# Supporting Information

## Terpenoids from the Soft Coral *Sinularia* sp. Collected in Yongxing Island

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# Experimental section

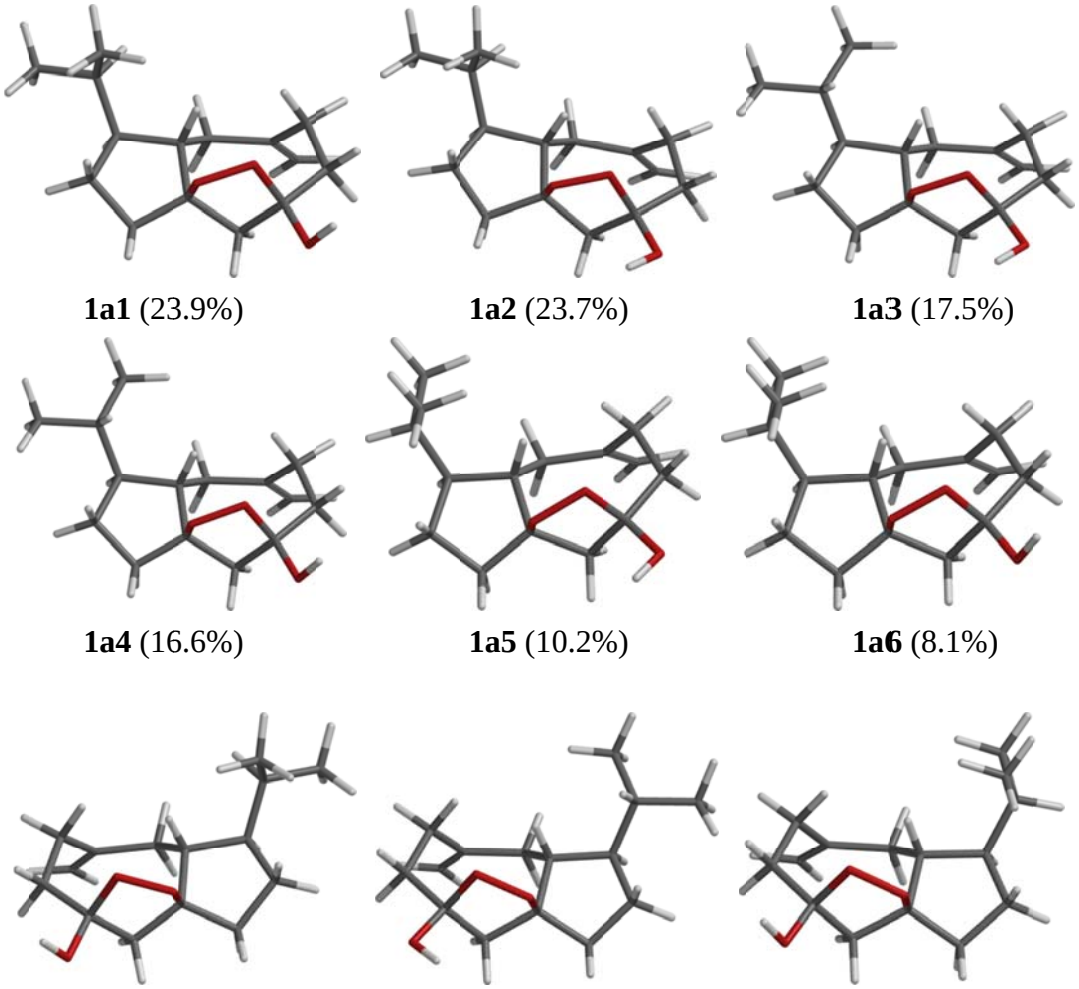
## 1. Animal material.

All collections of the soft coral *Sinularia* sp. were carried out in Yongxing Island of South China Sea in November 2012 and were frozen immediately. The specimen was identified by Dr. Leen van Ofwegen (Nationaal Natuurhistorisch Museum, Leiden, The Netherlands). The voucher specimen (No. XS-2012-04) was deposited at State Key Laboratory of Marine Drugs, Ocean University of China, P. R. China.

! sp.

# Computational details

## 1. Stable conformers of compounds of (1-3)



**1a1** (23.9%) **1a2** (23.7%) **1a3** (17.5%)

**1a4** (16.6%) **1a5** (10.2%) **1a6** (8.1%)

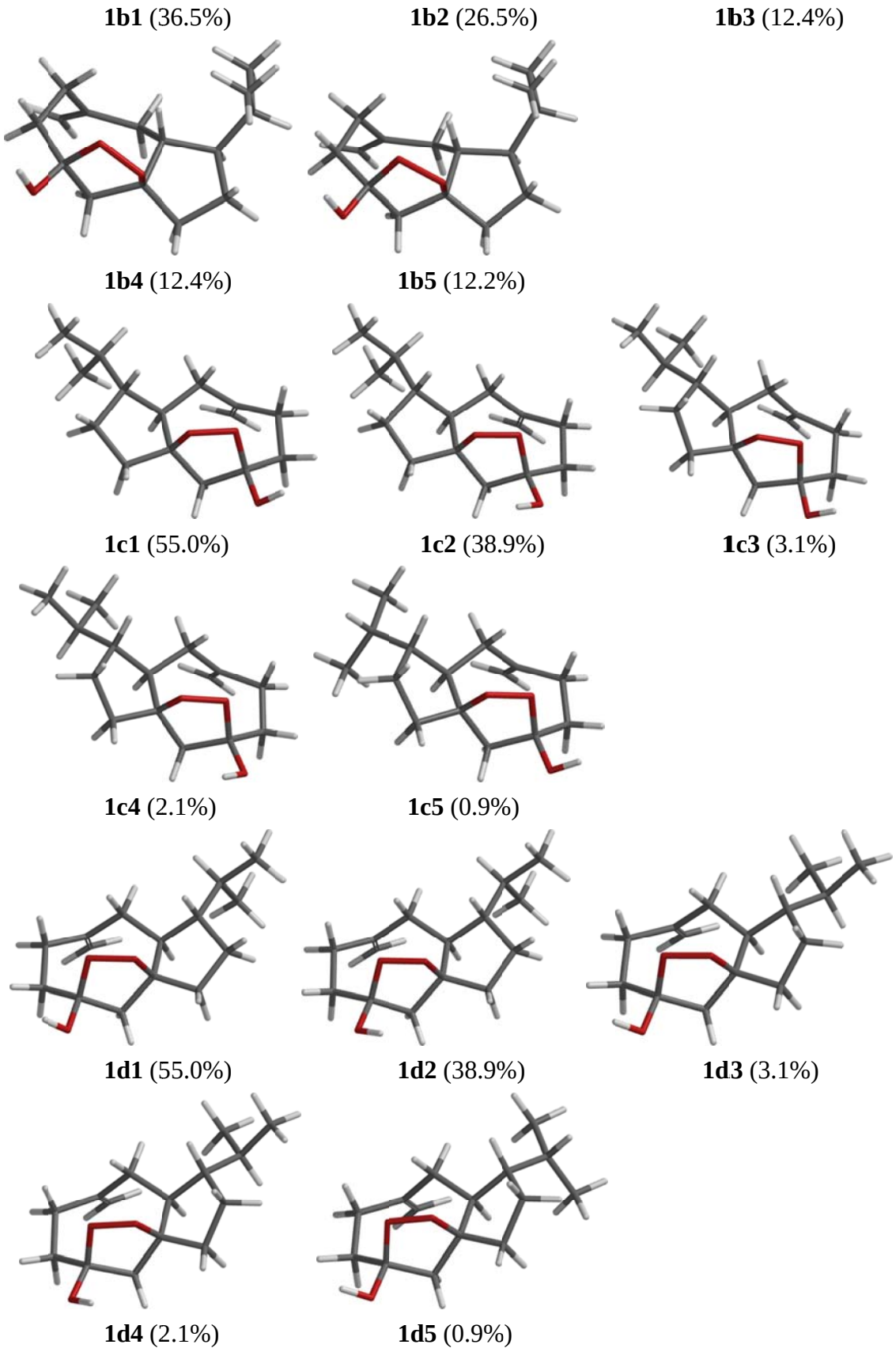
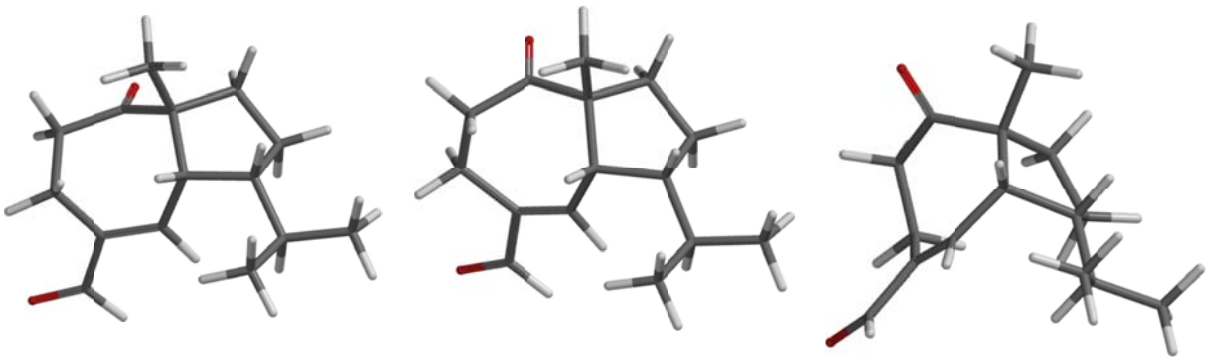
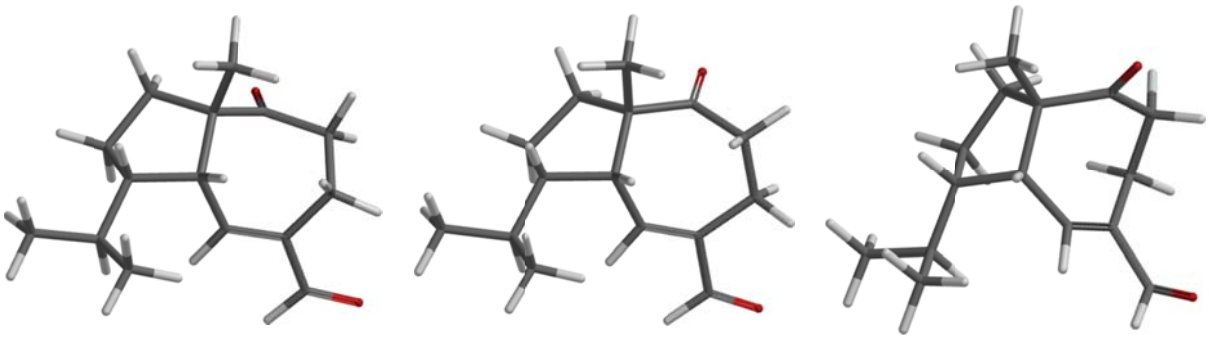


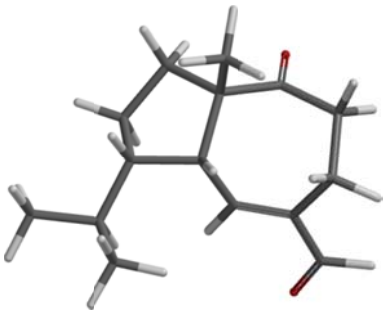

**Figure S1.** Stable conformers of compound **1** with **1a**, **1b**, **1c** and **1d** configurations, respectively.



**2a1** (59.5%) **2a2** (38.8%) **2a3** (1.6%)

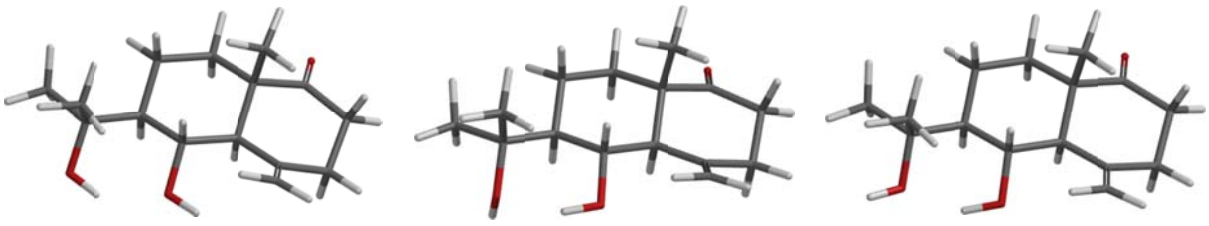


**2b1** (58.8%) **2b2** (38.5%) **2b3** (1.6%)

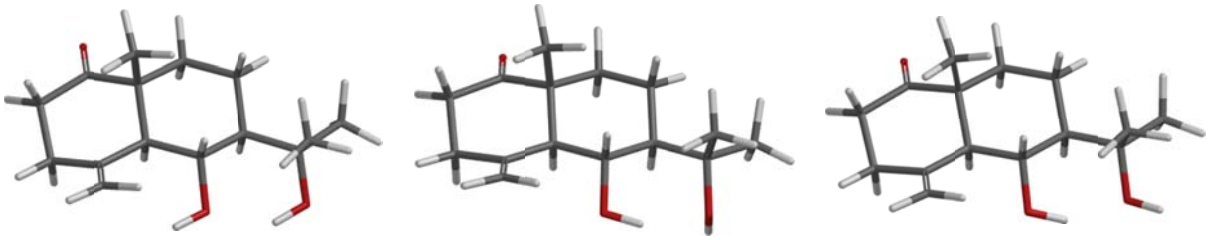


**2b4** (1.1%)

**Figure S2.** Stable conformers of compound **2** with 3*R*9*R*10*R* (**2a**) and 3*S*9*S*10*S* (**2b**) configurations, respectively.



**3a1** (51.1%) **3a2** (29.2%) **3a3** (19.7%)



**3b1** (51.1%) **3b2** (29.2%) **3b3** (19.7%)

**Figure S3.** Stable conformers of compound **3** with 5*R*6*S*7*S*10*S* (**3a**) and 5*S*3*R*9*R*10*R* (**3b**) configurations, respectively.

## 2. $^{13}$C NMR calculations details to support the assigned carbon and relative configuration of 1

**Table S1**. Important thermodynamic parameters (a.u.) of the optimized compound **1** with **1a**, **1b**, **1c** and **1d** at B3LYP/DGDZVP level in the gas phase.

| conformations | E+ZPE | G | conformations | E+ZPE | G |
|---|---|---|---|---|---|
| **1a1** | -811.279900 | -811.323160 | **1b1** | -811.279901 | -811.323163 |
| **1a2** | -811.279831 | -811.323152 | **1b2** | -811.280189 | -811.322862 |
| **1a3** | -811.280190 | -811.322864 | **1b3** | -811.278429 | -811.322143 |
| **1a4** | -811.280202 | -811.322817 | **1b4** | -811.278429 | -811.322142 |
| **1a5** | -811.278427 | -811.322358 | **1b5** | -811.278429 | -811.322133 |
| **1a6** | -811.278429 | -811.322145 | | | |
| **1c1** | -811.280859 | -811.324337 | **1d1** | -811.280859 | -811.324337 |
| **1c2** | -811.280504 | -811.324011 | **1d2** | -811.280504 | -811.324011 |
| **1c3** | -811.278638 | -811.321634 | **1d3** | -811.278638 | -811.321634 |
| **1c4** | -811.278212 | -811.321239 | **1d4** | -811.278212 | -811.321239 |
| **1c5** | -811.277544 | -811.320458 | **1d5** | -811.277544 | -811.320458 |

**Table S2**. Optimized Z-Matrixes of compound **1** in the Gas Phase (Å) at B3LYP/6-31G(d,p) level.

| **1a1** | | | | **1a2** | | | | **1a3** | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | 0.130217 | -0.891599 | -0.653646 | C | 0.128344 | -0.875207 | -0.668463 | C | -0.181202 | -1.028416 | 0.522675 |
| C | -0.605926 | 0.362887 | -0.083345 | C | -0.603844 | 0.372596 | -0.082932 | C | 0.626918 | 0.242758 | 0.110097 |
| C | 1.582973 | -0.728653 | -1.096476 | C | 1.58475 | -0.71988 | -1.091258 | C | -1.632326 | -0.852845 | 0.956419 |
| C | 2.361087 | -0.870219 | 0.225693 | C | 2.361483 | -0.874924 | 0.241528 | C | -2.397861 | -0.775145 | -0.38745 |
| C | 2.975563 | 0.411157 | 0.809325 | C | 2.982739 | 0.400104 | 0.81795 | C | -2.932552 | 0.6049 | -0.779702 |
| C | 2.011105 | 1.58797 | 1.086312 | C | 2.019227 | 1.576976 | 1.090164 | C | -1.905882 | 1.757706 | -0.846589 |
| C | 1.33867 | 2.161693 | -0.152533 | C | 1.349149 | 2.160002 | -0.145994 | C | -1.221625 | 2.096587 | 0.471136 |
| C | -0.08715 | 1.750902 | -0.509912 | C | -0.08129 | 1.762539 | -0.498839 | C | 0.182151 | 1.569753 | 0.759191 |
| C | 1.984735 | 3.054257 | -0.912455 | C | 1.999602 | 3.048642 | -0.90685 | C | -1.832017 | 2.8899 | 1.359716 |
| C | -2.107066 | 0.185599 | -0.490841 | C | -2.106449 | 0.202554 | -0.48869 | C | 2.12743 | -0.087345 | 0.433095 |
| C | -2.221297 | -1.258735 | -1.030459 | C | -2.223036 | -1.230911 | -1.056585 | C | 2.135971 | -1.571199 | 0.878841 |
| C | -0.844573 | -1.517857 | -1.65536 | C | -0.845422 | -1.481574 | -1.683293 | C | 0.740098 | -1.806906 | 1.462023 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -3.118537 | 0.591478 | 0.609259 | C | -3.113534 | 0.585567 | 0.623553 | C | 3.114911 | 0.203893 | -0.721332 |
| C | -3.132219 | -0.352583 | 1.822937 | C | -3.121268 | -0.382743 | 1.818013 | C | 4.550734 | -0.19945 | -0.347858 |
| C | -4.53622 | 0.749688 | 0.036947 | C | -4.533529 | 0.754737 | 0.060272 | C | 3.091602 | 1.670876 | -1.177078 |
| H | -0.515982 | 0.28688 | 1.002883 | H | -0.510479 | 0.286734 | 1.002097 | H | 0.509135 | 0.330416 | -0.973243 |
| O | 0.277989 | -1.868389 | 0.409436 | O | 0.268625 | -1.870587 | 0.381096 | O | -0.363733 | -1.867602 | -0.648593 |
| O | 1.381519 | -1.304078 | 1.188271 | O | 1.361811 | -1.318955 | 1.186183 | O | -1.414476 | -1.149975 | -1.378629 |
| O | 3.352236 | -1.850042 | 0.022746 | O | 3.40948 | -1.80912 | 0.150352 | O | -3.503526 | -1.644374 | -0.433326 |
| H | 1.870105 | -1.567062 | -1.735551 | H | 1.865057 | -1.546213 | -1.752481 | H | -1.963016 | -1.749159 | 1.491176 |
| H | 1.795159 | 0.203689 | -1.618206 | H | 1.815656 | 0.214015 | -1.602381 | H | -1.820671 | 0.009148 | 1.594662 |
| H | 3.465667 | 0.140399 | 1.75479 | H | 3.472352 | 0.115749 | 1.755437 | H | -3.407331 | 0.49314 | -1.760321 |
| H | 3.76476 | 0.733803 | 0.122173 | H | 3.772581 | 0.71791 | 0.129192 | H | -3.727041 | 0.85571 | -0.068815 |
| H | 2.603418 | 2.37912 | 1.558803 | H | 2.612871 | 2.364305 | 1.56702 | H | -2.451837 | 2.642686 | -1.190709 |
| H | 1.268845 | 1.269232 | 1.823218 | H | 1.274443 | 1.259962 | 1.825596 | H | -1.168479 | 1.528922 | -1.621203 |
| H | -0.763981 | 2.481892 | -0.04185 | H | -0.75158 | 2.491517 | -0.018433 | H | 0.893148 | 2.334904 | 0.419638 |
| H | -0.225872 | 1.882885 | -1.590636 | H | -0.226466 | 1.906351 | -1.577228 | H | 0.320383 | 1.513732 | 1.846888 |
| H | 1.544475 | 3.462734 | -1.818401 | H | 1.55891 | 3.463275 | -1.809854 | H | -1.381431 | 3.131553 | 2.318911 |
| H | 2.976079 | 3.415567 | -0.651166 | H | 2.995092 | 3.400594 | -0.648737 | H | -2.803204 | 3.33342 | 1.15599 |
| H | -2.286412 | 0.857638 | -1.343855 | H | -2.289388 | 0.891599 | -1.327071 | H | 2.432659 | 0.526904 | 1.294726 |
| H | -3.042471 | -1.378794 | -1.743444 | H | -3.042482 | -1.335031 | -1.773962 | H | 2.935178 | -1.794109 | 1.591187 |
| H | -2.383528 | -1.969552 | -0.214425 | H | -2.389289 | -1.957108 | -0.255126 | H | 2.279302 | -2.2215 | 0.00781 |
| H | -0.615134 | -2.573214 | -1.82873 | H | -0.619838 | -2.534751 | -1.876346 | H | 0.450527 | -2.860002 | 1.530012 |
| H | -0.750423 | -0.990596 | -2.61306 | H | -0.747603 | -0.937507 | -2.631096 | H | 0.660452 | -1.371851 | 2.466191 |
| H | -2.801859 | 1.582831 | 0.968265 | H | -2.795367 | 1.569581 | 1.000662 | H | 2.799278 | -0.417459 | -1.573153 |
| H | -3.720137 | 0.083268 | 2.637594 | H | -3.702648 | 0.037905 | 2.645193 | H | 5.239567 | 0.004758 | -1.174437 |
| H | -2.12741 | -0.553799 | 2.206495 | H | -2.114526 | -0.594086 | 2.190866 | H | 4.631019 | -1.263099 | -0.106508 |
| H | -3.587823 | -1.317089 | 1.574572 | H | -3.581257 | -1.34092 | 1.5535 | H | 4.902078 | 0.369019 | 0.522404 |
| H | -5.234077 | 1.100826 | 0.804662 | H | -5.228222 | 1.090519 | 0.837614 | H | 3.801907 | 1.831164 | -1.995247 |
| H | -4.558004 | 1.469479 | -0.788837 | H | -4.558698 | 1.49081 | -0.750942 | H | 2.10575 | 1.978576 | -1.53796 |
| H | -4.919756 | -0.204608 | -0.342148 | H | -4.918646 | -0.191925 | -0.336063 | H | 3.376804 | 2.343658 | -0.358693 |
| H | 3.76225 | -2.031372 | 0.880556 | H | 3.008657 | -2.664863 | -0.05996 | H | -3.158392 | -2.545318 | -0.354014 |
| **1a4** | | | | **1a5** | | | | **1a6** | | | |
| C | -0.181962 | -1.038321 | 0.510164 | C | -0.137875 | -0.967705 | 0.675118 | C | -0.142915 | -0.982156 | 0.660364 |
| C | 0.628287 | 0.236769 | 0.108507 | C | 0.700971 | 0.269178 | 0.219265 | C | 0.703181 | 0.256527 | 0.217001 |
| C | -1.630105 | -0.859602 | 0.962707 | C | -1.613251 | -0.760125 | 0.999834 | C | -1.614589 | -0.762783 | 1.007045 |
| C | -2.395261 | -0.777082 | -0.370069 | C | -2.290144 | -0.780934 | -0.392509 | C | -2.295018 | -0.77323 | -0.373254 |
| C | -2.926378 | 0.607215 | -0.772305 | C | -2.789562 | 0.567443 | -0.918882 | C | -2.785097 | 0.581451 | -0.90702 |
| C | -1.900572 | 1.762296 | -0.847664 | C | -1.753019 | 1.710064 | -1.003455 | C | -1.742619 | 1.71993 | -1.002049 |
| C | -1.215013 | 2.09775 | 0.470178 | C | -1.154997 | 2.145031 | 0.327917 | C | -1.139194 | 2.148043 | 0.328986 |
| C | 0.184579 | 1.561406 | 0.762875 | C | 0.225578 | 1.641753 | 0.741263 | C | 0.234675 | 1.628634 | 0.746141 |
| C | -1.822577 | 2.896803 | 1.355492 | C | -1.818272 | 2.99974 | 1.115969 | C | -1.794073 | 3.011634 | 1.114337 |
| C | 2.128002 | -0.096537 | 0.431796 | C | 2.172627 | -0.042349 | 0.664339 | C | 2.172399 | -0.06589 | 0.662153 |
| C | 2.135624 | -1.585447 | 0.860393 | C | 2.148401 | -1.485163 | 1.226296 | C | 2.142142 | -1.518651 | 1.196942 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | 0.739472 | -1.828737 | 1.439313 | C | 0.714911 | -1.673206 | 1.731158 | C | 0.709419 | -1.708556 | 1.70261 |
| C | 3.118858 | 0.206907 | -0.716739 | C | 3.285489 | 0.192013 | -0.391131 | C | 3.291479 | 0.18348 | -0.383475 |
| C | 4.553974 | -0.198371 | -0.342589 | C | 3.485516 | 1.68231 | -0.709941 | C | 3.510157 | 1.678591 | -0.665542 |
| C | 3.09603 | 1.677687 | -1.160107 | C | 3.107528 | -0.605741 | -1.693842 | C | 3.109877 | -0.579646 | -1.706369 |
| H | 0.513772 | 0.33061 | -0.974826 | H | 0.643428 | 0.281305 | -0.87092 | H | 0.649456 | 0.275963 | -0.873374 |
| O | -0.368197 | -1.861831 | -0.669144 | O | -0.249091 | -1.892054 | -0.439605 | O | -0.263939 | -1.88848 | -0.465489 |
| O | -1.428313 | -1.137102 | -1.375274 | O | -1.246751 | -1.229699 | -1.287282 | O | -1.271096 | -1.211368 | -1.287117 |
| O | -3.445129 | -1.714223 | -0.309899 | O | -3.396126 | -1.649155 | -0.445964 | O | -3.356379 | -1.697035 | -0.310818 |
| H | -1.966138 | -1.76291 | 1.477454 | H | -1.981565 | -1.615155 | 1.576105 | H | -1.990842 | -1.624596 | 1.563506 |
| H | -1.802745 | 0.000812 | 1.607182 | H | -1.837604 | 0.145954 | 1.560974 | H | -1.817429 | 0.142935 | 1.576535 |
| H | -3.401159 | 0.5062 | -1.758064 | H | -3.201169 | 0.384584 | -1.917205 | H | -3.199728 | 0.411977 | -1.910368 |
| H | -3.719691 | 0.863798 | -0.062264 | H | -3.626274 | 0.871388 | -0.280894 | H | -3.617168 | 0.894978 | -0.267732 |
| H | -2.446668 | 2.648066 | -1.189973 | H | -2.268507 | 2.567714 | -1.448861 | H | -2.253969 | 2.581418 | -1.44513 |
| H | -1.165332 | 1.530952 | -1.623267 | H | -0.966804 | 1.420754 | -1.706519 | H | -0.961233 | 1.423065 | -1.706956 |
| H | 0.900389 | 2.326334 | 0.433177 | H | 0.959593 | 2.378774 | 0.388329 | H | 0.976249 | 2.36328 | 0.404388 |
| H | 0.315331 | 1.498248 | 1.85107 | H | 0.297164 | 1.668476 | 1.836471 | H | 0.298976 | 1.646248 | 1.841937 |
| H | -1.373285 | 3.136592 | 2.315699 | H | -1.429125 | 3.310053 | 2.082346 | H | -1.403715 | 3.318145 | 2.08137 |
| H | -2.790118 | 3.346809 | 1.148467 | H | -2.772874 | 3.42656 | 0.819261 | H | -2.742841 | 3.449665 | 0.81511 |
| H | 2.430993 | 0.508053 | 1.301144 | H | 2.404202 | 0.623848 | 1.508577 | H | 2.40212 | 0.583627 | 1.519969 |
| H | 2.934435 | -1.816439 | 1.570685 | H | 2.901353 | -1.633482 | 2.006927 | H | 2.897373 | -1.685352 | 1.971729 |
| H | 2.280066 | -2.225509 | -0.018076 | H | 2.350039 | -2.214997 | 0.4363 | H | 2.337169 | -2.234303 | 0.392337 |
| H | 0.448158 | -2.881847 | 1.492183 | H | 0.413372 | -2.717163 | 1.86037 | H | 0.401501 | -2.752319 | 1.813948 |
| H | 0.659519 | -1.407048 | 2.449194 | H | 0.569655 | -1.161144 | 2.690633 | H | 0.569804 | -1.211782 | 2.671009 |
| H | 2.806632 | -0.407161 | -1.575097 | H | 4.214654 | -0.162328 | 0.080579 | H | 4.214815 | -0.192729 | 0.082682 |
| H | 5.245212 | 0.013789 | -1.165212 | H | 4.358772 | 1.827773 | -1.354981 | H | 4.388827 | 1.829274 | -1.302081 |
| H | 4.634403 | -1.263992 | -0.110377 | H | 3.640176 | 2.274498 | 0.198858 | H | 3.665944 | 2.247301 | 0.257942 |
| H | 4.90208 | 0.362675 | 0.533776 | H | 2.621158 | 2.098634 | -1.240092 | H | 2.653778 | 2.117197 | -1.190737 |
| H | 3.80939 | 1.845584 | -1.97415 | H | 3.985276 | -0.475409 | -2.33577 | H | 3.997266 | -0.454865 | -2.336089 |
| H | 2.111231 | 1.987414 | -1.522144 | H | 2.985405 | -1.67764 | -1.516929 | H | 2.959969 | -1.652087 | -1.55626 |
| H | 3.377419 | 2.343876 | -0.335028 | H | 2.235392 | -0.267357 | -2.263013 | H | 2.252349 | -0.206568 | -2.276165 |
| H | -3.848533 | -1.756077 | -1.188728 | H | -3.063381 | -2.542212 | -0.276137 | H | -3.706306 | -1.799672 | -1.2074 |
| **1b1** | | | | **1b2** | | | | **1b3** | | | |
| C | -0.130142 | -0.891437 | -0.653879 | C | 0.1812 | -1.028572 | 0.522589 | C | 0.142946 | -0.98218 | 0.660382 |
| C | 0.605844 | 0.363018 | -0.08345 | C | -0.6269 | 0.242721 | 0.110044 | C | -0.703165 | 0.256514 | 0.217017 |
| C | -1.582961 | -0.728683 | -1.09658 | C | 1.632288 | -0.852938 | 0.956482 | C | 1.614597 | -0.762716 | 1.00707 |
| C | -2.360922 | -0.870371 | 0.225739 | C | 2.397839 | -0.77518 | -0.387426 | C | 2.29504 | -0.773195 | -0.373207 |
| C | -2.97536 | 0.410925 | 0.80965 | C | 2.932655 | 0.604837 | -0.779641 | C | 2.78512 | 0.58149 | -0.906922 |
| C | -2.010976 | 1.587829 | 1.08654 | C | 1.906127 | 1.757749 | -0.846489 | C | 1.742605 | 1.719932 | -1.002037 |
| C | -1.338776 | 2.161675 | -0.15239 | C | 1.221706 | 2.096539 | 0.471161 | C | 1.139122 | 2.148133 | 0.32894 |
| C | 0.087014 | 1.751007 | -0.509975 | C | -0.182108 | 1.569677 | 0.7591 | C | -0.2347 | 1.62863 | 0.746185 |
| C | -1.985073 | 3.054187 | -0.912179 | C | 1.832008 | 2.889776 | 1.35987 | C | 1.793897 | 3.011887 | 1.114198 |
| C | 2.107054 | 0.185901 | -0.49081 | C | -2.12739 | -0.087326 | 0.4331 | C | -2.172384 | -0.065934 | 0.662137 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | 2.221386 | -1.258204 | -1.031035 | C | -2.136004 | -1.571178 | 0.878776 | C | -2.142126 | -1.518688 | 1.196977 |
| C | 0.844631 | -1.517263 | -1.65586 | C | -0.740158 | -1.807008 | 1.46195 | C | -0.709368 | -1.708627 | 1.702595 |
| C | 3.118275 | 0.59127 | 0.609673 | C | -3.114888 | 0.203973 | -0.721289 | C | -3.291443 | 0.183336 | -0.383541 |
| C | 3.131953 | -0.35366 | 1.822655 | C | -4.550745 | -0.199348 | -0.347871 | C | -3.109555 | -0.579573 | -1.706526 |
| C | 4.535981 | 0.75022 | 0.037655 | C | -3.09159 | 1.670974 | -1.177004 | C | -3.510443 | 1.678431 | -0.665451 |
| H | 0.515768 | 0.287055 | 1.002768 | H | -0.50917 | 0.330394 | -0.973326 | H | -0.649408 | 0.275941 | -0.873355 |
| O | -0.27763 | -1.868359 | 0.409071 | O | 0.363763 | -1.867579 | -0.648548 | O | 0.264006 | -1.888489 | -0.465485 |
| O | -1.381231 | -1.304263 | 1.188091 | O | 1.414275 | -1.149656 | -1.378688 | O | 1.271124 | -1.211351 | -1.287091 |
| O | -3.352091 | -1.850202 | 0.022885 | O | 3.503341 | -1.644452 | -0.43352 | O | 3.356391 | -1.697017 | -0.310789 |
| H | -1.795379 | 0.203557 | -1.618348 | H | 1.963062 | -1.749214 | 1.491267 | H | 1.817335 | 0.143072 | 1.576502 |
| H | -1.870009 | -1.567282 | -1.73545 | H | 1.82045 | 0.009075 | 1.594748 | H | 1.990929 | -1.624406 | 1.563672 |
| H | -3.764769 | 0.733571 | 0.122746 | H | 3.727248 | 0.855657 | -0.068854 | H | 3.617115 | 0.895017 | -0.267533 |
| H | -3.465192 | 0.139982 | 1.75521 | H | 3.407347 | 0.493059 | -1.760314 | H | 3.199891 | 0.412067 | -1.910218 |
| H | -1.268602 | 1.269183 | 1.823366 | H | 1.168824 | 1.529254 | -1.621281 | H | 2.25393 | 2.581405 | -1.445176 |
| H | -2.603339 | 2.378905 | 1.559094 | H | 2.452323 | 2.642676 | -1.190374 | H | 0.961251 | 1.422977 | -1.706944 |
| H | 0.22565 | 1.883052 | -1.590703 | H | -0.89307 | 2.334872 | 0.419582 | H | -0.976364 | 2.36323 | 0.404537 |
| H | 0.763848 | 2.482016 | -0.041924 | H | -0.320356 | 1.513663 | 1.846794 | H | -0.298903 | 1.646164 | 1.841987 |
| H | -1.544996 | 3.462755 | -1.818172 | H | 1.381373 | 3.13131 | 2.319079 | H | 2.742624 | 3.449975 | 0.814928 |
| H | -2.97642 | 3.415367 | -0.650728 | H | 2.803211 | 3.333303 | 1.156268 | H | 1.40348 | 3.318462 | 2.081187 |
| H | 2.286601 | 0.858385 | -1.343443 | H | -2.432563 | 0.526879 | 1.294783 | H | -2.402155 | 0.583604 | 1.519924 |
| H | 3.04249 | -1.377867 | -1.744158 | H | -2.279379 | -2.221429 | 0.007717 | H | -2.337231 | -2.234369 | 0.392414 |
| H | 2.383842 | -1.969337 | -0.215303 | H | -2.935245 | -1.794111 | 1.591092 | H | -2.897312 | -1.685329 | 1.971818 |
| H | 0.615378 | -2.572576 | -1.8297 | H | -0.450674 | -2.860143 | 1.529983 | H | -0.569722 | -1.211951 | 2.671037 |
| H | 0.750246 | -0.989586 | -2.61333 | H | -0.660499 | -1.371961 | 2.466115 | H | -0.401439 | -2.7524 | 1.813821 |
| H | 2.801233 | 1.582287 | 0.969282 | H | -2.799256 | -0.417347 | -1.573145 | H | -4.214724 | -0.193139 | 0.082504 |
| H | 2.127096 | -0.555557 | 2.205728 | H | -5.239584 | 0.005321 | -1.174335 | H | -3.9971 | -0.455289 | -2.336129 |
| H | 3.587997 | -1.317808 | 1.573697 | H | -4.901965 | 0.368806 | 0.522646 | H | -2.252342 | -0.205884 | -2.276393 |
| H | 3.71948 | 0.081811 | 2.637798 | H | -4.631216 | -1.263083 | -0.10696 | H | -2.958928 | -1.651931 | -1.556544 |
| H | 5.233685 | 1.101026 | 0.805667 | H | -3.801942 | 1.831278 | -1.995129 | H | -4.389067 | 1.828983 | -1.302086 |
| H | 4.919799 | -0.203724 | -0.342043 | H | -2.105775 | 1.978694 | -1.537975 | H | -2.654096 | 2.117295 | -1.190483 |
| H | 4.557655 | 1.470552 | -0.78766 | H | -3.376728 | 2.343764 | -0.358598 | H | -3.666485 | 2.246998 | 0.258079 |
| H | -3.762014 | -2.031652 | 0.880719 | H | 3.15831 | -2.545397 | -0.353848 | H | 3.705707 | -1.80027 | -1.207535 |
| **1b4** | | | | **1b5** | | | | **1c1** | | | |
| C | 0.142972 | -0.982209 | 0.660344 | C | 0.142952 | -0.982009 | 0.660623 | C | -0.190538 | -1.025399 | 0.396144 |
| C | -0.703187 | 0.256459 | 0.216983 | C | -0.703031 | 0.25664 | 0.217122 | C | 0.699994 | 0.226029 | 0.203053 |
| C | 1.614605 | -0.7627 | 1.00707 | C | 1.614681 | -0.762749 | 1.007101 | C | -1.512946 | -0.809392 | 1.136798 |
| C | 2.295088 | -0.77313 | -0.373174 | C | 2.294853 | -0.773143 | -0.373301 | C | -2.554186 | -0.668191 | 0.008591 |
| C | 2.785129 | 0.581573 | -0.906867 | C | 2.784957 | 0.581533 | -0.907144 | C | -3.275218 | 0.687255 | -0.090511 |
| C | 1.742571 | 1.71997 | -1.002016 | C | 1.742498 | 1.720023 | -1.002176 | C | -2.449383 | 1.866618 | -0.6534 |
| C | 1.139045 | 2.148152 | 0.328943 | C | 1.139301 | 2.148118 | 0.329001 | C | -1.079393 | 2.112448 | -0.041316 |
| C | -0.234746 | 1.62855 | 0.746211 | C | -0.234802 | 1.629181 | 0.745603 | C | 0.127022 | 1.386721 | -0.633347 |
| C | 1.793725 | 3.012001 | 1.114173 | C | 1.794586 | 3.011115 | 1.114666 | C | -0.927077 | 2.99632 | 0.952257 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -2.172387 | -0.066049 | 0.662099 | C | -2.172309 | -0.065648 | 0.662173 | C | 2.010912 | -0.386196 | -0.34963 |
| C | -2.142088 | -1.518842 | 1.196819 | C | -2.142095 | -1.518114 | 1.197719 | C | 2.195068 | -1.675576 | 0.495773 |
| C | -0.709351 | -1.708746 | 1.702503 | C | -0.709312 | -1.708088 | 1.70314 | C | 0.777981 | -2.065935 | 0.990543 |
| C | -3.29147 | 0.183281 | -0.38353 | C | -3.291221 | 0.182661 | -0.383892 | C | 3.241697 | 0.547123 | -0.426978 |
| C | -3.510591 | 1.678395 | -0.665228 | C | -3.512161 | 1.677538 | -0.665416 | C | 3.636146 | 1.192005 | 0.911422 |
| C | -3.1095 | -0.579434 | -1.706606 | C | -3.10773 | -0.579507 | -1.707149 | C | 4.442945 | -0.181553 | -1.052015 |
| H | -0.64944 | 0.275898 | -0.873389 | H | -0.64916 | 0.275819 | -0.873221 | H | 0.891027 | 0.607409 | 1.217536 |
| O | 0.264094 | -1.888511 | -0.465529 | O | 0.263842 | -1.888457 | -0.465117 | O | -0.62209 | -1.586137 | -0.868469 |
| O | 1.271225 | -1.211338 | -1.2871 | O | 1.270716 | -1.211277 | -1.287004 | O | -1.813505 | -0.806029 | -1.209308 |
| O | 3.356483 | -1.696905 | -0.3107 | O | 3.356145 | -1.696983 | -0.311096 | O | -3.476554 | -1.720806 | 0.18146 |
| H | 1.990931 | -1.624412 | 1.563648 | H | 1.990977 | -1.624655 | 1.56342 | H | -1.782341 | -1.69053 | 1.723314 |
| H | 1.817337 | 0.143061 | 1.576547 | H | 1.81761 | 0.14287 | 1.576666 | H | -1.483136 | 0.060619 | 1.794152 |
| H | 3.617085 | 0.895146 | -0.267448 | H | 3.617105 | 0.895037 | -0.267918 | H | -3.654585 | 0.924615 | 0.909107 |
| H | 3.199938 | 0.412175 | -1.910152 | H | 3.199592 | 0.411969 | -1.910459 | H | -4.157076 | 0.558436 | -0.731666 |
| H | 0.961245 | 1.422987 | -1.706942 | H | 0.960973 | 1.423034 | -1.706855 | H | -2.327644 | 1.71311 | -1.730555 |
| H | 2.253873 | 2.58146 | -1.445152 | H | 2.253773 | 2.581458 | -1.445451 | H | -3.057499 | 2.769664 | -0.529139 |
| H | -0.298884 | 1.645998 | 1.84202 | H | -0.300034 | 1.647861 | 1.841312 | H | -0.113282 | 1.014688 | -1.633091 |
| H | -0.976447 | 2.363172 | 0.404688 | H | -0.976168 | 2.363417 | 0.402412 | H | 0.928926 | 2.124297 | -0.754517 |
| H | 1.403274 | 3.318578 | 2.081147 | H | 1.404284 | 3.317477 | 2.081766 | H | 0.047536 | 3.213783 | 1.382607 |
| H | 2.742404 | 3.450191 | 0.814897 | H | 2.743581 | 3.448731 | 0.815592 | H | -1.770656 | 3.539791 | 1.369849 |
| H | -2.402148 | 0.583405 | 1.519954 | H | -2.402349 | 0.584325 | 1.519567 | H | 1.787314 | -0.7001 | -1.378634 |
| H | -2.33711 | -2.234477 | 0.392194 | H | -2.337556 | -2.234126 | 0.39351 | H | 2.656734 | -2.475433 | -0.089181 |
| H | -2.897321 | -1.685569 | 1.971601 | H | -2.897175 | -1.684291 | 1.972764 | H | 2.854545 | -1.490144 | 1.349911 |
| H | -0.569755 | -1.21214 | 2.670979 | H | -0.569454 | -1.211087 | 2.671389 | H | 0.71595 | -2.027704 | 2.082492 |
| H | -0.401373 | -2.752517 | 1.813643 | H | -0.401454 | -2.751833 | 1.814662 | H | 0.469205 | -3.069085 | 0.684056 |
| H | -4.214711 | -0.193348 | 0.082471 | H | -4.214218 | -0.195115 | 0.081678 | H | 2.975422 | 1.365022 | -1.111812 |
| H | -4.389193 | 1.828969 | -1.301889 | H | -4.390457 | 1.827067 | -1.302756 | H | 4.497024 | 1.85499 | 0.774221 |
| H | -2.654254 | 2.117418 | -1.190146 | H | -2.655999 | 2.117763 | -1.189622 | H | 2.825552 | 1.793207 | 1.335371 |
| H | -3.666735 | 2.246803 | 0.258381 | H | -3.669754 | 2.245636 | 0.258141 | H | 3.921355 | 0.442881 | 1.658525 |
| H | -3.997115 | -0.455297 | -2.336144 | H | -3.996395 | -0.458854 | -2.335864 | H | 5.277857 | 0.508183 | -1.215609 |
| H | -2.252419 | -0.205465 | -2.276492 | H | -2.252734 | -0.20205 | -2.277868 | H | 4.180818 | -0.625531 | -2.018642 |
| H | -2.958596 | -1.651771 | -1.55675 | H | -2.952276 | -1.65122 | -1.557493 | H | 4.804579 | -0.986838 | -0.402814 |
| H | 3.706095 | -1.799862 | -1.207366 | H | 3.704668 | -1.800812 | -1.208072 | H | -4.048572 | -1.735217 | -0.599247 |
| **1c2** | | | | **1c3** | | | | **1c4** | | | |
| C | -0.189187 | -1.022942 | 0.408078 | C | -0.201907 | -1.049877 | 0.363336 | C | -0.200753 | -1.049108 | 0.372215 |
| C | 0.698123 | 0.228272 | 0.204699 | C | 0.726535 | 0.177508 | 0.170366 | C | 0.724571 | 0.178509 | 0.170471 |
| C | -1.516669 | -0.808345 | 1.133647 | C | -1.485117 | -0.800287 | 1.159717 | C | -1.488683 | -0.802125 | 1.156126 |
| C | -2.561773 | -0.663966 | -0.00561 | C | -2.570195 | -0.623563 | 0.078085 | C | -2.579624 | -0.617178 | 0.066051 |
| C | -3.28397 | 0.686183 | -0.07873 | C | -3.247402 | 0.757021 | 0.007142 | C | -3.253604 | 0.760116 | 0.023374 |
| C | -2.456007 | 1.85722 | -0.65278 | C | -2.411134 | 1.896993 | -0.61881 | C | -2.416456 | 1.890668 | -0.61554 |
| C | -1.086038 | 2.110093 | -0.042314 | C | -1.005195 | 2.10428 | -0.078195 | C | -1.009085 | 2.102837 | -0.079668 |
| C | 0.124411 | 1.388707 | -0.63201 | C | 0.148294 | 1.315764 | -0.699097 | C | 0.145955 | 1.315963 | -0.700096 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | -0.935781 | 2.995563 | 0.950299 | C | -0.778149 | 3.008069 | 0.88295 | C | -0.780627 | 3.008183 | 0.879822 |
| C | 2.008626 | -0.385494 | -0.347678 | C | 2.07785 | -0.418148 | -0.345625 | C | 2.076433 | -0.417481 | -0.34446 |
| C | 2.196892 | -1.669855 | 0.504544 | C | 2.001859 | -1.946984 | -0.014871 | C | 2.003245 | -1.944788 | -0.007359 |
| C | 0.782326 | -2.055629 | 1.010398 | C | 0.757927 | -2.125508 | 0.872203 | C | 0.763066 | -2.119081 | 0.885706 |
| C | 3.238014 | 0.549035 | -0.432443 | C | 3.35475 | 0.230144 | 0.252654 | C | 3.353367 | 0.234139 | 0.250461 |
| C | 3.633919 | 1.202101 | 0.901512 | C | 4.619107 | -0.317661 | -0.431723 | C | 4.617141 | -0.313831 | -0.434927 |
| C | 4.438943 | -0.181623 | -1.055792 | C | 3.380883 | 1.765253 | 0.194686 | C | 3.377881 | 1.769103 | 0.189412 |
| H | 0.890752 | 0.612316 | 1.217939 | H | 0.894317 | 0.579376 | 1.18063 | H | 0.89283 | 0.58309 | 1.179613 |
| O | -0.6236 | -1.597675 | -0.851362 | O | -0.695289 | -1.574391 | -0.89483 | O | -0.698964 | -1.585365 | -0.880756 |
| O | -1.795123 | -0.795508 | -1.214486 | O | -1.89178 | -0.781686 | -1.172612 | O | -1.878072 | -0.771709 | -1.178352 |
| O | -3.563807 | -1.649887 | 0.069314 | O | -3.518204 | -1.645199 | 0.292259 | O | -3.613508 | -1.564946 | 0.187286 |
| H | -1.782487 | -1.681549 | 1.737324 | H | -1.754698 | -1.674722 | 1.756099 | H | -1.753724 | -1.671081 | 1.76621 |
| H | -1.497167 | 0.062308 | 1.790855 | H | -1.405133 | 0.066905 | 1.81633 | H | -1.417725 | 0.063377 | 1.816351 |
| H | -3.639613 | 0.926287 | 0.928923 | H | -3.559355 | 1.019873 | 1.023558 | H | -3.53821 | 1.025439 | 1.047116 |
| H | -4.172111 | 0.545344 | -0.702497 | H | -4.169136 | 0.655021 | -0.580626 | H | -4.182545 | 0.647976 | -0.544292 |
| H | -2.335356 | 1.694003 | -1.728563 | H | -2.348679 | 1.720224 | -1.697389 | H | -2.358143 | 1.704732 | -1.692747 |
| H | -3.064221 | 2.761045 | -0.536474 | H | -2.980903 | 2.82291 | -0.48148 | H | -2.985368 | 2.817785 | -0.484293 |
| H | -0.110877 | 1.019486 | -1.633799 | H | -0.158935 | 0.893207 | -1.658933 | H | -0.158992 | 0.894996 | -1.66115 |
| H | 0.925586 | 2.128087 | -0.746787 | H | 0.958097 | 2.01991 | -0.909539 | H | 0.956221 | 2.020489 | -0.907173 |
| H | 0.038454 | 3.217508 | 1.37943 | H | 0.219969 | 3.200046 | 1.268904 | H | 0.218276 | 3.202898 | 1.262611 |
| H | -1.780944 | 3.536794 | 1.367593 | H | -1.582707 | 3.595614 | 1.317739 | H | -1.584985 | 3.595175 | 1.31571 |
| H | 1.783591 | -0.705082 | -1.374515 | H | 2.11746 | -0.288113 | -1.435428 | H | 2.114684 | -0.291817 | -1.434705 |
| H | 2.653853 | -2.474037 | -0.07806 | H | 1.885942 | -2.531553 | -0.93188 | H | 1.8834 | -2.53348 | -0.921173 |
| H | 2.861158 | -1.480405 | 1.353933 | H | 2.905984 | -2.307714 | 0.483672 | H | 2.909201 | -2.303214 | 0.48931 |
| H | 0.725036 | -2.004304 | 2.102136 | H | 0.991434 | -1.917598 | 1.923045 | H | 0.999471 | -1.903511 | 1.934265 |
| H | 0.476281 | -3.064301 | 0.717707 | H | 0.310731 | -3.121798 | 0.816798 | H | 0.320711 | -3.118675 | 0.839972 |
| H | 2.968971 | 1.362333 | -1.121451 | H | 3.39161 | -0.059005 | 1.315257 | H | 3.392287 | -0.052729 | 1.31365 |
| H | 4.493905 | 1.865004 | 0.758845 | H | 5.523337 | 0.082233 | 0.039576 | H | 5.521622 | 0.087927 | 0.034193 |
| H | 2.823586 | 1.805256 | 1.323123 | H | 4.678787 | -1.408857 | -0.389795 | H | 4.678342 | -1.404912 | -0.391092 |
| H | 3.921335 | 0.457834 | 1.652628 | H | 4.640334 | -0.02567 | -1.488822 | H | 4.636378 | -0.023788 | -1.492557 |
| H | 5.272587 | 0.508345 | -1.224447 | H | 4.314306 | 2.144359 | 0.624952 | H | 4.311711 | 2.149475 | 0.617582 |
| H | 4.175686 | -0.630804 | -2.019693 | H | 2.557966 | 2.220505 | 0.752408 | H | 2.555608 | 2.22485 | 0.7476 |
| H | 4.803066 | -0.983028 | -0.403128 | H | 3.329308 | 2.125053 | -0.839912 | H | 3.324516 | 2.126993 | -0.845694 |
| H | -3.121807 | -2.509799 | 0.016331 | H | -4.126492 | -1.638017 | -0.460605 | H | -3.208165 | -2.441385 | 0.115746 |
| **1c5** | | | | **1d1** | | | | **1d2** | | | |
| C | -0.163128 | -1.078043 | 0.221025 | C | 0.190538 | -1.025399 | 0.396144 | C | 0.189187 | -1.022942 | 0.408078 |
| C | 0.789888 | 0.123975 | -0.014766 | C | -0.699994 | 0.226029 | 0.203053 | C | -0.698123 | 0.228272 | 0.204699 |
| C | -1.352875 | -0.812747 | 1.147019 | C | 1.512946 | -0.809392 | 1.136798 | C | 1.516669 | -0.808345 | 1.133647 |
| C | -2.527786 | -0.548961 | 0.183537 | C | 2.554186 | -0.668191 | 0.008591 | C | 2.561773 | -0.663966 | -0.00561 |
| C | -3.148605 | 0.858911 | 0.227734 | C | 3.275218 | 0.687255 | -0.090511 | C | 3.28397 | 0.686183 | -0.07873 |
| C | -2.331133 | 1.987725 | -0.441451 | C | 2.449383 | 1.866618 | -0.6534 | C | 2.456007 | 1.85722 | -0.65278 |
| C | -0.871915 | 2.123096 | -0.036502 | C | 1.079393 | 2.112448 | -0.041316 | C | 1.086038 | 2.110093 | -0.042314 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | 0.184032 | 1.315138 | -0.790636 | C | -0.127022 | 1.386721 | -0.633347 | C | -0.124411 | 1.388707 | -0.63201 |
| C | -0.513425 | 2.982426 | 0.925464 | C | 0.927077 | 2.99632 | 0.952257 | C | 0.935781 | 2.995563 | 0.950299 |
| C | 2.06588 | -0.501667 | -0.666776 | C | -2.010912 | -0.386196 | -0.34963 | C | -2.008626 | -0.385494 | -0.347678 |
| C | 1.949111 | -2.039932 | -0.412666 | C | -2.195068 | -1.675576 | 0.495773 | C | -2.196892 | -1.669855 | 0.504544 |
| C | 0.796074 | -2.212776 | 0.589998 | C | -0.777981 | -2.065935 | 0.990543 | C | -0.782326 | -2.055629 | 1.010398 |
| C | 3.431358 | 0.071112 | -0.192168 | C | -3.241697 | 0.547123 | -0.426978 | C | -3.238014 | 0.549035 | -0.432443 |
| C | 3.655651 | 1.534941 | -0.6014 | C | -3.636146 | 1.192005 | 0.911422 | C | -3.633919 | 1.202101 | 0.901512 |
| C | 3.701059 | -0.104167 | 1.312059 | C | -4.442945 | -0.181553 | -1.052015 | C | -4.438943 | -0.181623 | -1.055792 |
| H | 1.052597 | 0.487988 | 0.987364 | H | -0.891027 | 0.607409 | 1.217536 | H | -0.890752 | 0.612316 | 1.217939 |
| O | -0.796858 | -1.531539 | -1.001794 | O | 0.62209 | -1.586137 | -0.868469 | O | 0.6236 | -1.597675 | -0.851362 |
| O | -1.980751 | -0.684404 | -1.132613 | O | 1.813505 | -0.806029 | -1.209308 | O | 1.795123 | -0.795508 | -1.214486 |
| O | -3.494668 | -1.53985 | 0.452116 | O | 3.476554 | -1.720806 | 0.18146 | O | 3.563807 | -1.649887 | 0.069314 |
| H | -1.602023 | -1.699548 | 1.733936 | H | 1.782341 | -1.69053 | 1.723314 | H | 1.782487 | -1.681549 | 1.737324 |
| H | -1.173365 | 0.023046 | 1.82447 | H | 1.483136 | 0.060619 | 1.794152 | H | 1.497167 | 0.062308 | 1.790855 |
| H | -3.347262 | 1.096212 | 1.27833 | H | 3.654585 | 0.924615 | 0.909107 | H | 3.639613 | 0.926287 | 0.928923 |
| H | -4.127573 | 0.815159 | -0.267495 | H | 4.157076 | 0.558436 | -0.731666 | H | 4.172111 | 0.545344 | -0.702497 |
| H | -2.381691 | 1.847179 | -1.525925 | H | 2.327644 | 1.71311 | -1.730555 | H | 2.335356 | 1.694003 | -1.728563 |
| H | -2.846477 | 2.928956 | -0.219464 | H | 3.057499 | 2.769664 | -0.529139 | H | 3.064221 | 2.761045 | -0.536474 |
| H | -0.225256 | 0.944148 | -1.73371 | H | 0.113282 | 1.014688 | -1.633091 | H | 0.110877 | 1.019486 | -1.633799 |
| H | 1.002436 | 1.994301 | -1.046794 | H | -0.928926 | 2.124297 | -0.754517 | H | -0.925586 | 2.128087 | -0.746787 |
| H | 0.525832 | 3.120332 | 1.214131 | H | -0.047536 | 3.213783 | 1.382607 | H | -0.038454 | 3.217508 | 1.37943 |
| H | -1.244623 | 3.584617 | 1.458711 | H | 1.770656 | 3.539791 | 1.369849 | H | 1.780944 | 3.536794 | 1.367593 |
| H | 2.01514 | -0.32539 | -1.748432 | H | -1.787314 | -0.7001 | -1.378634 | H | -1.783591 | -0.705082 | -1.374515 |
| H | 1.696778 | -2.553299 | -1.344904 | H | -2.656734 | -2.475433 | -0.089181 | H | -2.653853 | -2.474037 | -0.07806 |
| H | 2.885807 | -2.475529 | -0.052016 | H | -2.854545 | -1.490144 | 1.349911 | H | -2.861158 | -1.480405 | 1.353933 |
| H | 1.140484 | -2.060567 | 1.619548 | H | -0.71595 | -2.027704 | 2.082492 | H | -0.725036 | -2.004304 | 2.102136 |
| H | 0.3011 | -3.186463 | 0.538304 | H | -0.469205 | -3.069085 | 0.684056 | H | -0.476281 | -3.064301 | 0.717707 |
| H | 4.188591 | -0.525439 | -0.722576 | H | -2.975422 | 1.365022 | -1.111812 | H | -2.968971 | 1.362333 | -1.121451 |
| H | 4.687674 | 1.838903 | -0.394167 | H | -4.497024 | 1.854991 | 0.774221 | H | -4.493905 | 1.865004 | 0.758845 |
| H | 3.471237 | 1.688872 | -1.670135 | H | -2.825552 | 1.793207 | 1.335371 | H | -2.823586 | 1.805256 | 1.323123 |
| H | 3.002127 | 2.216365 | -0.045666 | H | -3.921355 | 0.442881 | 1.658525 | H | -3.921335 | 0.457834 | 1.652628 |
| H | 4.724287 | 0.203278 | 1.552646 | H | -5.277857 | 0.508183 | -1.215609 | H | -5.272587 | 0.508345 | -1.224447 |
| H | 3.588445 | -1.143615 | 1.635809 | H | -4.180818 | -0.625531 | -2.018642 | H | -4.175686 | -0.630804 | -2.019693 |
| H | 3.02962 | 0.511345 | 1.921349 | H | -4.804579 | -0.986838 | -0.402814 | H | -4.803066 | -0.983028 | -0.403128 |
| H | -4.170776 | -1.478681 | -0.237806 | H | 4.048572 | -1.735217 | -0.599247 | H | 3.121807 | -2.509799 | 0.016331 |
| **1d3** | | | | **1d4** | | | | **1d5** | | | |
| C | 0.201907 | -1.049877 | 0.363336 | C | 0.200753 | -1.049108 | 0.372215 | C | 0.163128 | -1.078043 | 0.221025 |
| C | -0.726535 | 0.177508 | 0.170366 | C | -0.724571 | 0.178509 | 0.170471 | C | -0.789888 | 0.123975 | -0.014766 |
| C | 1.485117 | -0.800287 | 1.159717 | C | 1.488683 | -0.802125 | 1.156126 | C | 1.352875 | -0.812747 | 1.147019 |
| C | 2.570195 | -0.623563 | 0.078085 | C | 2.579624 | -0.617178 | 0.066051 | C | 2.527786 | -0.548961 | 0.183537 |
| C | 3.247402 | 0.757021 | 0.007142 | C | 3.253604 | 0.760116 | 0.023374 | C | 3.148605 | 0.858911 | 0.227734 |
| C | 2.411134 | 1.896993 | -0.61881 | C | 2.416456 | 1.890668 | -0.61554 | C | 2.331133 | 1.987725 | -0.441451 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | 1.005195 | 2.10428 | -0.078195 | C | 1.009085 | 2.102837 | -0.079668 | C | 0.871915 | 2.123096 | -0.036502 |
| C | -0.148294 | 1.315764 | -0.699097 | C | -0.145955 | 1.315963 | -0.700096 | C | -0.184032 | 1.315138 | -0.790636 |
| C | 0.778149 | 3.008069 | 0.88295 | C | 0.780627 | 3.008183 | 0.879822 | C | 0.513425 | 2.982426 | 0.925464 |
| C | -2.07785 | -0.418148 | -0.345625 | C | -2.076433 | -0.417481 | -0.34446 | C | -2.06588 | -0.501667 | -0.666776 |
| C | -2.001859 | -1.946984 | -0.014871 | C | -2.003245 | -1.944788 | -0.007359 | C | -1.949111 | -2.039932 | -0.412666 |
| C | -0.757927 | -2.125508 | 0.872203 | C | -0.763066 | -2.119081 | 0.885706 | C | -0.796074 | -2.212776 | 0.589998 |
| C | -3.35475 | 0.230144 | 0.252654 | C | -3.353367 | 0.234139 | 0.250461 | C | -3.431358 | 0.071112 | -0.192168 |
| C | -4.619107 | -0.317661 | -0.431723 | C | -4.617141 | -0.313831 | -0.434927 | C | -3.655651 | 1.534941 | -0.6014 |
| C | -3.380883 | 1.765253 | 0.194686 | C | -3.377881 | 1.769103 | 0.189412 | C | -3.701059 | -0.104167 | 1.312059 |
| H | -0.894317 | 0.579376 | 1.18063 | H | -0.89283 | 0.58309 | 1.179613 | H | -1.052597 | 0.487988 | 0.987364 |
| O | 0.695289 | -1.574391 | -0.89483 | O | 0.698964 | -1.585365 | -0.880756 | O | 0.796858 | -1.531539 | -1.001794 |
| O | 1.89178 | -0.781686 | -1.172612 | O | 1.878072 | -0.771709 | -1.178352 | O | 1.980751 | -0.684404 | -1.132613 |
| O | 3.518204 | -1.645199 | 0.292259 | O | 3.613508 | -1.564946 | 0.187286 | O | 3.494668 | -1.53985 | 0.452116 |
| H | 1.754698 | -1.674722 | 1.756099 | H | 1.753724 | -1.671081 | 1.76621 | H | 1.602023 | -1.699548 | 1.733936 |
| H | 1.405133 | 0.066905 | 1.81633 | H | 1.417725 | 0.063377 | 1.816351 | H | 1.173365 | 0.023046 | 1.82447 |
| H | 3.559355 | 1.019873 | 1.023558 | H | 3.53821 | 1.025439 | 1.047116 | H | 3.347262 | 1.096212 | 1.27833 |
| H | 4.169136 | 0.655021 | -0.580626 | H | 4.182545 | 0.647976 | -0.544292 | H | 4.127573 | 0.815159 | -0.267495 |
| H | 2.348679 | 1.720224 | -1.697389 | H | 2.358143 | 1.704732 | -1.692747 | H | 2.381691 | 1.847179 | -1.525925 |
| H | 2.980903 | 2.82291 | -0.48148 | H | 2.985368 | 2.817785 | -0.484293 | H | 2.846477 | 2.928956 | -0.219464 |
| H | 0.158935 | 0.893207 | -1.658933 | H | 0.158992 | 0.894996 | -1.66115 | H | 0.225256 | 0.944148 | -1.73371 |
| H | -0.958097 | 2.01991 | -0.909539 | H | -0.956221 | 2.020489 | -0.907173 | H | -1.002436 | 1.994301 | -1.046794 |
| H | -0.219969 | 3.200046 | 1.268904 | H | -0.218276 | 3.202898 | 1.262611 | H | -0.525832 | 3.120332 | 1.214131 |
| H | 1.582707 | 3.595614 | 1.317739 | H | 1.584985 | 3.595175 | 1.31571 | H | 1.244623 | 3.584617 | 1.458711 |
| H | -2.11746 | -0.288113 | -1.435428 | H | -2.114684 | -0.291817 | -1.434705 | H | -2.01514 | -0.32539 | -1.748432 |
| H | -1.885942 | -2.531553 | -0.93188 | H | -1.8834 | -2.53348 | -0.921173 | H | -1.696778 | -2.553299 | -1.344904 |
| H | -2.905984 | -2.307714 | 0.483672 | H | -2.909201 | -2.303214 | 0.48931 | H | -2.885807 | -2.475529 | -0.052016 |
| H | -0.991434 | -1.917598 | 1.923045 | H | -0.999471 | -1.903511 | 1.934265 | H | -1.140484 | -2.060567 | 1.619548 |
| H | -0.310731 | -3.121798 | 0.816798 | H | -0.320711 | -3.118675 | 0.839972 | H | -0.3011 | -3.186463 | 0.538304 |
| H | -3.39161 | -0.059005 | 1.315257 | H | -3.392287 | -0.052729 | 1.31365 | H | -4.188591 | -0.525439 | -0.722576 |
| H | -5.523337 | 0.082233 | 0.039576 | H | -5.521622 | 0.087927 | 0.034193 | H | -4.687674 | 1.838903 | -0.394167 |
| H | -4.678787 | -1.408857 | -0.389795 | H | -4.678342 | -1.404912 | -0.391092 | H | -3.471237 | 1.688872 | -1.670135 |
| H | -4.640334 | -0.02567 | -1.488822 | H | -4.636378 | -0.023788 | -1.492557 | H | -3.002127 | 2.216365 | -0.045666 |
| H | -4.314306 | 2.144359 | 0.624952 | H | -4.311711 | 2.149475 | 0.617582 | H | -4.724287 | 0.203278 | 1.552646 |
| H | -2.557966 | 2.220505 | 0.752408 | H | -2.555608 | 2.22485 | 0.7476 | H | -3.588445 | -1.143615 | 1.635809 |
| H | -3.329308 | 2.125053 | -0.839912 | H | -3.324516 | 2.126993 | -0.845694 | H | -3.02962 | 0.511345 | 1.921349 |
| H | 4.126492 | -1.638017 | -0.460605 | H | 3.208165 | -2.441385 | 0.115746 | H | 4.170776 | -1.478681 | -0.237806 |

**Table S3.** Calculated $^{13}$C NMR chemical shifts for **1a**.

| No. | **1a1** | **1a2** | **1a3** | **1a4** | **1a5** | **1a6** |
|---|---|---|---|---|---|---|
| 1 | 35.2523 | 35.41 | 26.1684 | 26.2986 | 32.6373 | 32.9805 |
| 2 | 37.0144 | 36.7614 | 38.0516 | 37.9095 | 36.3566 | 36.0586 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 3 | 104.9012 | 105.2844 | 104.2063 | 104.6173 | 105.3647 | 105.6498 |
| 4 | 54.3011 | 51.2485 | 54.3891 | 51.1147 | 54.1606 | 50.919 |
| 5 | 115.088 | 113.7436 | 115.3219 | 113.8164 | 114.9313 | 113.6122 |
| 6 | 42.3717 | 45.2555 | 42.4407 | 45.2173 | 42.1852 | 45.0658 |
| 7 | 32.0634 | 33.0684 | 31.8604 | 32.8861 | 32.0003 | 32.9953 |
| 8 | 165.3782 | 165.3066 | 165.4338 | 165.3587 | 165.5551 | 165.5259 |
| 9 | 45.2072 | 45.0963 | 44.4643 | 44.3267 | 46.2978 | 46.1964 |
| 10 | 52.75 | 53.4826 | 50.8691 | 51.6025 | 45.0695 | 45.7676 |
| 11 | 59.4167 | 59.4525 | 59.4519 | 59.4799 | 57.883 | 58.0145 |
| 12 | 42.581 | 42.6586 | 34.8496 | 34.7622 | 35.8356 | 35.939 |
| 13 | 22.8103 | 22.831 | 23.5171 | 23.5212 | 15.7807 | 15.8377 |
| 14 | 22.4086 | 22.4504 | 16.2172 | 16.2323 | 24.3689 | 24.4718 |
| 15 | 115.8088 | 115.8888 | 115.9306 | 115.9952 | 115.5483 | 115.6679 |

**Table S4.** Experimental and calculated $^{13}$C NMR chemical shifts of **1a**.

| No. | $\delta_{exp}$ | $\delta_{calc}$ | $\delta_{scalc}$ |
|---|---|---|---|
| 1 | 28.0 | 30.5 | 28.2 |
| 2 | 33.2 | 37.3 | 34.5 |
| 3 | 98.0 | 104.8 | 97.4 |
| 4 | 49.2 | 52.8 | 48.9 |
| 5 | 107.4 | 114.5 | 106.4 |
| 6 | 39.3 | 43.7 | 40.5 |
| 7 | 29.1 | 32.4 | 30.0 |
| 8 | 149.4 | 165.4 | 153.8 |
| 9 | 40.8 | 45.0 | 41.7 |
| 10 | 46.8 | 50.8 | 47.1 |
| 11 | 54.3 | 59.2 | 54.9 |
| 12 | 32.8 | 37.7 | 34.8 |
| 13 | 22.0 | 21.9 | 20.1 |
| 14 | 20.1 | 19.8 | 18.2 |
| 15 | 113.0 | 115.9 | 107.6 |

$\delta_{calc}$: unscaled chemical shifts of **1a** relative to TMS at the same level of theory;
$\delta_{scalc}$: calculated chemical shifts of **1a** after linear scaling.

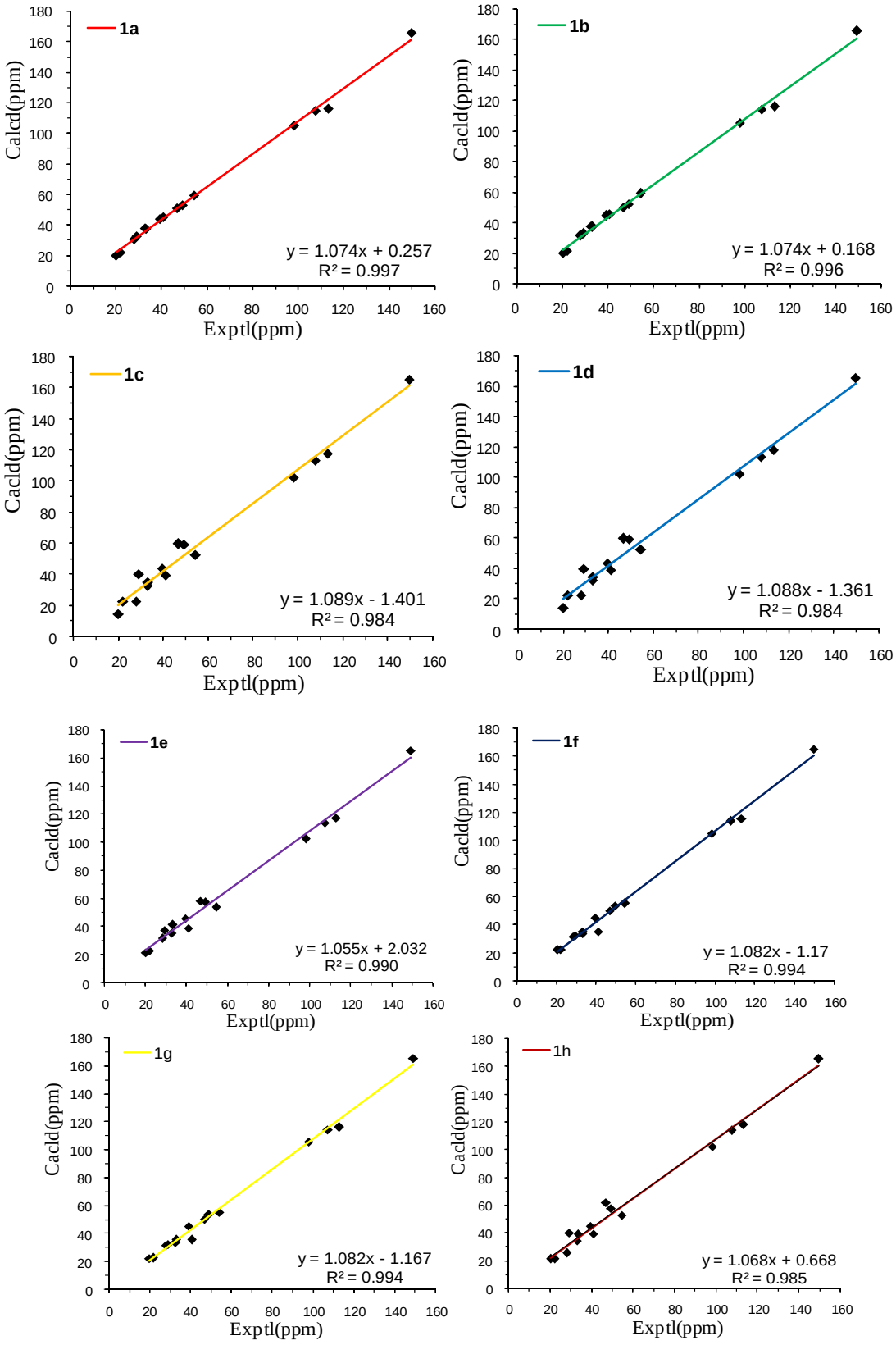



**Figure S4.** Correlation of experimental and calculated chemical shifts of compound **1** with **1a-1h**

**NOTE: 1a:** 3*R*,5*R*,10*S*,11*S*; **1b**: 3*S*,5*S*,10*R*,11*R*; **1c:** 3*R*,5*R*,10*R*,11*R*; **1d**: 3*S*,5*S*,10*S*,11*S*; **1e:** 3*R*,5*R*,10*R*,11*S*; **1f**: 3*R*,5*R*,10*S*,11*R*; **1g:** 3*S*,5*S*,10*R*,11*S*; **1h**: 3*S*,5*S*,10*S*,11*R*

## 3. ECD calculations details for 1 to determine the absolute configuration

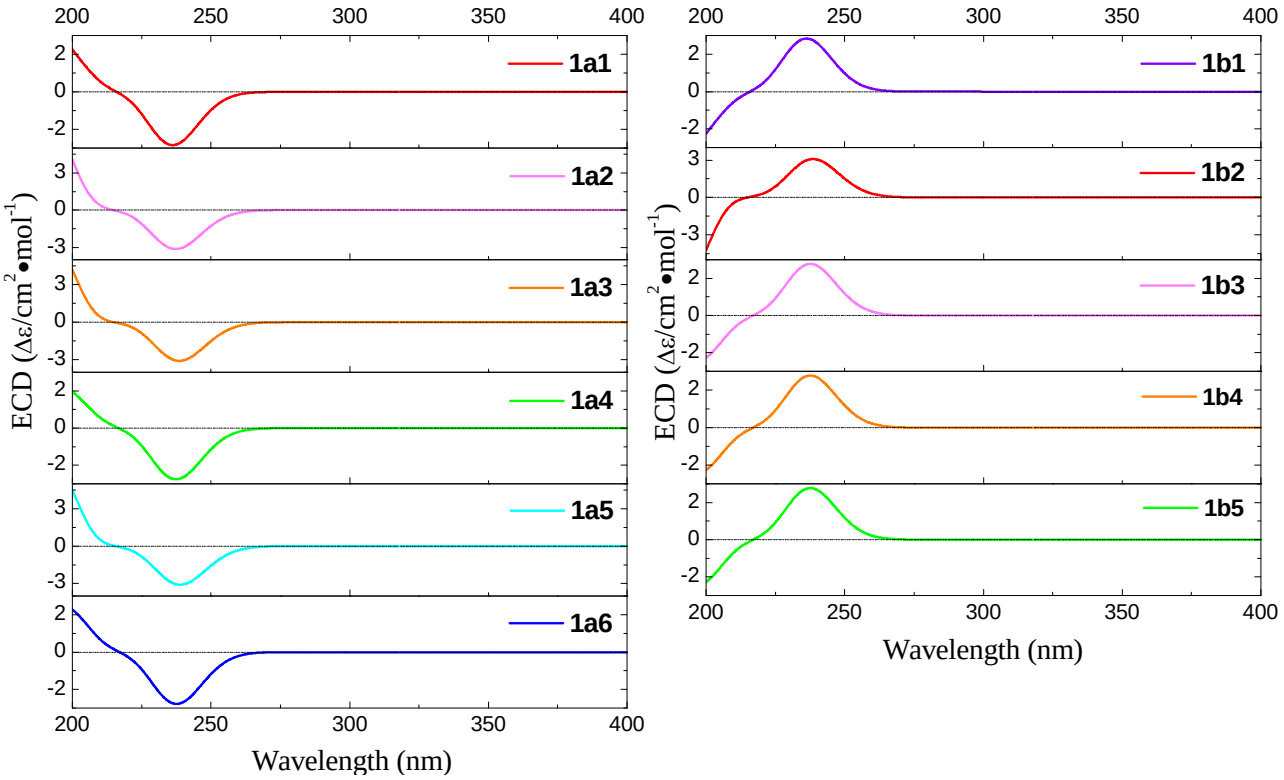



**Figure S5.** The corresponding calculated ECD of structural candidates with respective **1a** and **1b** configurations.

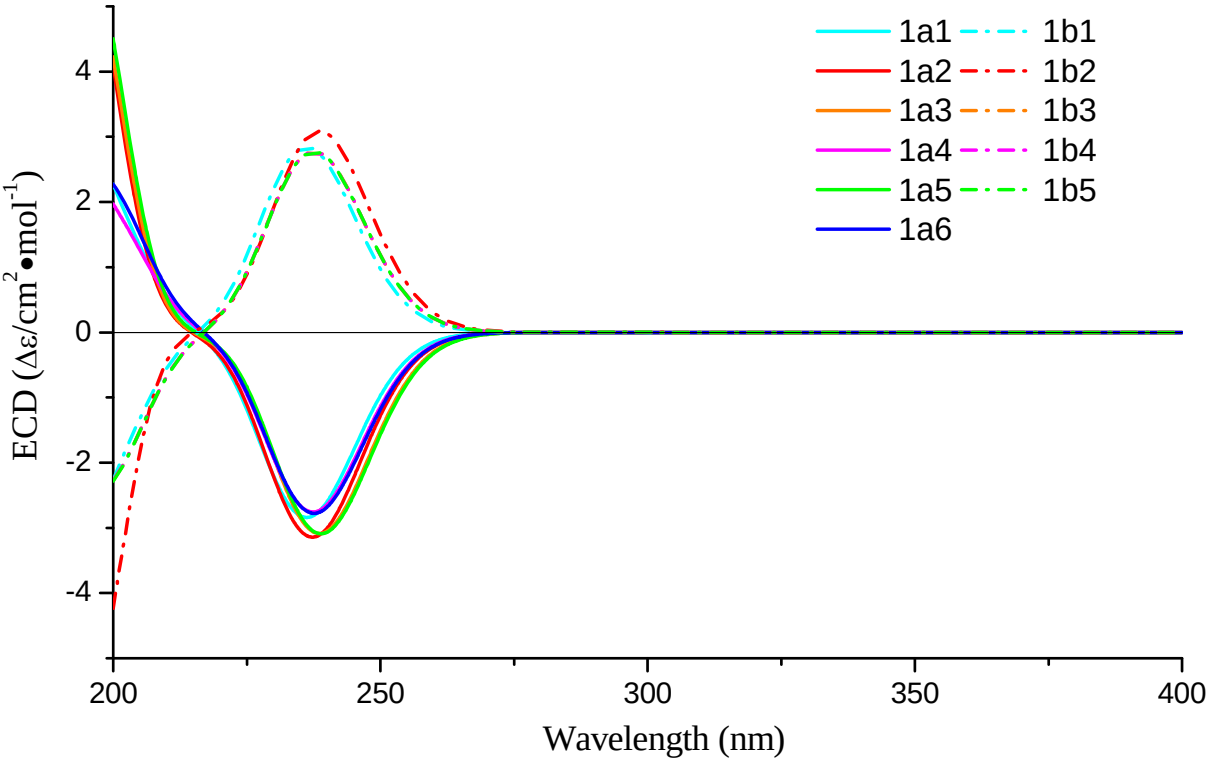



**Figure S6.** The overlaid ECD calculated for all the structural candidates.

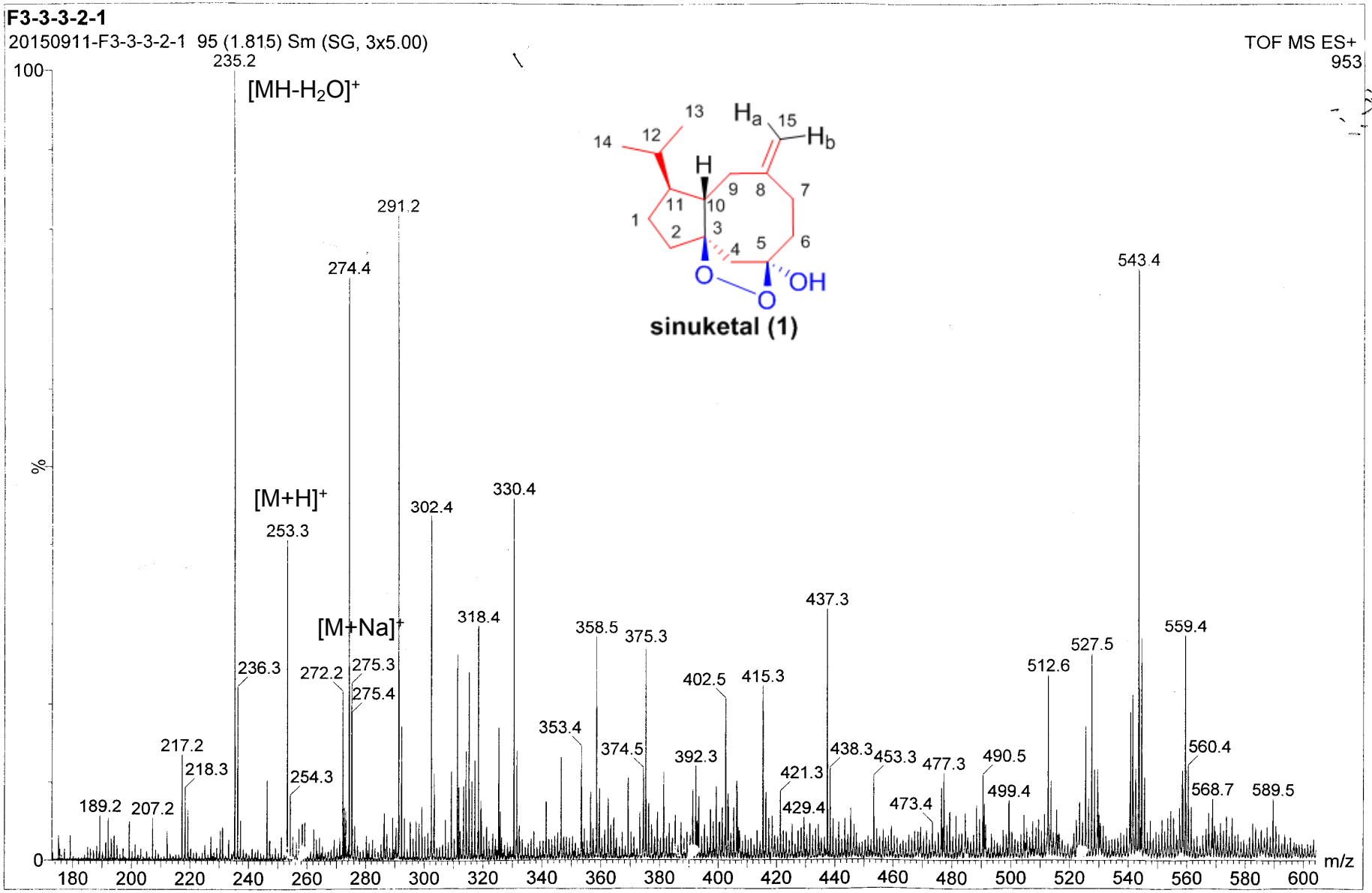



**Figure SS1 The positive ESIMS spectrum of sinuketal (1)**

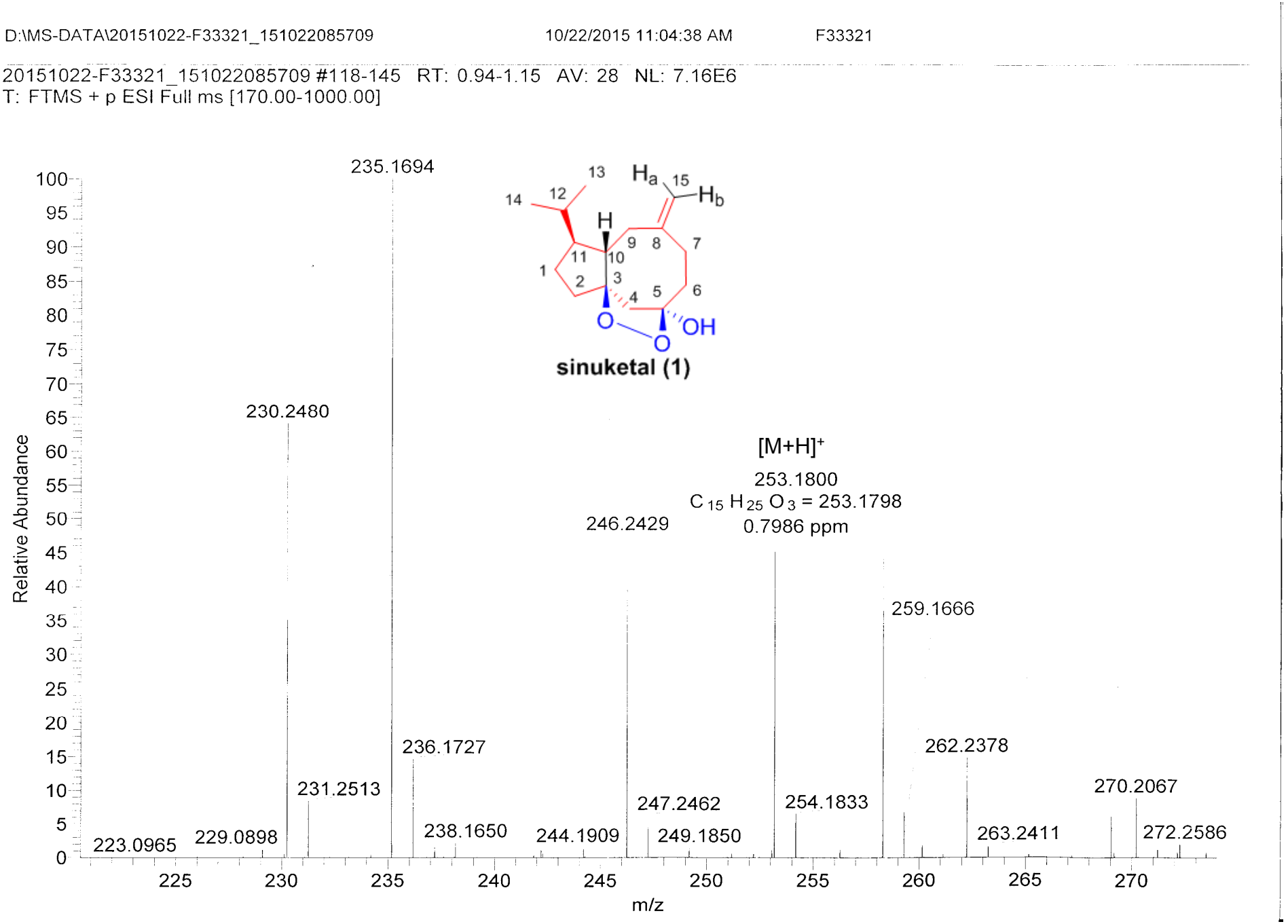



**Figure SS2 The positive HRESIMS spectrum of sinuketal (1)**

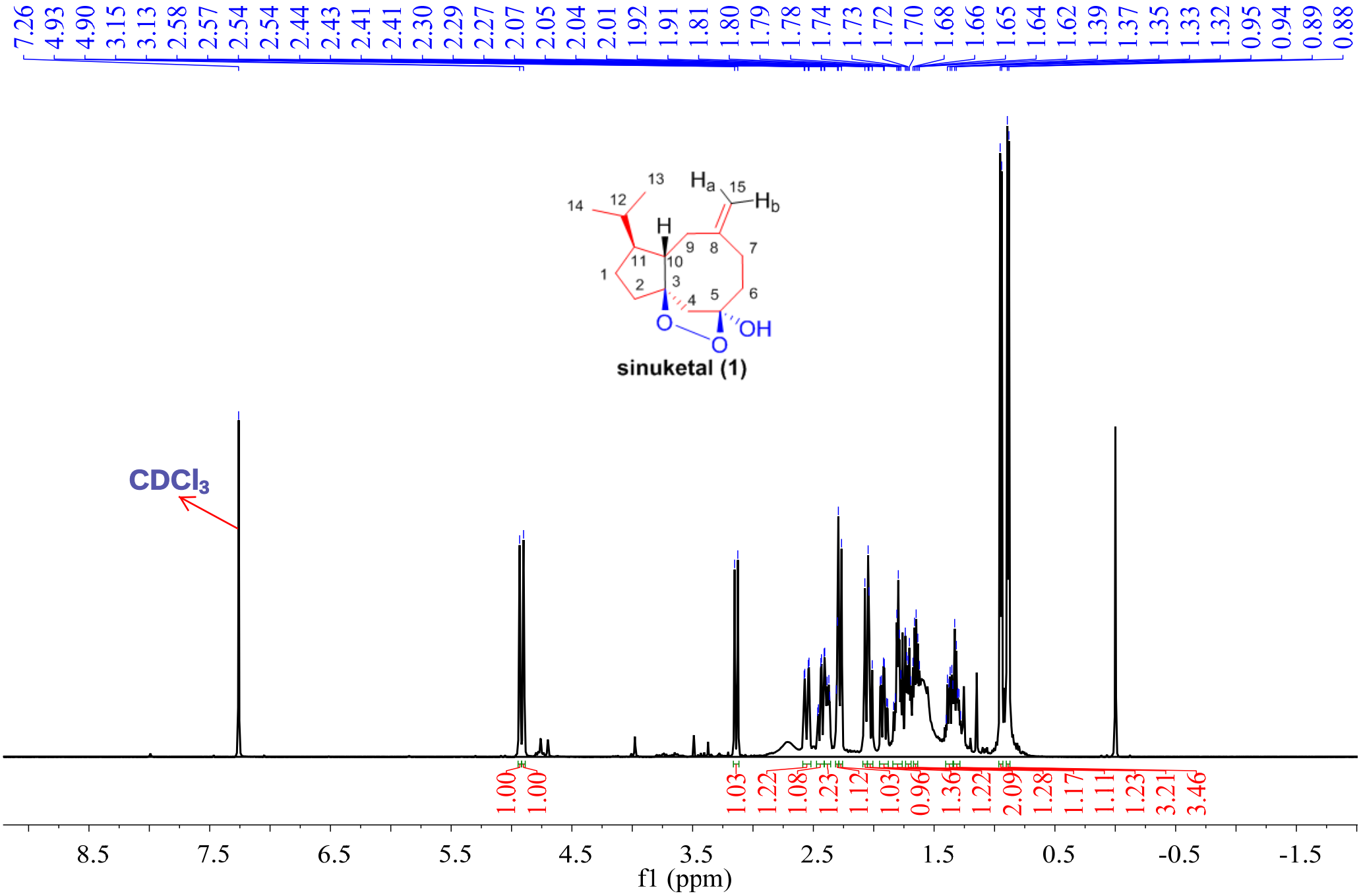



**Figure SS3 $^{1}$H NMR (500MHz, $CDCl_3$) spectrum of sinuketal (1)**

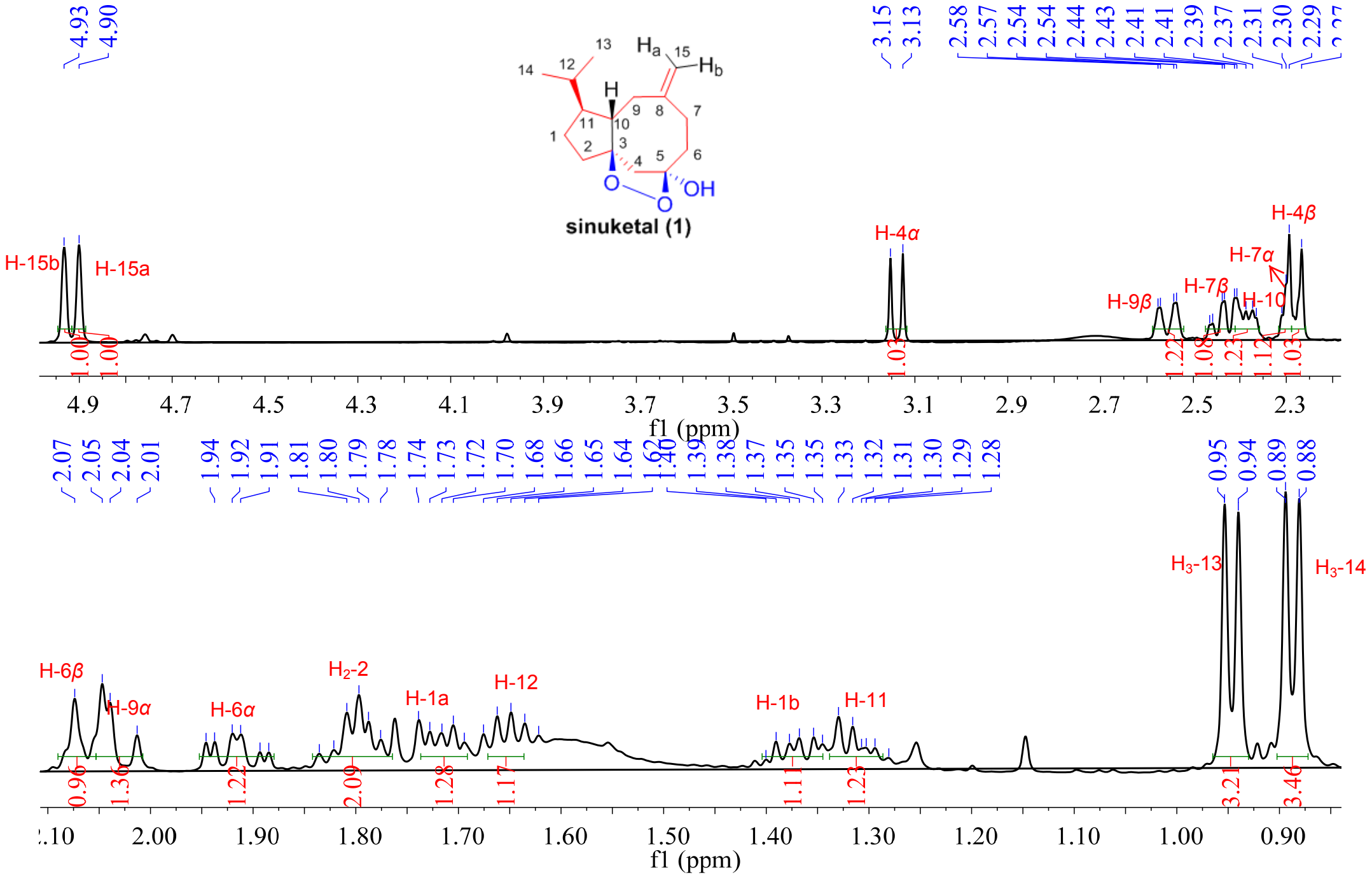



**Figure SS4 Amplificatory $^{1}$H NMR spectrum of sinuketal (1)**

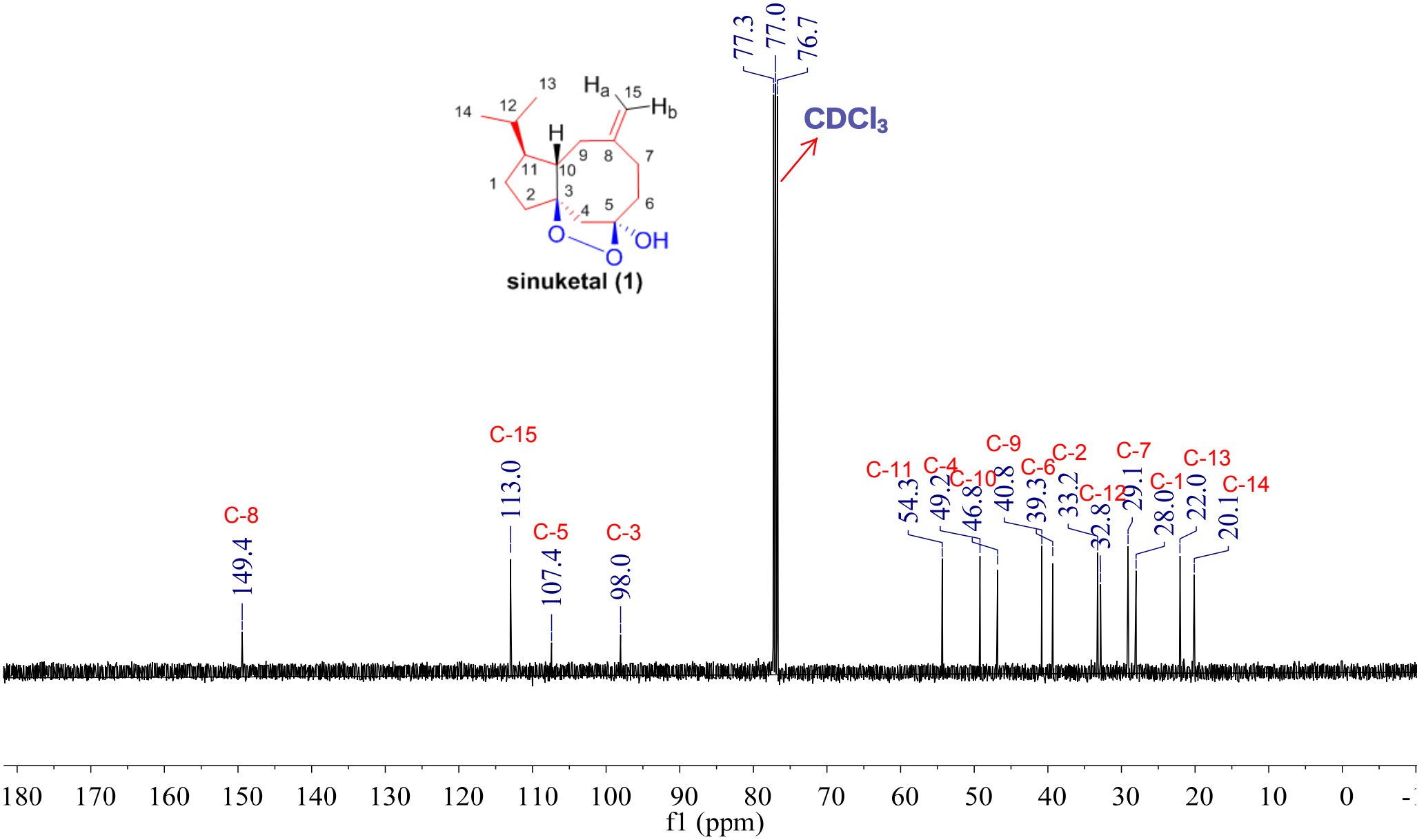



**Figure SS5 $^{13}C$ NMR (125MHz, $CDCl_3$) spectrum of sinuketal (1)**

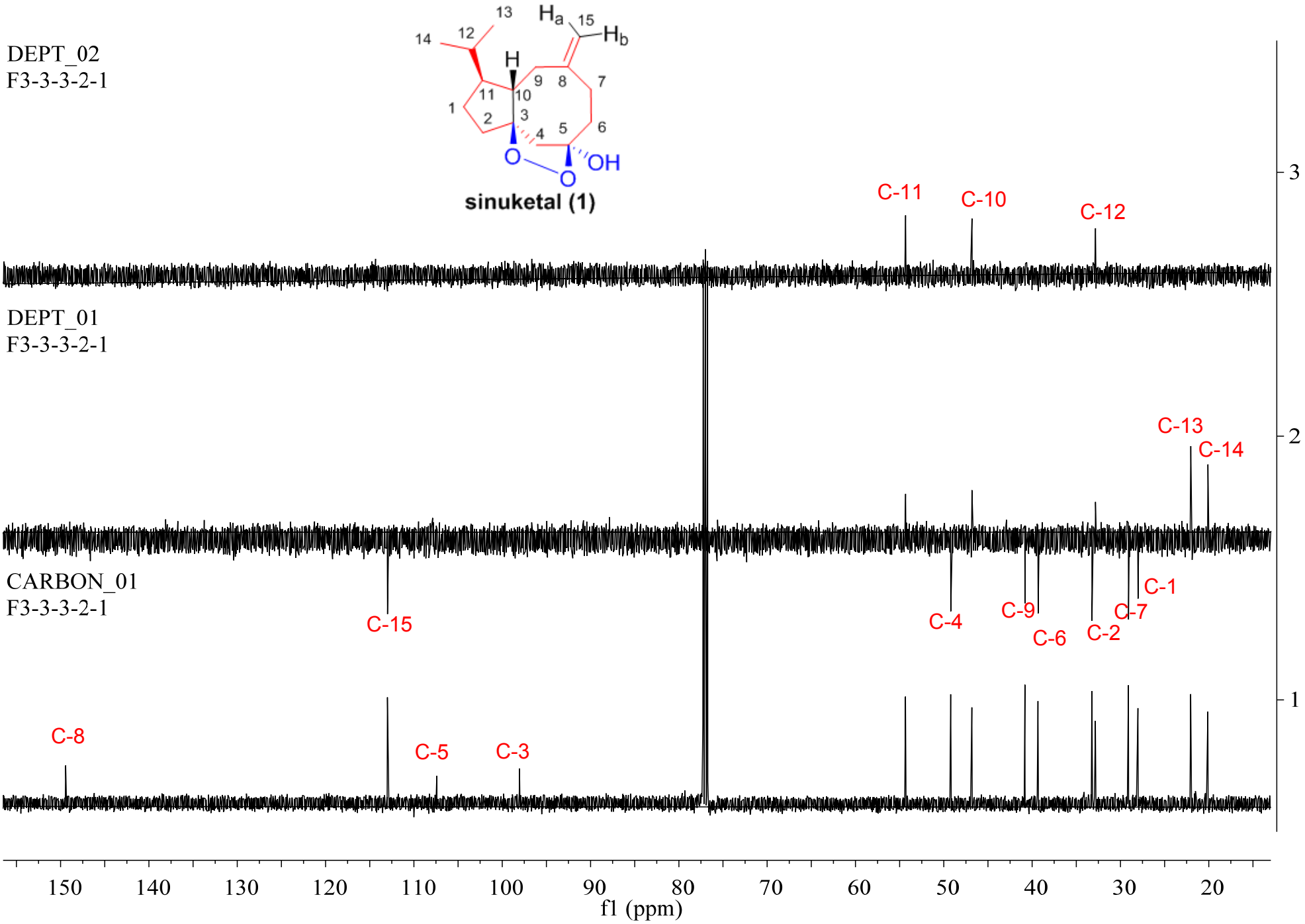



**Figure SS6 DEPT spectrum of sinuketal (1)**

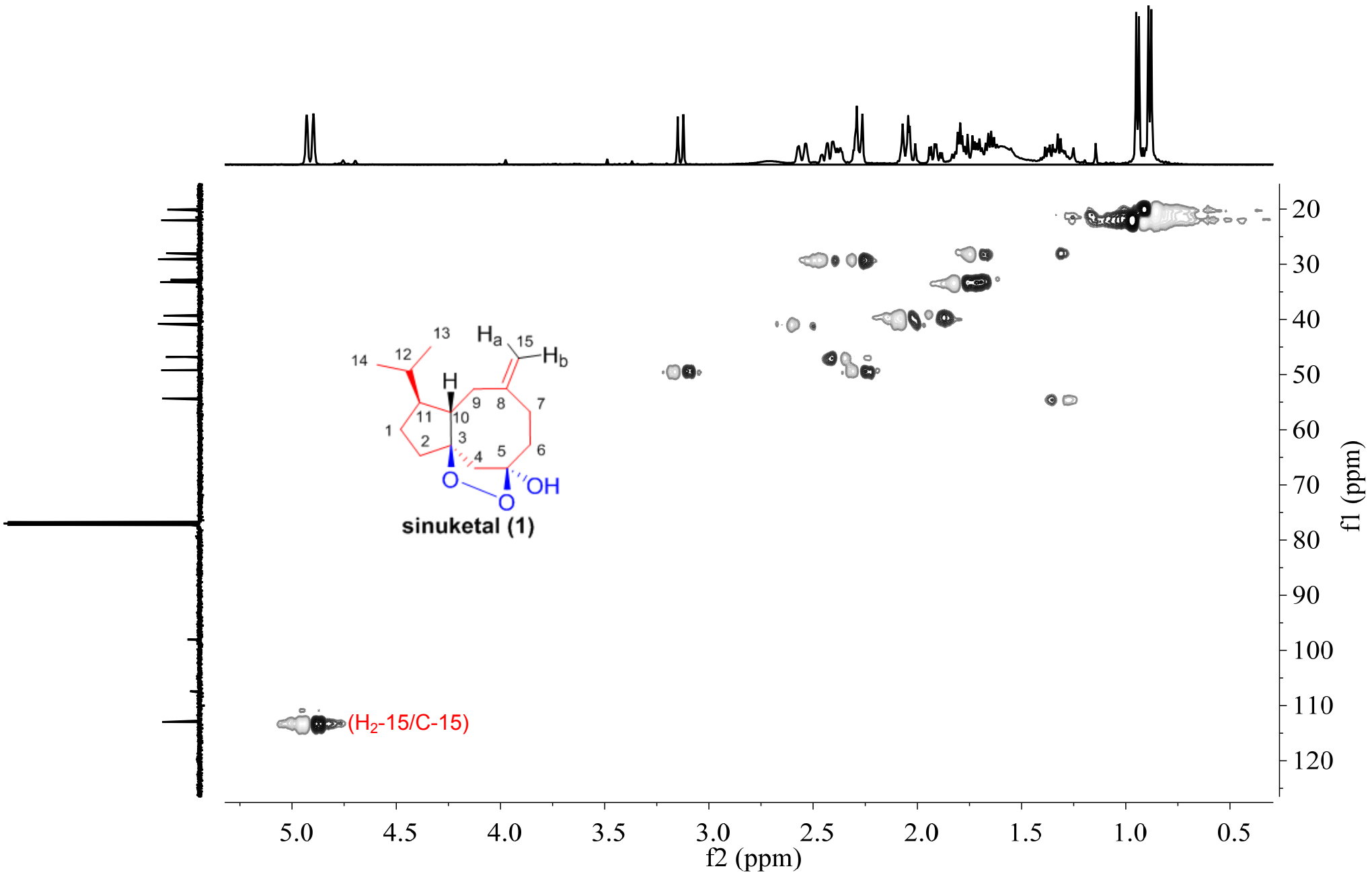



**Figure SS7 HMQC spectrum of sinuketal (1)**

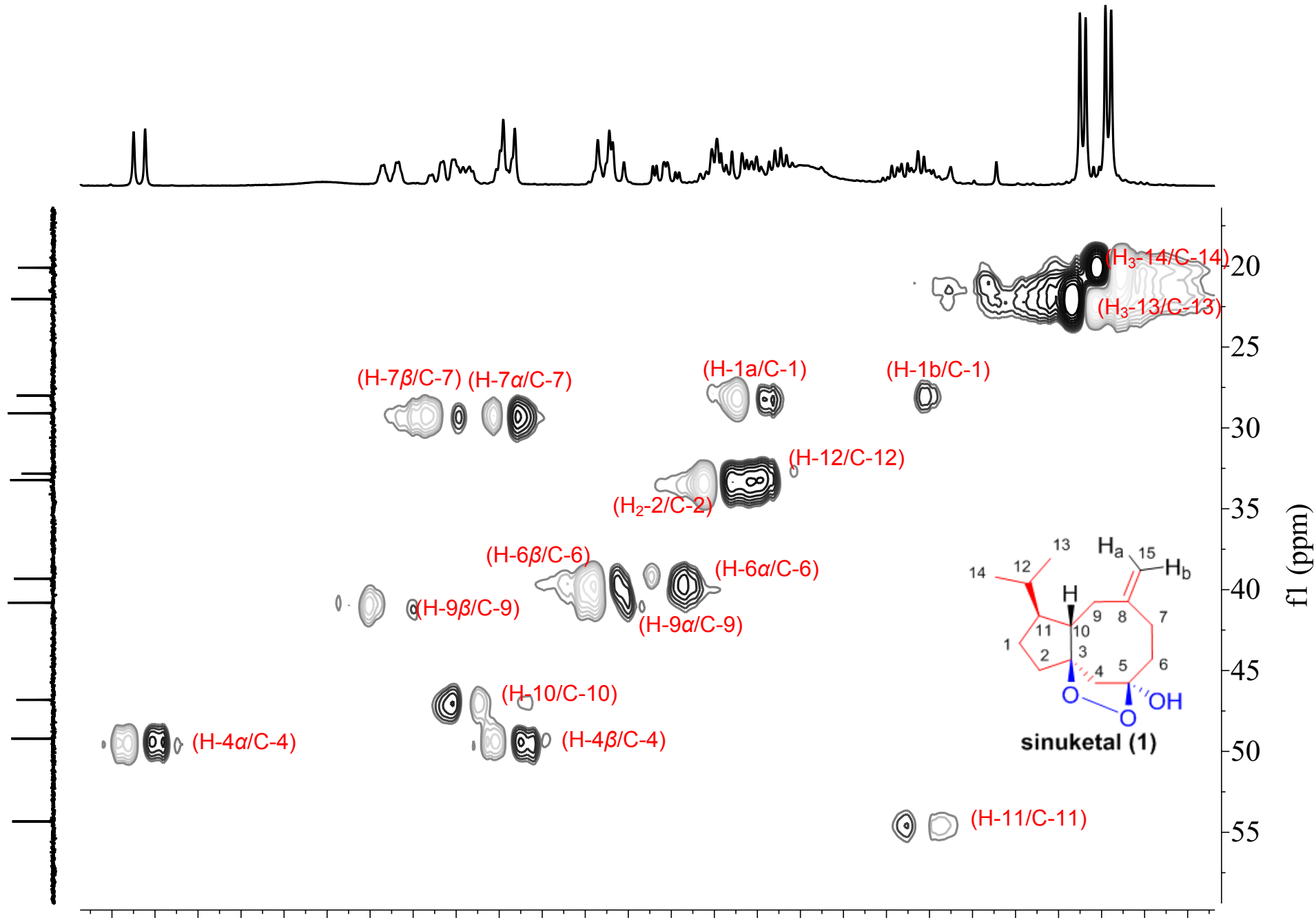



**Figure SS8 Partial HMQC spectrum of sinuketal (1)**

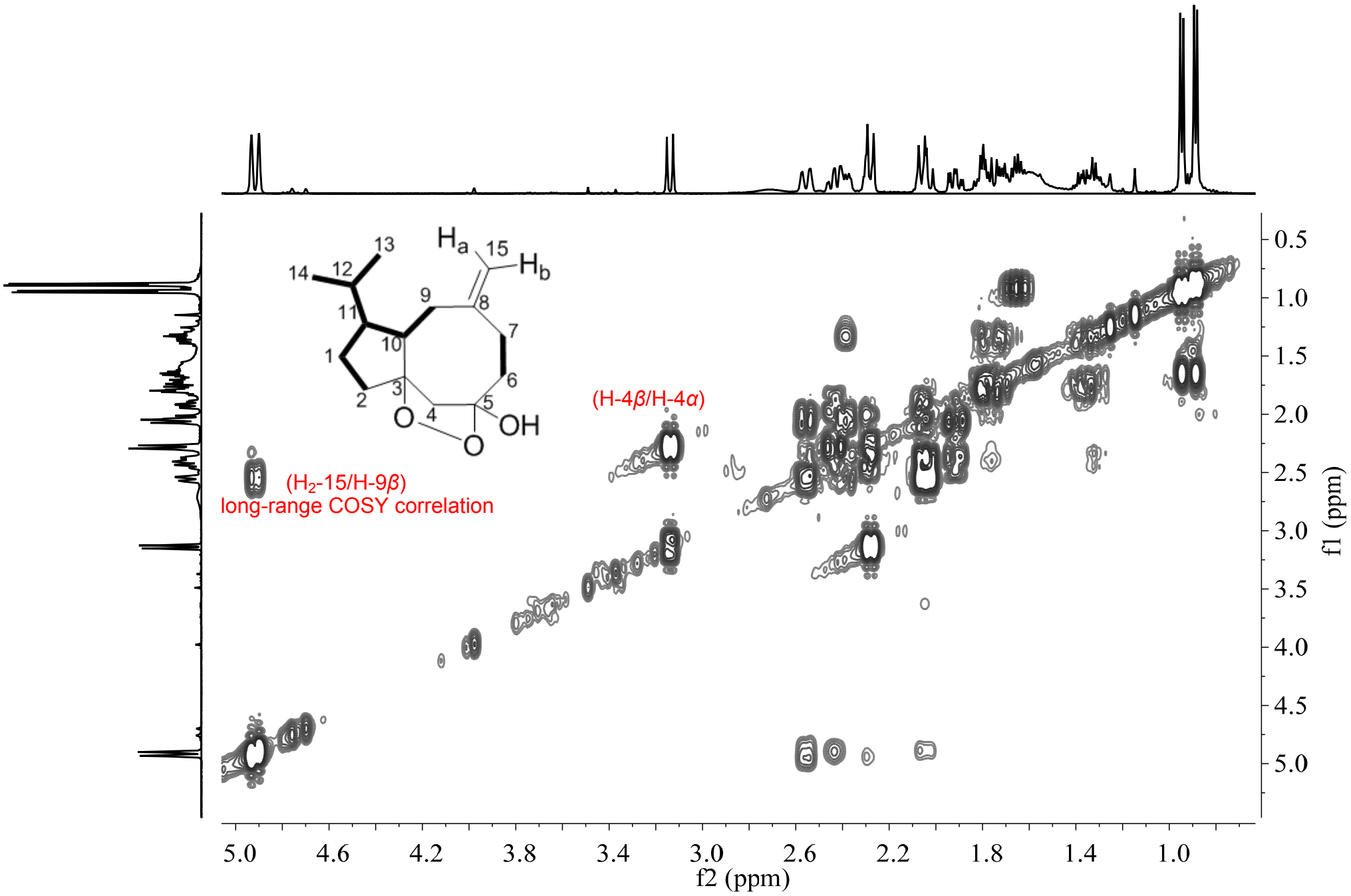



**Figure SS9 $^{1}$H-$^{1}$H COSY spectrum of sinuketal (1)**

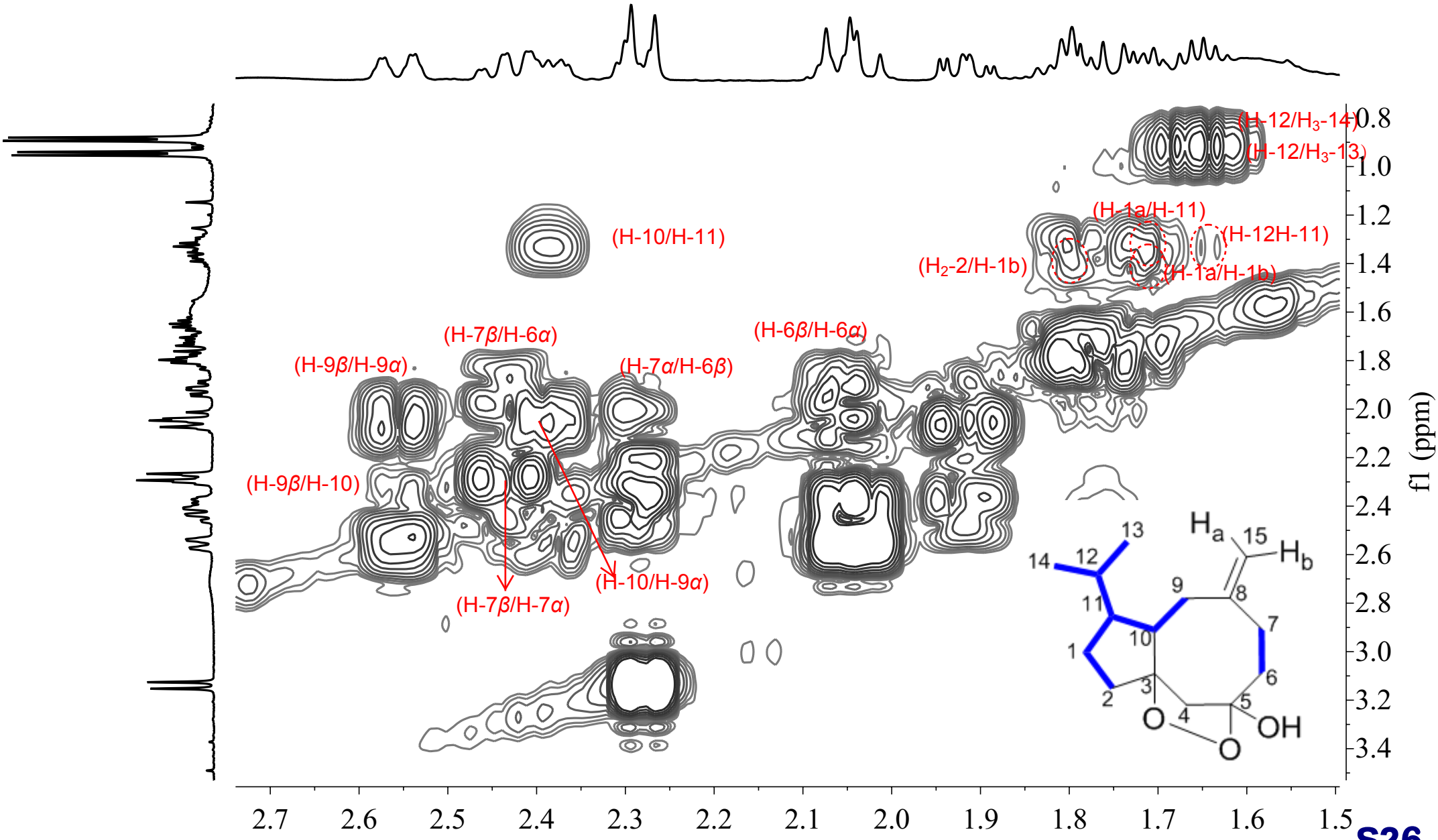



**Figure SS10 Partial $^{1}H$-$^{1}H$ COSY spectrum of sinuketal (1)**

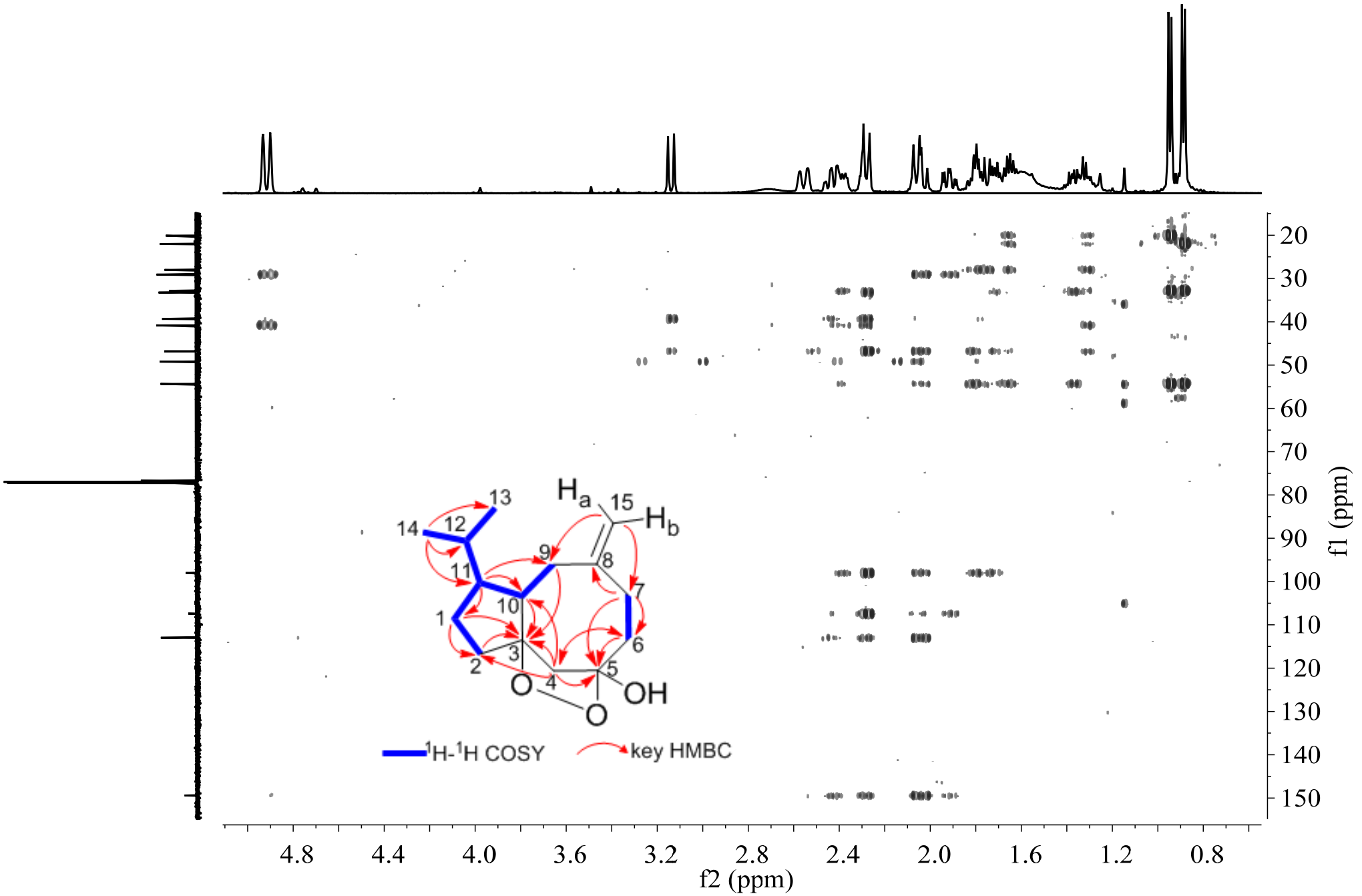



**Figure SS11 Key HMBC spectrum of sinuketal (1)**

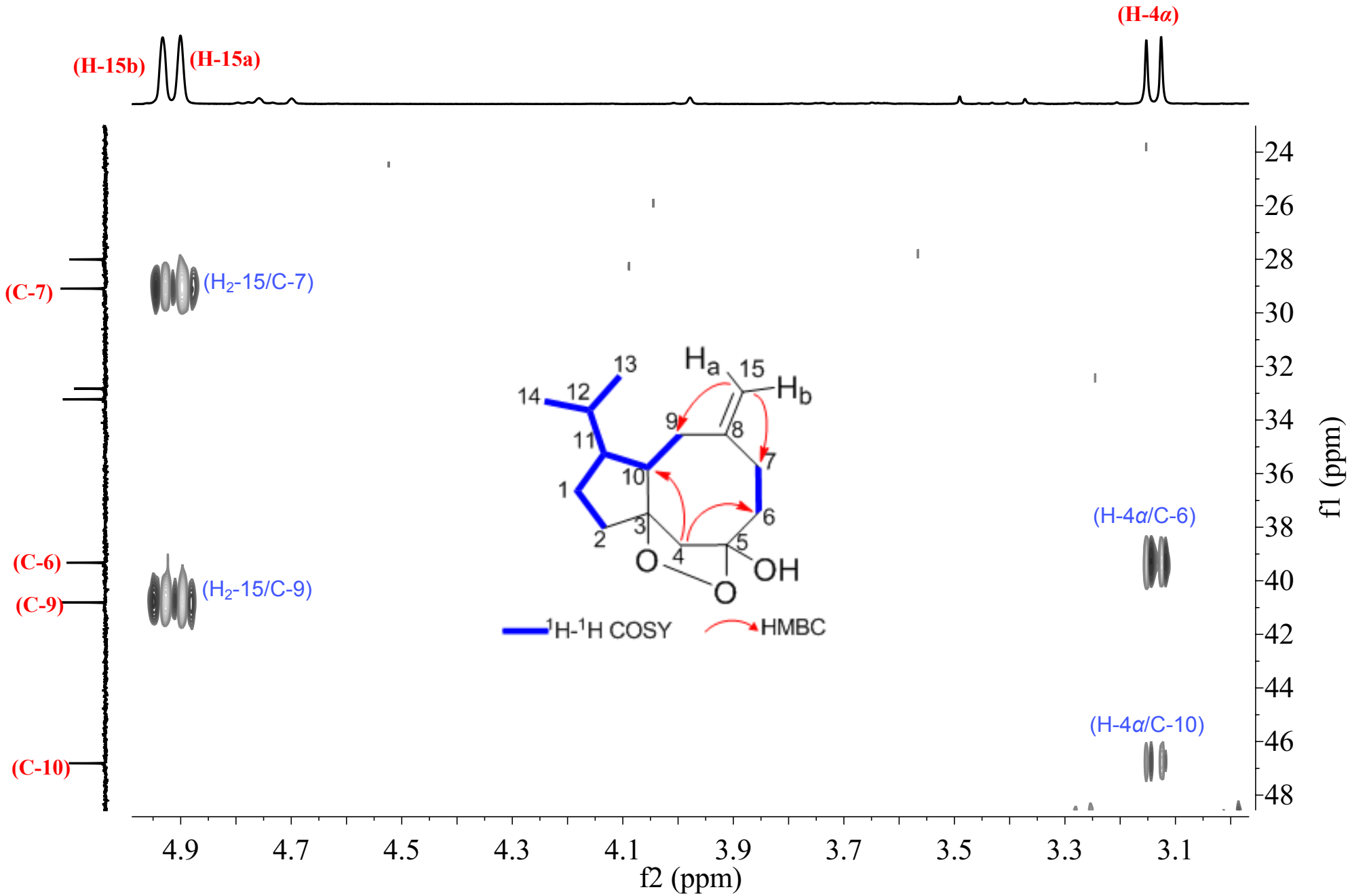



**Figure SS12 Partial HMBC spectrum of sinuketal (1) (A)**

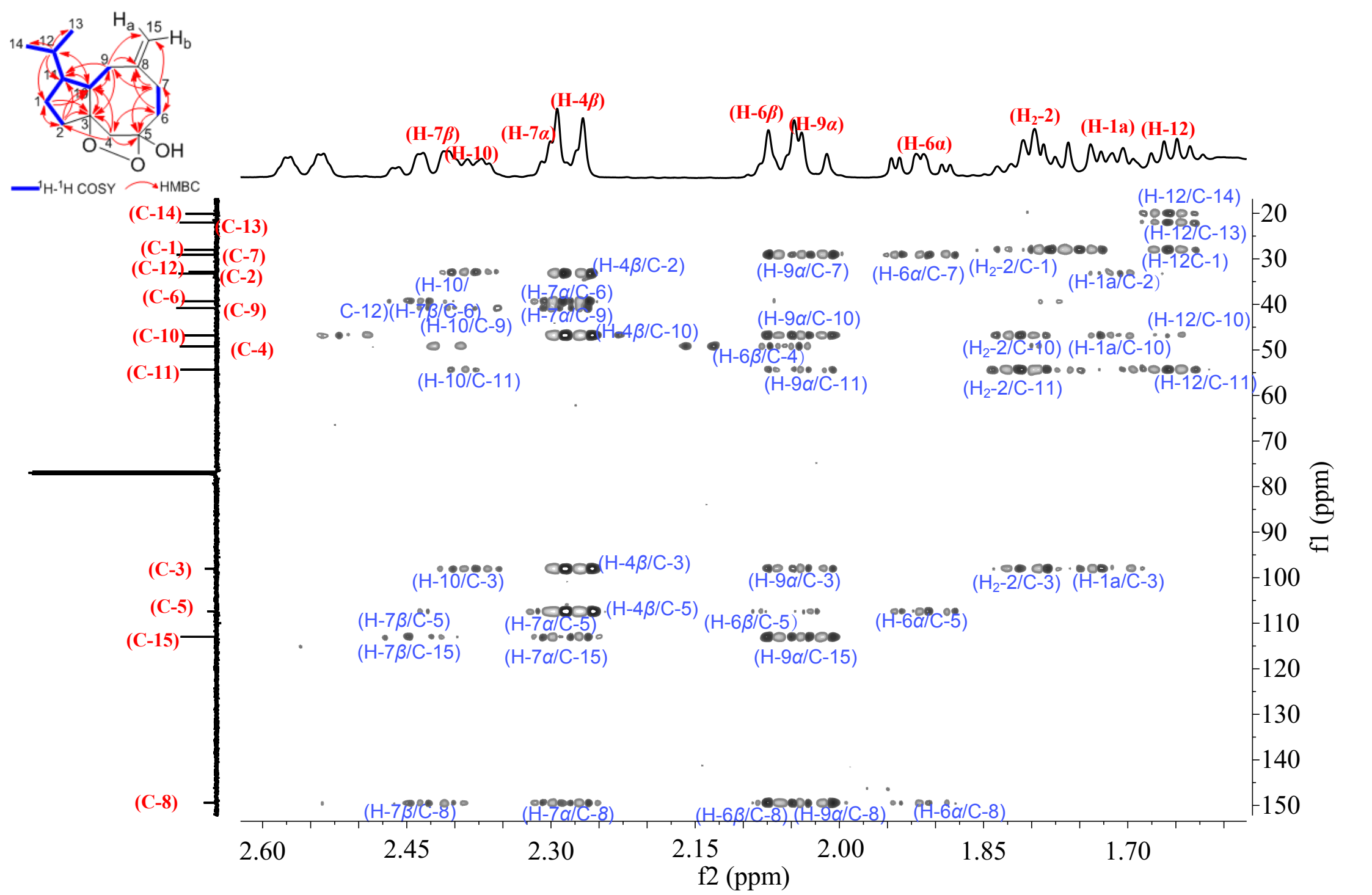



**Figure SS13 Partial HMBC spectrum of sinuketal (1) (B)**

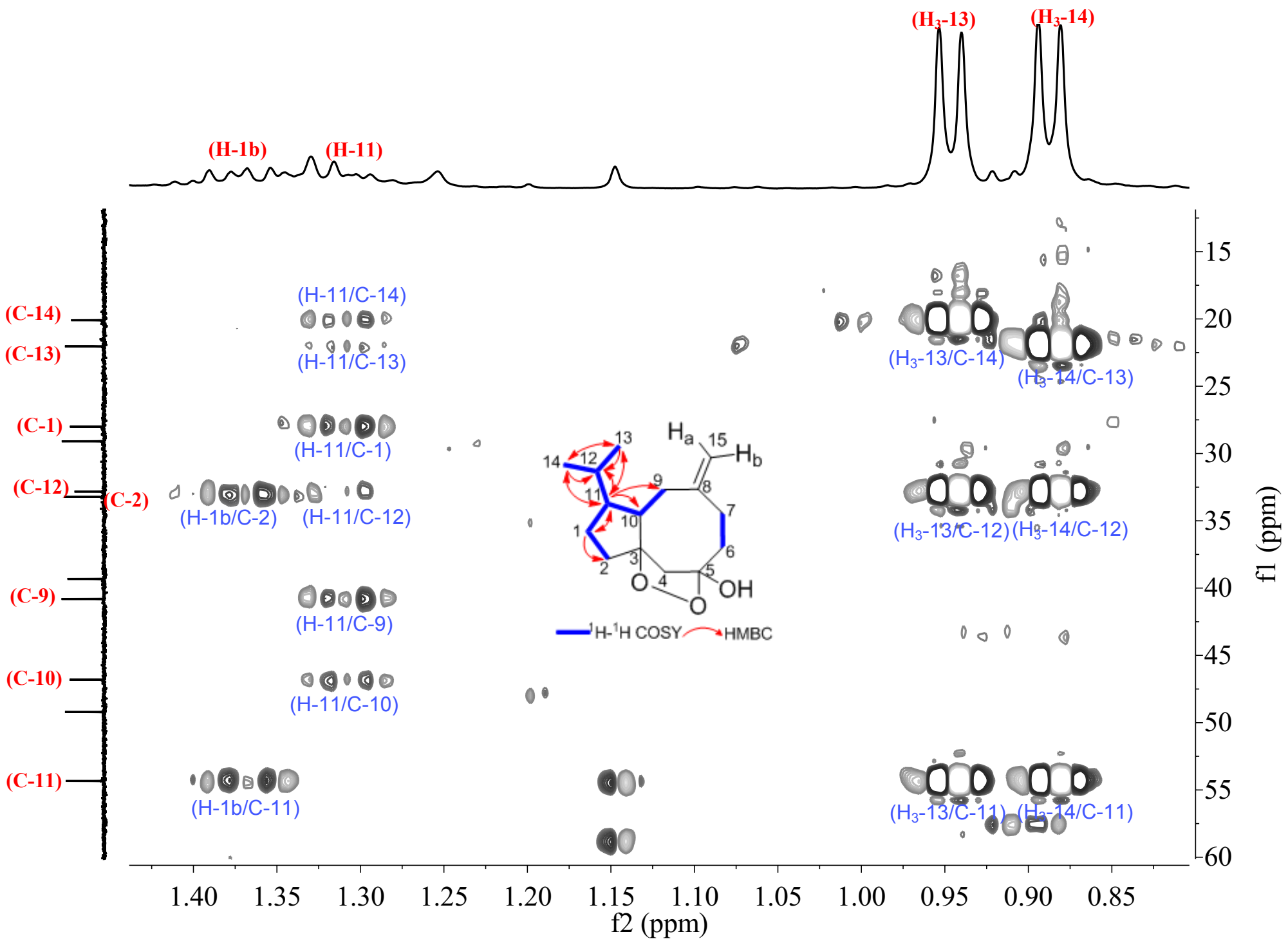



**Figure SS14 Partial HMBC spectrum of sinuketal (1) (C)**

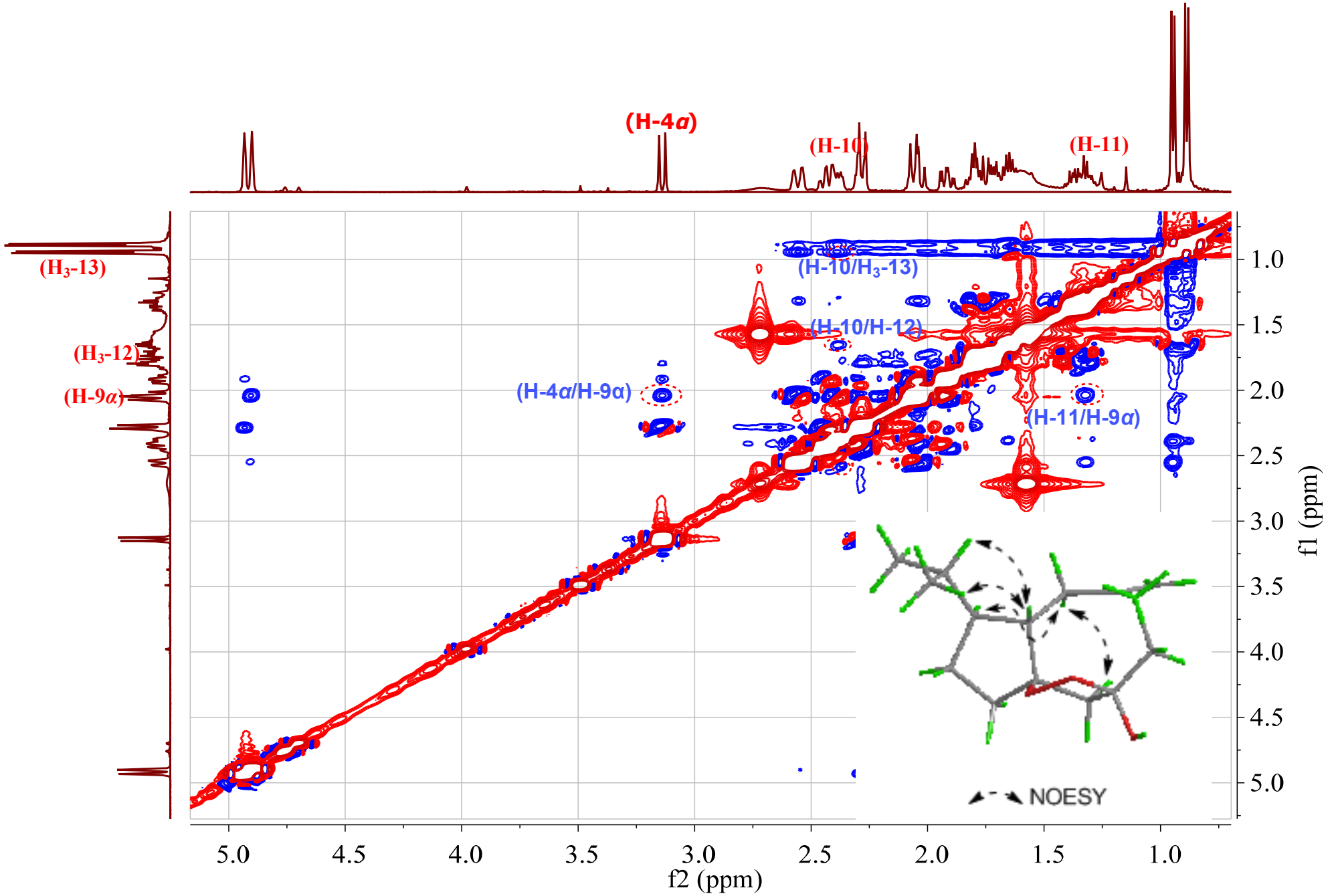



**Figure SS15 NOESY spectrum of sinuketal (1)**

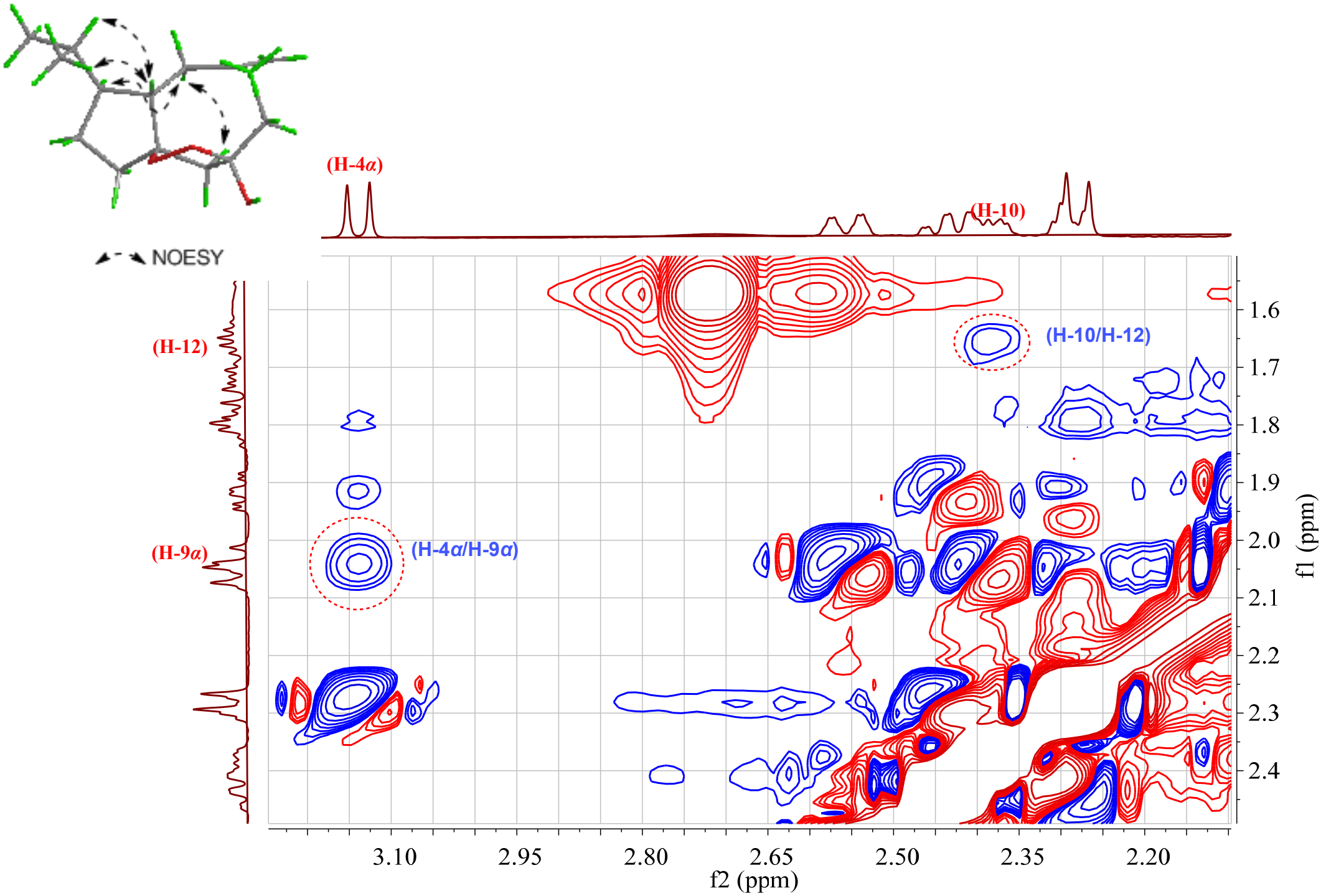



**Figure SS16 Key amplificatory NOESY spectrum of sinuketal (1)**

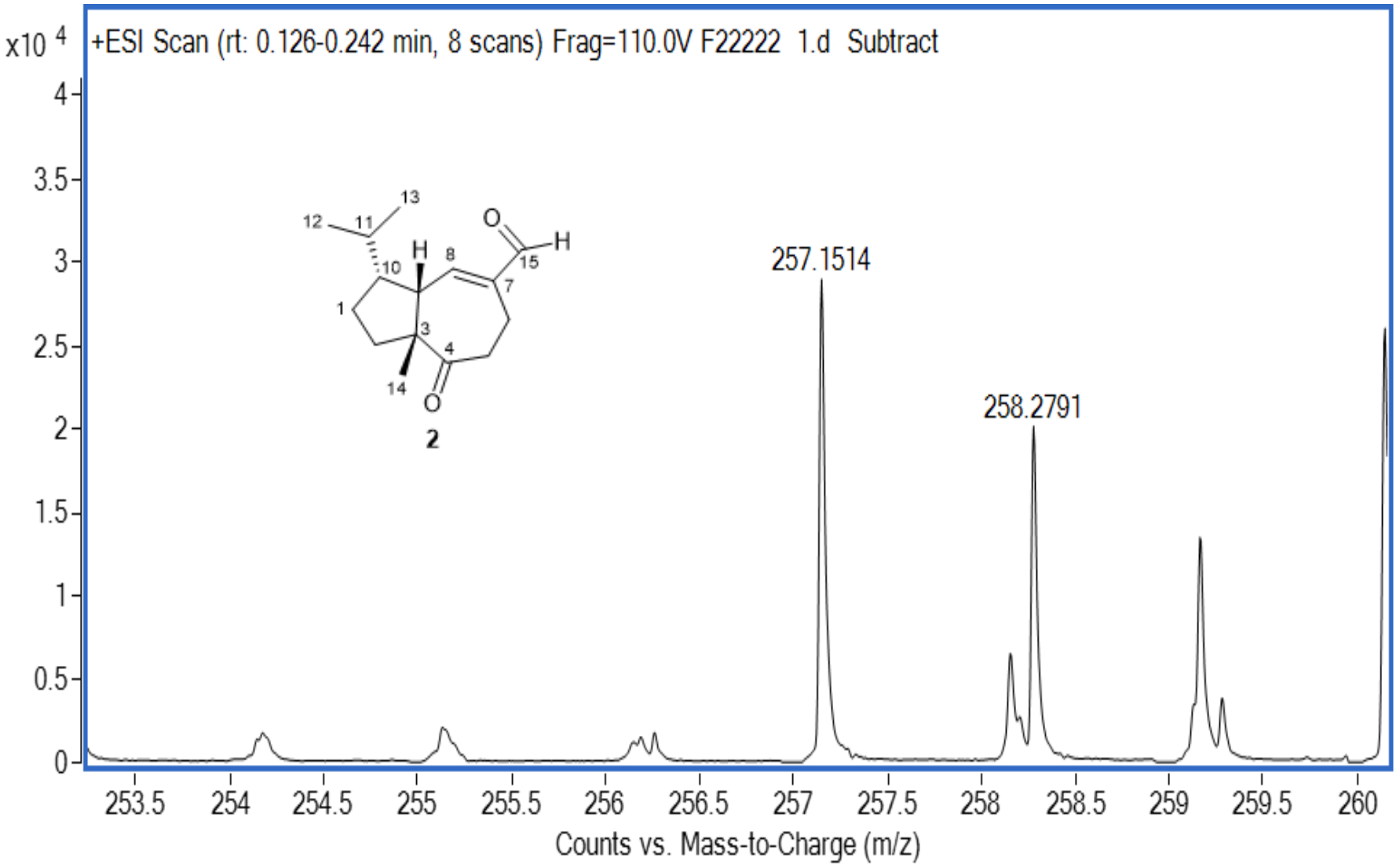



**Figure SS17 The positive HRESIMS spectrum of sinulin A (2)**

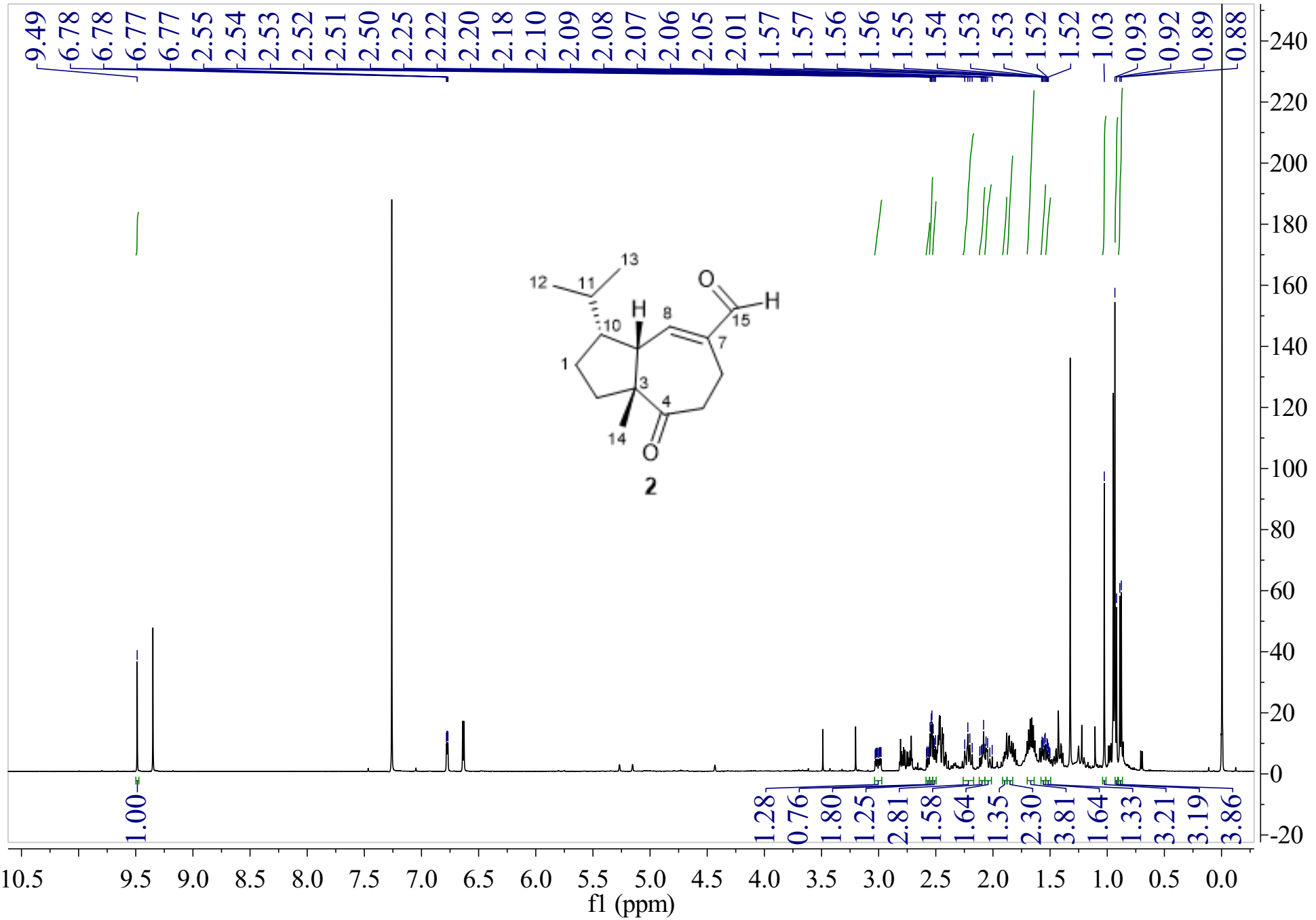



**Figure SS18 $^{1}H$ NMR (500MHz, $CDCl_3$) spectrum of sinulin A (2) and compound (6)**

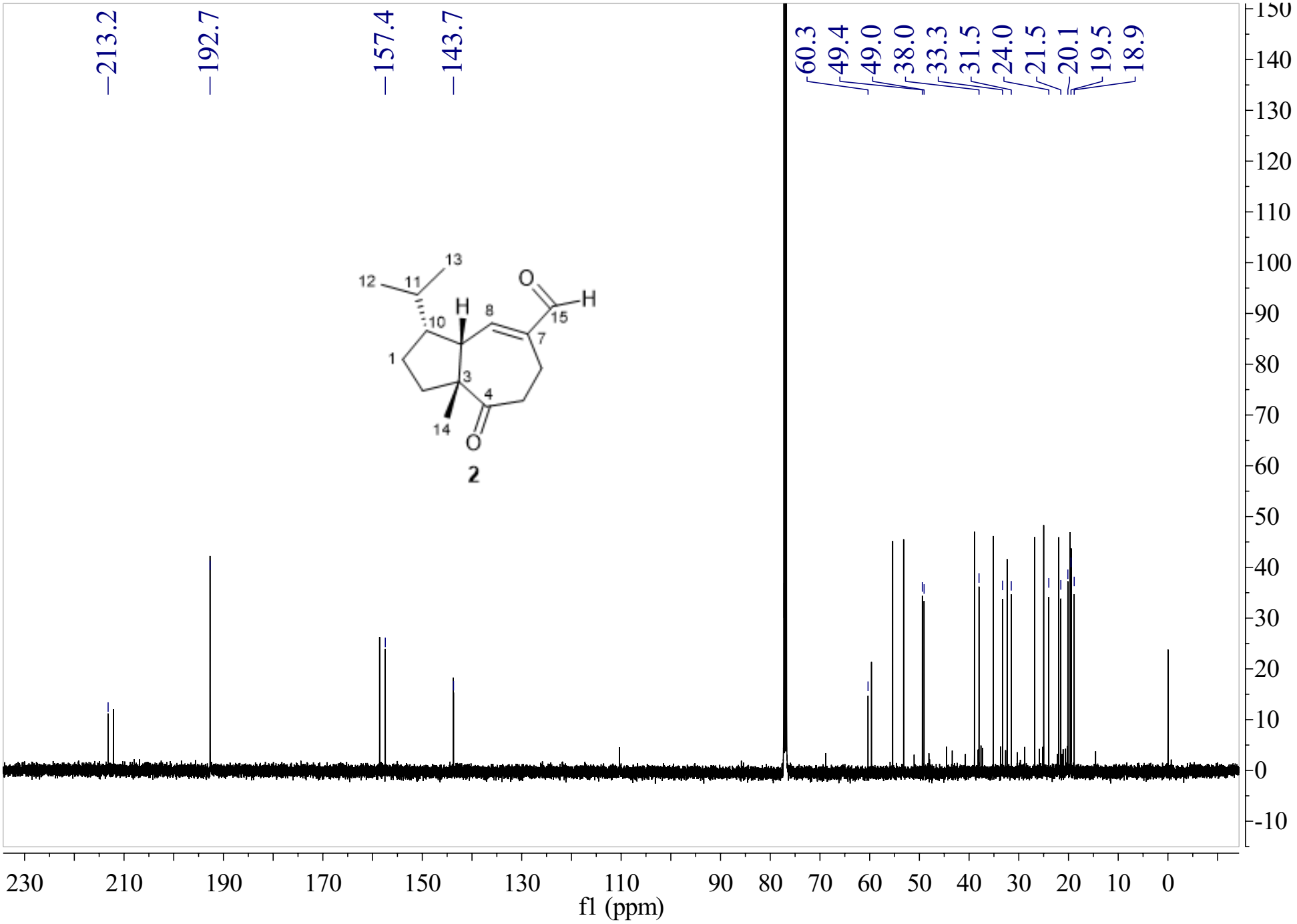



**Figure SS19 $^{13}C$ NMR (125MHz, $CDCl_3$) spectrum of sinulin A (2) and compound (6)**

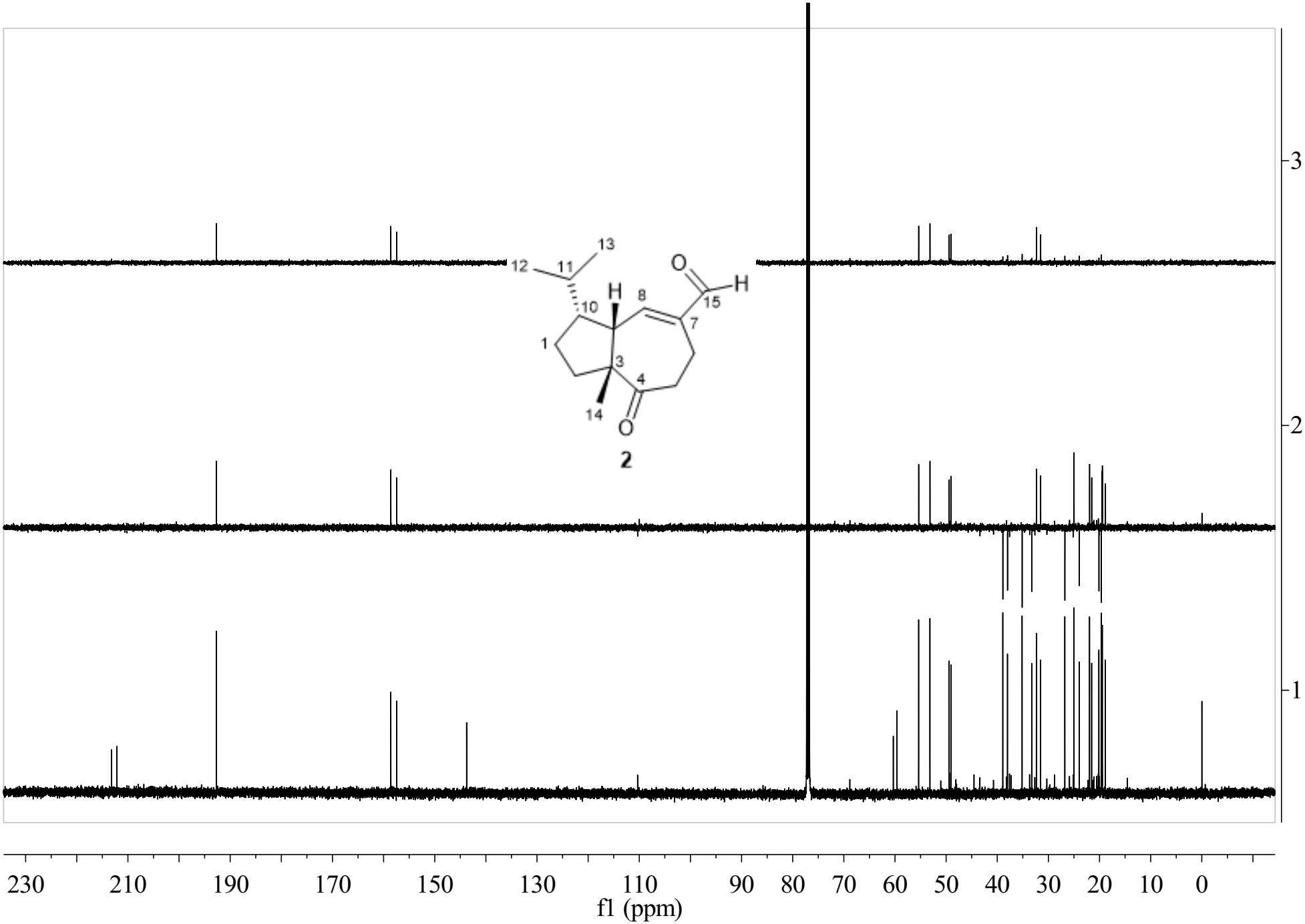



**Figure SS20 DEPT spectrum of sinulin A (2) and compound (6)**

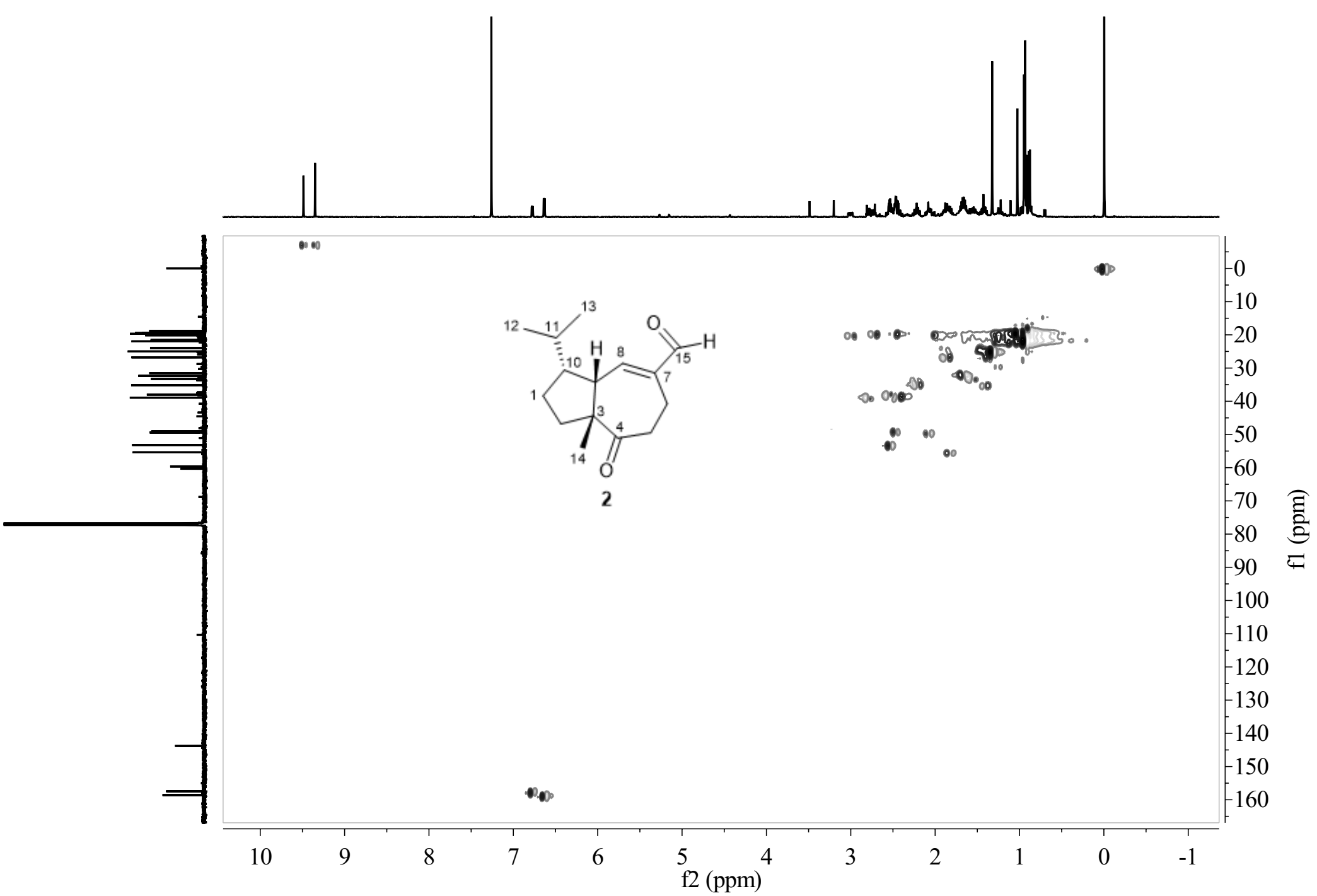



**Figure SS21 HMQC spectrum of sinulin A (2) and compound (6)**

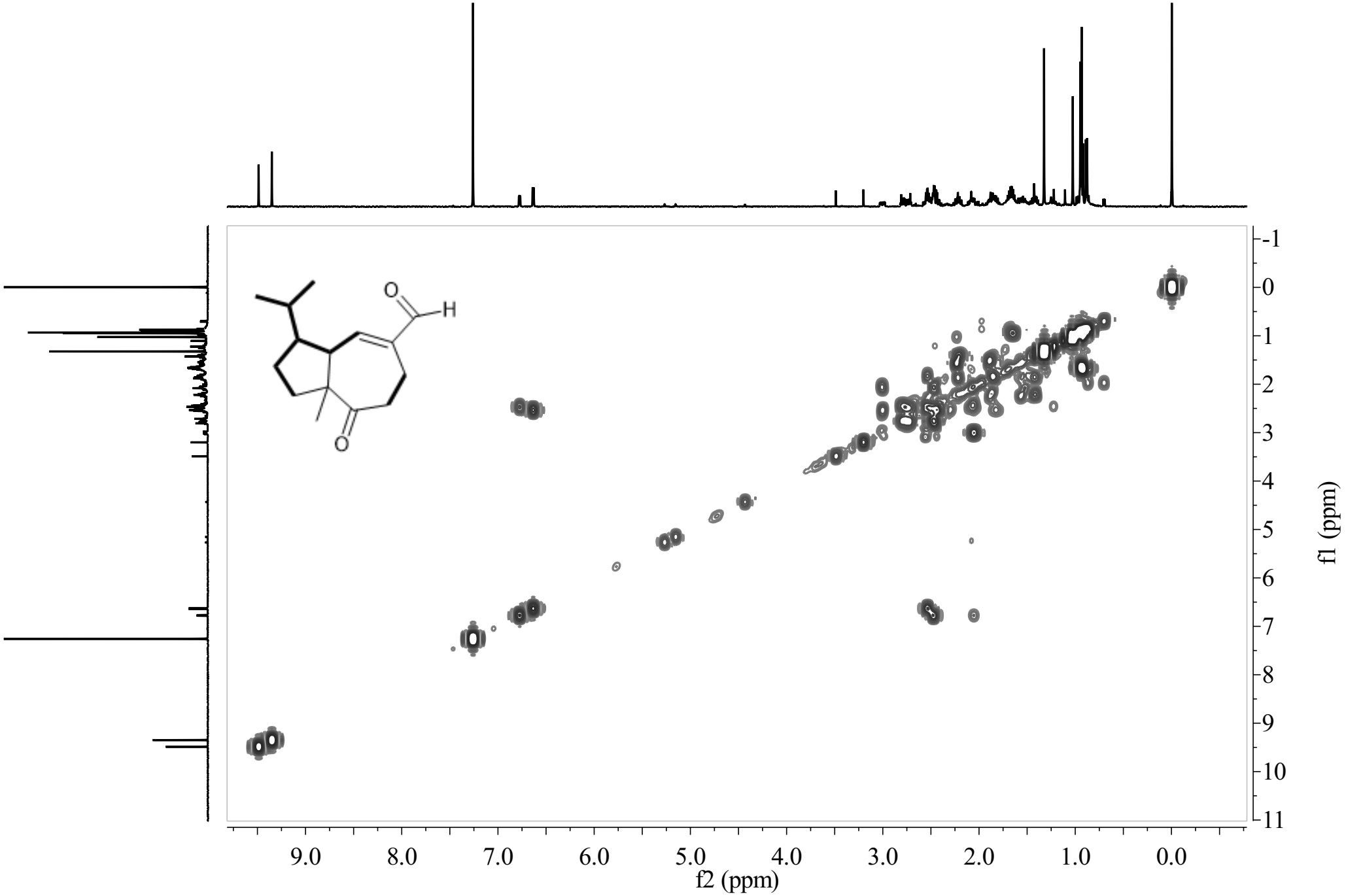



**Figure SS22 $^{1}$H-$^{1}$H COSY spectrum of sinulin A (2) and compound (6)**

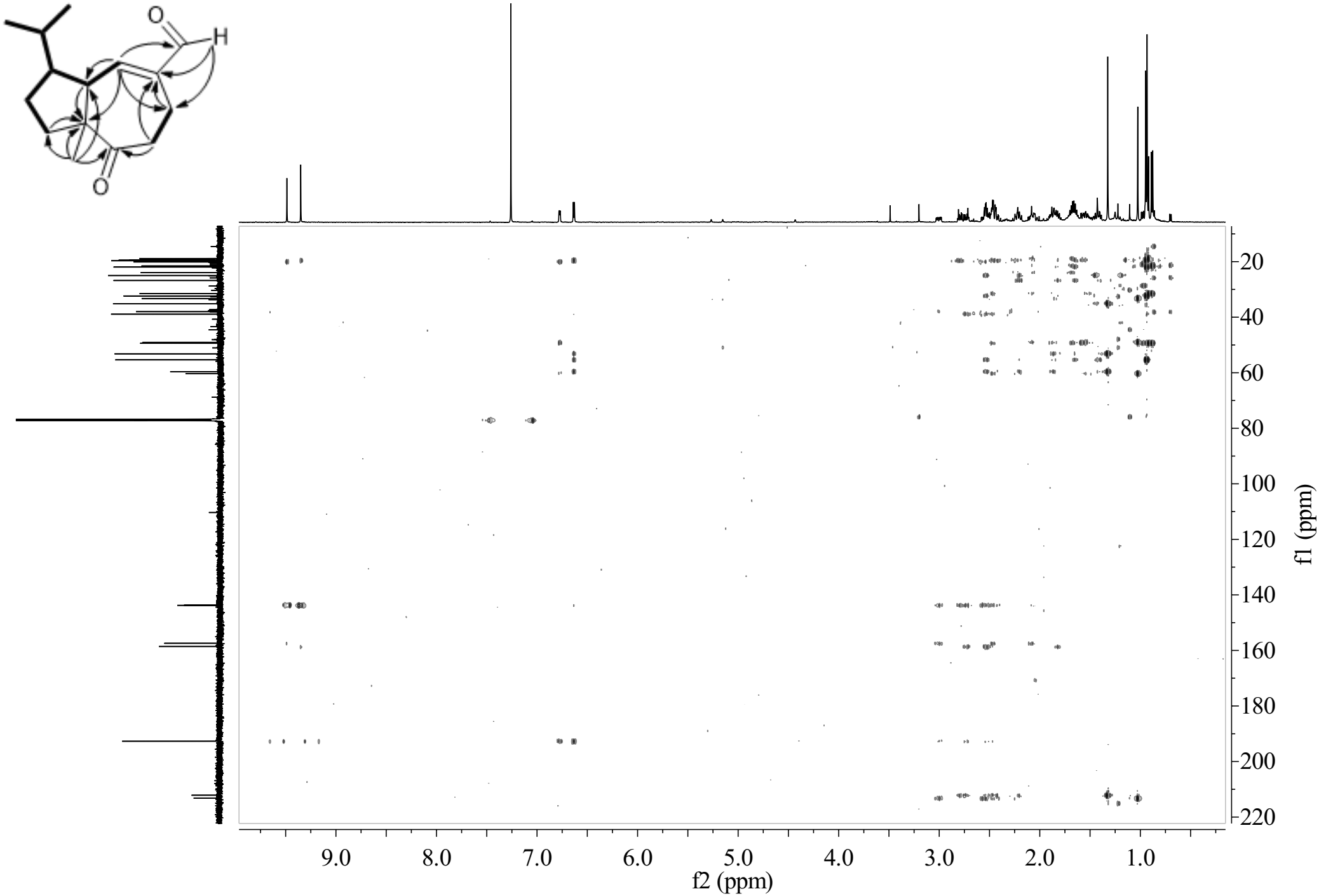



**Figure SS23 HMBC spectrum of sinulin A (2) and compound (6)**

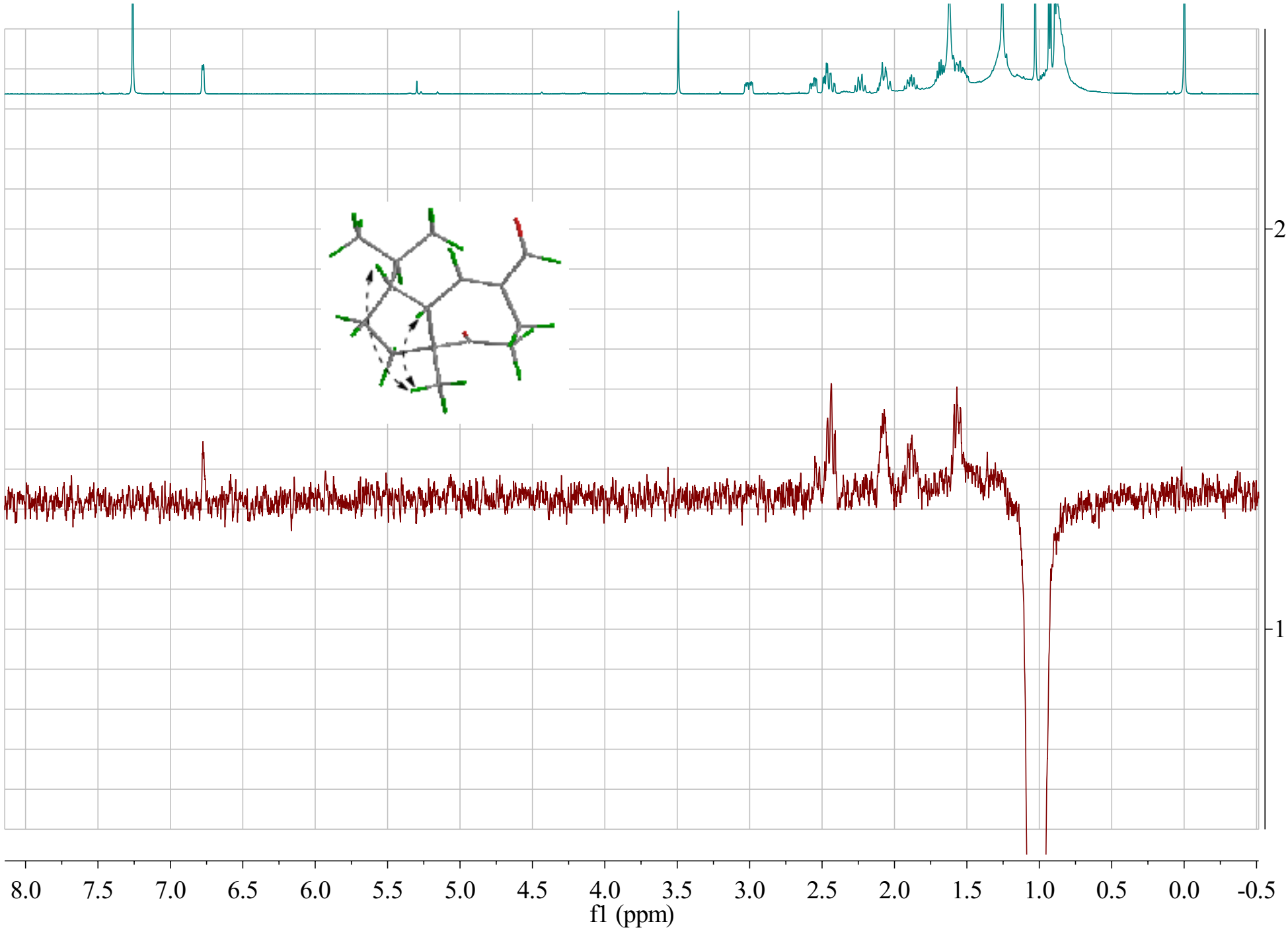



**Figure SS24 NOE spectrum of sinulin A (2)**

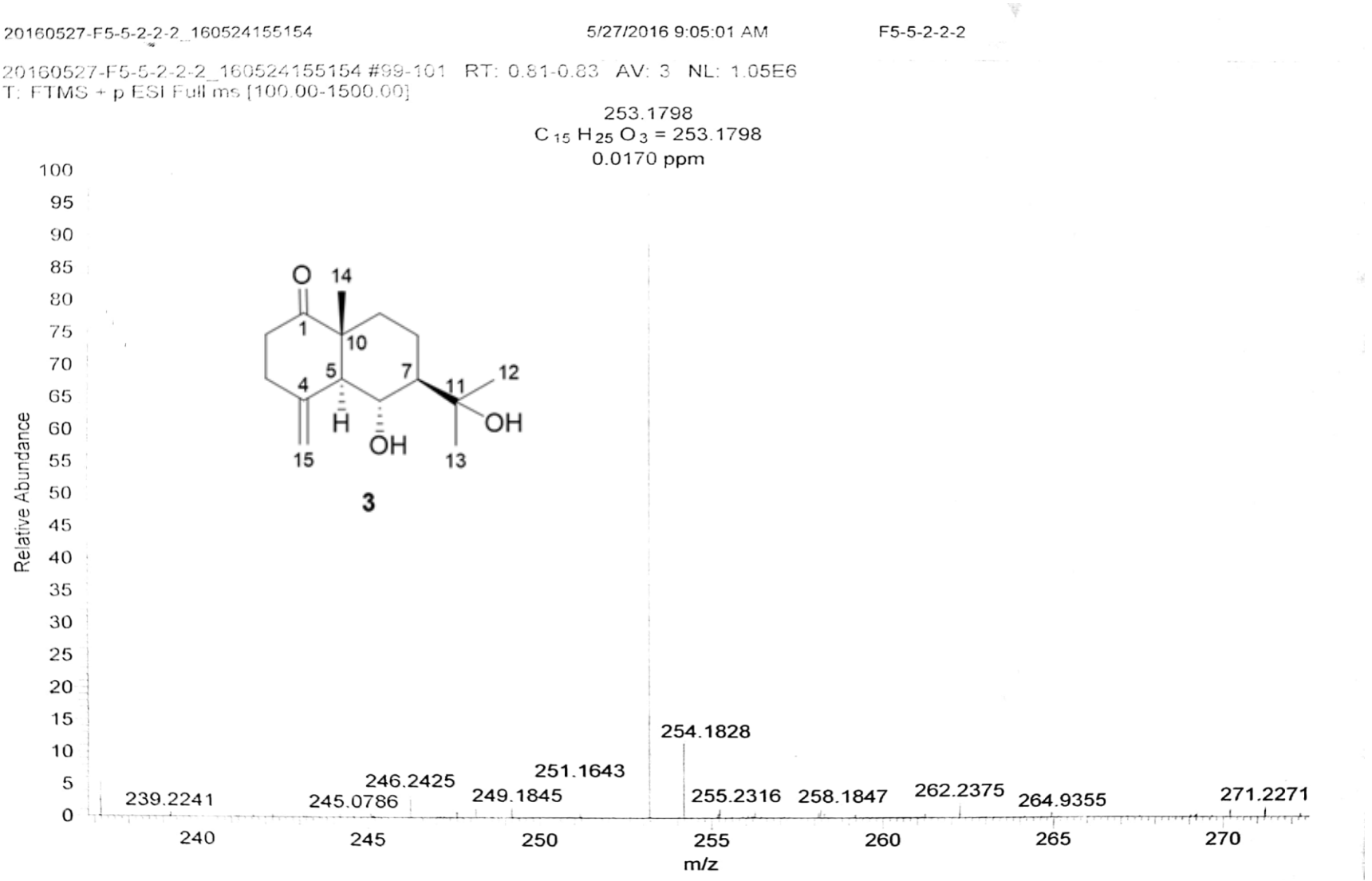



**Figure SS25 The positive HRESIMS spectrum of sinulin B (3)**

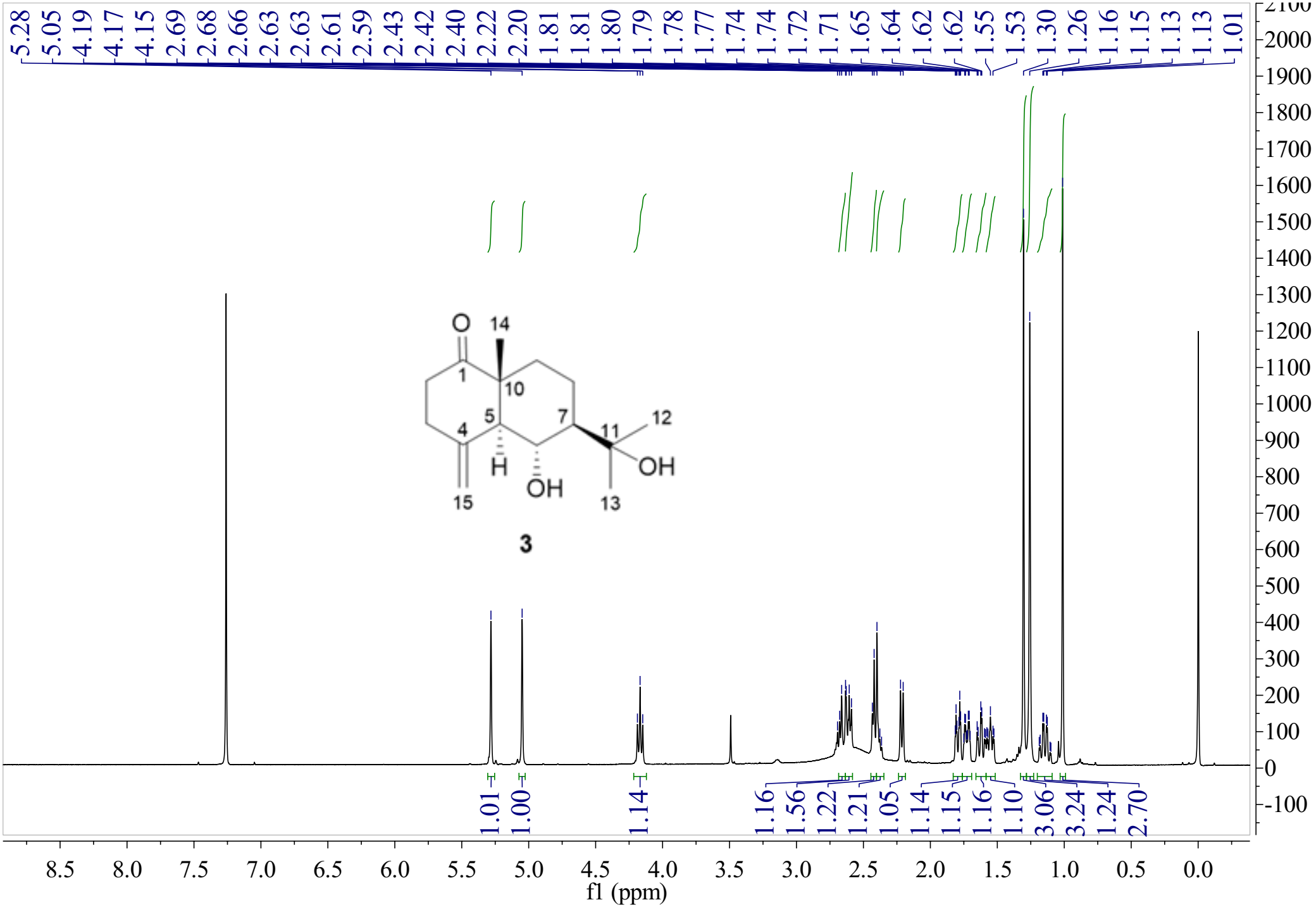



**Figure SS26 $^{1}$H NMR (500MHz, $CDCl_3$) spectrum of sinulin B (3)**

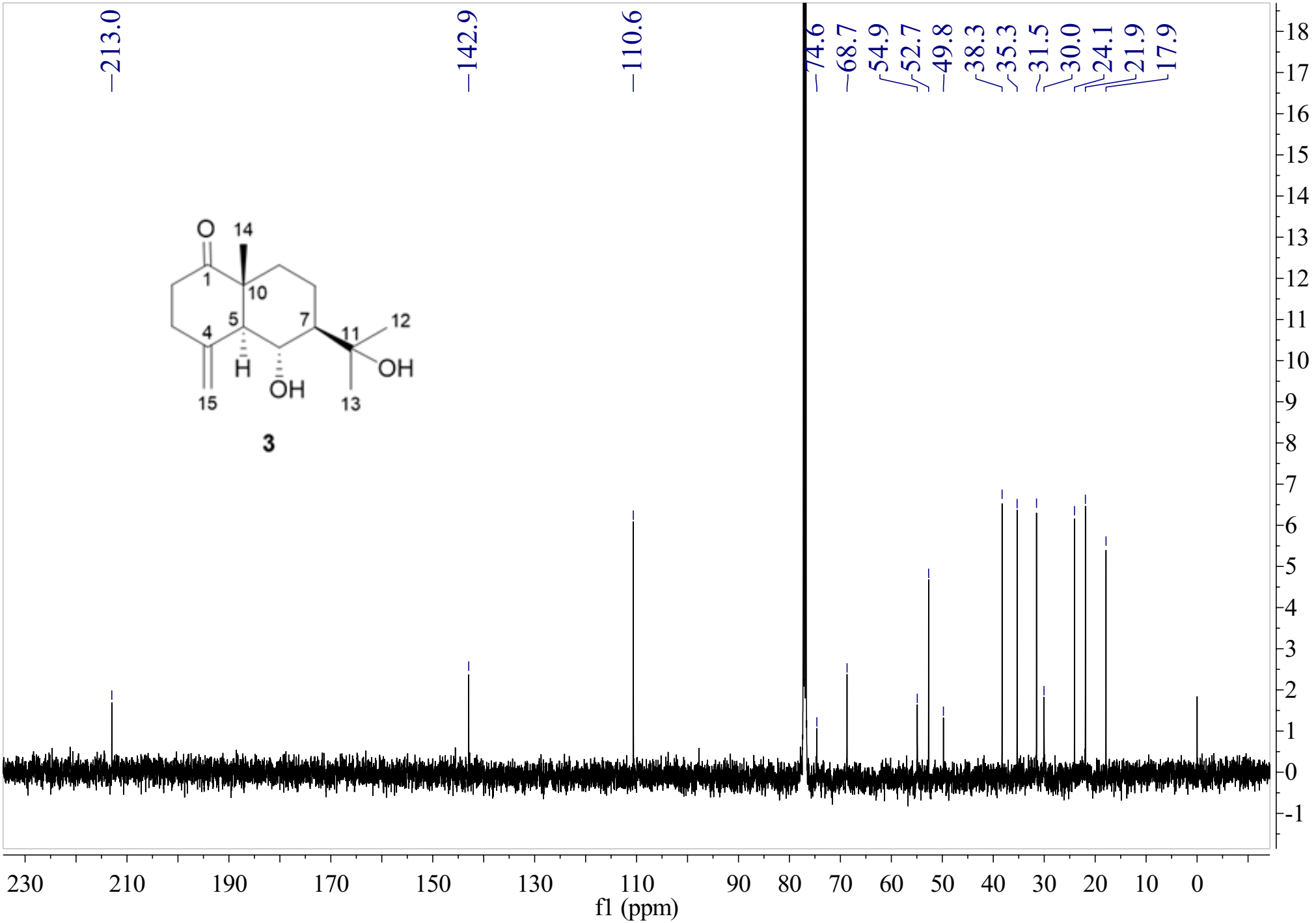



**Figure SS27 $^{13}C$ NMR (125MHz, $CDCl_3$) spectrum of sinulin B (3)**

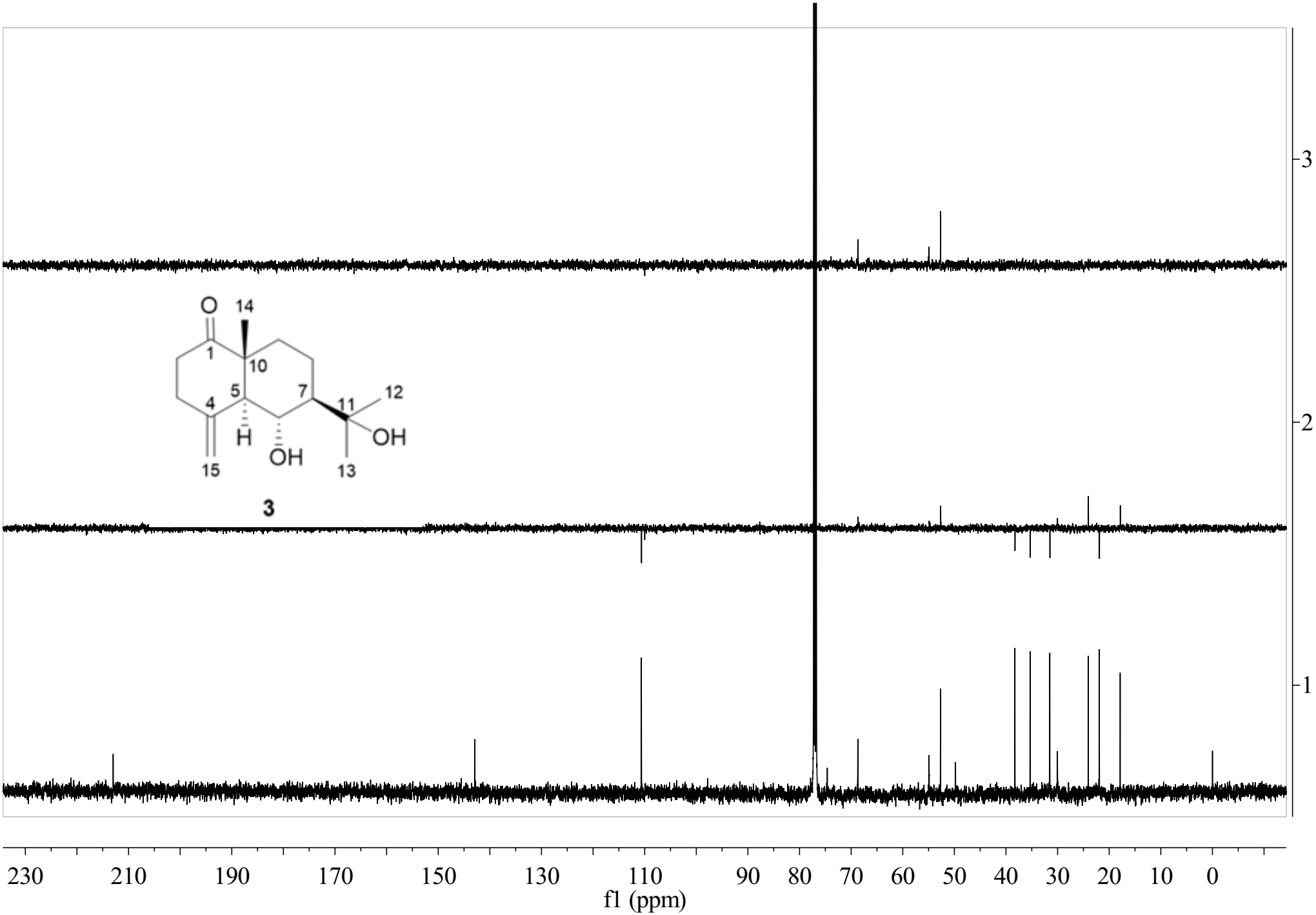



**Figure SS28 DEPT spectrum of sinulin B (3)**

3

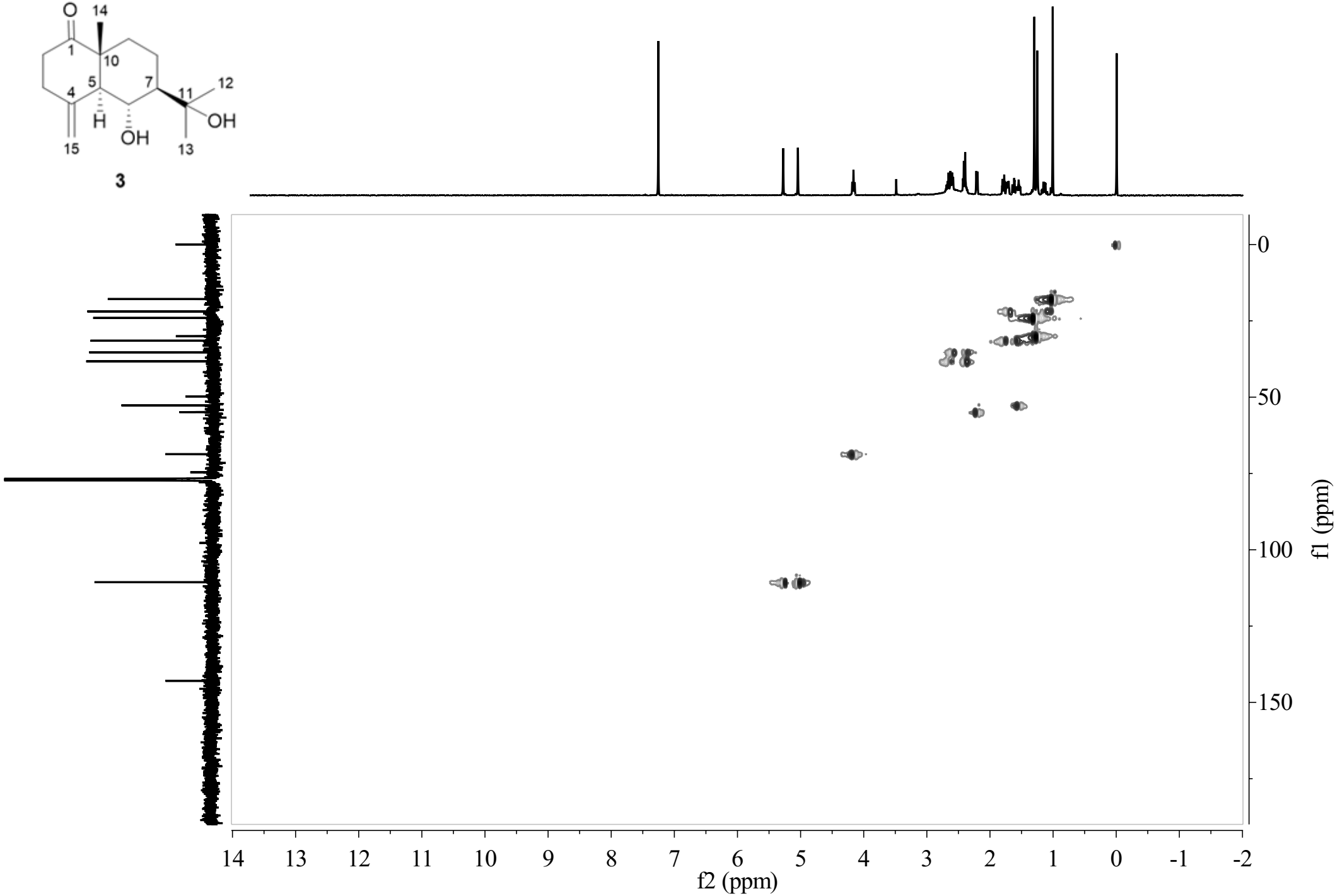



**Figure SS29 HMQC spectrum of sinulin B (3)**

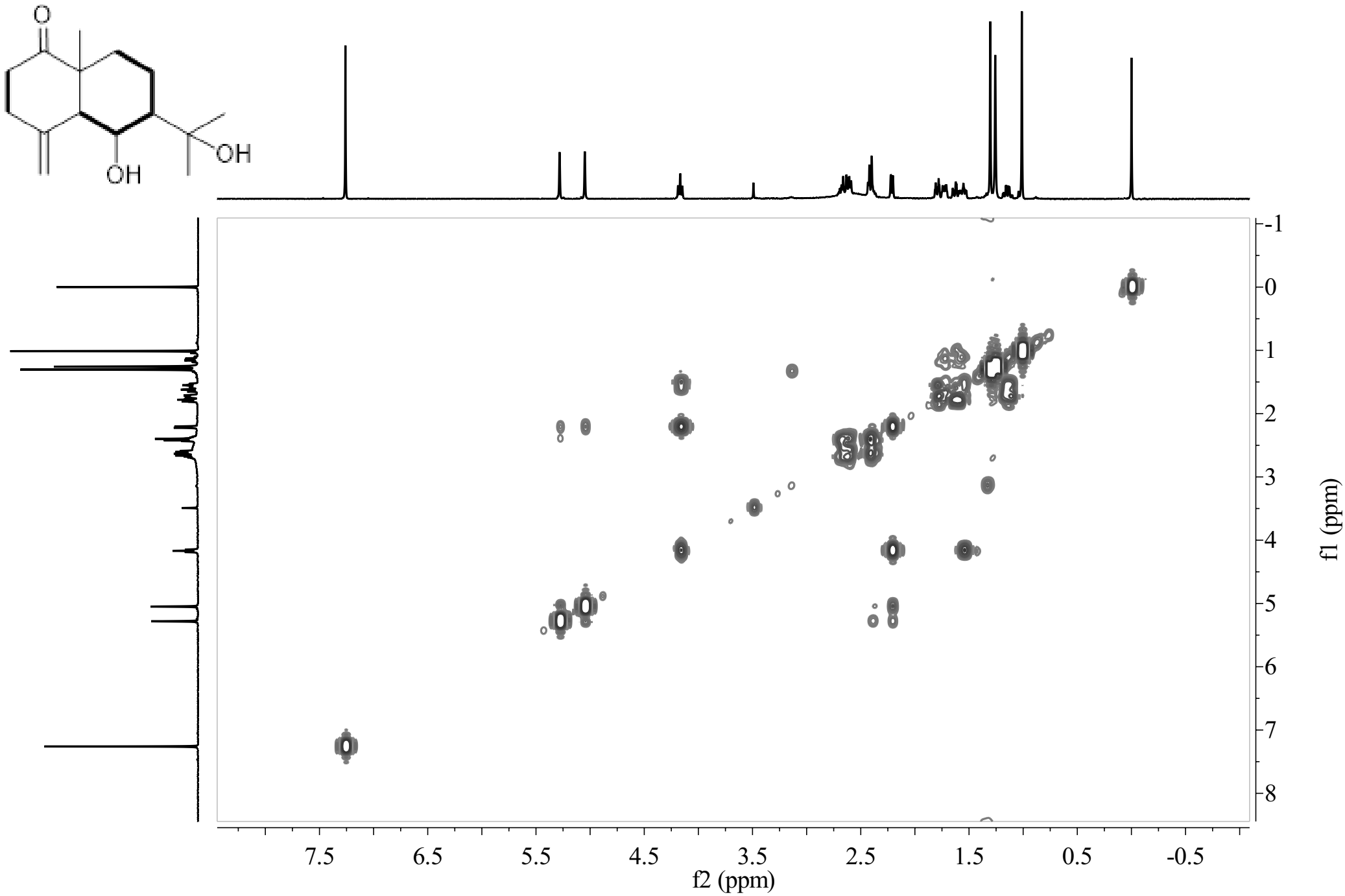



**Figure SS30 $^{1}$H-$^{1}$H COSY spectrum of sinulin B (3)**

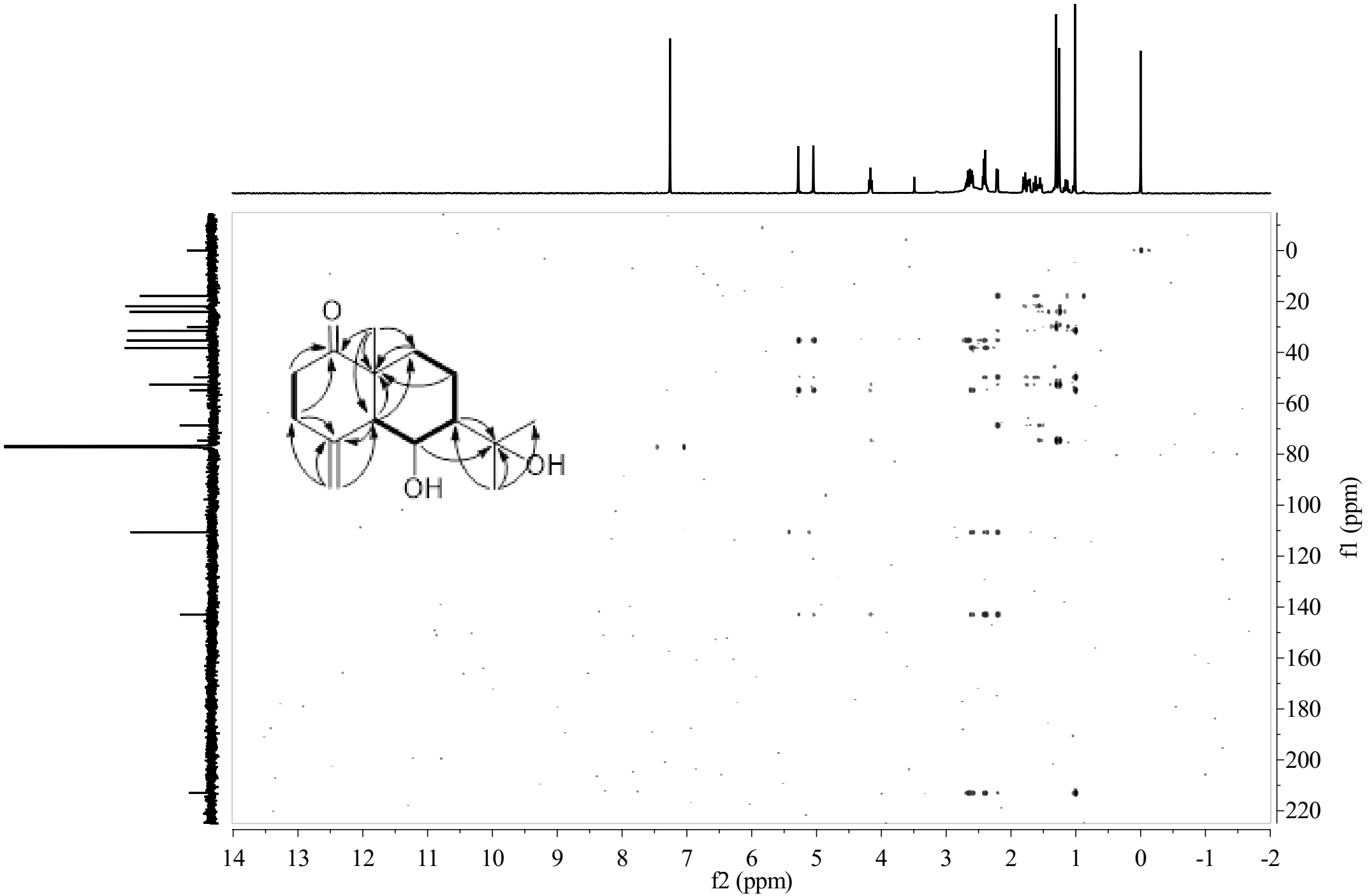



**Figure SS31 HMBC spectrum of sinulin B (3)**

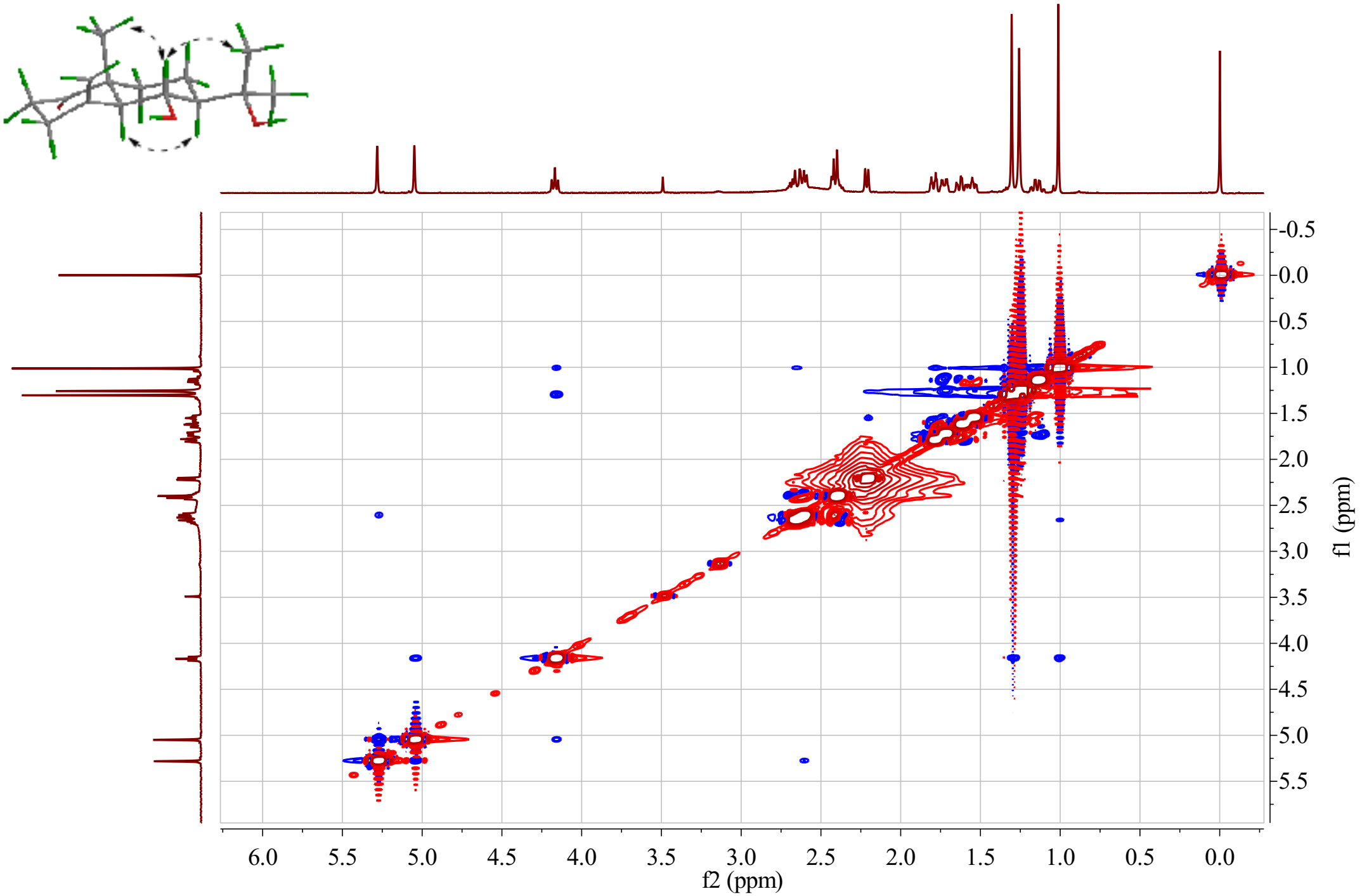



**Figure SS32 NOESY spectrum of sinulin B (3)**

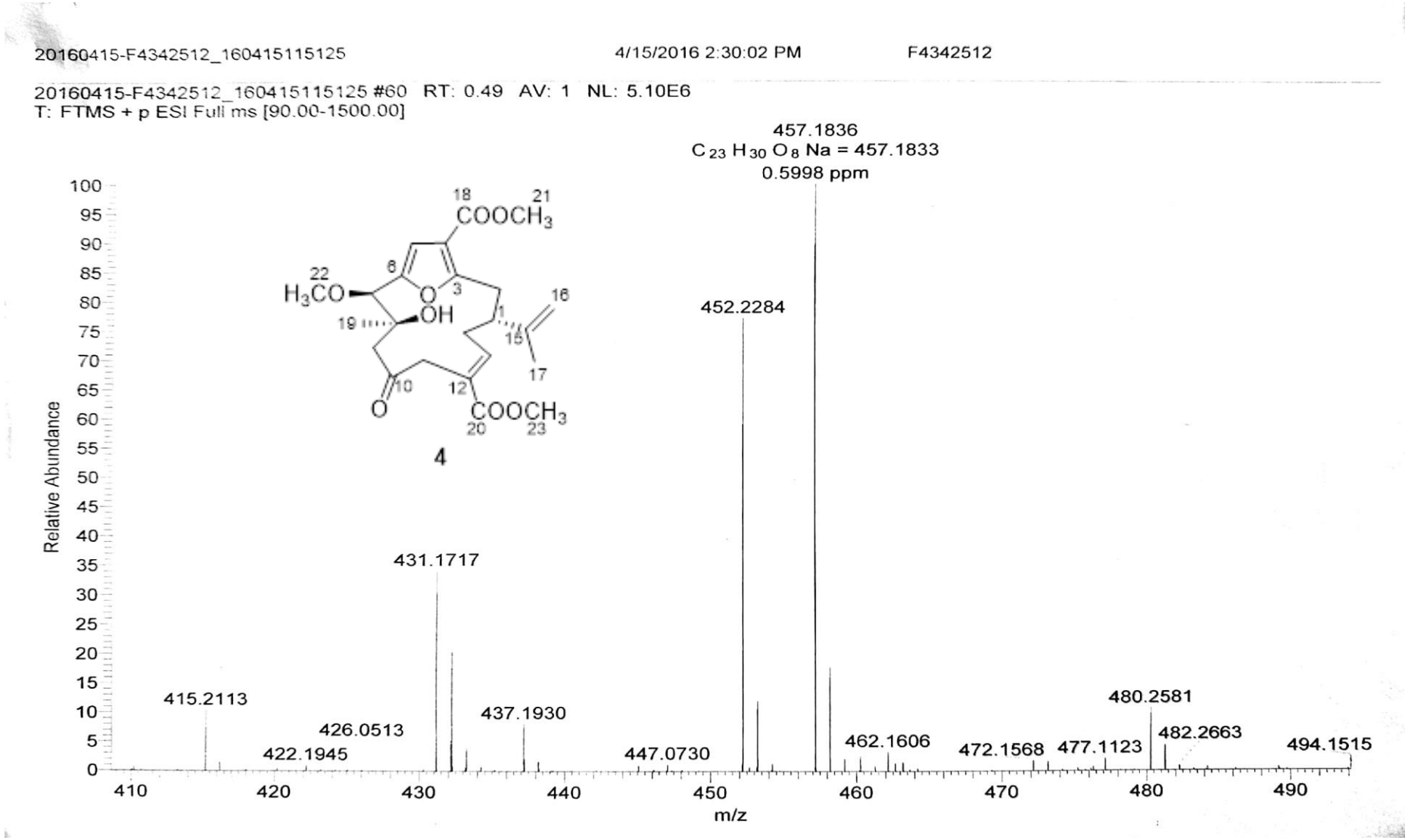



**Figure SS33 The positive HRESIMS spectrum of sinulin C (4)**

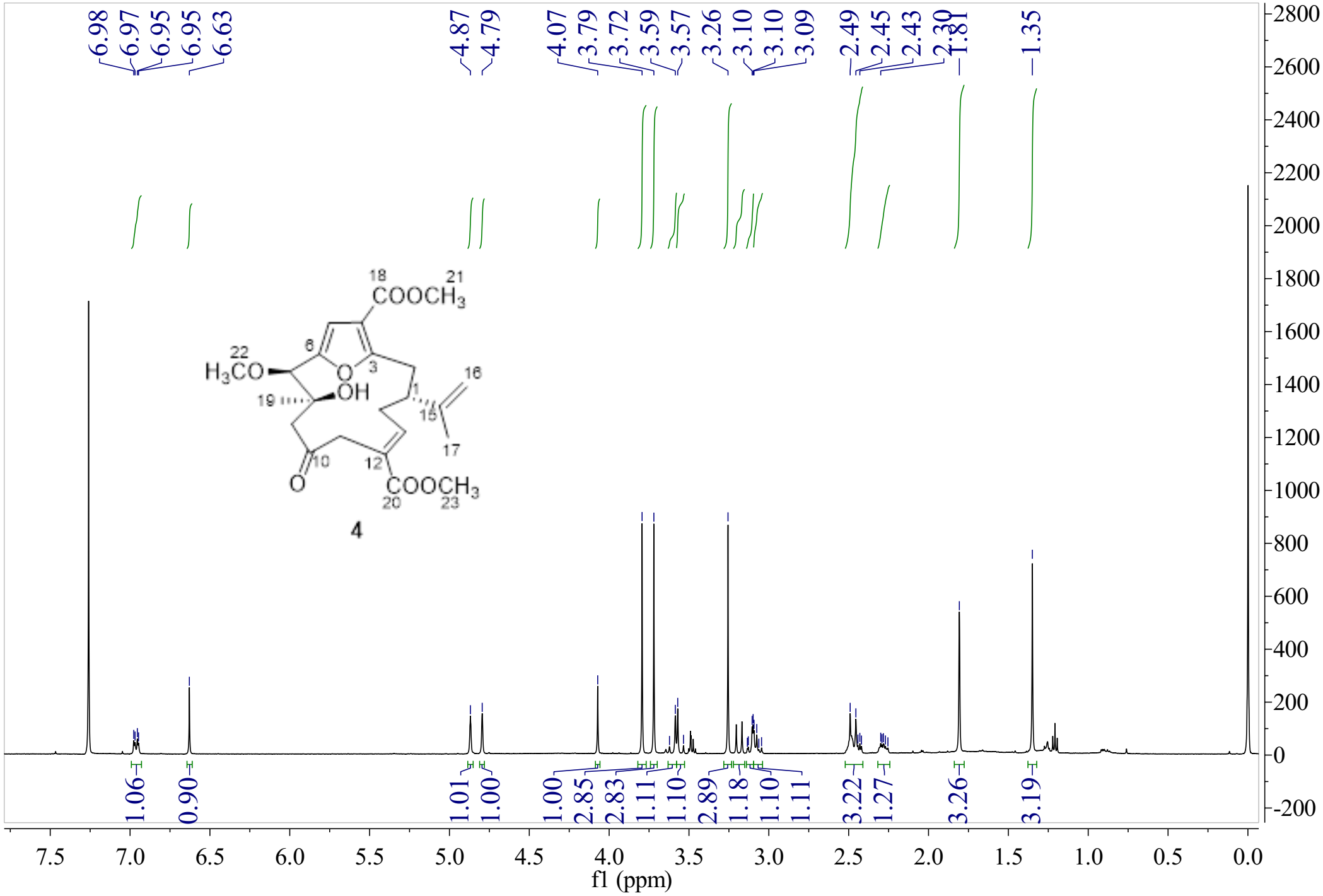



**Figure SS34 $^{1}H$ NMR (500MHz, $CDCl_3$) spectrum of sinulin C (4)**

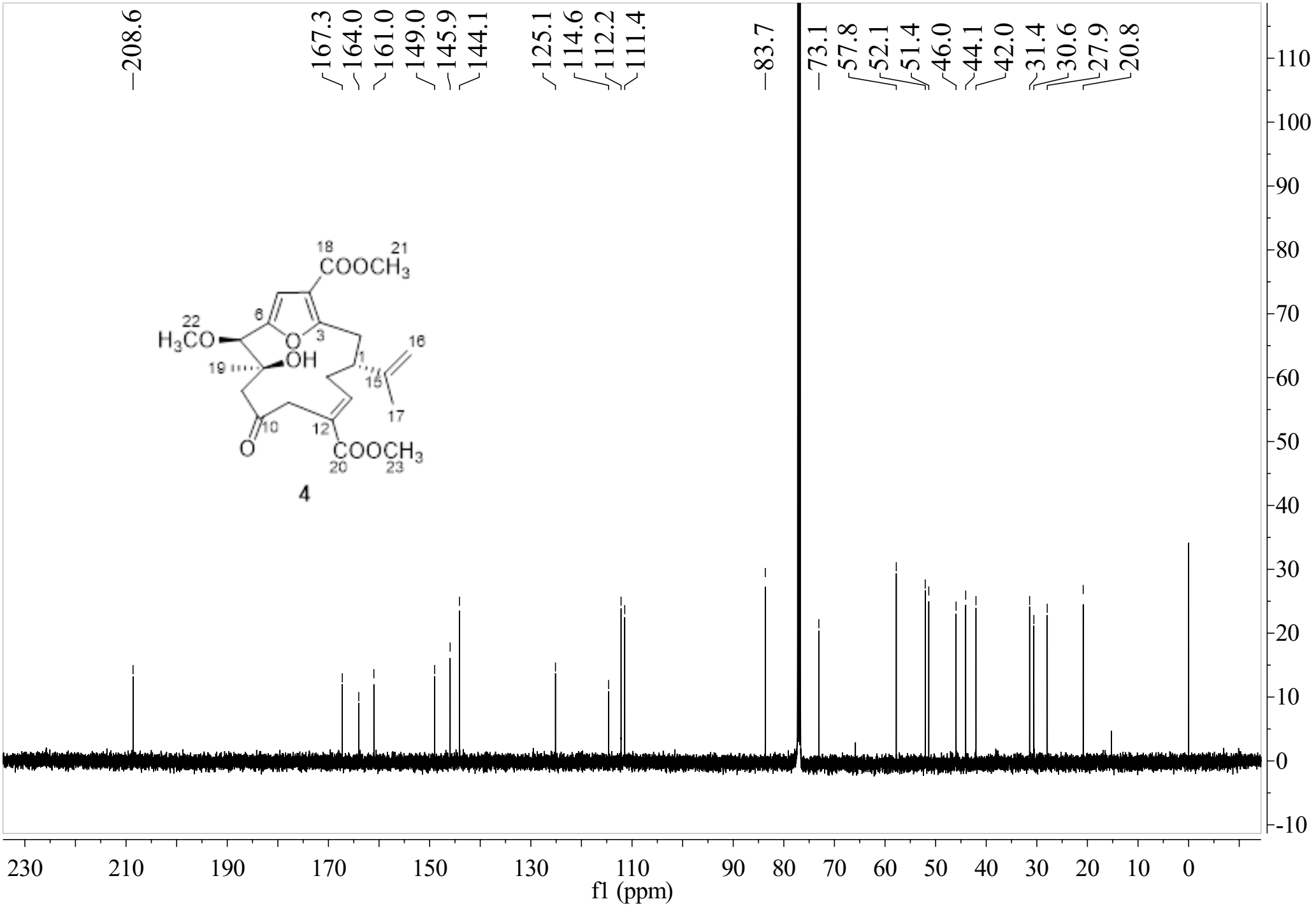



**Figure SS35 $^{13}C$ NMR (125MHz, $CDCl_3$) spectrum of sinulin C (4)**

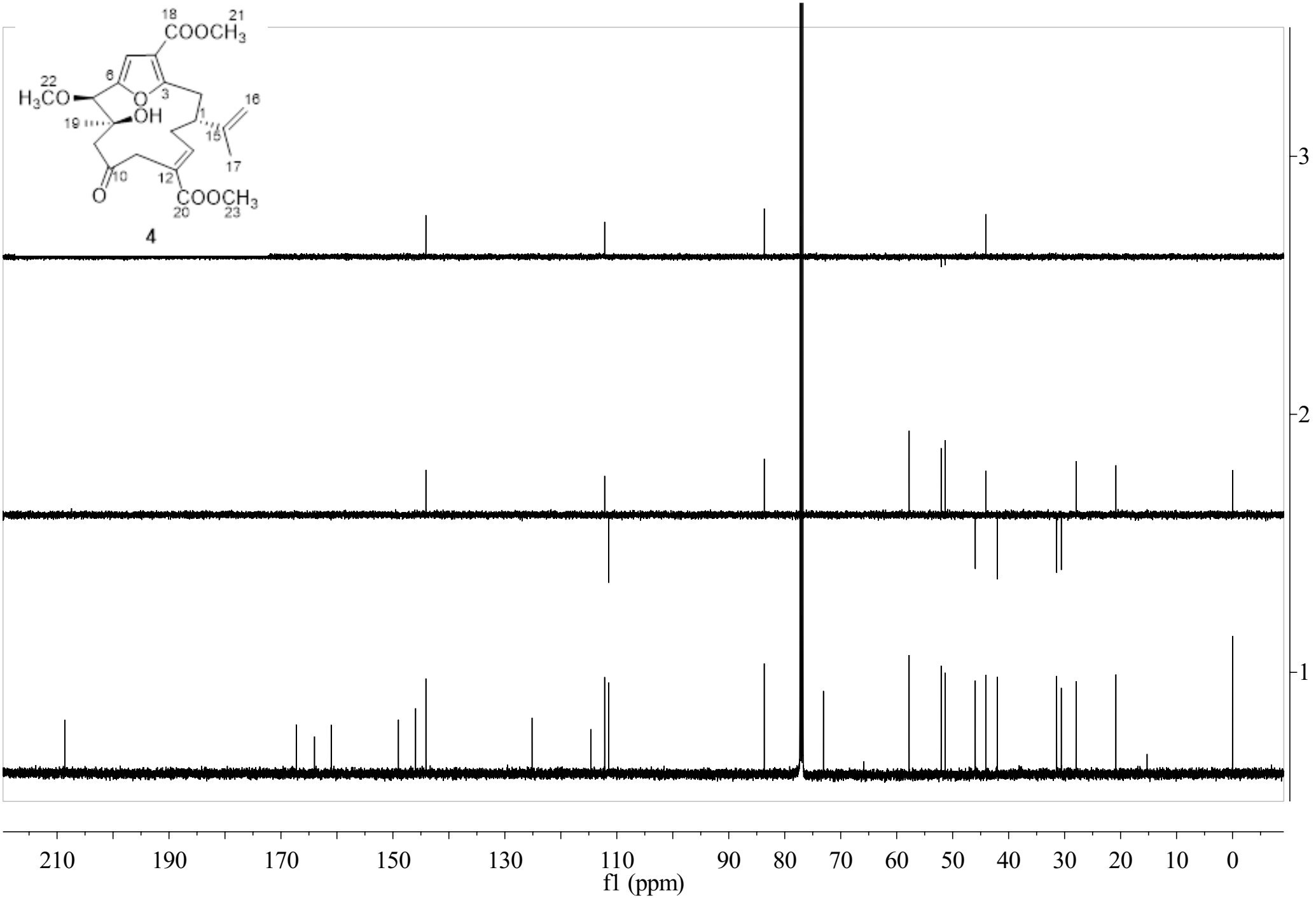



**Figure SS36 DEPT spectrum of sinulin C (4)**

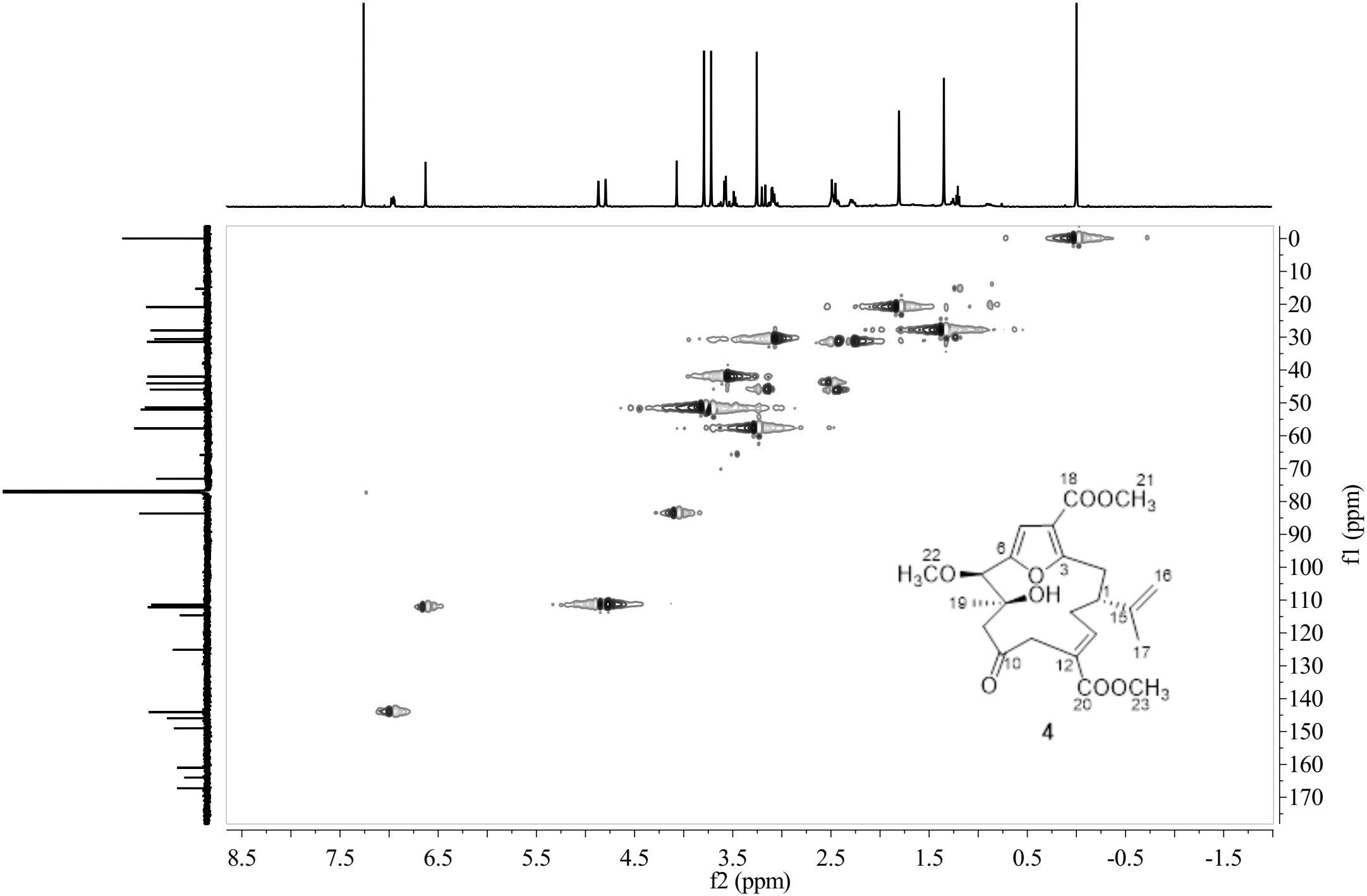



**Figure SS37 HMQC spectrum of sinulin C (4)**

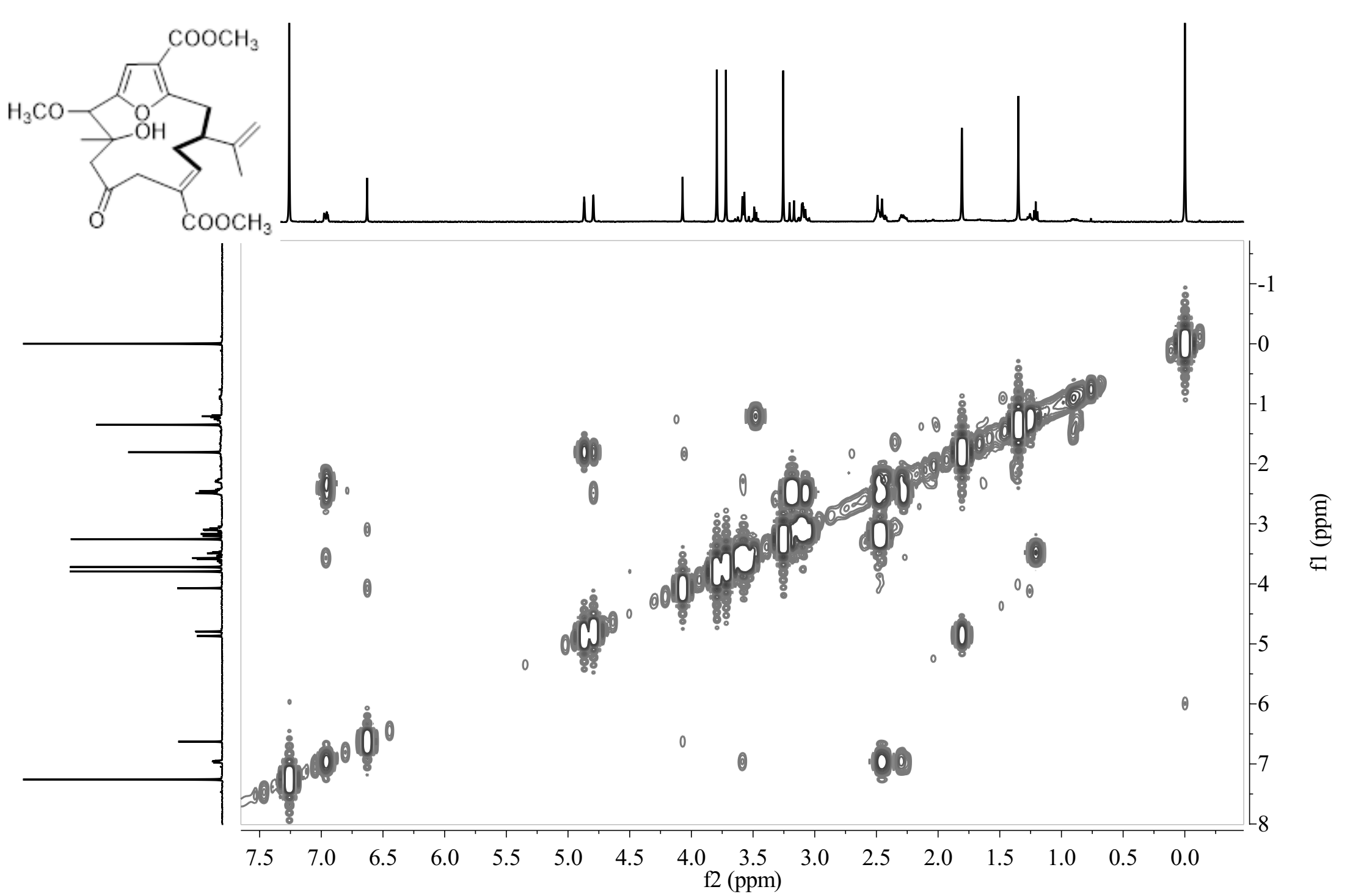



**Figure SS38 $^{1}$H-$^{1}$H COSY spectrum of sinulin C (4)**

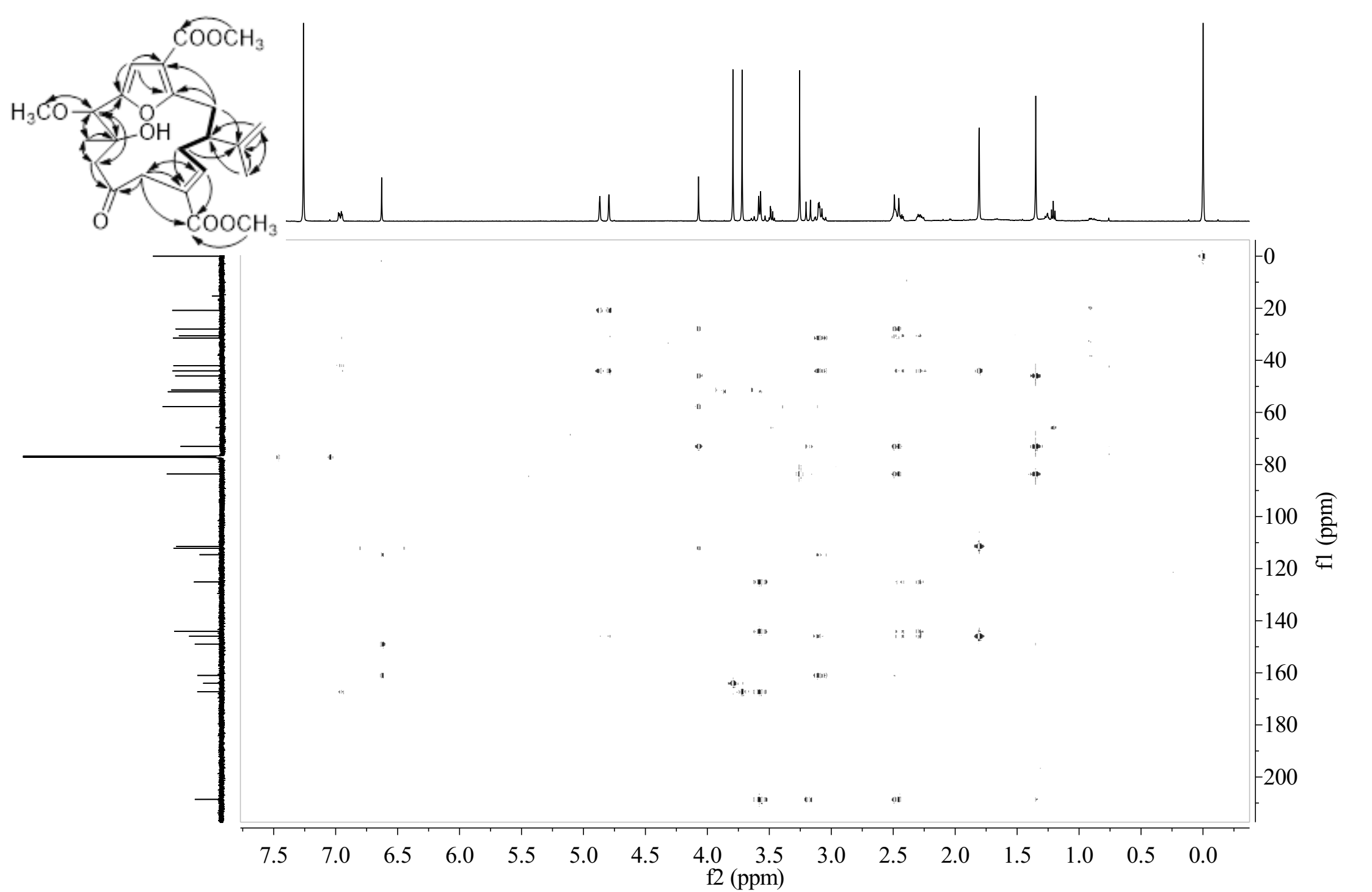



**Figure SS39 HMBC spectrum of sinulin C (4)**

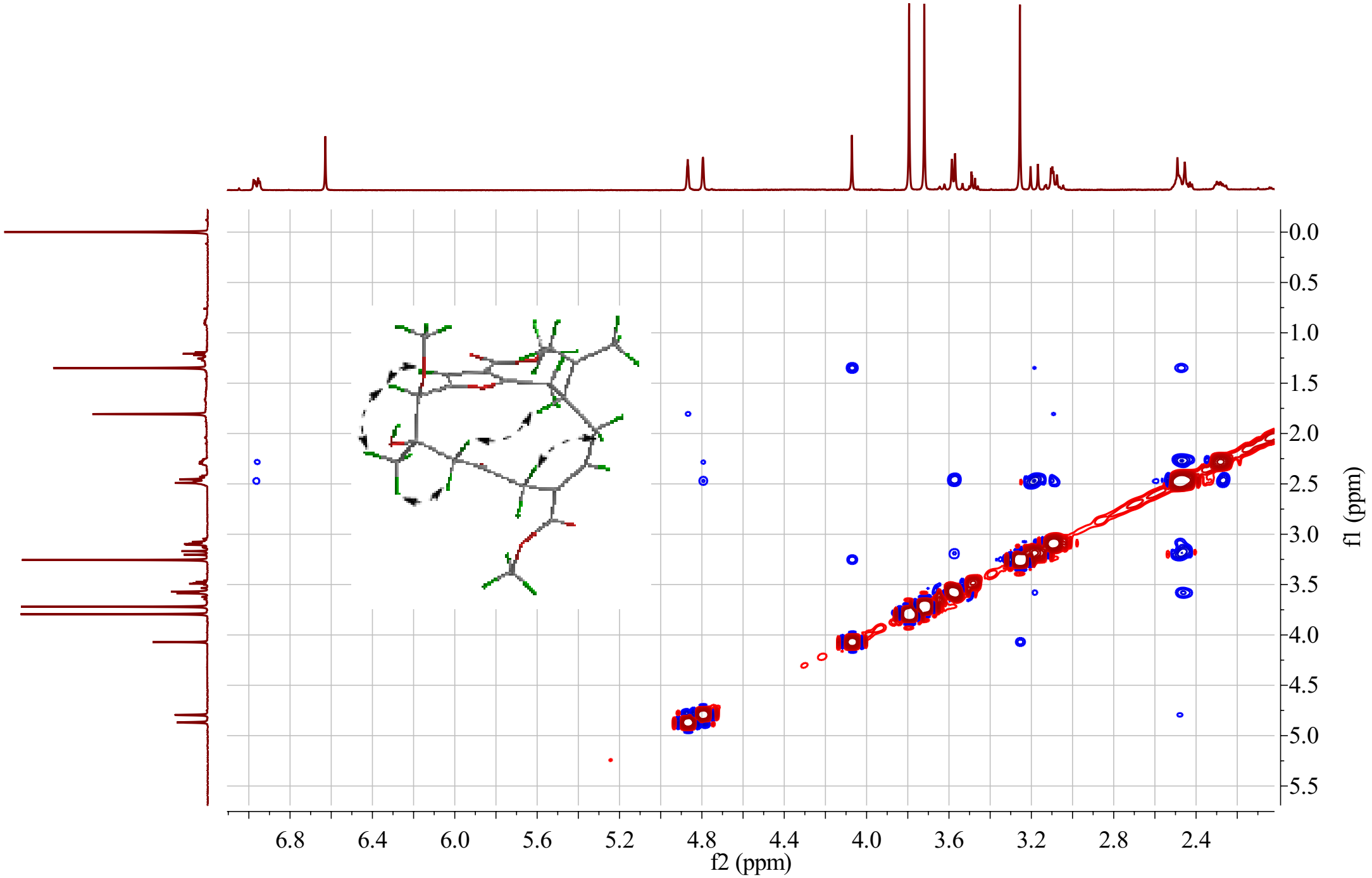



**Figure SS40 NOESY spectrum of sinulin C (4)**

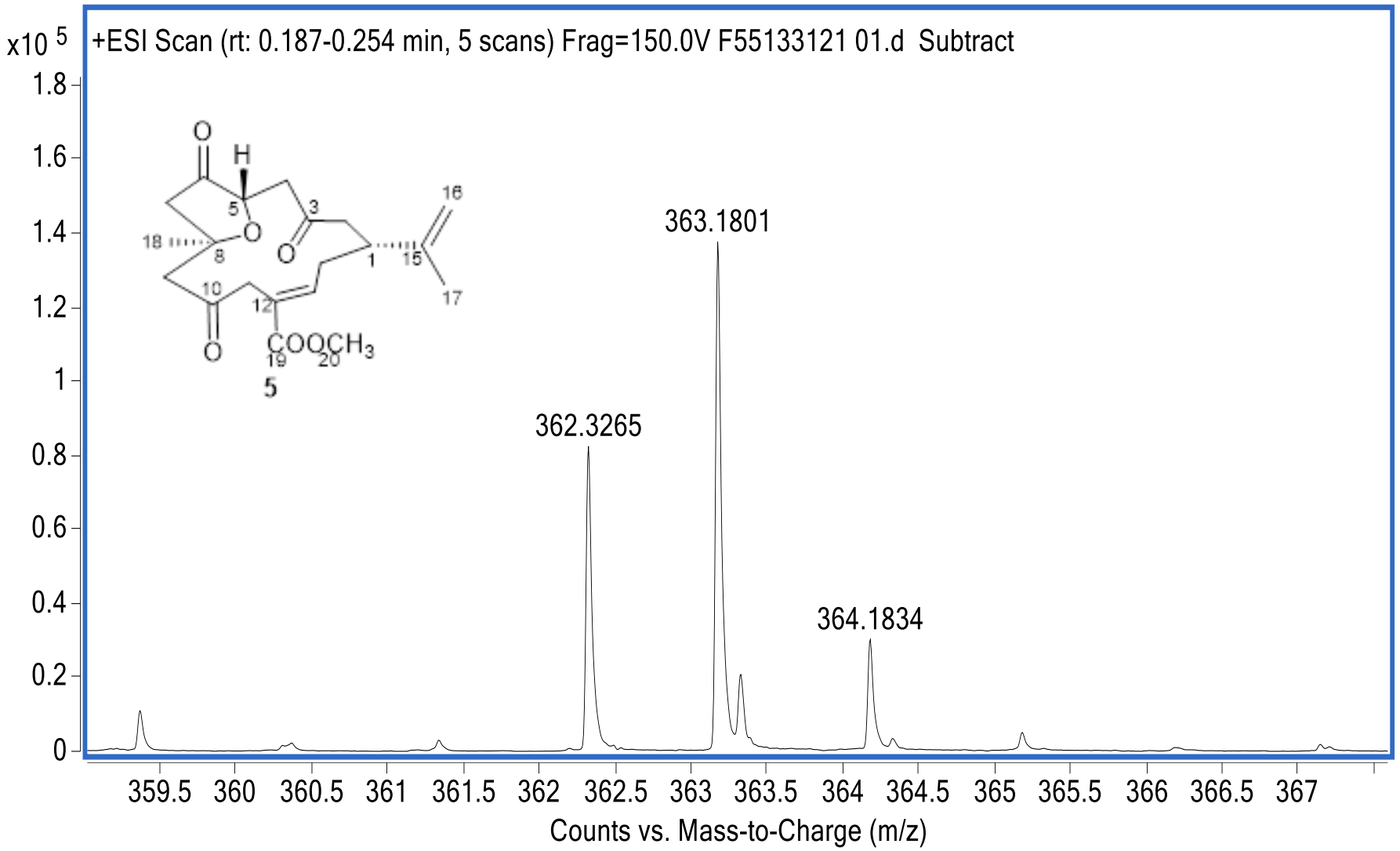
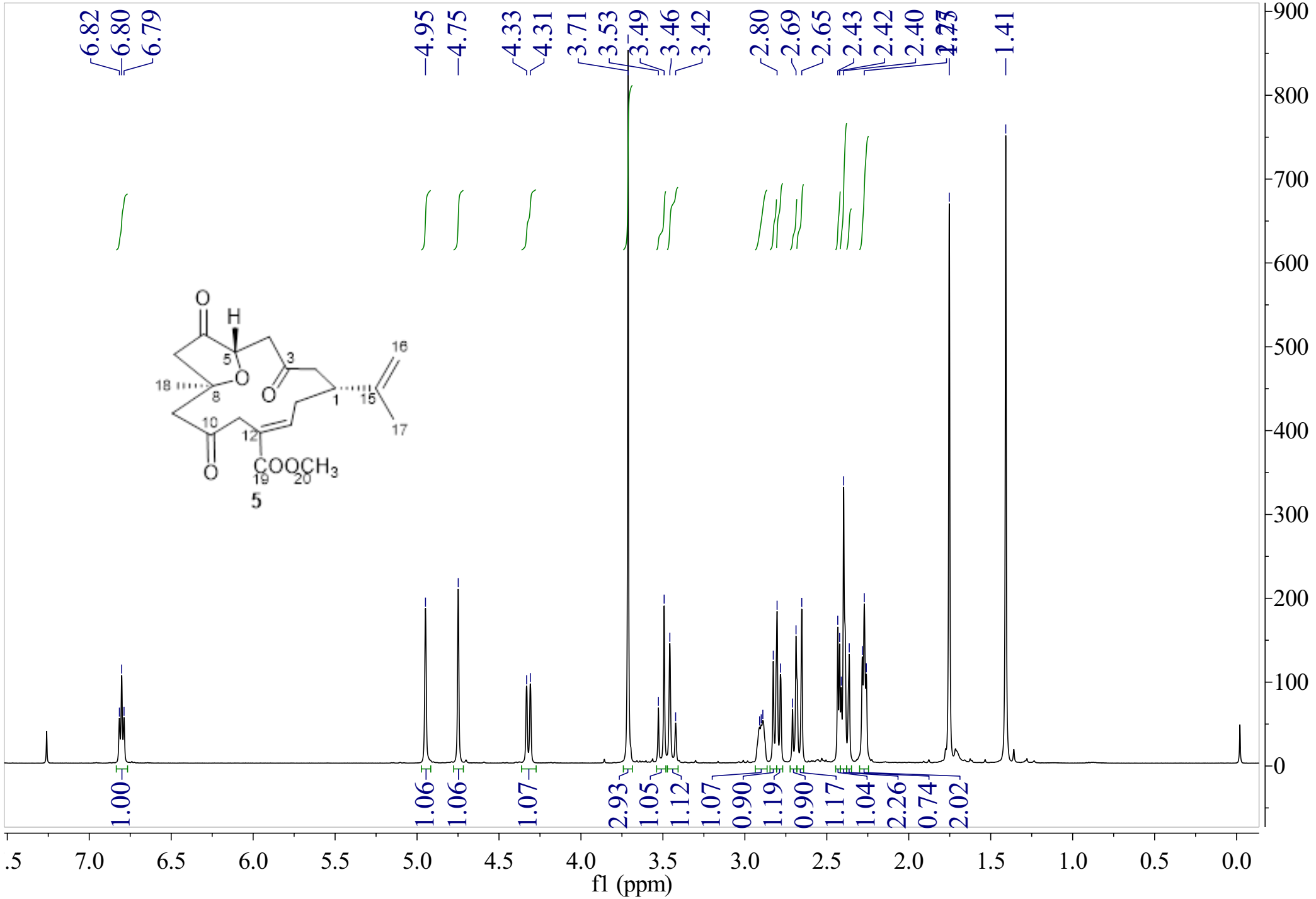



**Figure SS41 The positive HRESIMS spectrum of sinulin D (5)**




5

**Figure SS42 $^{1}$H NMR (500MHz, $CDCl_3$) spectrum of sinulin D (5)**

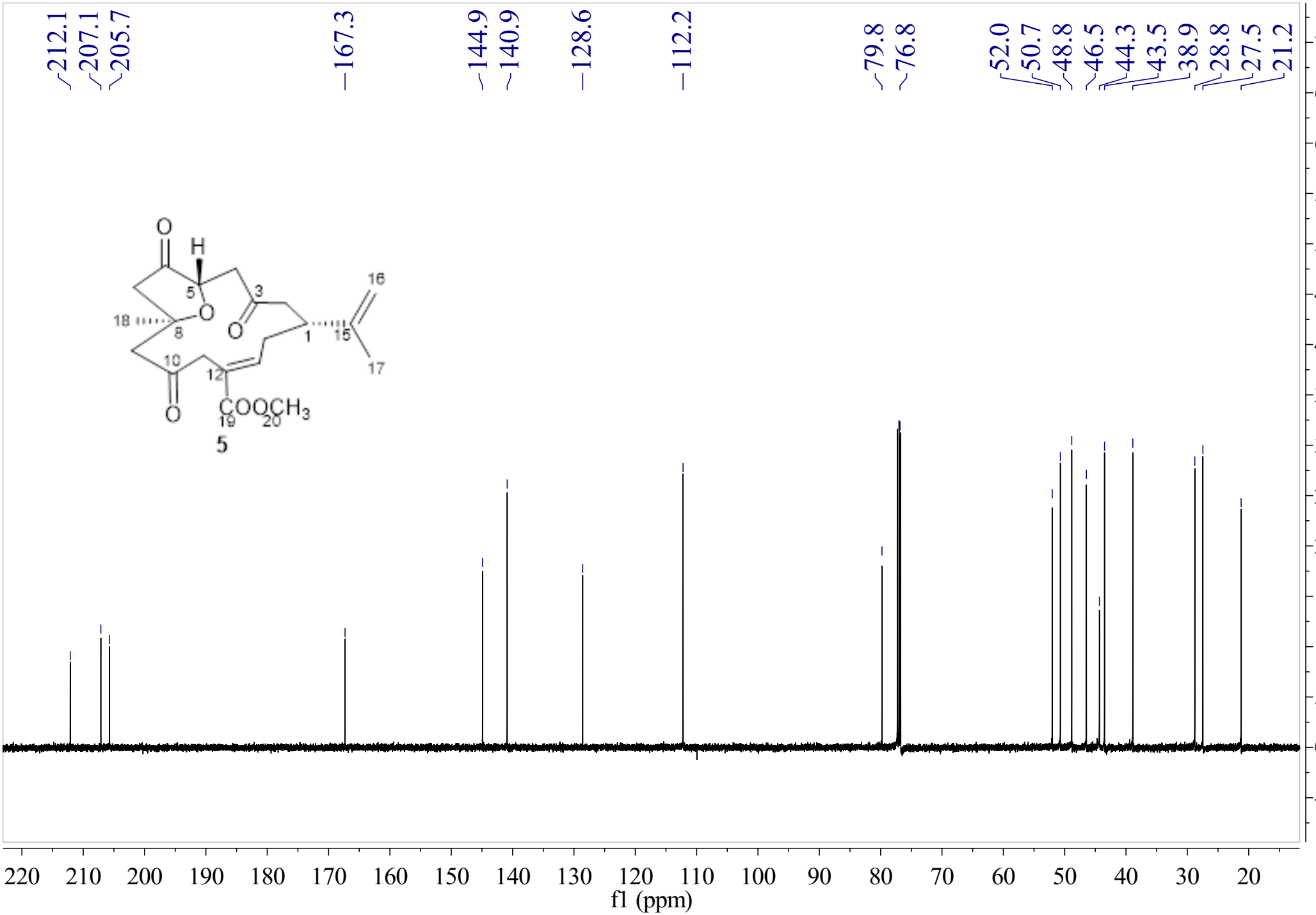



**Figure SS43 $^{13}C$ NMR (125MHz, $CDCl_3$) spectrum of sinulin D (5)**

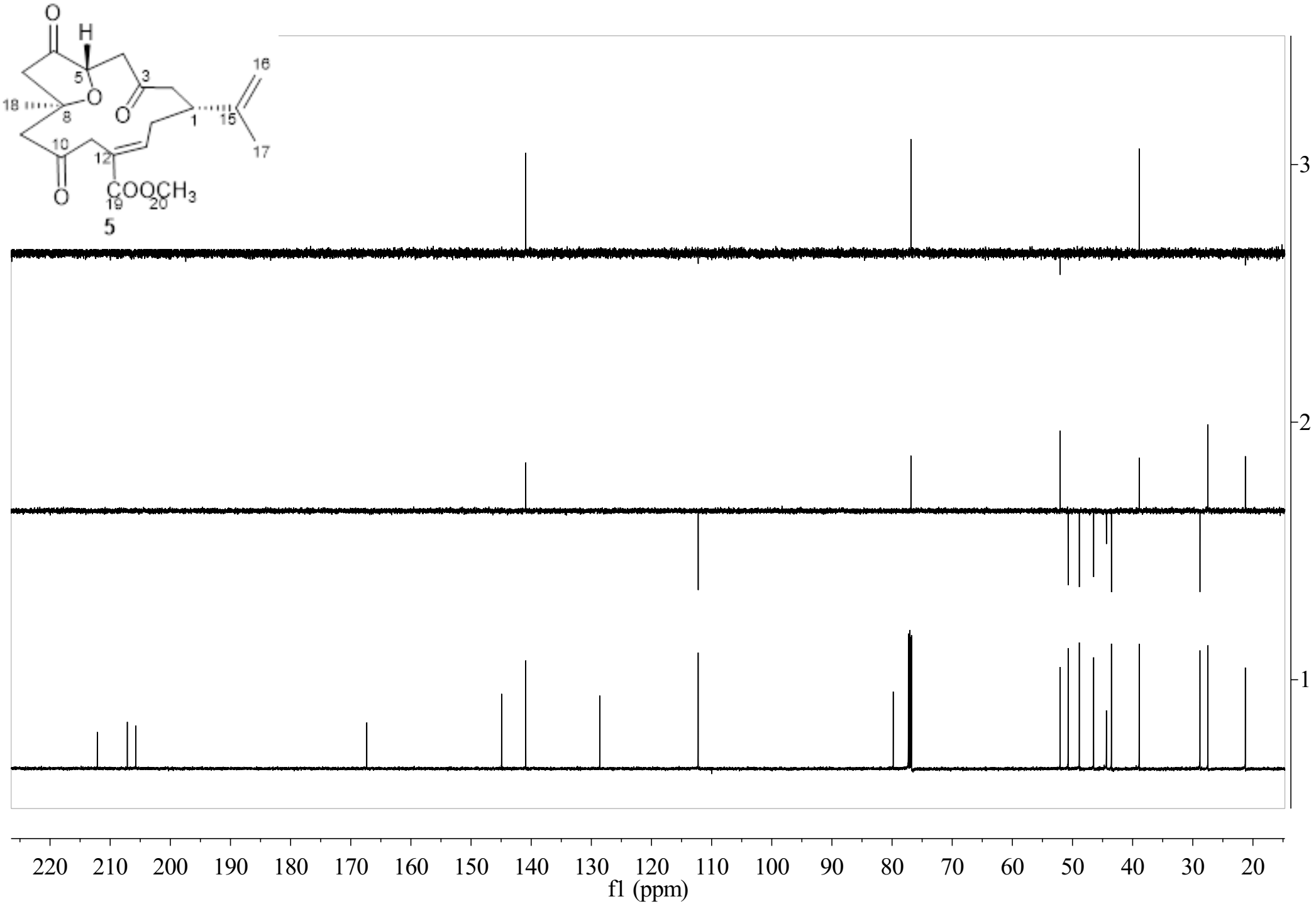



**Figure SS44 DEPT spectrum of sinulin D (5)**

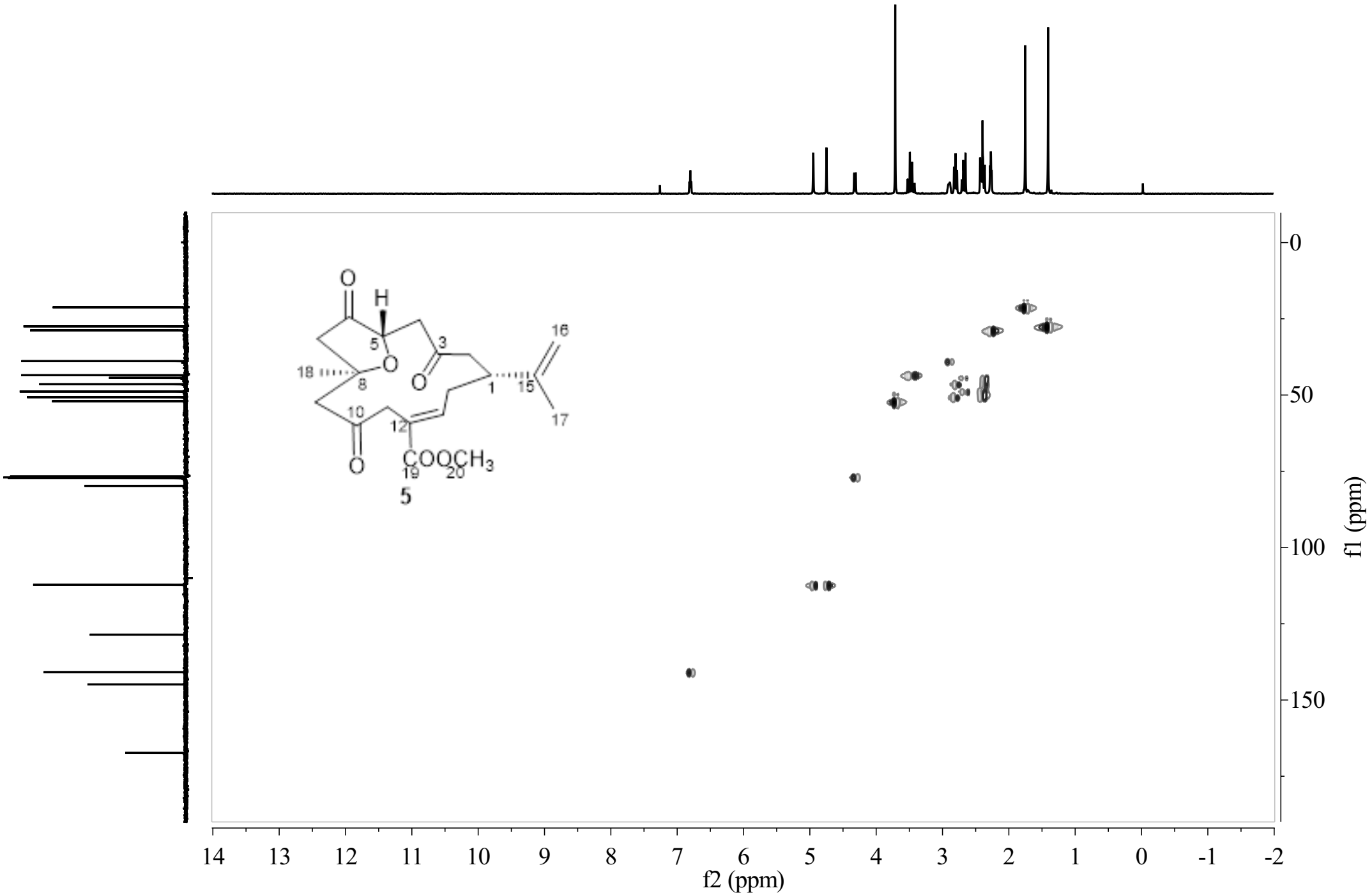



**Figure SS45 HMQC spectrum of sinulin D (5)**

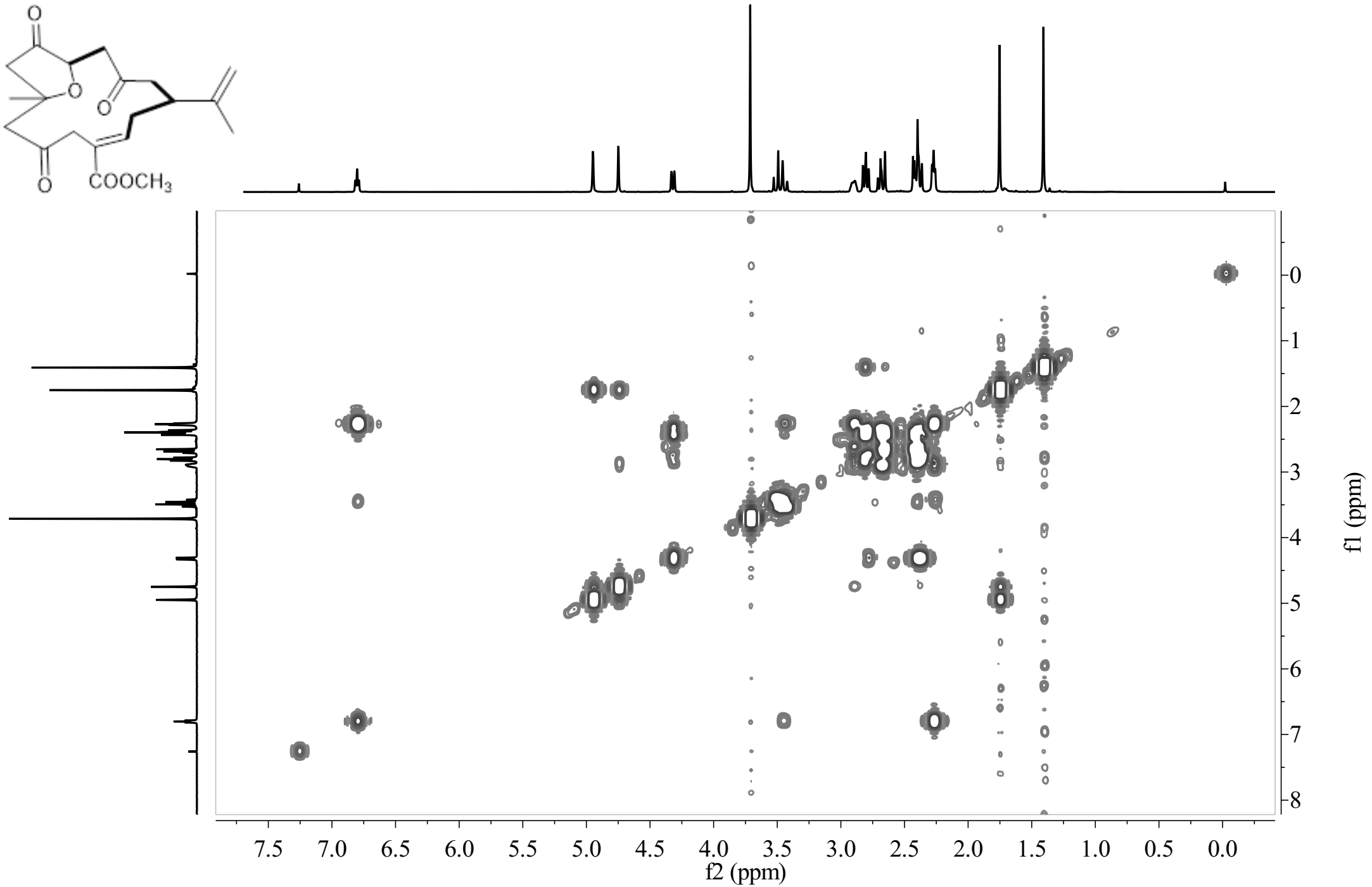



**Figure SS46 $^{1}$H-$^{1}$H COSY spectrum of sinulin D (5)**

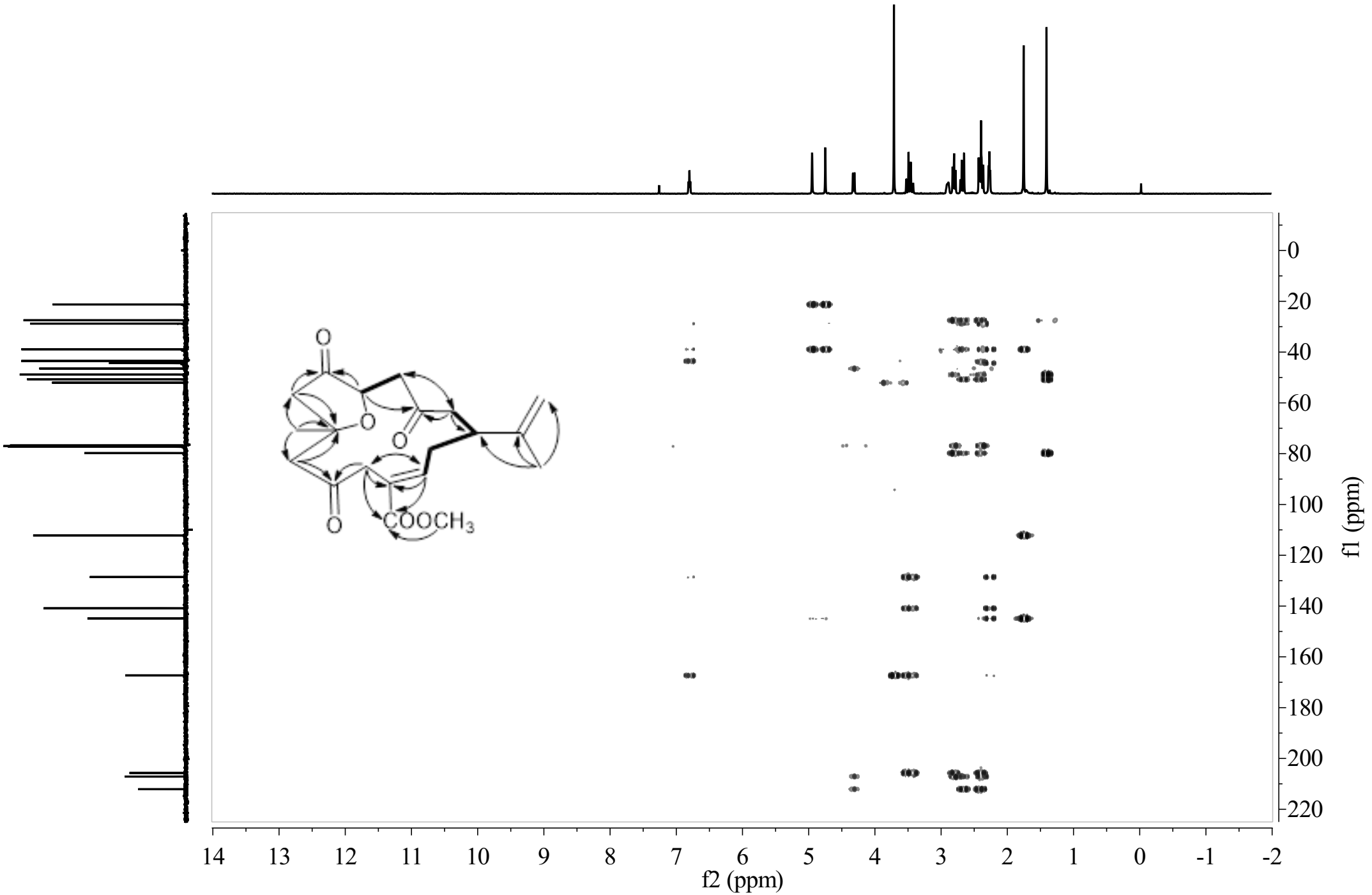



**Figure SS47 HMBC spectrum of sinulin D (5)**

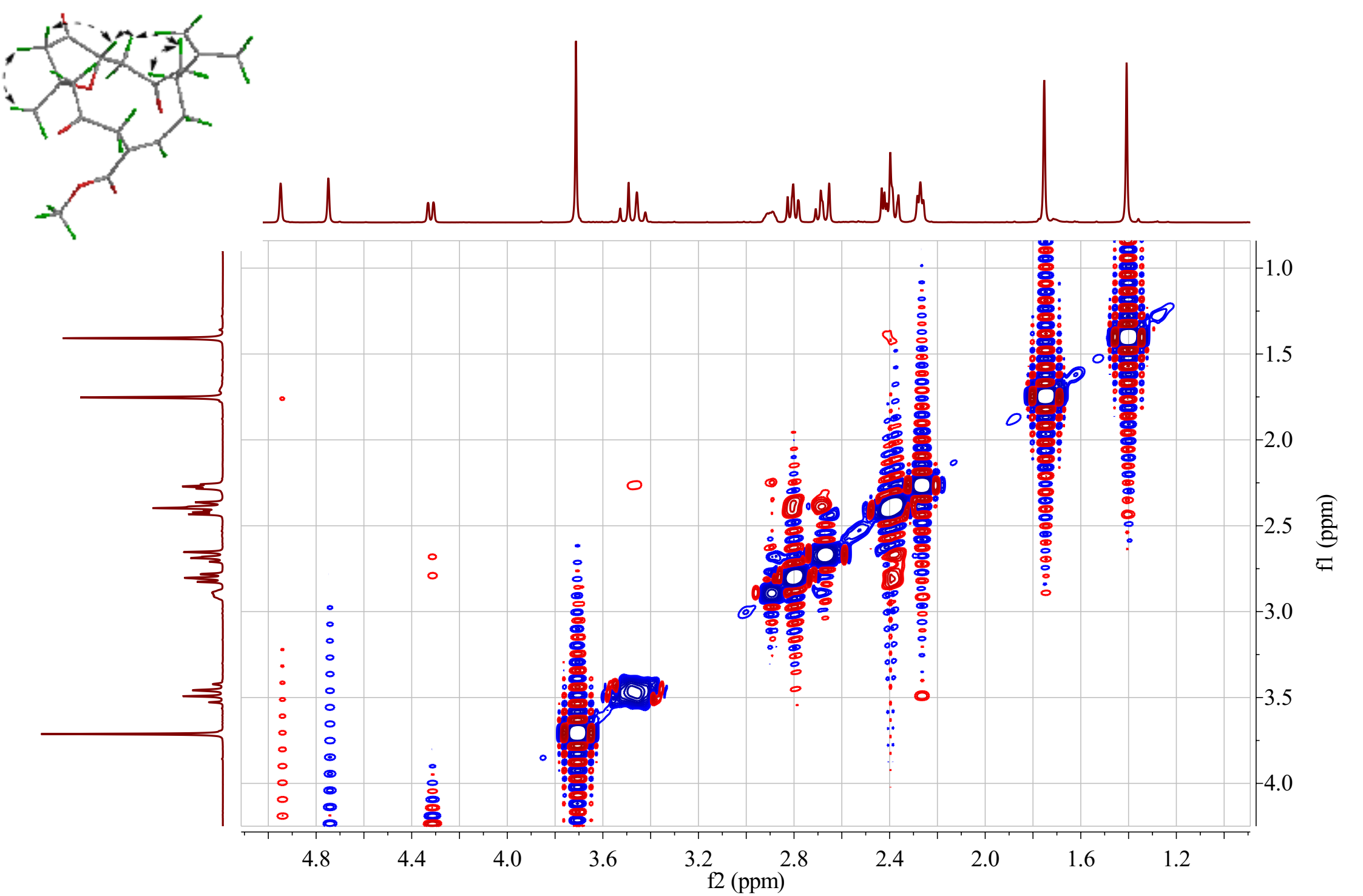



**Figure SS48 NOESY spectrum of sinulin D (5)**