

Supporting Information

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Expremental section

¹³C NMR Calculation Methods

For the calculations of ¹³C NMR chemical shifts, B3LYP/6-31G(d,p) method was used to optimize the selected conformations. For all optimized structures, vibrational spectra were calculated to ensure that no imaginary frequencies for energy minimum were obtained. NMR calculations were performed at the levels of mPW1PW91/6-31G(d,p) with the gauge-independent atomic orbital (GIAO) method.¹ The solvent effect was considered by using chloroform for **1** and **2** in the calculations to resemble the experimental condition. The polarized continuum model (PCM) of Tomasi et al. was used.² The calculated ¹³C NMR chemical shifts were analyzed by subtracting the isotopic shifts for TMS calculated with the same methods.¹ Different conformers for structures **1** were considered. The ¹³C NMR chemical shifts in each compound were considered as the average values of the same atoms in the different conformers. The average values were obtained by the Boltzmann distributions, using the relative Gibbs free energies as weighting factors.³ The differences $\Delta\delta$ were determined by subtracting the experimental chemical shifts δ_{exptl} from the calculated chemical shifts δ_{calcd} .

ECD Calculation Methods

The theoretical calculations of **1** and **2** were performed using Gaussian 09⁴ and figured using GaussView 5.0.⁵ Conformation search using molecular mechanics calculations was performed in Discovery Studio 3.5 Client with MMFF force field with 20 kcal mol⁻¹ upper energy limit.⁶ The optimized conformation geometries and thermodynamic parameters of all selected conformations were provided. The predominant conformers were optimized at B3LYP/6-31G(d,p) level. The theoretical calculation of ECD was performed using time dependent Density Functional Theory (TDDFT) at B3LYP/6-31G(d,p) level in MeOH with PCM model.¹ The ECD spectra of **1** and **2** were obtained by weighing the Boltzmann distribution rate of each geometric conformation.³ The ECD spectra were simulated by overlapping Gaussian functions for each transition according to:

$$\Delta\varepsilon(E) = \frac{1}{2.297 \times 10^{-39}} \times \frac{1}{\sqrt{2\pi\sigma}} \sum_i^A \Delta E_i R_i e^{-[(E-E_i)/(2\sigma)]^2} \quad (1)$$

The σ represented the width of the band at 1/e height, and ΔE_i and R_i were the excitation energies and rotational strengths for transition i , respectively. R_{vel} was used in this work.

References:

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- (2) (a) Ditchfield, R. *Mol. Phys.* **1974**, *27*, 789. (b) Rohlfing, C. M.; Allen, L. C.; Ditchfield, R. *Chem. Phys.* **1984**, *87*, 9. (c) Wolinski, K.; Hinton, J. F.; Pulay, P. *J. Am. Chem. Soc.* **1990**, *112*, 8251.
- (3) Tähtinen, P.; Bagno, A.; Klika, K. D.; Pihlaja, K. *J. Am. Chem. Soc.* **2003**, *125*, 4609–4618.
- (4) Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.
- (5) GaussView, Version 5, Dennington, R.; Keith, T.; Millam, J. *Semichem Inc.*, Shawnee Mission, KS, **2009**.
- (6) Smith, S. G.; Goodman, J. M. *J. Am. Chem. Soc.* **2010**, *132*, 12946–12959.

Table S1. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **1** at B3LYP/6-31G(d,p) level in the gas phase

Compound	SCF	G	Zero-point	%
1-a	-1081.141005	0.409978	0.459809	49.98
1-b	-1081.141006	0.409975	0.459810	49.98
1-c	-1081.1133865	0.409837	0.459785	0.03
1-d	-1081.133565	0.409598	0.459705	0.02

SCF, G: self consistent field (SCF) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

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

1-a				1-b			
C	3.114	-2.261	0.65	C	2.314	-1.188	0.837
C	2.314	-1.188	0.837	C	2.738	-0.161	-0.109
C	2.738	-0.161	-0.109	C	2.199	1.081	-0.198
C	2.199	1.081	-0.198	C	1.109	1.472	0.823
C	4.062	-1.944	-0.42	C	0.262	0.224	1.29
C	-6.273	-0.816	-1.158	C	1.193	-0.913	1.786
C	2.772	2.083	-1.122	C	0.145	2.571	0.299
C	-4.941	-0.896	-1.2	C	-0.905	2.089	-0.702
C	1.193	-0.913	1.786	C	-1.744	0.977	-0.063
C	-0.905	2.089	-0.702	C	-0.874	-0.262	0.306
C	0.145	2.571	0.3	C	-2.994	0.618	-0.884
C	-3.09	-1.616	0.295	C	-3.938	-0.398	-0.175
C	-1.808	-1.249	1.065	C	-3.09	-1.616	0.295
C	-2.994	0.618	-0.883	C	-1.808	-1.249	1.065
C	0.262	0.224	1.29	C	-4.642	0.26	1.026
C	-1.745	0.977	-0.063	H	-2.101	1.388	0.893
C	1.109	1.472	0.824	H	-0.278	0.578	2.178
C	-3.938	-0.398	-0.175	C	1.852	2.083	2.046
C	-0.874	-0.262	0.306	C	-0.322	-0.971	-0.952
C	1.852	2.083	2.046	C	3.113	-2.261	0.65
C	-4.642	0.259	1.026	C	4.062	-1.944	-0.42
C	-0.322	-0.971	-0.952	O	3.782	-0.636	-0.859
O	4.952	-2.581	-0.929	C	2.773	2.083	-1.122
O	3.521	1.836	-2.057	H	2.492	3.131	-0.914
O	3.782	-0.635	-0.859	O	4.952	-2.581	-0.929
H	3.105	-3.213	1.163	O	3.521	1.836	-2.057

H	-6.882	-1.216	-1.965	C	-4.941	-0.896	-1.2
H	-6.81	-0.358	-0.333	C	-6.273	-0.817	-1.158
H	2.491	3.131	-0.914	H	1.633	-0.618	2.748
H	-4.482	-1.374	-2.069	H	0.639	-1.832	1.99
H	1.633	-0.618	2.747	H	-0.385	2.965	1.177
H	0.639	-1.832	1.99	H	0.707	3.42	-0.102
H	-1.552	2.932	-0.976	H	-1.552	2.932	-0.976
H	-0.437	1.746	-1.635	H	-0.437	1.746	-1.635
H	-0.385	2.965	1.178	H	-3.558	1.537	-1.093
H	0.707	3.42	-0.101	H	-2.698	0.218	-1.863
H	-3.714	-2.263	0.927	H	-3.714	-2.263	0.927
H	-2.825	-2.222	-0.58	H	-2.826	-2.222	-0.58
H	-2.076	-0.806	2.035	H	-2.076	-0.806	2.035
H	-1.279	-2.183	1.293	H	-1.279	-2.182	1.293
H	-3.558	1.537	-1.093	H	-5.225	1.132	0.712
H	-2.698	0.218	-1.862	H	-3.927	0.596	1.782
H	-0.278	0.578	2.178	H	-5.324	-0.447	1.512
H	-2.101	1.388	0.894	H	2.373	3.002	1.753
H	2.373	3.002	1.753	H	1.139	2.343	2.837
H	1.139	2.343	2.838	H	2.601	1.403	2.463
H	2.601	1.403	2.463	H	-1.13	-1.323	-1.598
H	-3.927	0.595	1.782	H	0.316	-0.325	-1.559
H	-5.324	-0.447	1.512	H	0.266	-1.853	-0.677
H	-5.226	1.132	0.712	H	3.104	-3.213	1.163
H	0.266	-1.853	-0.678	H	-4.482	-1.373	-2.069
H	-1.13	-1.323	-1.598	H	-6.882	-1.215	-1.965
H	0.316	-0.325	-1.559	H	-6.81	-0.358	-0.332

Table S3. Cytotoxic assay results for tagalide A (1), tagalsin C and its two analogs against human breast cancer cells [IC_{50} (μM)]

Compound	Cell Lines					
	MD-MBA-453	MD-MBA-231	SK-BR-3	MCF-7	MT-1	ZR-75-1
 <p>Tagalide A (1)</p>	1.73	8.12	2.45	12.03	3.75	1.97
 <p>tagalsin C</p>	4.06	43.51	1.85	17.26	2.17	3.55
 <p><i>ent</i>-5α,3,15-dioxodolabr-1,4(18)-diene-2,16-diol</p>	2.58	10.99	2.08	20.65	3.92	5.87
 <p>(5S,8S,9S,10R,13S)-2-hydroxy-16-nor-3-oxodolabr-1,4(18)-dien-15-oic acid</p>	7.98	50.97	4.20	34.93	8.07	12.40
Cisplatin (the positive control)	4.37	3.73	8.42	3.21	7.90	20.65

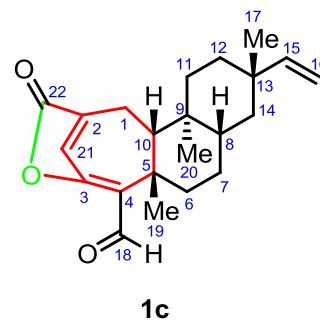
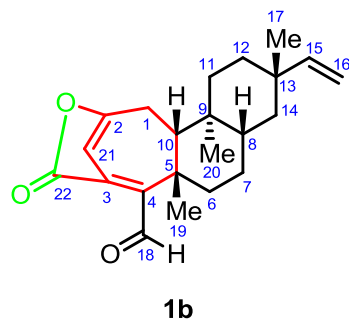
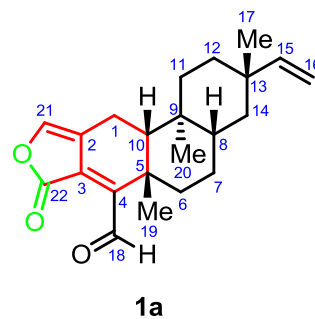
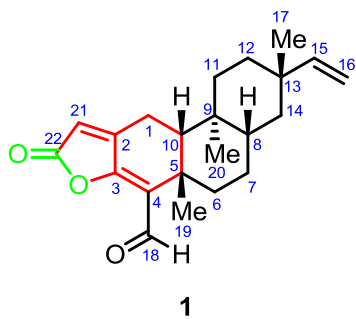
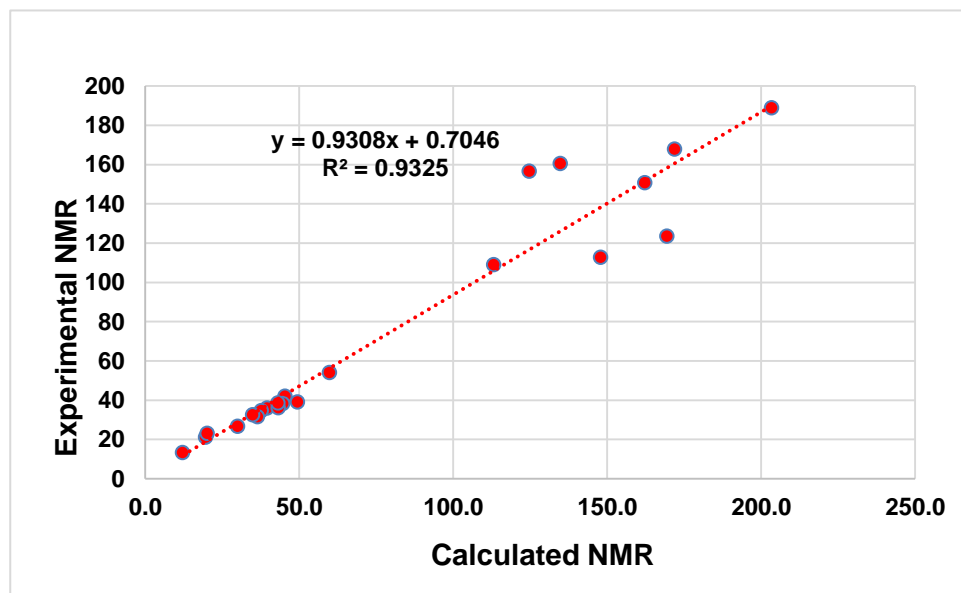
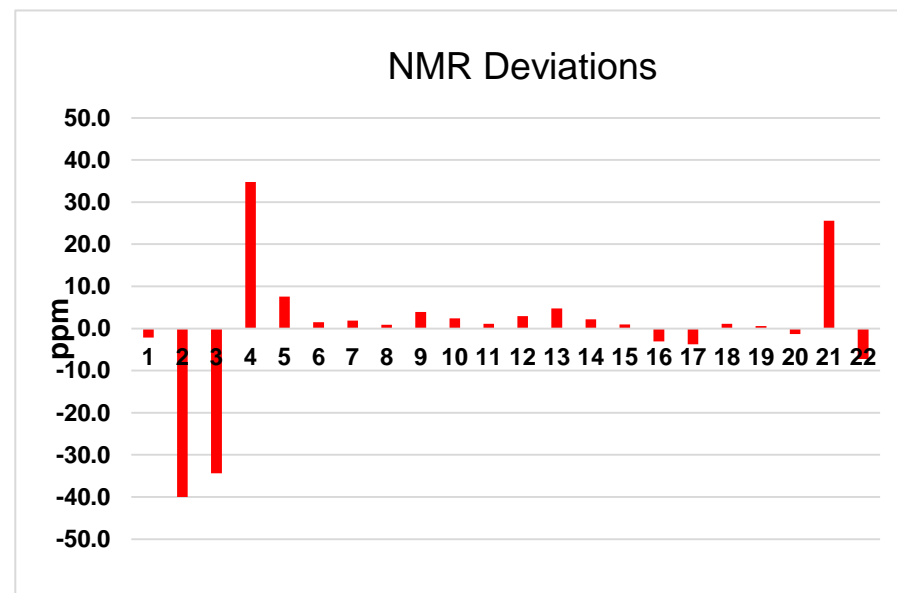


Figure S1. Four possible structures for compound **1**.



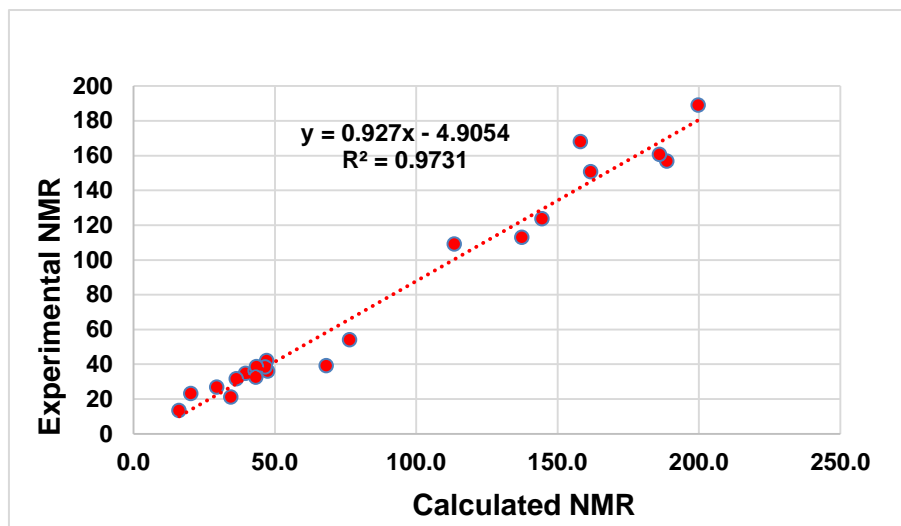
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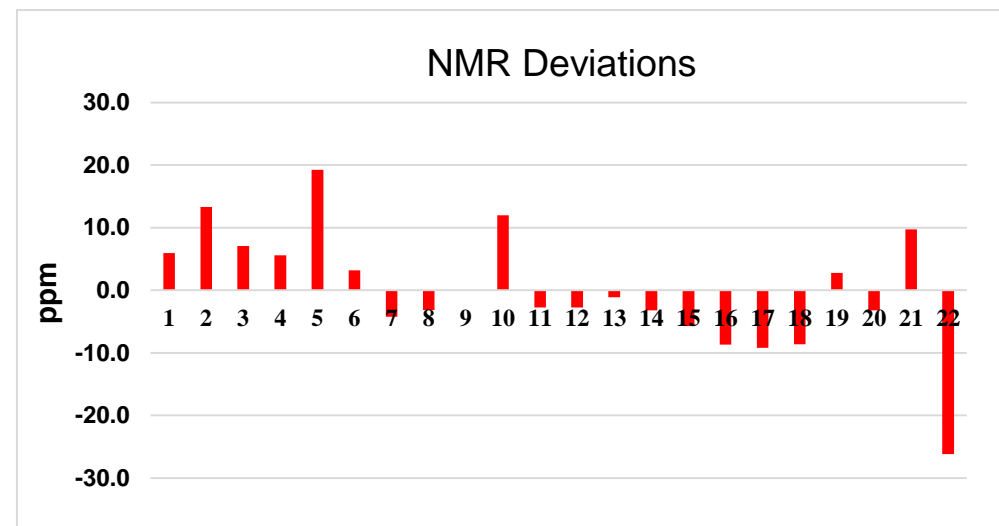
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Figure S2. Calculated ^{13}C NMR chemical shifts for the structure of **1a**.

(A) Linear correlations between the experimental and calculated ^{13}C NMR chemical shifts of **1a**. (B) Individual deviations between the calculated and experimental ^{13}C chemical shifts.



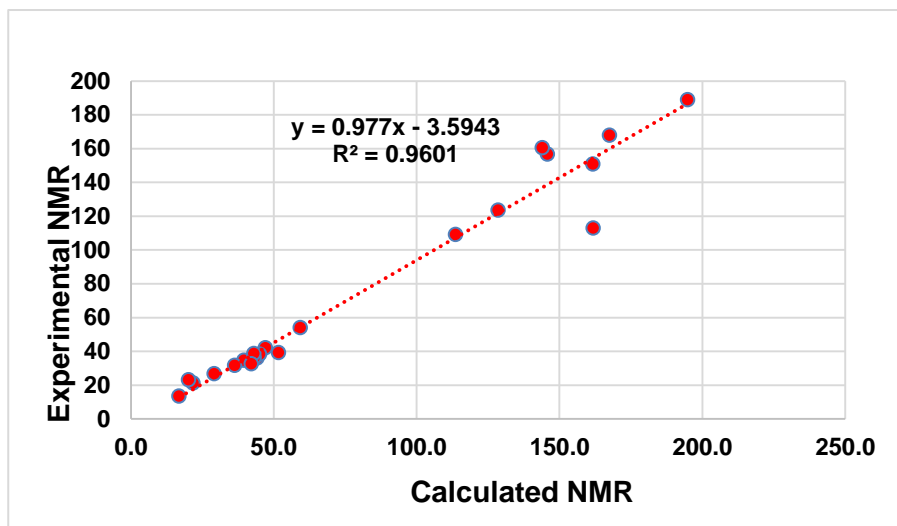
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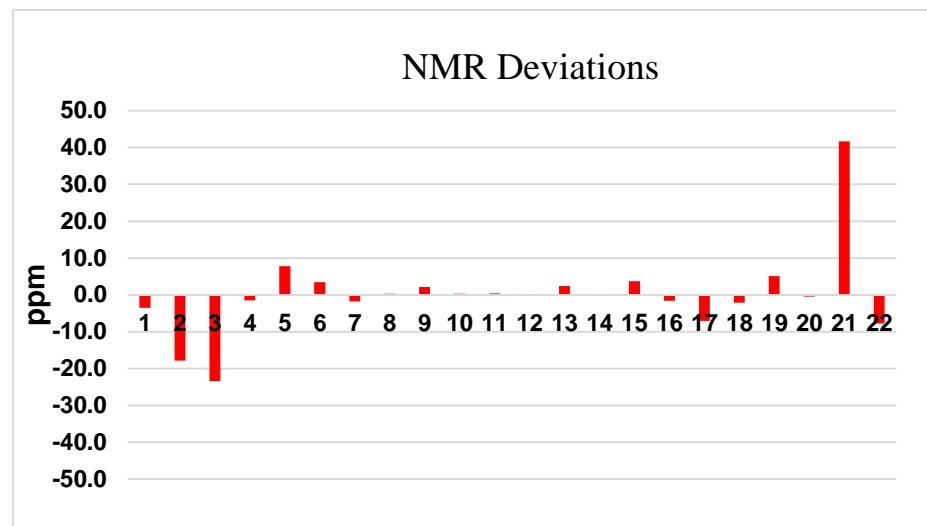
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Figure S3. Calculated ^{13}C NMR chemical shifts for the structure of **1b**.

(A) Linear correlations between the experimental and calculated ^{13}C NMR chemical shifts of **1b**. (B) Individual deviations between the calculated and experimental ^{13}C chemical shifts.



A



B

Figure S4. Calculated ^{13}C NMR chemical shifts for the structure of of **1c**.

(A) Linear correlations between the experimental and calculated ^{13}C NMR chemical shifts of **1c**. (B) Individual deviations between the calculated and experimental ^{13}C chemical shifts.

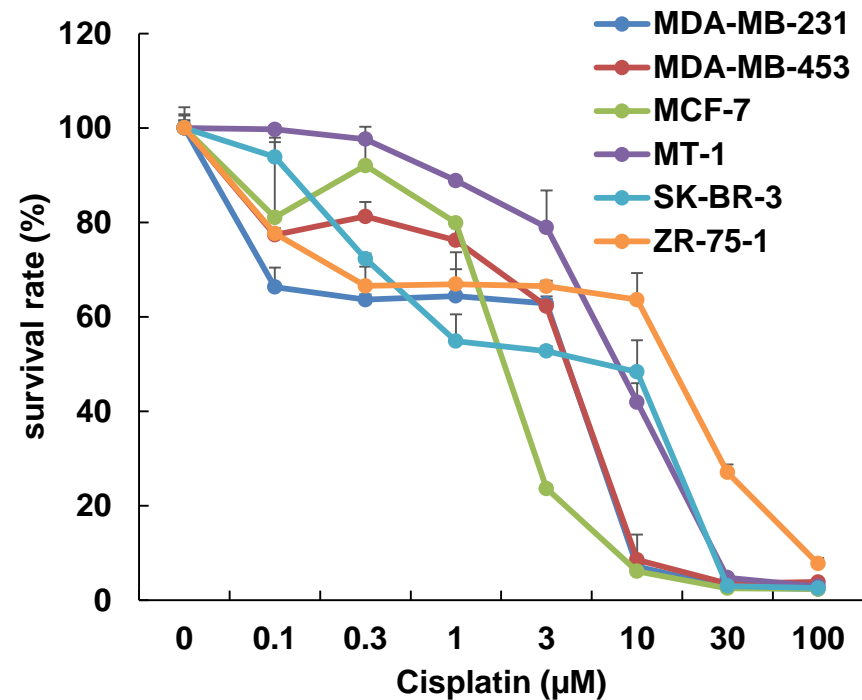
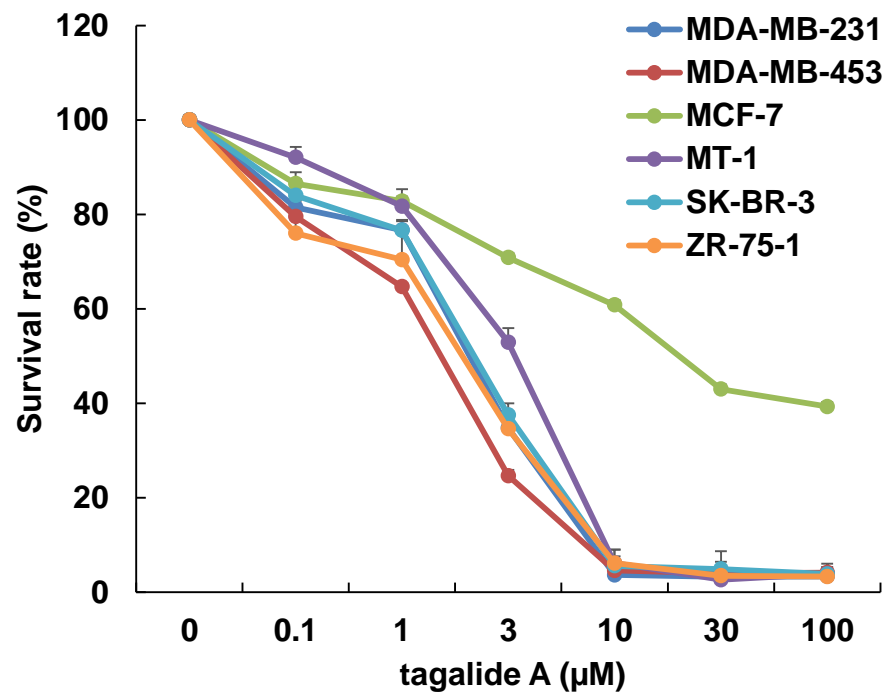


Figure S5. Tagalide A (1) inhibits the growth of six human breast cancer cell lines *in vitro*.

Summary of IC_{50} of Tagalide A (1) and cisplatin against breast cancer cells was shown. Cells were grown in 96-well plates for 24 h and treated with the indicated concentrations of tagalide A (1) and cisplatin for 72 h. Cell survival was measured by MTT assay. The representative growth curves of cells treated with tagalide A (1) are shown.

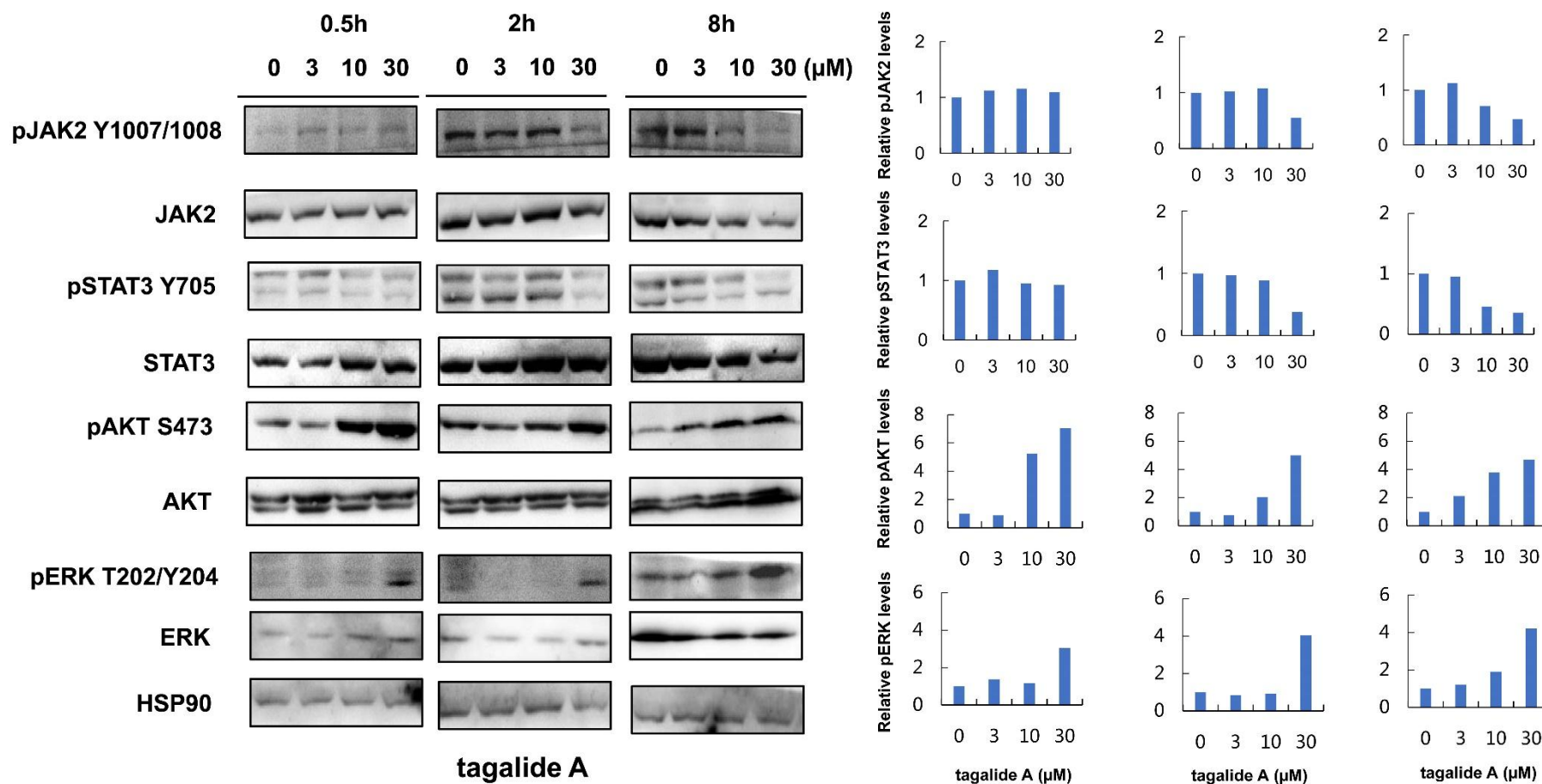


Figure S6. Tagalide A (1) inhibits phosphorylation of JAK2 and STAT3, but enhances that of AKT and ERK in MDA-MB-453 cells.

Human breast cancer MDA-MB-453 cells were treated with 1 at the indicated time and concentrations. The protein expression was examined by Western blot after lysing cells, and HSP90 was used as loading control. The representative Western blot results and quantified results were shown.

HRESIMS for tagalide A (1)

Mass Spectrum SmartFormula Report

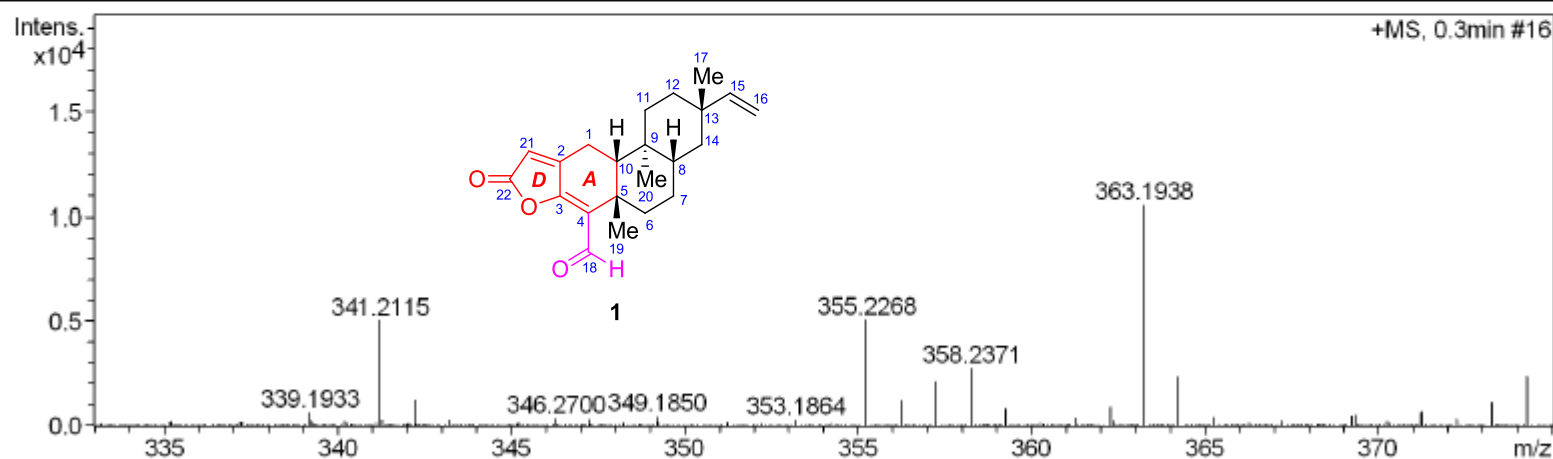
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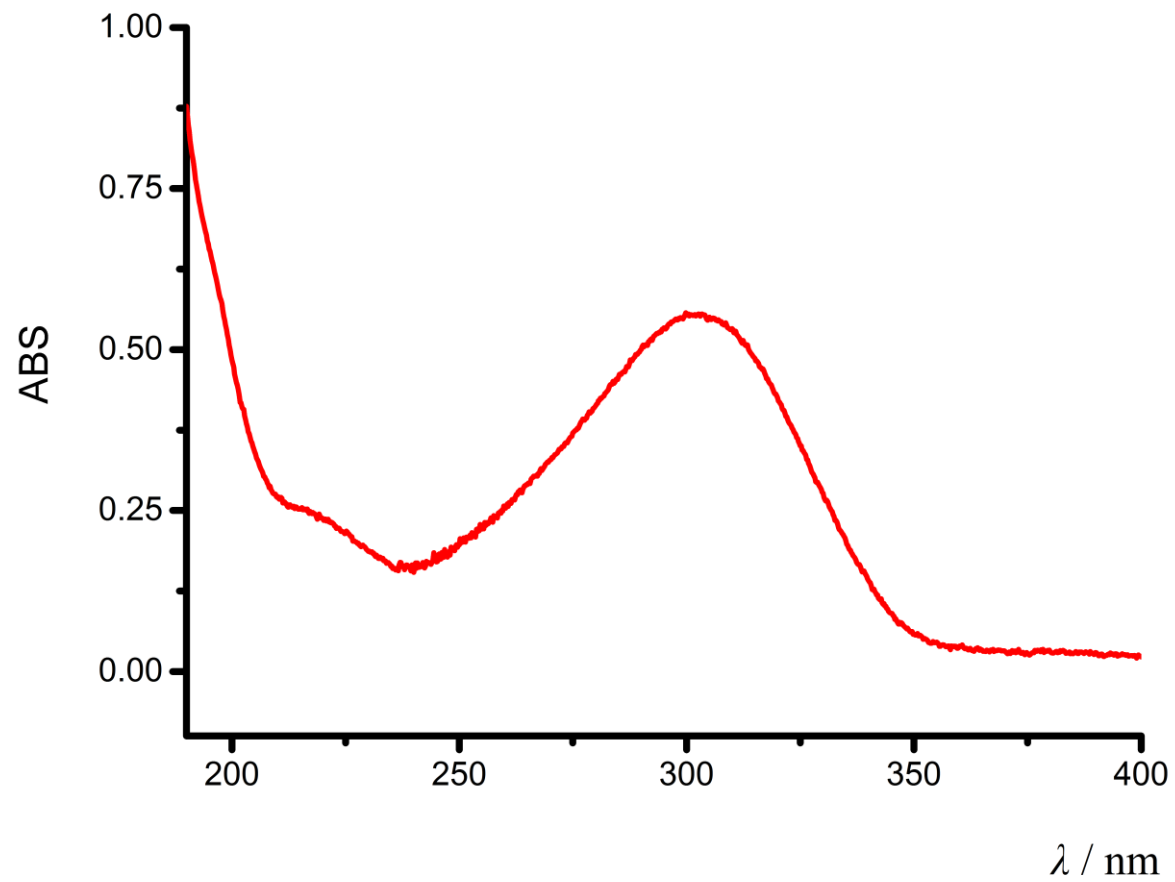
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363.1938	1	C ₂₂ H ₂₈ NaO ₃	100.00	363.1931	-2.0	-0.7	10.3	8.5	even	ok
703.3990	1	C ₄₄ H ₅₆ NaO ₆	27.04	703.3969	-3.0	-2.1	41.9	16.5	even	ok

UV spectrum for tagalide A (1) (recorded in MeCN at 250 $\mu\text{g/mL}$)



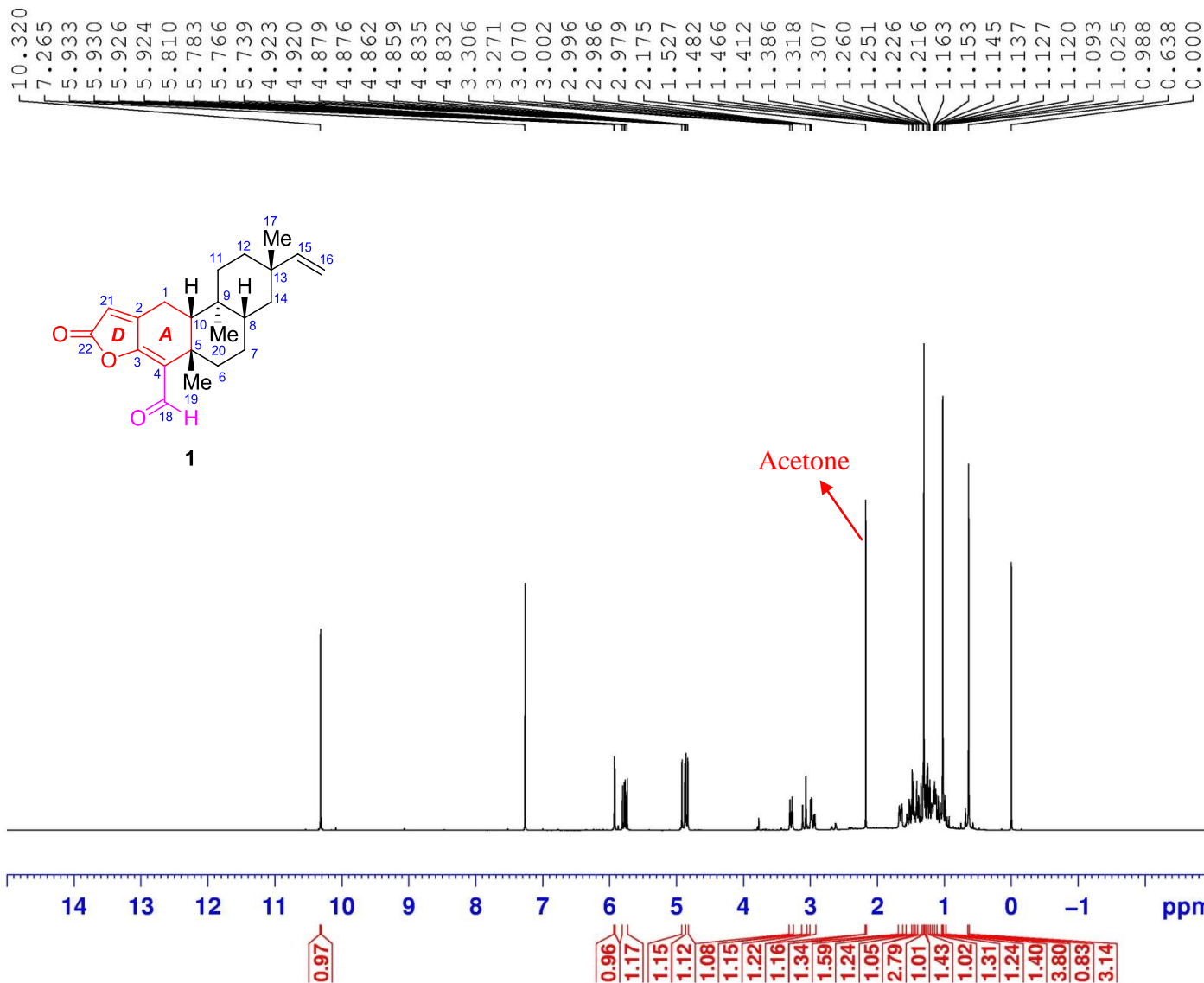
¹H (400 MHz) NMR spectrum of tagalide A (1) in CDCl₃



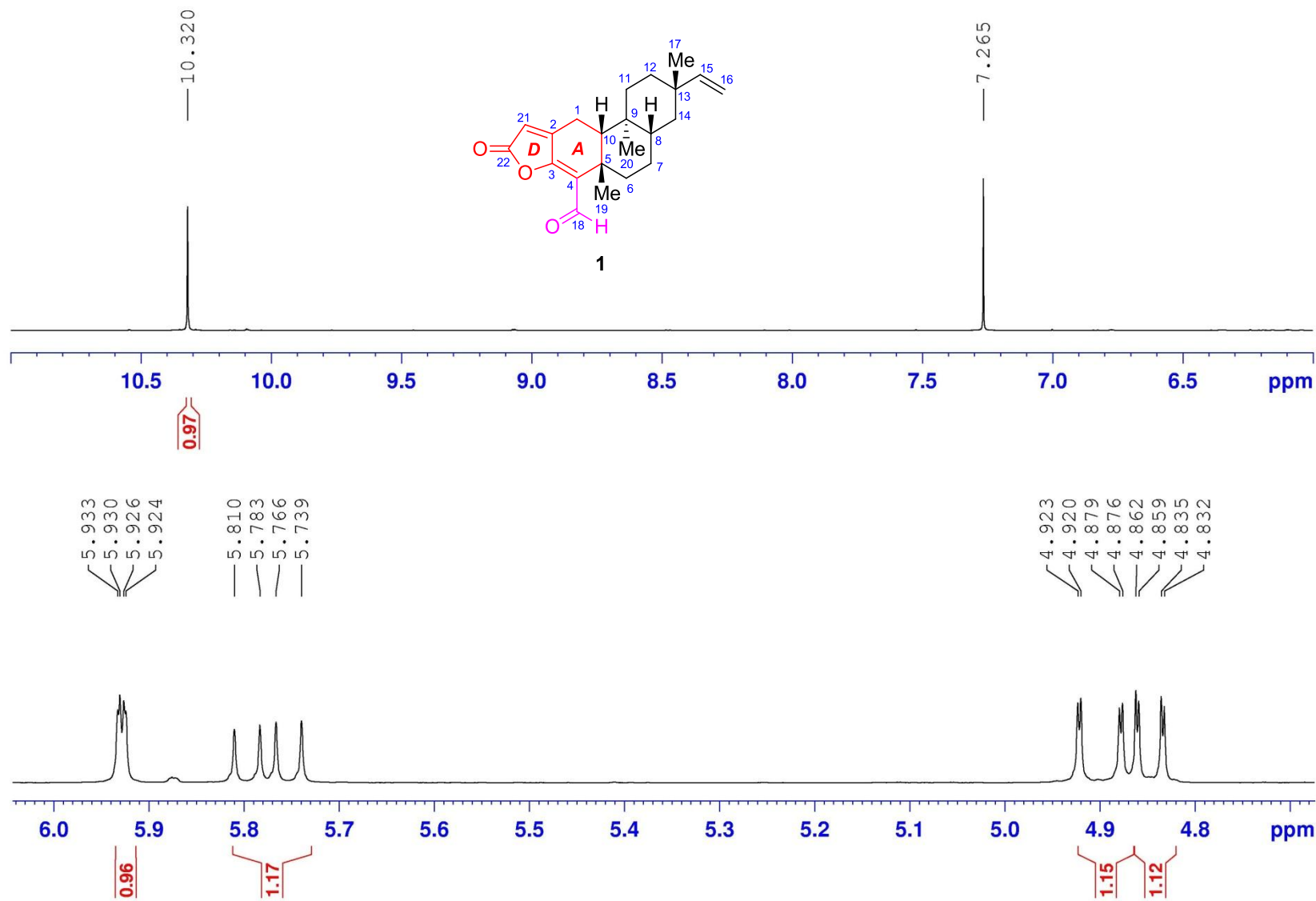
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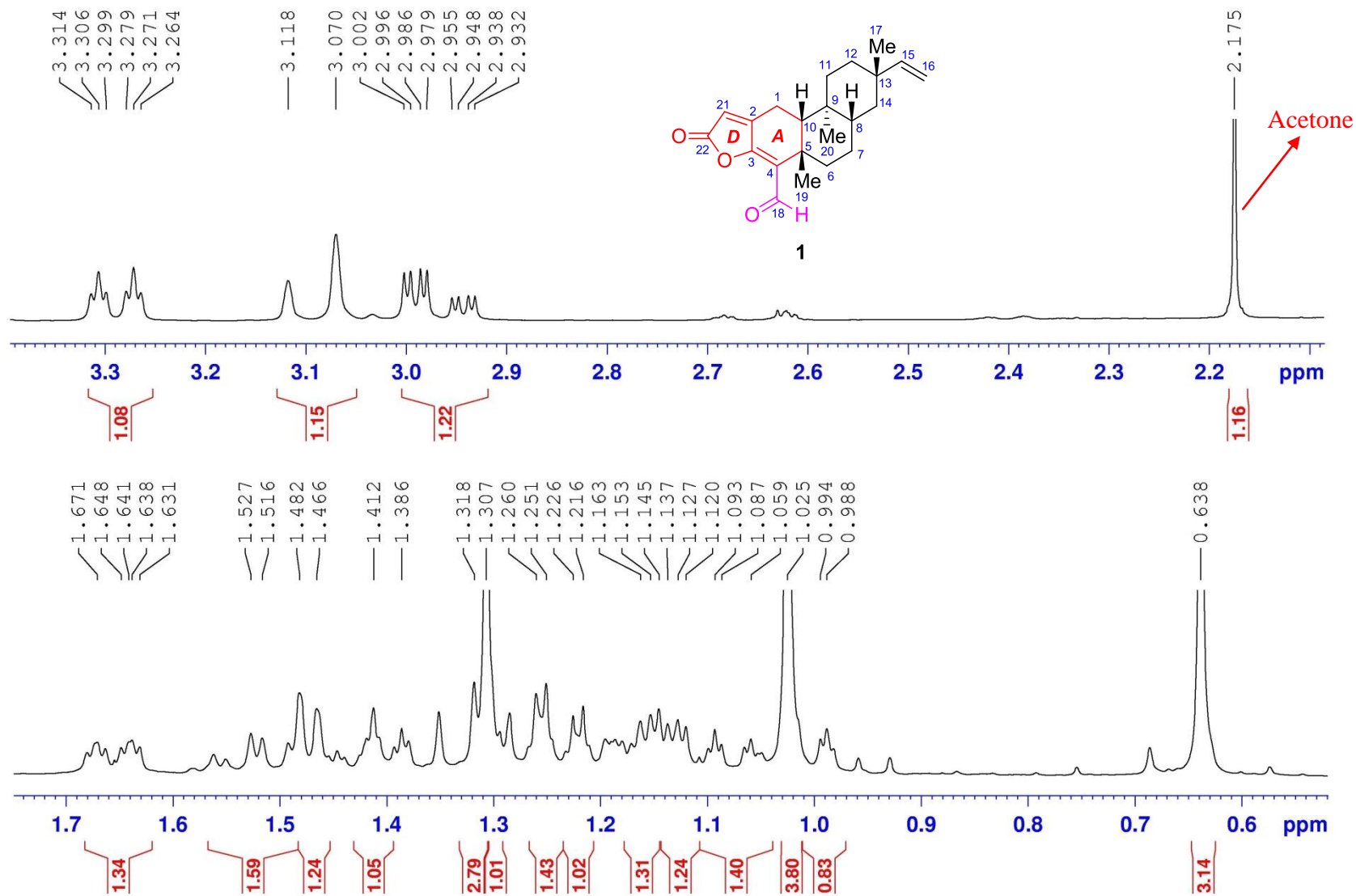
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¹H (400 MHz) NMR spectrum of tagalide A (1) in CDCl₃



¹H (400 MHz) NMR spectrum of tagalide A (1) in CDCl₃



¹³C (100 MHz) NMR spectrum of tagalide A (1) in CDCl₃

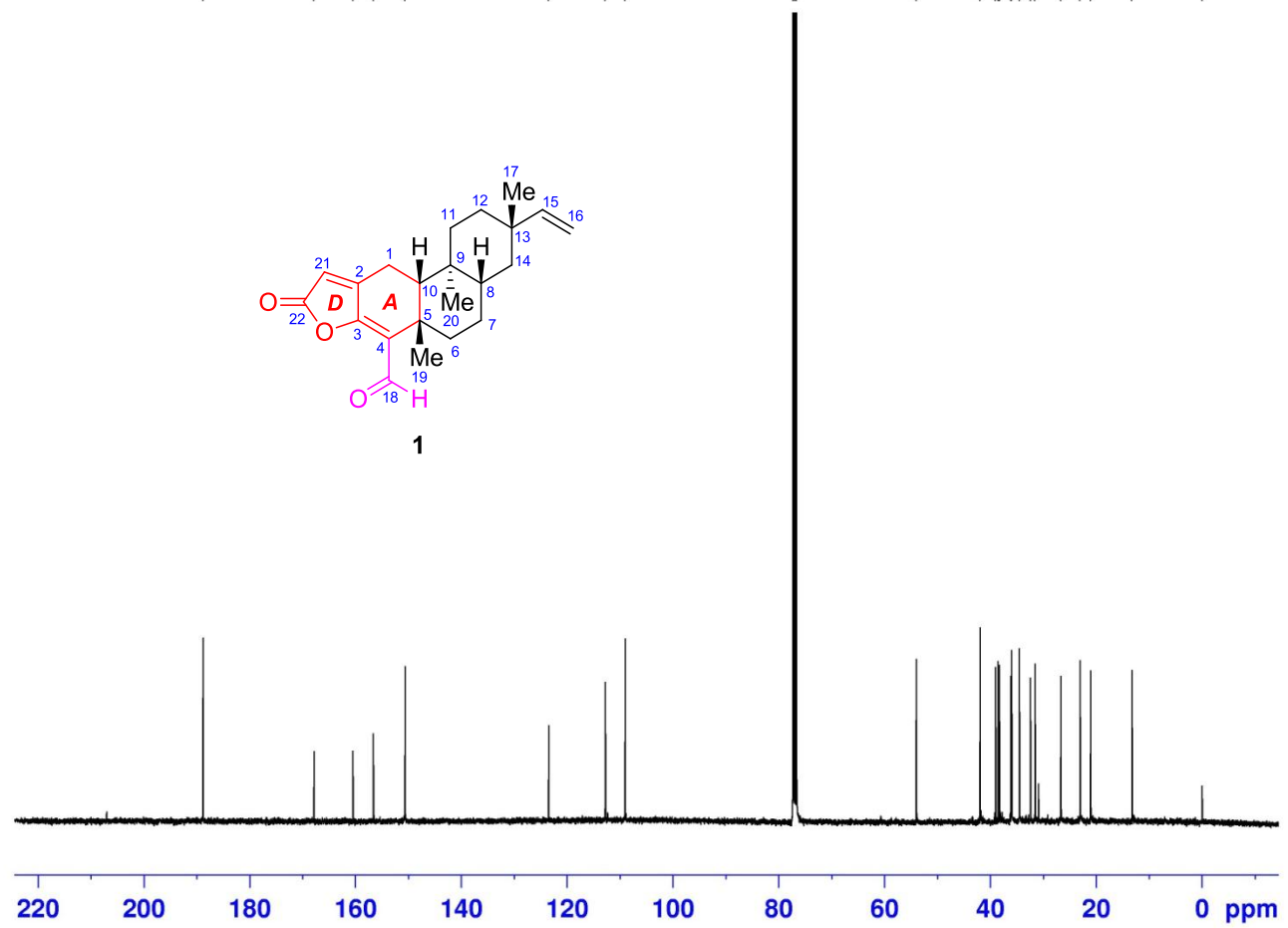
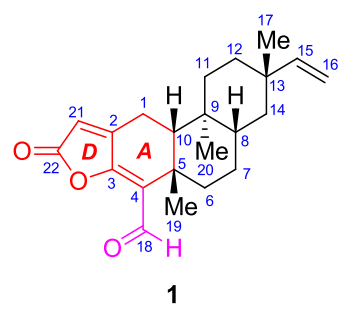


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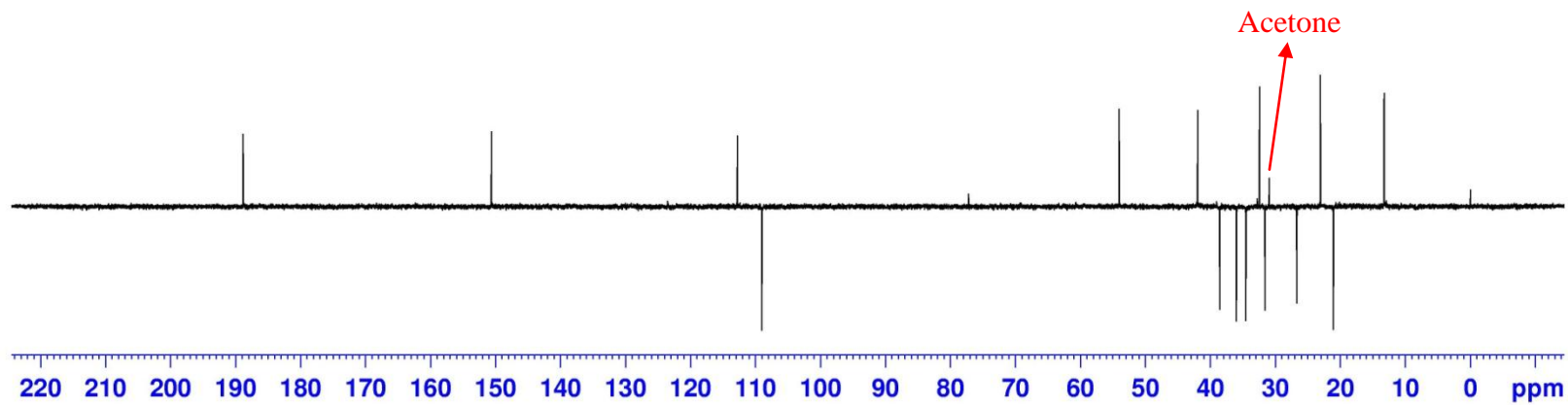
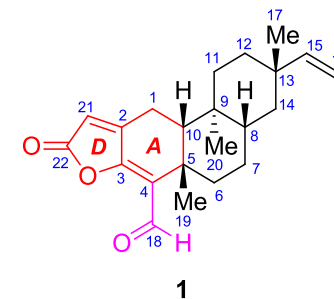
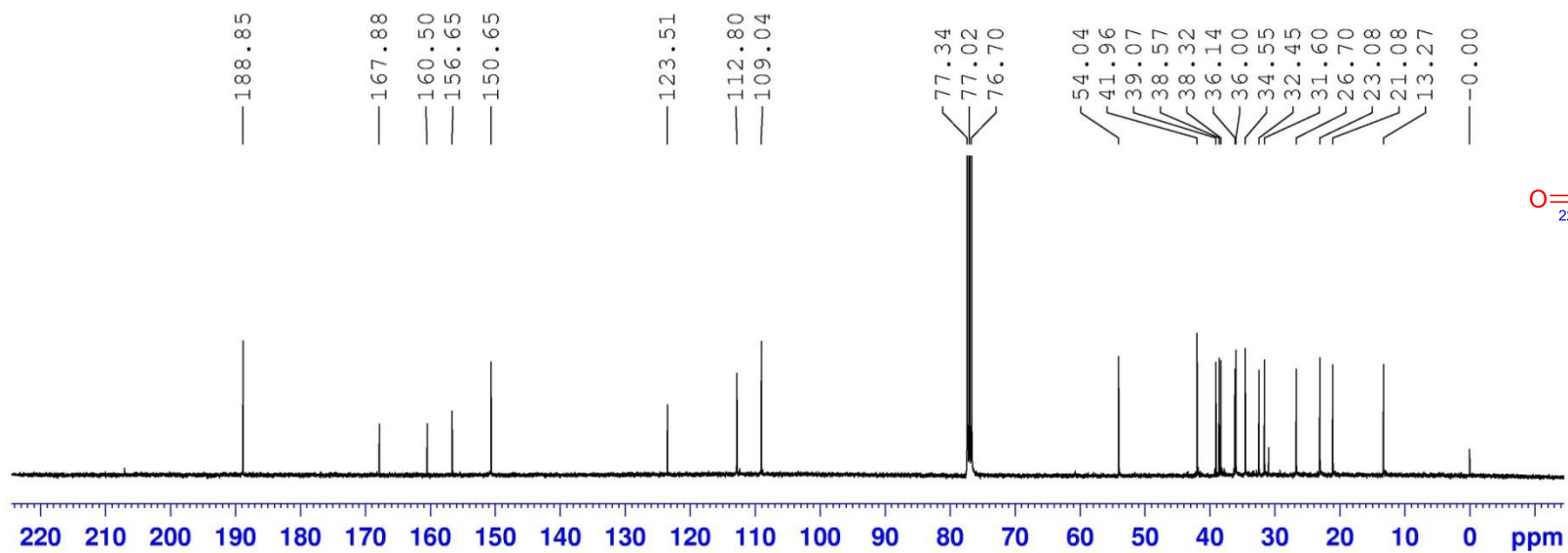
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LB            1.00 Hz
GB            0
PC            1.40
    
```

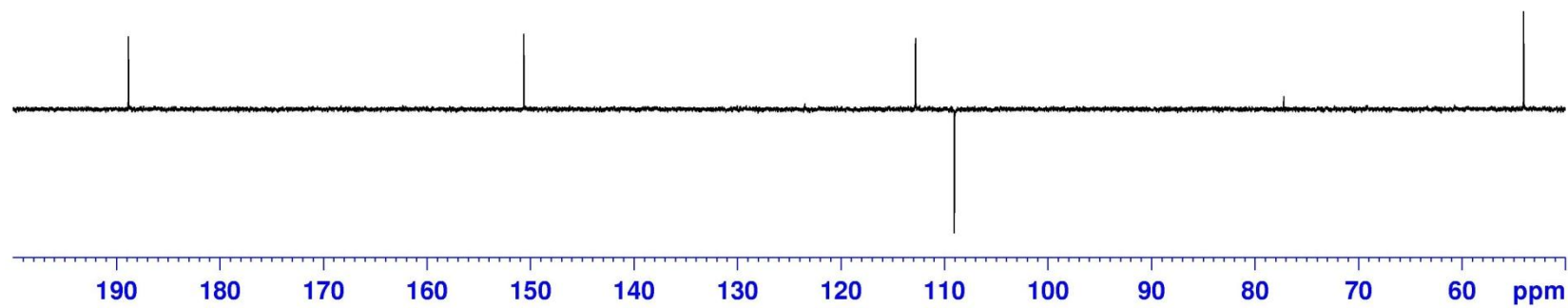
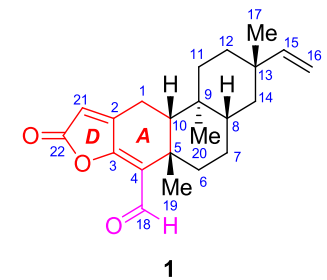
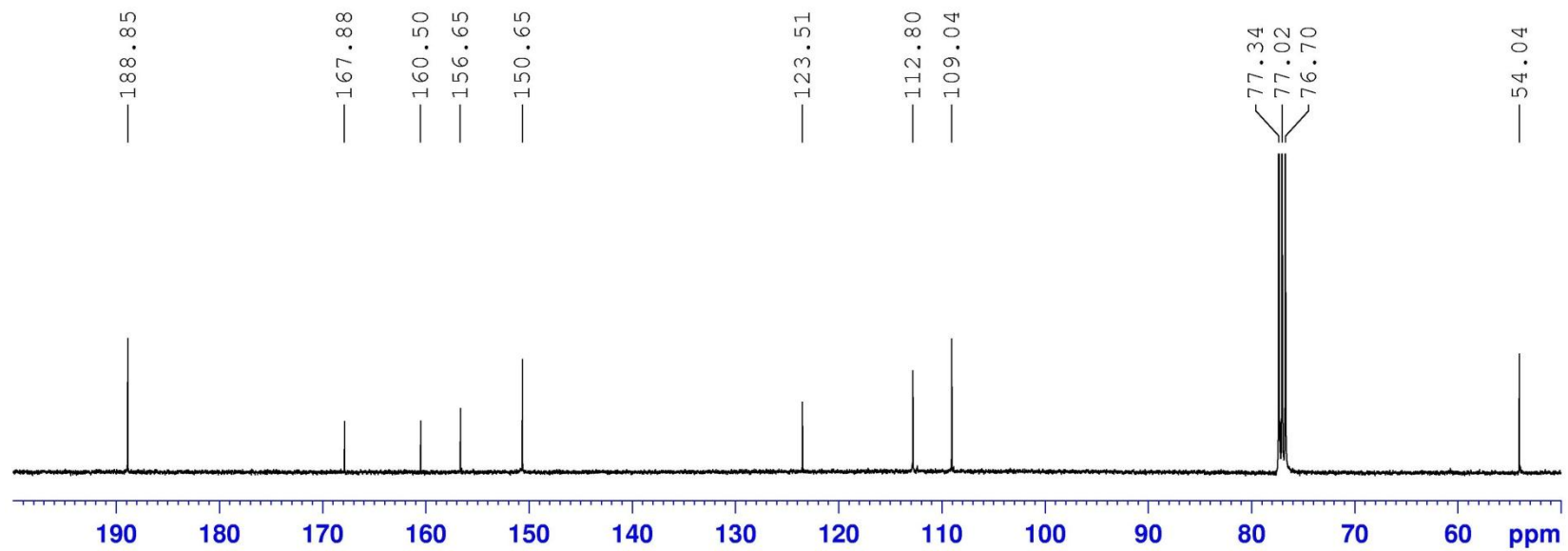
— 188.85
 — 167.88
 — 160.50
 — 156.65
 — 150.65
 — 123.51
 — 112.80
 — 109.04
 77.34
 77.02
 76.70
 54.04
 41.96
 39.07
 38.57
 38.32
 36.14
 36.00
 34.55
 32.45
 31.60
 26.70
 23.08
 21.08
 13.27
 -0.00



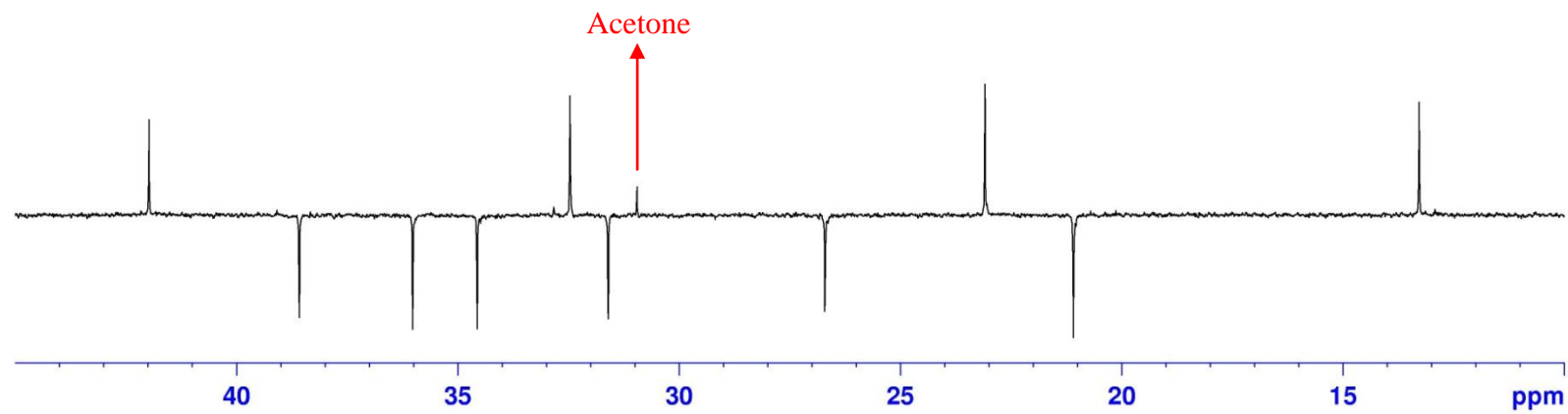
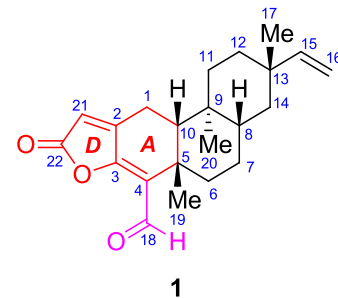
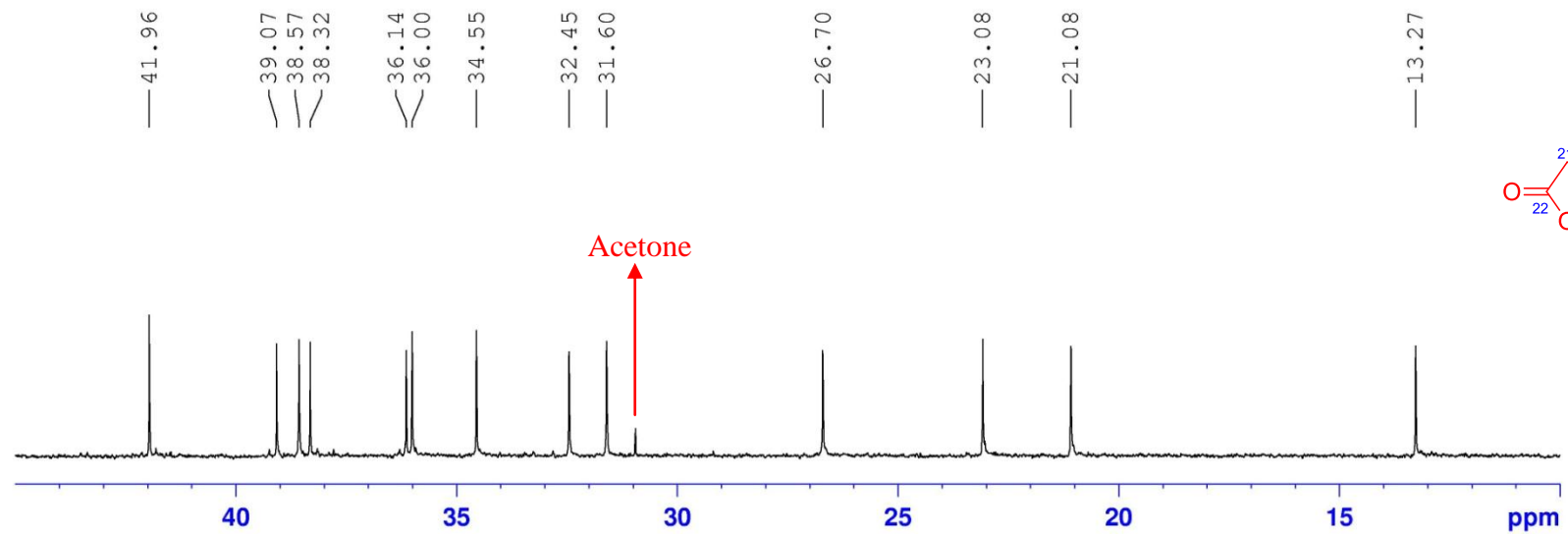
DEPT135 (100 MHz) spectrum of tagalide A (1) in CDCl₃



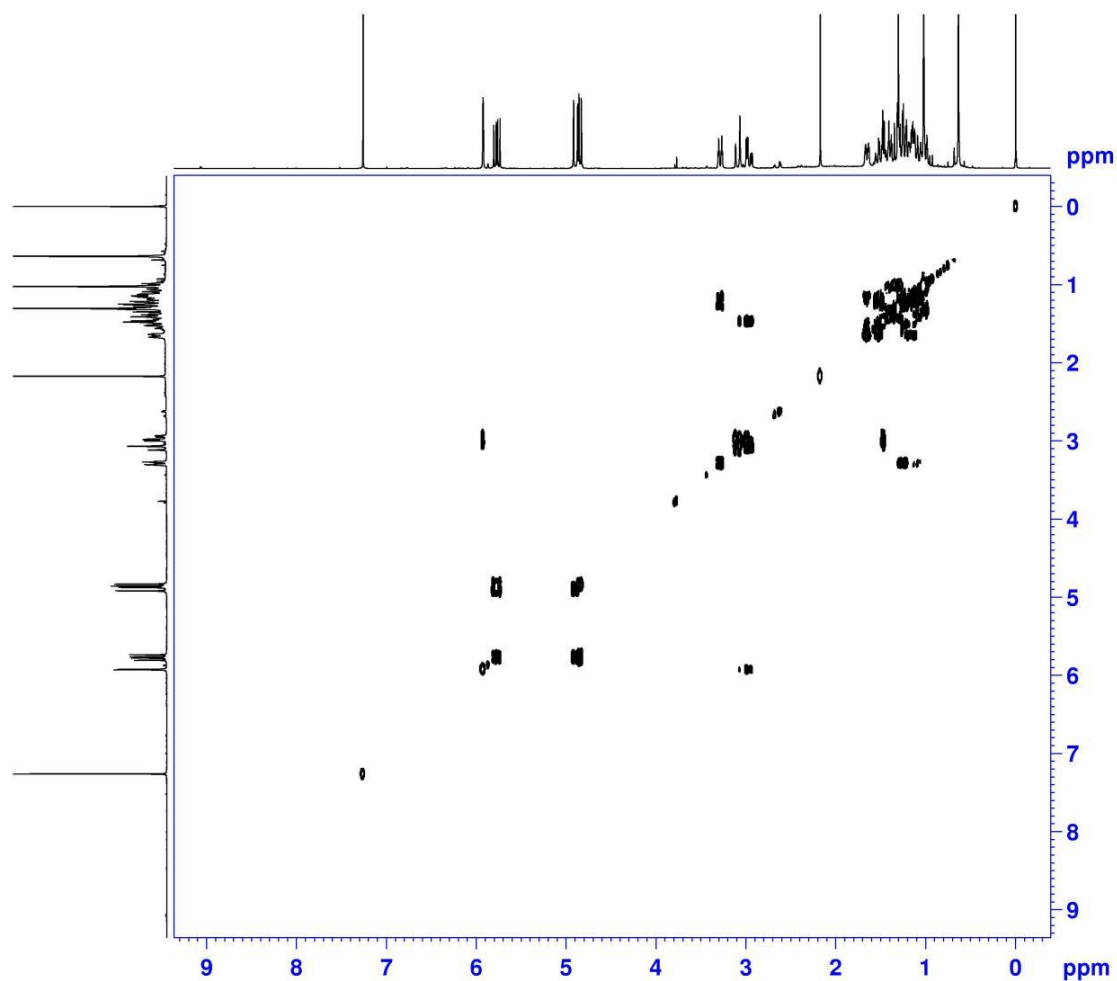
DEPT135 (100 MHz) experiment of tagalide A (1) in CDCl₃



DEPT135 (100 MHz) experiment of tagalide A (1) in CDCl₃



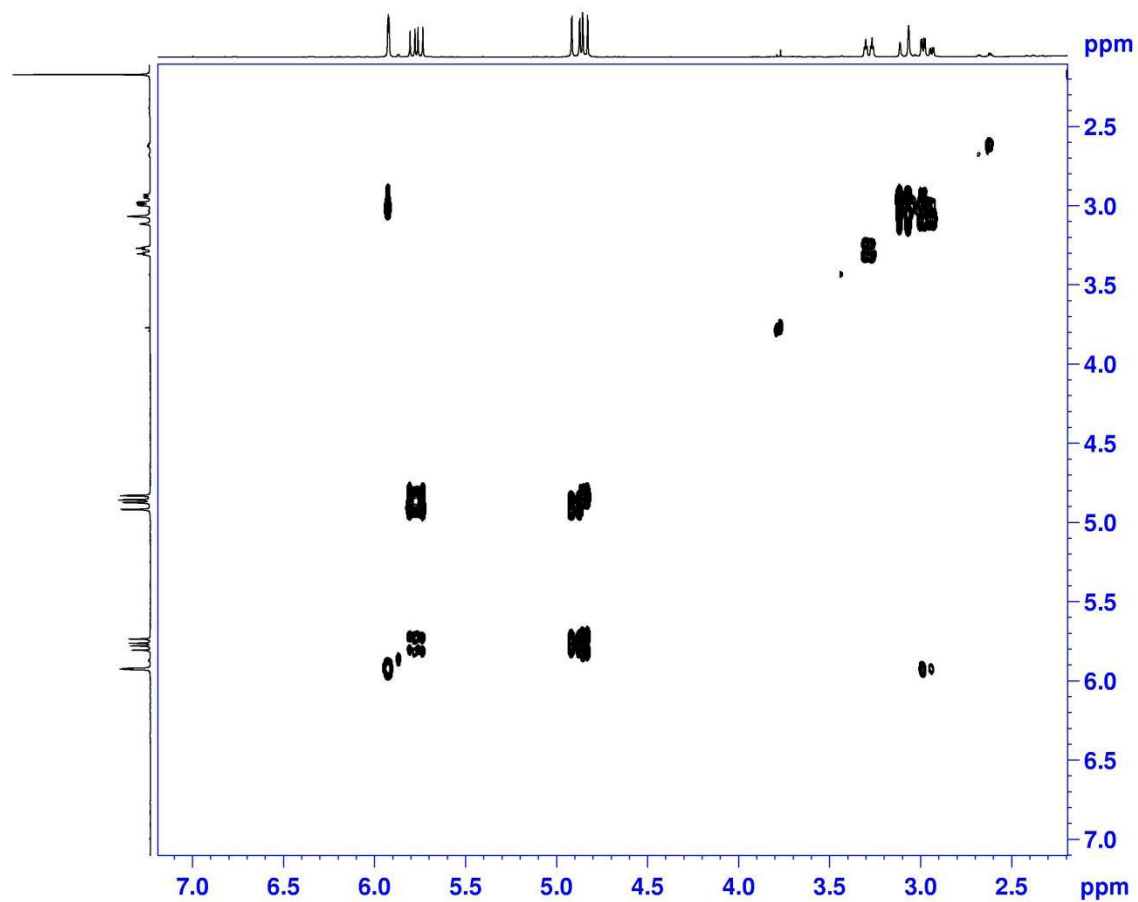
^1H - ^1H COSY (400 MHz) spectrum of tagalide A (1) in CDCl_3



```
NAME R-36-1-1
EXPNO 4
PROCNO 1
Date_ 20160203
Time 21.07
INSTRUM spect
PROBHD 5 mm CFPBBO BB
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 8
DS 8
SMH 3906.250 Hz
FIDRES 1.907349 Hz
AQ 0.2621940 sec
RG 208.5
DW 128.000 usec
DE 10.00 usec
TE 297.0 K
D0 0.00000300 sec
D1 1.89678097 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00004000 sec
D16 0.00020000 sec
IN0 0.00025600 sec
```

```
===== CHANNEL f1 =====
SF01 400.1318006 MHz
NUC1 1H
P0 11.50 usec
P1 11.50 usec
P17 2500.00 usec
ND0 1
TD 128
SF01 400.1318 MHz
FIDRES 30.517578 Hz
SW 9.762 ppm
FhMODE QF
SI 1024
SF 400.1300080 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
```

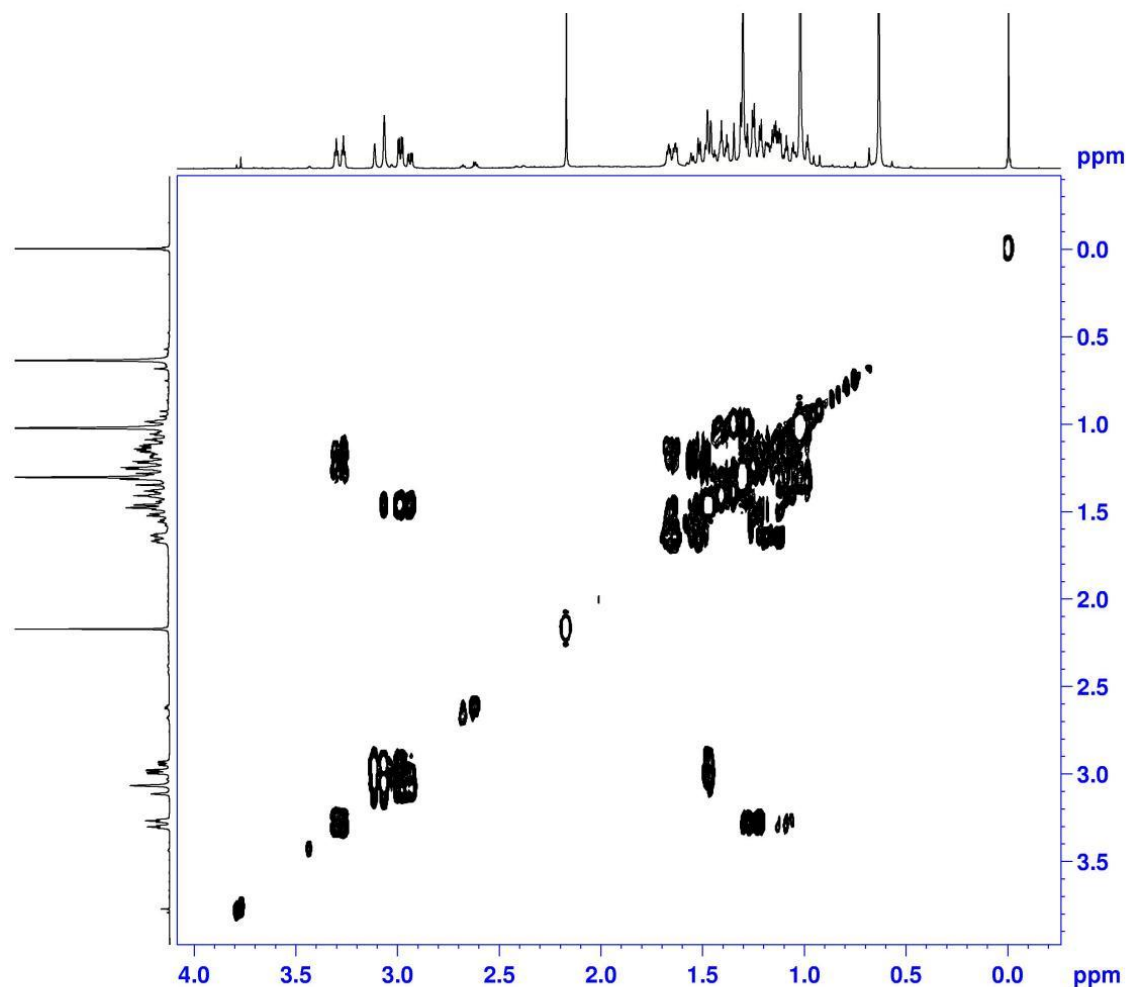
^1H - ^1H COSY (400 MHz) spectrum of tagalide A (1) in CDCl_3



```
NAME          R-36-1-1
EXPNO         4
PROCNO        1
Date_         20160203
Time         21.07
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       cosygpppqf
TD            2048
SOLVENT       CDC13
NS            8
DS            8
SWH           3906.250 Hz
FIDRES        1.907349 Hz
AQ            0.2621940 sec
RG            208.5
DW            128.000 usec
DE            10.00 usec
TE            297.0 K
D0            0.00000300 sec
D1            1.89678097 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00025600 sec
```

```
----- CHANNEL f1 -----
SF01         400.1318006 MHz
NUC1          1H
P0            11.50 usec
P1            11.50 usec
P17           2500.00 usec
ND0           1
TD            128
SF01         400.1318 MHz
FIDRES        30.517578 Hz
SW            9.762 ppm
FnMODE        QF
SI            1024
SF           400.1300080 MHz
WDW           QSINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF           400.1300098 MHz
WDW           QSINE
SSB           0
LB            0.00 Hz
GB            0
```

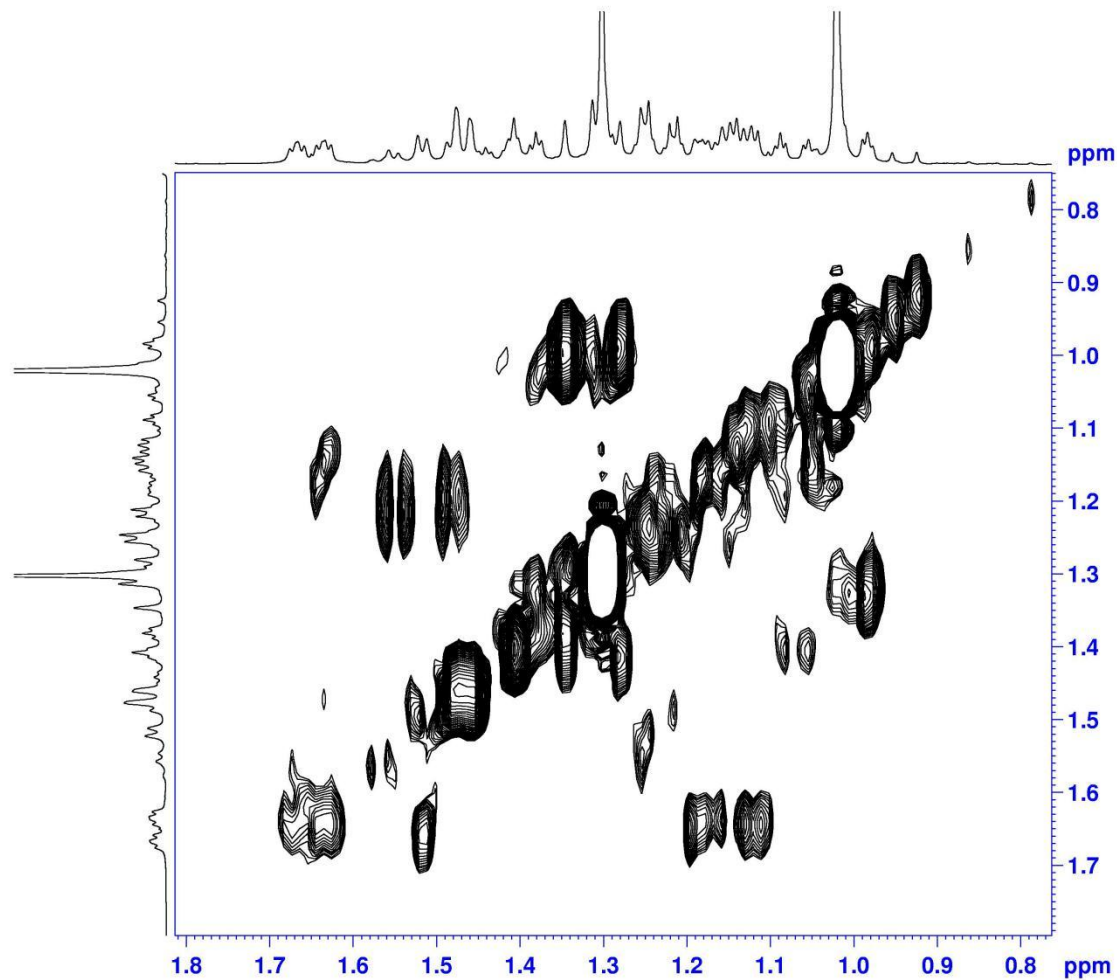
^1H - ^1H COSY (400 MHz) spectrum of tagalide A (1) in CDCl_3



```
NAME R-36-1-1
EXPNO 4
PROCNO 1
Date_ 20160203
Time 21.07
INSTRUM spect
PROBHD 5 mm CPMASQ BB
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 8
DS 8
SWH 3906.250 Hz
FIDRES 1.907349 Hz
AQ 0.2621940 sec
RG 208.5
DW 128.000 usec
DE 10.00 usec
TE 297.0 K
D0 0.00000300 sec
D1 1.89678097 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00004000 sec
D16 0.00020000 sec
IN0 0.00025600 sec
```

```
----- CHANNEL f1 -----
SFO1 400.1318006 MHz
NUC1 1H
P0 11.50 usec
P1 11.50 usec
P17 2500.00 usec
ND0 1
TD 128
SFO1 400.1318 MHz
FIDRES 30.517578 Hz
SW 9.762 ppm
FnMODE QF
SI 1024
SF 400.1300080 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
```

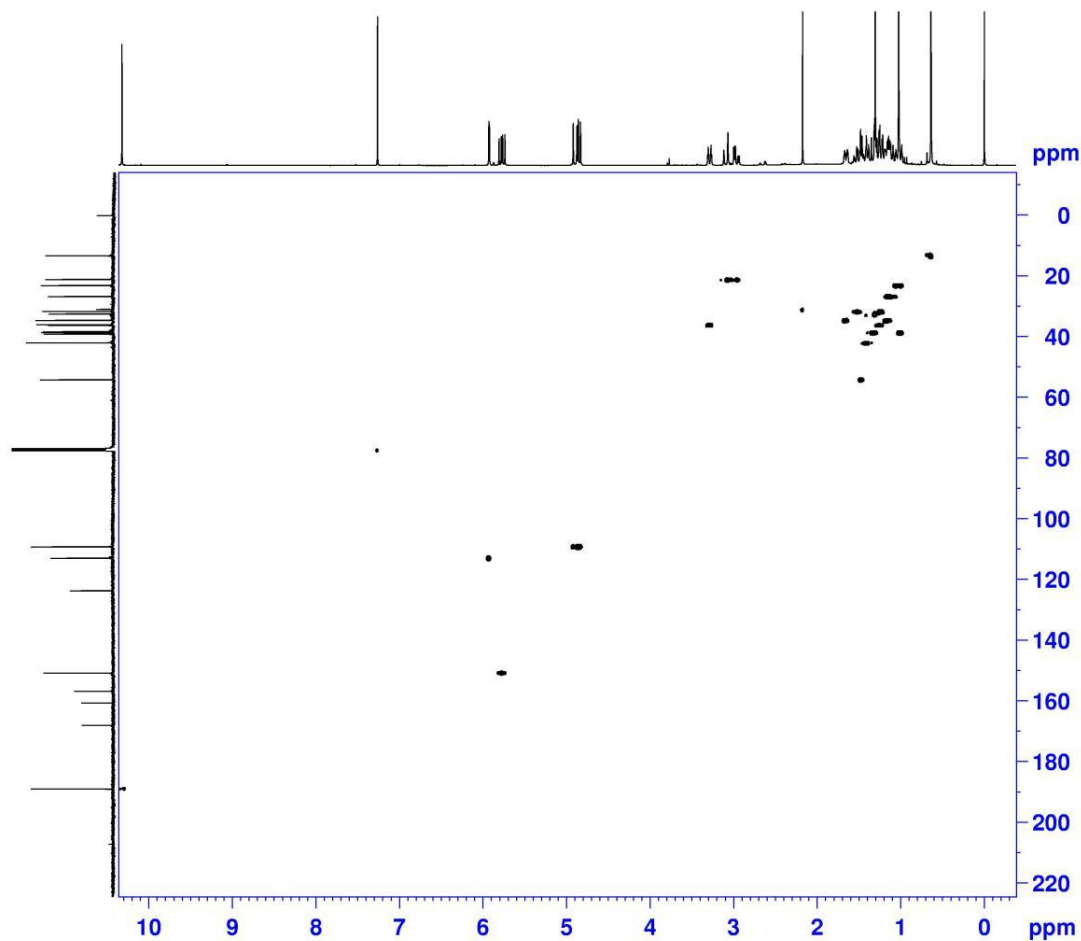
^1H - ^1H COSY (400 MHz) spectrum of tagalide A (1) in CDCl_3



```
NAME          R-36-1-1
EXPNO         4
PROCNO        1
Date_         20160203
Time          21.07
INSTRUM       spect
PROBHD        5 mm CYPBBO BB
PULPROG       cosygpppqf
TD            2048
SOLVENT       CDC13
NS            8
DS            8
SWH           3906.250 Hz
FIDRES        1.907349 Hz
AQ            0.2621940 sec
RG            208.5
DW            128.000 usec
DE            10.00 usec
TE            297.0 K
DO            0.00000300 sec
D1            1.89678097 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00025600 sec
```

```
----- CHANNEL f1 -----
SFO1          400.1318006 MHz
NUC1          1H
P0            11.50 usec
P1            11.50 usec
P17           2500.00 usec
ND0           1
TD            128
SFO1          400.1318 MHz
FIDRES        30.517578 Hz
SW            9.762 ppm
F1MODE        QF
SI            1024
SF            400.1300080 MHz
WDW           QSINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            400.1300098 MHz
WDW           QSINE
SSB           0
LB            0.00 Hz
GB            0
```

HSQC (400 MHz) spectrum of tagalide A (1) in CDCl₃



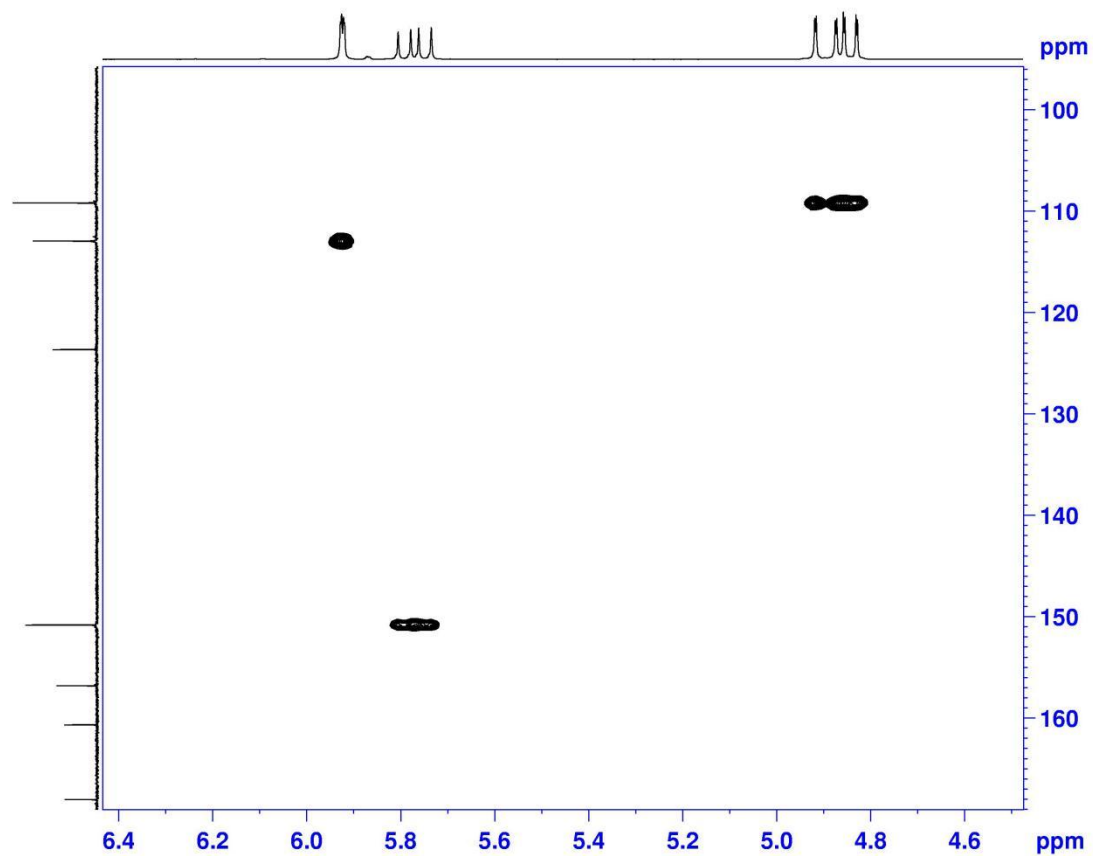
```

NAME          R-36-1-1
EXPNO         5
PROCNO        1
Date_         20160203
Time          21.47
INSTRUM       spect
PROBHD        5 mm CPBPR3 BB
PULPROG       hsqcetgpai2
TD            1024
SOLVENT       CDCl3
NS            16
DS            16
SWH           4302.926 Hz
FIDRES        4.202076 Hz
AQ            0.1190388 sec
RG            208.5
DW            116.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
DO            0.0000300 sec
D1            1.46497905 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
TNO           0.00002000 sec
ZGPTNS
    
```

```

----- CHANNEL f1 -----
SF01         400.1320007 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
F28           0.00 usec
ND0           2
TD            256
SF01         100.6233 MHz
FIDRES        93.900238 Hz
SW            238.896 ppm
FmMODE        Echo-Antiecho
SI            1024
SF            400.1300070 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
EC            1.40
SI            1024
MC2           echo-antiecho
SF            100.6127465 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
    
```

HSQC (400 MHz) spectrum of tagalide A (1) in CDCl₃

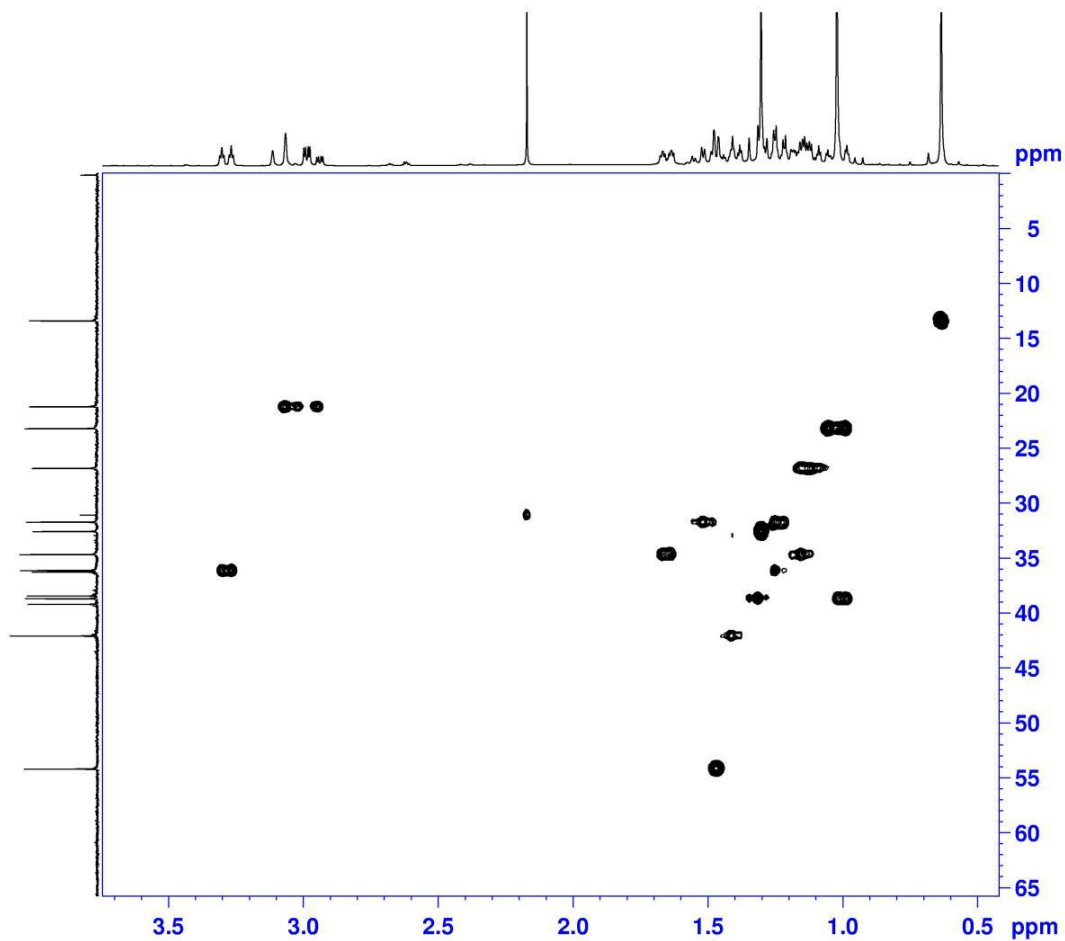


```

NAME          R-36-1-1
EXPNO         5
PROCNO        1
Date_         20160203
Time          21.47
INSTRUM       spect
PROBHD        5 mm CPBPBBO BB
PULPROG       hsqcetppr12
TD            1024
SOLVENT       CDCl3
NS            16
DS            16
SWH           4302.926 Hz
FIDRES        4.202076 Hz
AQ            0.1190388 sec
RG            208.5
DW            116.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
D0            0.00000300 sec
D1            1.46497905 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00002080 sec
ZGOPTNS

***** CHANNEL f1 *****
SF01          400.1320007 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
P28           0.00 usec
ND0           2
TD            256
SF01          100.6233 MHz
FIDRES        93.900238 Hz
SW            238.896 ppm
F1MODE        Echo-Antiecho
SI            1024
SF            400.1300070 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           echo-antiecho
SF            100.6127465 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
    
```

HSQC (400 MHz) spectrum of tagalide A (1) in CDCl₃



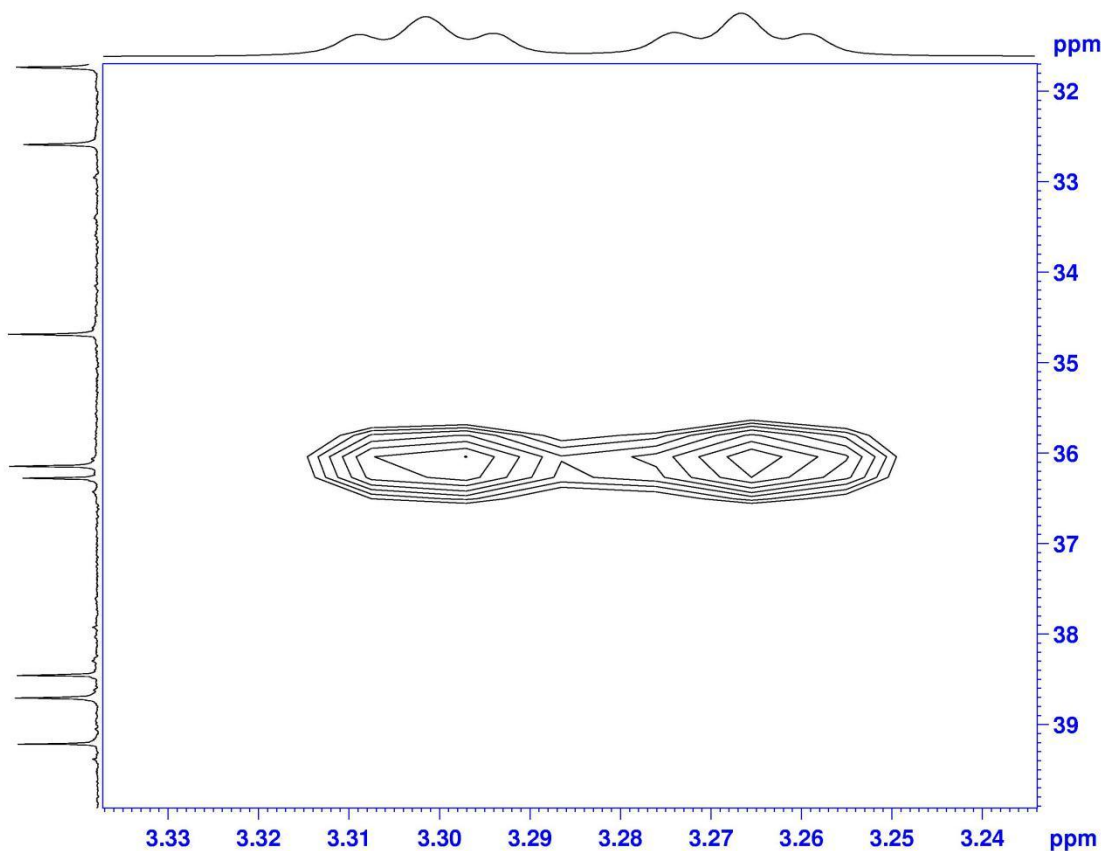
```

NAME          R-36-1-1
EXPNO         5
PROCNO        1
Date_         20160203
Time          21.47
INSTRUM       spect
PROBHD        5 mm CPBPRB0 BB
PULPROG       hsqcetgps12
TD            1024
SOLVENT       CDCl3
NS            16
DS            16
SWH           4302.926 Hz
FIDRES        4.202076 Hz
AQ            0.1190388 sec
RG            208.5
DW            116.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
D0            0.0000000 sec
D1            1.46497905 sec
D4            0.0012434 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
TNO           0.00002080 sec
ZGPG-TNS
    
```

```

----- CHANNEL f1 -----
SF01         400.1320007 MHz
NUC1         1H
P1           11.50 usec
P2           23.00 usec
P28          0.00 usec
NDO          2
TD           256
SF01         100.6233 MHz
FIDRES        93.900238 Hz
SW           238.896 ppm
FmMODE       Echo-Antiecho
SI           1024
SF           400.1300070 MHz
WDW          QSINE
SSB          2
GB           0.00 Hz
PC           1.40
SI           1024
MC2          echo-antiecho
SF           100.6127465 MHz
WDW          QSINE
SSB          2
GB           0.00 Hz
    
```

HSQC (400 MHz) spectrum of tagalide A (1) in CDCl₃

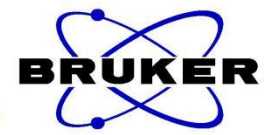
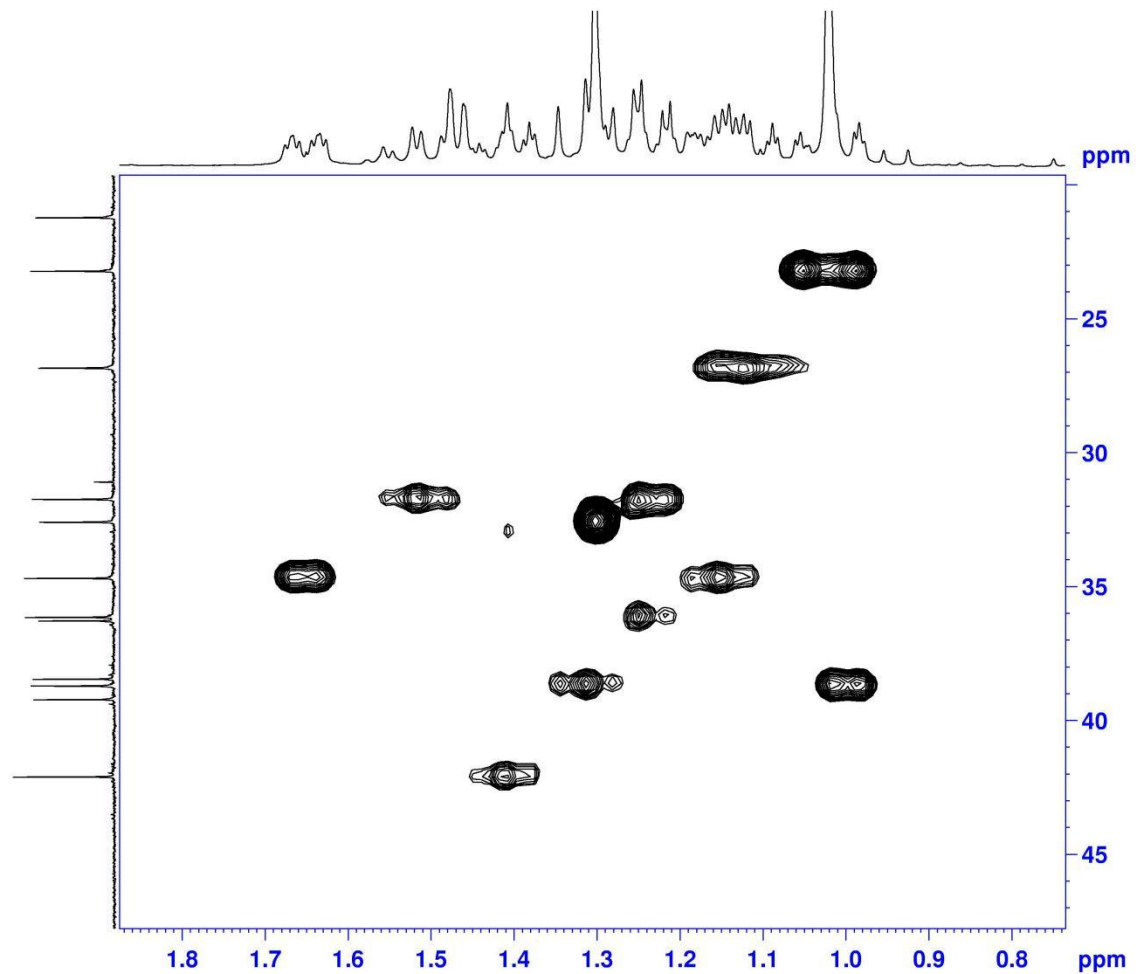


```

NAME          R-36-1-1
EXPNO         5
PROCNO        1
Date_         20160203
Time          21.47
INSTRUM       spect
PROBHD        5 mm CBBBO BB
PULPROG       hsqcetgps12
TD            1024
SOLVENT       CDCl3
NS            16
DS            16
SWH           4302.926 Hz
FIDRES        4.202076 Hz
AQ            0.1190388 sec
RG            208.5
DW            116.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
DO            0.00000300 sec
D1            1.46497905 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
LN0           0.00002080 sec
ZGOPTNS

===== CHANNEL f1 =====
SF01          400.1320007 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
P28           0.00 usec
ND0           2
TD            256
SF01          100.6233 MHz
FIDRES        93.900238 Hz
SW            238.896 ppm
FrMODE        Echo-Antiecho
SI            1024
SF            400.1300070 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           echo-antiecho
SF            100.6127465 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
    
```


HSQC (400 MHz) spectrum of tagalide A (1) in CDCl₃

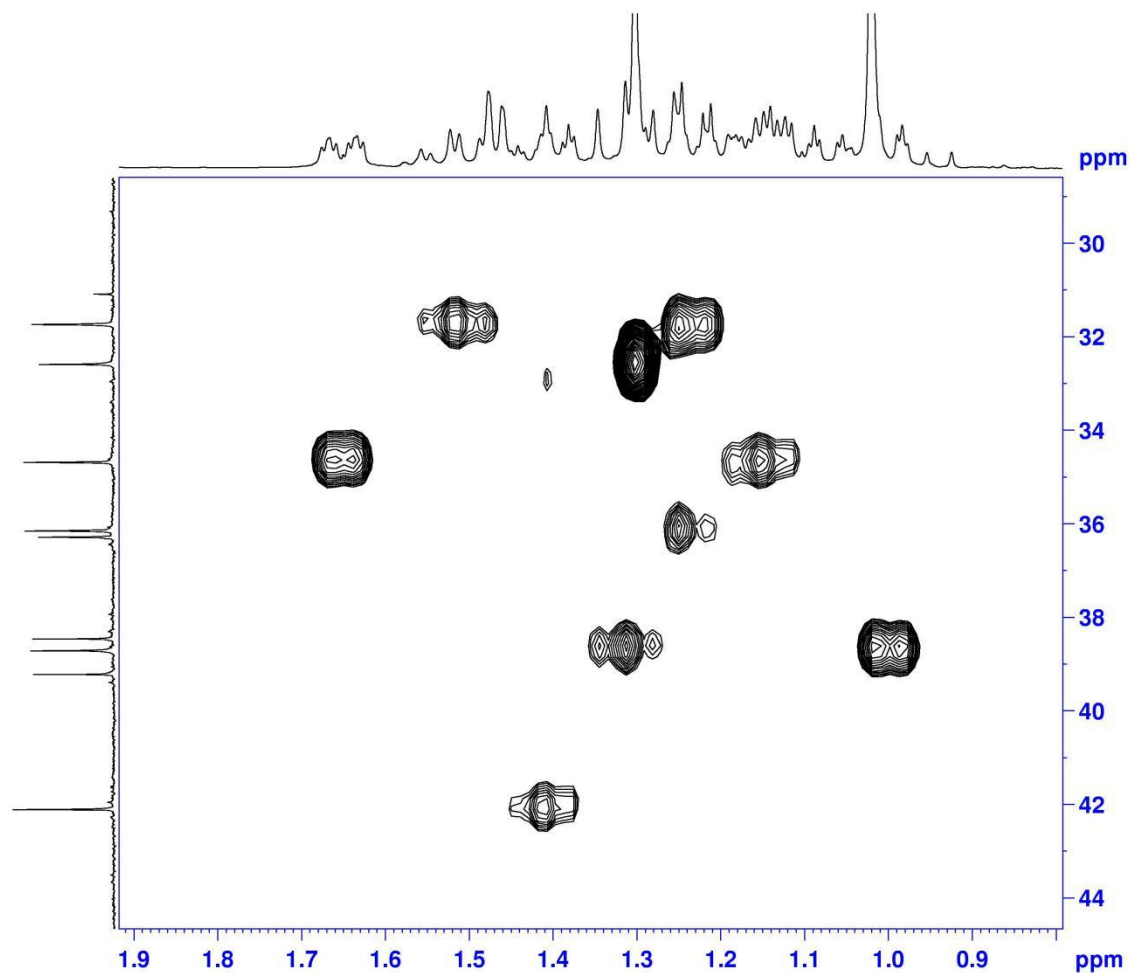


```

NAME          R-36-1-1
EXPNO         5
PROCNO        1
Date_         20160203
Time          21.47
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       hsqcetgps12
TD            1024
SOLVENT       CDCl3
NS            16
DS            16
SWH           4302.926 Hz
FIDRES        4.202076 Hz
AQ            0.1190388 sec
RG            208.5
DW            116.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
D0            0.00000300 sec
D1            1.46497905 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
INO           0.00002080 sec
ZGPTNS

===== CHANNEL f1 =====
SF01          400.1320007 MHz
NUC1          1H
F1            11.50 usec
P2            23.00 usec
P28           0.00 usec
ND0           2
TD            256
SF01          100.6233 MHz
FIDRES        93.900238 Hz
SW            238.896 ppm
FrMODE        Echo-Antiecho
SI            1024
SF            400.1300070 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           echo-antiecho
SF            100.6127465 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
    
```

HSQC (400 MHz) spectrum of tagalide A (1) in CDCl₃

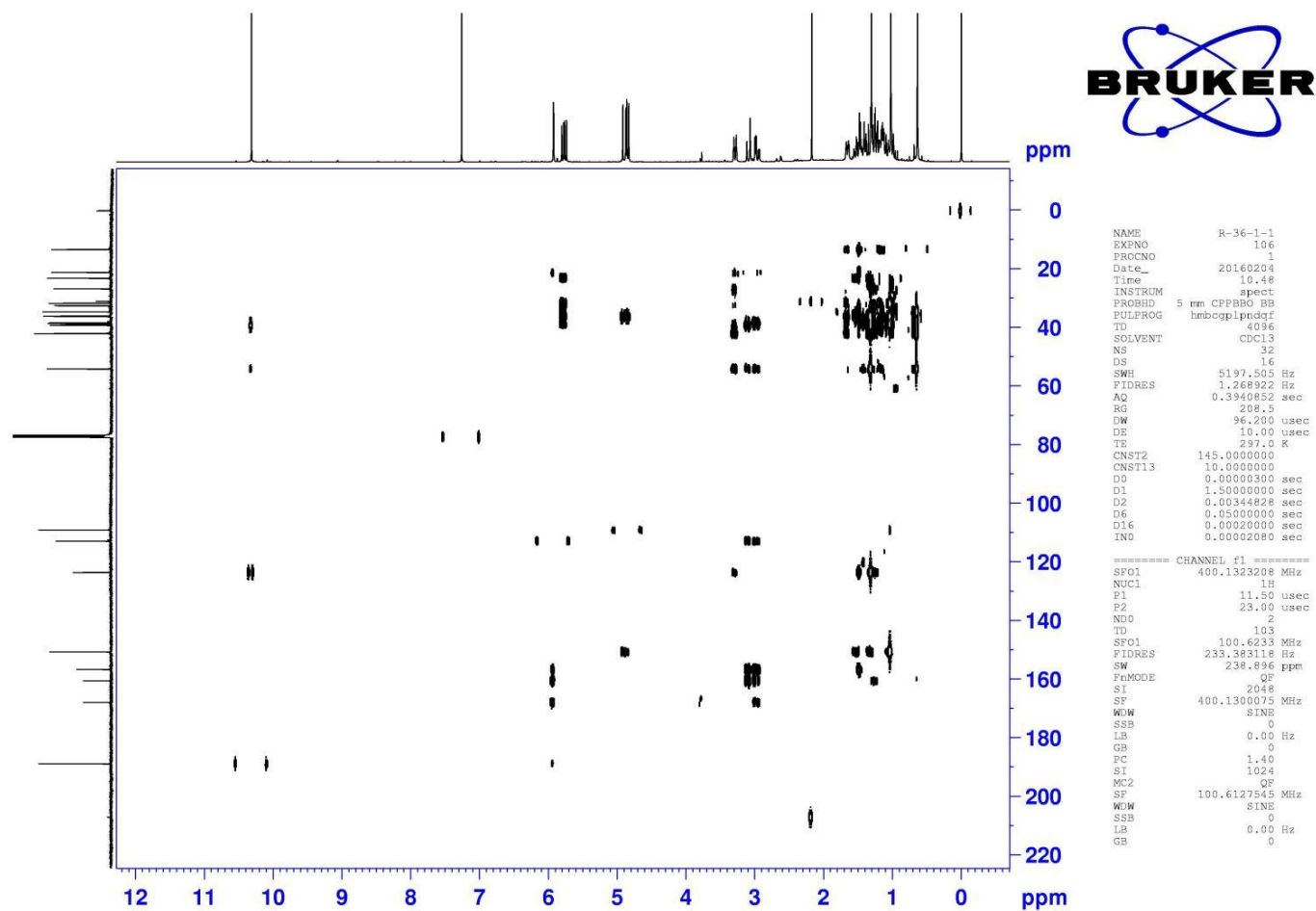


```

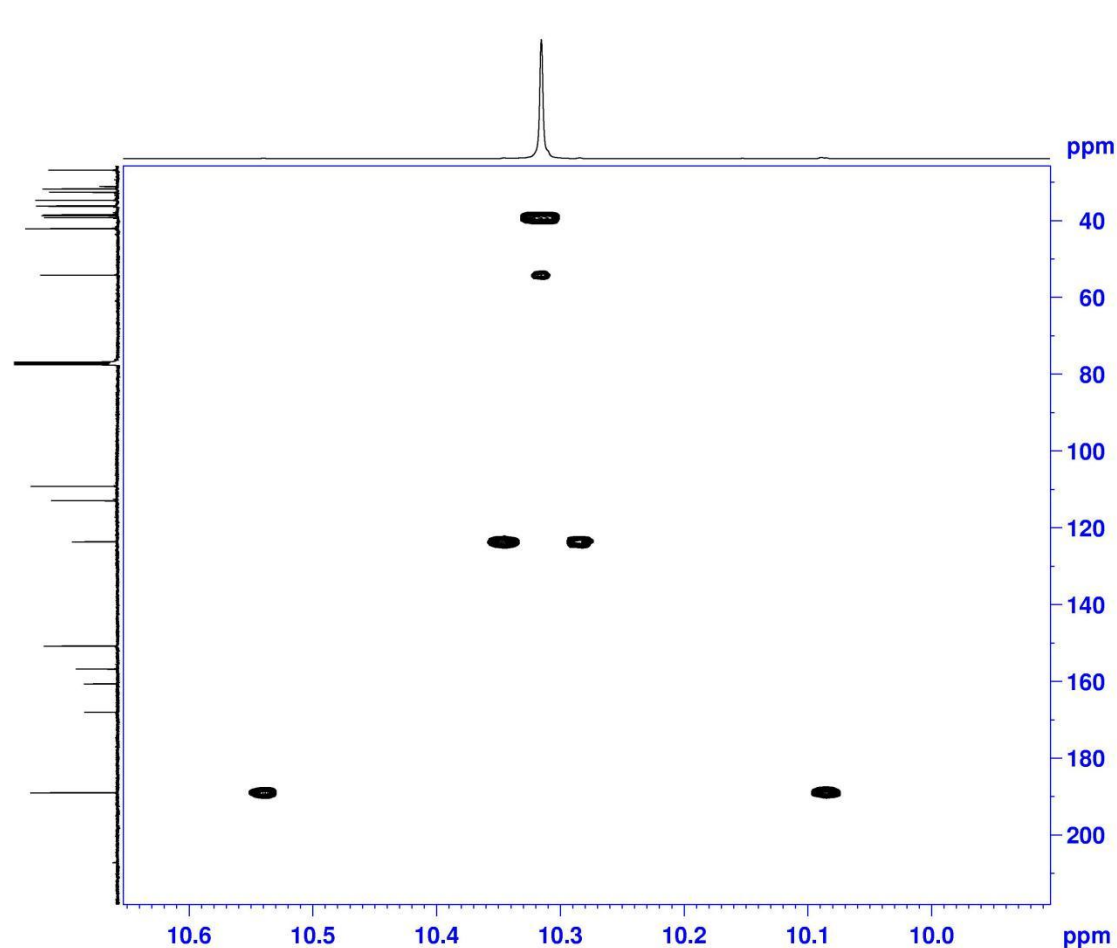
NAME          R-36-1-1
EXPNO         5
PROCNO        1
Date_         20160203
Time          21.47
INSTRUM       spect
PROBHD        5 mm CPMAS BB
PULPROG       hsqcetgpsi2
TD            1024
SOLVENT       CDCl3
NS            16
DS            16
SWH           4302.926 Hz
FIDRES        4.202076 Hz
AQ            0.1130388 sec
RG            208.5
DW            116.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
D0            0.00000300 sec
D1            1.46497905 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
INO           0.00002080 sec
ZGOPTNS

===== CHANNEL f1 =====
SF01          400.1320007 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
P28           0.00 usec
NDO           2
TD            256
SF01          100.6233 MHz
FIDRES        93.900238 Hz
SW            238.896 ppm
FnMODE        Echo-Antiecho
SI            1024
SF            400.1300070 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           echo-antiecho
SF            100.6127465 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
    
```

HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃



HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃



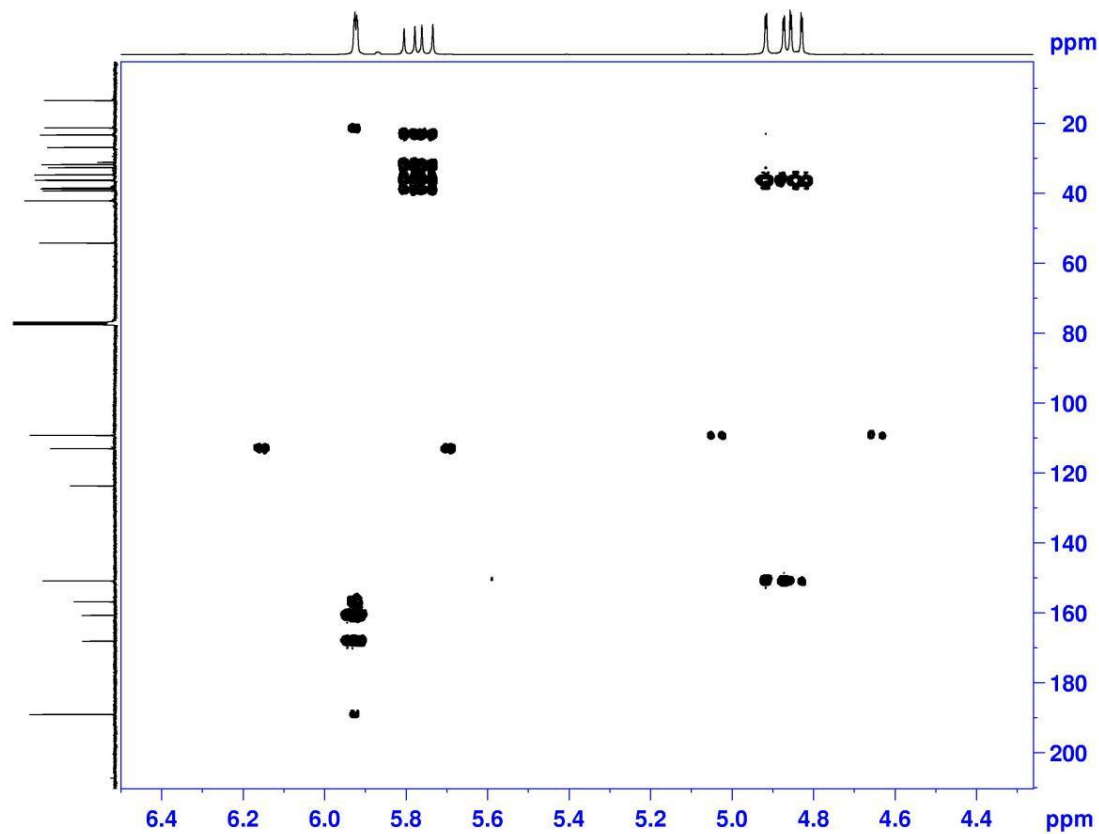
```

NAME           R-36-1-1
EXPNO          106
PROCNO         1
Date_          20160204
Time          10.48
INSTRUM        spect
PROBHD         5 mm CFPBBO BB
PULPROG        hmbcgp1pndqf
TD             4096
SOLVENT        CDCl3
NS             32
DS             16
SWH            5197.505 Hz
FIDRES         1.268922 Hz
AQ             0.3940852 sec
RG             208.5
DW             96.200 usec
DE             10.00 usec
TE             297.0 K
CNST2          145.0000000
CNST13         10.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D2             0.00344828 sec
D6             0.05000000 sec
D16            0.00020000 sec
IN0            0.00002080 sec
    
```

```

----- CHANNEL f1 -----
SFO1          400.1323208 MHz
NUC1           1H
P1             11.50 usec
P2             23.00 usec
ND0            2
TD             103
SFO1          100.6233 MHz
FIDRES         233.383118 Hz
SW             238.896 ppm
FhMODE         QF
SI             2048
SF            400.1300075 MHz
WDW            SINE
SSB            0
LB             0.00 Hz
GB             0
PC             1.40
SI             1024
MC2            QF
SF            100.6127545 MHz
WDW            SINE
SSB            0
LB             0.00 Hz
GB             0
    
```

HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃

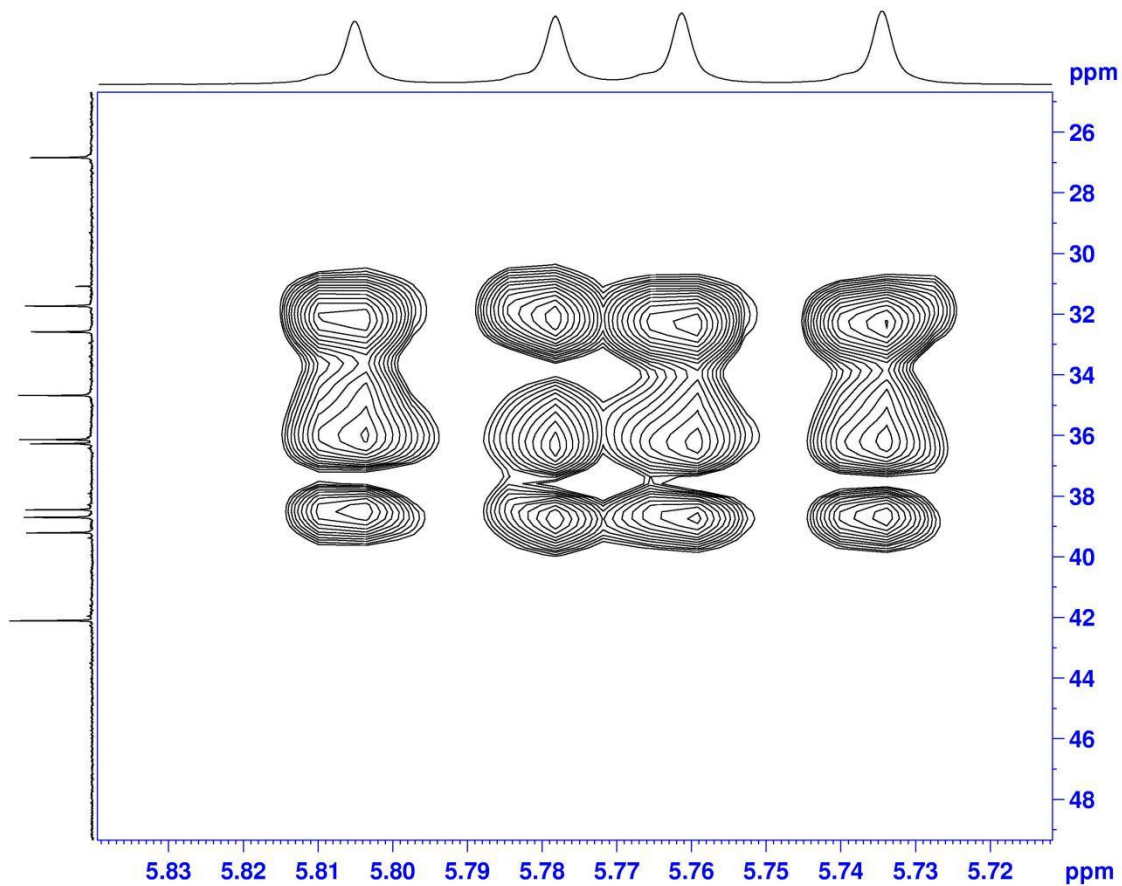


```

NAME           R-36-1-1
EXPNO           106
PROCNO          1
Date_           20160204
Time            10.48
INSTRUM         spect
PROBHD          5 mm CPPBBO BB
PULPROG         hmbcggplpndgf
TD              4096
SOLVENT         CDCl3
NS              32
DS              16
SWH             5197.505 Hz
FIDRES         1.268922 Hz
AQ             0.3940852 sec
RG             208.5
DW             96.200 usec
DE             10.00 usec
TE             297.0 K
CNST2          145.0000000
CNST13         10.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D2             0.00344828 sec
D6             0.05000000 sec
D16            0.00020000 sec
IN0            0.00002080 sec

----- CHANNEL f1 -----
SF01           400.1323208 MHz
NUC1           1H
P1             11.50 usec
P2             23.00 usec
ND0            2
TD             103
SF01           100.6233 MHz
FIDRES         233.383118 Hz
SW             238.896 ppm
FrMODE         QF
SI             2048
SF             400.1300075 MHz
WDW            SINE
SSB            0
LB             0.00 Hz
GB             0
PC             1.40
SI             1024
MC2            QF
SF             100.6127545 MHz
WDW            SINE
SSB            0
LB             0.00 Hz
GB             0
    
```

HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃

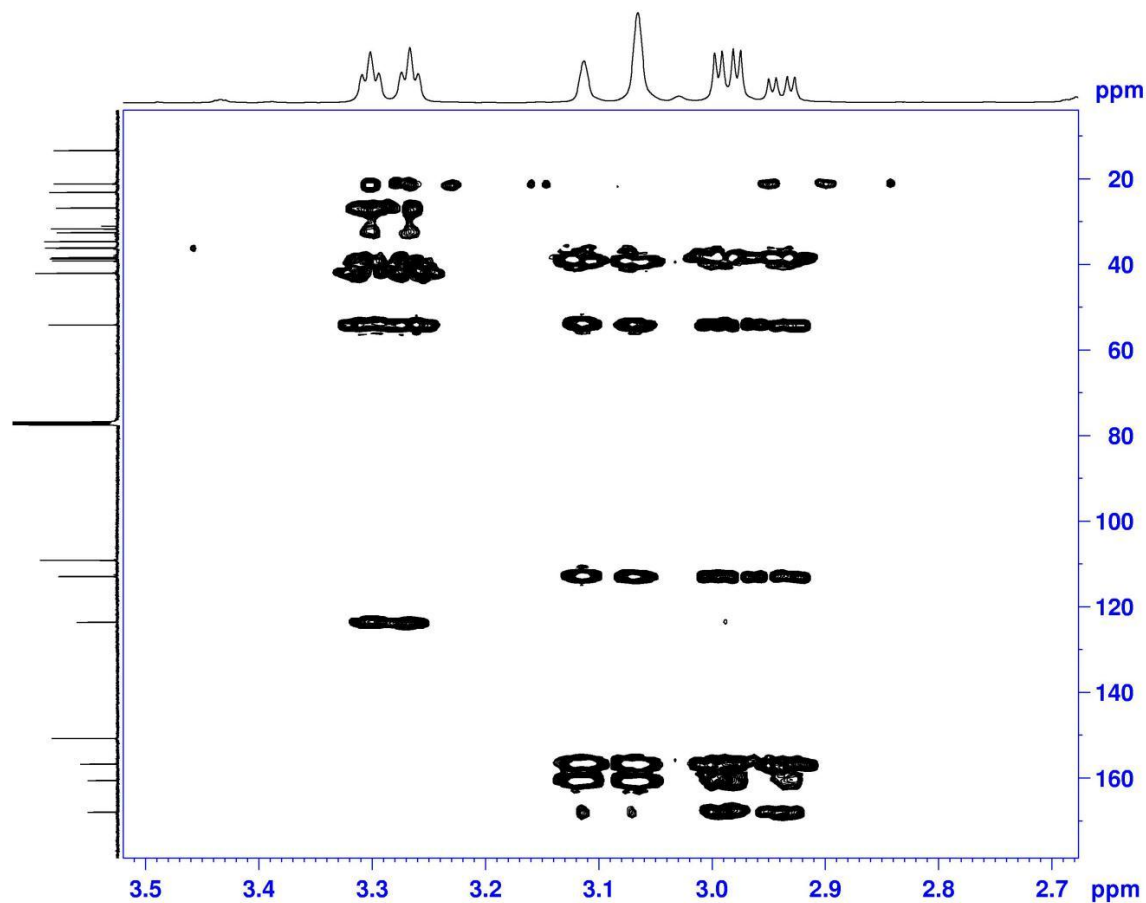


```

NAME          R-36-1-1
EXPNO         106
PROCNO        1
Date_         20160204
Time          10.48
INSTRUM       spect
PROBHD        5 mm CFPBBO BB
PULPROG       hmbcgp1p0d4f
TD            4096
SOLVENT       CDCl3
NS            32
DS            16
SWH           5197.505 Hz
FIDRES        1.268922 Hz
AQ            0.3940852 sec
RG            208.5
DW            96.200 usec
DE            10.00 usec
TE            297.0 K
CNSTZ         145.0000000
CNSTI3        10.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00020000 sec
IN0           0.00002080 sec

----- CHANNEL f1 -----
SF01          400.1323208 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
ND0           2
TD            103
SF01          100.6233 MHz
FIDRES        233.383118 Hz
SW            238.896 ppm
FmMODE        QF
SI            2048
SF            400.1300075 MHz
WEW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            100.6127545 MHz
WEW           SINE
SSB           0
LB            0.00 Hz
GB            0
    
```

HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃

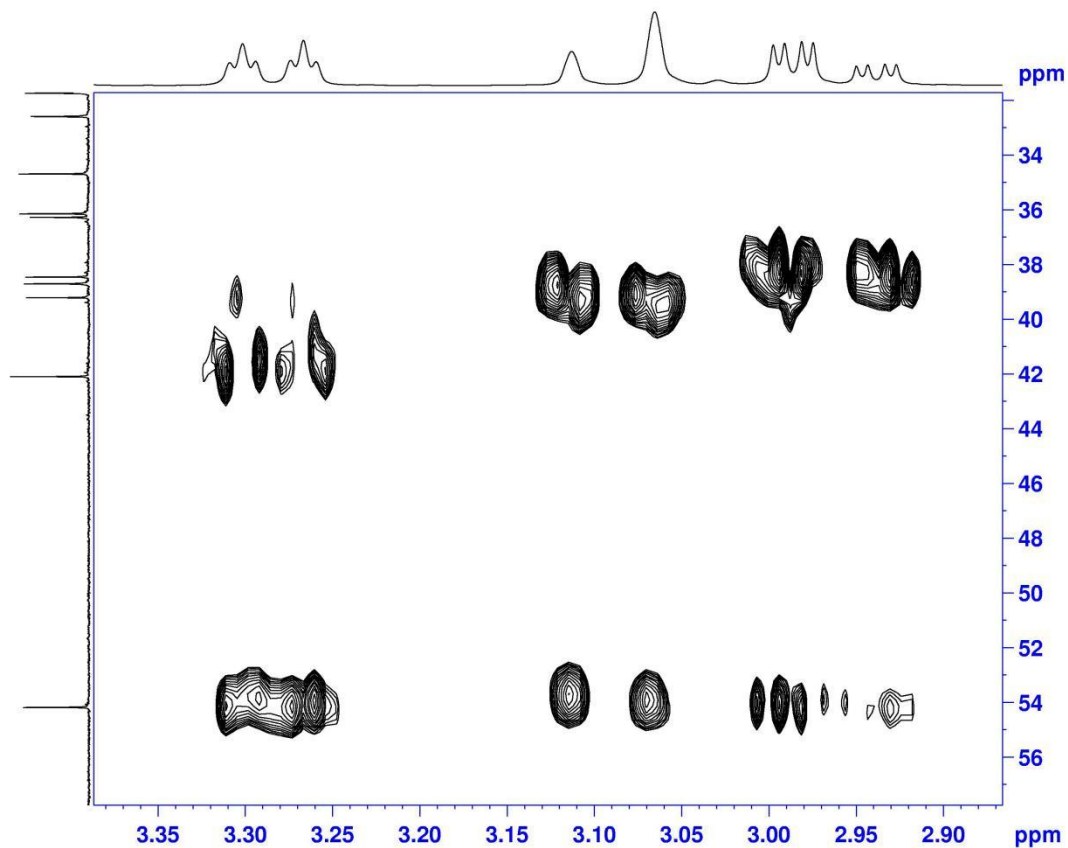


```

NAME          R-36-1-1
EXPNO         106
PROCNO        1
Date_         20160204
Time          10.48
INSTRUM       spect
PROBHD        5 mm CDPBBO BB
PULPROG       hmbcgp1pndef
TD            4096
SOLVENT       CDCl3
NS            32
DS            16
SWH           5197.505 Hz
FIDRES        1.268922 Hz
AQ            0.3940852 sec
RG            208.5
DW            96.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
CNST3         10.0000000
D0            0.0000000 sec
D1            1.5000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00020000 sec
TNO           0.0002080 sec

===== CHANNEL f1 =====
SF01          400.1323208 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
ND0           2
TD            163
SF01          100.62333 MHz
FIDRES        233.383118 Hz
SW            238.896 ppm
FmMODE        QF
SI            2048
SF            400.1300075 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            100.6127545 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
    
```

HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃

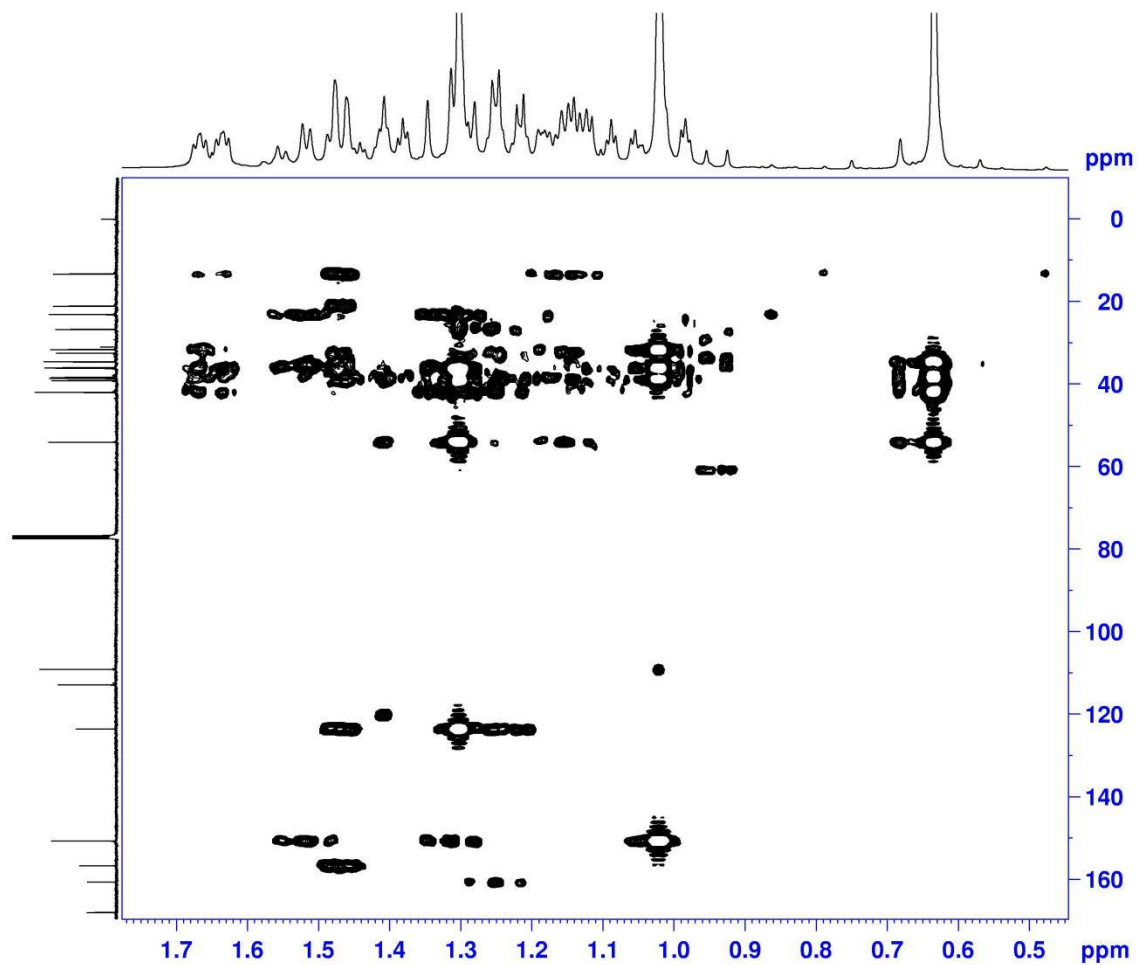


```

NAME          R-36-1-1
EXPNO         1
PROCNO        1
Date_         20160204
Time          10.48
INSTRUM       spect
PROBHD        5 mm CPMBO BB
PULPROG       hmcgplprdgf
TD            4096
SOLVENT       CDCl3
NS            32
DS            16
SWH           5197.505 Hz
FIDRES        1.268922 Hz
AQ            0.3940852 sec
RG            298.5
DW            96.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.000000
CNST13        10.000000
D0            0.00000300 sec
D1            1.50000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00020000 sec
IN0           0.00002080 sec

===== CHANNEL f1 =====
SFO1          400.1323208 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
ND0           2
TD            103
SFO1          100.6233 MHz
FIDRES        233.383118 Hz
SW            238.896 ppm
FEMODE        QF
SI            2048
SF            400.1300075 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
EC            1.40
SI            1024
MC2           QF
SF            100.6127545 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
    
```

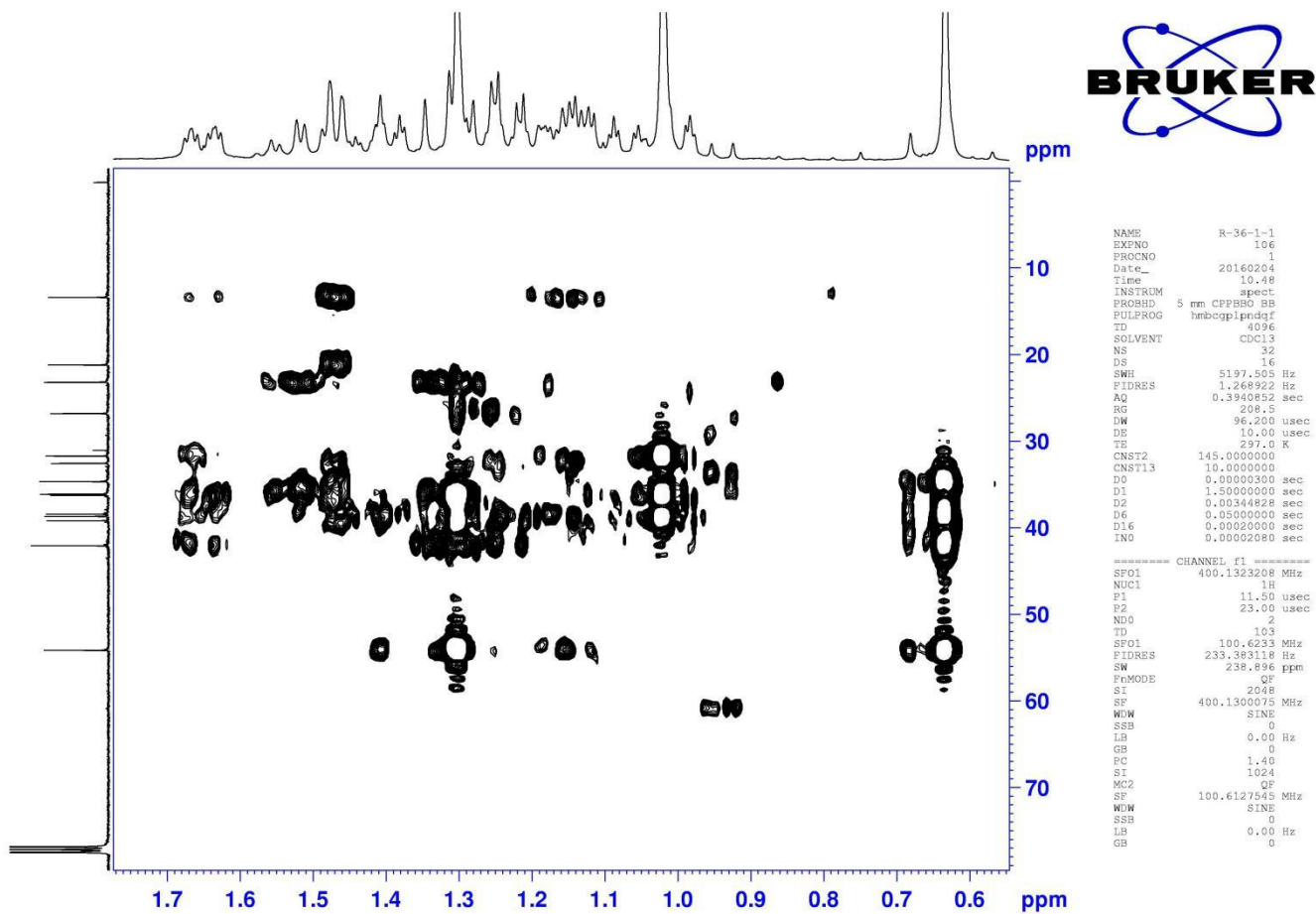

HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃



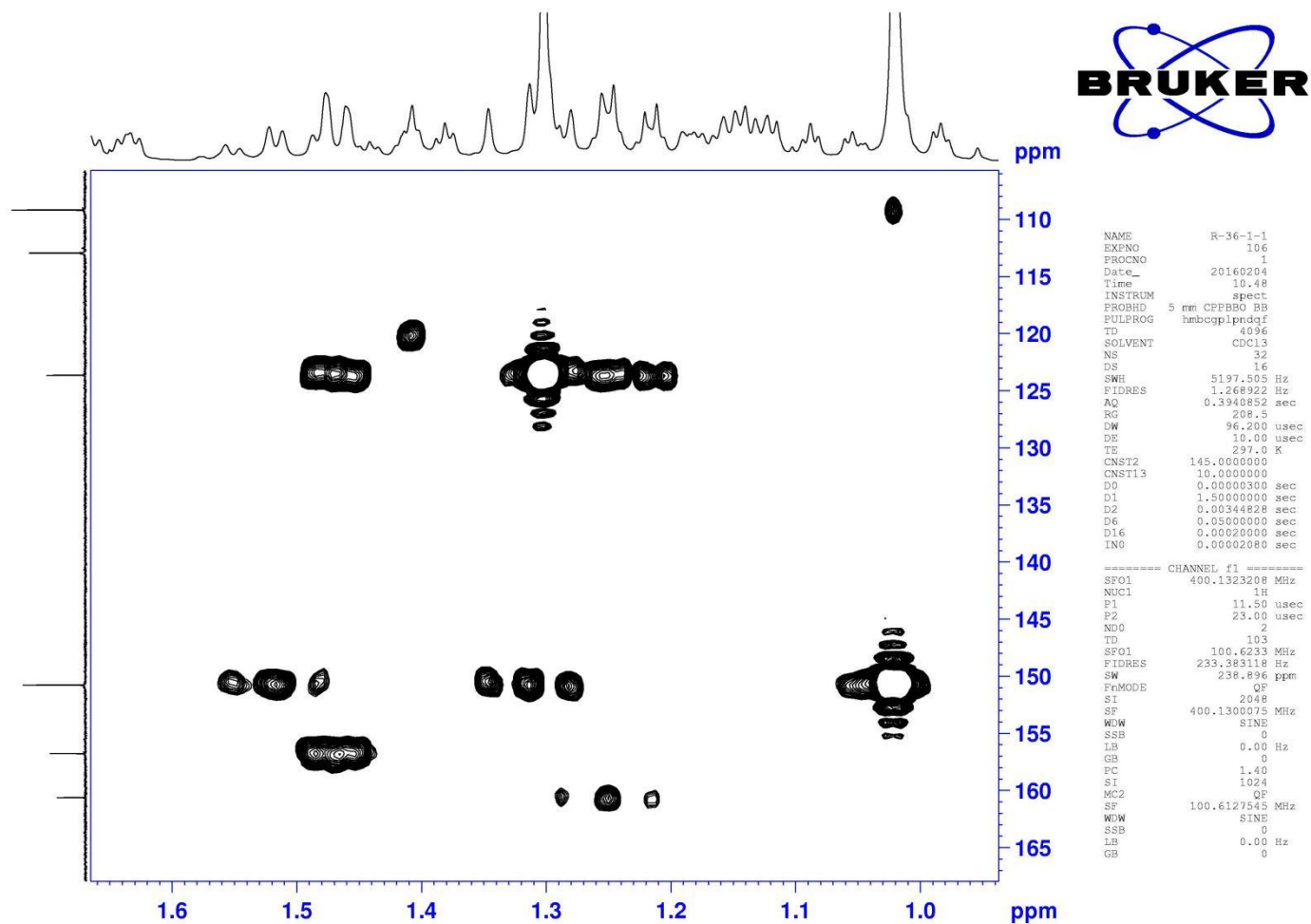
```
NAME R-36-1-1
EXPNO 106
PROCNO 1
Date_ 20160204
Time 10.48
INSTRUM spect
PROBHD 5 mm CFPBBO BB
PULPROG hmbcsp1pndt1f
TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 5197.505 Hz
FIDRES 1.268922 Hz
AQ 0.3940852 sec
RG 208.5
DW 96.200 usec
DE 10.00 usec
TE 297.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.0000300 sec
D1 1.5000000 sec
D2 0.00344828 sec
D6 0.0500000 sec
D16 0.0002000 sec
IN0 0.0002080 sec
```

```
===== CHANNEL f1 =====
SF01 400.1323208 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
ND0 2
TD 103
SF01 100.6233 MHz
FIDRES 233.383118 Hz
SW 238.896 ppm
FMODE QF
SI 2048
SF 400.1300075 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6127545 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```

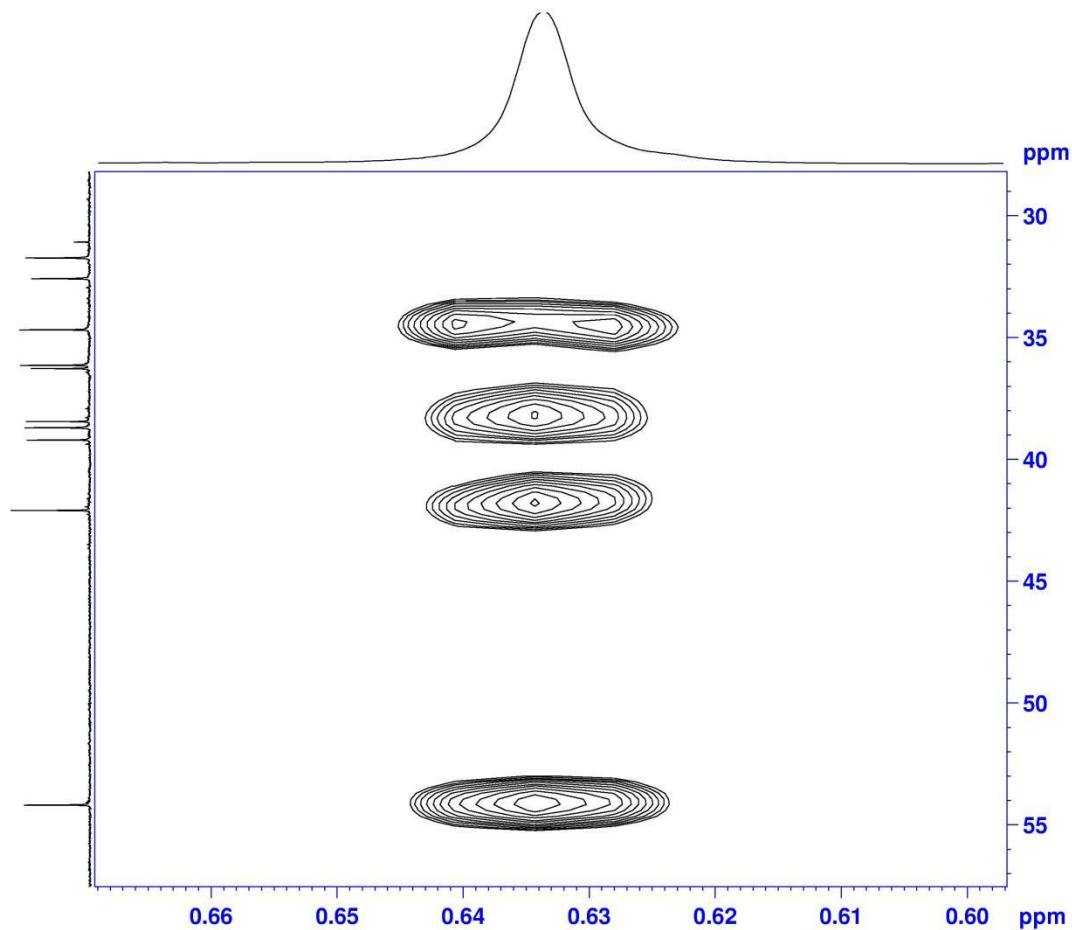
HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃



HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃



HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃

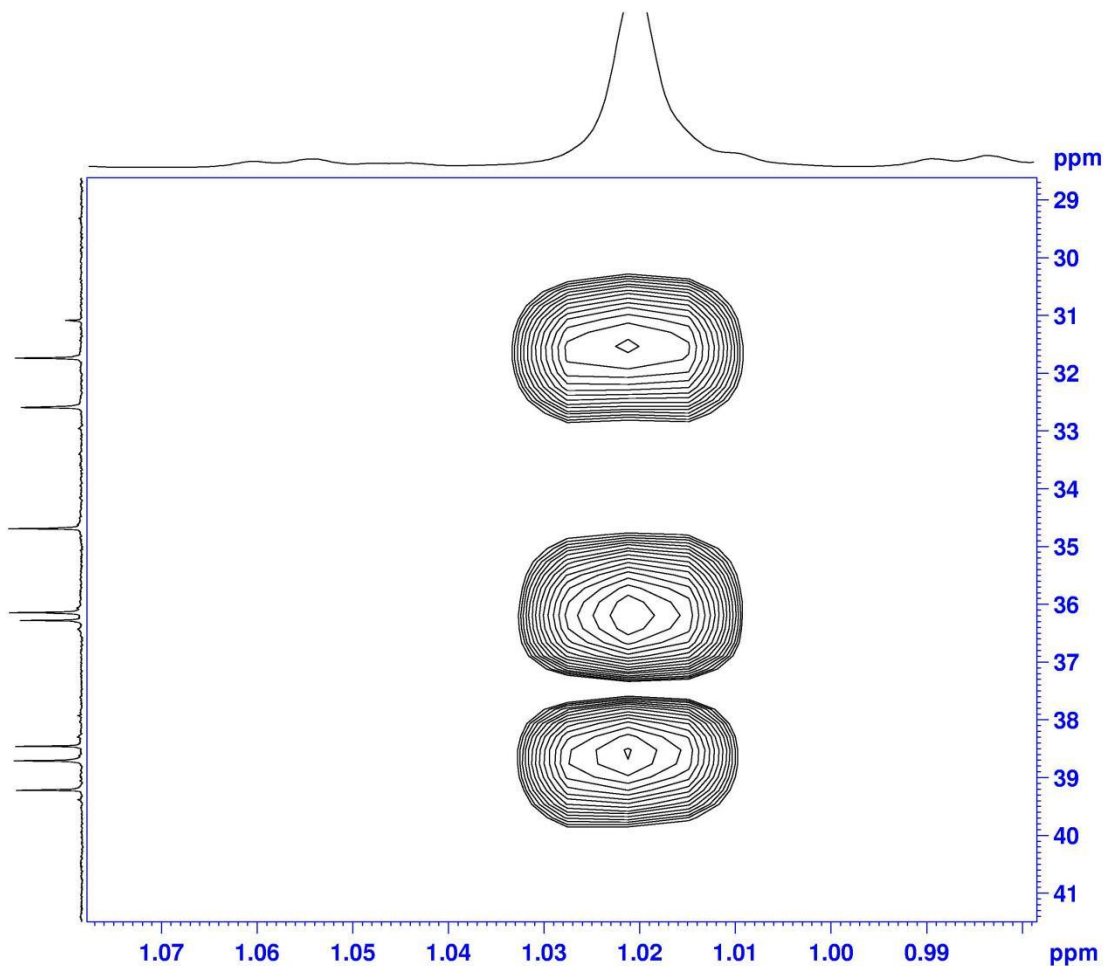


```

NAME          R-36-1-1
EXPNO         106
PROCNO        1
Date_         20160204
Time          10.48
INSTRUM       spect
PROBHD        5 mm CPMBO BB
PULPROG       hmbcsp1prdgf
TD            4096
SOLVENT       CDCl3
NS            32
DS            16
SWH           5197.505 Hz
FIDRES        1.268922 Hz
AQ            0.3940852 sec
RG            208.5
DW            96.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
CNST13        10.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00020000 sec
IN0           0.00002080 sec

===== CHANNEL f1 =====
SF01          400.1323208 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
ND0           2
TD            103
SF01          100.6233 MHz
FIDRES        233.383118 Hz
SW            238.896 ppm
F1MODE        QF
SI            2048
SF            400.1300075 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            100.6127545 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
    
```

HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃



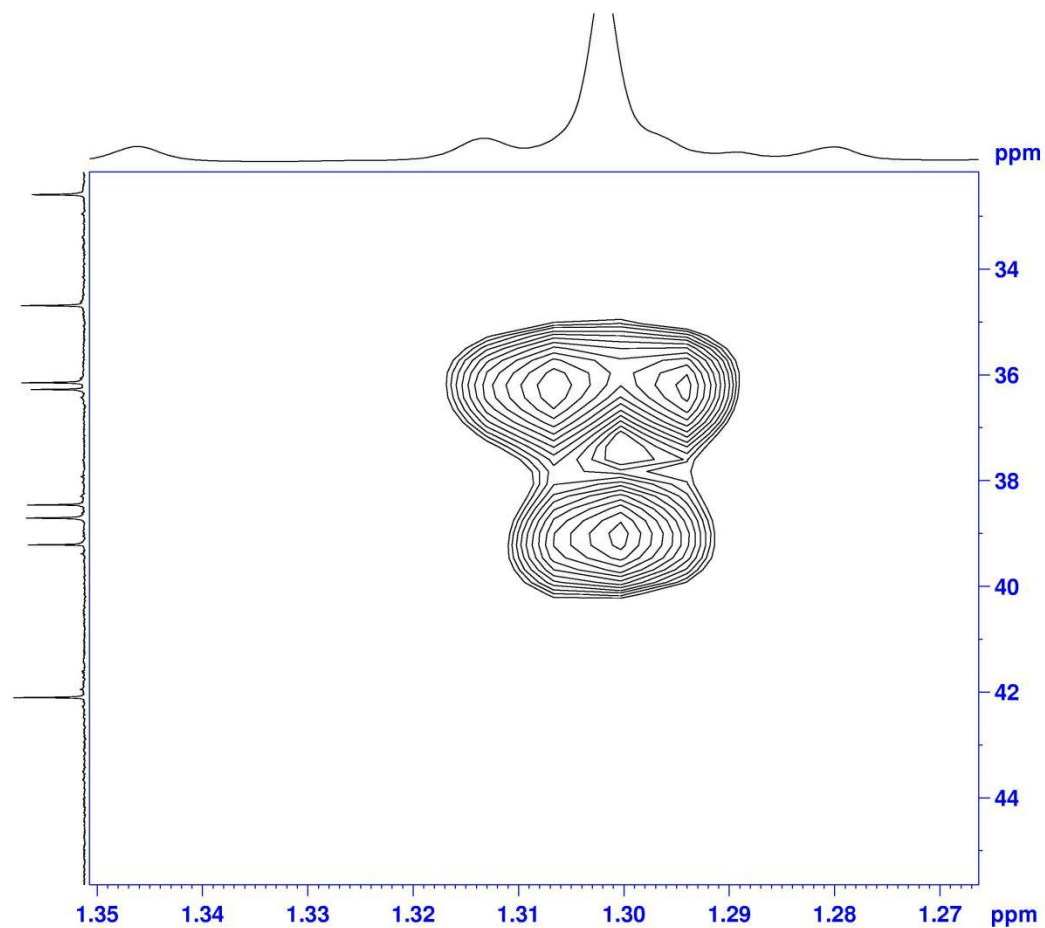
```

NAME          R-36-1-1
EXPNO         106
PROCNO        1
Date_         20160204
Time          10.48
INSTRUM       spect
PROBHD        5 mm CFPBBO BB
PULPROG       hmbcgp1p0d9f
TD            4096
SOLVENT       CDCl3
NS            32
DS            16
SWH           5197.505 Hz
FIDRES        1.268922 Hz
AQ            0.3940852 sec
RG            208.5
DW            96.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
CNST13        10.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00020000 sec
IN0           0.00002080 sec
  
```

```

===== CHANNEL f1 =====
SP01         400.1323298 MHz
NUC1         1H
P1           11.50 usec
P2           23.00 usec
ND0          2
TD           103
SP01         100.6233 MHz
FIDRES        233.383118 Hz
SW           238.896 ppm
F0MODE        QF
SI           2048
SF           400.1300075 MHz
WDW           SINE
SSB           0
LB           0.00 Hz
GB           0
PC           1.40
SI           1024
MC2           QF
SF           100.6127545 MHz
WDW           SINE
SSB           0
LB           0.00 Hz
GB           0
  
```

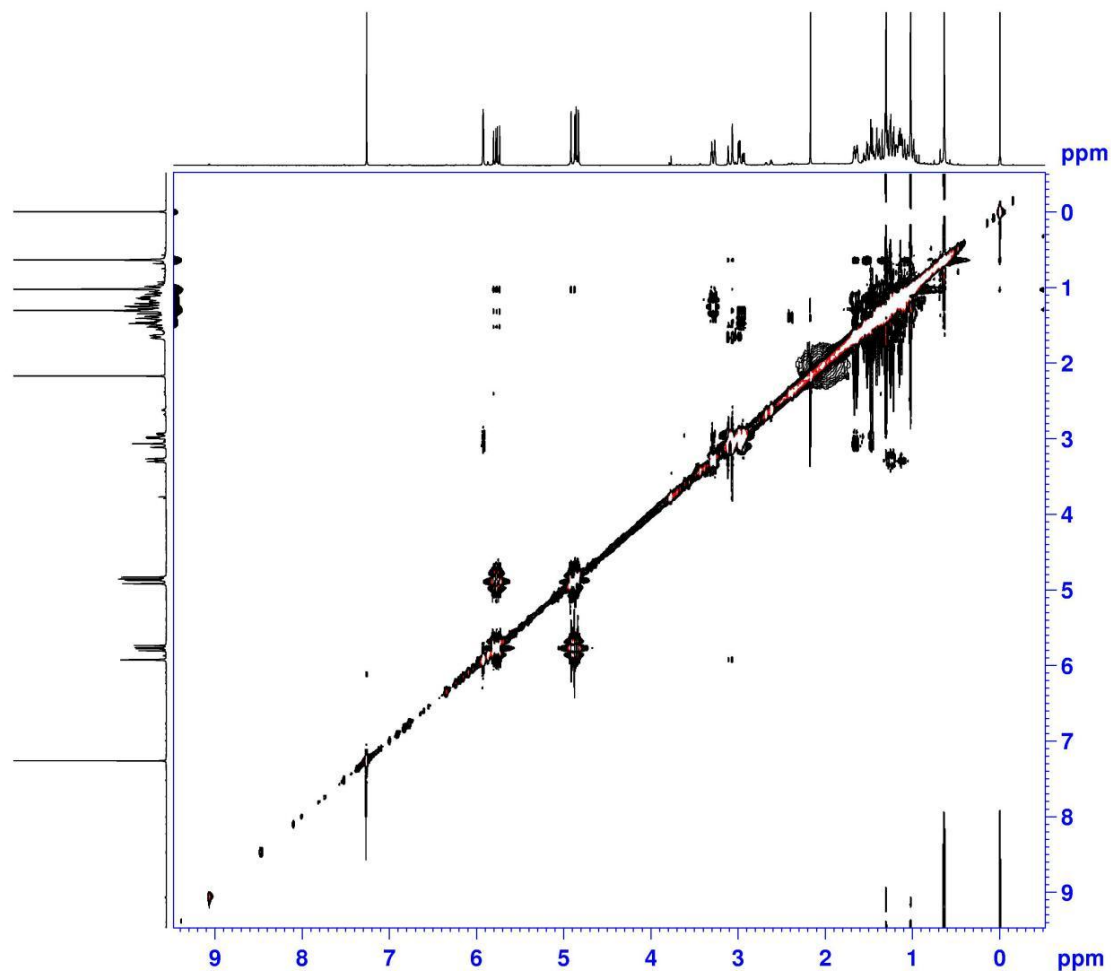
HMBC (400 MHz) spectrum of tagalide A (1) in CDCl₃



```
NAME R-36-1-1
EXPNO 106
PROCNO 1
Date_ 20160204
Time 10.48
INSTRUM spect
PROBHD 5 mm CFPBBO BB
PULPROG hmbcgp1prdgf
TD 4096
SOLVENT CDCl3
NS 32
DS 16
SWH 5197.505 Hz
FIDRES 1.268922 Hz
AQ 0.3940852 sec
RG 208.5
DW 96.200 usec
DE 10.00 usec
TE 297.0 K
CNST2 145.000000
CNST13 10.000000
DC 0.0000000 sec
D1 1.5000000 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.0002080 sec

----- CHANNEL f1 -----
SF01 400.1323208 MHz
NUC1 1H
F1 11.50 usec
P2 23.00 usec
NDO 2
TD 103
SF01 100.6233 MHz
FIDRES 233.383118 Hz
SW 238.896 ppm
PQMODE QF
SI 2048
SF 400.1300075 MHz
WDW SINE
SBB 0
LB 0.00 Hz
GB 0
FC 1.40
SI 1024
MC2 QF
SF 100.6127545 MHz
WDW SINE
SBB 0
LB 0.00 Hz
GB 0
```

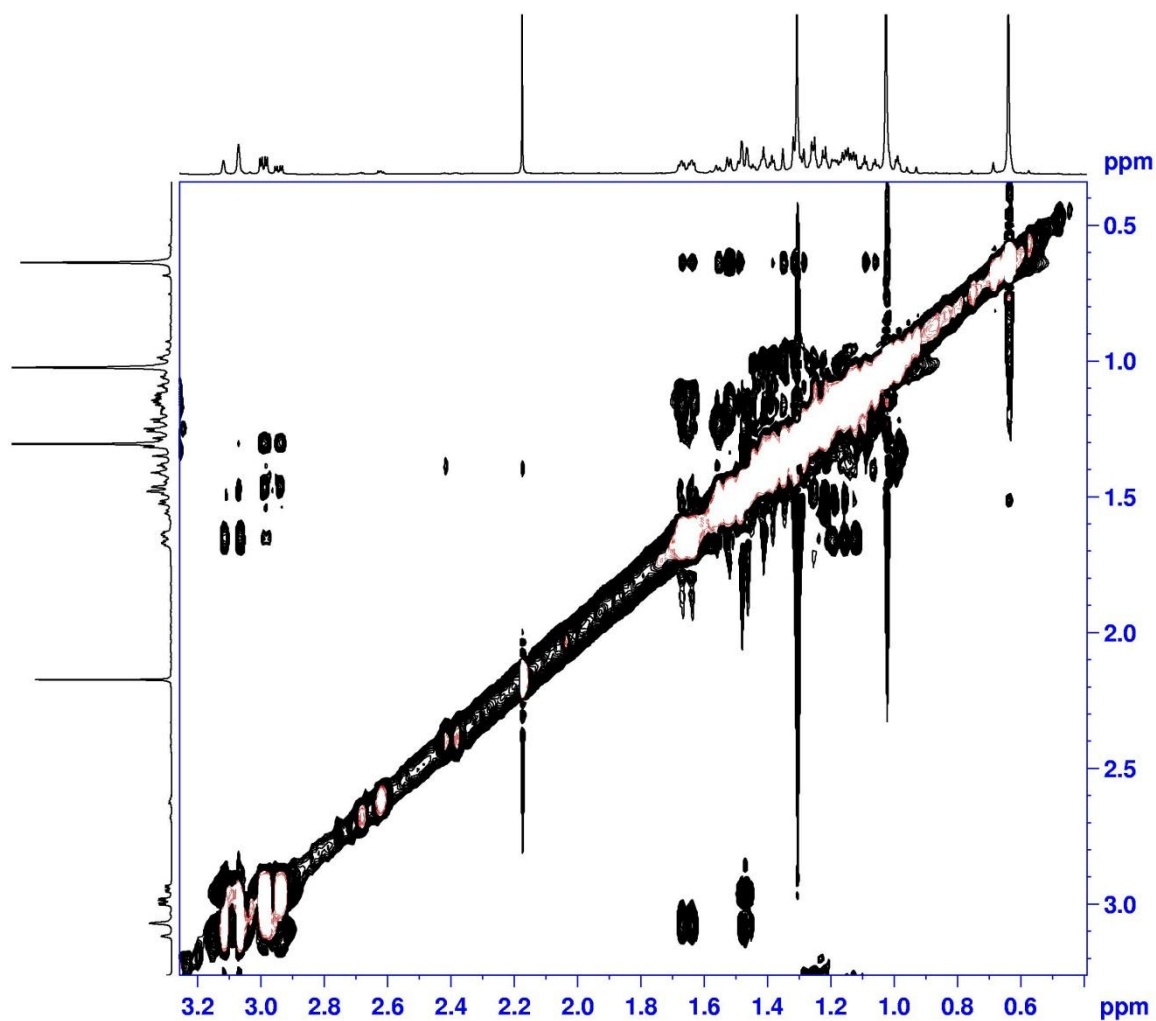
NOESY (400 MHz) spectrum of tagalide A (1) in CDCl₃



```
NAME R-36-1-1
EXPNO 7
PROCNO 1
Date_ 20160216
Time 0.40
INSTRUM spect
PROBHD 5 mm CPMAS
PULPROG noesypphpp
TD 2048
SOLVENT CDCl3
NS 16
DS 32
SWH 4000.000 Hz
FIDRES 1.953125 Hz
AQ 0.2560500 sec
RG 208.5
DW 125.000 usec
DE 10.00 usec
TE 297.0 K
DO 0.00011036 sec
D1 1.99385595 sec
DB 0.30000001 sec
D11 0.03000000 sec
D12 0.00020000 sec
D16 0.00020000 sec
IN0 0.00025000 sec

===== CHANNEL f1 =====
SFO1 400.1318006 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
P17 2500.00 usec
ND0 1
TD 256
SFO1 400.1318 MHz
FIDRES 15.625000 Hz
SW 9.997 ppm
EnMODE States-TFPI
SI 1024
SF 400.1300098 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 States-TFPI
SF 400.1300098 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
```

NOESY (400 MHz) spectrum of tagalide A (1) in CDCl₃



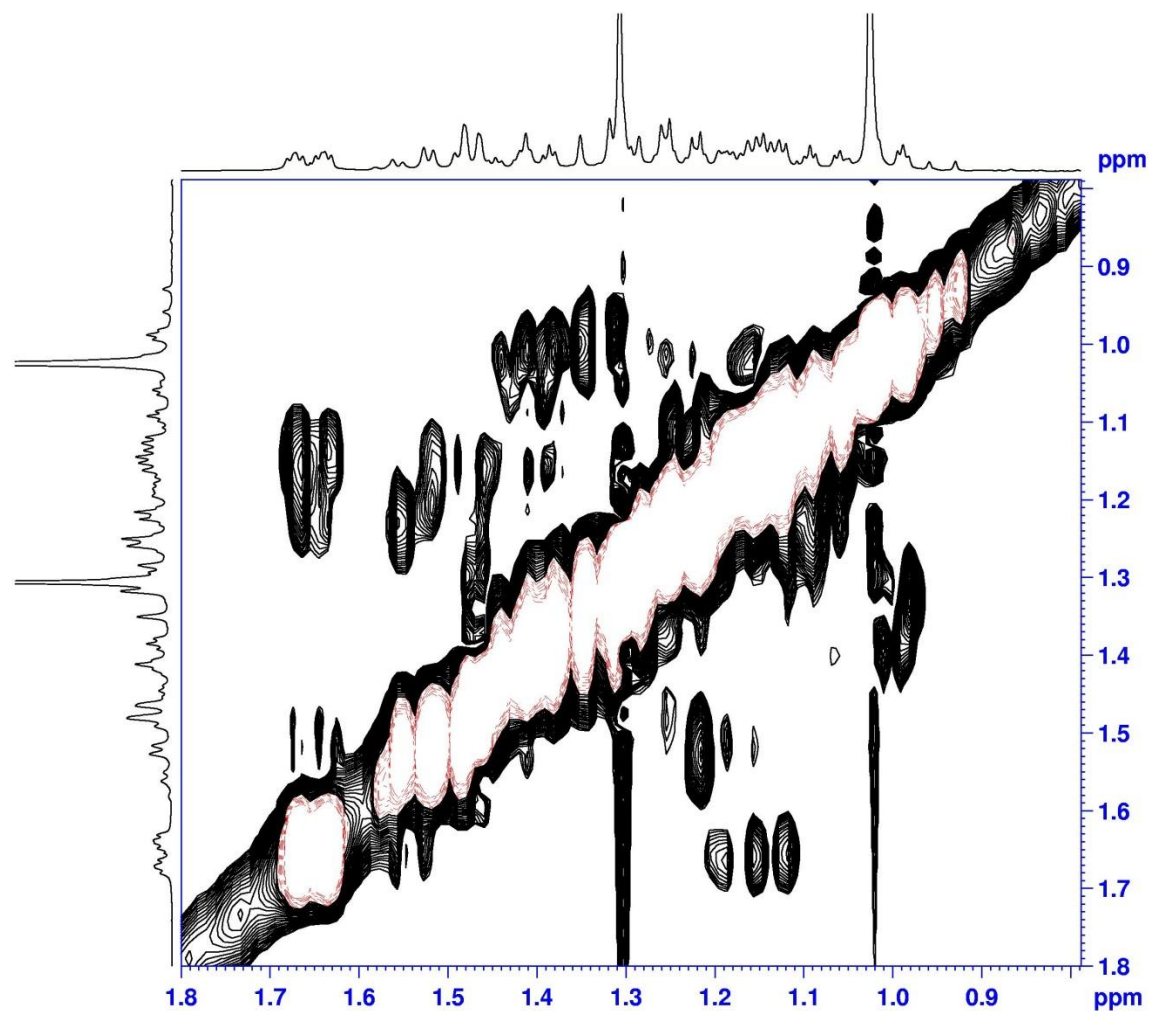
```

NAME      ZXH-13  K-36-1-1
EXPNO     7
PROCNO    1
Date_     20160216
Time      0.40
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   noesygpphpp
TD        2048
SOLVENT   CDC13
NS        16
DS        32
SWH       4000.000 Hz
FIDRES    1.953125 Hz
AQ        0.2560500 sec
RG        208.5
DW        125.000 usec
DE        10.00 usec
TE        297.0 K
D0        0.00011036 sec
D1        1.99385595 sec
D8        0.30000001 sec
D11       0.03000000 sec
D12       0.00002000 sec
D16       0.00020000 sec
IN0       0.00025000 sec
    
```

```

===== CHANNEL f1 =====
SFO1    400.1318006 MHz
NUC1     1H
P1       11.50 usec
P2       23.00 usec
P17     2500.00 usec
ND0      1
TD       256
SFO1    400.1318 MHz
FIDRES   15.625000 Hz
SW       9.997 ppm
FnMODE   States-TPPI
SI       1024
SF       400.1300080 MHz
WDW      QSINE
SSB      2
LB       0.00 Hz
GB       0
PC       1.00
SI       1024
MC2     States-TPPI
SF       400.1300080 MHz
WDW      QSINE
SSB      2
LB       0.00 Hz
GB       0
    
```


NOESY (400 MHz) spectrum of tagalide A (1) in CDCl₃



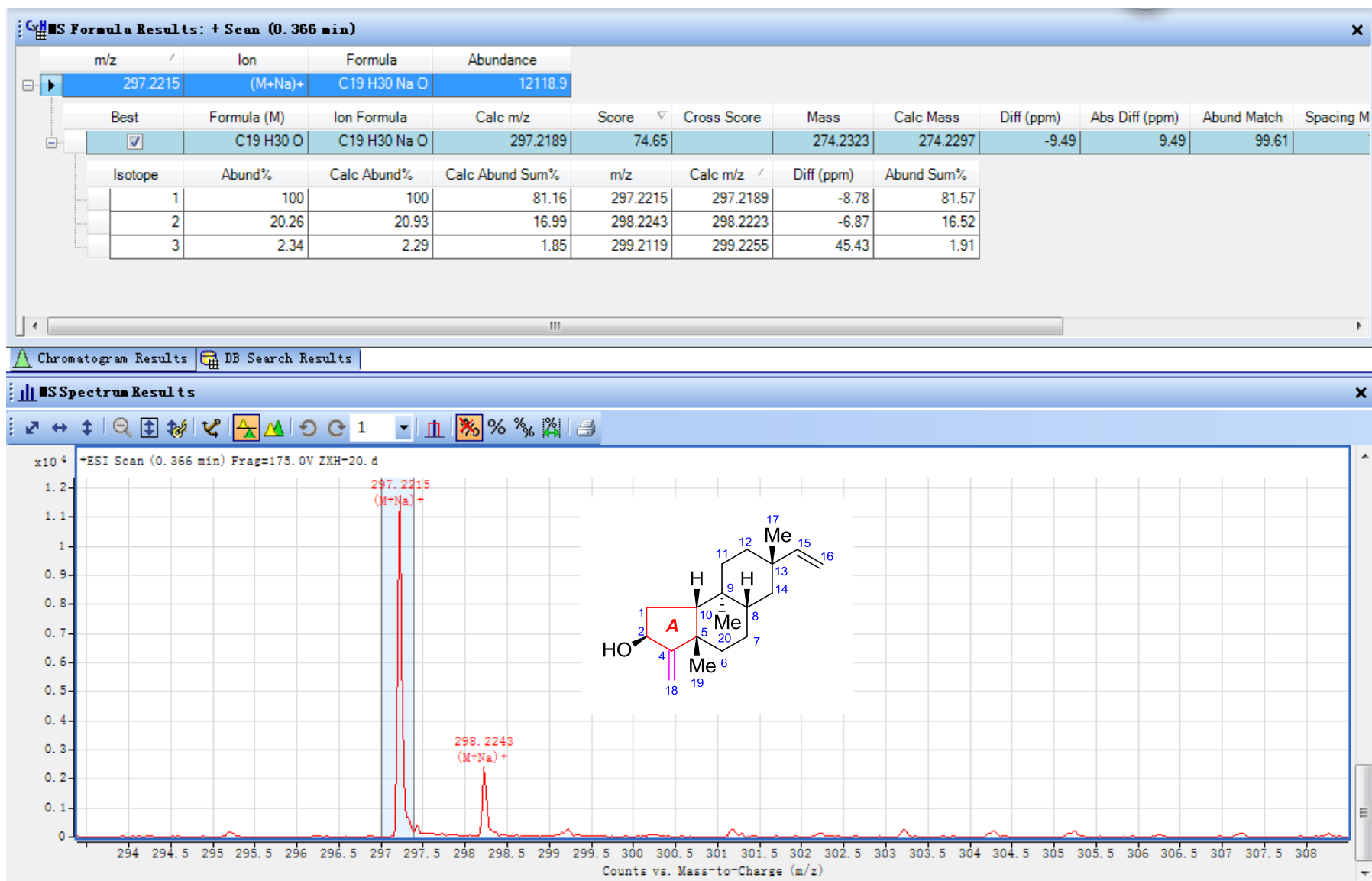
```

NAME      ZXU-13  K-36-1-1
EXPNO     7
PROCNO    1
Date_     20160216
Time      0.40
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   noesygpphpp
TD        2048
SOLVENT   CDCl3
NS        16
DS        32
SWH       4000.000 Hz
FIDRES    1.953125 Hz
AQ        0.2560500 sec
RG        208.5
DW        125.000 usec
DE        10.00 usec
TE        297.0 K
D0        0.00011036 sec
D1        1.99385595 sec
D8        0.30000001 sec
D11       0.03000000 sec
D12       0.00020000 sec
D16       0.00020000 sec
IN0       0.00025000 sec
    
```

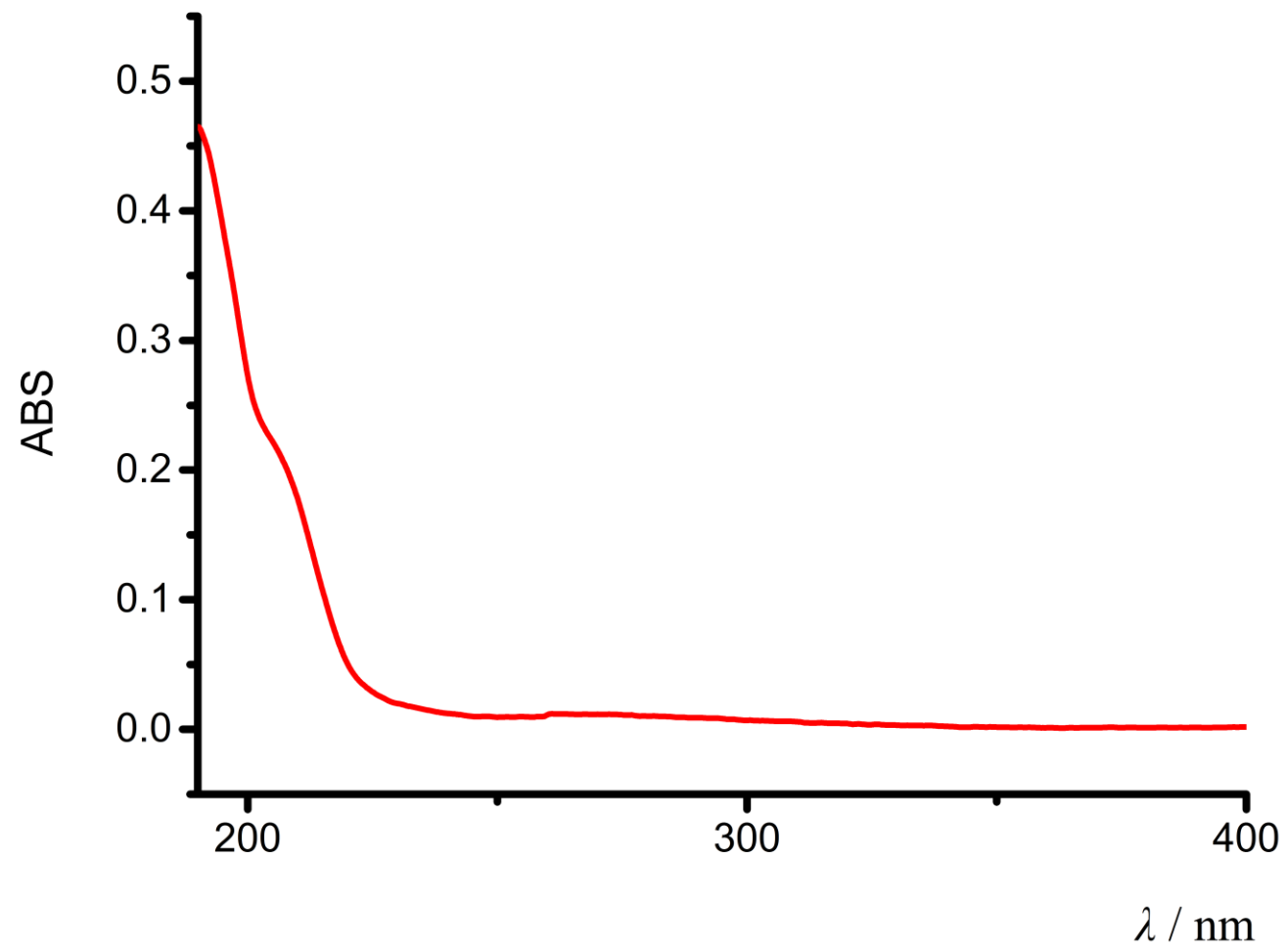
```

===== CHANNEL f1 =====
SFO1    400.1318006 MHz
NUC1     1H
P1       11.50 usec
P2       23.00 usec
P17     2500.00 usec
ND0      1
TD       256
SFO1    400.1318 MHz
FIDRES   15.625000 Hz
SW       9.997 ppm
FnMODE   States-TPPI
SI       1024
SF      400.1300080 MHz
WDW      QSINE
SSB      2
LB       0.00 Hz
GB       0
PC       1.00
SI       1024
MC2     States-TPPI
SF      400.1300080 MHz
WDW      QSINE
SSB      2
LB       0.00 Hz
GB       0
    
```

HRESIMS for tagalol A (2)

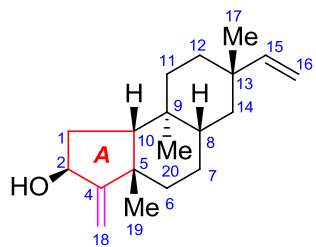


UV spectrum for tagalol A (2) (recorded in MeCN at 100 $\mu\text{g}/\text{mL}$)



¹H (400 MHz) NMR spectrum of tagalol A (2) in CDCl₃

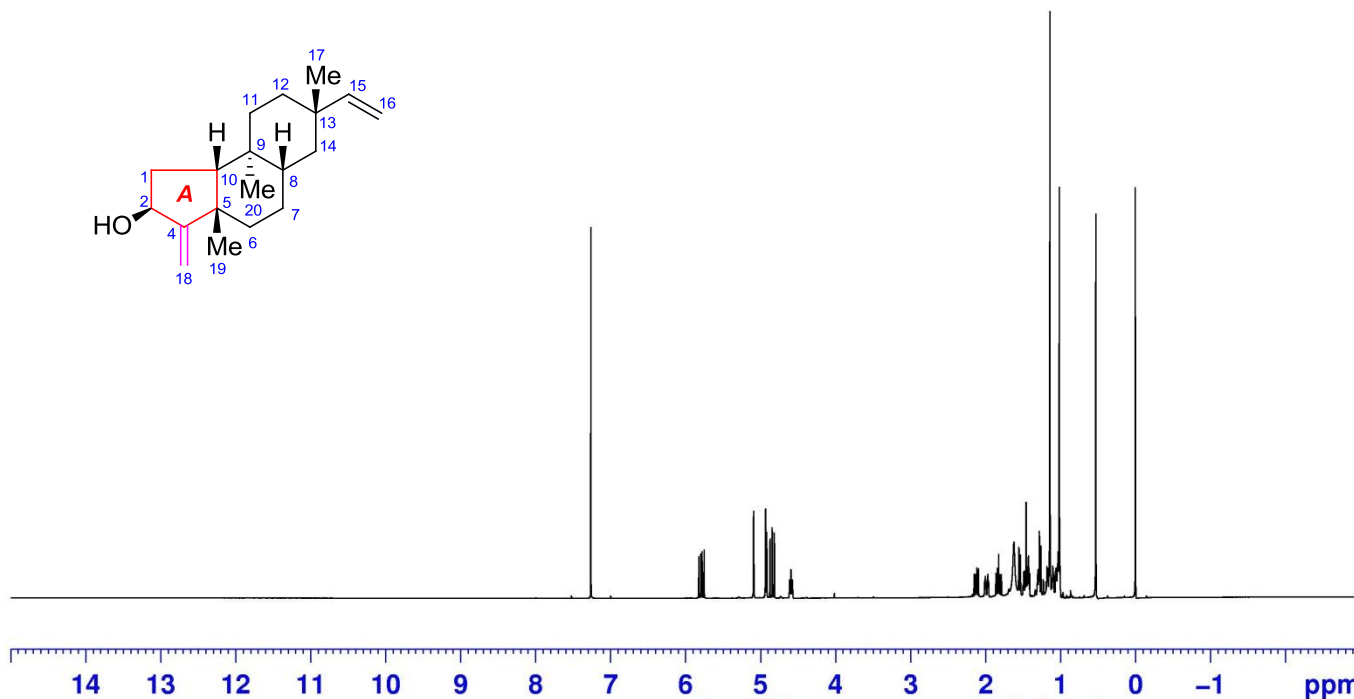
7.262
5.822
5.795
5.778
5.751
5.092
5.089
4.934
4.930
4.919
4.915
4.875
4.872
4.844
4.840
4.817
4.814
4.594
2.114
2.093
1.838
1.823
1.620
1.553
1.533
1.457
1.444
1.433
1.428
1.423
1.418
1.301
1.289
1.281
1.278
1.258
1.180
1.174
1.170
1.140
1.101
1.058
1.033
1.027
1.014
0.527
0.000



```

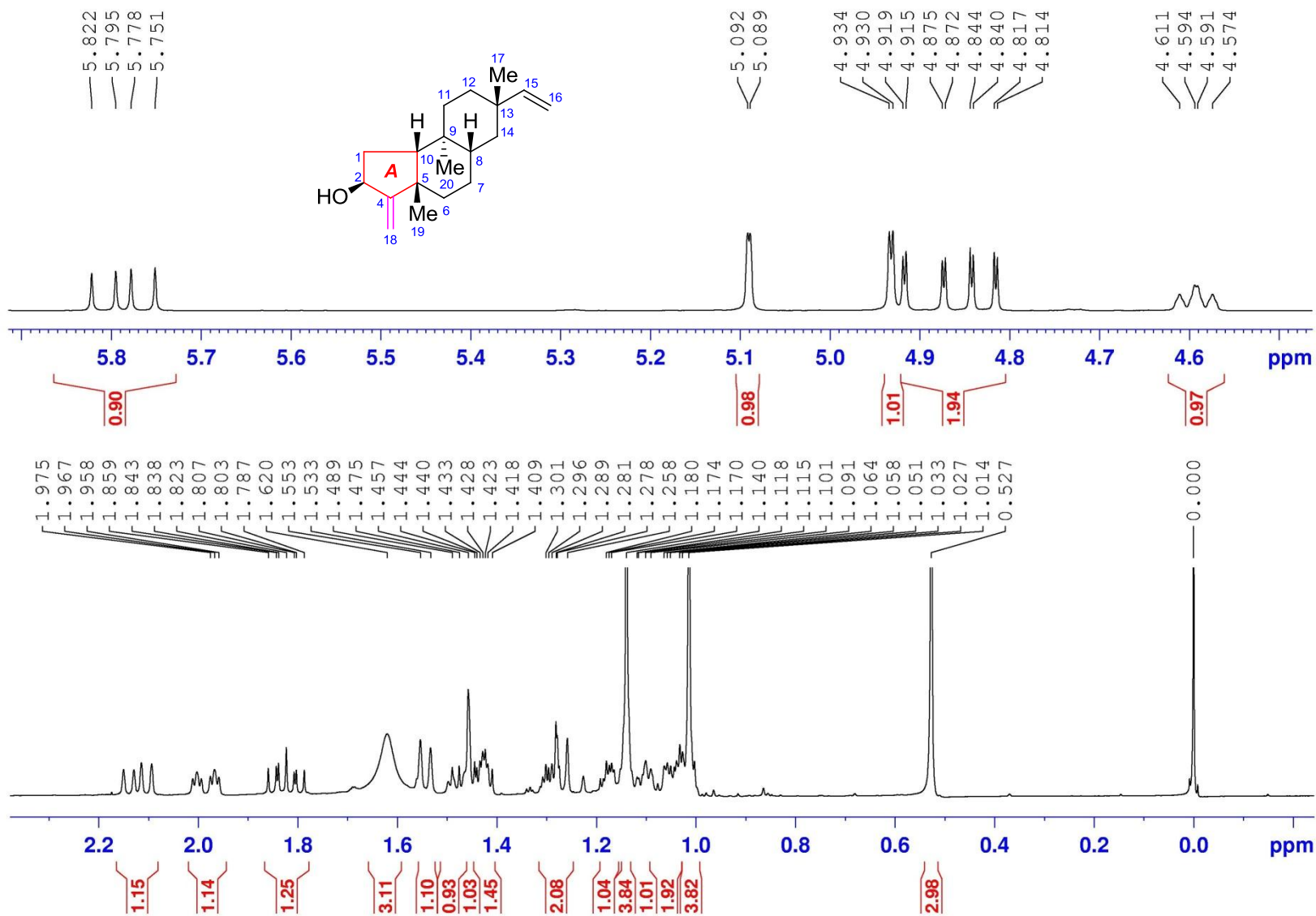
NAME          R-36-3-3
EXPNO         1
PROCNO        1
Date_         20160227
Time          3.35
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG            208.5
DW            60.800 usec
DE            10.00 usec
TE            297.0 K
D1            1.0000000 sec
TD0           1

===== CHANNEL f1 =====
SF01          400.1324710 MHz
NUC1          1H
P1            11.50 usec
SI            65536
SF            400.1300089 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

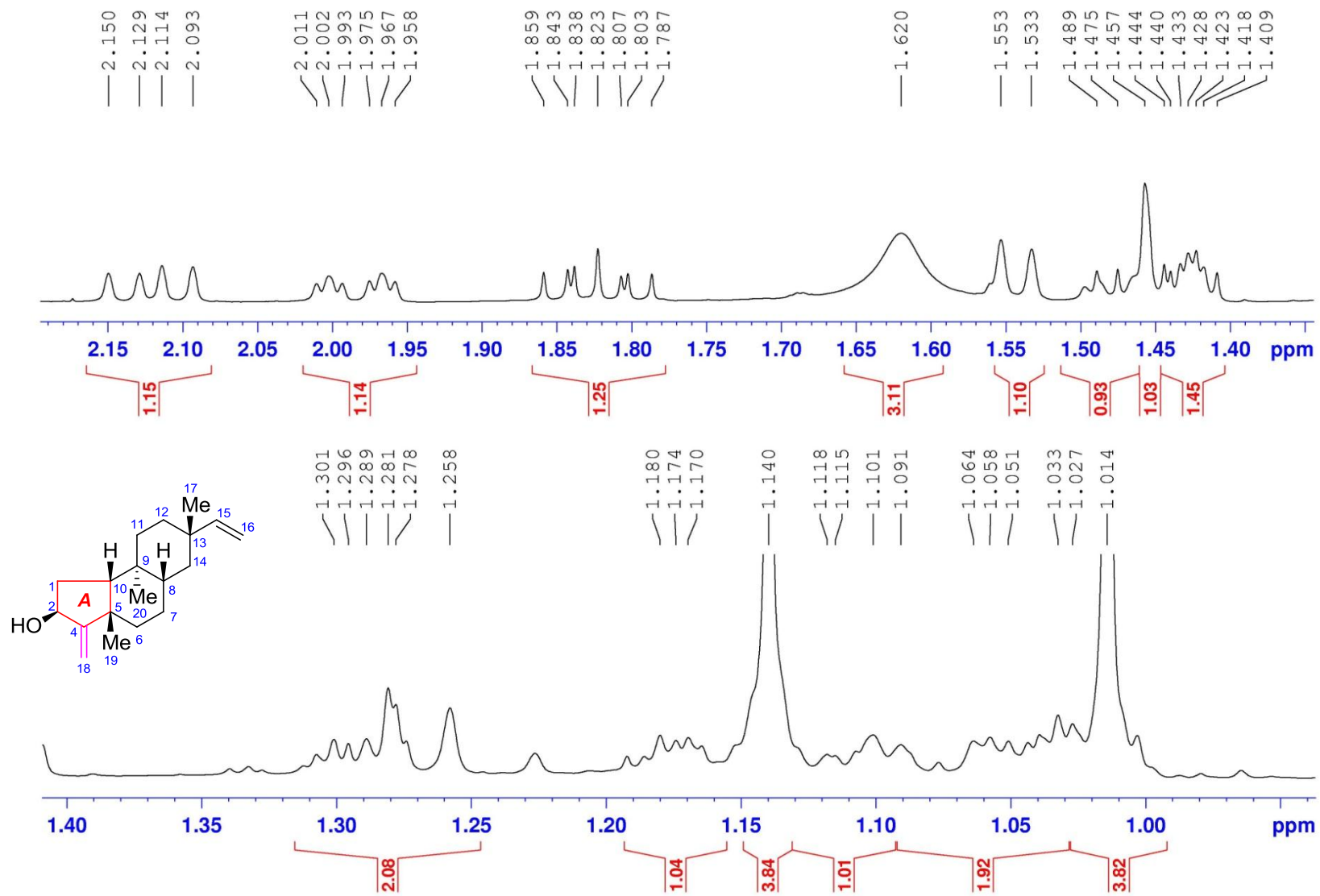


0.90
0.98
1.01
1.94
0.97
1.15
1.14
1.25
3.11
1.10
0.93
1.03
1.45
2.08
1.04
3.84
1.01
1.92
3.82
2.98

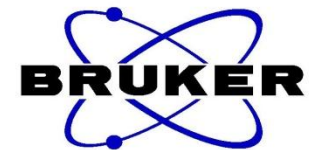
¹H (400 MHz) NMR spectrum of tagalol A (2) in CDCl₃



¹H (400 MHz) NMR spectrum of tagalol A (2) in CDCl₃



¹³C (100 MHz) NMR spectrum of tagalol A (2) in CDCl₃

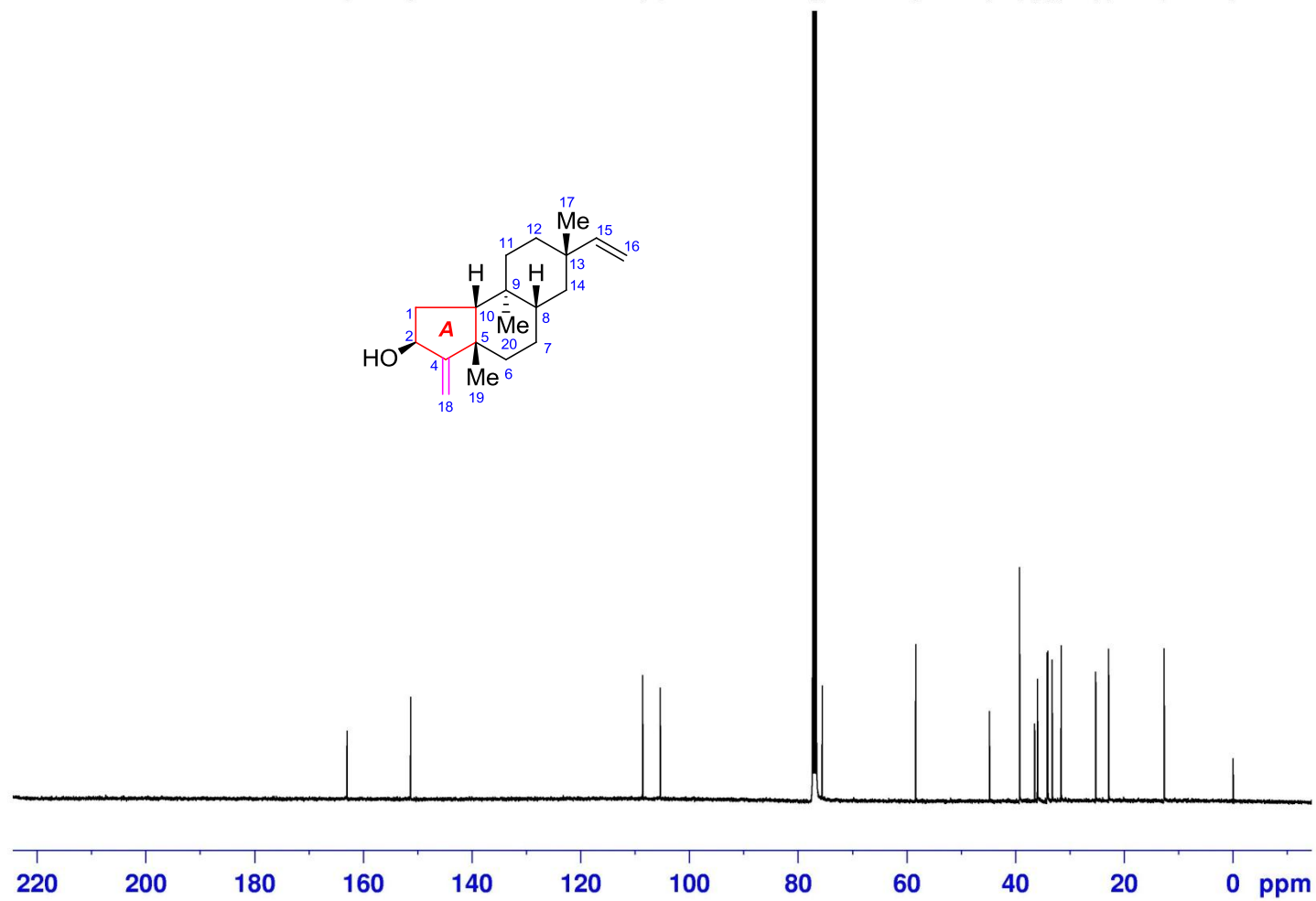
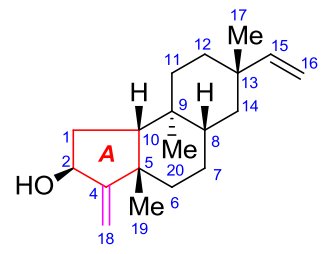


```

NAME           R-36-3-3
EXPNO          2
PROCNO         1
Date_          20160227
Time           7.25
INSTRUM        spect
PROBHD         5 mm CPPBBO HB
PULPROG        zgpg30
TD             65536
SOLVENT        CDCl3
NS             4000
DS             4
SWH            24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG            117.37
DW            20.800 usec
DE            18.00 usec
TE            297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

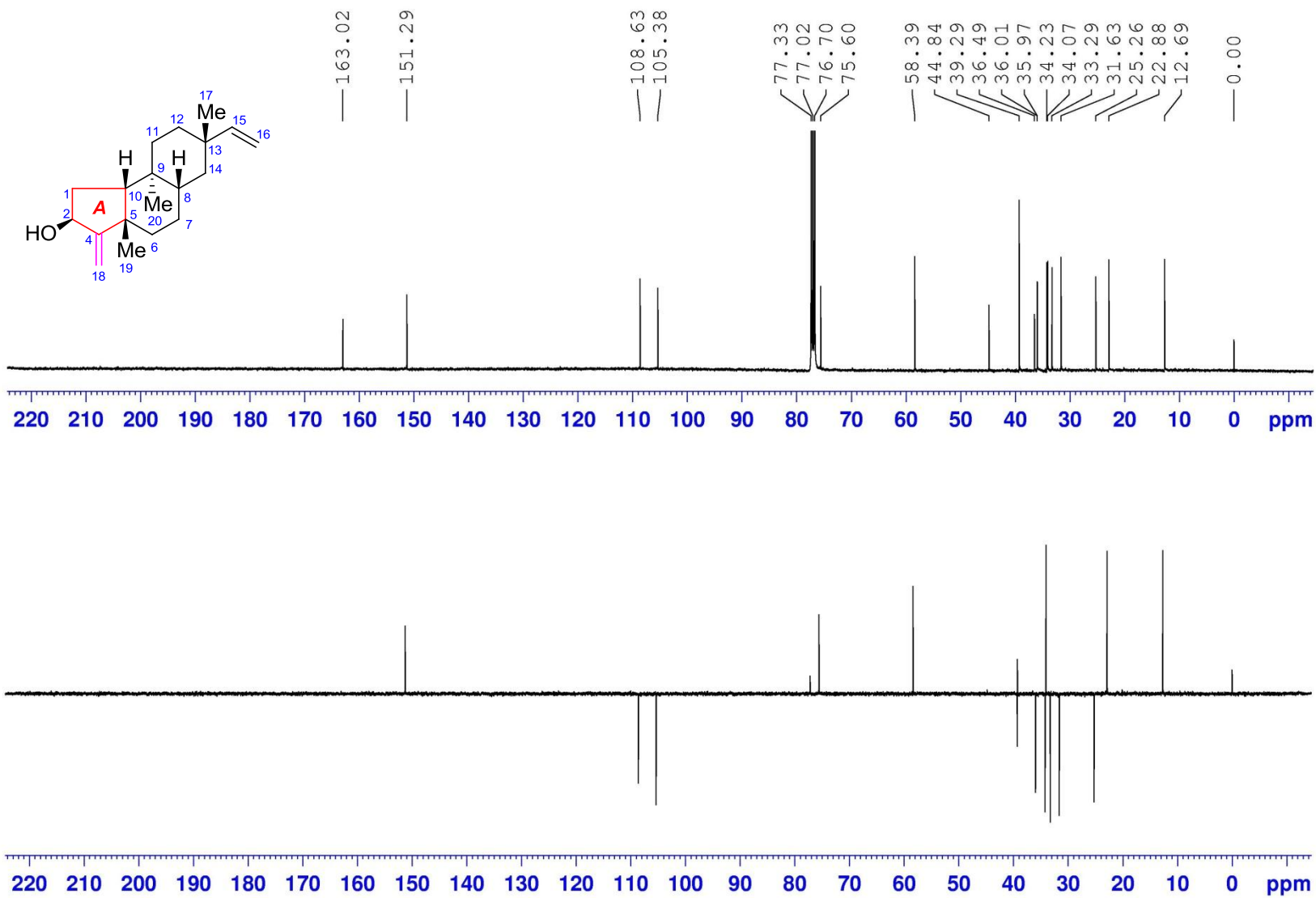
===== CHANNEL f1 =====
SFO1          100.6233324 MHz
NUC1           13C
P1            10.00 usec
SI            32768
SF            100.6127694 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

— 163.02
 — 151.29
 — 108.63
 — 105.38
 77.33
 77.02
 76.70
 75.60
 58.39
 44.84
 39.29
 36.49
 36.01
 35.97
 34.23
 34.07
 33.29
 31.63
 25.26
 22.88
 12.69
 — 0.00

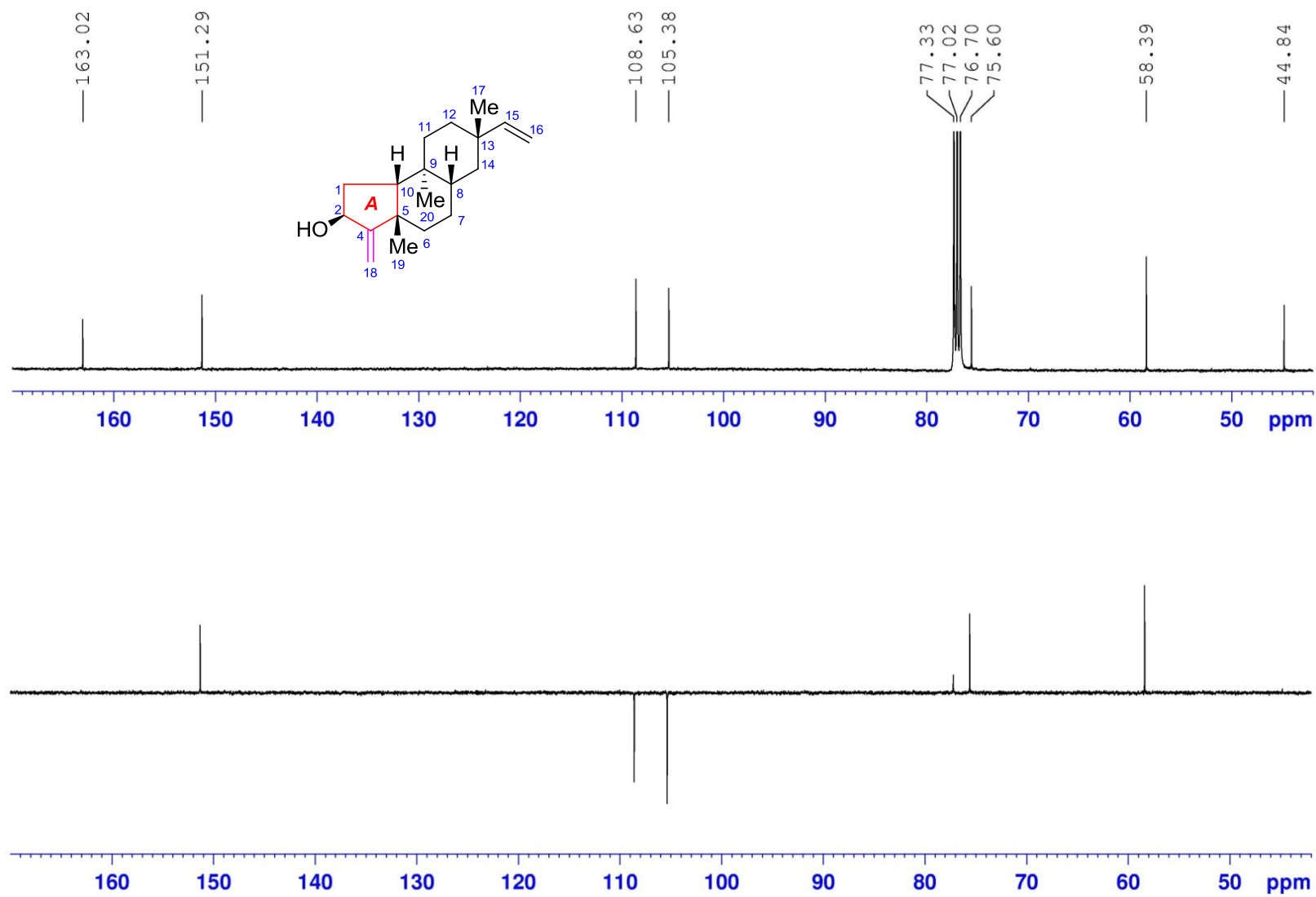


S55

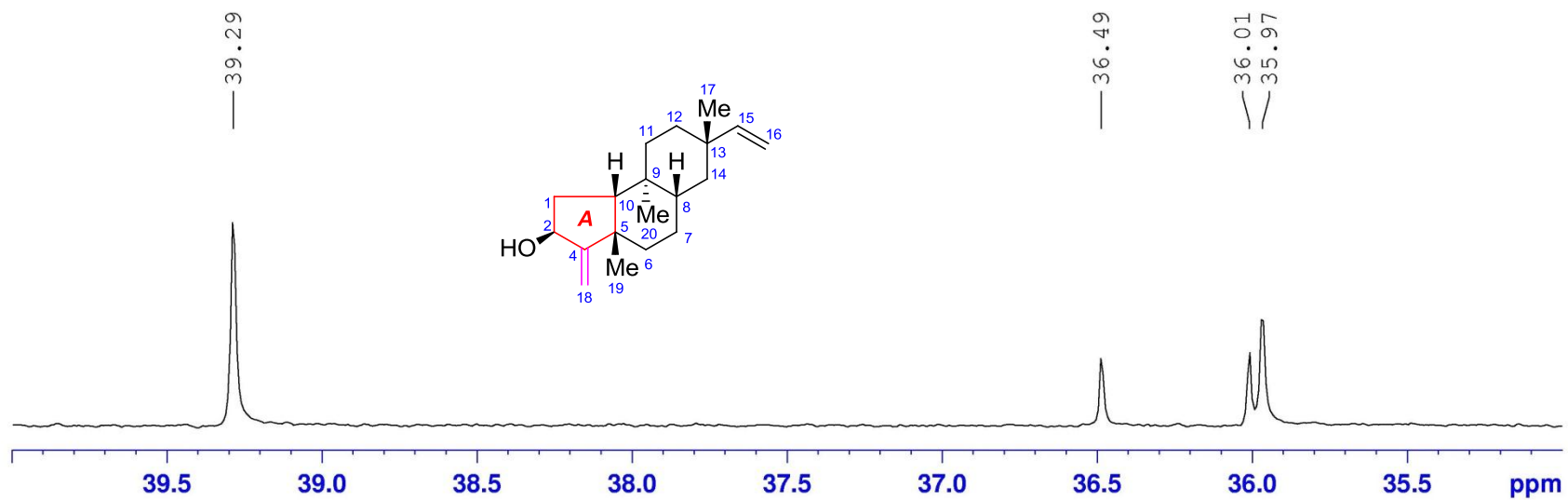
DEPT135 (100 MHz) experiment of tagalol A (2) in CDCl₃



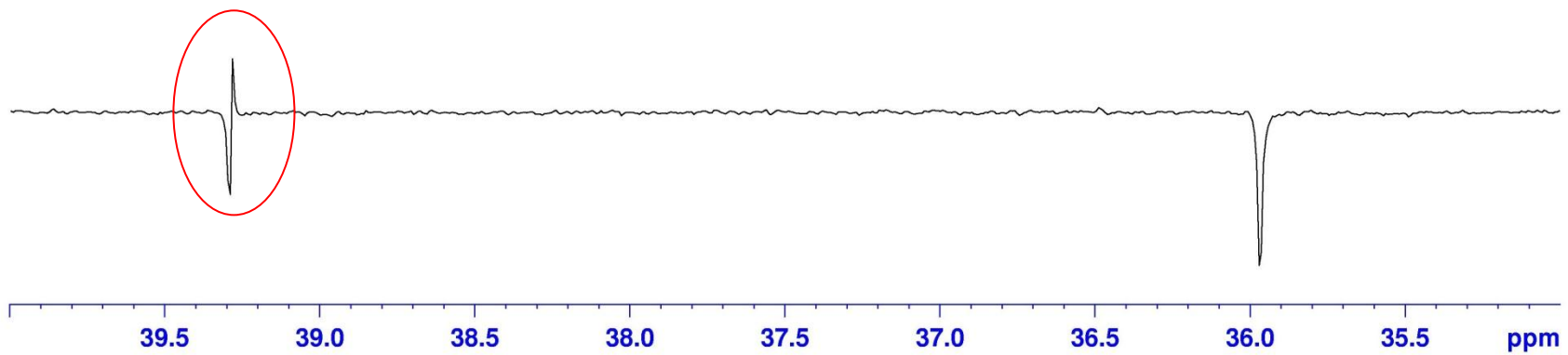
DEPT135 (100 MHz) experiment of tagalol A (2) in CDCl₃



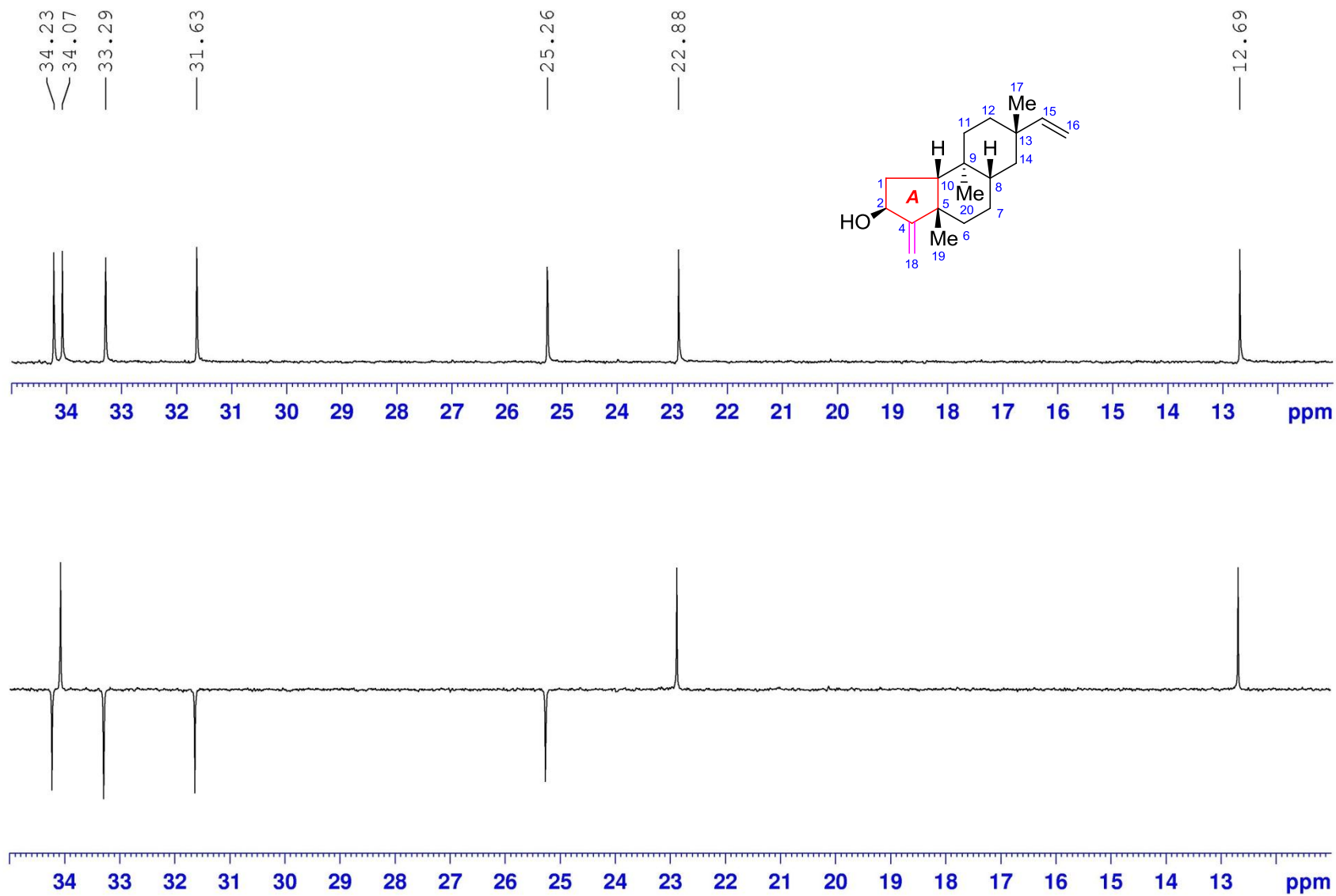
DEPT135 (100 MHz) experiment of tagalol A (2) in CDCl₃



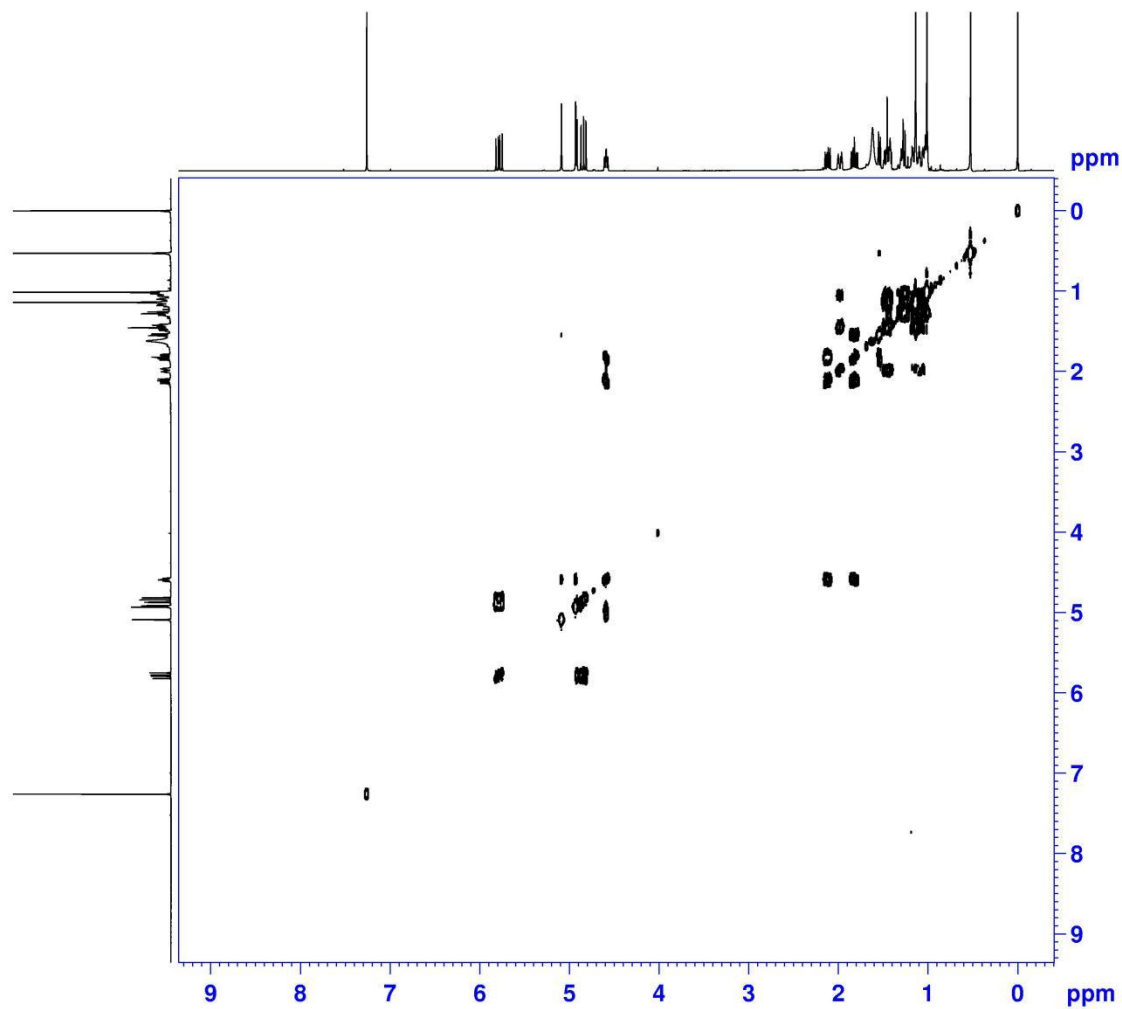
Overlapped ¹³C signals



DEPT135 (100 MHz) experiment of tagalol A (2) in CDCl₃



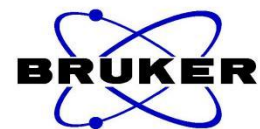
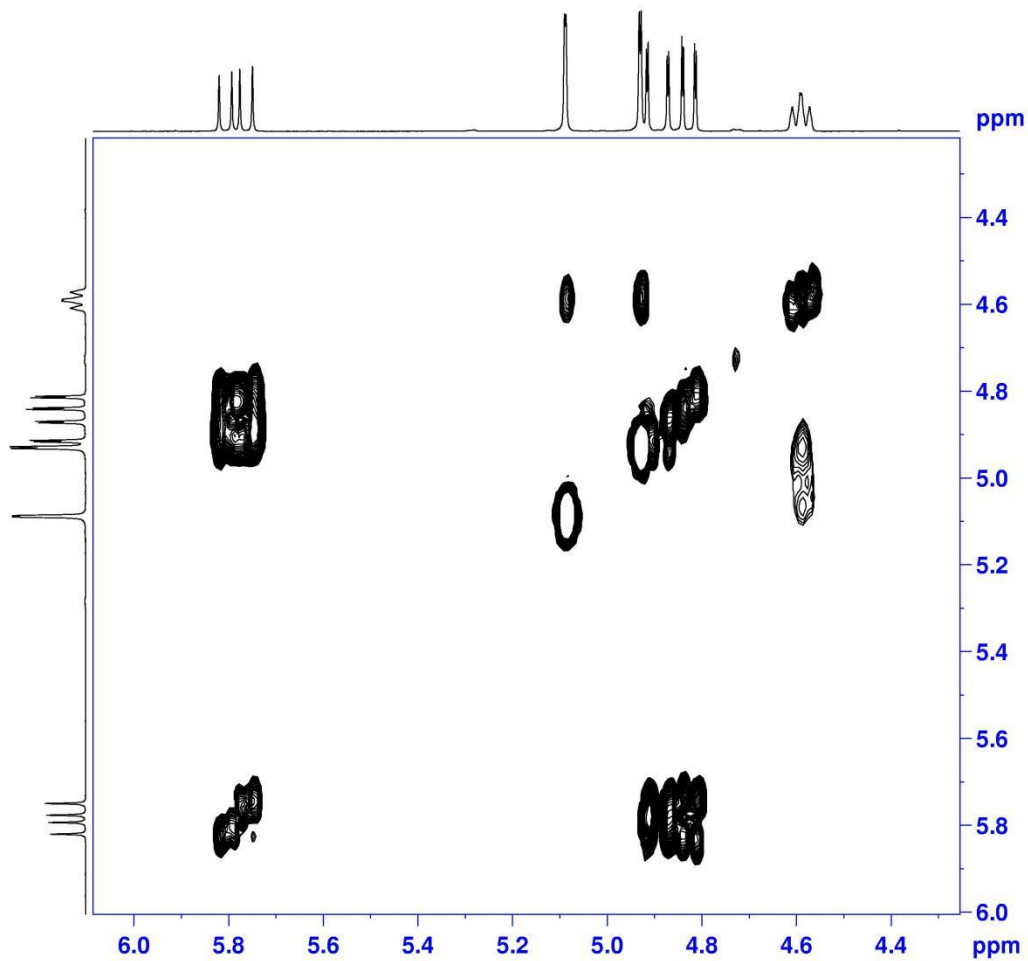
^1H - ^1H COSY (400 MHz) spectrum of tagalol A (2) in CDCl_3



```
NAME R-36-3-3
EXPNO 4
PROCNO 1
Date_ 20160305
Time 22.57
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG cosygpppf
TD 2048
SOLVENT CDCl3
NS 16
DS 8
SWH 3906.250 Hz
FIDRES 1.907349 Hz
AQ 0.2621940 sec
RG 208.5
DW 128.000 usec
DE 10.00 usec
TE 297.0 K
D0 0.00000300 sec
D1 1.89678097 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00025600 sec
```

```
----- CHANNEL f1 -----
SFO1 400.1318006 MHz
NUC1 1H
P0 11.50 usec
P1 11.50 usec
P17 2500.00 usec
ND0 1
TD 128
SFO1 400.1318 MHz
FIDRES 30.517578 Hz
SW 9.762 ppm
FnMODE QF
SI 1024
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
```

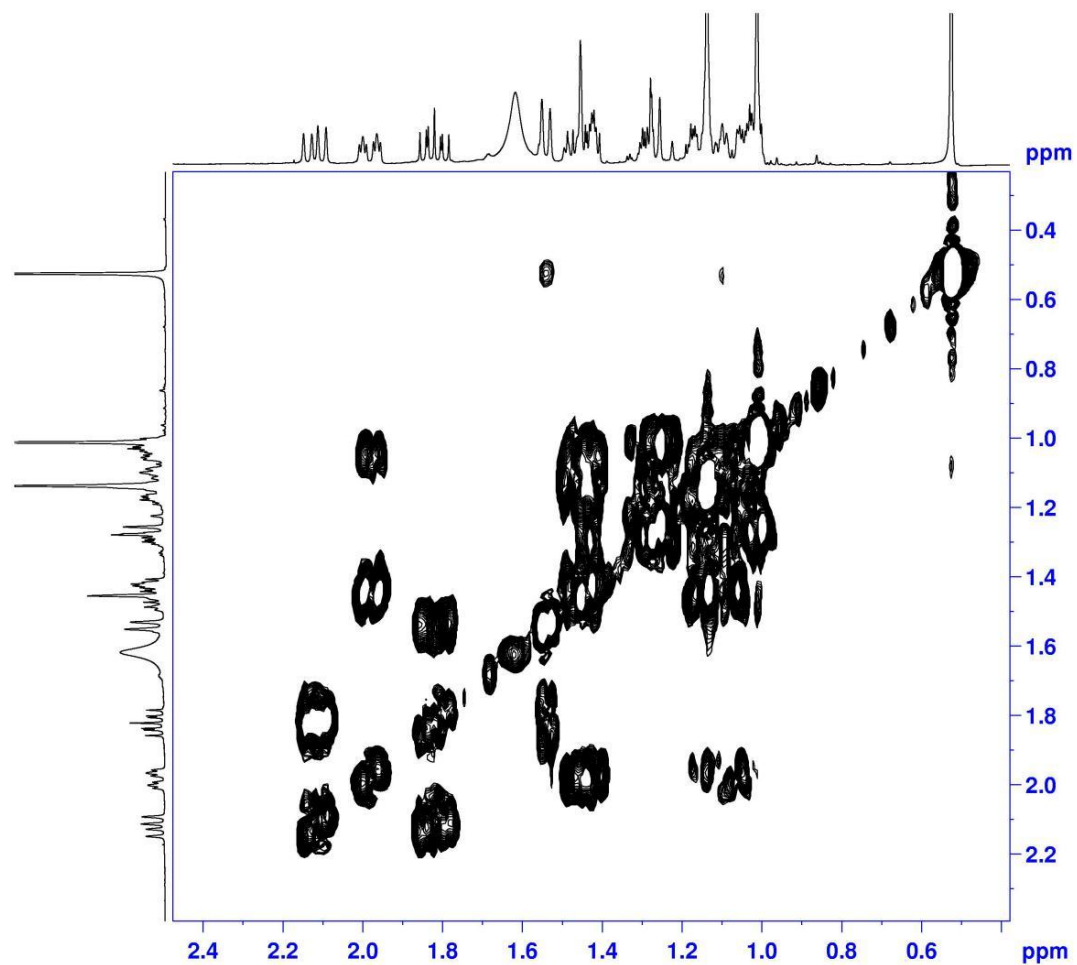
^1H - ^1H COSY (400 MHz) spectrum of tagalol A (2) in CDCl_3



```
NAME R-36-3-3
EXFNO 4
PROCNO 1
Date_ 20160305
Time 22.57
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 16
DS 8
SWH 3906.250 Hz
FIDRES 1.907349 Hz
AQ 0.2621940 sec
RG 208.5
DW 128.000 usec
DE 10.00 usec
TE 297.0 K
D0 0.0000300 sec
D1 1.89678097 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00004000 sec
D16 0.00020000 sec
IN0 0.00025600 sec
```

```
----- CHANNEL f1 -----
SFO1 400.1318006 MHz
NUC1 1H
P0 11.50 usec
P1 11.50 usec
P17 2500.00 usec
ND0 1
TD 128
SFO1 400.1318 MHz
FIDRES 30.517578 Hz
SW 9.762 ppm
PnMODE QF
SI 1024
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
```

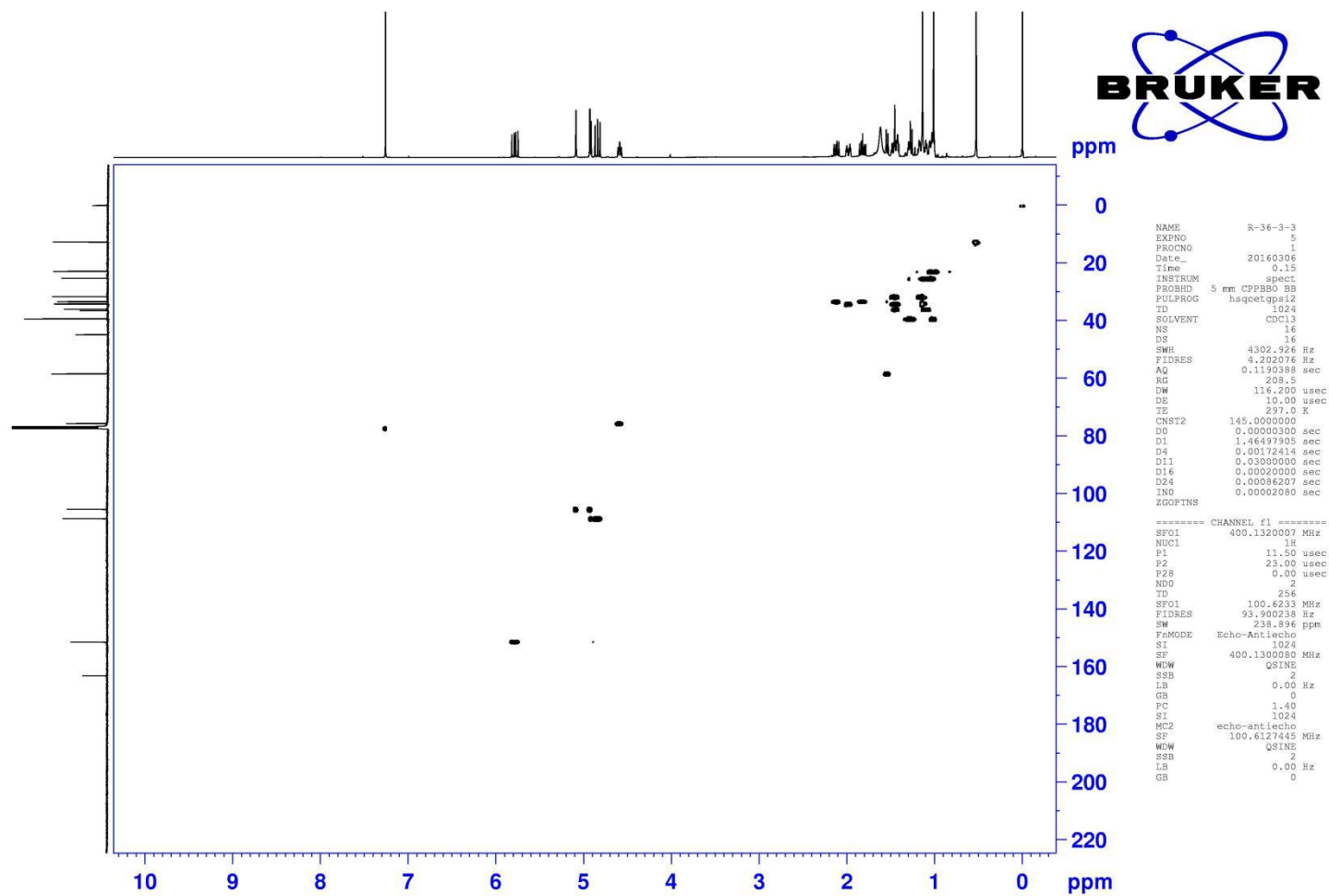
^1H - ^1H COSY (400 MHz) spectrum of tagalol A (2) in CDCl_3



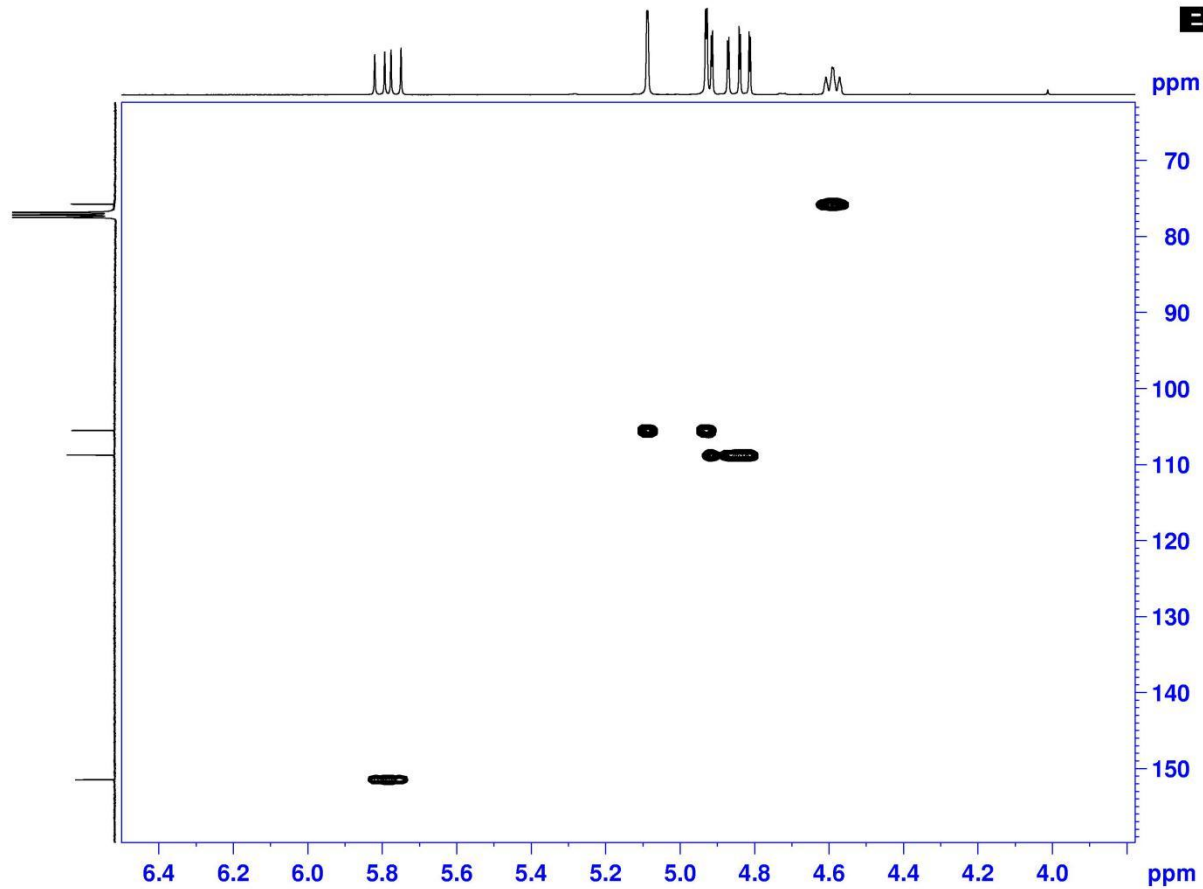
```
NAME R-36-3-3
EXPNO 4
PROCNO 1
Date_ 20160305
Time 22.57
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG cosygpppgf
TD 2048
SOLVENT CDCl3
NS 16
DS 8
SWH 3906.250 Hz
FIDRES 1.907349 Hz
AQ 0.2621940 sec
RG 208.5
DW 128.000 usec
DE 10.00 usec
TE 297.0 K
D0 0.00000300 sec
D1 1.89678097 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00025600 sec

----- CHANNEL f1 -----
SFO1 400.1318006 MHz
NUC1 1H
P0 11.50 usec
P1 11.50 usec
P17 2500.00 usec
ND0 1
TD 128
SFO1 400.1318 MHz
FIDRES 30.517578 Hz
SW 9.762 ppm
FhMODE QF
SI 1024
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0
```

HSQC (400 MHz) spectrum of tagalol A (2) in CDCl₃



HSQC (400 MHz) spectrum of tagalol A (2) in CDCl₃

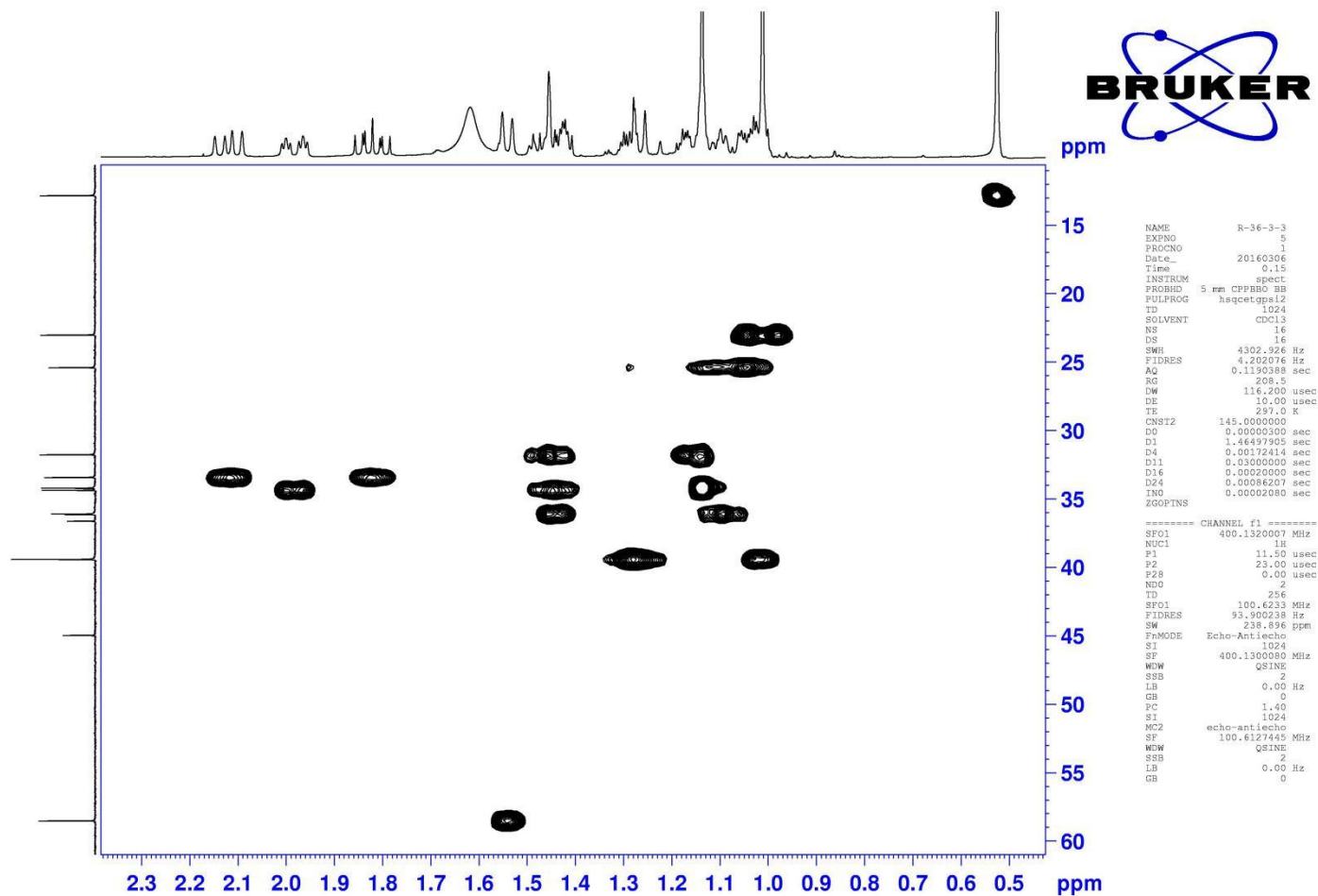


```

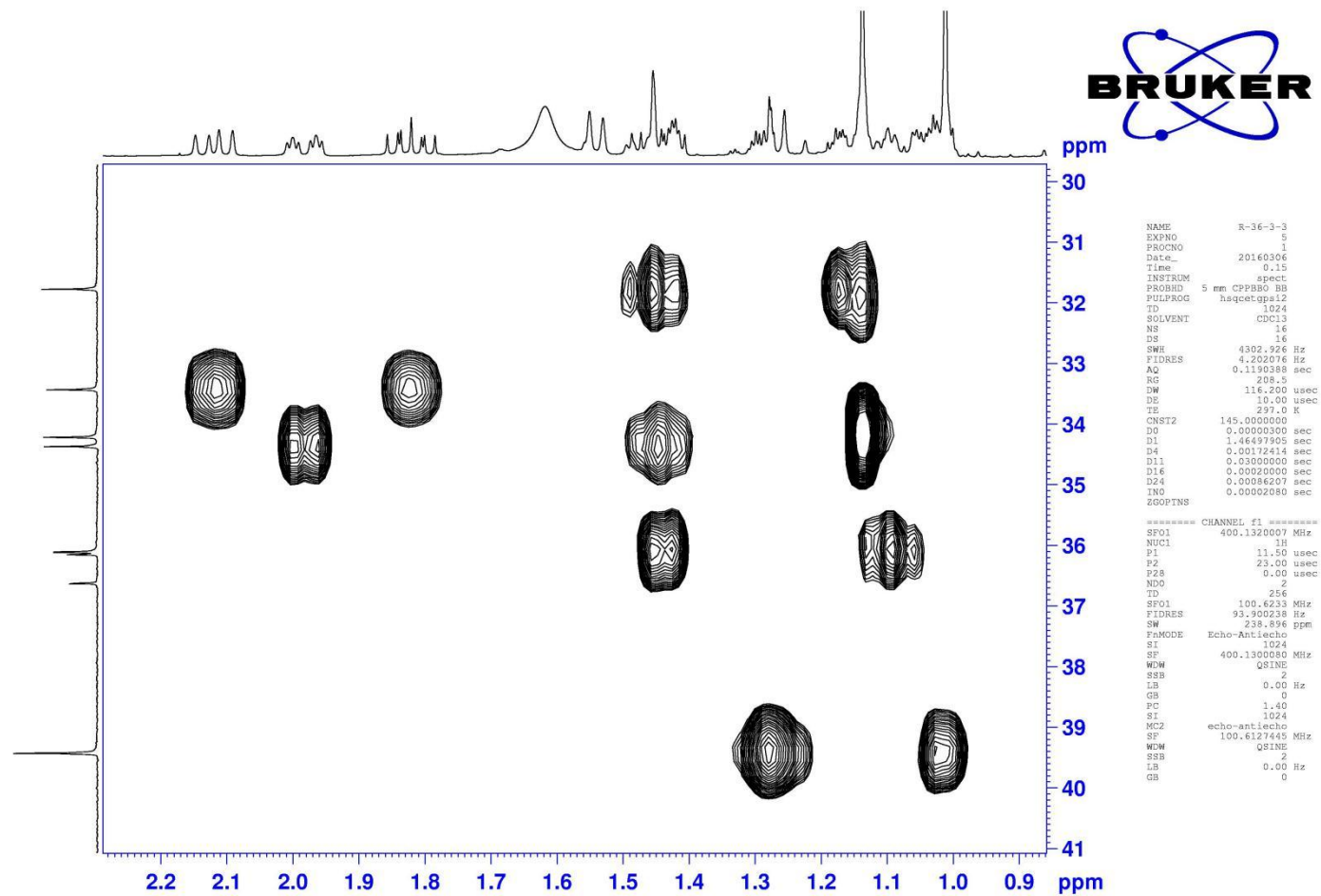
NAME          R-36-3-3
EXPNO         5
PROCNO        1
Date_         20160306
Time          0.15
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       hsqcetaps12
TD            1024
SOLVENT       CDCl3
NS            16
DS            16
SWH           4302.926 Hz
FIDRES        4.202076 Hz
AQ            0.1190388 sec
RG            208.5
DW            116.200 usec
DE            10.00 usec
TE            297.0 K
CNST2         145.0000000
D0            0.0000000 sec
D1            1.46497905 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00002080 sec
ZGPGPNS

===== CHANNEL f1 =====
SFO1         400.1320007 MHz
NUC1         1H
P1           11.50 usec
P2           23.00 usec
P28          0.00 usec
NDD          2
TD           256
SFO1         100.6233 MHz
FIDRES       93.900238 Hz
SW           238.896 ppm
FAMODE       Echo-Antiecho
SI           1024
SF           400.1300080 MHz
WOW          QSIINE
SSB          2
LB           0.00 Hz
GB           0
PC           1.40
SI           1024
WFX         echo-antiecho
SF           100.6127445 MHz
WDW          QSIINE
SSB          2
LB           0.00 Hz
GB           0
    
```

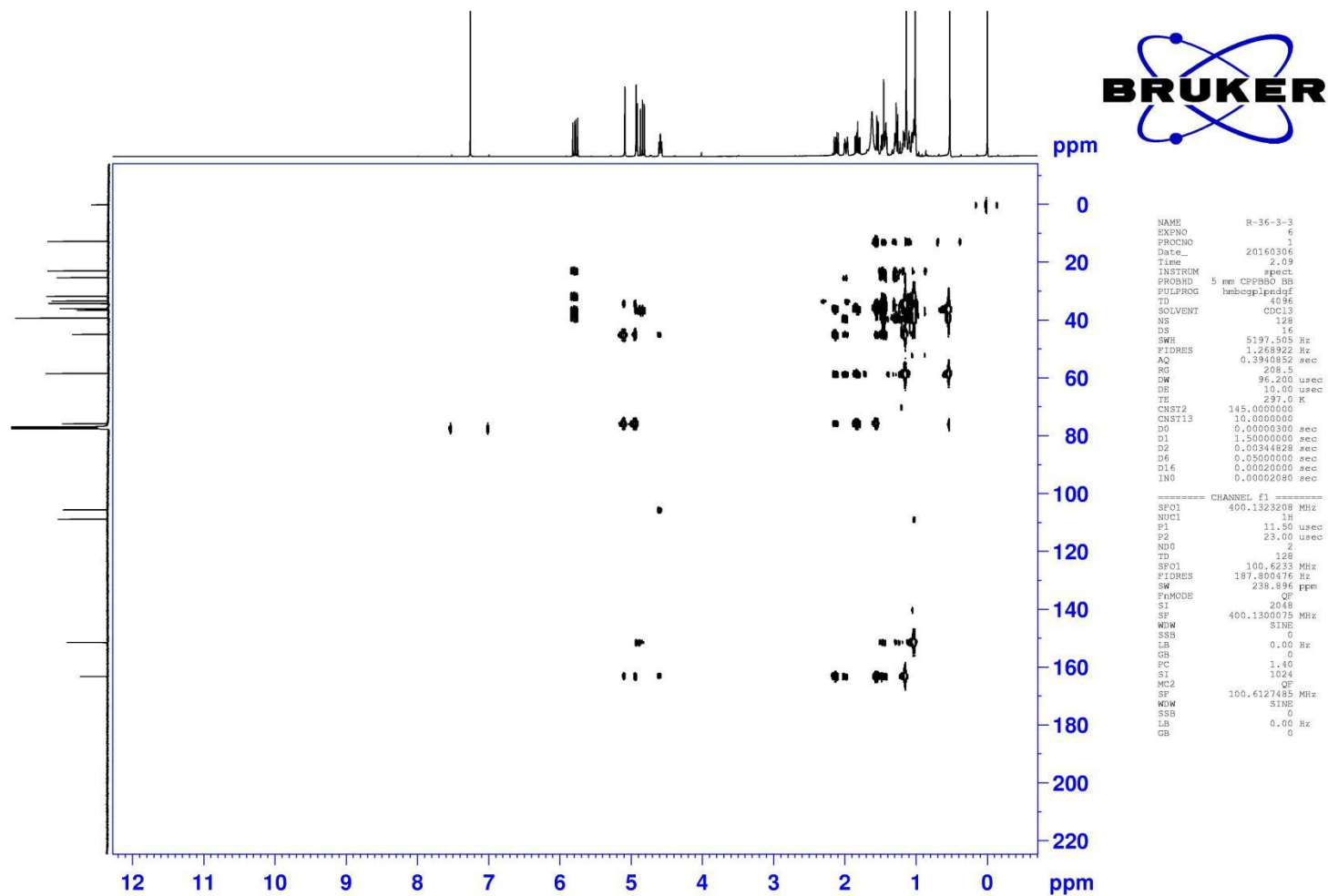

HSQC (400 MHz) spectrum of tagalol A (2) in CDCl₃



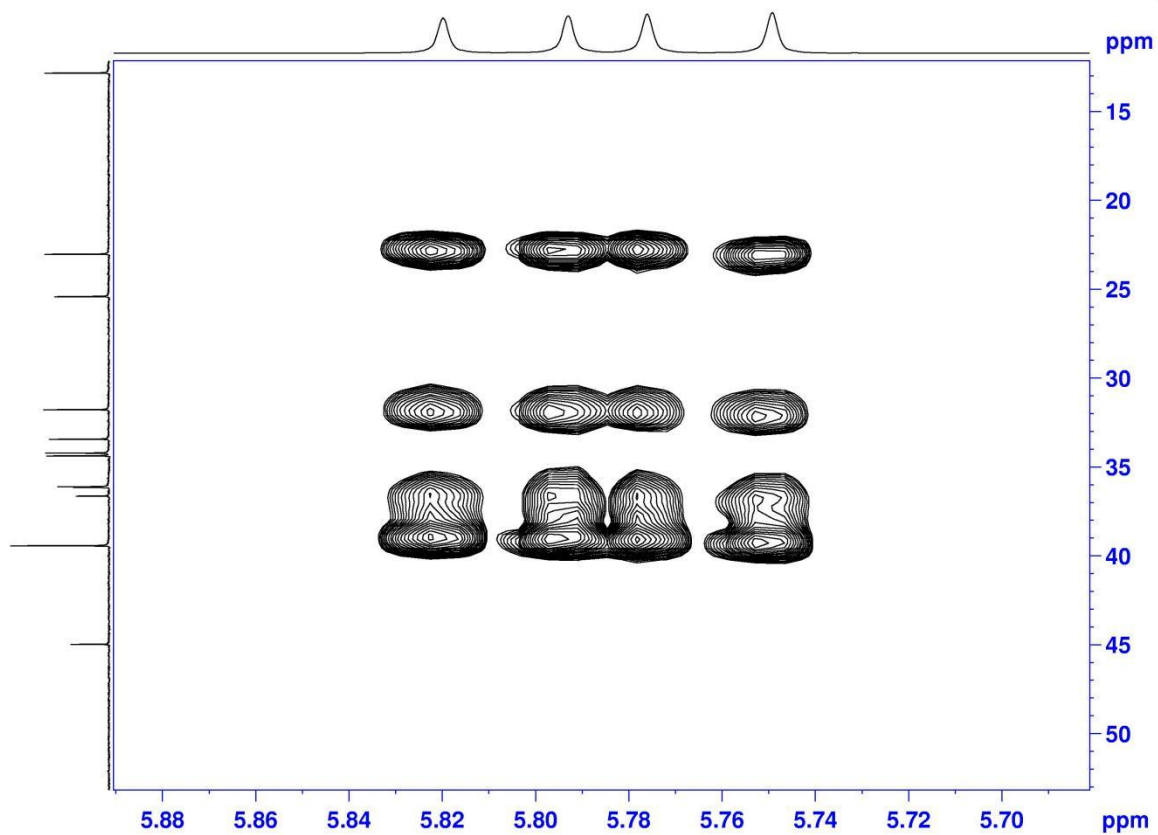
HSQC (400 MHz) spectrum of tagalol A (2) in CDCl₃



HMBC (400 MHz) spectrum of tagalol A (2) in CDCl₃



HMBC (400 MHz) spectrum of tagalol A (2) in CDCl₃

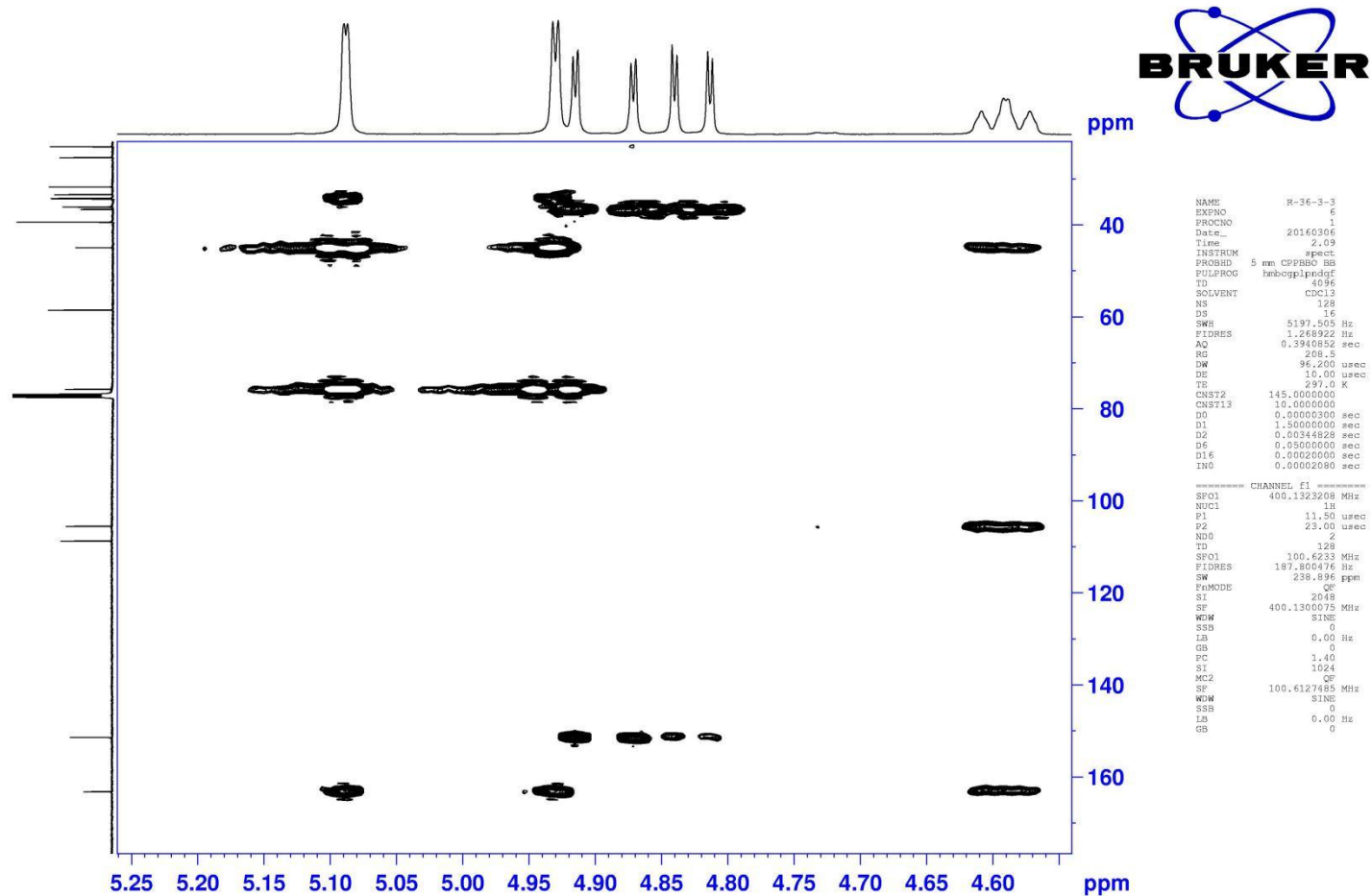


```

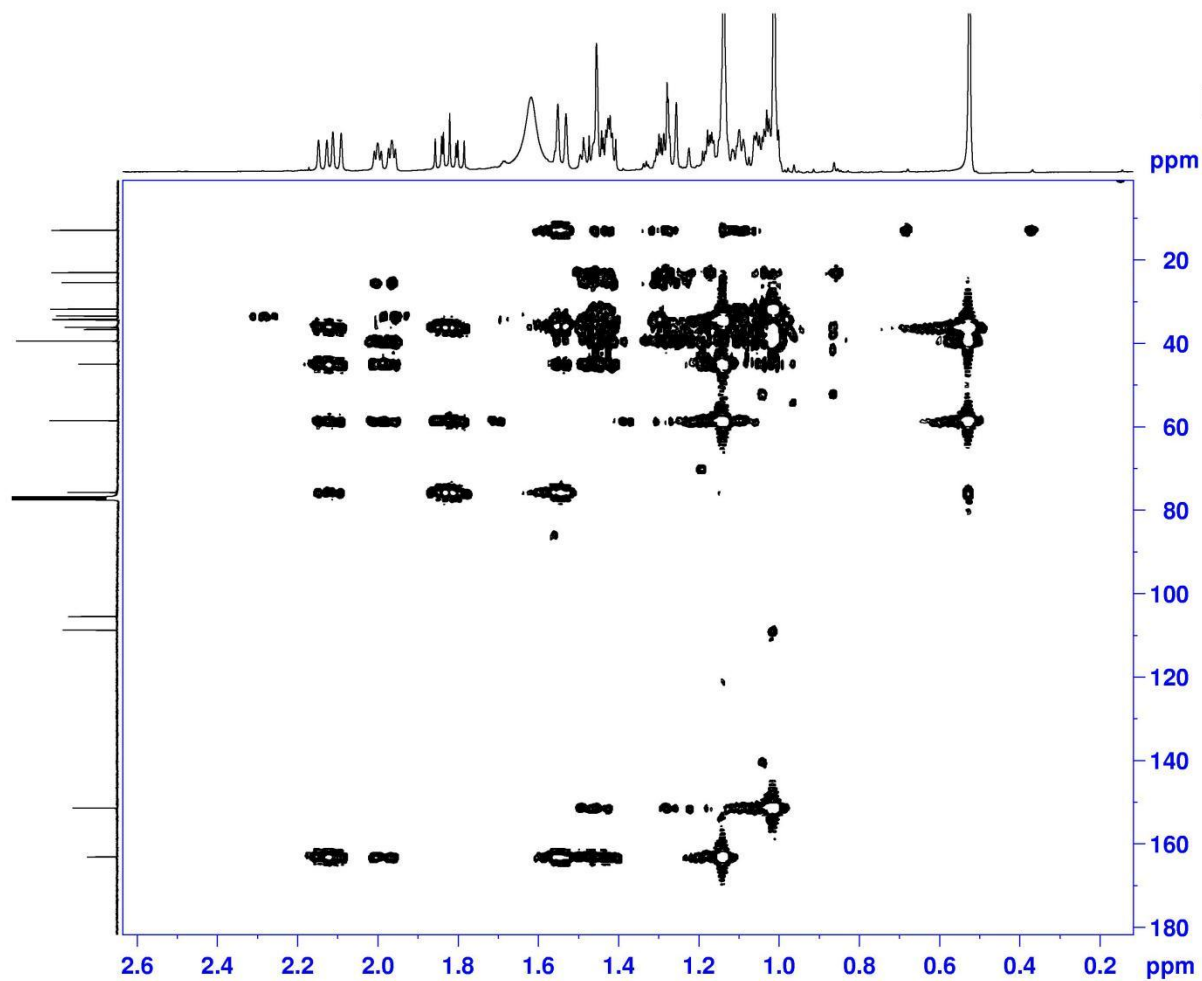
NAME          R-36-3-3
EXPNO         6
PROCNO        1
Date_         20160306
Time          2.09
INSTRUM       spect
PROBHD        5 mm CPBPRBO BB
PULPROG       hmbcgp1pndgf
TD            4096
SOLVENT       CDCl3
NS            128
DS            16
SWH           5197.505 Hz
FIDRES        1.268922 Hz
AQ            0.3940852 sec
RG            208.5
DW            96.200 usec
DE            10.00 usec
TE            297.0 K
CNSTZ         145.0000000
CNST13        10.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00020000 sec
TNO           0.00002080 sec

----- CHANNEL f1 -----
SF01          400.1323208 MHz
NUC1          13
P1            11.50 usec
P2            23.00 usec
ND0           2
TD            128
SF01          100.6233 MHz
FIDRES        187.800476 Hz
SW            238.896 ppm
PRMCDDE       QF
SI            2048
SF            400.1300075 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            100.6127485 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
    
```

HMBC (400 MHz) spectrum of tagalol A (2) in CDCl₃



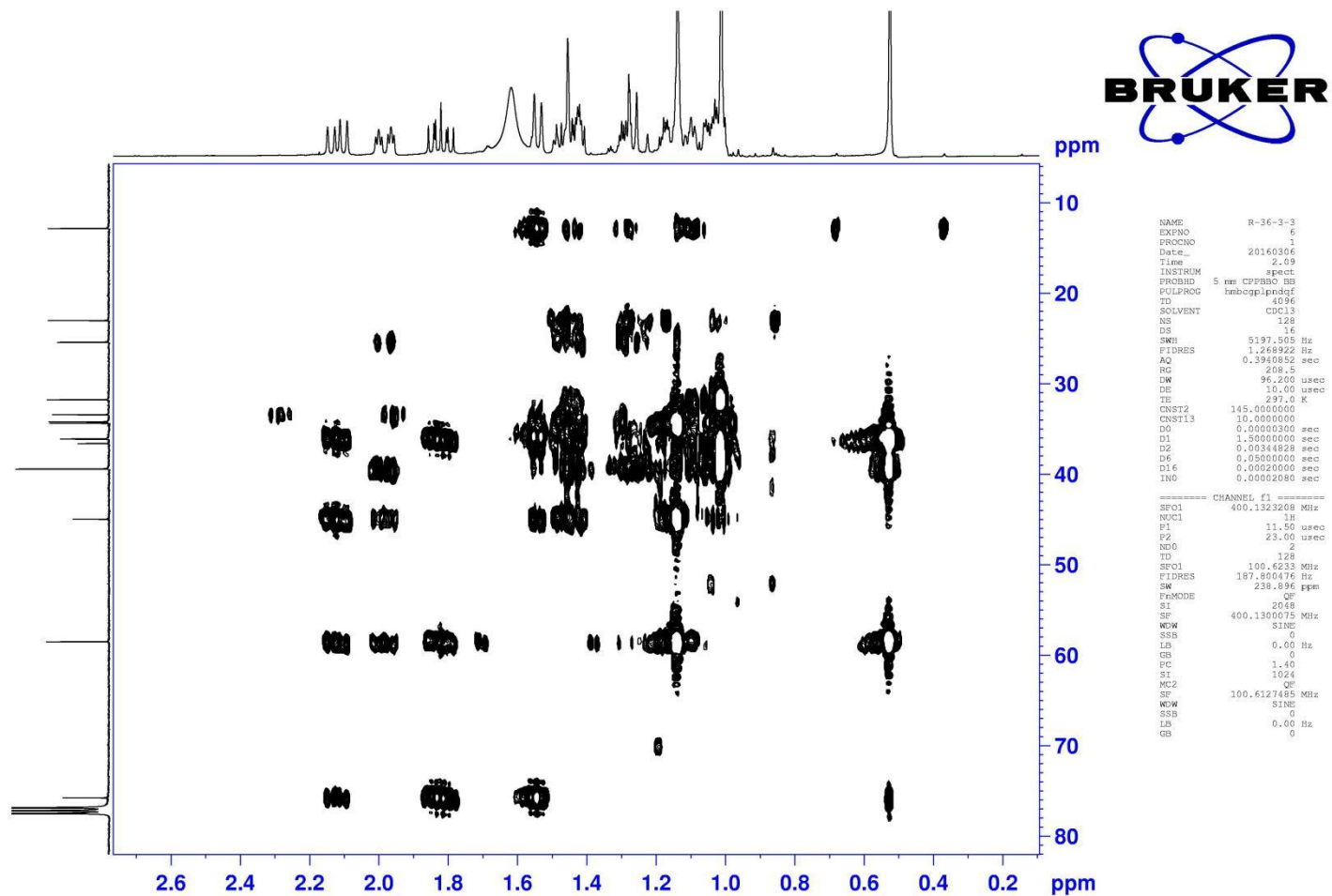
HMBC (400 MHz) spectrum of tagalol A (2) in CDCl₃



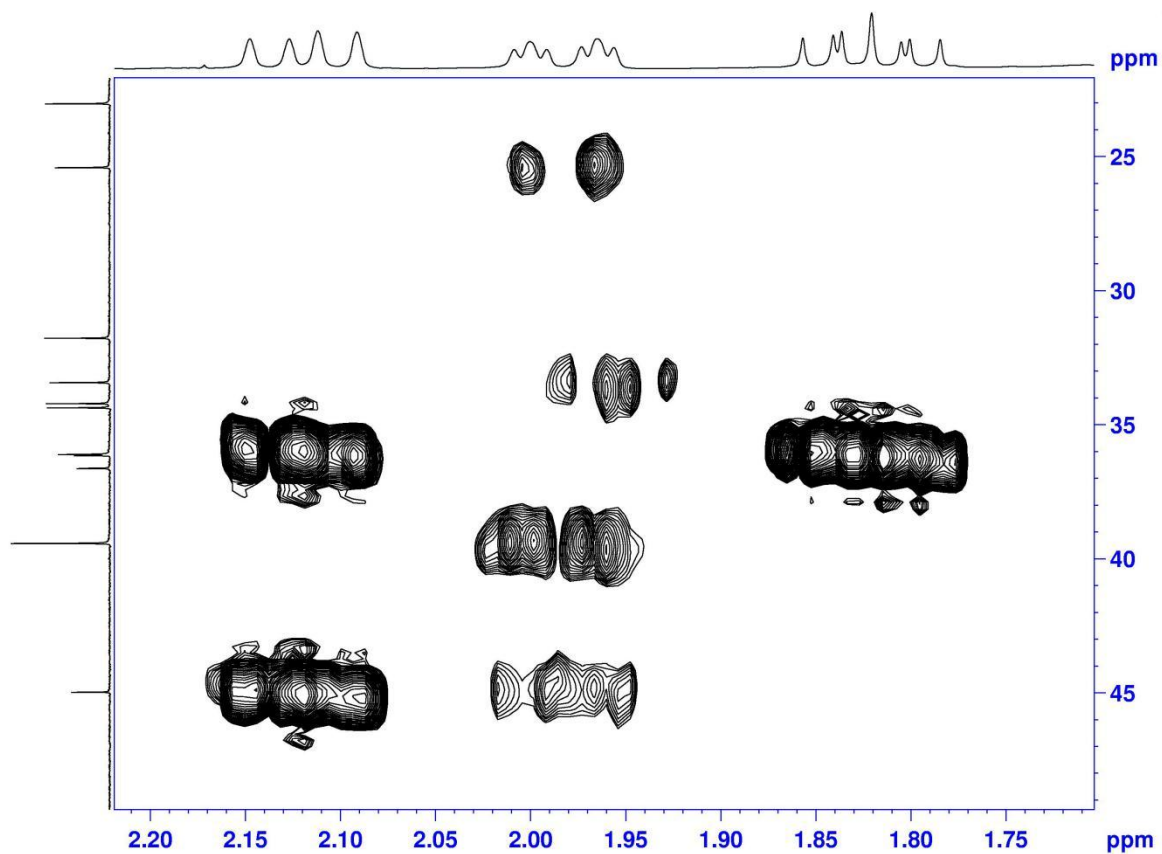
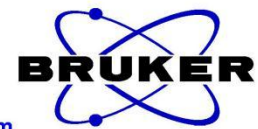
```
NAME R-36-3-3
EXPNO 6
PROCNO 1
Date_ 20160306
Time 2.09
INSTRUM spect
PROBHD 5 mm CPPBBO B3
PULPROG hmcgpp1pndgf
TD 4096
SOLVENT cdcl3
NS 128
DS 16
SWH 5197.505 Hz
FIDRES 1.268922 Hz
AQ 0.3940852 sec
RG 208.5
DW 96.200 usec
DE 10.00 usec
TE 297.0 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.00002080 sec

----- CHANNEL f1 -----
SFO1 400.1323208 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
ND0 2
TD 128
SFO1 100.6233 MHz
FIDRES 107.800476 Hz
SW 238.896 ppm
EnMODE QF
SI 2048
SF 400.1300075 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6127485 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```

HMBC (400 MHz) spectrum of tagalol A (2) in CDCl₃



HMBC (400 MHz) spectrum of tagalol A (2) in CDCl₃

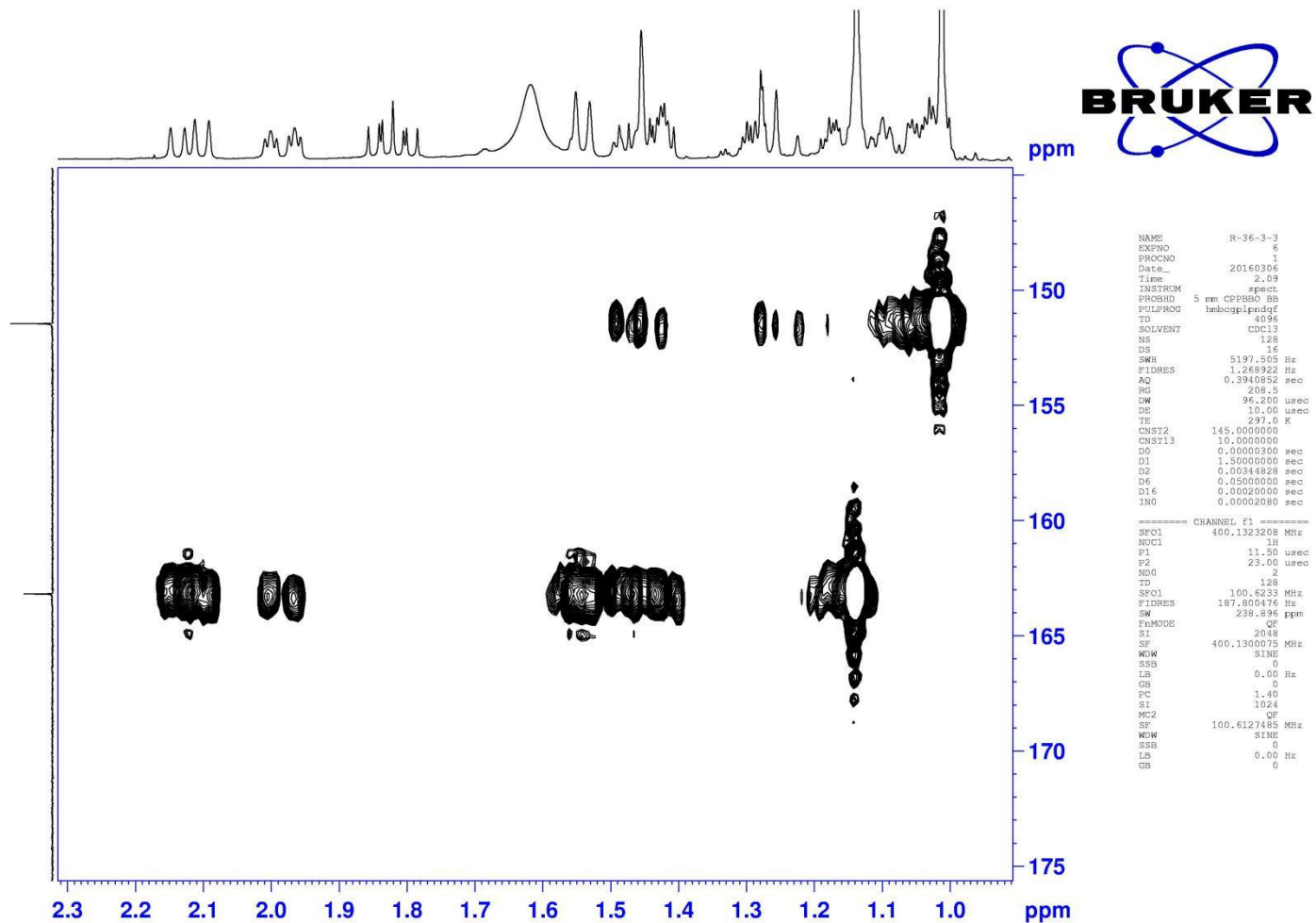


```

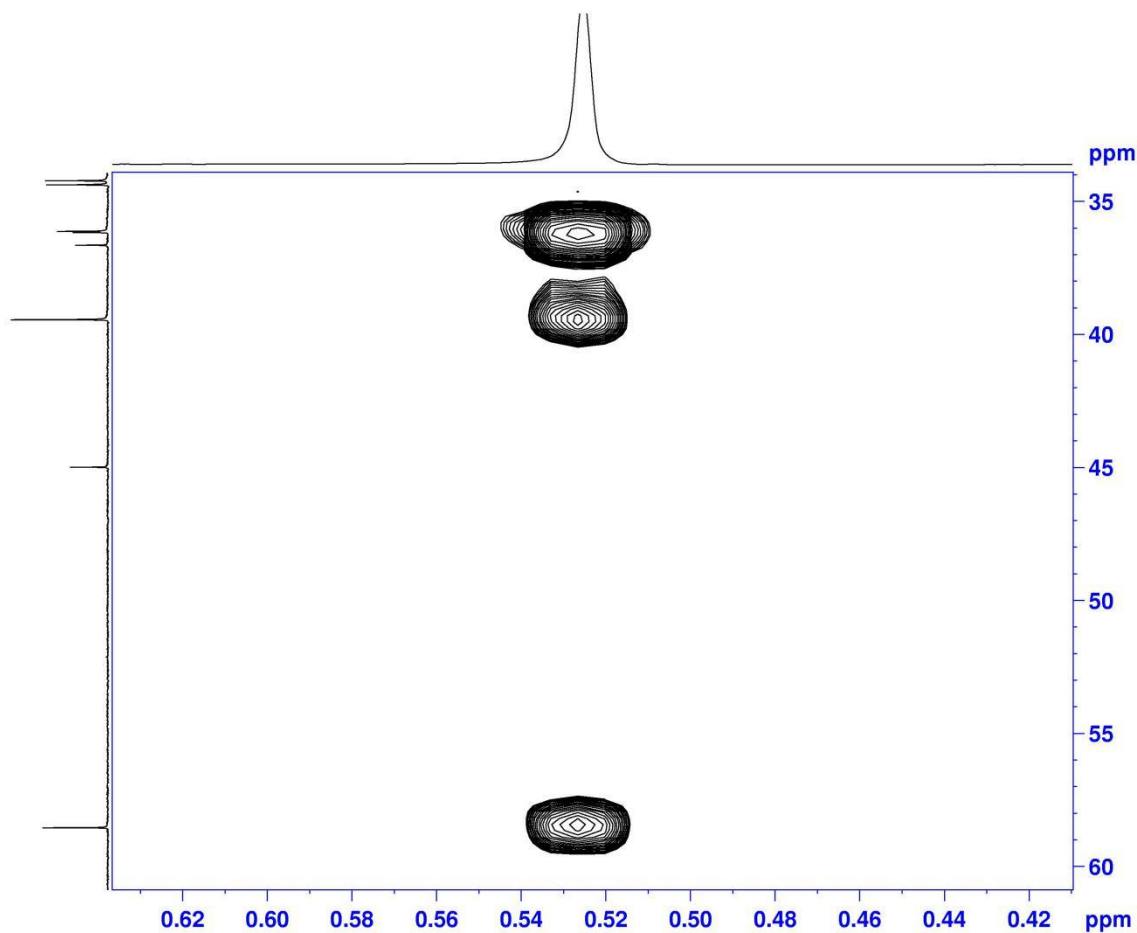
NAME R-36-3-3
EXPNO 6
PROCNO 1
Date_ 20160306
Time 2.09
INSTRUM spect
PROBHD 5 mm CP131 BBO
PULPROG hmczgpg1p0d0f
TD 4096
SOLVENT CDCl3
NS 128
DS 16
SWH 5197.505 Hz
FIDRES 1.268922 Hz
AQ 0.3940852 sec
RG 208.5
DW 96.200 usec
DE 10.00 usec
TE 297.0 K
CNS12 145.000000
CNS13 10.000000
D0 0.0000300 sec
D1 1.5000000 sec
D2 0.00344828 sec
D6 0.0000000 sec
D16 0.0002000 sec
IN0 0.00002090 sec

===== CHANNEL f1 =====
SFO1 400.1323208 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
ND0 2
TD 128
SFO1 100.6223 MHz
FIDRES 187.804476 Hz
SW 238.896 ppm
FHM0DE QF
SI 2048
SF 400.1300075 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
FC 1.40
SI 1024
MC2 QF
SF 100.6127485 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
    
```


HMBC (400 MHz) spectrum of tagalol A (2) in CDCl₃



HMBC (400 MHz) spectrum of tagalol A (2) in CDCl₃

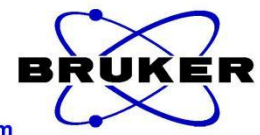
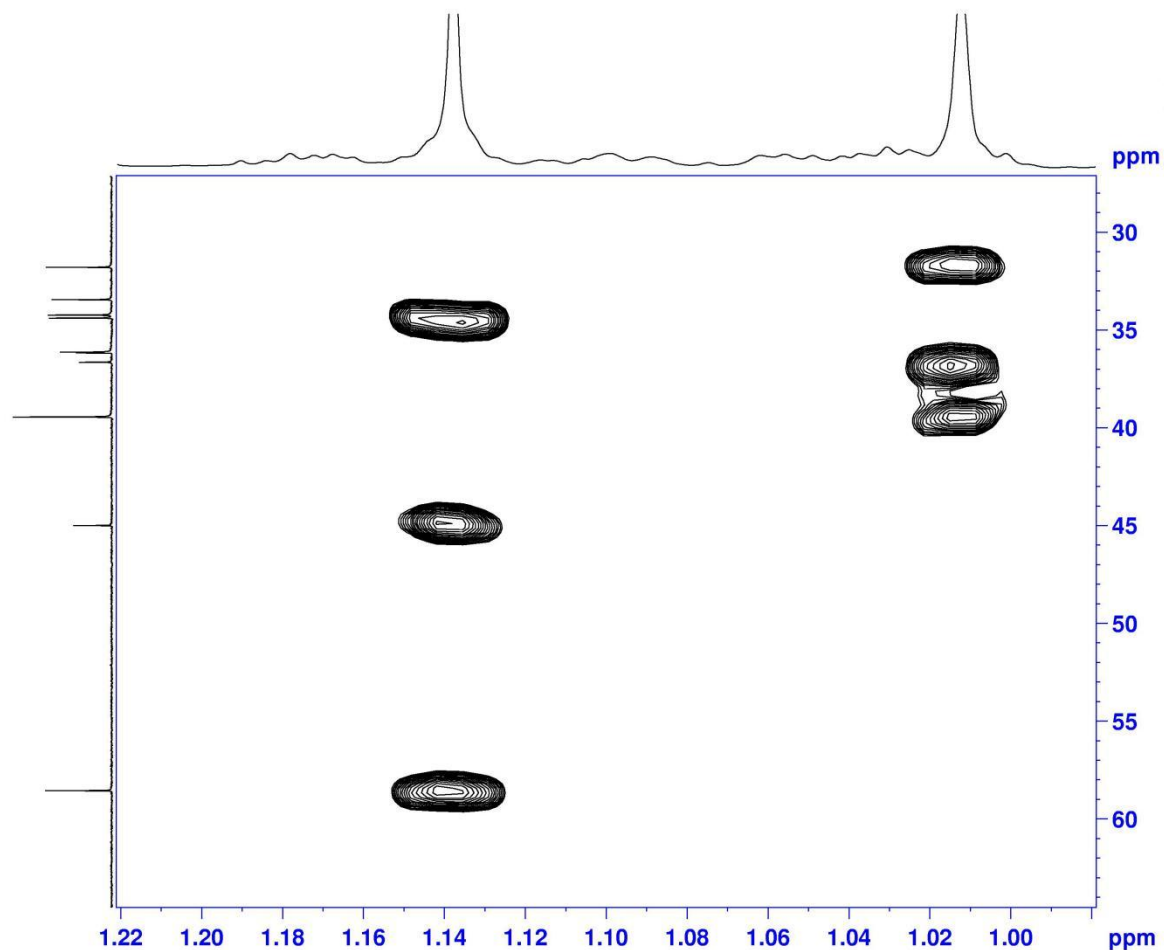


```

NAME          R-36-3-3
EXPNO         6
PROCNO        1
Date_         20160306
Time          2.09
INSTRUM       spect
PROBHD        5 mm CPBPRNO BB
PULPROG       hmbcgp1pndqf
TD            4096
SOLVENT       CDCl3
NS            128
DS            16
SWH           5197.505 Hz
FIDRES        1.268922 Hz
AQ            0.3960852 sec
RG            208.5
DW            96.200 usec
DE            10.00 usec
TE            297.0 K
CNS12         145.0000000
CNS13         10.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00200000 sec
RG            0.00020000 sec

===== CHANNEL f1 =====
SF01          400.1323208 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
ND0           2
TD            128
SF01          100.6233 MHz
FIDRES        187.800476 Hz
SW            238.496 ppm
FIMODE        QF
SI            2048
SF            400.1300075 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            100.6127485 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
    
```

HMBC (400 MHz) spectrum of tagalol A (2) in CDCl₃

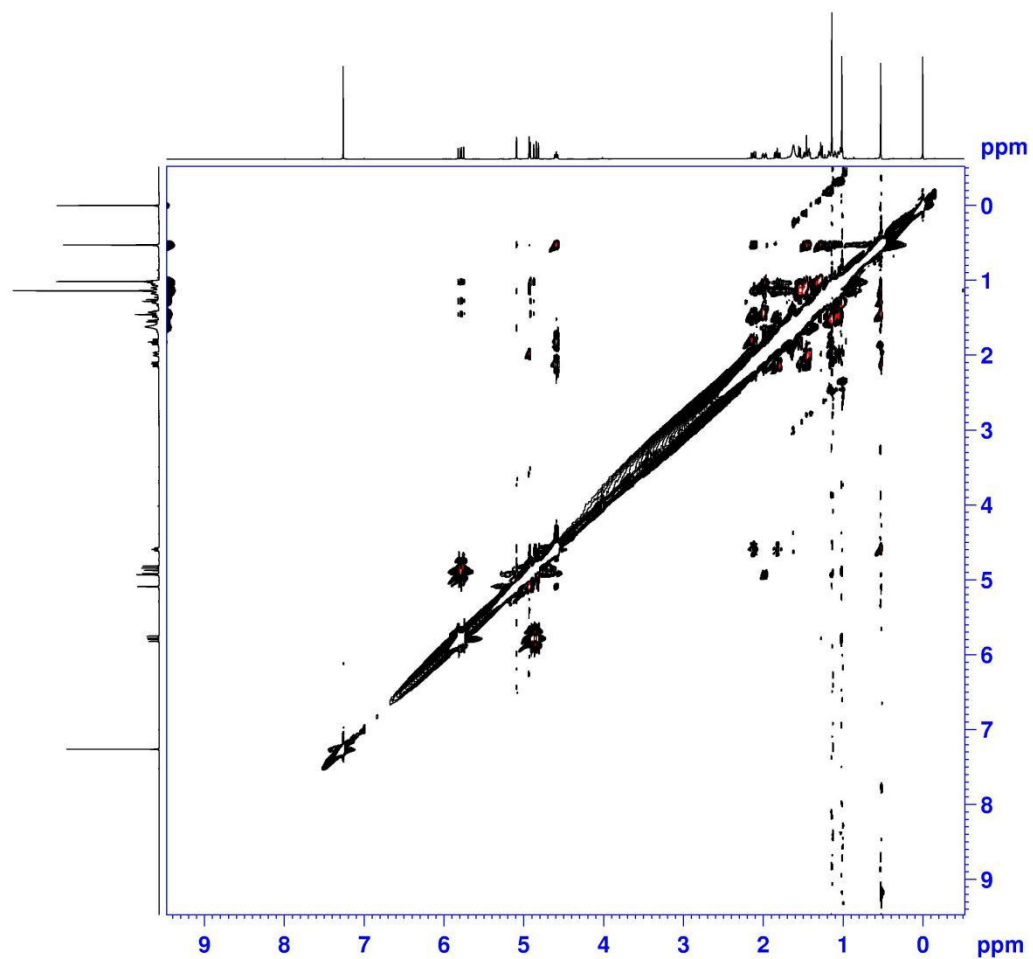


```

NAME          R-36-3-3
EXPNO         6
PROCNO        1
Date_         20160306
Time          2.09
INSTRUM       spect
PROBHD        5 mm CDPABO BB
PULPROG       hmcpgpprdgf
TD            4096
SOLVENT       CDCl3
NS           128
DS            16
SWH           5197.505 Hz
FIDRES        1.268922 Hz
AQ            0.3940852 sec
RG            208.5
DW            96.200 usec
DE            10.00 usec
TE            297.0 K
CNS12         145.000000
CNS13         10.000000
D0            0.0000300 sec
D1            1.5000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00020000 sec
IN0           0.00002090 sec

----- CHANNEL f1 -----
SFO1         400.1323208 MHz
NUC1         1H
P1           11.50 usec
P2           23.00 usec
ND0          2
TD           128
SFO1         100.6223 MHz
FIDRES        187.804476 Hz
SW           238.896 ppm
FHM0DE       QF
SI           2048
SF           400.1300075 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
FC           1.40
SI           1024
MC2          QF
SF           100.6127485 MHz
WDW          SINE
SSB          0
LB           0.00 Hz
GB           0
    
```

NOESY (400 MHz) spectrum of tagalol A (2) in CDCl₃



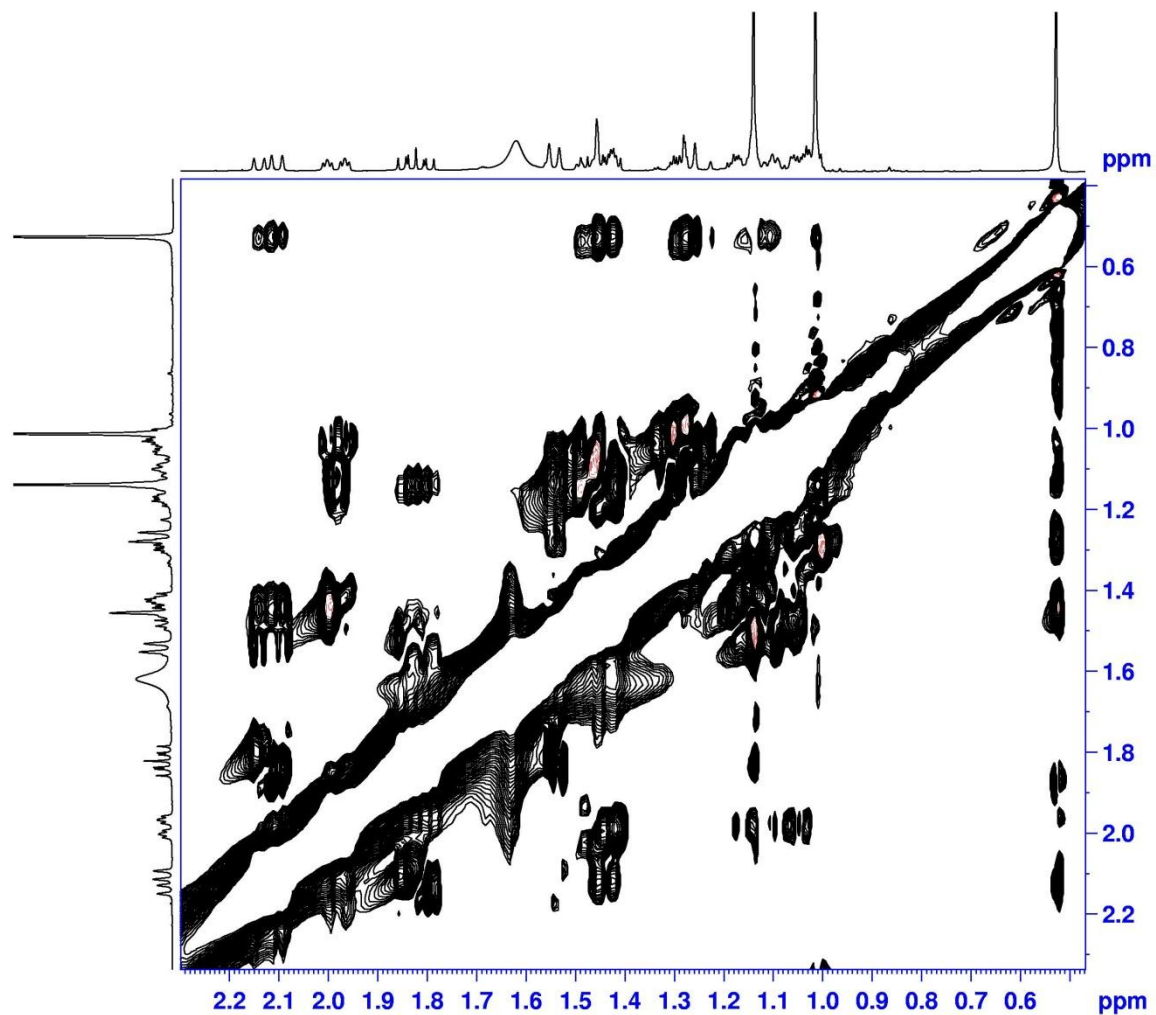
```

NAME          R-36-3-3
EXPNO         7
PROCNO        1
Date_         20160306
Time         11.03
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       noesygpphpp
TD            2048
SOLVENT       cdcl3
NS            32
DS            32
SWH           4000.000 Hz
FIDRES        1.953125 Hz
AQ            0.2560500 sec
RG            208.5
DW            125.000 usec
DE            10.00 usec
TE            297.0 K
DO            0.00011036 sec
D1            1.99385395 sec
DS            0.30000001 sec
D11           0.03000000 sec
D12           0.00002000 sec
D16           0.00020000 sec
INO           0.00025000 sec
    
```

```

===== CHANNEL f1 =====
SFO1         400.1318006 MHz
NUC1         1H
P1           11.50 usec
P2           23.00 usec
P17          2500.00 usec
ND0          1
TD           256
SFO1         400.1318 MHz
FIDRES        15.625000 Hz
SW           9.997 ppm
FrMODE       States-TPPI
SI           1024
SF           400.1300098 MHz
WDW          QSINE
SSB          2
LB           0.00 Hz
GB           0
PC           1.00
SI           1024
WC2          States-TPPI
SF           400.1300098 MHz
WDW          QSINE
SSB          2
LB           0.00 Hz
GB           0
    
```

NOESY (400 MHz) spectrum of tagalol A (2) in CDCl₃



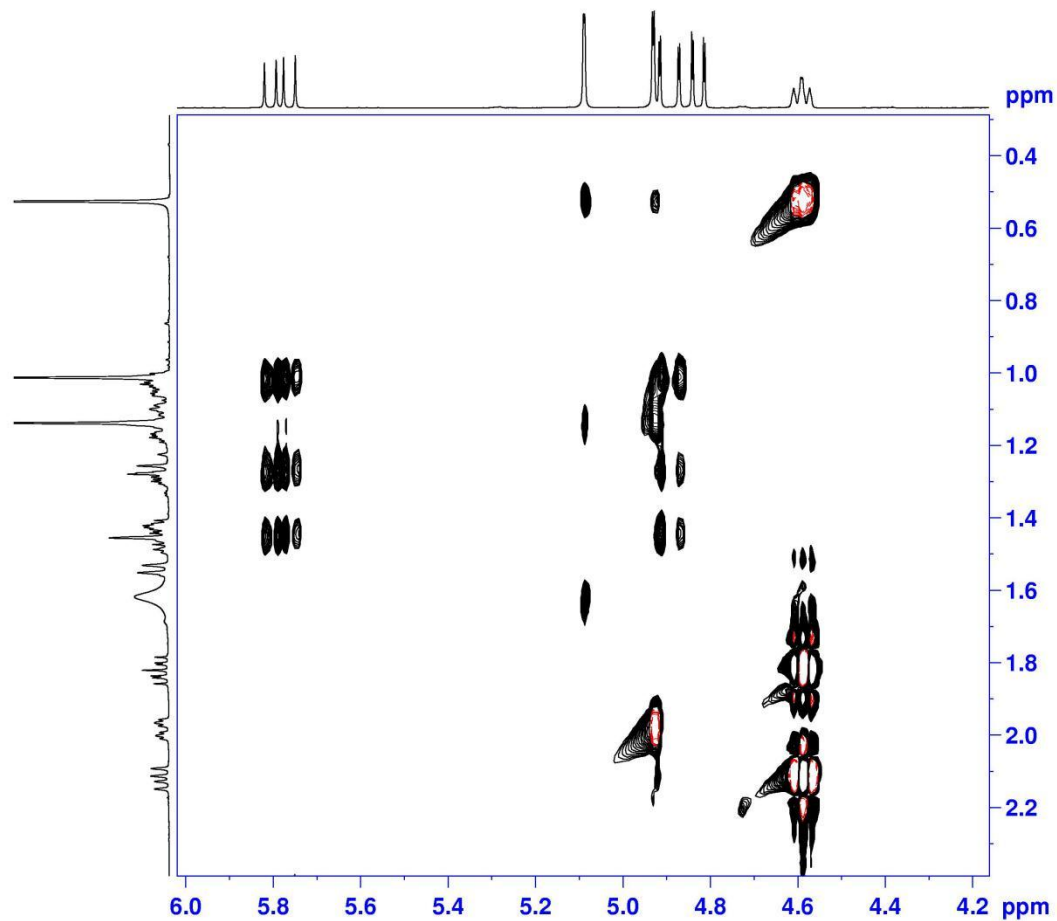
```

NAME      zzh-16  R-36-3-3
EXPNO     7
PROCNO    1
Date_     20160306
Time      11.03
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   noesygpphpp
TD         2048
SOLVENT   CDCl3
NS         32
DS         32
SWH        4000.000 Hz
FIDRES     1.953125 Hz
AQ         0.2560500 sec
RG         208.5
DW         125.000 usec
DE         10.00 usec
TE         297.0 K
D0         0.00011036 sec
D1         1.99385595 sec
D8         0.30000001 sec
D11        0.03000000 sec
D12        0.00002000 sec
D16        0.00020000 sec
IN0        0.00025000 sec
    
```

```

===== CHANNEL f1 =====
SF01      400.1318006 MHz
NUC1       1H
P1         11.50 usec
P2         23.00 usec
P17        2500.00 usec
ND0        1
TD         256
SF01      400.1318 MHz
FIDRES     15.625000 Hz
SW         9.997 ppm
FnMODE     States-TPPI
SI         1024
SF         400.1300089 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00
SI         1024
MC2        States-TPPI
SF         400.1300089 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
    
```

NOESY (400 MHz) spectrum of tagalol A (2) in CDCl₃



```

NAME          R-36-3-3
EXPNO         7
PROCNO        1
Date_         20160306
Time          11.03
INSTRUM       spect
PROBHD        5 mm CPPBBO BB
PULPROG       noesygpphph
TD            2048
SOLVENT       CDCl3
NS            32
DS            32
SWH           4000.000 Hz
FIDRES        1.953125 Hz
AQ            0.2560500 sec
RG            208.5
DW            125.000 usec
DE            10.00 usec
TE            297.0 K
D0            0.00011036 sec
D1            1.99385595 sec
D8            0.30000001 sec
D11           0.03000000 sec
D12           0.00020000 sec
D16           0.00020000 sec
IN0           0.00025000 sec

===== CHANNEL f1 =====
SFO1          400.1318006 MHz
NUC1          1H
P1            11.50 usec
P2            23.00 usec
P17           2500.00 usec
ND0           1
TD            256
SFO1          400.1318 MHz
FIDRES        15.625000 Hz
SW            9.997 ppm
FMODE         States-TPPI
SI            1024
SF            400.1300098 MHz
WVW           QSINE
SBB           2
LB            0.00 Hz
GB            0
PC            1.00
SI            1024
MC2           States-TPPI
SF            400.1300098 MHz
WVW           QSINE
SBB           2
LB            0.00 Hz
GB            0
    
```