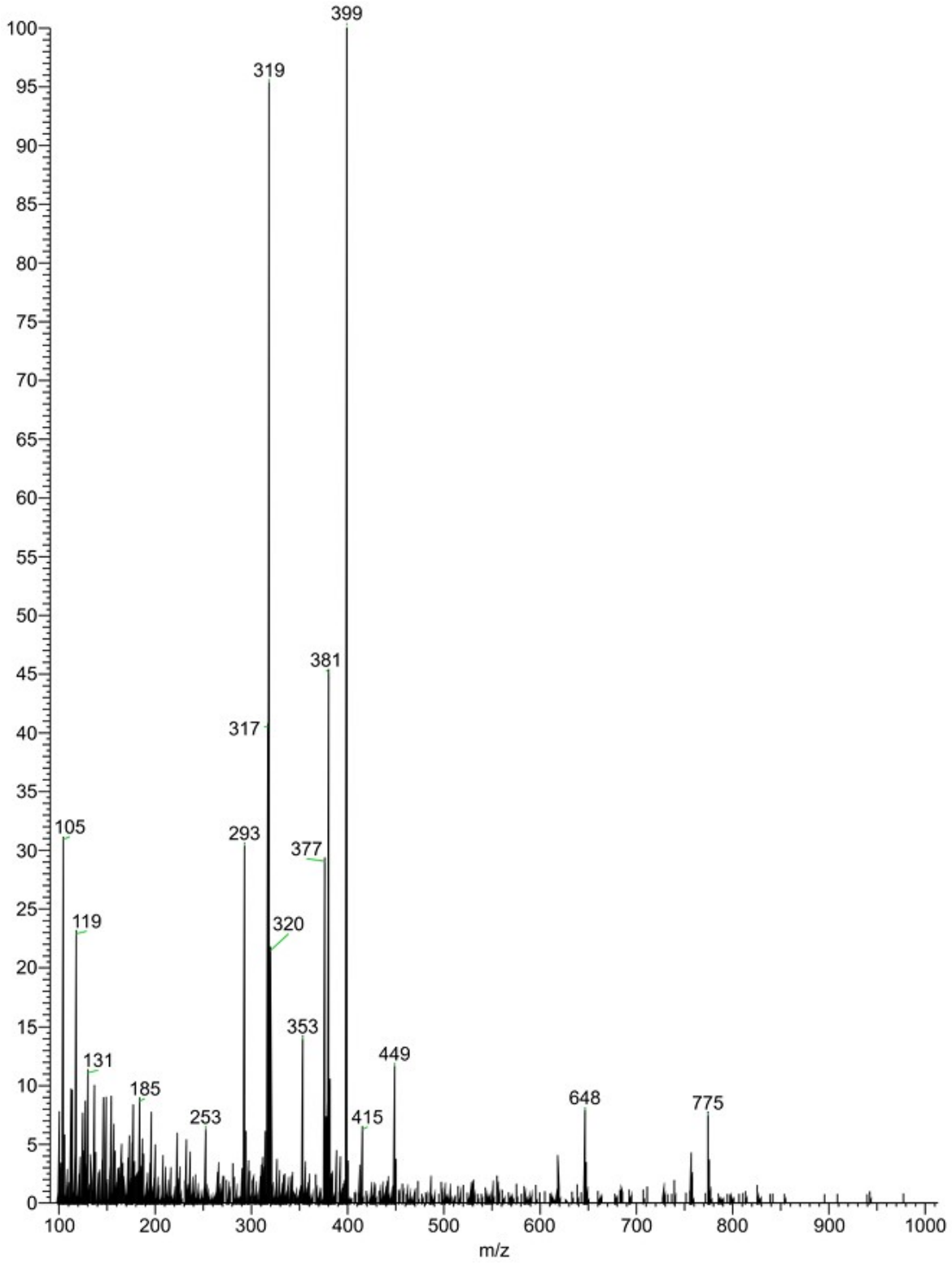
# Supporting Information

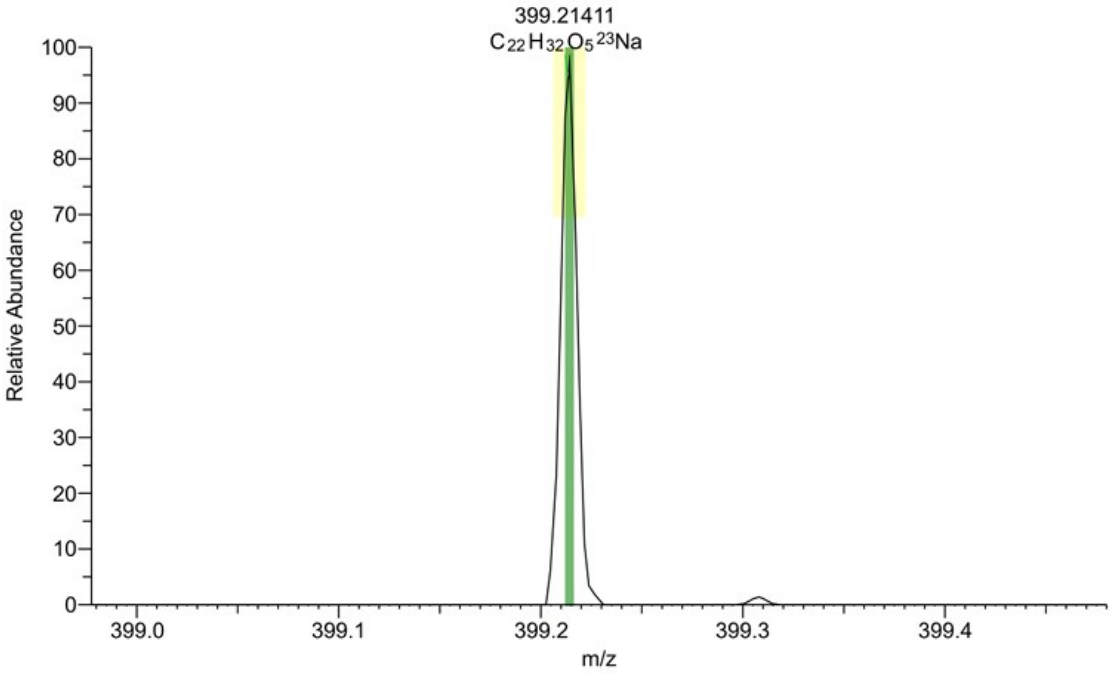
Sarcoglaucone A, a novel sarsolenane-related diterpenoid from the soft coral *Sarcophyton glaucum*

Yue-Wen Chuang,[ab] Atallah F. Ahmed,[cd] Hsiao-Ling Chung,[ab] Yueh-Wen Liu, Su-Ying Chien,[f] Yu-Chi Lin,[g] Chia-Ching Liaw,[ghijk] Yu-Jen Wu,[l] Jing-Ru Weng,[a] Quoc Vu Pham,[m] Jui-Hsin Su,*[abn] Jyh-Horng Sheu*[ao] and Ping-Jyun Sung*[abhpqrs]

[a] *Department of Marine Biotechnology and Resources, National Sun Yat-sen University, Kaohsiung 804201, Taiwan*
[b] *National Museum of Marine Biology and Aquarium, Pingtung 944401, Taiwan*
[c] *Department of Pharmacognosy, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia*
[d] *Department of Pharmacognosy, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt*
[e] *Department of Cosmetics and Fashion Styling, Cheng Shiu University, Kaohsiung 833301, Taiwan*
[f] *X-Ray Laboratory, the Institute of Chemistry, Academia Sinica, Taipei 115201, Taiwan*
[g] *National Research Institute of Chinese Medicine, MOHW, Taipei 112026, Taiwan*
[h] *Graduate Institute of Natural Products, Kaohsiung Medical University, Kaohsiung 807378, Taiwan*
[i] *Department of Pharmacy, College of Pharmaceutical Sciences, National Yang Ming Chian Tung University, Taipei 112304, Taiwan*
[j] *School of Chinese Medicine, College of Medicine, National Yang Ming Chian Tung University, Taipei 112304, Taiwan*
[k] *Department of Biochemical Science and Technology, National Chiayi University, Chiayi 600355, Taiwan*
[l] *Yu Jun Biotechnology Co., Ltd, Donggang, Pingtung 928003, Taiwan*
[m] *Graduate Institute of Pharmacognosy, College of Pharmacy, Taipei Medical University, Taipei 110301, Taiwan*
[n] *Graduate Institute of Marine Biology, National Dong Hwa University, Pingtung 944401, Taiwan*
[o] *Department of Medical Research, China Medical University Hospital, China Medical University, Taichung 404327, Taiwan*
[p] *Chinese Medicine Research and Development Center, China Medical University Hospital, China Medical University, Taichung 404327, Taiwan*
[q] *Ph.D. Program in Pharmaceutical Biotechnology, Fu Jen Catholic University, New Taipei City 242062, Taiwan*
[r] *Department of Biochemistry and Molecular Medicine, National Dong Hwa University, Hualien 974301, Taiwan*
[s] *School of Medicine, Kaohsiung Medical University, Kaohsiung 807378, Taiwan*

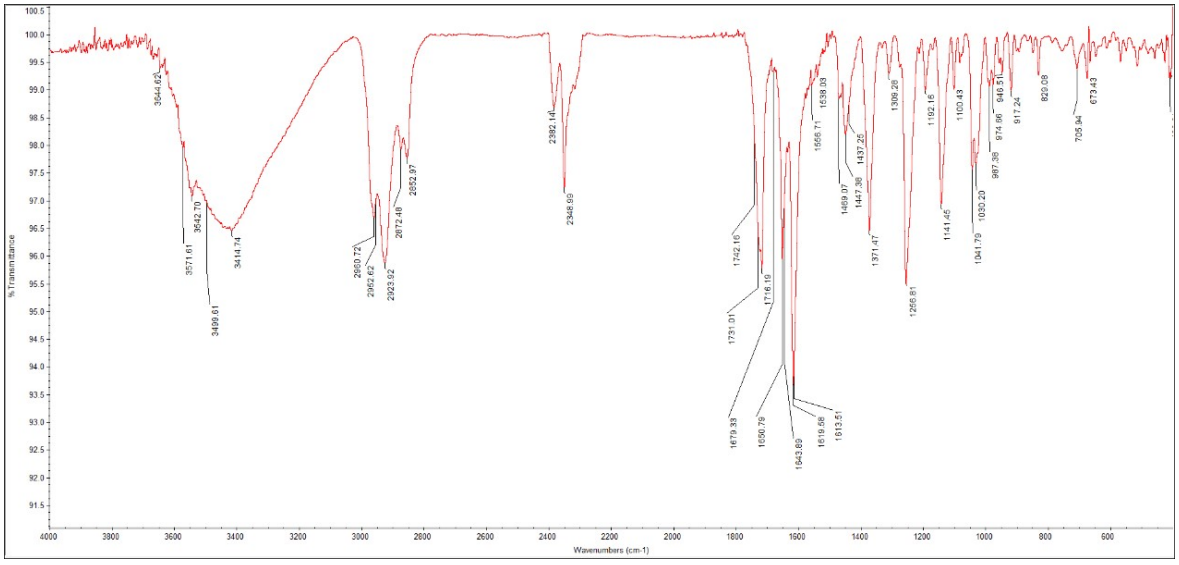



S1. ESIMS spectrum of compound **1**

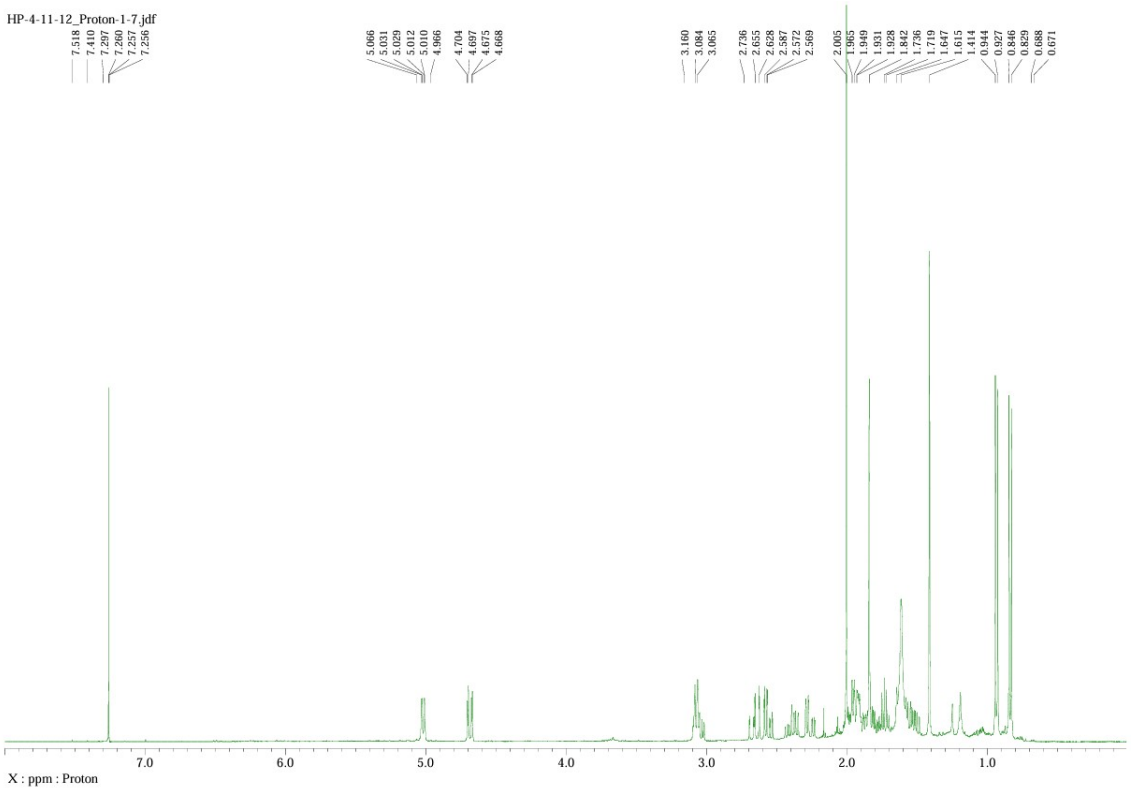



| Peak Mass | Display Formula | S Fit | RDB | Delta [ppm] | Theo. mass | Pattern Cov. [%] | MSMS Matched... |
|---|---|---|---|---|---|---|---|
| 399.21411 | $C_{22}H_{32}O_5{}^{23}Na$ | 85.37273237161 34 | 6.50 | -0.21 | 399.21420 | 100 | (Collection) |

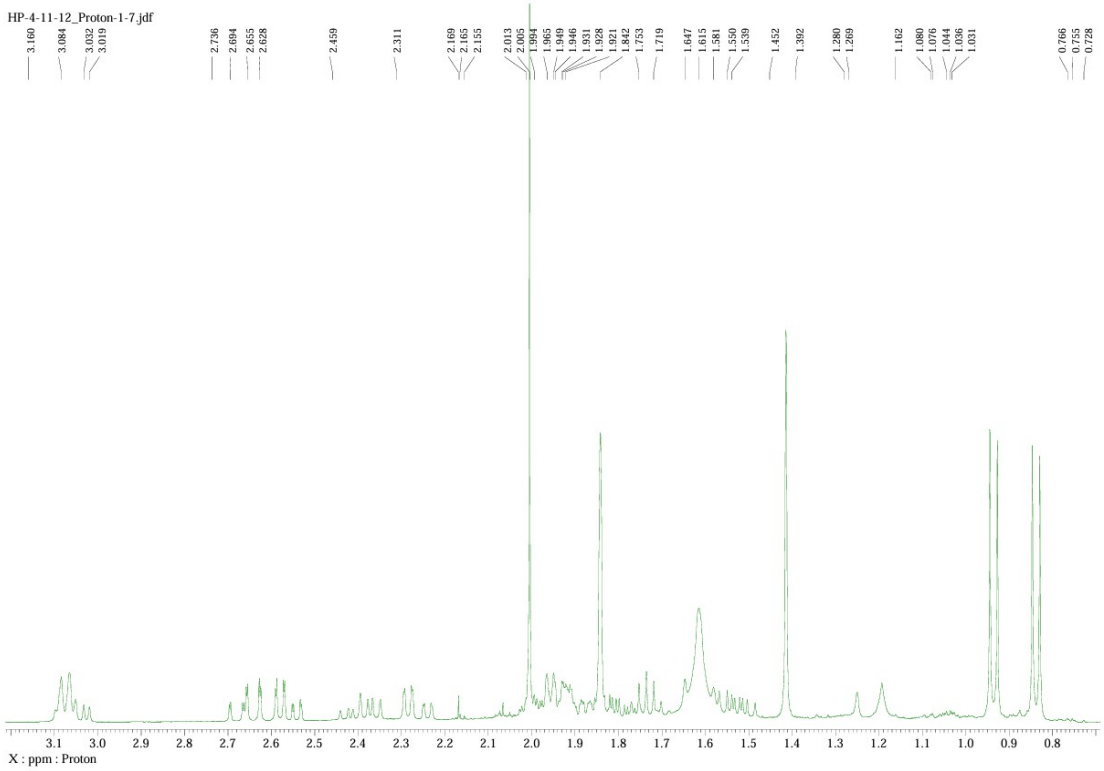
S2. HRESIMS spectrum of compound **1**



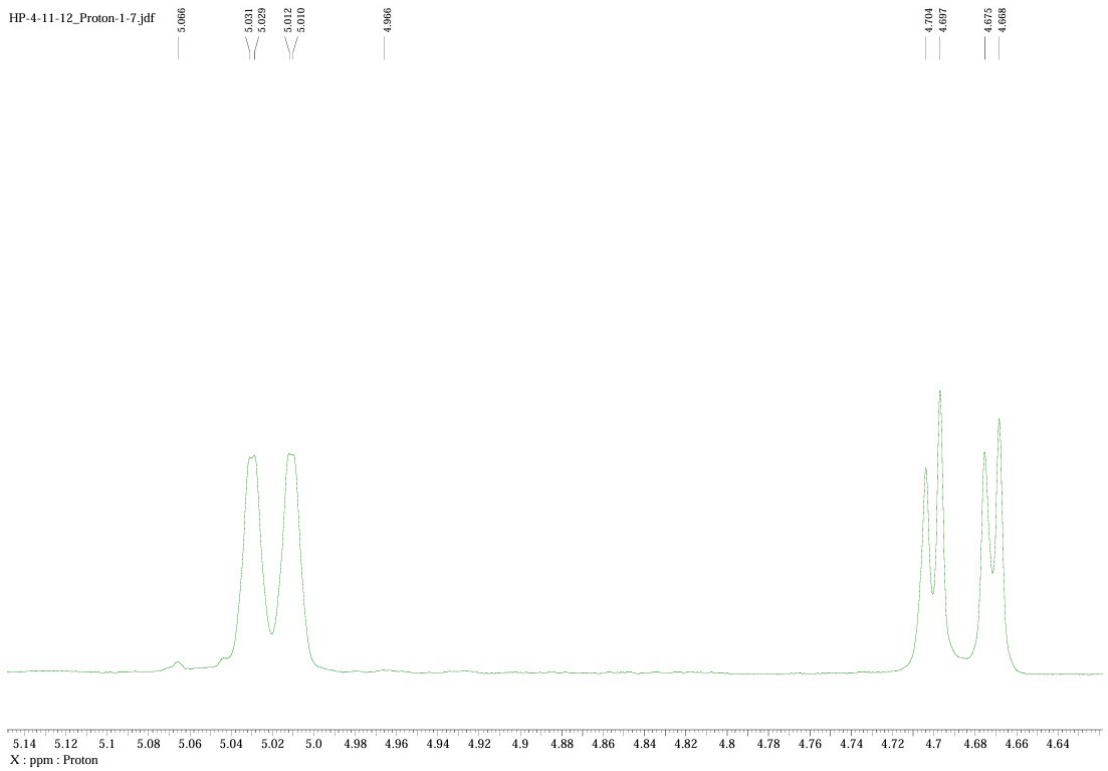

S3. IR spectrum of compound **1**



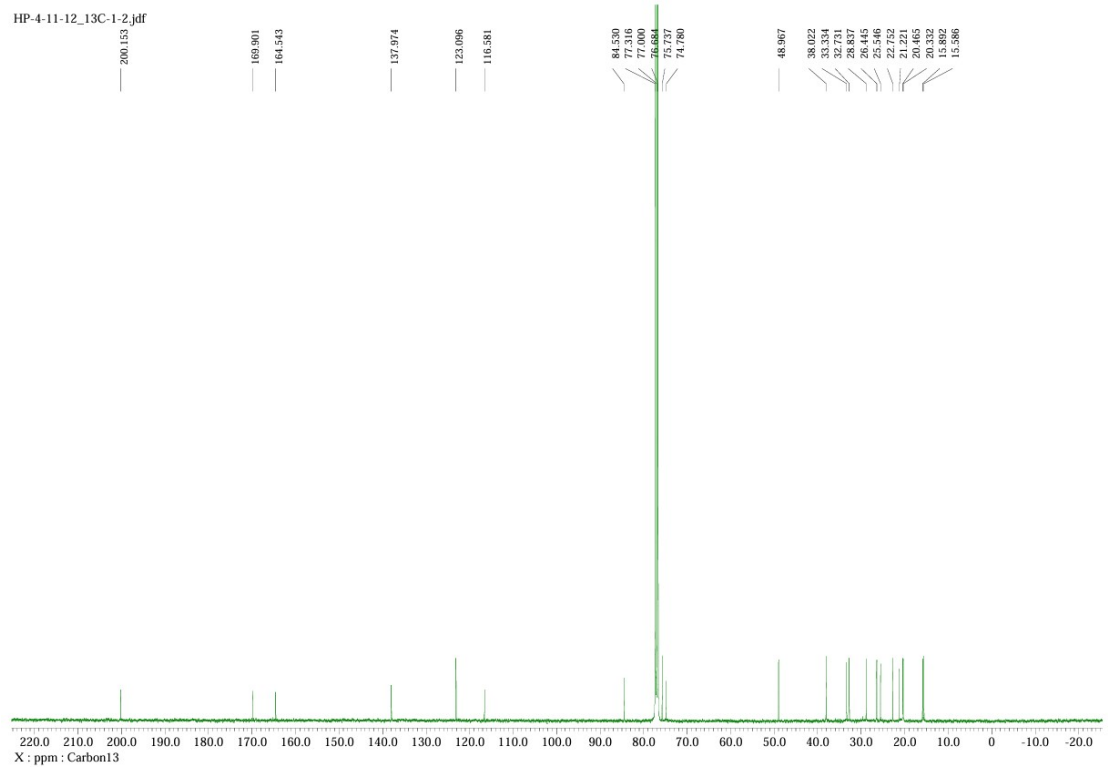

S4. $^{1}H$ NMR spectrum (400 MHz) of compound **1** in $CDCl_3$



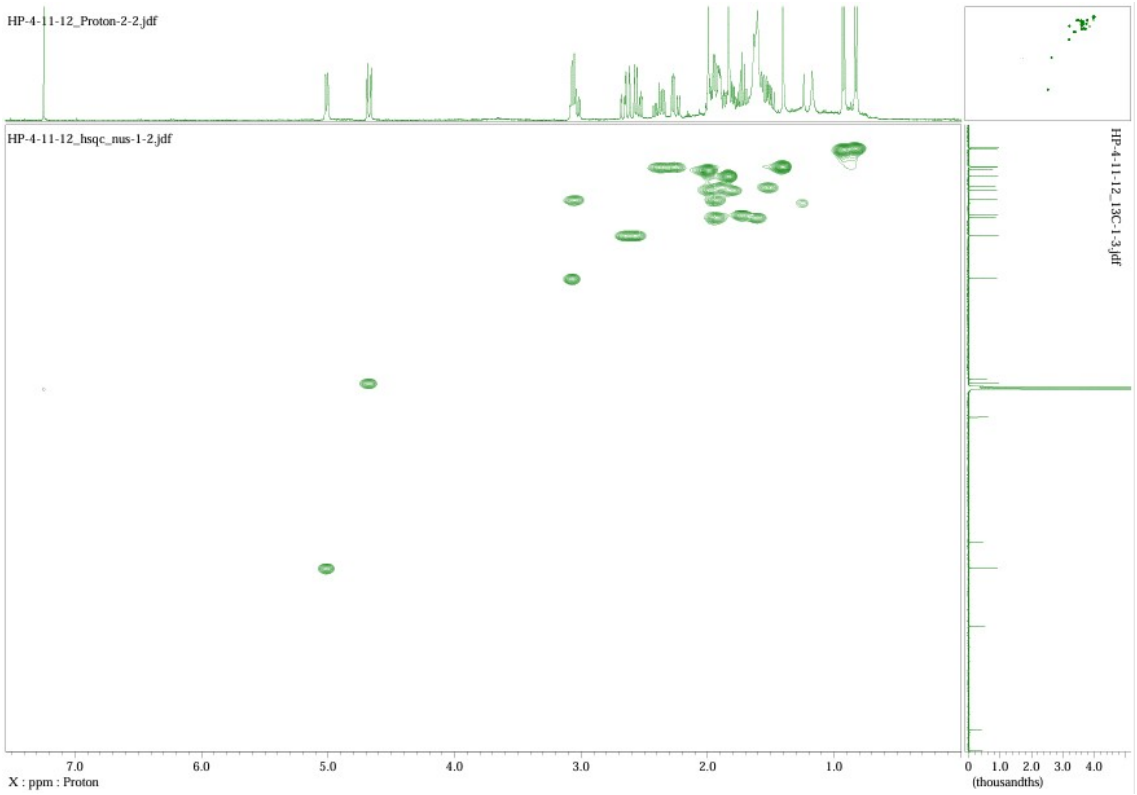

S5. Zoomed-in region of compound **1** from 0.8-3.3 ppm



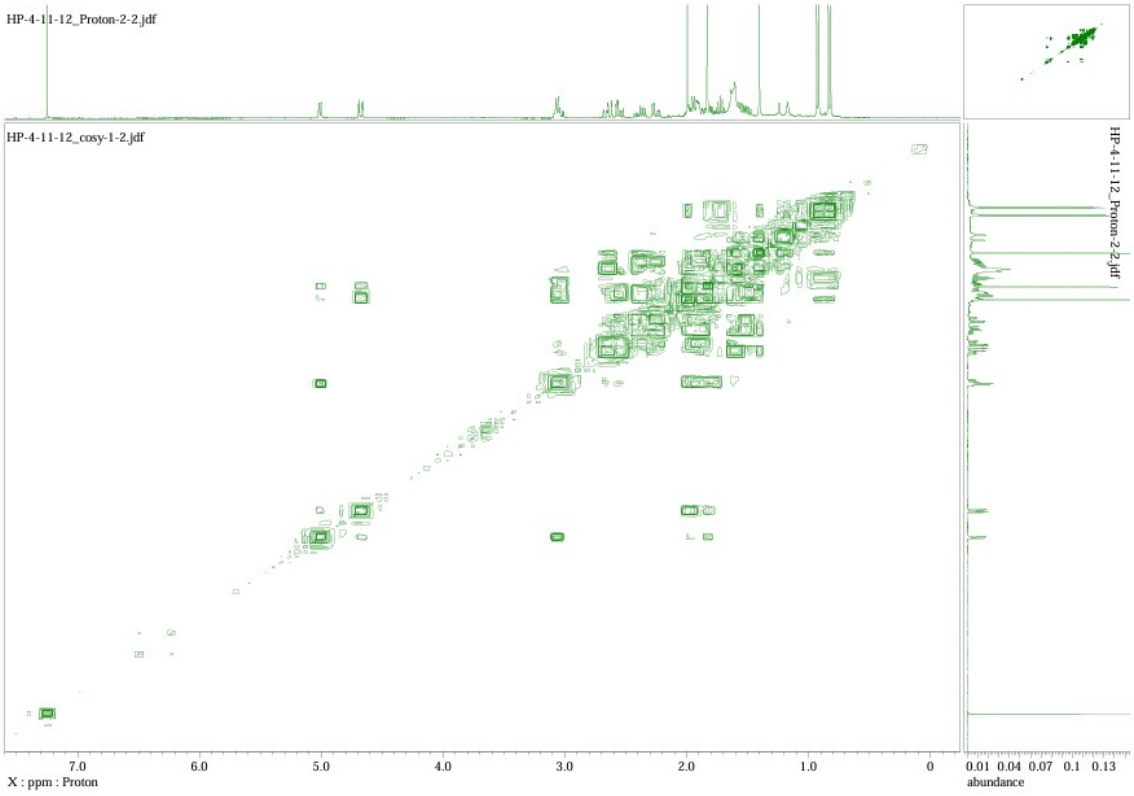

S6. Zoomed-in region of compound **1** from 4.64-5.14 ppm



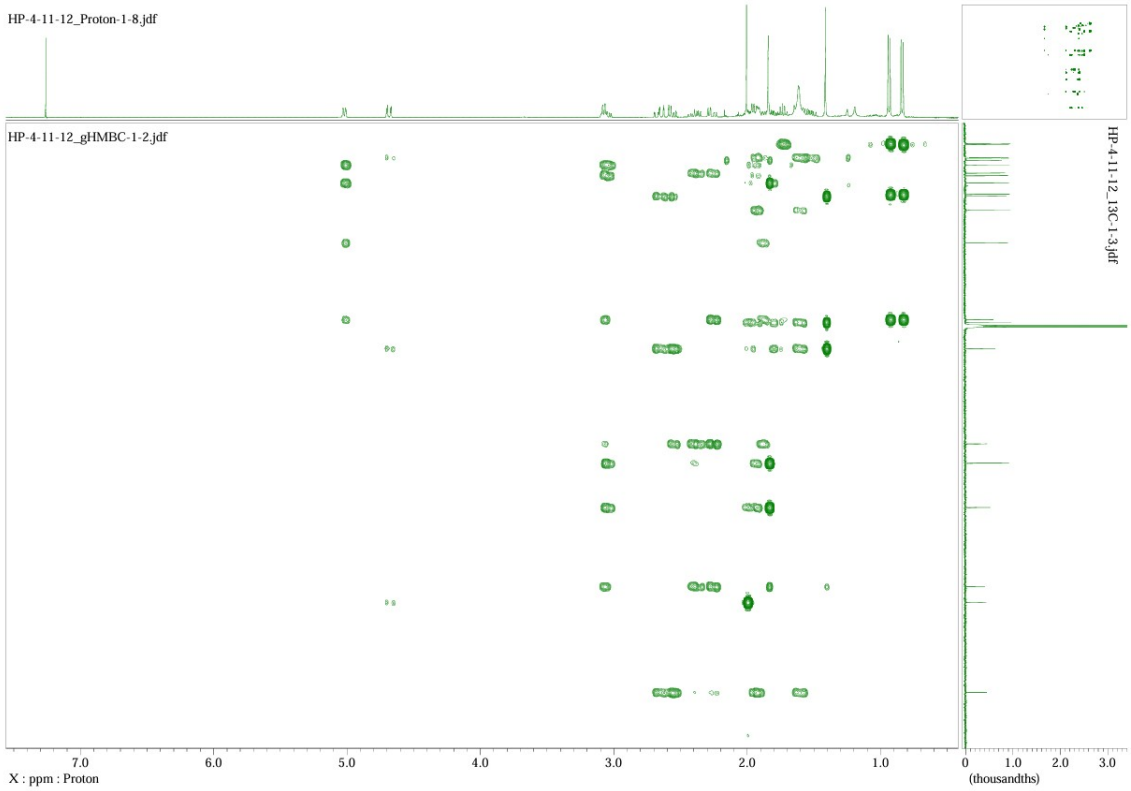

S7. $^{13}C$ NMR spectrum (100 MHz) of compound **1** in $CDCl_3$



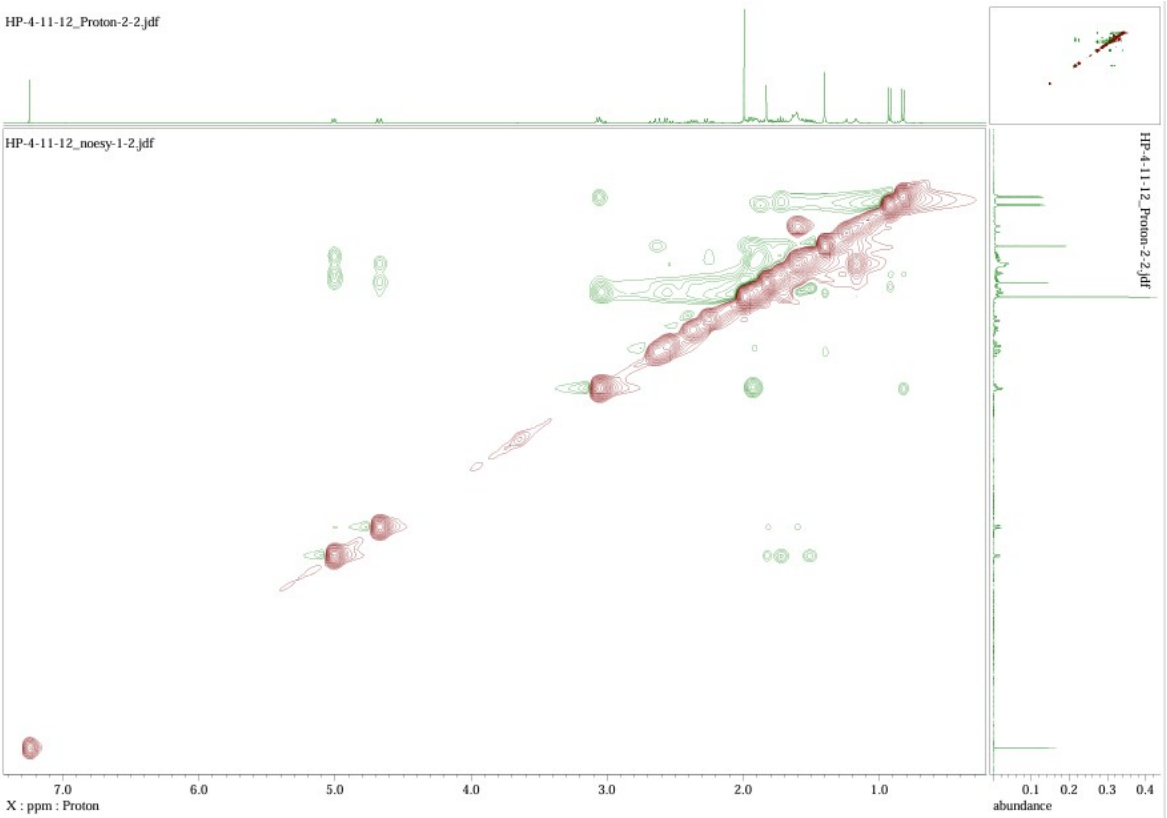

S8. HSQC spectrum of compound **1**




S9. COSY spectrum of compound **1**

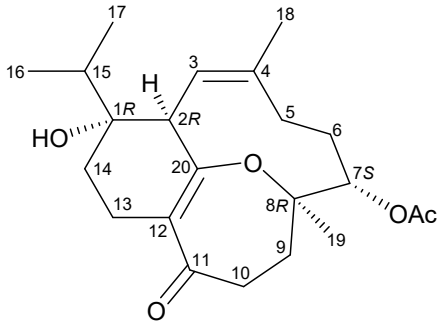



S10. HMBC spectrum of compound **1**




S11. NOESY spectrum of compound **1**

1. Crystal data and structure refinement for dihydrosarsolenone (**1**) (CCDC number: 2496063)



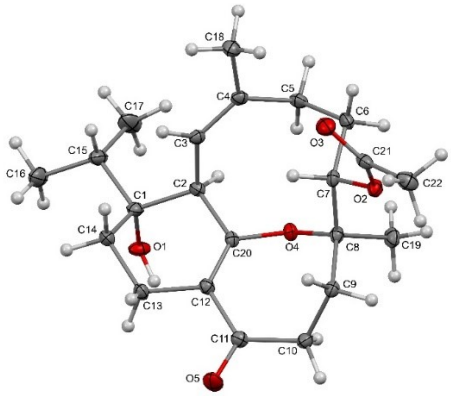




Table 1. Crystal data and structure refinement for . i19811

| | | |
|---|---|---|
| Identification code | i19811 | |
| Empirical formula | C22 H32 O5 | |
| Formula weight | 376.47 | |
| Temperature | 100(2) K | |
| Wavelength | 1.54178 Å | |
| Crystal system | Monoclinic | |
| Space group | C2 | |
| Unit cell dimensions | a = 18.2228(7) Å | α= 90°. |
| | b = 5.8415(2) Å | β= 90.551(2)°. |
| | c = 18.7272(7) Å | γ = 90°. |
| Volume | 1993.39(13) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.254 $Mg/m^3$ | |
| Absorption coefficient | 0.706 $mm^{-1}$ | |
| F(000) | 816 | |
| Crystal size | 0.190 x 0.080 x 0.036 $mm^3$ | |
| Theta range for data collection | 2.359 to 74.644°. | |
| Index ranges | -22<=h<=21, -7<=k<=7, -23<=l<=23 | |
| Reflections collected | 18724 | |
| Independent reflections | 4026 [R(int) = 0.0786] | |
| Completeness to theta = 67.679° | 99.6 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.9819 and 0.6502 | |

| | |
|---|---|
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4026 / 1 / 251 |
| Goodness-of-fit on $F^2$ | 1.040 |
| Final R indices [I>2sigma(I)] | R1 = 0.0405, wR2 = 0.1026 |
| R indices (all data) | R1 = 0.0431, wR2 = 0.1049 |
| Absolute structure parameter | 0.02(11) |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.302 and -0.257 e.$Å^{-3}$ |

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

| | *x* | *y* | *z* | *U(eq)* |
|---|---|---|---|---|
| O(1) | 8860(1) | 4898(3) | 3195(1) | 19(1) |
| O(2) | 5264(1) | 5235(3) | 1415(1) | 16(1) |
| O(3) | 4783(1) | 8197(3) | 2023(1) | 21(1) |
| O(4) | 7067(1) | 3538(3) | 2088(1) | 13(1) |
| O(5) | 8322(1) | 7798(3) | 764(1) | 26(1) |
| C(1) | 8275(1) | 6437(4) | 3376(1) | 15(1) |
| C(2) | 7536(1) | 5399(4) | 3118(1) | 13(1) |
| C(3) | 6873(1) | 6614(4) | 3427(1) | 14(1) |
| C(4) | 6198(1) | 5781(4) | 3512(1) | 14(1) |
| C(5) | 5960(1) | 3430(4) | 3270(1) | 16(1) |
| C(6) | 5473(1) | 3541(4) | 2592(1) | 17(1) |
| C(7) | 5812(1) | 4865(4) | 1975(1) | 13(1) |
| C(8) | 6452(1) | 3705(4) | 1581(1) | 14(1) |
| C(9) | 6651(1) | 5038(4) | 907(1) | 14(1) |
| C(10) | 7463(1) | 4765(4) | 723(1) | 16(1) |
| C(11) | 7918(1) | 6539(4) | 1104(1) | 15(1) |
| C(12) | 7879(1) | 6768(4) | 1887(1) | 14(1) |
| C(13) | 8381(1) | 8578(4) | 2203(1) | 16(1) |
| C(14) | 8364(1) | 8767(4) | 3017(1) | 17(1) |
| C(15) | 8312(1) | 6616(5) | 4200(1) | 21(1) |
| C(16) | 9062(1) | 7448(5) | 4471(1) | 28(1) |
| C(17) | 8120(2) | 4363(6) | 4563(1) | 32(1) |
| C(18) | 5603(1) | 7227(4) | 3837(1) | 18(1) |
| C(19) | 6297(1) | 1213(4) | 1398(1) | 19(1) |
| C(20) | 7490(1) | 5354(4) | 2310(1) | 12(1) |
| C(21) | 4802(1) | 7032(4) | 1494(1) | 16(1) |
| C(22) | 4337(1) | 7347(5) | 841(1) | 22(1) |

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

| | |
|---|---|
| *O(1)-C(1)* | *1.437(3)* |
| *O(2)-C(21)* | *1.353(3)* |
| *O(2)-C(7)* | *1.458(3)* |
| *O(3)-C(21)* | *1.203(3)* |
| *O(4)-C(20)* | *1.374(3)* |
| *O(4)-C(8)* | *1.465(3)* |
| *O(5)-C(11)* | *1.223(3)* |
| *C(1)-C(14)* | *1.527(3)* |
| *C(1)-C(15)* | *1.548(3)* |
| *C(1)-C(2)* | *1.550(3)* |
| *C(2)-C(20)* | *1.515(3)* |
| *C(2)-C(3)* | *1.521(3)* |
| *C(3)-C(4)* | *1.333(3)* |
| *C(4)-C(18)* | *1.507(3)* |
| *C(4)-C(5)* | *1.509(3)* |
| *C(5)-C(6)* | *1.544(3)* |
| *C(6)-C(7)* | *1.525(3)* |
| *C(7)-C(8)* | *1.542(3)* |
| *C(8)-C(19)* | *1.522(3)* |
| *C(8)-C(9)* | *1.530(3)* |
| *C(9)-C(10)* | *1.531(3)* |
| *C(10)-C(11)* | *1.503(3)* |
| *C(11)-C(12)* | *1.475(3)* |
| *C(12)-C(20)* | *1.351(3)* |
| *C(12)-C(13)* | *1.515(3)* |
| *C(13)-C(14)* | *1.529(3)* |
| *C(15)-C(17)* | *1.523(4)* |
| *C(15)-C(16)* | *1.532(3)* |
| *C(21)-C(22)* | *1.492(3)* |
| | |
| *C(21)-O(2)-C(7)* | *117.32(17)* |
| *C(20)-O(4)-C(8)* | *124.59(16)* |
| *O(1)-C(1)-C(14)* | *111.82(17)* |
| *O(1)-C(1)-C(15)* | *104.66(18)* |
| *C(14)-C(1)-C(15)* | *112.02(19)* |
| *O(1)-C(1)-C(2)* | *109.00(17)* |

| | |
|---|---|
| *C(14)-C(1)-C(2)* | *107.86(18)* |
| *C(15)-C(1)-C(2)* | *111.47(16)* |
| *C(20)-C(2)-C(3)* | *110.60(17)* |
| *C(20)-C(2)-C(1)* | *110.93(16)* |
| *C(3)-C(2)-C(1)* | *112.98(17)* |
| *C(4)-C(3)-C(2)* | *127.8(2)* |
| *C(3)-C(4)-C(18)* | *120.8(2)* |
| *C(3)-C(4)-C(5)* | *124.0(2)* |
| *C(18)-C(4)-C(5)* | *115.20(19)* |
| *C(4)-C(5)-C(6)* | *111.76(18)* |
| *C(7)-C(6)-C(5)* | *114.18(17)* |
| *O(2)-C(7)-C(6)* | *109.80(16)* |
| *O(2)-C(7)-C(8)* | *103.73(16)* |
| *C(6)-C(7)-C(8)* | *116.94(18)* |
| *O(4)-C(8)-C(19)* | *102.77(17)* |
| *O(4)-C(8)-C(9)* | *112.54(16)* |
| *C(19)-C(8)-C(9)* | *110.26(18)* |
| *O(4)-C(8)-C(7)* | *107.22(16)* |
| *C(19)-C(8)-C(7)* | *112.84(18)* |
| *C(9)-C(8)-C(7)* | *110.95(17)* |
| *C(8)-C(9)-C(10)* | *111.72(17)* |
| *C(11)-C(10)-C(9)* | *110.60(18)* |
| *O(5)-C(11)-C(12)* | *119.8(2)* |
| *O(5)-C(11)-C(10)* | *120.0(2)* |
| *C(12)-C(11)-C(10)* | *120.17(18)* |
| *C(20)-C(12)-C(11)* | *124.0(2)* |
| *C(20)-C(12)-C(13)* | *121.05(19)* |
| *C(11)-C(12)-C(13)* | *114.66(18)* |
| *C(12)-C(13)-C(14)* | *114.95(17)* |
| *C(1)-C(14)-C(13)* | *112.19(18)* |
| *C(17)-C(15)-C(16)* | *109.6(2)* |
| *C(17)-C(15)-C(1)* | *112.2(2)* |
| *C(16)-C(15)-C(1)* | *112.42(18)* |
| *C(12)-C(20)-O(4)* | *126.24(19)* |
| *C(12)-C(20)-C(2)* | *123.48(19)* |
| *O(4)-C(20)-C(2)* | *109.92(17)* |
| *O(3)-C(21)-O(2)* | *123.5(2)* |
| *O(3)-C(21)-C(22)* | *125.7(2)* |

*O(2)-C(21)-C(22)* *110.79(19)*

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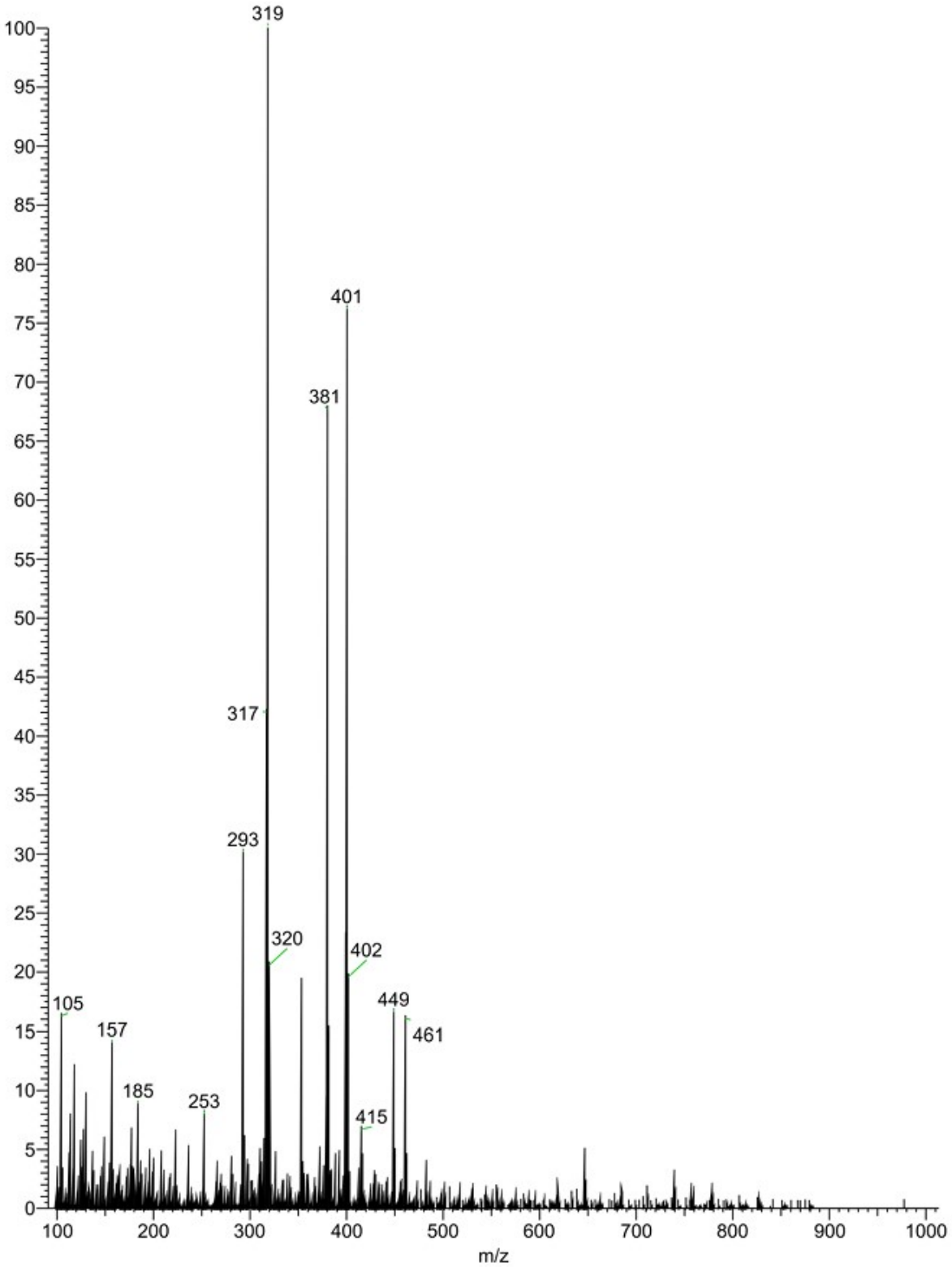
*Symmetry transformations used to generate equivalent atoms:*

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

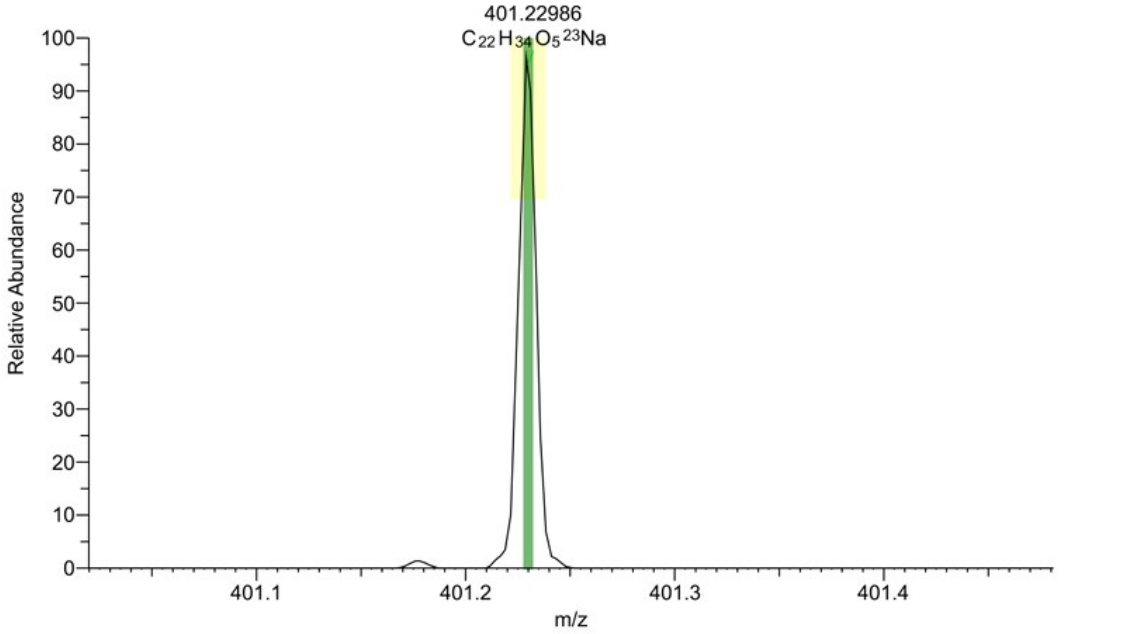
| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| O(1) | 13(1) | 30(1) | 14(1) | 2(1) | 2(1) | 6(1) |
| O(2) | 12(1) | 18(1) | 18(1) | -4(1) | -2(1) | 1(1) |
| O(3) | 20(1) | 19(1) | 25(1) | -4(1) | 4(1) | 1(1) |
| O(4) | 13(1) | 11(1) | 16(1) | 0(1) | -2(1) | -1(1) |
| O(5) | 29(1) | 31(1) | 17(1) | 7(1) | 1(1) | -13(1) |
| C(1) | 11(1) | 21(1) | 13(1) | -1(1) | 2(1) | 0(1) |
| C(2) | 11(1) | 14(1) | 14(1) | 1(1) | 1(1) | -1(1) |
| C(3) | 15(1) | 16(1) | 11(1) | 0(1) | 0(1) | 1(1) |
| C(4) | 15(1) | 18(1) | 10(1) | 2(1) | 0(1) | 0(1) |
| C(5) | 16(1) | 15(1) | 17(1) | 3(1) | 4(1) | -2(1) |
| C(6) | 14(1) | 15(1) | 21(1) | -2(1) | 2(1) | -5(1) |
| C(7) | 12(1) | 13(1) | 14(1) | -2(1) | -2(1) | -1(1) |
| C(8) | 11(1) | 14(1) | 15(1) | -2(1) | -2(1) | 0(1) |
| C(9) | 14(1) | 14(1) | 14(1) | -2(1) | -2(1) | 1(1) |
| C(10) | 16(1) | 19(1) | 13(1) | -2(1) | 1(1) | 0(1) |
| C(11) | 14(1) | 17(1) | 15(1) | 2(1) | -1(1) | 0(1) |
| C(12) | 12(1) | 14(1) | 14(1) | 1(1) | -1(1) | 0(1) |
| C(13) | 16(1) | 17(1) | 15(1) | 2(1) | 0(1) | -5(1) |
| C(14) | 14(1) | 20(1) | 16(1) | -2(1) | 2(1) | -5(1) |
| C(15) | 14(1) | 36(1) | 13(1) | -2(1) | 1(1) | -2(1) |
| C(16) | 21(1) | 47(2) | 16(1) | -3(1) | -3(1) | -6(1) |
| C(17) | 28(1) | 54(2) | 14(1) | 10(1) | -3(1) | -12(1) |
| C(18) | 14(1) | 22(1) | 20(1) | -1(1) | 2(1) | 1(1) |
| C(19) | 20(1) | 14(1) | 24(1) | -5(1) | 0(1) | -2(1) |
| C(20) | 10(1) | 10(1) | 14(1) | -1(1) | -1(1) | 1(1) |
| C(21) | 12(1) | 13(1) | 22(1) | 1(1) | 6(1) | -1(1) |
| C(22) | 16(1) | 26(1) | 25(1) | 5(1) | 1(1) | 2(1) |

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

| | *x* | *y* | *z* | *U(eq)* |
|---|---|---|---|---|
| H(1) | 8922(13) | 4910(40) | 2742(18) | 28 |
| H(2) | 7521 | 3776 | 3287 | 16 |
| H(3) | 6948 | 8151 | 3577 | 16 |
| H(5A) | 5684 | 2676 | 3657 | 19 |
| H(5B) | 6400 | 2491 | 3171 | 19 |
| H(6A) | 5367 | 1960 | 2430 | 20 |
| H(6B) | 5000 | 4265 | 2715 | 20 |
| H(7) | 5982 | 6388 | 2157 | 16 |
| H(9A) | 6540 | 6680 | 979 | 17 |
| H(9B) | 6346 | 4483 | 502 | 17 |
| H(10A) | 7632 | 3218 | 863 | 19 |
| H(10B) | 7526 | 4926 | 201 | 19 |
| H(13A) | 8245 | 10081 | 1996 | 19 |
| H(13B) | 8891 | 8242 | 2057 | 19 |
| H(14A) | 8825 | 9486 | 3189 | 20 |
| H(14B) | 7952 | 9771 | 3156 | 20 |
| H(15) | 7939 | 7772 | 4349 | 25 |
| H(16A) | 9439 | 6326 | 4346 | 42 |
| H(16B) | 9049 | 7628 | 4991 | 42 |
| H(16C) | 9177 | 8924 | 4250 | 42 |
| H(17A) | 7613 | 3944 | 4442 | 48 |
| H(17B) | 8170 | 4535 | 5082 | 48 |
| H(17C) | 8453 | 3160 | 4398 | 48 |
| H(18A) | 5809 | 8697 | 3990 | 28 |
| H(18B) | 5397 | 6430 | 4250 | 28 |
| H(18C) | 5214 | 7493 | 3481 | 28 |
| H(19A) | 5830 | 1104 | 1136 | 29 |
| H(19B) | 6267 | 317 | 1840 | 29 |
| H(19C) | 6693 | 612 | 1102 | 29 |
| H(22A) | 4602 | 6787 | 423 | 33 |
| H(22B) | 4225 | 8976 | 779 | 33 |
| H(22C) | 3879 | 6485 | 893 | 33 |

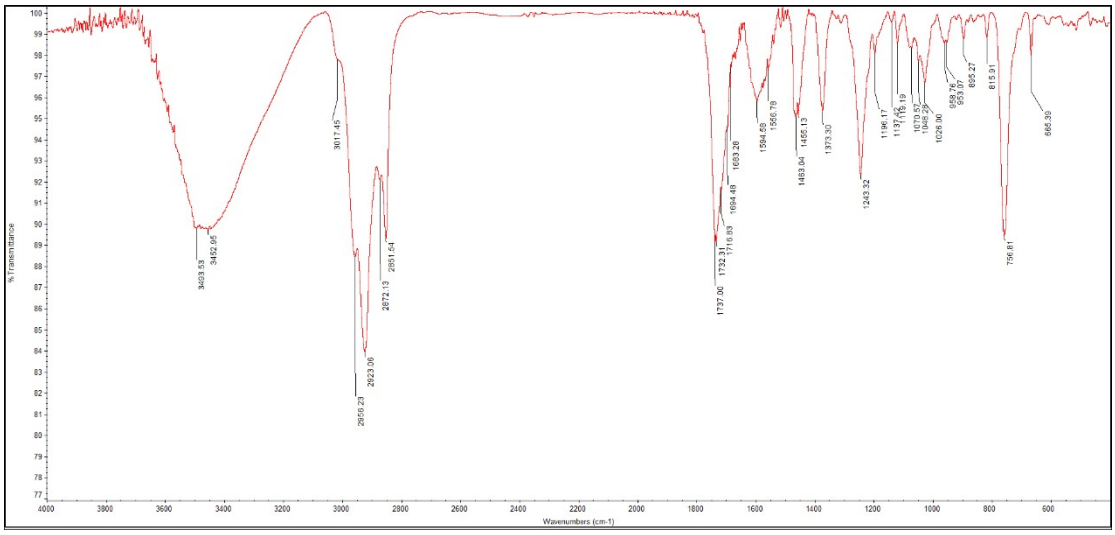



S12. ESIMS spectrum of compound **2**

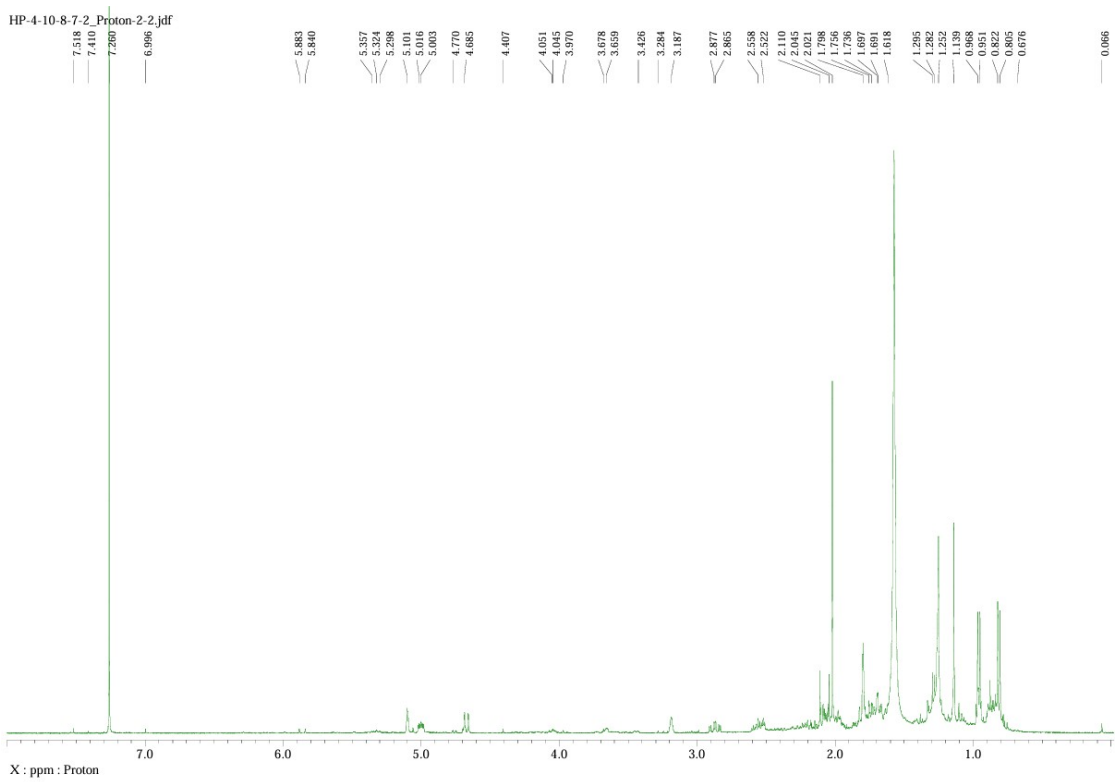



| Peak Mass | Display Formula | S Fit | RDB | Delta [ppm] | Theo. mass | Pattern Cov. [%] | MSMS Matched... |
|---|---|---|---|---|---|---|---|
| 401.22986 | $C_{22}H_{34}O_5{}^{23}Na$ | 73.28197114804 98 | 5.50 | 0.03 | 401.22985 | 100 | (Collection) |

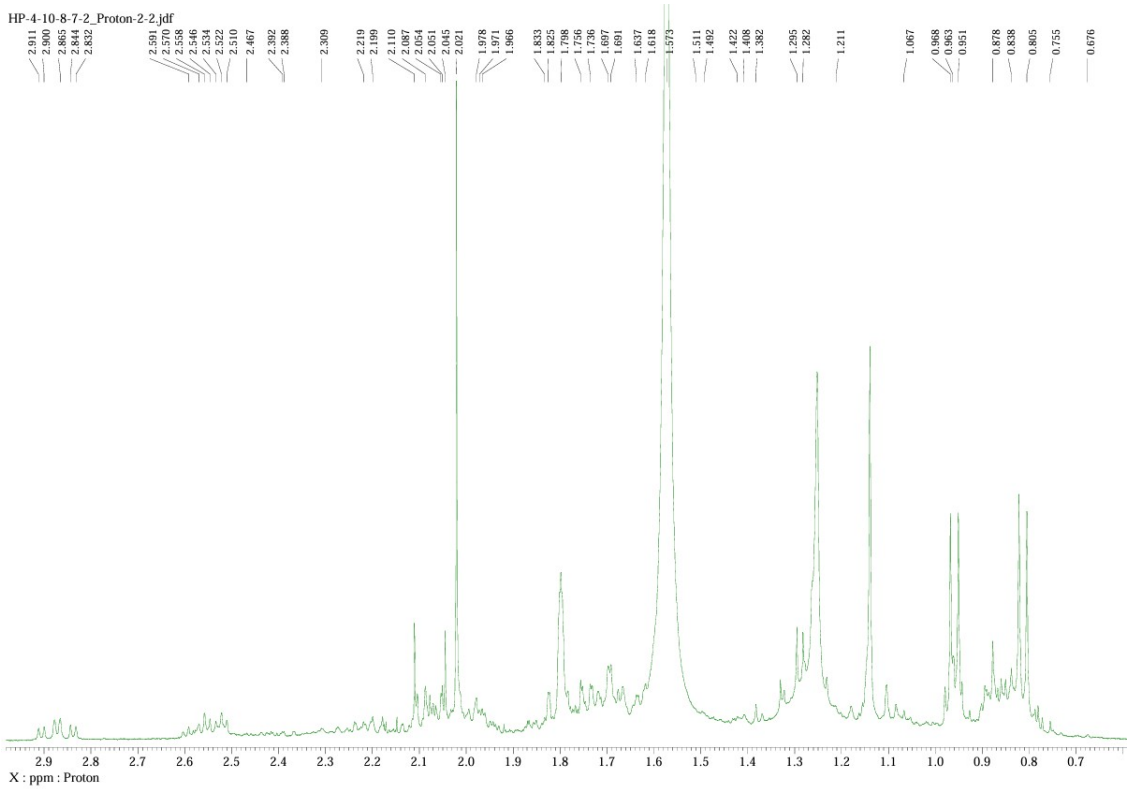
S13. HRESIMS spectrum of compound **2**



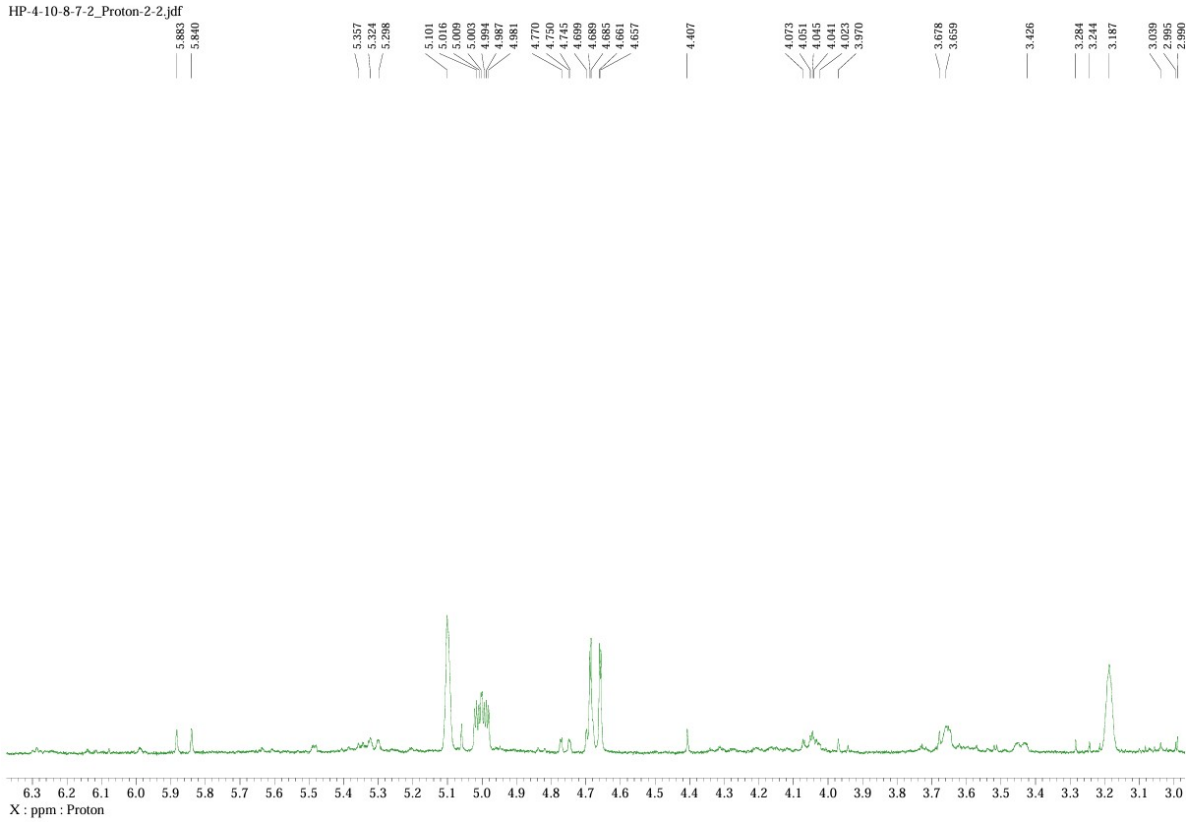

S14. IR spectrum of compound **2**



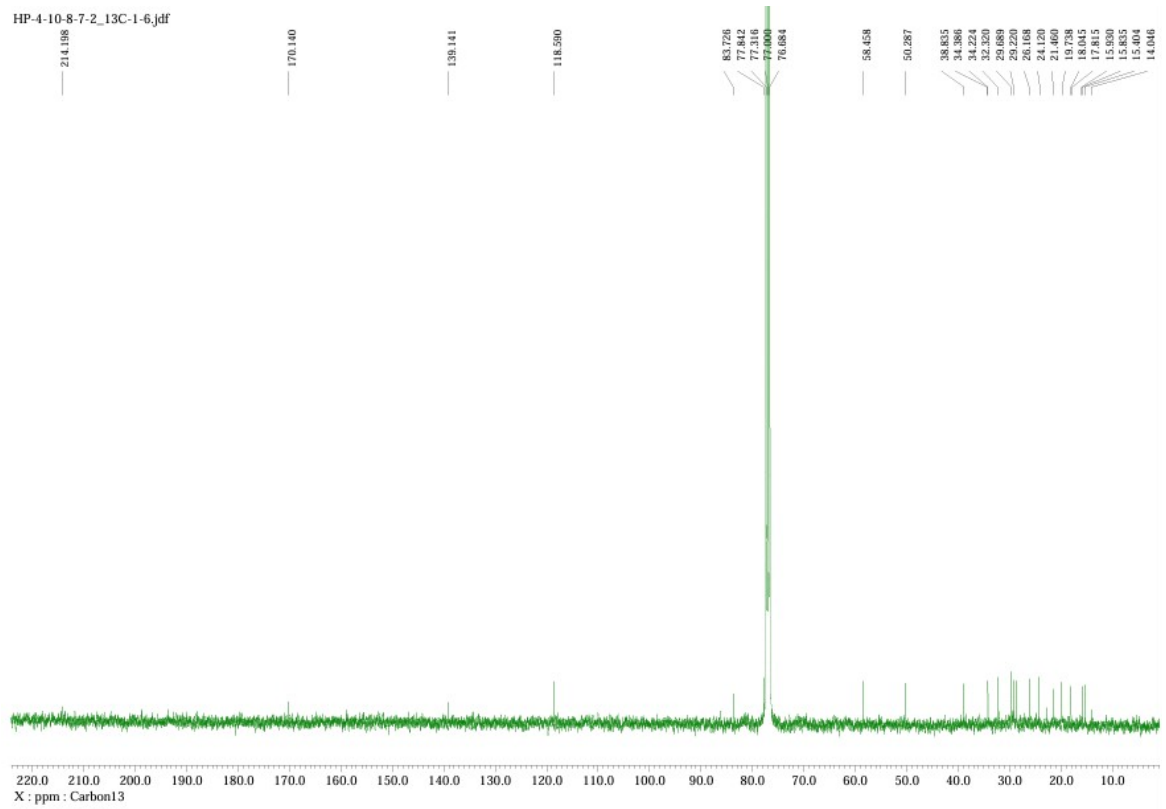

S15. $^{1}H$ NMR spectrum (400 MHz) of compound **2** in $CDCl_3$



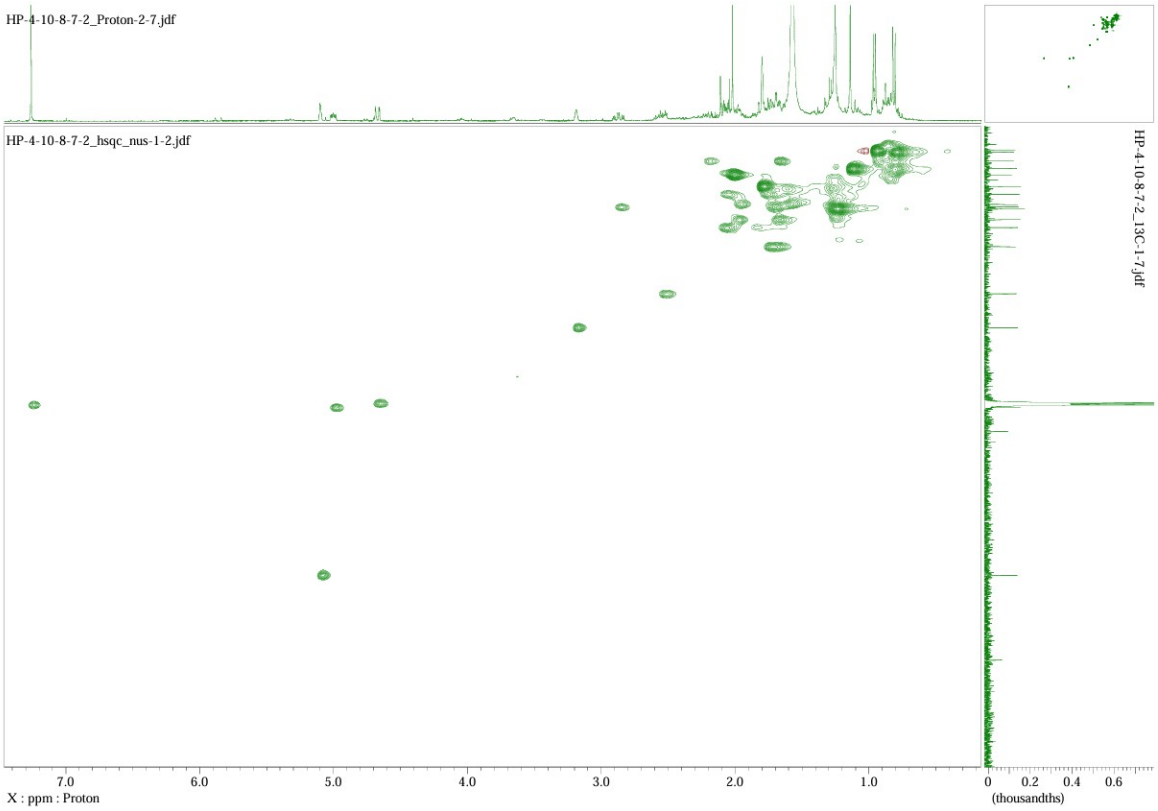

S16. Zoomed-in region of compound **2** from 0.7-2.97 ppm



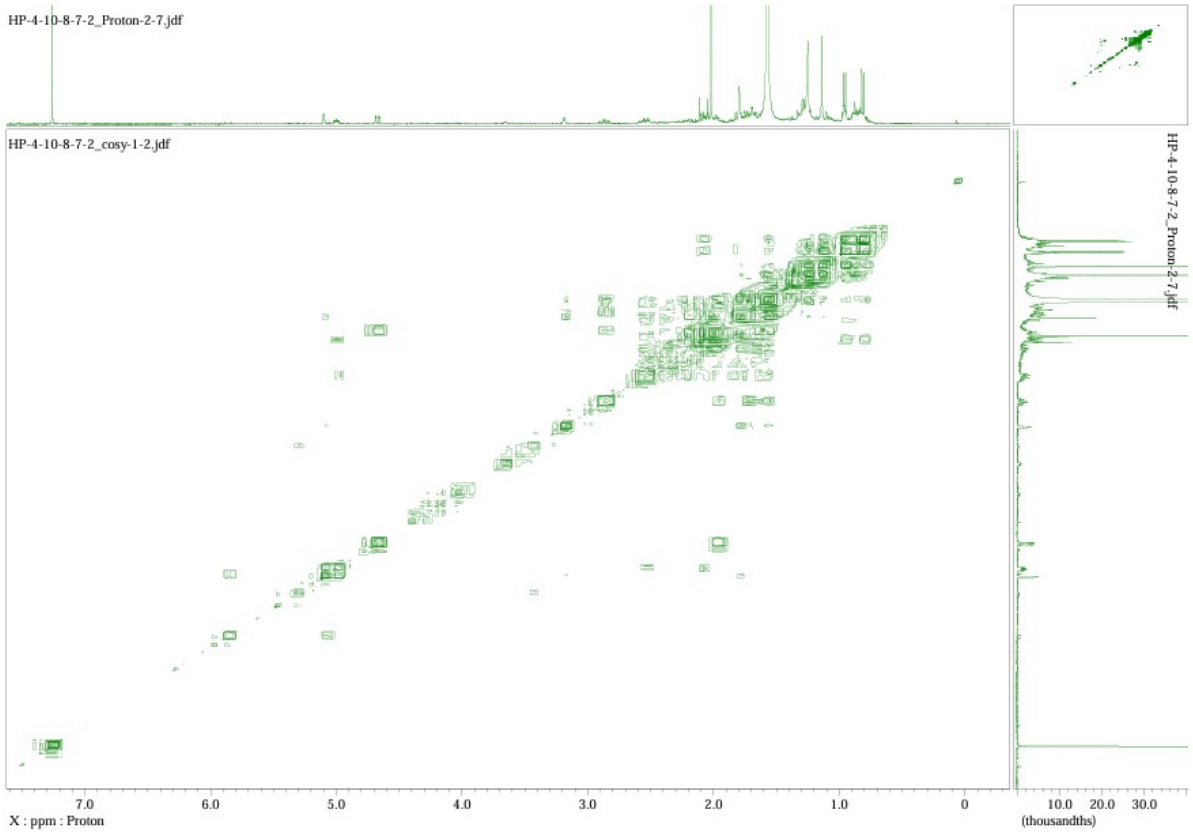

S17. Zoomed-in region of compound **2** from 3.0-6.3 ppm



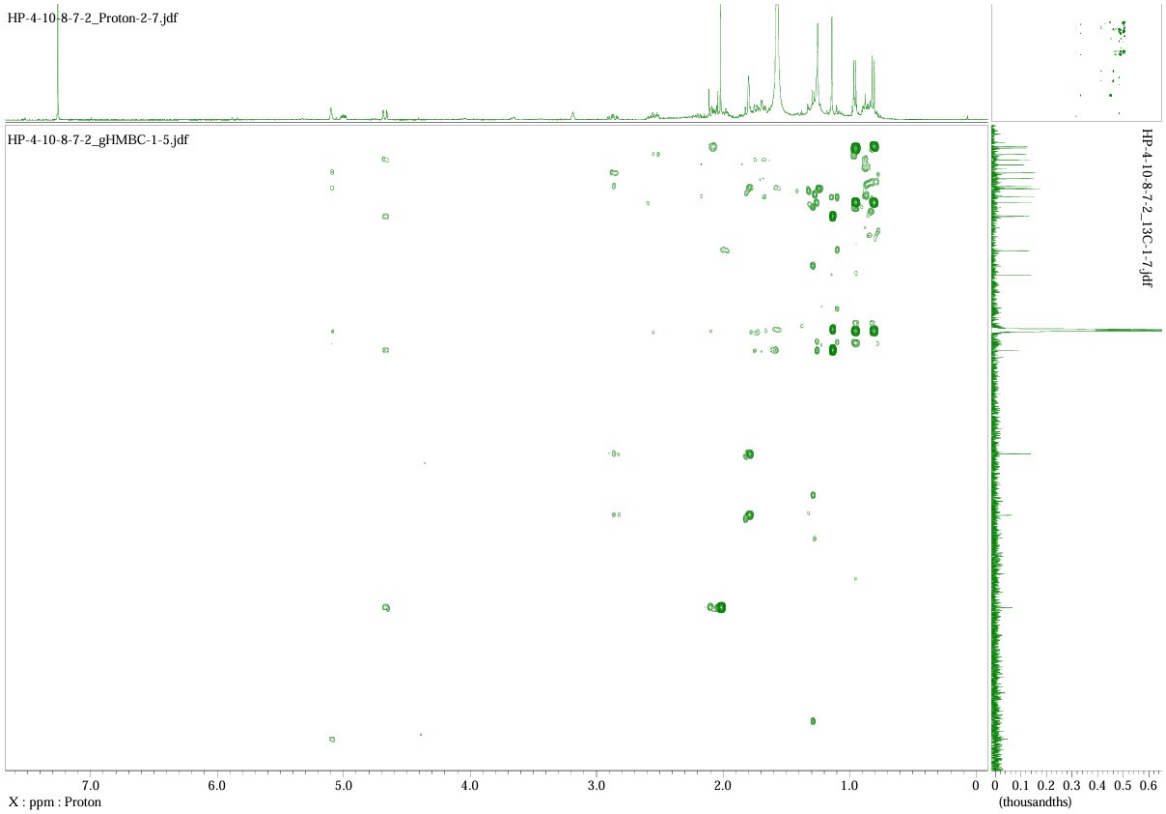

S18. $^{13}C$ NMR spectrum (100 MHz) of compound **2** in $CDCl_3$



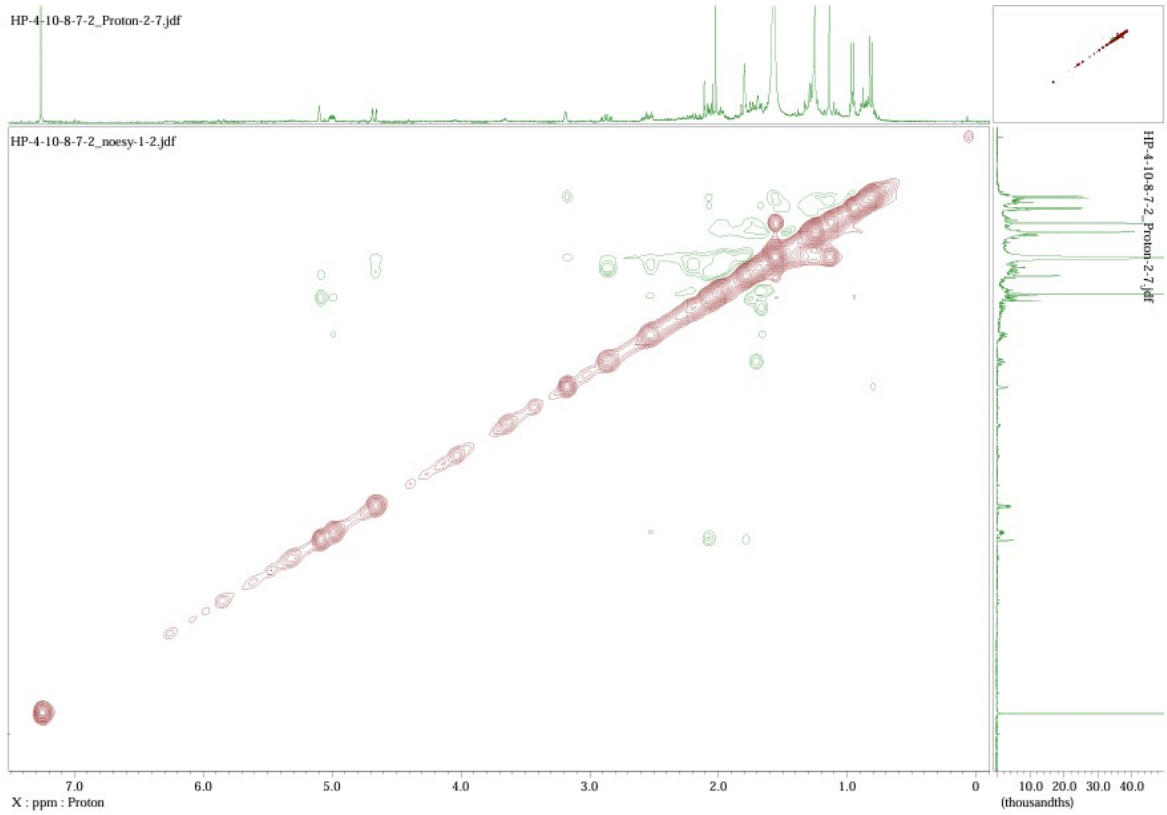

S19. HSQC spectrum of compound **2**



S20. COSY spectrum of compound **2**

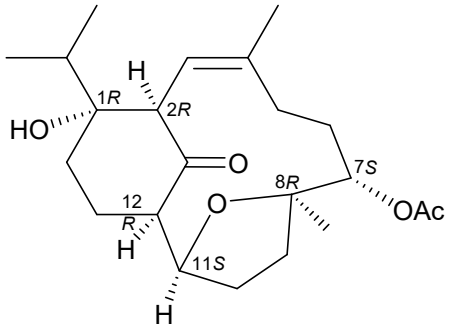



S21. HMBC spectrum of compound **2**



S22. NOESY spectrum of compound **2**

2. Crystal data and structure refinement for sarcoglaucone A (**2**) (CCDC number: 2496064)



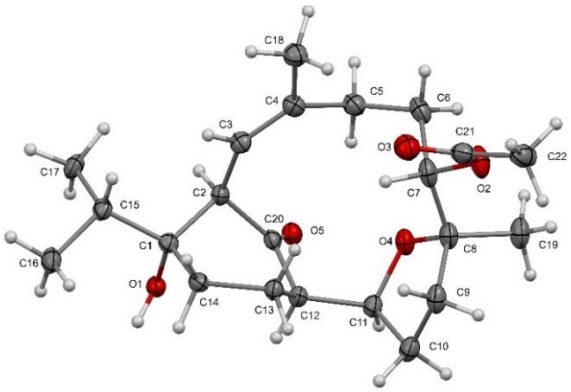




Table 1. Crystal data and structure refinement for i19812.

| | | |
|---|---|---|
| Identification code | i19812 | |
| Empirical formula | $C_{22}$ $H_{34}$ $O_5$ | |
| Formula weight | 378.49 | |
| Temperature | 100(2) K | |
| Wavelength | 1.54178 Å | |
| Crystal system | Orthorhombic | |
| Space group | $P2_12_12_1$ | |
| Unit cell dimensions | a = 6.6754(4) Å | α= 90°. |
| | b = 12.6299(8) Å | β= 90°. |
| | c = 24.3212(15) Å | γ = 90°. |
| Volume | 2050.5(2) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.226 $Mg/m^3$ | |
| Absorption coefficient | 0.687 $mm^{-1}$ | |
| F(000) | 824 | |
| Crystal size | 0.149 x 0.026 x 0.017 $mm^3$ | |
| Theta range for data collection | 3.635 to 66.599°. | |
| Index ranges | -7<=h<=7, -12<=k<=15, -28<=l<=27 | |
| Reflections collected | 28706 | |
| Independent reflections | 3586 [R(int) = 0.1776] | |
| Completeness to theta = 66.599° | 99.7 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.9819 and 0.6176 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3586 / 0 / 250 | |

| | |
|---|---|
| Goodness-of-fit on $F^2$ | 1.042 |
| Final R indices [I>2sigma(I)] | R1 = 0.0638, wR2 = 0.1229 |
| R indices (all data) | R1 = 0.1207, wR2 = 0.1448 |
| Absolute structure parameter | -0.4(5) |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.162 and -0.220 e.$Å^{-3}$ |

Table 2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for i19812. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| O(1) | 5852(5) | 6982(3) | 5356(1) | 45(1) |
| O(2) | 3621(7) | 2909(4) | 3013(2) | 69(1) |
| O(3) | 2010(6) | 2138(4) | 3716(2) | 66(1) |
| O(4) | 5611(5) | 5457(3) | 3395(1) | 51(1) |
| O(5) | 8059(6) | 6519(3) | 4224(1) | 48(1) |
| C(1) | 5304(8) | 5871(5) | 5356(2) | 43(1) |
| C(2) | 6810(8) | 5404(5) | 4943(2) | 43(1) |
| C(3) | 6519(8) | 4203(5) | 4881(2) | 46(1) |
| C(4) | 6945(8) | 3529(5) | 4488(2) | 48(2) |
| C(5) | 7926(9) | 3767(5) | 3946(2) | 54(2) |
| C(6) | 6829(9) | 3298(5) | 3444(2) | 60(2) |
| C(7) | 4661(9) | 3657(6) | 3371(2) | 58(2) |
| C(8) | 4333(9) | 4727(6) | 3106(2) | 50(2) |
| C(9) | 2206(8) | 5157(6) | 3196(2) | 58(2) |
| C(10) | 2506(9) | 6330(6) | 3315(2) | 58(2) |
| C(11) | 4540(8) | 6369(5) | 3599(2) | 47(2) |
| C(12) | 4502(8) | 6333(5) | 4230(2) | 44(1) |
| C(13) | 2979(8) | 5635(5) | 4515(2) | 44(1) |
| C(14) | 3141(8) | 5723(5) | 5140(2) | 44(1) |
| C(15) | 5547(8) | 5439(5) | 5948(2) | 46(2) |
| C(16) | 4097(9) | 5989(5) | 6350(2) | 59(2) |
| C(17) | 7707(8) | 5517(6) | 6156(2) | 59(2) |
| C(18) | 6538(9) | 2357(5) | 4585(2) | 60(2) |
| C(19) | 4922(9) | 4754(6) | 2496(2) | 65(2) |
| C(20) | 6591(8) | 6096(5) | 4442(2) | 41(1) |
| C(21) | 2258(9) | 2237(6) | 3231(3) | 60(2) |
| C(22) | 1117(10) | 1697(6) | 2785(3) | 72(2) |

Table 3. Bond lengths [Å] and angles [°] for i19812.

| | |
|---|---|
| O(1)-C(1) | 1.450(7) |
| O(2)-C(21) | 1.353(8) |
| O(2)-C(7) | 1.461(7) |
| O(3)-C(21) | 1.197(7) |
| O(4)-C(8) | 1.439(7) |
| O(4)-C(11) | 1.444(7) |
| O(5)-C(20) | 1.235(6) |
| C(1)-C(2) | 1.539(7) |
| C(1)-C(14) | 1.548(7) |
| C(1)-C(15) | 1.548(7) |
| C(2)-C(20) | 1.507(8) |
| C(2)-C(3) | 1.537(8) |
| C(3)-C(4) | 1.311(8) |
| C(4)-C(5) | 1.502(8) |
| C(4)-C(18) | 1.523(9) |
| C(5)-C(6) | 1.543(8) |
| C(6)-C(7) | 1.527(8) |
| C(7)-C(8) | 1.513(9) |
| C(8)-C(9) | 1.536(8) |
| C(8)-C(19) | 1.537(8) |
| C(9)-C(10) | 1.524(9) |
| C(10)-C(11) | 1.524(8) |
| C(11)-C(12) | 1.536(7) |
| C(12)-C(13) | 1.513(8) |
| C(12)-C(20) | 1.516(7) |
| C(13)-C(14) | 1.527(7) |
| C(15)-C(17) | 1.531(8) |
| C(15)-C(16) | 1.541(8) |
| C(21)-C(22) | 1.492(9) |

| | |
|---|---|
| C(21)-O(2)-C(7) | 119.4(5) |
| C(8)-O(4)-C(11) | 112.7(4) |
| O(1)-C(1)-C(2) | 101.8(4) |
| O(1)-C(1)-C(14) | 110.5(5) |
| C(2)-C(1)-C(14) | 109.9(4) |
| O(1)-C(1)-C(15) | 108.4(4) |

| | |
|---|---|
| C(2)-C(1)-C(15) | 113.9(4) |
| C(14)-C(1)-C(15) | 111.8(5) |
| C(20)-C(2)-C(3) | 118.7(4) |
| C(20)-C(2)-C(1) | 104.1(4) |
| C(3)-C(2)-C(1) | 111.1(5) |
| C(4)-C(3)-C(2) | 133.2(5) |
| C(3)-C(4)-C(5) | 127.2(6) |
| C(3)-C(4)-C(18) | 118.7(5) |
| C(5)-C(4)-C(18) | 114.1(5) |
| C(4)-C(5)-C(6) | 114.3(5) |
| C(7)-C(6)-C(5) | 115.3(5) |
| O(2)-C(7)-C(8) | 104.8(5) |
| O(2)-C(7)-C(6) | 109.1(5) |
| C(8)-C(7)-C(6) | 116.9(5) |
| O(4)-C(8)-C(7) | 106.2(4) |
| O(4)-C(8)-C(9) | 104.6(5) |
| C(7)-C(8)-C(9) | 112.9(5) |
| O(4)-C(8)-C(19) | 107.8(5) |
| C(7)-C(8)-C(19) | 113.2(6) |
| C(9)-C(8)-C(19) | 111.5(5) |
| C(10)-C(9)-C(8) | 104.4(5) |
| C(9)-C(10)-C(11) | 103.5(5) |
| O(4)-C(11)-C(10) | 105.1(5) |
| O(4)-C(11)-C(12) | 109.2(5) |
| C(10)-C(11)-C(12) | 115.9(5) |
| C(13)-C(12)-C(20) | 110.3(4) |
| C(13)-C(12)-C(11) | 119.1(5) |
| C(20)-C(12)-C(11) | 109.3(5) |
| C(12)-C(13)-C(14) | 111.5(5) |
| C(13)-C(14)-C(1) | 114.4(4) |
| C(17)-C(15)-C(16) | 110.8(5) |
| C(17)-C(15)-C(1) | 112.5(4) |
| C(16)-C(15)-C(1) | 111.4(5) |
| O(5)-C(20)-C(2) | 121.4(5) |
| O(5)-C(20)-C(12) | 119.9(5) |
| C(2)-C(20)-C(12) | 118.6(5) |
| O(3)-C(21)-O(2) | 123.0(6) |
| O(3)-C(21)-C(22) | 126.8(7) |

| | |
|---|---|
| O(2)-C(21)-C(22) | 110.1(6) |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for i19812. 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) | 54(2) | 43(3) | 38(2) | -2(2) | 2(2) | 2(2) |
| O(2) | 85(3) | 74(4) | 47(2) | -20(2) | 4(2) | -25(3) |
| O(3) | 76(3) | 57(3) | 67(3) | 0(3) | 5(2) | -4(2) |
| O(4) | 54(2) | 63(3) | 36(2) | -9(2) | 1(2) | -8(2) |
| O(5) | 51(2) | 51(3) | 42(2) | -5(2) | -1(2) | -1(2) |
| C(1) | 50(3) | 37(4) | 41(3) | -1(3) | -1(2) | 0(3) |
| C(2) | 50(3) | 44(4) | 34(3) | -3(3) | -6(3) | 4(3) |
| C(3) | 49(3) | 43(4) | 46(3) | 4(3) | 4(3) | -4(3) |
| C(4) | 47(3) | 47(4) | 51(3) | -2(3) | 2(3) | 1(3) |
| C(5) | 57(3) | 51(4) | 52(3) | -3(3) | 6(3) | 2(3) |
| C(6) | 73(4) | 56(5) | 50(3) | -16(3) | 15(3) | -3(3) |
| C(7) | 65(4) | 73(5) | 37(3) | -17(4) | 3(3) | -10(4) |
| C(8) | 55(3) | 62(5) | 34(3) | -5(3) | 4(3) | -9(3) |
| C(9) | 54(3) | 81(6) | 38(3) | -6(3) | -1(3) | -14(3) |
| C(10) | 61(4) | 73(5) | 39(3) | 5(3) | -6(3) | 0(4) |
| C(11) | 56(3) | 50(4) | 35(3) | 2(3) | 1(3) | 1(3) |
| C(12) | 49(3) | 49(4) | 34(3) | 1(3) | -1(2) | 7(3) |
| C(13) | 46(3) | 49(4) | 36(3) | -1(3) | -2(2) | 0(3) |
| C(14) | 49(3) | 41(4) | 43(3) | -2(3) | 4(3) | 6(3) |
| C(15) | 59(3) | 45(4) | 35(3) | 5(3) | 0(3) | -3(3) |
| C(16) | 80(4) | 59(5) | 37(3) | 1(3) | 2(3) | -2(4) |
| C(17) | 67(4) | 70(5) | 39(3) | 7(3) | -15(3) | 2(3) |
| C(18) | 68(4) | 51(5) | 60(4) | 2(3) | 4(3) | 3(3) |
| C(19) | 70(4) | 88(6) | 38(3) | -6(3) | 5(3) | -14(4) |
| C(20) | 51(3) | 39(4) | 34(3) | -9(3) | 1(3) | 0(3) |
| C(21) | 56(4) | 54(5) | 71(5) | -6(4) | -3(4) | 13(4) |
| C(22) | 68(4) | 62(5) | 86(5) | -22(4) | -22(4) | 13(4) |

Table 5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^{-3}$) for i19812.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | 4912 | 7340 | 5490 | 67 |
| H(2) | 8184 | 5523 | 5095 | 51 |
| H(3) | 5903 | 3883 | 5192 | 55 |
| H(5A) | 9311 | 3487 | 3954 | 64 |
| H(5B) | 8010 | 4545 | 3902 | 64 |
| H(6A) | 7587 | 3489 | 3109 | 72 |
| H(6B) | 6846 | 2517 | 3475 | 72 |
| H(7) | 3991 | 3655 | 3739 | 70 |
| H(9A) | 1374 | 5054 | 2863 | 69 |
| H(9B) | 1552 | 4799 | 3511 | 69 |
| H(10A) | 1437 | 6605 | 3558 | 69 |
| H(10B) | 2518 | 6748 | 2970 | 69 |
| H(11) | 5259 | 7024 | 3480 | 56 |
| H(12) | 4197 | 7072 | 4352 | 53 |
| H(13A) | 3193 | 4890 | 4404 | 52 |
| H(13B) | 1614 | 5845 | 4398 | 52 |
| H(14A) | 2569 | 5075 | 5307 | 53 |
| H(14B) | 2320 | 6331 | 5264 | 53 |
| H(15) | 5184 | 4671 | 5940 | 56 |
| H(16A) | 4240 | 5676 | 6716 | 88 |
| H(16B) | 2717 | 5895 | 6221 | 88 |
| H(16C) | 4410 | 6746 | 6367 | 88 |
| H(17A) | 7762 | 5303 | 6543 | 88 |
| H(17B) | 8177 | 6249 | 6120 | 88 |
| H(17C) | 8566 | 5049 | 5937 | 88 |
| H(18A) | 7744 | 1947 | 4498 | 89 |
| H(18B) | 5434 | 2126 | 4348 | 89 |
| H(18C) | 6175 | 2244 | 4971 | 89 |
| H(19A) | 4109 | 4241 | 2291 | 98 |
| H(19B) | 6342 | 4572 | 2458 | 98 |
| H(19C) | 4691 | 5465 | 2348 | 98 |
| H(22A) | 244 | 1155 | 2945 | 108 |

| | | | | |
|---|---|---|---|---|
| H(22B) | 2056 | 1363 | 2528 | 108 |
| H(22C) | 300 | 2218 | 2588 | 108 |