Supporting Information

Smart and concise entry to chiral spiro[cyclopentane-indolizidine]-tetraol diastereomers as new aza-spirocyclic framework

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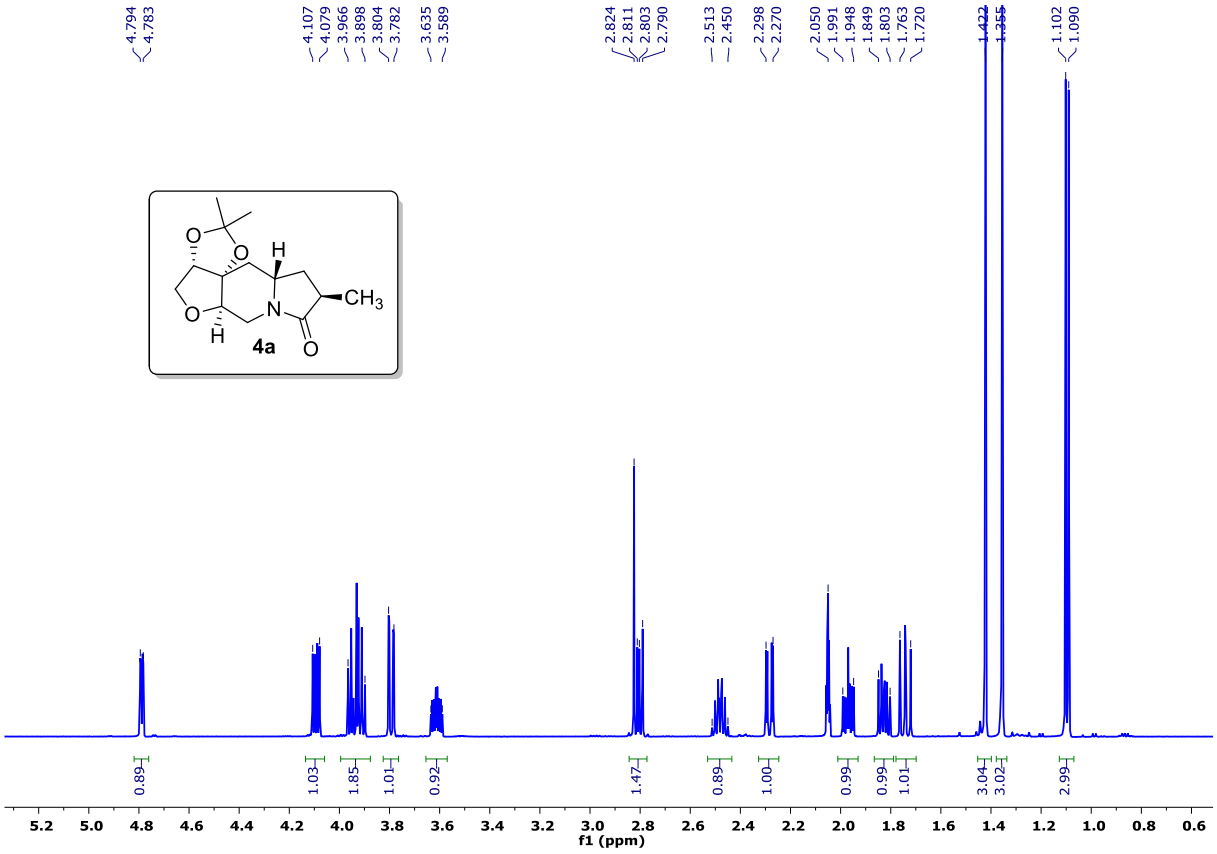
1. General methods

NMR spectra were recorded on a VNMRS 600 NMR spectrometer (Varian) with operating frequencies 599.76 MHz for ^{1}H and 150.82 MHz for ^{13}C. NMR spectra from all samples were measured in acetone-d_6 at 25 °C. Chemical shifts (δ) are quoted in ppm; the chemical shift axes were calculated using the reference signals of TMS (for ^{1}H and ^{13}C NMR). Depending on the possibilities and amount of information needed to provide the best possible structural proof ^{1}H, standard ^{13}C, quantitative ^{13}C,^{13}C-attached proton test, within versegated ^{1}H decoupling, supported by ^{1}H-^{1}HCOSY (with gradient coherence selection and with/without zero quantum filtering), ^{1}H-^{13}C HSQC (with varied use of gradient coherence selection, adiabatic 180° pulses on the ^{13}C channel and non-uniform sampling). For the precise extraction of chemical shift and *J*-coupling values manual spin simulation was preformed if needed in the spin simulation package built in the MestReNova software (version 11.0.2–18153).

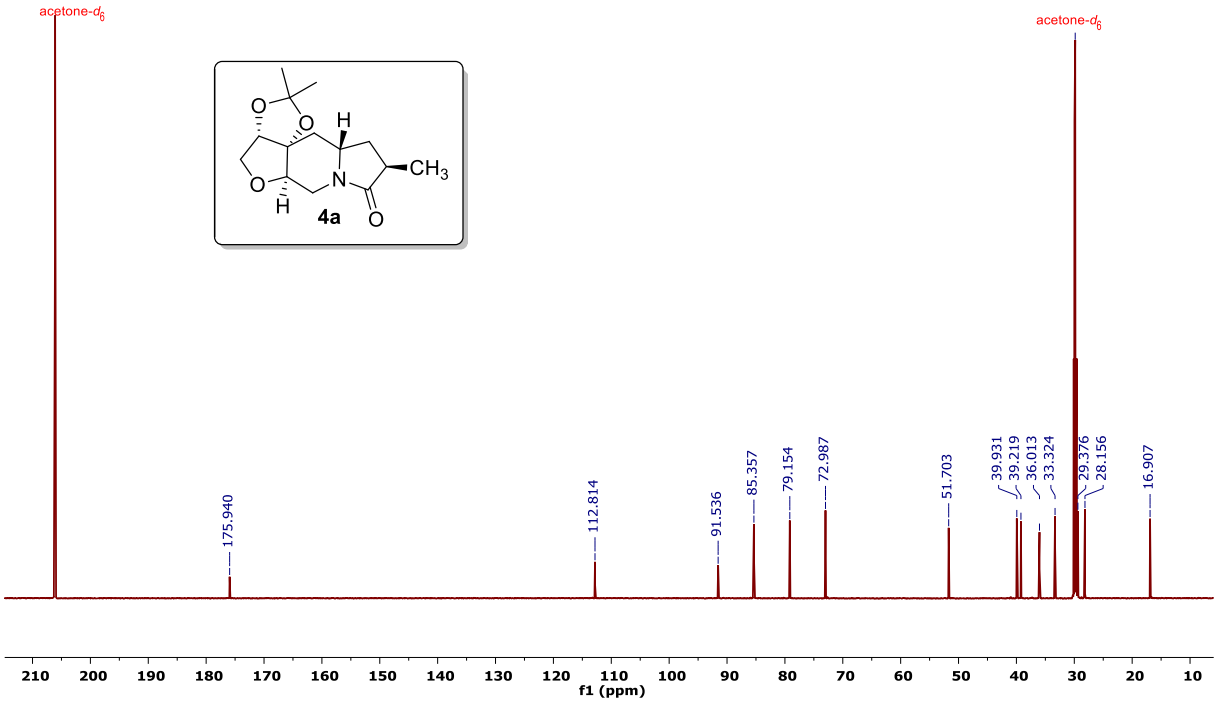
MS analysis was performed using a Thermo Scientific LTQ Orbitrap with ETD, mass spectrometer, a syringe pump, and an ESI source in the positive ion source mode, run by Xcalibur 2.0 software (Thermo Electron Corporation). The spray needle voltage was set at 5.0 kV and the spray was stabilized with a nitrogen sheath gas (30 psi). The capillary temperature was 275 °C. A syringe pump delivering 6 µl/min was used for the direct injections of compounds diluted in methanol (c = 1 mg/mL). Mass spectra were acquired in full mass scan mode and recorded with a limited mass range from m/z 80-600. All the samples were diluted in methanol (LC-MS quality, Sigma Aldrich). High-resolution spectrometry was performed on Micromass Q-Tof Micro MS system with ESI^{+}ionization (measured mass represents $M+1^{+}$) and LC-MS chromatographic separation was performed on Agilent 1260B LC-MS system using HALO C18 column (2.1 × 50 mm, 5.0 µm particle size). A 10 min gradient elution was performed at 1.5 mL/min flow rate as follows: maintain H_2O/MeOH with 0.1 % formic acid from 5 % to 100 %. MS detector used combine dionization (ESI + APCI) in positive mode, 50 % scan and 50 % SIM.

All samples for analysis and NMR spectroscopy were dried at room temperature for 48 hours at Laboratory Freeze Dryer Alpha 2–4 LD plus Lyophilizer.

2. Copy of ^{1}H and ^{13}C NMR, HMBC, HSQC, COSY, NOESY and TOCSY spectra



^{1}H NMR spectrum of compound **4a**



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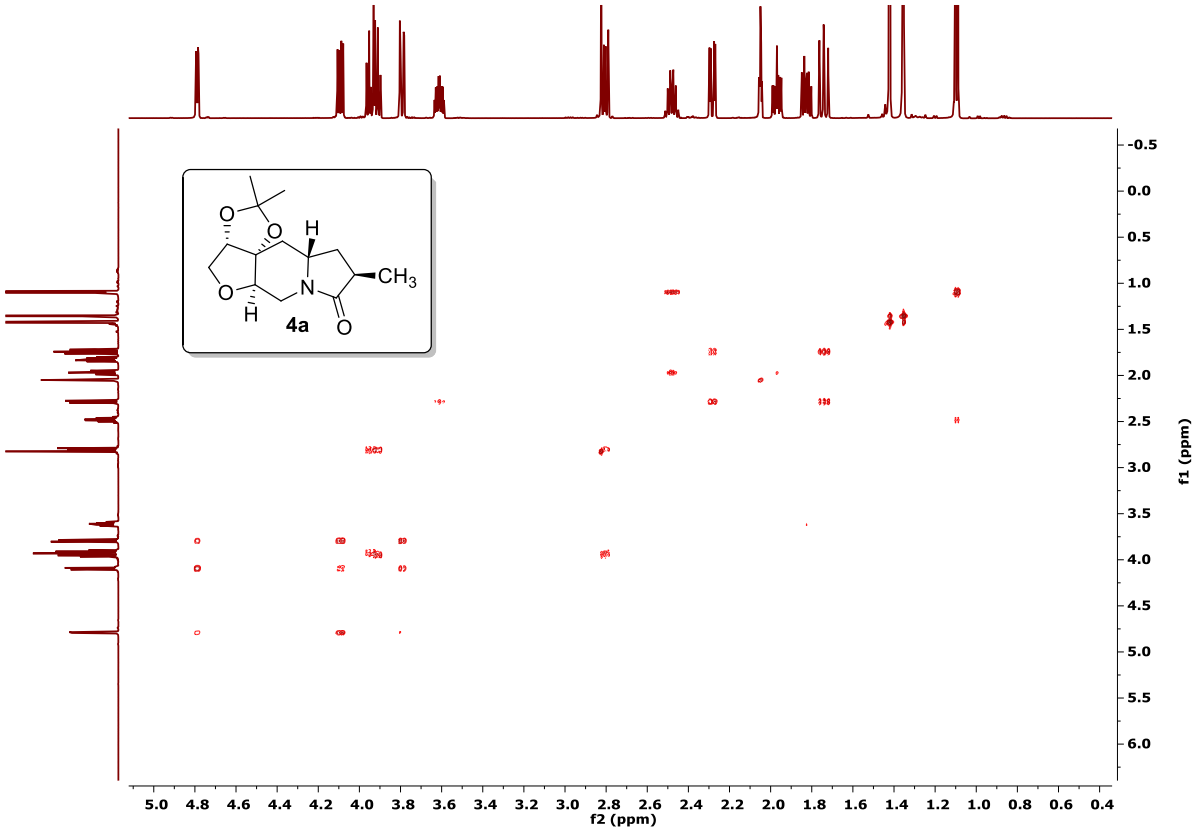
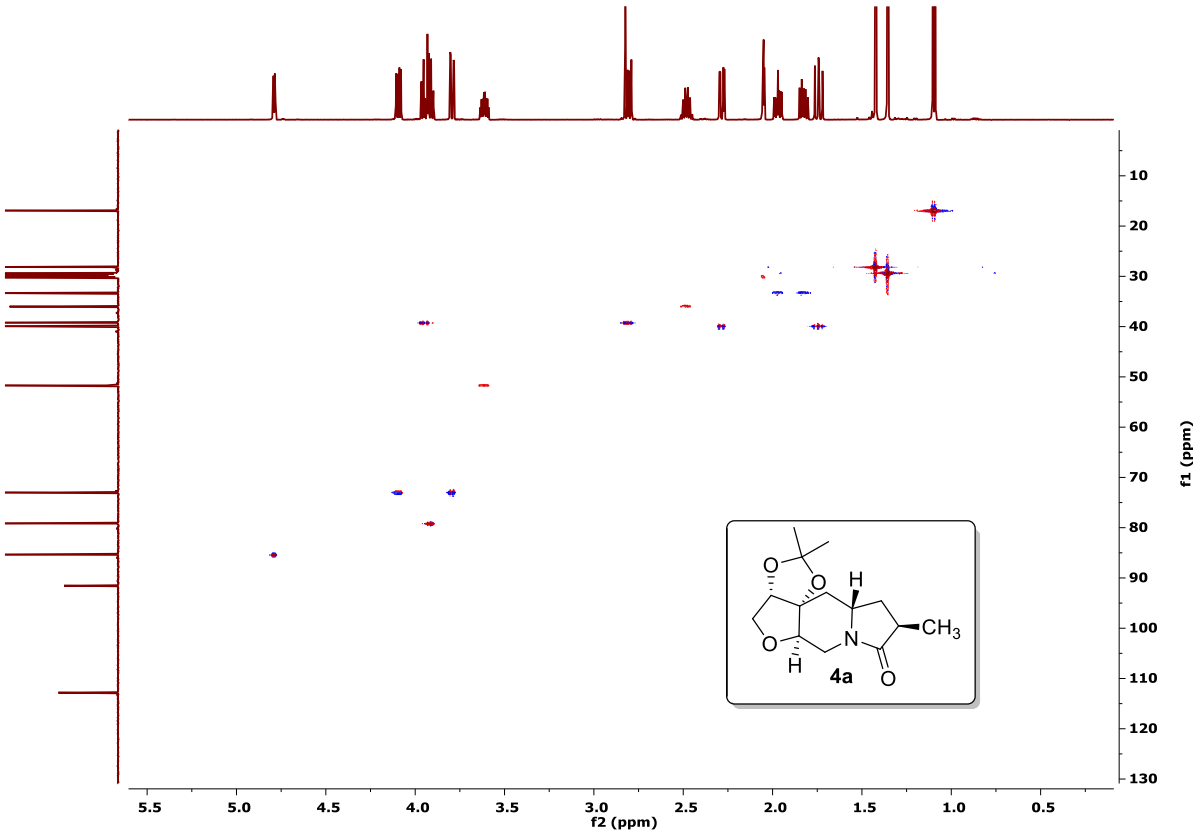


COSY spectrum of compound **4a**



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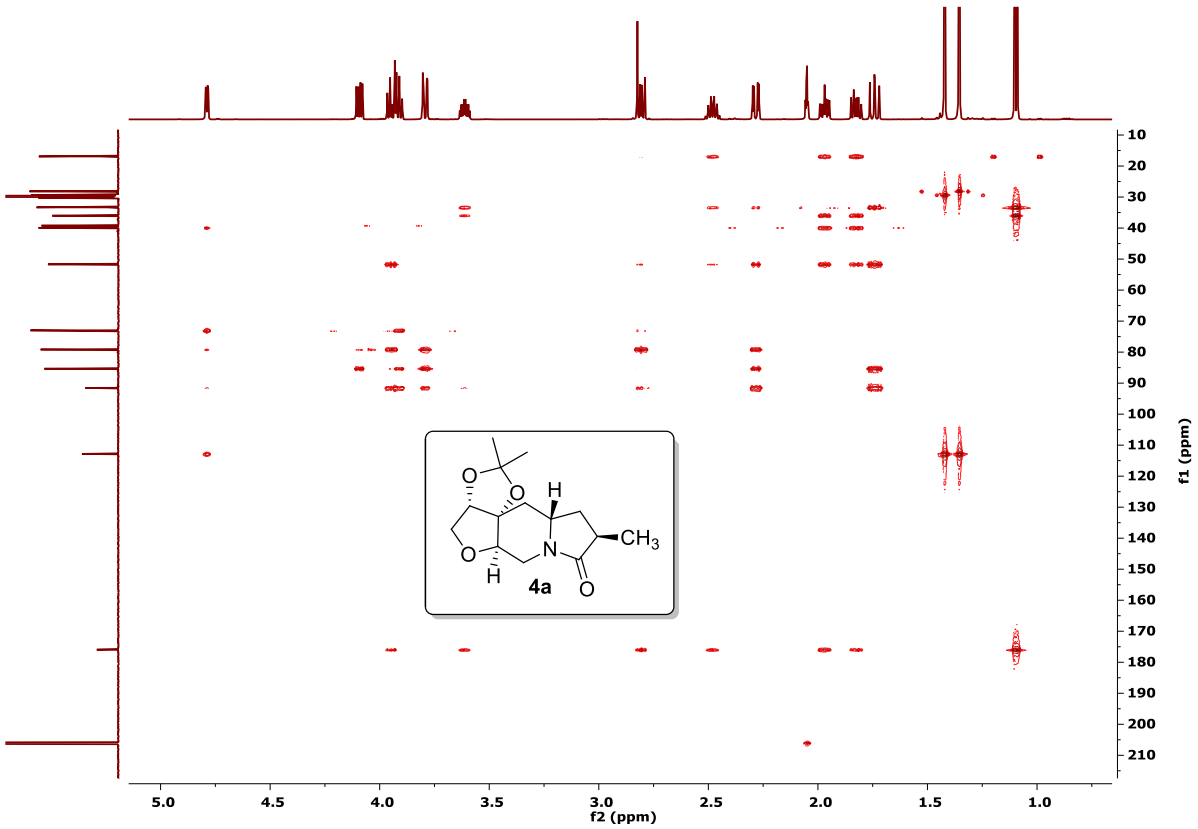

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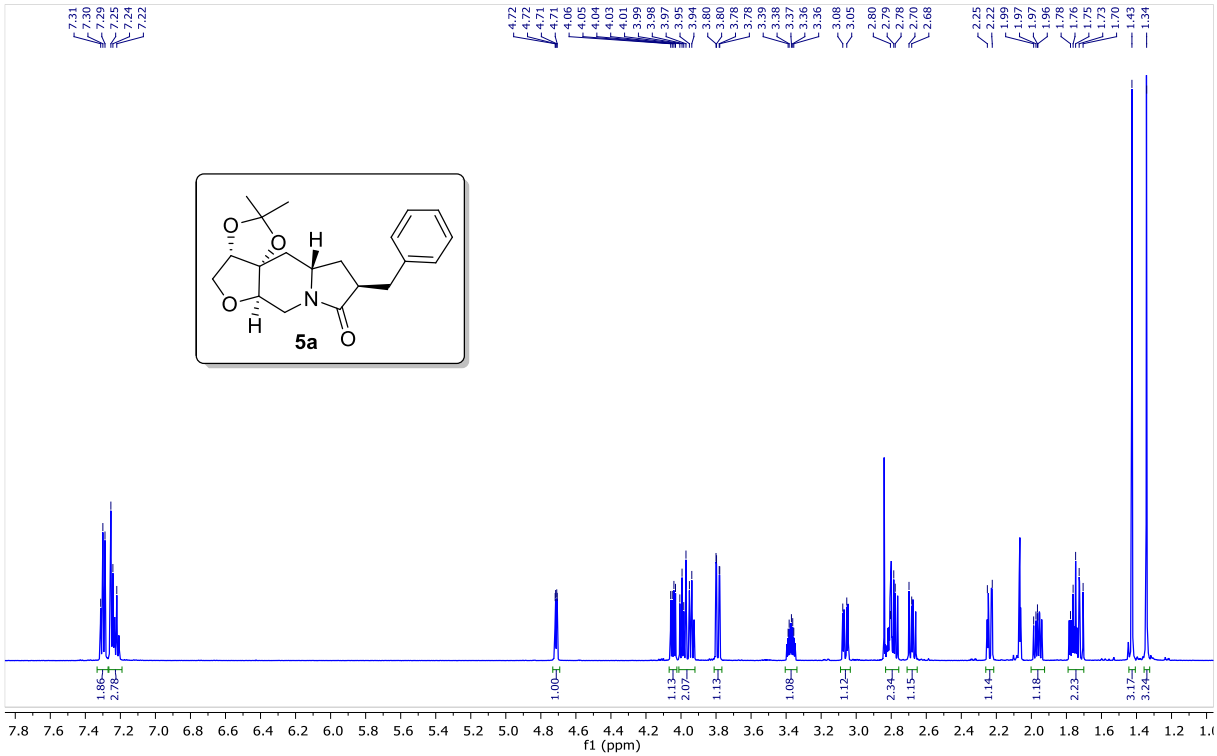

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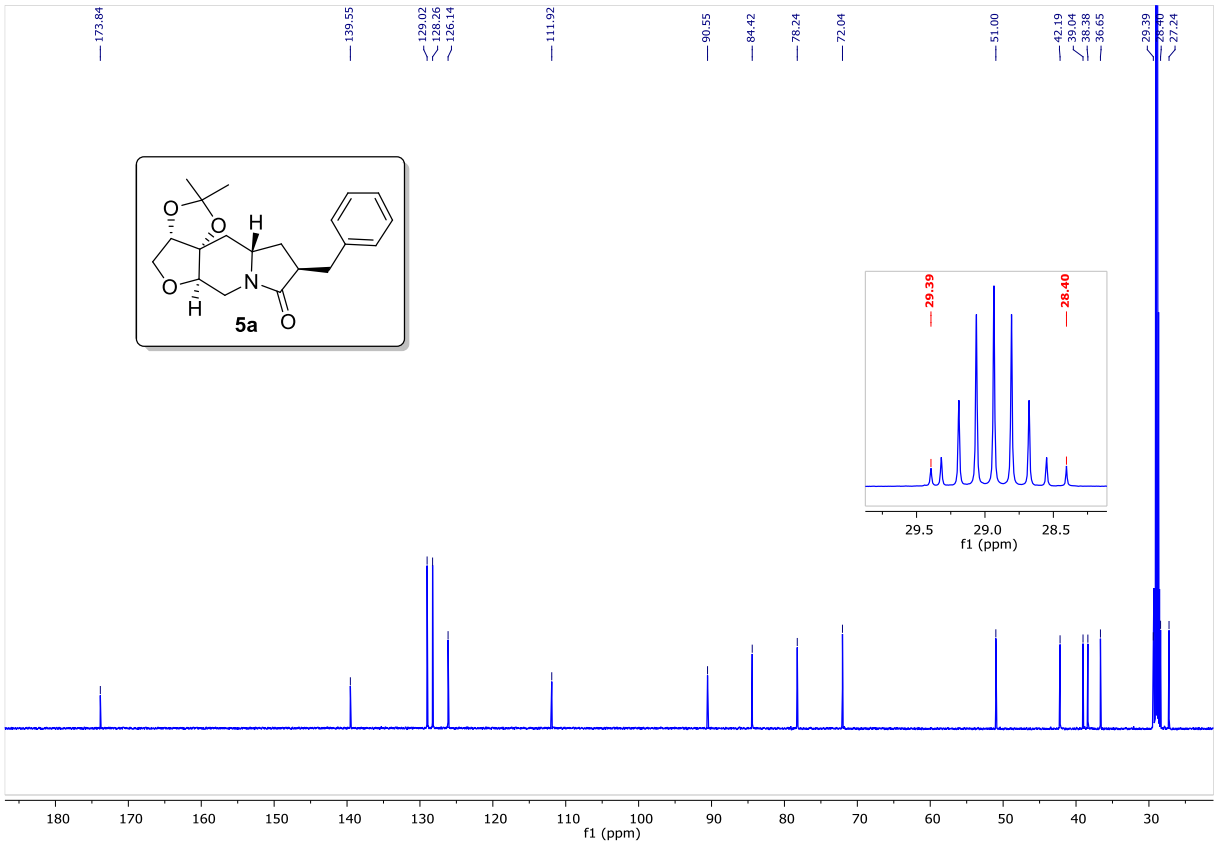

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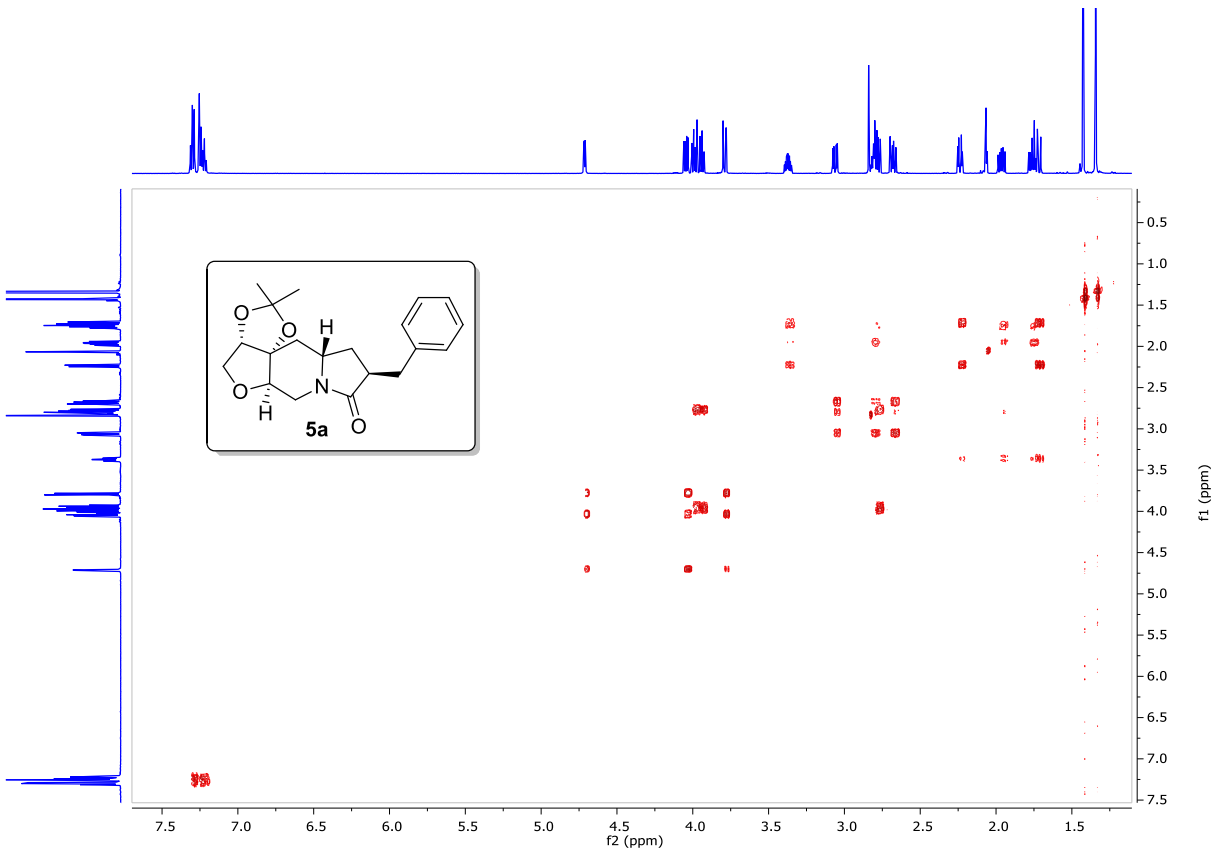

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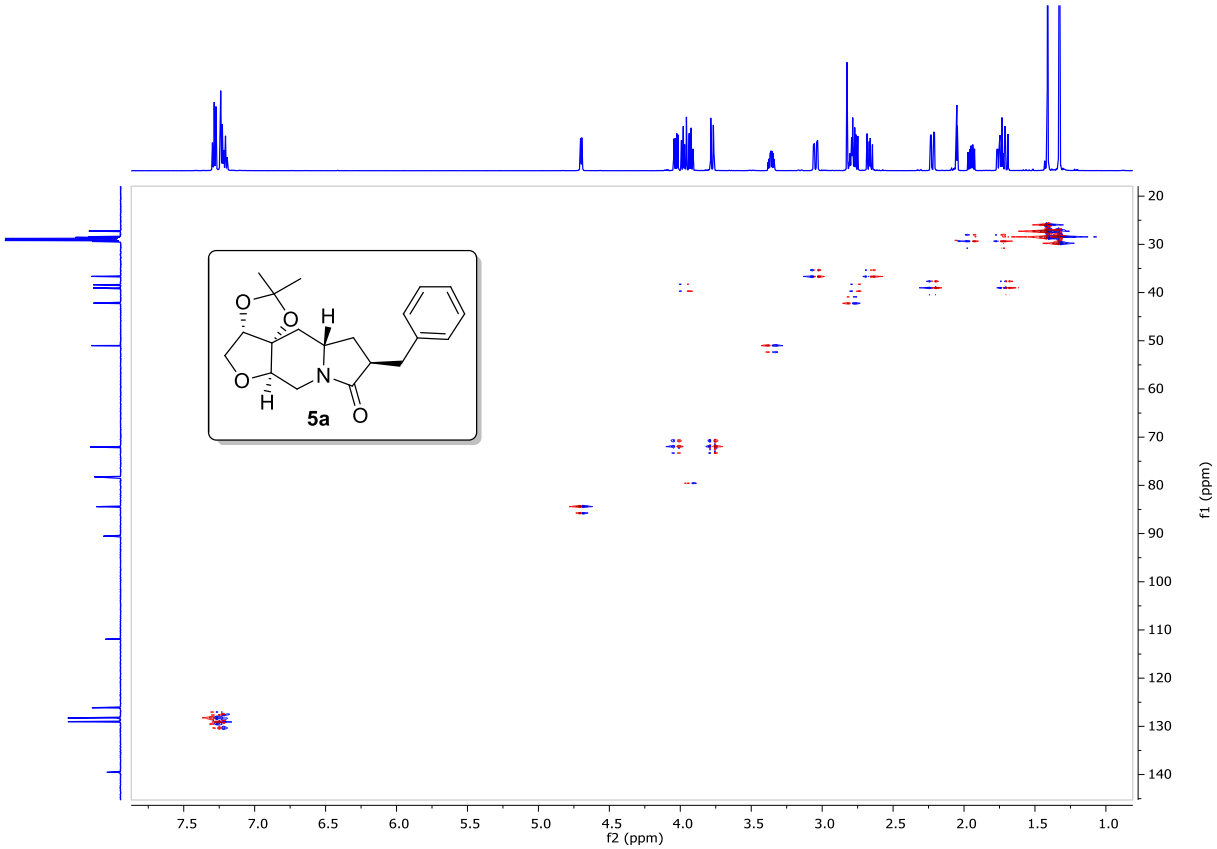

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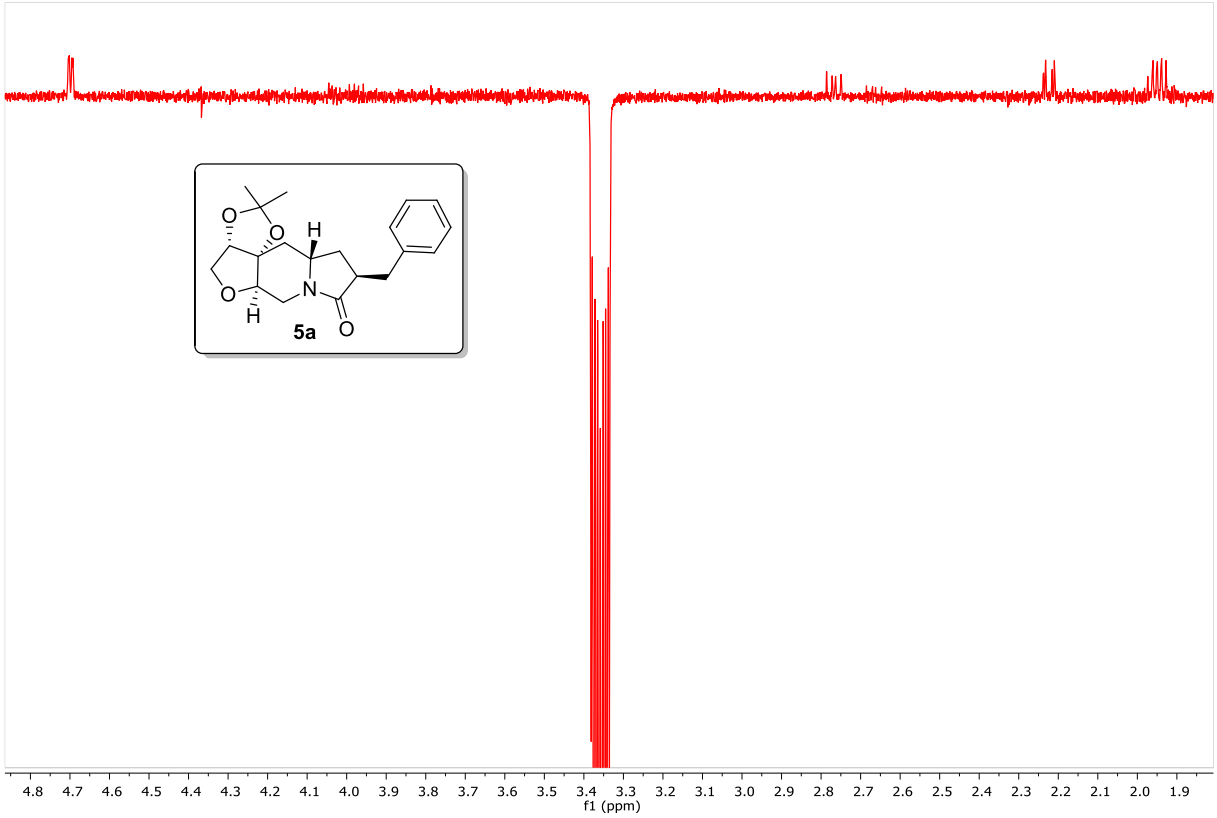

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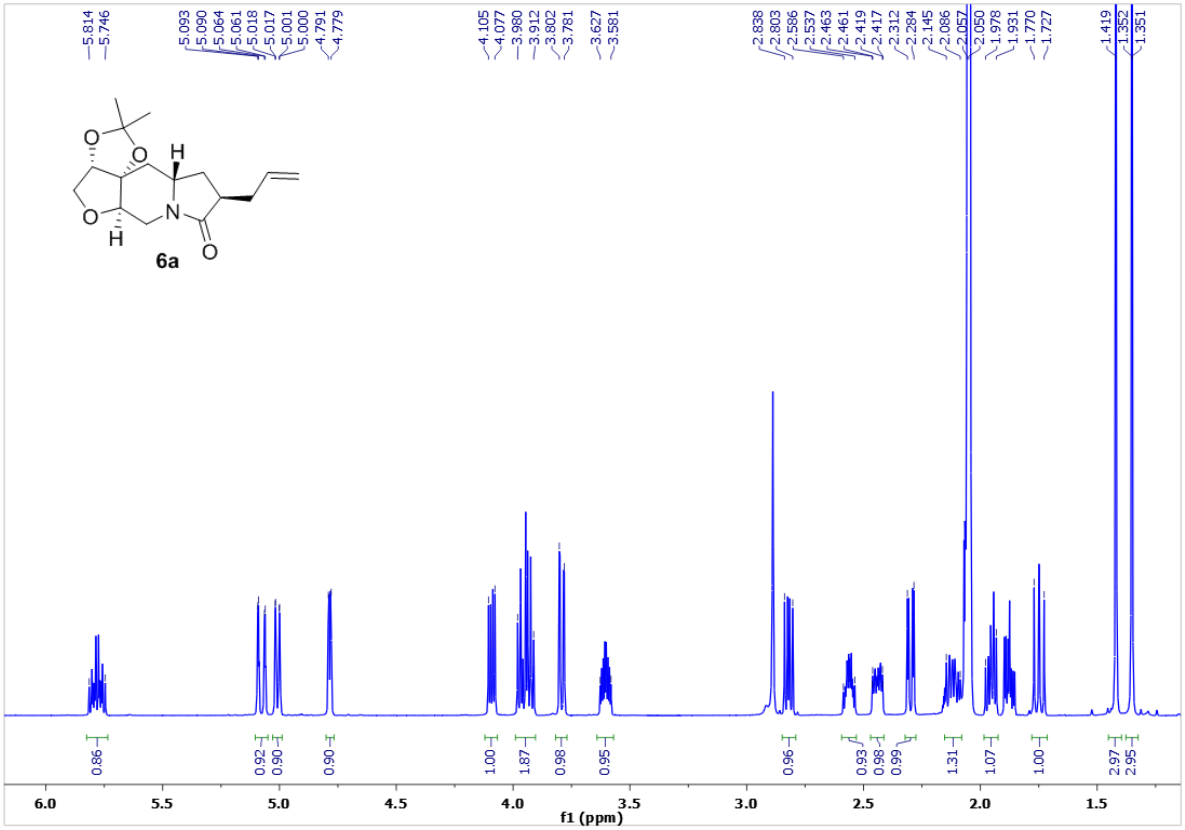

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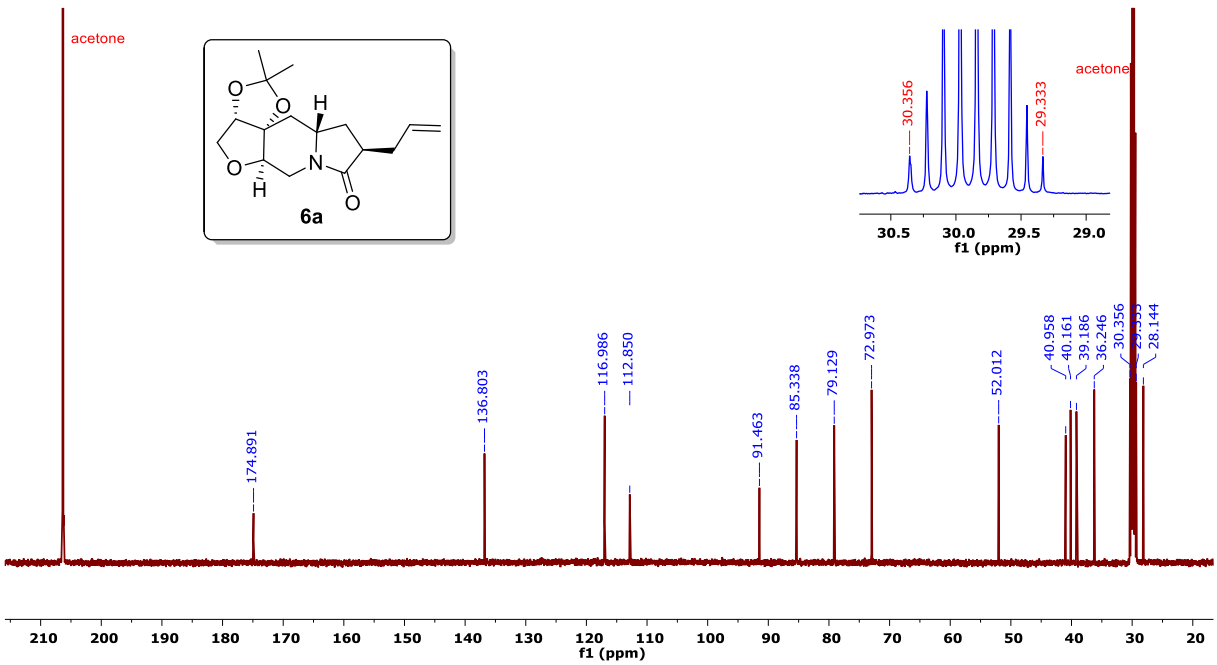

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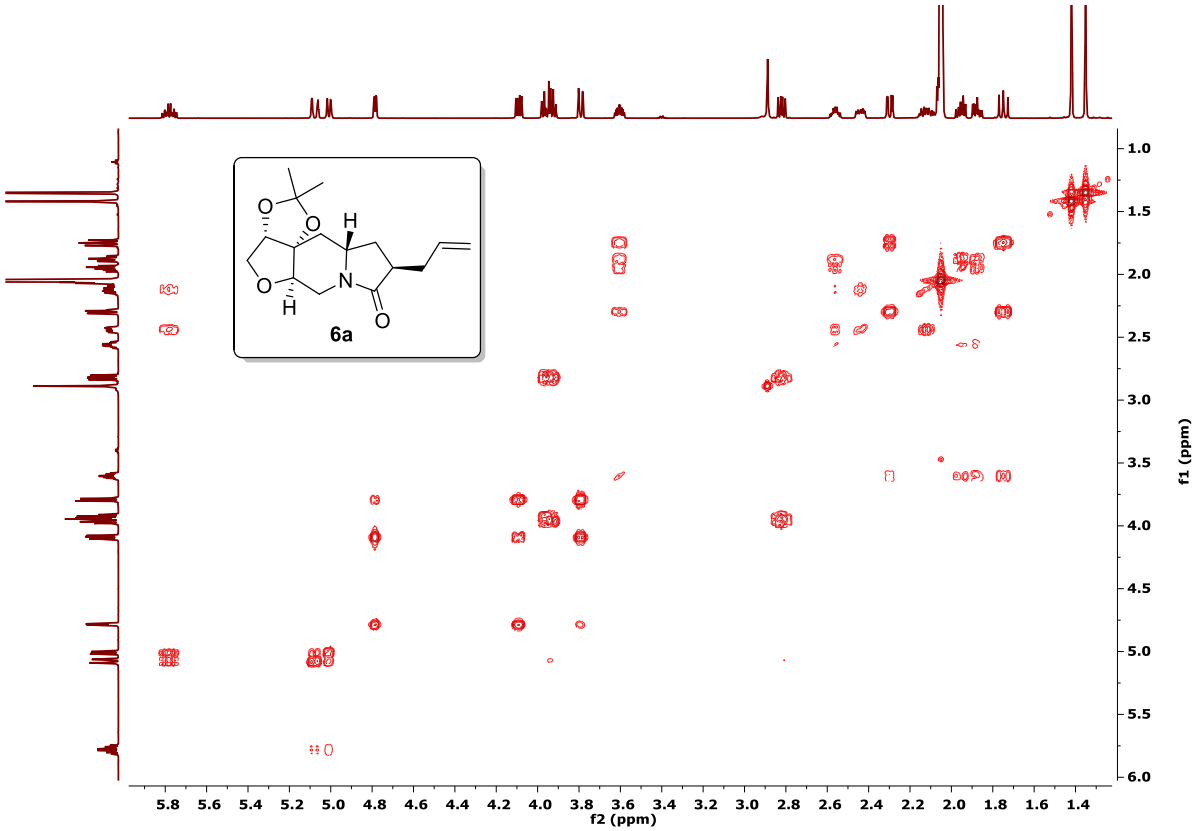

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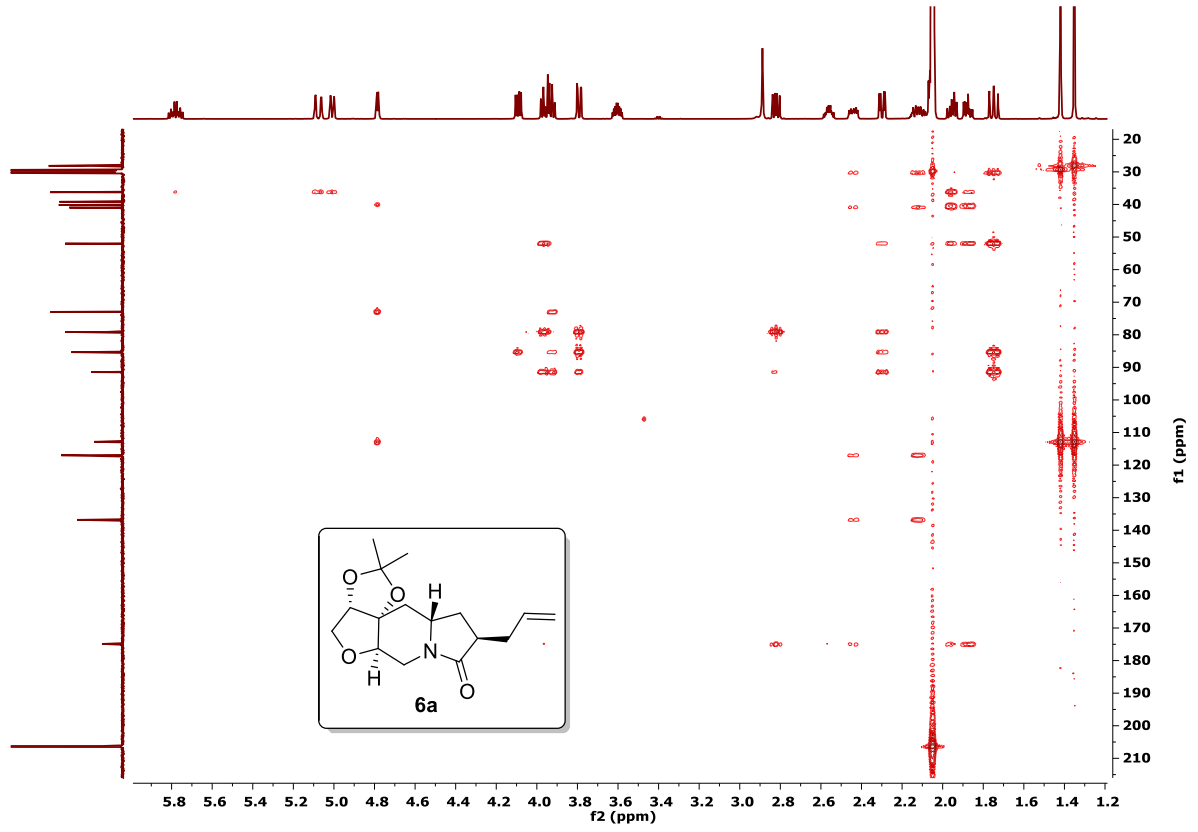

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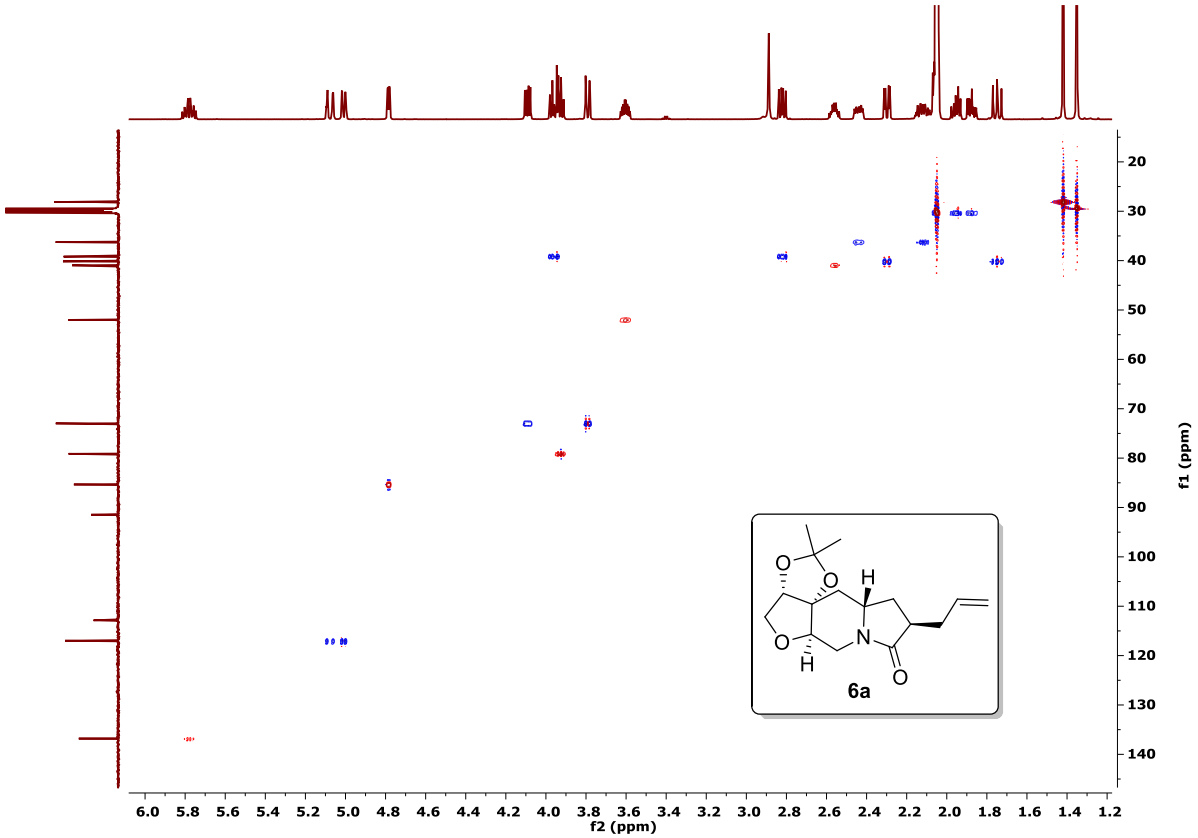

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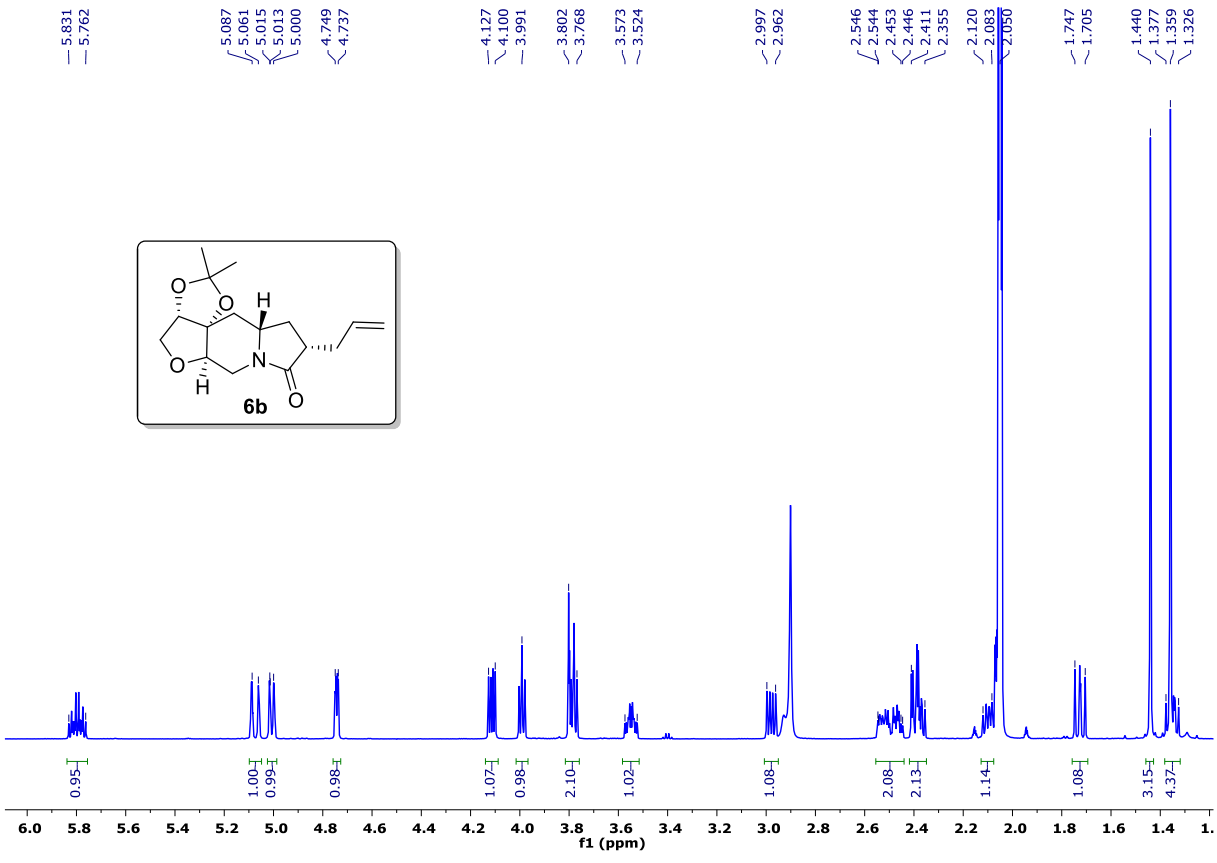

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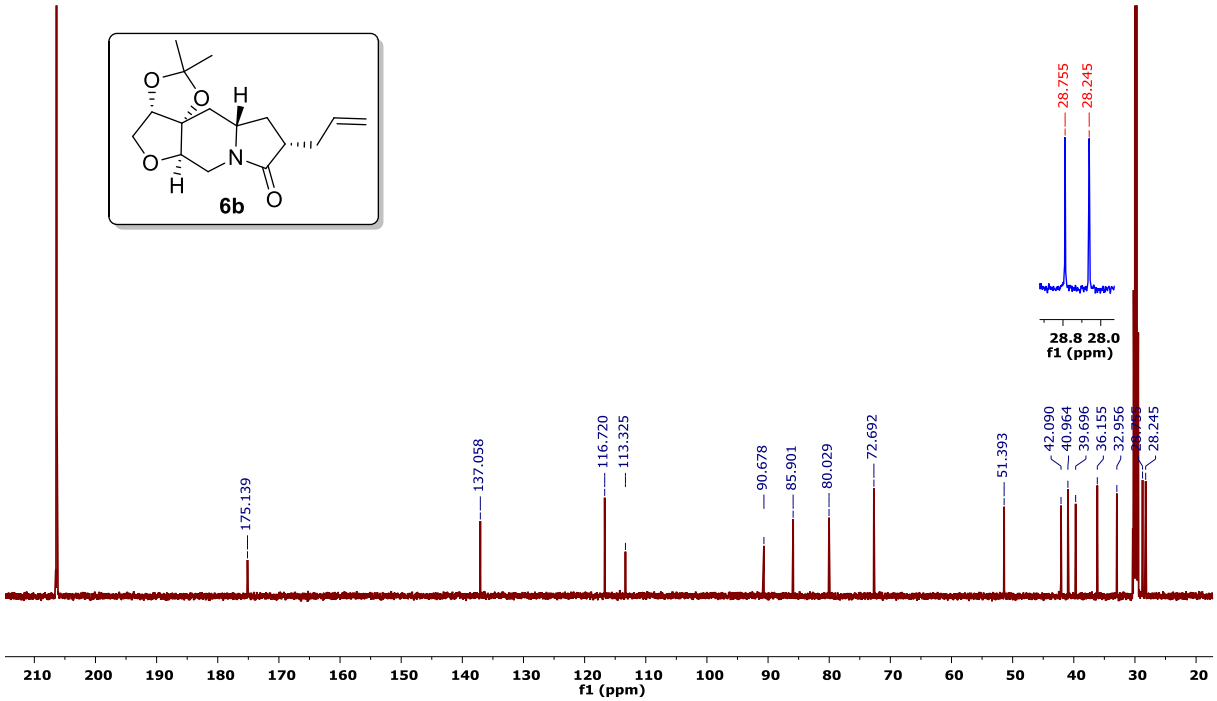

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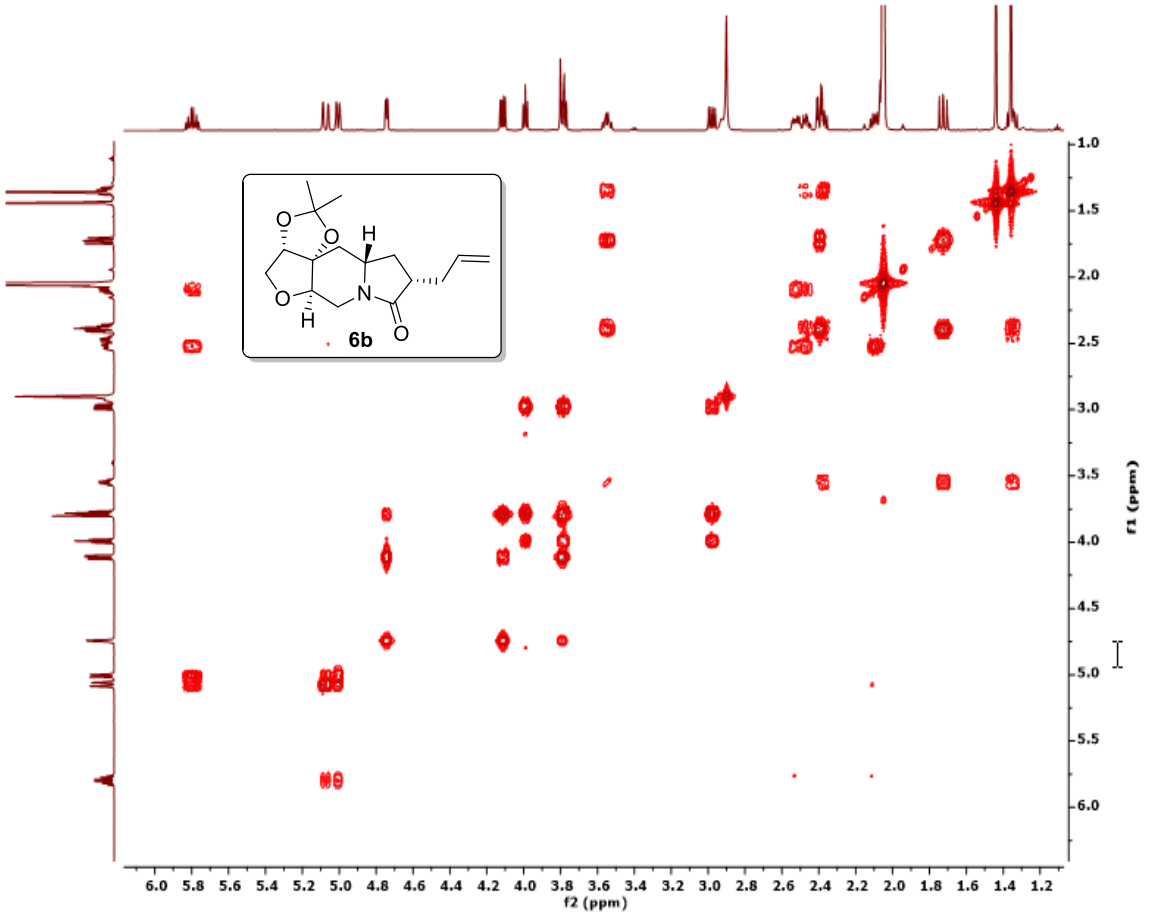

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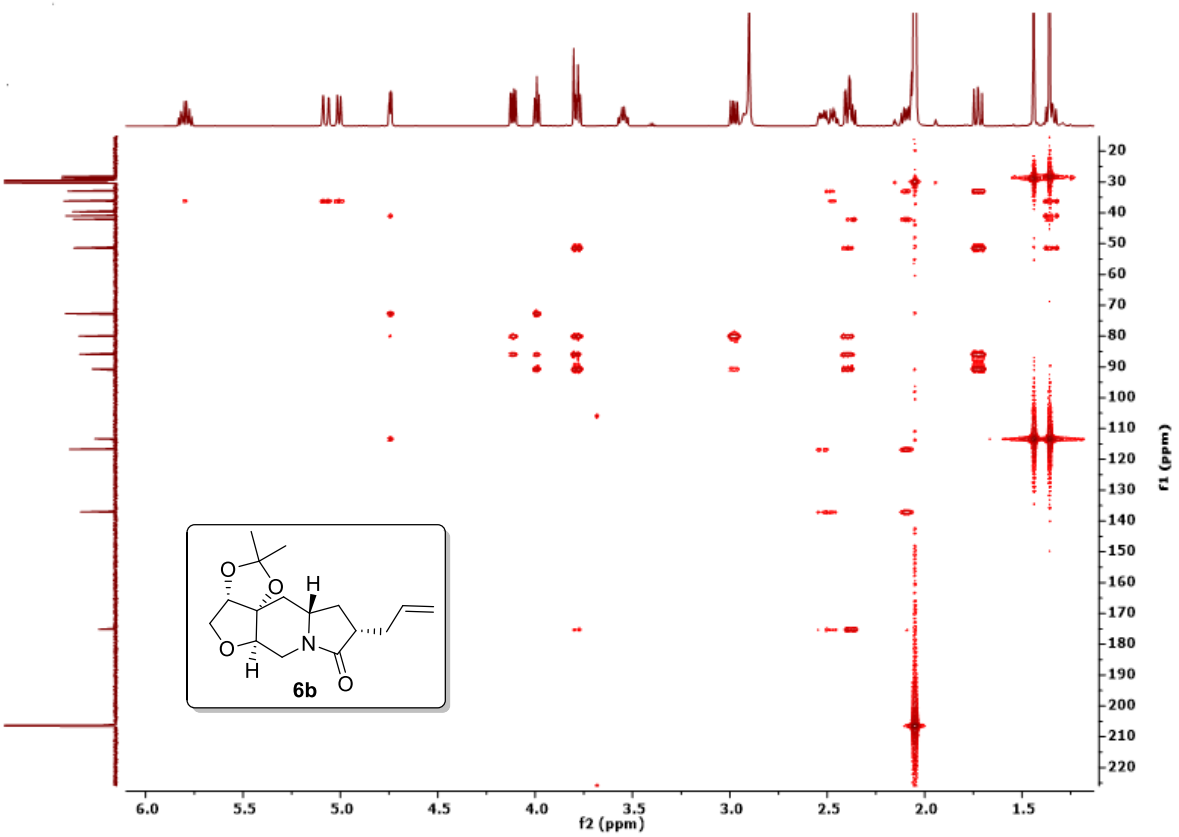

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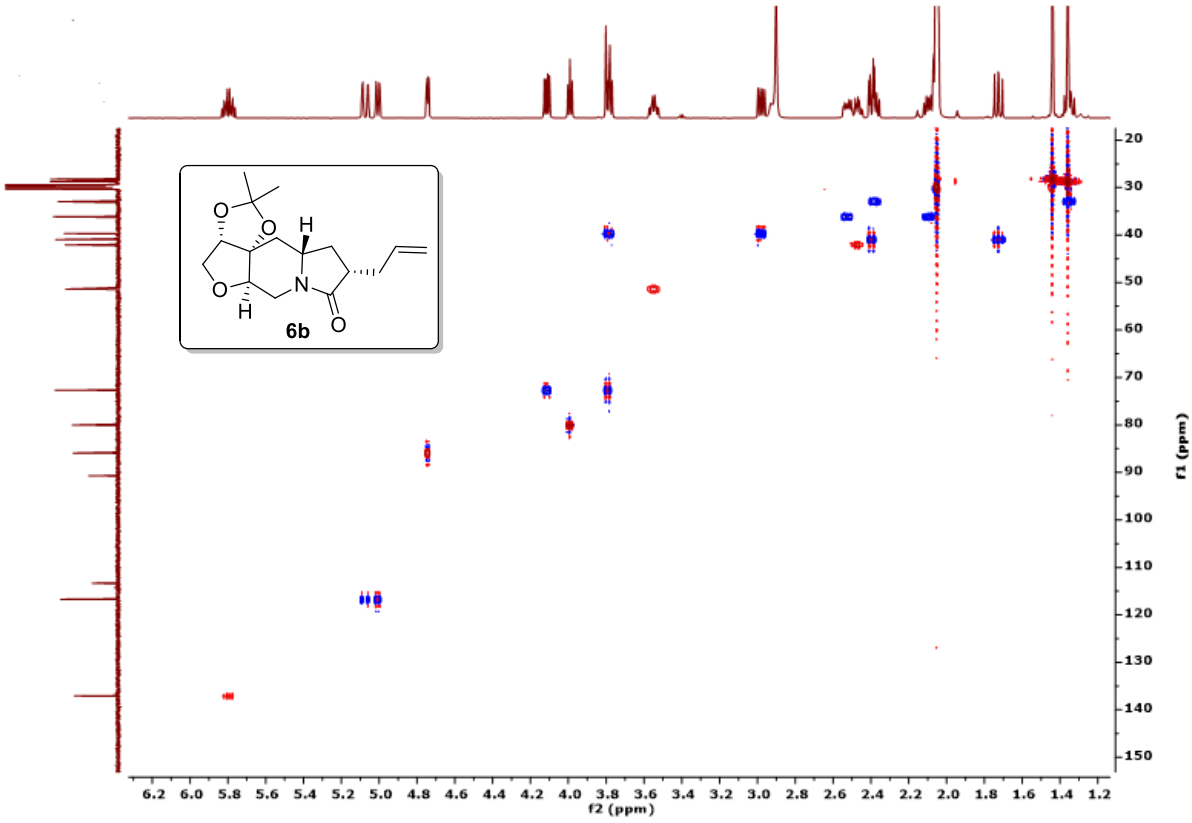

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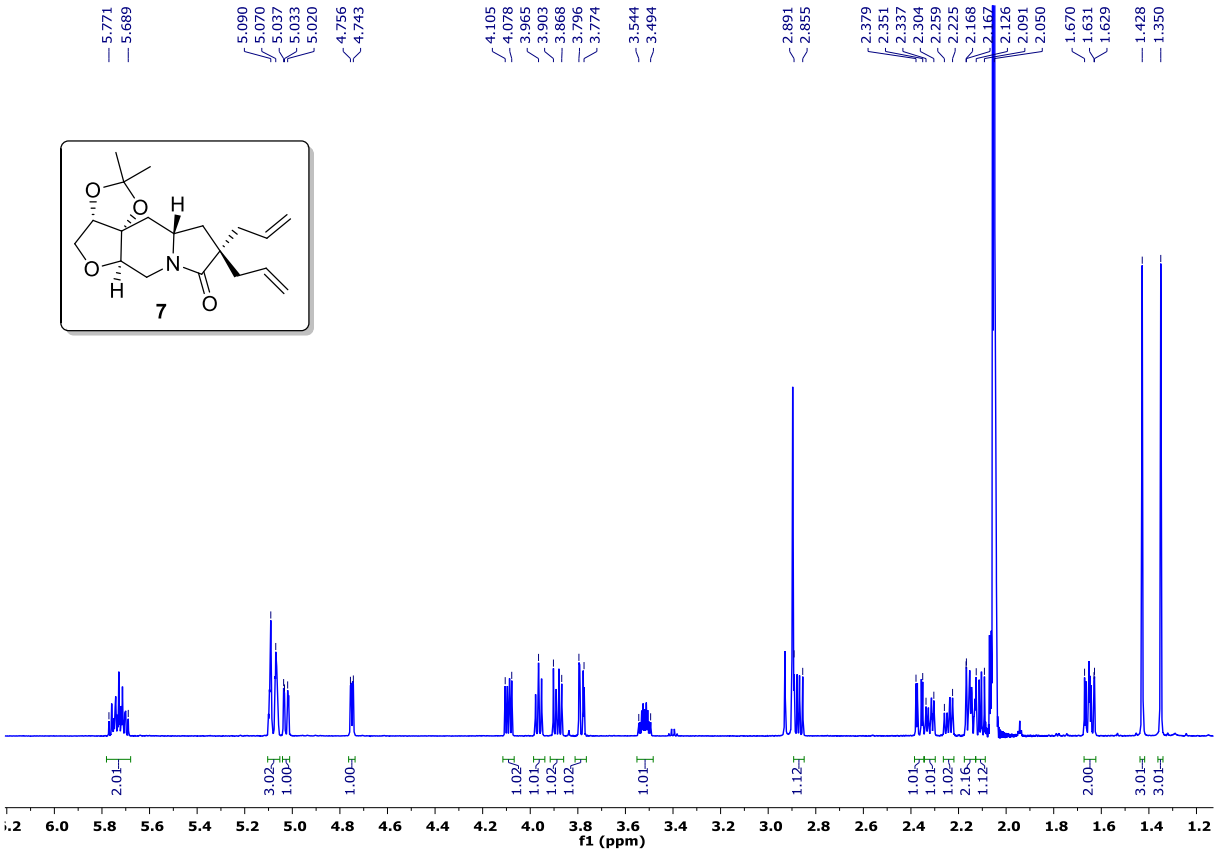

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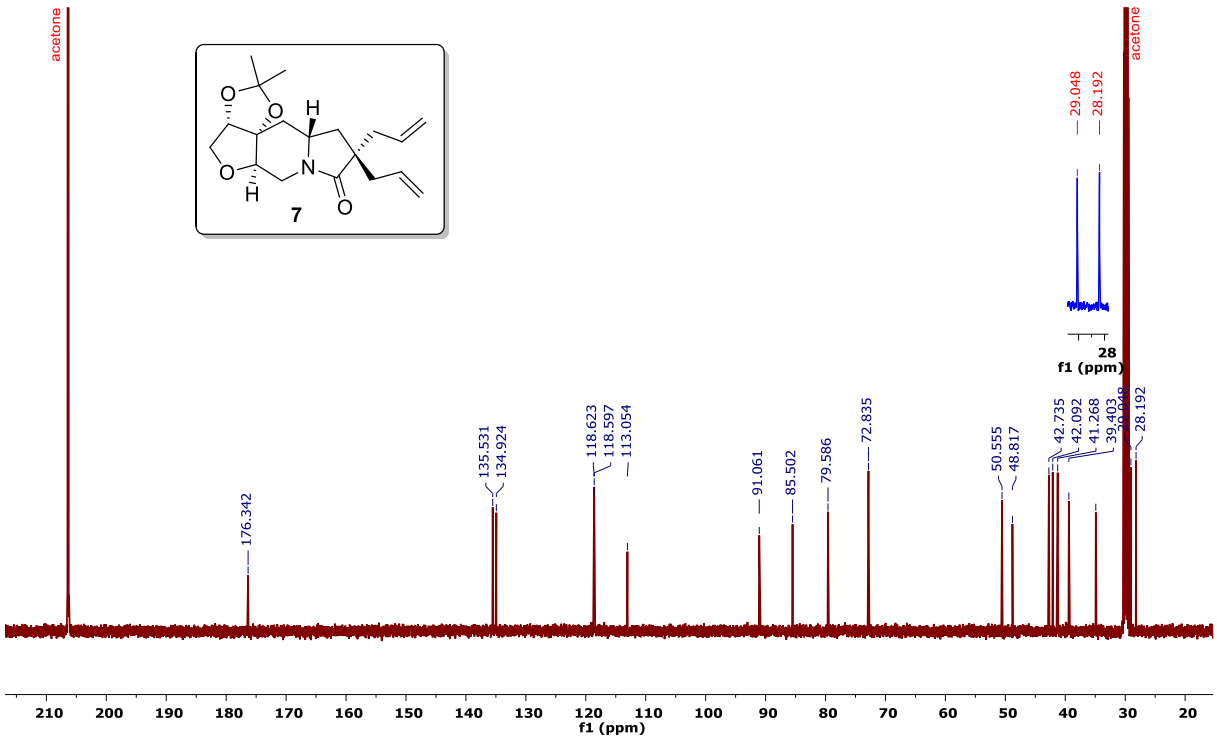

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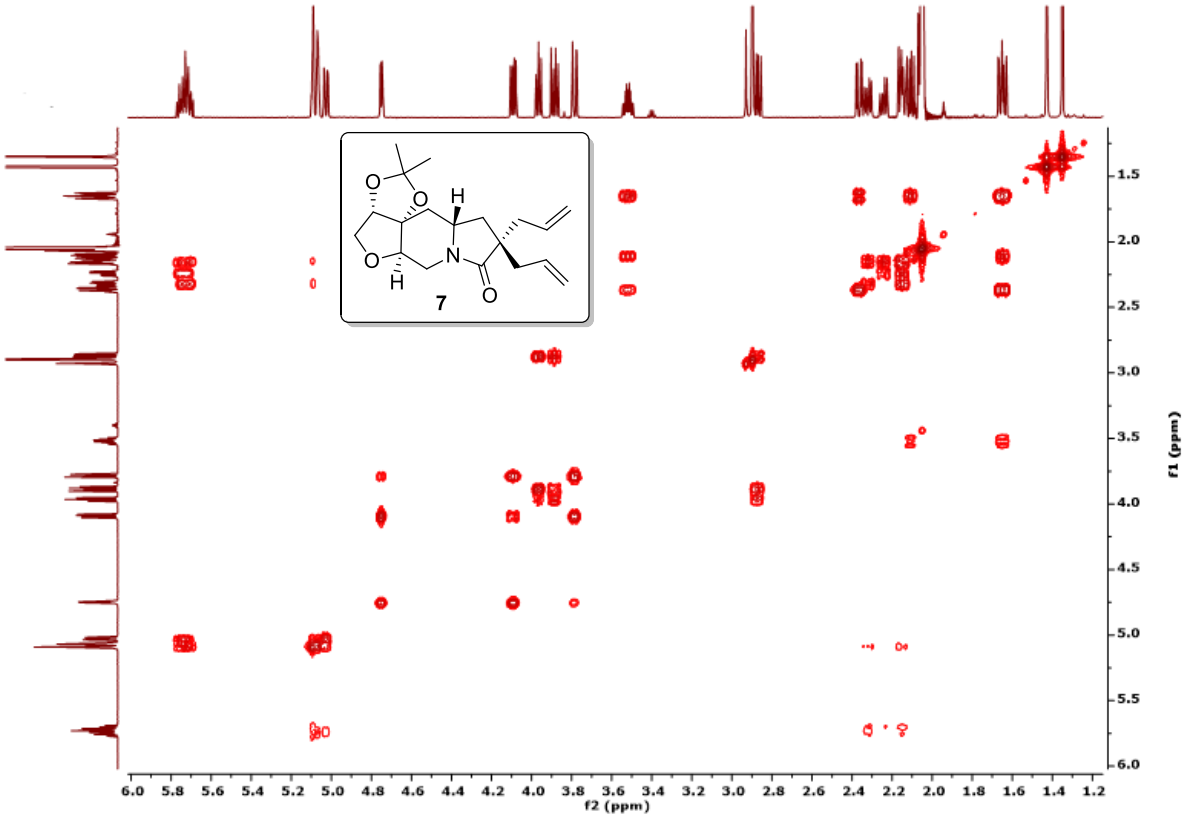

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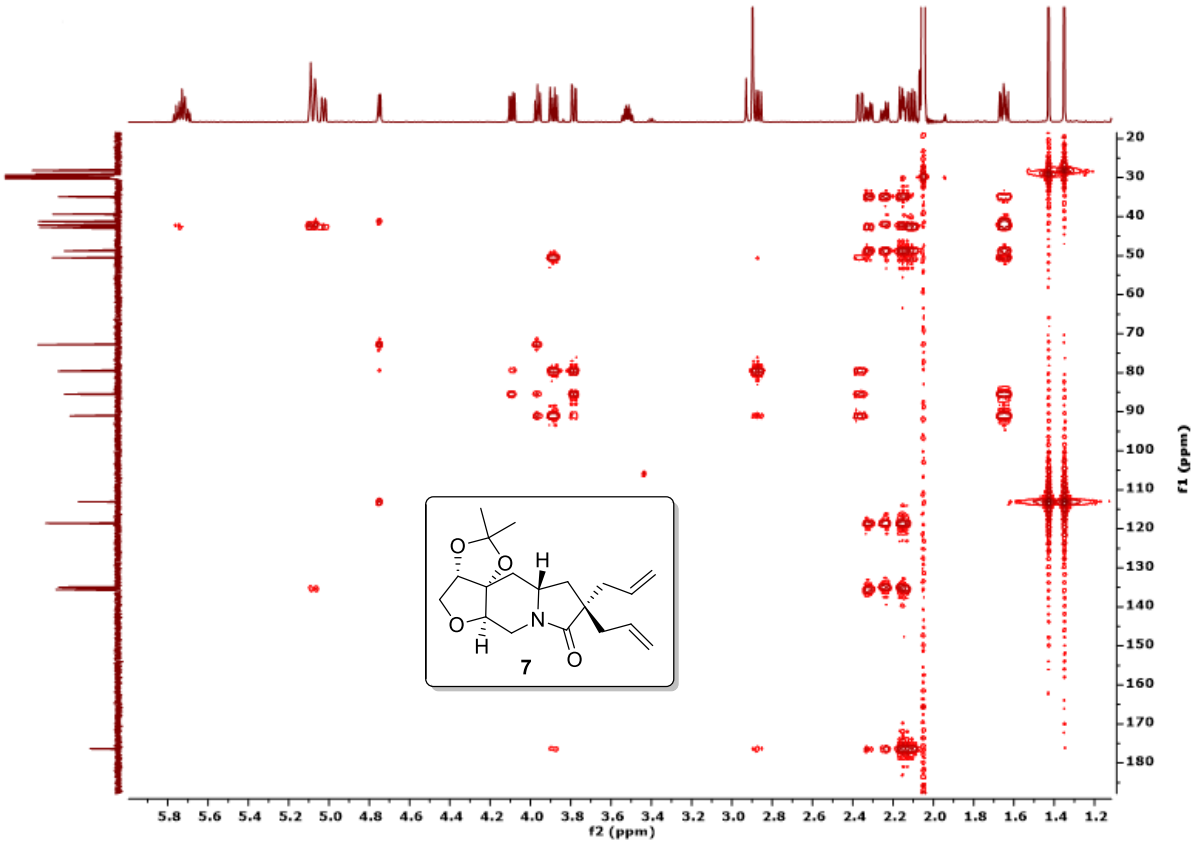

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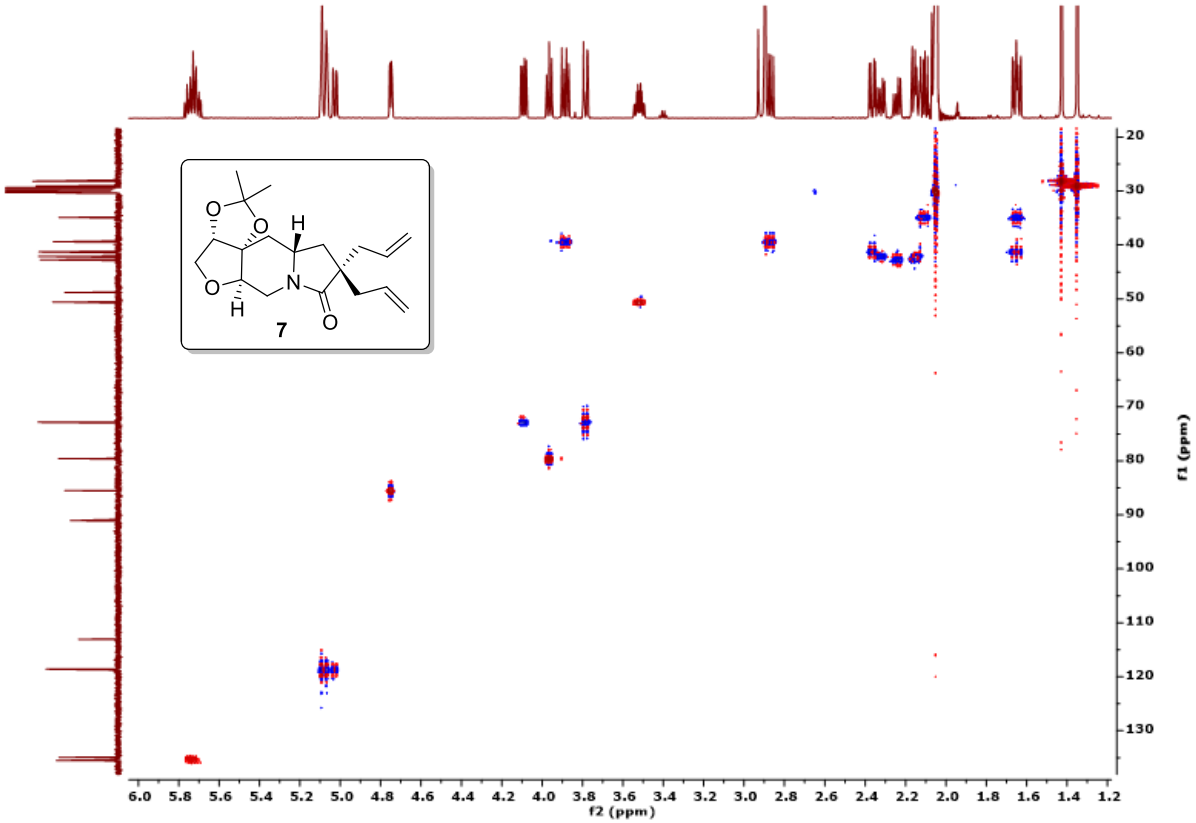

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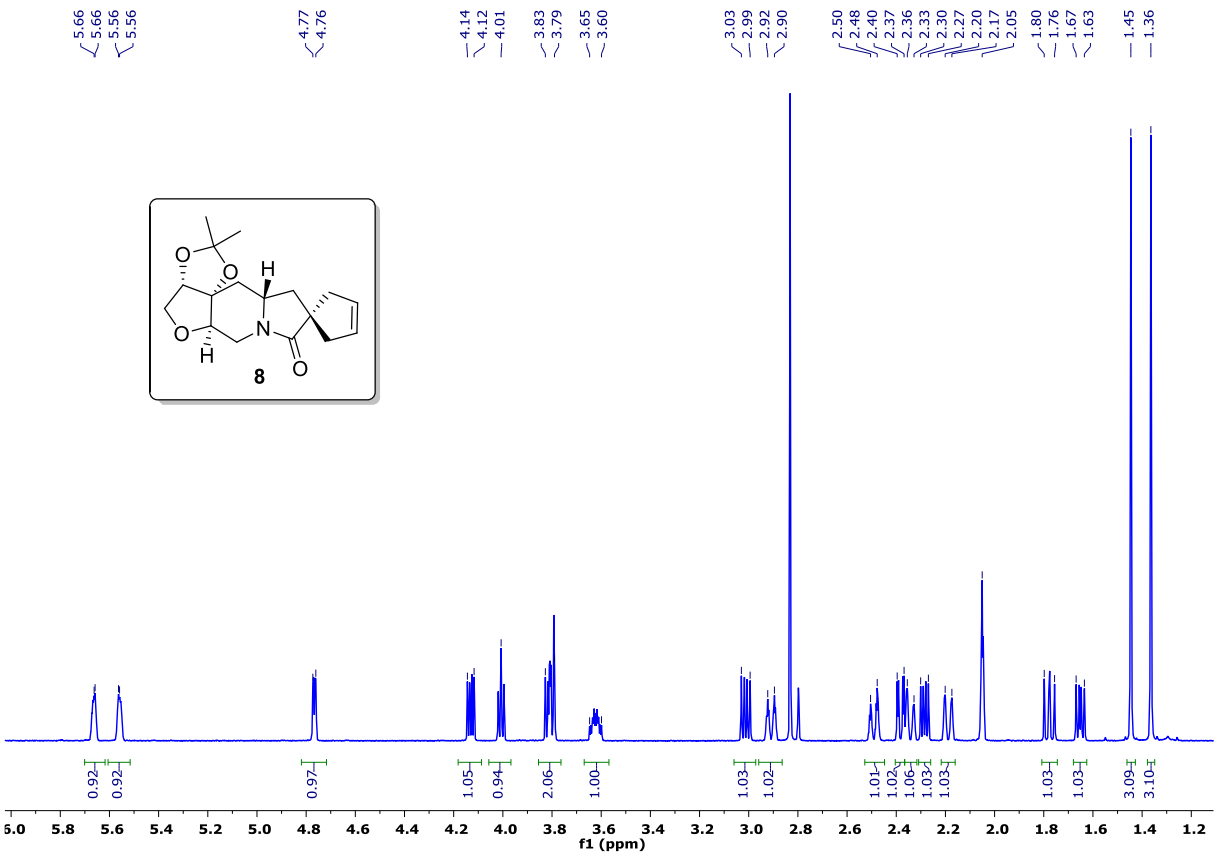

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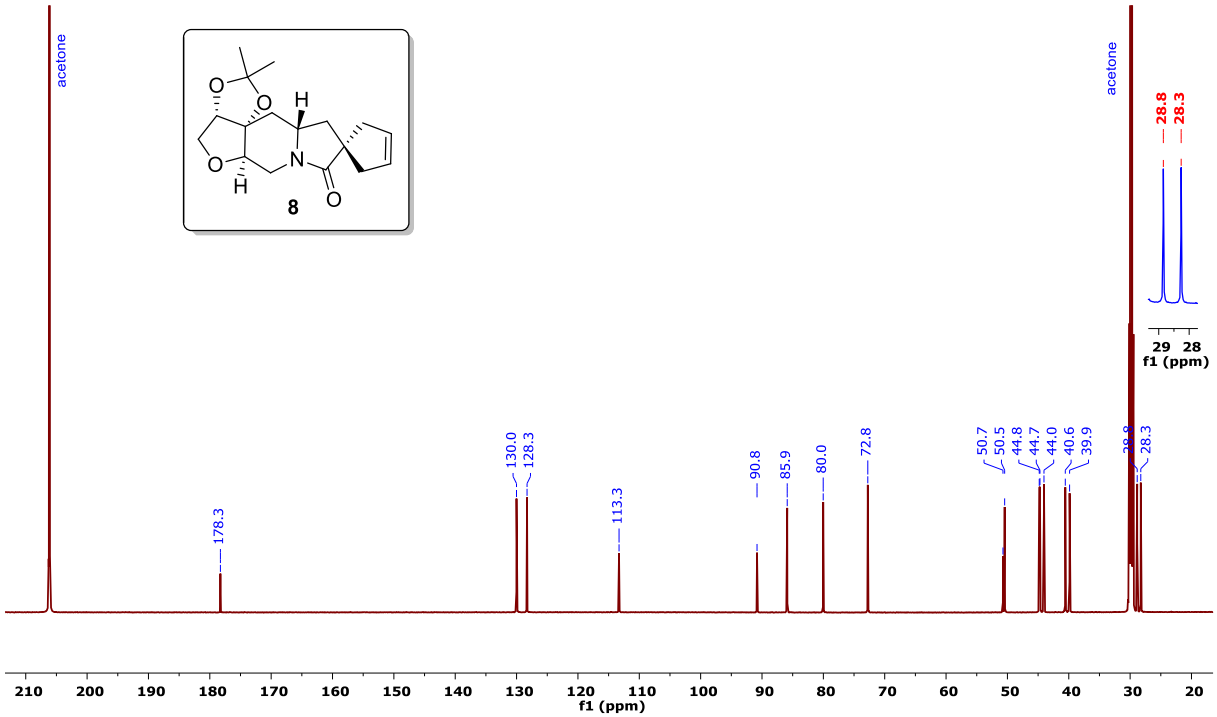

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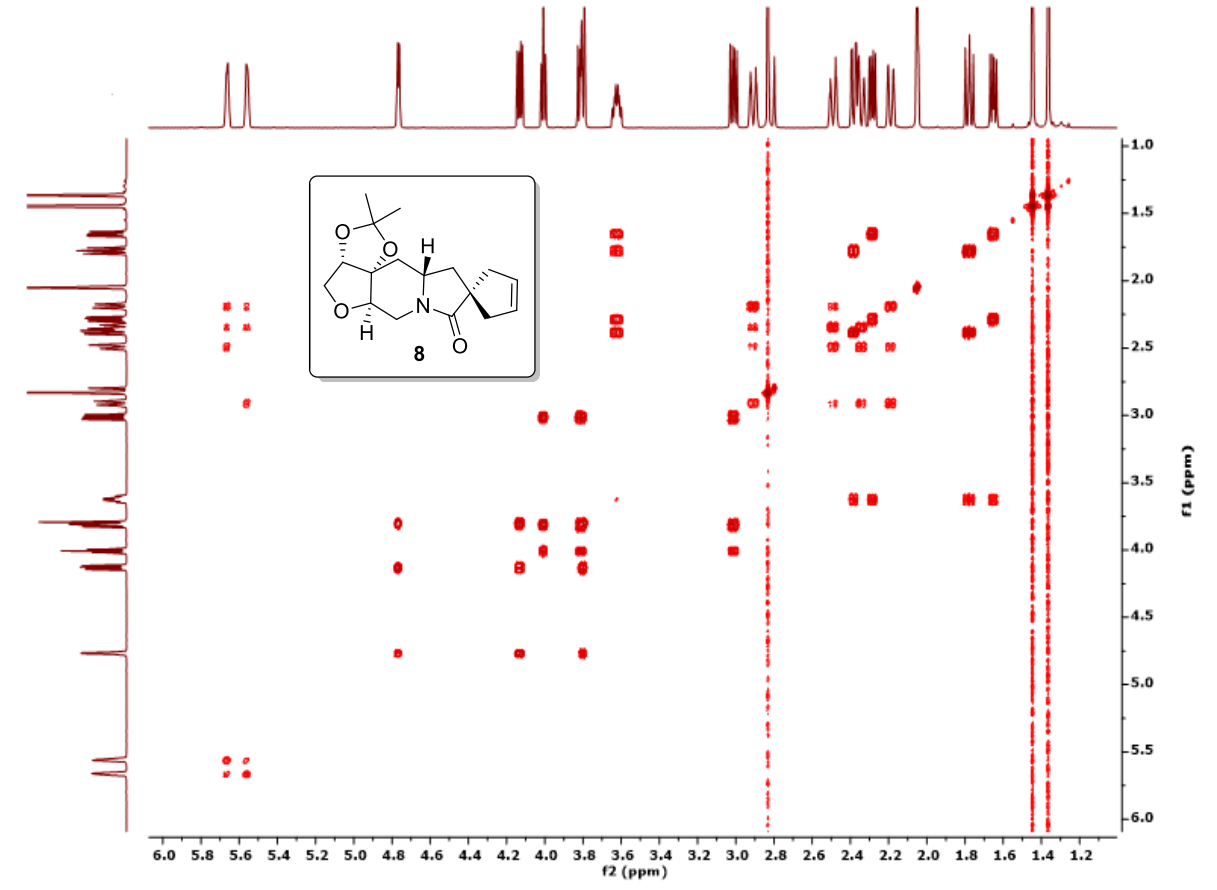

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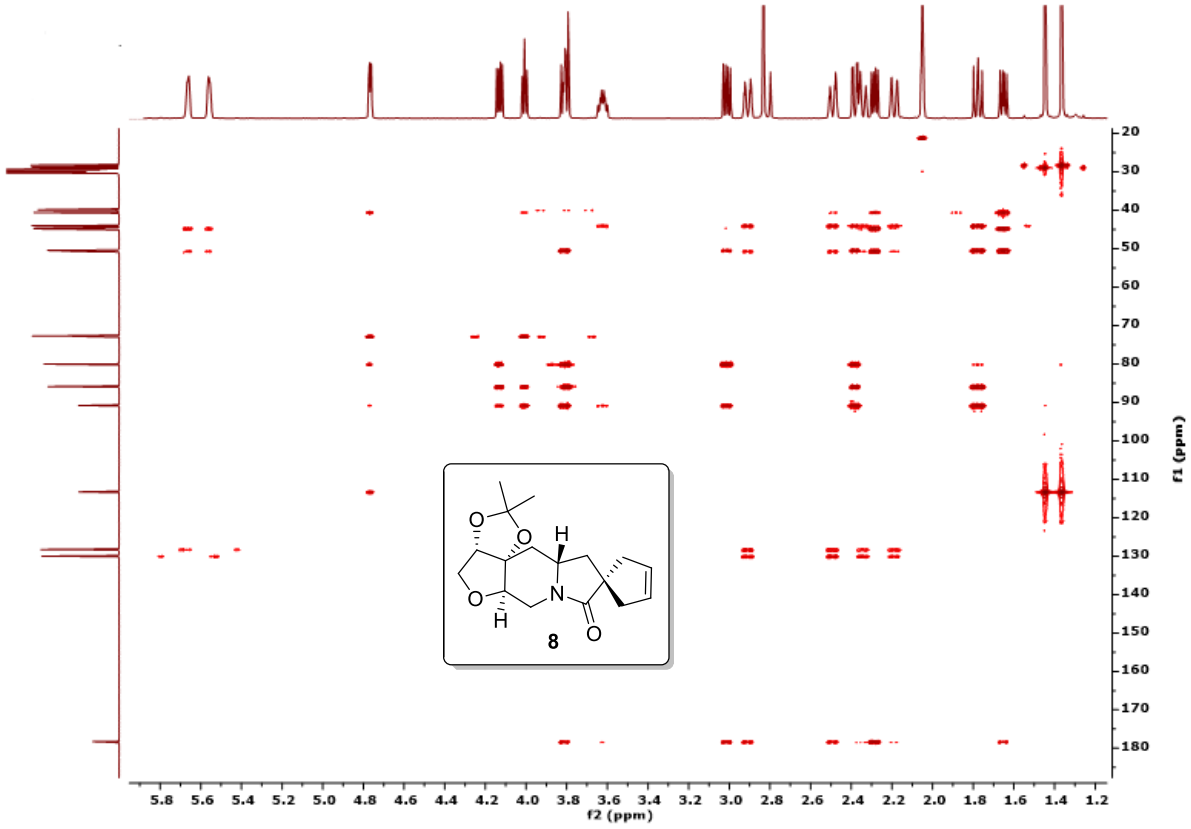

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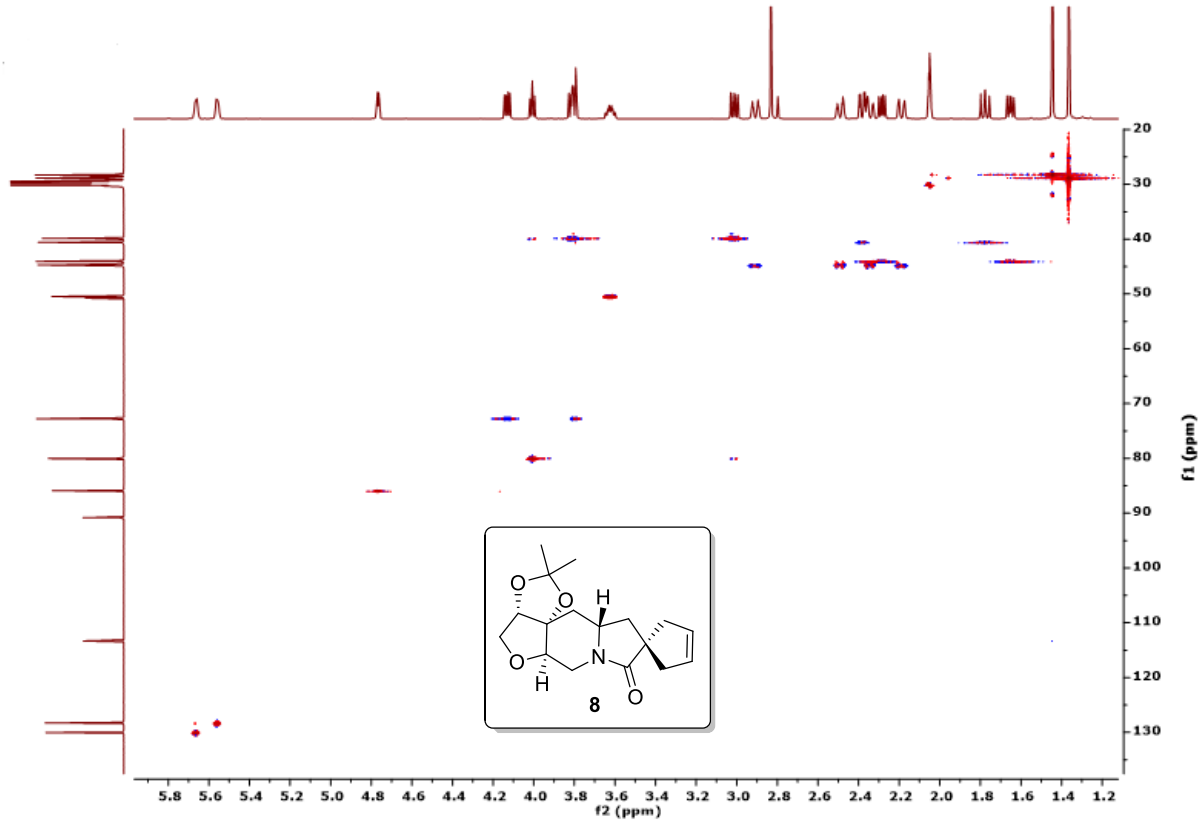

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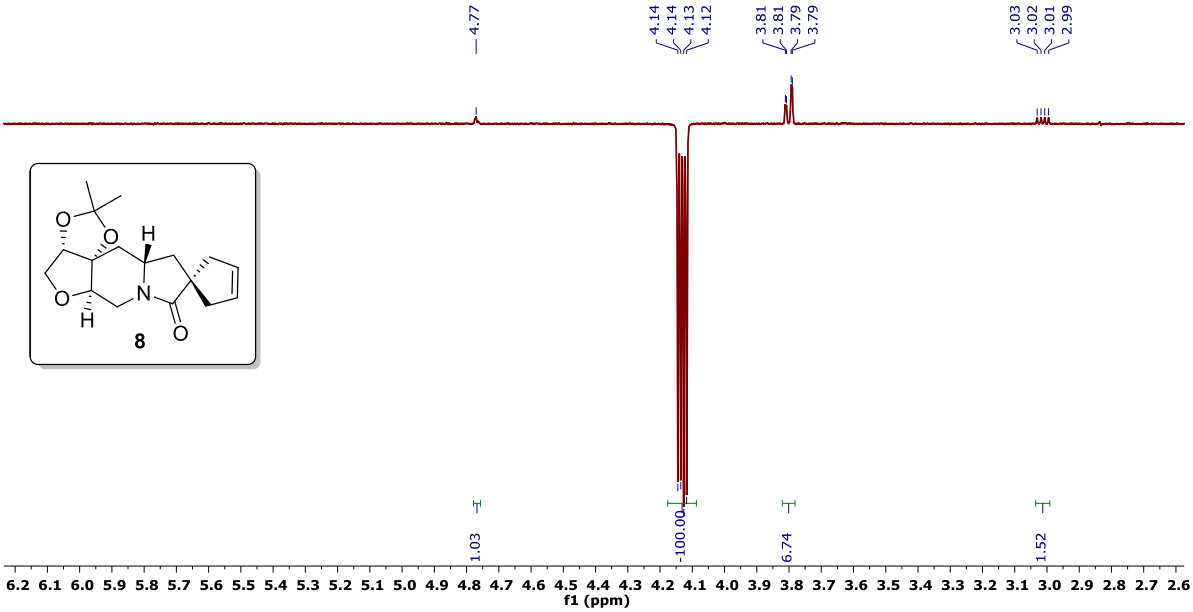

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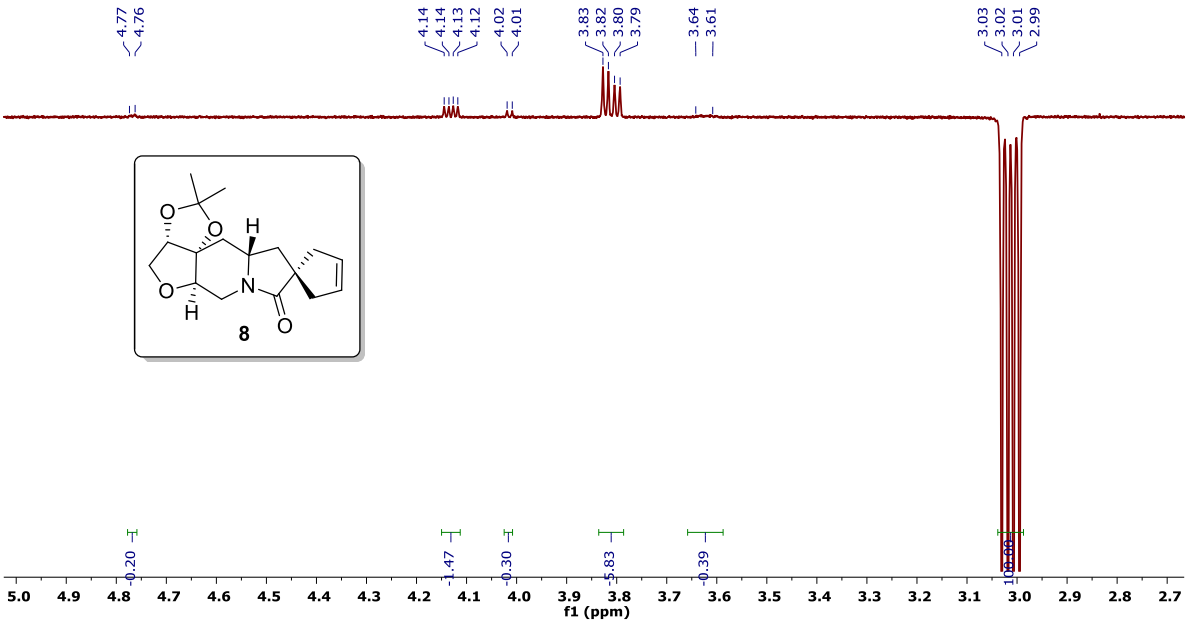

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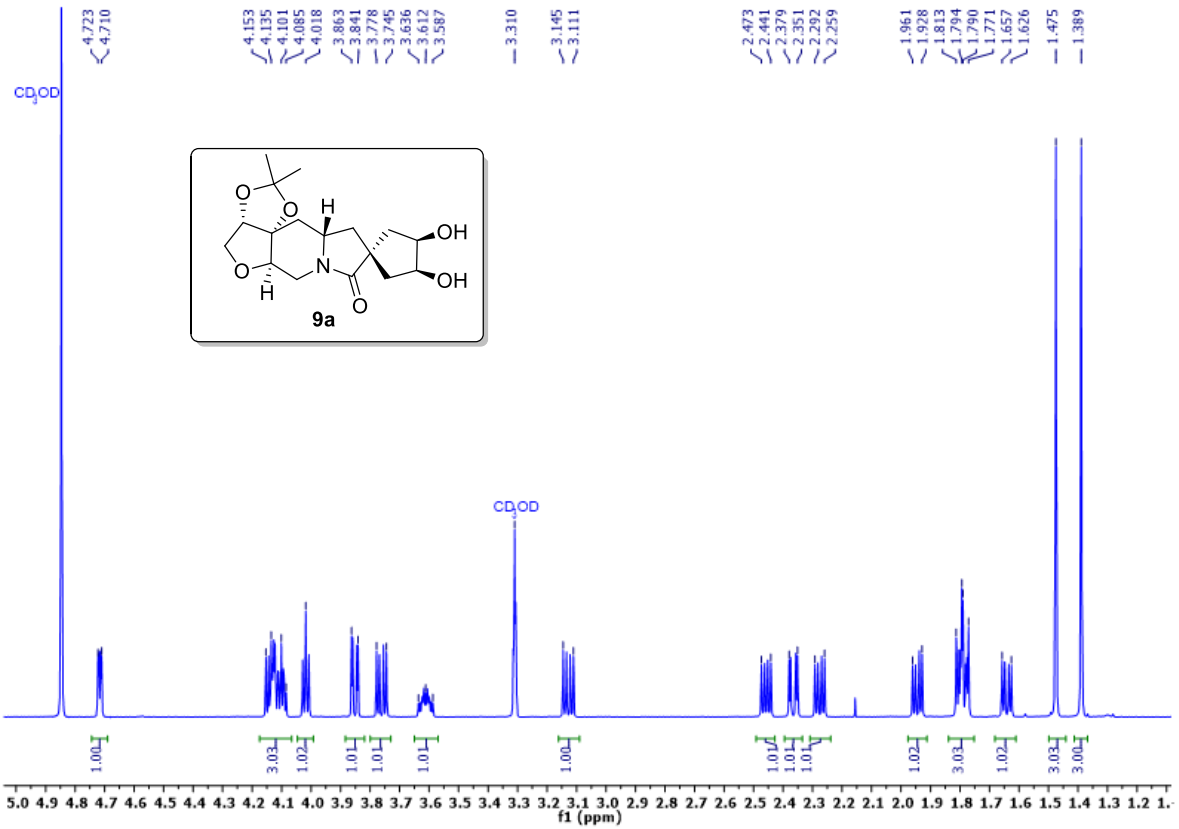

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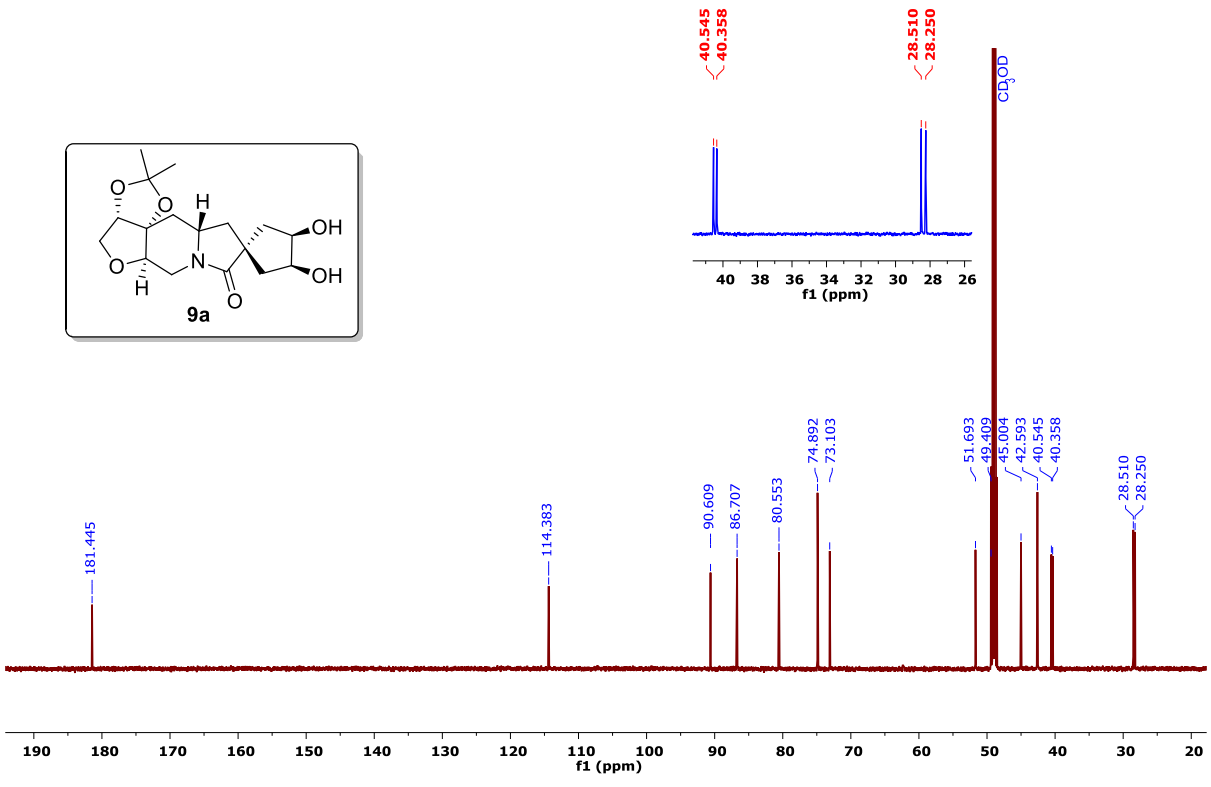

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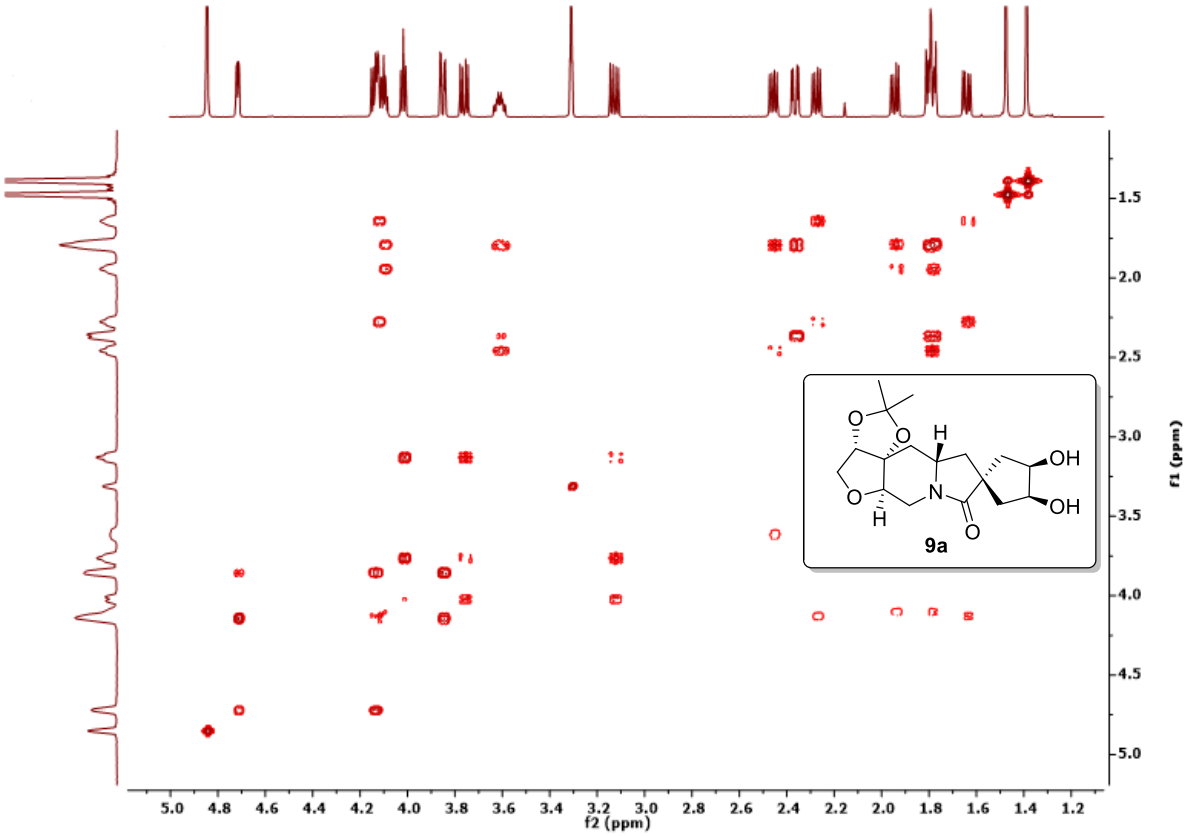

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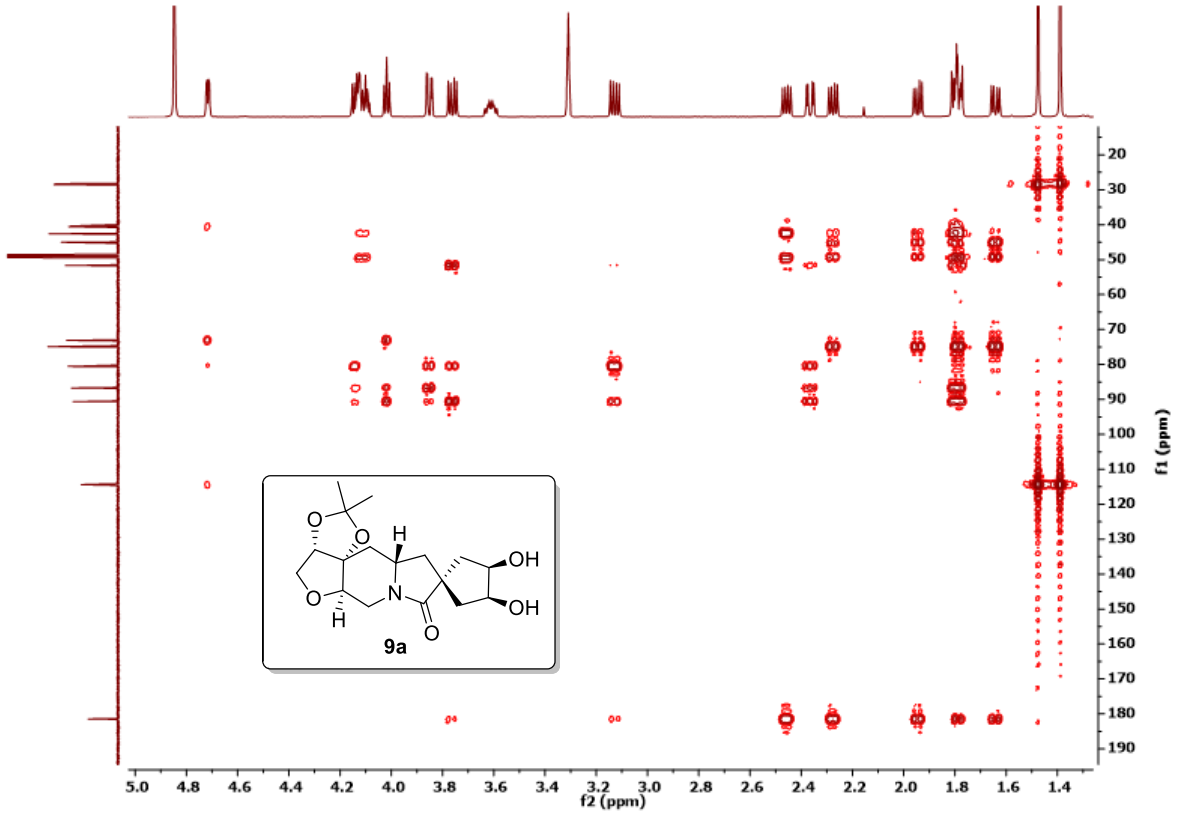

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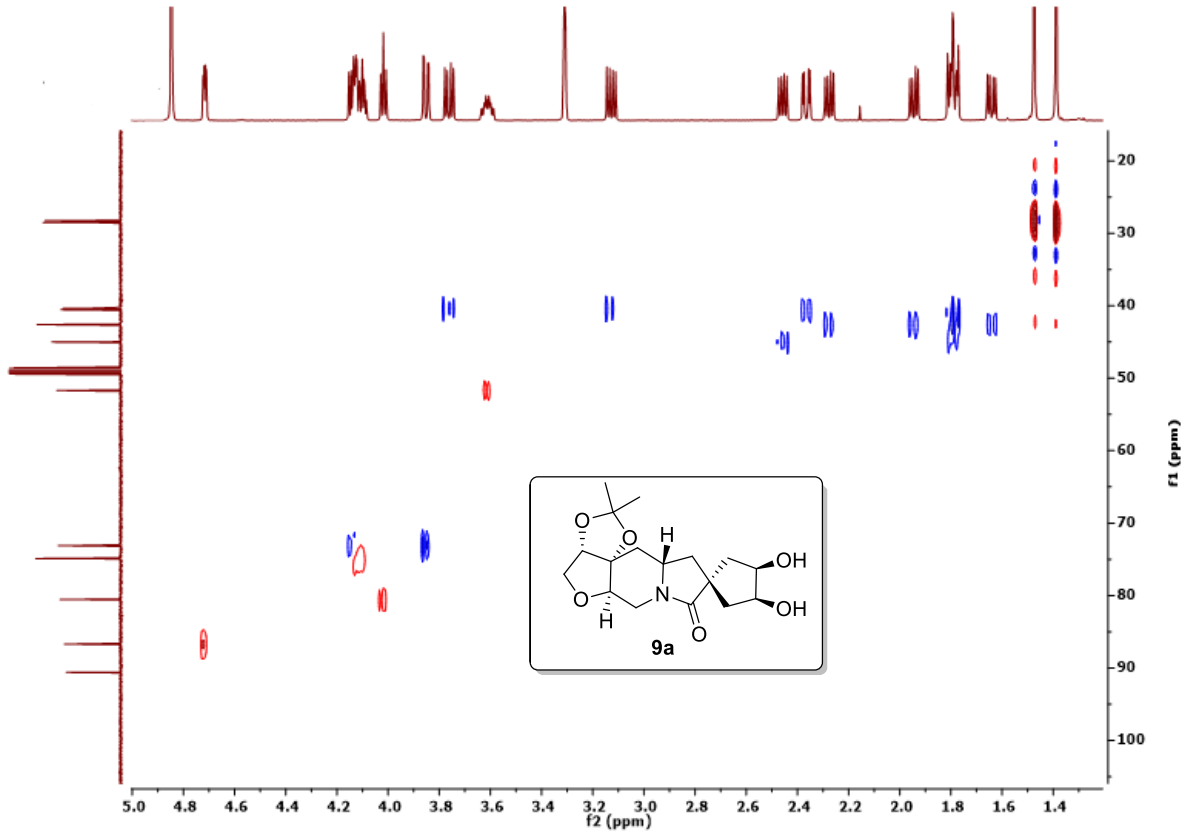

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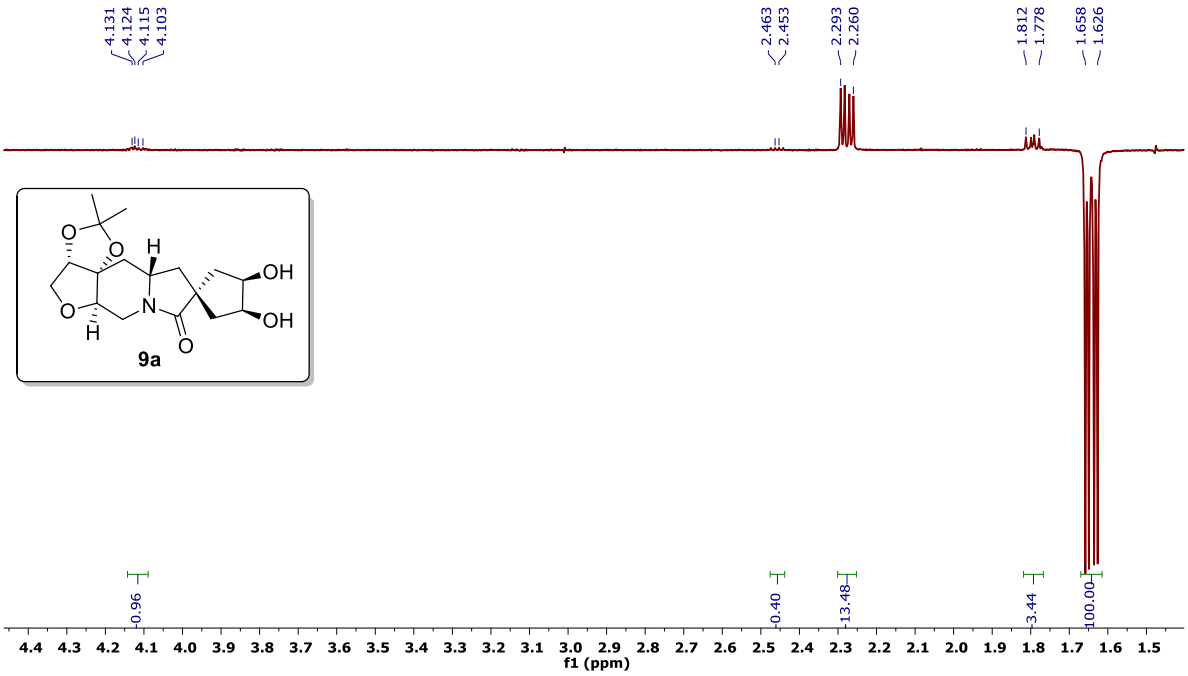
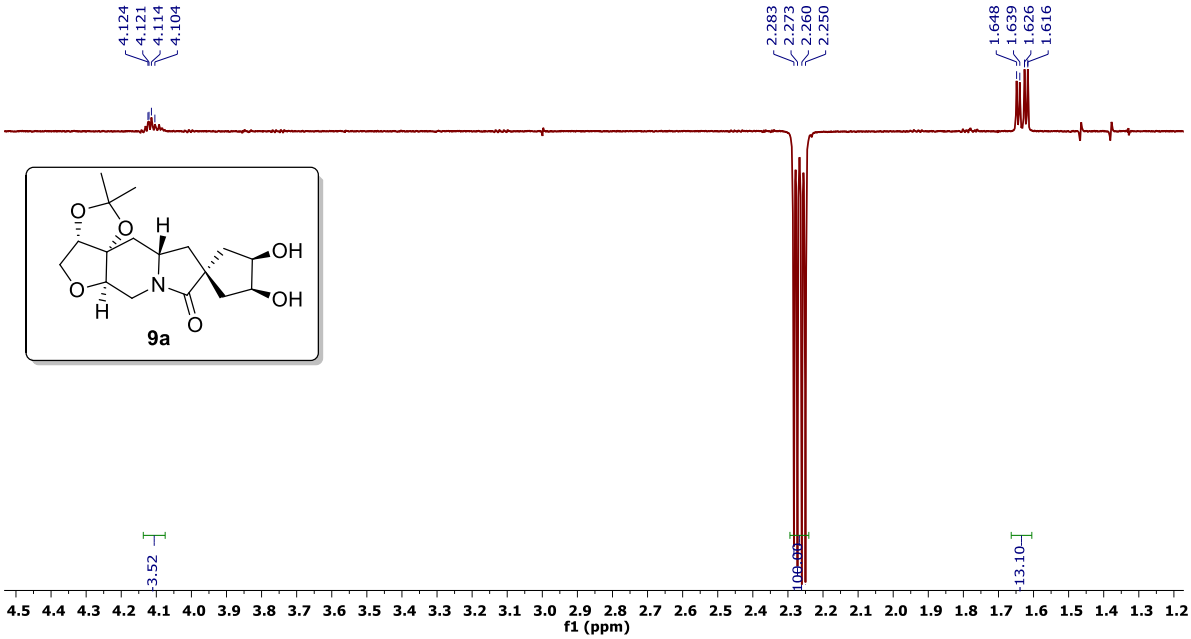
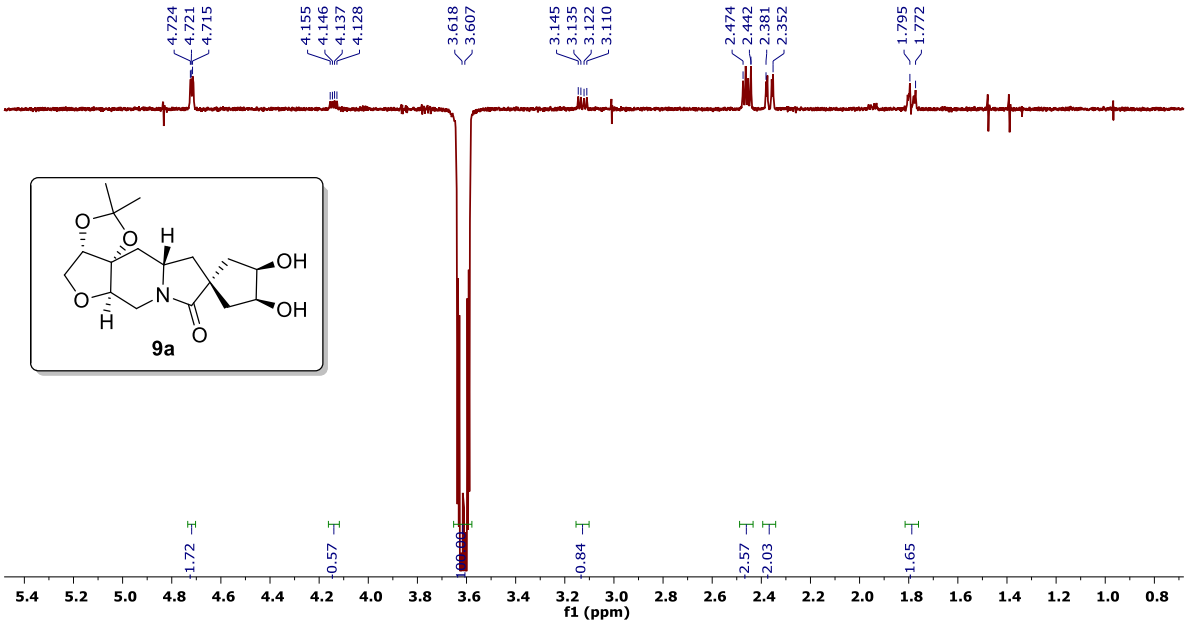
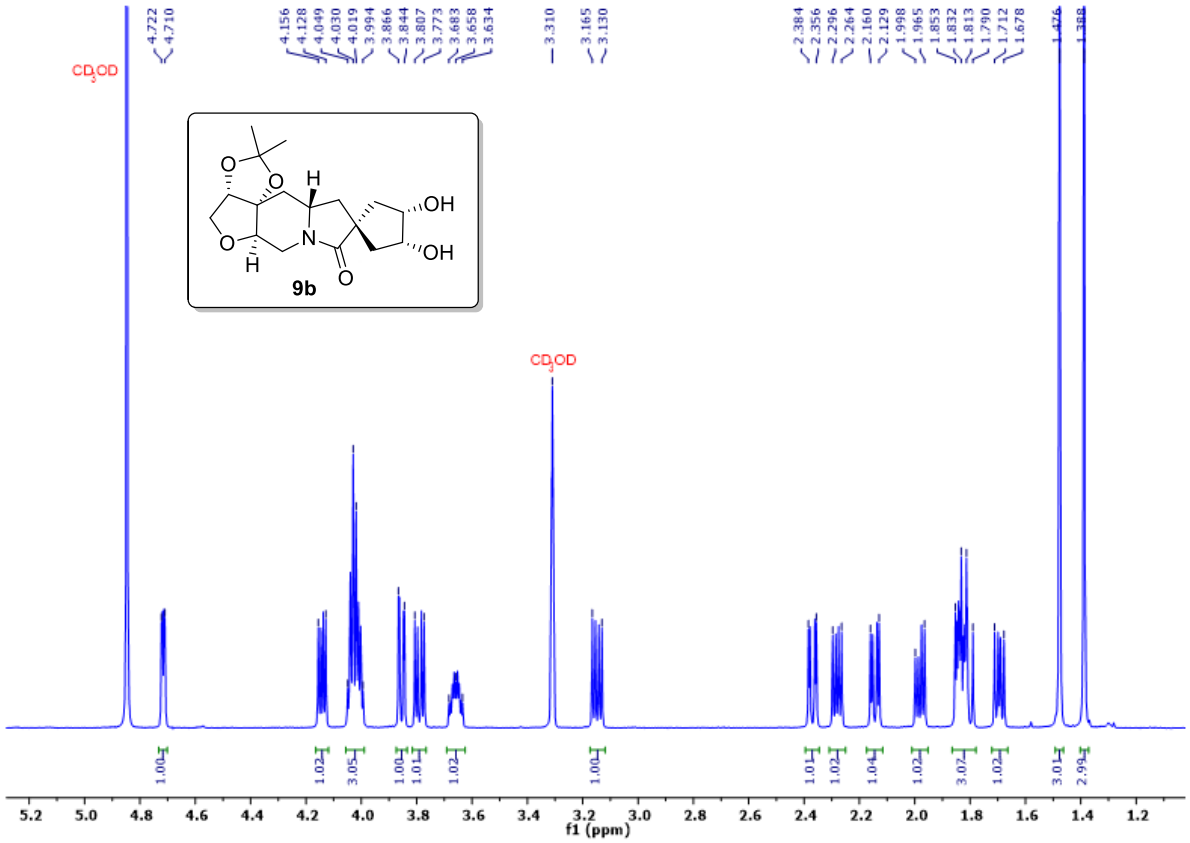






NOESY spectra of compounds **9a**



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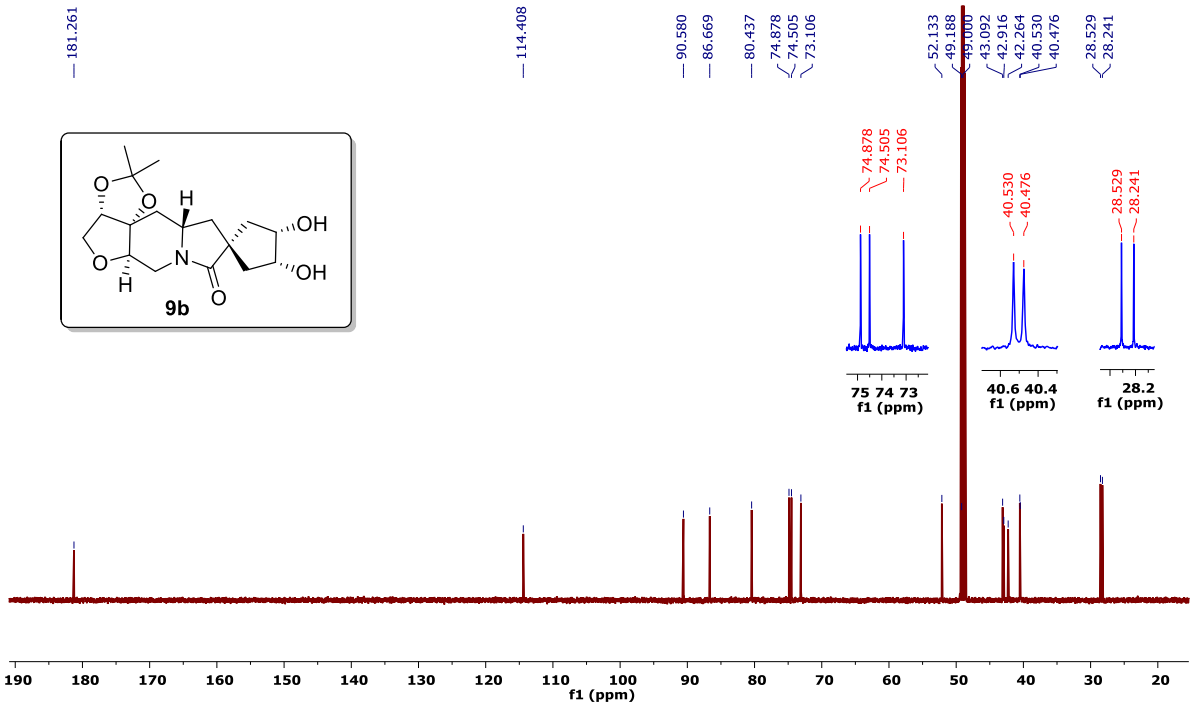

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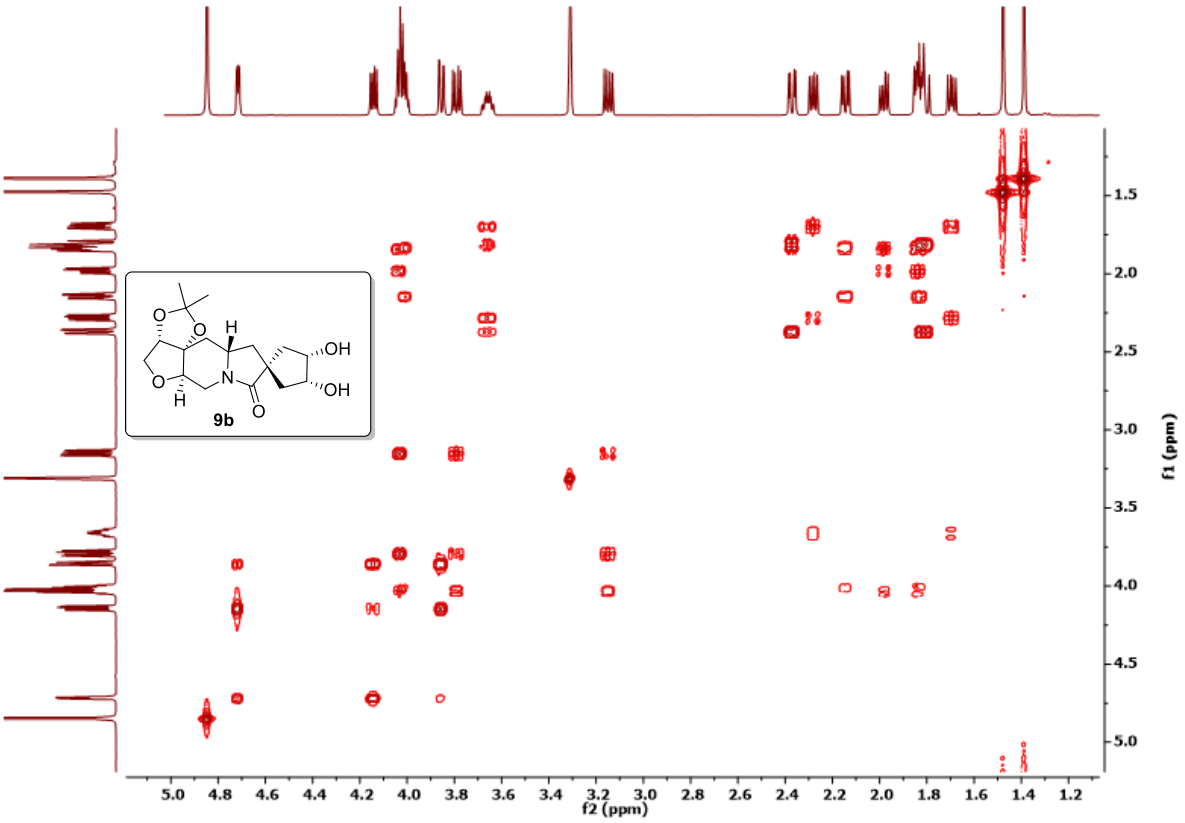

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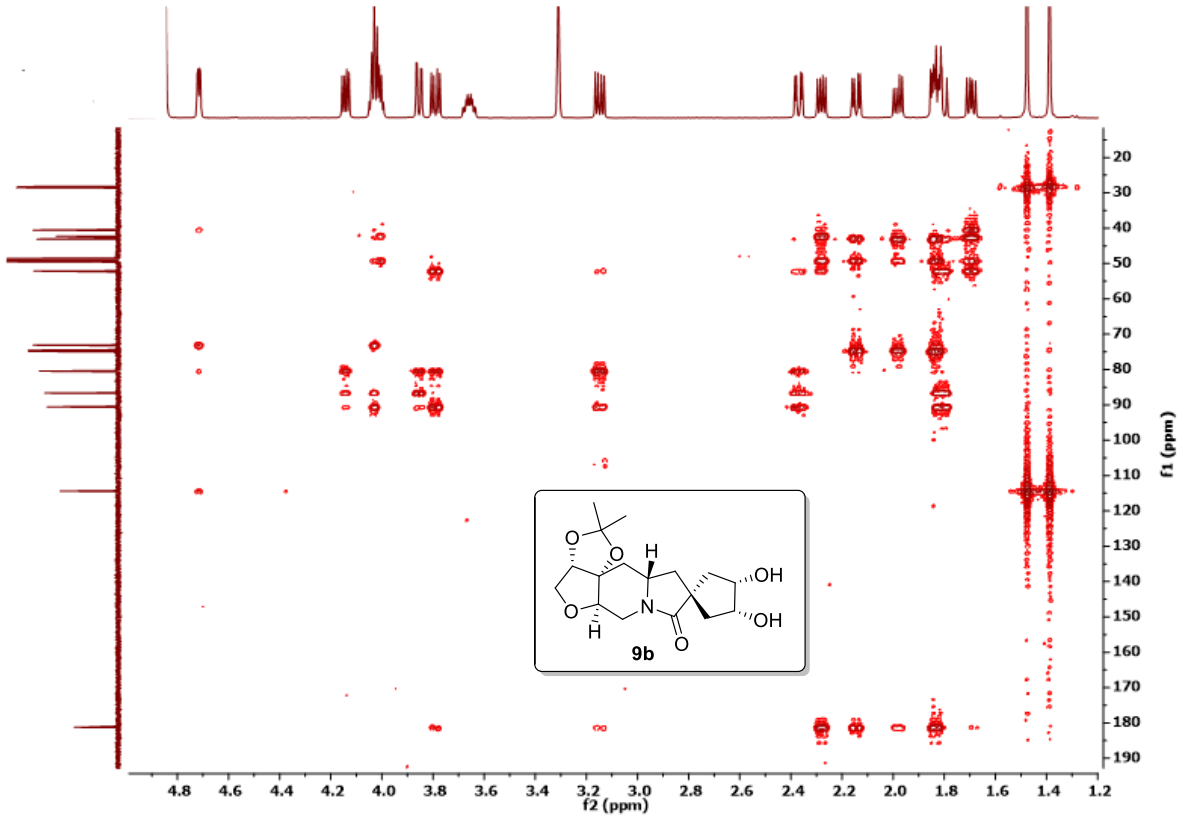

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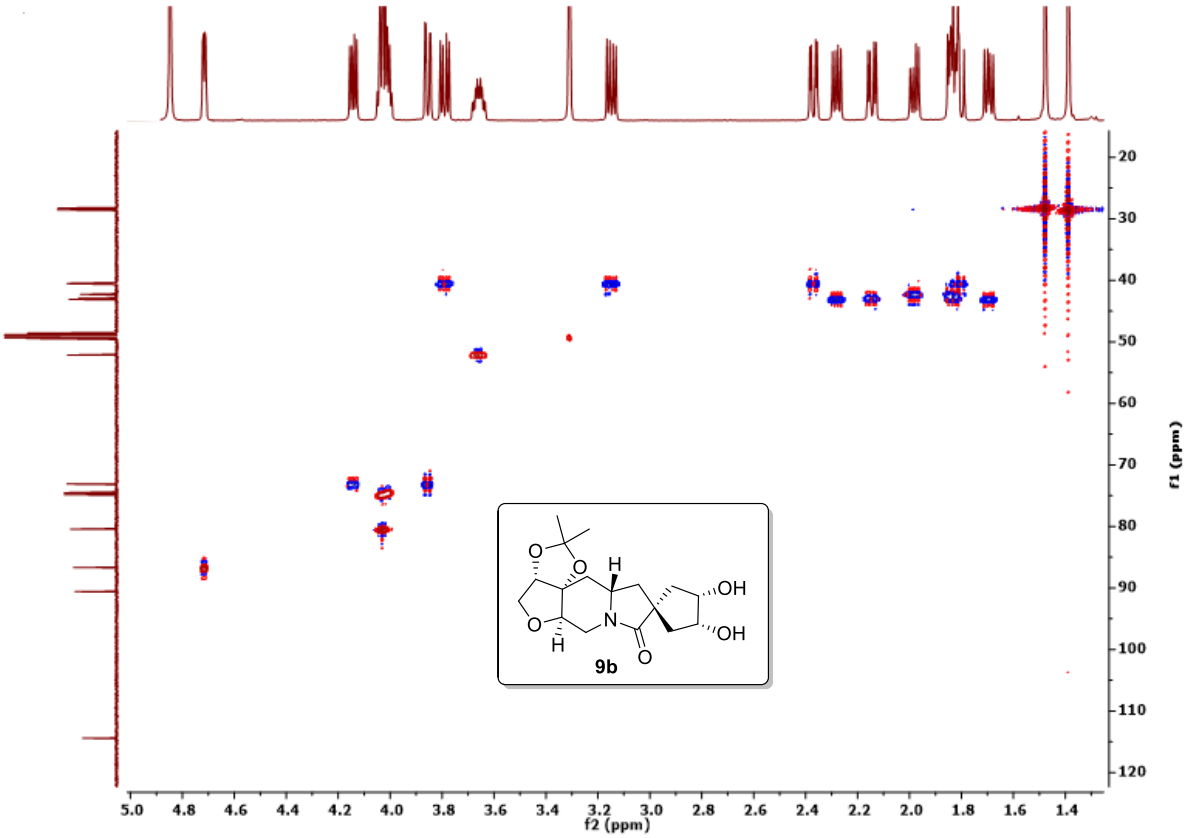

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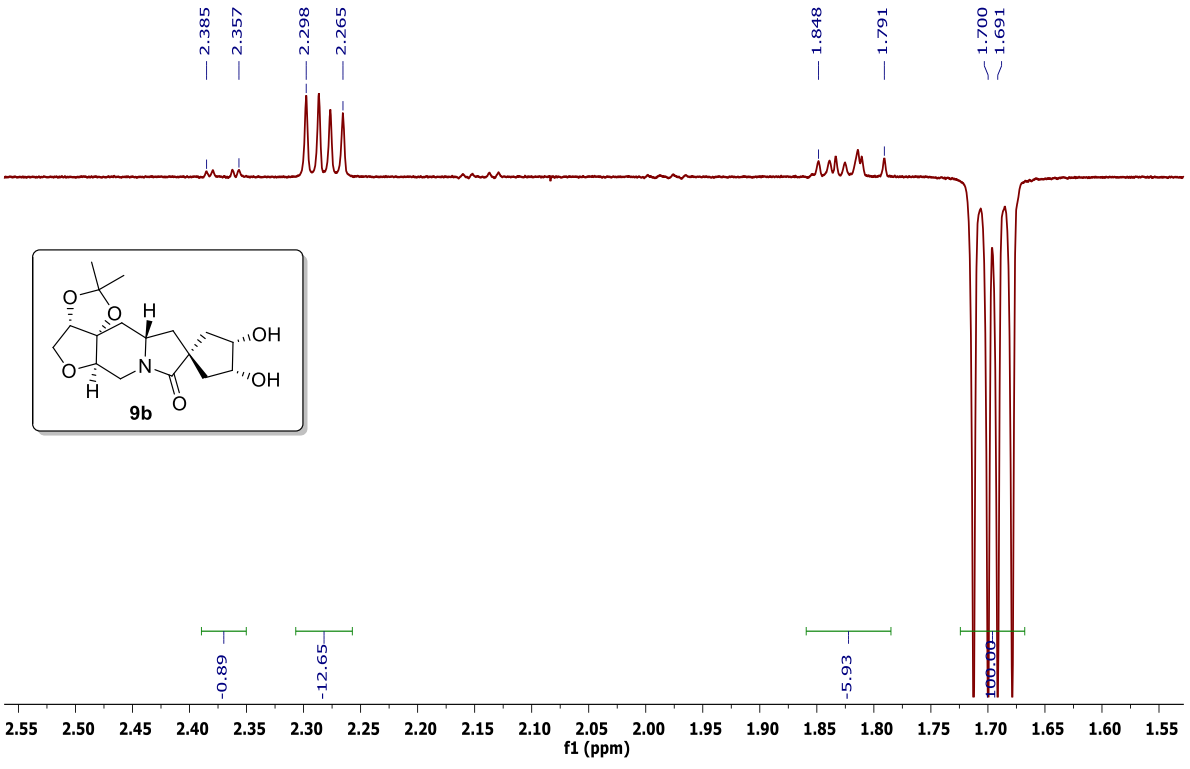
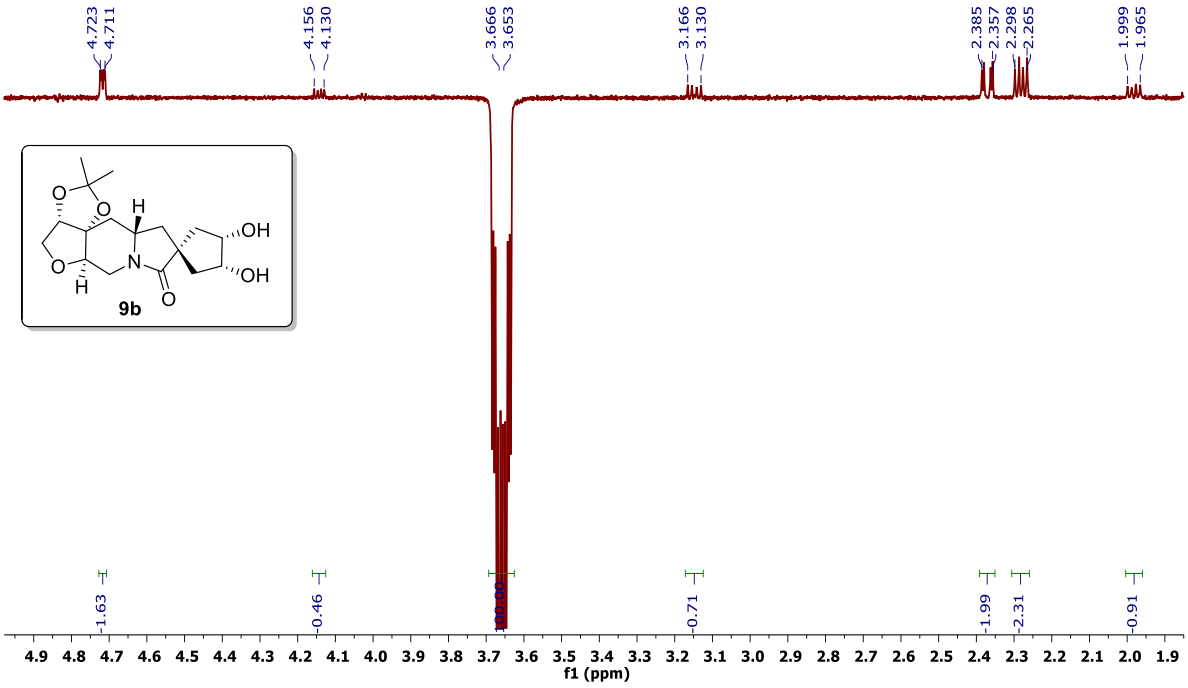
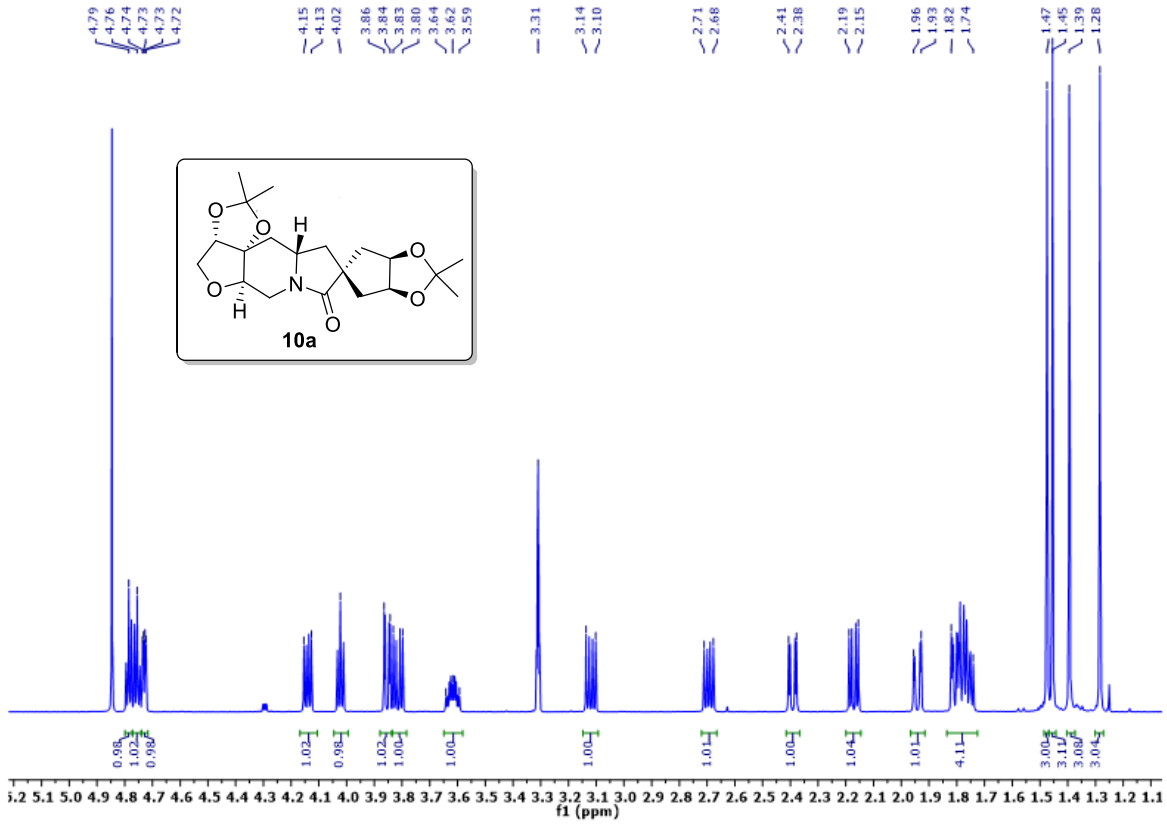


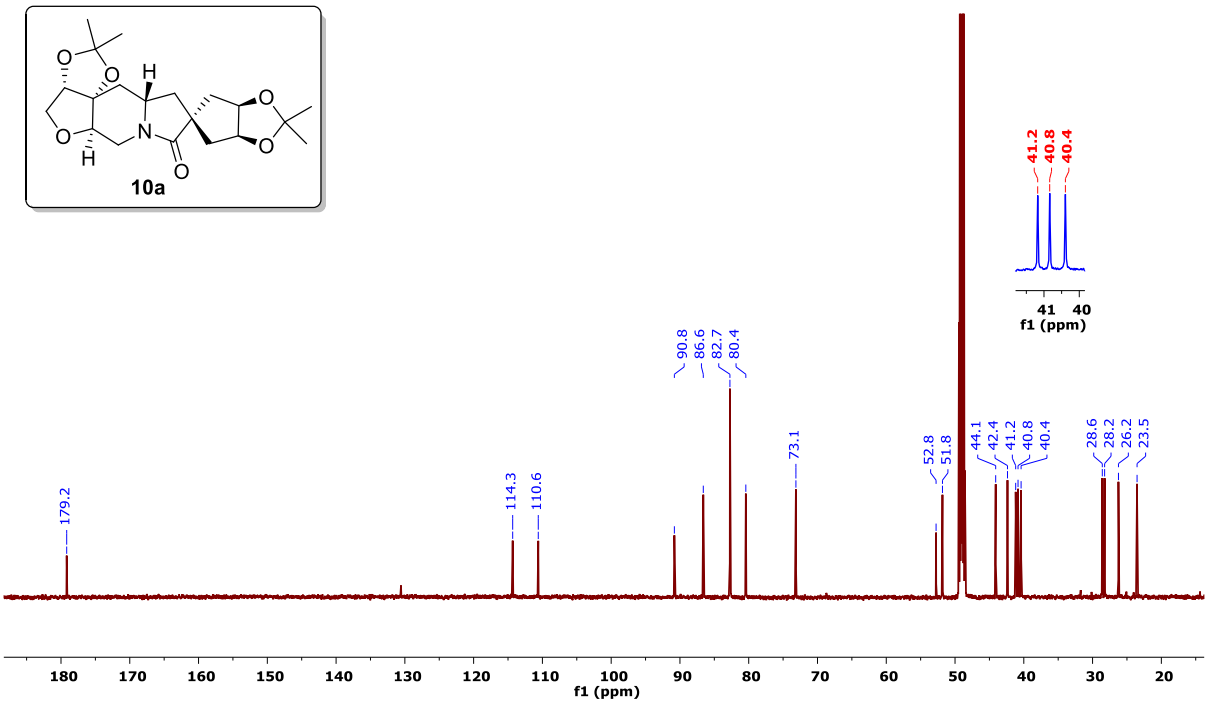
NOESY spectrum of compound **9b**



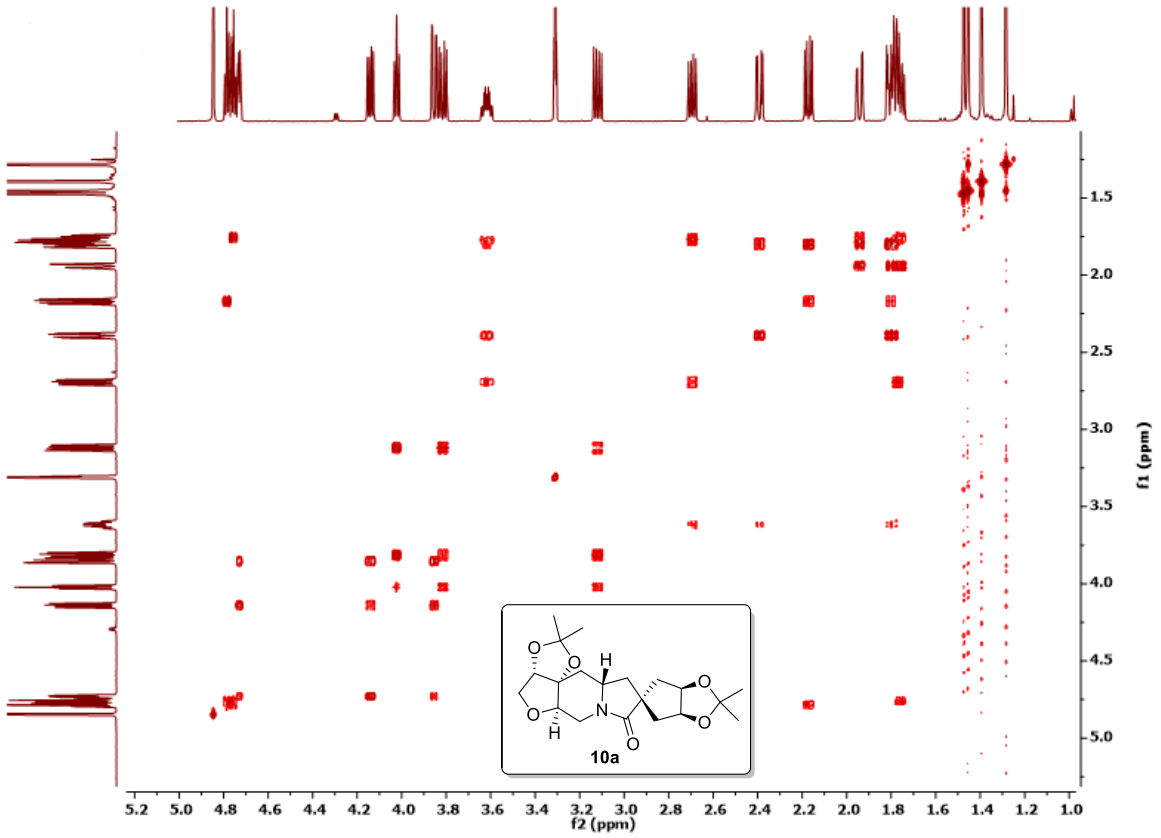
NOESY spectrum of compound **9b**



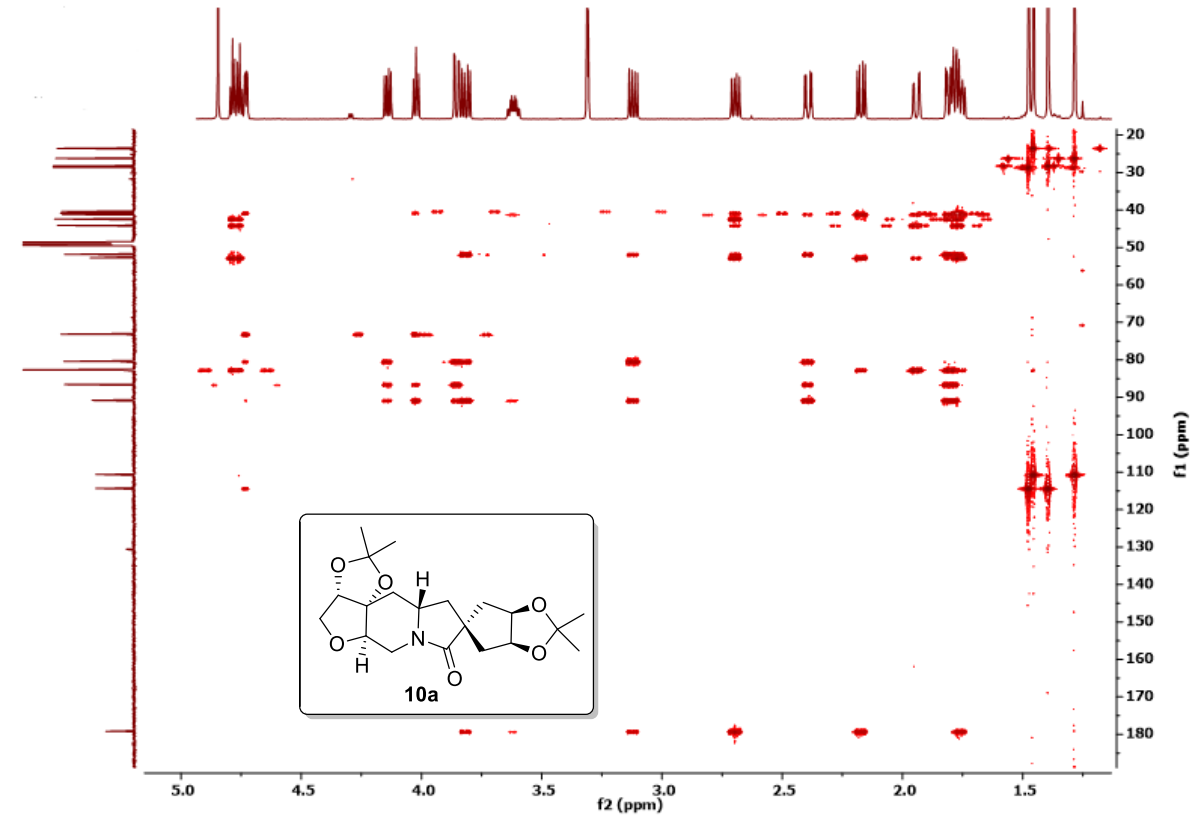
^{1}H NMR spectrum of compound **10a**



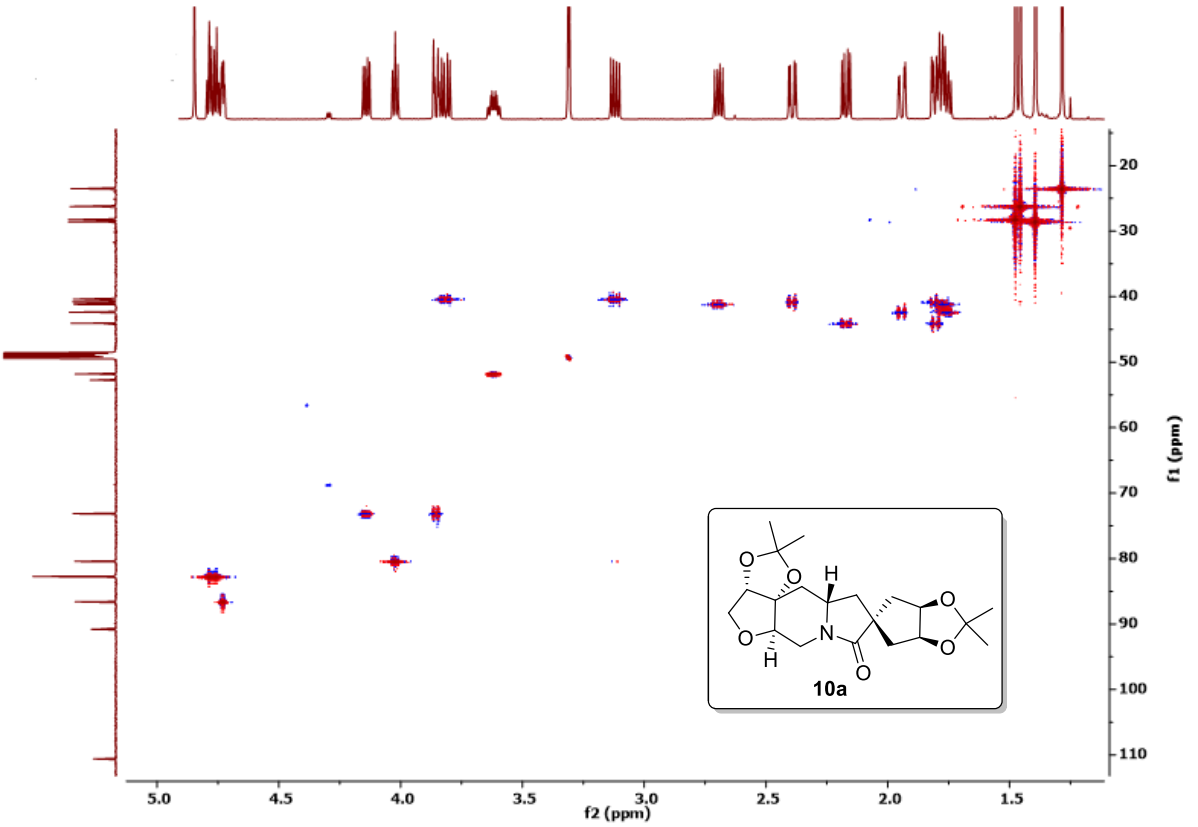
^{13}C NMR spectrum of compound **10a**



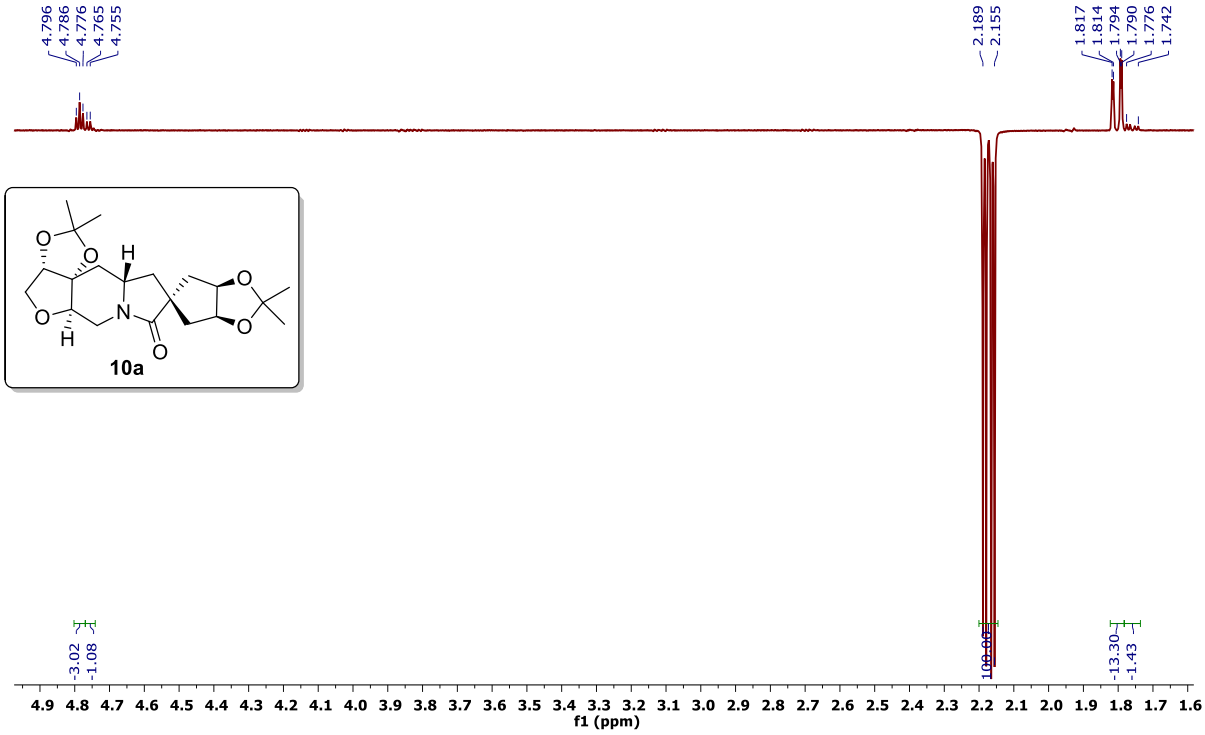
COSY spectrum of compound **10a**



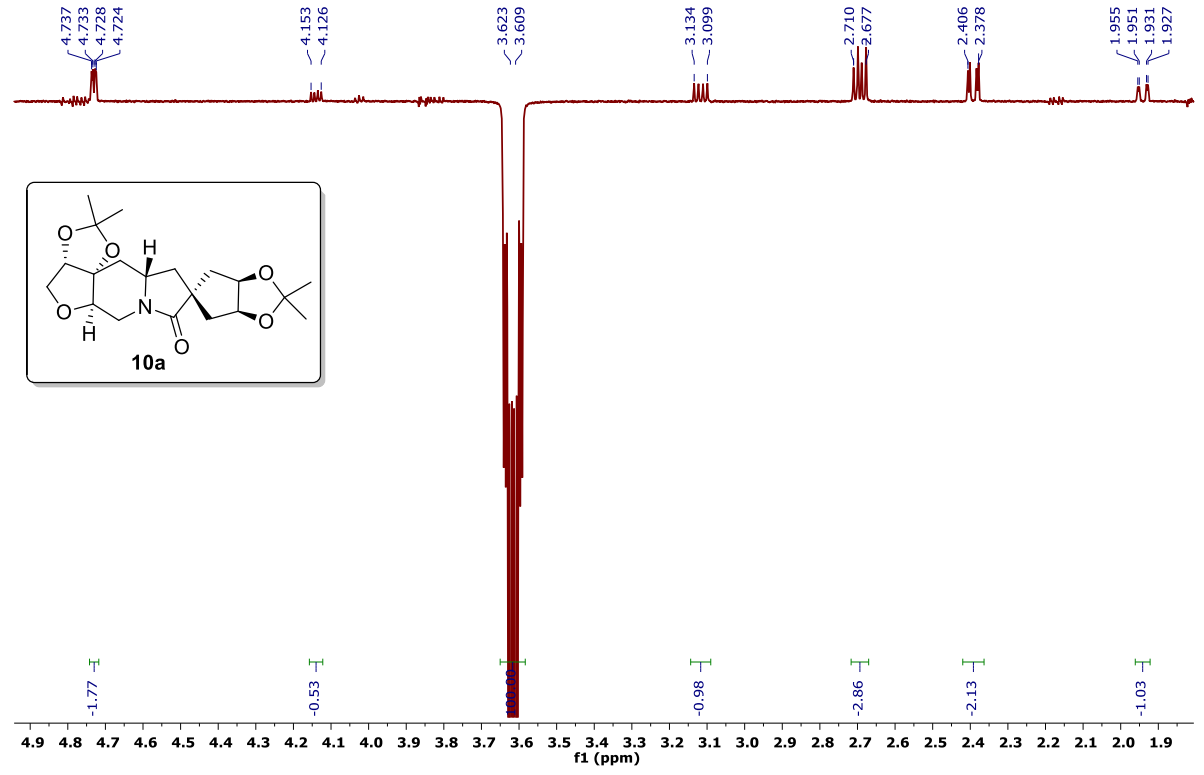
HMBCAD spectrum of compound **10a**



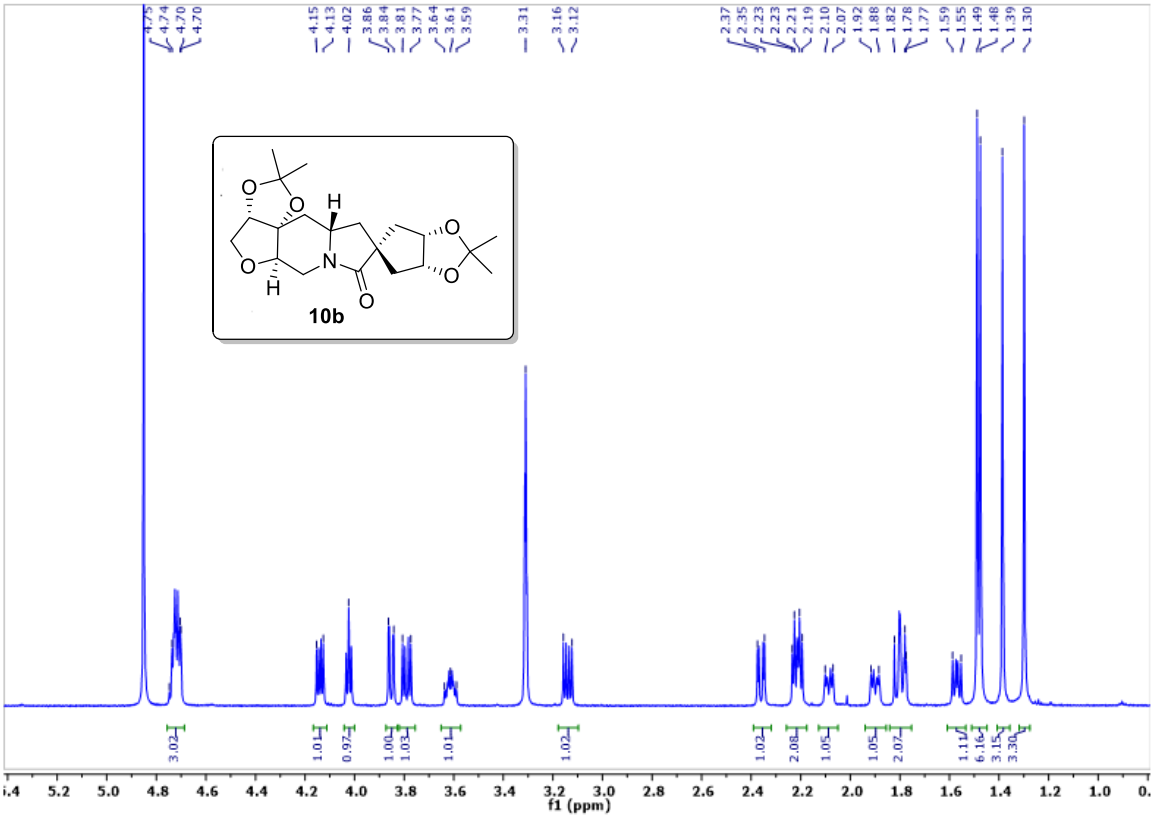
HSQCAD spectrum of compound **10a**



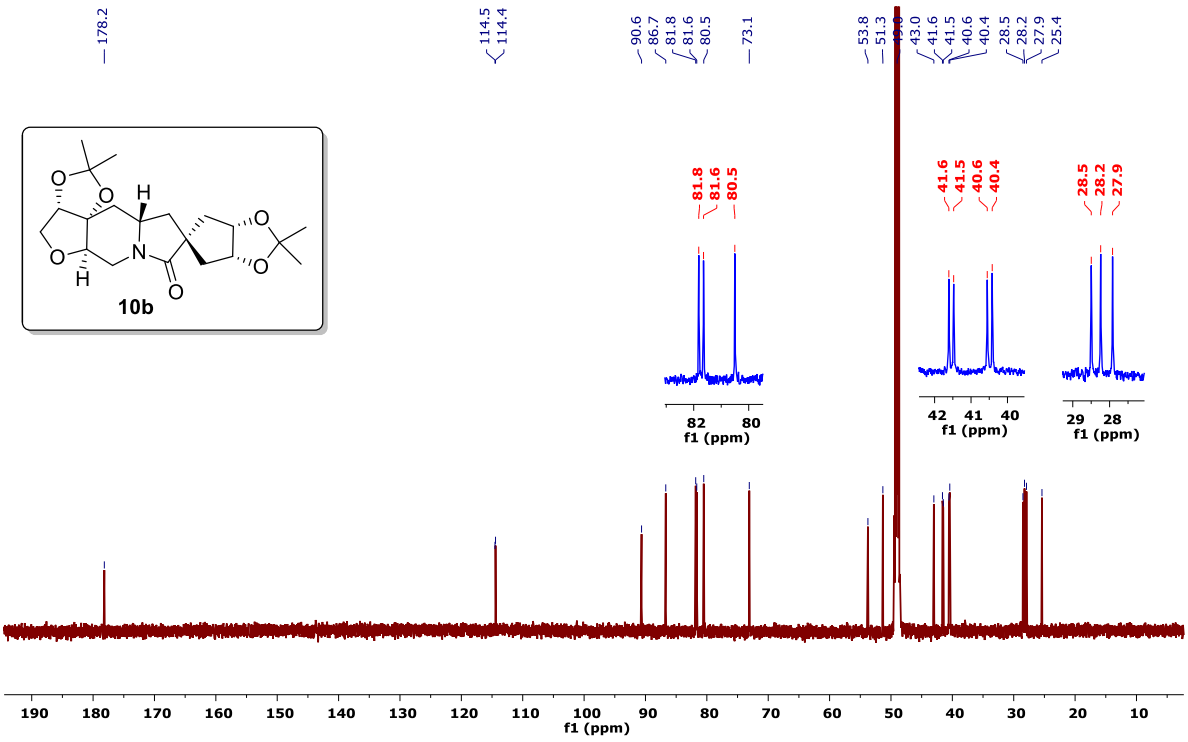
NOESY spectrum of compound **10a**



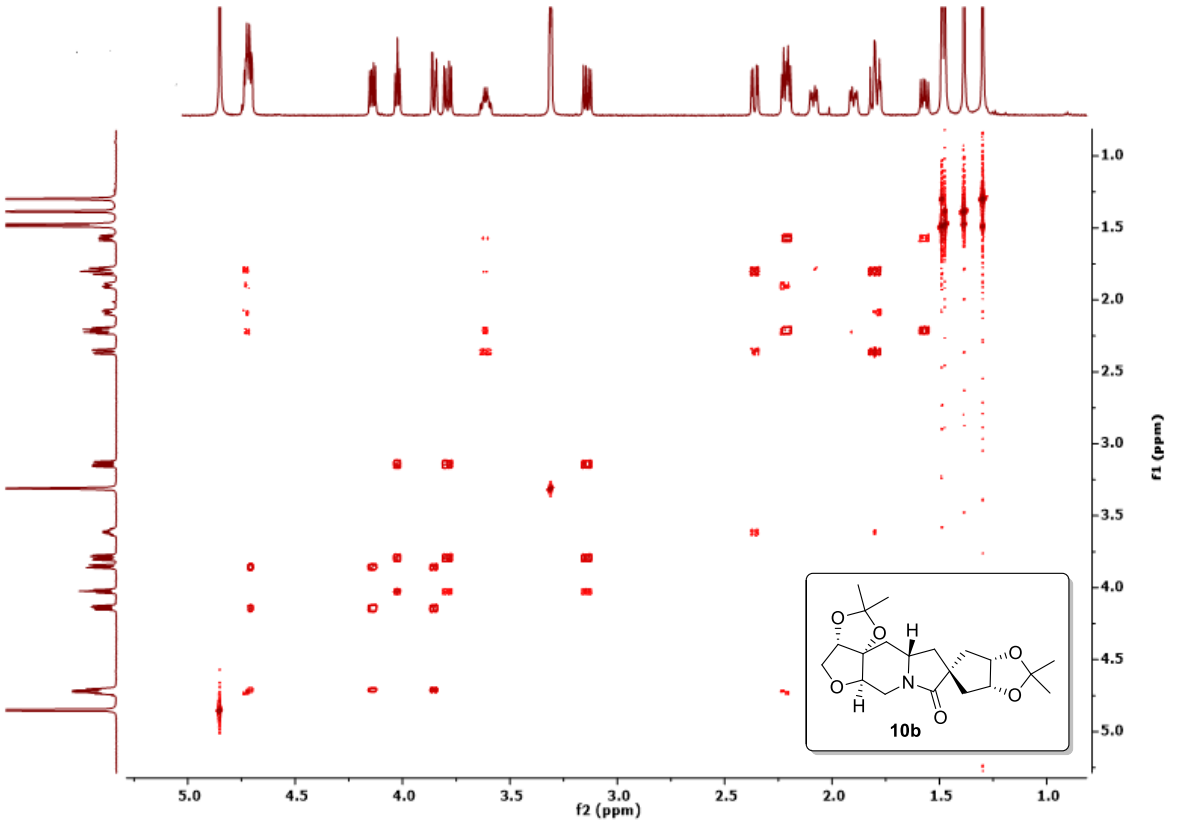
NOESY spectrum of compound **10a**



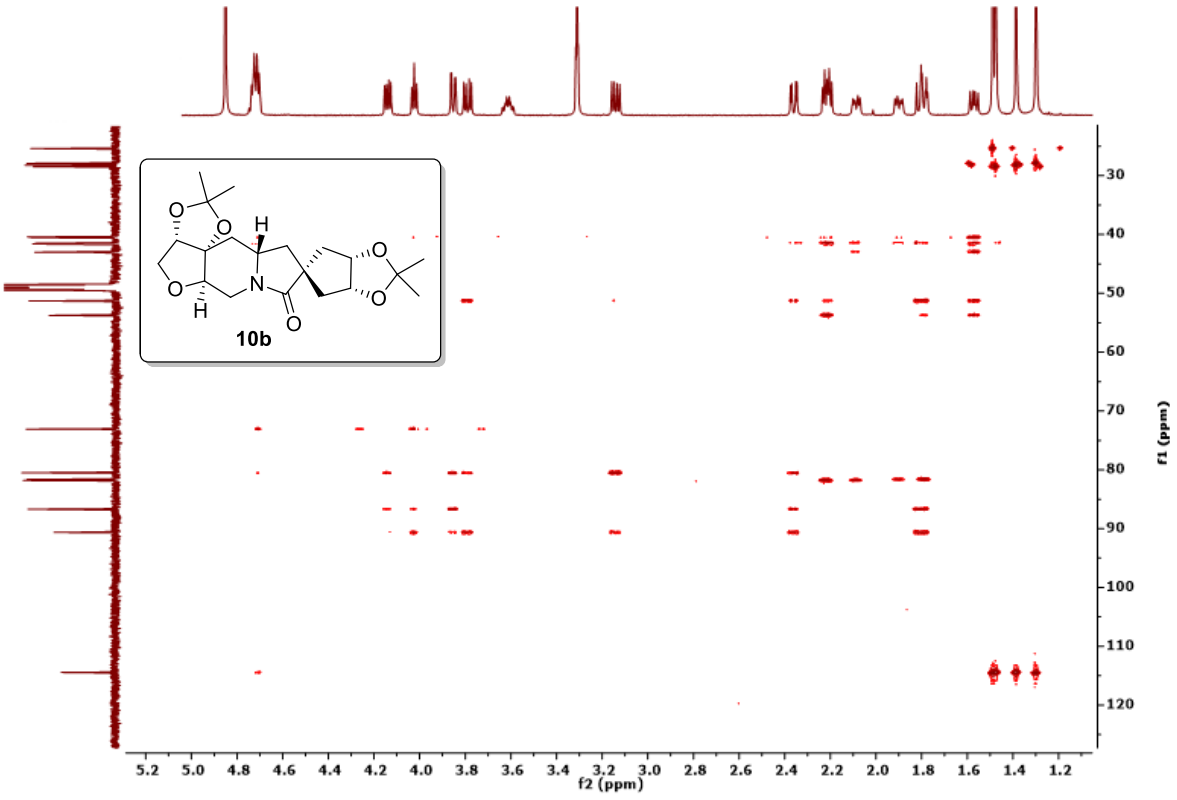
^{1}H NMR spectrum of compound **10b**



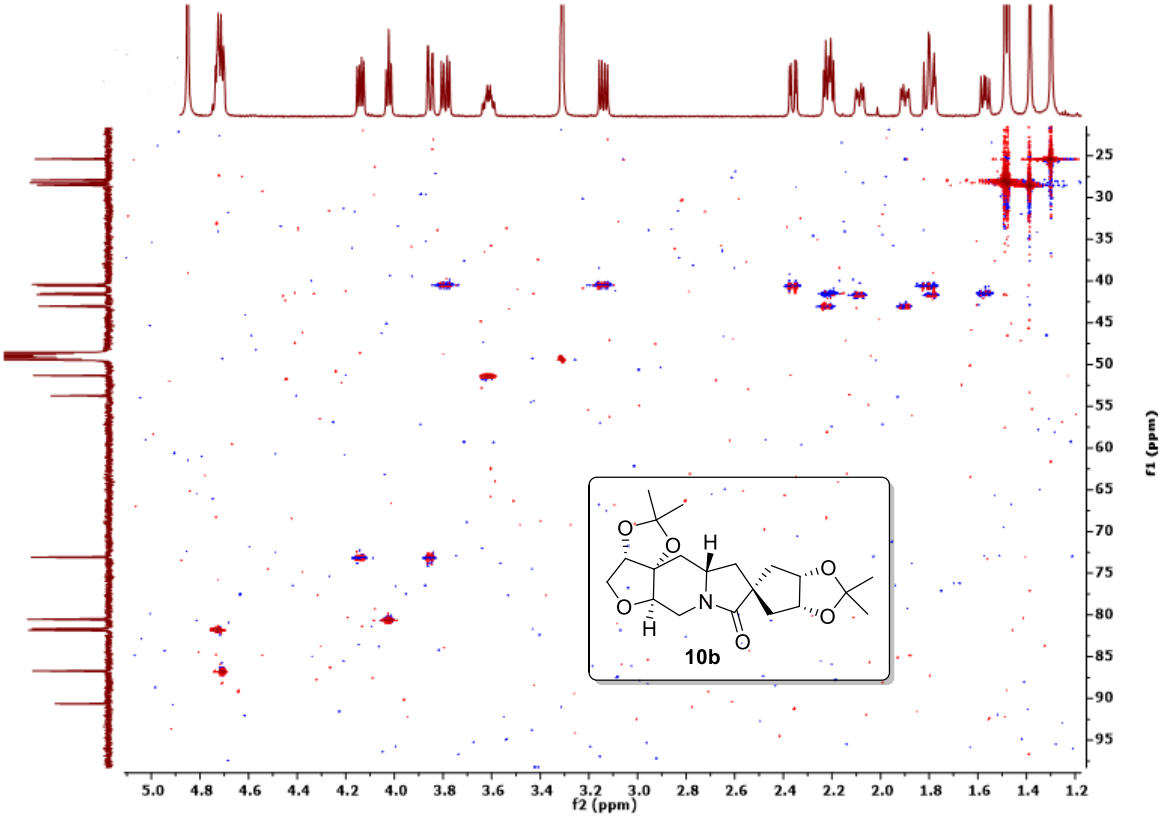
^{13}C NMR spectrum of compound **10b**



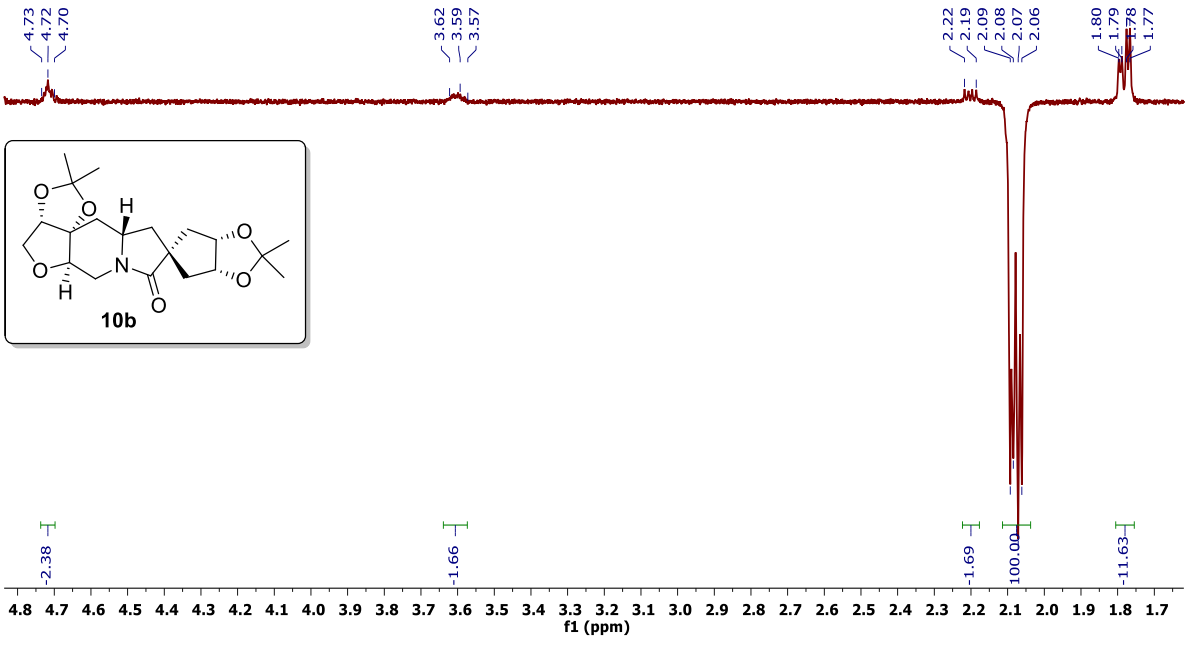
COSY spectrum of compound **10b**



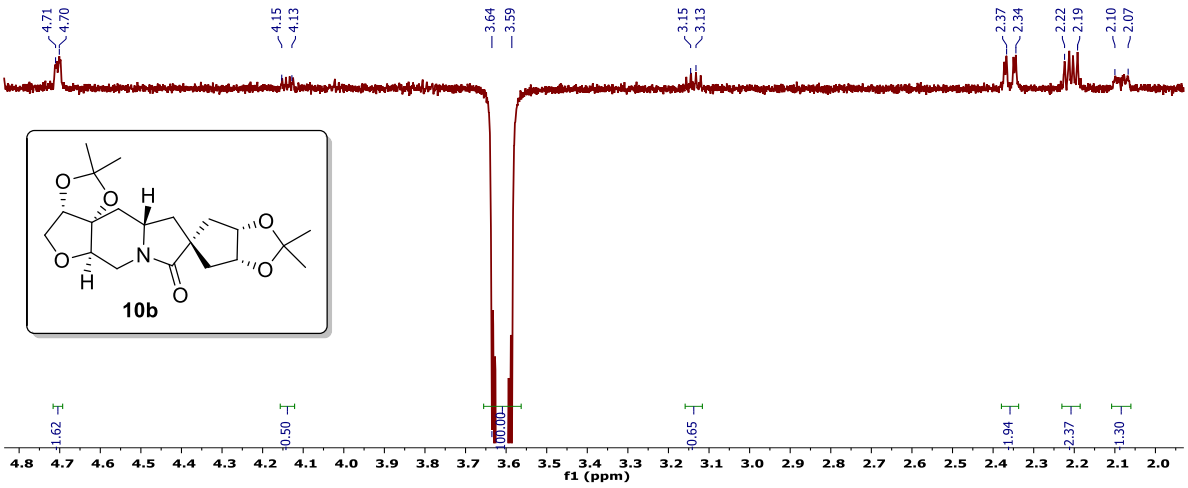
HMBCAD spectrum of compound **10b**

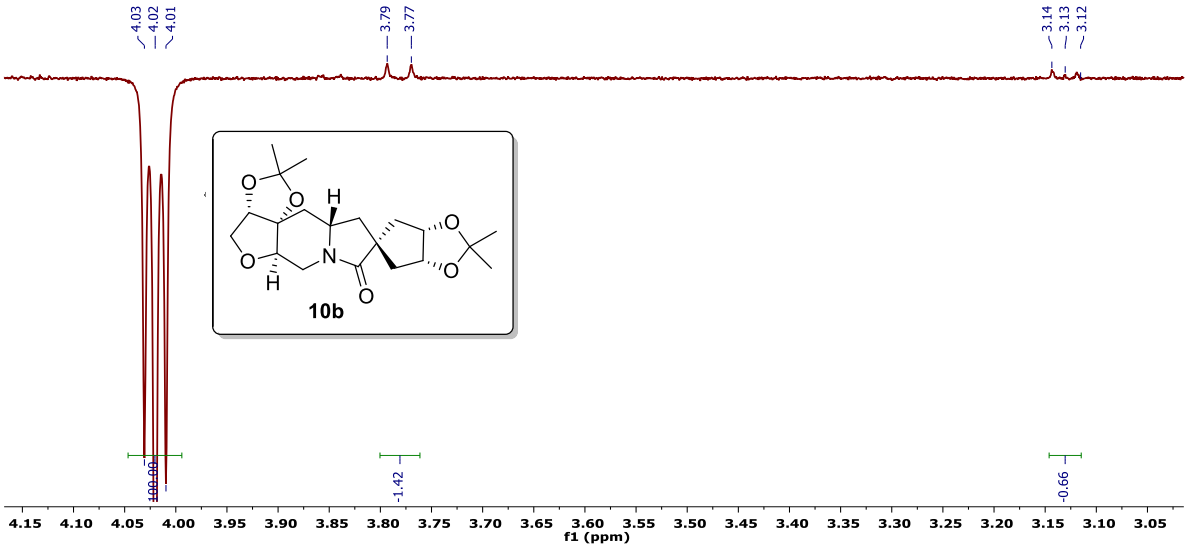


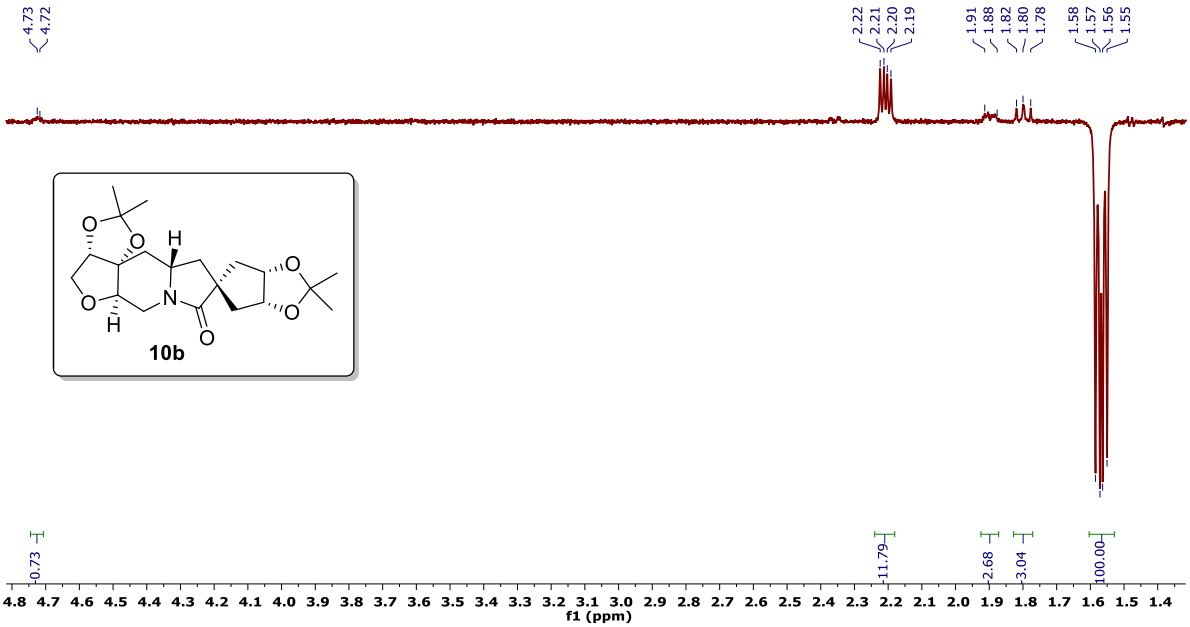
HSQCAD spectrum of compound **10b**



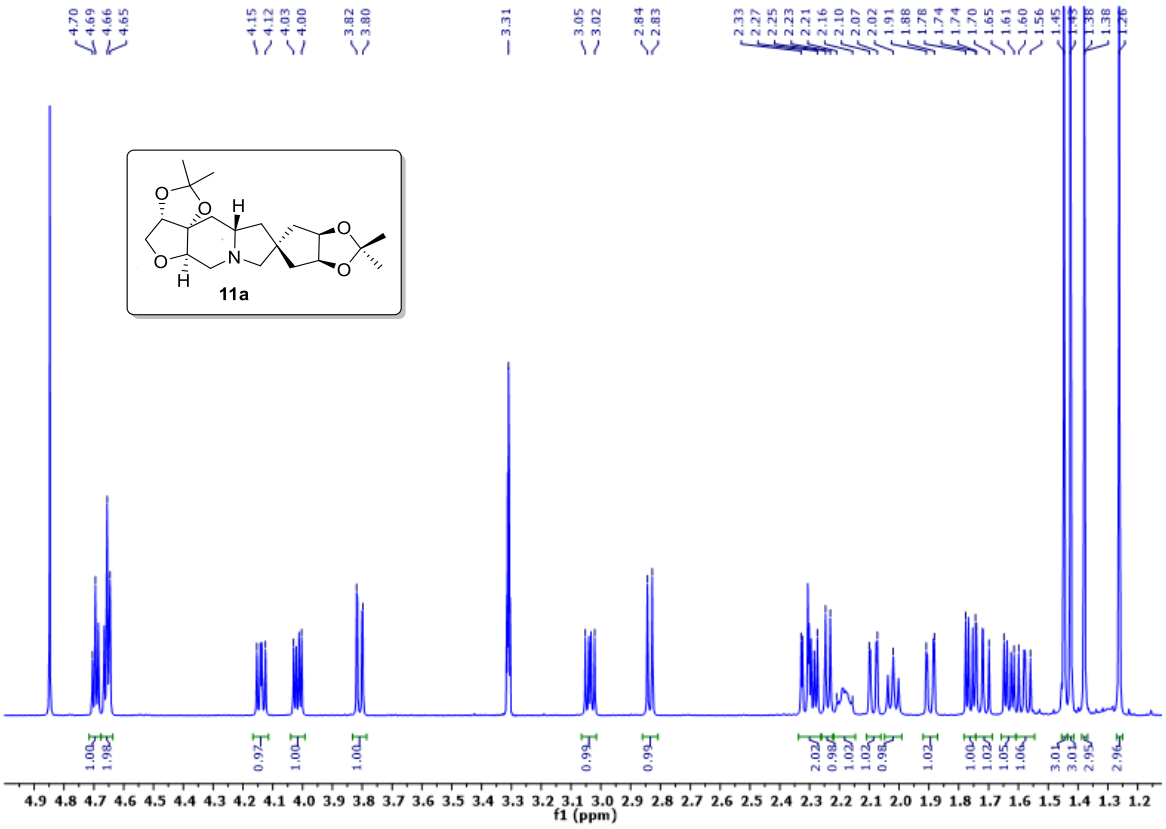
NOESY spectrum of compound **10b**



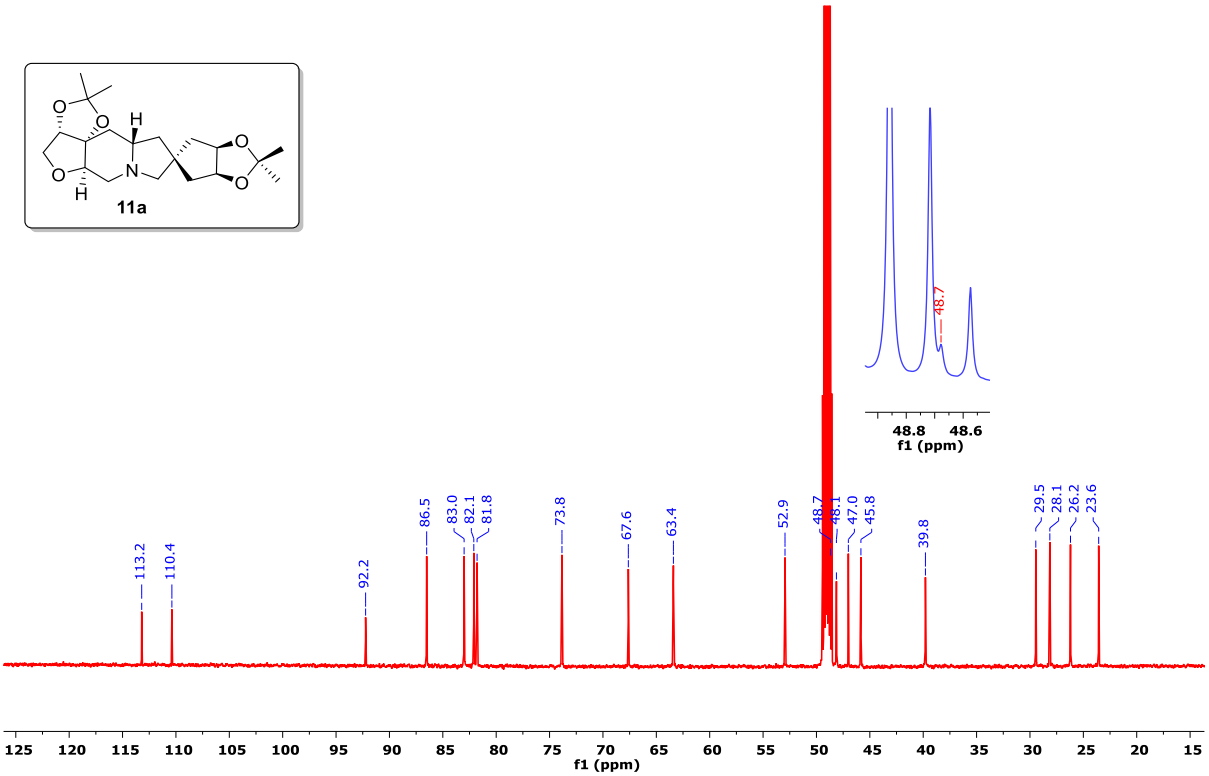




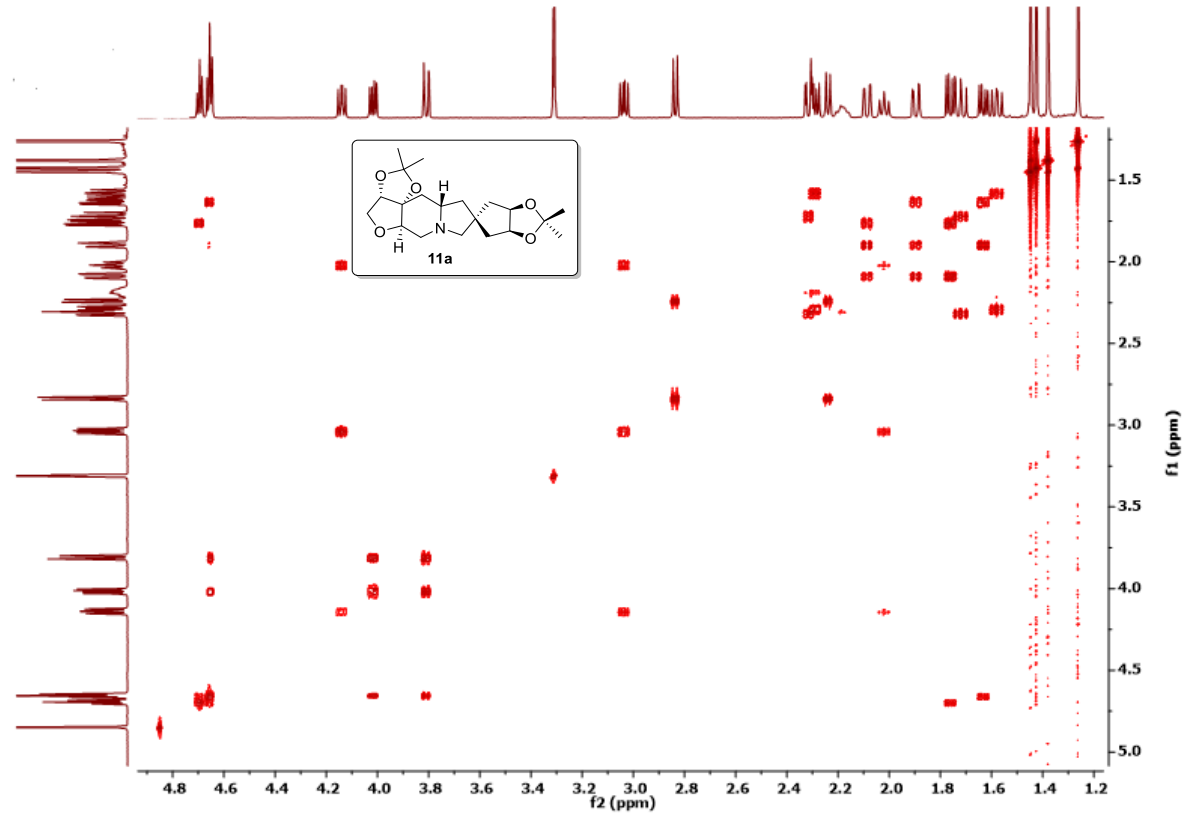
NOESY spectra of compound **10b**



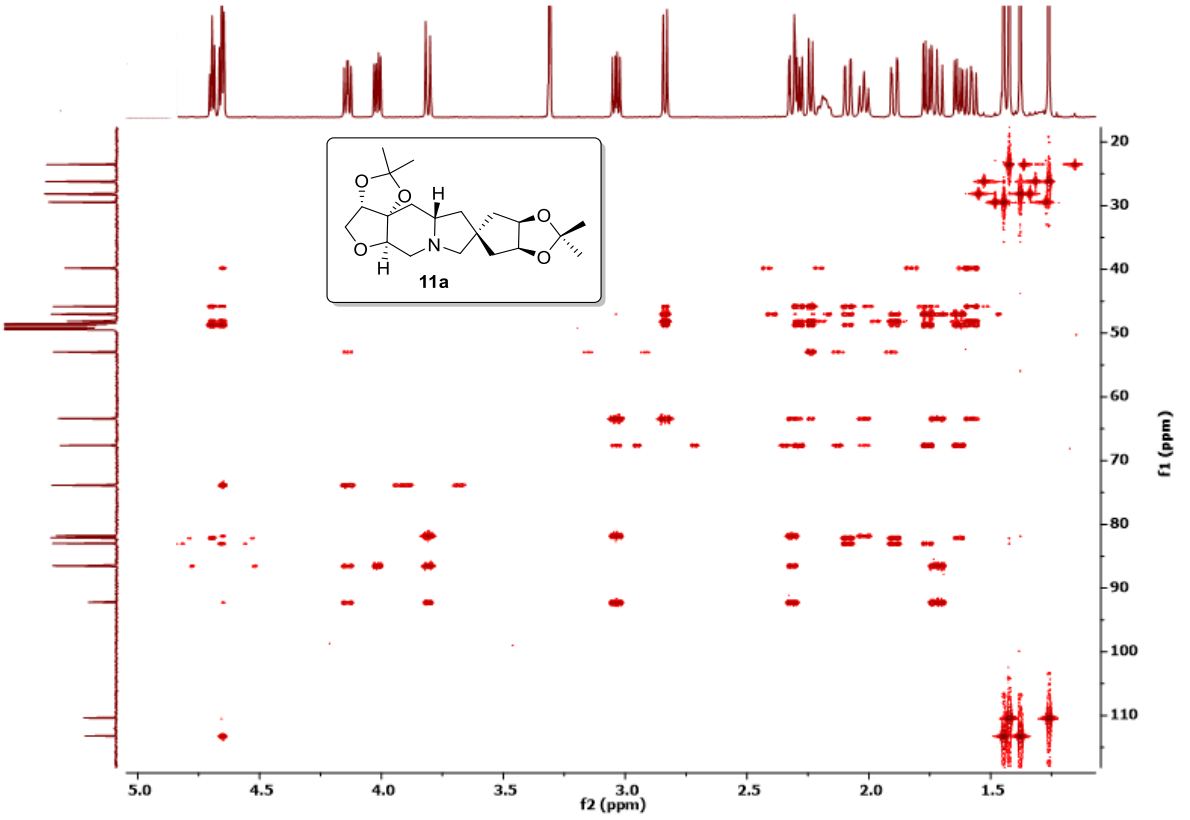
^{1}H NMR spectrum of compound **11a**



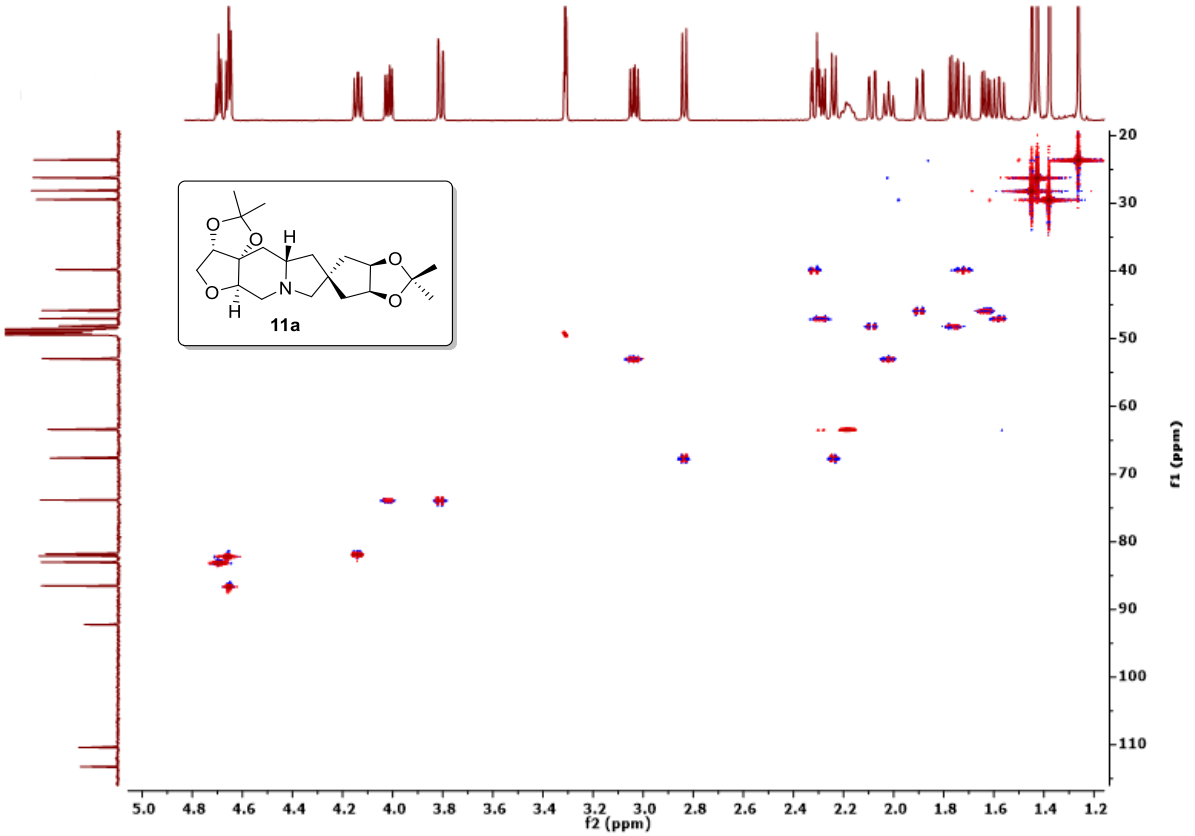
^{13}C NMR spectrum of compound **11a**



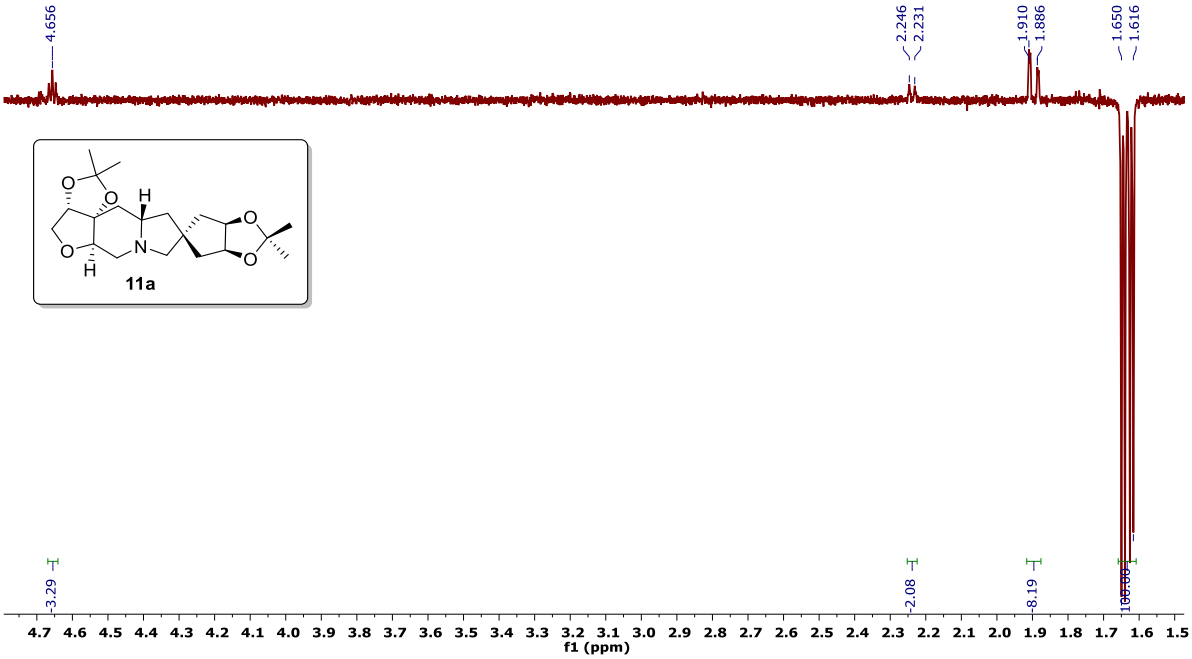
COSY spectrum of compound **11a**



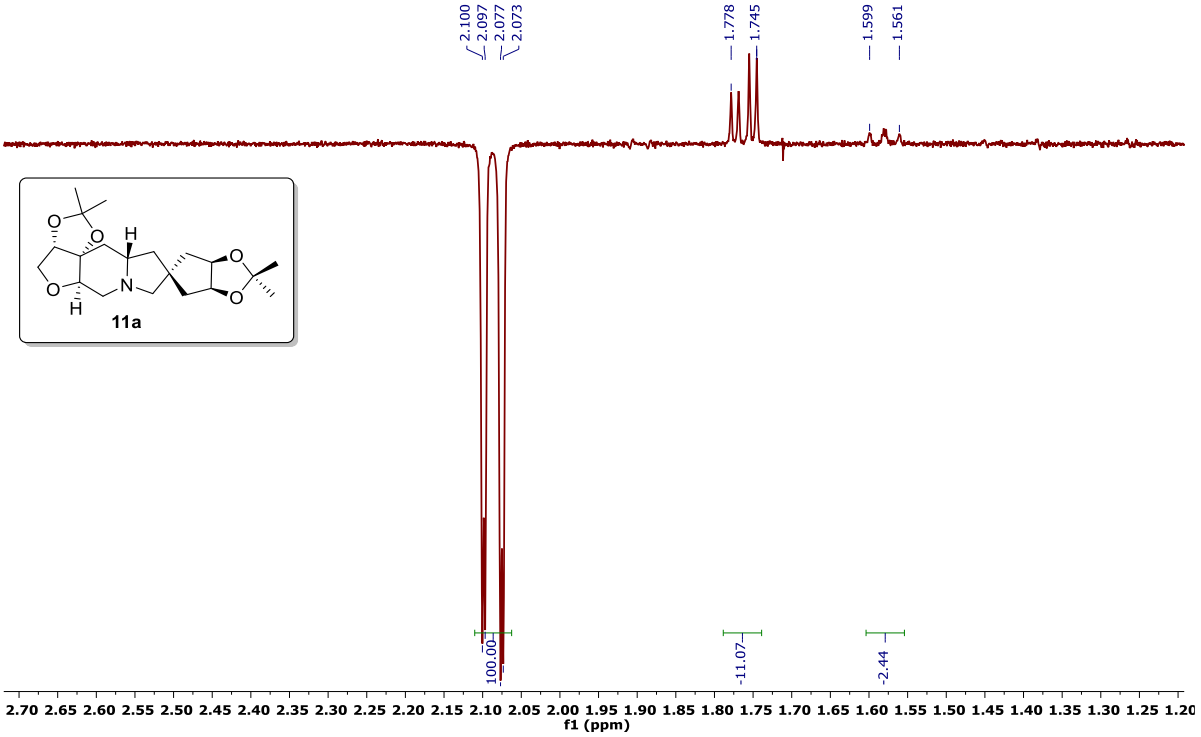
HMBCAD spectrum of compound **11a**



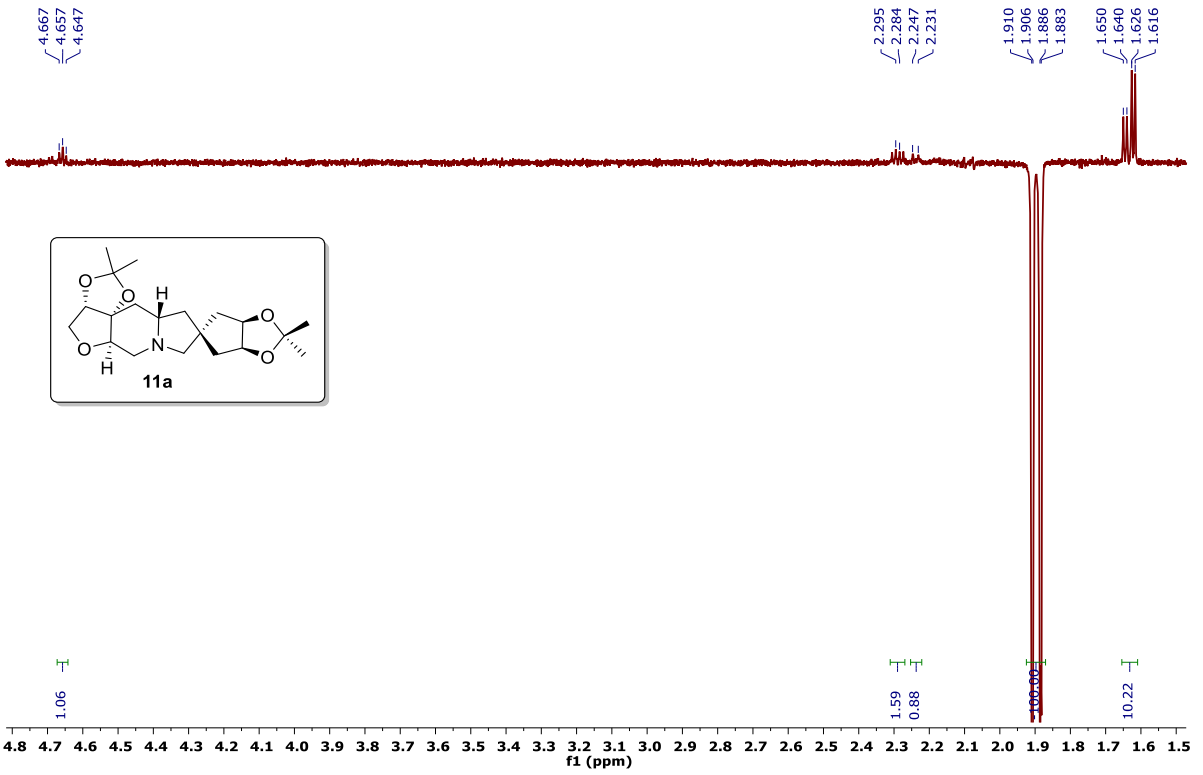
HSQCAD spectrum of compound **11a**



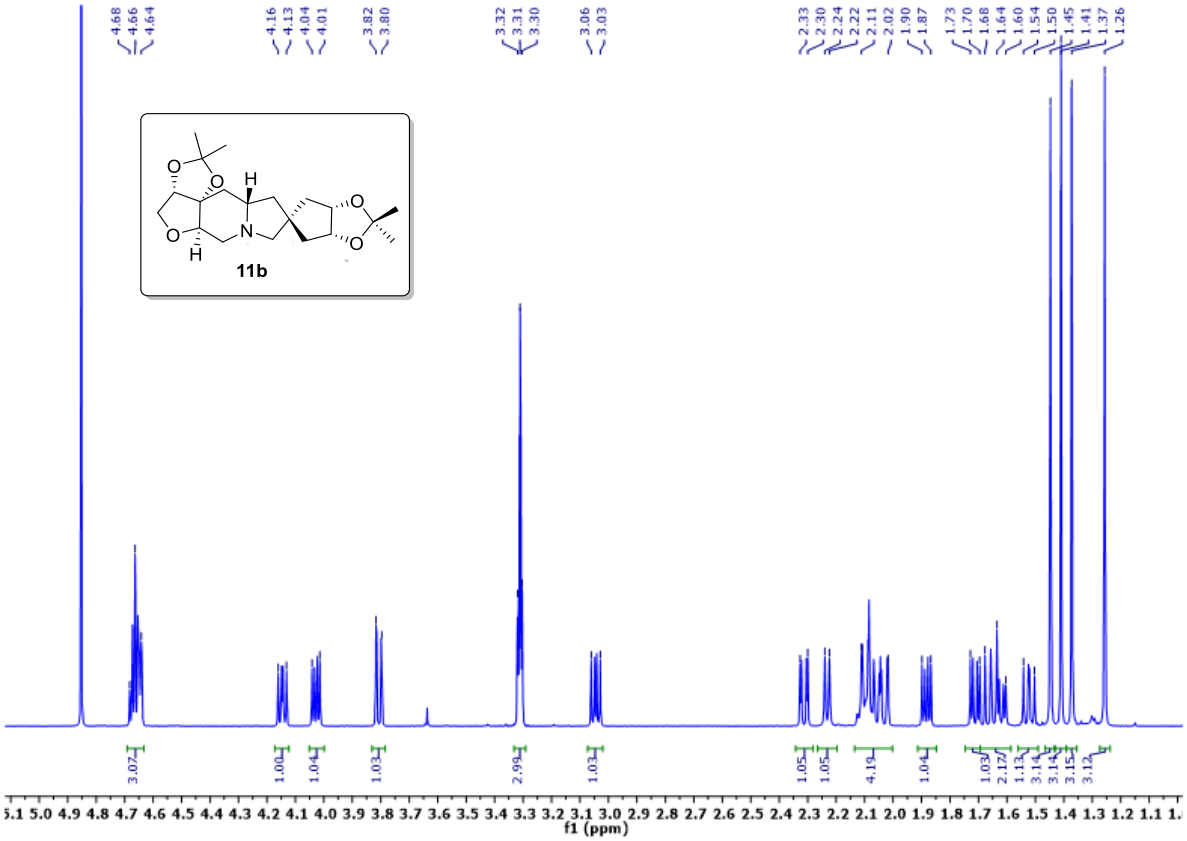
NOESY spectrum of compound **11a**



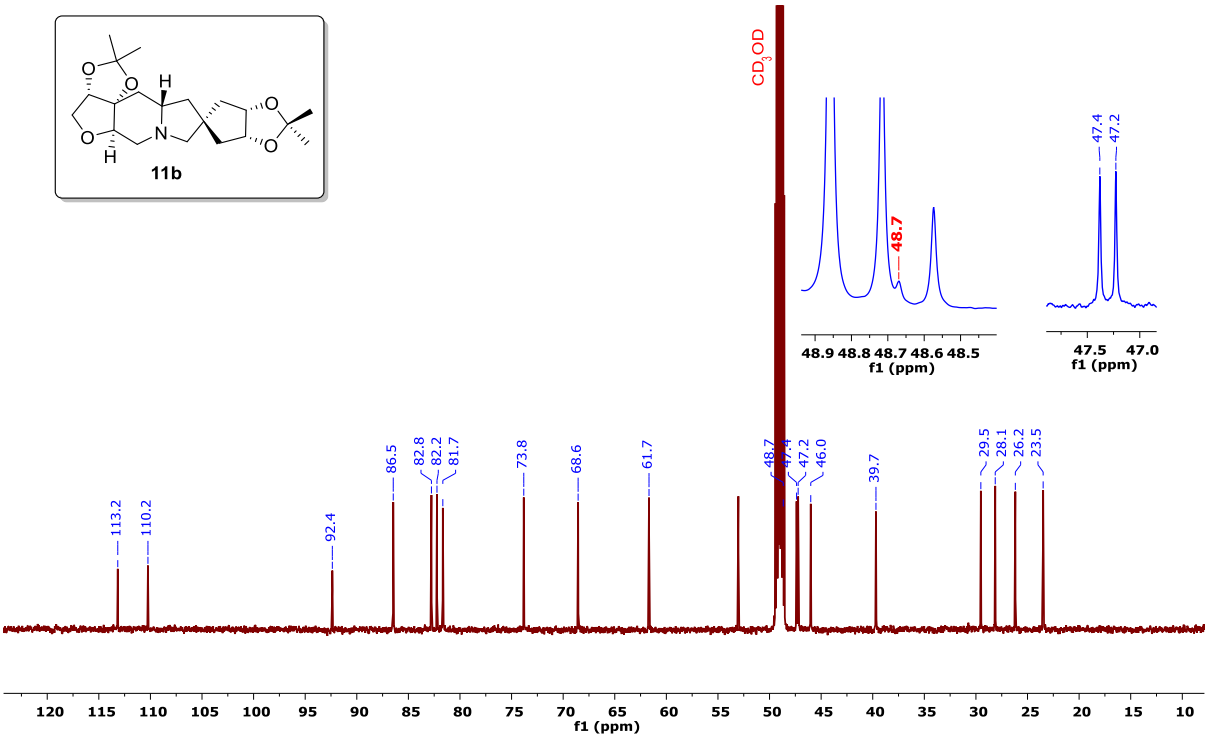
NOESY spectrum of compound **11a**



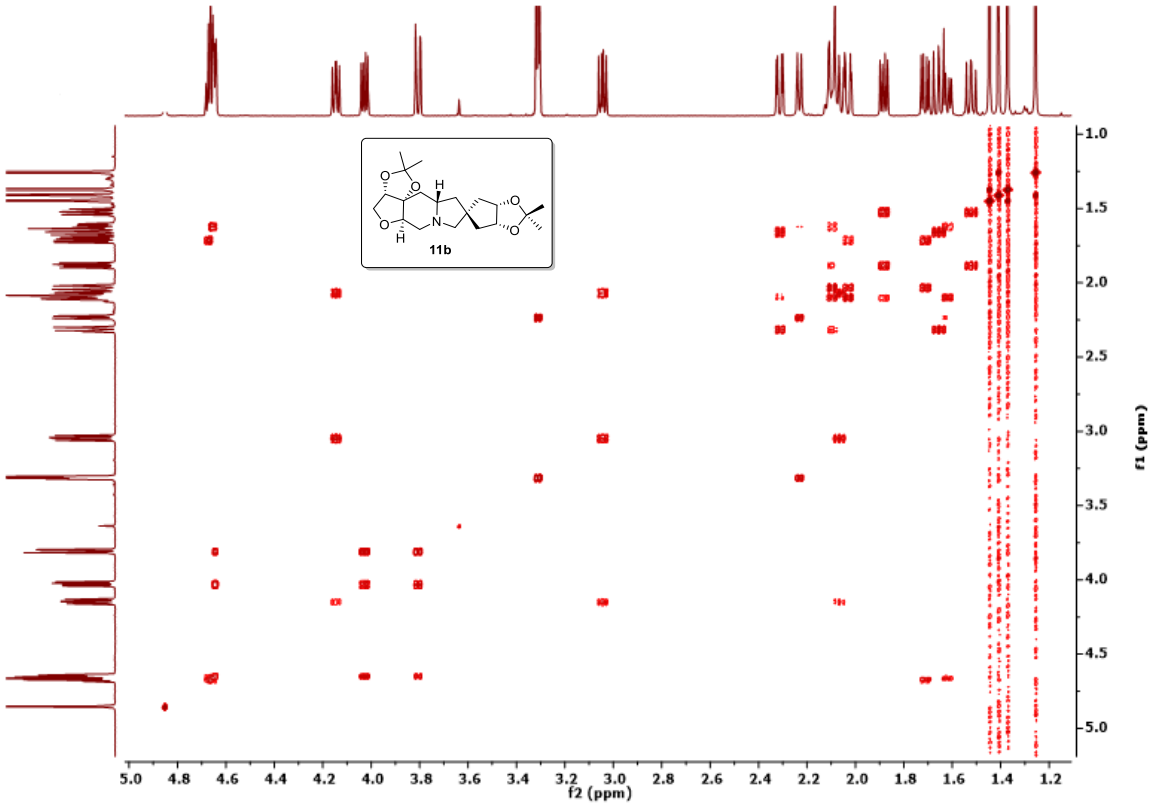
NOESY spectrum of compound **11a**



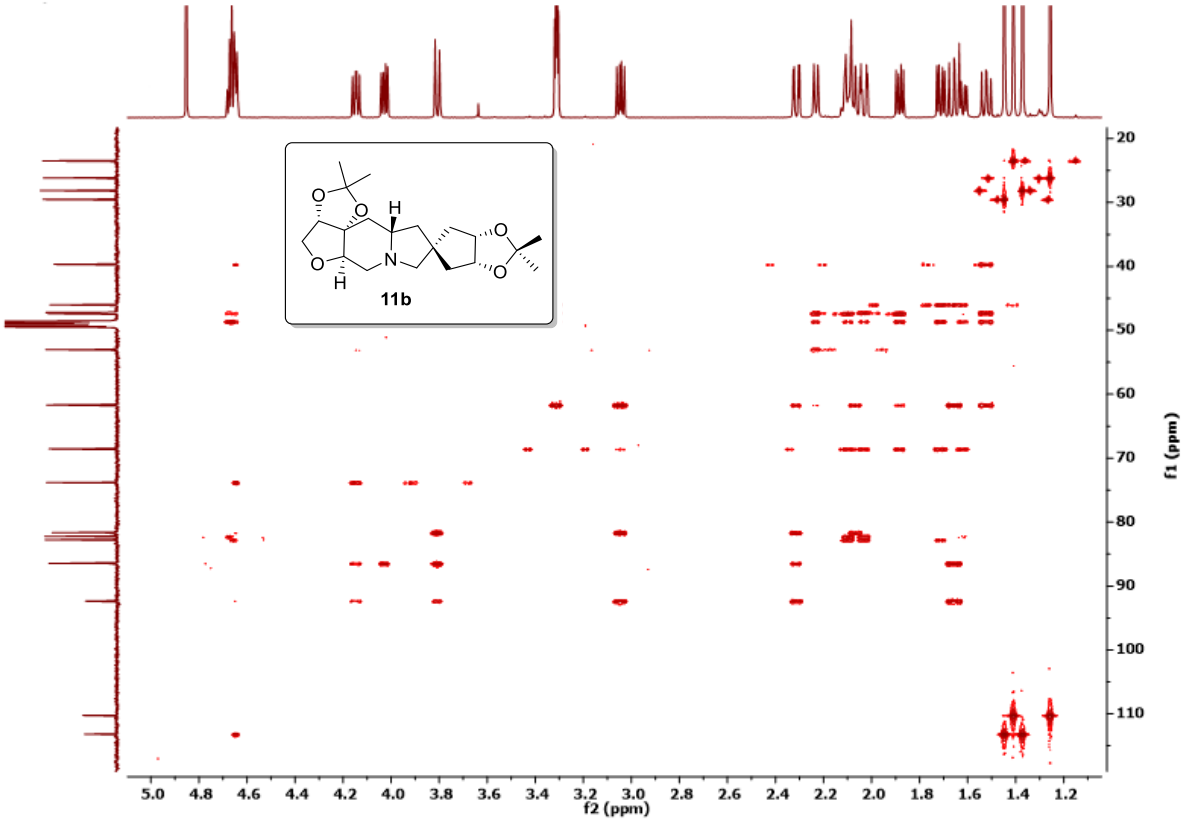
^{1}H NMR spectrum of compound **11b**



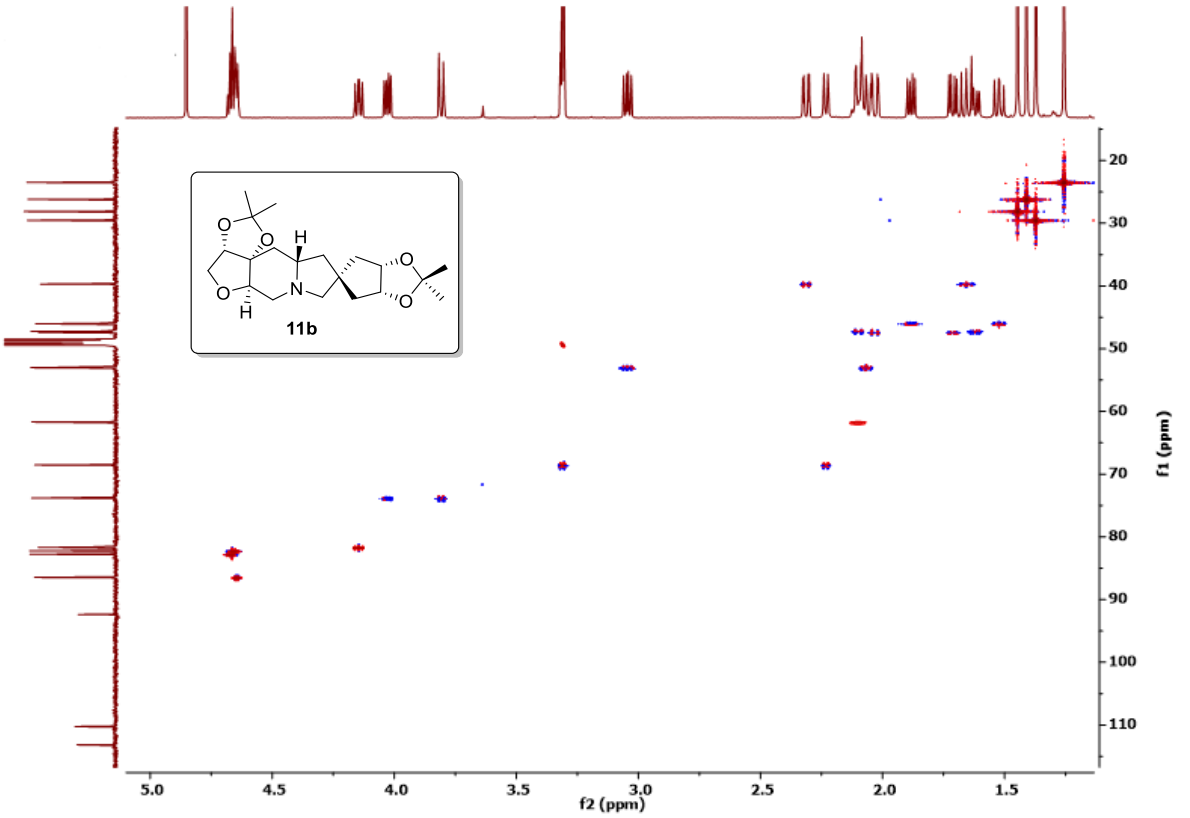
^{13}C NMR spectrum of compound **11b**



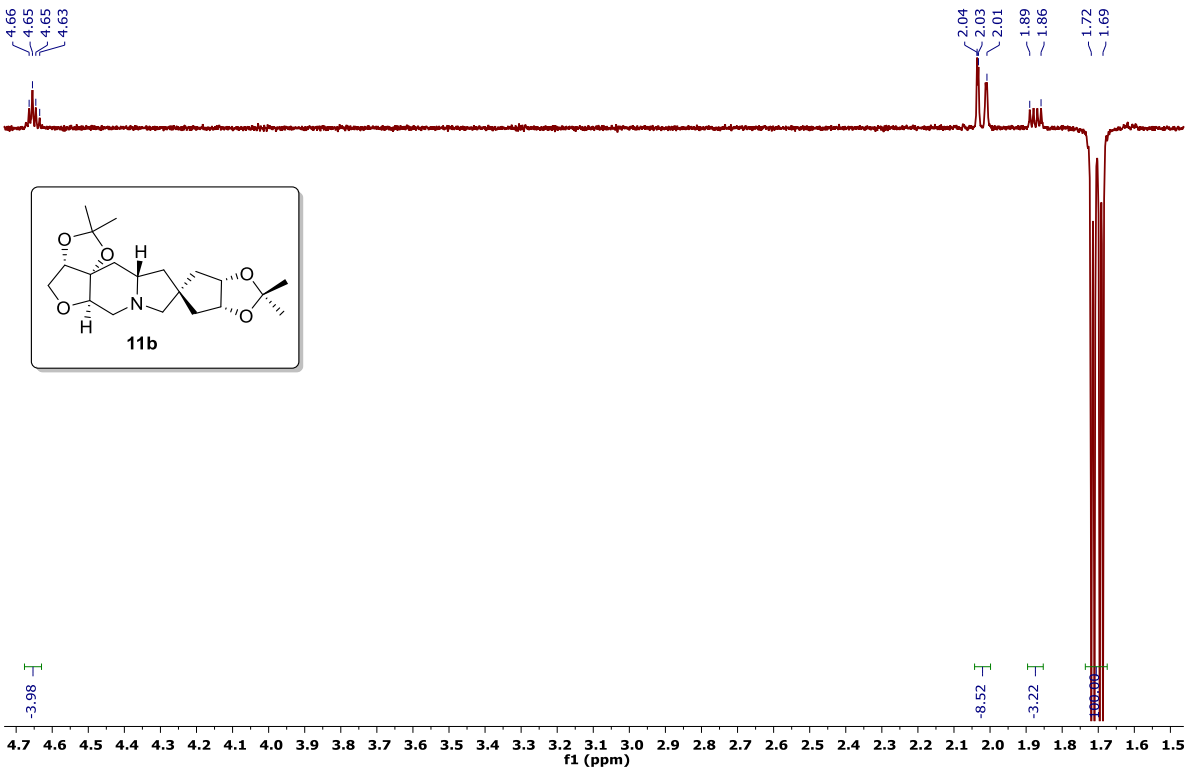
COSY spectrum of compound **11b**



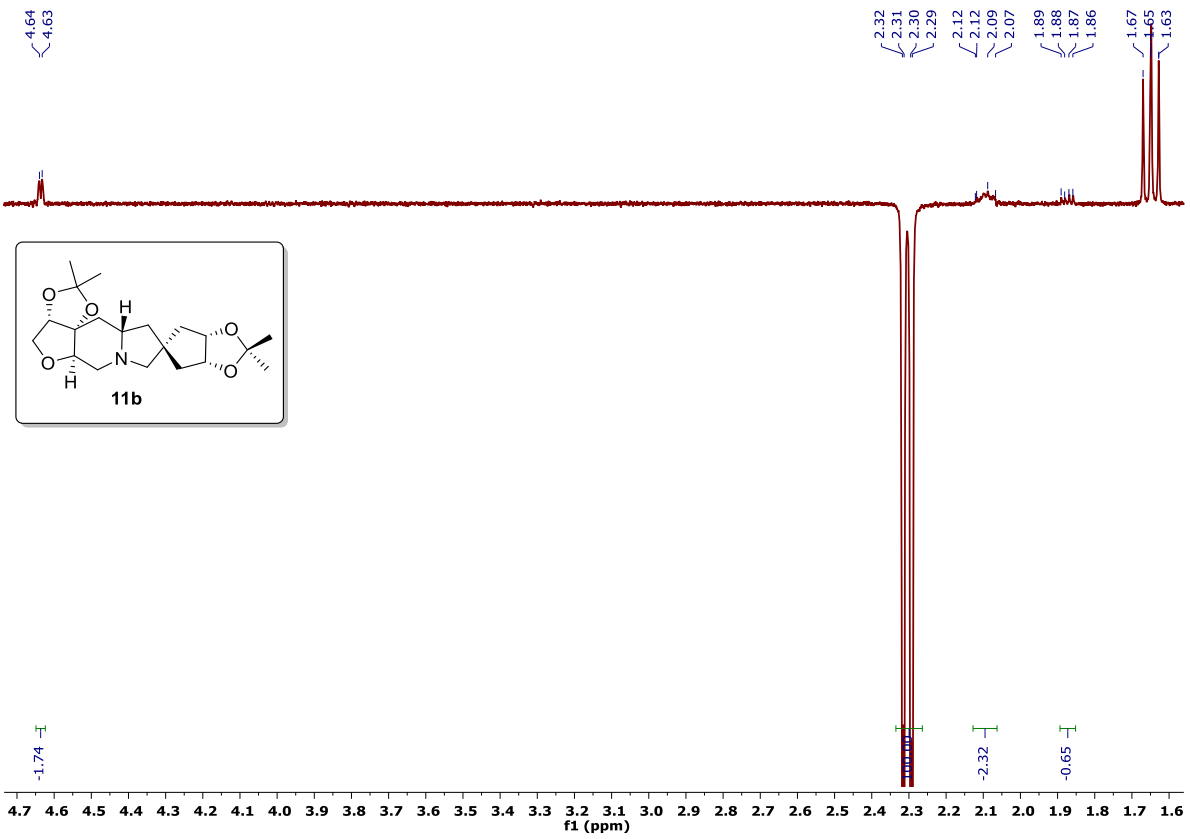
HMBCAD spectrum of compound **11b**



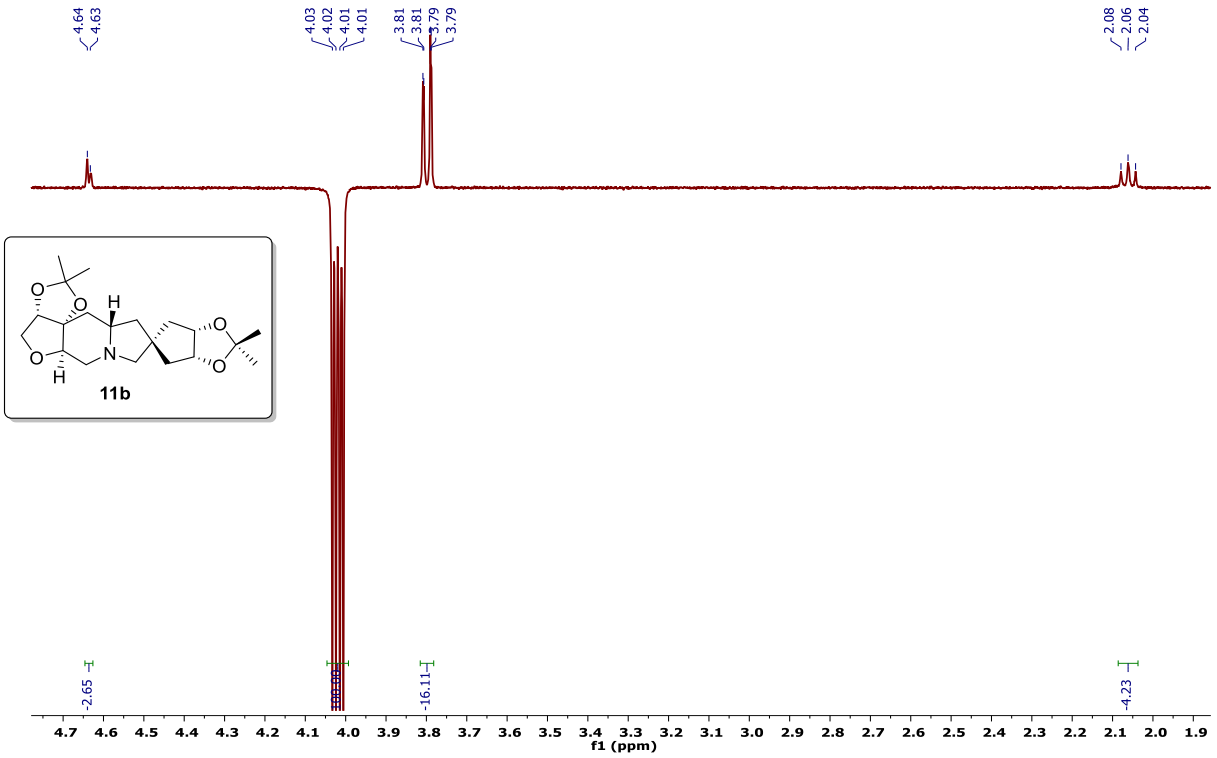
HSQCAD spectrum of compound **11b**



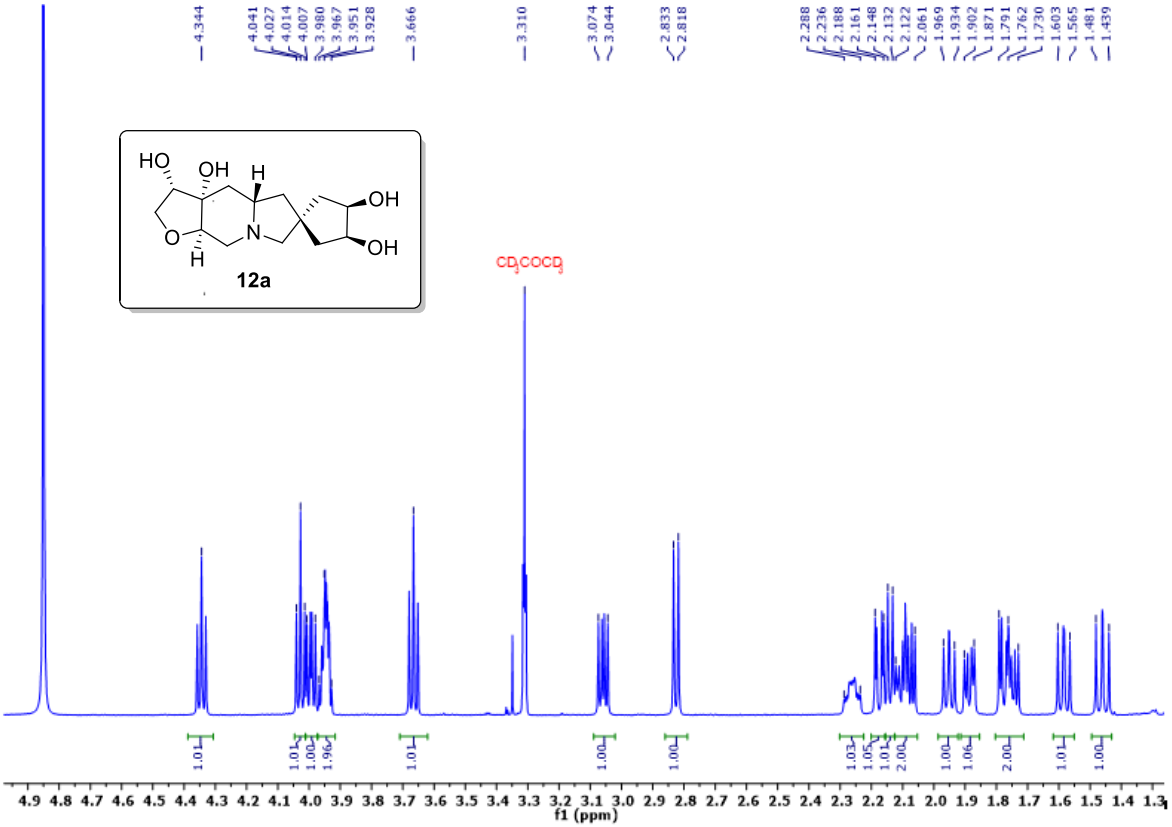
NOESY spectrum of compound **11b**



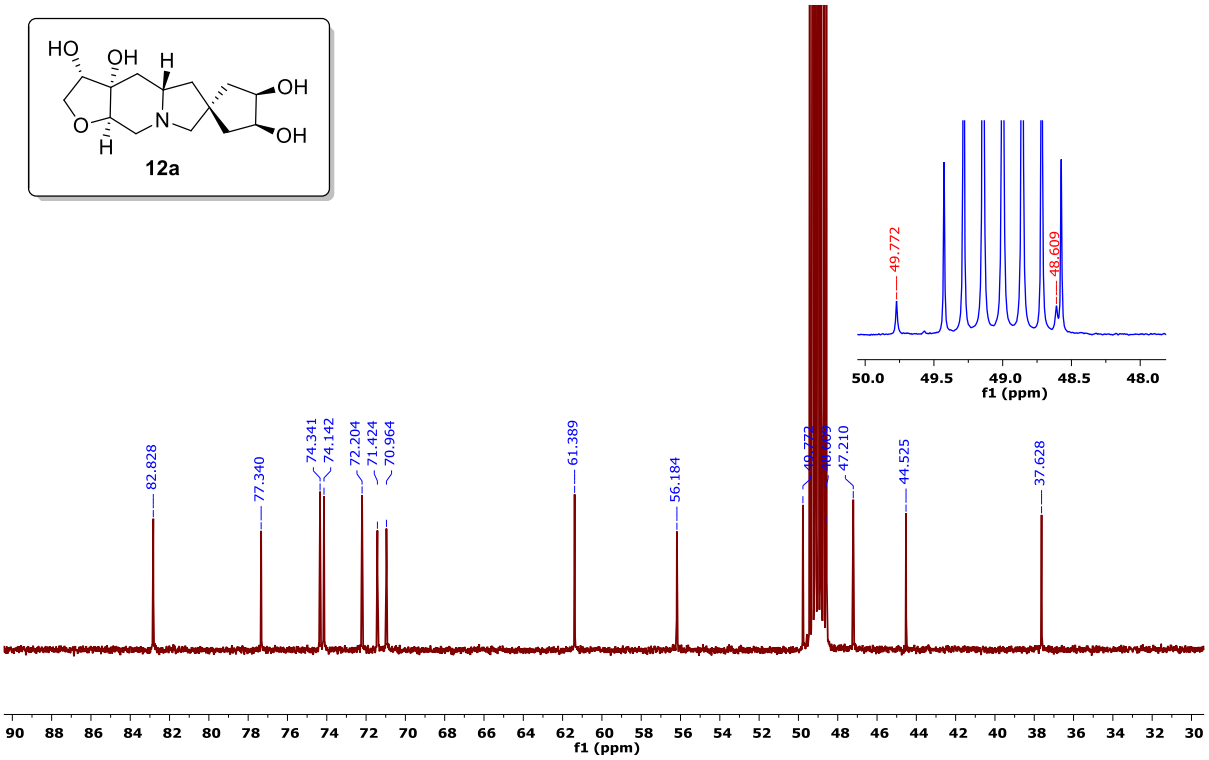
NOESY spectrum of compound **11b**



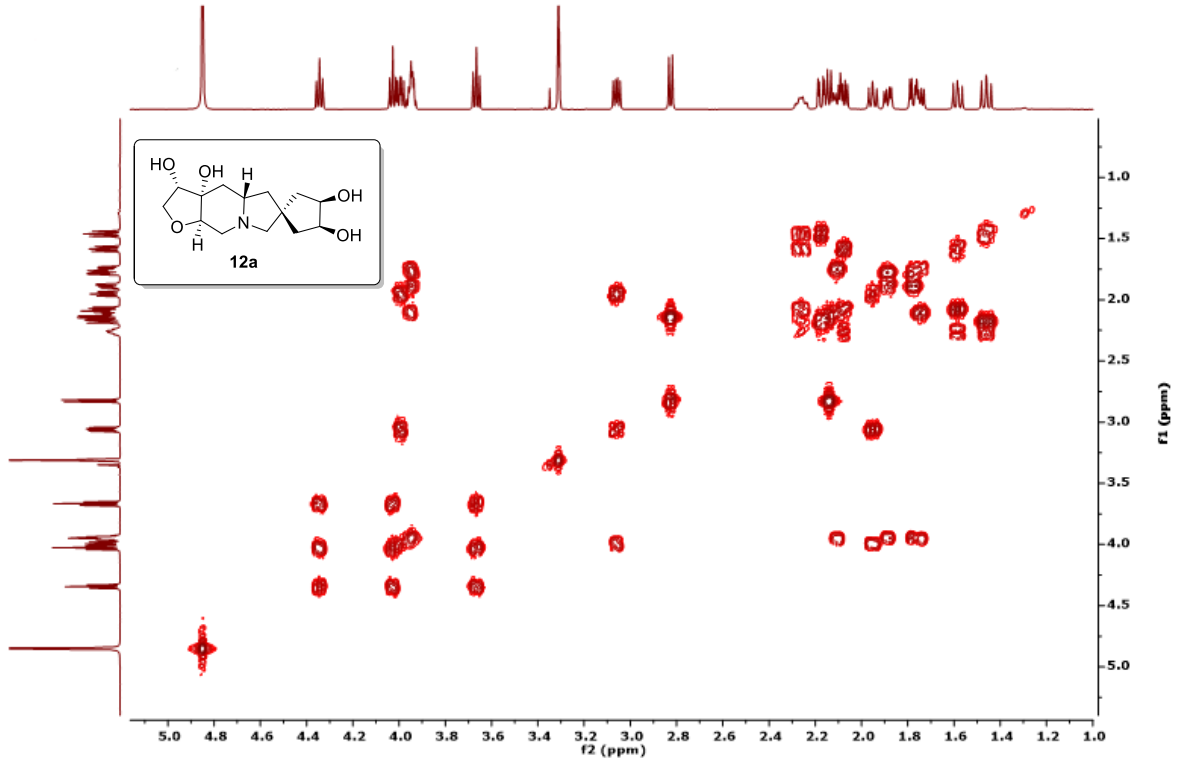
NOESY spectrum of compound **11b**



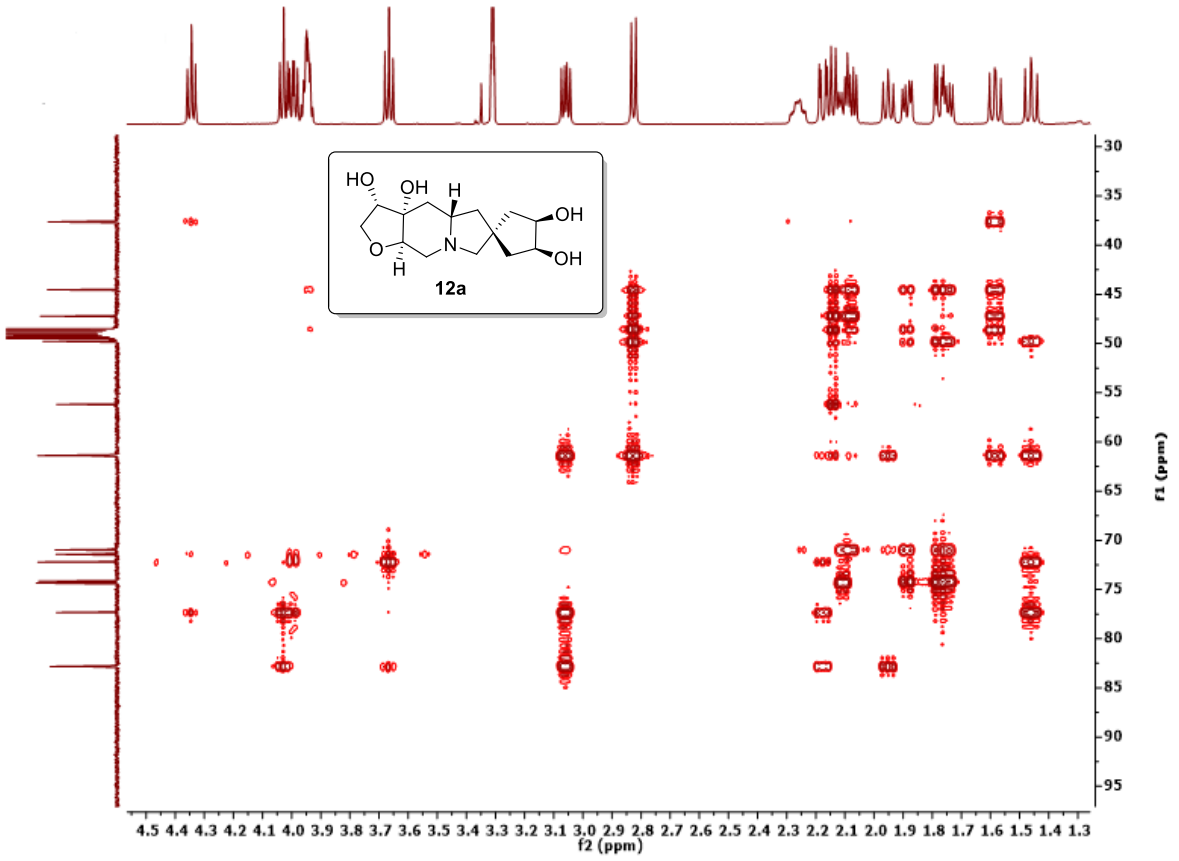
^{1}H NMR spectrum of compound **12a**



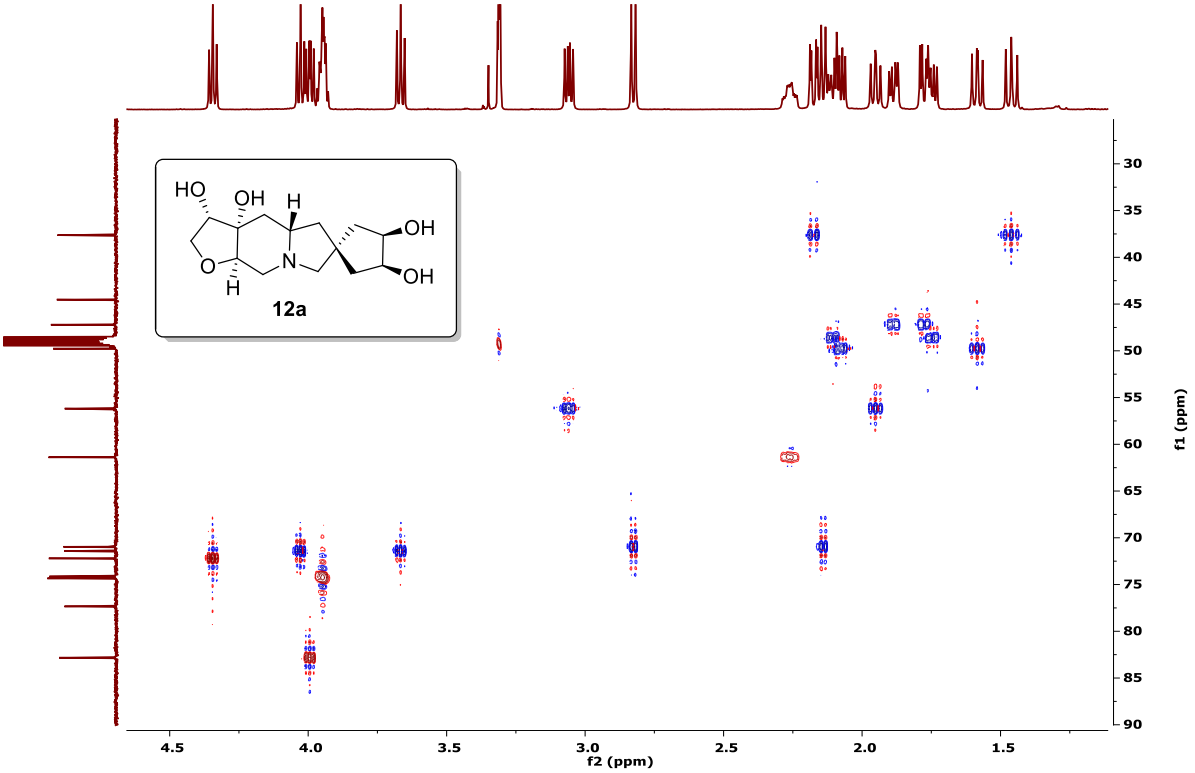
^{13}C NMR spectrum of compound **12a**



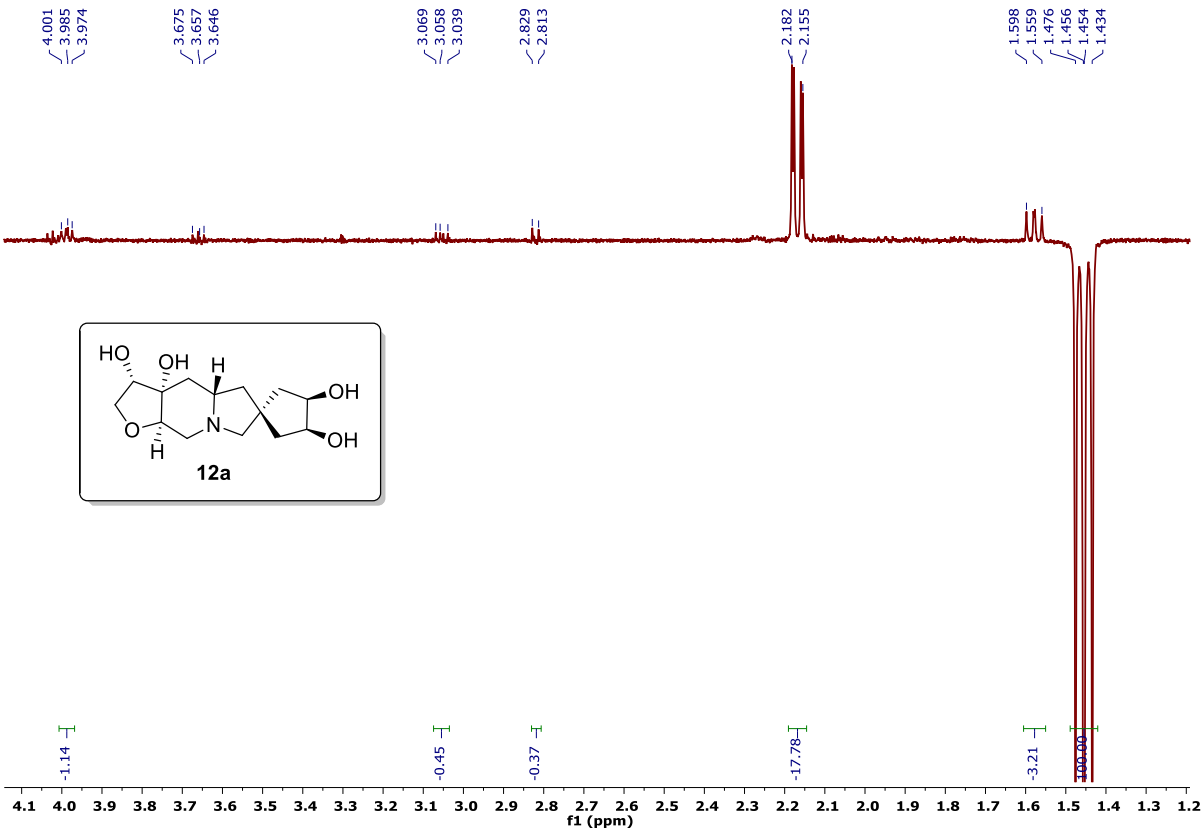
COSY spectrum of compound **12a**



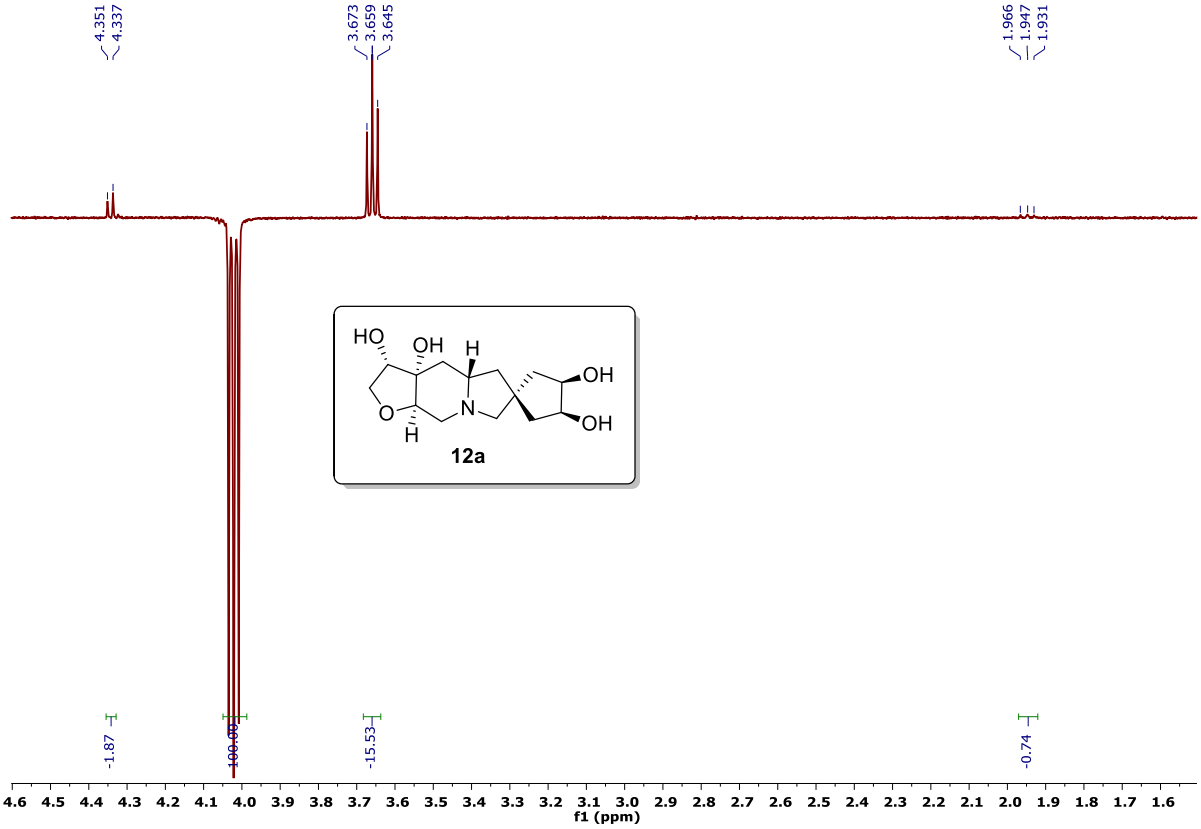
HMBCAD spectrum of compound **12a**



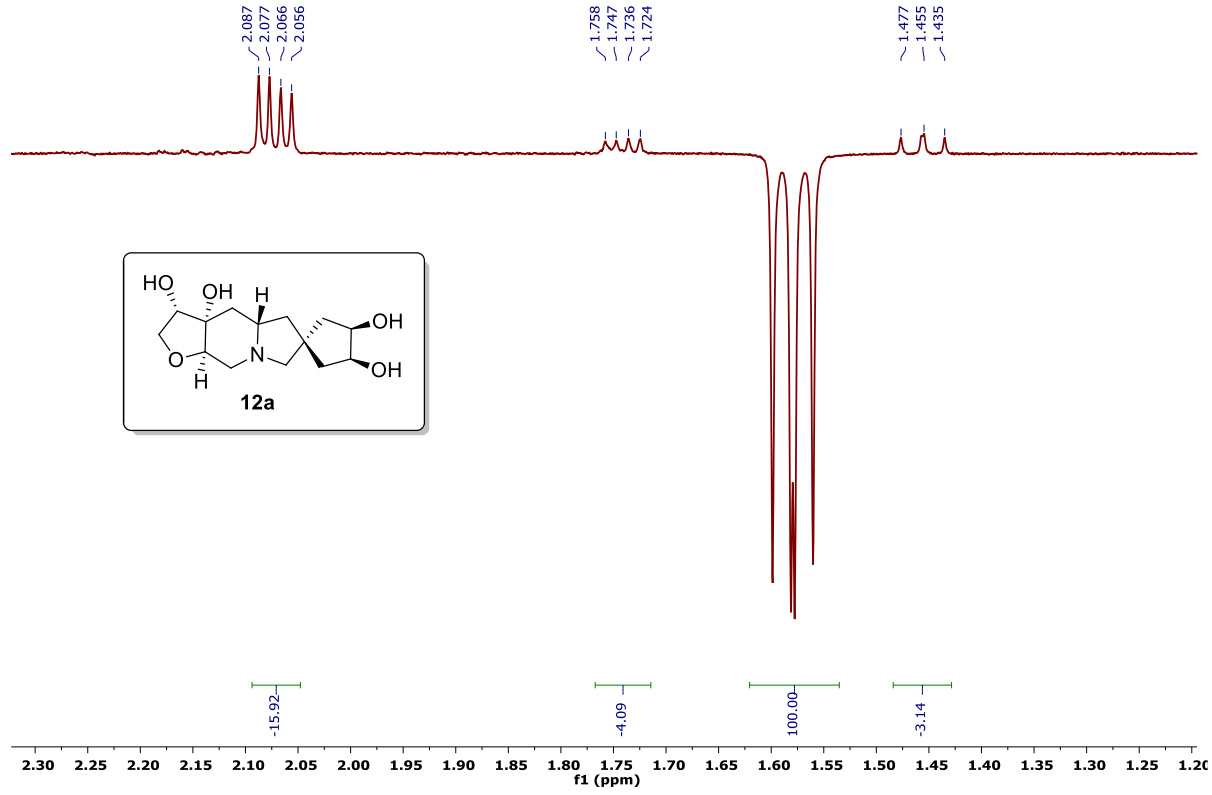
HSQCAD spectrum of compound **12a**



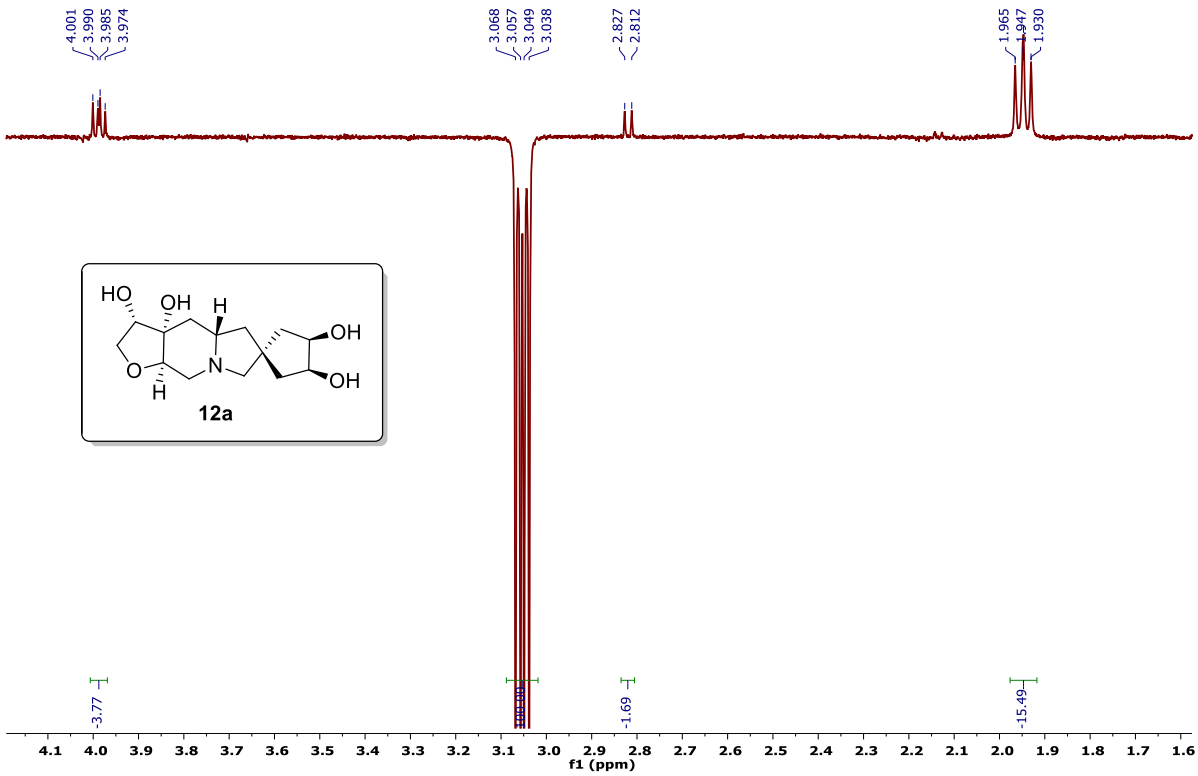
NOESY spectrum of compound **12a**



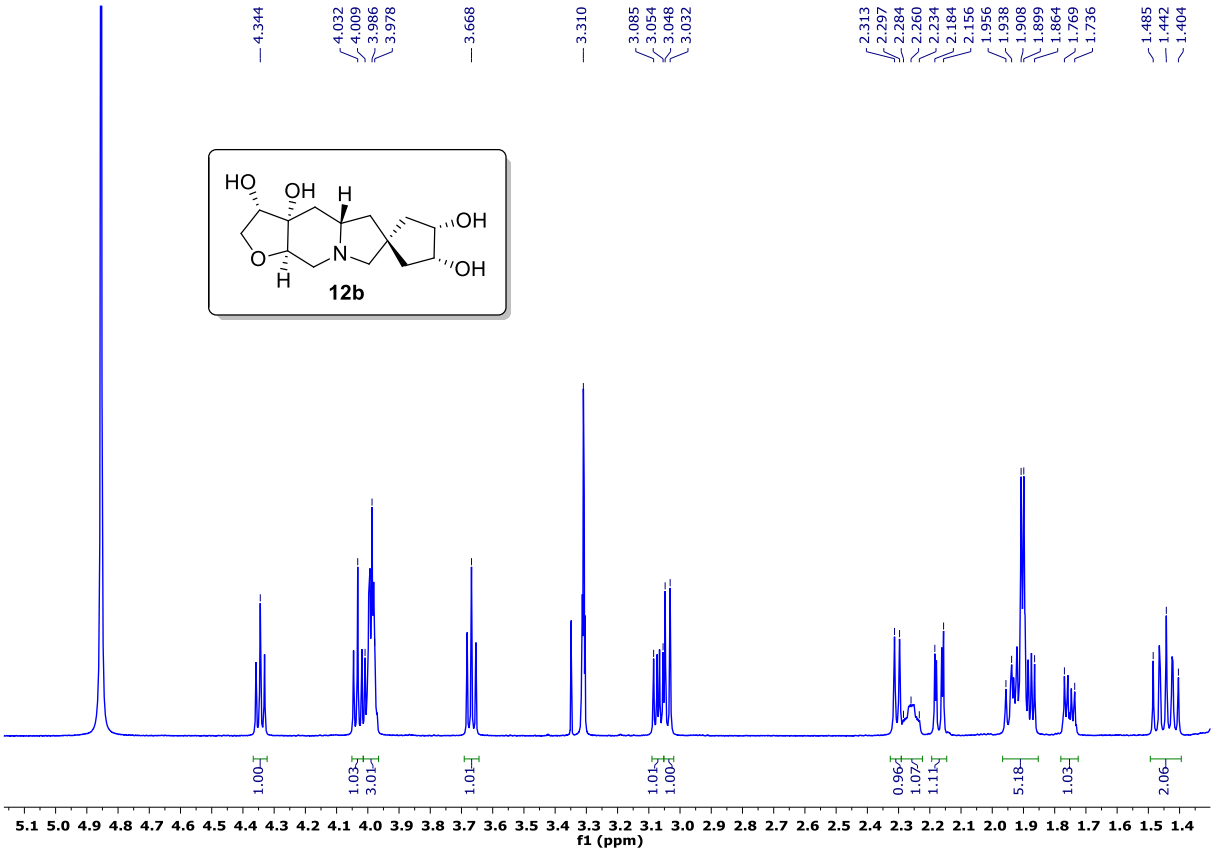
NOESY spectrum of compound **12a**



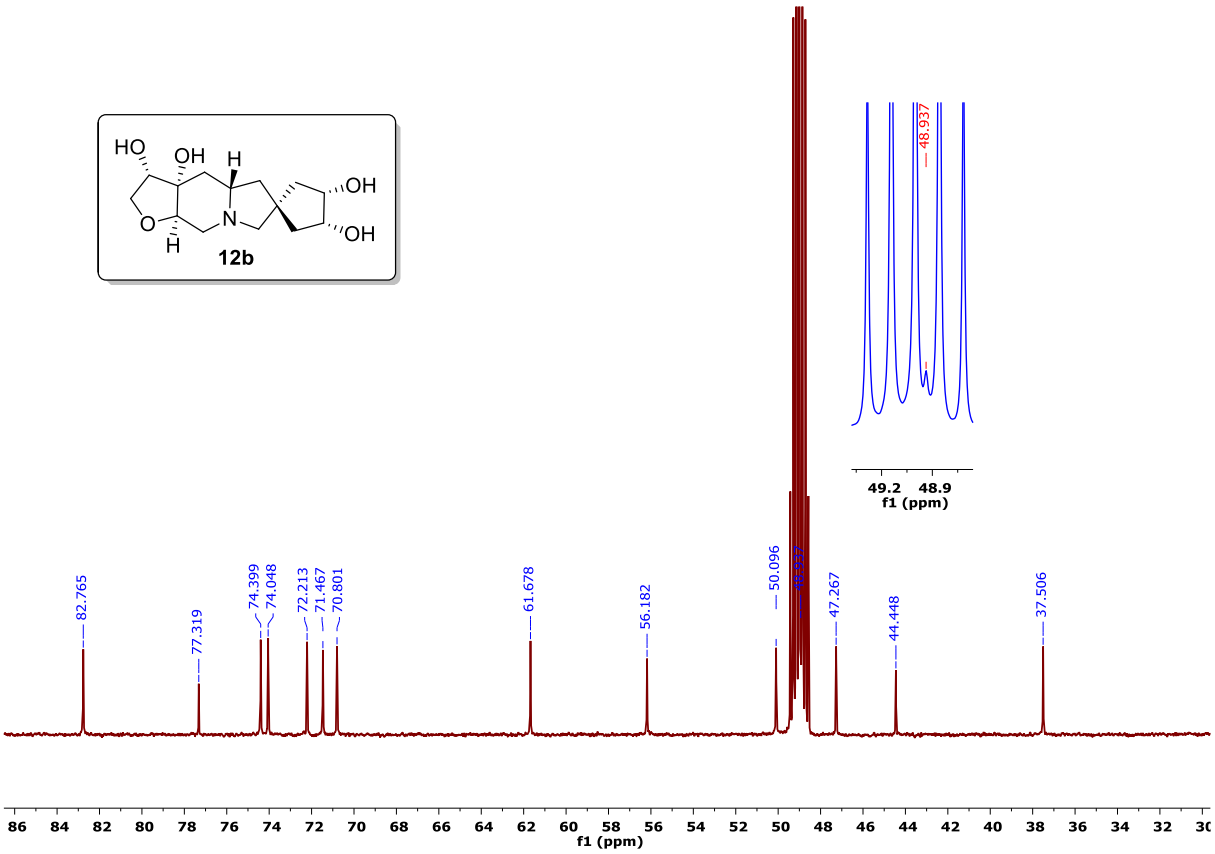
NOESY spectrum of compound **12a**



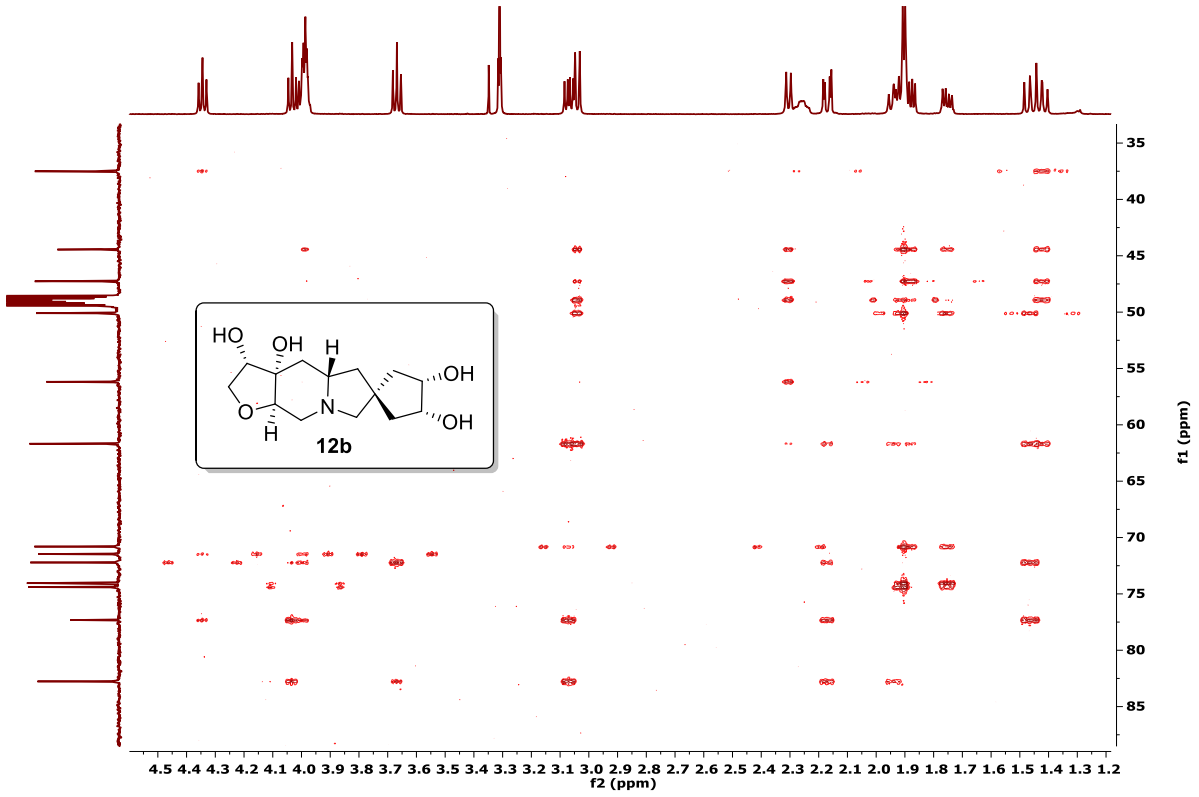
NOESY spectrum of compound **12a**



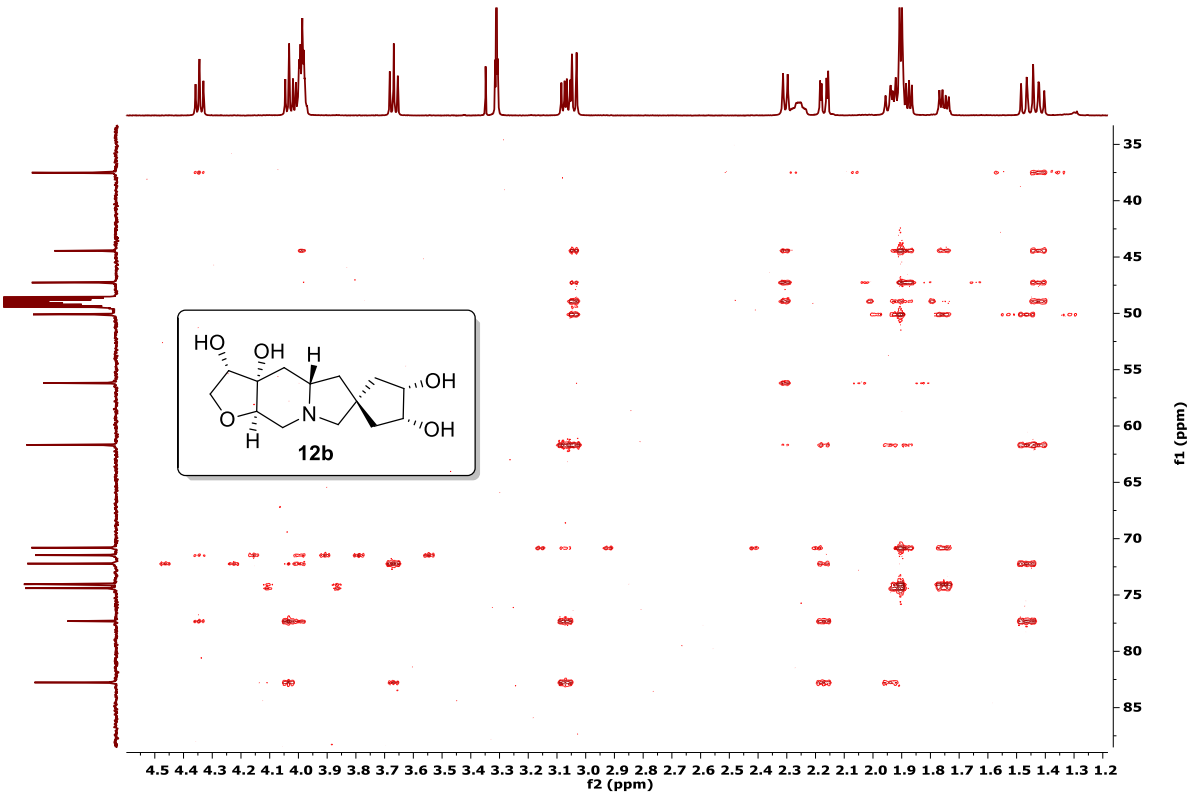
^{1}H NMR spectrum of compound **12b**



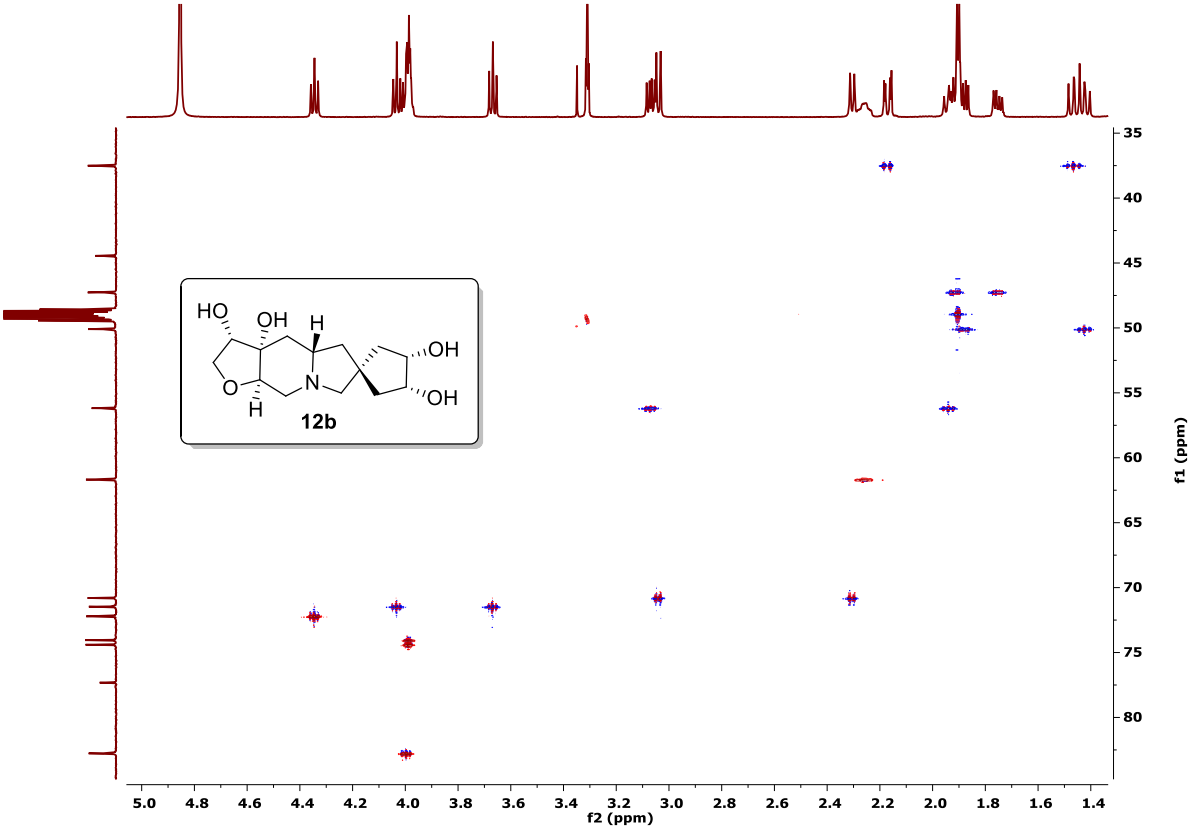
^{13}C NMR spectrum of compound **12b**



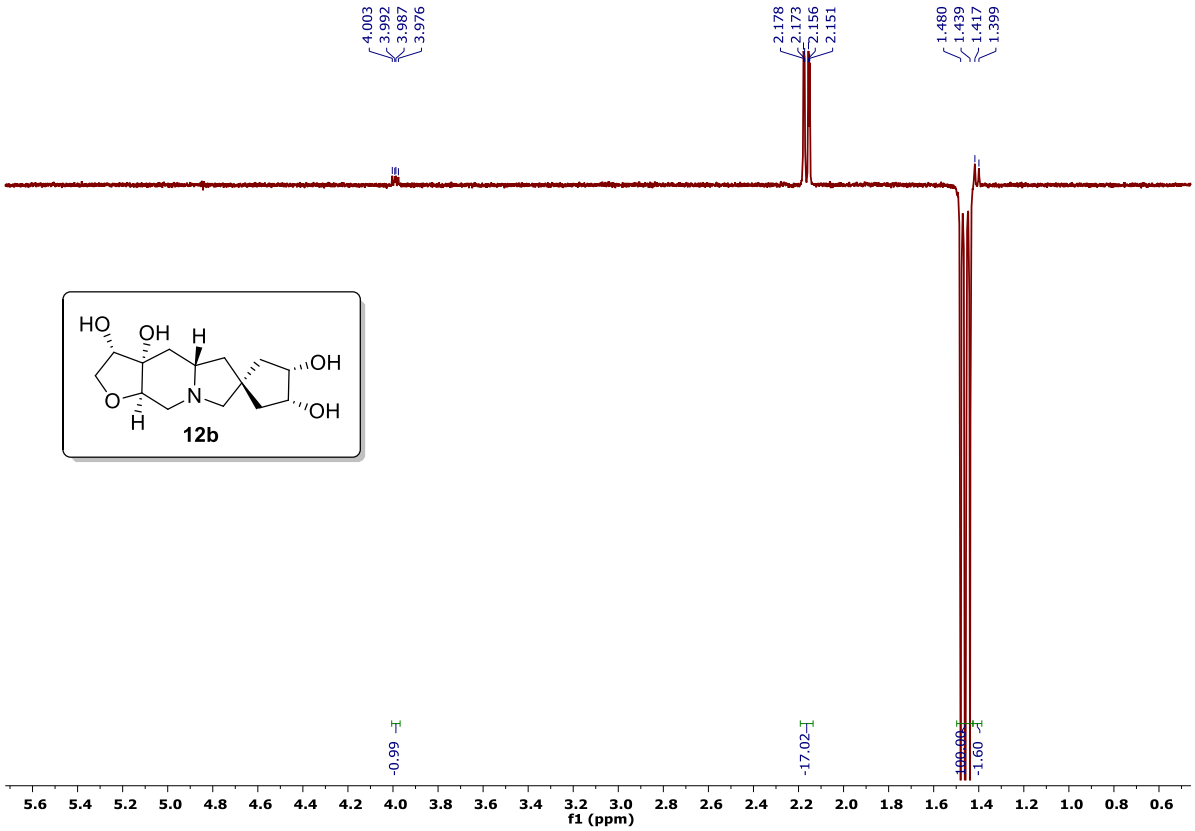
COSY spectrum of compound **12b**



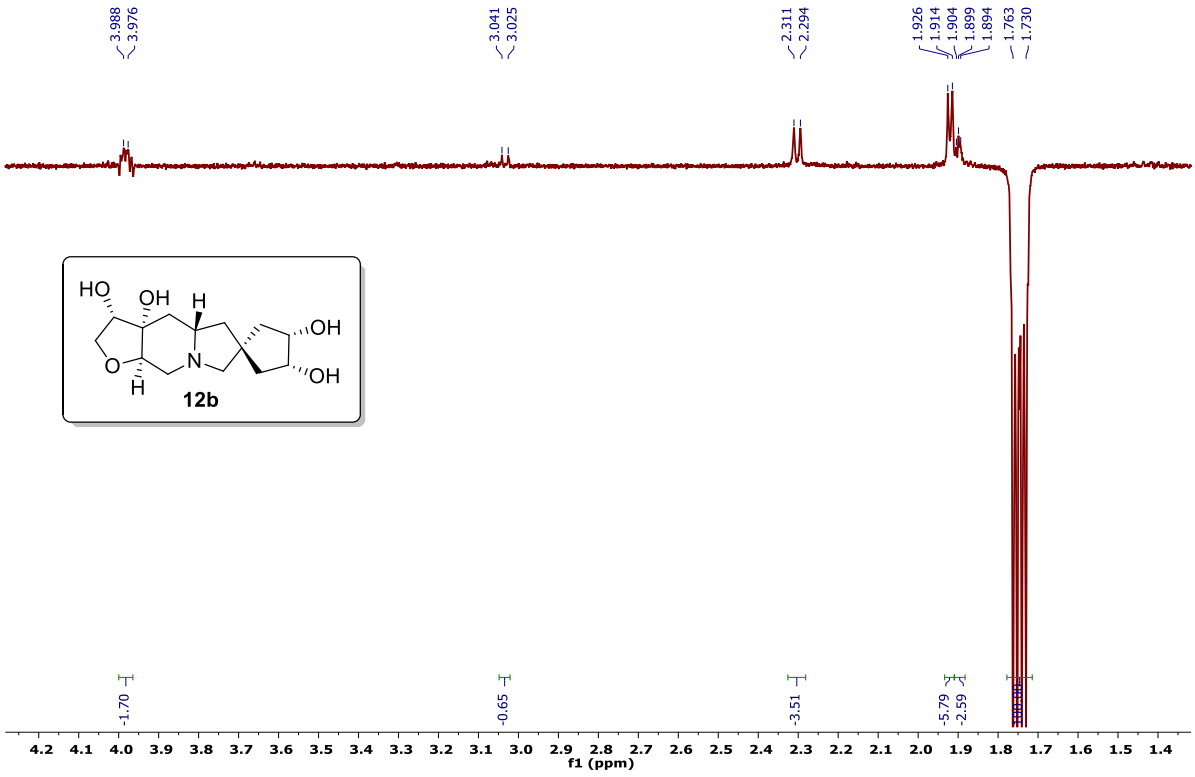
HMBCAD spectrum of compound **12b**



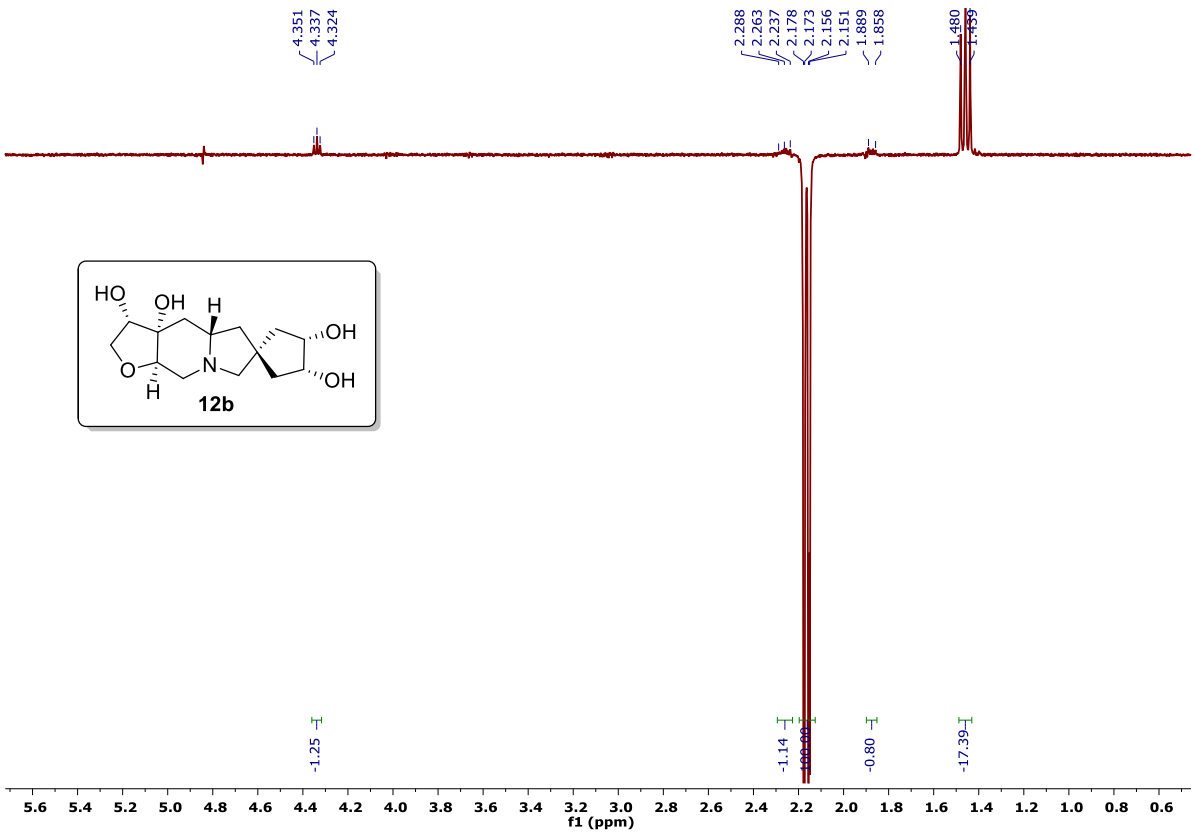
HSQCAD spectrum of compound **12b**



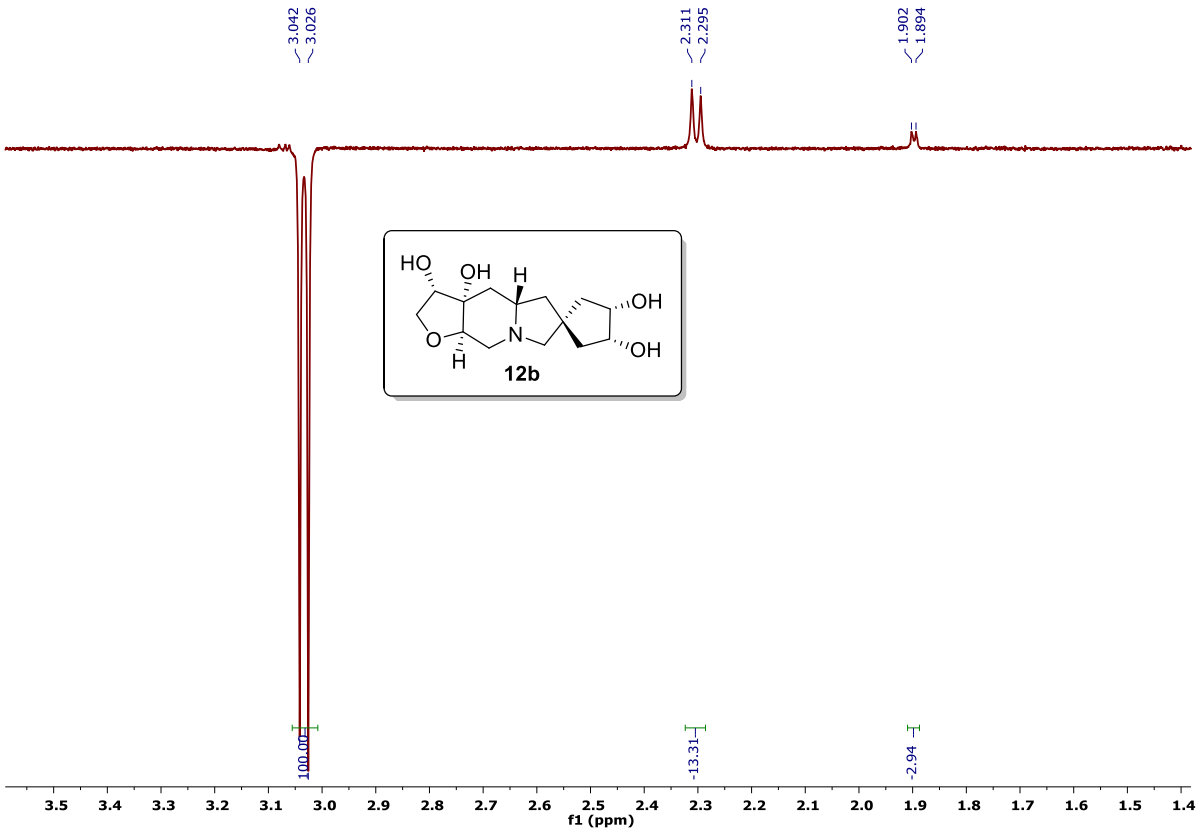
NOESY spectrum of compound **12b**



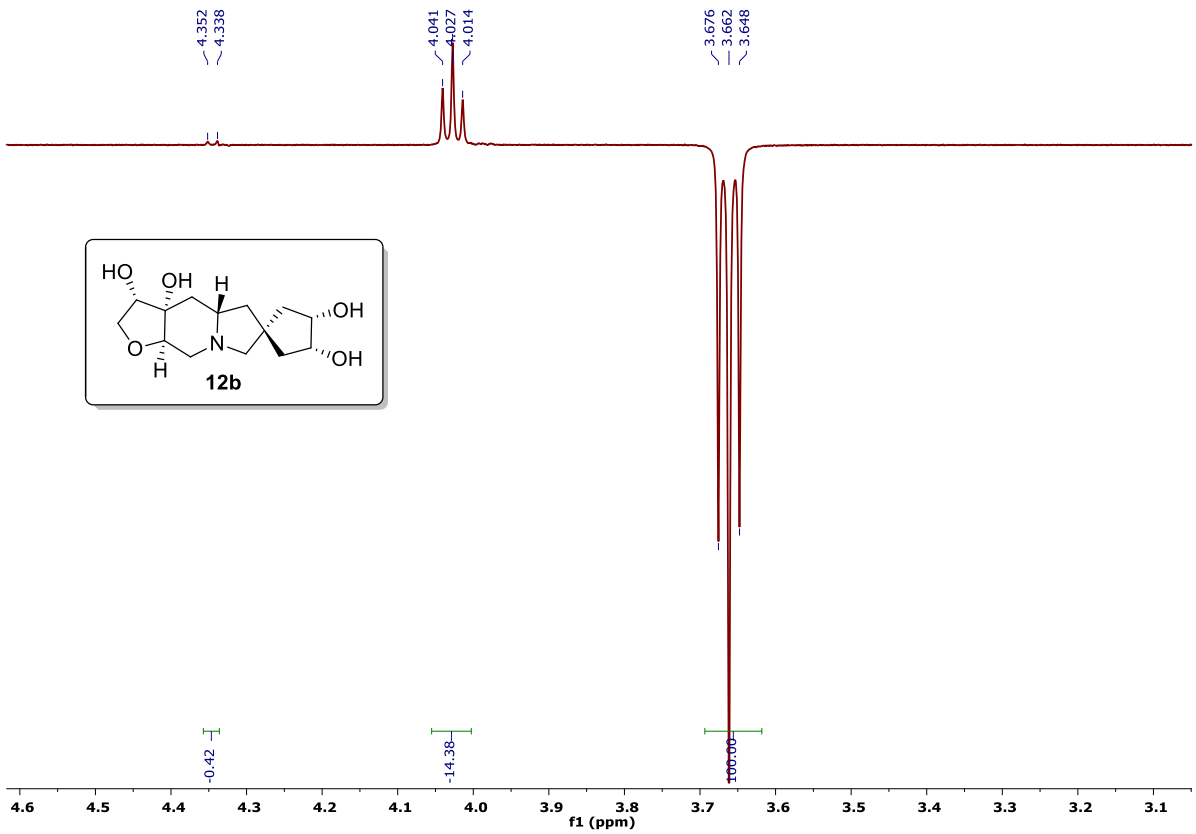
NOESY spectrum of compound **12b**



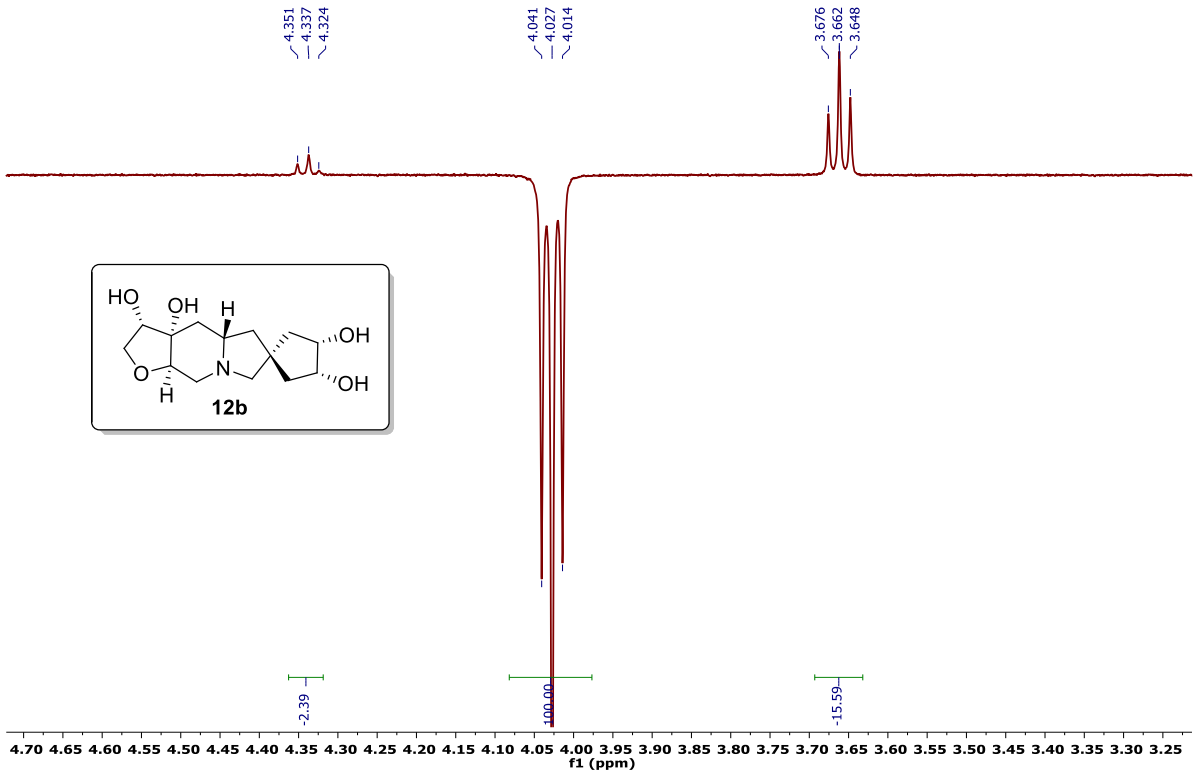
NOESY spectrum of compound **12b**



NOESY spectrum of compound **12b**



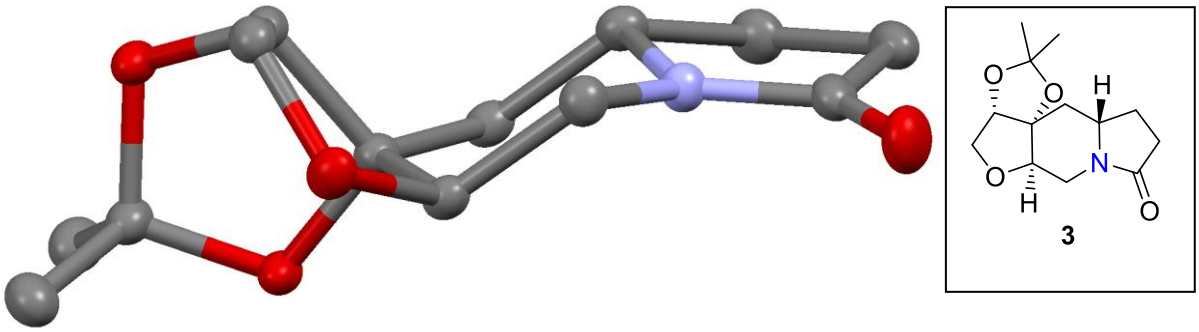
NOESY spectrum of compound **12b**



NOESY spectrum of compound **12b**

3. X-ray Crystallographic Data of compound 4a and 10b.

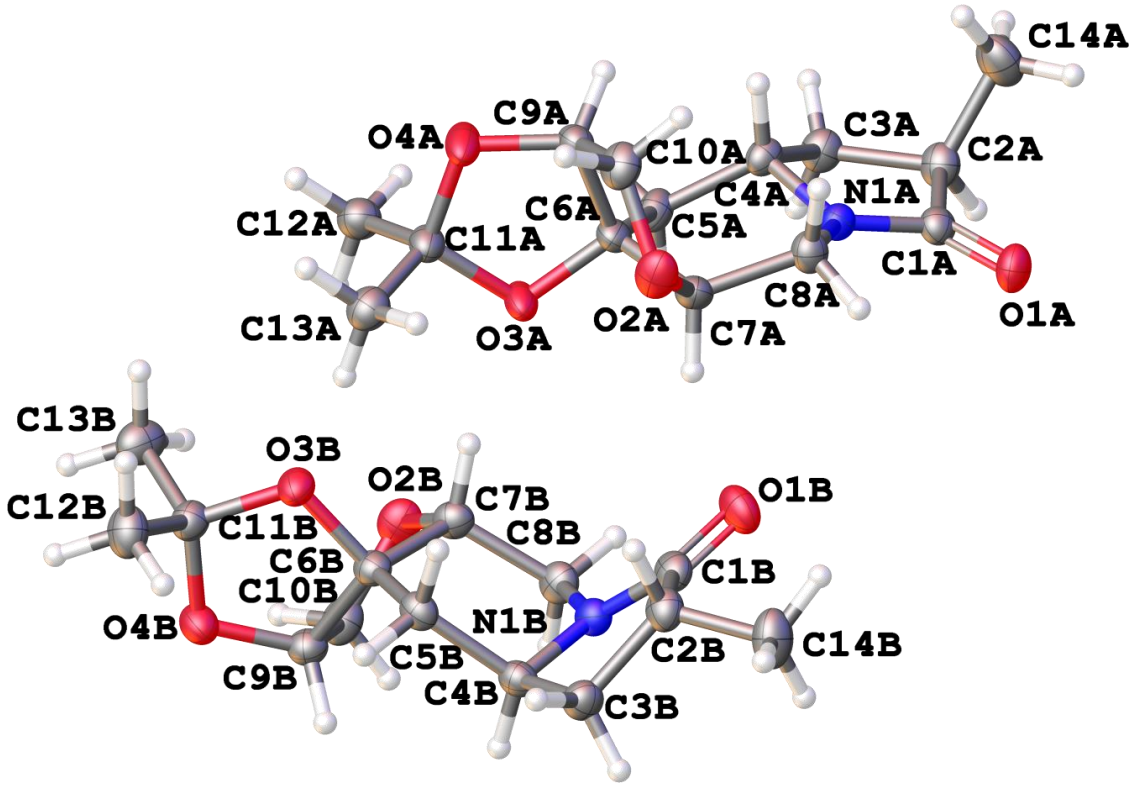
Known product 3 used in this paper.[1]



Stick plot of protected diol **3** (hydrogen atoms were omitted for clarity)[1]

Crystal data for product 4a

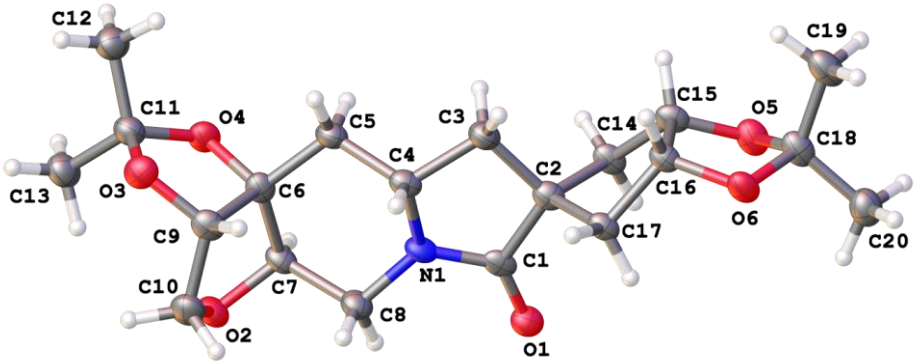
Product 4a (CCDC reference number 2070168)**:** $C_{14}H_{21}NO_4$ (M = 267.32 g/mol), orthorhombic space group $P2_12_12_1$, a = 11.1457(2), b = 19.5658(3), c = 12.5717(2)Å, V = 2741.57(8) Å^3, Z = 8, D_c = 1.295 g/cm^3, μ = 0.777 mm^{-1}, N_{ref} = 5314, R_1 = 0.0336[$I > 2\sigma(I)$] and wR_2 = 0.0861, N_{par} = 349, S = 1.027 for all 61940 reflections, Data completeness = 0.999.[2]

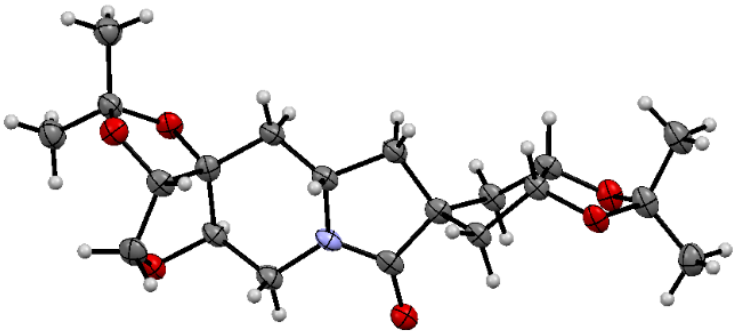


ORTEP plot of **4a**.

Crystal data for product 10b

Product 10b (CCDC reference number 2070169)**:** $C_{20}H_{29}NO_6$ (M = 379.44 g/mol), monoclinic space group $P2_1$, a = 6.5826(2), b = 9.0483(1), c = 16.3477(4) Å, β = 98.638(2)°. V = 962.65(4) Å^3, Z = 2, D_c = 1.308 g/cm^3, μ = 0.792 mm^{-1}, N_{ref} = 3471, R_1 = 0.0893 [$I > 2\sigma(I)$] and wR_2 = 0.2477, N_{par} = 248, S = 1.165 for all 36055 reflections. Data completeness = 0.999.[2]





Or

ORTEP plot of **10b**.

---

1 P. Šafář, Š. Marchalín, M. Cvečko, J. Moncol, V. Dujnič, M. Šoral and A. Daïch, *Org. Biomol. Chem.*, **2020**, *18*, 6384–6393.

2 Crystal structure determination of compounds **4a** and **10b** was accomplished on a StadiVari four-circle diffractometer by Stoe & Cie GmbH using a Pilatus3 R 300K HPC detector by Dectris Ltd. X-ray radiation (Cu-Kα, λ = 1.54186 Å) was generated by microfocus sources Xenocs Genix3D Cu HF with graded multilayer mirror optic. Using Olex2 the structures were solved with the Sir14 or ShelXT structure solution programs and refined with ShelXL (ver. 2018/3) against F^2 with the full-matrix least squares method.[3] The non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in geometrically calculated positions and each was assigned a fixed isotropic displacement parameter based on a riding model. Absolute structure of compound **4a** were confirmed by Parsons (x = 0.09(7)) and Hooft (y = 0.07(3)) methods, and for compound **10b** using only Hooft (y = -0.06(3)) method.[4]

3 (a) O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, **2009**, *42*, 339–341. (b) G. M. Sheldrick, *Acta Crystallogr.*, **2015**, *A71*, 3–8; (c) M. C. Burla, R. Caliandro, B. Carrozzini, G. L. Cascarano, C. Cuocci, C. Giacovazzo, M. Mallamo, A. Mazzone, G. Polidori and R. Spagna, *J. Appl. Crystallogr.*, **2015**, *48*, 306–309; (d) G. M. Sheldrick, *Acta Crystallogr.*, **2015**, *C71*, 3–8.

4 (a) S. Parsons, H. D. Flack and T. Wagner, *Acta Crystallogr.*, **2013**, *B69*, 249–259; (b) R. W. Hooft, L. H. Straver and A. L. Spek, *J. Appl. Crystallogr.*, **2008**, *41*, 96–103.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4a and 10b

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 4a

```
Bond precision:  C-C = 0.0030 A          Wavelength=1.54186

Cell:            a=11.1457(2)     b=19.5658(3)     c=12.5717(2)
                 alpha=90         beta=90          gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	2741.57(8)	2741.57(8)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C14 H21 N O4	C14 H21 N O4
Sum formula	C14 H21 N O4	C14 H21 N O4
Mr	267.32	267.32
Dx,g cm-3	1.295	1.295
Z	8	8
Mu (mm-1)	0.777	0.777
F000	1152.0	1152.0
F000'	1155.69	
h,k,lmax	13,24,15	13,23,14
Nref	5409[3052]	5314
Tmin,Tmax	0.823,0.969	0.283,0.814
Tmin'	0.823	

```
Correction method= # Reported T Limits: Tmin=0.283 Tmax=0.814
AbsCorr = MULTI-SCAN

Data completeness= 1.74/0.98      Theta(max)= 72.139

R(reflections)= 0.0336( 5082)     wR2(reflections)= 0.0861( 5314)

S = 1.027                 Npar= 349
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level G

```
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O2A           105.9 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O2B           106.3 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O4B           109.8 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....            12 Note
PLAT791_ALERT_4_G Model has Chirality at C2A         (Sohnke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at C2B         (Sohnke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at C4A         (Sohnke SpGr)        S Verify
PLAT791_ALERT_4_G Model has Chirality at C4B         (Sohnke SpGr)        S Verify
PLAT791_ALERT_4_G Model has Chirality at C6A         (Sohnke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at C6B         (Sohnke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at C7A         (Sohnke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at C7B         (Sohnke SpGr)        R Verify
PLAT791_ALERT_4_G Model has Chirality at C9A         (Sohnke SpGr)        S Verify
PLAT791_ALERT_4_G Model has Chirality at C9B         (Sohnke SpGr)        S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        17 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        11 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  16 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Datablock: 10b

```
Bond precision:  C-C = 0.0073 A          Wavelength=1.54186

Cell:            a=6.5826(2)     b=9.0483(1)         c=16.3477(4)
                 alpha=90        beta=98.638(2)      gamma=90
Temperature:     100 K
```

	Calculated	Reported
Volume	962.65(4)	962.65(4)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C20 H29 N O6	C20 H29 N O6
Sum formula	C20 H29 N O6	C20 H29 N O6
Mr	379.44	379.44
Dx,g cm-3	1.309	1.309
Z	2	2
Mu (mm-1)	0.792	0.792
F000	408.0	408.0
F000'	409.32	
h,k,lmax	8,11,20	8,11,19
Nref	3772[2013]	3471
Tmin,Tmax	0.835,0.939	0.163,0.808
Tmin'	0.820	

Correction method= # Reported T Limits: Tmin=0.163 Tmax=0.808
AbsCorr = MULTI-SCAN

Data completeness= 1.72/0.92 Theta(max)= 71.914

R(reflections)= 0.0893(3399) wR2(reflections)= 0.2477(3471)

S = 1.165 Npar= 248

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 0.80 eA-3
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00728 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C20 H29 N O6
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 14.96 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.96A From O1 0.54 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.95A From O1 0.50 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.83A From O2 0.47 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.96A From O6 -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H17A -0.36 eA-3

Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.500 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.18 Report
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O2 106.5 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O3 109.0 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O5 107.3 Degree

```
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O6             107.4 Degree
PLAT791_ALERT_4_G Model has Chirality at C4          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C6          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C7          (Sohnke SpGr)          R Verify
PLAT791_ALERT_4_G Model has Chirality at C9          (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C15         (Sohnke SpGr)          S Verify
PLAT791_ALERT_4_G Model has Chirality at C16         (Sohnke SpGr)          R Verify
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          7 Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.20 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          5 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  17 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  14 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   9 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

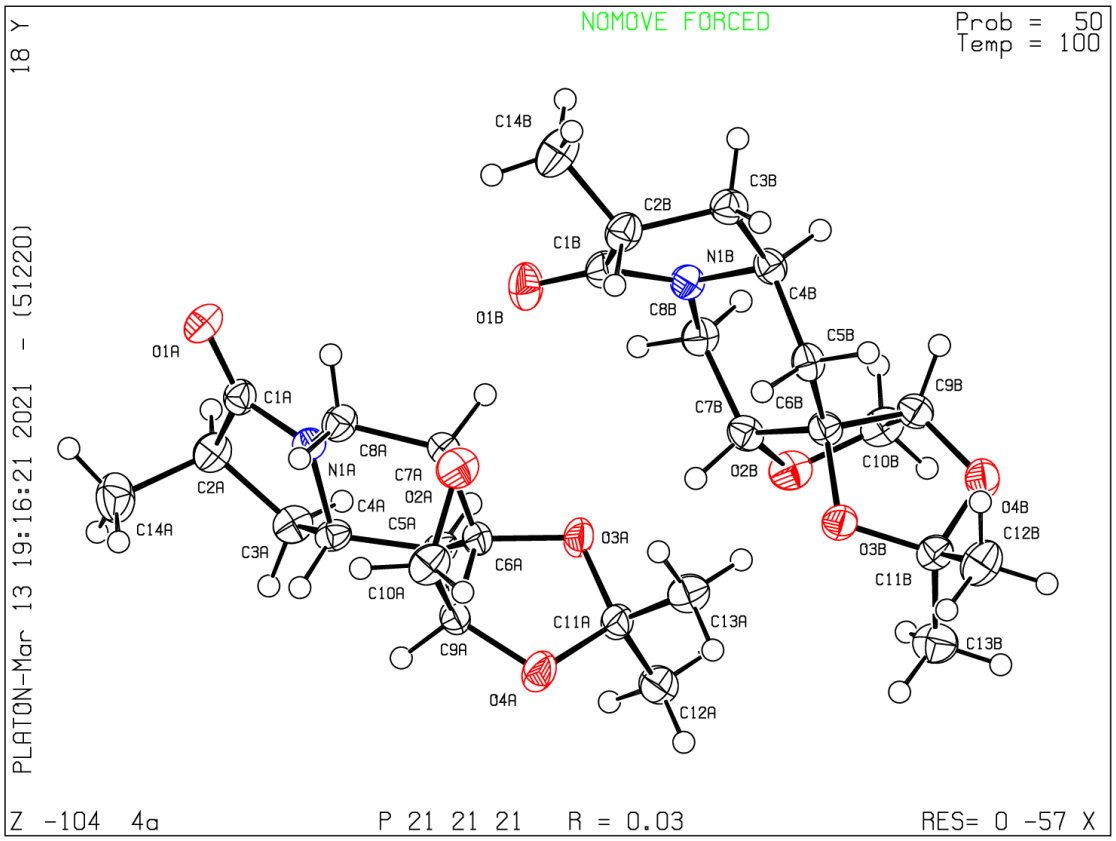
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 05/12/2020; check.def file version of 05/12/2020

Datablock 4a - ellipsoid plot



Datablock 10b - ellipsoid plot