# Supplementary Materials

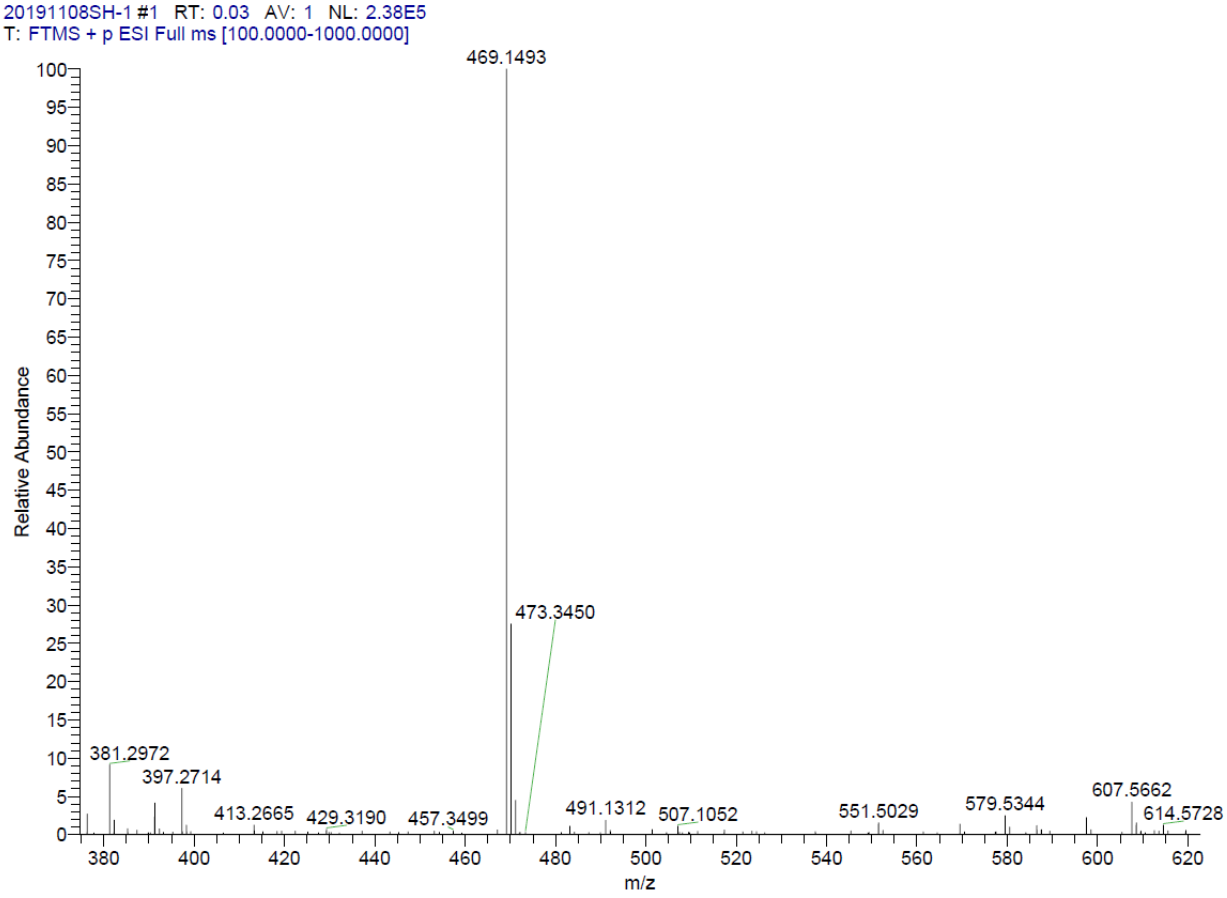


Figure S1. The HR-MS of compound **1**

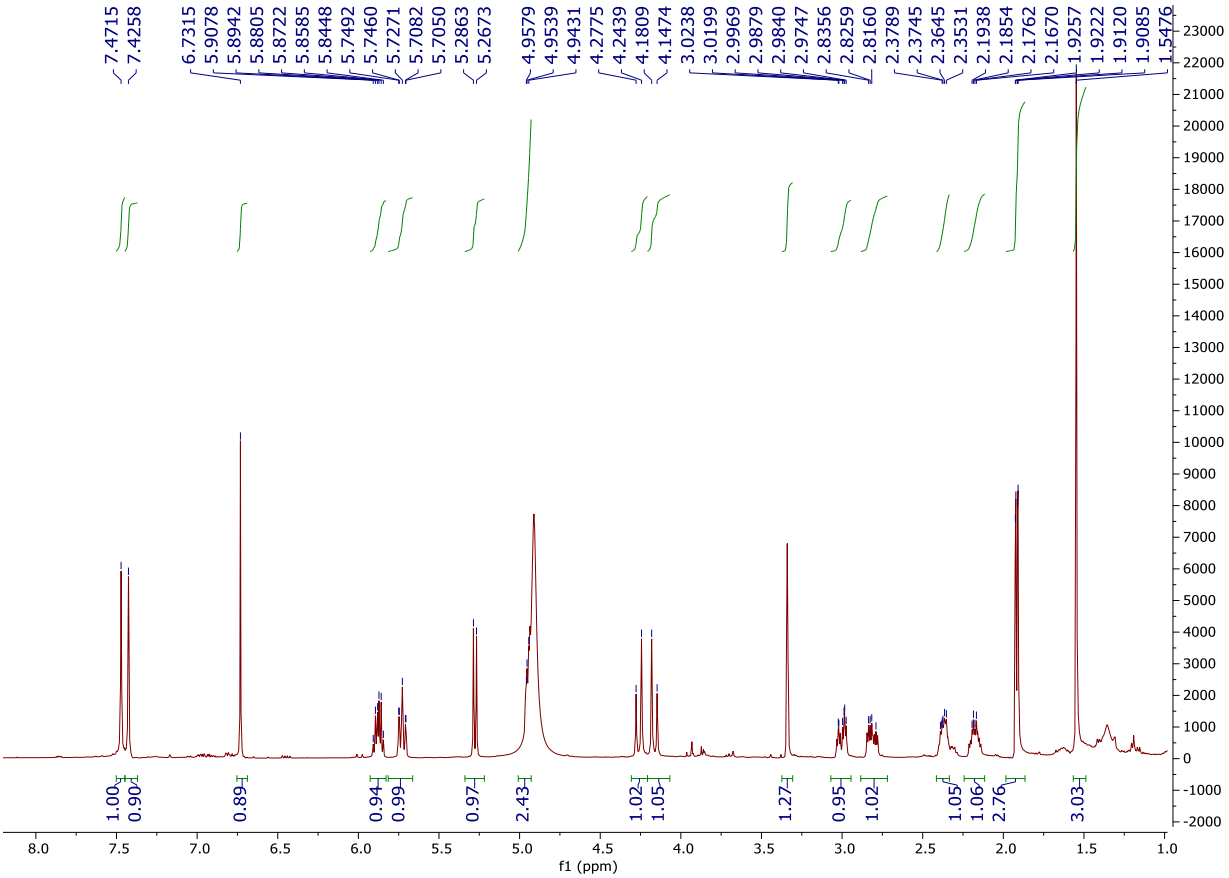


Figure S2. The $^{1}$H-NMR of compound **1**

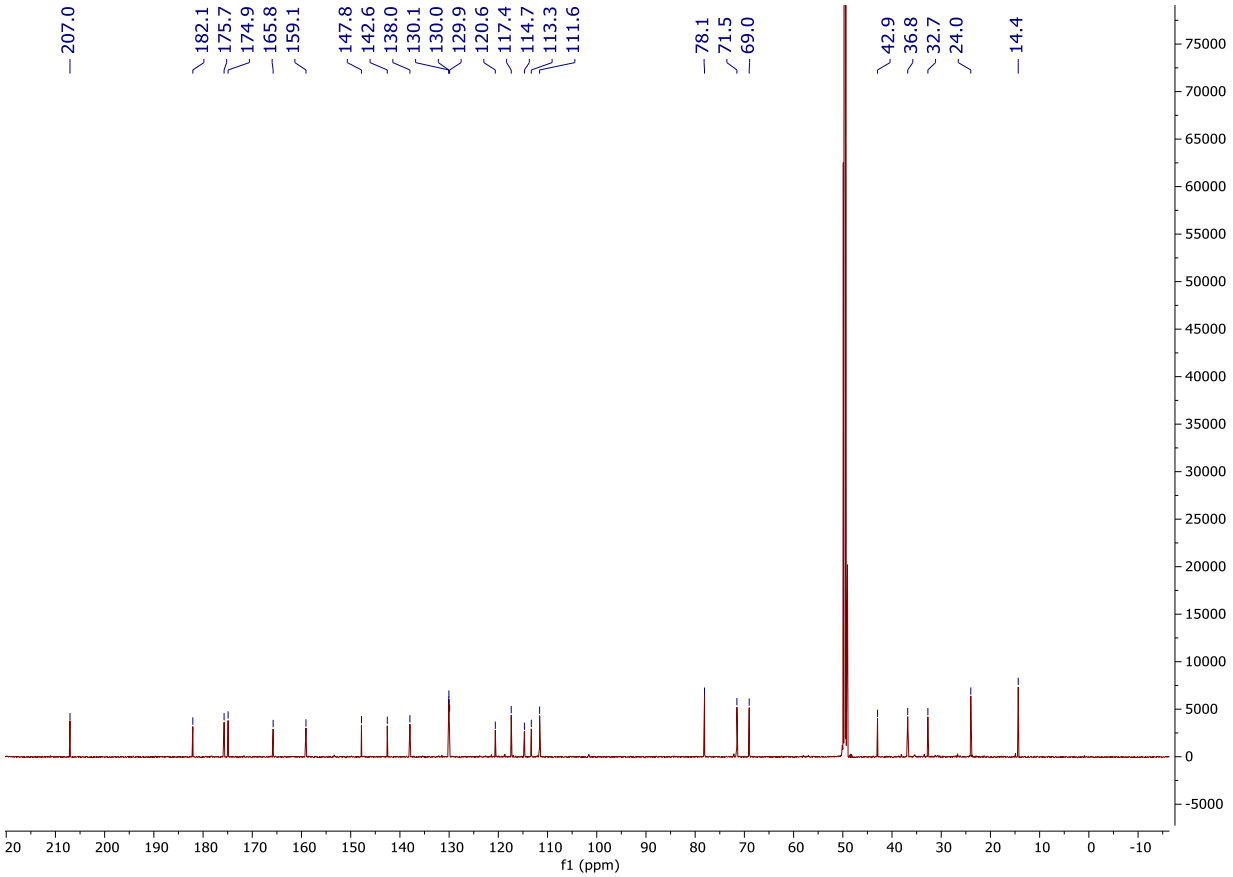


Figure S3. The $^{13}$C-NMR of compound **1**

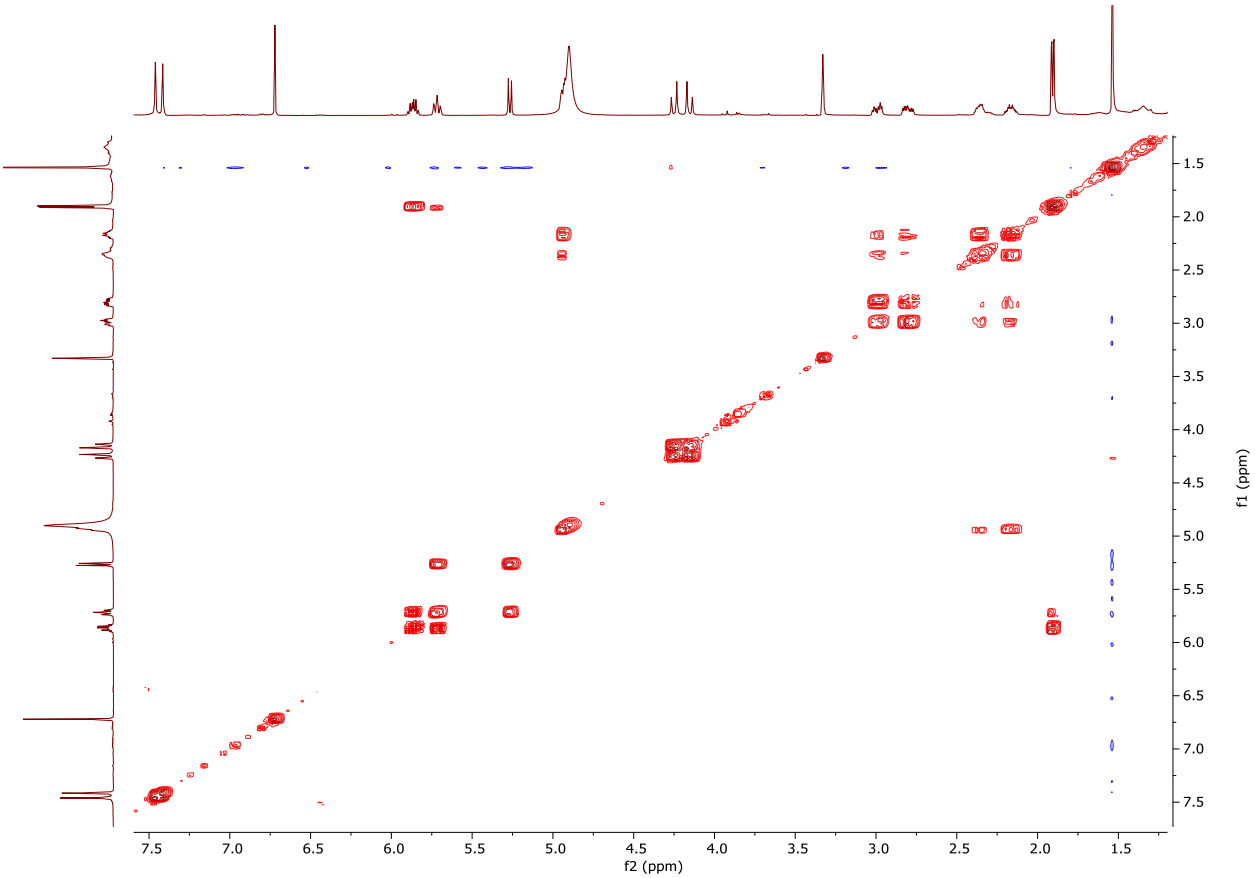


Figure S4. The $^{1}$H-$^{1}$H COSY of compound **1**

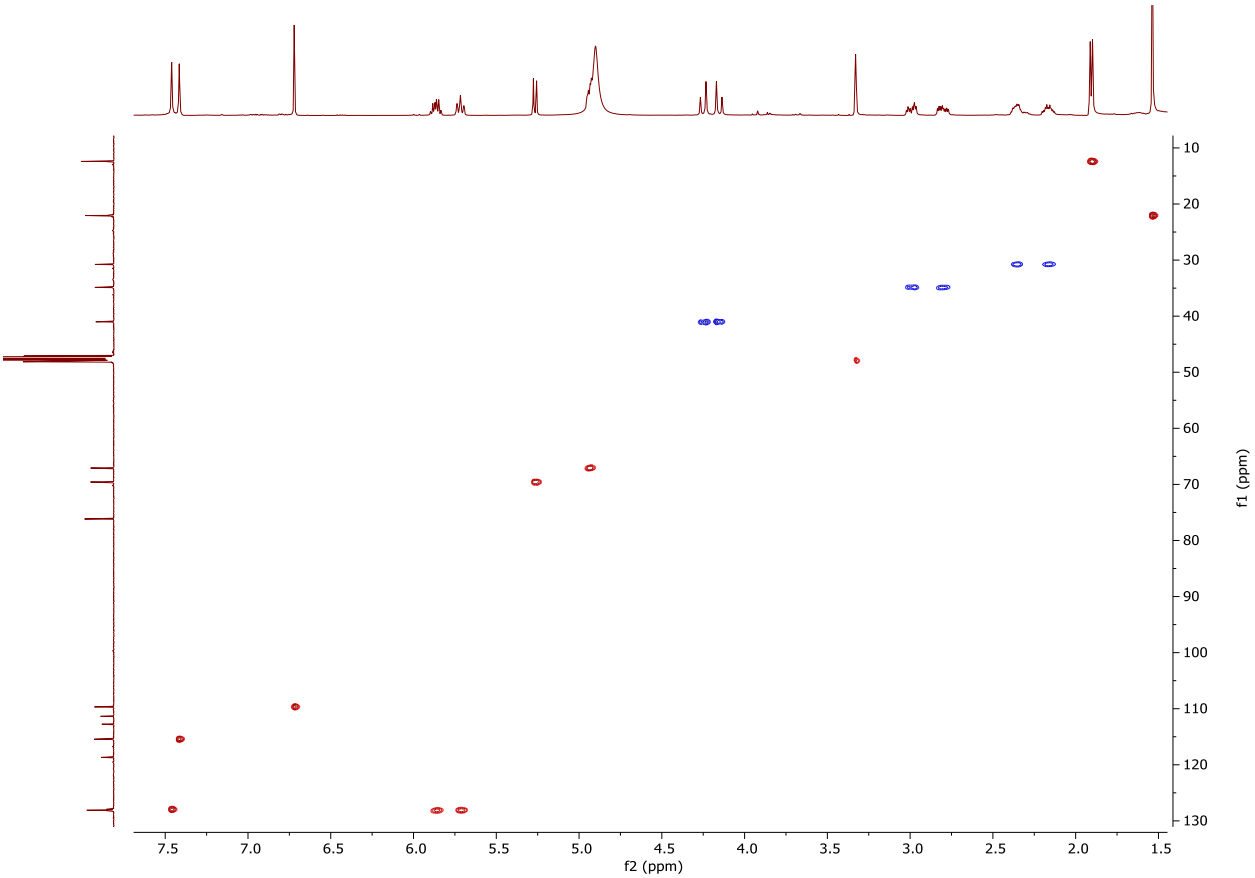


Figure S5. The HSQC of compound **1**

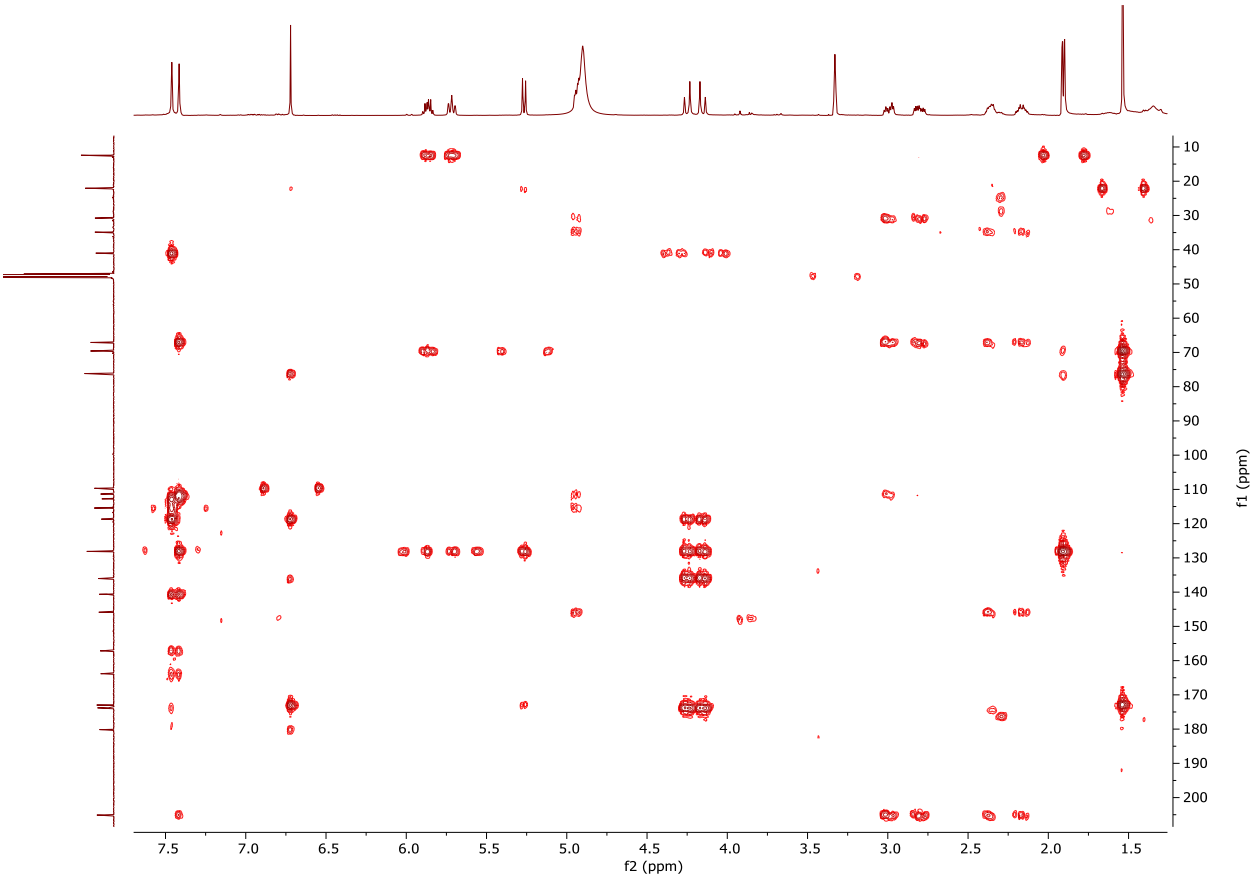


Figure S6. The HMBC of compound **1**

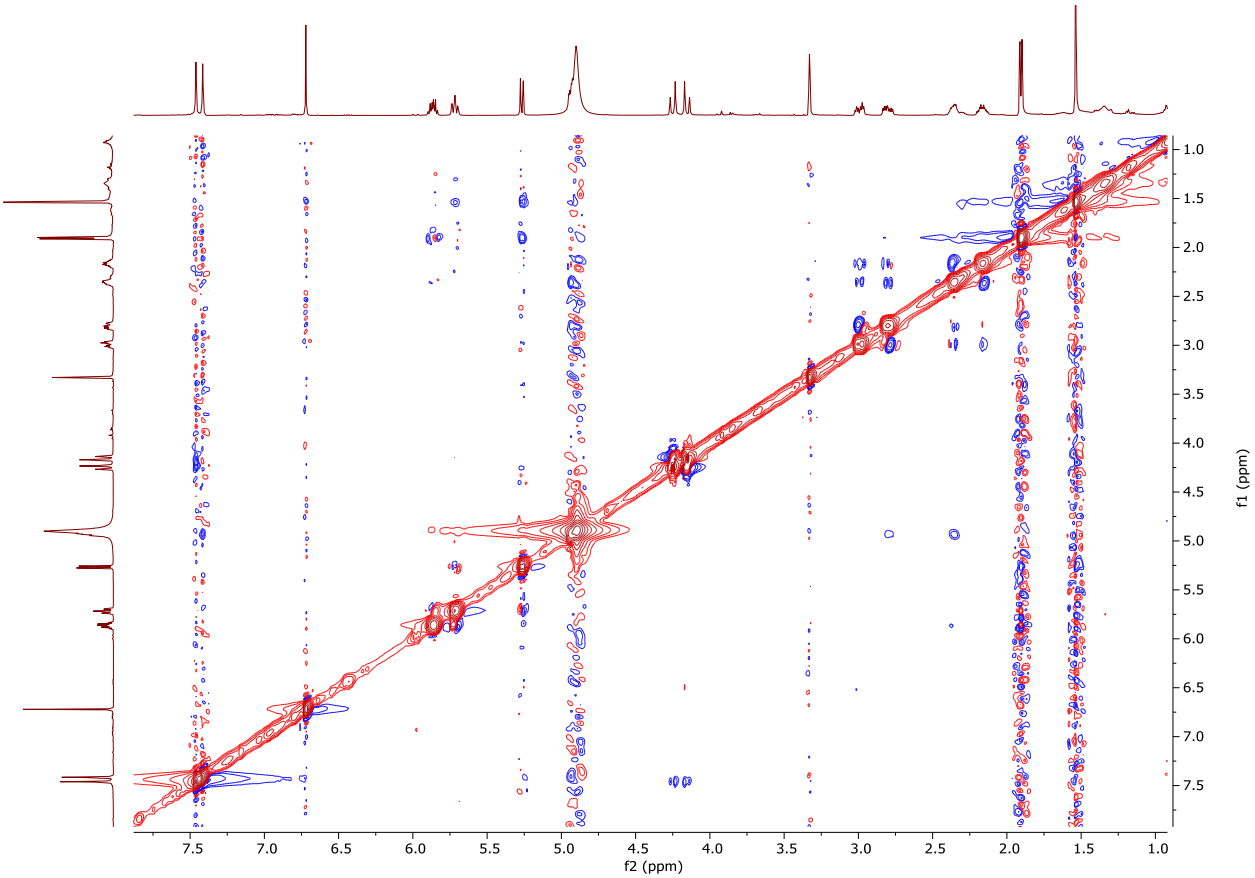


Figure S7. The NOESY of compound **1**

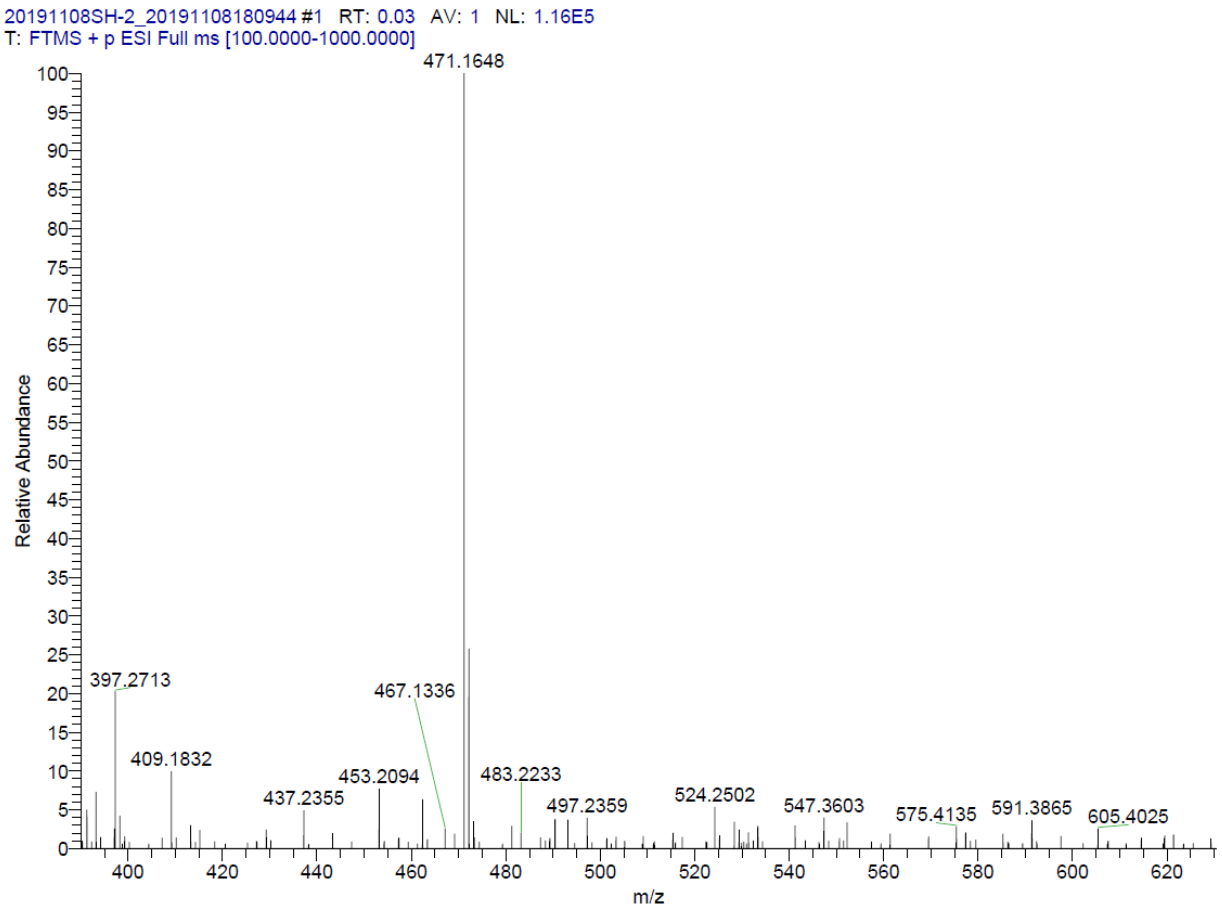


Figure S8. The HR-MS of compound **2**

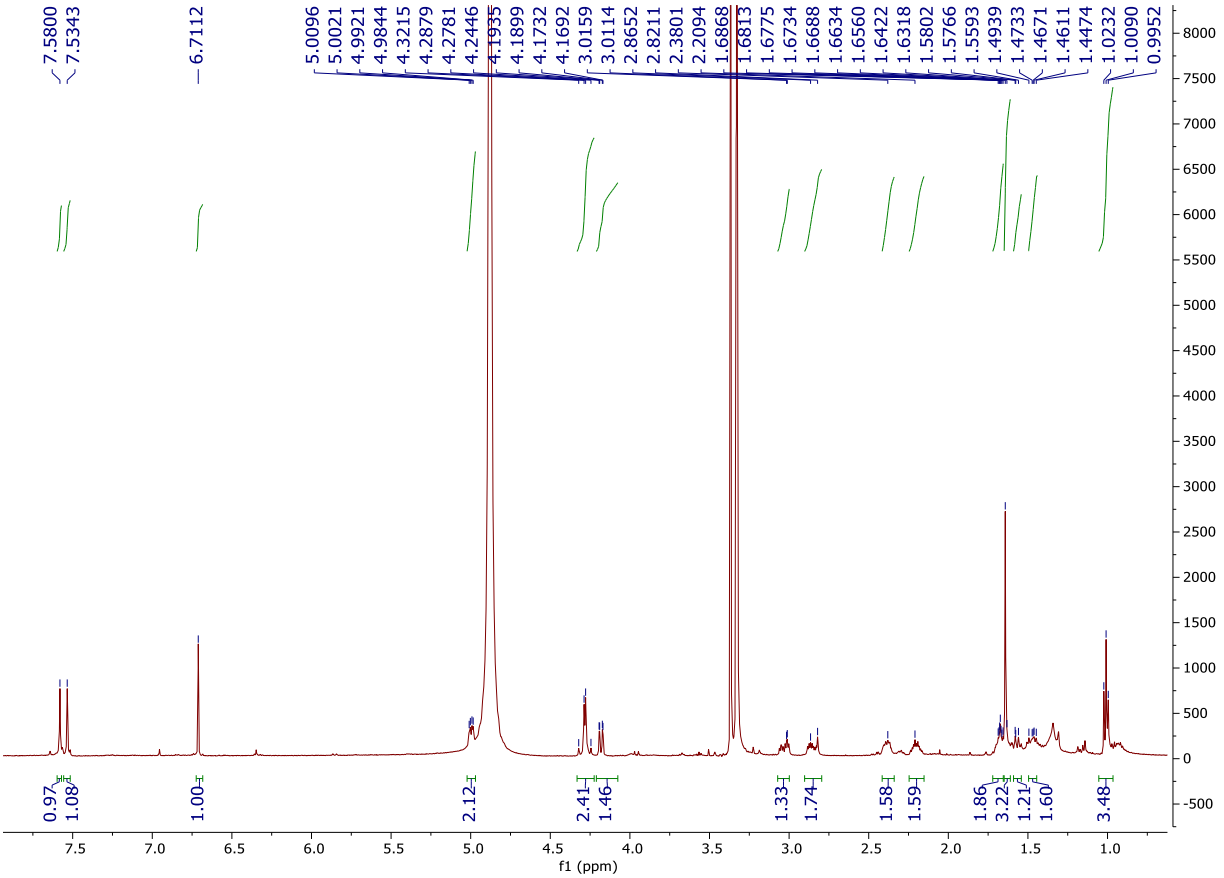


Figure S9. The $^{1}$H-NMR of compound **2**

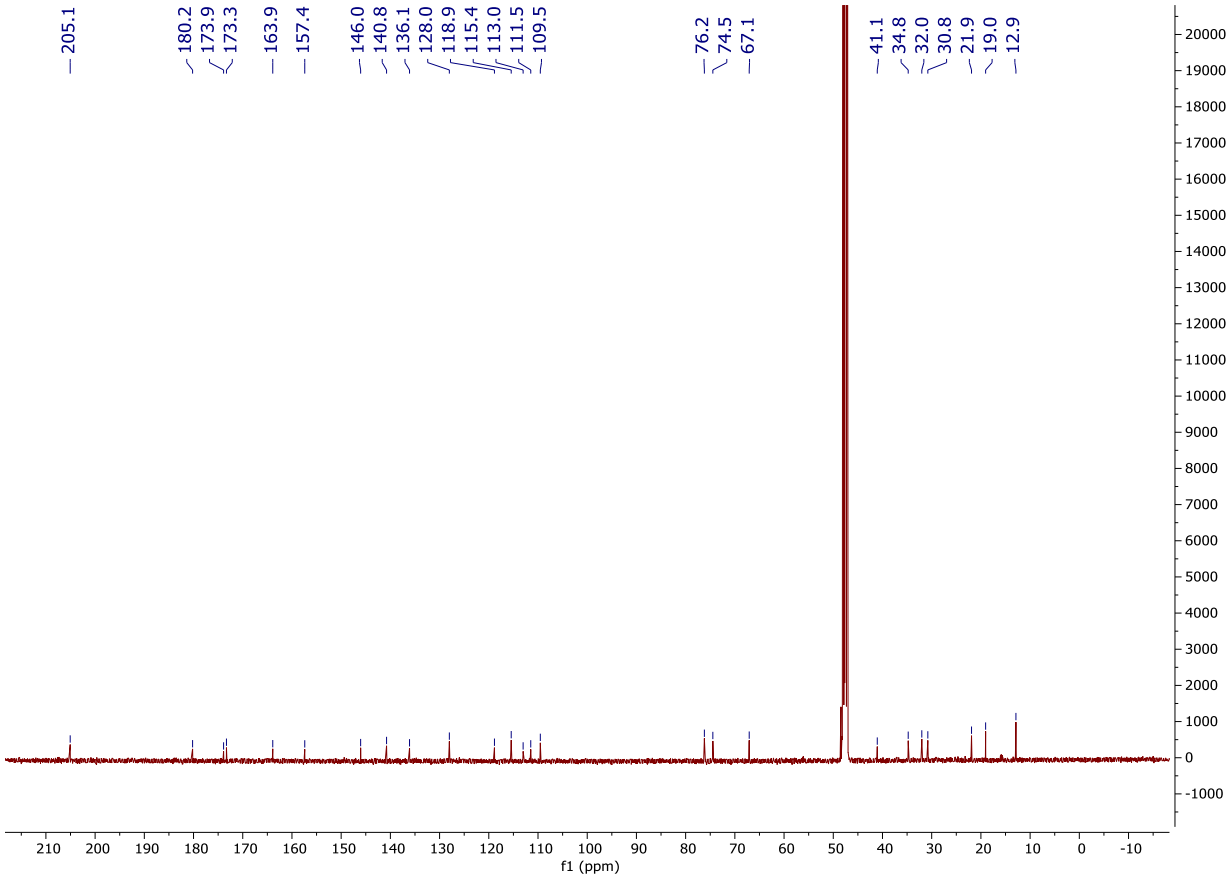


Figure S10. The $^{13}$C-NMR of compound **2**

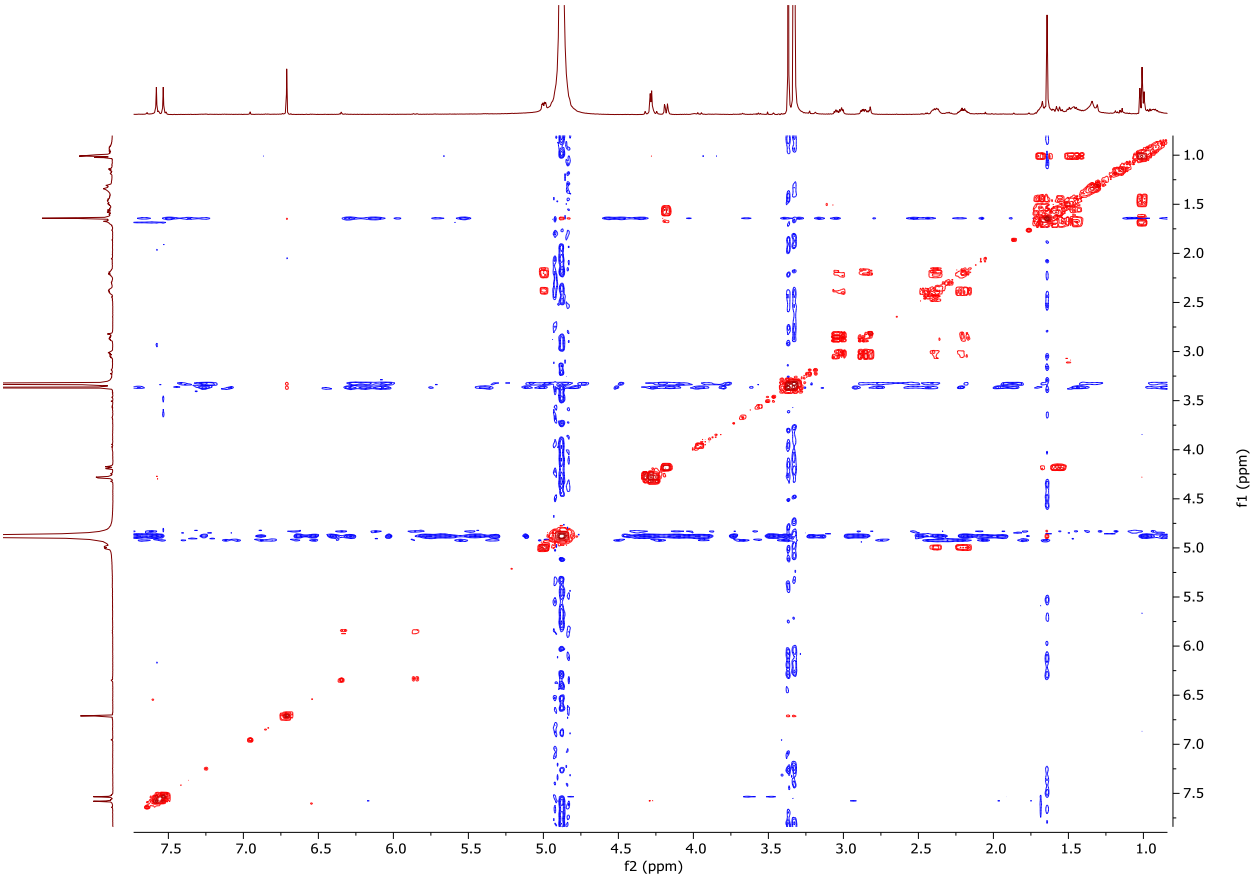


Figure S11. The $^{1}$H-$^{1}$H COSY of compound **2**

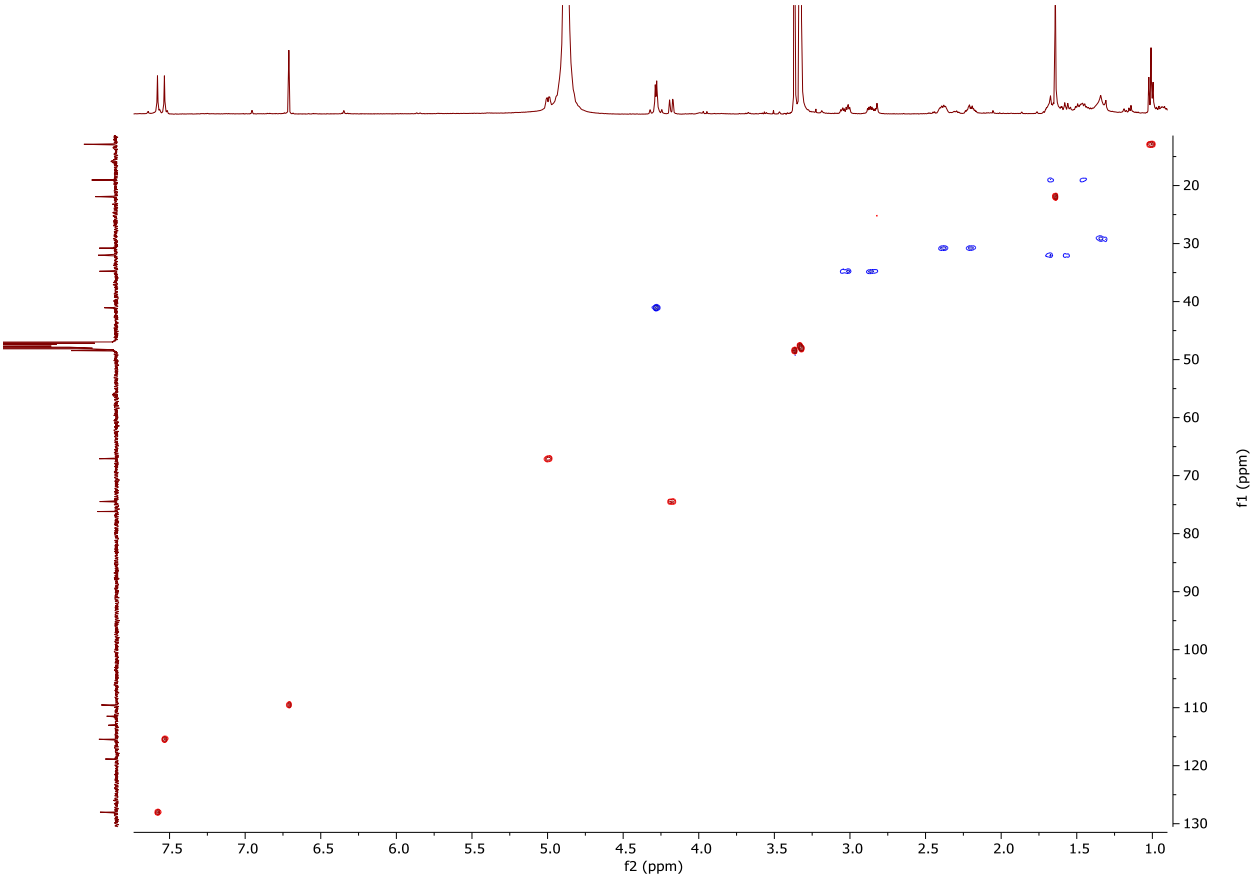


Figure S12. The HSQC of compound **2**

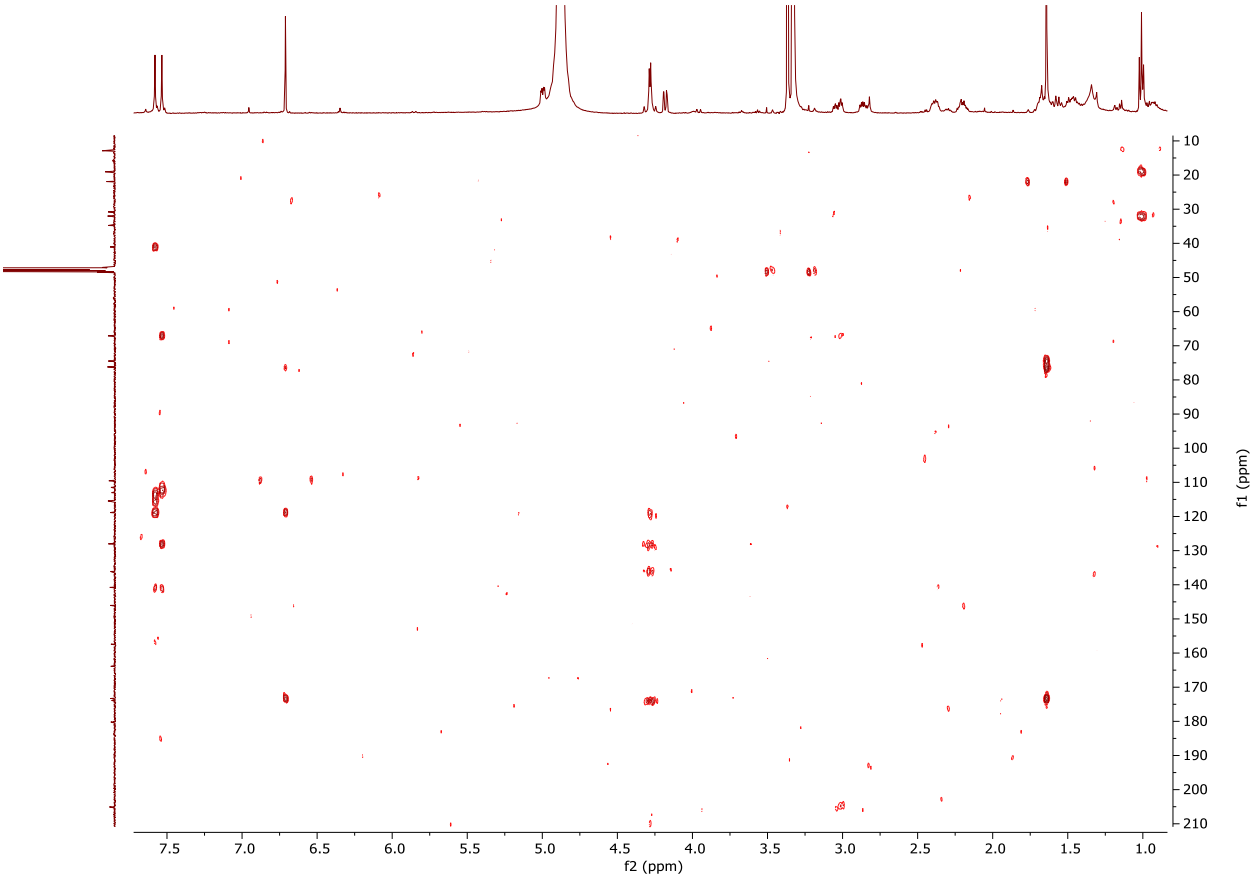


Figure S13. The HMBC of compound **2**

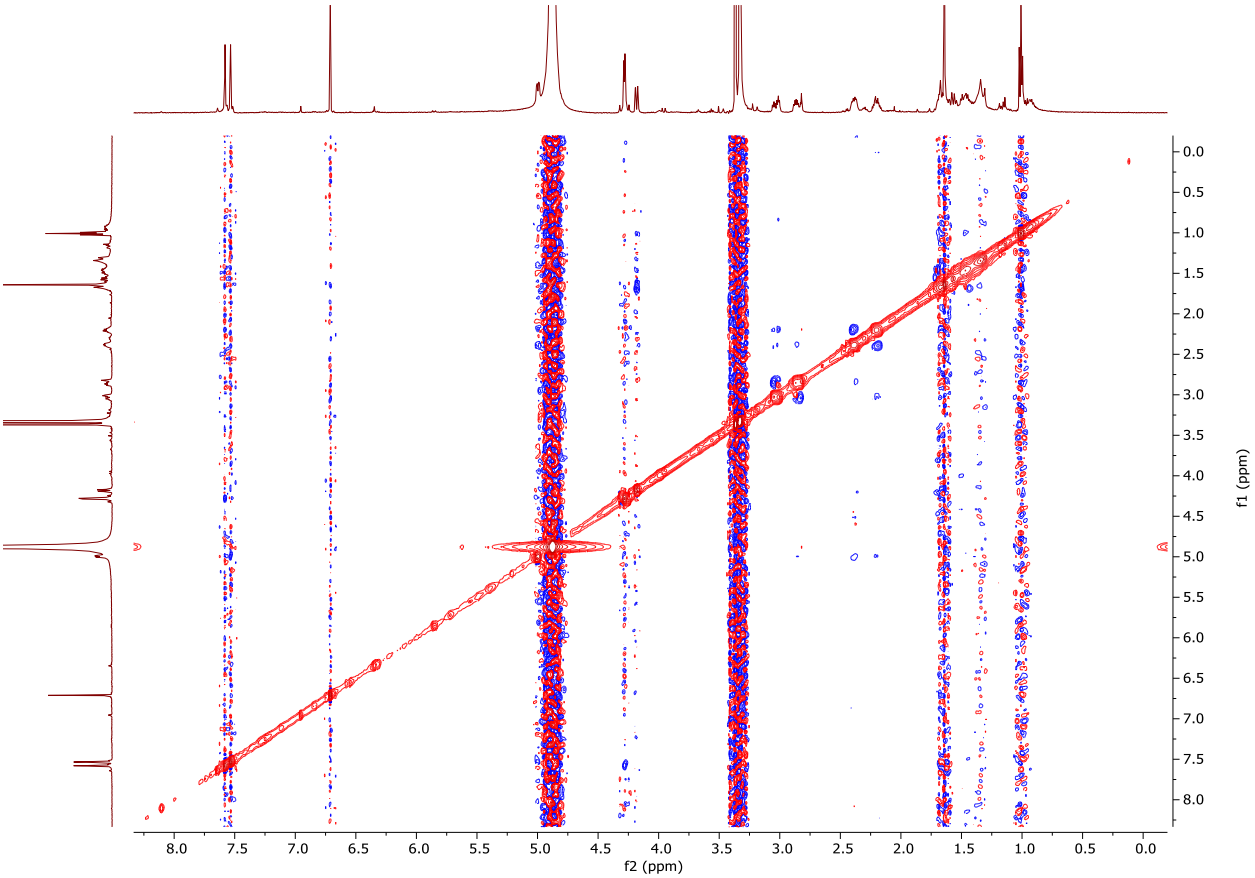


Figure S14. The NOESY of compound **2**

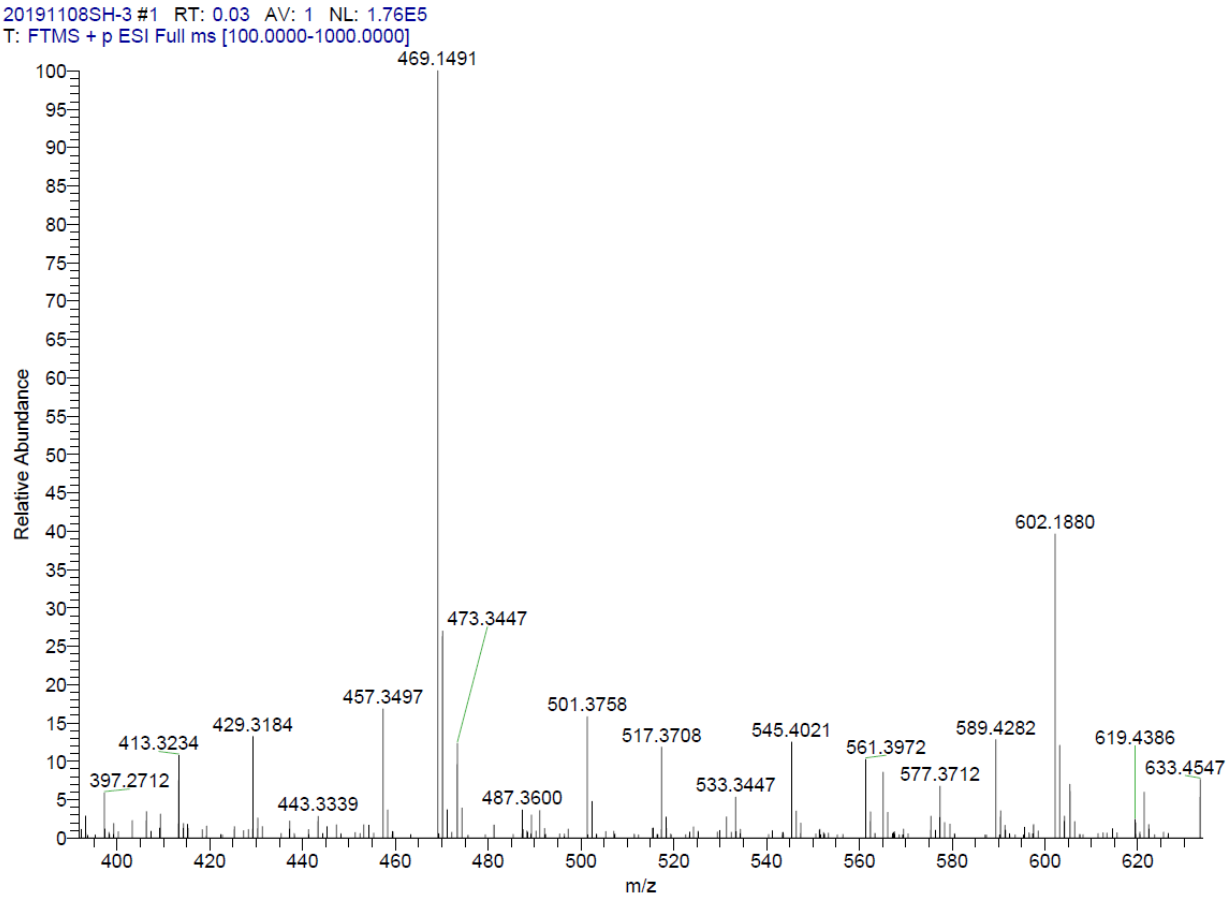


Figure S15. The HR-MS of compound **3**

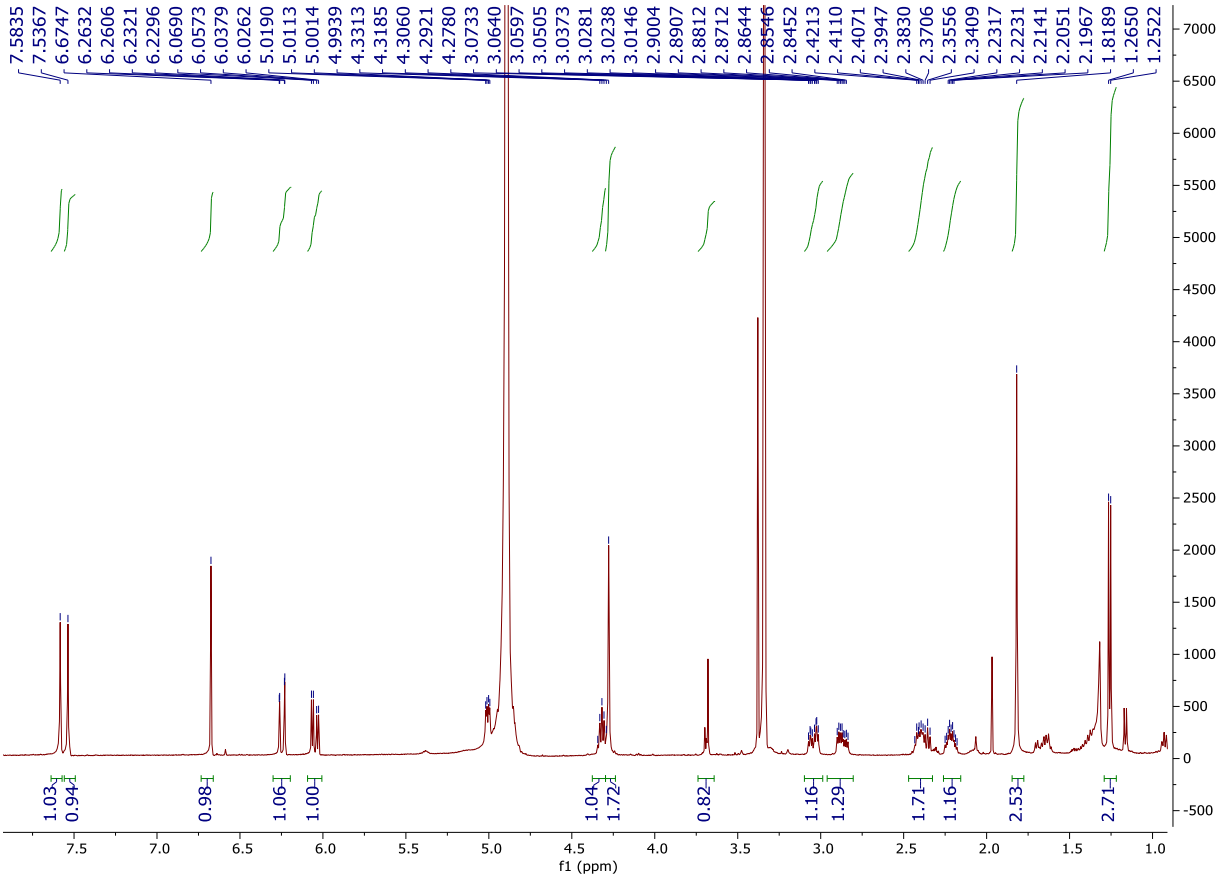


Figure S23. The $^{1}$H-NMR of compound **3**

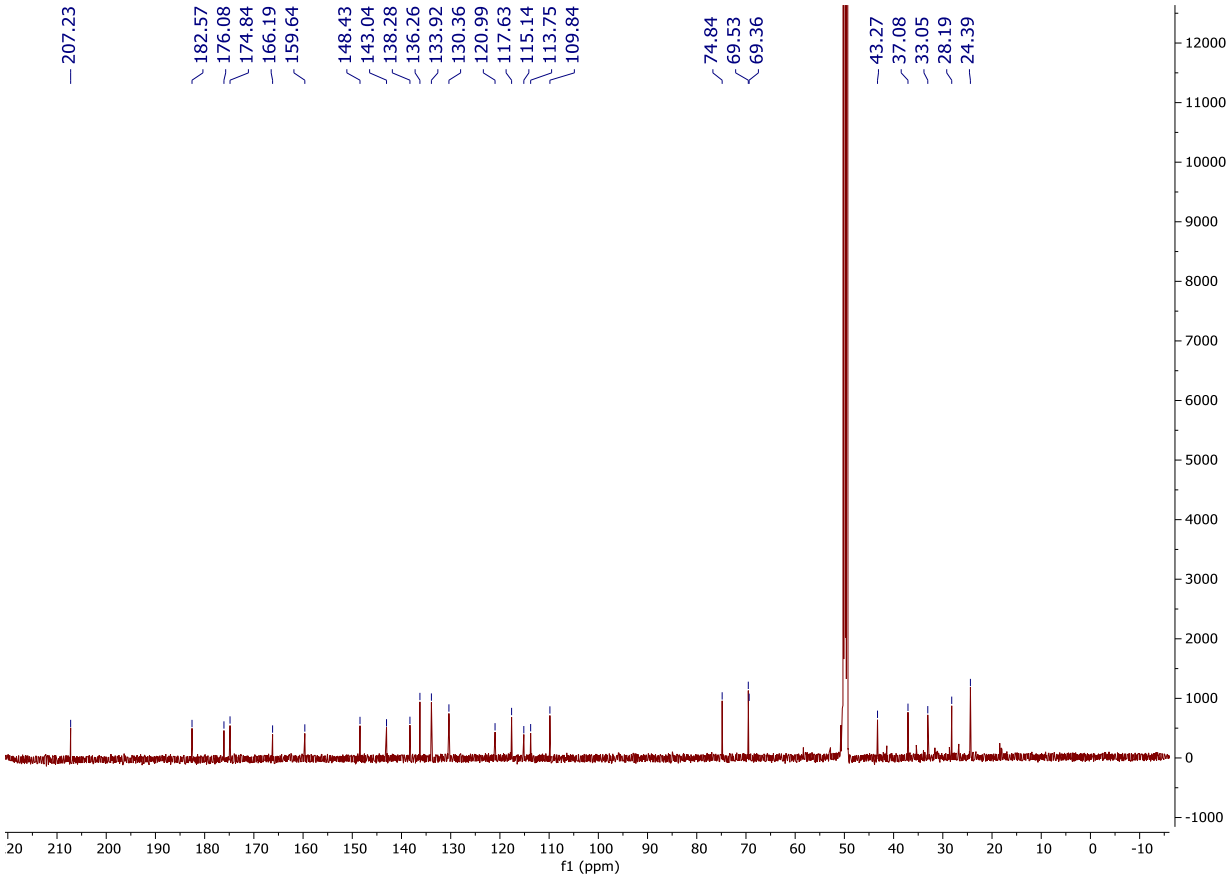


Figure S24. The $^{13}$C-NMR of compound **3**

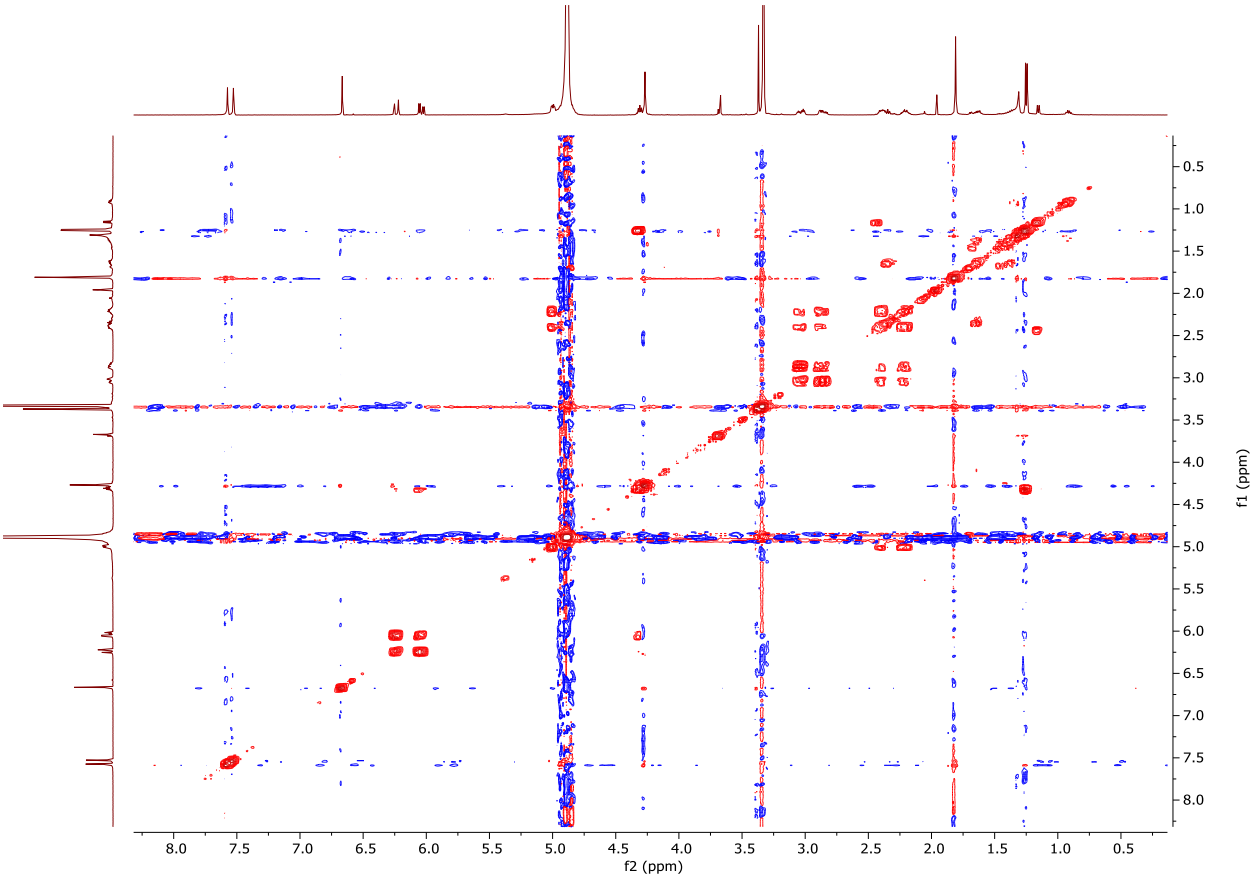


Figure S25. The $^{1}$H-$^{1}$H COSY of compound **3**

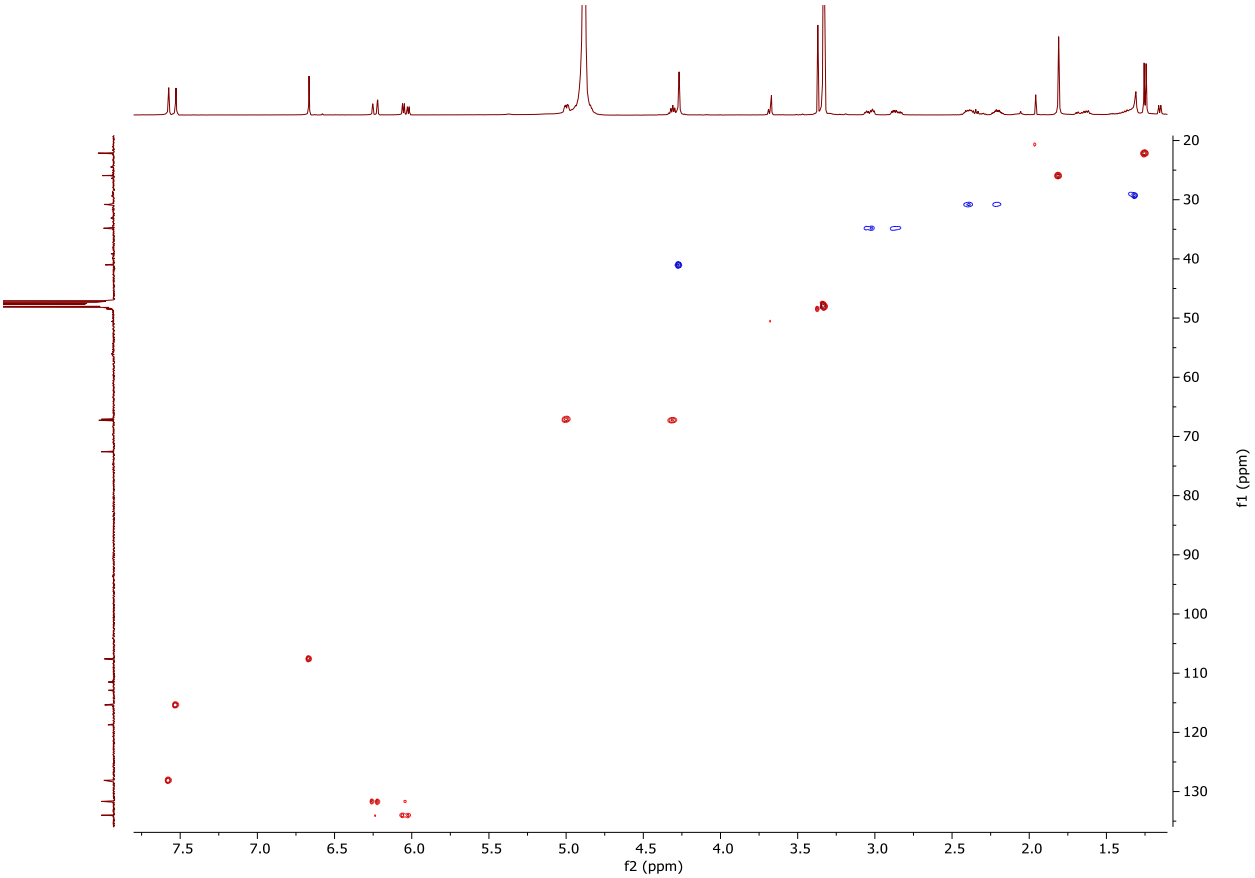


Figure S26. The HSQC of compound **3**

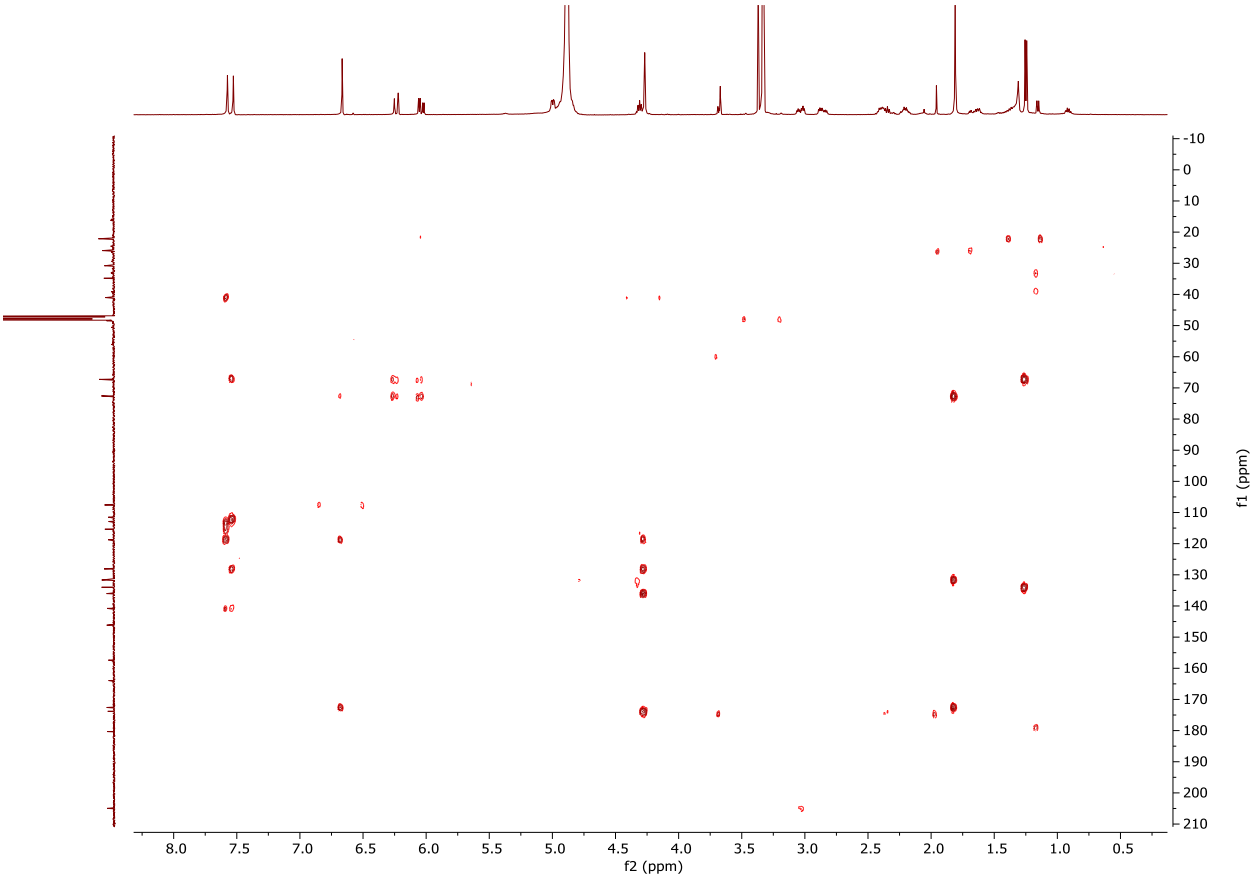


Figure S27. The HMBC of compound **3**

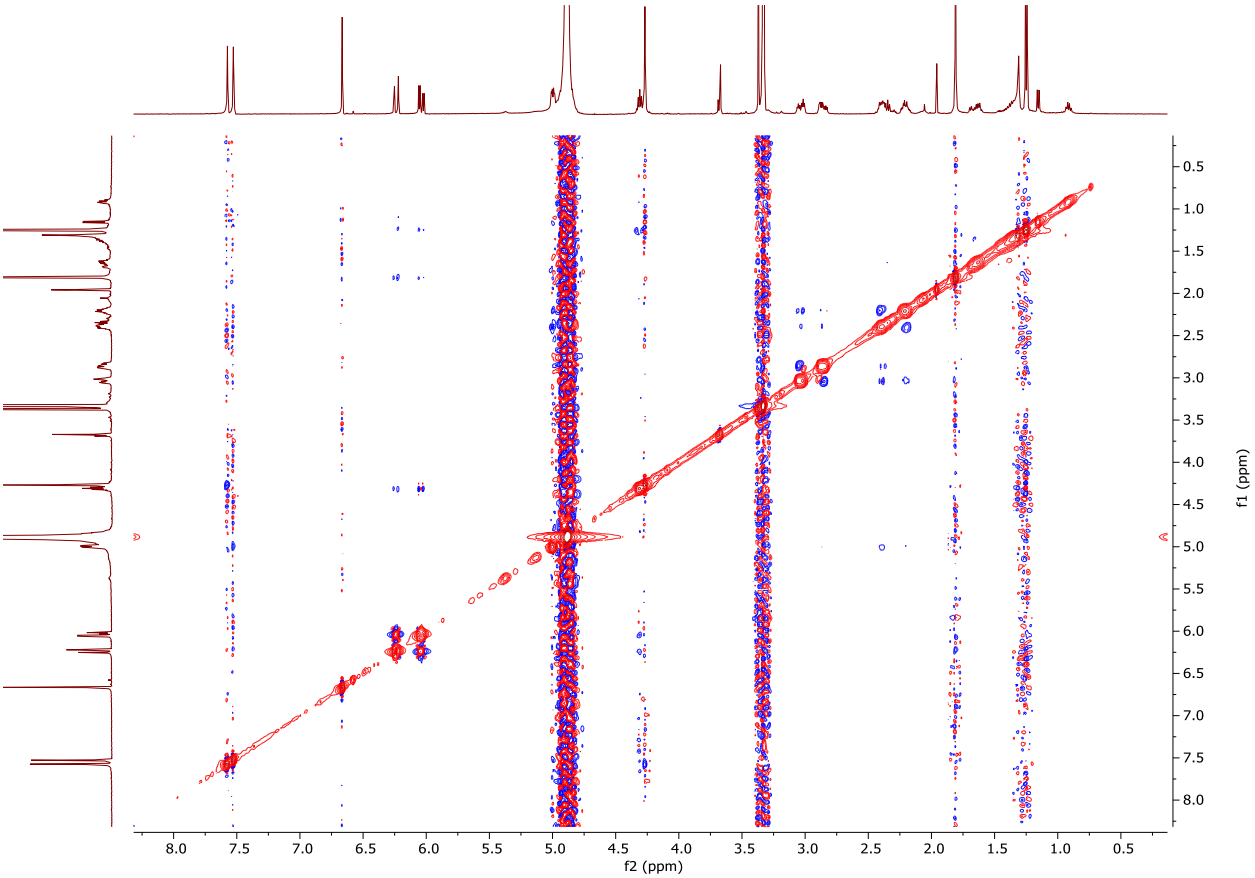


Figure S28. The NOESY of compound **3**

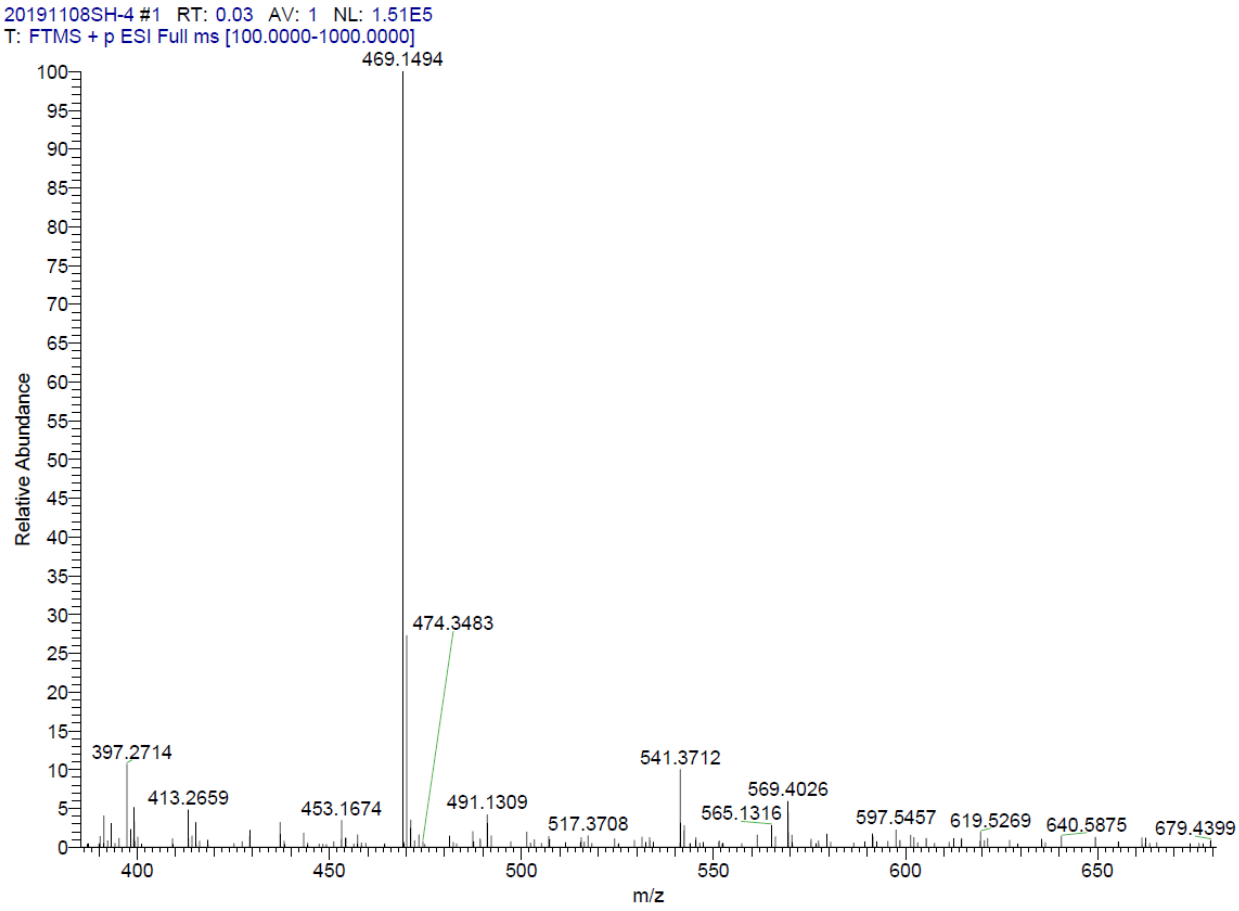


Figure S22. The HR-MS of compound **4**

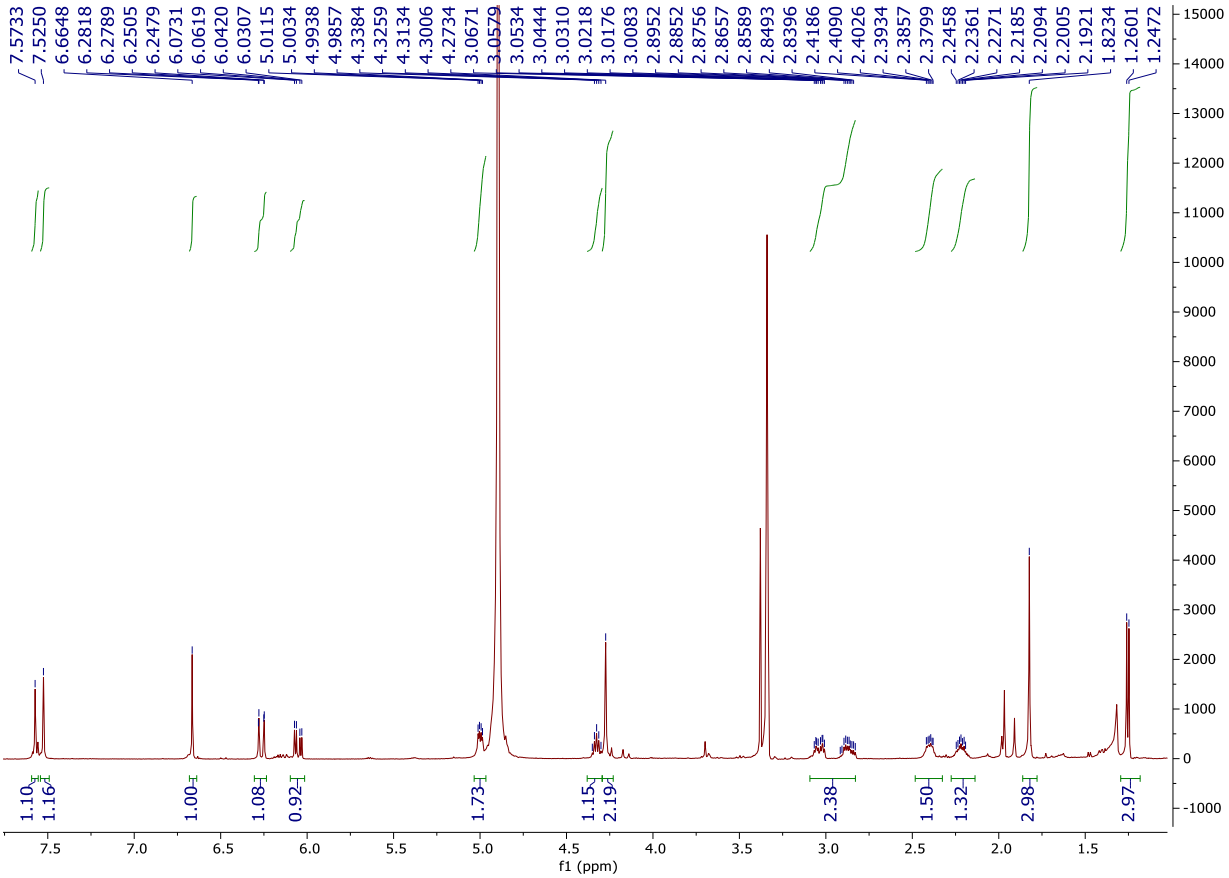


Figure S16. The $^{1}$H-NMR of compound **4**

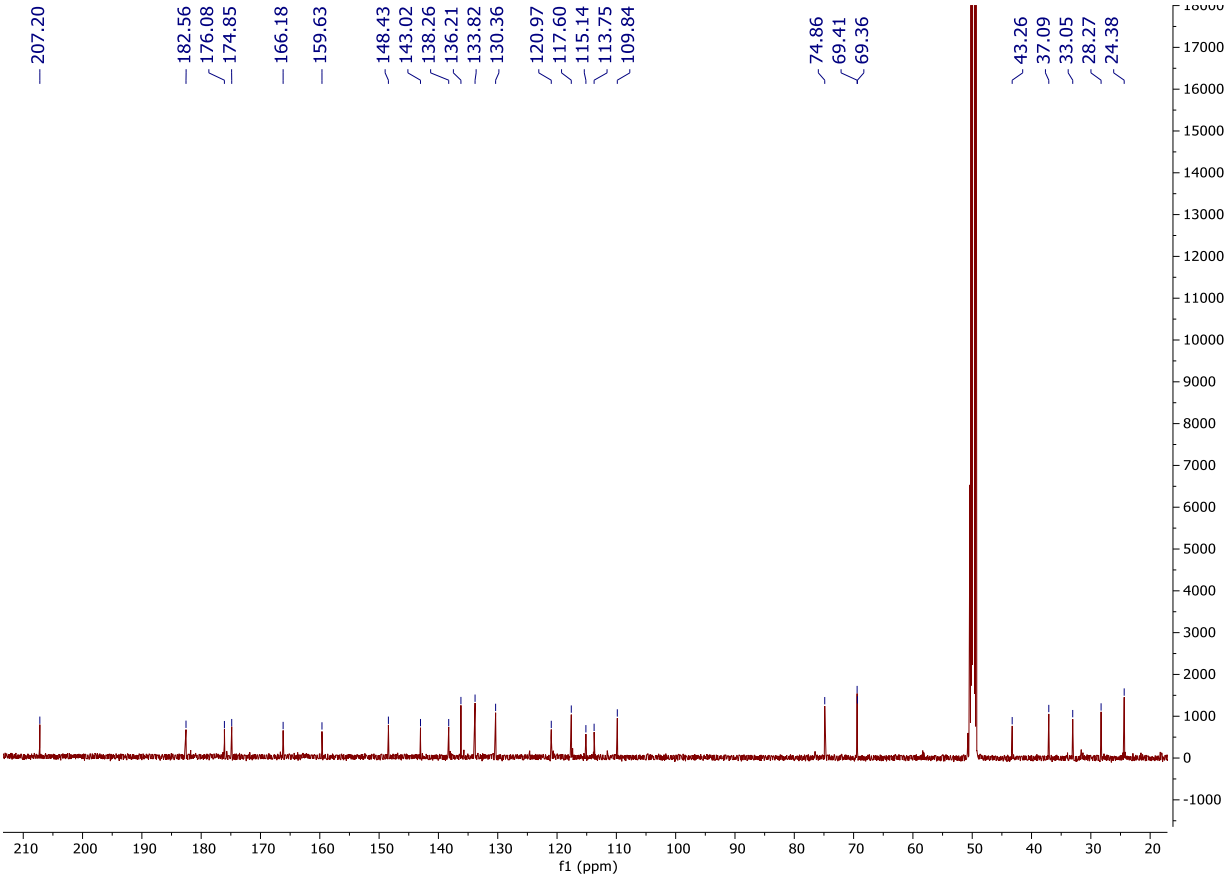


Figure S17. The $^{13}$C-NMR of compound **4**

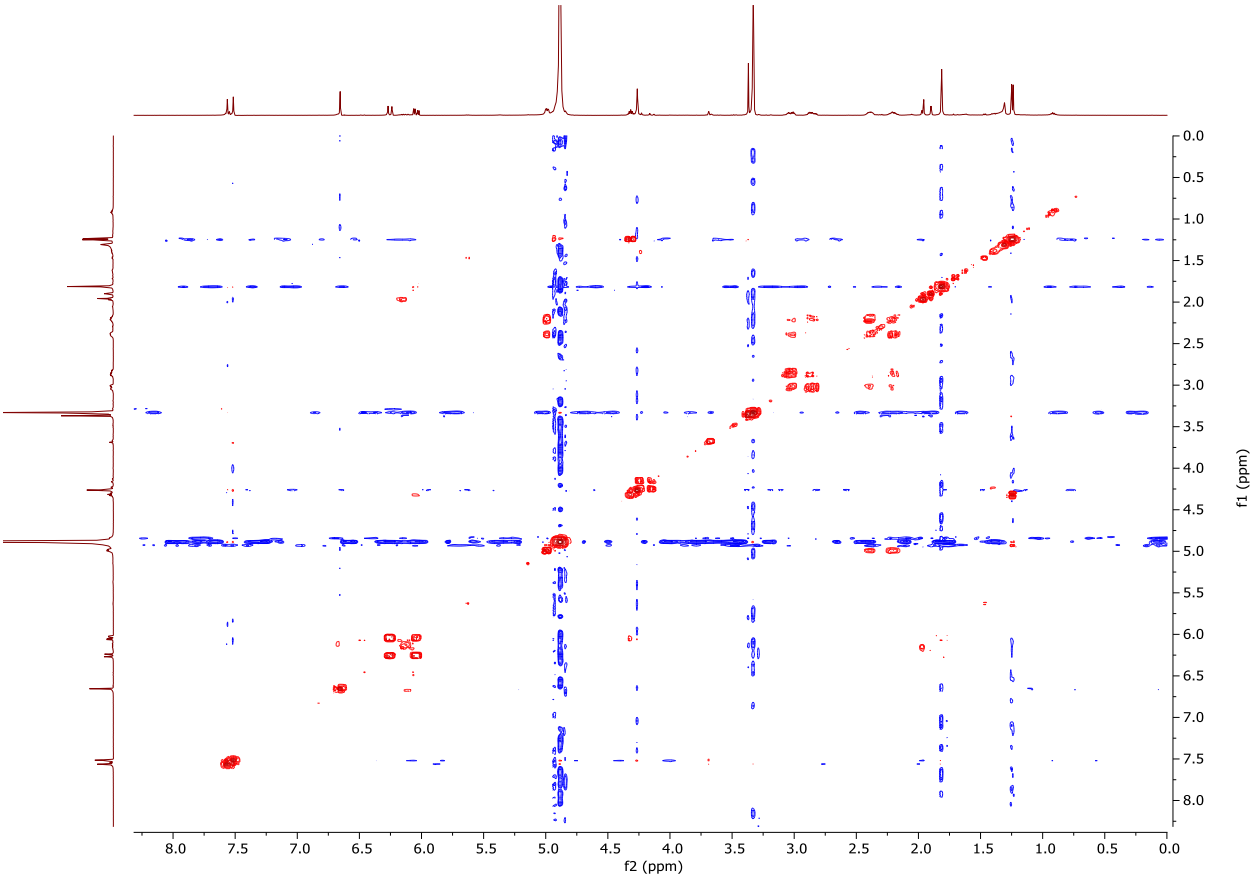


Figure S18. The $^{1}$H-$^{1}$H COSY of compound **4**

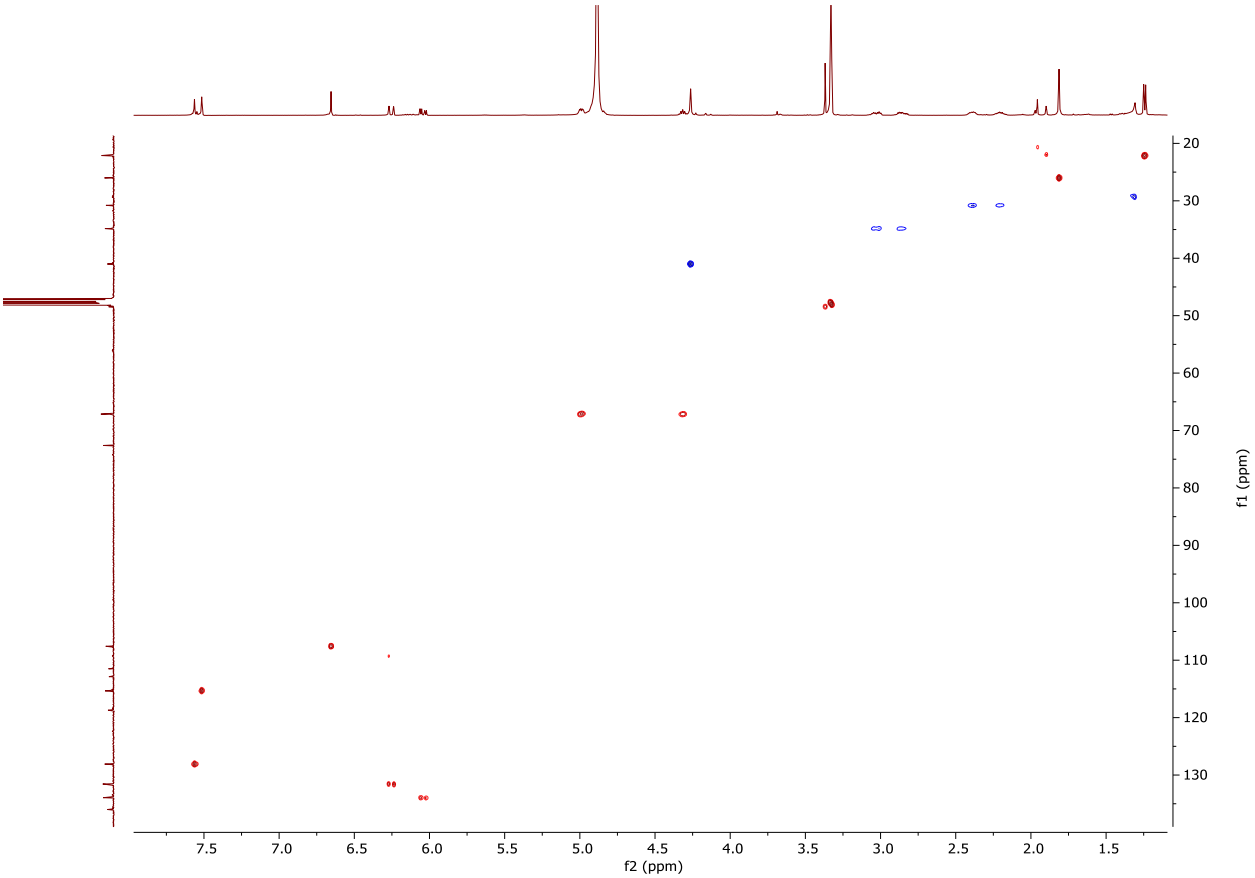


Figure S19. The HSQC of compound **4**

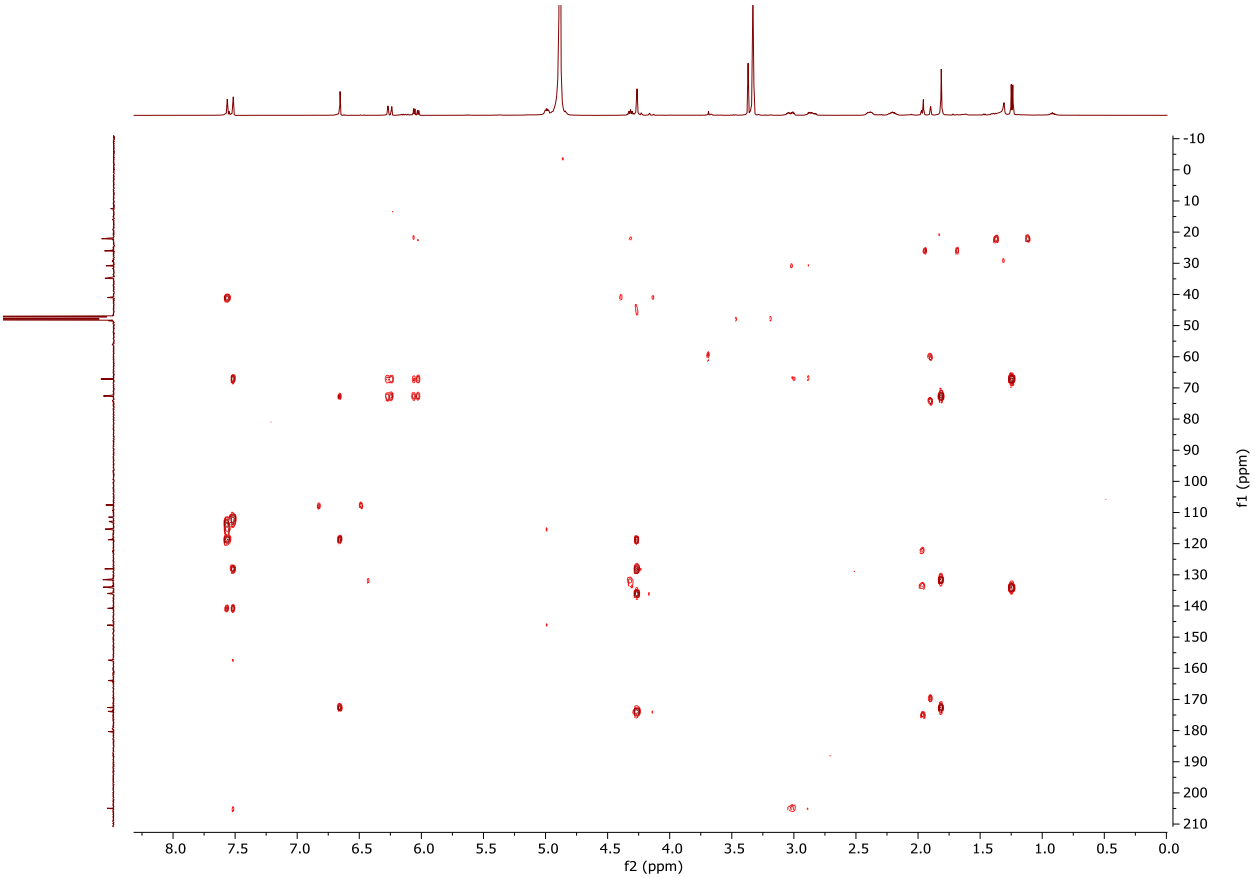


Figure S20. The HMBC of compound **4**

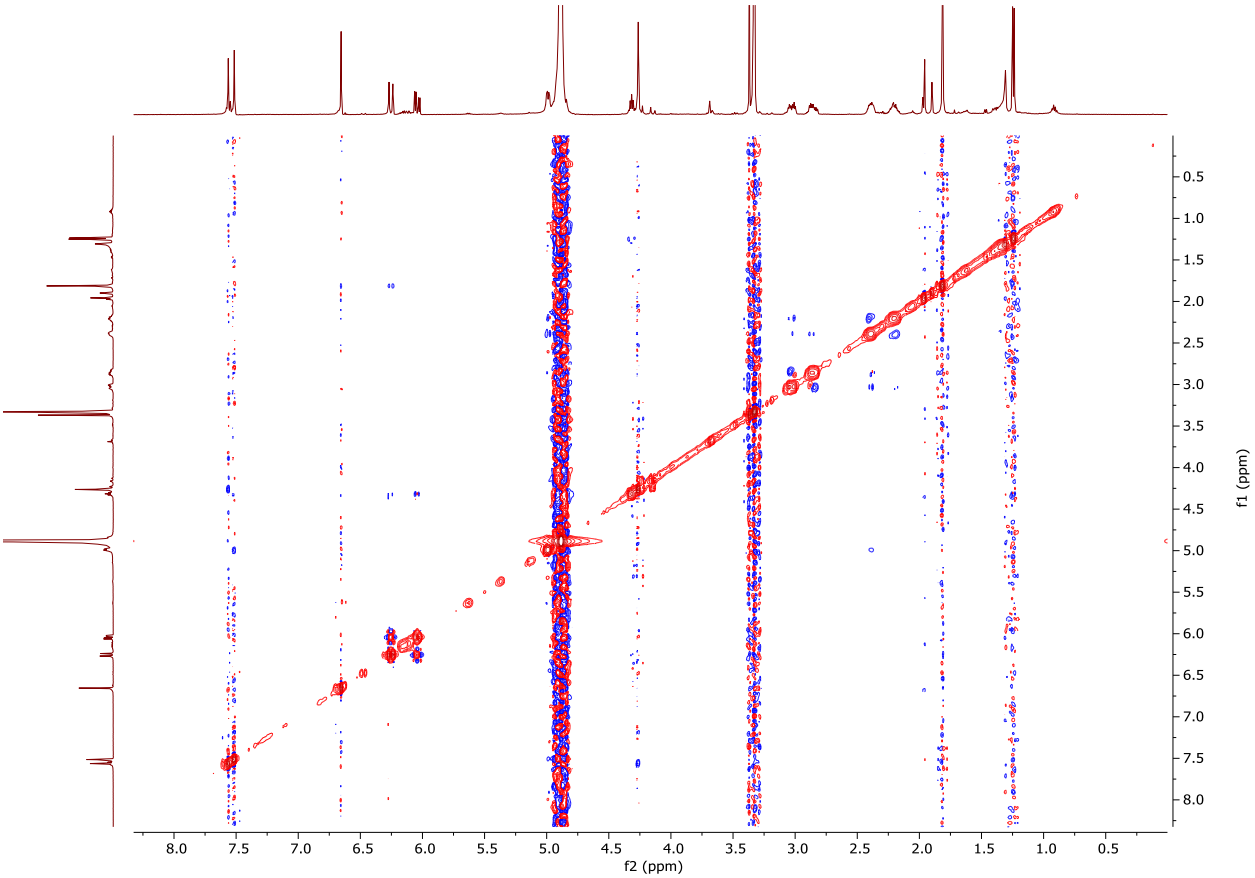


Figure S21. The NOESY of compound **4**

16S ribosomal RNA of *Streptomyces* sp. shell-016, partial sequence

ATGCAGTCGACGATGAACCGGTTTCGGCCGGGGATTAGTGGCGAACGGGTGAGTAA
CACGTGGGCAATCTGCCCTGCACTCTGGGACAAGCCCTGGAAACGGGGTCTAATAC
CGGATATGAACCTGGAAGGCATCTTCCGGGTTGTAAAGCTCCGGCGGTGCAGGATG
AGCCCGCGGCCTATCAGCTTGTTGGTGAGGTAACGGCTCACCAAGGCGACGACGGG
TAGCCGGCCTGAGAGGGCGACCGGCCACACTGGGACTGAGACACGGCCCAGACTCC
TACGGGGAGGCAGCAGTGGGGAATATTGCACAATGGGCGAAAGCCTGATGCAGCGA
CGCCGCGTGAGGGATGACGGCCTTCGGGTTGTAAACCTCTTTCAGCAGGGAAGAAG
CGAAAGTGACGGTACCTGCAGAAGAAGCGCCGGCTAACTACGTGCCAGCAGCCGCG
GTAATACGTAGGGCGCAAGCGTTGTCCGGAATTATTGGGCGTAAAGAGCTCGTAGG
CGGCTTGTCACGTCGGTTGTGAAAGCCCGGGGCTTAACCCCGGGTCTGCAGTCGATA
CGGGCAGGCTAGAGTTCGGTAGGGGAGATCGGAATTCcTGGTGTAGCGGTGAAATG
CGCAGATATCAGGAGGAACACCGGTGGCGAAGGCGGATCTCTGGGCCGATACTGAC
GCTGAGGAGCGAAAGCGTGGGGAGCGAACAGGATTAGATACCCTGGTAGTCCACGC
CGTAAACGGTGGGCACTAGGTGTGGGCAACATTCCACGTTGTCCGTGCCGCAGCTAA
CGCATTAAGTGCCCCGCCTGGGGAGTACGGCCGCAAGGCTAAAACTCAAAGGAATT
GACGGGGGCCCGCACAAGCGGCGGAGCATGTGGCTTAATTCGACGCAACGCGAAGA
ACCTTACCAAGGCTTGACATACACCGGAAAGCATTAGAGATAGTGCCCCCCTTGTGG
TCGGTGTACAGGTGGTGCATGGCTGTCGTCAGCTCGTGTCGTGAGATGTTGGGTTAA
GTCCCGCAACGAGCGCAACCCTTGTCCCGTGTTGCCAGCAGGCCCTTGTGGTGCTGG
GGACTCACGGGAGACCGCCGGGGTCAACTCGGAGGAAGGTGGGGACGACGTCAAG
TCATCATGCCCCTTATGTCTTGGGCTGCACACGTGCTACAATGGCCGGTACAATGAG
CTGCGATACCGCGAGGTGGAGCGAATCTCAAAAAGCCGGTCTCAGTTCGGATTGGG
GTCTGCAACTCGACCCCATGAAGTCGGAGTCGCTAGTAATCGCAGATCAGCATTGCT
GCGGTGAATACGTTCCCGGGCCTTGTACACACCGCCCGTCACGTCACGAAAGTCGGT
AACACCCGAAGCCGGTGGCCCAACCCCTTGTGGGAGGGAGC

Crystal Structure Reports

**Experimental Summary**

The single crystal X-ray diffraction studies were carried out on a Bruker Kappa Photon II CPAD diffractometer equipped with Cu $K_\alpha$ radiation ($\lambda$ = 1.54178). A 0.217 x 0.114 x 0.096 mm piece of an orange rod was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using $\phi$ and $\varpi$ scans. Crystal-to-detector distance was 50 mm using variable exposure time (10s-60s) depending on $\theta$ with a scan width of 1.0°. Data collection was 89.2% complete to 59.031° in $\theta$, (0.90 Å). A total of 14220 reflections were collected covering the indices, -10<=h<=10, -12<=k<=12, -13<=l<=12. 5334 reflections were found to be symmetry independent, with a $R_{int}$ of 0.0251. Indexing and unit cell refinement indicated a primitive, triclinic lattice. The space group was found to be *P*1. The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model for refinement.

All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. The absolute stereochemistry of the molecule was established by anomalous dispersion using the Parson's method with a Flack parameter of 0.020(73). Crystallographic data are summarized in Table 1.

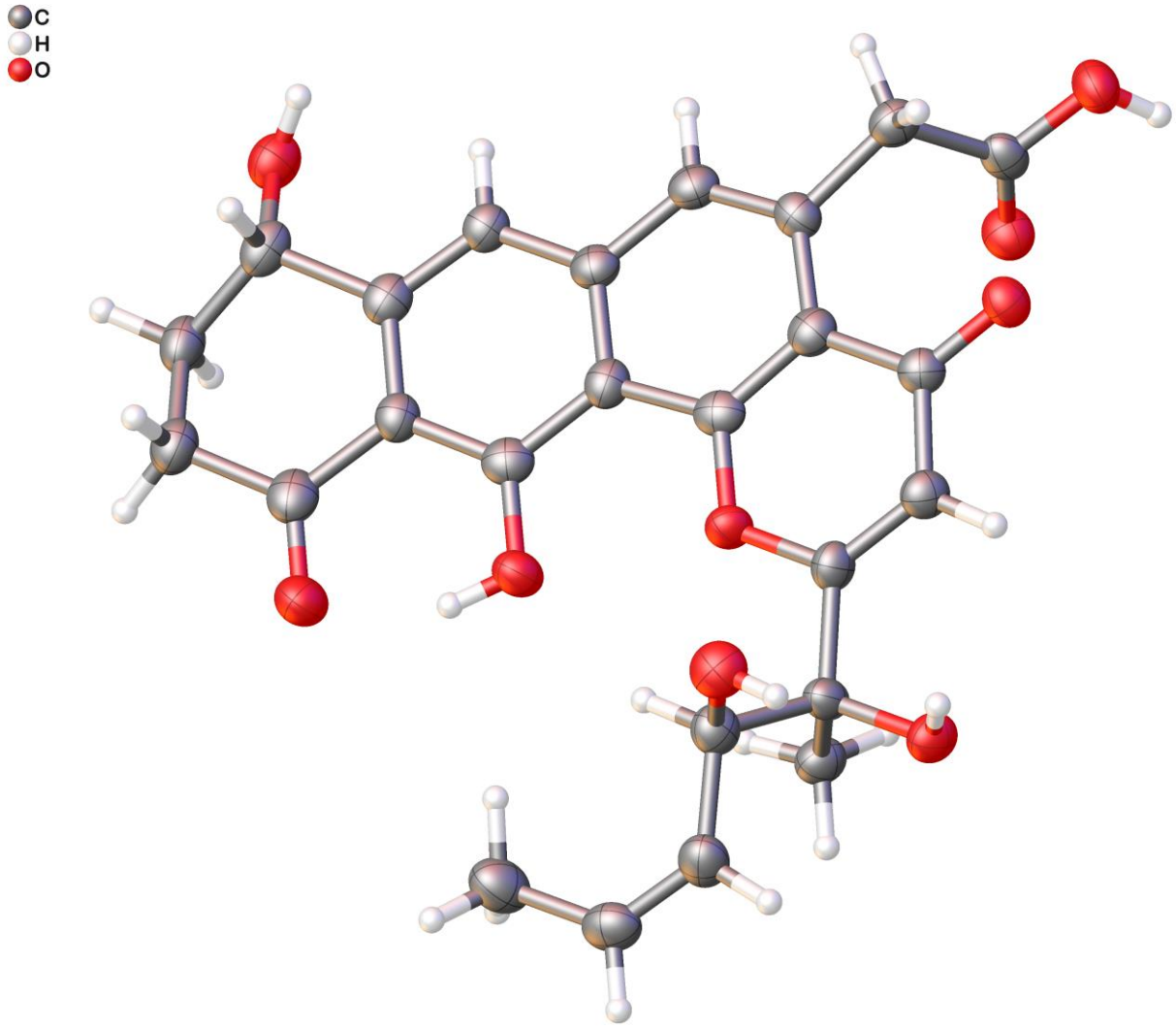
C
H
O

Table 1. Crystal data and structure refinement for SHELLMYCINA.

| | | |
|---|---|---|
| Report date | 2019-12-05 | |
| Identification code | SHELLMYCINA | |
| Empirical formula | C26.20 H28.40 O10 | |
| Molecular formula | C25 H24 O9, 0.8(C H4 O), 0.2(C2 H6 O) | |
| Formula weight | 503.29 | |
| Temperature | 100 K | |
| Wavelength | 1.54178 Å | |
| Crystal system | Triclinic | |
| Space group | P1 | |
| Unit cell dimensions | a = 9.5749(5) Å | $\alpha$= 65.634(3)°. |
| | b = 11.5552(6) Å | $\beta$= 89.720(3)°. |
| | c = 11.8417(6) Å | $\gamma$ = 79.122(3)°. |
| Volume | 1168.12(11) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.431 $Mg/m^3$ | |
| Absorption coefficient | 0.927 $mm^{-1}$ | |
| F(000) | 531 | |
| Crystal size | 0.217 x 0.114 x 0.096 $mm^3$ | |
| Crystal color, habit | Orange Rod | |
| Theta range for data collection | 4.112 to 59.031°. | |
| Index ranges | -10<=h<=10, -12<=k<=12, -13<=l<=12 | |
| Reflections collected | 14220 | |
| Independent reflections | 5334 [R(int) = 0.0251, R(sigma) = 0.0313] | |
| Completeness to theta = 59.031° | 89.2 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.152328 and 0.065793 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5334 / 21 / 676 | |
| Goodness-of-fit on $F^2$ | 1.078 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0274, wR2 = 0.0745 | |
| R indices (all data) | R1 = 0.0282, wR2 = 0.0753 | |
| Absolute structure parameter | 0.02(7) | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.190 and -0.168 $e.Å^{-3}$ | |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for SHELLMYCINA. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| O(1) | 5155(3) | 1211(3) | 459(3) | 43(1) |
| O(2) | 3957(3) | 3950(3) | -229(3) | 36(1) |
| O(3) | 3163(3) | 1557(3) | 2654(3) | 30(1) |
| O(4) | 5564(3) | 3248(3) | 4091(3) | 33(1) |
| O(5) | 1705(3) | -132(3) | 2856(3) | 35(1) |
| O(6) | 598(3) | -2020(3) | 3175(3) | 44(1) |
| O(7) | 576(3) | -3325(3) | 8164(3) | 40(1) |
| O(8) | 3095(3) | 3812(3) | 5609(3) | 37(1) |
| O(9) | 5141(3) | 3801(3) | 6524(3) | 38(1) |
| C(1) | 1505(5) | 467(5) | -571(5) | 48(1) |
| C(2) | 2164(5) | 1551(4) | -1385(5) | 40(1) |
| C(3) | 3081(5) | 2098(4) | -1044(4) | 38(1) |
| C(4) | 3656(4) | 1747(4) | 245(4) | 34(1) |
| C(5) | 3291(4) | 2938(4) | 552(4) | 30(1) |
| C(6) | 3751(4) | 2570(4) | 1898(4) | 30(1) |
| C(7) | 4546(4) | 3138(4) | 2341(4) | 32(1) |
| C(8) | 4793(4) | 2742(4) | 3657(4) | 28(1) |
| C(9) | 4077(4) | 1709(4) | 4464(5) | 32(1) |
| C(10) | 3302(4) | 1149(4) | 3907(4) | 30(1) |
| C(11) | 2592(4) | 107(4) | 4608(5) | 30(1) |
| C(12) | 1866(4) | -545(4) | 4085(5) | 32(1) |
| C(13) | 1362(4) | -1658(4) | 4878(5) | 30(1) |
| C(14) | 753(4) | -2398(4) | 4317(5) | 38(1) |
| C(15) | 362(5) | -3645(4) | 5155(5) | 40(1) |
| C(16) | -43(4) | -3681(4) | 6415(5) | 38(1) |
| C(17) | 1083(4) | -3360(4) | 7041(5) | 35(1) |
| C(18) | 1495(4) | -2077(4) | 6183(4) | 32(1) |
| C(19) | 2073(4) | -1377(4) | 6678(4) | 29(1) |
| C(20) | 2668(4) | -316(4) | 5914(4) | 30(1) |
| C(21) | 3411(4) | 318(4) | 6458(5) | 32(1) |
| C(22) | 4115(4) | 1273(4) | 5781(4) | 29(1) |

| | | | | |
|---|---|---|---|---|
| C(23) | 4909(4) | 1842(4) | 6454(4) | 34(1) |
| C(24) | 4268(5) | 3257(4) | 6122(4) | 31(1) |
| C(25) | 1689(4) | 3486(4) | 349(4) | 35(1) |
| O(1') | 8545(3) | 5724(2) | 9707(3) | 32(1) |
| O(2') | 5680(3) | 5848(3) | 10063(3) | 32(1) |
| O(3') | 6643(3) | 8192(2) | 7226(3) | 29(1) |
| O(4') | 4501(3) | 6364(3) | 5760(3) | 34(1) |
| O(5') | 8220(3) | 9776(3) | 7073(3) | 32(1) |
| O(6') | 9556(3) | 11522(3) | 6795(3) | 40(1) |
| O(7') | 8592(3) | 13335(3) | 1740(3) | 36(1) |
| O(8') | 7010(3) | 5833(3) | 4291(3) | 36(1) |
| O(9') | 5030(3) | 5842(3) | 3279(3) | 38(1) |
| C(1') | 8459(6) | 9000(5) | 10517(5) | 48(1) |
| C(2') | 8181(5) | 7691(4) | 11355(5) | 34(1) |
| C(3') | 7862(4) | 6809(4) | 11024(4) | 32(1) |
| C(4') | 7720(4) | 6894(4) | 9732(4) | 32(1) |
| C(5') | 6155(4) | 7012(4) | 9321(4) | 33(1) |
| C(6') | 6009(4) | 7210(4) | 7974(4) | 27(1) |
| C(7') | 5316(4) | 6582(4) | 7505(4) | 30(1) |
| C(8') | 5189(4) | 6918(4) | 6188(4) | 31(1) |
| C(9') | 5909(4) | 7953(4) | 5407(4) | 28(1) |
| C(10') | 6612(4) | 8545(4) | 5979(4) | 27(1) |
| C(11') | 7365(4) | 9554(4) | 5299(4) | 28(1) |
| C(12') | 8137(4) | 10172(4) | 5844(4) | 29(1) |
| C(13') | 8764(4) | 11209(4) | 5082(5) | 29(1) |
| C(14') | 9456(4) | 11876(4) | 5656(5) | 31(1) |
| C(15') | 10047(4) | 13039(4) | 4824(5) | 37(1) |
| C(16') | 9299(5) | 13705(4) | 3524(4) | 35(1) |
| C(17') | 9335(4) | 12750(4) | 2957(4) | 31(1) |
| C(18') | 8679(4) | 11621(4) | 3770(4) | 30(1) |
| C(19') | 8006(5) | 10979(4) | 3255(4) | 33(1) |
| C(20') | 7340(4) | 9955(4) | 3997(4) | 29(1) |
| C(21') | 6599(4) | 9355(4) | 3431(5) | 31(1) |
| C(22') | 5916(4) | 8380(4) | 4089(4) | 30(1) |
| C(23') | 5196(4) | 7780(4) | 3401(4) | 31(1) |
| C(24') | 5858(5) | 6381(4) | 3729(4) | 31(1) |

| | | | | |
|---|---|---|---|---|
| C(25') | 5181(5) | 8119(4) | 9491(4) | 35(1) |
| O(2S) | 6938(3) | 13273(3) | -115(3) | 50(1) |
| C(2S) | 7785(6) | 13331(6) | -1134(6) | 62(2) |
| C(4S) | 8130(30) | 13590(30) | -2480(30) | 62(2) |
| O(1S) | 2532(3) | -3496(3) | 9875(3) | 48(1) |
| C(1S) | 2174(6) | -3475(6) | 11081(6) | 65(2) |
| C(3S) | 1980(30) | -4030(30) | 12370(30) | 65(2) |

Table 3. Bond lengths [Å] and angles [°] for SHELLMYCINA.

| | | | |
|---|---|---|---|
| O(1)-H(1) | 0.8400 | C(11)-C(12) | 1.423(7) |
| O(1)-C(4) | 1.430(5) | C(11)-C(20) | 1.414(7) |
| O(2)-H(2) | 0.8400 | C(12)-C(13) | 1.415(6) |
| O(2)-C(5) | 1.418(5) | C(13)-C(14) | 1.474(7) |
| O(3)-C(6) | 1.367(5) | C(13)-C(18) | 1.414(7) |
| O(3)-C(10) | 1.357(6) | C(14)-C(15) | 1.490(6) |
| O(4)-C(8) | 1.251(5) | C(15)-H(15A) | 0.9900 |
| O(5)-H(5) | 0.8400 | C(15)-H(15B) | 0.9900 |
| O(5)-C(12) | 1.330(6) | C(15)-C(16) | 1.526(7) |
| O(6)-C(14) | 1.237(6) | C(16)-H(16A) | 0.9900 |
| O(7)-H(7) | 0.8400 | C(16)-H(16B) | 0.9900 |
| O(7)-C(17) | 1.426(6) | C(16)-C(17) | 1.496(7) |
| O(8)-C(24) | 1.207(5) | C(17)-H(17) | 1.0000 |
| O(9)-H(9) | 0.8400 | C(17)-C(18) | 1.536(6) |
| O(9)-C(24) | 1.330(5) | C(18)-C(19) | 1.367(6) |
| C(1)-H(1A) | 0.9800 | C(19)-H(19) | 0.9500 |
| C(1)-H(1B) | 0.9800 | C(19)-C(20) | 1.410(6) |
| C(1)-H(1C) | 0.9800 | C(20)-C(21) | 1.432(6) |
| C(1)-C(2) | 1.481(7) | C(21)-H(21) | 0.9500 |
| C(2)-H(2A) | 0.9500 | C(21)-C(22) | 1.364(6) |
| C(2)-C(3) | 1.326(6) | C(22)-C(23) | 1.507(6) |
| C(3)-H(3) | 0.9500 | C(23)-H(23A) | 0.9900 |
| C(3)-C(4) | 1.487(6) | C(23)-H(23B) | 0.9900 |
| C(4)-H(4) | 1.0000 | C(23)-C(24) | 1.516(6) |
| C(4)-C(5) | 1.542(6) | C(25)-H(25A) | 0.9800 |
| C(5)-C(6) | 1.514(6) | C(25)-H(25B) | 0.9800 |
| C(5)-C(25) | 1.524(6) | C(25)-H(25C) | 0.9800 |
| C(6)-C(7) | 1.327(6) | O(1')-H(1') | 0.8400 |
| C(7)-H(7A) | 0.9500 | O(1')-C(4') | 1.443(5) |
| C(7)-C(8) | 1.439(7) | O(2')-H(2') | 0.8400 |
| C(8)-C(9) | 1.472(6) | O(2')-C(5') | 1.429(5) |
| C(9)-C(10) | 1.394(7) | O(3')-C(6') | 1.367(5) |
| C(9)-C(22) | 1.426(7) | O(3')-C(10') | 1.359(5) |
| C(10)-C(11) | 1.442(6) | O(4')-C(8') | 1.238(5) |

| | | | |
|---|---|---|---|
| O(5')-H(5') | 0.8400 | C(16')-H(16C) | 0.9900 |
| O(5')-C(12') | 1.331(6) | C(16')-H(16D) | 0.9900 |
| O(6')-C(14') | 1.236(6) | C(16')-C(17') | 1.506(7) |
| O(7')-H(7') | 0.8400 | C(17')-H(17') | 1.0000 |
| O(7')-C(17') | 1.437(5) | C(17')-C(18') | 1.513(6) |
| O(8')-C(24') | 1.207(5) | C(18')-C(19') | 1.377(7) |
| O(9')-H(9') | 0.8400 | C(19')-H(19') | 0.9500 |
| O(9')-C(24') | 1.328(5) | C(19')-C(20') | 1.414(6) |
| C(1')-H(1'A) | 0.9800 | C(20')-C(21') | 1.417(6) |
| C(1')-H(1'B) | 0.9800 | C(21')-H(21') | 0.9500 |
| C(1')-H(1'C) | 0.9800 | C(21')-C(22') | 1.361(6) |
| C(1')-C(2') | 1.501(7) | C(22')-C(23') | 1.507(6) |
| C(2')-H(2'A) | 0.9500 | C(23')-H(23C) | 0.9900 |
| C(2')-C(3') | 1.317(6) | C(23')-H(23D) | 0.9900 |
| C(3')-H(3') | 0.9500 | C(23')-C(24') | 1.505(6) |
| C(3')-C(4') | 1.497(6) | C(25')-H(25D) | 0.9800 |
| C(4')-H(4') | 1.0000 | C(25')-H(25E) | 0.9800 |
| C(4')-C(5') | 1.542(6) | C(25')-H(25F) | 0.9800 |
| C(5')-C(6') | 1.518(7) | O(2S)-H(2S) | 0.8400 |
| C(5')-C(25') | 1.519(6) | O(2S)-C(2S) | 1.436(7) |
| C(6')-C(7') | 1.339(6) | C(2S)-H(2SA) | 0.9800 |
| C(7')-H(7'A) | 0.9500 | C(2S)-H(2SB) | 0.9800 |
| C(7')-C(8') | 1.443(7) | C(2S)-H(2SC) | 0.9800 |
| C(8')-C(9') | 1.467(6) | C(2S)-H(2SD) | 0.9900 |
| C(9')-C(10') | 1.393(6) | C(2S)-H(2SE) | 0.9900 |
| C(9')-C(22') | 1.430(7) | C(2S)-C(4S) | 1.54(3) |
| C(10')-C(11') | 1.436(6) | C(4S)-H(4SA) | 0.9800 |
| C(11')-C(12') | 1.434(7) | C(4S)-H(4SB) | 0.9800 |
| C(11')-C(20') | 1.414(7) | C(4S)-H(4SC) | 0.9800 |
| C(12')-C(13') | 1.408(6) | O(1S)-H(1S) | 0.8400 |
| C(13')-C(14') | 1.458(7) | O(1S)-C(1S) | 1.475(8) |
| C(13')-C(18') | 1.423(7) | C(1S)-H(1SA) | 0.9800 |
| C(14')-C(15') | 1.512(6) | C(1S)-H(1SB) | 0.9800 |
| C(15')-H(15C) | 0.9900 | C(1S)-H(1SC) | 0.9800 |
| C(15')-H(15D) | 0.9900 | C(1S)-H(1SD) | 0.9900 |
| C(15')-C(16') | 1.517(6) | C(1S)-H(1SE) | 0.9900 |

| | | | |
|---|---|---|---|
| C(1S)-C(3S) | 1.42(3) | C(7)-C(6)-O(3) | 122.5(4) |
| C(3S)-H(3SA) | 0.9800 | C(7)-C(6)-C(5) | 127.8(4) |
| C(3S)-H(3SB) | 0.9800 | C(6)-C(7)-H(7A) | 119.4 |
| C(3S)-H(3SC) | 0.9800 | C(6)-C(7)-C(8) | 121.2(4) |
| | | C(8)-C(7)-H(7A) | 119.4 |
| C(4)-O(1)-H(1) | 109.5 | O(4)-C(8)-C(7) | 122.0(4) |
| C(5)-O(2)-H(2) | 109.5 | O(4)-C(8)-C(9) | 122.0(4) |
| C(10)-O(3)-C(6) | 120.2(4) | C(7)-C(8)-C(9) | 116.0(4) |
| C(12)-O(5)-H(5) | 109.5 | C(10)-C(9)-C(8) | 118.2(4) |
| C(17)-O(7)-H(7) | 109.5 | C(10)-C(9)-C(22) | 118.5(4) |
| C(24)-O(9)-H(9) | 109.5 | C(22)-C(9)-C(8) | 123.3(4) |
| H(1A)-C(1)-H(1B) | 109.5 | O(3)-C(10)-C(9) | 121.8(4) |
| H(1A)-C(1)-H(1C) | 109.5 | O(3)-C(10)-C(11) | 115.3(4) |
| H(1B)-C(1)-H(1C) | 109.5 | C(9)-C(10)-C(11) | 122.9(5) |
| C(2)-C(1)-H(1A) | 109.5 | C(12)-C(11)-C(10) | 124.7(5) |
| C(2)-C(1)-H(1B) | 109.5 | C(20)-C(11)-C(10) | 117.1(4) |
| C(2)-C(1)-H(1C) | 109.5 | C(20)-C(11)-C(12) | 118.1(4) |
| C(1)-C(2)-H(2A) | 116.3 | O(5)-C(12)-C(11) | 119.9(4) |
| C(3)-C(2)-C(1) | 127.4(5) | O(5)-C(12)-C(13) | 120.4(4) |
| C(3)-C(2)-H(2A) | 116.3 | C(13)-C(12)-C(11) | 119.6(5) |
| C(2)-C(3)-H(3) | 116.6 | C(12)-C(13)-C(14) | 118.5(5) |
| C(2)-C(3)-C(4) | 126.8(4) | C(18)-C(13)-C(12) | 120.5(4) |
| C(4)-C(3)-H(3) | 116.6 | C(18)-C(13)-C(14) | 121.0(4) |
| O(1)-C(4)-C(3) | 113.1(4) | O(6)-C(14)-C(13) | 121.3(4) |
| O(1)-C(4)-H(4) | 107.5 | O(6)-C(14)-C(15) | 120.0(5) |
| O(1)-C(4)-C(5) | 111.1(3) | C(13)-C(14)-C(15) | 118.6(5) |
| C(3)-C(4)-H(4) | 107.5 | C(14)-C(15)-H(15A) | 109.0 |
| C(3)-C(4)-C(5) | 109.9(3) | C(14)-C(15)-H(15B) | 109.0 |
| C(5)-C(4)-H(4) | 107.5 | C(14)-C(15)-C(16) | 112.9(4) |
| O(2)-C(5)-C(4) | 111.2(3) | H(15A)-C(15)-H(15B) | 107.8 |
| O(2)-C(5)-C(6) | 109.3(3) | C(16)-C(15)-H(15A) | 109.0 |
| O(2)-C(5)-C(25) | 106.9(3) | C(16)-C(15)-H(15B) | 109.0 |
| C(6)-C(5)-C(4) | 110.6(3) | C(15)-C(16)-H(16A) | 109.2 |
| C(6)-C(5)-C(25) | 107.9(4) | C(15)-C(16)-H(16B) | 109.2 |
| C(25)-C(5)-C(4) | 110.8(3) | H(16A)-C(16)-H(16B) | 107.9 |
| O(3)-C(6)-C(5) | 109.6(3) | C(17)-C(16)-C(15) | 112.1(4) |

| | | | |
|---|---|---|---|
| C(17)-C(16)-H(16A) | 109.2 | H(25A)-C(25)-H(25C) | 109.5 |
| C(17)-C(16)-H(16B) | 109.2 | H(25B)-C(25)-H(25C) | 109.5 |
| O(7)-C(17)-C(16) | 108.4(3) | C(4')-O(1')-H(1') | 109.5 |
| O(7)-C(17)-H(17) | 108.3 | C(5')-O(2')-H(2') | 109.5 |
| O(7)-C(17)-C(18) | 111.8(4) | C(10')-O(3')-C(6') | 120.7(3) |
| C(16)-C(17)-H(17) | 108.3 | C(12')-O(5')-H(5') | 109.5 |
| C(16)-C(17)-C(18) | 111.6(4) | C(17')-O(7')-H(7') | 109.5 |
| C(18)-C(17)-H(17) | 108.3 | C(24')-O(9')-H(9') | 109.5 |
| C(13)-C(18)-C(17) | 120.0(4) | H(1'A)-C(1')-H(1'B) | 109.5 |
| C(19)-C(18)-C(13) | 119.7(4) | H(1'A)-C(1')-H(1'C) | 109.5 |
| C(19)-C(18)-C(17) | 120.2(4) | H(1'B)-C(1')-H(1'C) | 109.5 |
| C(18)-C(19)-H(19) | 119.6 | C(2')-C(1')-H(1'A) | 109.5 |
| C(18)-C(19)-C(20) | 120.7(4) | C(2')-C(1')-H(1'B) | 109.5 |
| C(20)-C(19)-H(19) | 119.6 | C(2')-C(1')-H(1'C) | 109.5 |
| C(11)-C(20)-C(21) | 118.8(4) | C(1')-C(2')-H(2'A) | 116.4 |
| C(19)-C(20)-C(11) | 120.9(4) | C(3')-C(2')-C(1') | 127.3(5) |
| C(19)-C(20)-C(21) | 120.2(5) | C(3')-C(2')-H(2'A) | 116.4 |
| C(20)-C(21)-H(21) | 118.5 | C(2')-C(3')-H(3') | 116.4 |
| C(22)-C(21)-C(20) | 123.0(5) | C(2')-C(3')-C(4') | 127.2(4) |
| C(22)-C(21)-H(21) | 118.5 | C(4')-C(3')-H(3') | 116.4 |
| C(9)-C(22)-C(23) | 121.9(4) | O(1')-C(4')-C(3') | 108.9(3) |
| C(21)-C(22)-C(9) | 119.4(4) | O(1')-C(4')-H(4') | 109.6 |
| C(21)-C(22)-C(23) | 118.7(4) | O(1')-C(4')-C(5') | 107.9(3) |
| C(22)-C(23)-H(23A) | 109.1 | C(3')-C(4')-H(4') | 109.6 |
| C(22)-C(23)-H(23B) | 109.1 | C(3')-C(4')-C(5') | 111.2(3) |
| C(22)-C(23)-C(24) | 112.7(4) | C(5')-C(4')-H(4') | 109.6 |
| H(23A)-C(23)-H(23B) | 107.8 | O(2')-C(5')-C(4') | 110.0(3) |
| C(24)-C(23)-H(23A) | 109.1 | O(2')-C(5')-C(6') | 107.7(3) |
| C(24)-C(23)-H(23B) | 109.1 | O(2')-C(5')-C(25') | 107.3(3) |
| O(8)-C(24)-O(9) | 123.8(4) | C(6')-C(5')-C(4') | 110.7(3) |
| O(8)-C(24)-C(23) | 124.9(4) | C(6')-C(5')-C(25') | 110.0(3) |
| O(9)-C(24)-C(23) | 111.2(4) | C(25')-C(5')-C(4') | 111.1(4) |
| C(5)-C(25)-H(25A) | 109.5 | O(3')-C(6')-C(5') | 111.1(4) |
| C(5)-C(25)-H(25B) | 109.5 | C(7')-C(6')-O(3') | 121.4(4) |
| C(5)-C(25)-H(25C) | 109.5 | C(7')-C(6')-C(5') | 127.4(4) |
| H(25A)-C(25)-H(25B) | 109.5 | C(6')-C(7')-H(7'A) | 119.1 |

| | | | |
|---|---|---|---|
| C(6')-C(7')-C(8') | 121.7(4) | O(7')-C(17')-H(17') | 108.3 |
| C(8')-C(7')-H(7'A) | 119.1 | O(7')-C(17')-C(18') | 108.3(3) |
| O(4')-C(8')-C(7') | 121.2(4) | C(16')-C(17')-H(17') | 108.3 |
| O(4')-C(8')-C(9') | 122.9(4) | C(16')-C(17')-C(18') | 111.1(4) |
| C(7')-C(8')-C(9') | 115.9(4) | C(18')-C(17')-H(17') | 108.3 |
| C(10')-C(9')-C(8') | 118.3(4) | C(13')-C(18')-C(17') | 119.9(4) |
| C(10')-C(9')-C(22') | 118.8(4) | C(19')-C(18')-C(13') | 119.4(4) |
| C(22')-C(9')-C(8') | 122.9(4) | C(19')-C(18')-C(17') | 120.7(4) |
| O(3')-C(10')-C(9') | 121.9(3) | C(18')-C(19')-H(19') | 119.3 |
| O(3')-C(10')-C(11') | 115.5(4) | C(18')-C(19')-C(20') | 121.3(5) |
| C(9')-C(10')-C(11') | 122.6(4) | C(20')-C(19')-H(19') | 119.3 |
| C(12')-C(11')-C(10') | 124.9(4) | C(11')-C(20')-C(19') | 120.5(4) |
| C(20')-C(11')-C(10') | 117.0(4) | C(11')-C(20')-C(21') | 119.5(4) |
| C(20')-C(11')-C(12') | 118.1(4) | C(19')-C(20')-C(21') | 119.9(4) |
| O(5')-C(12')-C(11') | 119.1(4) | C(20')-C(21')-H(21') | 118.5 |
| O(5')-C(12')-C(13') | 120.6(4) | C(22')-C(21')-C(20') | 122.9(5) |
| C(13')-C(12')-C(11') | 120.3(5) | C(22')-C(21')-H(21') | 118.5 |
| C(12')-C(13')-C(14') | 118.9(5) | C(9')-C(22')-C(23') | 122.1(4) |
| C(12')-C(13')-C(18') | 120.3(4) | C(21')-C(22')-C(9') | 119.2(4) |
| C(18')-C(13')-C(14') | 120.8(4) | C(21')-C(22')-C(23') | 118.7(4) |
| O(6')-C(14')-C(13') | 121.7(4) | C(22')-C(23')-H(23C) | 108.7 |
| O(6')-C(14')-C(15') | 119.7(4) | C(22')-C(23')-H(23D) | 108.7 |
| C(13')-C(14')-C(15') | 118.6(4) | H(23C)-C(23')-H(23D) | 107.6 |
| C(14')-C(15')-H(15C) | 109.1 | C(24')-C(23')-C(22') | 114.0(4) |
| C(14')-C(15')-H(15D) | 109.1 | C(24')-C(23')-H(23C) | 108.7 |
| C(14')-C(15')-C(16') | 112.5(4) | C(24')-C(23')-H(23D) | 108.7 |
| H(15C)-C(15')-H(15D) | 107.8 | O(8')-C(24')-O(9') | 124.4(4) |
| C(16')-C(15')-H(15C) | 109.1 | O(8')-C(24')-C(23') | 124.5(4) |
| C(16')-C(15')-H(15D) | 109.1 | O(9')-C(24')-C(23') | 111.1(3) |
| C(15')-C(16')-H(16C) | 109.5 | C(5')-C(25')-H(25D) | 109.5 |
| C(15')-C(16')-H(16D) | 109.5 | C(5')-C(25')-H(25E) | 109.5 |
| H(16C)-C(16')-H(16D) | 108.1 | C(5')-C(25')-H(25F) | 109.5 |
| C(17')-C(16')-C(15') | 110.6(3) | H(25D)-C(25')-H(25E) | 109.5 |
| C(17')-C(16')-H(16C) | 109.5 | H(25D)-C(25')-H(25F) | 109.5 |
| C(17')-C(16')-H(16D) | 109.5 | H(25E)-C(25')-H(25F) | 109.5 |
| O(7')-C(17')-C(16') | 112.3(3) | C(2S)-O(2S)-H(2S) | 109.5 |

| | | | |
|---|---|---|---|
| O(2S)-C(2S)-H(2SA) | 109.5 | H(3SB)-C(3S)-H(3SC) | 109.5 |
| O(2S)-C(2S)-H(2SB) | 109.5 | | |
| O(2S)-C(2S)-H(2SC) | 109.5 | | |
| O(2S)-C(2S)-H(2SD) | 96.7 | | |
| O(2S)-C(2S)-H(2SE) | 96.7 | | |
| O(2S)-C(2S)-C(4S) | 158.4(12) | | |
| H(2SA)-C(2S)-H(2SB) | 109.5 | | |
| H(2SA)-C(2S)-H(2SC) | 109.5 | | |
| H(2SB)-C(2S)-H(2SC) | 109.5 | | |
| H(2SD)-C(2S)-H(2SE) | 103.5 | | |
| C(4S)-C(2S)-H(2SD) | 96.7 | | |
| C(4S)-C(2S)-H(2SE) | 96.7 | | |
| C(2S)-C(4S)-H(4SA) | 109.5 | | |
| C(2S)-C(4S)-H(4SB) | 109.5 | | |
| C(2S)-C(4S)-H(4SC) | 109.5 | | |
| H(4SA)-C(4S)-H(4SB) | 109.5 | | |
| H(4SA)-C(4S)-H(4SC) | 109.5 | | |
| H(4SB)-C(4S)-H(4SC) | 109.5 | | |
| C(1S)-O(1S)-H(1S) | 109.5 | | |
| O(1S)-C(1S)-H(1SA) | 109.5 | | |
| O(1S)-C(1S)-H(1SB) | 109.5 | | |
| O(1S)-C(1S)-H(1SC) | 109.5 | | |
| O(1S)-C(1S)-H(1SD) | 97.5 | | |
| O(1S)-C(1S)-H(1SE) | 97.5 | | |
| H(1SA)-C(1S)-H(1SB) | 109.5 | | |
| H(1SA)-C(1S)-H(1SC) | 109.5 | | |
| H(1SB)-C(1S)-H(1SC) | 109.5 | | |
| H(1SD)-C(1S)-H(1SE) | 103.6 | | |
| C(3S)-C(1S)-O(1S) | 155.5(14) | | |
| C(3S)-C(1S)-H(1SD) | 97.5 | | |
| C(3S)-C(1S)-H(1SE) | 97.5 | | |
| C(1S)-C(3S)-H(3SA) | 109.5 | | |
| C(1S)-C(3S)-H(3SB) | 109.5 | | |
| C(1S)-C(3S)-H(3SC) | 109.5 | | |
| H(3SA)-C(3S)-H(3SB) | 109.5 | | |
| H(3SA)-C(3S)-H(3SC) | 109.5 | | |

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for SHELLMYCINA. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| O(1) | 40(2) | 43(2) | 45(2) | -19(2) | 5(2) | -6(1) |
| O(2) | 35(2) | 37(2) | 32(2) | -9(1) | 5(1) | -13(1) |
| O(3) | 32(2) | 34(2) | 24(2) | -11(1) | 5(1) | -10(1) |
| O(4) | 30(2) | 36(2) | 36(2) | -18(1) | 4(1) | -11(1) |
| O(5) | 38(2) | 41(2) | 31(2) | -17(2) | 2(1) | -13(1) |
| O(6) | 49(2) | 46(2) | 39(3) | -16(2) | -3(2) | -17(1) |
| O(7) | 38(2) | 38(2) | 40(2) | -12(2) | 7(2) | -10(1) |
| O(8) | 32(2) | 39(2) | 43(2) | -19(1) | 2(2) | -6(1) |
| O(9) | 39(2) | 35(2) | 44(2) | -20(2) | -1(2) | -10(1) |
| C(1) | 45(3) | 61(3) | 44(4) | -24(3) | 4(2) | -20(2) |
| C(2) | 44(3) | 45(2) | 32(3) | -19(2) | 2(2) | -3(2) |
| C(3) | 46(3) | 39(2) | 34(3) | -19(2) | 9(2) | -13(2) |
| C(4) | 32(2) | 36(2) | 35(3) | -15(2) | 6(2) | -10(2) |
| C(5) | 32(2) | 34(2) | 25(3) | -11(2) | 2(2) | -12(2) |
| C(6) | 29(2) | 29(2) | 32(3) | -11(2) | 7(2) | -9(2) |
| C(7) | 29(2) | 35(2) | 31(3) | -12(2) | 5(2) | -9(2) |
| C(8) | 26(2) | 31(2) | 29(3) | -13(2) | 4(2) | -4(2) |
| C(9) | 29(2) | 29(2) | 33(3) | -11(2) | 2(2) | -2(2) |
| C(10) | 26(2) | 31(2) | 31(3) | -14(2) | 0(2) | 2(2) |
| C(11) | 24(2) | 28(2) | 35(3) | -11(2) | 3(2) | -4(2) |
| C(12) | 25(2) | 35(2) | 33(3) | -14(2) | 1(2) | -1(2) |
| C(13) | 27(2) | 28(2) | 35(3) | -12(2) | 3(2) | -6(2) |
| C(14) | 29(2) | 34(2) | 45(4) | -13(2) | -2(2) | -3(2) |
| C(15) | 40(2) | 30(2) | 44(3) | -10(2) | 2(2) | -7(2) |
| C(16) | 33(2) | 29(2) | 47(3) | -9(2) | 2(2) | -9(2) |
| C(17) | 28(2) | 31(2) | 40(3) | -9(2) | 8(2) | -4(2) |
| C(18) | 24(2) | 31(2) | 36(3) | -11(2) | 4(2) | -3(2) |
| C(19) | 26(2) | 29(2) | 31(3) | -11(2) | 5(2) | -5(2) |
| C(20) | 27(2) | 29(2) | 29(3) | -10(2) | -1(2) | -1(2) |
| C(21) | 29(2) | 31(2) | 29(3) | -9(2) | -1(2) | -2(2) |
| C(22) | 26(2) | 31(2) | 32(3) | -17(2) | 2(2) | -4(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(23) | 34(2) | 34(2) | 30(3) | -11(2) | 4(2) | -7(2) |
| C(24) | 35(3) | 38(2) | 27(3) | -18(2) | 9(2) | -13(2) |
| C(25) | 36(2) | 36(2) | 30(3) | -10(2) | 3(2) | -10(2) |
| O(1') | 28(1) | 33(1) | 33(2) | -12(1) | 6(1) | -7(1) |
| O(2') | 32(2) | 29(1) | 32(2) | -10(1) | 4(1) | -8(1) |
| O(3') | 28(1) | 31(1) | 29(2) | -12(1) | 4(1) | -9(1) |
| O(4') | 33(2) | 39(2) | 34(2) | -18(1) | 5(1) | -11(1) |
| O(5') | 38(2) | 34(2) | 28(2) | -14(1) | 2(1) | -15(1) |
| O(6') | 49(2) | 42(2) | 30(2) | -13(2) | 2(2) | -19(1) |
| O(7') | 37(2) | 33(2) | 32(2) | -7(1) | 4(1) | -10(1) |
| O(8') | 34(2) | 36(2) | 41(2) | -20(1) | 1(2) | -6(1) |
| O(9') | 42(2) | 36(1) | 42(2) | -20(1) | 0(1) | -12(1) |
| C(1') | 60(3) | 54(3) | 40(3) | -25(2) | 9(2) | -23(2) |
| C(2') | 33(2) | 44(2) | 27(2) | -16(2) | 0(2) | -9(2) |
| C(3') | 28(2) | 38(2) | 26(2) | -9(2) | 3(2) | -7(2) |
| C(4') | 35(2) | 30(2) | 31(2) | -12(2) | 5(2) | -8(2) |
| C(5') | 31(2) | 28(2) | 37(3) | -8(2) | 4(2) | -9(2) |
| C(6') | 26(2) | 26(2) | 28(3) | -8(2) | 4(2) | -6(2) |
| C(7') | 26(2) | 31(2) | 30(3) | -10(2) | 3(2) | -7(2) |
| C(8') | 25(2) | 31(2) | 37(3) | -15(2) | 4(2) | -5(2) |
| C(9') | 24(2) | 28(2) | 30(3) | -11(2) | 1(2) | 1(2) |
| C(10') | 23(2) | 31(2) | 28(3) | -13(2) | 5(2) | -6(2) |
| C(11') | 26(2) | 28(2) | 29(3) | -13(2) | 2(2) | -1(2) |
| C(12') | 29(2) | 29(2) | 27(3) | -11(2) | 2(2) | -4(2) |
| C(13') | 23(2) | 31(2) | 35(3) | -15(2) | 2(2) | -4(2) |
| C(14') | 28(2) | 34(2) | 32(3) | -15(2) | 2(2) | -6(2) |
| C(15') | 36(2) | 33(2) | 43(3) | -16(2) | 2(2) | -10(2) |
| C(16') | 32(2) | 30(2) | 38(3) | -9(2) | 4(2) | -8(2) |
| C(17') | 30(2) | 32(2) | 29(3) | -10(2) | 4(2) | -7(2) |
| C(18') | 28(2) | 31(2) | 31(3) | -13(2) | 7(2) | -5(2) |
| C(19') | 33(2) | 33(2) | 28(3) | -11(2) | 4(2) | -2(2) |
| C(20') | 26(2) | 29(2) | 30(3) | -13(2) | 5(2) | -2(2) |
| C(21') | 31(2) | 36(2) | 26(3) | -15(2) | 2(2) | -3(2) |
| C(22') | 25(2) | 30(2) | 34(3) | -14(2) | 3(2) | 0(2) |
| C(23') | 30(2) | 37(2) | 30(3) | -17(2) | 2(2) | -12(2) |
| C(24') | 33(2) | 33(2) | 29(3) | -12(2) | 7(2) | -11(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(25') | 33(2) | 33(2) | 35(3) | -12(2) | 5(2) | -3(2) |
| O(2S) | 40(2) | 62(2) | 43(2) | -19(2) | 2(2) | -11(2) |
| C(2S) | 49(3) | 74(4) | 73(4) | -41(3) | 9(3) | -10(3) |
| C(4S) | 49(3) | 74(4) | 73(4) | -41(3) | 9(3) | -10(3) |
| O(1S) | 37(2) | 48(2) | 58(2) | -21(2) | 9(2) | -9(1) |
| C(1S) | 54(3) | 67(3) | 68(3) | -24(3) | 13(3) | -8(3) |
| C(3S) | 54(3) | 67(3) | 68(3) | -24(3) | 13(3) | -8(3) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for SHELLMYCINA.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | 5593 | 1743 | -49 | 64 |
| H(2) | 4845 | 3679 | -142 | 54 |
| H(5) | 1396 | -679 | 2685 | 53 |
| H(7) | 1272 | -3426 | 8648 | 60 |
| H(9) | 4841 | 4609 | 6214 | 57 |
| H(1A) | 1978 | 85 | 271 | 72 |
| H(1B) | 1614 | -195 | -898 | 72 |
| H(1C) | 489 | 794 | -548 | 72 |
| H(2A) | 1899 | 1894 | -2252 | 48 |
| H(3) | 3404 | 2787 | -1691 | 46 |
| H(4) | 3161 | 1070 | 823 | 41 |
| H(7A) | 4959 | 3819 | 1778 | 38 |
| H(15A) | 1179 | -4368 | 5287 | 48 |
| H(15B) | -451 | -3781 | 4744 | 48 |
| H(16A) | -950 | -3053 | 6298 | 46 |
| H(16B) | -200 | -4558 | 6957 | 46 |
| H(17) | 1951 | -4070 | 7262 | 42 |
| H(19) | 2075 | -1608 | 7547 | 35 |
| H(21) | 3414 | 62 | 7330 | 38 |
| H(23A) | 5915 | 1762 | 6245 | 41 |
| H(23B) | 4903 | 1337 | 7362 | 41 |
| H(25A) | 1469 | 4177 | 637 | 53 |
| H(25B) | 1183 | 2793 | 817 | 53 |
| H(25C) | 1385 | 3838 | -539 | 53 |
| H(1') | 9196 | 5910 | 9226 | 48 |
| H(2') | 6216 | 5213 | 10005 | 48 |
| H(5') | 8681 | 10227 | 7266 | 48 |
| H(7') | 8910 | 13992 | 1289 | 54 |
| H(9') | 5358 | 5039 | 3558 | 57 |
| H(1'A) | 7606 | 9668 | 10410 | 72 |
| H(1'B) | 8689 | 9012 | 9705 | 72 |

| | | | | |
|---|---|---|---|---|
| H(1'C) | 9262 | 9173 | 10888 | 72 |
| H(2'A) | 8241 | 7475 | 12222 | 41 |
| H(3') | 7705 | 6033 | 11677 | 38 |
| H(4') | 8085 | 7662 | 9142 | 38 |
| H(7'A) | 4898 | 5897 | 8054 | 36 |
| H(15C) | 11077 | 12755 | 4770 | 44 |
| H(15D) | 9944 | 13669 | 5202 | 44 |
| H(16C) | 8295 | 14095 | 3561 | 42 |
| H(16D) | 9774 | 14411 | 2997 | 42 |
| H(17') | 10354 | 12405 | 2883 | 38 |
| H(19') | 7989 | 11229 | 2383 | 39 |
| H(21') | 6579 | 9645 | 2554 | 37 |
| H(23C) | 4181 | 7844 | 3582 | 37 |
| H(23D) | 5226 | 8287 | 2497 | 37 |
| H(25D) | 4195 | 8173 | 9223 | 53 |
| H(25E) | 5475 | 8937 | 8990 | 53 |
| H(25F) | 5244 | 7961 | 10370 | 53 |
| H(2S) | 7460 | 13214 | 482 | 75 |
| H(2SA) | 7222 | 13233 | -1765 | 93 |
| H(2SB) | 8635 | 12631 | -831 | 93 |
| H(2SC) | 8077 | 14170 | -1500 | 93 |
| H(2SD) | 8326 | 12423 | -739 | 74 |
| H(2SE) | 8447 | 13831 | -995 | 74 |
| H(4SA) | 7970 | 12863 | -2658 | 93 |
| H(4SB) | 9128 | 13665 | -2578 | 93 |
| H(4SC) | 7507 | 14393 | -3059 | 93 |
| H(1S) | 3406 | -3808 | 9912 | 72 |
| H(1SA) | 2931 | -3201 | 11403 | 98 |
| H(1SB) | 2087 | -4346 | 11672 | 98 |
| H(1SC) | 1268 | -2865 | 10968 | 98 |
| H(1SD) | 2814 | -2901 | 11099 | 78 |
| H(1SE) | 1228 | -2885 | 10797 | 78 |
| H(3SA) | 1428 | -4707 | 12552 | 98 |
| H(3SB) | 1468 | -3352 | 12605 | 98 |
| H(3SC) | 2915 | -4405 | 12845 | 98 |

Table 6. Hydrogen bonds for SHELLMYCINA [Å and °].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| O(1)-H(1)...O(2S)#1 | 0.84 | 2.35 | 3.040(4) | 139.4 |
| O(2)-H(2)...O(2S)#1 | 0.84 | 1.97 | 2.802(4) | 172.4 |
| O(5)-H(5)...O(6) | 0.84 | 1.74 | 2.492(4) | 148.4 |
| O(7)-H(7)...O(1S) | 0.84 | 1.86 | 2.687(5) | 168.2 |
| O(9)-H(9)...O(4') | 0.84 | 1.83 | 2.659(4) | 167.6 |
| O(1')-H(1')...O(7)#2 | 0.84 | 1.90 | 2.729(4) | 167.8 |
| O(2')-H(2')...O(2S)#3 | 0.84 | 2.28 | 3.084(5) | 160.2 |
| O(5')-H(5')...O(6') | 0.84 | 1.74 | 2.497(4) | 148.8 |
| O(7')-H(7')...O(1')#4 | 0.84 | 2.07 | 2.809(4) | 146.4 |
| O(9')-H(9')...O(4) | 0.84 | 1.87 | 2.687(4) | 164.2 |
| O(2S)-H(2S)...O(7') | 0.84 | 1.91 | 2.747(5) | 172.1 |
| O(1S)-H(1S)...O(2')#1 | 0.84 | 2.13 | 2.952(4) | 164.8 |

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 x+1,y+1,z #3 x,y-1,z+1 #4 x,y+1,z-1