

Supplementary Data

Identification, structural modification, and dichotomous effects on human immunodeficiency virus type 1 (HIV-1) replication of ingenane esters from *Euphorbia kansui*

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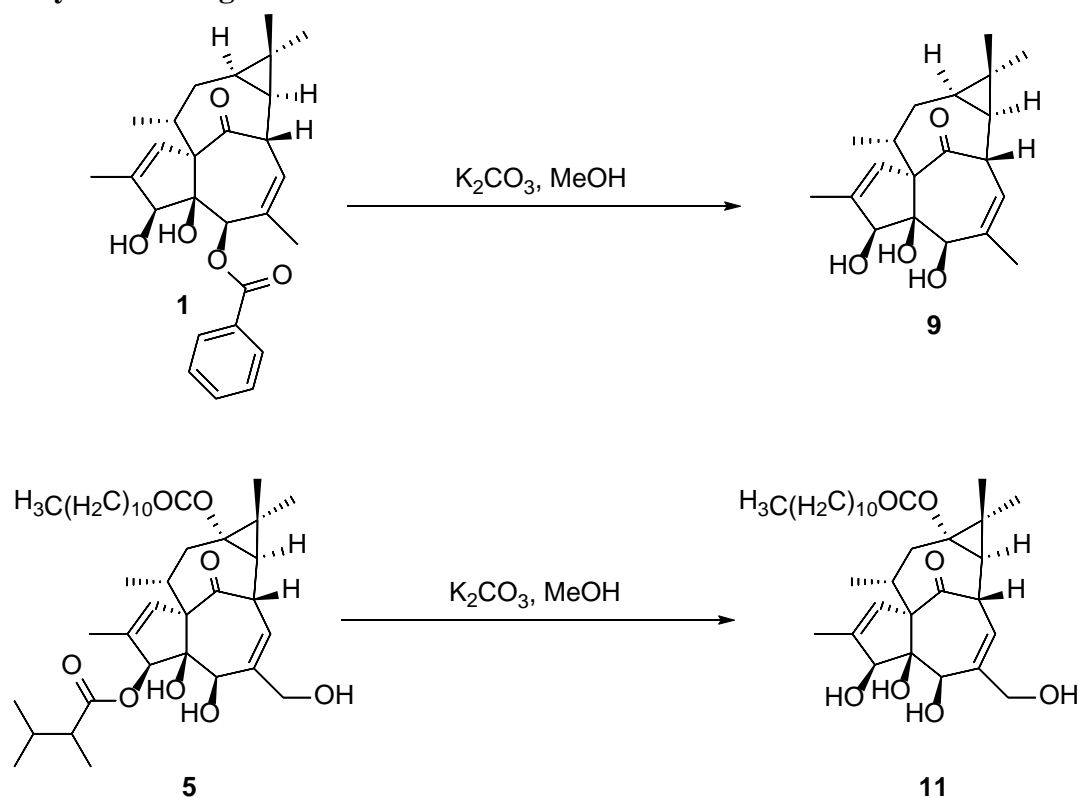
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Anti-HIV activities of *E. kansui* MeOH extract and fractions (E1-4)

TableS1. Anti-HIV activities of *E. kansui* MeOH extract and fractions

Extract	anti-HIV EC ₅₀ (μg/ml)	cytotoxicity CC ₅₀ (μg/ml)
MeOH extract	0.15	>10
EtOAc fraction	0.11	>10
H ₂ O fraction	>10	>10
E1	1.3	>10
E2	>10	>10
E3	0.028	9.4
E4	0.86	>10

Selective deacylation of ingenane esters **1** and **5**.



A solution of **1** (4 mg, 9 μmol) or **5** (4 mg, 6 μmol) and potassium carbonate (3 mg, 15 μmol) in 3 mL of anhydrous methanol was stirred at room temperature for 3 h, diluted with diethyl ether, washed with water. After removal of solvent *in vacuo*, the residue was purified by RP-HPLC (YMC Pack Pro C₁₈, MeCN-H₂O, 50:50 and 90:10, 5 mL/min) to give **9** (2.6 mg, 82%, t_R = 22.0 min) and **11** (2.3 mg, 70%, t_R = 25.5 min).

20-Deoxyingenol (**9**): colorless oil; $[\alpha]_D^{25}$ -13.5 (c 0.2, MeOH); UV (MeCN) λ_{max} (log ϵ): 205 (4.34) nm; IR (KBr) max: 2923, 1707, 1449, 1379, 1460, 1261, 1168, 1100, 1098, 801 cm^{-1} ; ¹H NMR (pyridine-*d*₅,

500 MHz) δ 6.23 (1H, q, $J = 1.2$ Hz, H-1), 5.02 (1H, d, $J = 5.8$ Hz, H-3), 3.87 (1H, d, $J = 10.9$ Hz, H-5), 5.90 (1H, dq, $J = 4.8, 1.4$ Hz, H-7), 4.60 (1H, ddq, $J = 11.2, 4.8, 2.0$ Hz, H-8), 2.80 (1H, qdd, $J = 7.2, 4.6, 3.0$ Hz, H-11), 2.63 (1H, ddd, $J = 15.4, 8.9, 3.0$ Hz, H₂-12a), 1.75 (1H, ddd, $J = 15.4, 6.3, 4.6$ Hz, H₂-12b), 0.75 (1H, ddd, $J = 8.9, 8.6, 6.3$ Hz, H-13), 1.17 (dd, $J = 12.1, 8.6$ Hz, H-14), 1.06 (3H, s, H₃-16), 1.24 (3H, s, H₃-17), 1.14 (3H, d, $J = 7.2$ Hz, H₃-18), 1.89 (3H, d, $J = 1.2$ Hz, H₃-19), 1.96 (3H, brs, H₃-20); ¹³C NMR (pyridine-*d*₅, 125 MHz) δ 129.5 (C-1), 140.3 (C-2), 80.6 (C-3), 85.9 (C-4), 77.0 (C-5), 140.4 (C-6), 123.1 (C-7), 44.4 (C-8), 207.4 (C-9), 73.3 (C-10), 39.9 (C-11), 31.4 (C-12), 23.7 (C-13), 24.3 (C-14), 24.1 (C-15), 28.7 (C-16), 15.8 (C-17), 17.5 (C-18), 15.7 (C-19), 22.8 (C-20); positive-ion HRESIMS m/z 355.1878 [M+Na]⁺, (calcd for C₂₀H₂₈O₄Na, 355.1885).

13-Oxyingenol-13-dodecanoate (**11**): colorless oil; $[\alpha]_D^{25}$ -41.4 (*c* 0.2, CHCl₃); UV (MeCN) λ_{\max} (log ϵ): 203 (4.31); IR (KBr) max: 2926, 1727, 1605, 1458, 1379, 1260, 1021, 800 cm⁻¹; ¹H NMR (CDCl₃, 500 MHz) δ 5.90 (1H, brq, $J = 1.6$ Hz, H-1), 4.40 (1H, s, H-3), 3.82 (1H, brs, H-5), 5.90 (1H, dd, $J = 4.9, 1.4$ Hz, H-7), 4.06 (1H, brdd, $J = 11.7, 4.0$ Hz, H-8), 2.42 (1H, m, H-11), 2.63 (1H, dd, $J = 16.6, 4.2$ Hz, CH₂-12a), 2.18 (1H, overlap, CH₂-12b), 1.28 (1H, overlap, H-14), 1.05 (3H, s, H₃-16), 1.20 (H, s, CH₃-17), 0.95 (3H, d, $J = 7.2$ Hz, H₃-18), 1.84 (3H, d, $J = 1.5$ Hz, H₃-19), 4.16 (1H, d, $J = 12.6$ Hz, H₂-20a), 4.11 (1H, d, $J = 12.6$ Hz, H₂-20b), 2.18 (2H, t, $J = 6.9$ Hz, H₂-2'), 1.55 (2H, overlap, H₂-3'), 1.27-1.21 (16H, m, H₂-4'-H₂-11'), 0.86 (3H, t, $J = 6.9$ Hz, H₃-12') ppm; ¹³C NMR (CDCl₃, 125 MHz) δ 129.3 (C-1), 139.3 (C-2), 80.4 (C-3), 84.1 (C-4), 75.3 (C-5), 140.8 (C-6), 126.1 (C-7), 43.3 (C-8), 206.2 (C-9), 72.6 (C-10), 38.7 (C-11), 35.1 (C-12), 68.9 (C-13), 28.3 (C-14), 30.3 (C-15), 22.5 (C-16), 16.7 (C-17), 18.4 (C-18), 15.3 (C-19), 66.8 (C-20), 174.0 (C-1'), 34.4 (C-2'), 24.8 (C-3'), 29.7-29.2 (C-4'-C-11'), 14.1 (C-12'); positive-ion HRESIMS m/z 569.3475 [M+Na]⁺, (calcd for C₃₂H₅₀O₇Na, 569.3454).

ESI-MS fragmentation behavior of isolated ingenane esters (1–5) and monitoring deacylation by LC-MS analysis

The reference solutions of **1–5** were prepared by dissolving them in LC-MS grade acetonitrile, and were made up at a concentration of 0.1 mg/mL. The samples (E3-fraction and E3-fraction after deacylation of *E. kansui* MeOH extract) used for LC-MS analysis were prepared by dissolving in MeOH at a concentration of 2.5 mg/mL. All the samples were filtered on 0.45 μm filter.

LC-MS analysis was performed on a Shimadzu LCMS-8040 Triple Quadrupole LC/MS/MS Mass Spectrometer. Nitrogen was used as the dry, nebulizer and auxiliary heated gas, and ultrapure helium was used as the collision gas. The ESI parameters were set as follows: interface voltage (4.5 kV in the positive-ion mode and -3.5 kV in the negative-ion mode); collision voltage, 15 V; dry gas, 15 L/min; dry temperature, 350 °C. Both the positive and negative ionization modes were checked, data reported in the range of m/z 100-800 Da.

HPLC was performed using a Shimadzu 8040 system (Shimadzu, Kyoto, Japan), which was equipped with a binary solvent delivery system and an auto-sampler. Separation was performed on a YMC-Triart C₁₈ column (150 mm \times 20 mm) maintained at 35°C, and the flow rate was 0.2 mL/min. The mobile phase was composed of A (0.1% formic acid in aqueous solution) and B (acetonitrile) with a gradient elution: 0-30 min, 50%-100% B, and the column was equilibrated for 20 min under the initial conditions. A volume of 2 μL was injected for LC-MS analysis. ESI-MS fragmentation behavior of **1-5** in positive ion mode was shown in Figure S1.

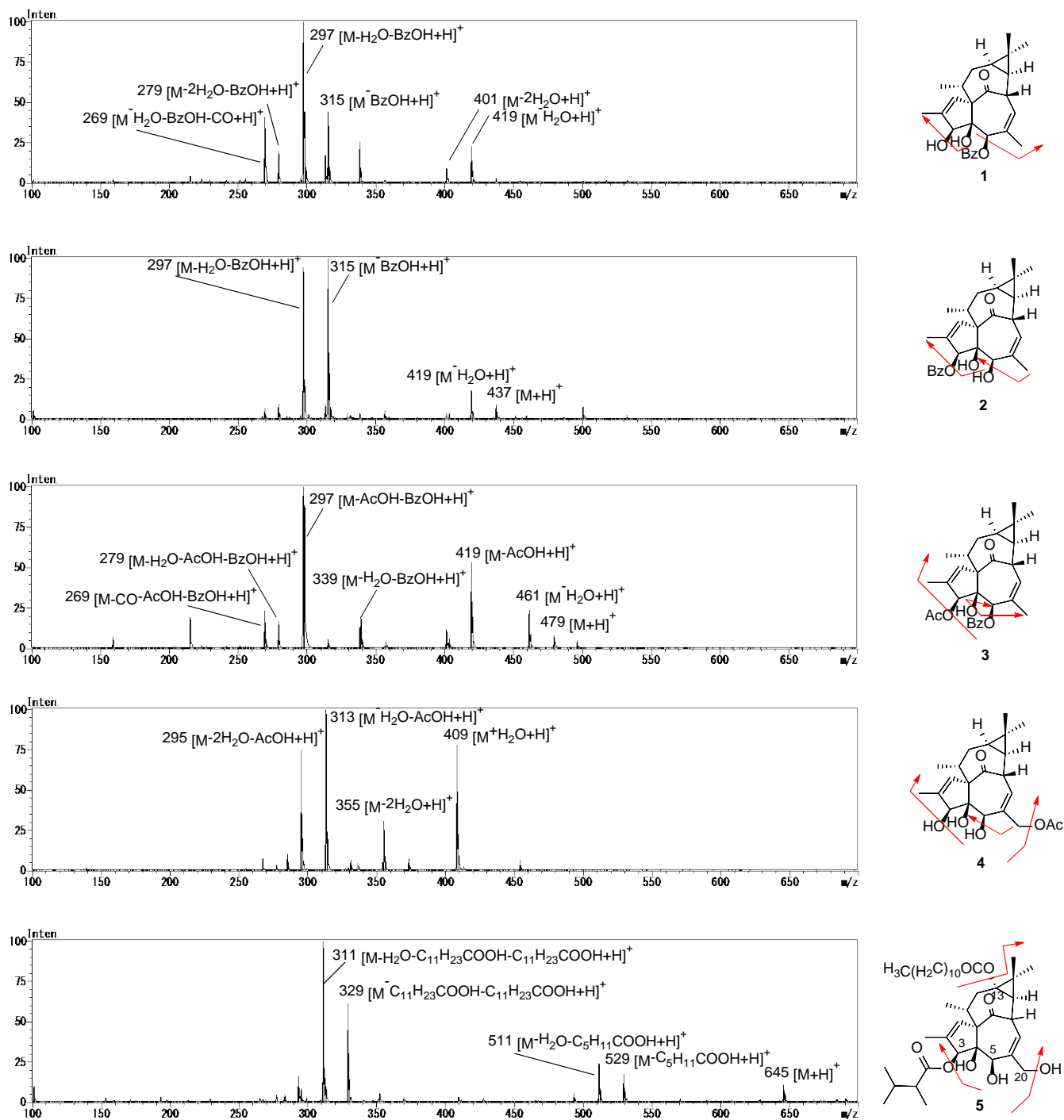
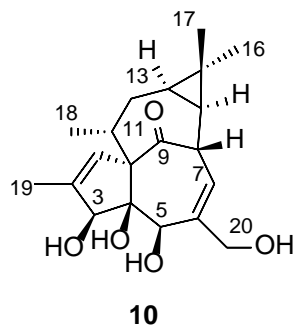


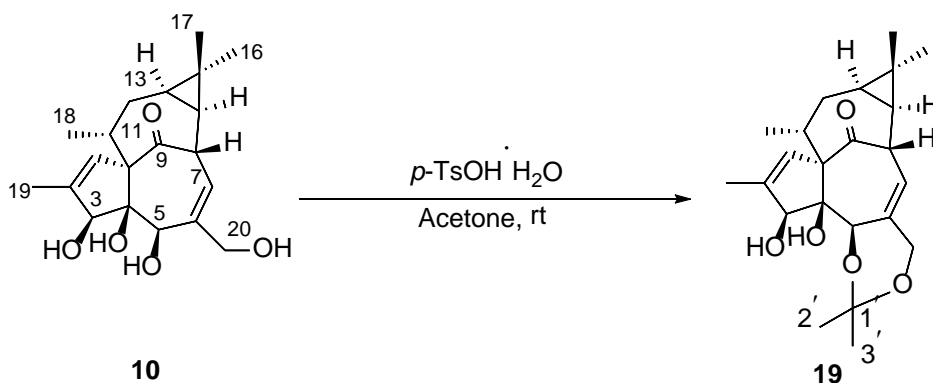
Figure S1. Proposed main ESI-MS fragmentation behavior of **1-5** in positive ion mode.

Physical and spectroscopic data of ingenol (10).



Ingenol (10): colorless oil; $[\alpha]_D^{25} -44.6$ (c 0.4, CHCl_3); UV (MeCN) λ_{max} ($\log \epsilon$): 203 (4.31) nm; IR (KBr) max: 2935, 1710, 1454, 1379, 1460, 1150, 1017, 756 cm^{-1} ; ^1H NMR (CDCl_3 , 500 MHz) δ 6.03 (1H, brd, $J = 4.3$ Hz, H-1), 4.37 (1H, s, H-3), 3.79 (1H, brs, H-5), 5.90 (1H, dd, $J = 3.1, 1.7$ Hz, H-7), 4.10 (1H, overlap, H-8), 2.32 (1H, m, H-11), 2.26 (1H, ddd, $J = 15.5, 8.9, 2.8$ Hz, H₂-12a), 1.74 (1H, ddd, $J = 15.5, 6.3, 5.1$ Hz, H₂-12b), 0.68 (1H, ddd, $J = 8.9, 8.9, 6.3$ Hz, H-13), 0.92 (1H, dd, $J = 12.0, 8.9$ Hz, H-14), 1.04 (3H, s, H₃-16), 1.10 (3H, s, H₃-17), 0.95 (3H, d, $J = 6.8$ Hz, H₃-18), 1.83 (3H, d, $J = 1.5$ Hz, H₃-19), 4.15 (1H, d, $J = 12.6$ Hz, H₂-20a), 4.10 (1H, d, $J = 12.6$ Hz, H₂-20b) ppm; ^{13}C NMR (CDCl_3 , 125 MHz) δ 129.8 (C-1), 138.9 (C-2), 80.5 (C-3), 84.3 (C-4), 75.3 (C-5), 140.4 (C-6), 127.4 (C-7), 44.1 (C-8), 207.2 (C-9), 72.6 (C-10), 39.7 (C-11), 30.9 (C-12), 23.2 (C-13), 23.0 (C-14), 23.9 (C-15), 28.5 (C-16), 15.5 (C-17), 17.3 (C-18), 15.4 (C-19), 66.9 (C-20); positive-ion HRESIMS m/z 371.1823 $[\text{M}+\text{Na}]^+$, (calcd for $\text{C}_{20}\text{H}_{28}\text{O}_5\text{Na}$, 371.1834).

Preparation of ingenol-5,20-acetonide (19).

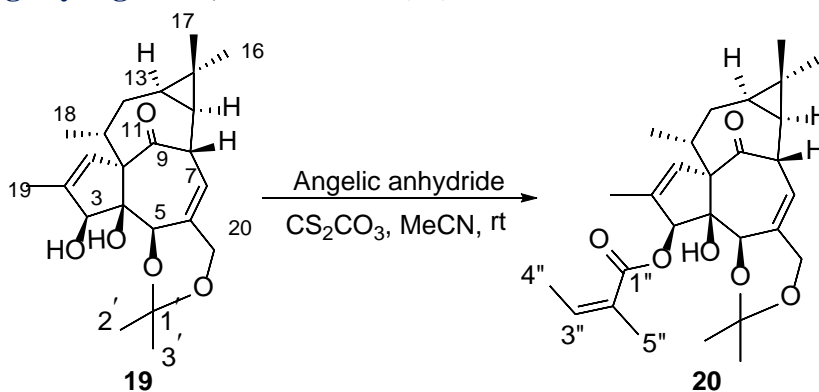


To a stirred solution of **10** (11 mg, 32 μmol) in acetone (6 mL) was added $p\text{-TsOH} \cdot \text{H}_2\text{O}$ (0.5 mg, 2.6 μmol) at room temperature for 2 h. After removal of solvent *in vacuo*, the residue passed through a Sep-

Pak C18 cartridge (Waters) using MeCN-H₂O (10:90 and 100:0, each 10.0 ml) as solvents. Then, CH₃CN-H₂O (100:0) eluate was purified by RP-HPLC (YMC Pack Pro C₁₈, MeCN-H₂O, 60:40, 5 mL/min) to give **19** (8.3 mg, 66.8%, *t_R* = 21.0 min).

Ingenol-5,20-acetonide (19): colorless oil; [α]_D²⁵ -26.1 (*c* 0.3, CHCl₃); UV (MeCN) λ _{max} (log ϵ): 204 (4.14) nm; IR (KBr) max: 2924, 1724, 1469, 1379, 1261, 1222, 1157, 1077 cm⁻¹; ¹H NMR (CDCl₃, 500 MHz) δ 5.90 (1H, q, *J* = 1.7 Hz, H-1), 4.23 (1H, s, H-3), 3.91 (1H, brs, H-5), 5.78 (1H, dq, *J* = 4.0, 1.7 Hz, H-7), 4.10 (1H, overlap, H-8), 2.47 (1H, m, H-11), 2.24 (1H, ddd, *J* = 15.8, 8.3, 3.1 Hz, H₂-12a), 1.76 (1H, ddd, *J* = 15.8, 6.3, 5.5 Hz, H₂-12b), 0.69 (1H, ddd, *J* = 8.3, 8.3, 6.3 Hz, H-13), 0.91 (1H, dd, *J* = 11.8, 8.3 Hz, H-14), 1.03 (3H, s, H₃-16), 1.10 (3H, s, H₃-17), 0.95 (3H, d, *J* = 7.2 Hz, H₃-18), 1.83 (3H, d, *J* = 1.7 Hz, H₃-19), 4.15 (1H, d, *J* = 12.6 Hz, H₂-20a), 4.10 (1H, d, *J* = 12.6 Hz, H₂-20b), 1.39 (3H, s, H₃-2'), 1.33 (3H, s, H₃-3'); ¹³C NMR (CDCl₃, 125 MHz) δ 129.5 (C-1), 136.1 (C-2), 80.0 (C-3), 83.3 (C-4), 73.8 (C-5), 139.6 (C-6), 122.3 (C-7), 44.0 (C-8), 207.6 (C-9), 72.9 (C-10), 38.3 (C-11), 31.2 (C-12), 23.6 (C-13), 23.0 (C-14), 23.8 (C-15), 28.6 (C-16), 15.6 (C-17), 17.8 (C-18), 15.6 (C-19), 64.2 (C-20), 100.6 (C-1'), 26.6 (C-2'), 21.1 (C-3'); positive-ion HRESIMS *m/z* 411.2147 [M+Na]⁺, (calcd for C₂₃H₃₂O₅Na, 411.2159).

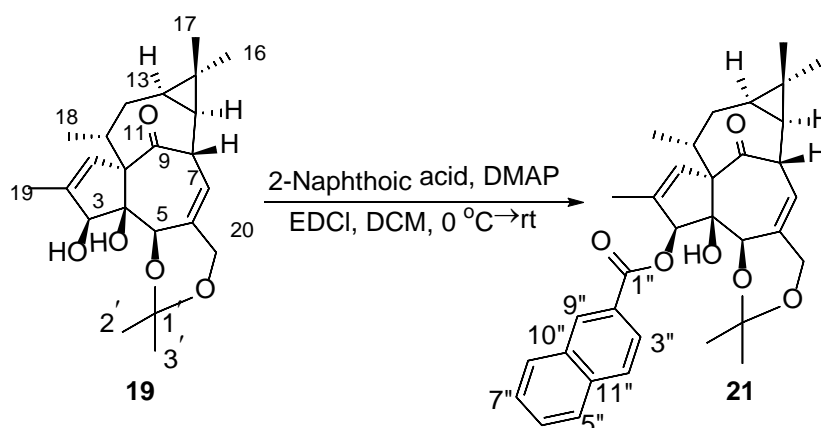
Preparation of 3-angeloylingenol-5,20-acetonide (**20**).



To a stirred solution of diol **19** (2.7 mg, 7 μ mol) in MeCN (2.0 ml) were added Cs₂CO₃ (9 mg, 27.6 μ mol) and angelic anhydride (5 μ L, 28 μ mol) at room temperature for 4 h. After removal of solvent *in vacuo*, the residue passed through a Sep-Pak C18 cartridge (Waters) using MeCN-H₂O (10:90 and 100:0, each 10 mL) as solvents to obtain **20** (3 mg, 95.7%, *t_R* = 21.0 min).

3-Angeloylingenol-5,20-acetonide (20): colorless oil; ^1H NMR (CDCl_3 , 500 MHz) δ 6.03 (1H, brq, $J = 1.5$ Hz, H-1), 5.64 (1H, s, H-3), 4.00 (1H, brs, H-5), 5.78 (1H, dq, $J = 4.0, 2.0$ Hz, H-7), 4.15 (1H, m, H-8), 2.59 (1H, m, H-11), 2.25 (1H, ddd, $J = 15.7, 8.9, 2.8$ Hz, CH_2 -12a), 1.73 (1H, ddd, $J = 15.7, 6.3, 5.5$ Hz, CH_2 -12b), 0.67 (1H, ddd, $J = 8.9, 8.3, 6.5$ Hz, H-13), 0.89 (1H, dd, $J = 12.0, 8.3$ Hz, H-14), 1.05 (3H, s, H_3 -16), 1.15 (3H, s, H_3 -17), 0.95 (3H, d, $J = 7.1$ Hz, H_3 -18), 1.76 (3H, d, $J = 1.7$ Hz, H_3 -19), 4.19 (1H, d, $J = 12.6$ Hz, H_2 -20a), 4.13 (1H, d, $J = 12.6$ Hz, H_2 -20b), 1.44 (3H, s, CH_3 -2'), 1.40 (3H, s, CH_3 -3'), 6.06 (1H, qq, $J = 7.1, 1.5$ Hz, H-3''), 2.00 (1H, dq, $J = 7.2, 1.5$ Hz, H-4''), 1.91 (3H, qui, $J = 1.5$ Hz, CH_3 -5''); ^{13}C NMR (CDCl_3 , 125 MHz) δ 132.5 (C-1), 136.8 (C-2), 81.5 (C-3), 84.1 (C-4), 74.0 (C-5), 136.2 (C-6), 122.2 (C-7), 43.6 (C-8), 208.0 (C-9), 72.3 (C-10), 37.5 (C-11), 30.9 (C-12), 23.2 (C-13), 22.8 (C-14), 23.9 (C-15), 28.3 (C-16), 15.4 (C-17), 17.2 (C-18), 15.5 (C-19), 64.2 (C-20), 100.5 (C-1'), 26.5 (C-2'), 21.1 (C-3'), 168.5 (C-1''), 128.1 (C-2''), 138.2 (C-3''), 15.5 (C-4''), 20.6 (C-5'').

Preparation of 3-(2-naphthoyl)ingenol-5,20-acetonide (21).



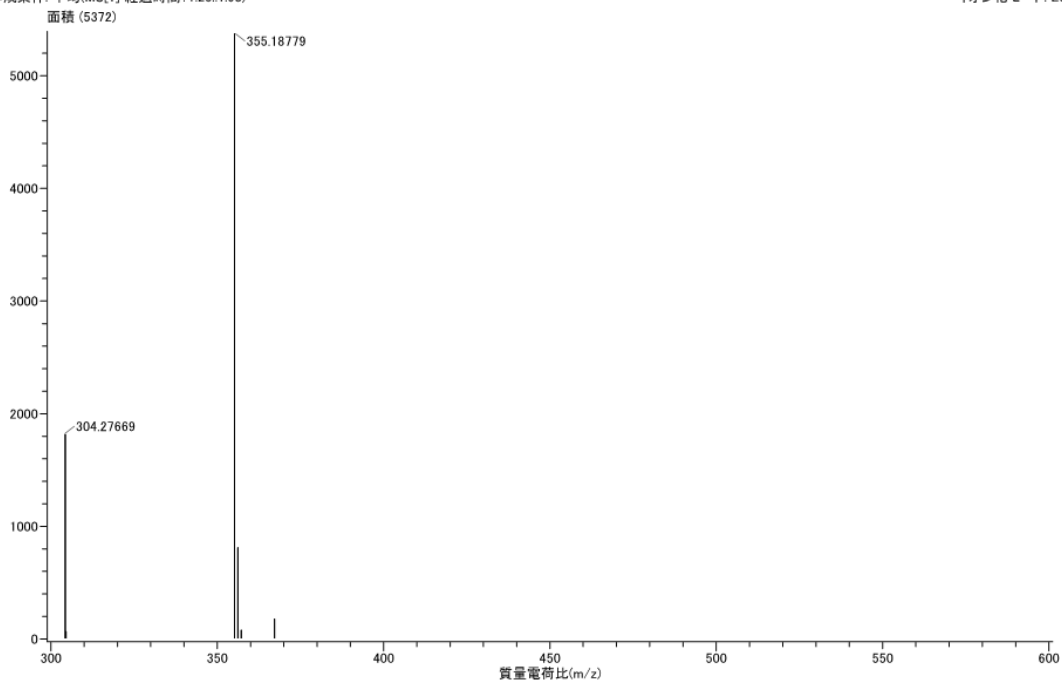
To a stirred solution of diol **19** (2.7 mg, 7 μmol) in dehydrated DCM (3 mL) were added DMAP (3 mg, 25 μmol) and 2-naphthoic acid (5 mg, 29 μmol), and chilled to 0 $^\circ\text{C}$. A solution of EDCI (4 mg, 20 μmol) dissolved in dehydrated DCM (0.5 mL) was added dropwise, and the reaction mixture was stirred at room temperature for 4 h under protection of argon. After removal of solvent *in vacuo*, the residue was purified by RP-HPLC (YMC Pack Pro C_{18} , $\text{MeCN-H}_2\text{O}$, 80:20, 5.0 mL/min) to give **21** (2.6 mg, 68.6%, $t_R = 28.5$ min).

3-(2-naphthoyl)ingenol-5,20-acetonide (21): colorless oil; ^1H NMR (CDCl_3 , 500 MHz) δ 6.14 (1H,

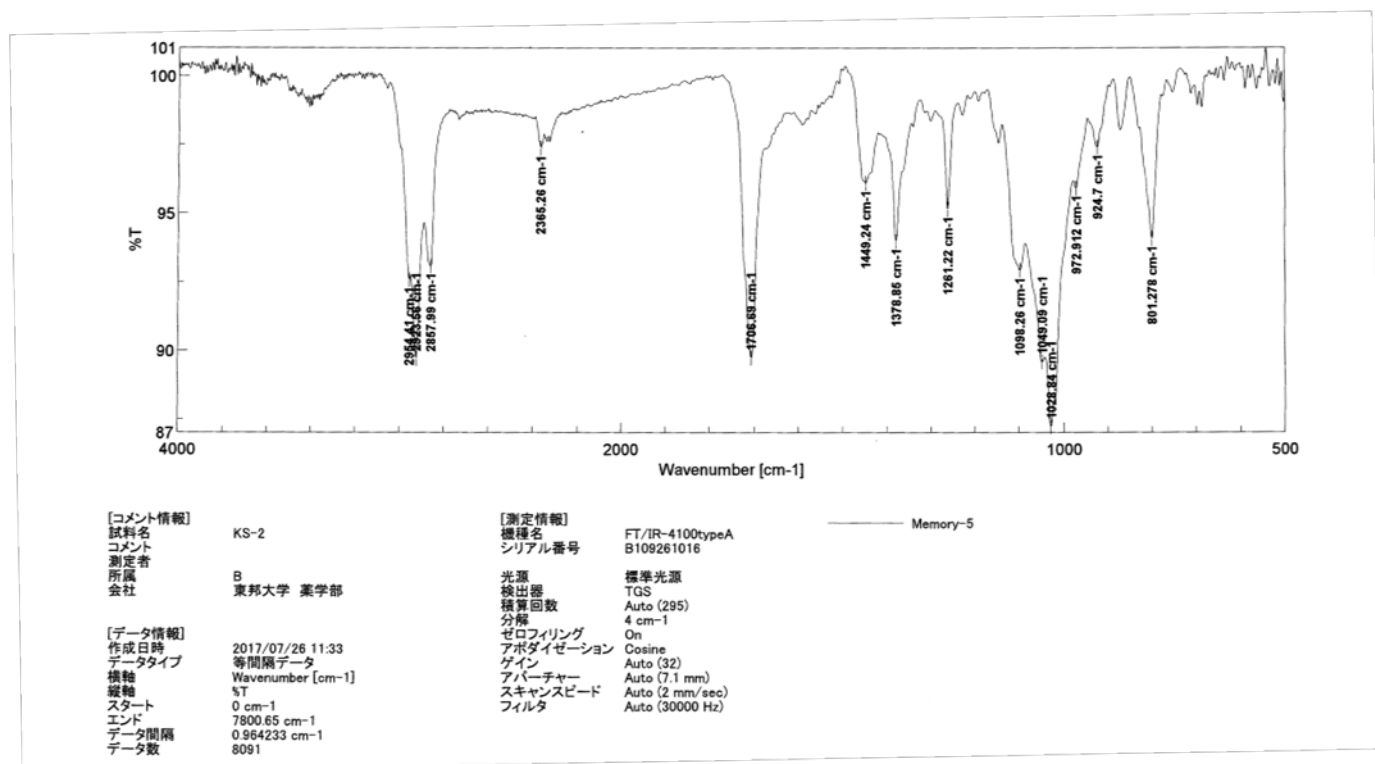
brq, $J = 1.5$ Hz, H-1), 5.84 (1H, s, H-3), 4.08 (1H, brs, H-5), 5.78 (1H, dq, $J = 4.0, 1.7$ Hz, H-7), 4.18 (1H, ddq, $J = 11.7, 4.0, 2.3$ Hz, H-8), 2.74 (1H, m, H-11), 2.26 (1H, ddd, $J = 15.8, 8.9, 3.2$ Hz, H₂-12a), 1.73 (1H, ddd, $J = 15.8, 8.3, 6.3$ Hz, H₂-12b), 0.67 (1H, ddd, $J = 8.9, 8.6, 6.0$ Hz, H-13), 0.91 (1H, dd, $J = 11.8, 8.3$ Hz, H-14), 1.03 (3H, s, H₃-16), 1.05 (3H, s, H₃-17), 1.08 (3H, d, $J = 7.1$ Hz, H₃-18), 1.80 (3H, d, $J = 1.2$ Hz, H₃-19), 4.23 (1H, d, $J = 12.6$ Hz, H₂-20a), 4.15 (1H, d, $J = 12.6$ Hz, H₂-20b), 1.50 (3H, s, H₃-2'), 1.47 (3H, s, H₃-3'), 8.03 (1H, dd, $J = 8.6, 1.5$ Hz, H-3''), 7.89 (1H, d, $J = 8.6$ Hz, H-4''), 7.87 (1H, brd, $J = 8.0$ Hz, H-5''), 7.58 (1H, ddd, $J = 8.0, 6.9, 1.2$ Hz, H-6''), 7.53 (1H, ddd, $J = 8.0, 6.9, 1.2$ Hz, H-7''), 7.95 (1H, brd, $J = 8.0$ Hz, H-8''), 8.58 (1H, brs, H-9''); ¹³C NMR (CDCl₃, 125 MHz) δ 132.7 (C-1), 136.5 (C-2), 82.7 (C-3), 84.3 (C-4), 74.1 (C-5), 135.8 (C-6), 124.2 (C-7), 43.4 (C-8), 207.5 (C-9), 72.4 (C-10), 37.9 (C-11), 31.3 (C-12), 23.6 (C-13), 23.0 (C-14), 24.0 (C-15), 28.5 (C-16), 15.5 (C-17), 17.6 (C-18), 15.6 (C-19), 64.4 (C-20), 100.5 (C-1'), 26.8 (C-2'), 20.9 (C-3'), 167.6 (C-1''), 127.5 (C-2''), 125.3 (C-3''), 128.3 (C-4''), 127.7 (C-5''), 128.4 (C-6''), 126.7 (C-7''), 129.4 (C-8''), 131.3 (C-9''), 132.5 (C-10''), 135.6 (C-11'').

測定データ名: KS-2
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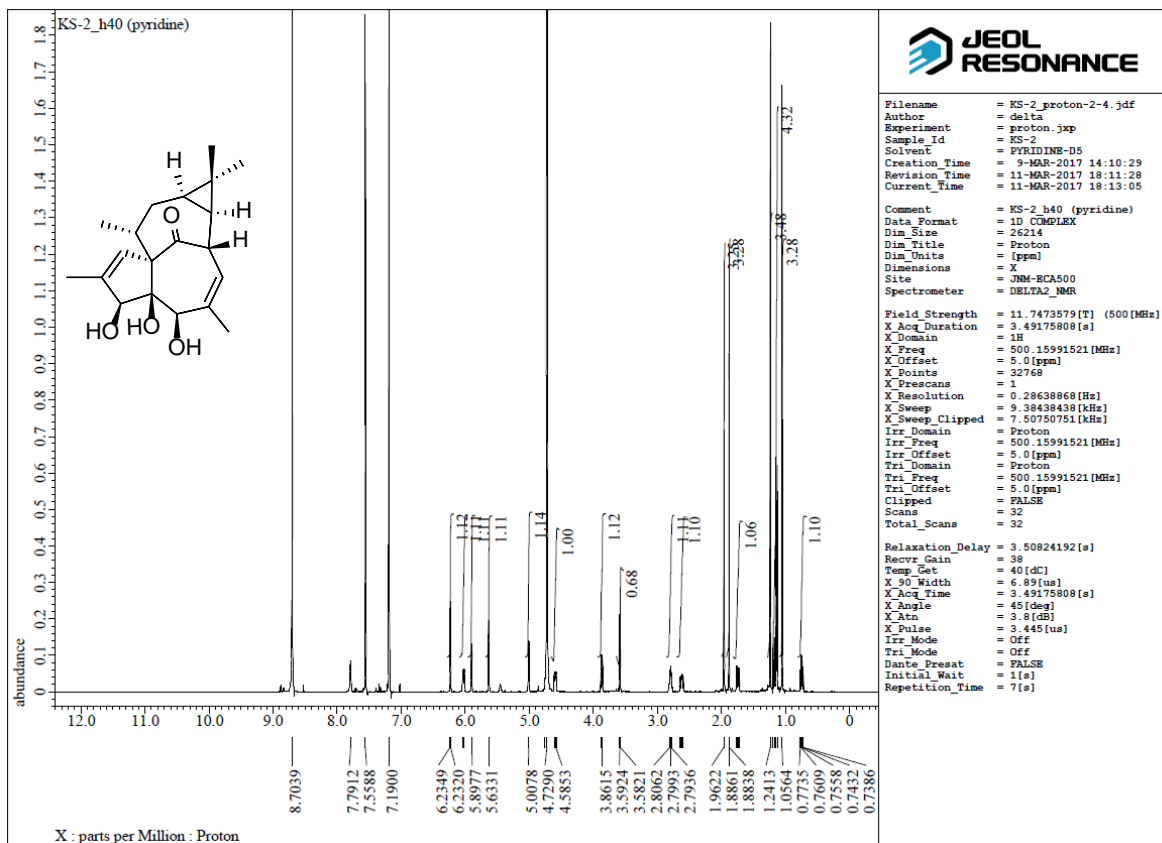
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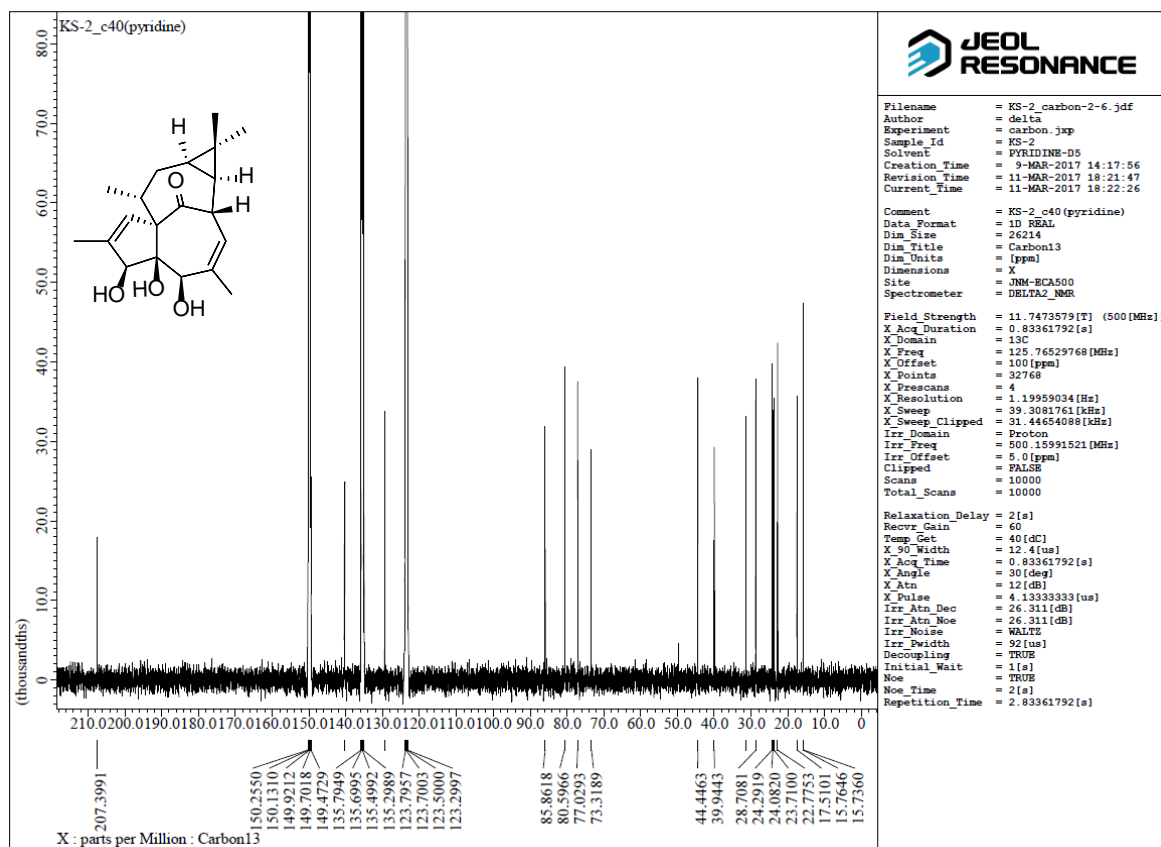
The HRESIMS spectrum of compound 9



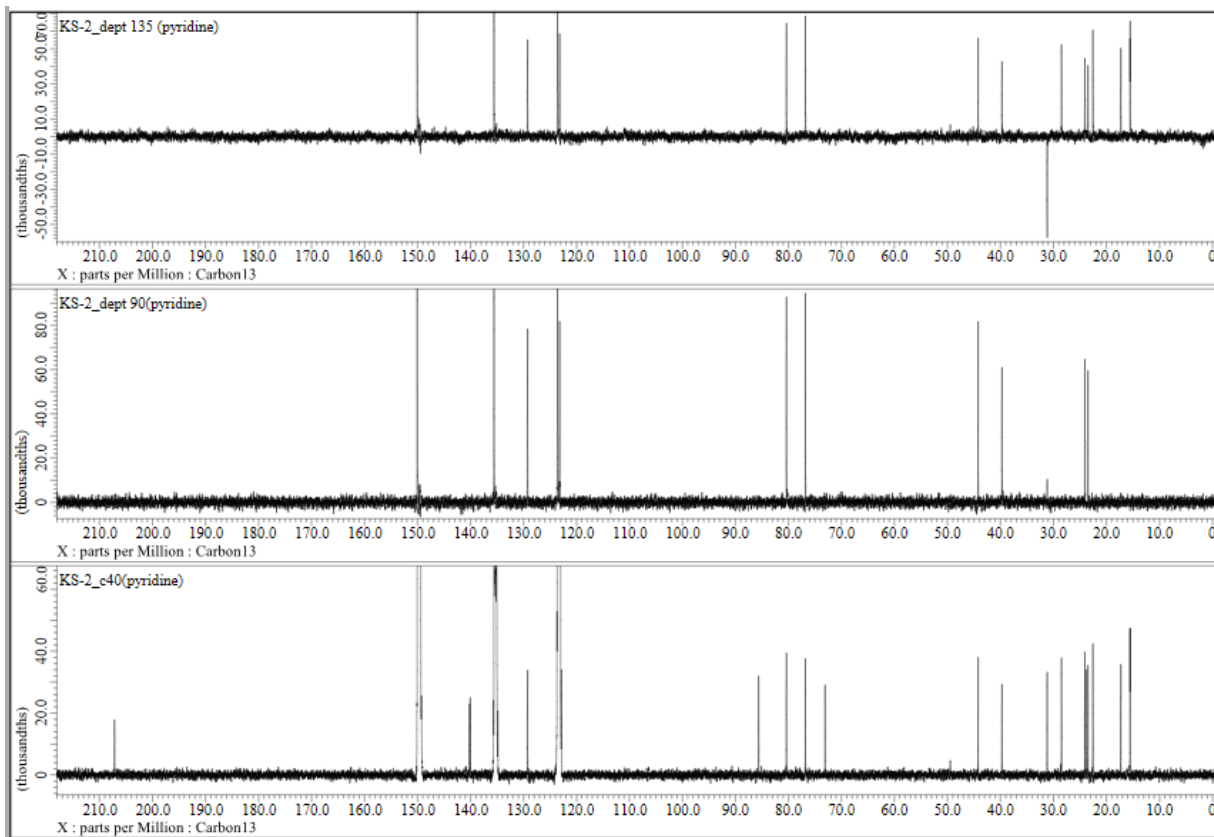
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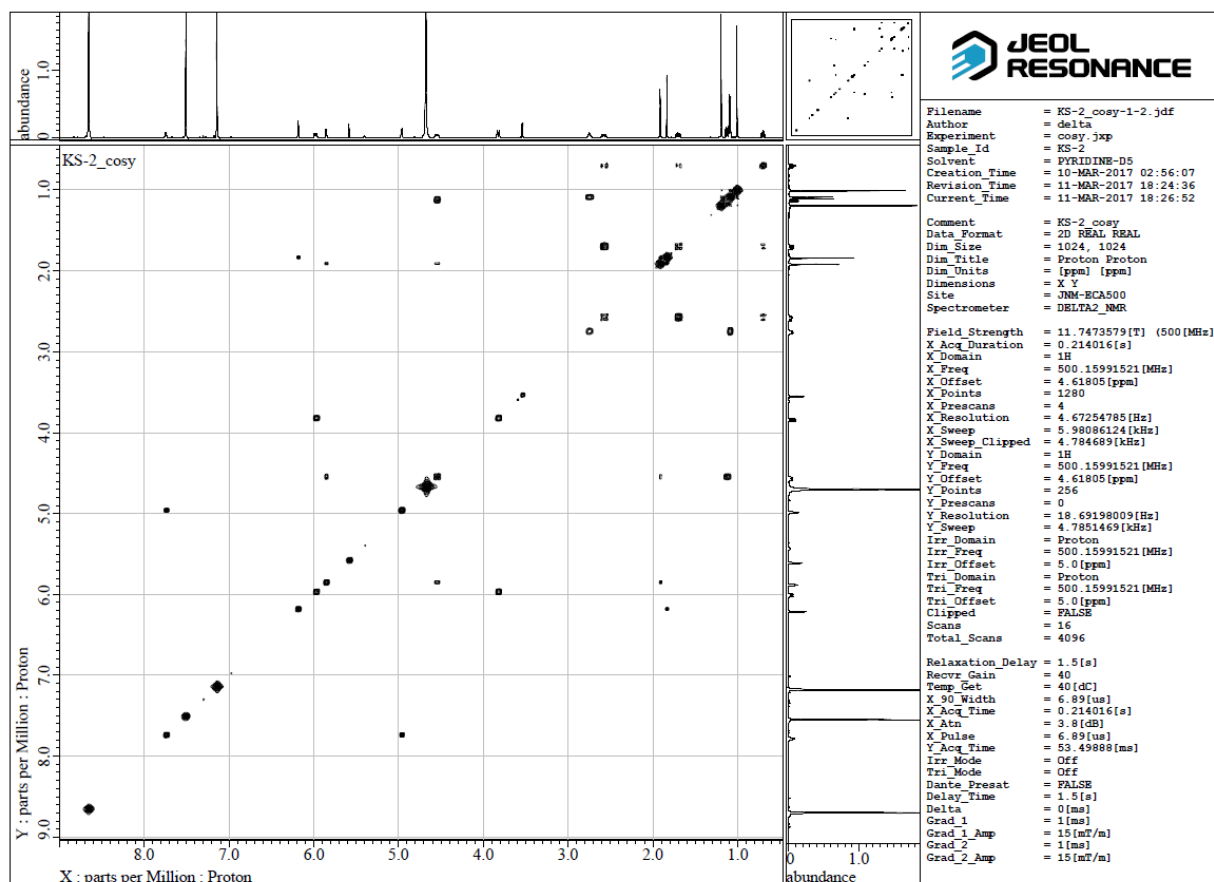
The ^1H spectrum of compound 9



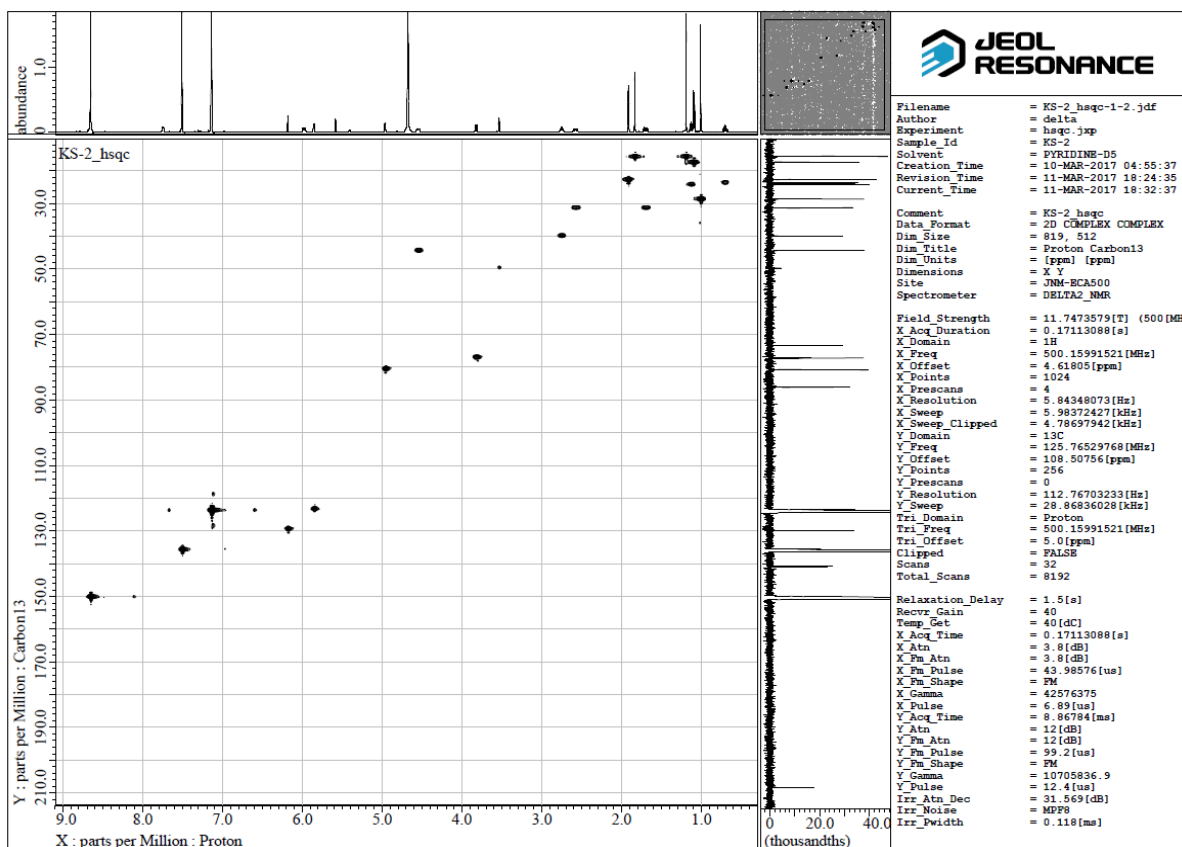
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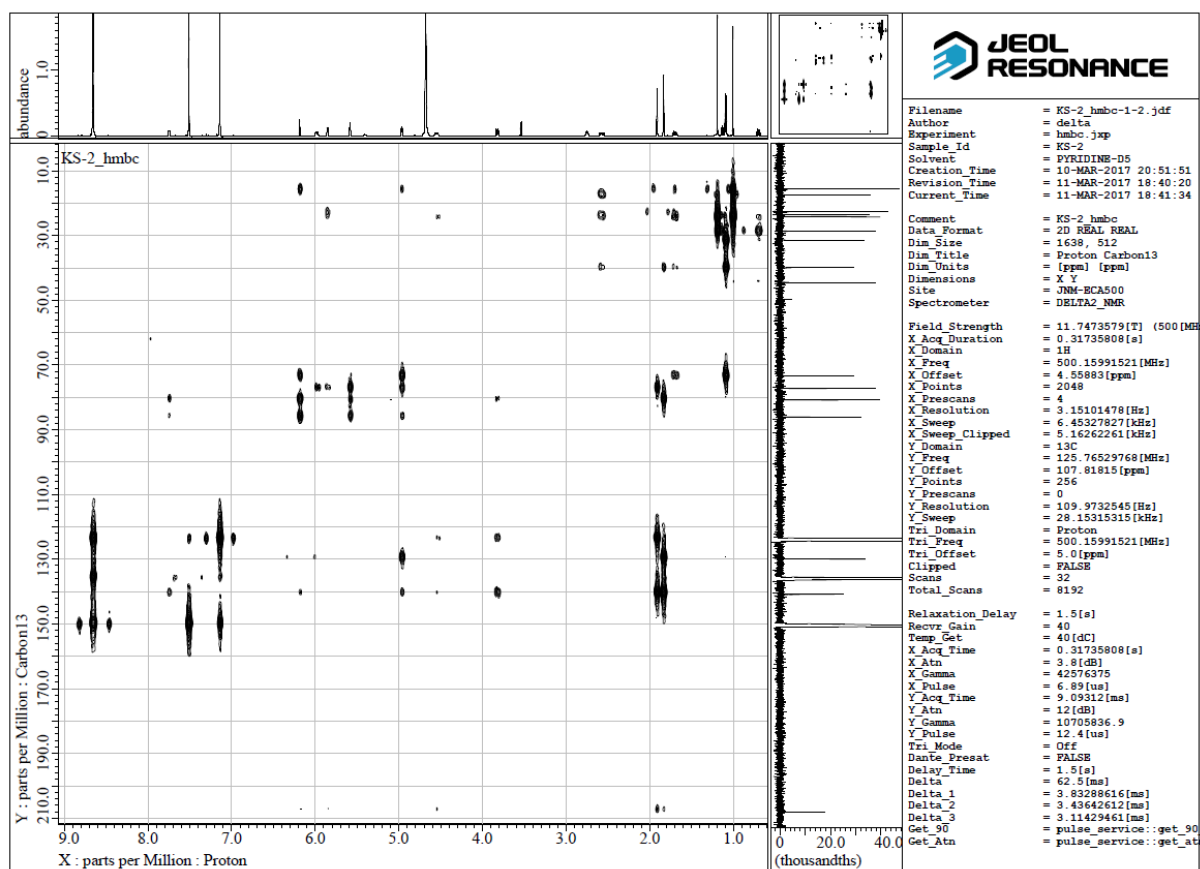
The DEPT spectrum of compound 9



The DQF_COSY spectrum of compound 9



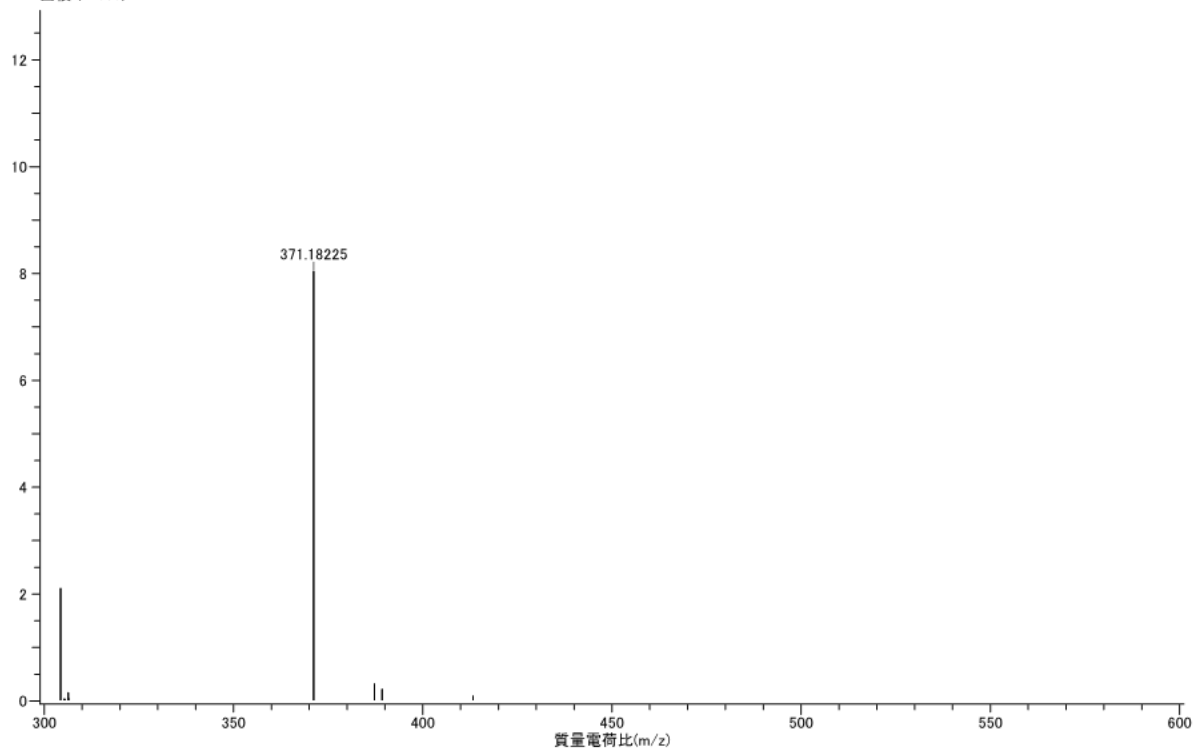
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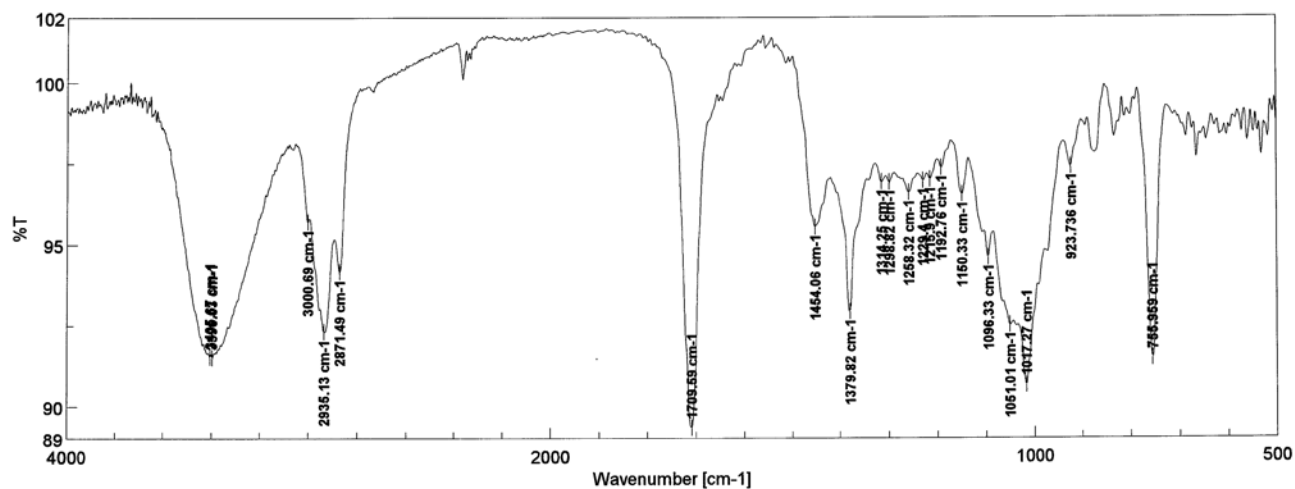
The HMBC spectrum of compound 9

測定データ名: KS-7.02
 作成条件: 平均(MS[1] 経過時間: 0.47..0.86)
 x10³ 面積 (12868)

実験日時: 2017/10/13 21:25:51
 イオン化モード: ESI+



The HRESIMS spectrum of compound **10**



[コメント情報]
 試料名
 コメント
 測定者
 所属
 会社

KS-7
 B
 東邦大学 薬学部

[測定情報]
 機種名
 シリアル番号

FT/IR-4100typeA
 B109261016

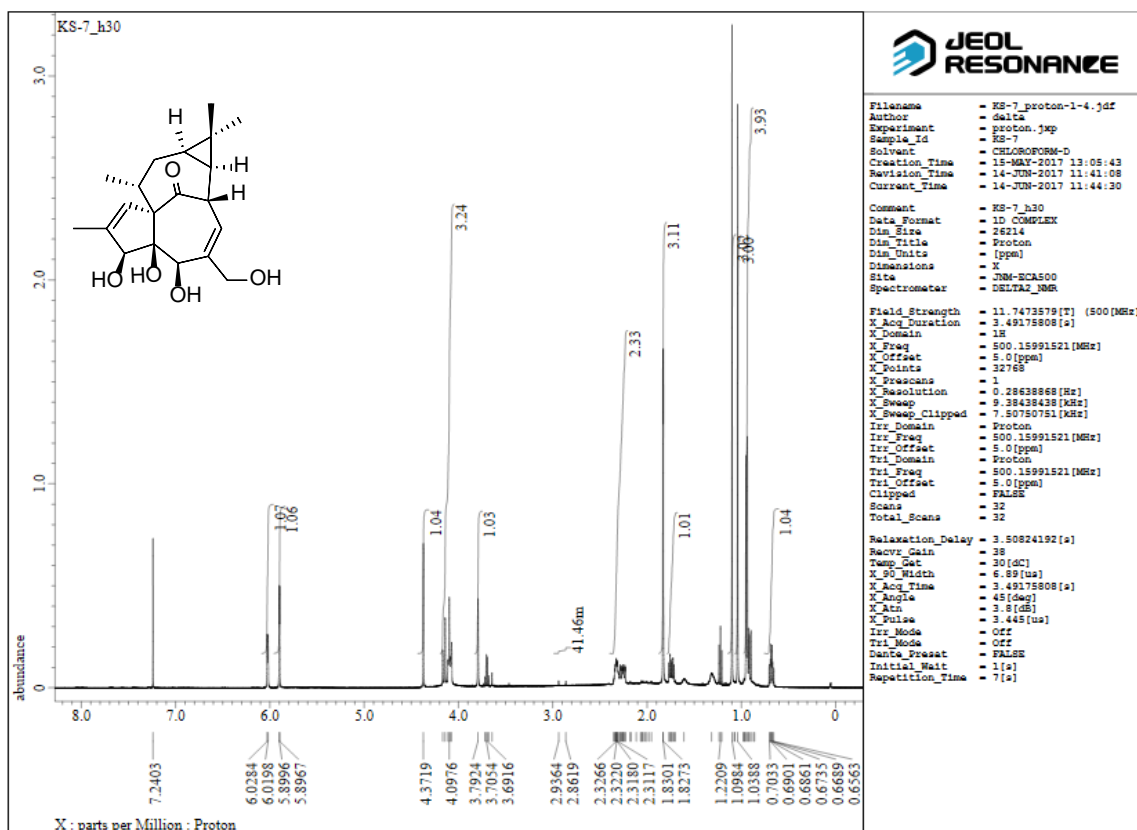
光源 標準光源
 検出器 TGS
 積算回数 Auto (186)
 分解 4 cm⁻¹
 ゼロファイリング On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャ Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

Memory-2

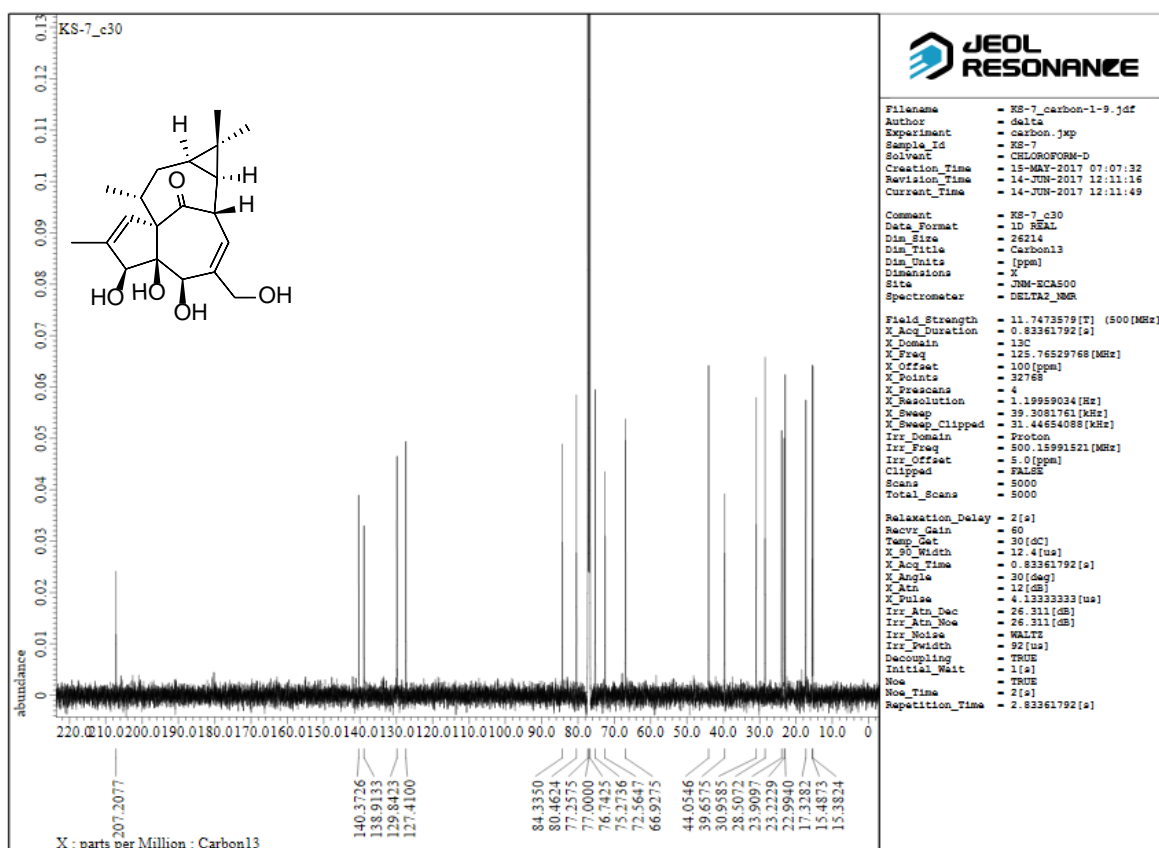
[データ情報]
 作成日時
 データタイプ
 横軸
 縦軸
 スタート
 エンド
 データ間隔
 データ数

2017/07/26 14:22
 等間隔データ
 Wavenumber [cm⁻¹]
 %T
 0 cm⁻¹
 7800.65 cm⁻¹
 0.964233 cm⁻¹
 8091

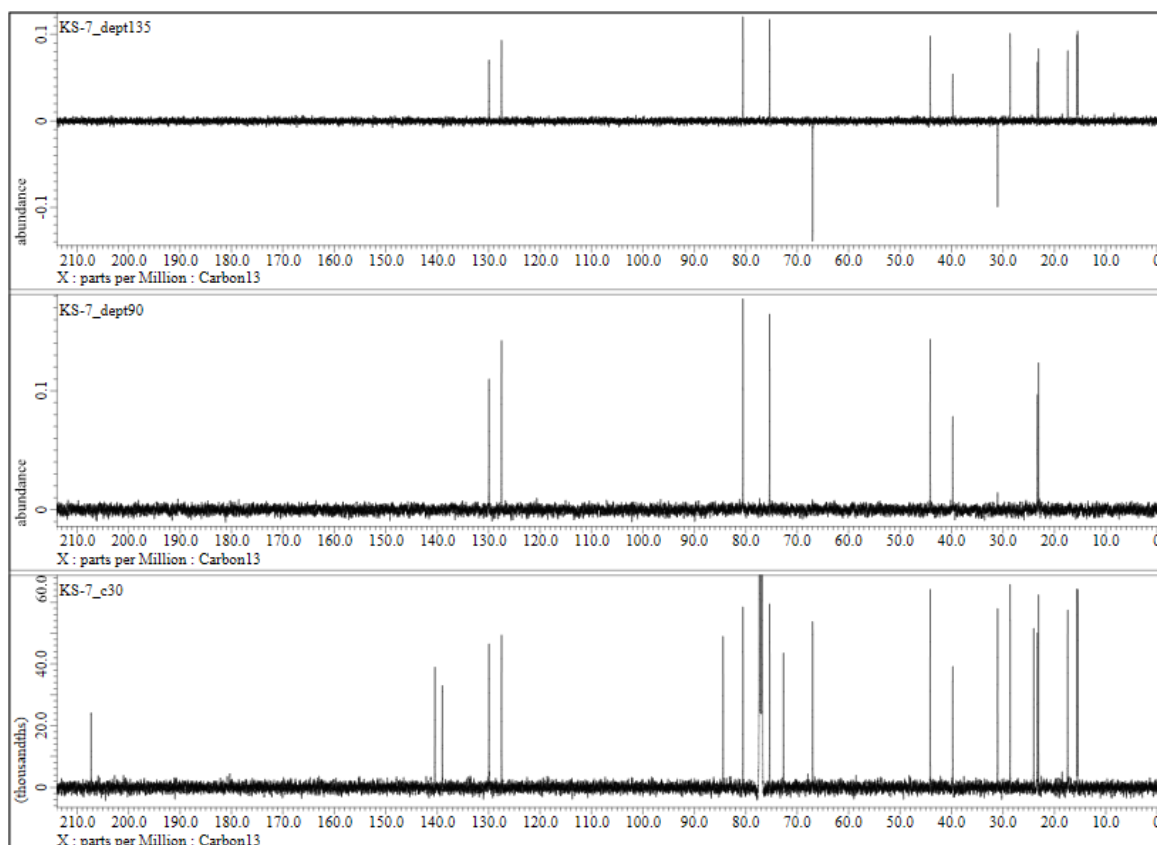
The IR spectrum of compound **10**



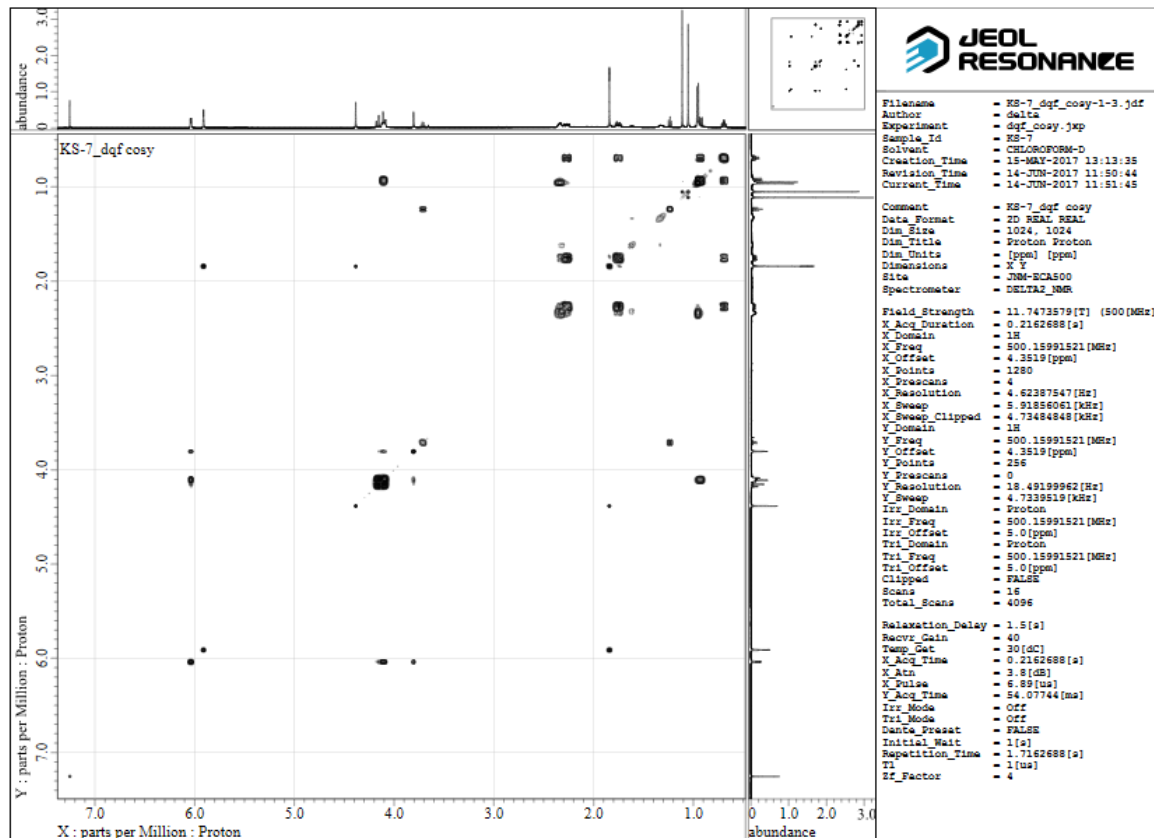
The ^1H spectrum of compound 10



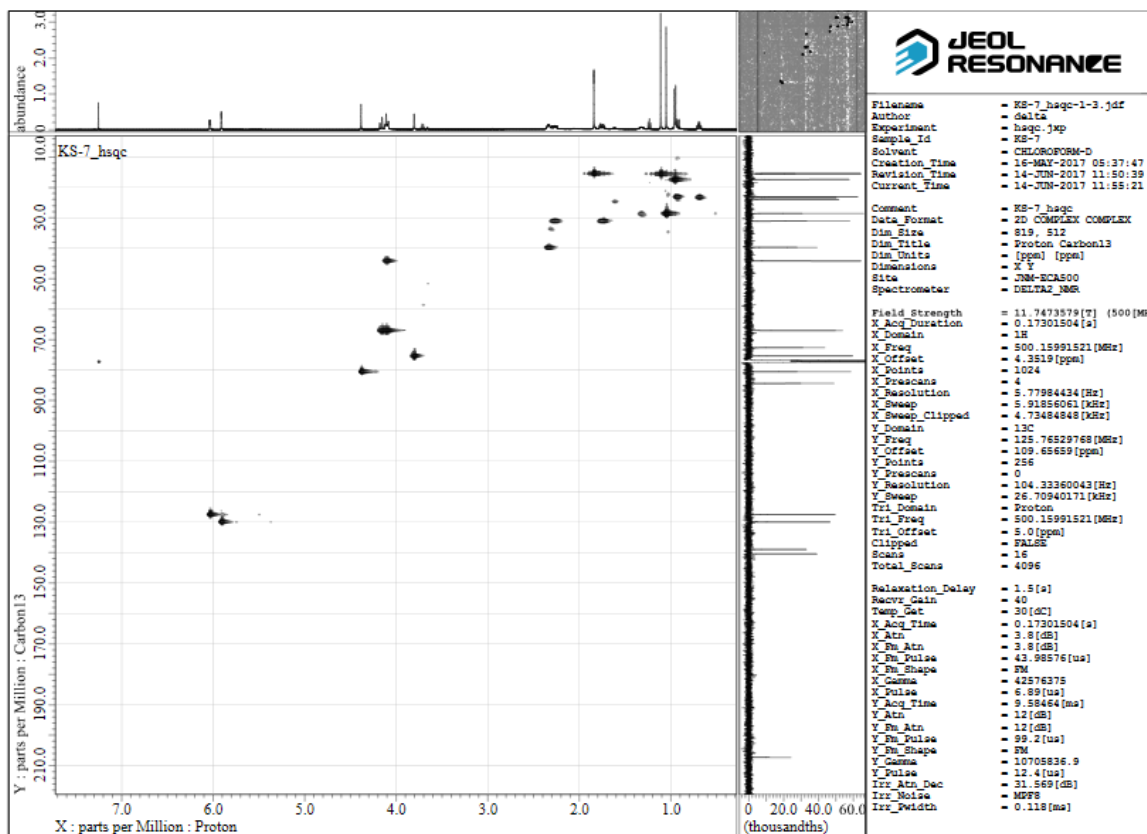
The ^{13}C spectrum of compound 10



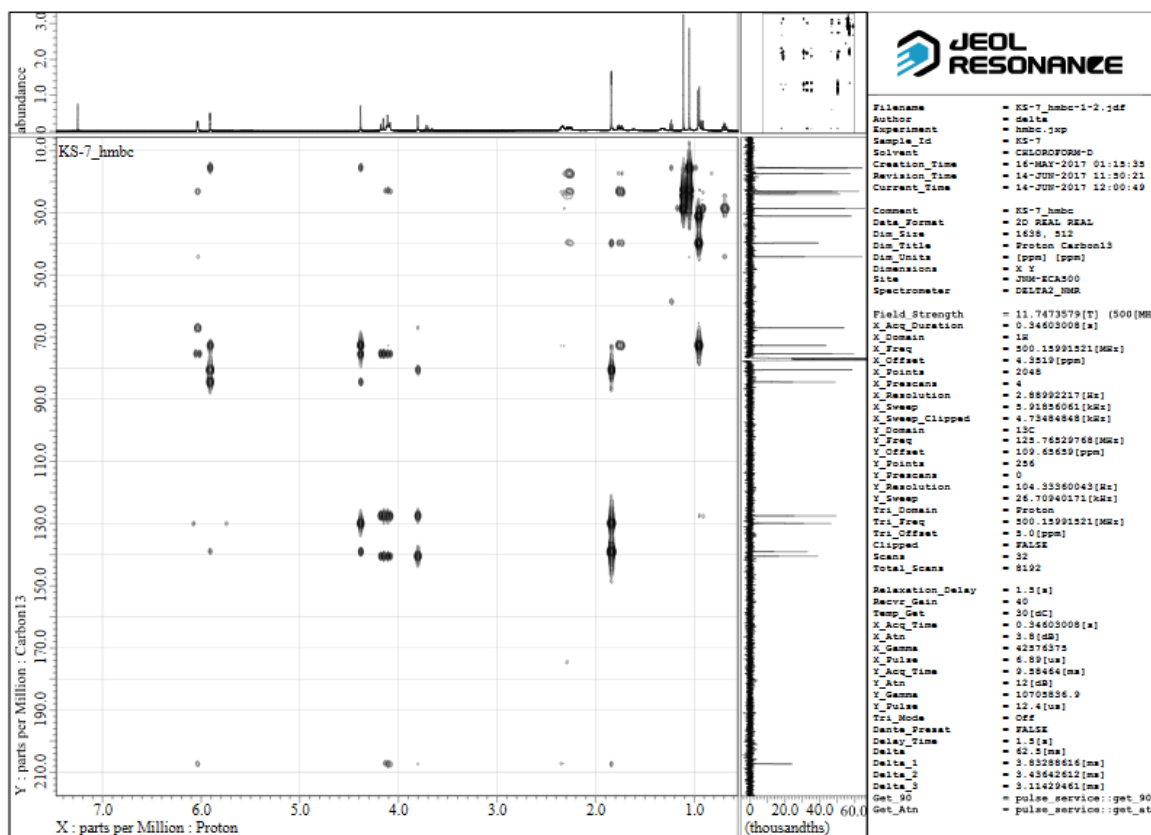
The DEPT spectrum of compound 10



The DQF-COSY spectrum of compound 10



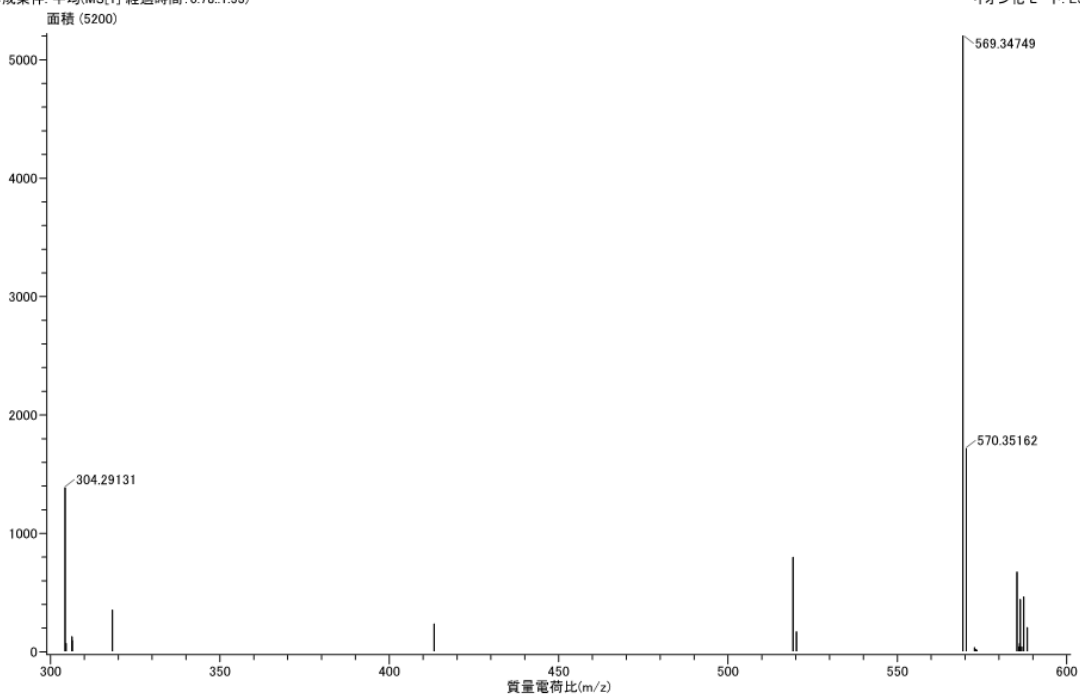
The HSQC spectrum of compound 10



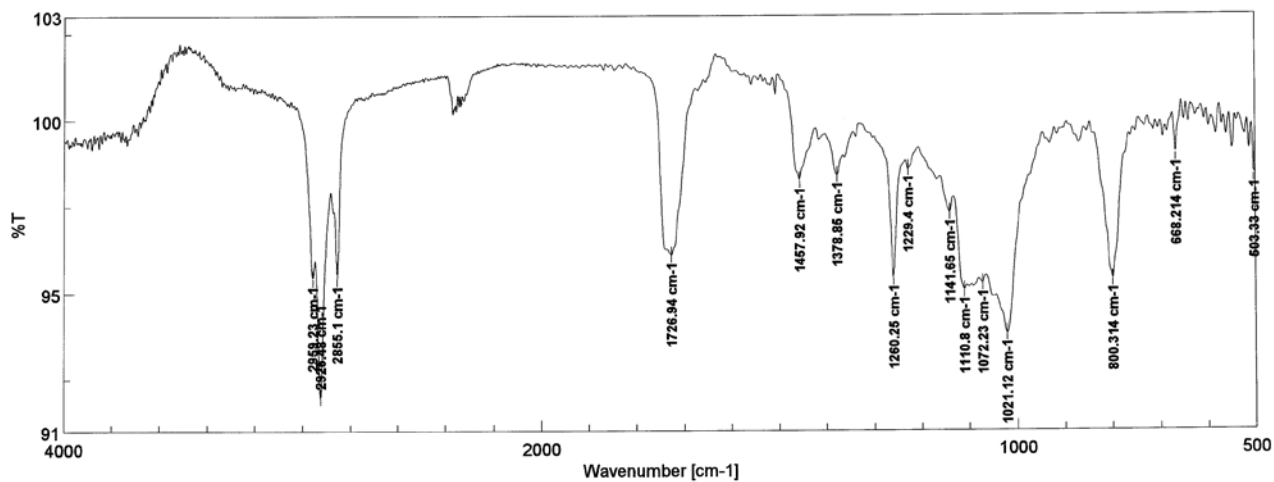
The HMBC spectrum of compound 10

測定データ名: ks-1
 作成条件: 平均(MS[1]) 経過時間: 0.78..1.53

実験日時: 2017/10/07 15:50:45
 イオン化モード: ESI+



The HRESIMS spectrum of compound **11**



[コメント情報]
 試料名 KS-1
 コメント
 測定者 B
 所属 東邦大学 薬学部
 会社

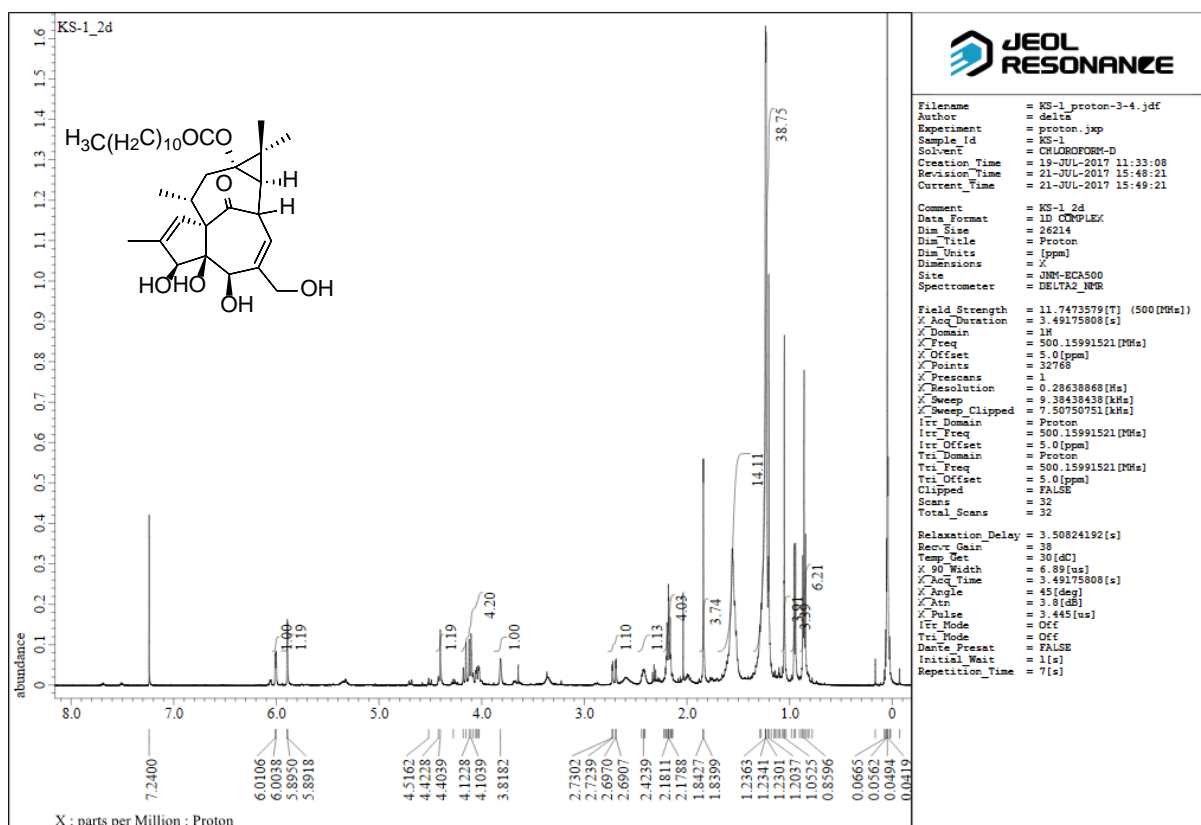
[データ情報]
 作成日時 2017/07/26 11:03
 データタイプ 等間隔データ
 横軸 Wavenumber [cm-1]
 縦軸 %T
 スタート 0 cm-1
 エンド 7800.65 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

[測定情報] FT/IR-4100typeA
 機種名 B109261016
 シリアル番号

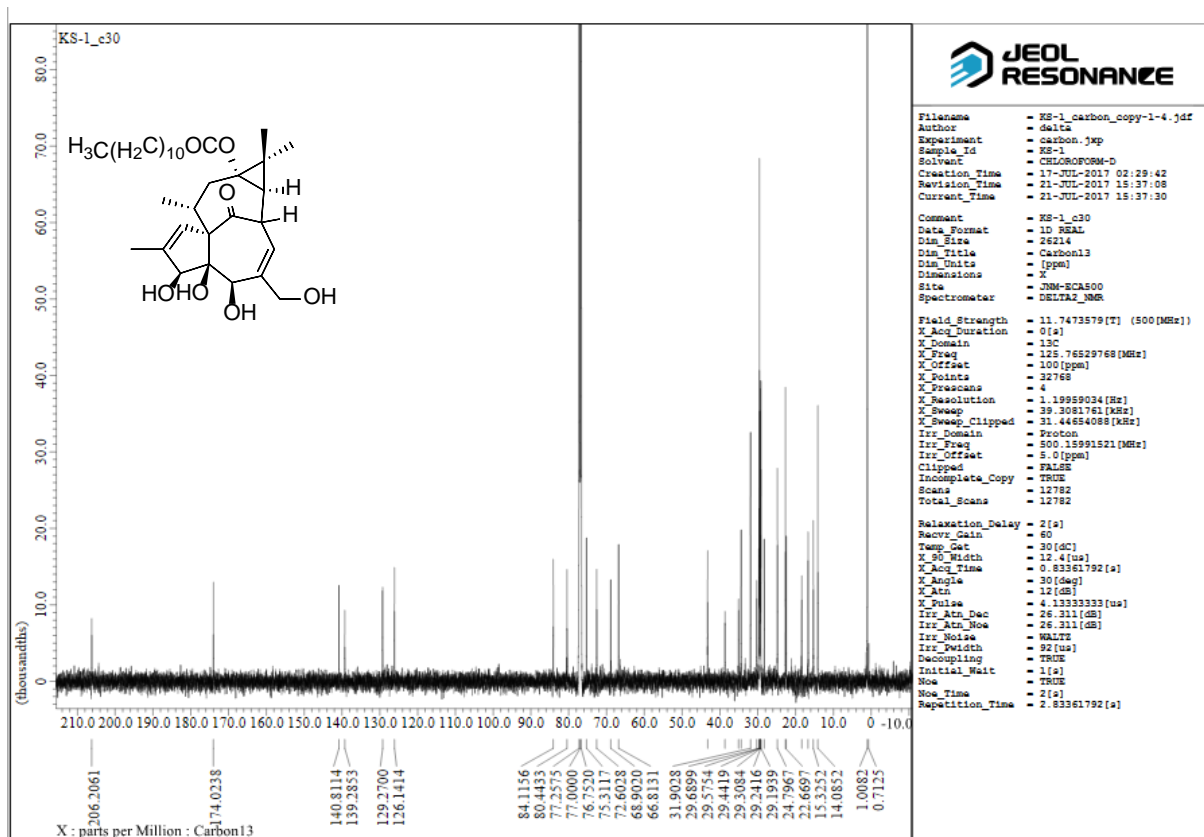
光源 標準光源
 検出器 TGS
 積算回数 Auto (206)
 分解 4 cm-1
 ゼロフィリング On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャー Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

KS-1,2

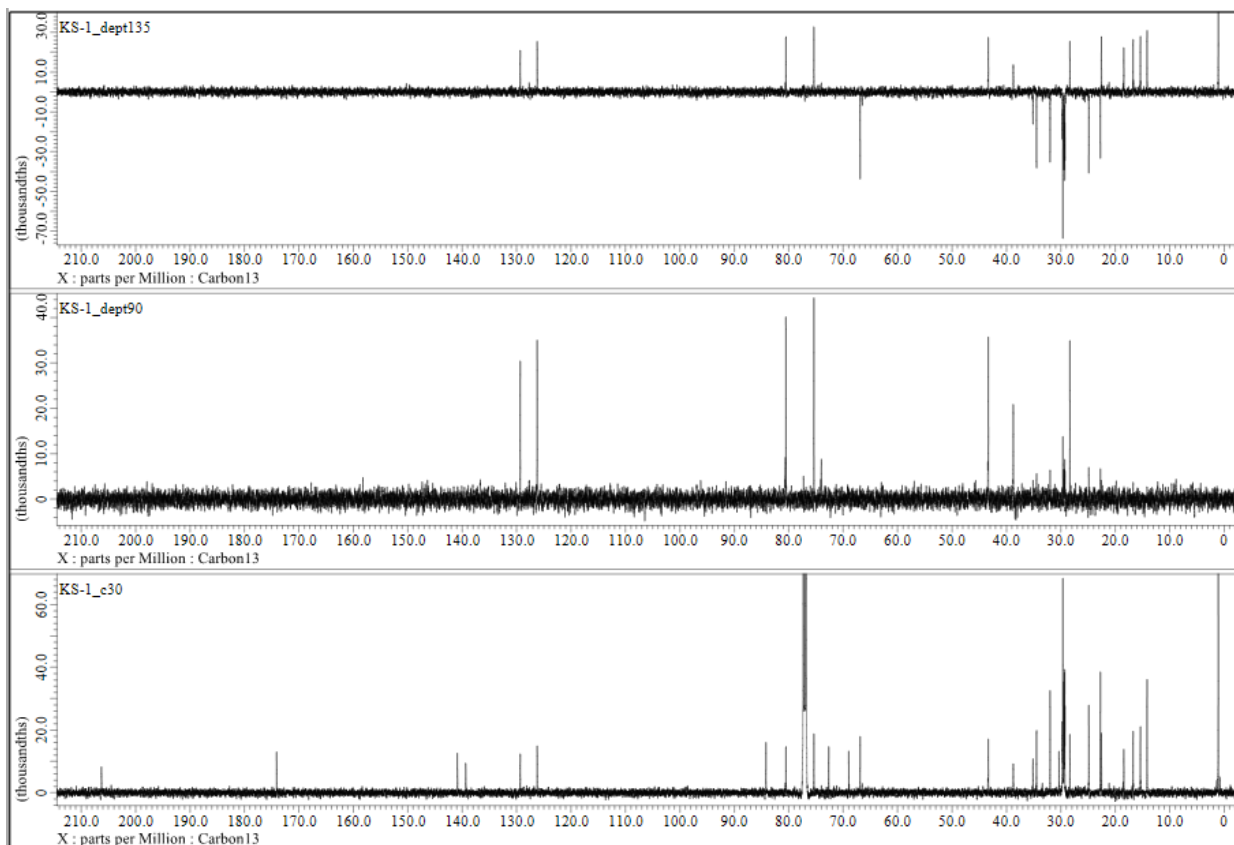
The IR spectrum of compound **11**



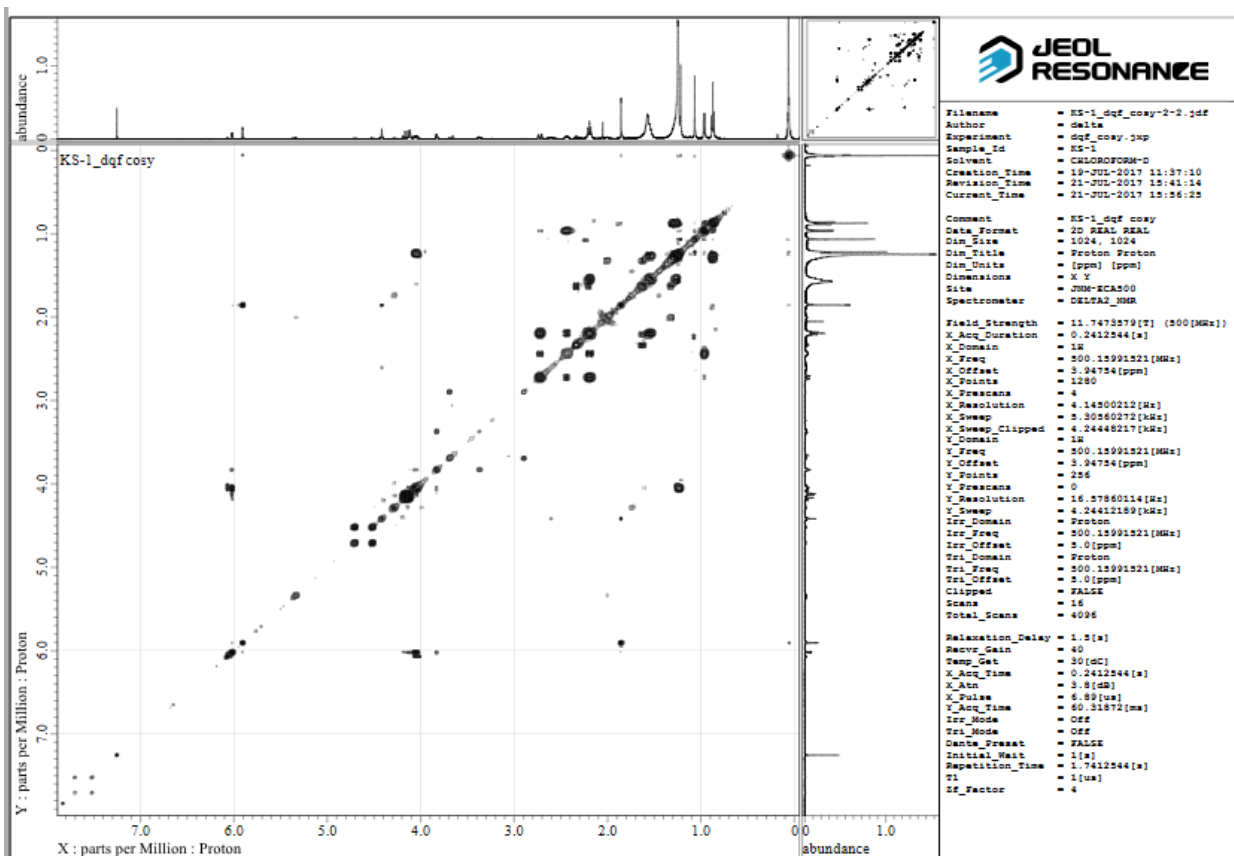
The ^1H spectrum of compound **11**



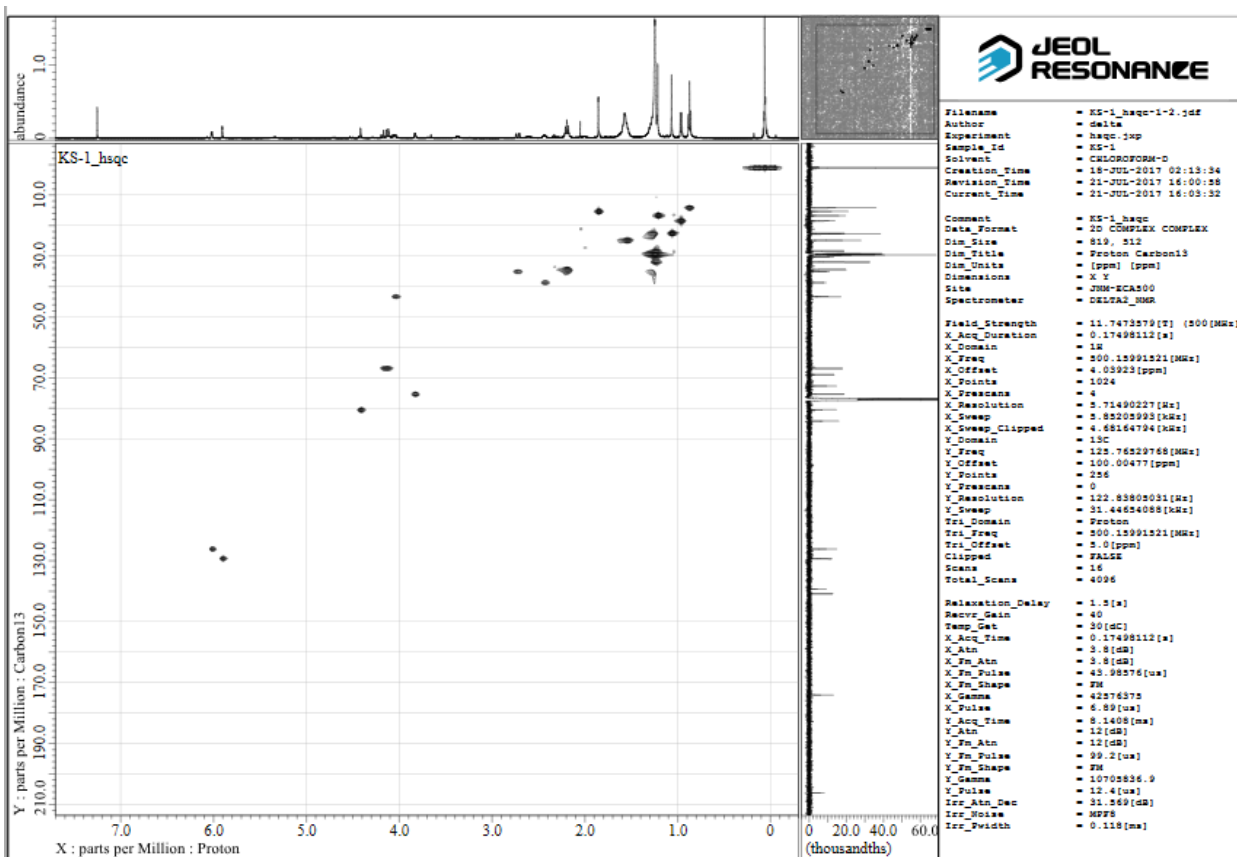
The ^{13}C spectrum of compound **11**



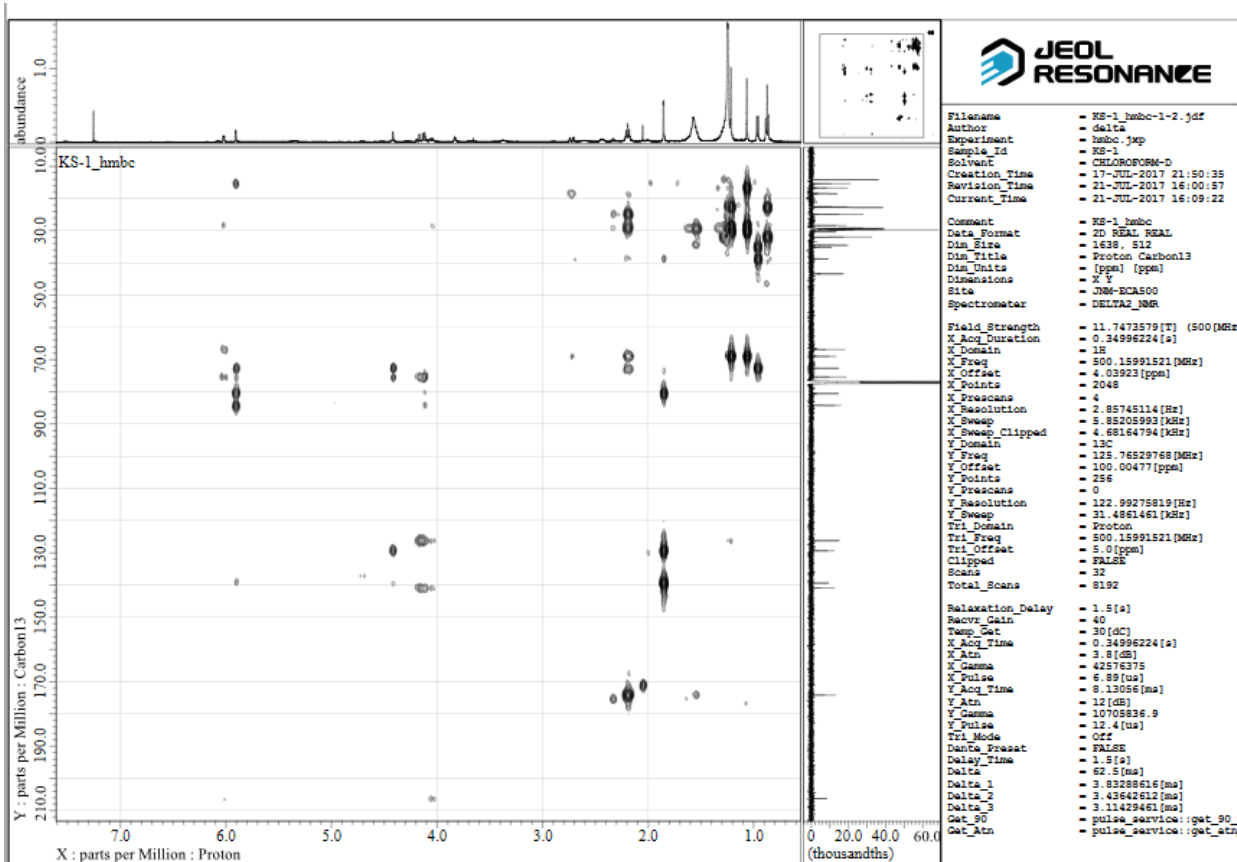
The DEPT spectrum of compound 11



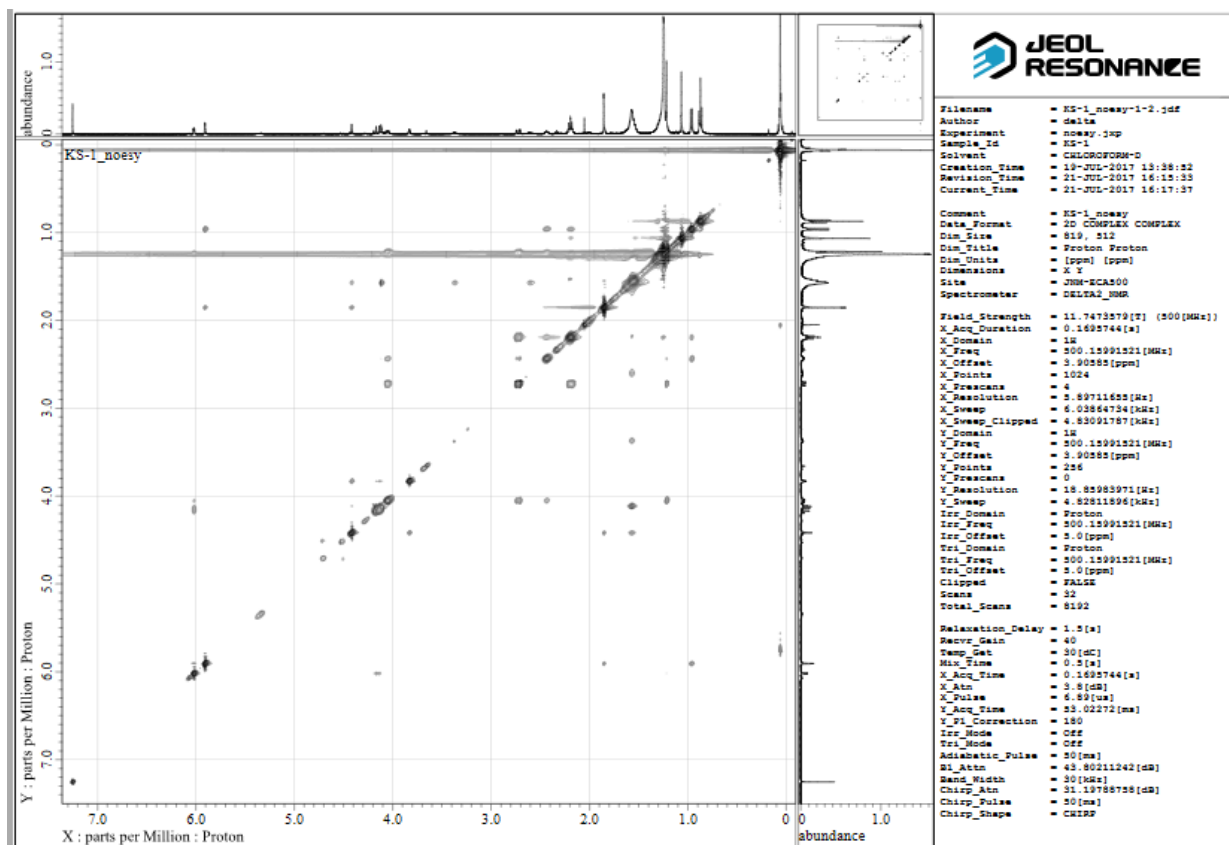
The DQF-COSY spectrum of compound 11



The HSQC spectrum of compound **11**

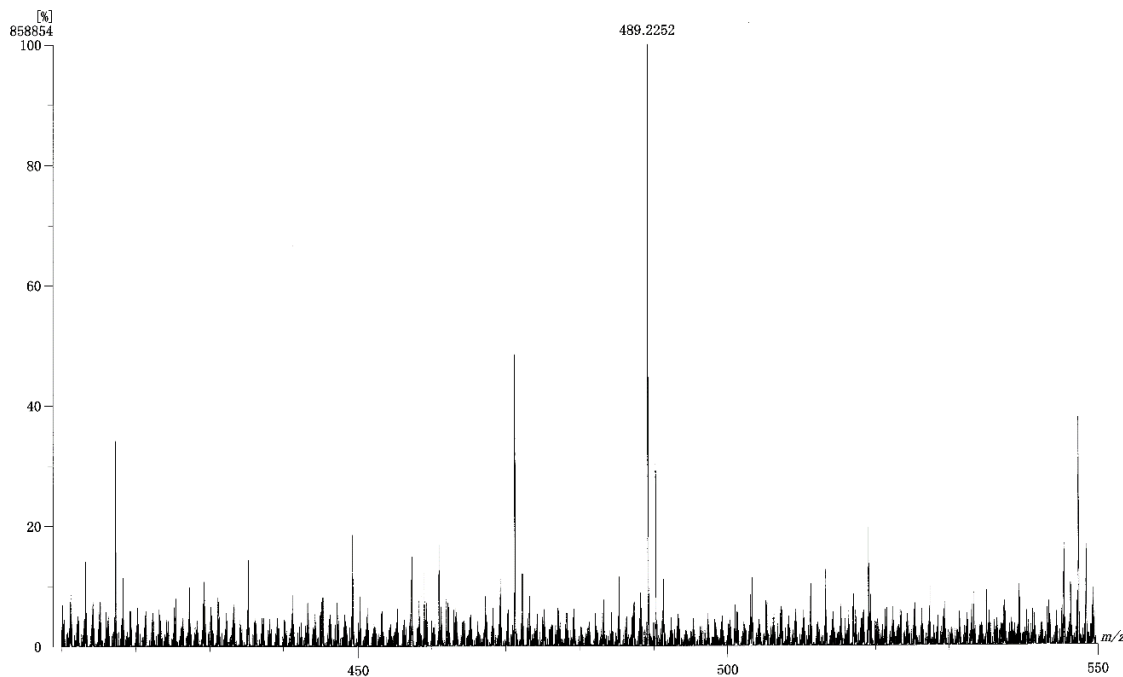


The HMBC spectrum of compound **11**

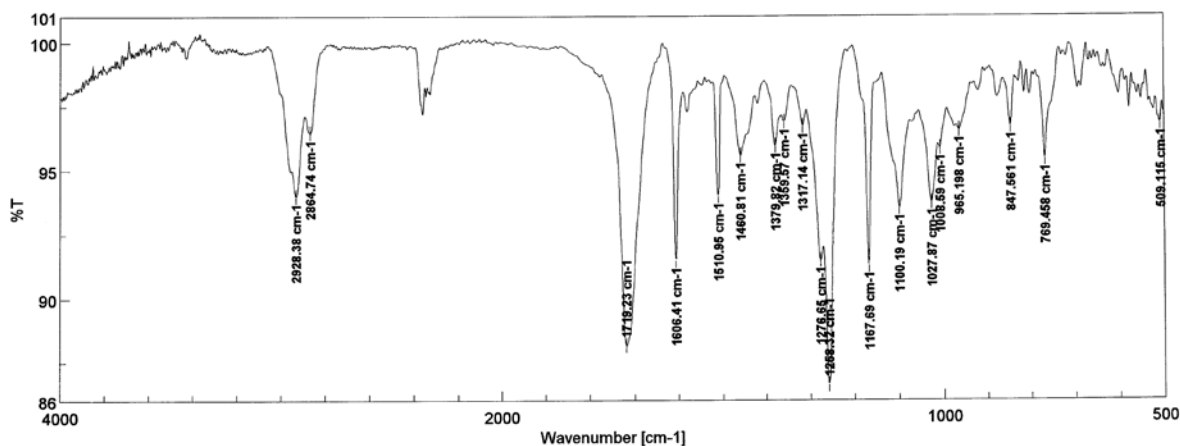


The NOESY spectrum of compound **11**

[Mass Spectrum]
 Data : KS-6+Na-FABpHR2-NBA Date : 22-Aug-2017 17:01
 Instrument : MSStation
 Sample : KS-6
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [EP-Linear]
 RT : 3.69 min Scan# : 14 Temp : 3276.7 deg.C
 BP : m/z 499.2252 Int. : 81.91 (858854)
 Output m/z range : 410 to 550 Cut Level : 0.00 %

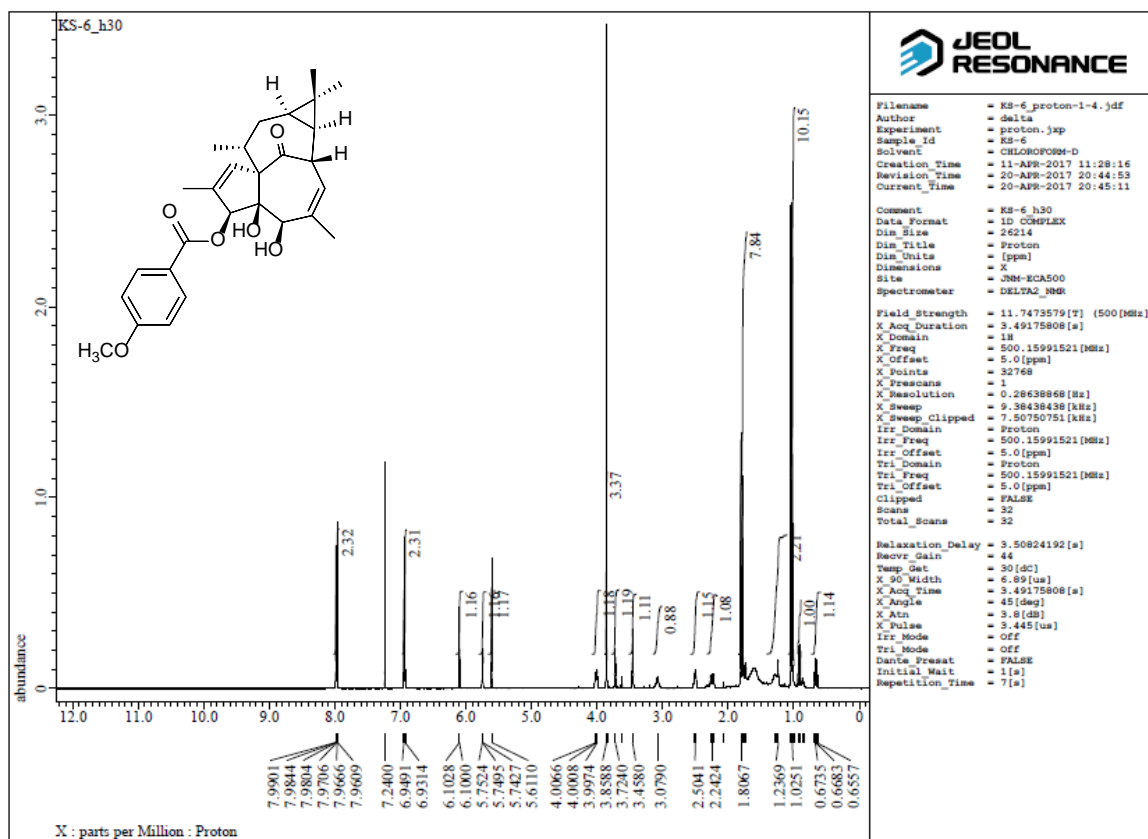


The HRFABMS spectrum of compound **12a**

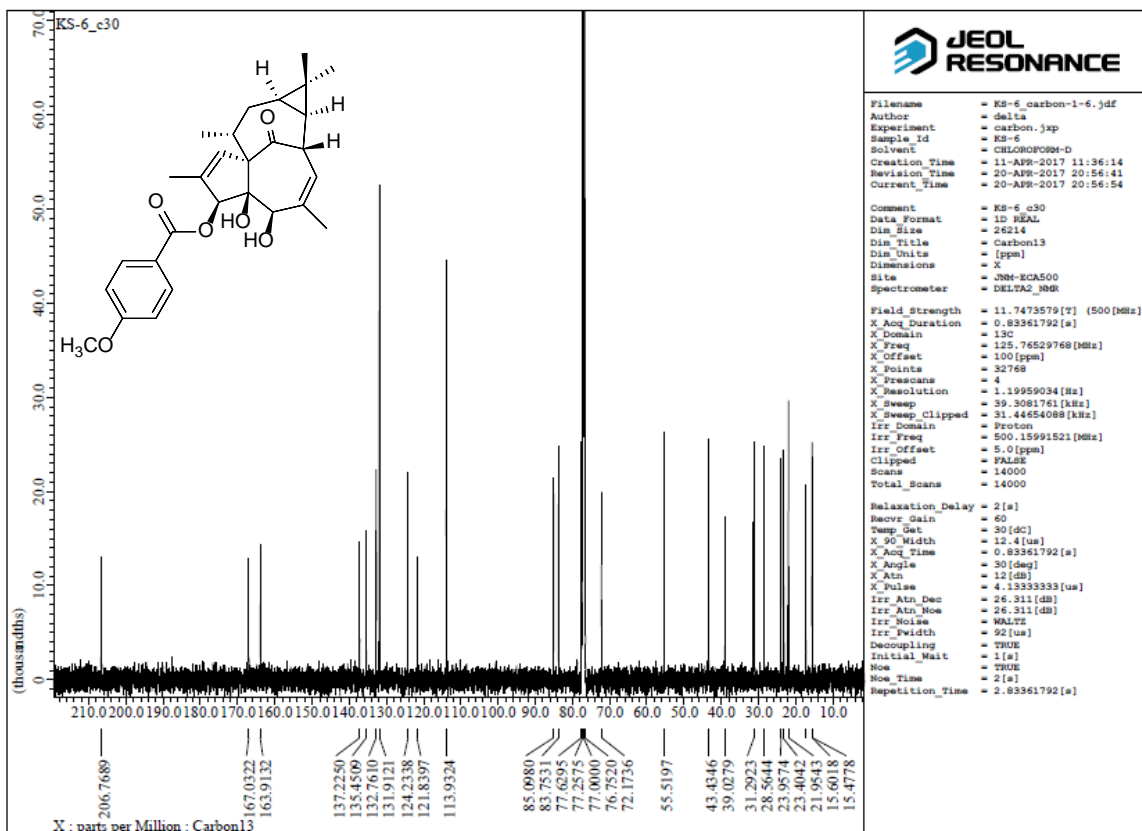


<p>[コメント情報] 試料名 KS-6 コメント 測定者 B 所属 東邦大学 薬学部 会社</p> <p>[データ情報] 作成日時 2017/07/26 14:08 データタイプ 等間隔データ 横軸 Wavenumber [cm-1] 縦軸 %T スタート 0 cm-1 エンド 7800.65 cm-1 データ間隔 0.964233 cm-1 データ数 8091</p>	<p>[測定情報] 機種名 FT/IR-4100typeA シリアル番号 B109261016</p> <p>光源 標準光源 検出器 TGS 積算回数 Auto (174) 分解 4 cm-1 ゼロフリンク On アボダイゼーション Cosine ゲイン Auto (16) アパーチャー Auto (7.1 mm) スキャンスピード Auto (2 mm/sec) フィルタ Auto (30000 Hz)</p>	<p>KS-6.2</p>
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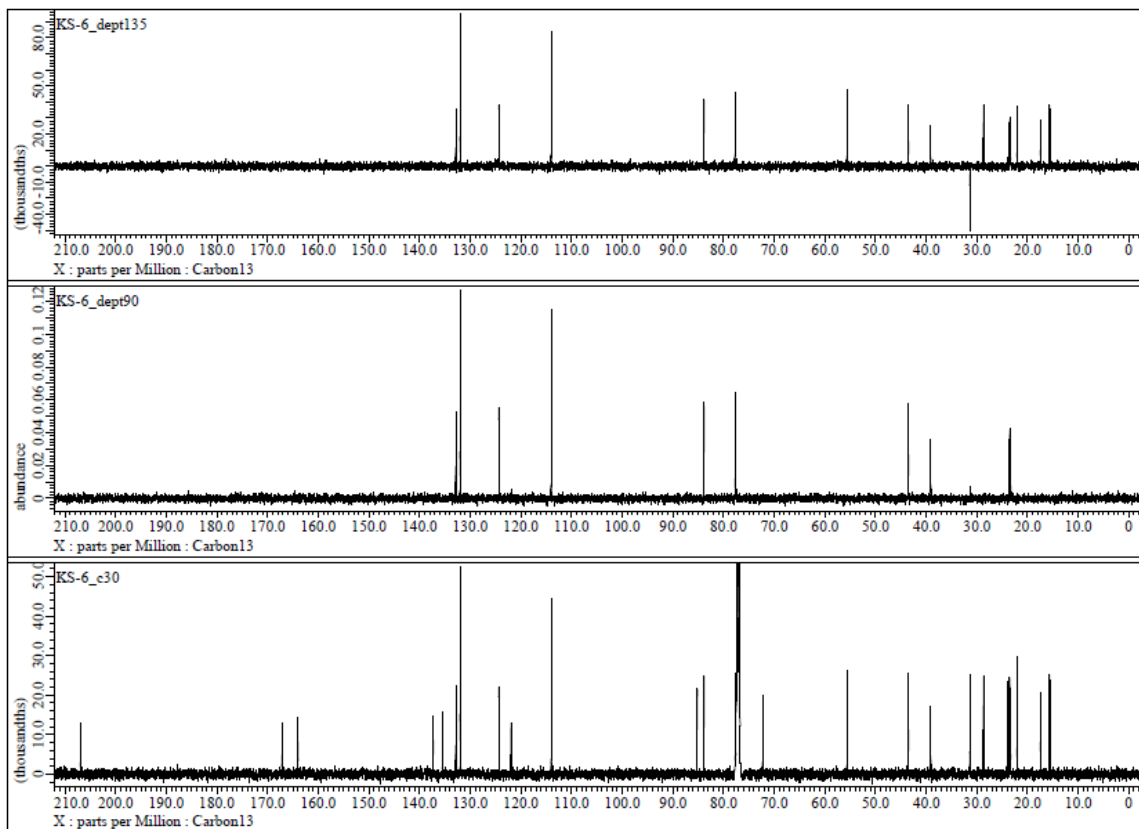
The IR spectrum of compound 12a



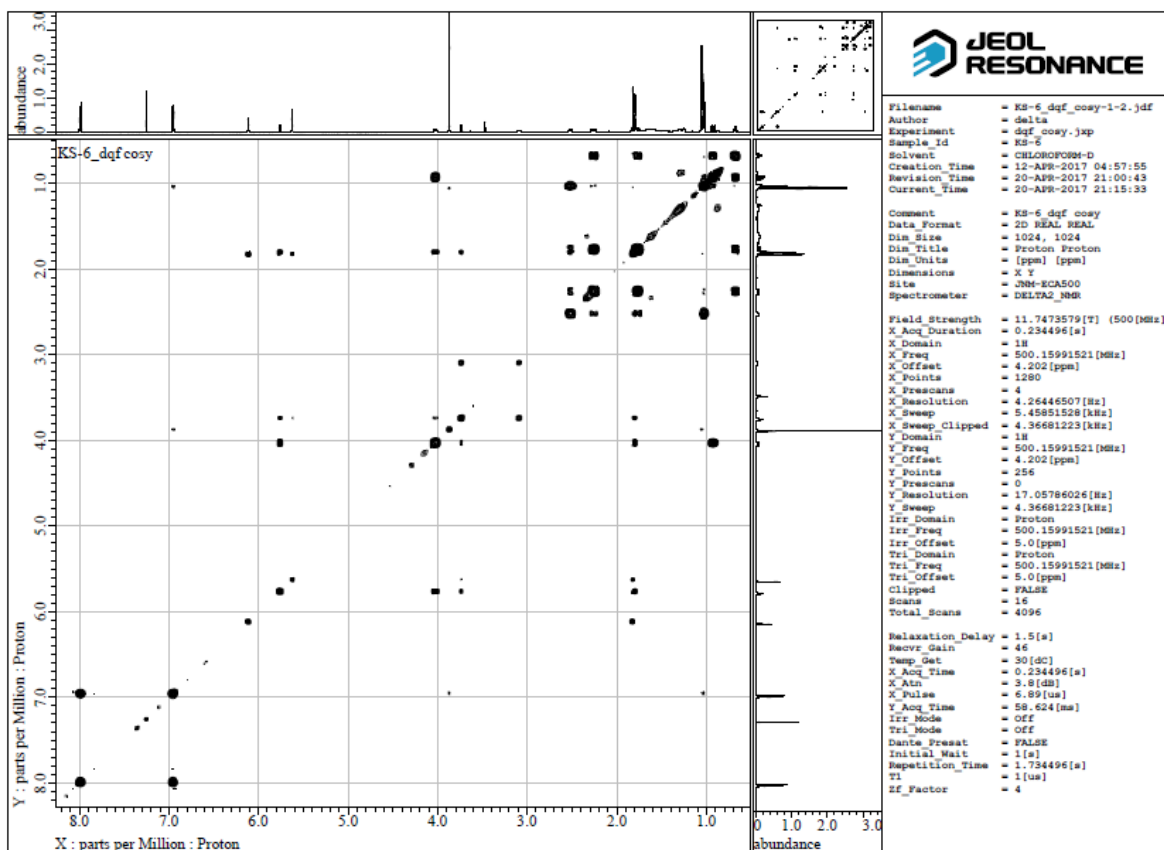
The ¹H spectrum of compound 12a



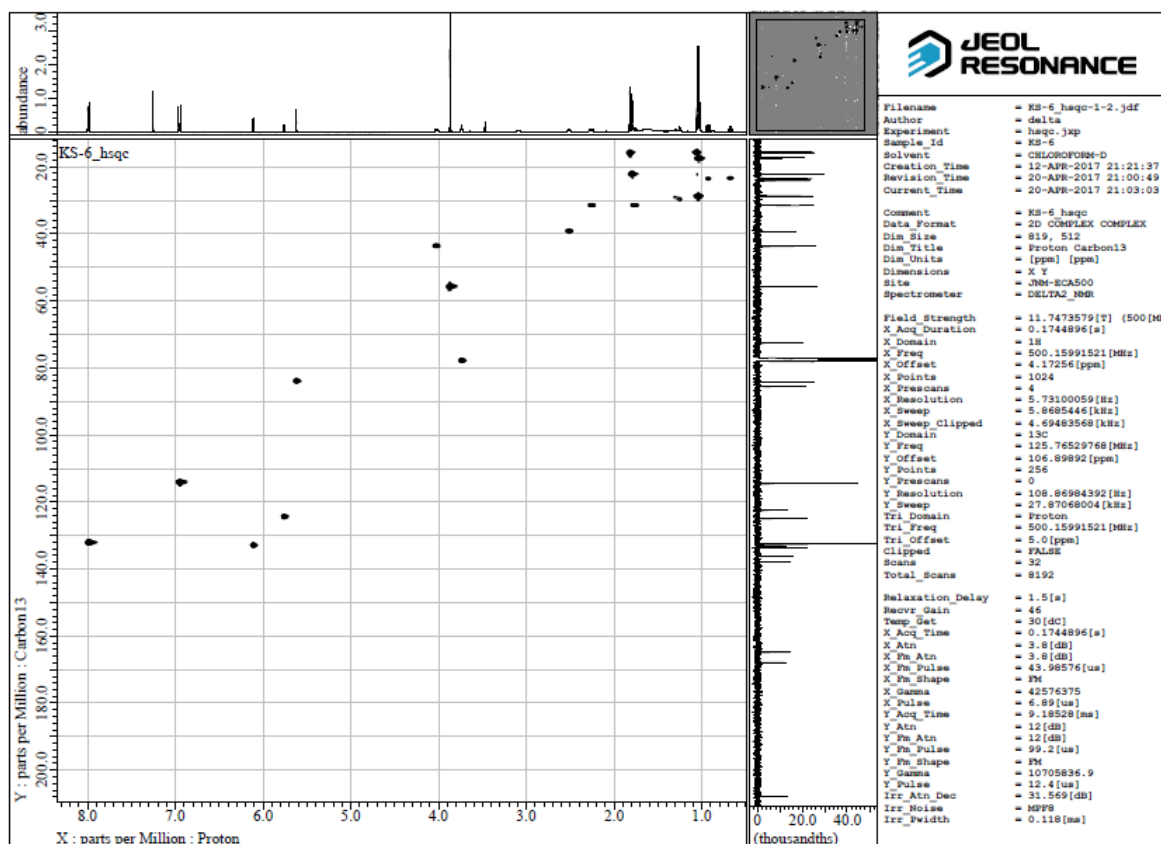
The ¹³C spectrum of compound 12a



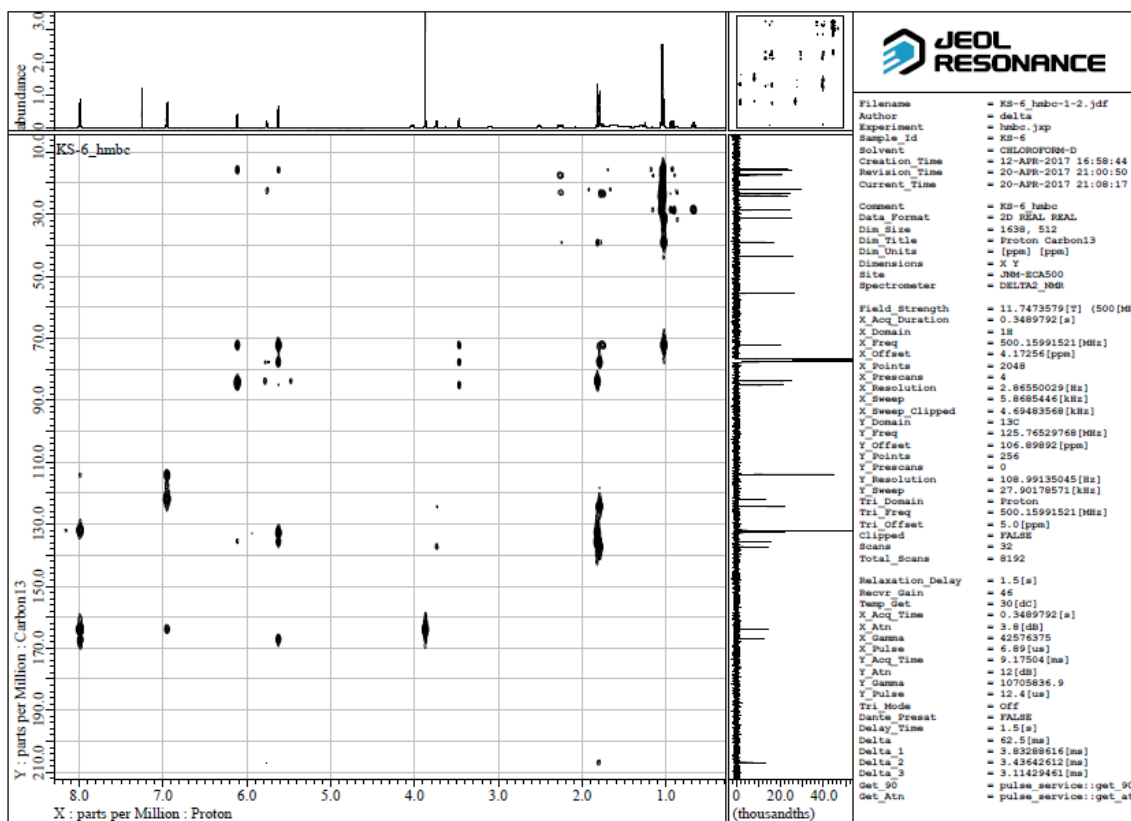
The DEPT spectrum of compound 12a



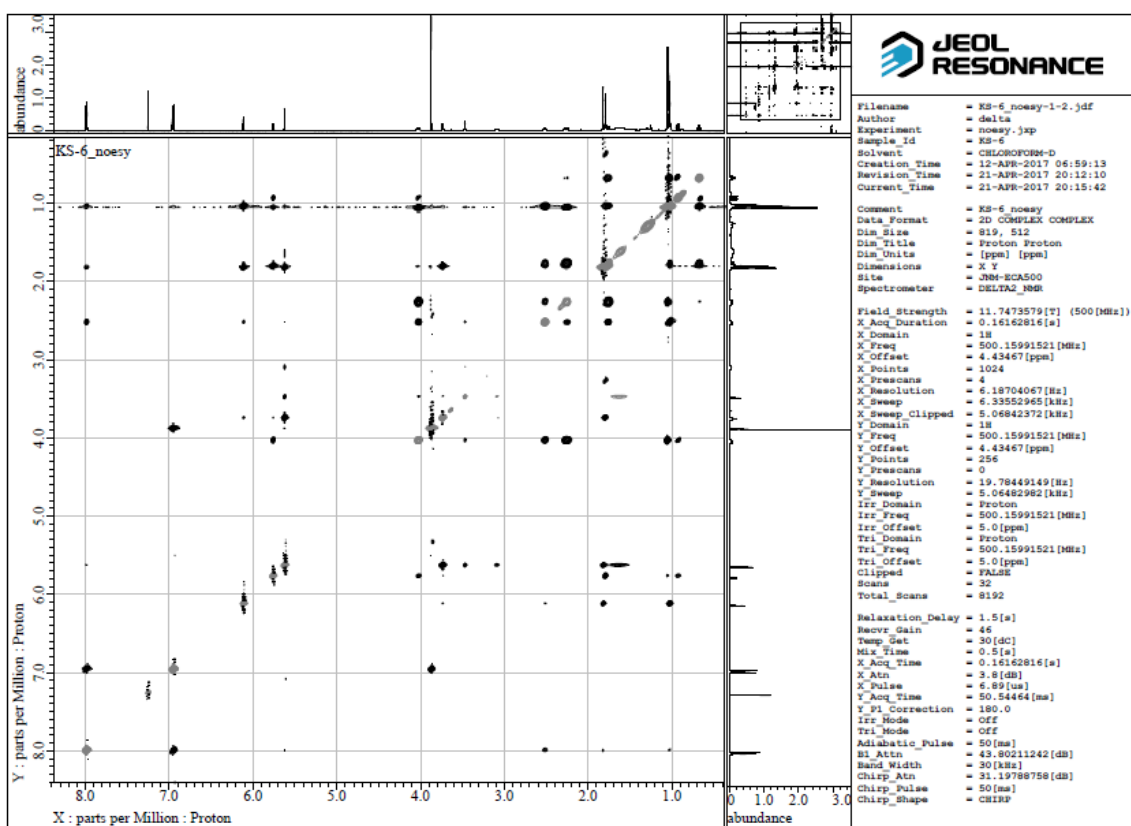
The DQF_COSY spectrum of compound 12a



The HSQC spectrum of compound 12a

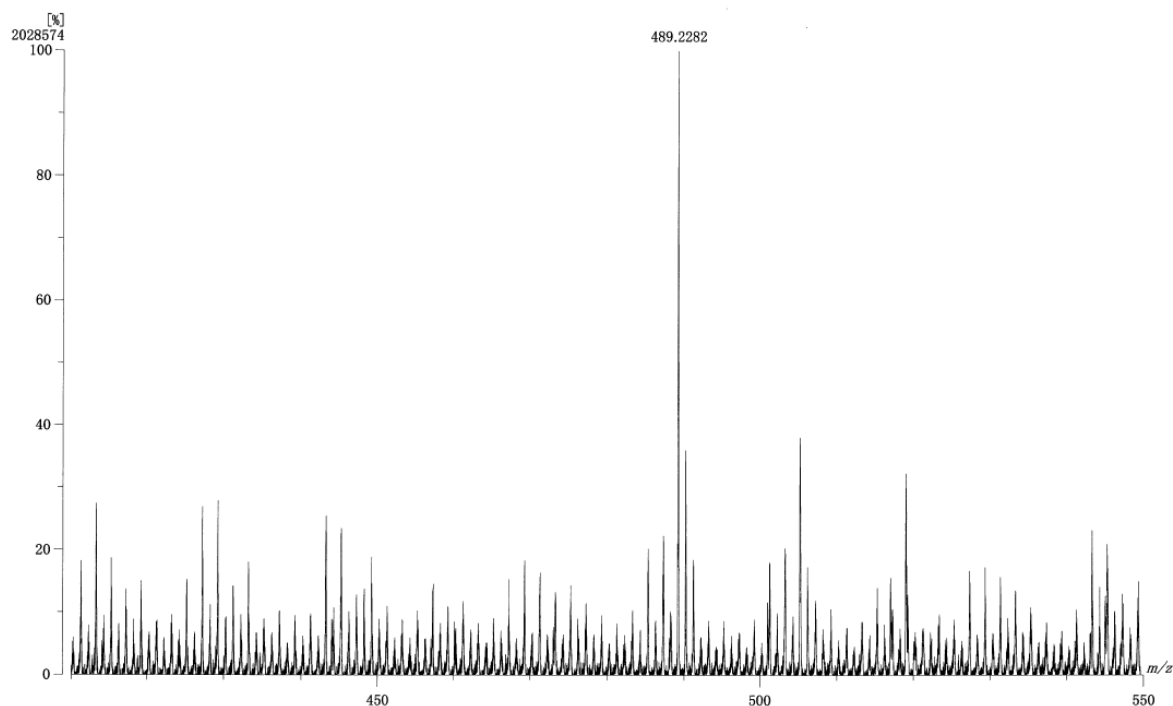


The HMBC spectrum of compound 12a

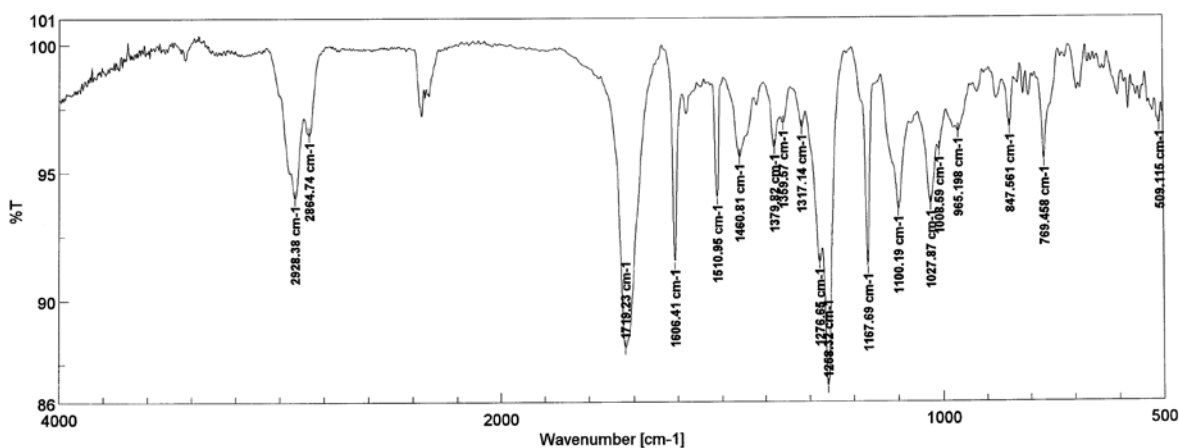


The NOESY spectrum of compound 12a

[Mass Spectrum]
 Data : KS-5+Na-FABpHR-NBA Date : 22-Aug-2017 13:55
 Instrument : MStation
 Sample : KS-5
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 5.37 min Scan# : 20 Temp : 3276.7 deg.C
 BP : m/z 489.2282 Int. : 193.46 (2028574)
 Output m/z range : 410 to 550 Cut Level : 0.00 %



The HRFABMS spectrum of compound **12b**



[コメント情報]
 試料名 KS-6
 コメント
 測定者
 所属 B
 会社 東邦大学 薬学部

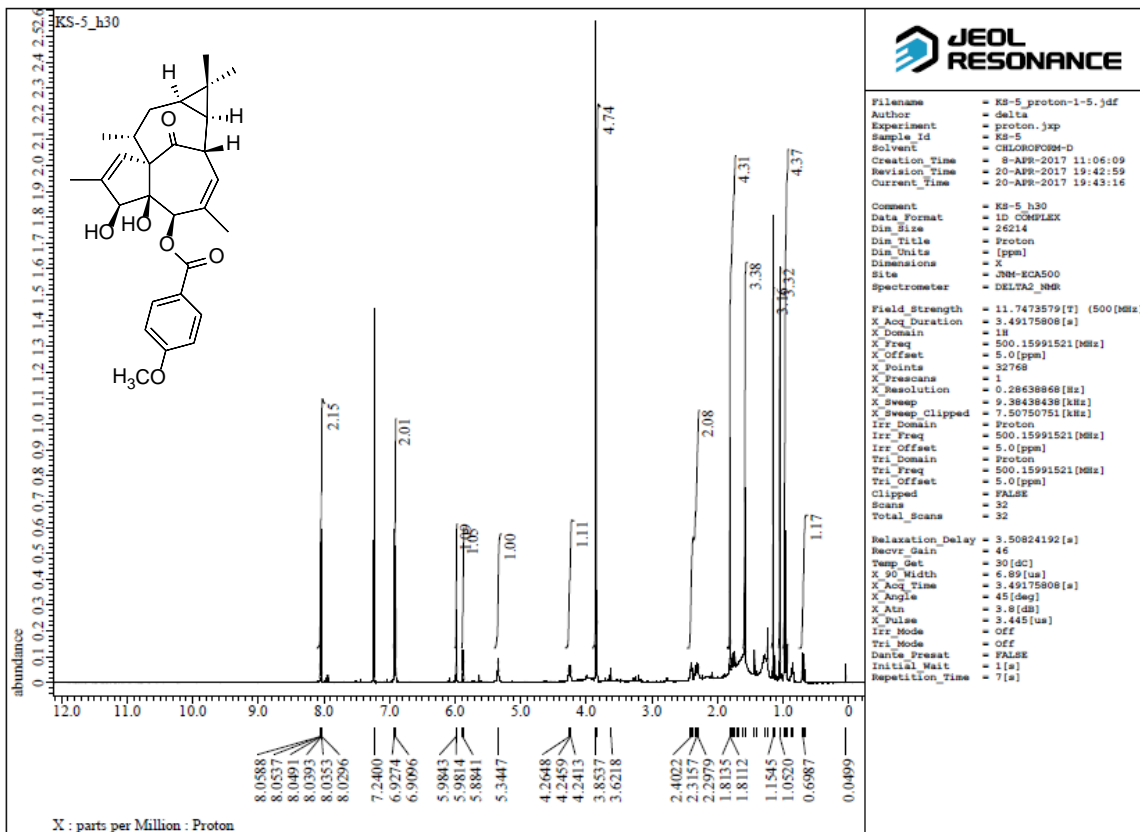
[データ情報]
 作成日時 2017/07/26 14:08
 データタイプ 等間隔データ
 横軸 Wavenumber [cm-1]
 縦軸 %T
 スタート 0 cm-1
 エンド 7800.65 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

[測定情報]
 機種名 FT/IR-4100typeA
 シリアル番号 B109261016

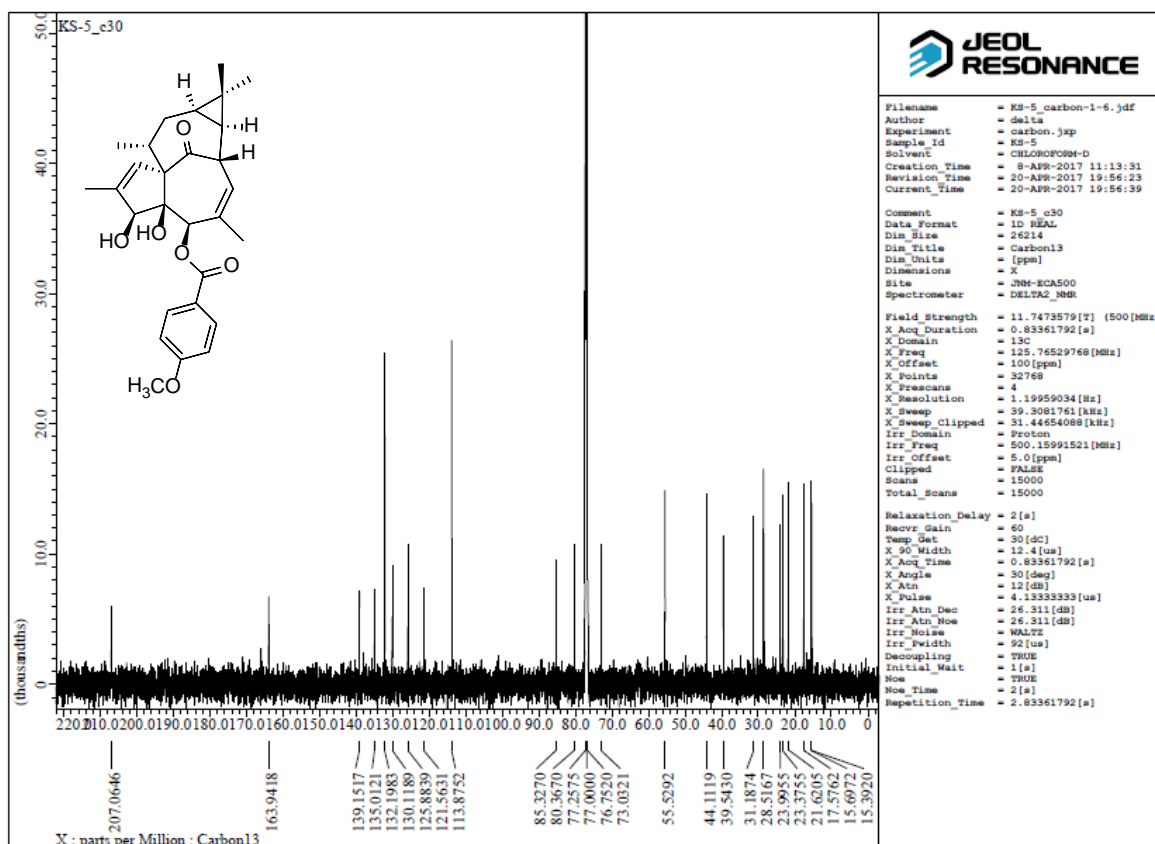
光源 標準光源
 検出器 TGS
 積算回数 Auto (174)
 分解 4 cm-1
 ゼロフリンギング On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャー Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

KS-6_2

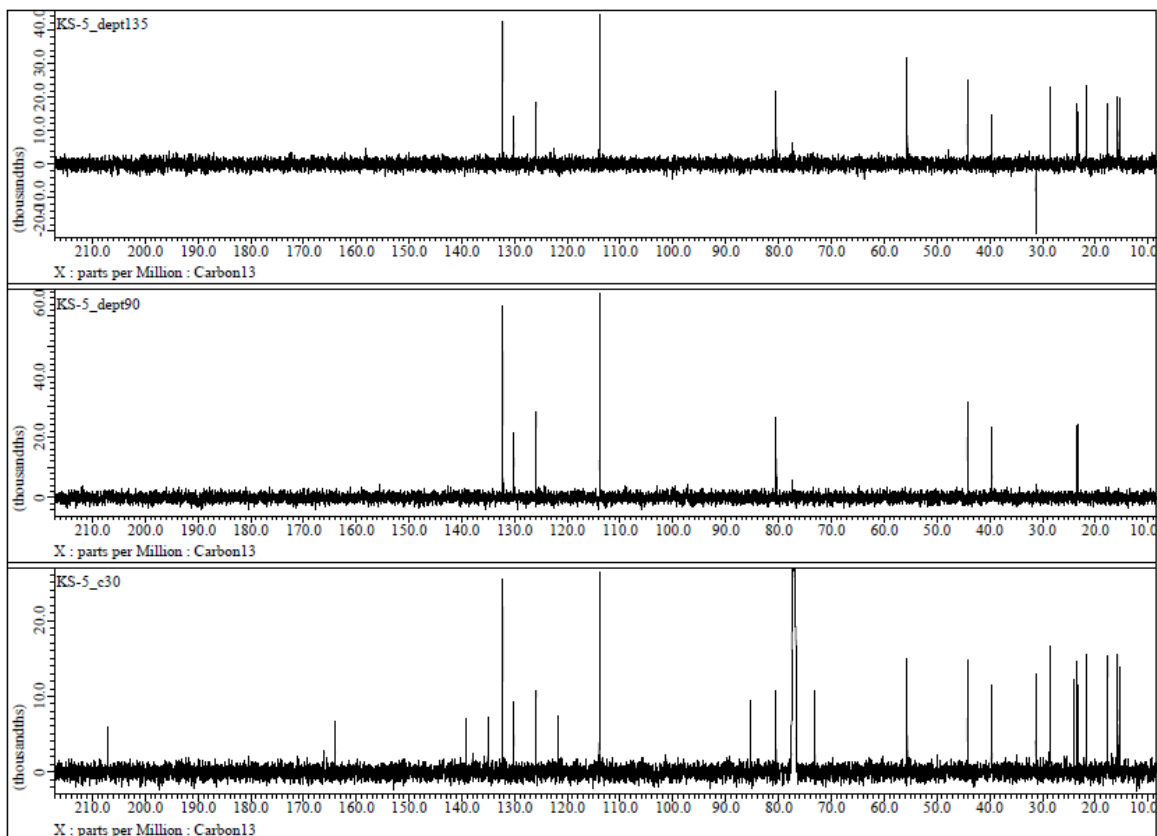
The IR spectrum of compound **12b**



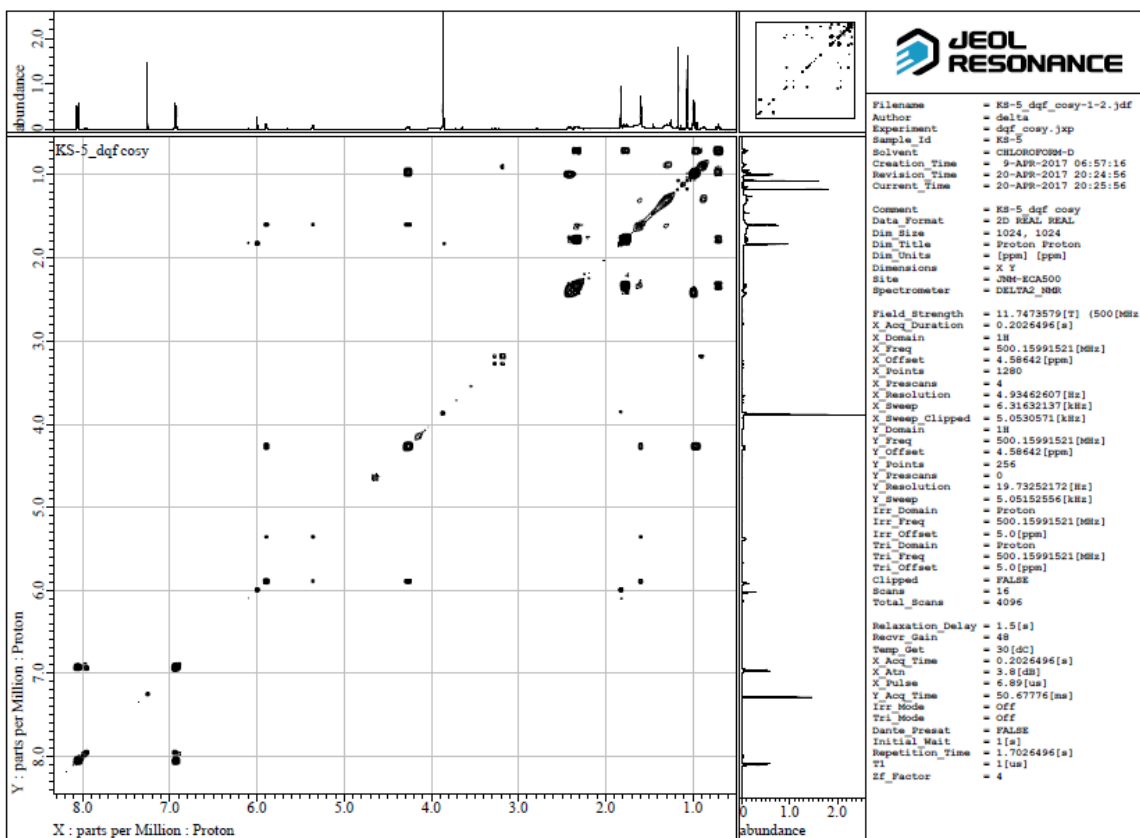
The ^1H spectrum of compound 12b



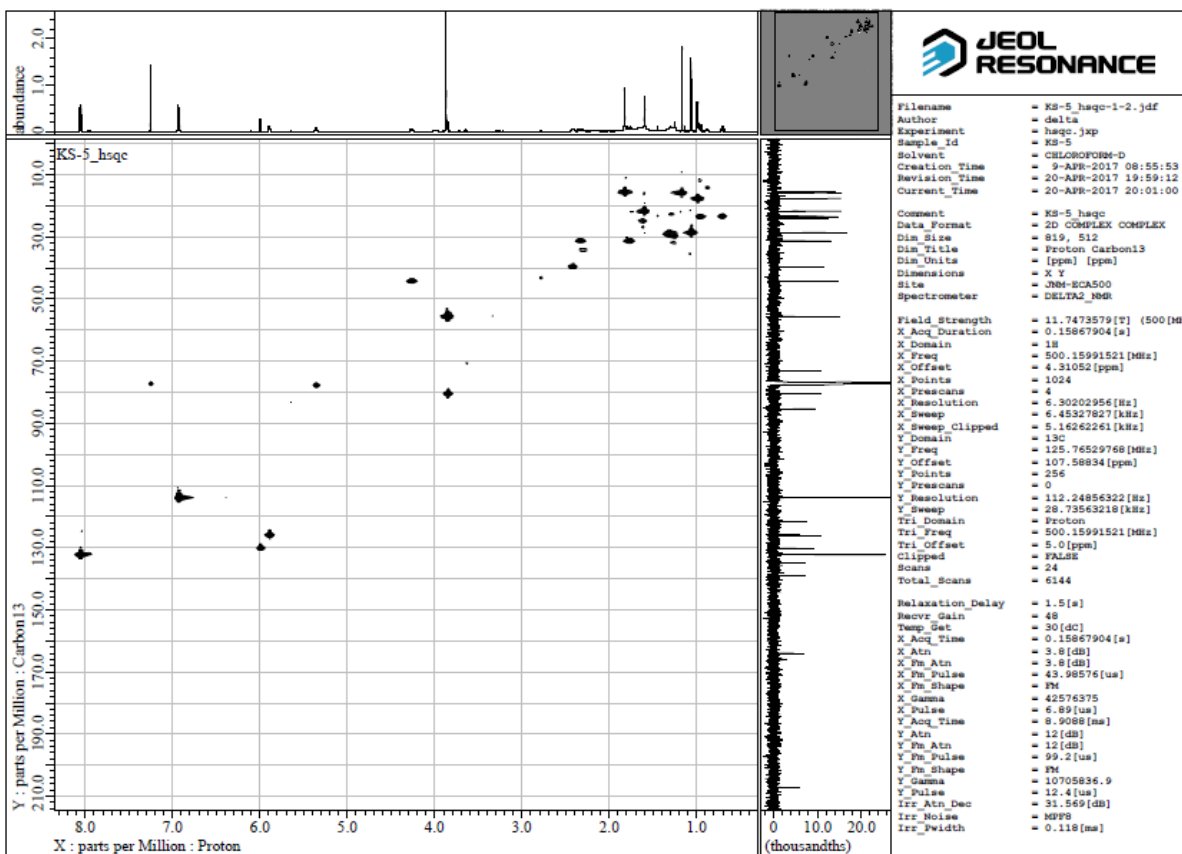
The ^{13}C spectrum of compound 12b



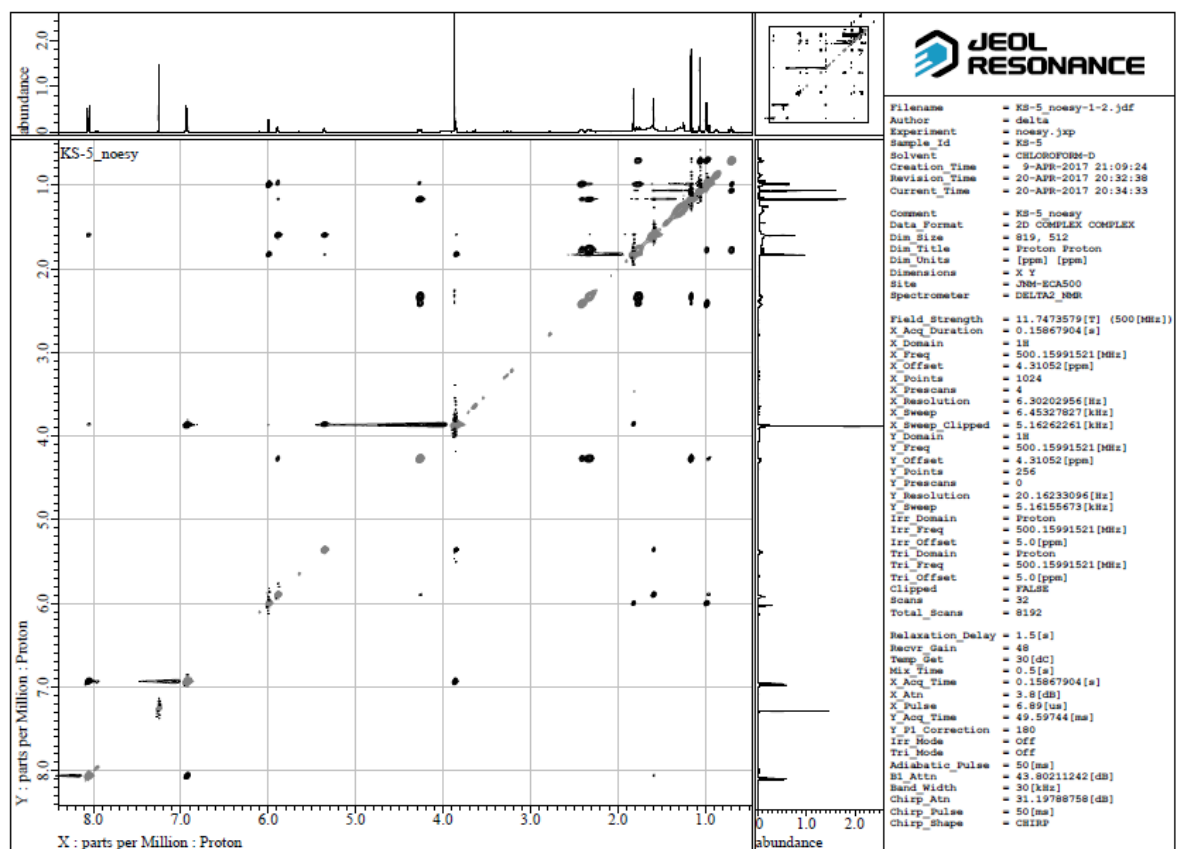
The DEPT spectrum of compound **12b**



The DQF-COSY spectrum of compound **12b**



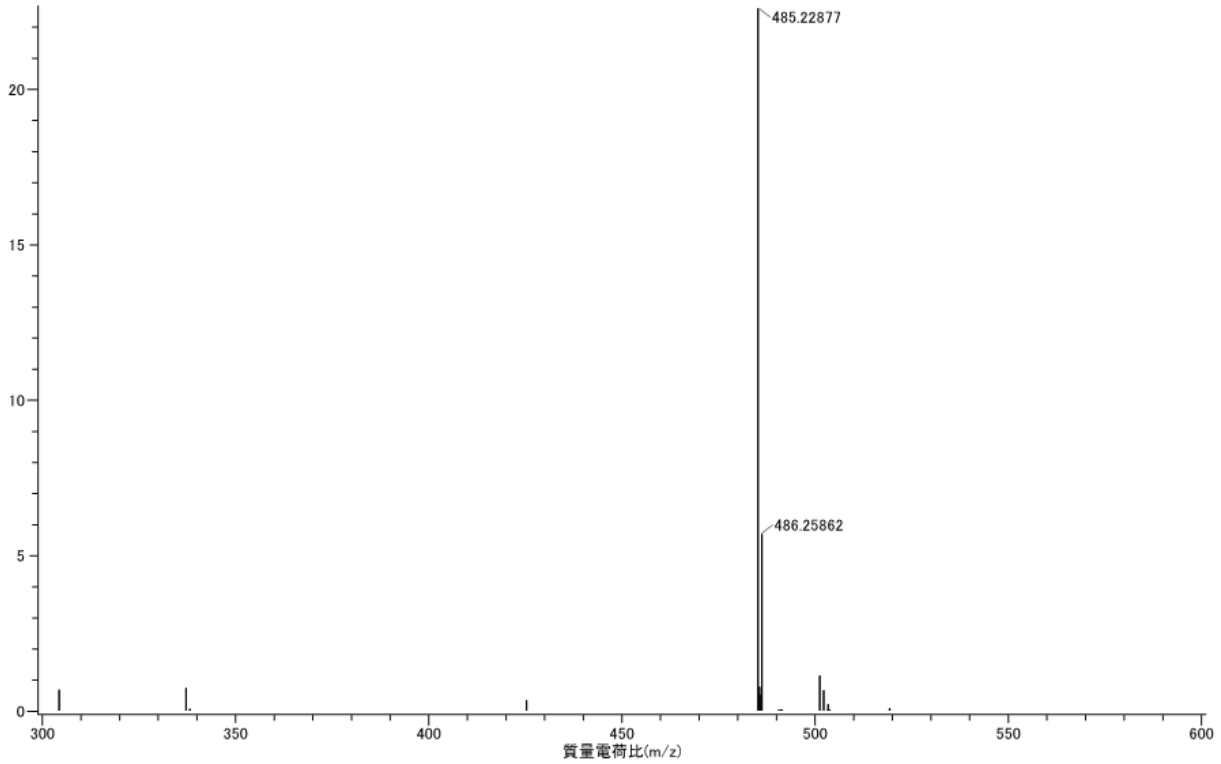
The HSQC spectrum of compound 12b



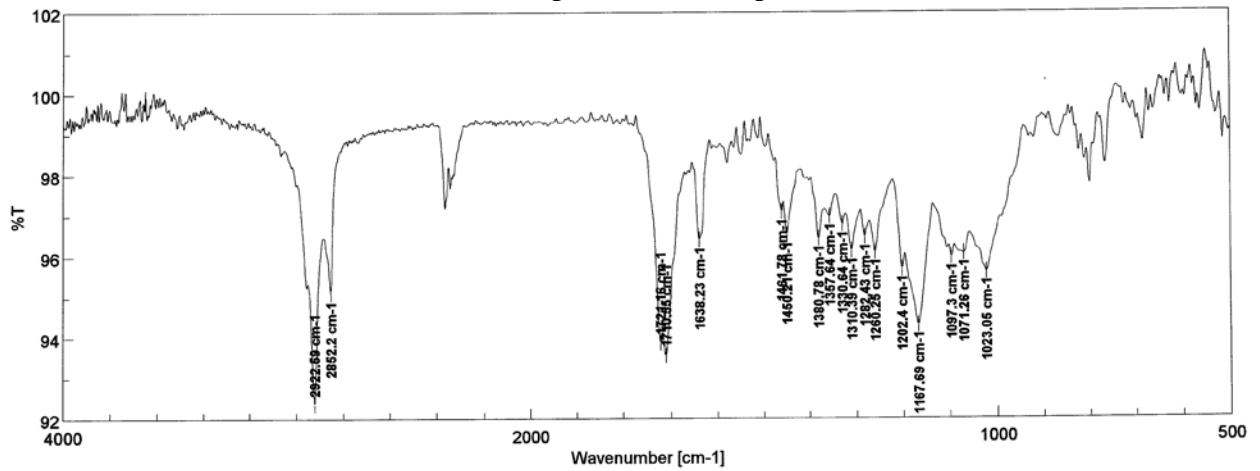
The NOESY spectrum of compound 12b

測定データ名: KS-14.01
 作成条件: 平均(MS[1]) 経過時間: 0.66.0.82)
 x10³ 面積 (22590)

実験日時: 2017/10/13 21:52:53
 イオン化モード: ESI+



The HRESIMS spectrum of compound 13a



【コメント情報】
 試料名 KS-14
 コメント
 測定者 B
 所属 東邦大学 薬学部
 会社

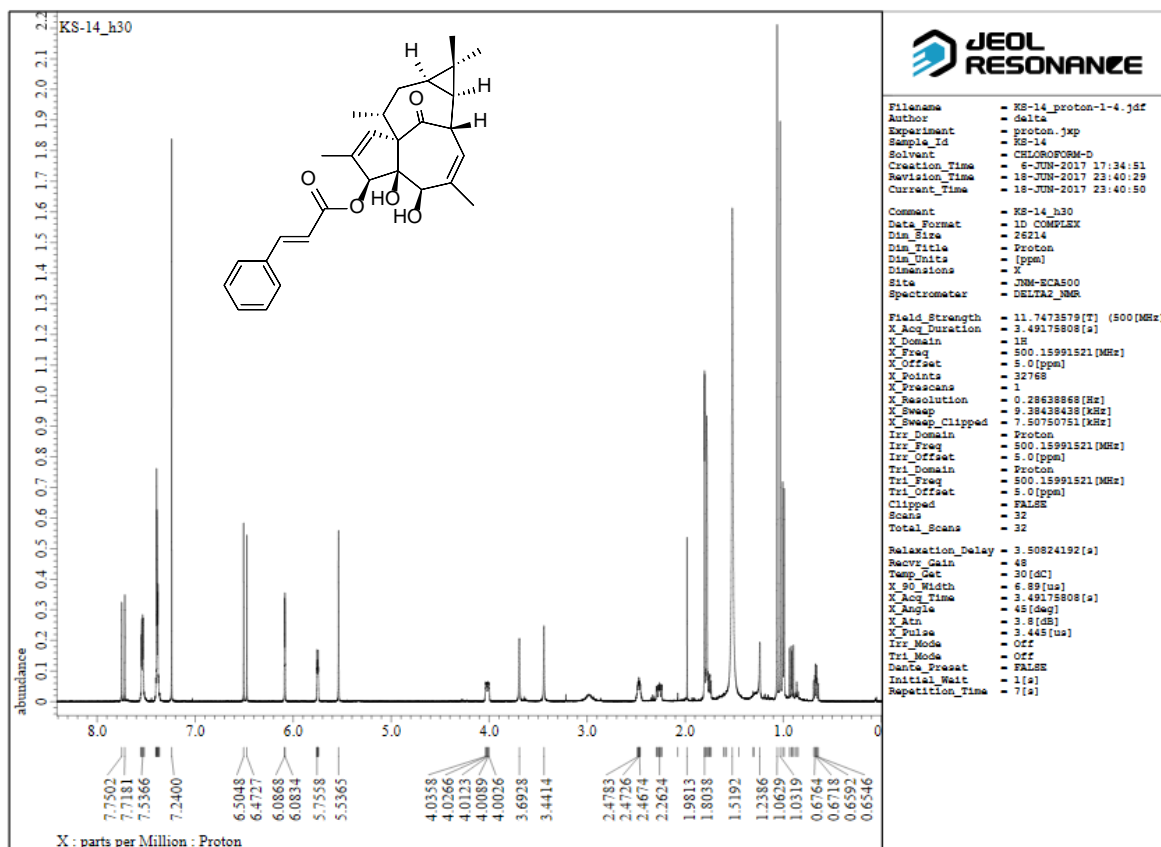
【データ情報】
 作成日時 2017/07/26 15:57
 データタイプ 等間隔データ
 横軸 Wavenumber [cm-1]
 縦軸 %T
 スタート 0 cm-1
 エンド 7800.85 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

【測定情報】
 機種名 FT/IR-4100typeA
 シリアル番号 B109261016

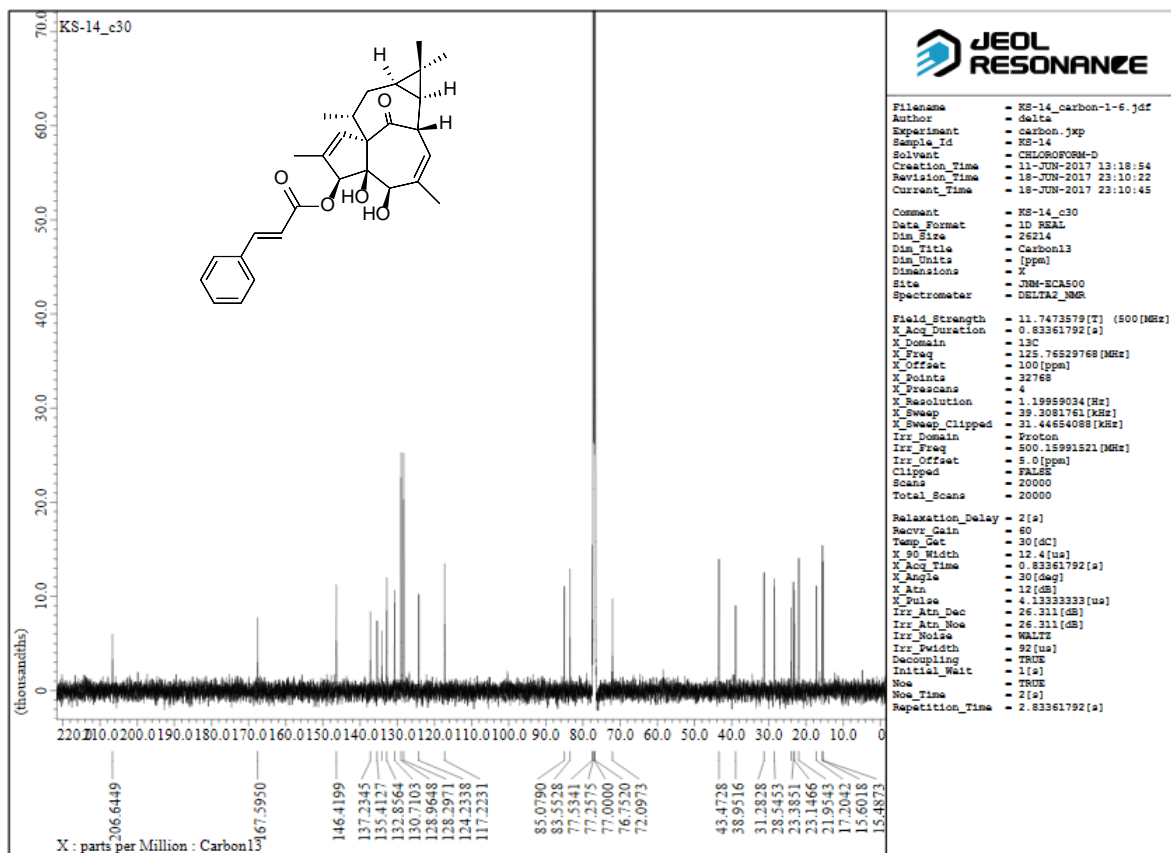
光源 標準光源
 検出器 TGS
 積算回数 Auto (223)
 分解 4 cm-1
 ゼロフリンギング On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャ Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

Memory-2

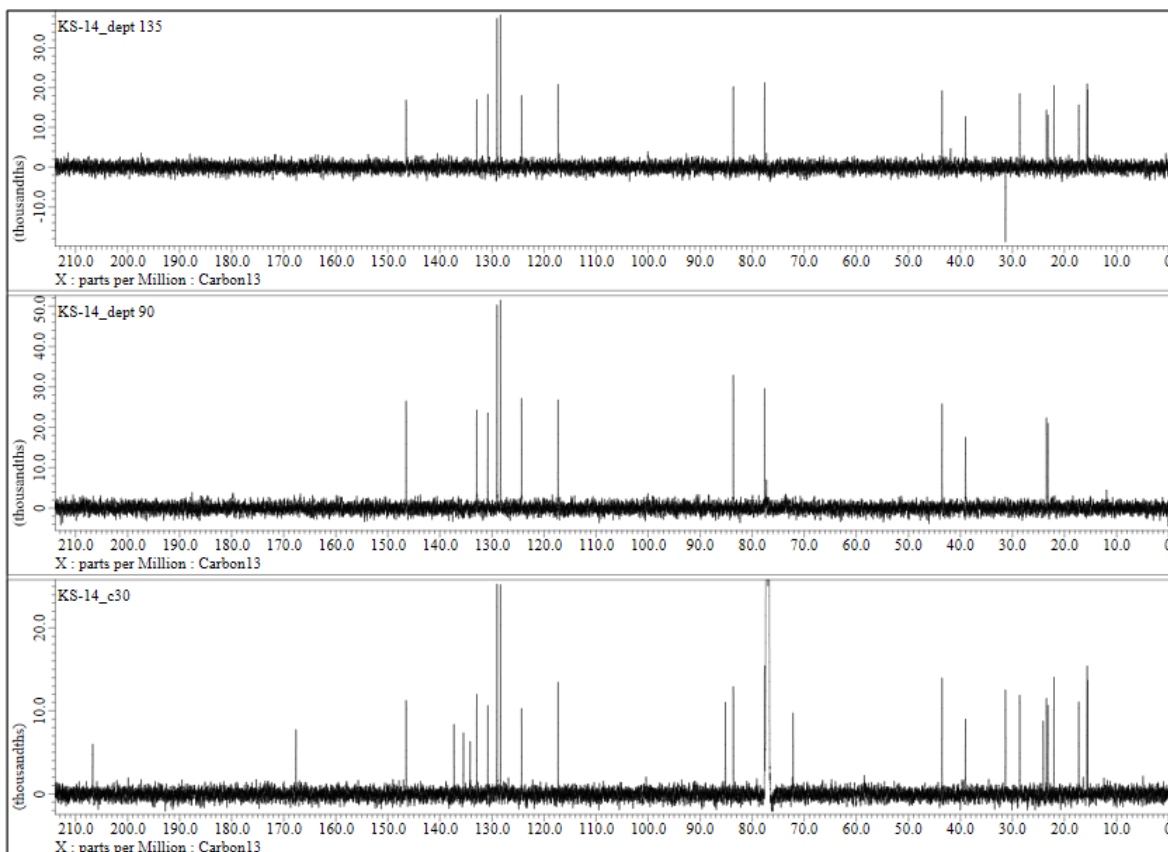
The IR spectrum of compound 13a



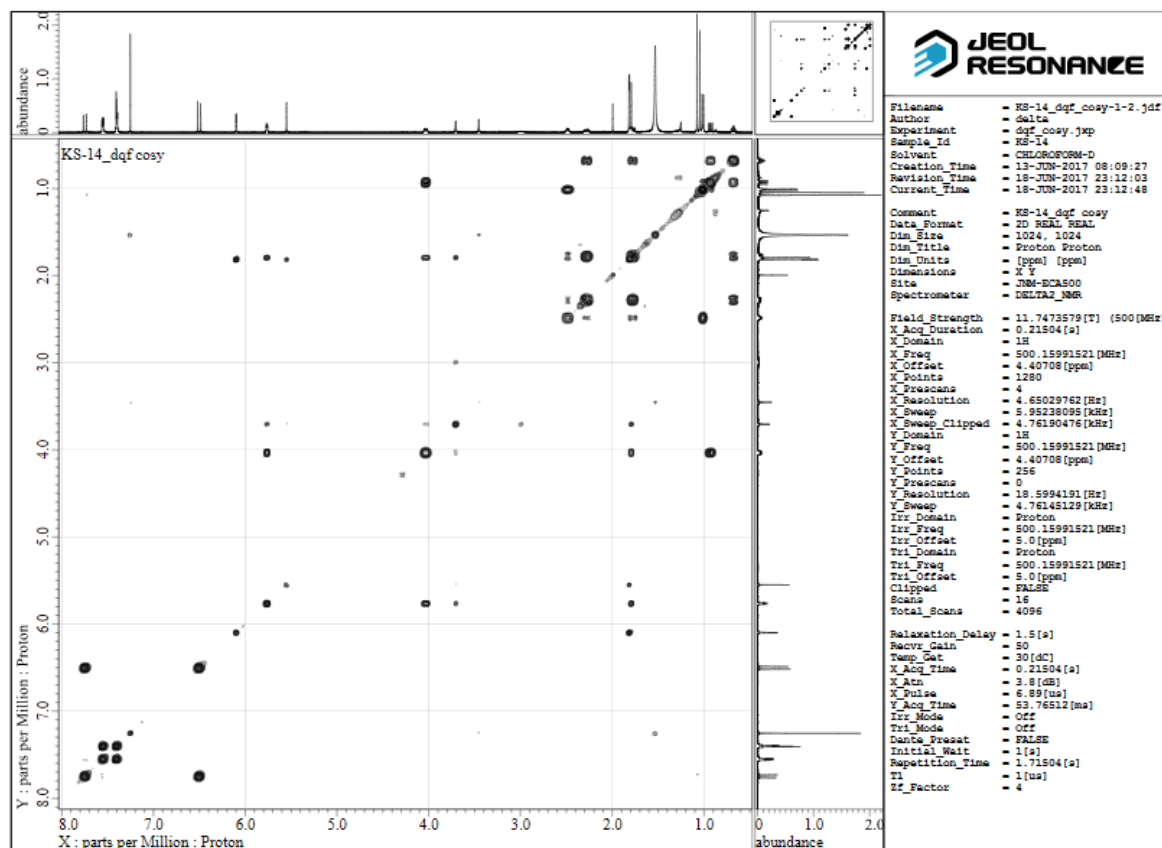
The ¹H spectrum of compound 13a



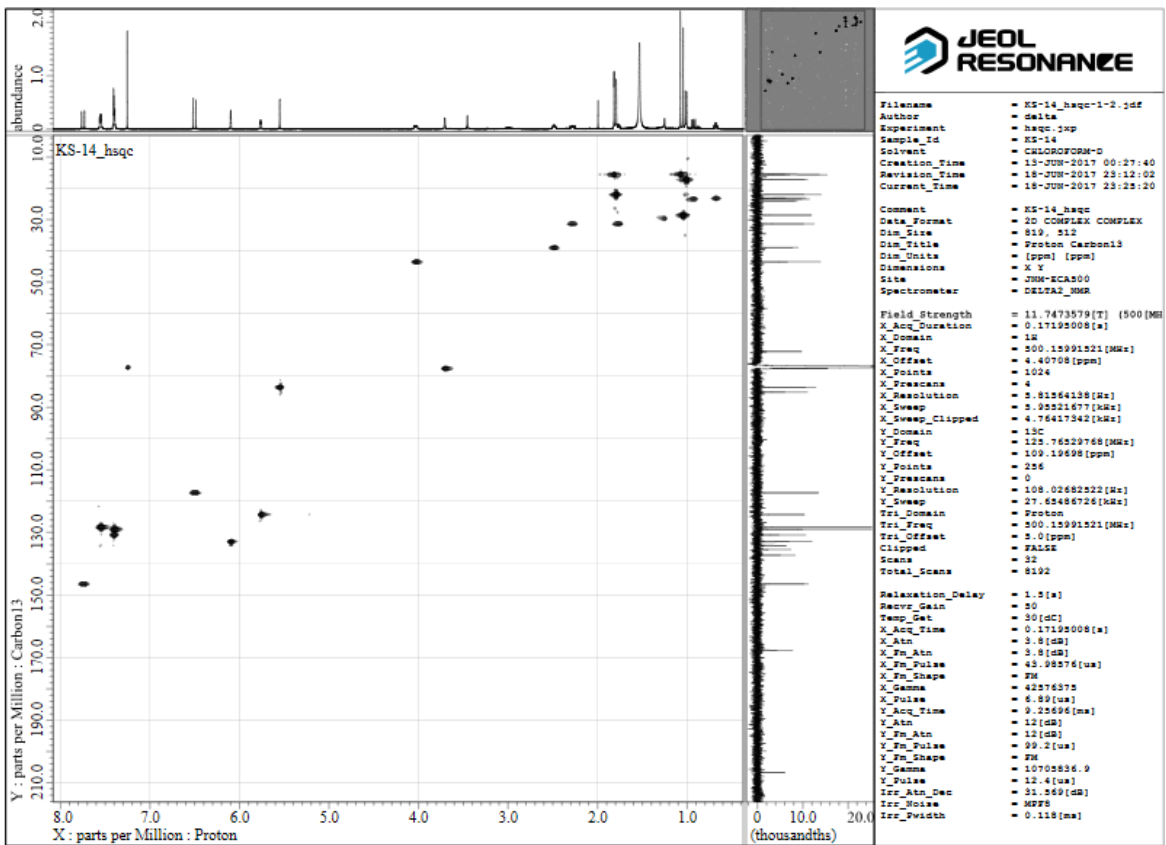
The ¹³C spectrum of compound 13a



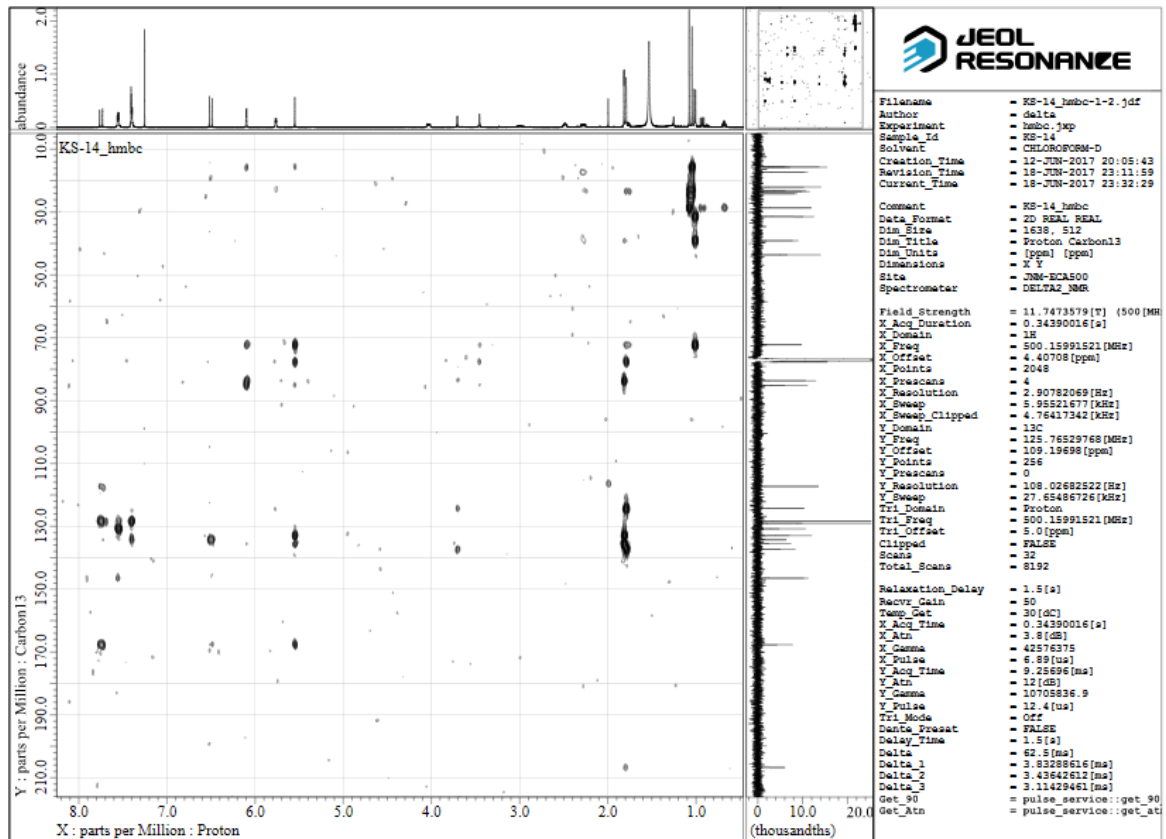
The DEPT spectrum of compound 13a



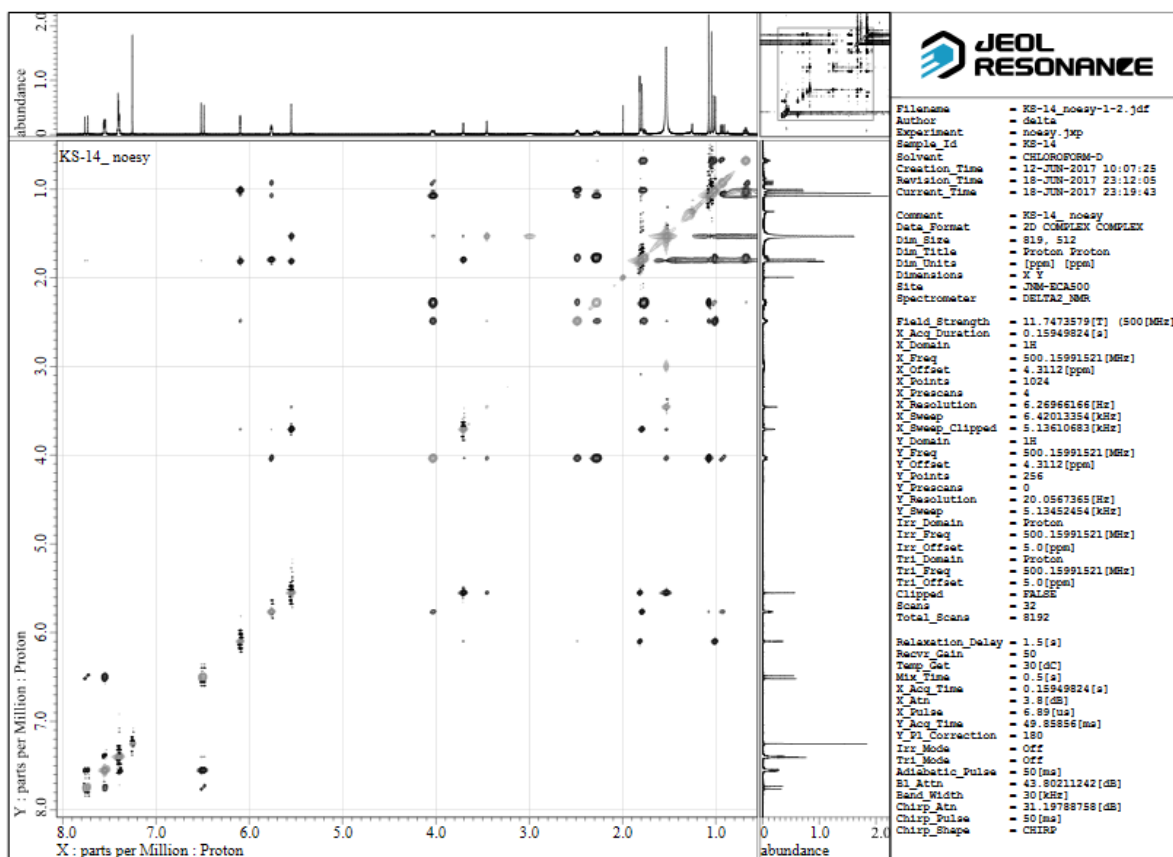
The DQF-COSY spectrum of compound 13a



The HSQC spectrum of compound 13a



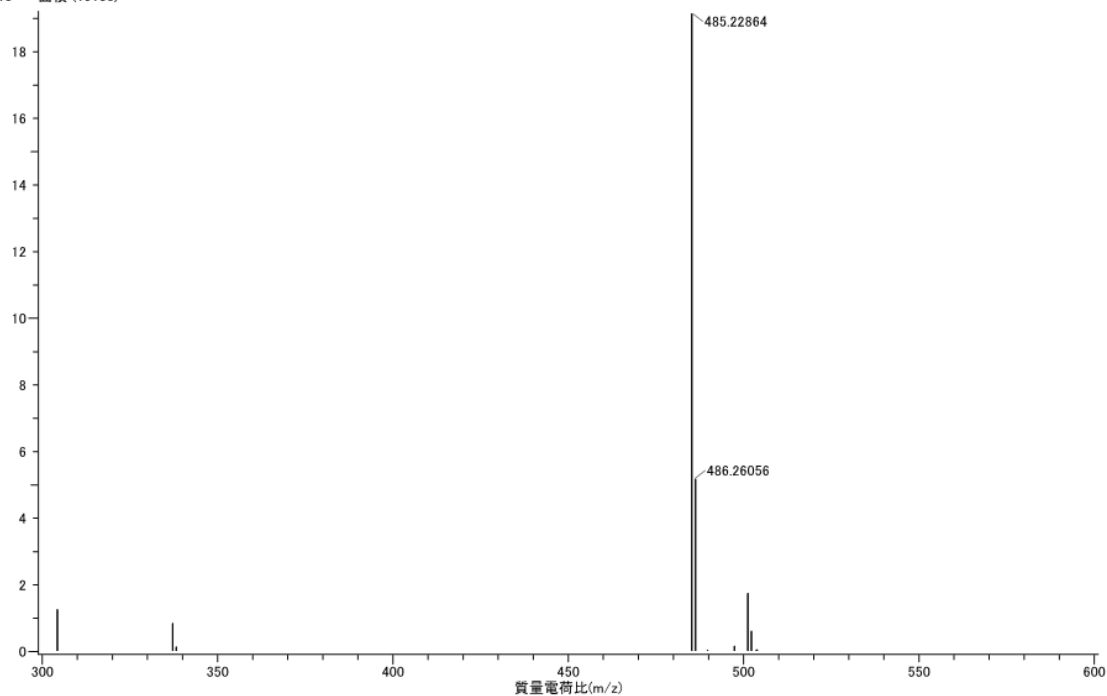
The HMBC spectrum of compound 13a



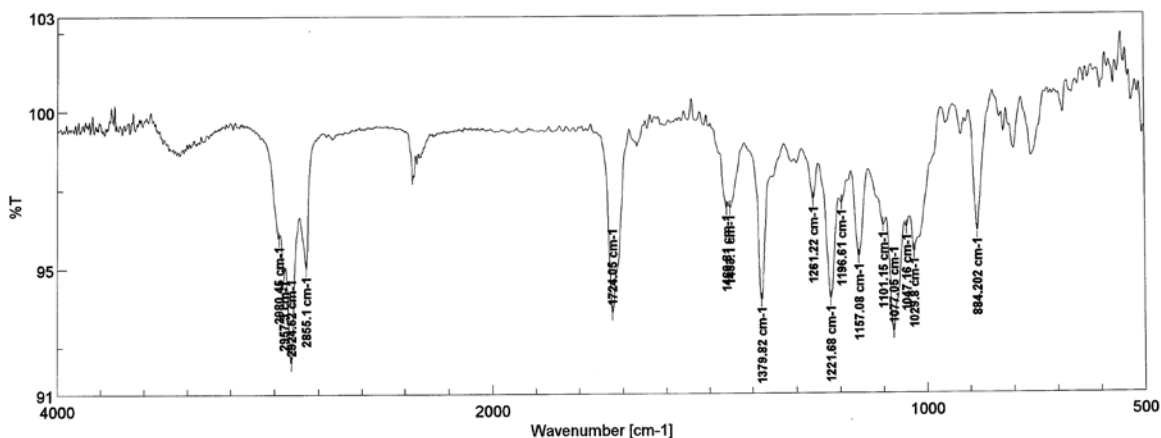
The NOESY spectrum of compound **13a**

測定データ名: KS-13.02
作成条件: 平均(MS[1] 経過時間: 0.64.0.96)
×10³ 面積 (19136)

実験日時: 2017/10/13 21:44:25
イオン化モード: ESI+



The HRESIMS spectrum of compound **13b**

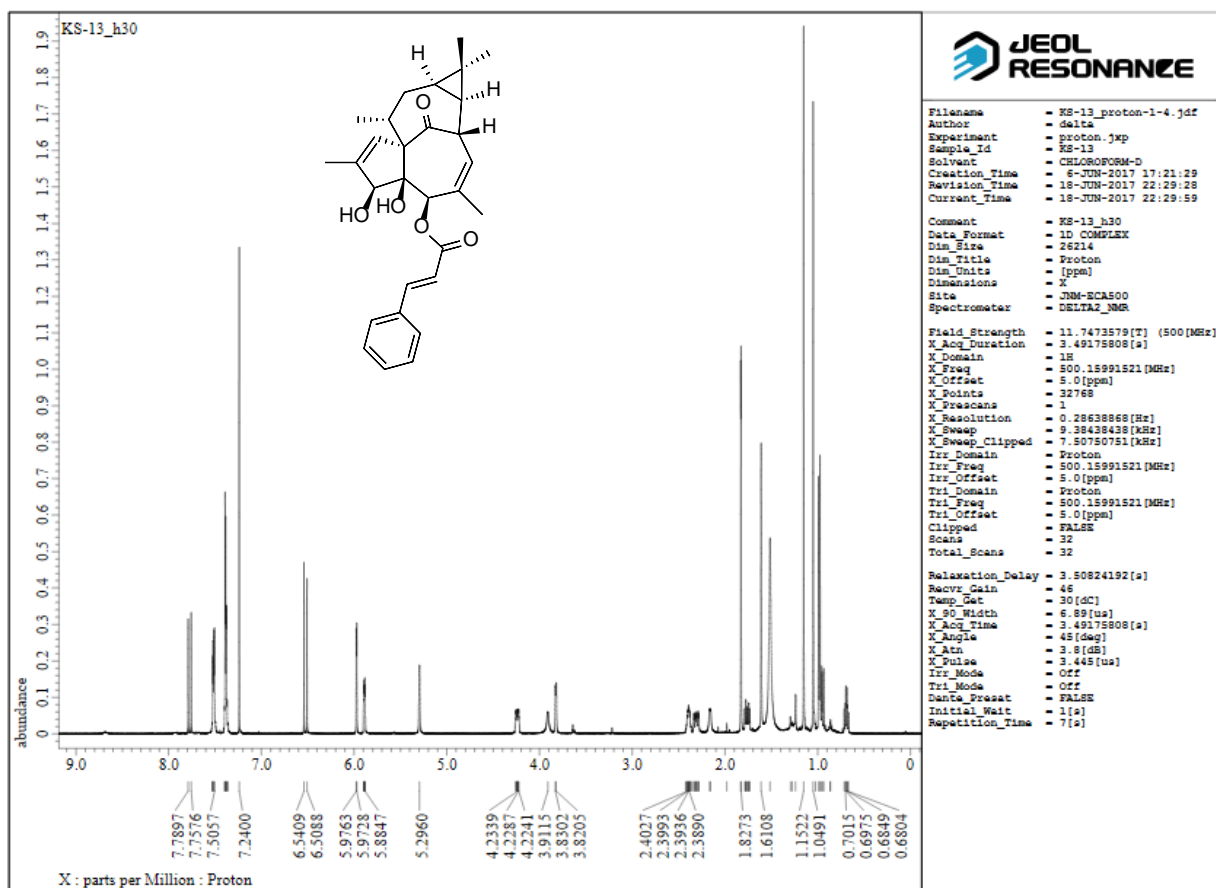


[コメント情報]
 試料名 KS-12
 コメント
 測定者 B
 所属会社 東邦大学 薬学部
 [データ情報]
 作成日時 2017/07/26 15:14
 データタイプ 等間隔データ
 横軸 Wavenumber [cm-1]
 縦軸 %T
 スタート 0 cm-1
 エンド 7800.65 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

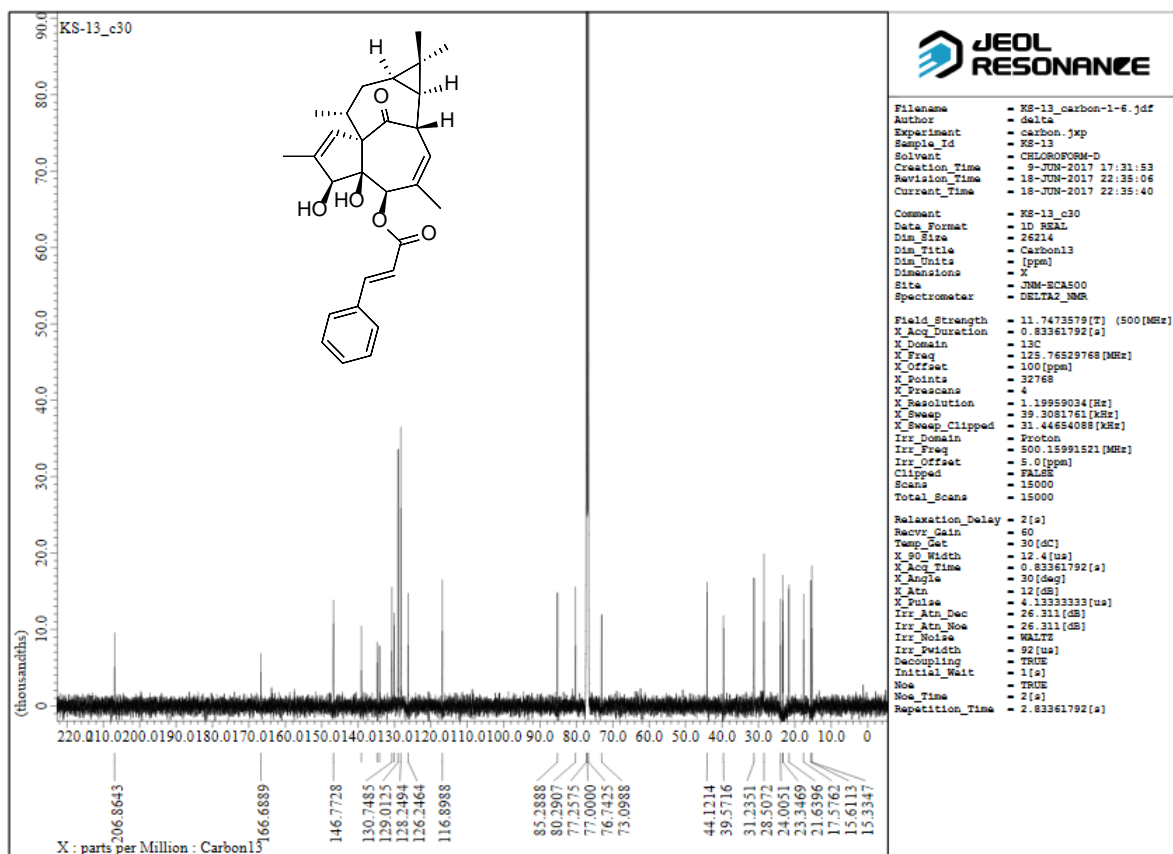
[測定情報]
 機種名 FT/IR-4100typeA
 シリアル番号 B109261016
 光源 標準光源
 検出器 TGS
 積算回数 Auto (190)
 分解 4 cm-1
 ゼロフリンギング On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャー Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

Memory-2

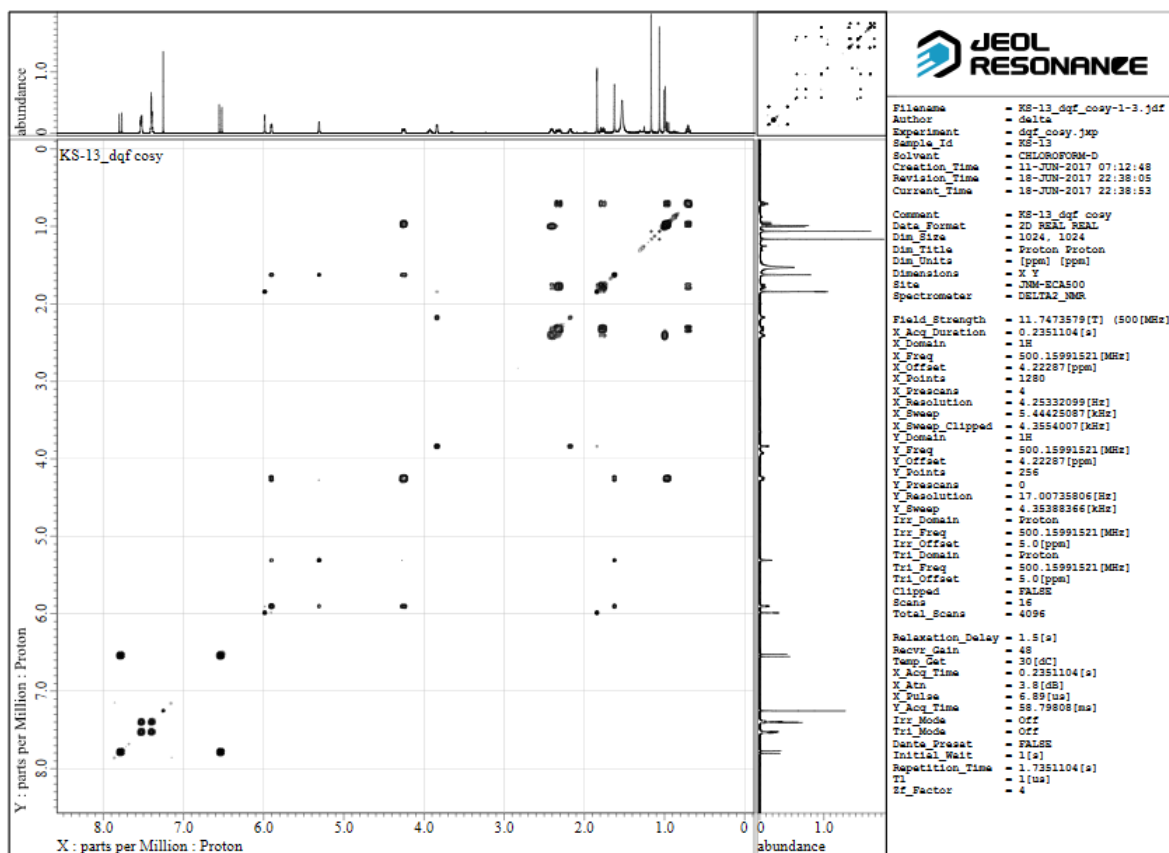
The HRESIMS spectrum of compound 13b



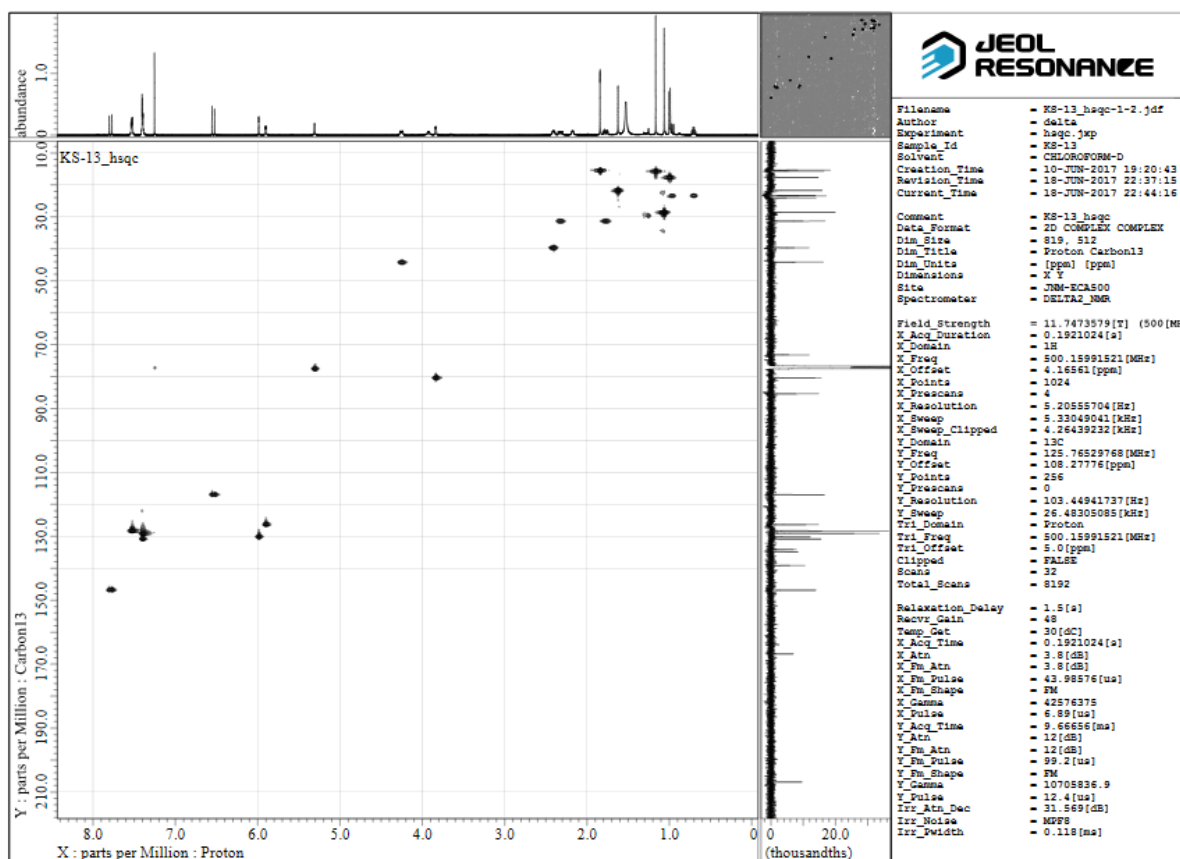
The ¹H spectrum of compound 13b



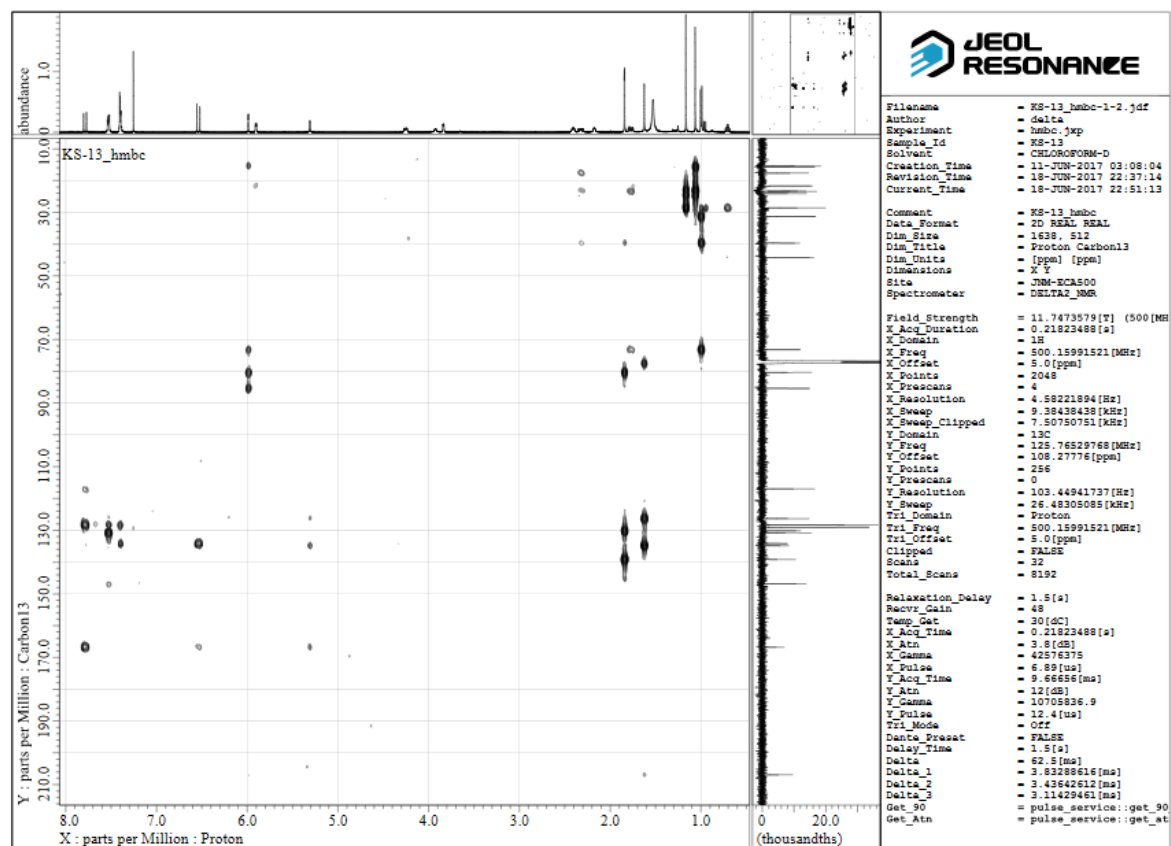
The ^{13}C spectrum of compound 13b



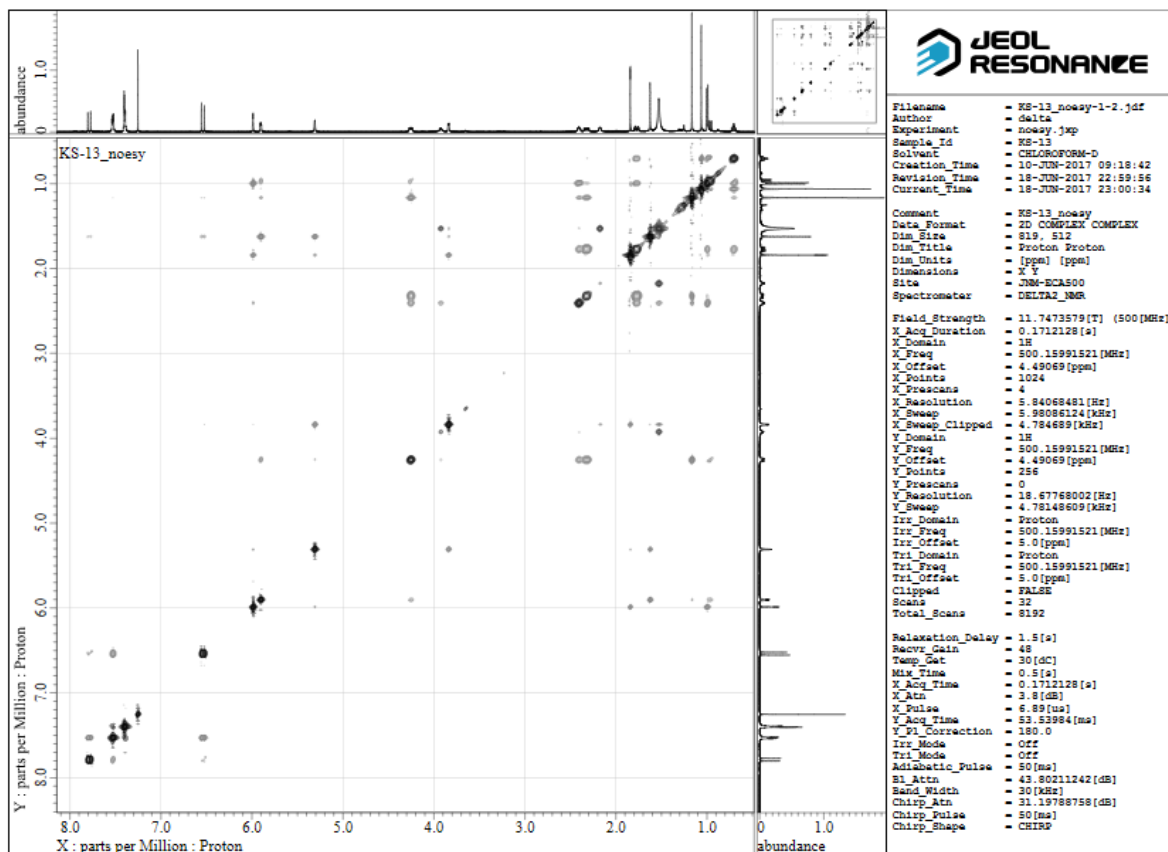
The DQF-COSY spectrum of compound 13b



The HSQC spectrum of compound **13b**



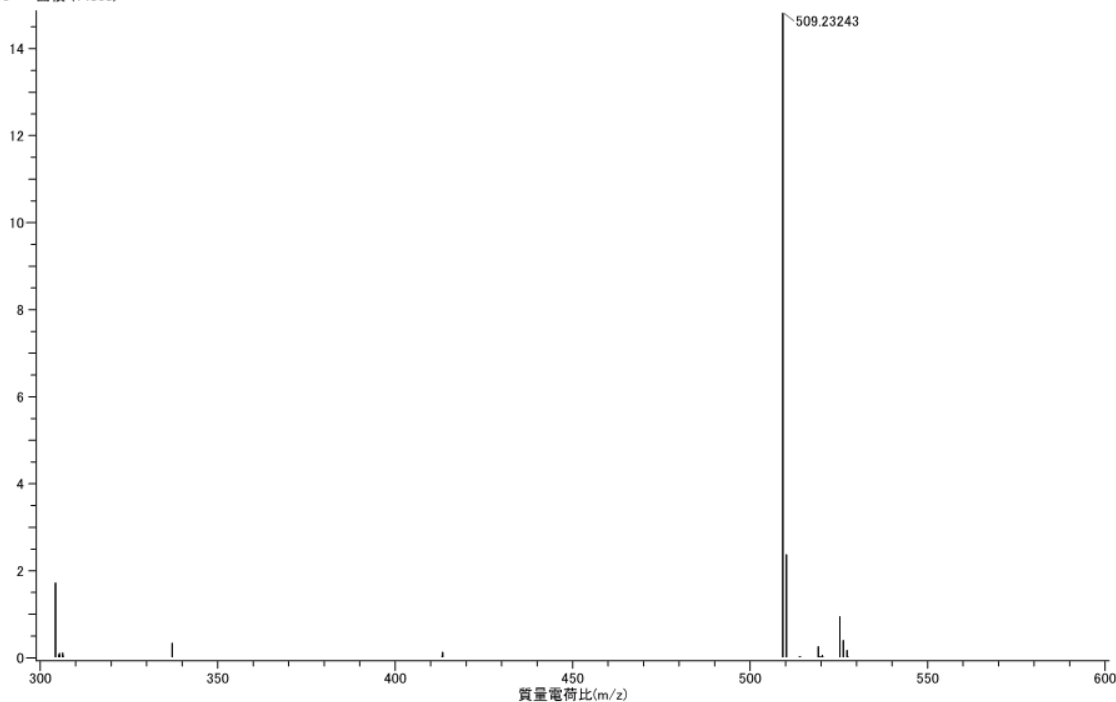
The HMBC spectrum of compound **13b**



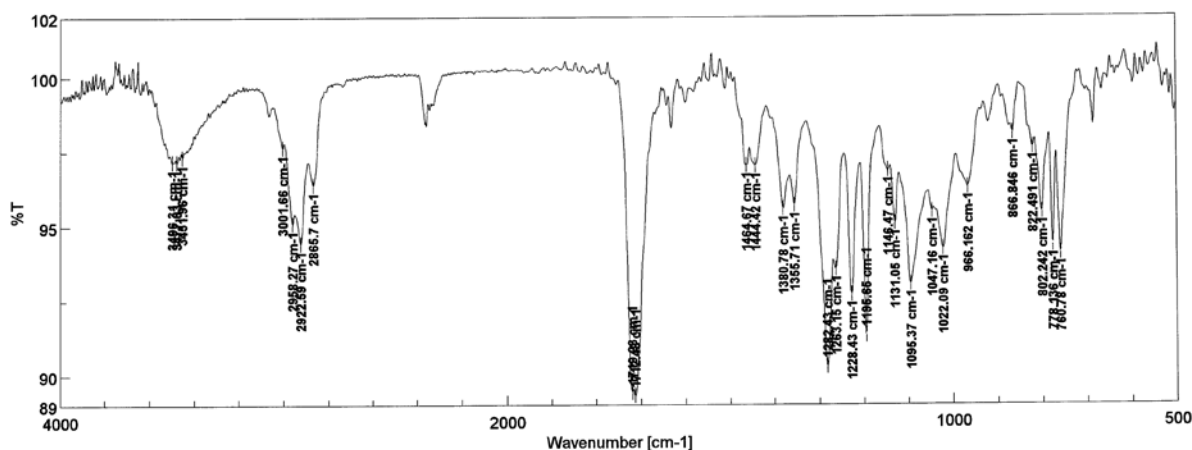
The NOESY spectrum of compound **13b**

測定データ名: KS-16.01
作成条件: 平均(MS[1]) 経過時間: 0.43.0.52
x10³ 面積 (14808)

実験日時: 2017/10/13 22:06:09
イオン化モード: ESI+

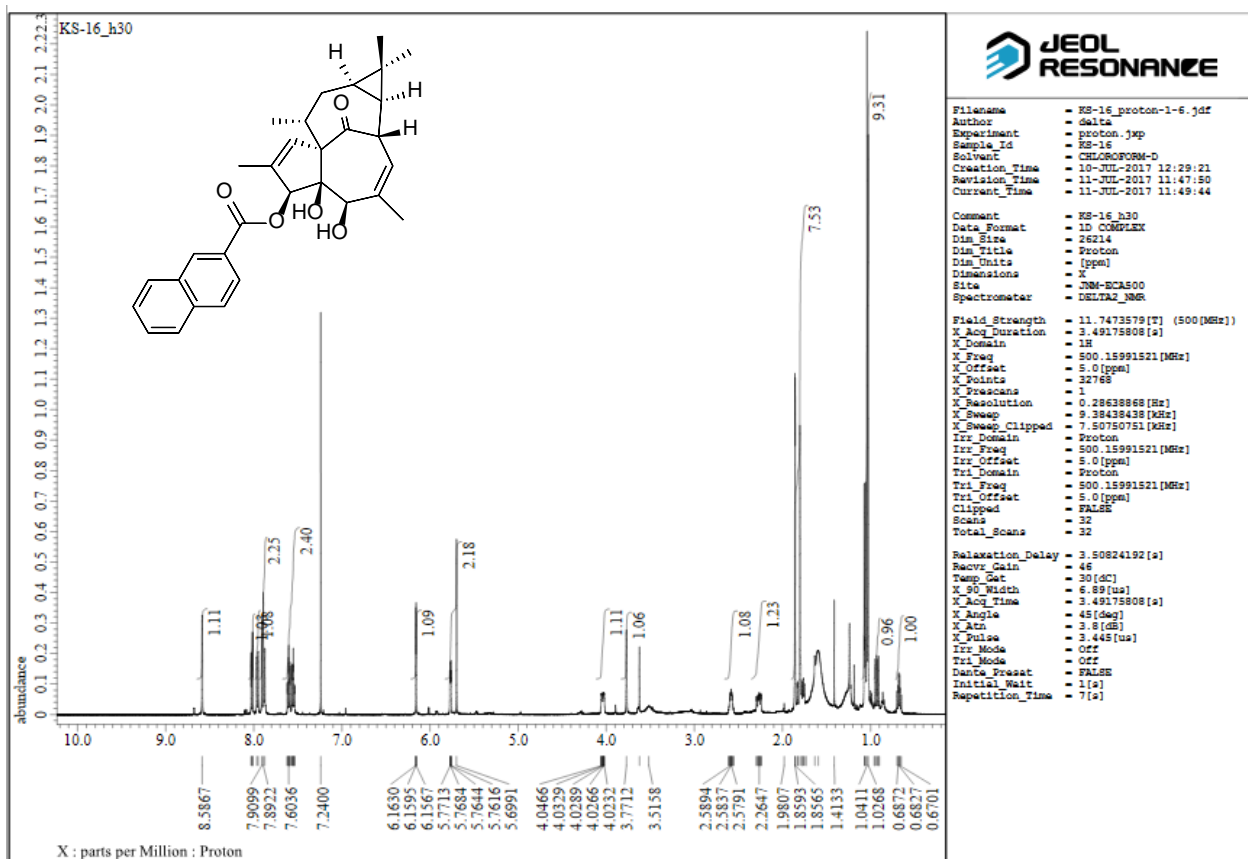


The HRESIMS spectrum of compound **14a**

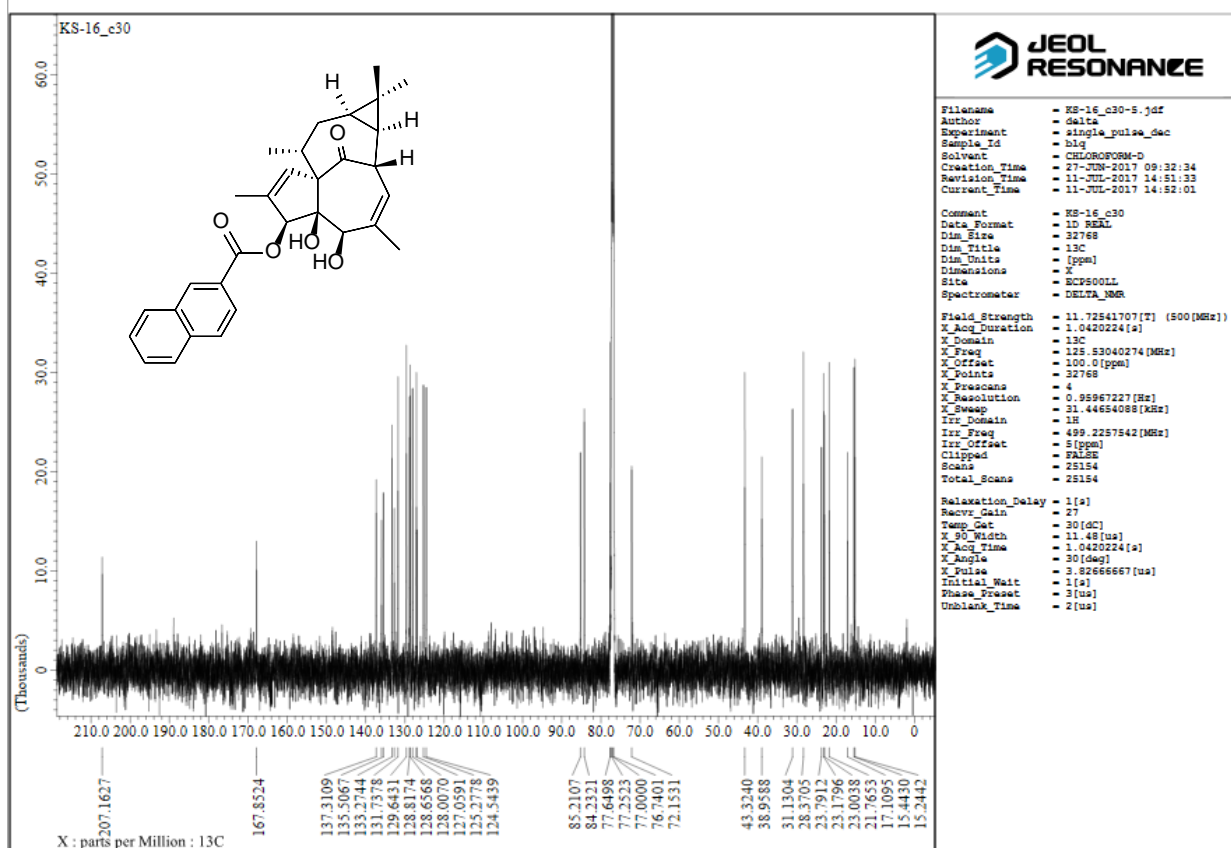


[コメント情報]	KS-16	[測定情報]	機種名 FT/IR-4100typeA	Memory-2
試料名		シリアル番号	B109261016	
測定者	B	光源	標準光源	
所属会社	東邦大学 薬学部	検出器	TGS	
		積算回数	Auto (221)	
[データ情報]		分解	4 cm-1	
作成日時	2017/07/26 16:23	ゼロフリンギング	On	
データタイプ	等間隔データ	アポダイゼーション	Cosine	
横軸	Wavenumber [cm-1]	ゲイン	Auto (16)	
縦軸	%T	アパーチャー	Auto (7.1 mm)	
スタート	0 cm-1	スキャンスピード	Auto (2 mm/sec)	
エンド	7800.65 cm-1	フィルタ	Auto (30000 Hz)	
データ間隔	0.964233 cm-1			
データ数	8091			

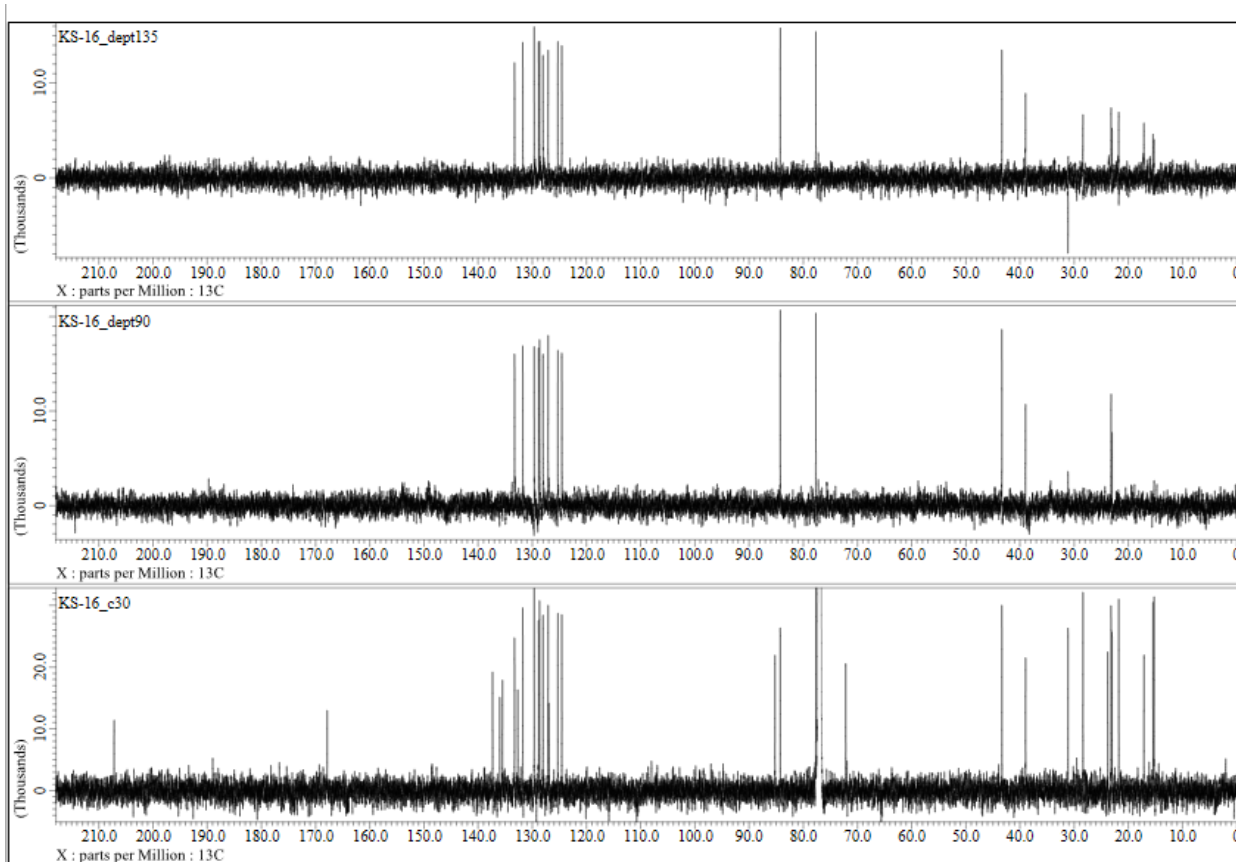
The IR spectrum of compound 14a



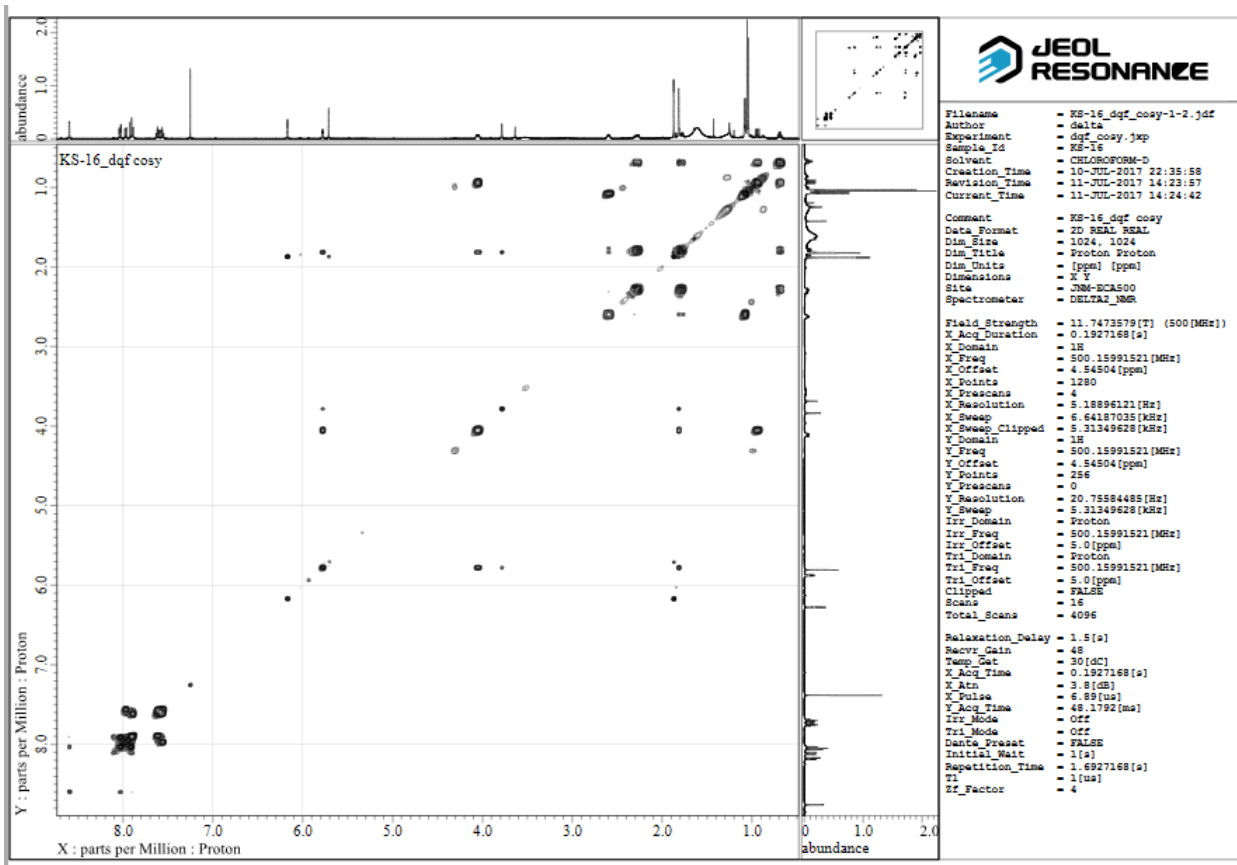
The ¹H spectrum of compound 14a



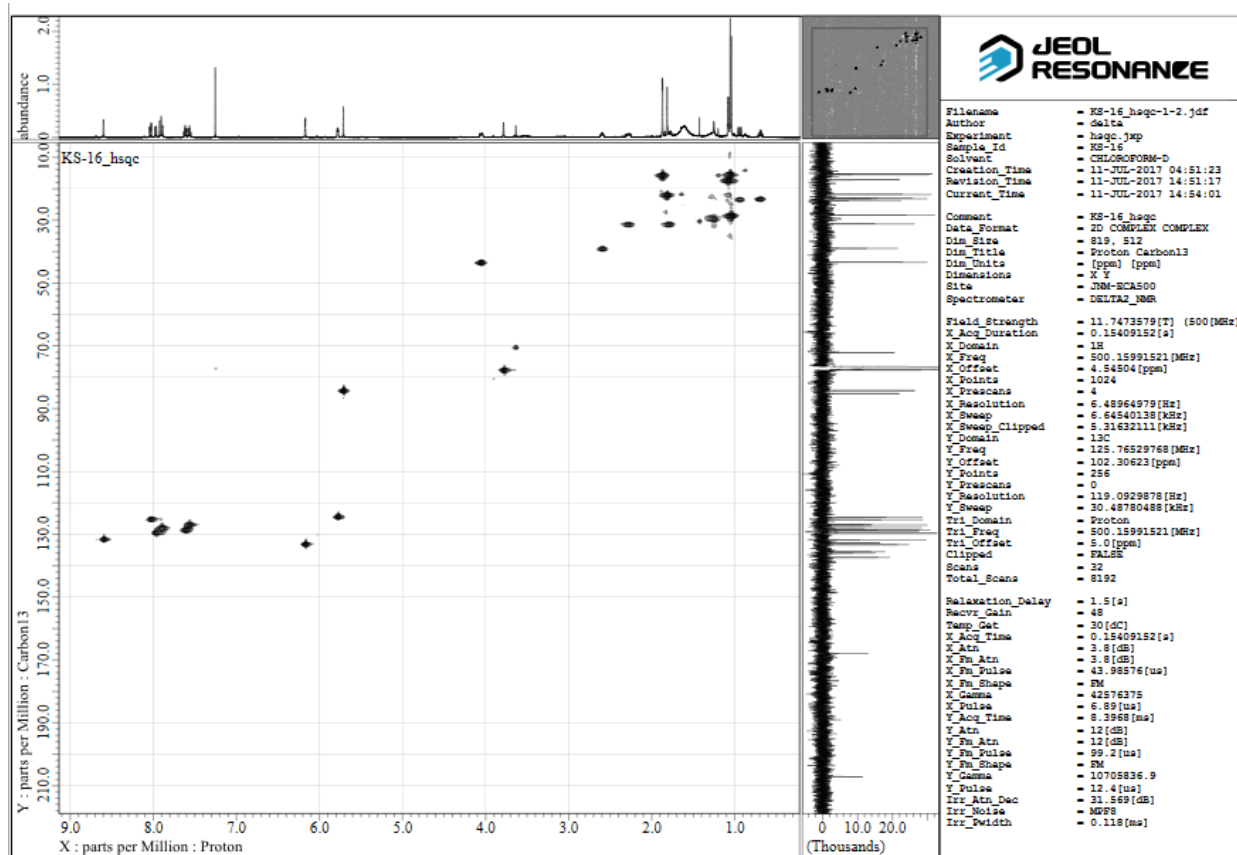
The ^{13}C spectrum of compound 14a



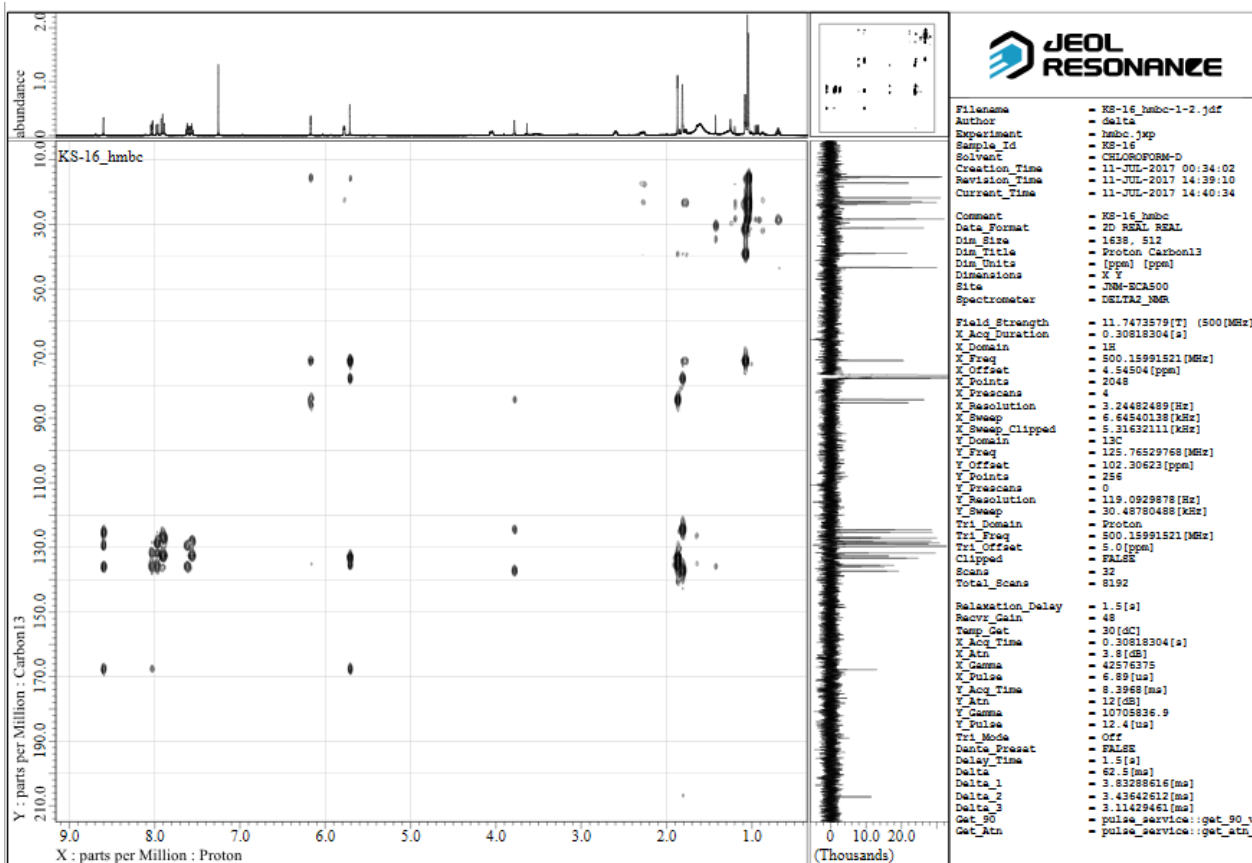
The DEPT spectrum of compound 14a



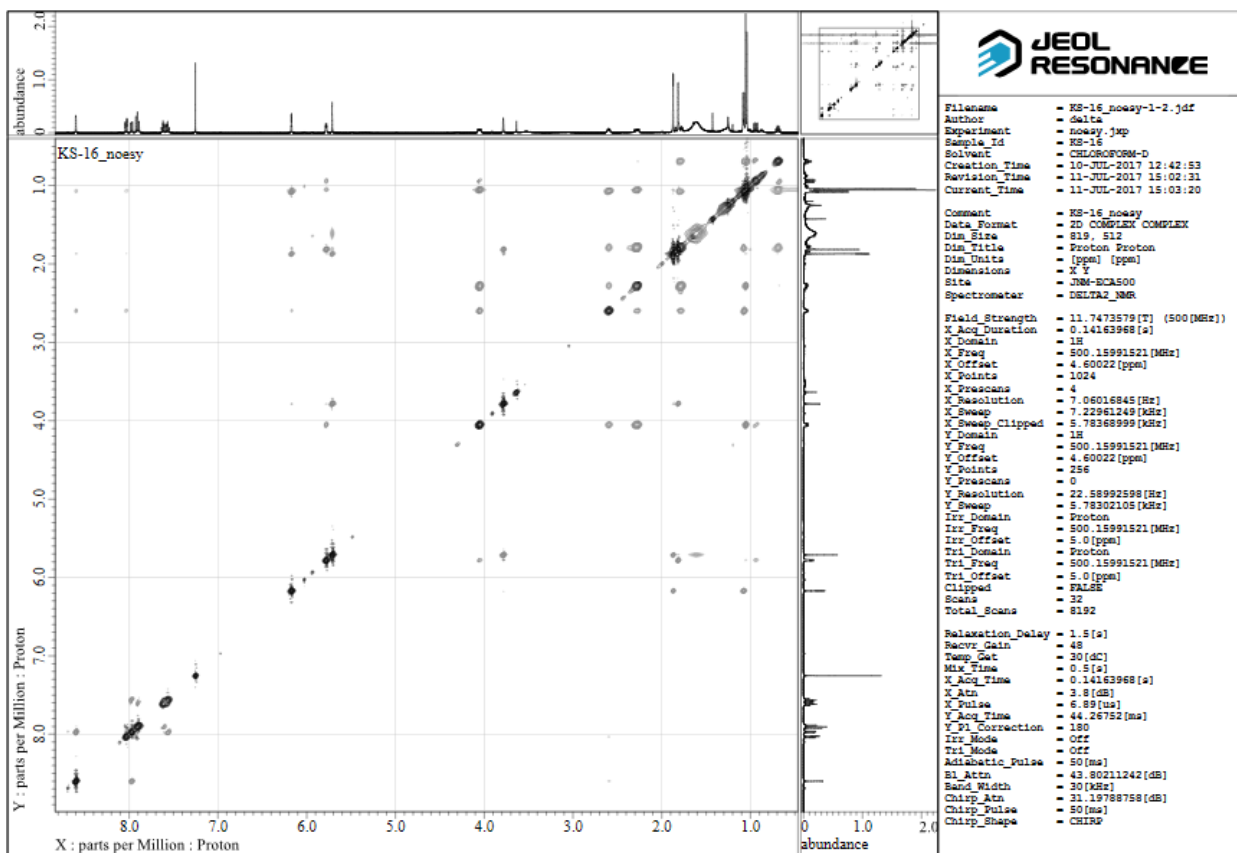
The DQF_COSY spectrum of compound 14a



The HSQC spectrum of compound 14a



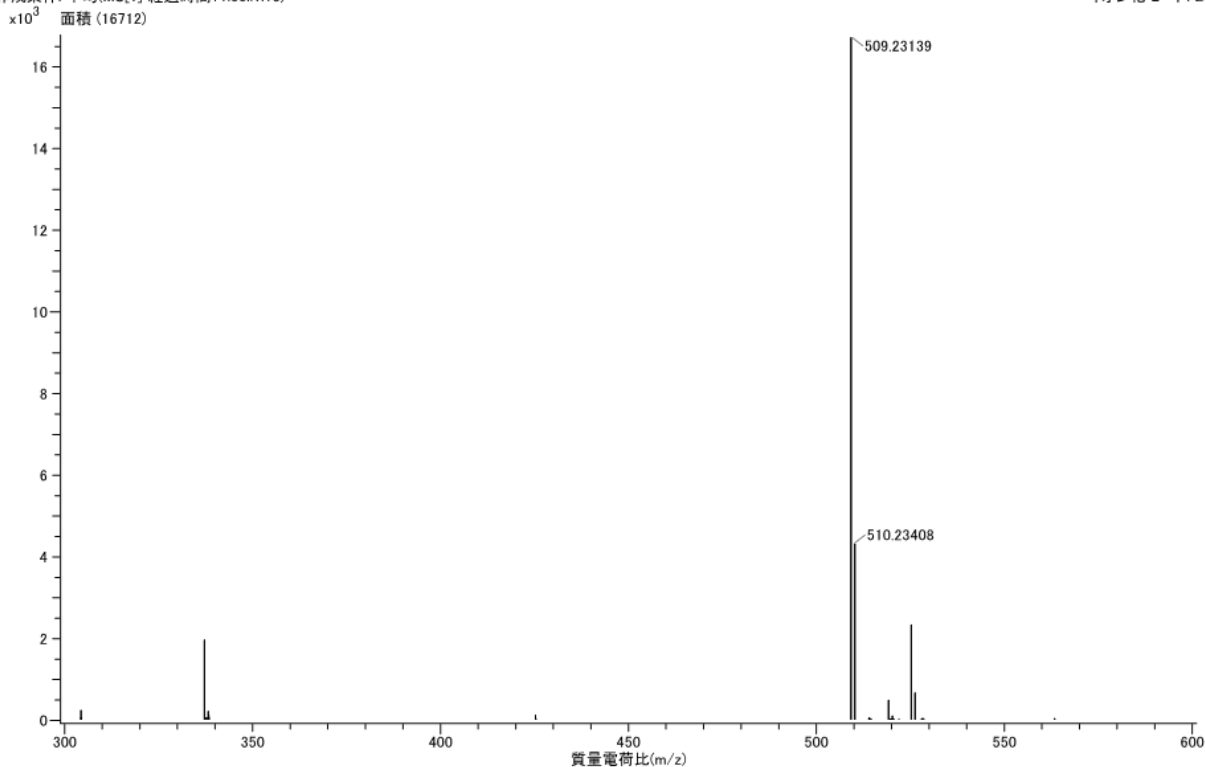
The HMBC spectrum of compound **14a**



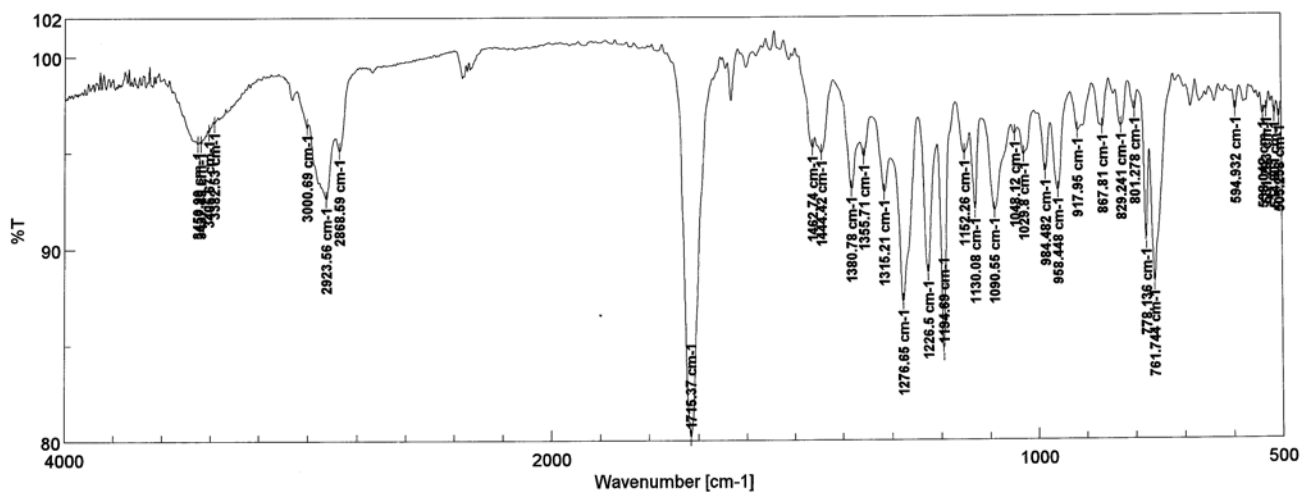
The NOESY spectrum of compound **14a**

測定データ名: KS-15_01
 作成条件: 平均(MS1) 経過時間: 1.00.1.13

実験日時: 2017/10/13 21:59:57
 イオン化モード: ESI+



The HRESIMS spectrum of compound **14b**



[コメント情報]

試料名 KS-15
 コメント
 測定者 B
 所属 東邦大学 薬学部
 会社

[測定情報]

機種名 FT/IR-4100typeA
 シリアル番号 B109261016

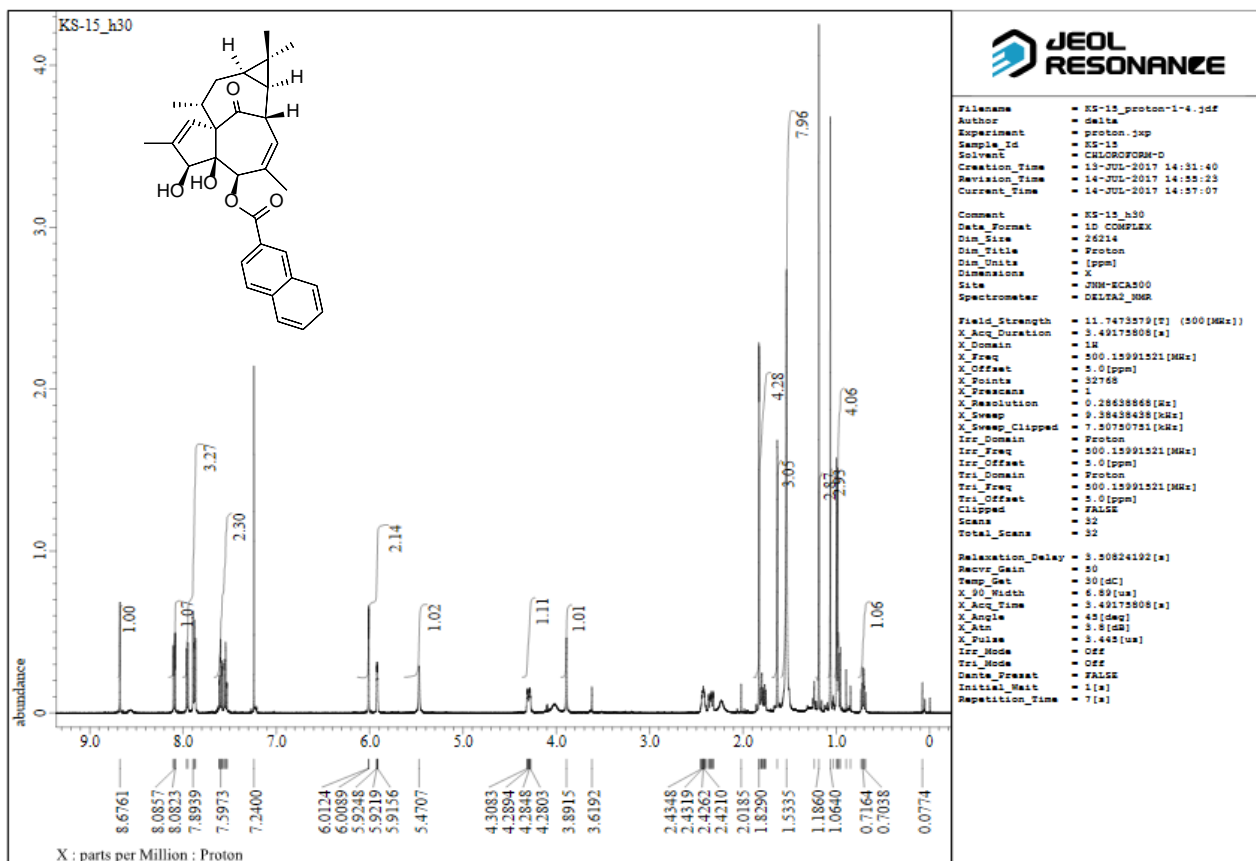
光源 標準光源
 検出器 TGS
 積算回数 Auto (221)
 分解 4 cm-1
 ゼロフィリング On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャ Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

Memory-2

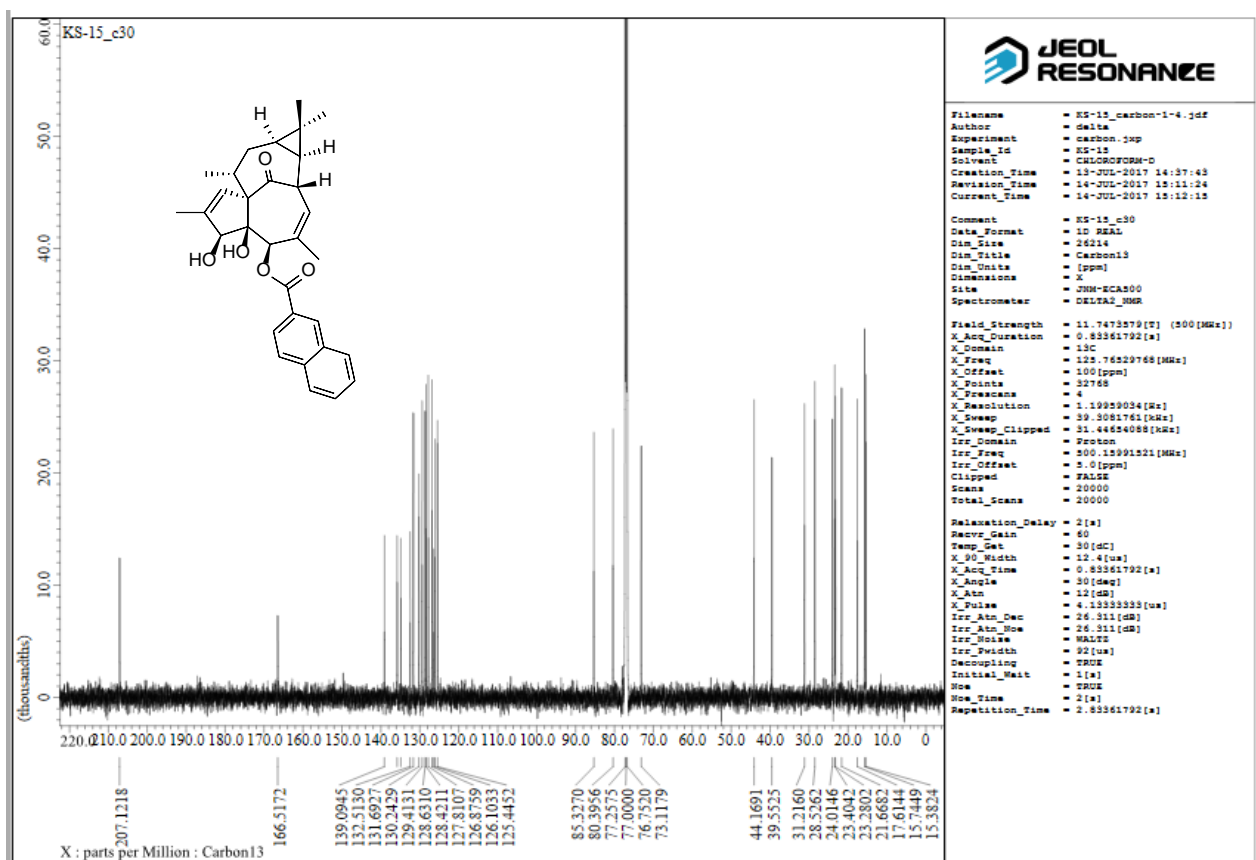
[データ情報]

作成日時 2017/07/26 16:12
 データタイプ 等間隔データ
 縦軸 Wavenumber [cm-1]
 横軸 %T
 スタート 0 cm-1
 エンド 7800.65 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

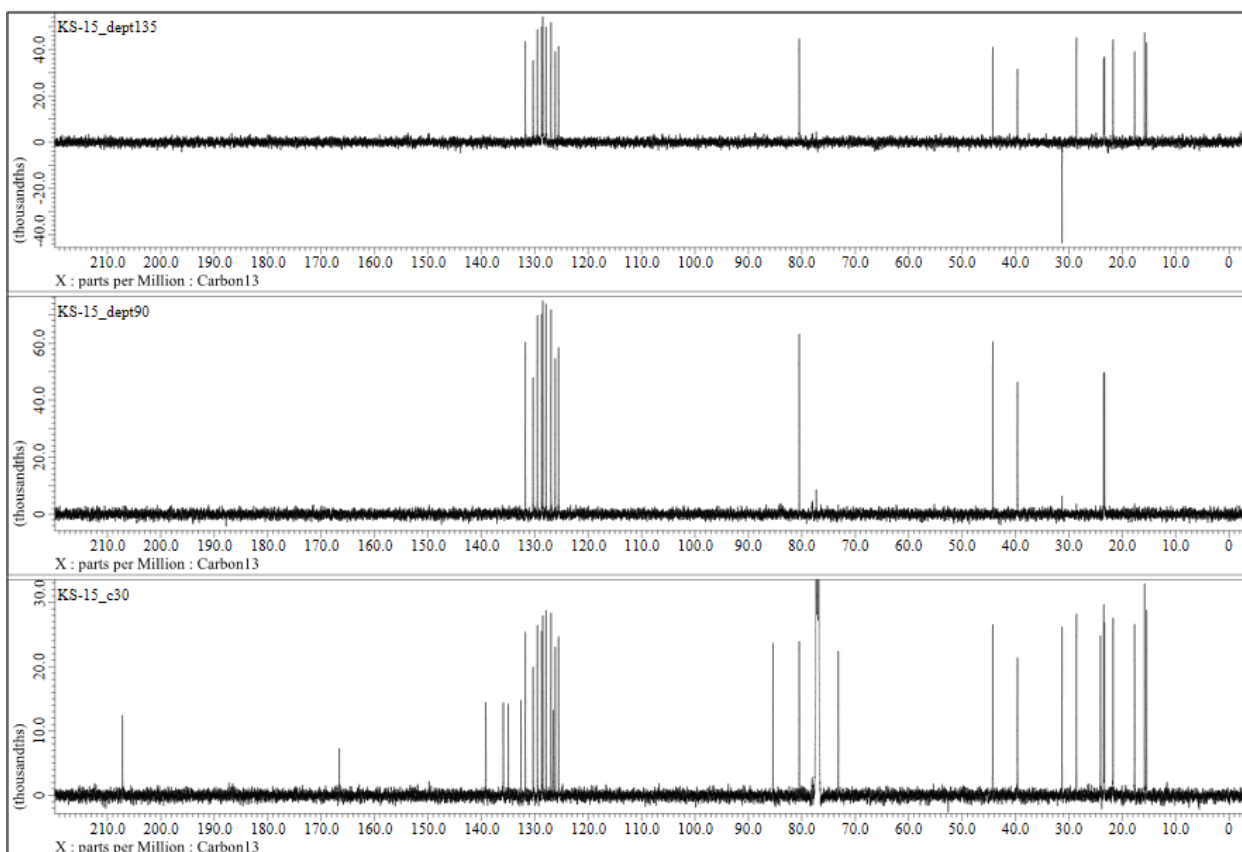
The IR spectrum of compound **14b**



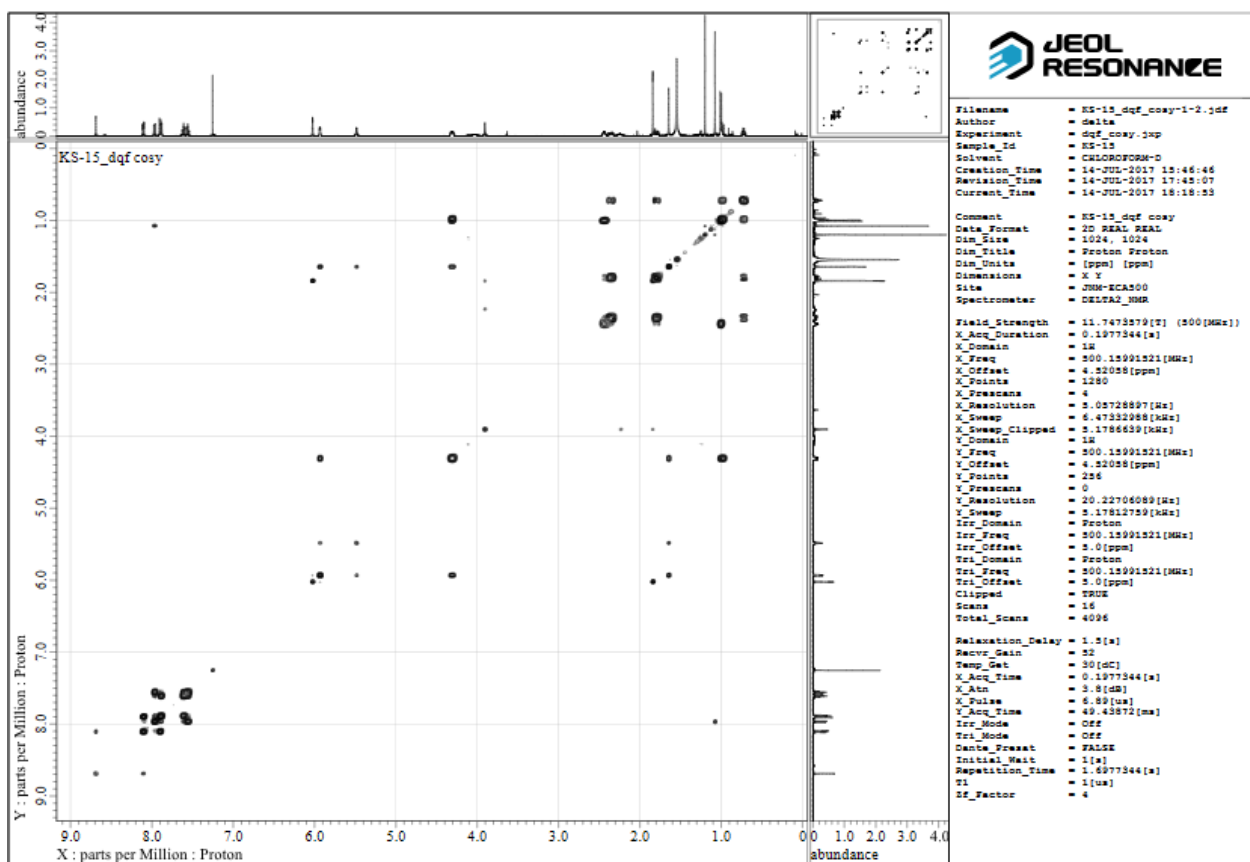
The ^1H spectrum of compound **14b**



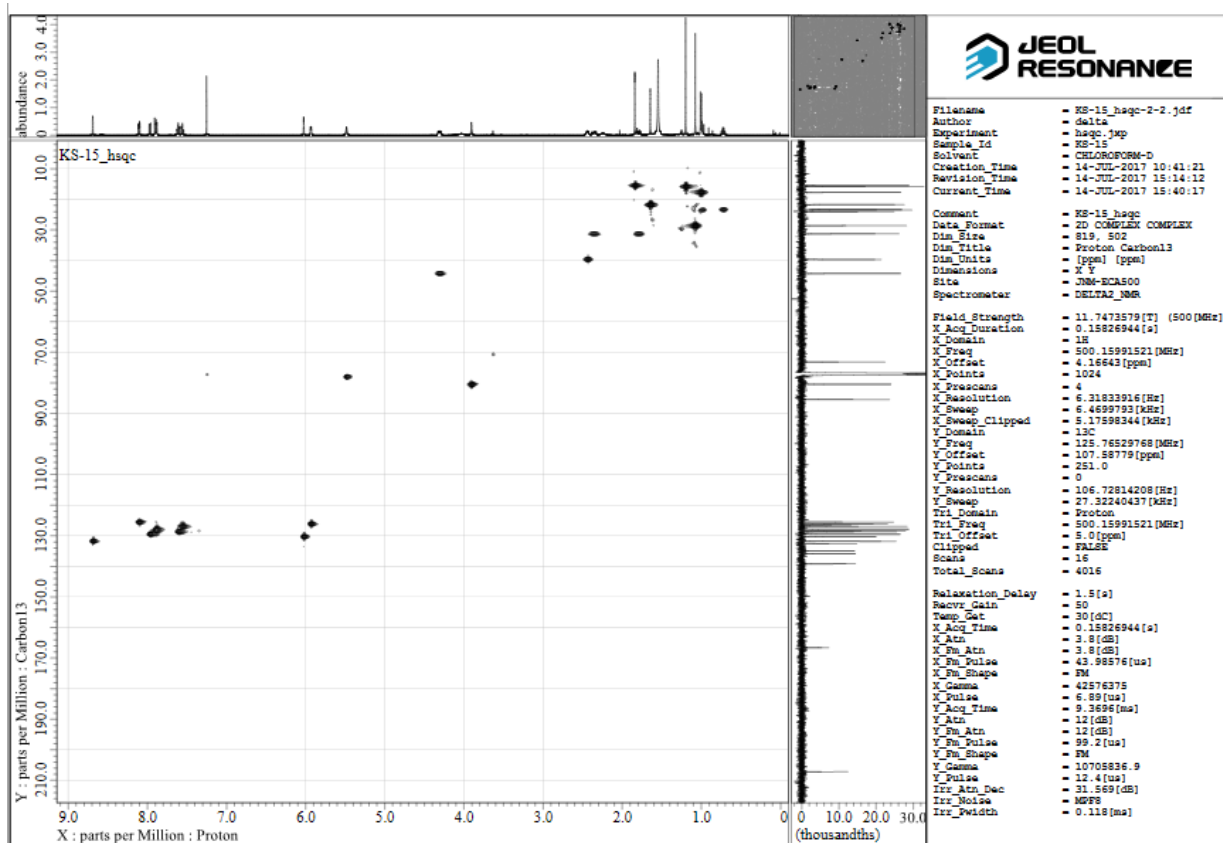
The ^{13}C spectrum of compound **14b**



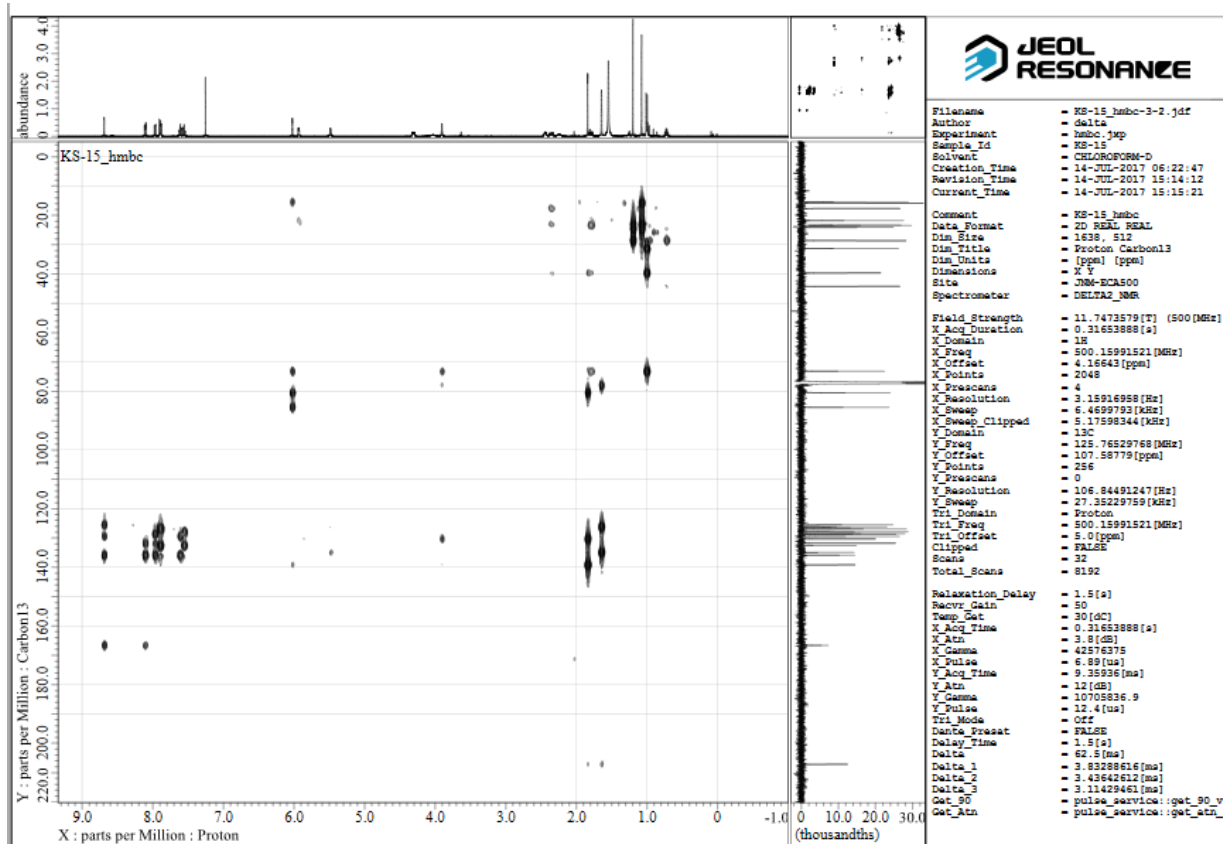
The DEPT spectrum of compound **14b**



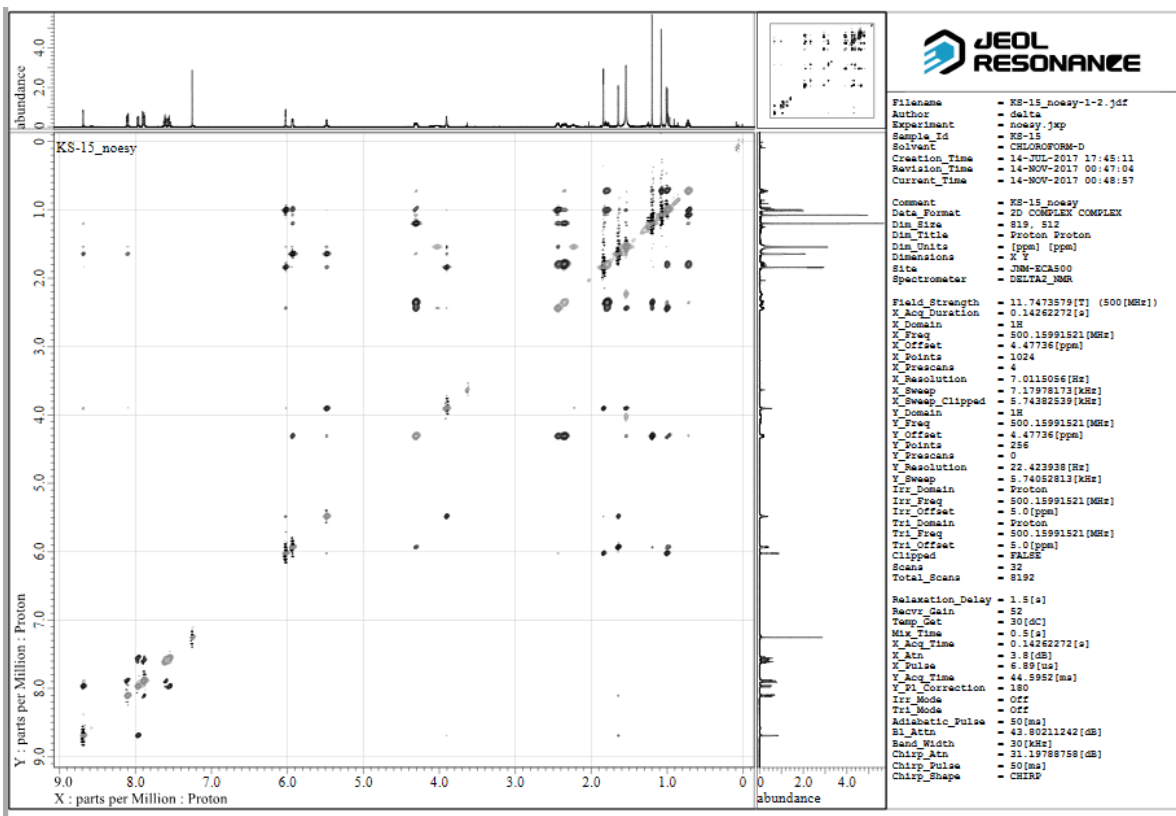
The DQF-COSY spectrum of compound **14b**



The HSQC spectrum of compound **14b**

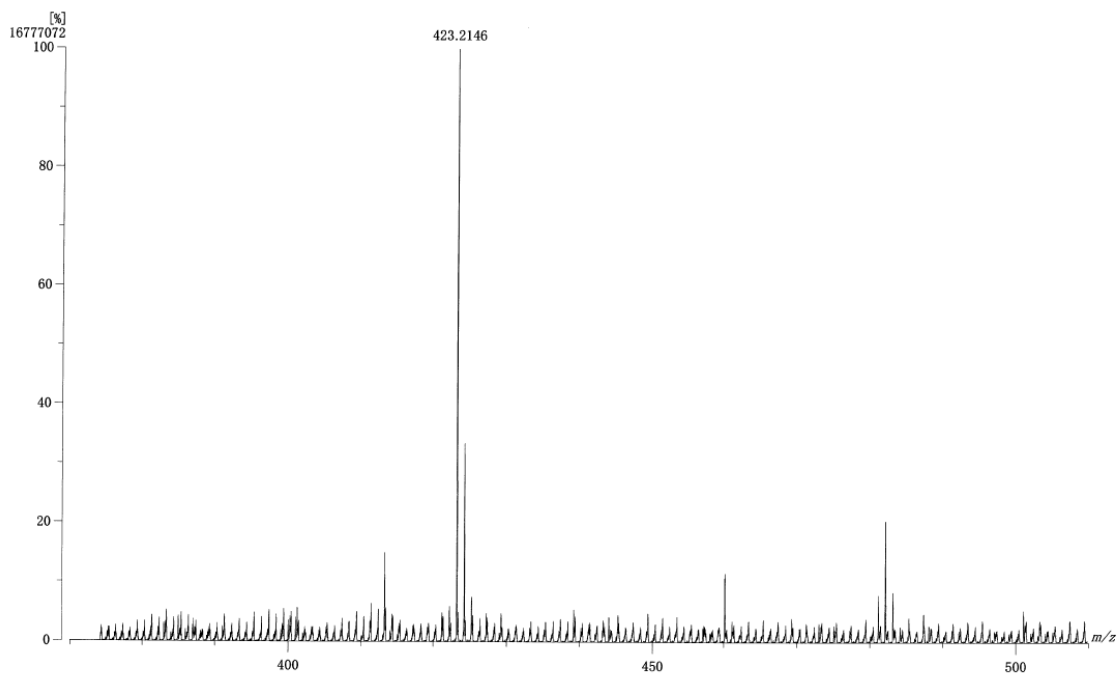


The HMBC spectrum of compound **14b**

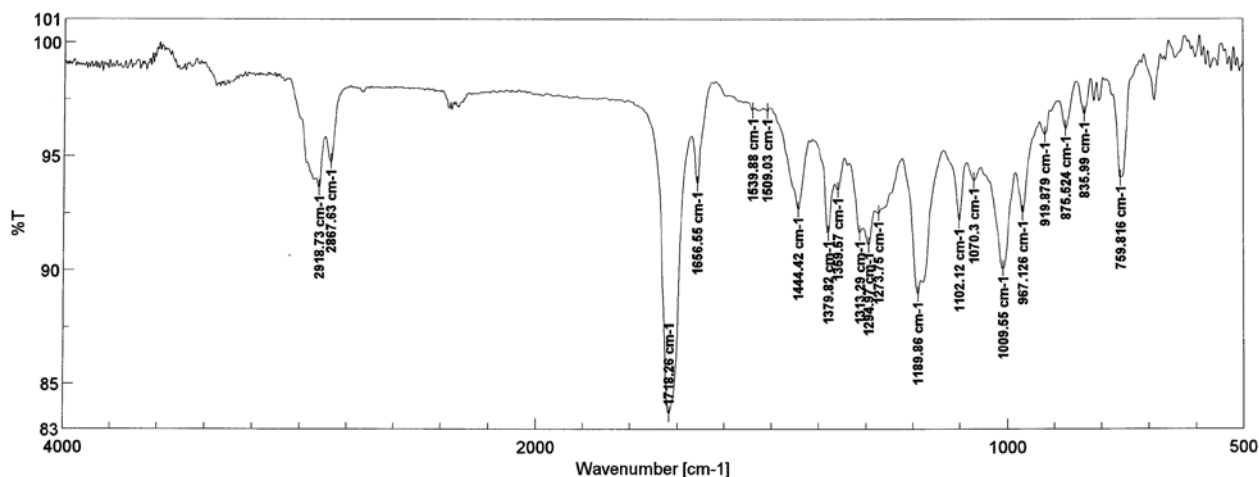


The NOESY spectrum of compound **14b**

[Mass Spectrum]
 Data : KS-3Na-FABpHRI-NBA Date : 18-Aug-2017 15:27
 Instrument : MStation
 Sample : KS-3
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 3.94 min Scan# : 14 Temp : 3276.7 deg.C
 BP : m/z 423.2146 Int. : 1599.99 (16777072)
 Output m/z range : 370 to 510 Cut Level : 0.00 %

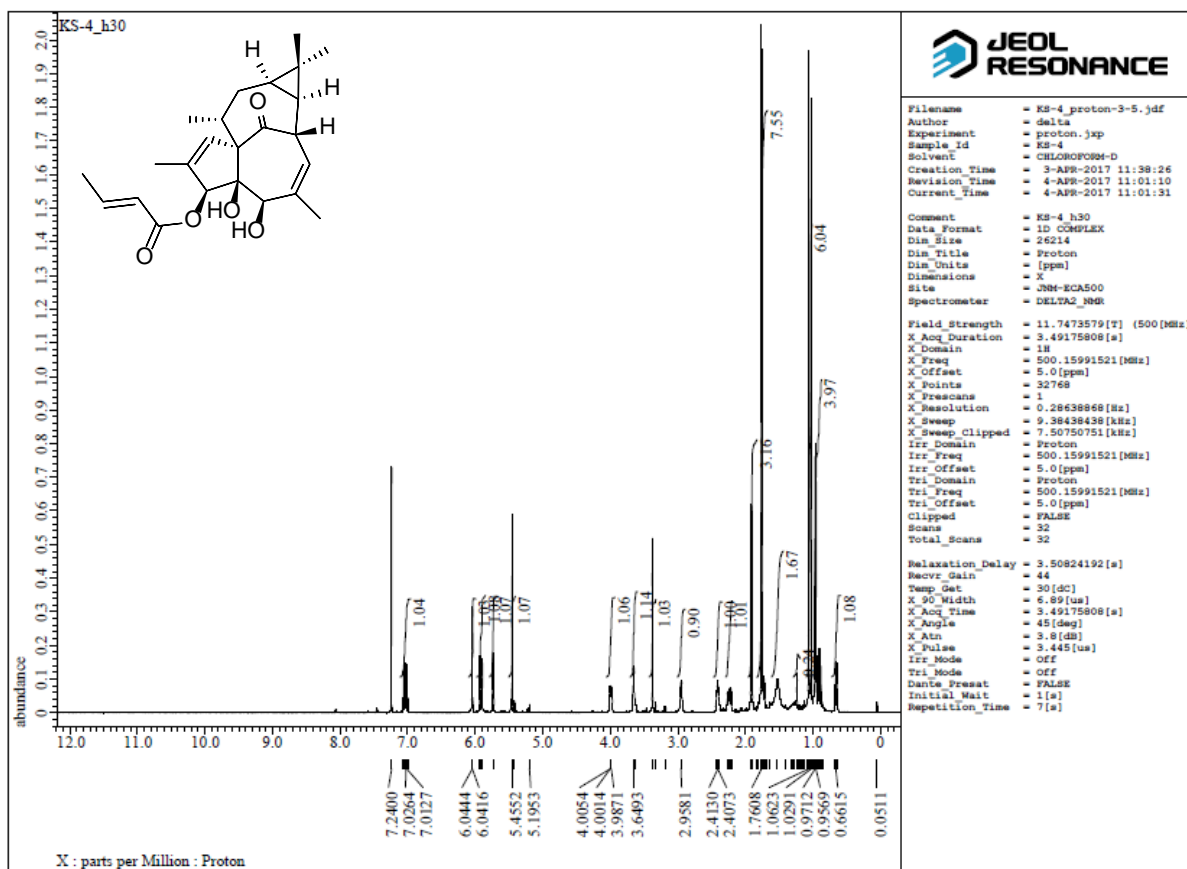


The HRFABMS spectrum of compound **15a**

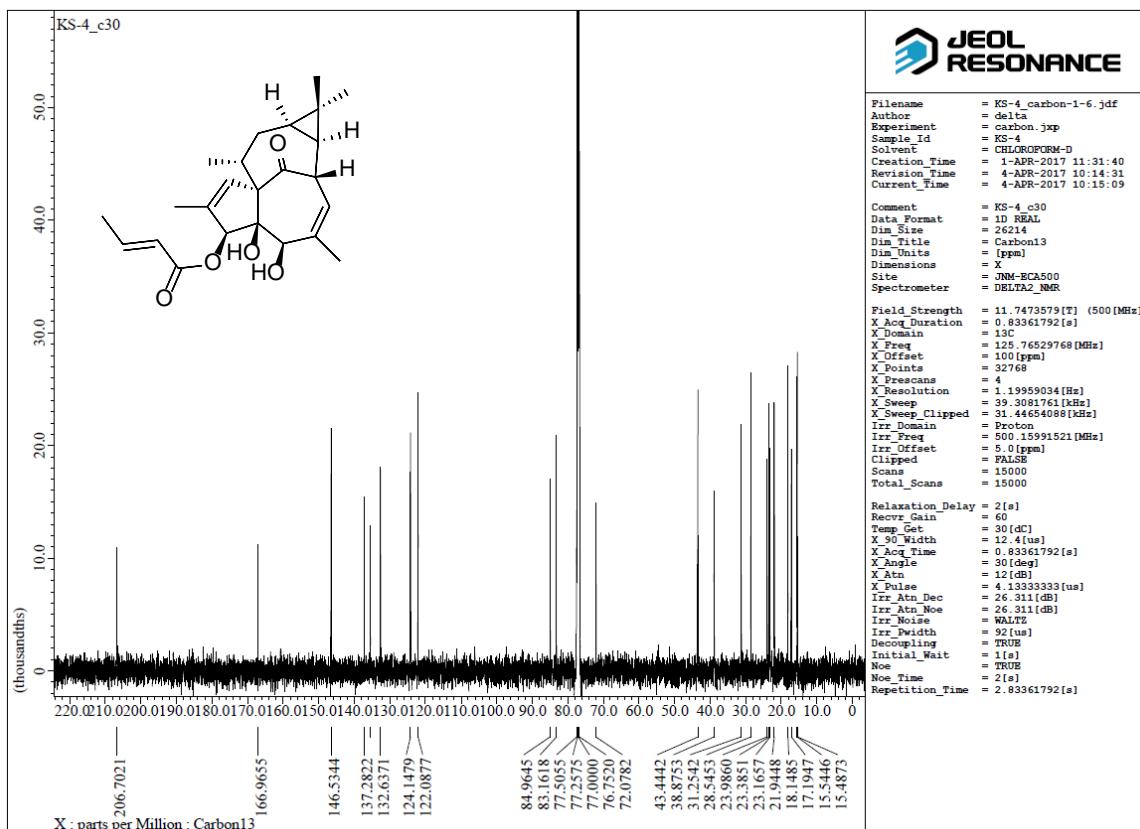


<p>[コメント情報] 試料名 KS-4 コメント 測定者 所属 会社</p> <p>[データ情報] 作成日時 2017/07/26 13:08 データタイプ 等間隔データ 横軸 Wavenumber [cm-1] 縦軸 %T スタート 0 cm-1 エンド 7800.65 cm-1 データ間隔 0.964233 cm-1 データ数 8091</p>	<p>[測定情報] 機種名 FT/IR-4100typeA シリアル番号 B109261016</p> <p>光源 標準光源 検出器 TGS 積算回数 Auto (178) 分解 4 cm-1 ゼロファイリング On アポダイゼーション Cosine ゲイン Auto (16) アパーチャ Auto (7.1 mm) スキャンスピード Auto (2 mm/sec) フィルタ Auto (30000 Hz)</p>	<p>Memory-5</p>
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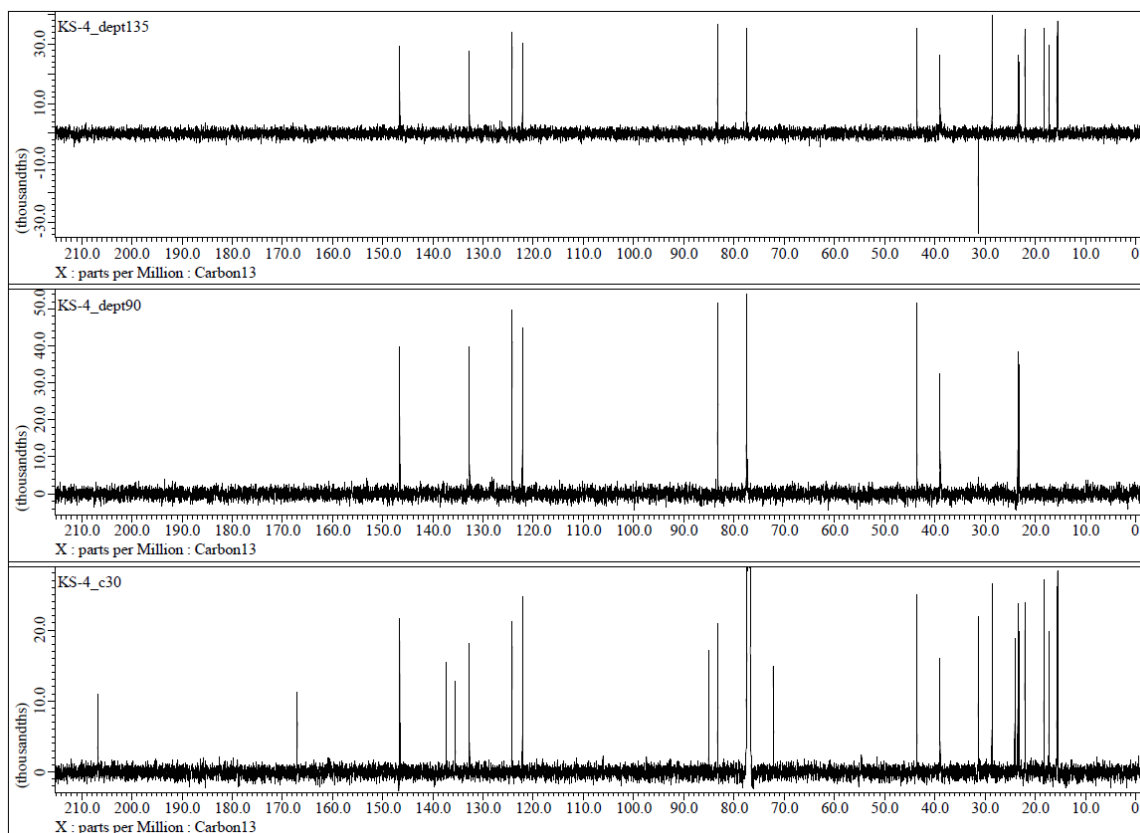
The IR spectrum of compound 15a



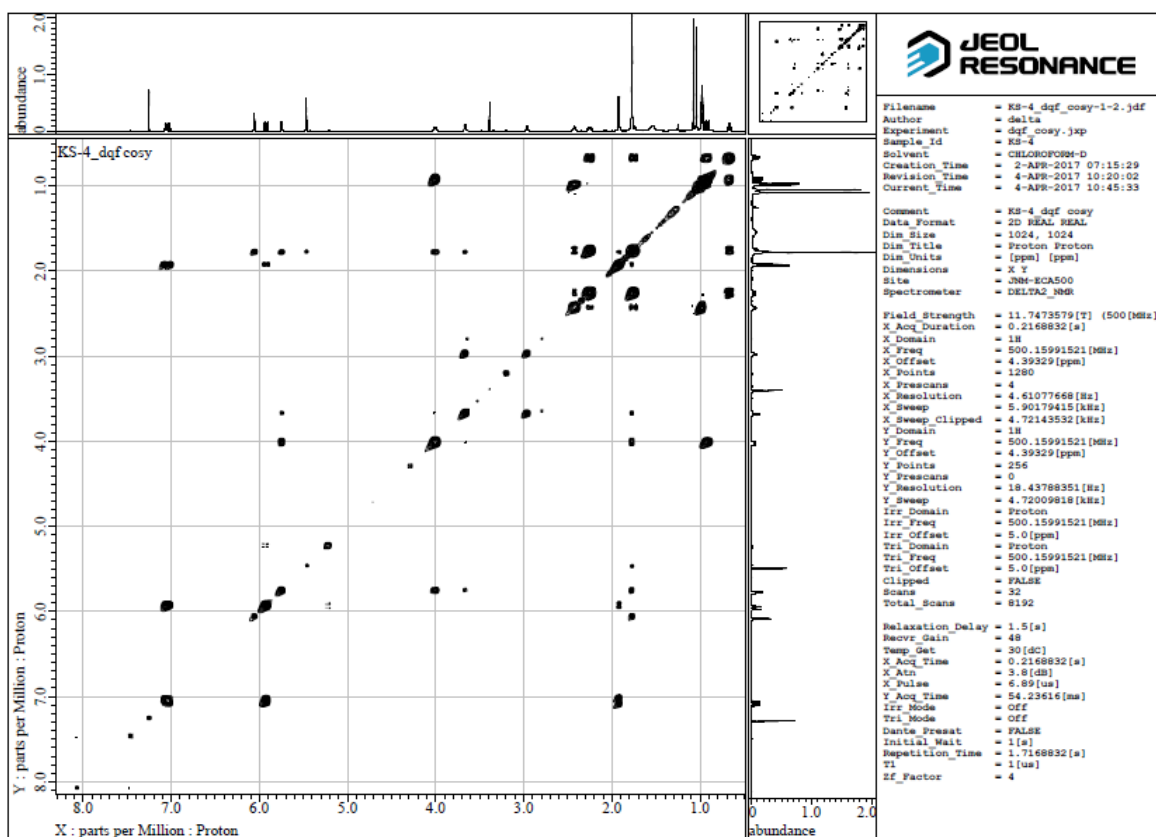
The ¹H spectrum of compound 15a



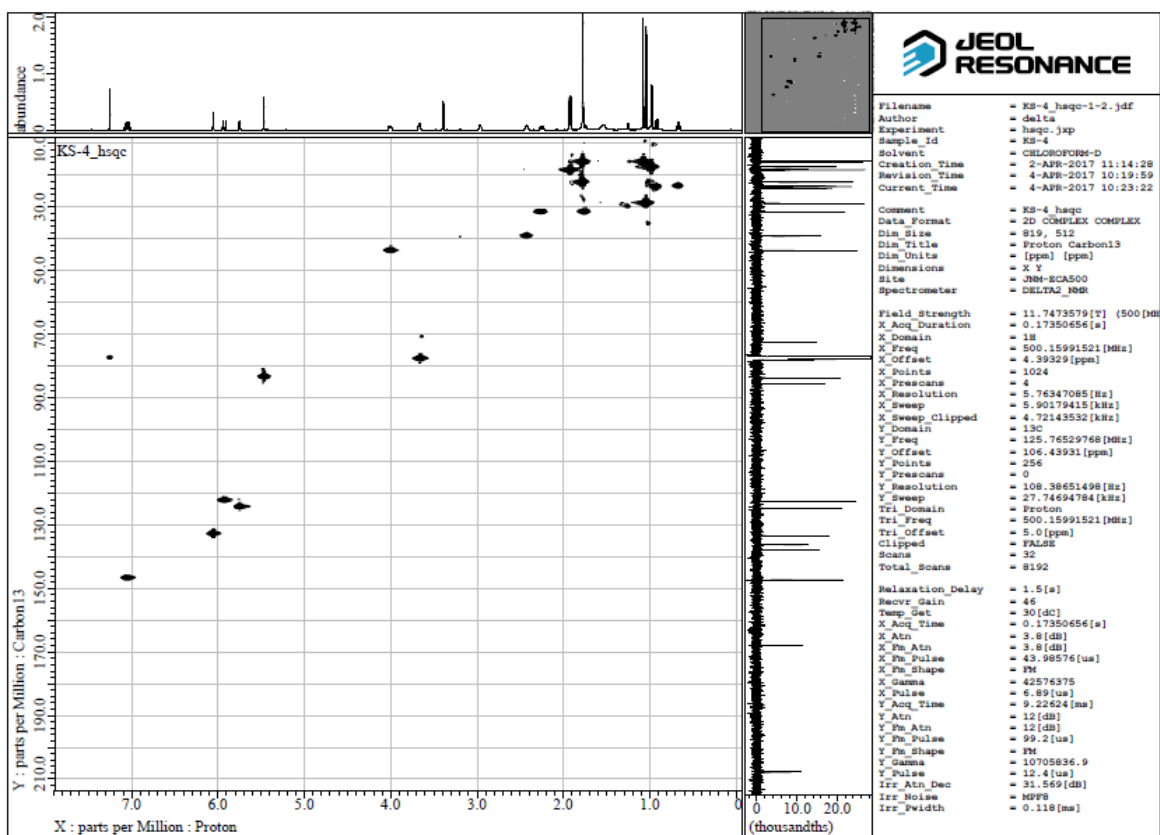
The ^{13}C spectrum of compound 15a



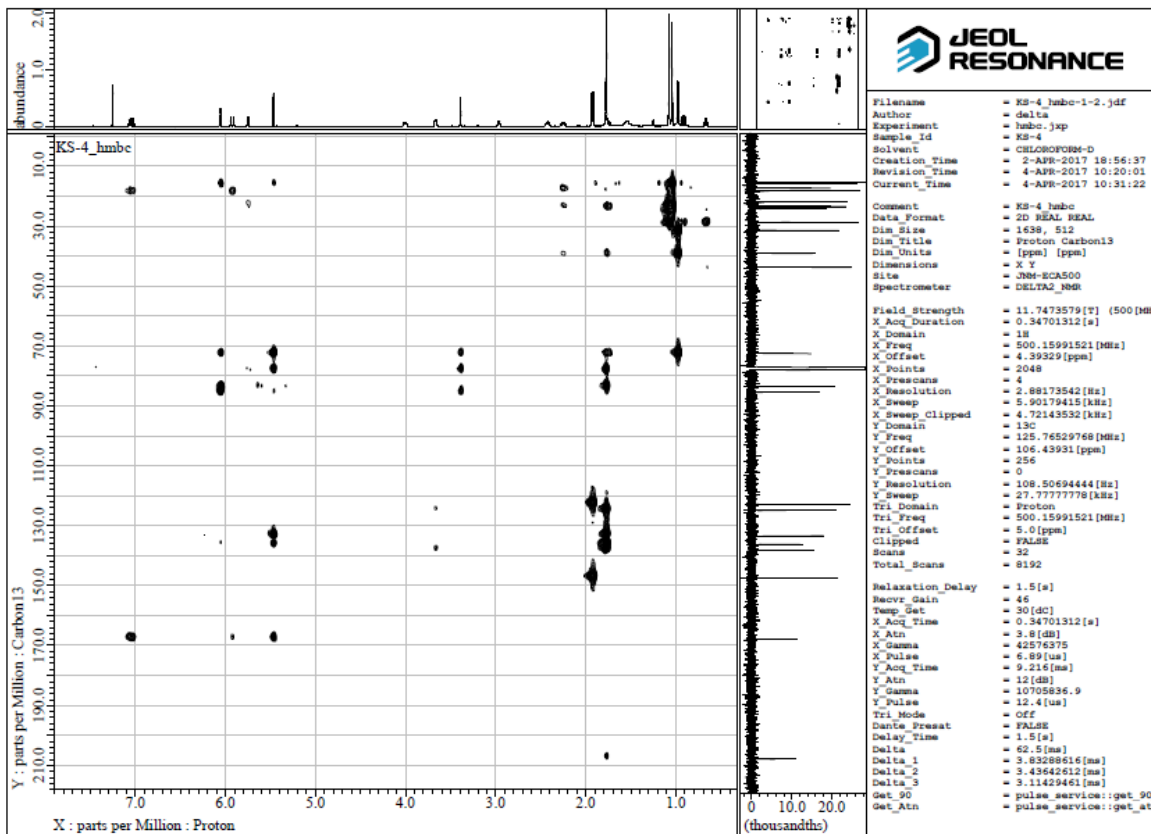
The DEPT of compound 15a



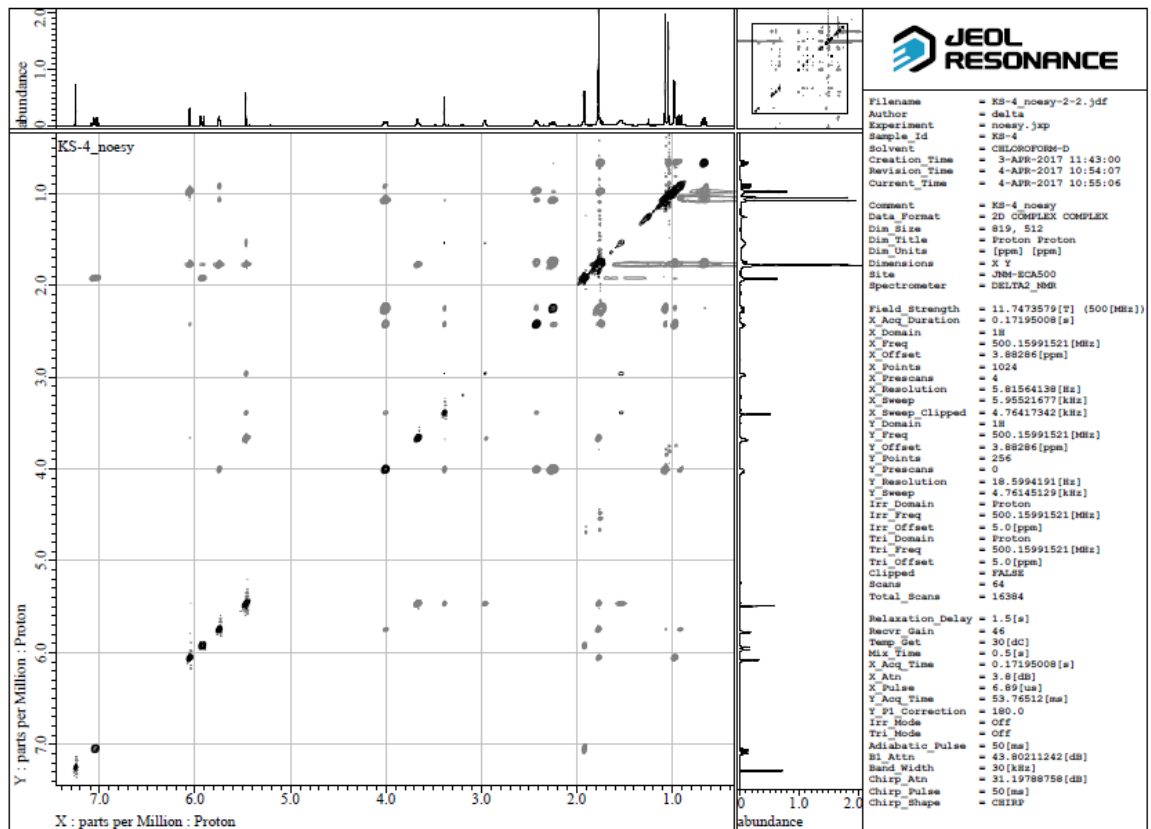
The DQF_COSY of compound 15a



The HSQC of compound 15a

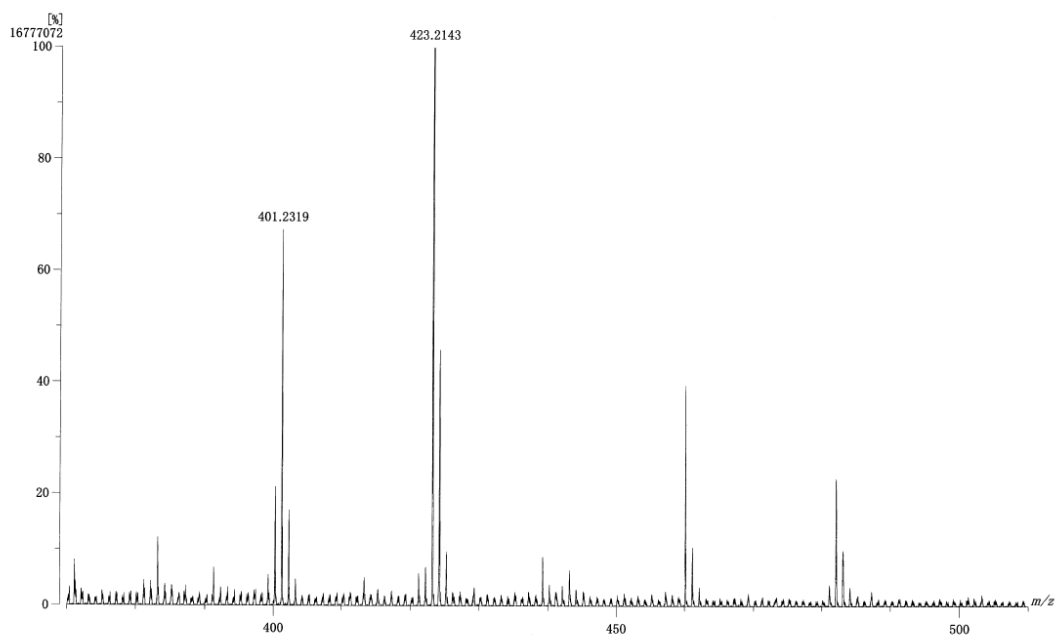


The HMBC of compound 15a

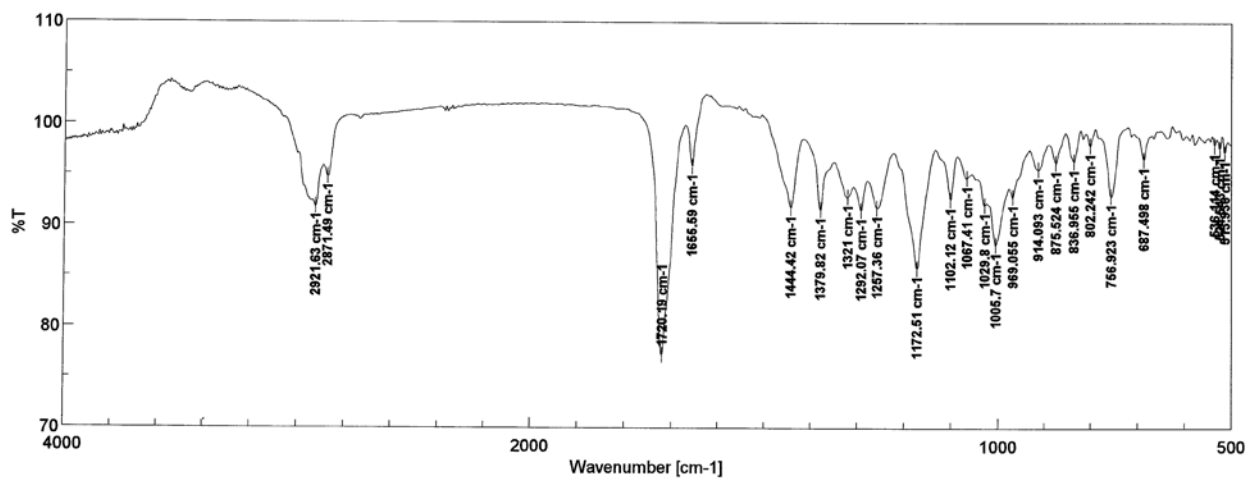


The NOESY of compound 15a

[Mass Spectrum]
 Data : KS-4+Na-FABpHR1-NBA Date : 18-Aug-2017 12:24
 Instrument : MStation
 Sample : KS-4
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [EF-Linear]
 RT : 5.15 min Scan# : 18 Temp : 327.6 deg.C
 BP : m/z 423.2143 Int. : 1599.99 (16777072)
 Output m/z range : 370 to 510 Cut Level : 0.00 %



The HRFABMS spectrum of compound **15b**

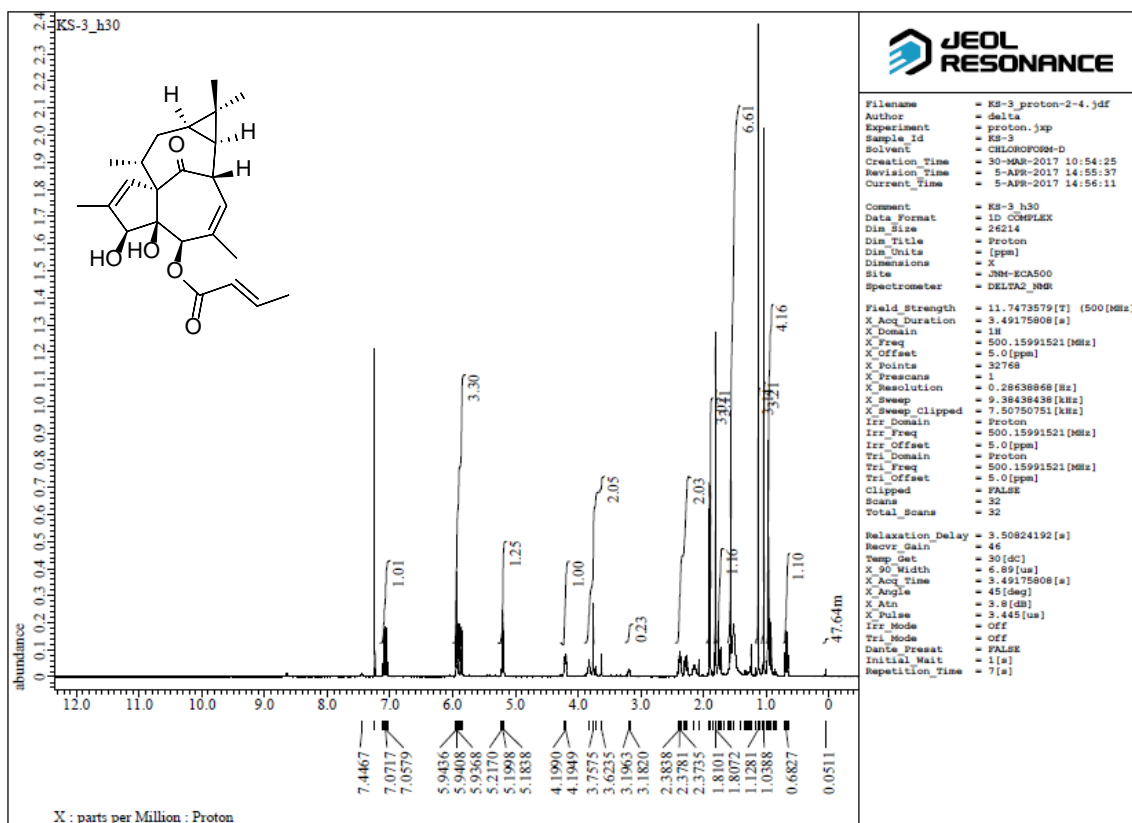


[コメント情報]
 試料名 KS-3
 コメント
 測定者 B
 所属 東邦大学 薬学部
 会社
 [データ情報]
 作成日時 2017/07/26 12:54
 データタイプ 等間隔データ
 横軸 Wavenumber [cm-1]
 縦軸 %T
 スタート 0 cm-1
 エンド 7800.65 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

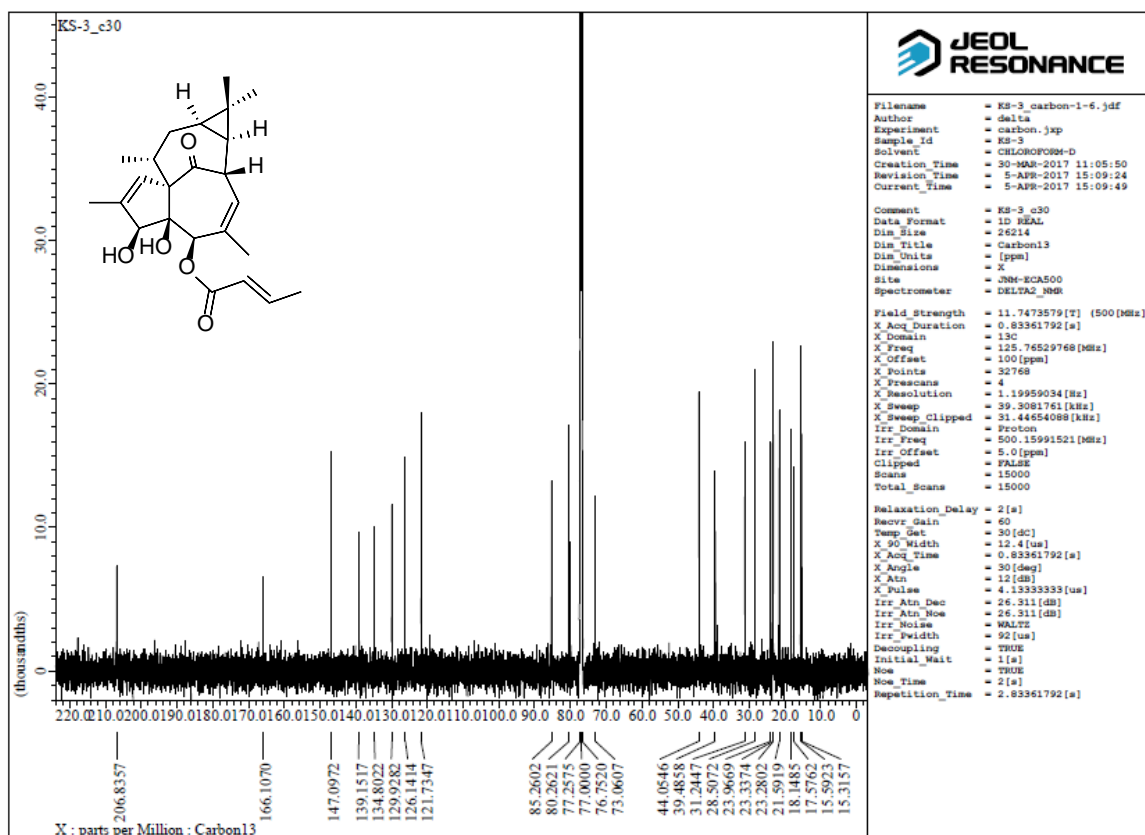
[測定情報]
 機種名 FT/IR-4100typeA
 シリアル番号 B109261016
 光源 標準光源
 検出器 TGS
 積算回数 Auto (188)
 分解 4 cm-1
 ゼロフライング On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャ Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

Memory-2

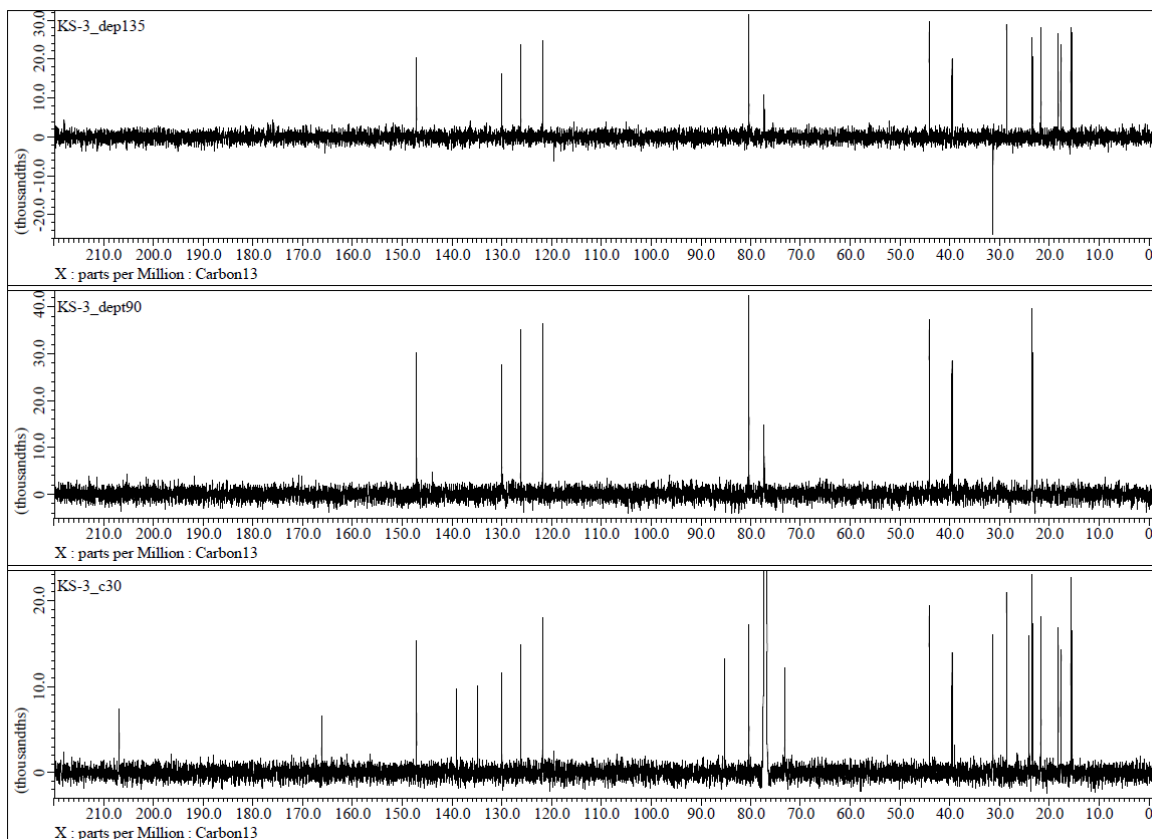
The IR spectrum of compound **KS-3**



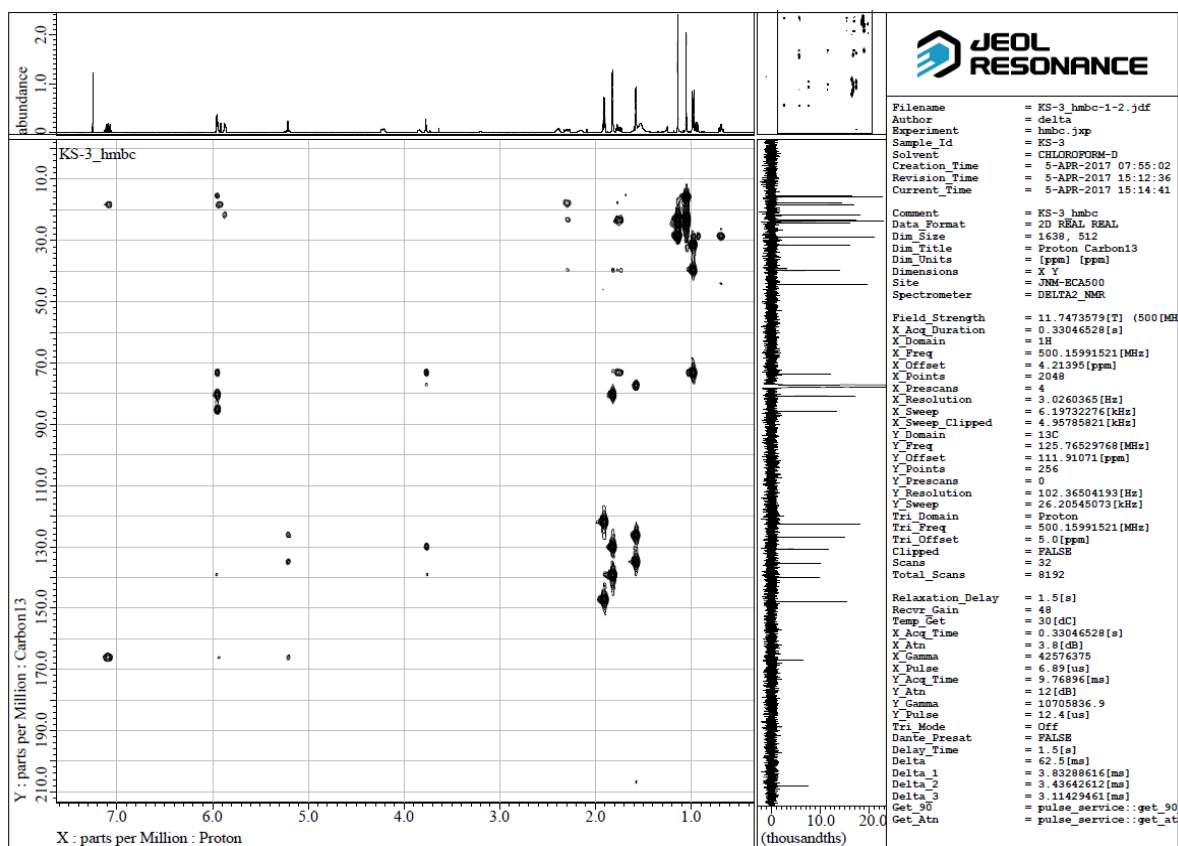
The ^1H spectrum of compound 15b



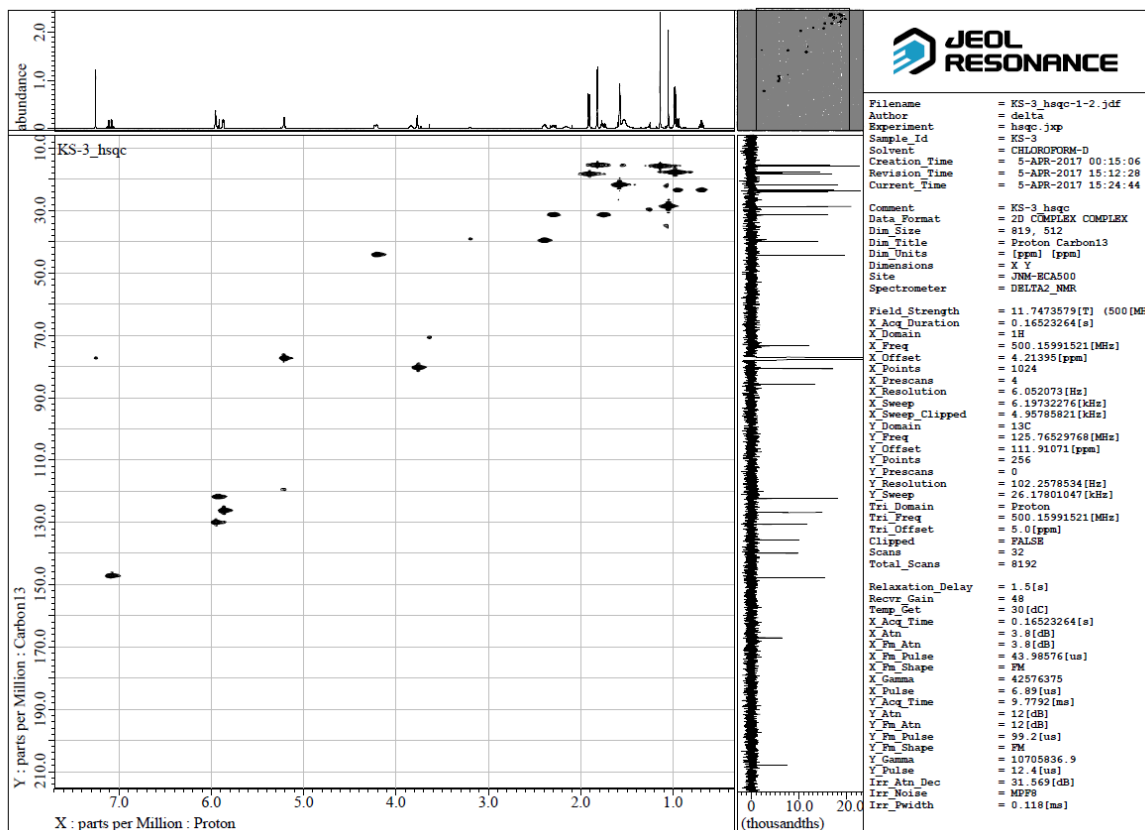
The ^{13}C spectrum of compound 15b



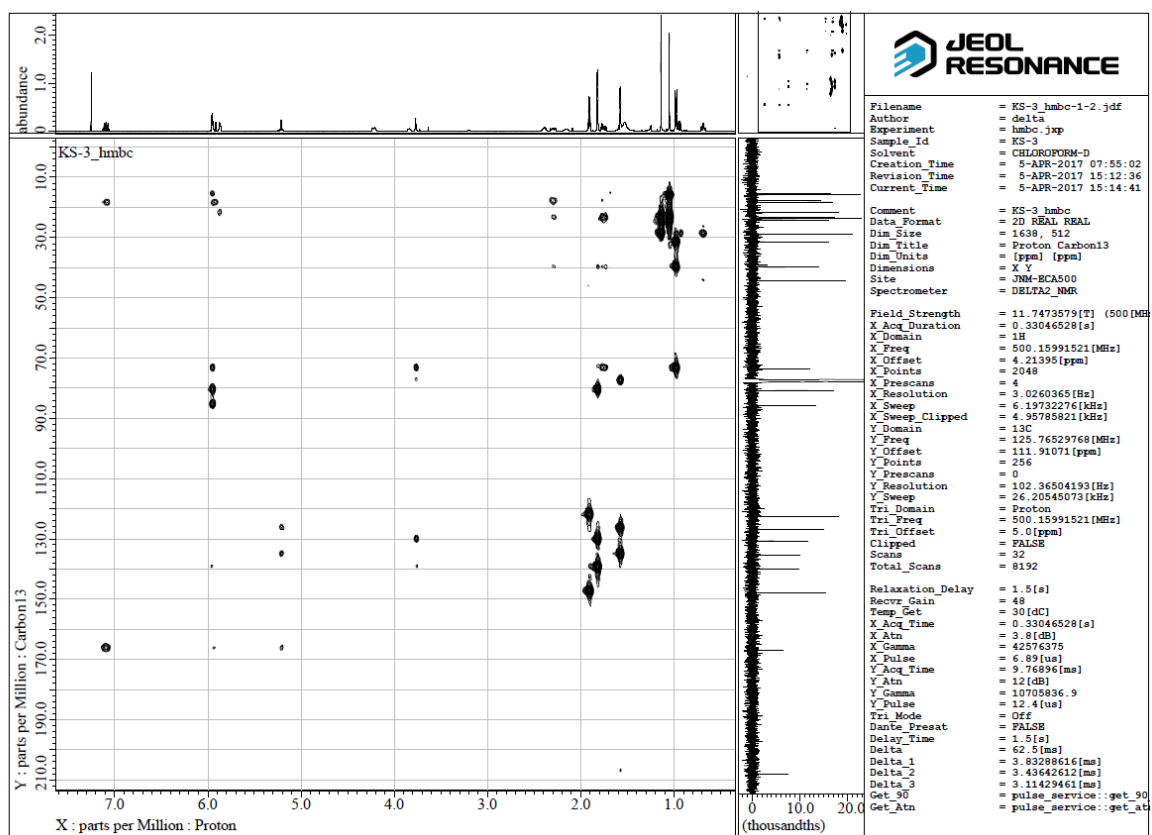
The DEPT spectrum of compound **15b**



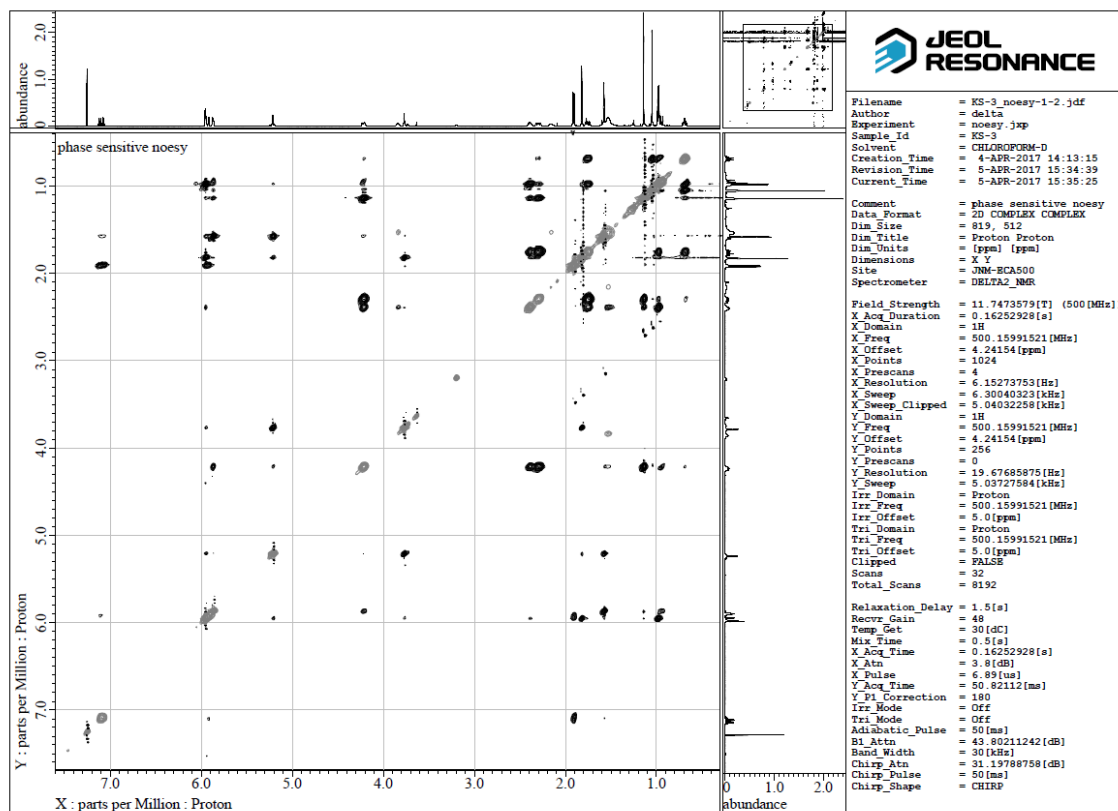
The DQF_COSY spectrum of compound **15b**



The HSQC spectrum of compound **15b**



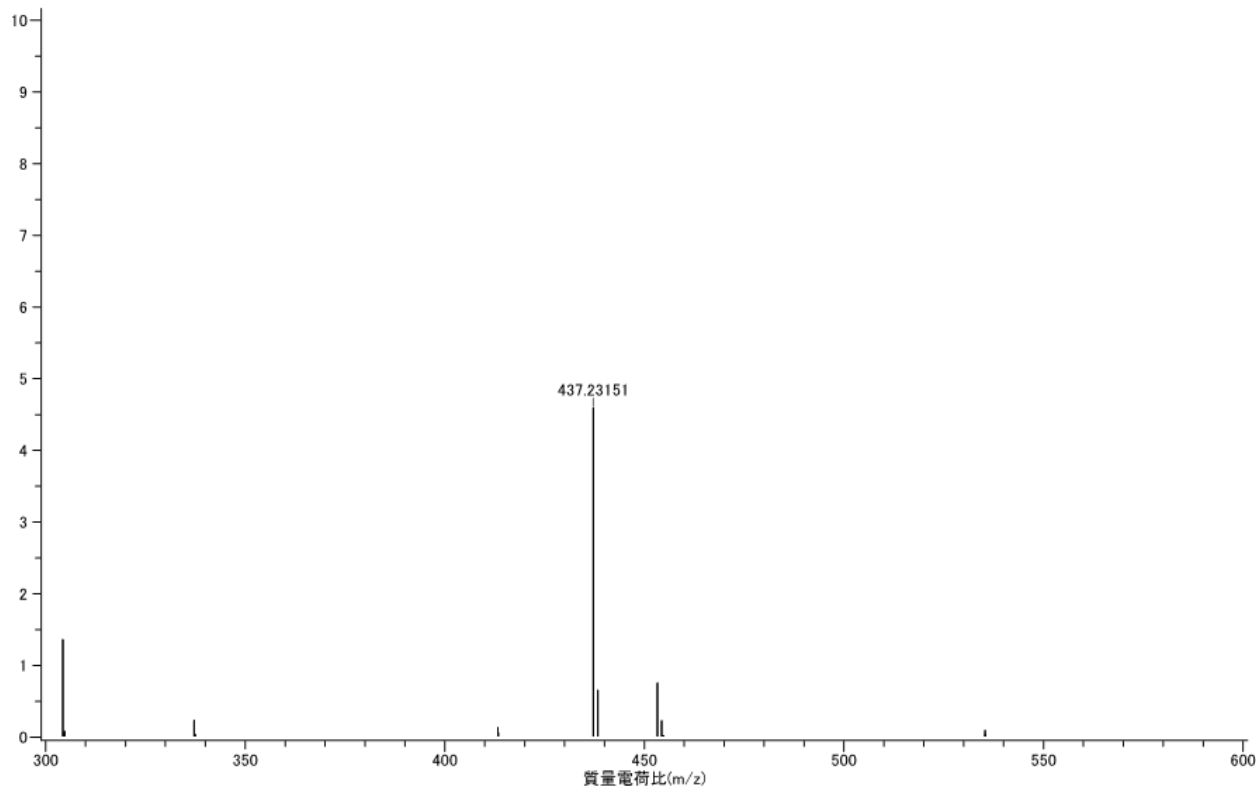
The HMBC spectrum of compound **15b**



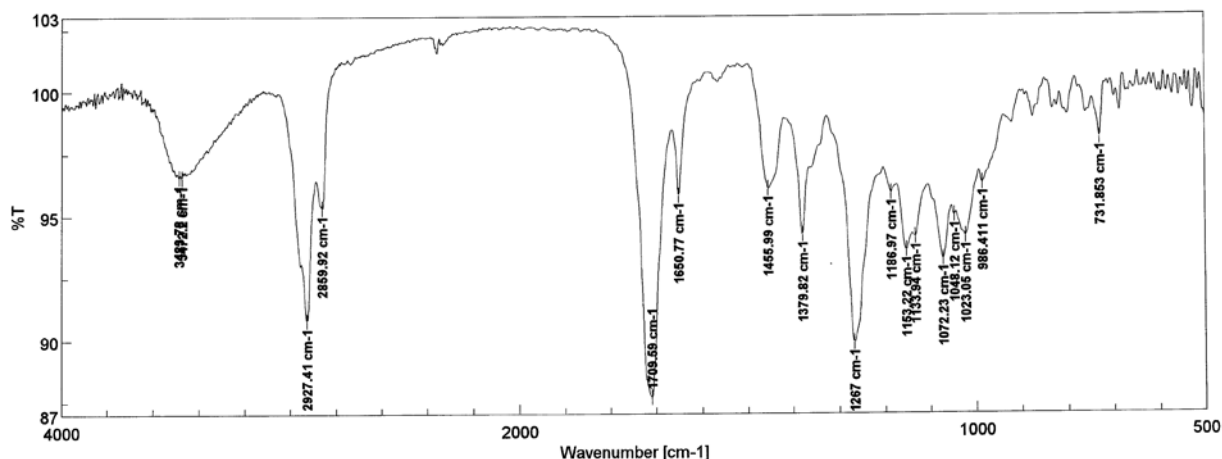
The NOESY spectrum of compound **15b**

測定データ名: KS-8.02
 作成条件: 平均(MS[1]) 経過時間: 0.62..0.83
 x10³ 面積 (10121)

実験日時: 2017/10/07 17:13:26
 イオン化モード: ESI+



The HRESIMS spectrum of compound **16**



[コメント情報]

試料名 KS-8
 コメント
 測定者 B
 所属 東邦大学 薬学部
 会社

[データ情報]

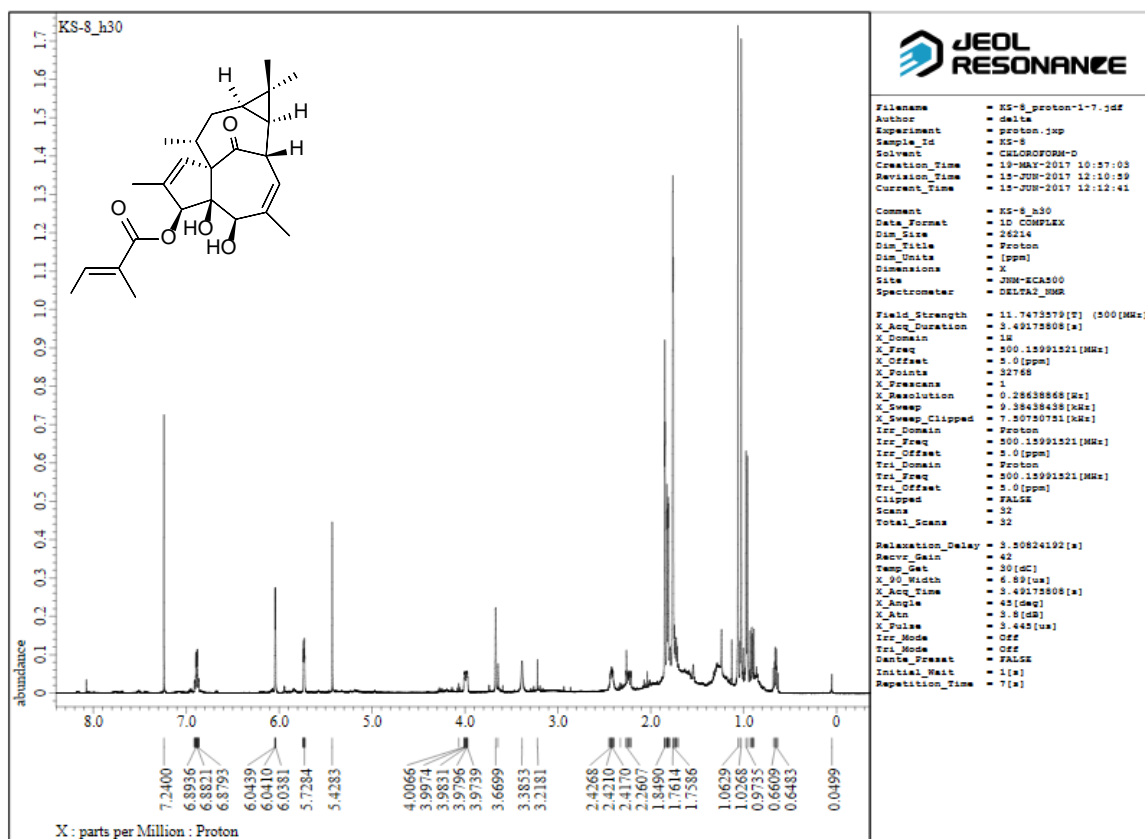
作成日時 2017/07/26 14:35
 データタイプ 等間隔データ
 横軸 Wavenumber [cm-1]
 縦軸 %T
 スタート 0 cm-1
 エンド 7800.65 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

[測定情報]

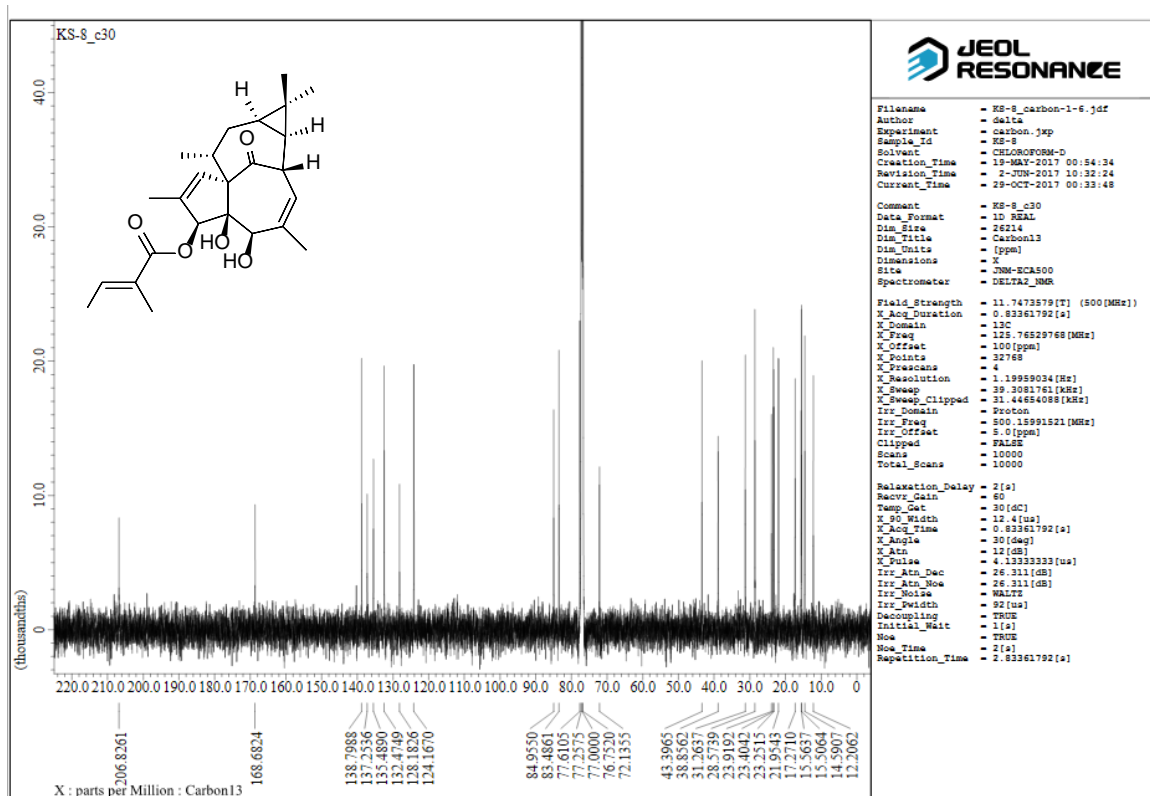
機種名 FT/IR-4100typeA
 シリアル番号 B109261016
 光源 標準光源
 検出器 TGS
 積算回数 Auto (174)
 分解 4 cm-1
 ゼロフリンジ On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャー Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

Memory-2

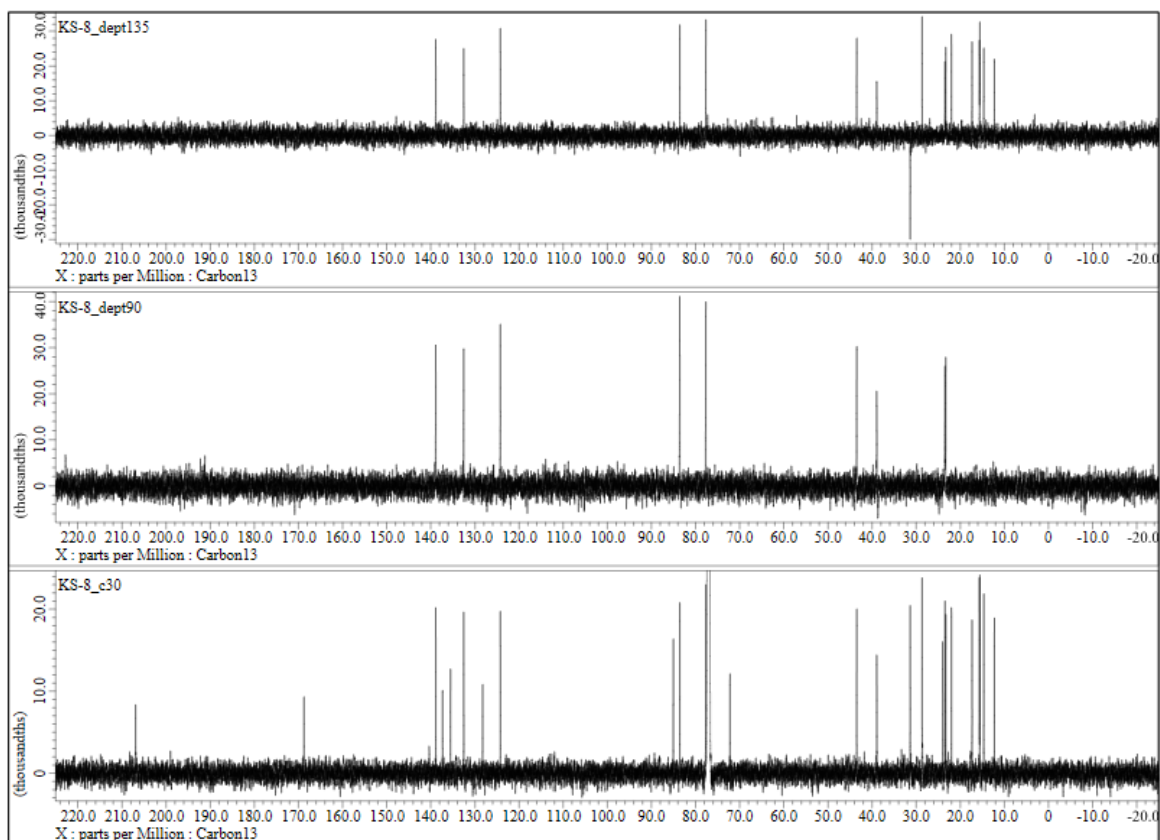
The IR spectrum of compound 16



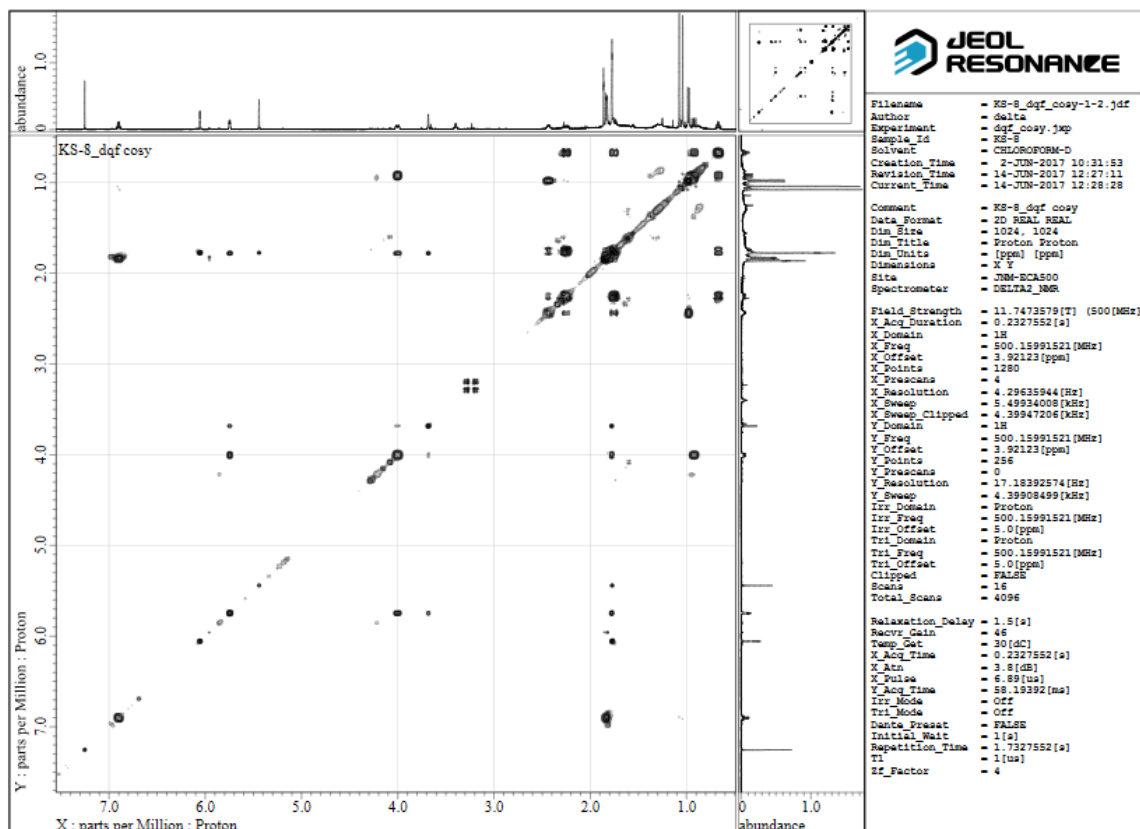
The ¹H spectrum of compound 16



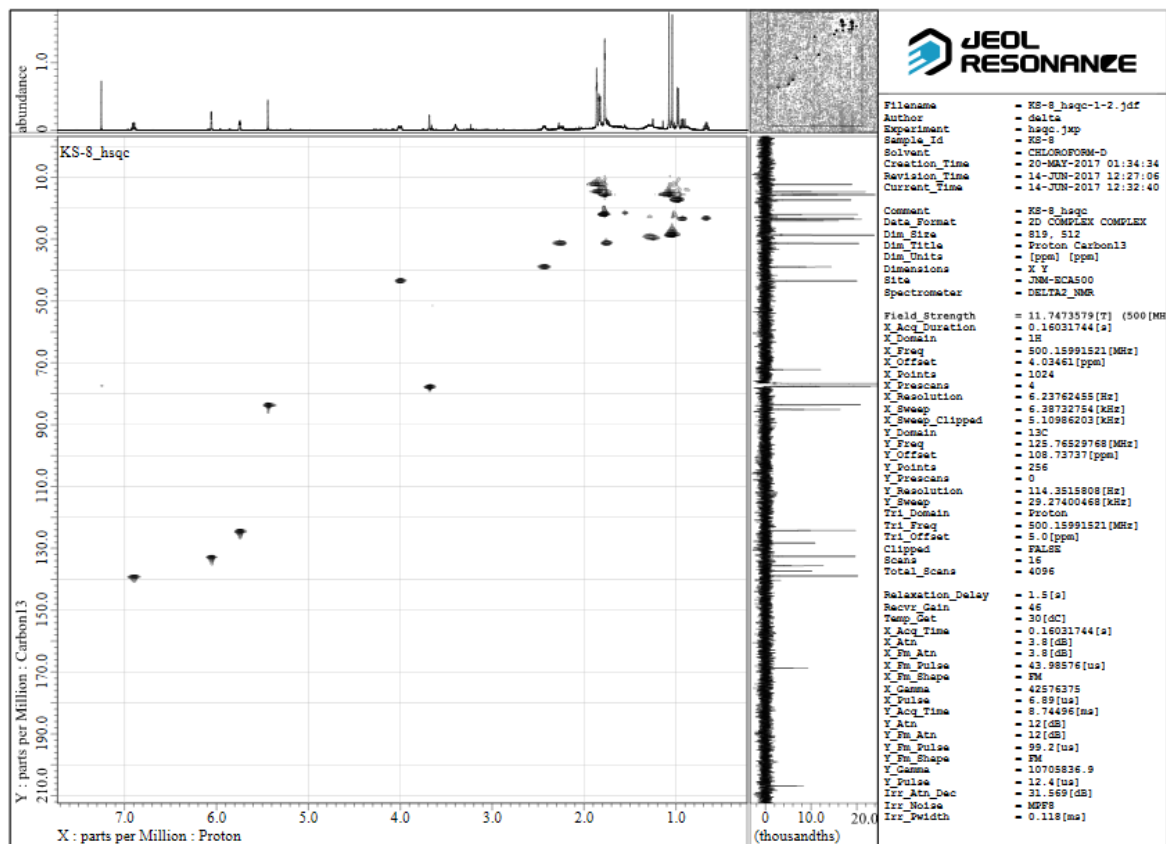
The ^{13}C spectrum of compound 16



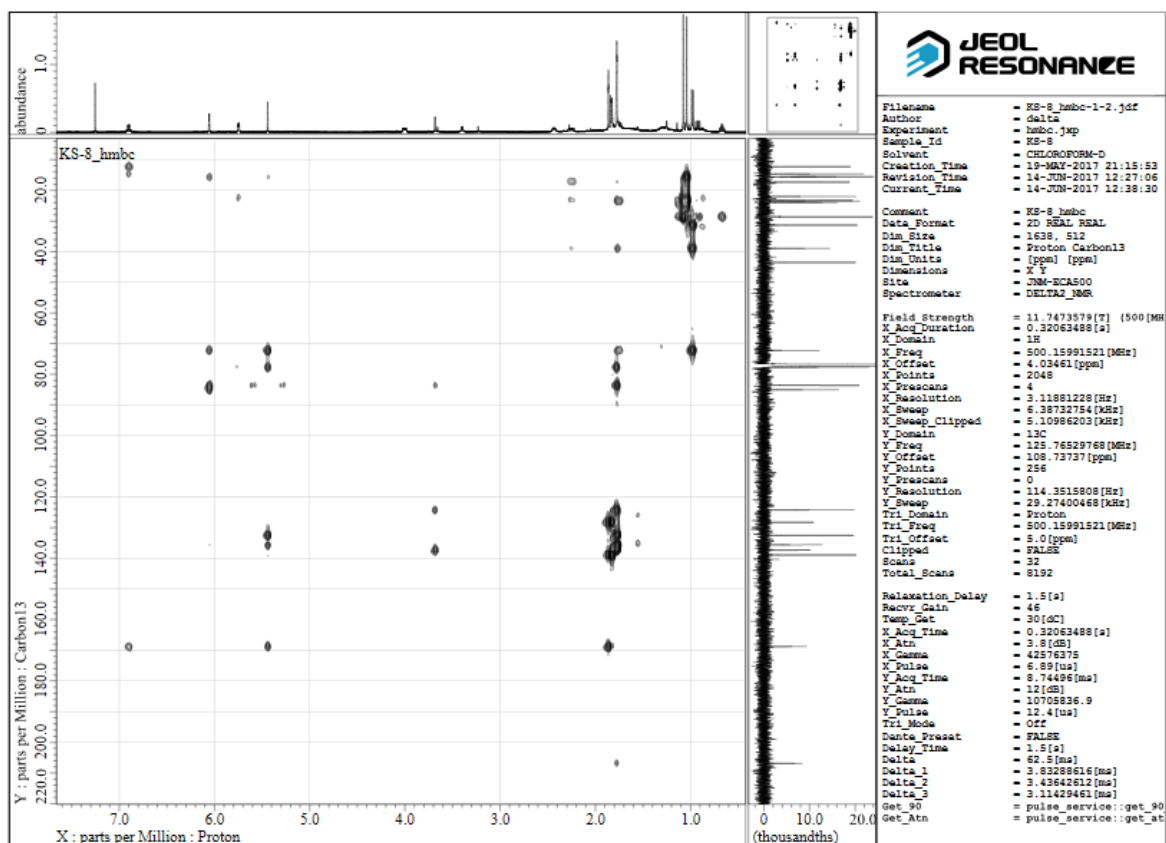
The DEPT spectrum of compound 16



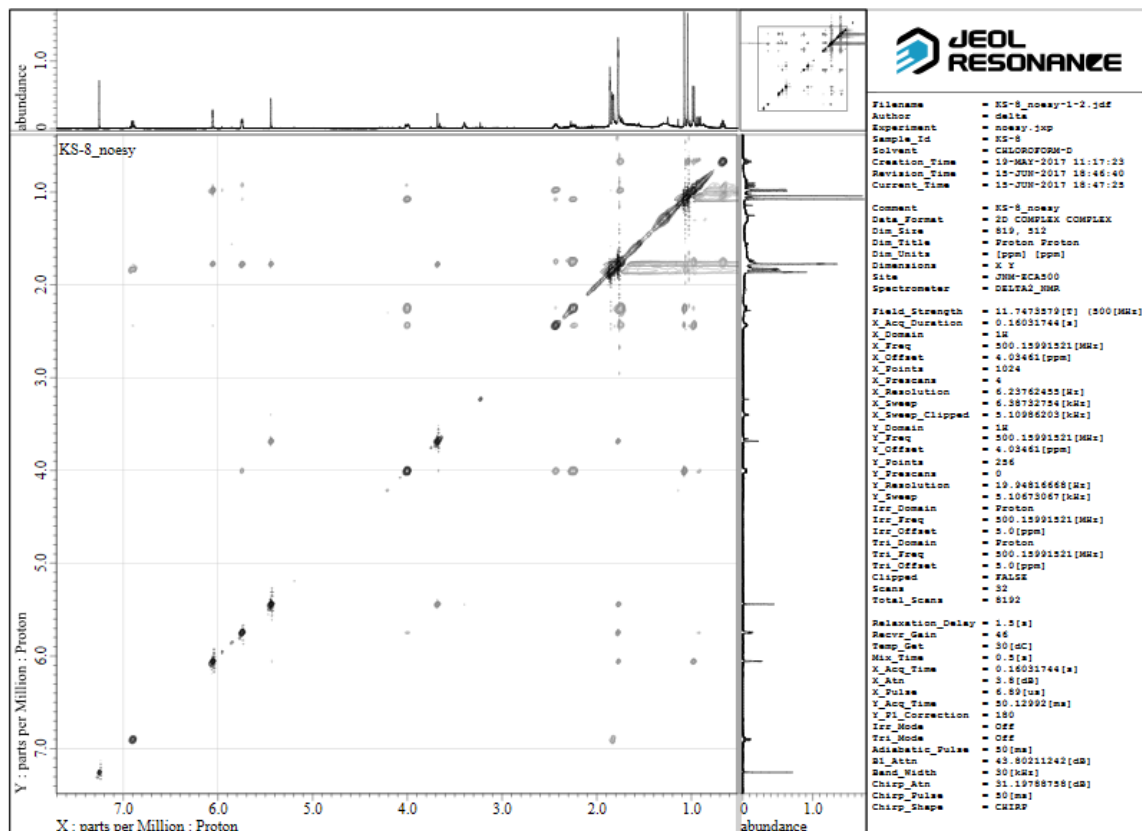
The DQF_COSY spectrum of compound 16



The HSQC spectrum of compound 16



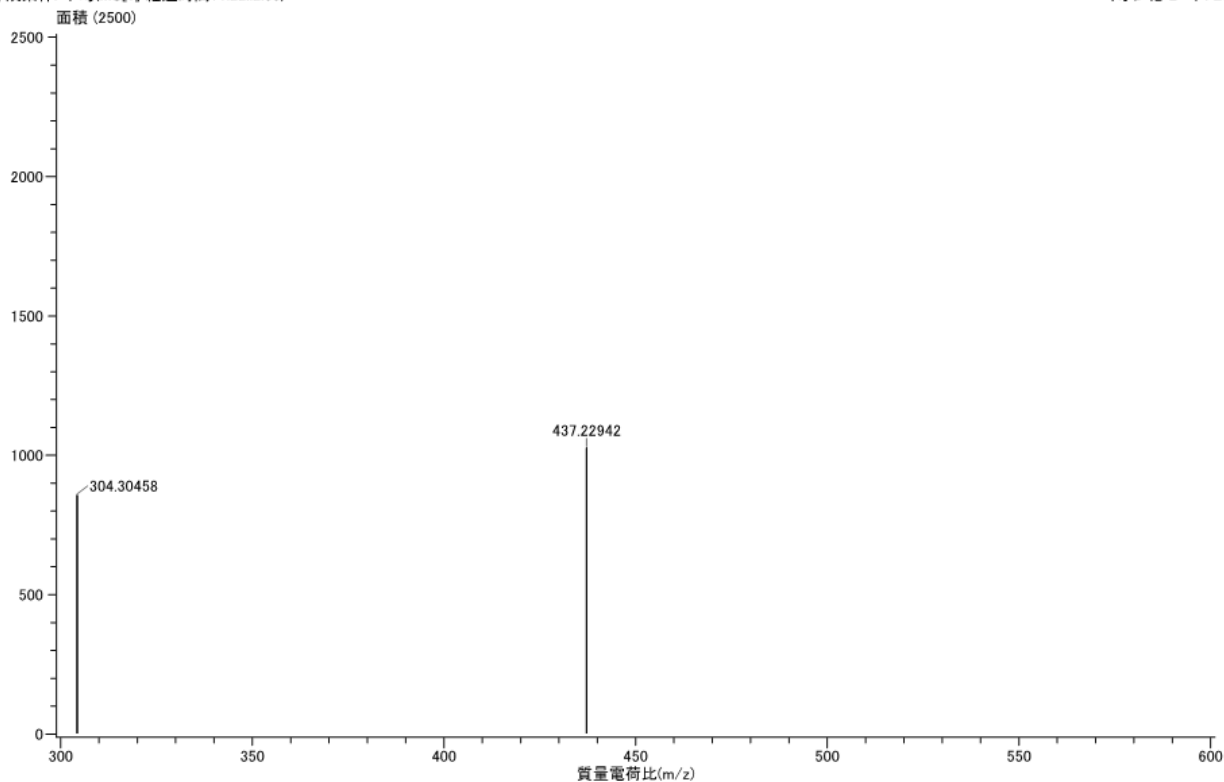
The HMBC spectrum of compound 16



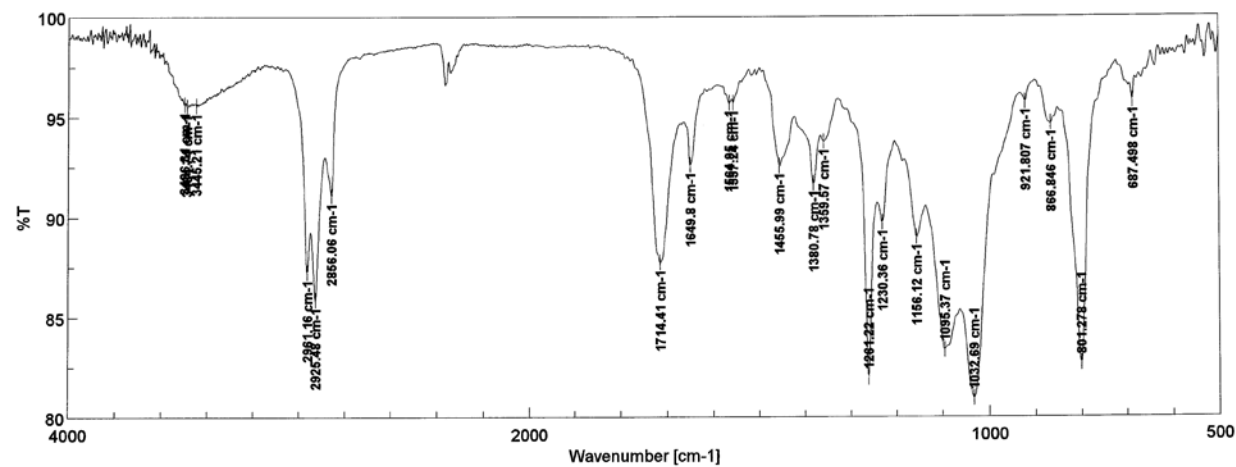
The NOESY spectrum of compound 16

測定データ名: KS-9_04
 作成条件: 平均(MS[1] 経過時間: 1.22.2.65)

実験日時: 2017/10/07 21:09:03
 イオン化モード: ESI+



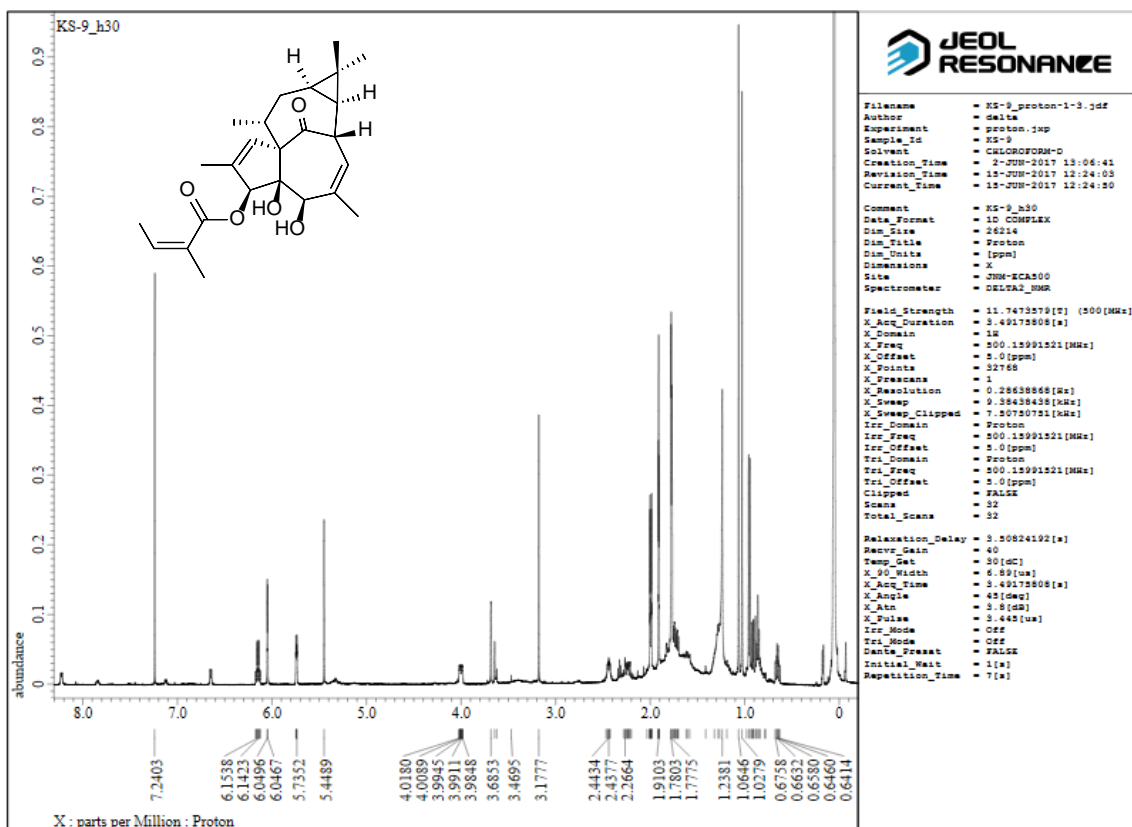
The HRESIMS spectrum of compound 17



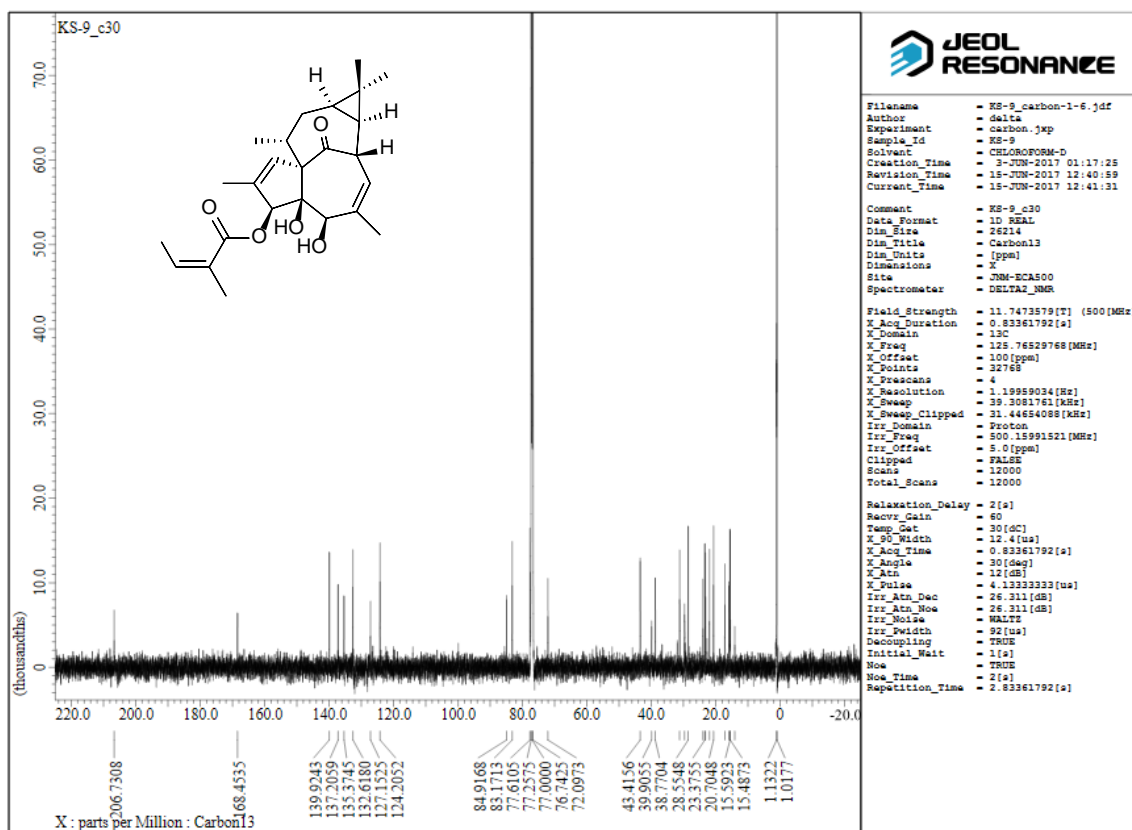
[コメント情報]
 試料名 KS-9
 コメント
 測定者 B
 所属 東邦大学 薬学部
 会社
 [データ情報]
 作成日時 2017/07/26 14:49
 データタイプ 等間隔データ
 横軸 Wavenumber [cm-1]
 縦軸 %T
 スタート 0 cm-1
 エンド 7800.65 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

[測定情報]
 機種名 FT/IR-4100typeA
 シリアル番号 B109261016
 光源 標準光源
 検出器 TGS
 積算回数 Auto (204)
 分解 4 cm-1
 ゼロフライング On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャ Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

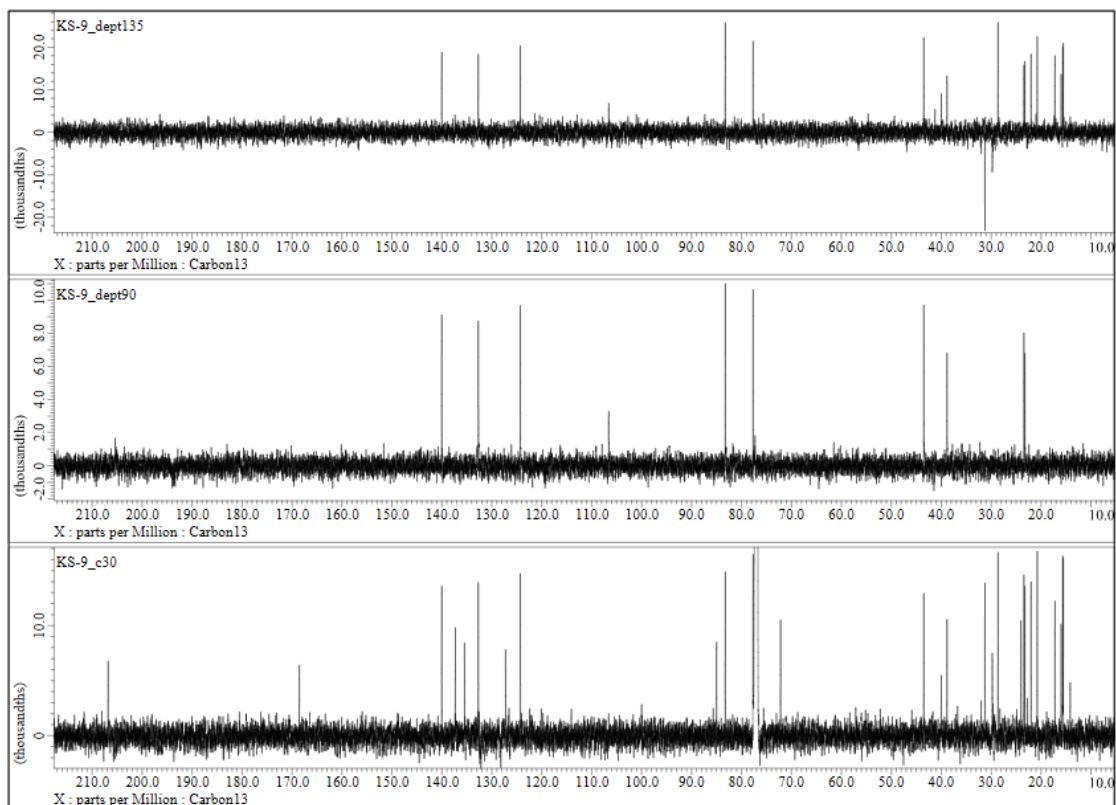
The IR spectrum of compound 17



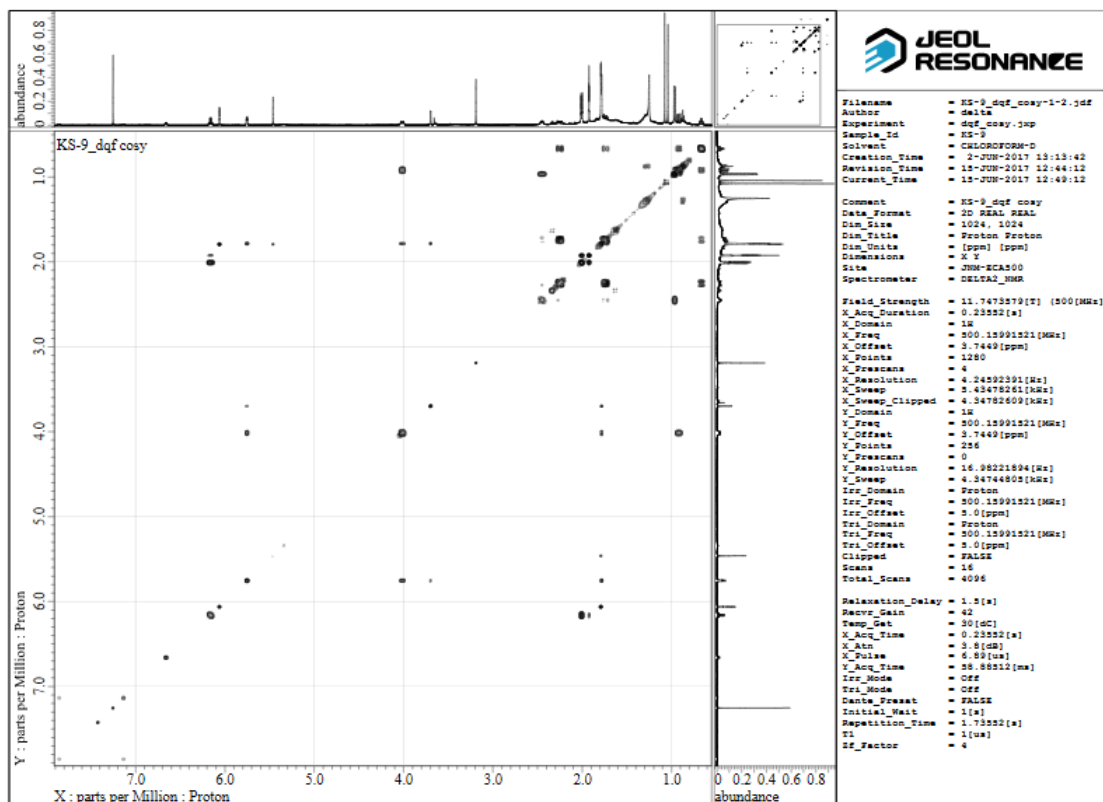
The ^1H spectrum of compound 17



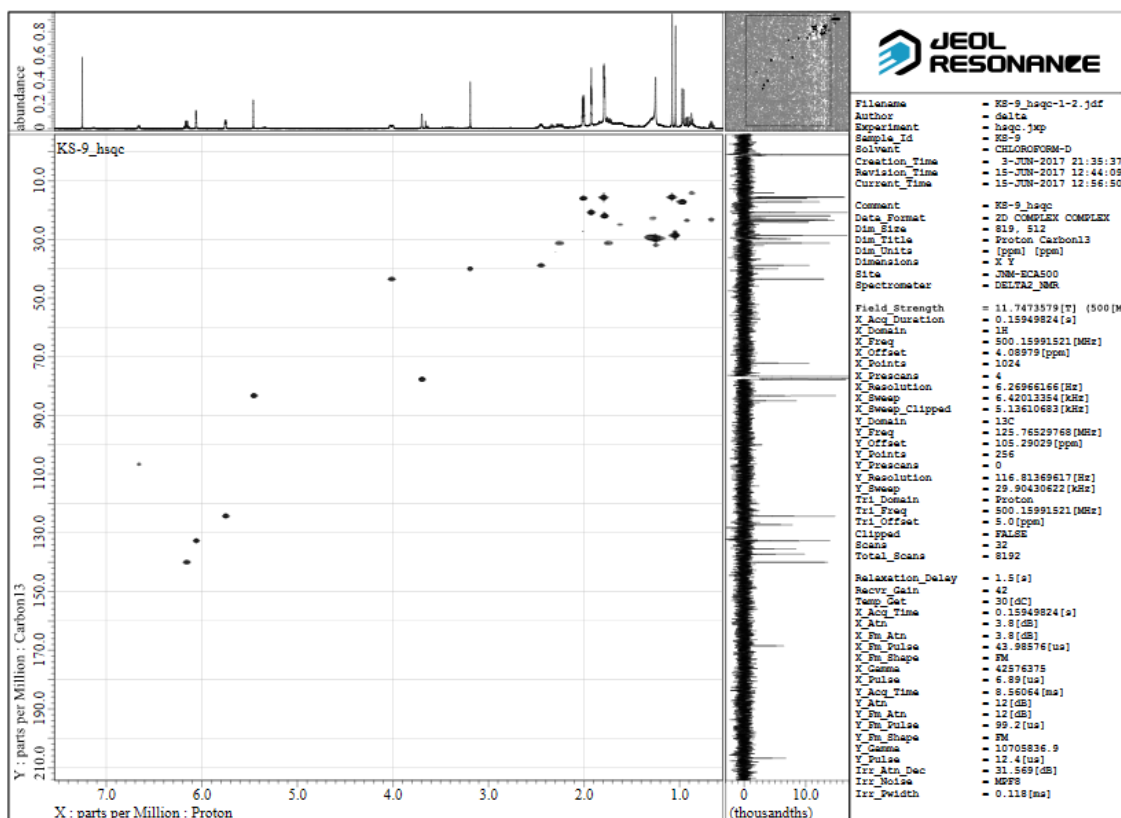
The ^{13}C spectrum of compound 17



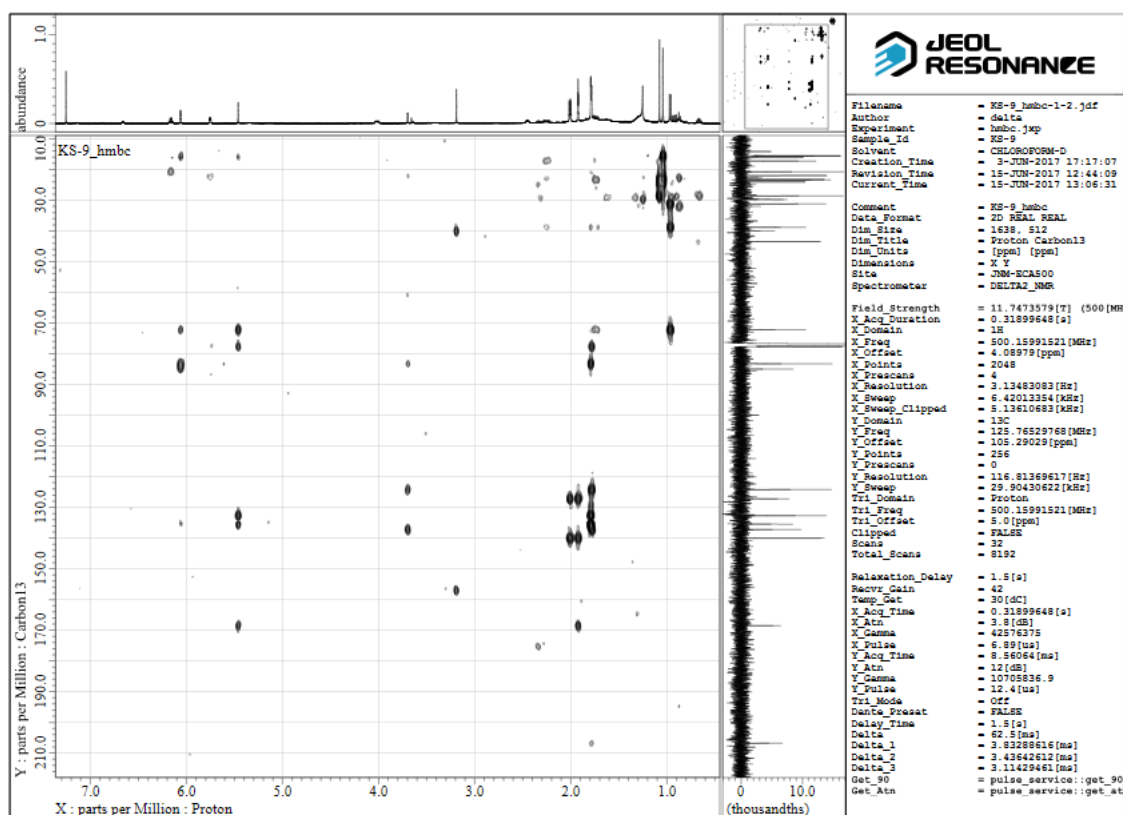
The DEPT spectrum of compound 17



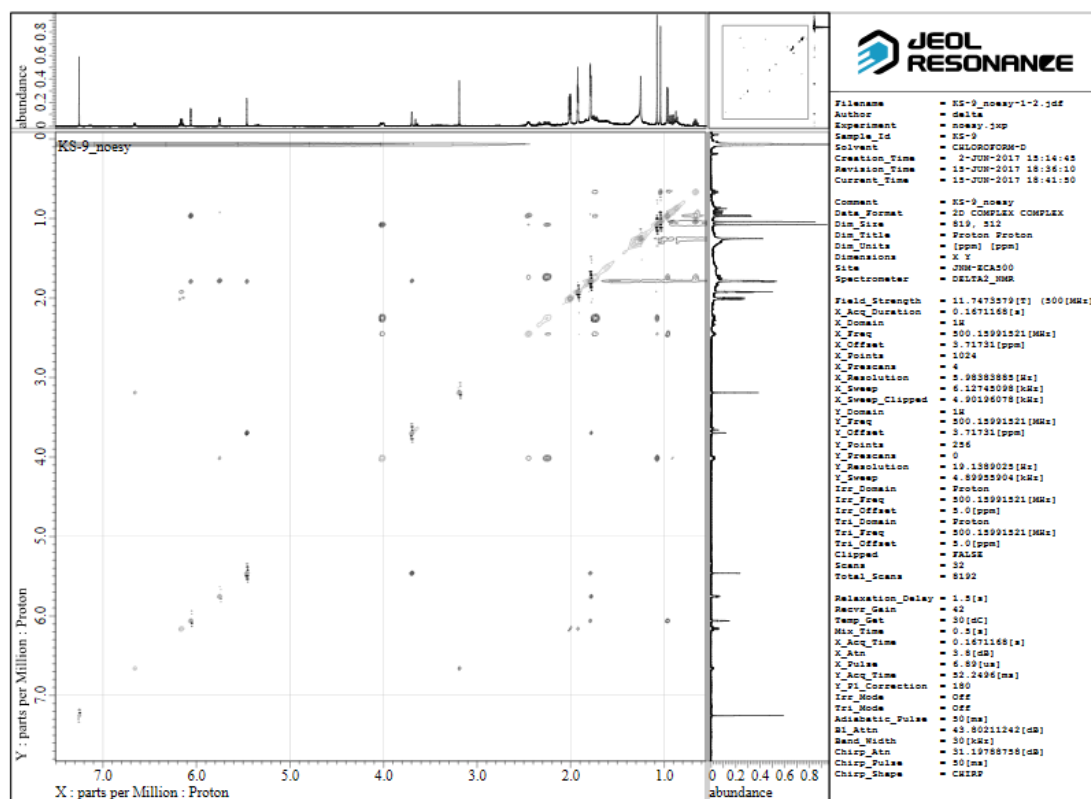
The DQF-COSY spectrum of compound 17



The HSQC spectrum of compound 17



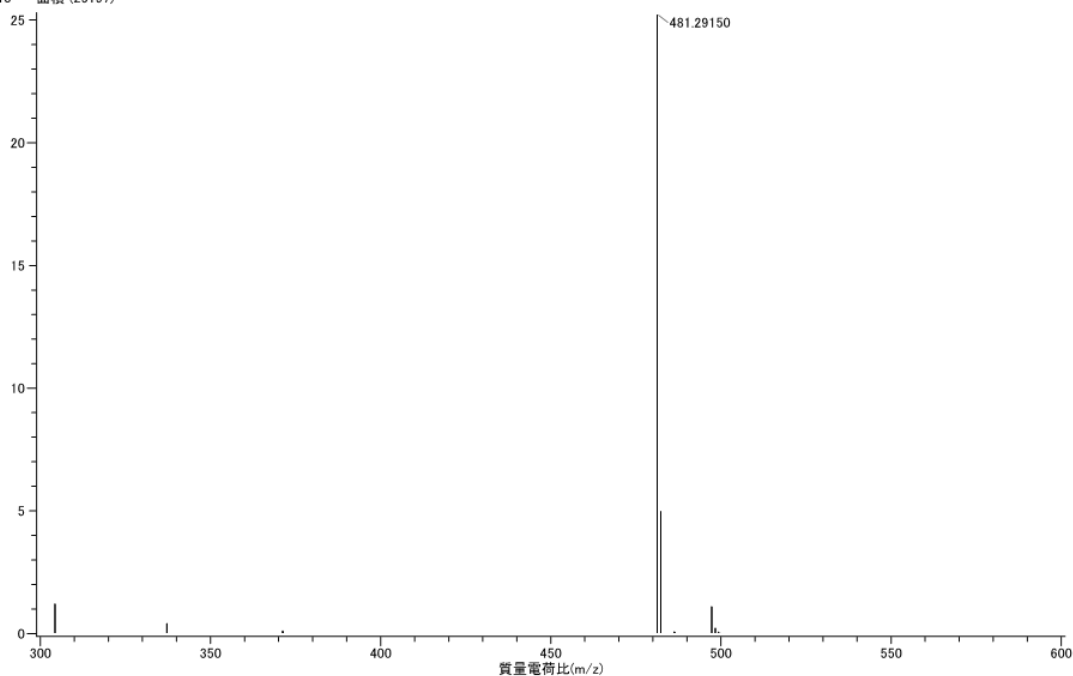
The HMBC spectrum of compound 17



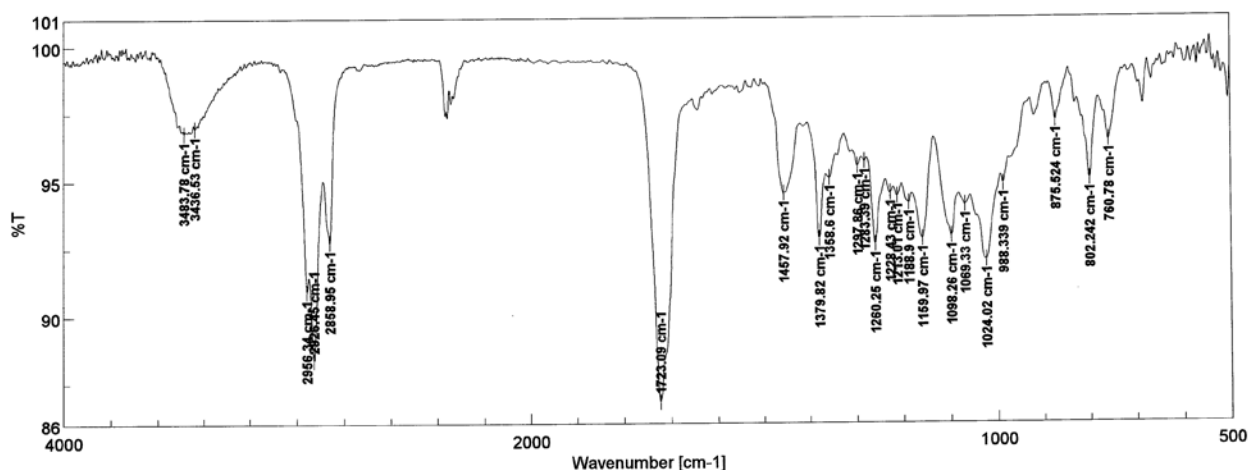
The NOESY spectrum of compound 17

測定データ名: KS-11
 作成条件: 平均(MS[1]) 経過時間: 0.47-0.65
 x10³ 面積 (25197)

実験日時: 2017/10/13 21:33:15
 イオン化モード: ESI+



The HRESIMS spectrum of compound 18



【コメント情報】
 試料名
 コメント
 測定者
 所属
 会社

KS-11
 B
 東邦大学 薬学部

【データ情報】
 作成日時
 データタイプ
 横軸
 縦軸
 スタート
 エンド
 データ間隔
 データ数

2017/07/26 15:01
 等間隔データ
 Wavenumber [cm-1]
 %T
 0 cm-1
 7800.65 cm-1
 0.964233 cm-1
 8091

【測定情報】
 機種名
 シリアル番号

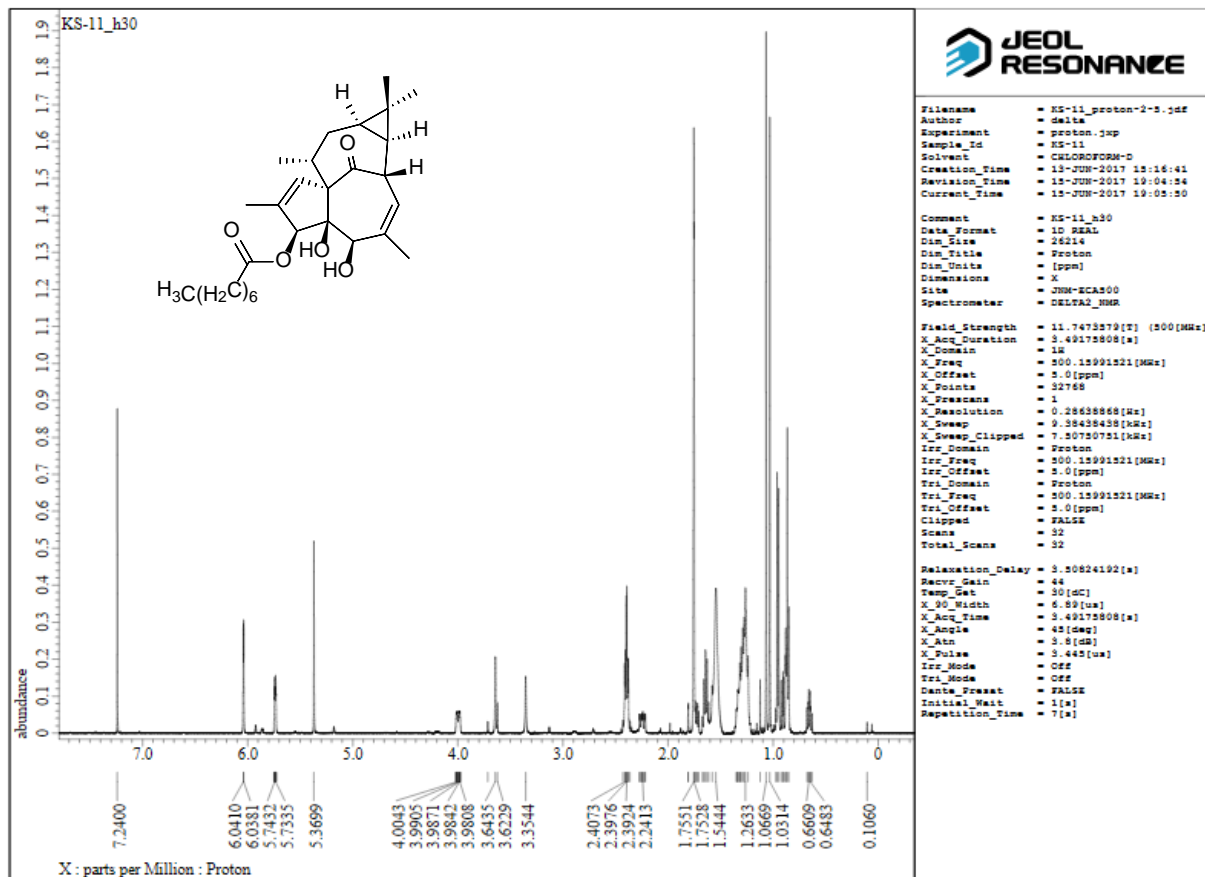
FT/IR-4100typeA
 B109261016

光源
 検出器
 積算回数
 分解
 ゼロフリンギ
 アボタイゼーション
 ゲイン
 アパーチャー
 スキャンスピード
 フィルタ

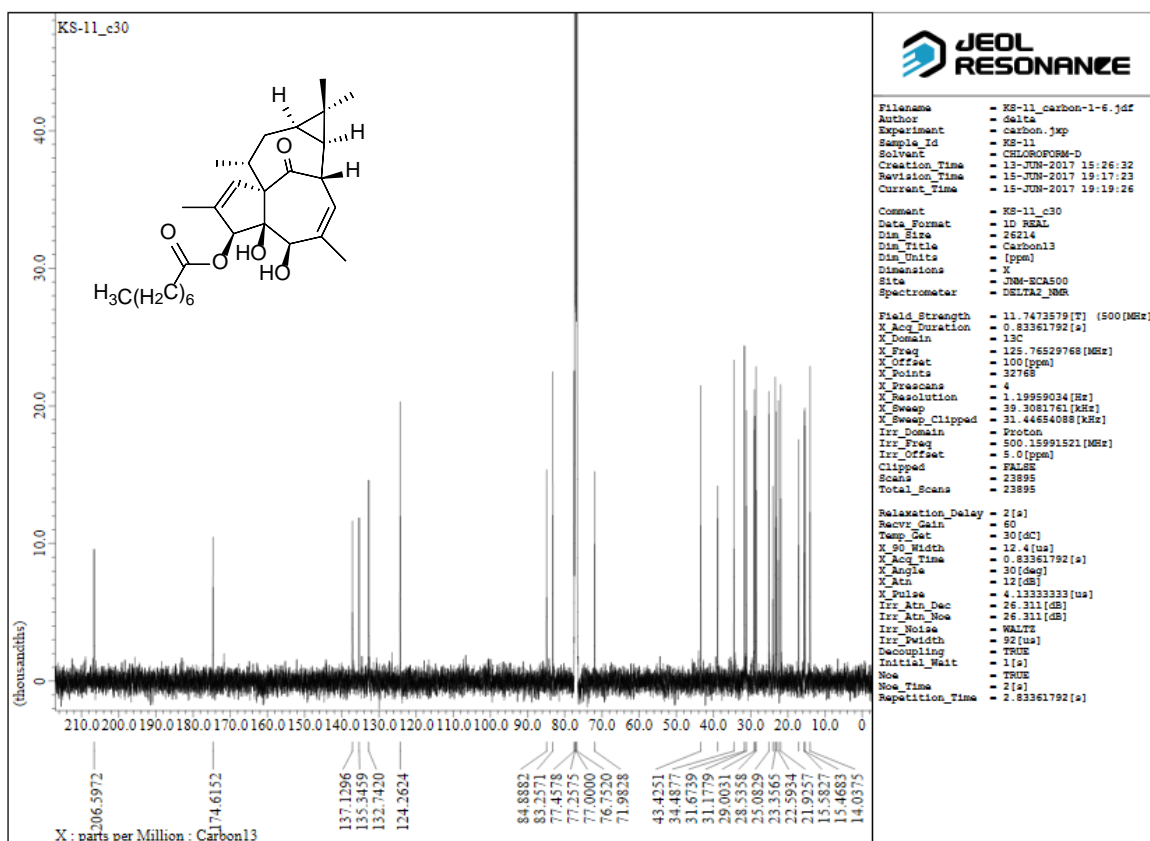
標準光源
 TGS
 Auto (178)
 4 cm-1
 On
 Cosine
 Auto (16)
 Auto (7.1 mm)
 Auto (2 mm/sec)
 Auto (30000 Hz)

Memory-2

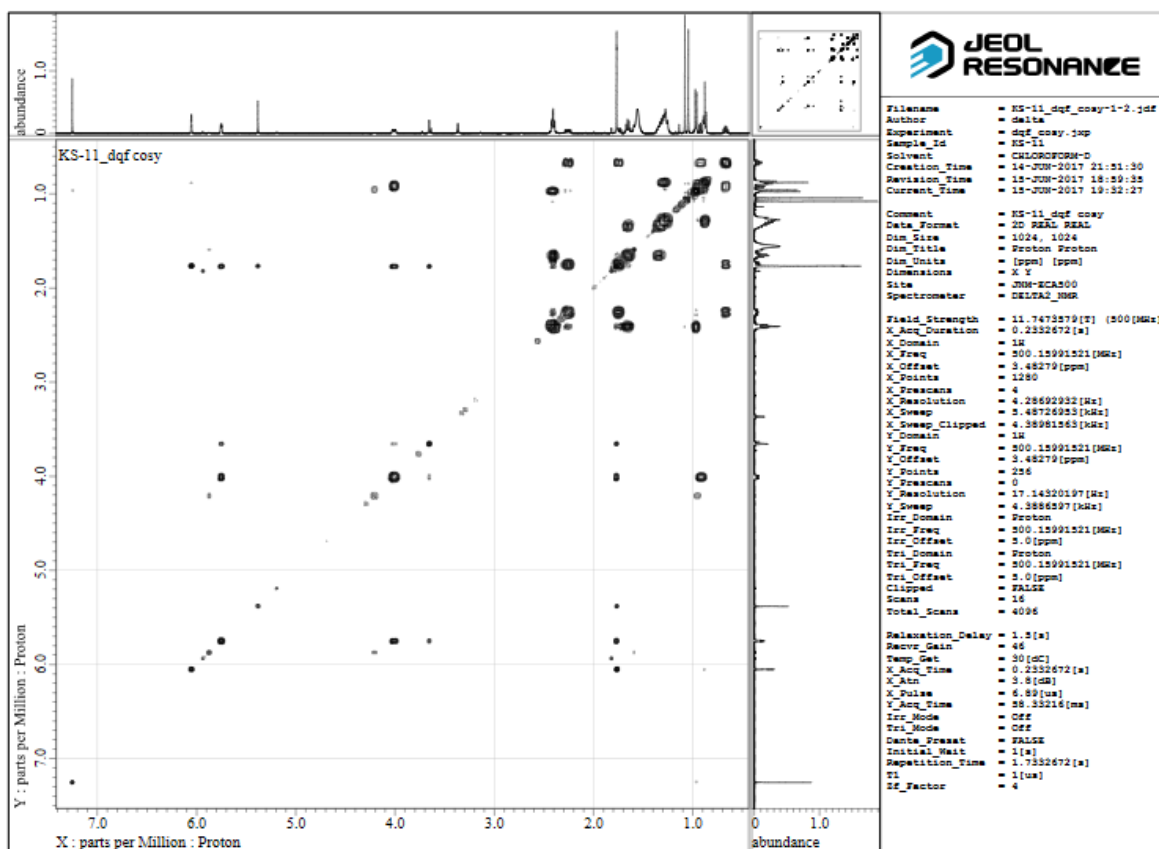
The IR spectrum of compound 18



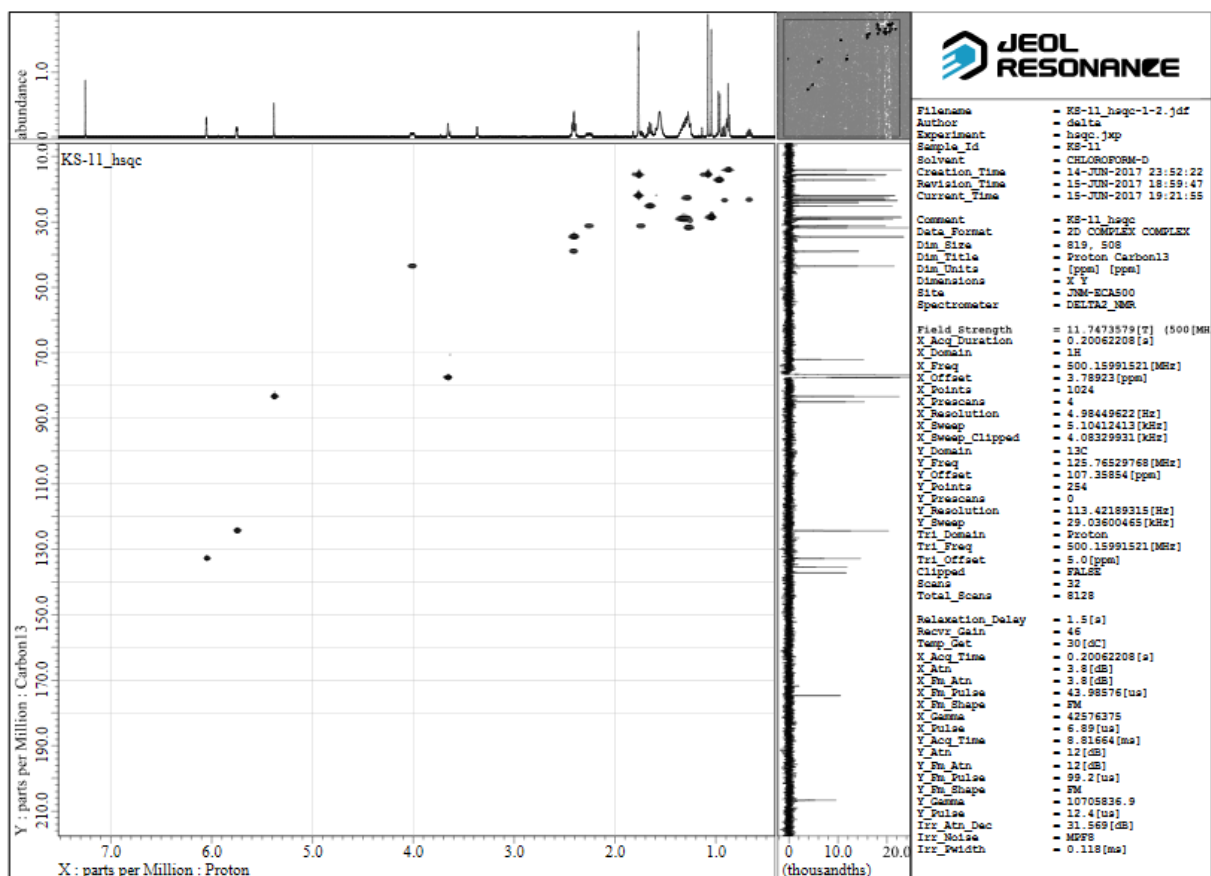
The ¹H spectrum of compound 18



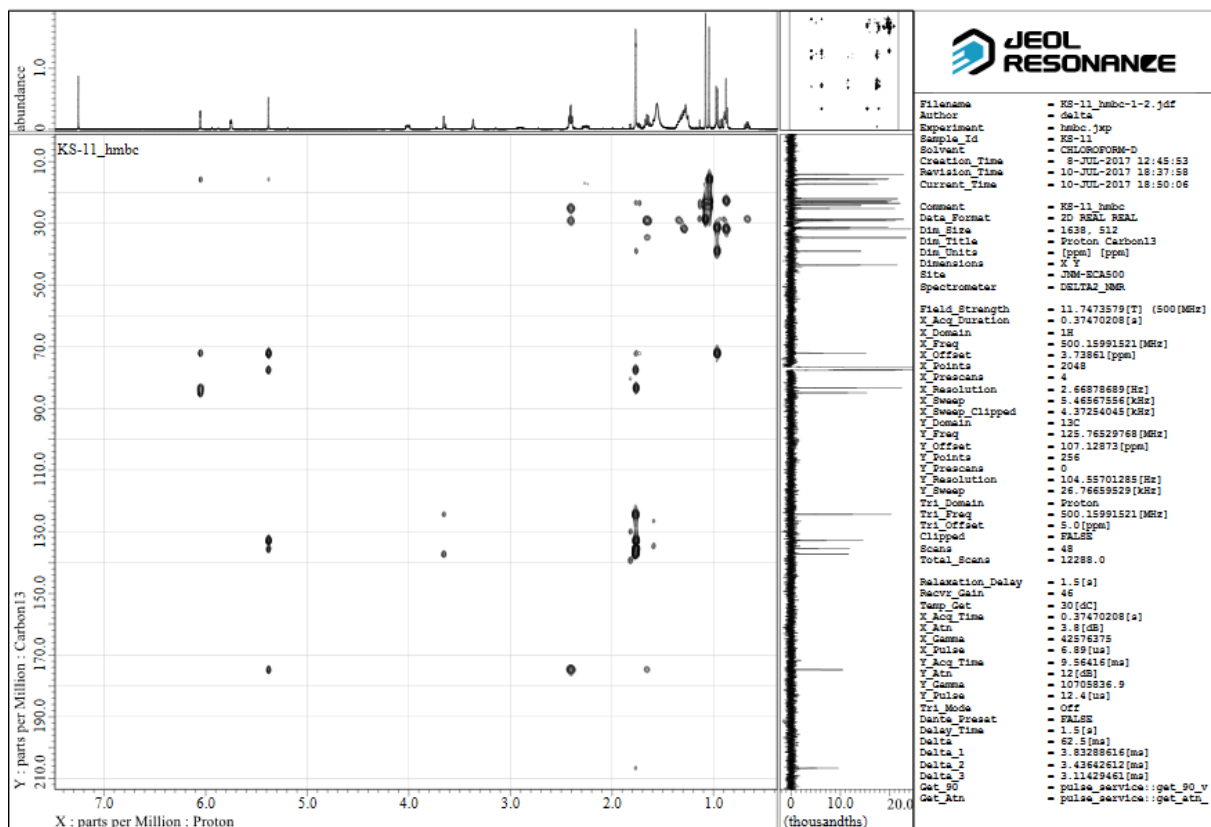
The ^{13}C spectrum of compound 18



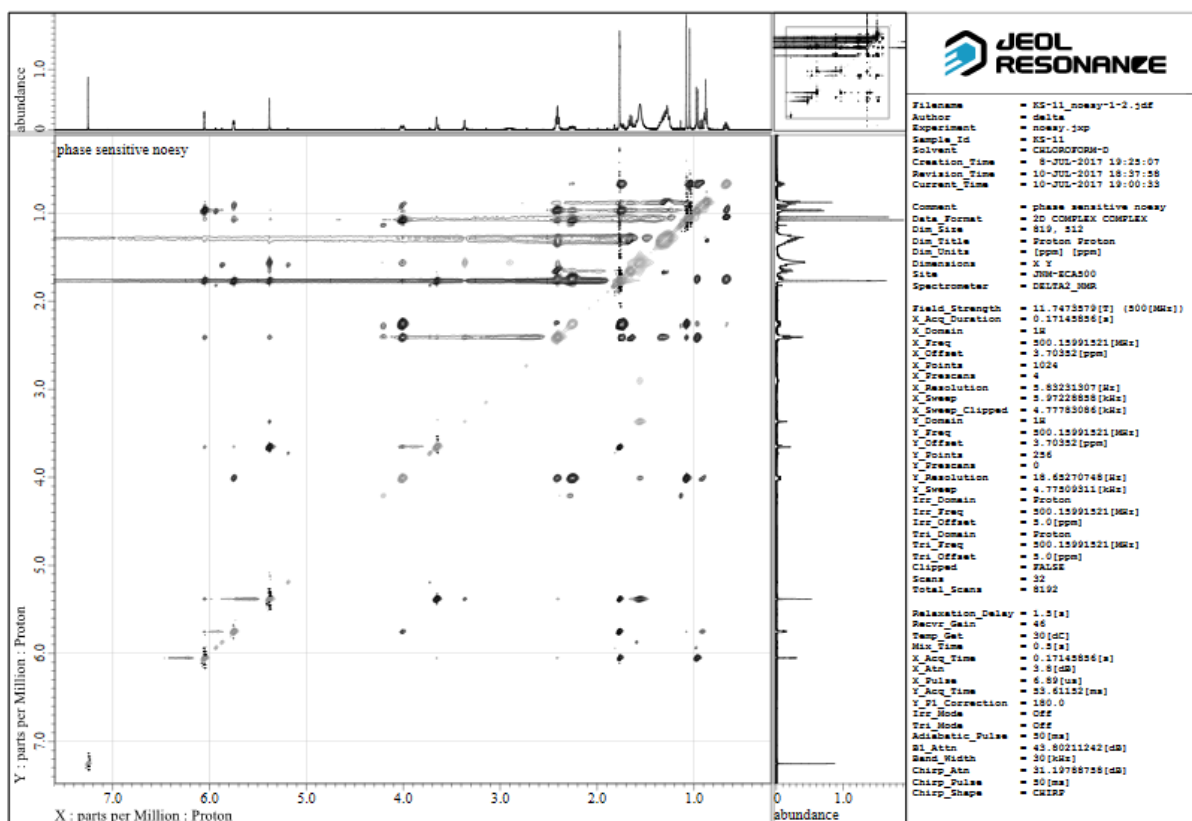
The DQF-COSY spectrum of compound 18



The HSQC spectrum of compound 18



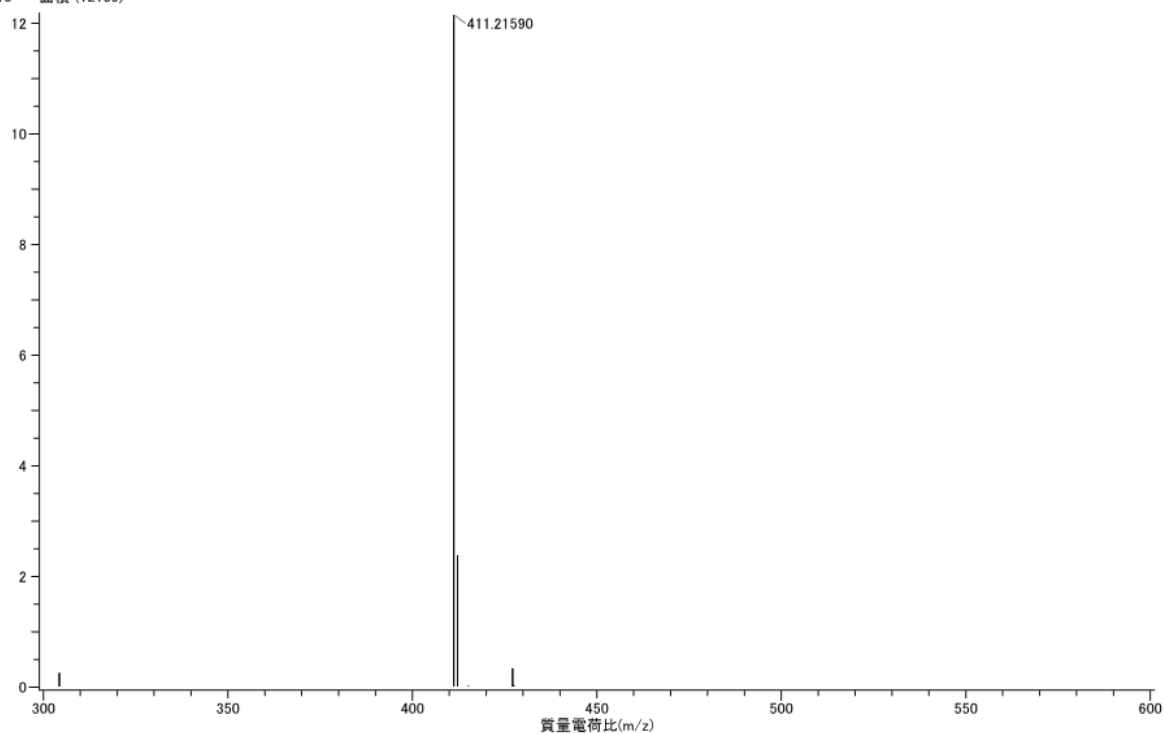
The HMBC spectrum of compound 18



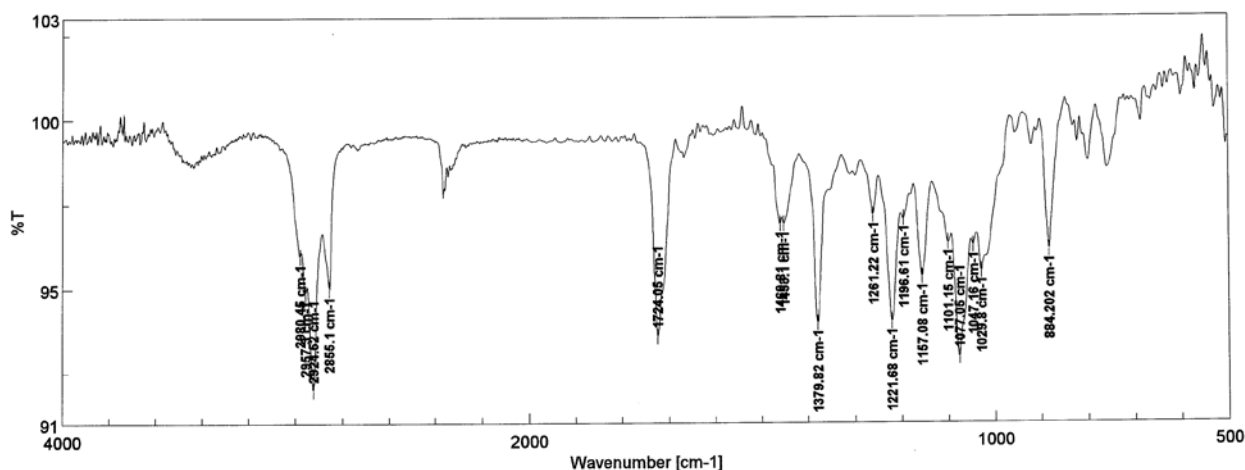
The NOESY spectrum of compound 18

測定データ名: KS-12.02
 作成条件: 平均(MS[1] 経過時間: 0.76..1.03)
 x10³ 面積 (12139)

実験日時: 2017/10/13 22:37:12
 イオン化モード: ESI+



The HRMS spectrum of compound 19



[コメント情報]
 試料名 KS-12
 コメント
 測定者 B
 所属 東邦大学 薬学部
 会社

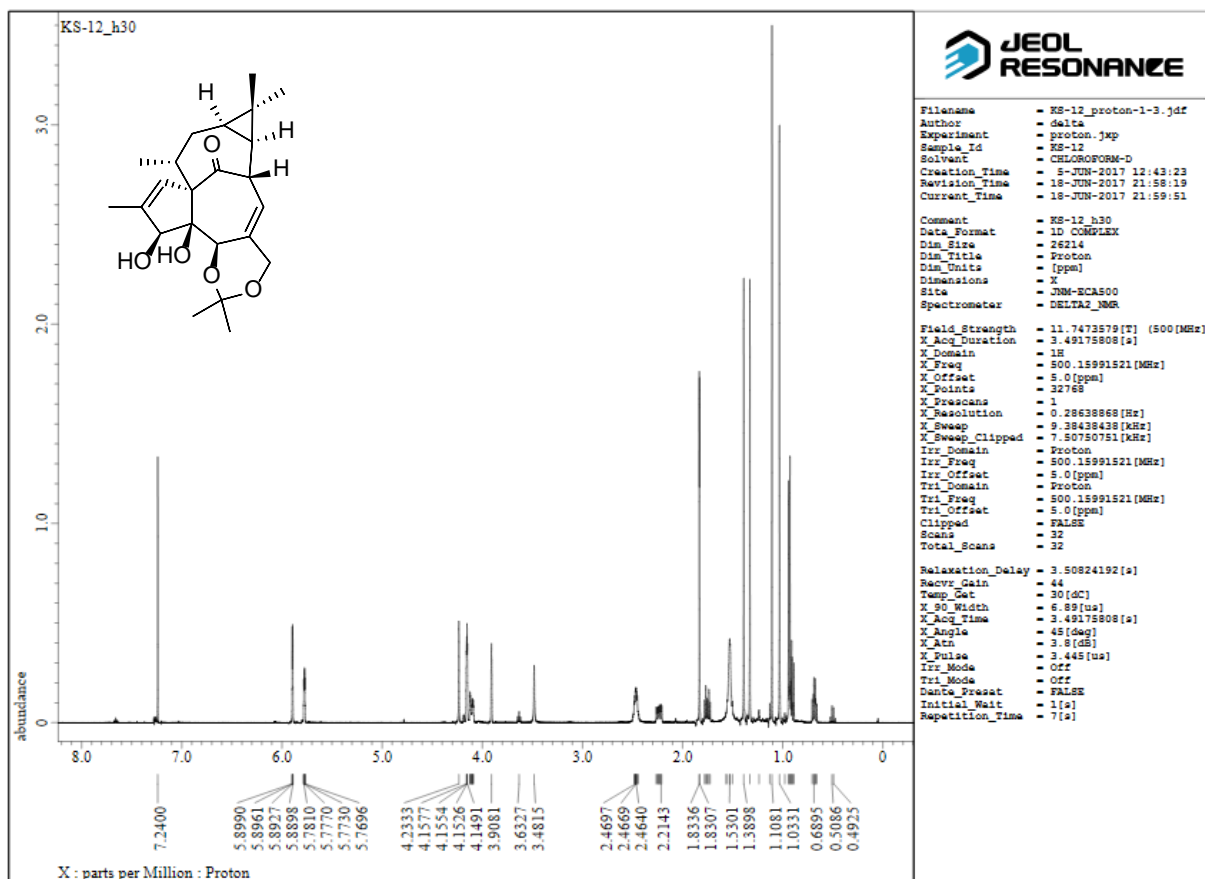
[データ情報]
 作成日時 2017/07/26 15:14
 データタイプ 等間隔データ
 横軸 Wavenumber [cm-1]
 縦軸 %T
 スタート 0 cm-1
 エンド 7800.65 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

[測定情報]
 機種名 FT/IR-4100typeA
 シリアル番号 B109261016

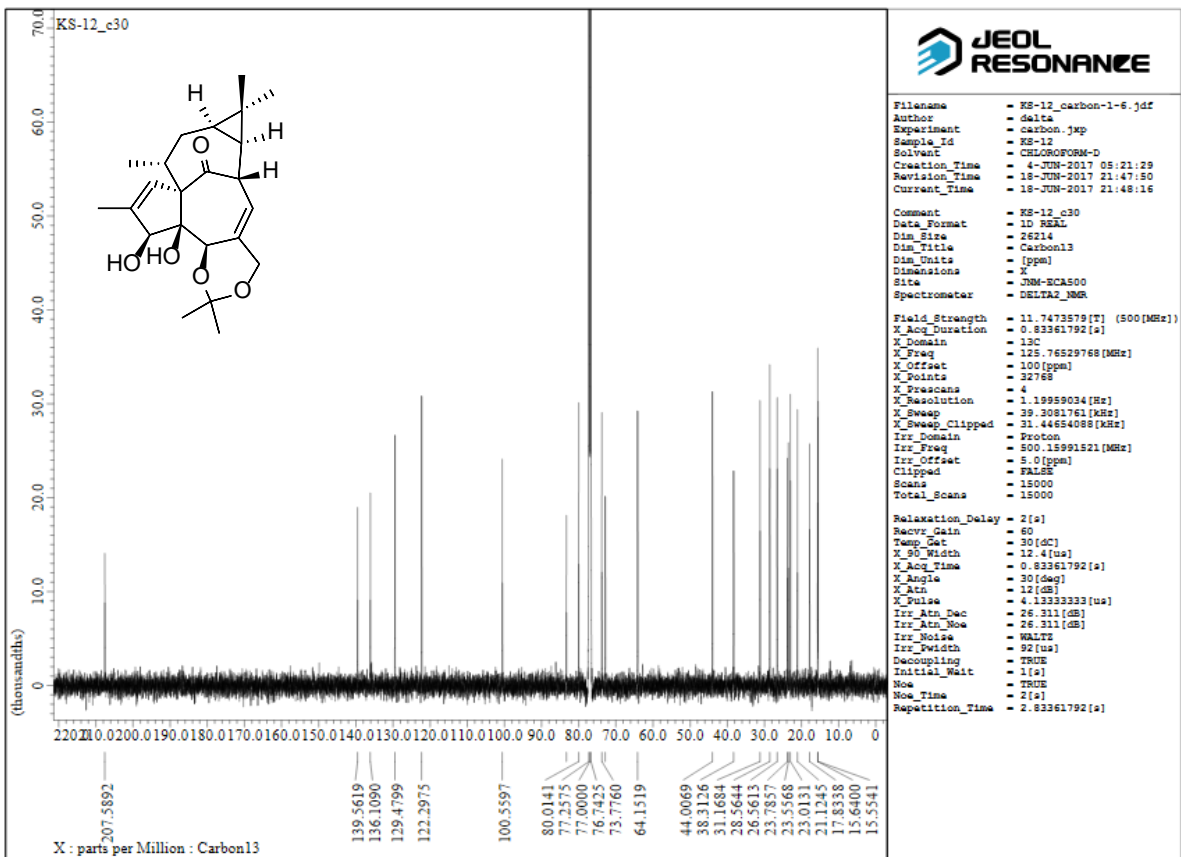
光源 標準光源
 検出器 TGS
 積算回数 Auto (190)
 分解 4 cm-1
 ゼロフリング On
 アボタイゼーション Cosine
 ゲイン Auto (16)
 アパーチャー Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

Memory-2

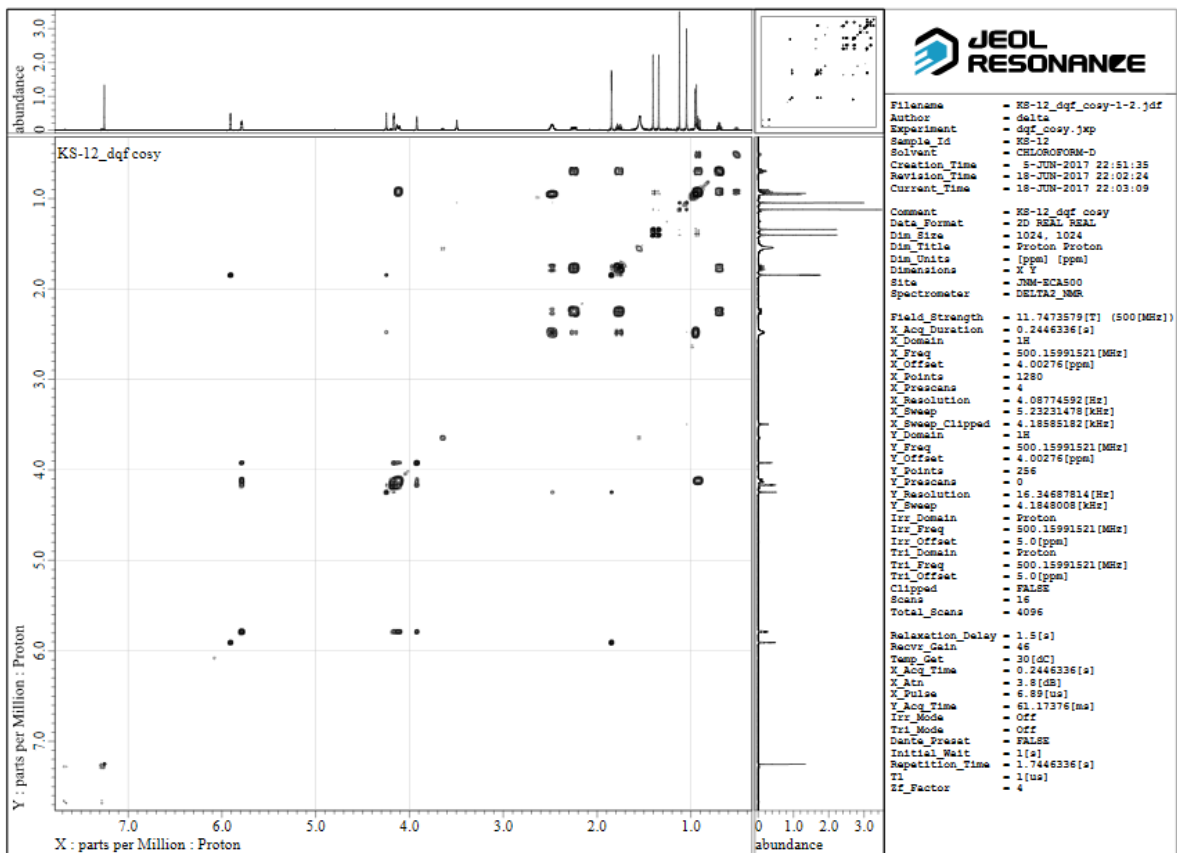
The IR spectrum of compound 19



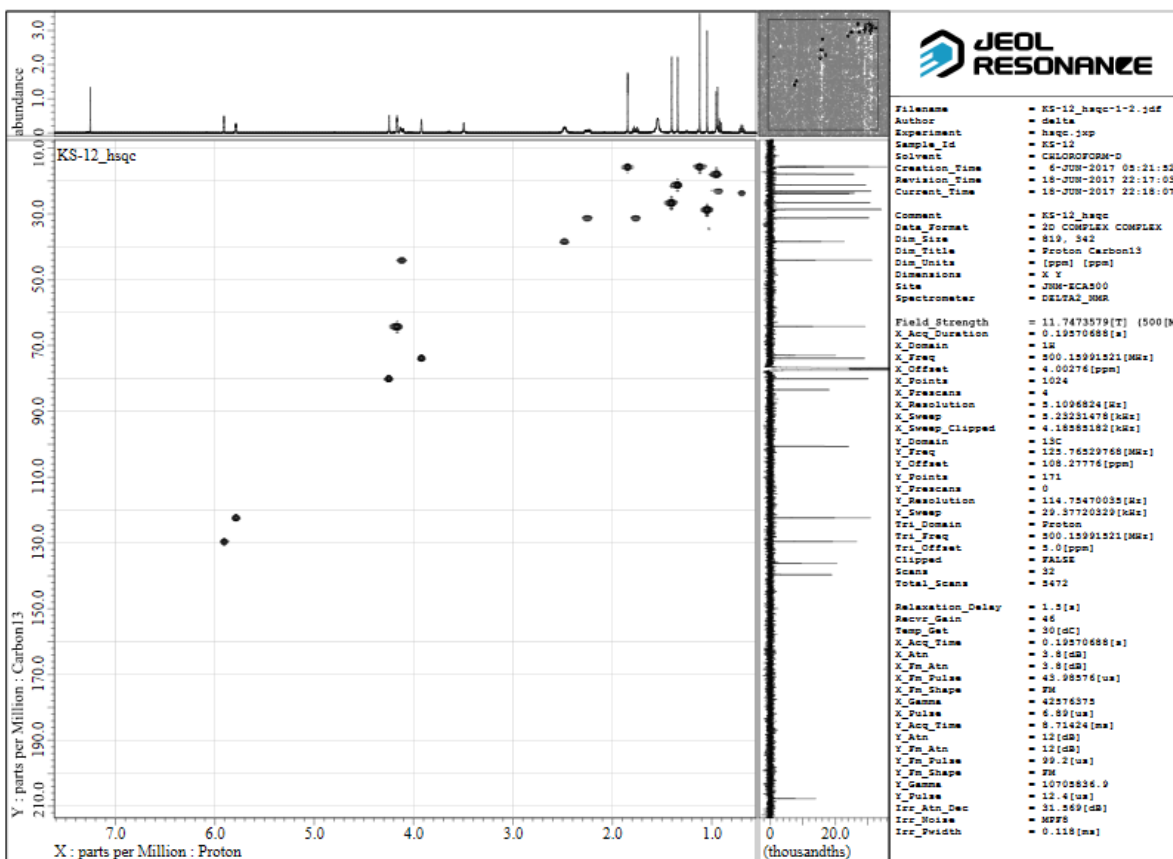
The ^1H spectrum of compound 19



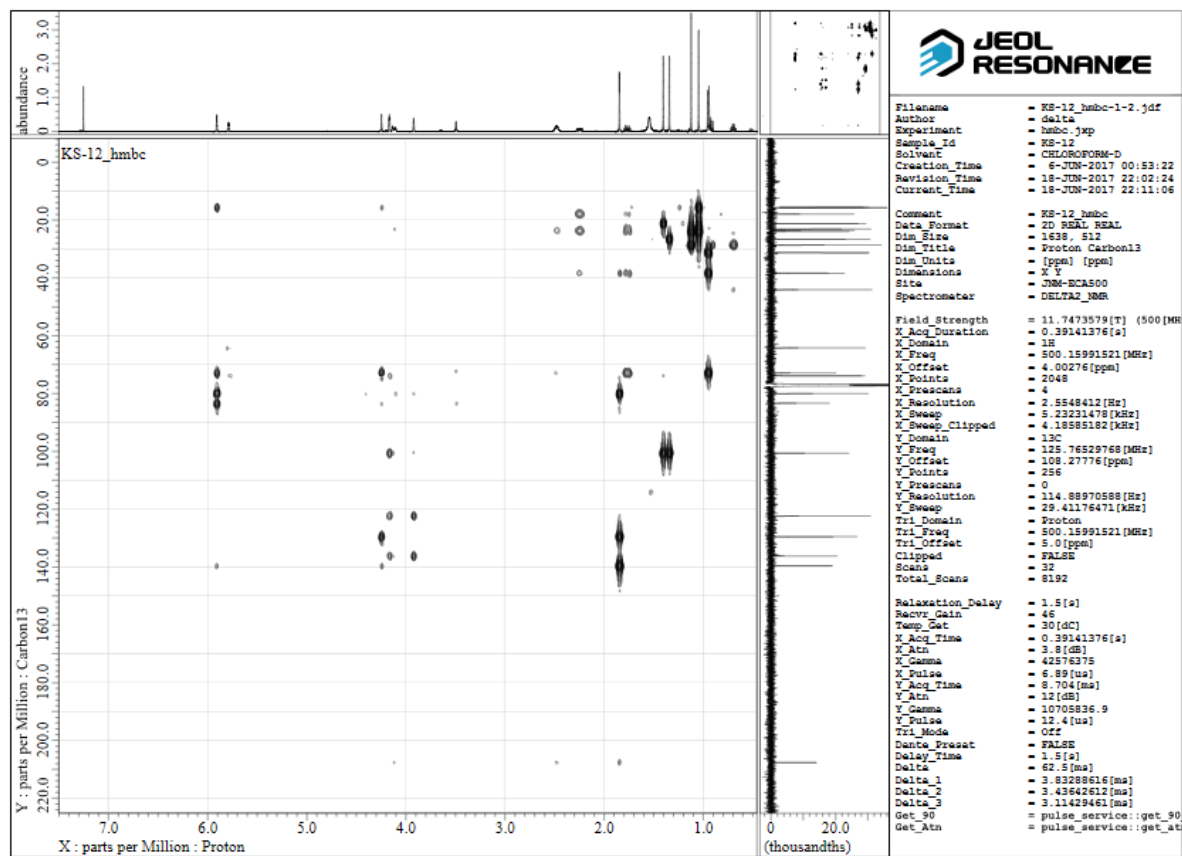
The ¹³C spectrum of compound 19



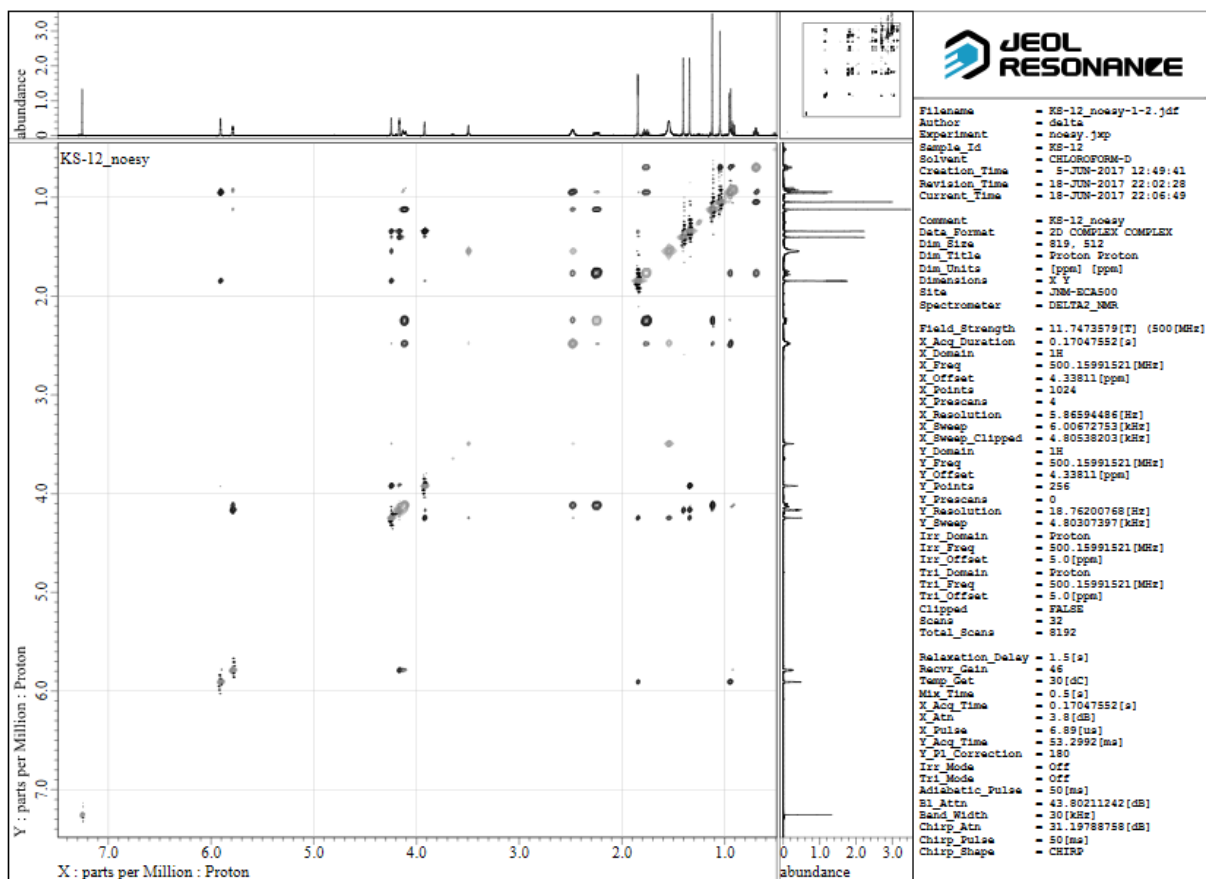
The DQF-COSY spectrum of compound 19



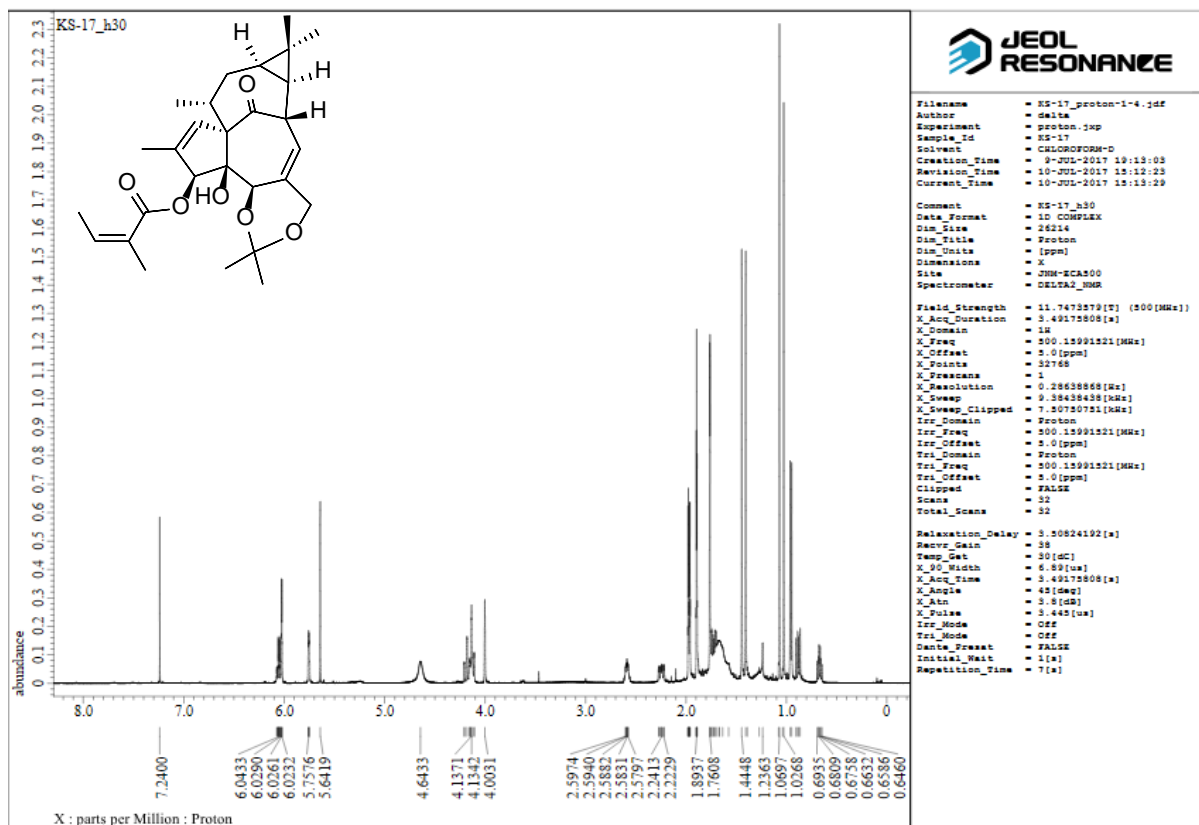
The HSQC spectrum of compound 19



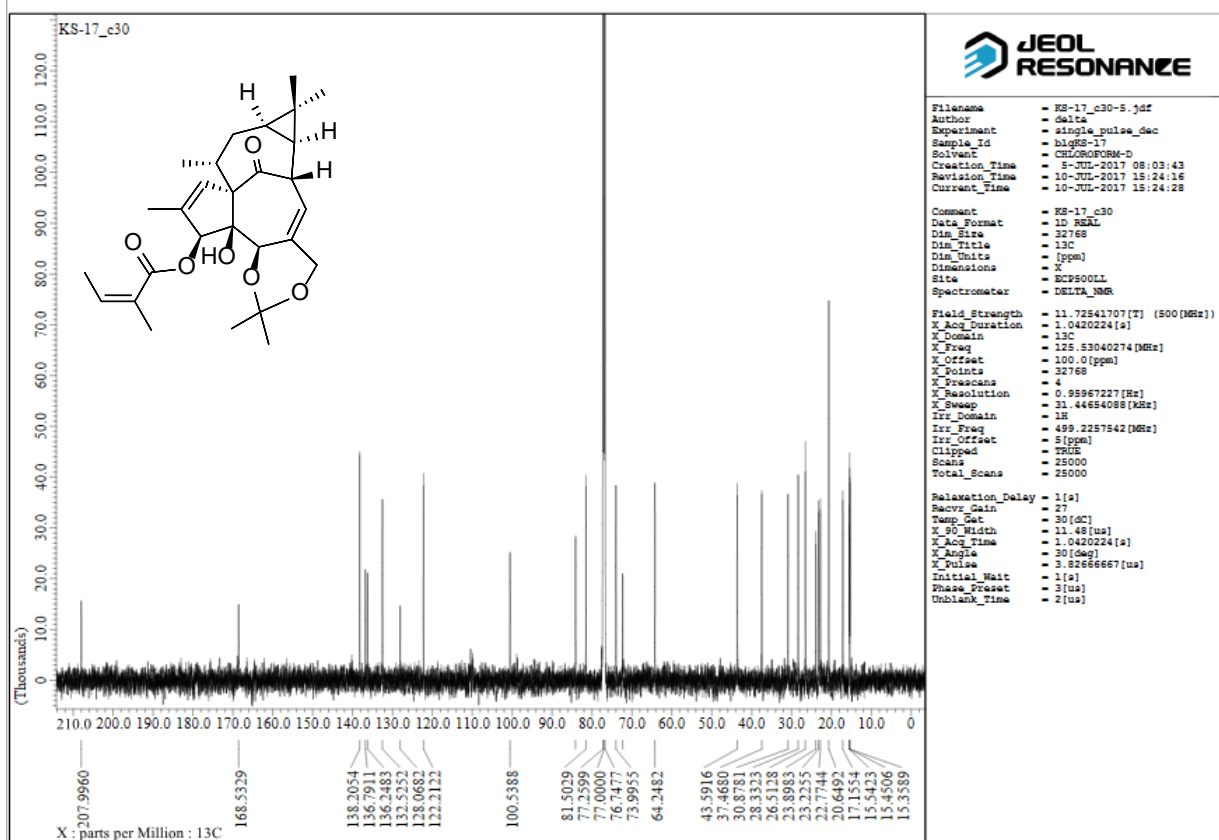
The HMBC spectrum of compound 19



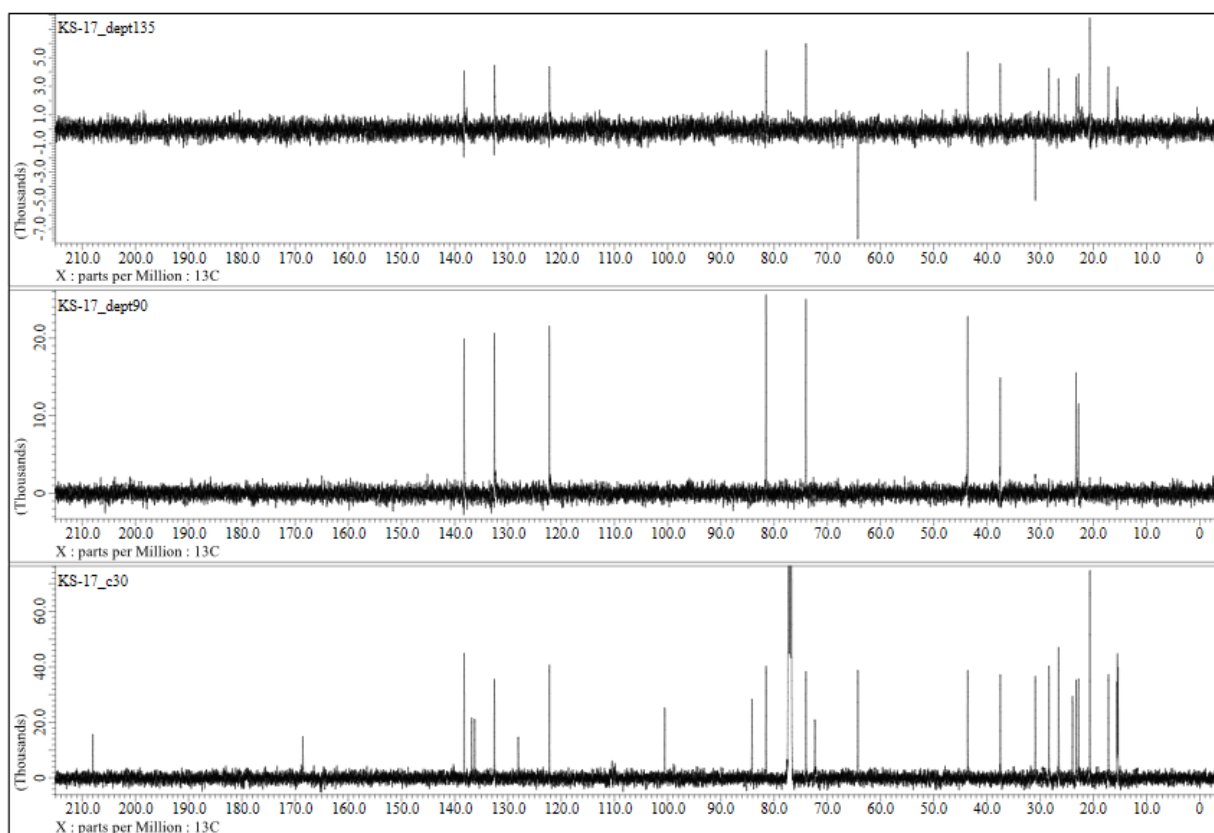
The NOESY spectrum of compound 19



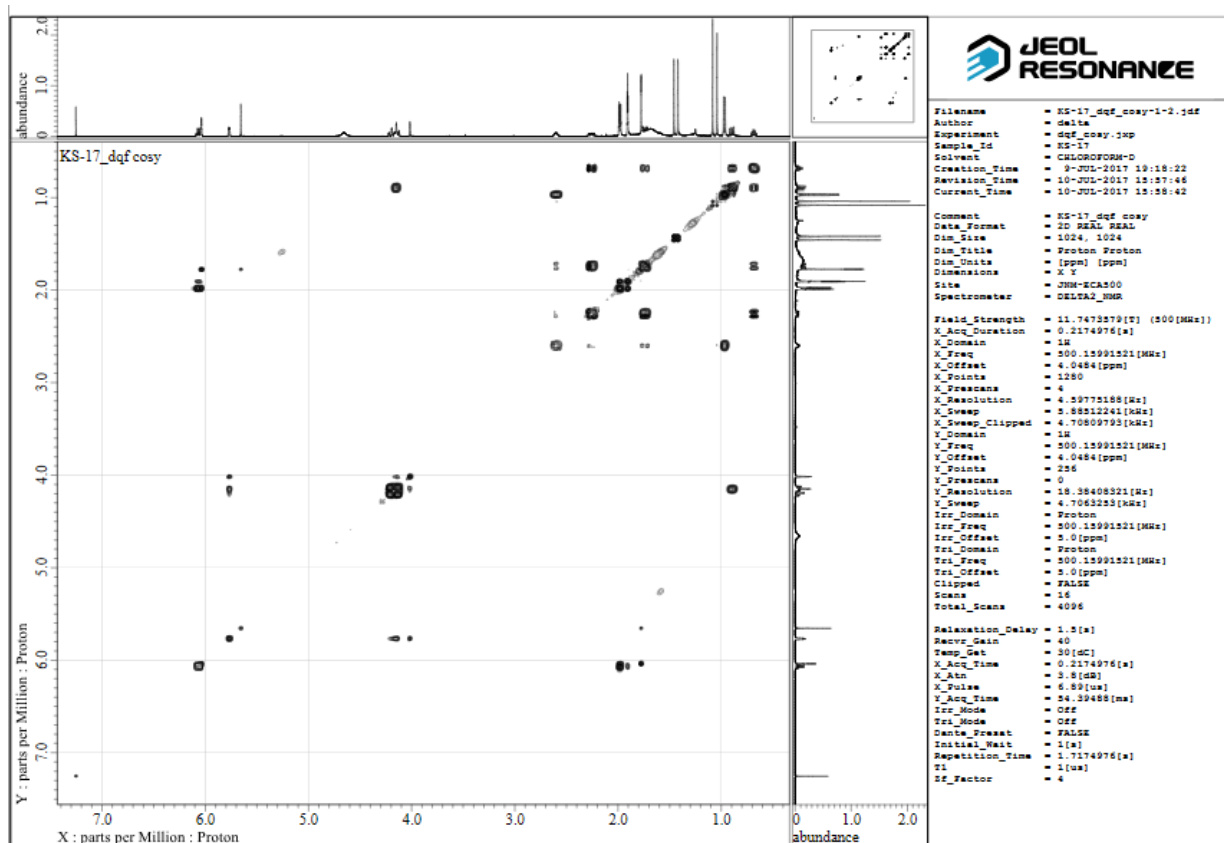
The ^1H spectrum of compound 20



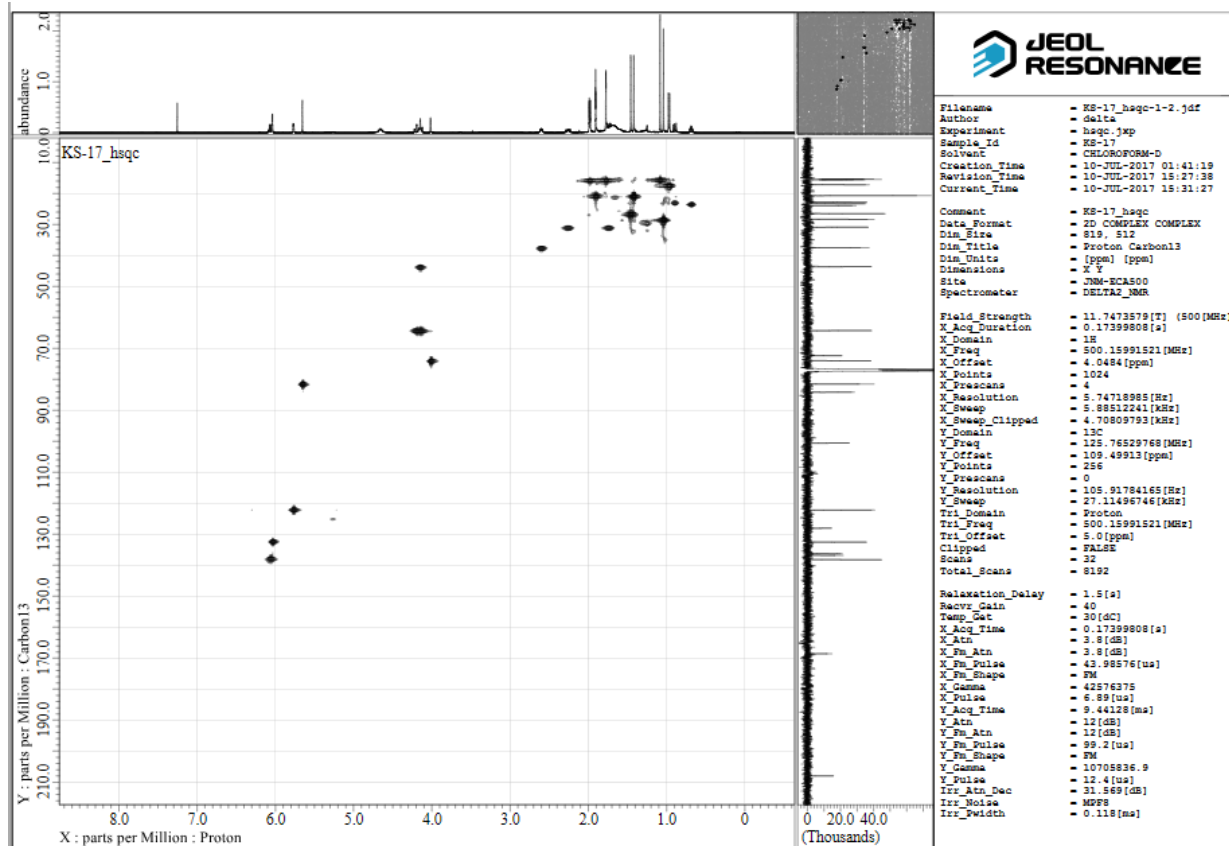
The ^{13}C spectrum of compound 20



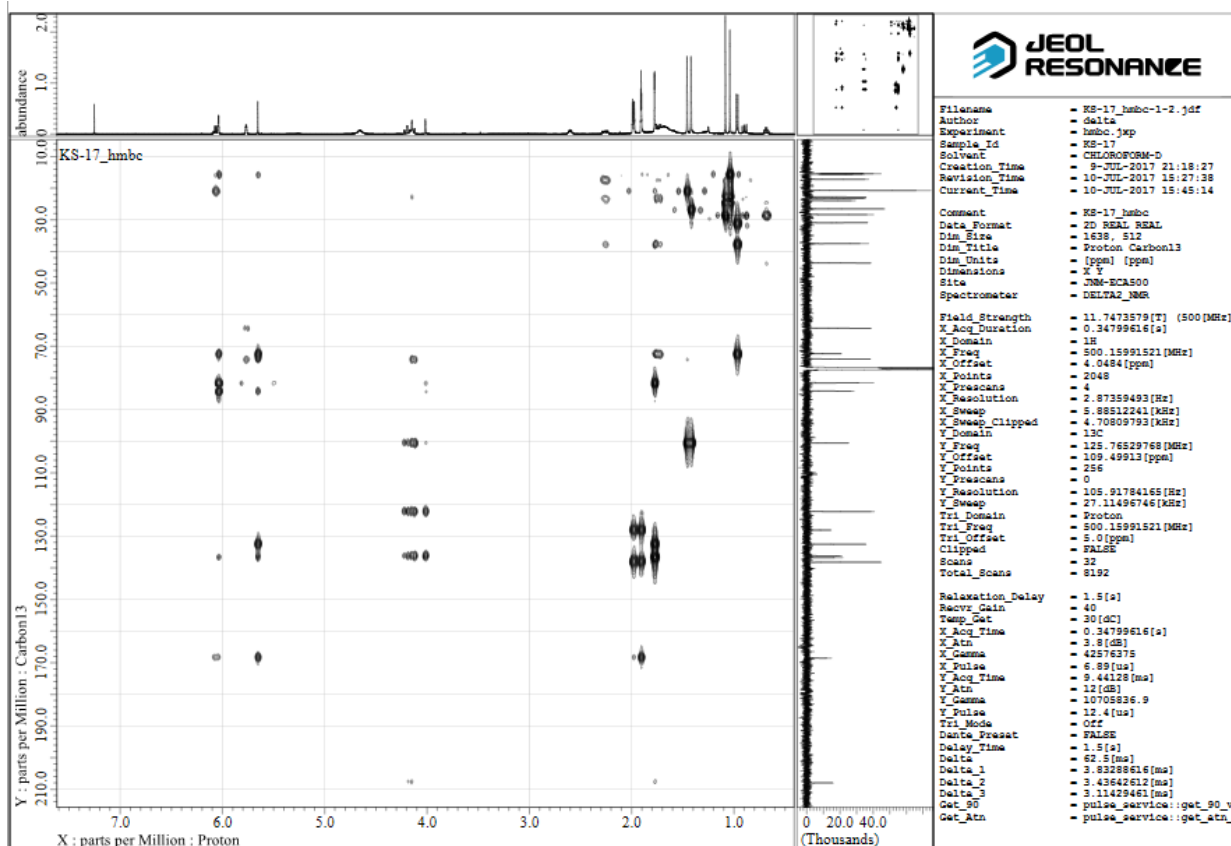
The DEPT spectrum of compound 20



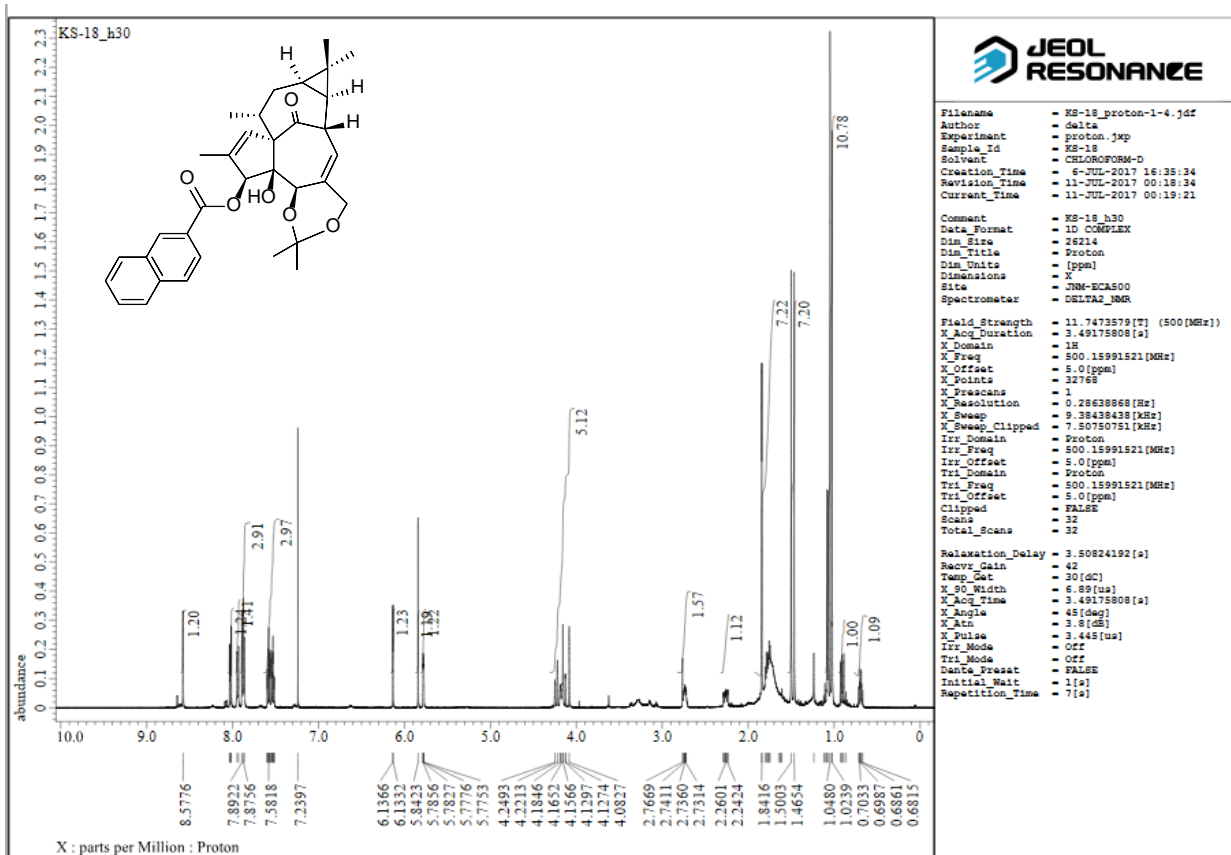
The DQF_COSY spectrum of compound 20



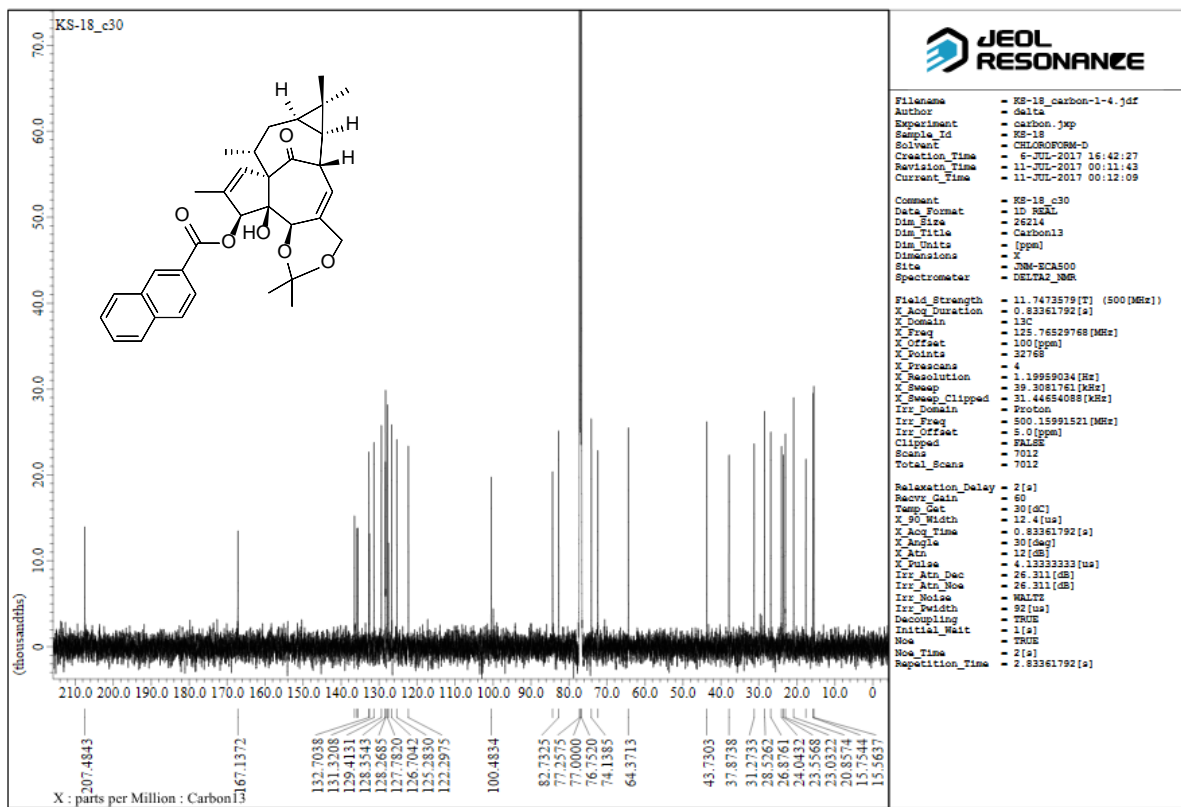
The HSQC spectrum of compound 20



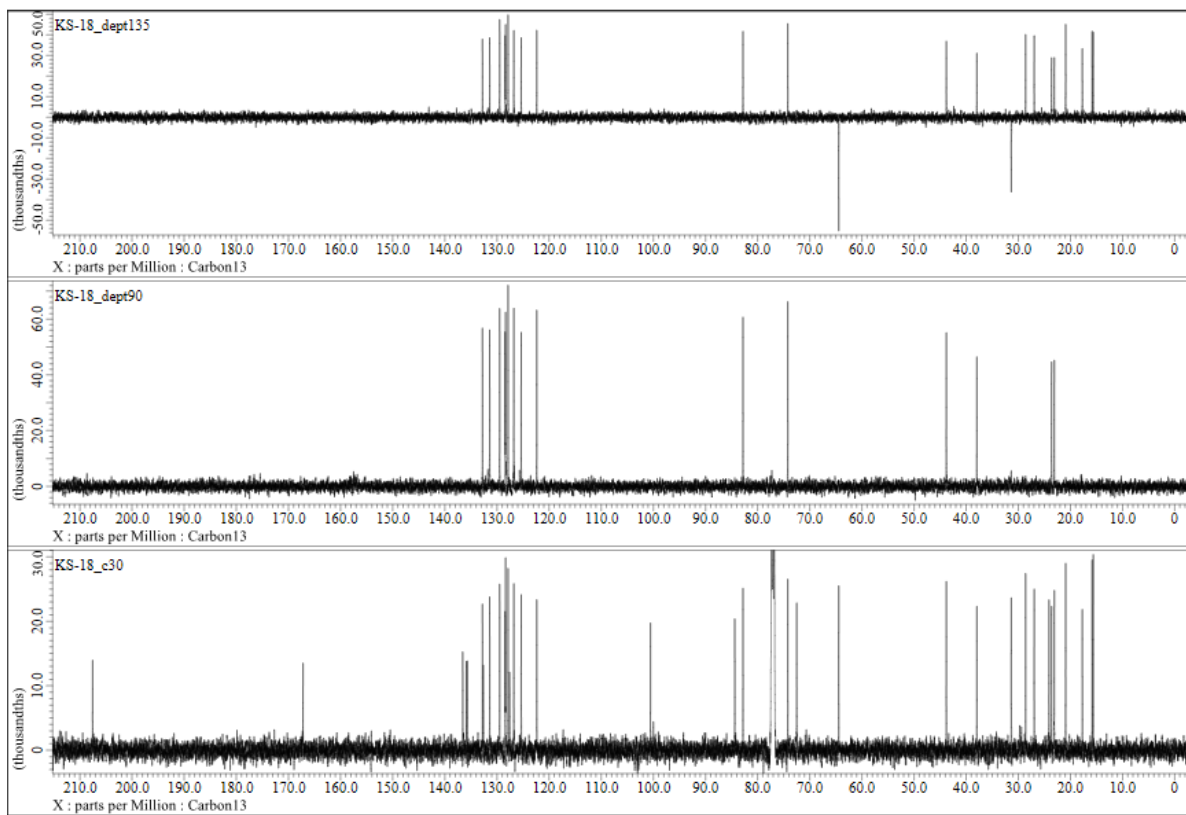
The HMBC spectrum of compound 20



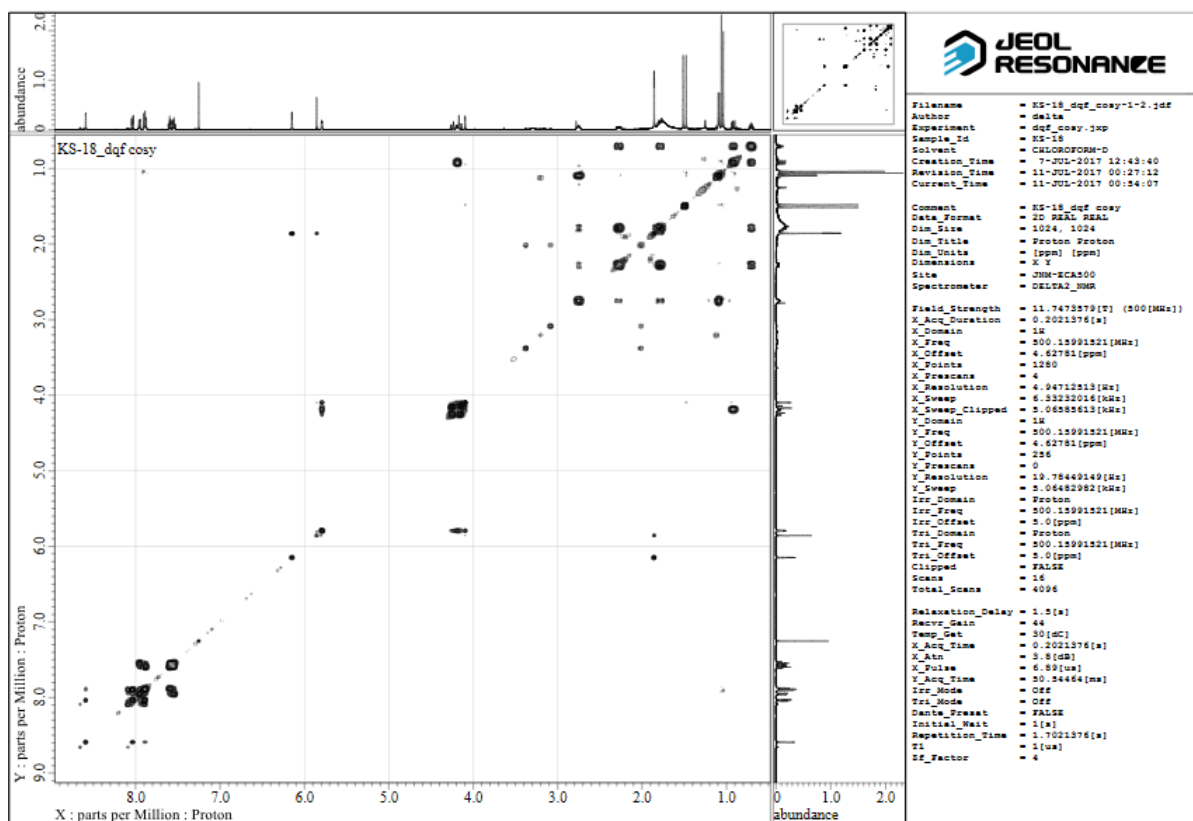
The ¹H spectrum of compound 21



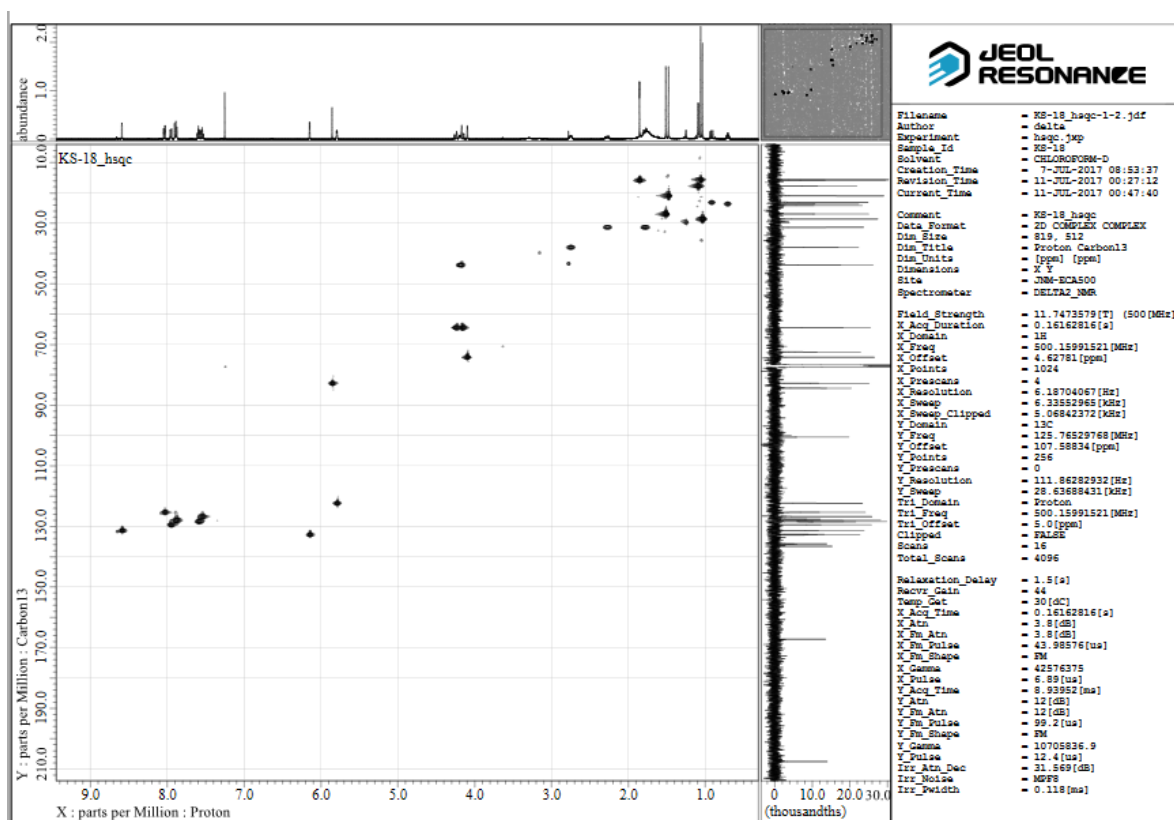
The ^{13}C spectrum of compound 21



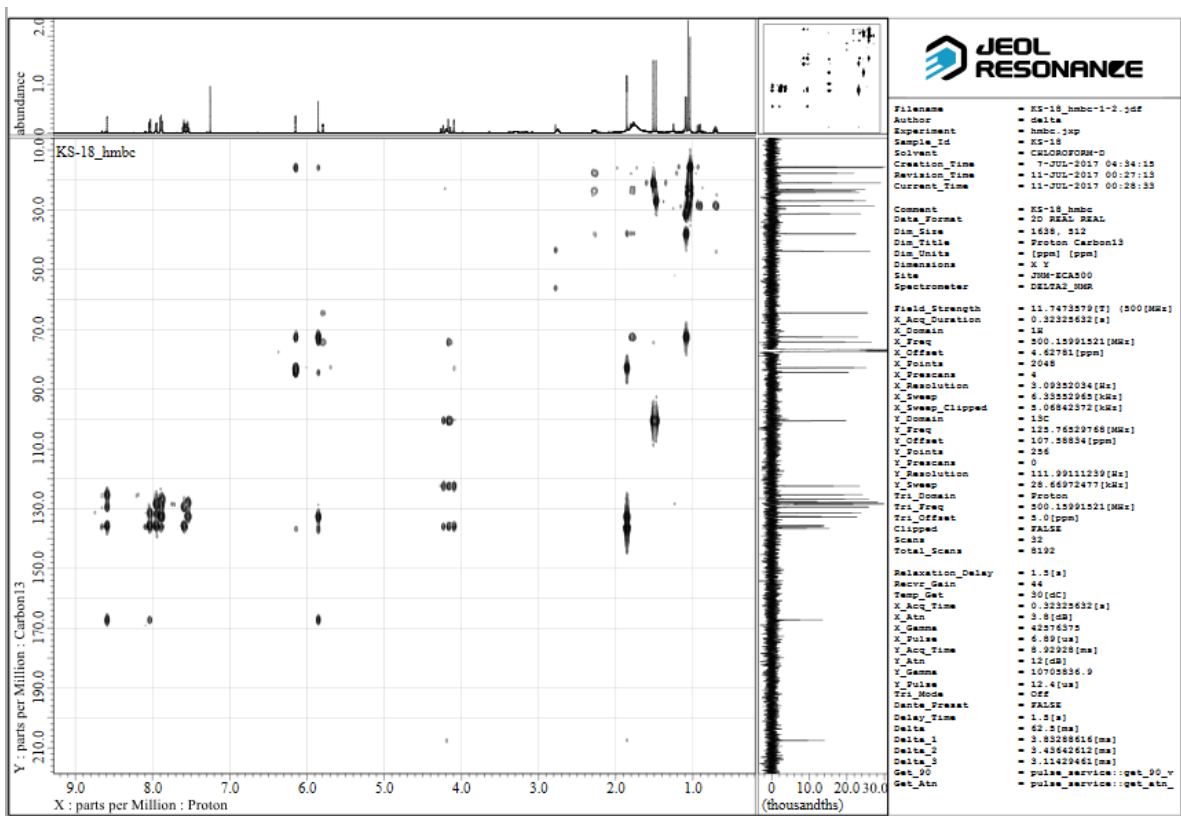
The DEPT spectrum of compound 21



The DQF_COSY spectrum of compound 21



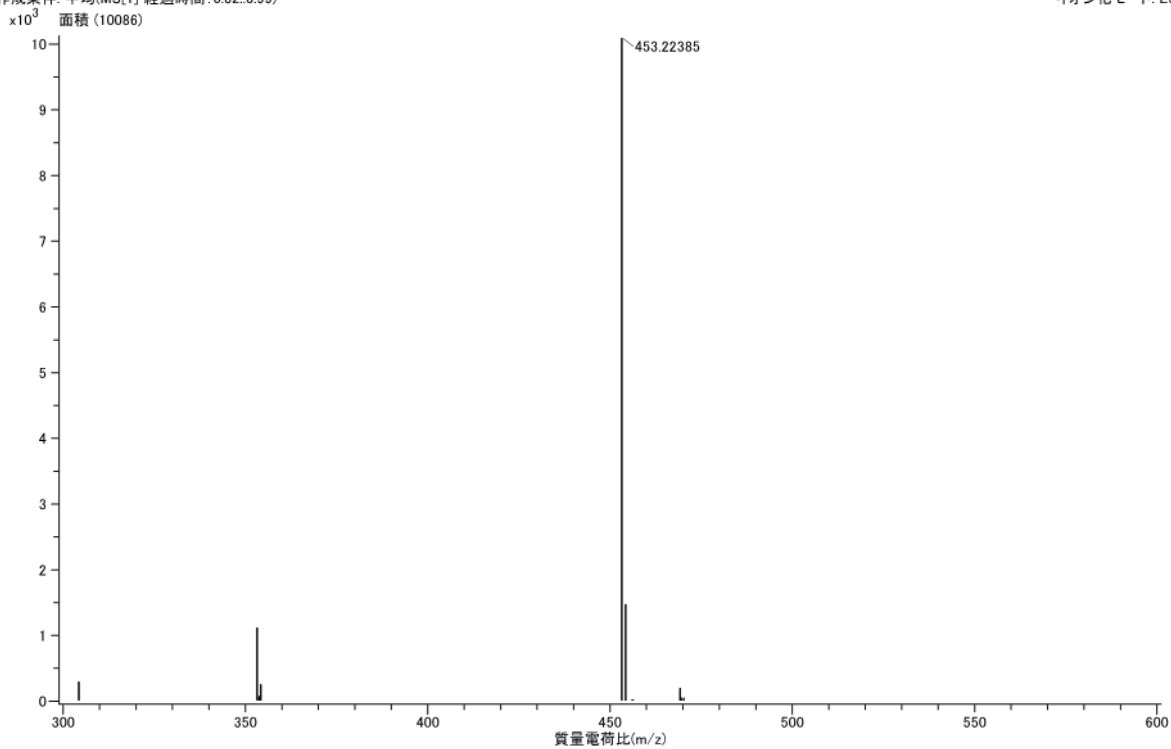
The HSQC spectrum of compound 21



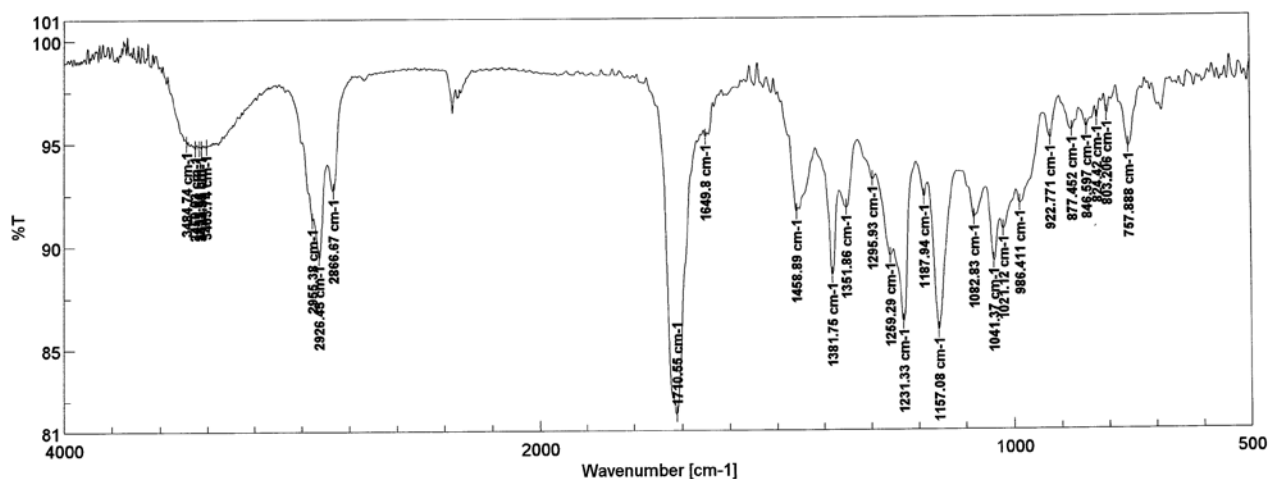
The HMBC spectrum of compound 21

測定データ名: KS-19
作成条件: 平均(MS[1]) 経過時間: 0.82.0.99

実験日時: 2017/10/13 22:13:47
イオン化モード: ESI+

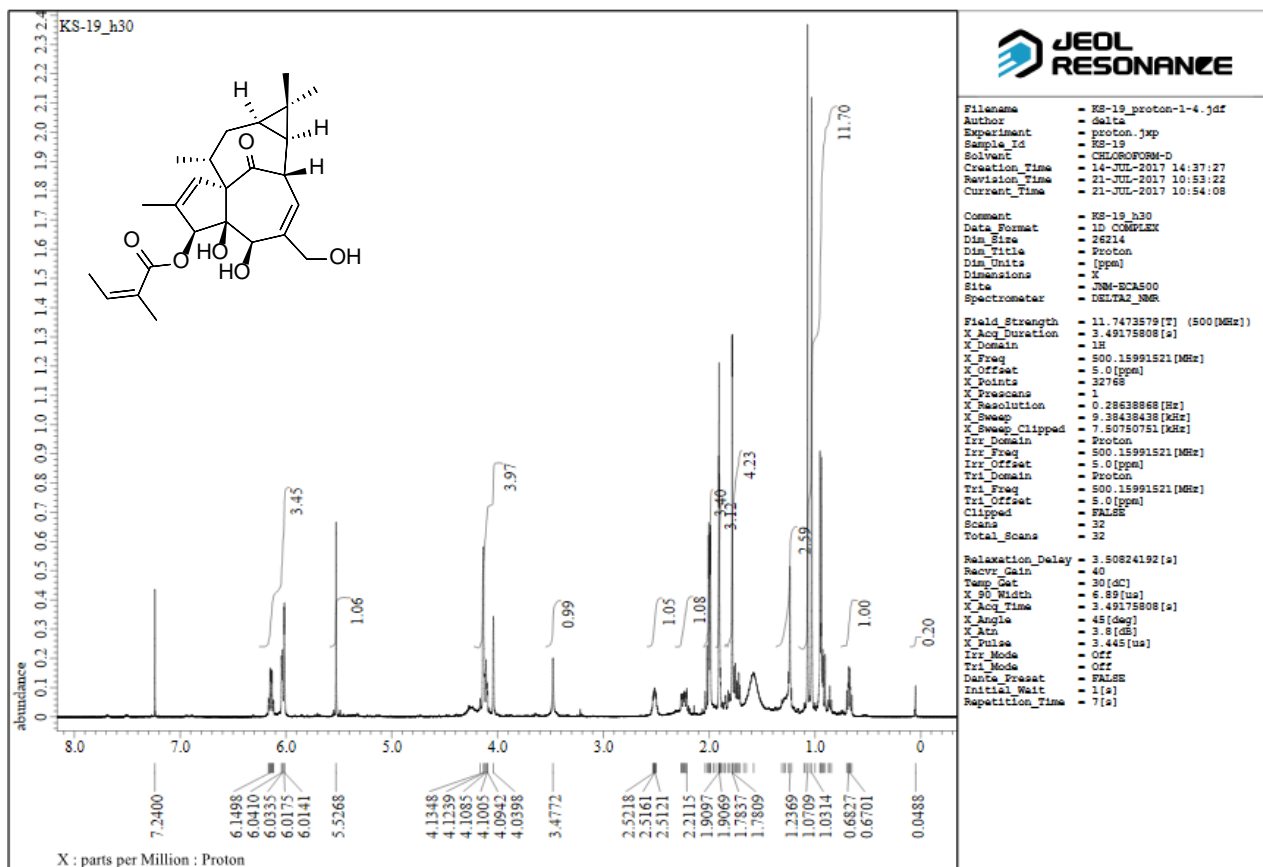


The HRESIMS spectrum of compound 22

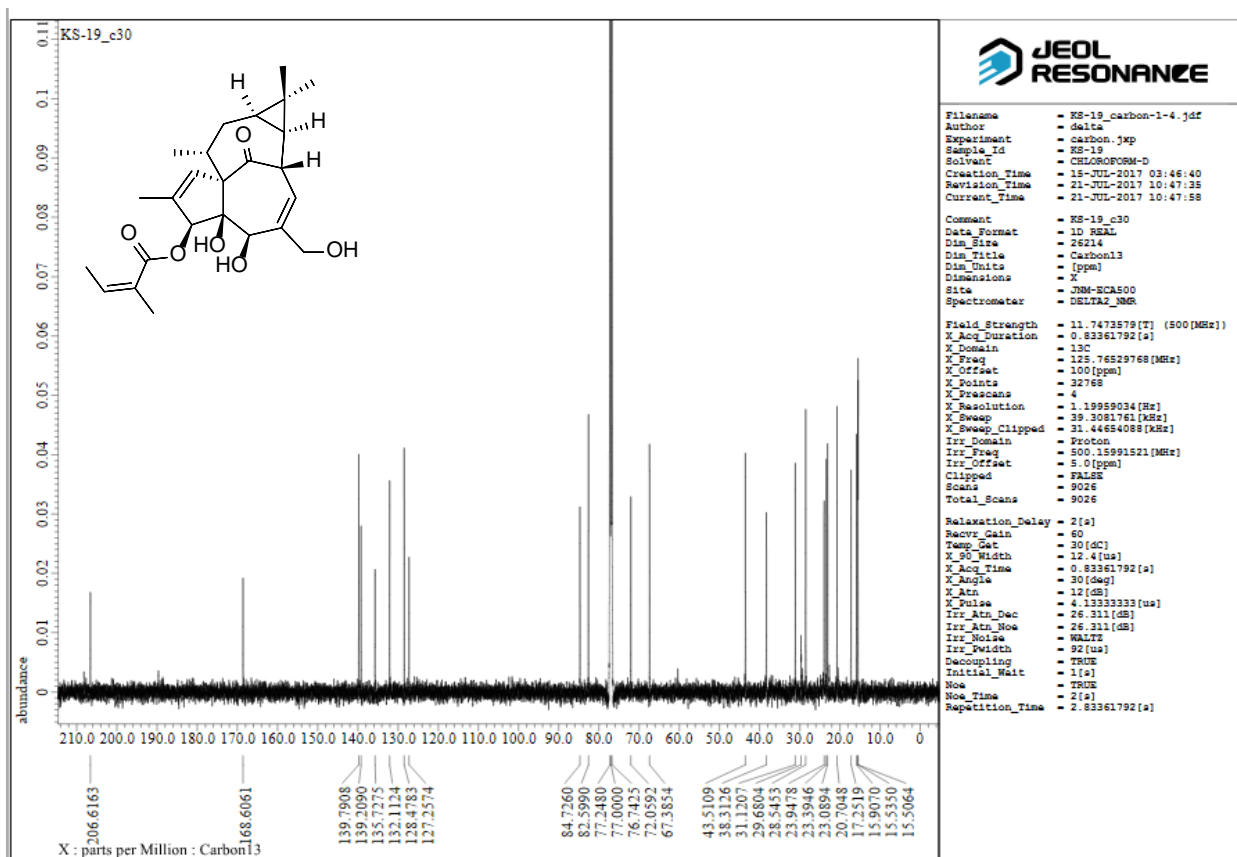


[コメント情報]		[測定情報]		Memory-2
試料名	KS-19	機種名	FT/IR-4100typeA	
コメント		シリアル番号	B109261016	
測定者		光源	標準光源	
所属	B	検出器	TGS	
会社	東邦大学 薬学部	積算回数	Auto (204)	
		分解	4 cm-1	
		ゼロフライング	On	
[データ情報]		アポダイゼーション	Cosine	
作成日時	2017/07/26 16:37	ゲイン	Auto (16)	
データタイプ	等間隔データ	アパーチャ	Auto (7.1 mm)	
横軸	Wavenumber [cm-1]	スキャンスピード	Auto (2 mm/sec)	
縦軸	%T	フィルタ	Auto (30000 Hz)	
スタート	0 cm-1			
エンド	7800.65 cm-1			
データ間隔	0.964233 cm-1			
データ数	8091			

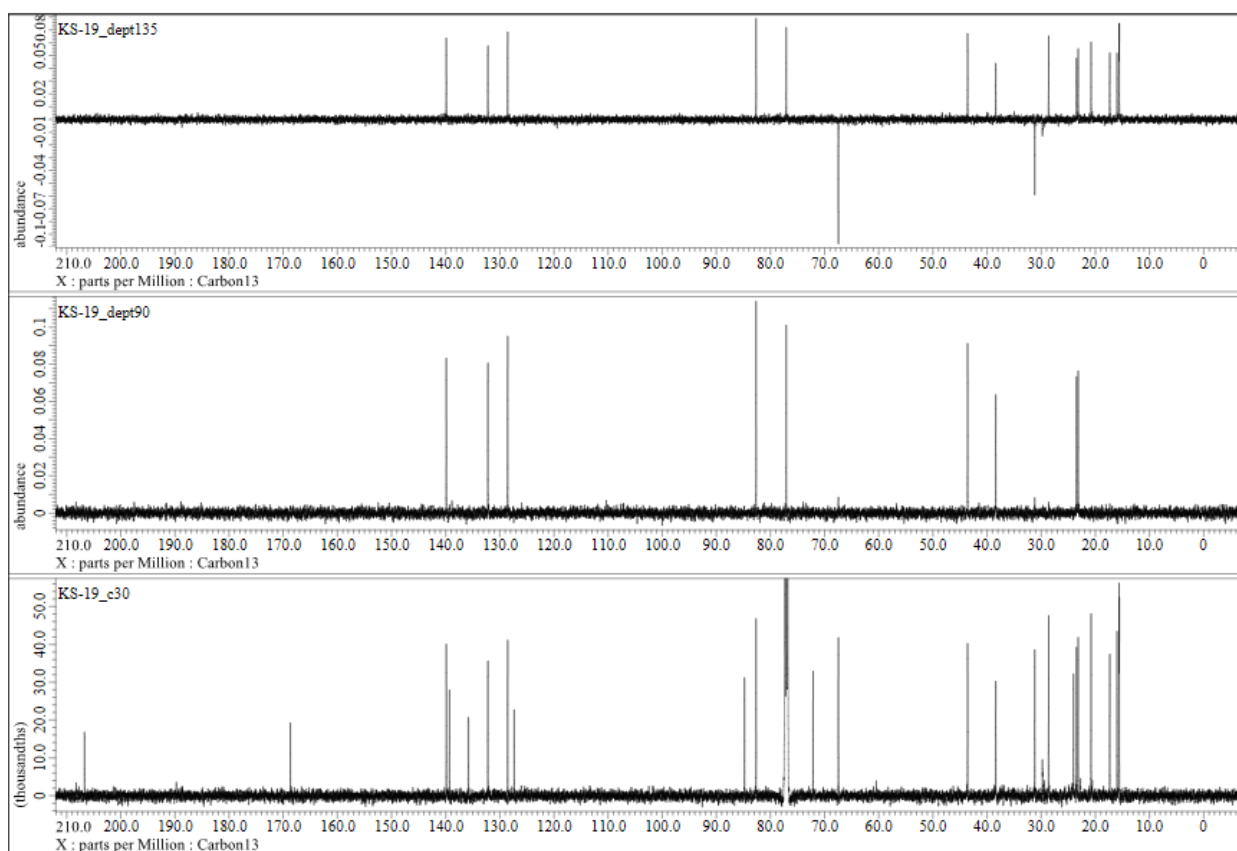
The IR spectrum of compound 22



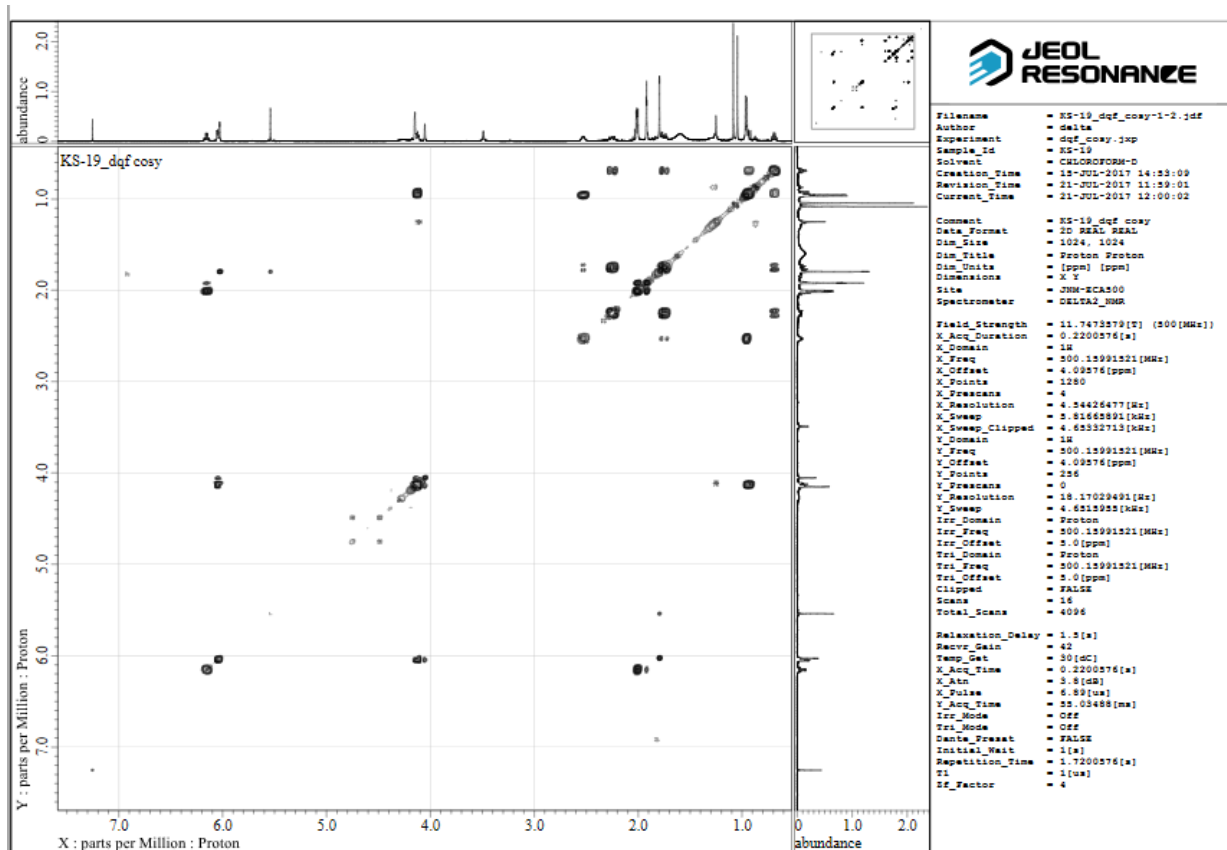
The ¹H spectrum of compound 22



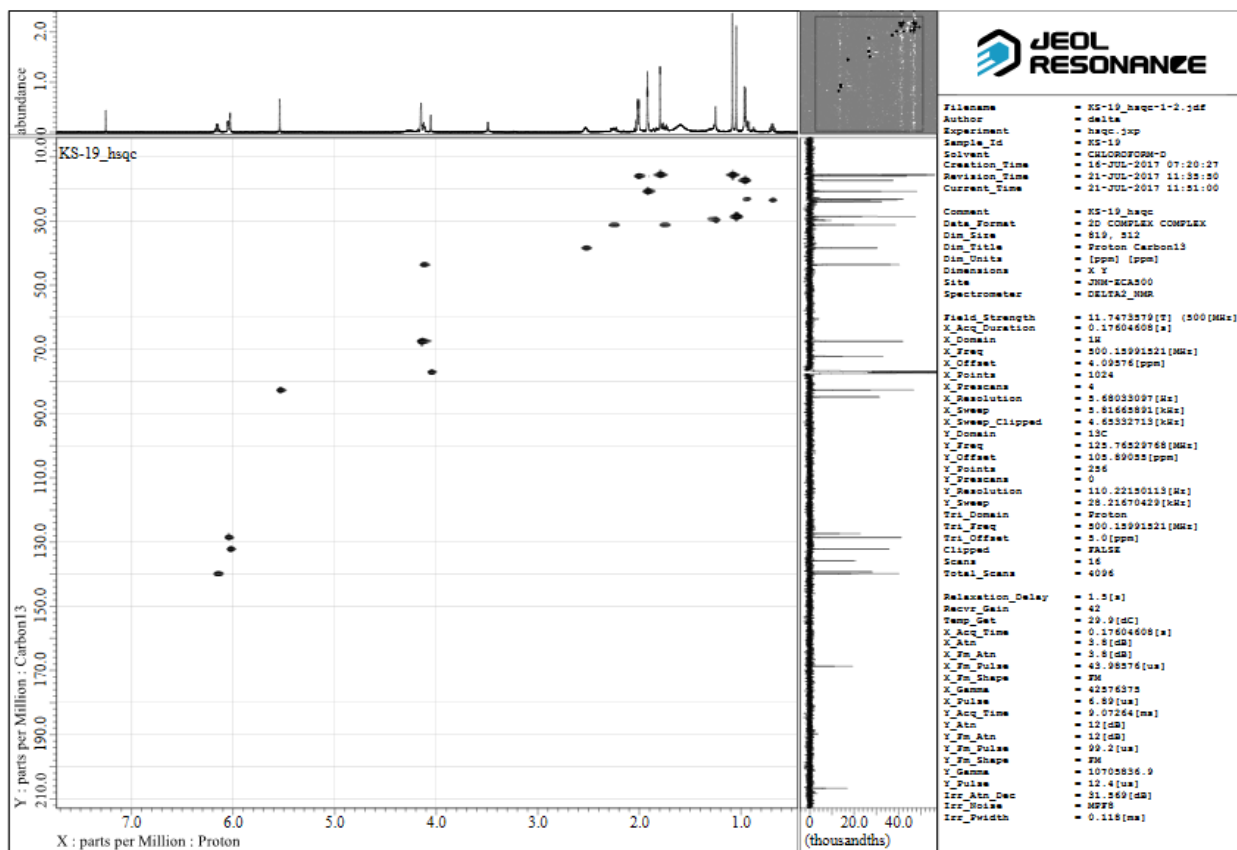
The ^{13}C spectrum of compound 22



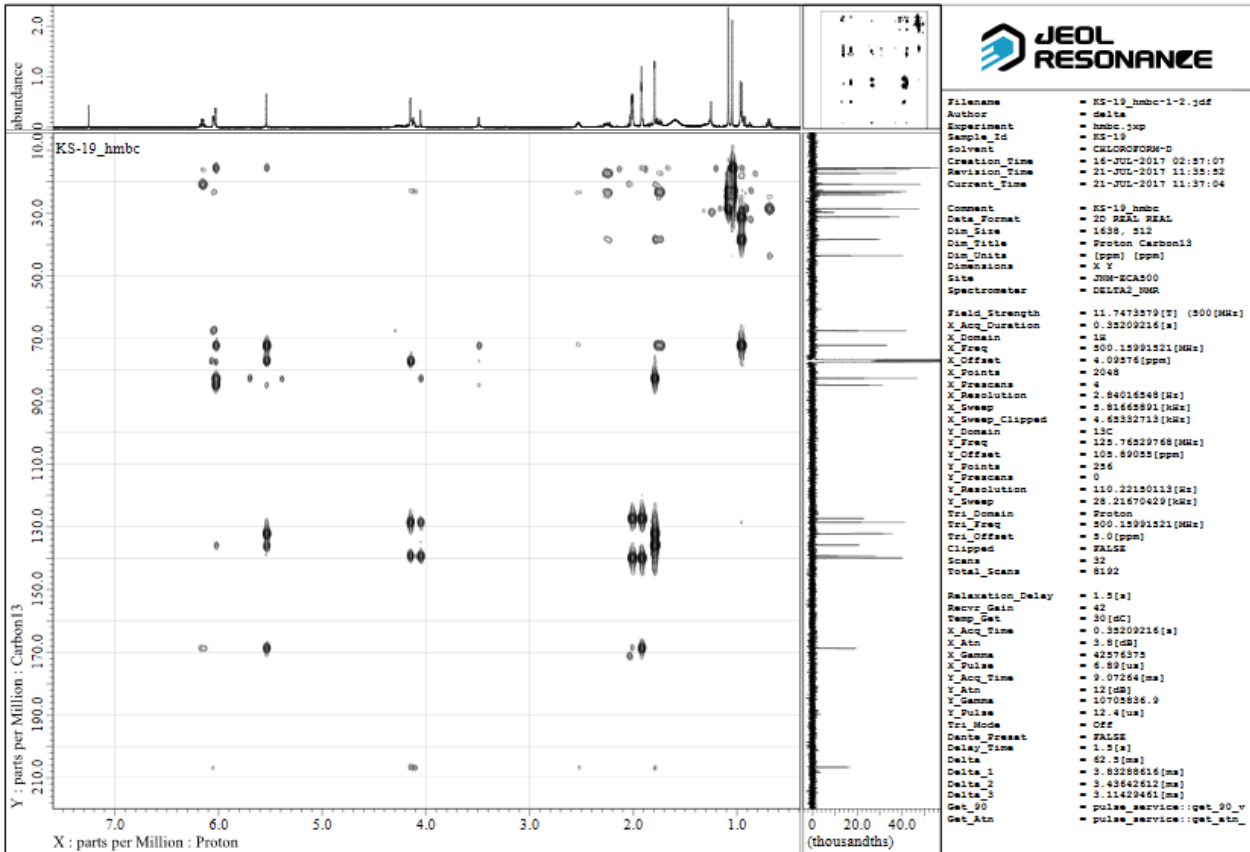
The DEPT spectrum of compound 22



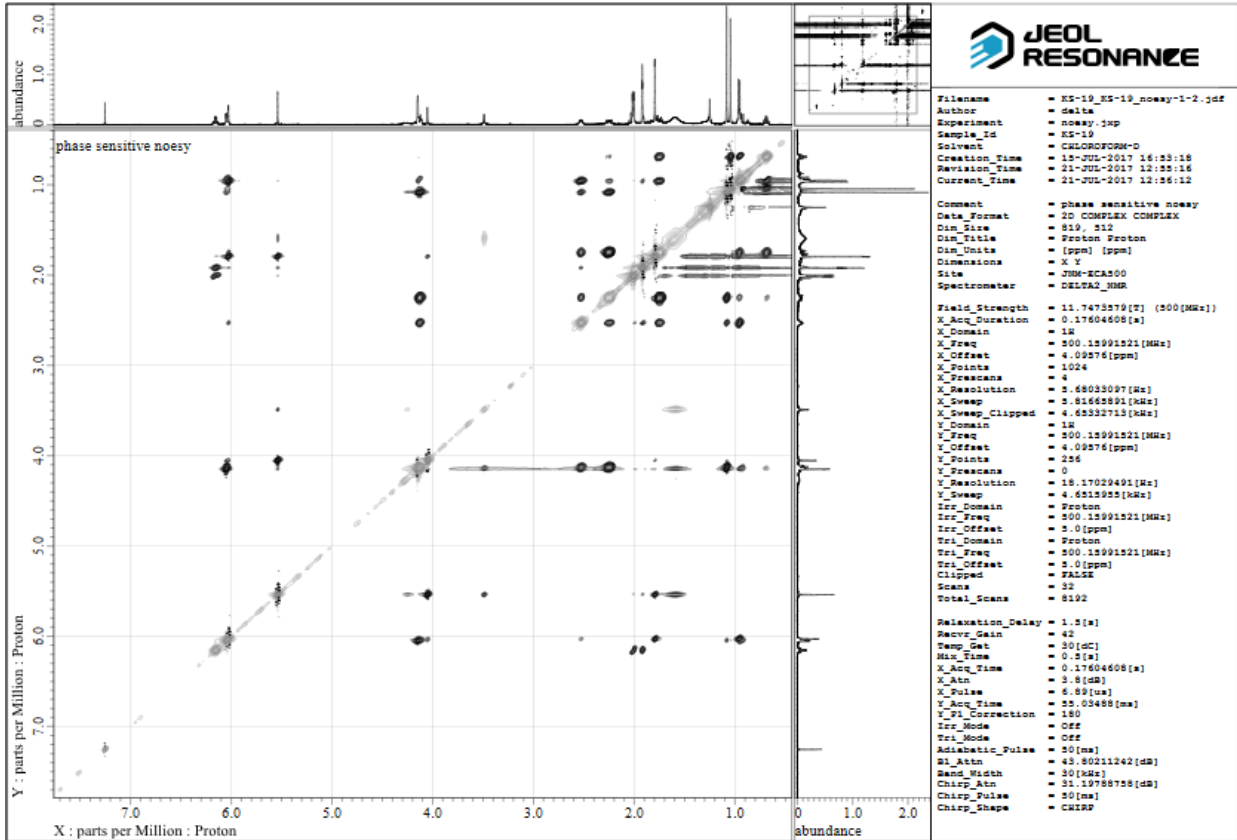
The DQF_COSY spectrum of compound 22



The HSQC spectrum of compound 22



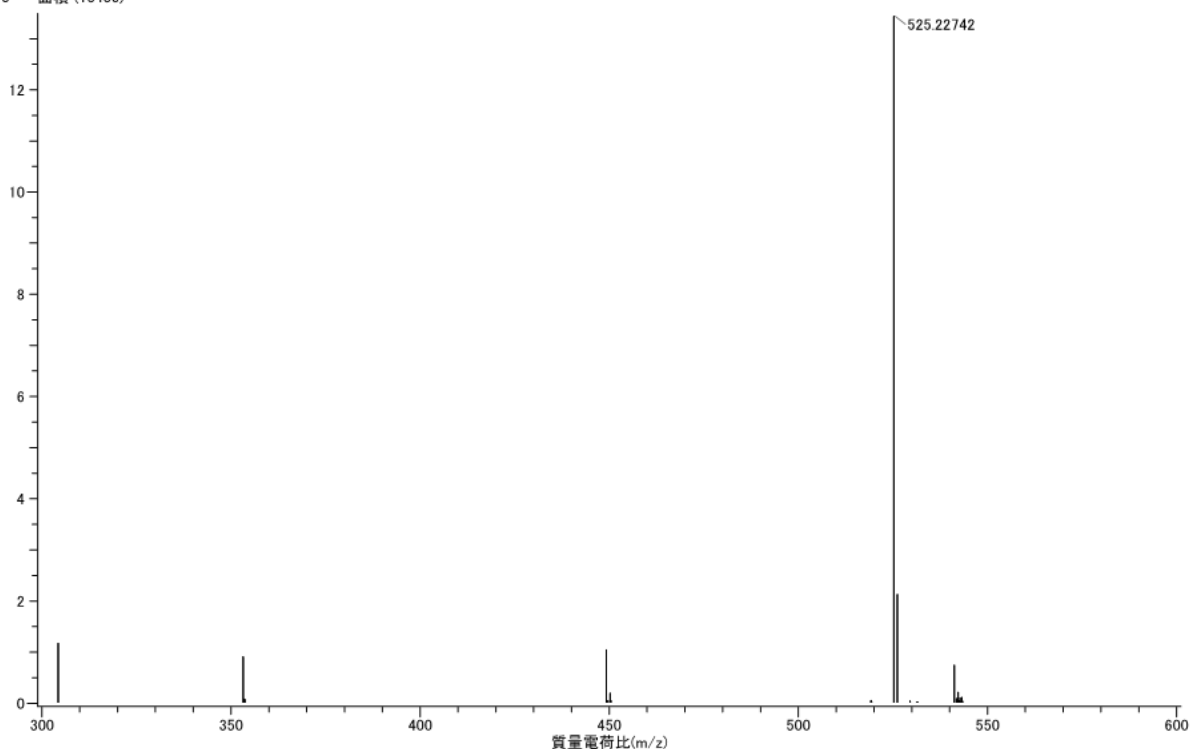
The HMBC spectrum of compound 22



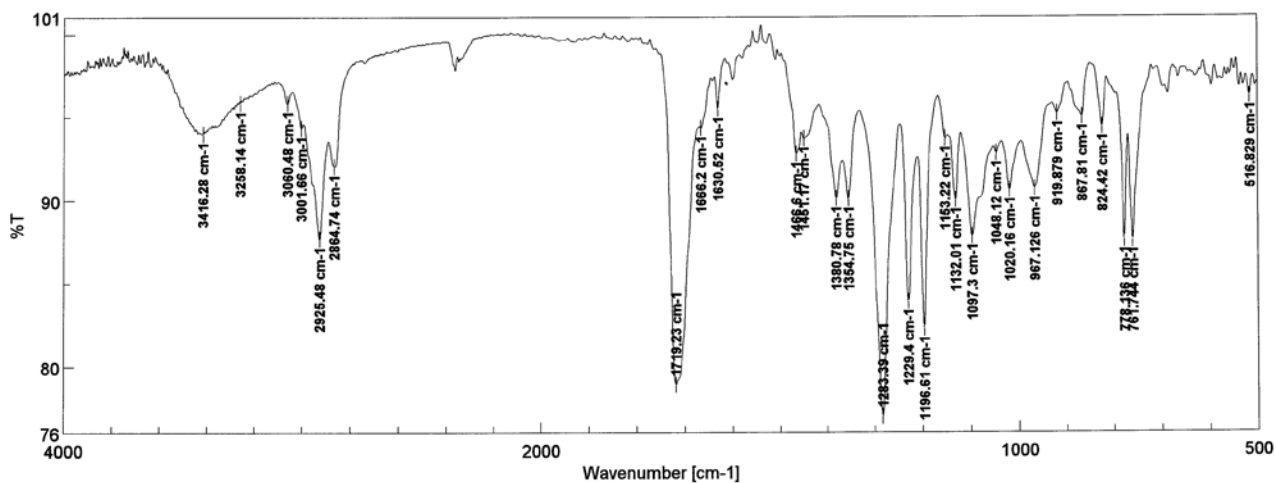
The NOESY spectrum of compound 22

測定データ名: KS-20
 作成条件: 平均(MS[1]) 経過時間: 1.44..1.52
 x10³ 面積 (13436)

実験日時: 2017/10/13 22:18:36
 イオン化モード: ESI+



The HRESIMS spectrum of compound 23



[コメント情報]

試料名 KS-20
 コメント
 測定者 B
 所属 東邦大学 薬学部
 会社

[データ情報]

作成日時 2017/07/26 16:50
 データタイプ 等間隔データ
 横軸 Wavenumber [cm-1]
 縦軸 %T
 スタート 0 cm-1
 エンド 7800.65 cm-1
 データ間隔 0.964233 cm-1
 データ数 8091

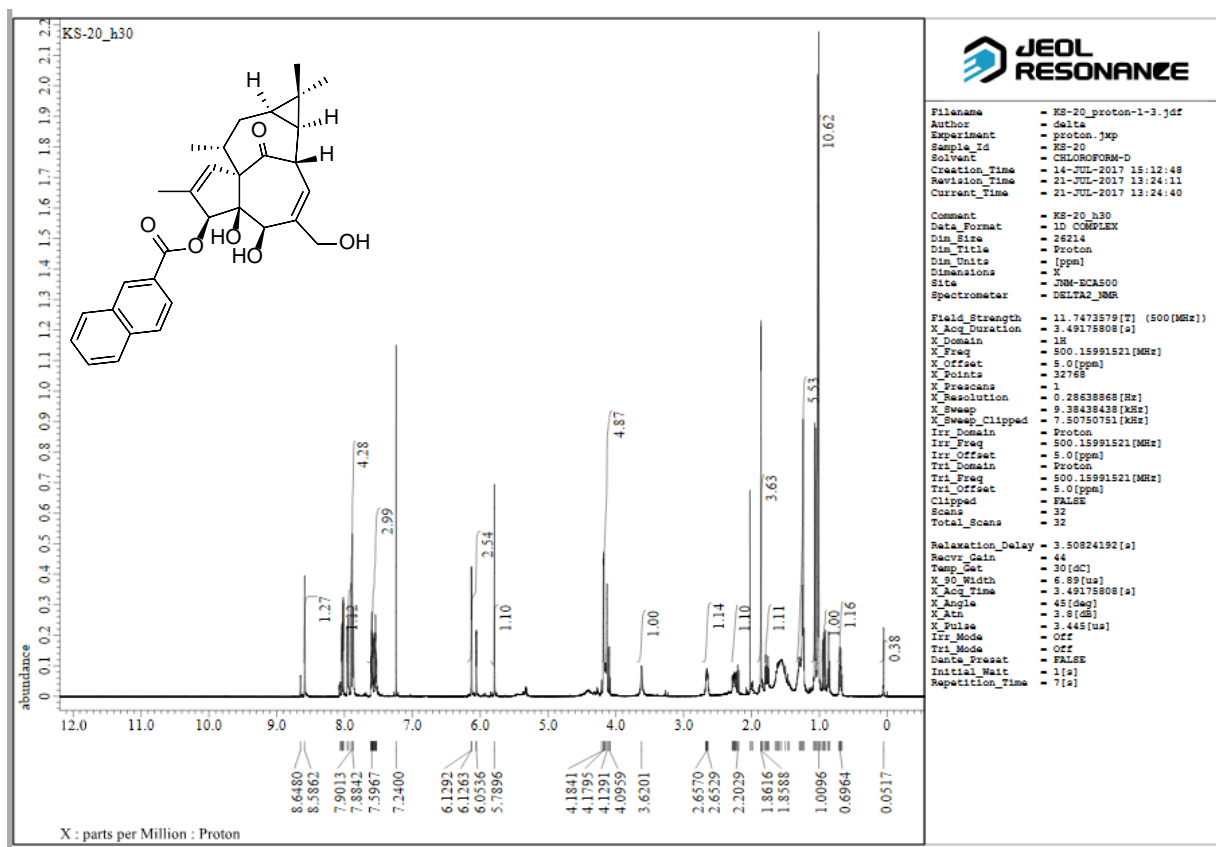
[測定情報]

機種名 FT/IR-4100typeA
 シリアル番号 B109261016

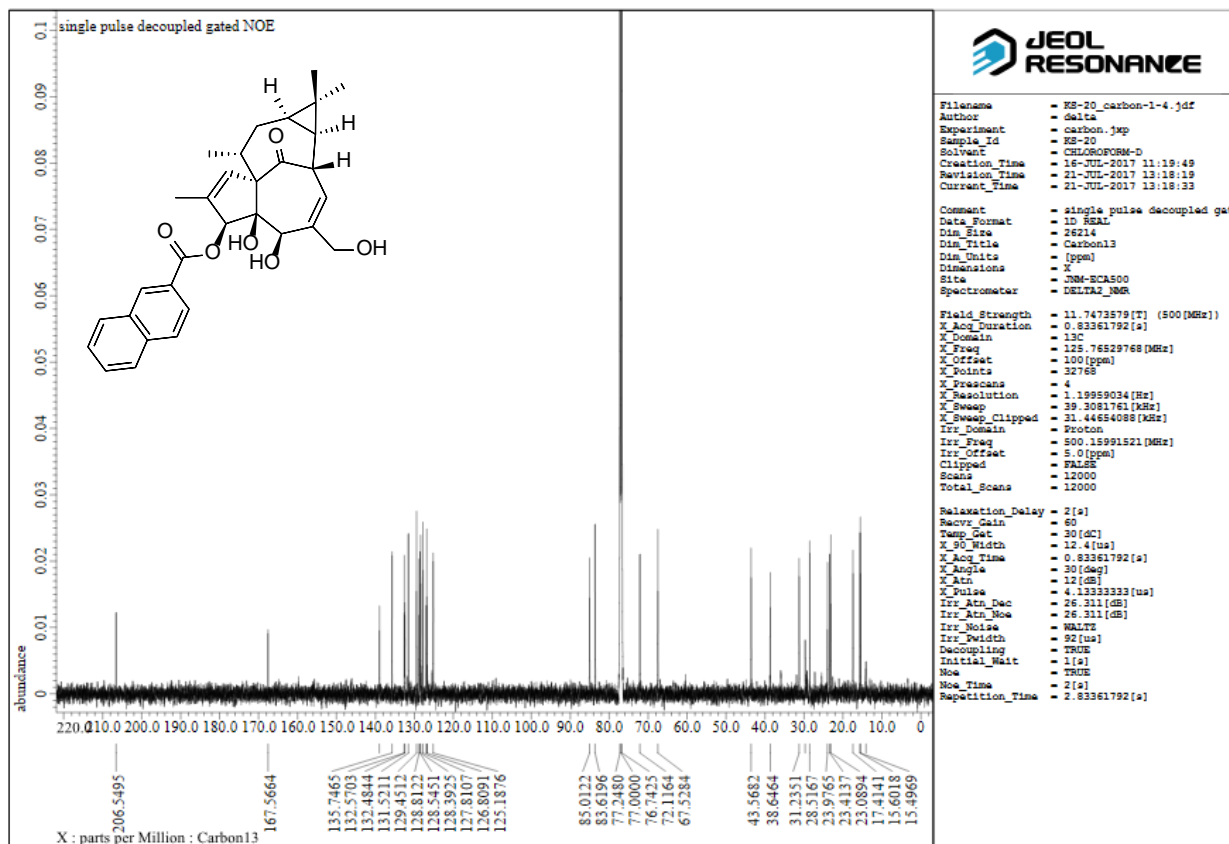
光源 標準光源
 検出器 TGS
 積算回数 Auto (210)
 分解 4 cm-1
 ゼロフリンク On
 アポダイゼーション Cosine
 ゲイン Auto (16)
 アパーチャー Auto (7.1 mm)
 スキャンスピード Auto (2 mm/sec)
 フィルタ Auto (30000 Hz)

Memory-2

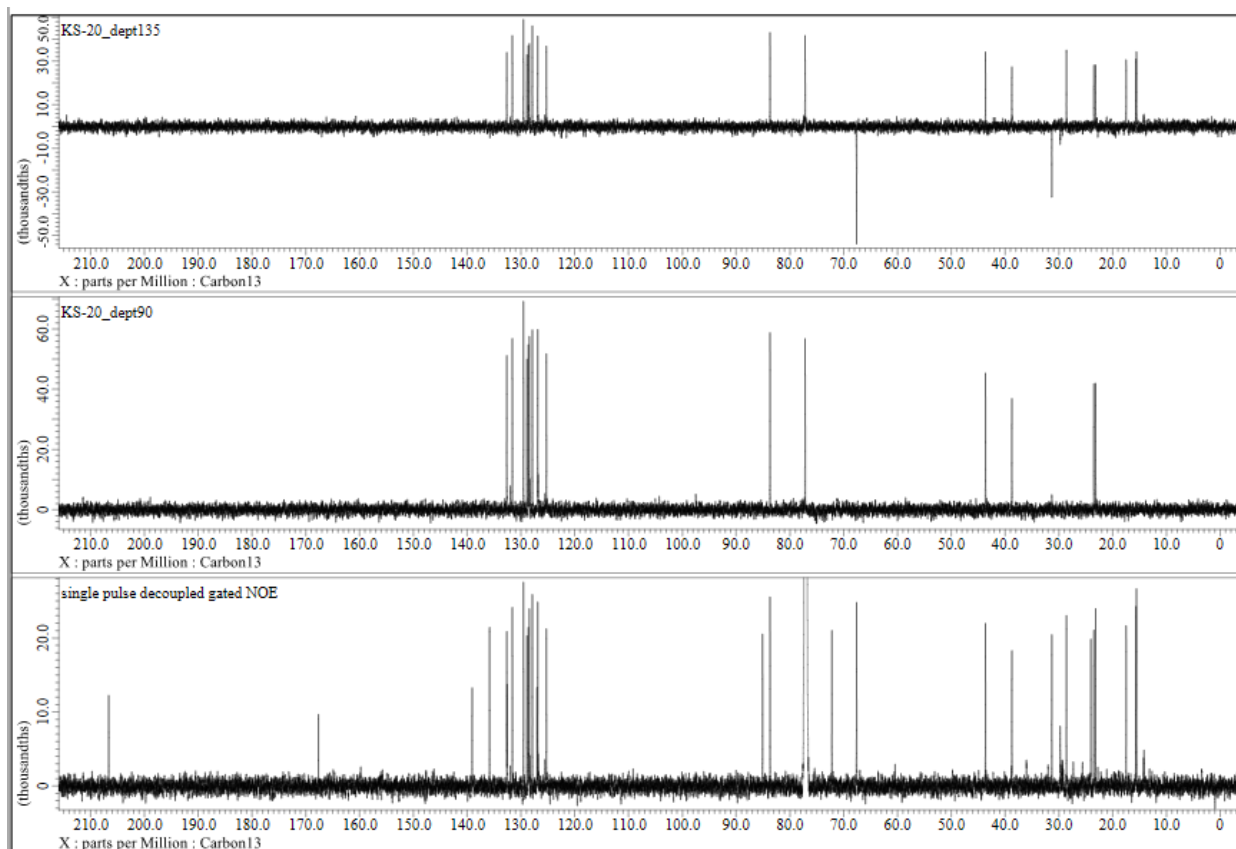
The IR spectrum of compound 23



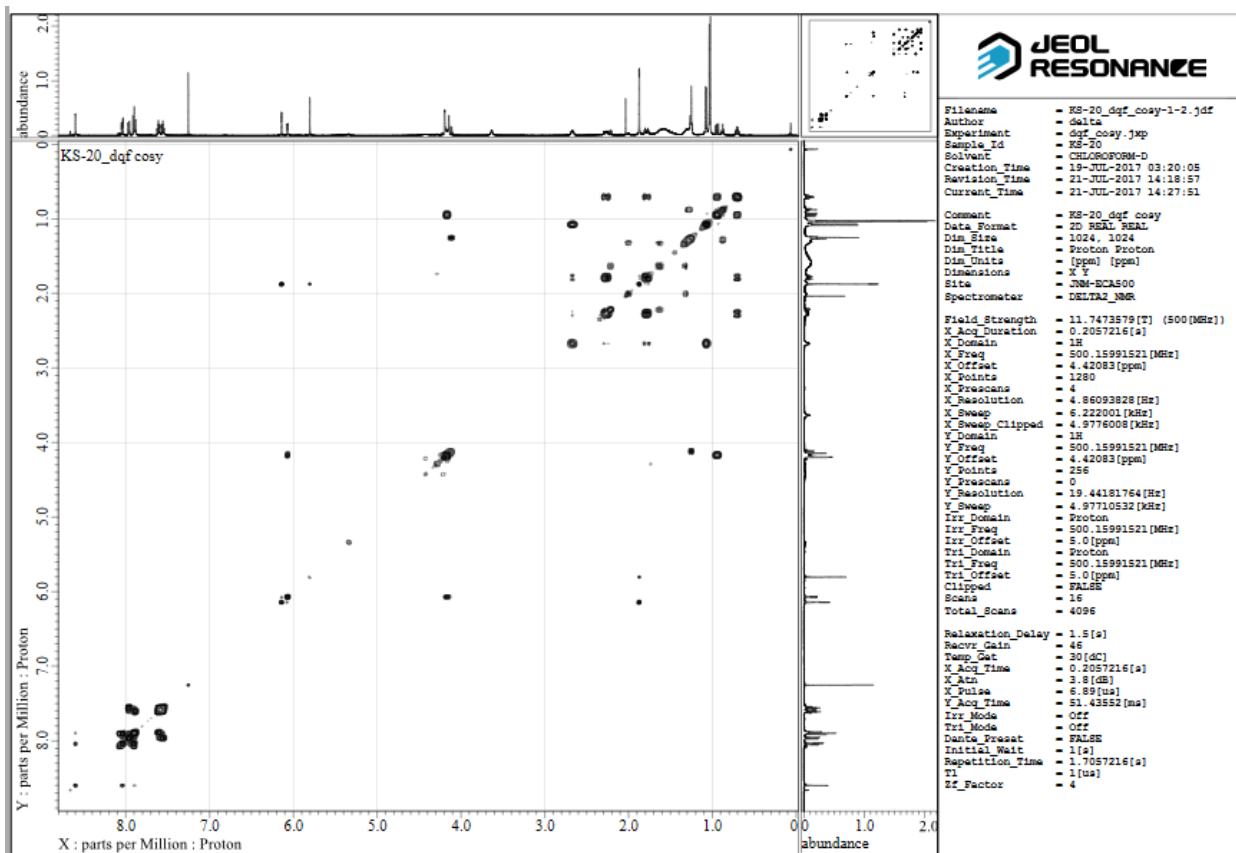
The ^1H spectrum of compound 23



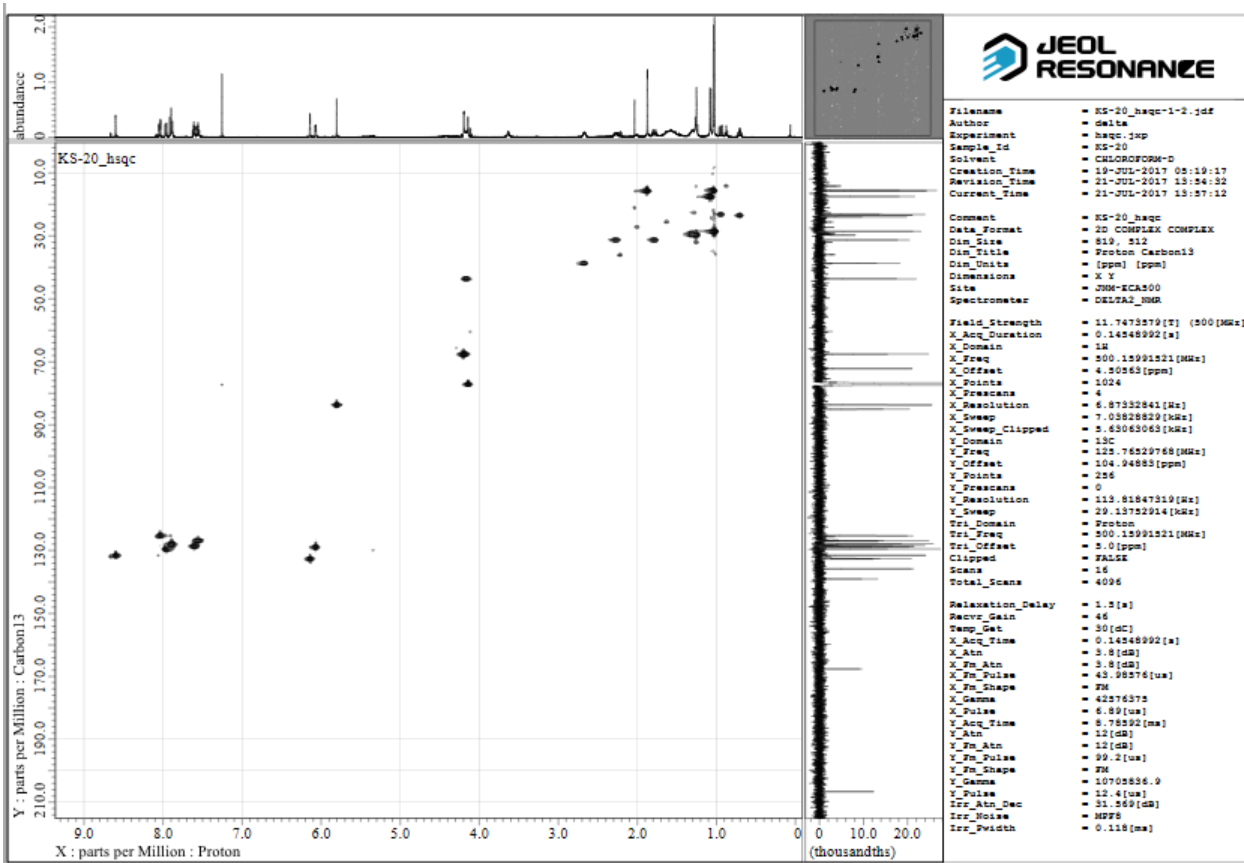
The ^{13}C spectrum of compound 23



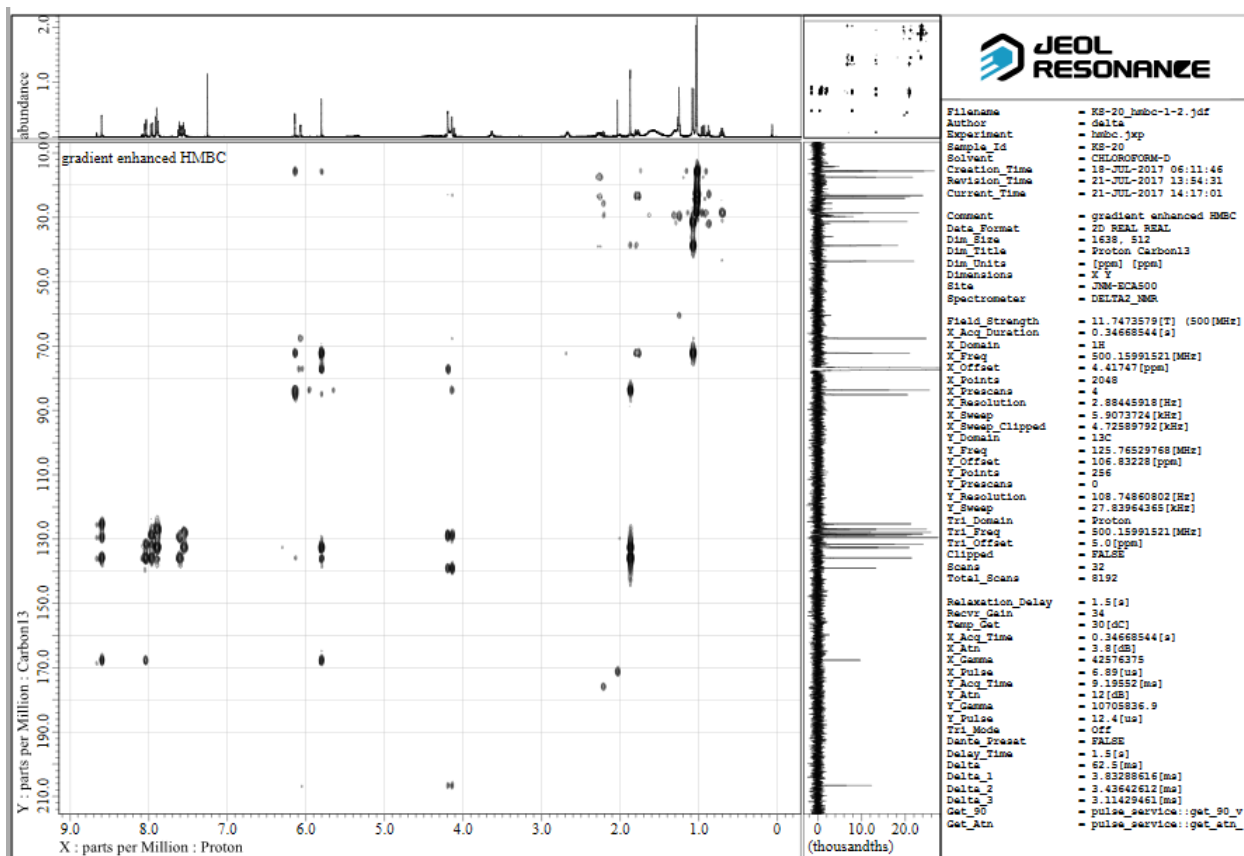
The DEPT spectrum of compound 23



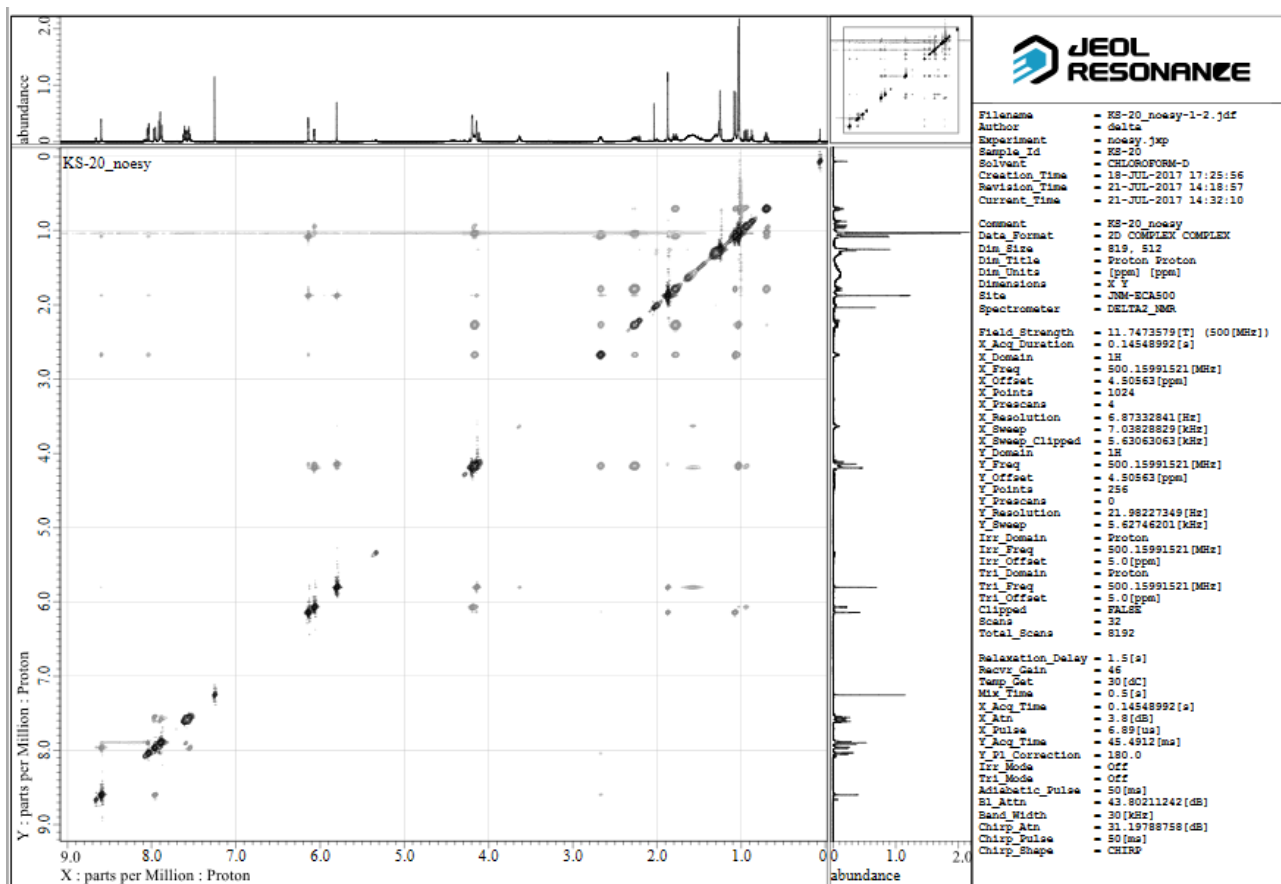
The DQF-COSY spectrum of compound 23



The HSQC spectrum of compound 23



The HMBC spectrum of compound 23



The NOESY spectrum of compound **23**