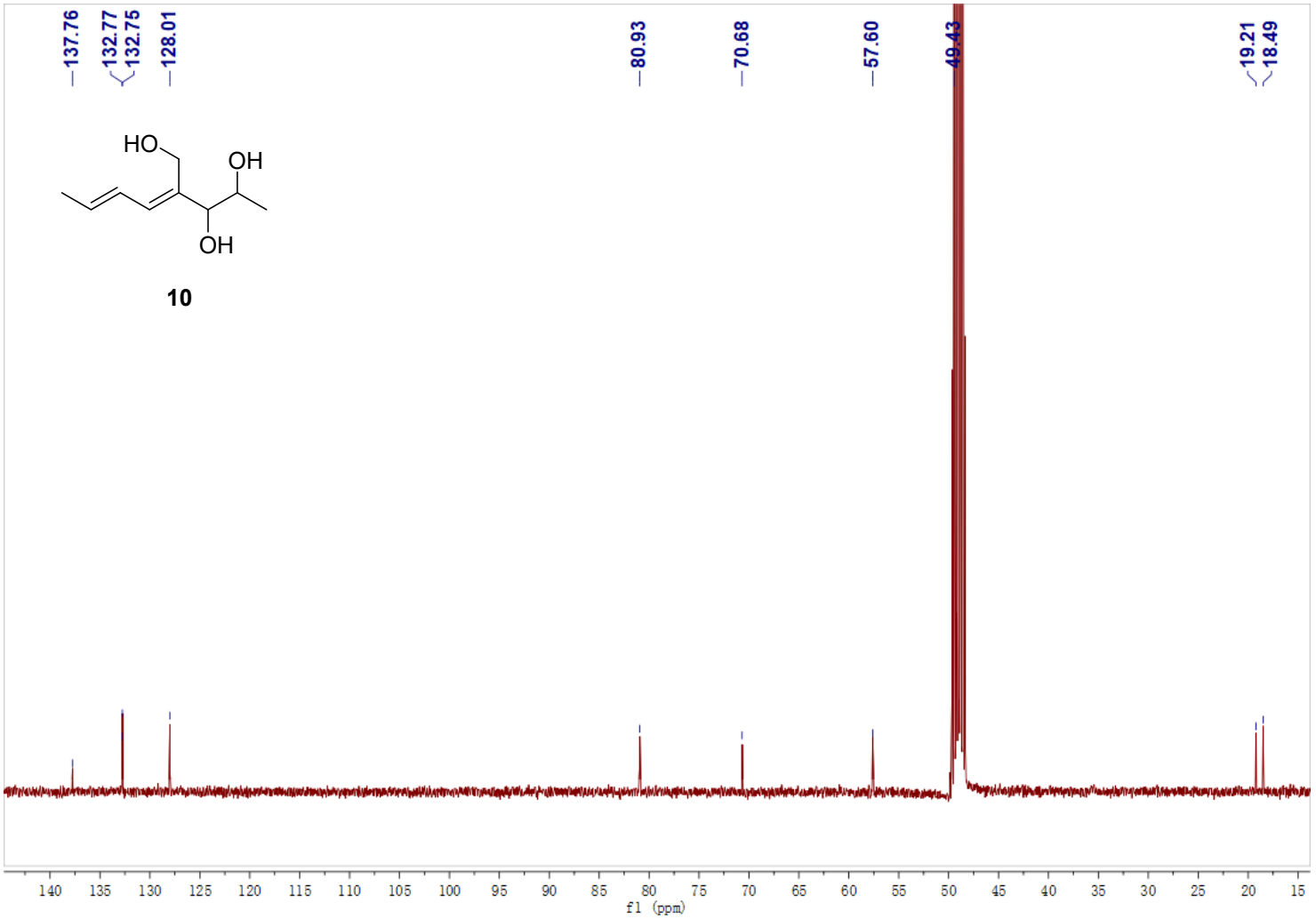


**Figure S43.** $^{1}$H NMR spectrum of compound **11** in methanol-$d_4$ (600 MHz)

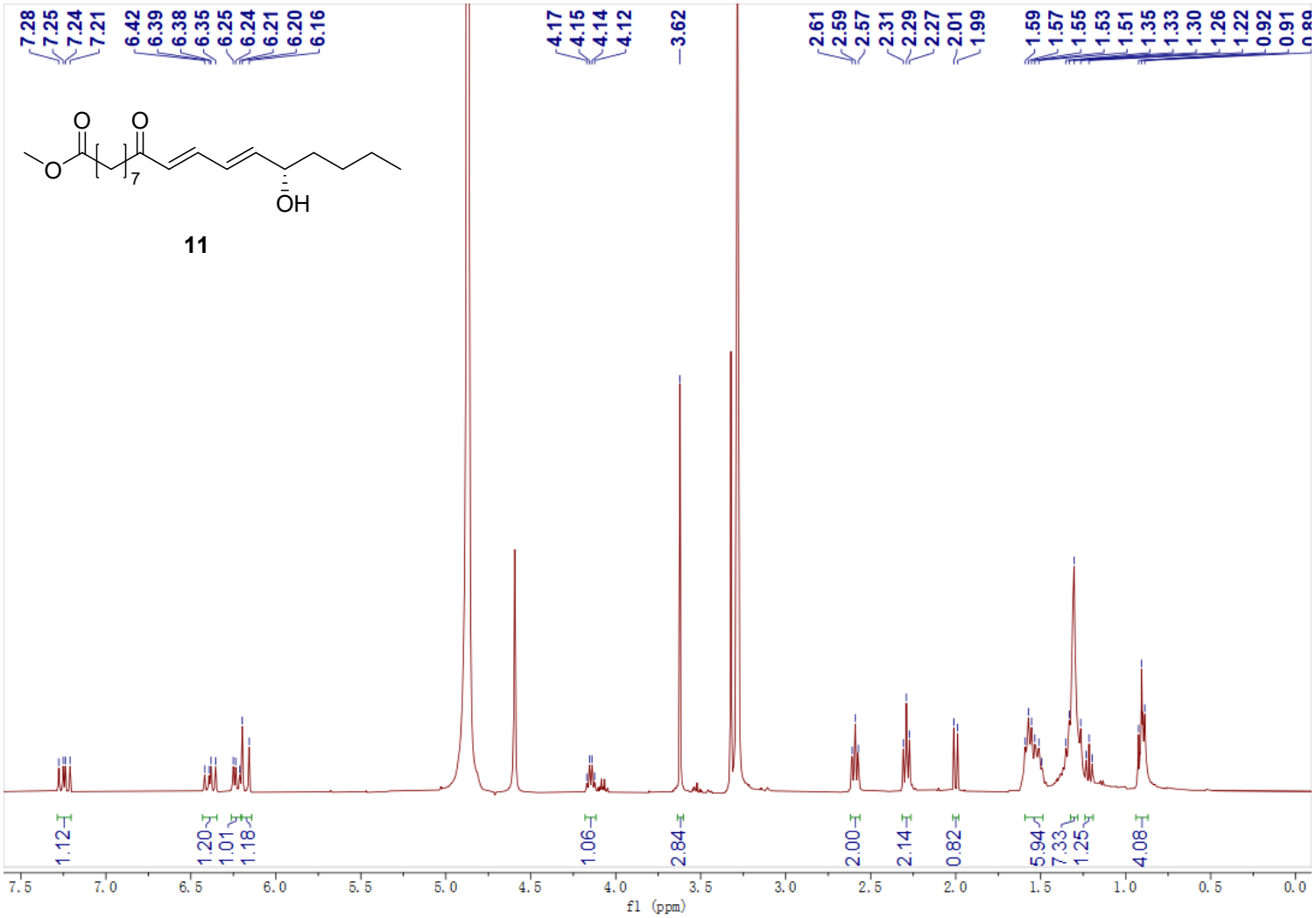


**Figure S44.** $^{13}$C NMR spectrum of compound **11** in methanol-$d_4$ (125 MHz)

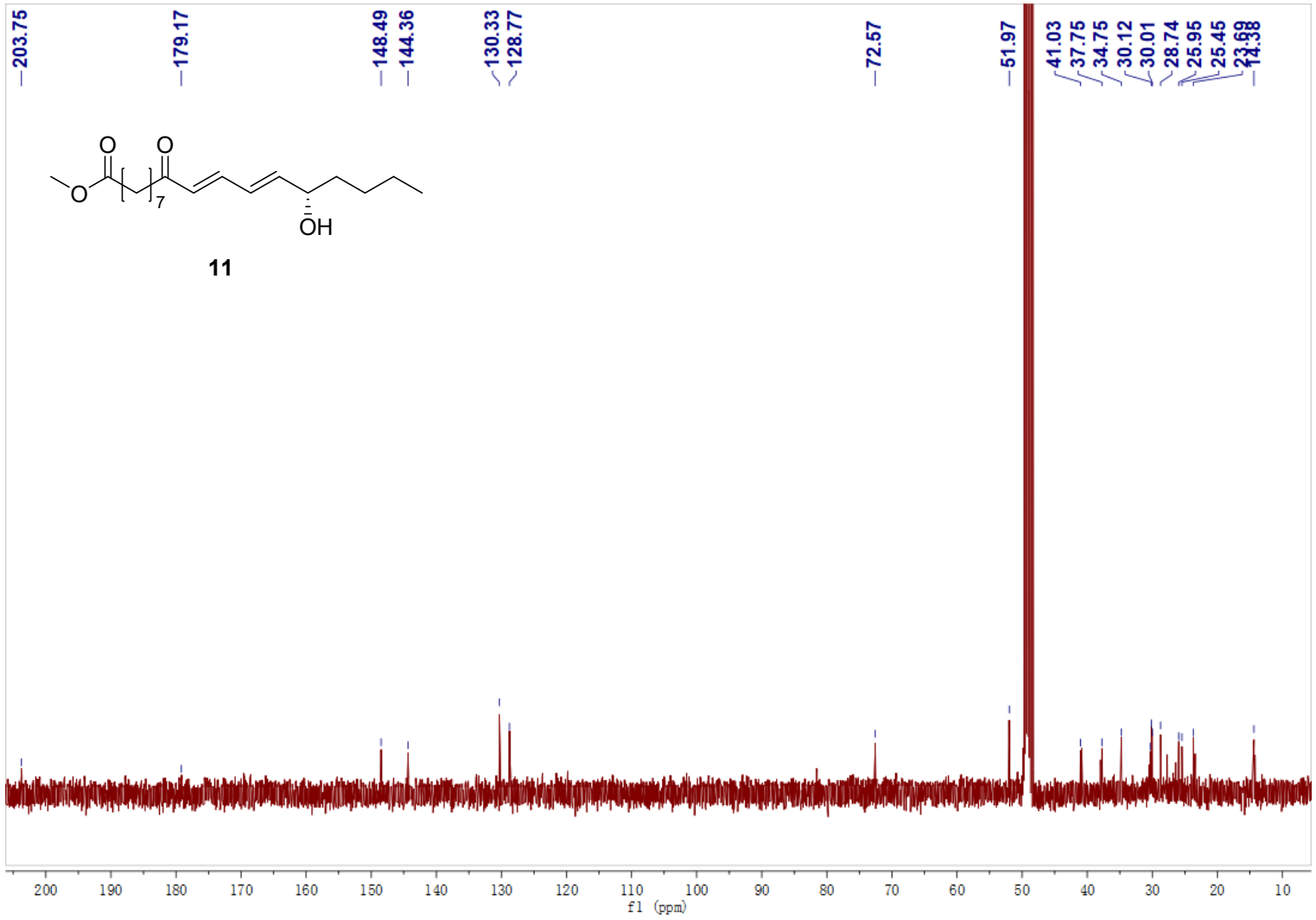


**Figure S45.** $^{1}$H NMR spectrum of compound **12** in methanol-$d_4$ (600 MHz)

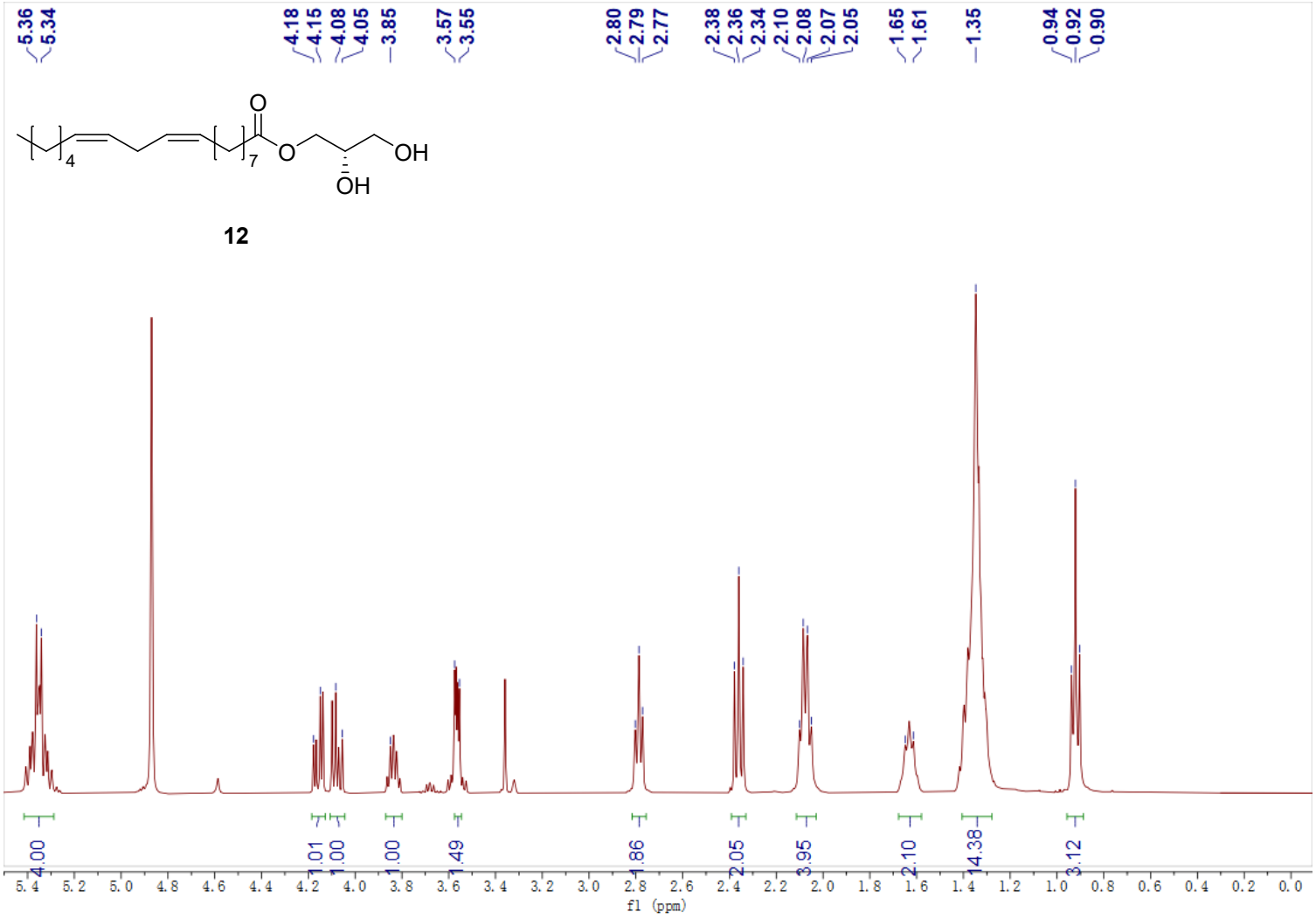


**Figure S46.** $^{13}C$ NMR spectrum of compound **12** in methanol-$d_4$ (125 MHz)

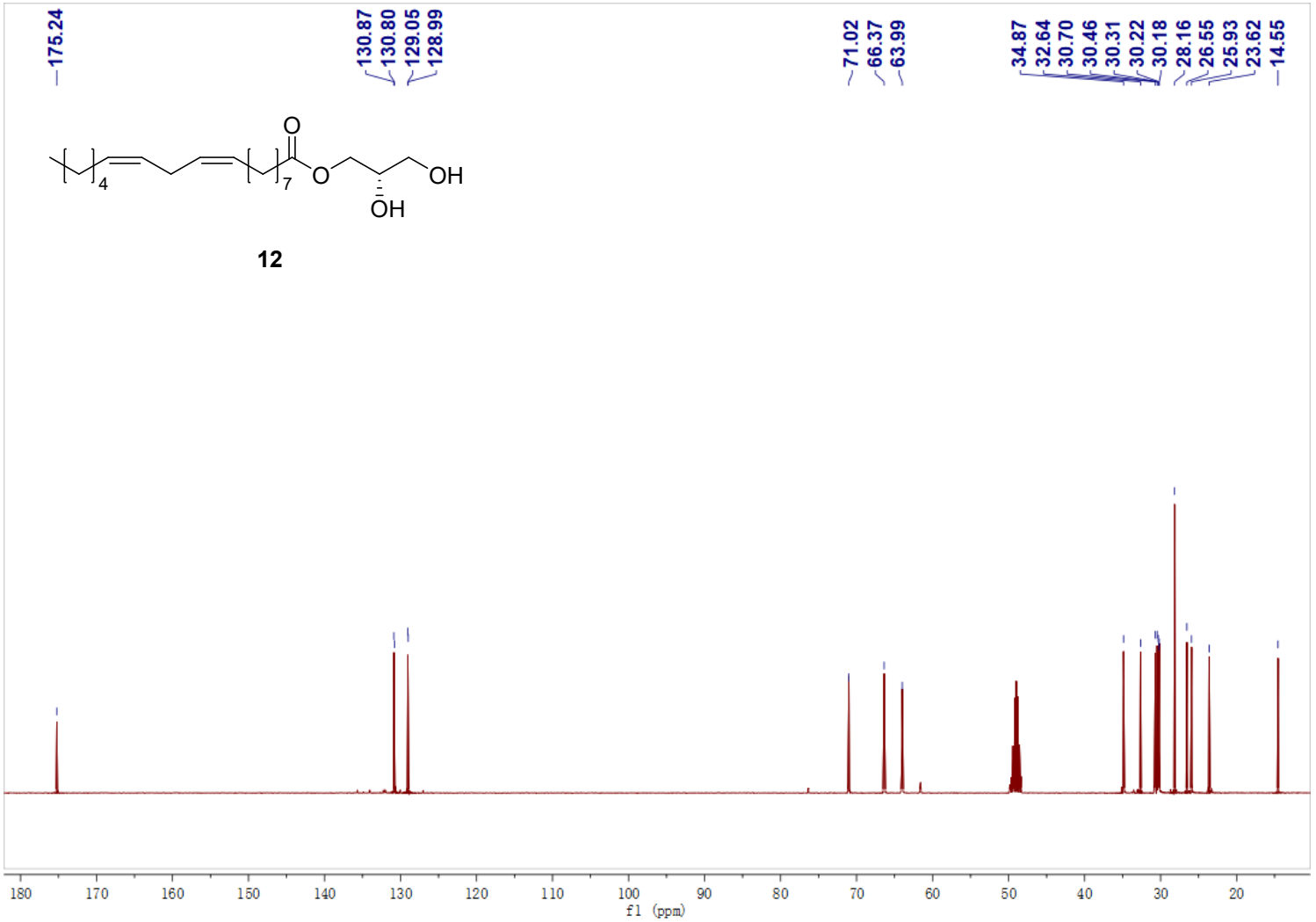


**Figure S47.** [1]H NMR spectrum of compound **13** in methanol-$d_4$ (600 MHz)

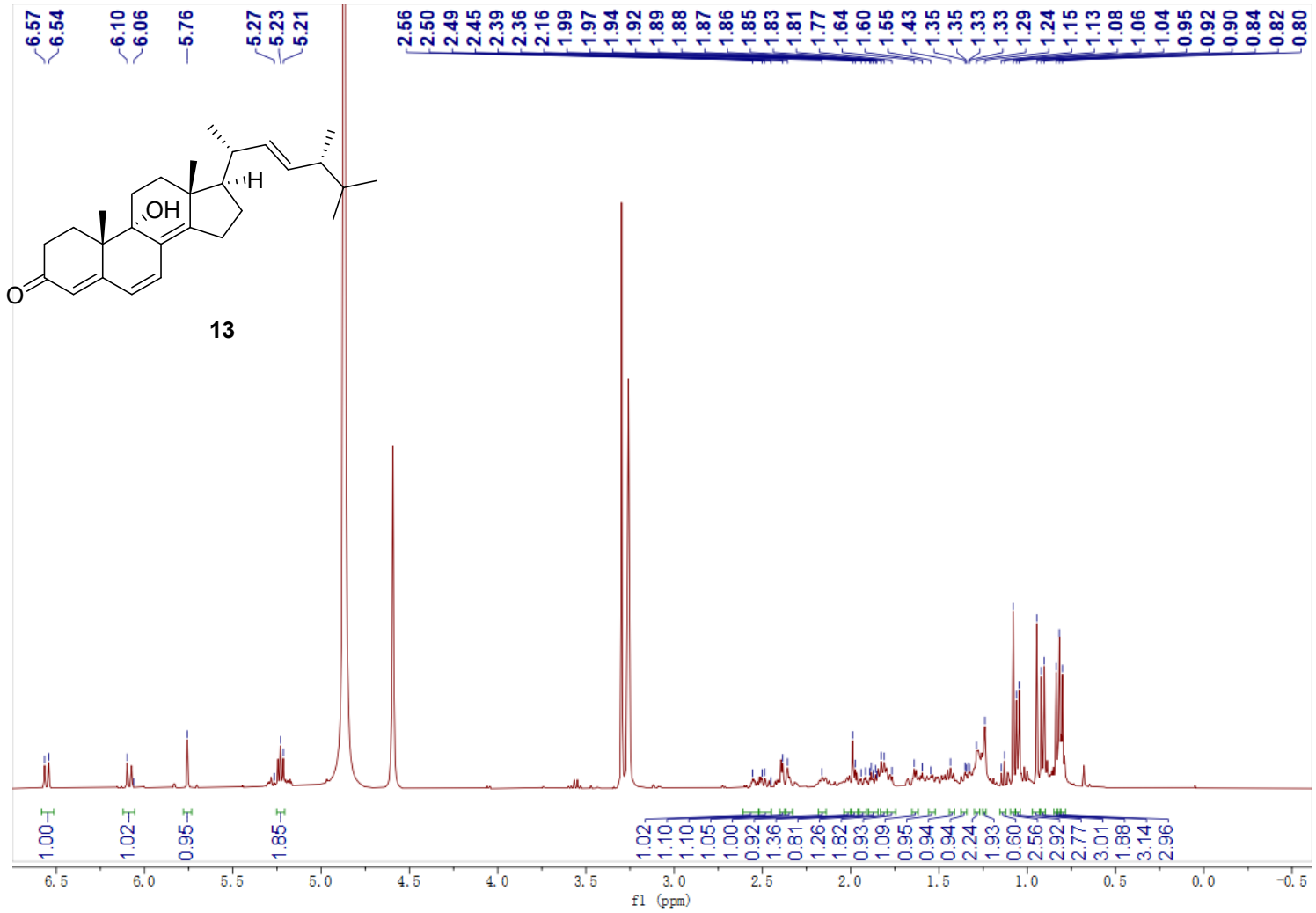


**Figure S48.** $^{13}$C NMR spectrum of compound **13** in methanol-$d_4$ (125 MHz)