Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

^{13}C NMR and ECD Calculation Methods, Table S1-S3, Figure S1-S6, HRESIMS, 1D and 2D NMR Spectra for Tagalide A (**1**) and Tagalol A (**2**).

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Expremental section

^{13}C NMR Calculation Methods

For the calculations of ^{13}C 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 Tomasiet al. was used.[2] The calculated ^{13}C 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 ^{13}C 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 09[4] 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:

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

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:

(1) (a) Miertus, S.; Scrocc, E.; Tomasi, J. *J. Chem. Phys.* **1981**, *55*, 117. (b) Miertus, S.; Tomasi, J. *J. Chem. Phys.* **1982**, *65*, 239. (c) Cossi, M.; Barone, V.; Cammi, R.; Tomasi, J. *Chem. Phys. Lett.* **1996**, *255*, 327.

(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**

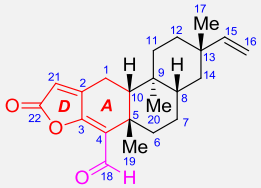
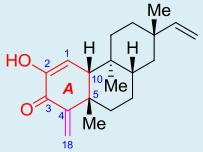
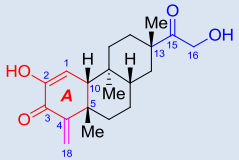
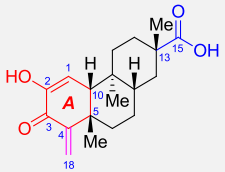
SCF, G: self consistent field (SCF) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level., %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

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 anologs against human breast cancer cells [$\mathbf{IC_{50}}$ (μM)]

Compound	Cell Lines					
	MD-MBA-453	MD-MBA-231	SK-BR-3	MCF-7	MT-1	ZR-75-1
 Tagalide A (**1**)	**1.73**	**8.12**	**2.45**	**12.03**	**3.75**	**1.97**
 tagalsin C	**4.06**	**43.51**	**1.85**	**17.26**	**2.17**	**3.55**
 *ent*-5α,3,15-dioxodolabr-1,4(18)-diene-2,16-diol	**2.58**	**10.99**	**2.08**	**20.65**	**3.92**	**5.87**
 (5*S*,8*S*,9*S*,10*R*,13*S*)-2-hydroxy-16-nor-3-oxodolabr-1,4(18)-dien-15-oic acid	**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**

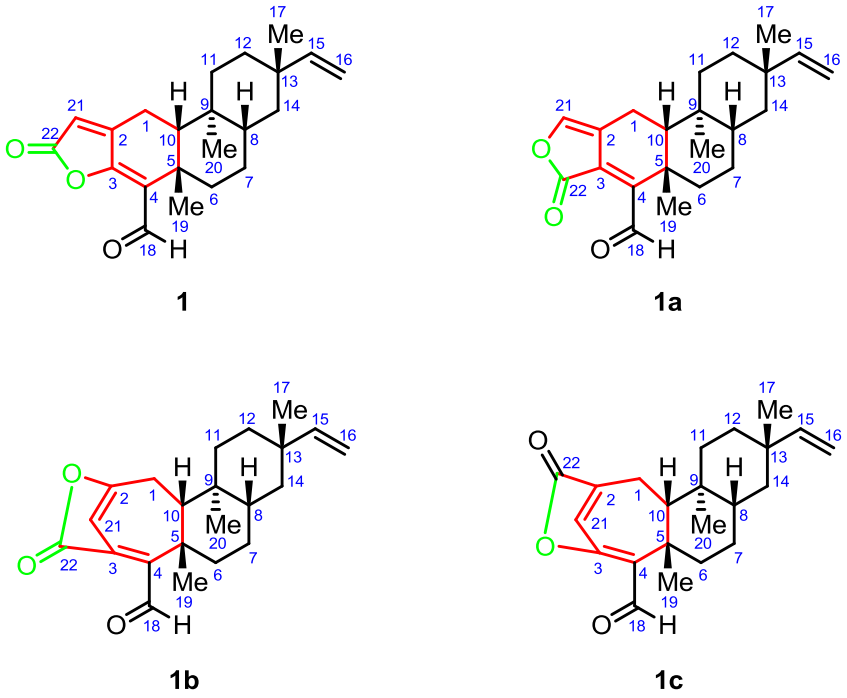
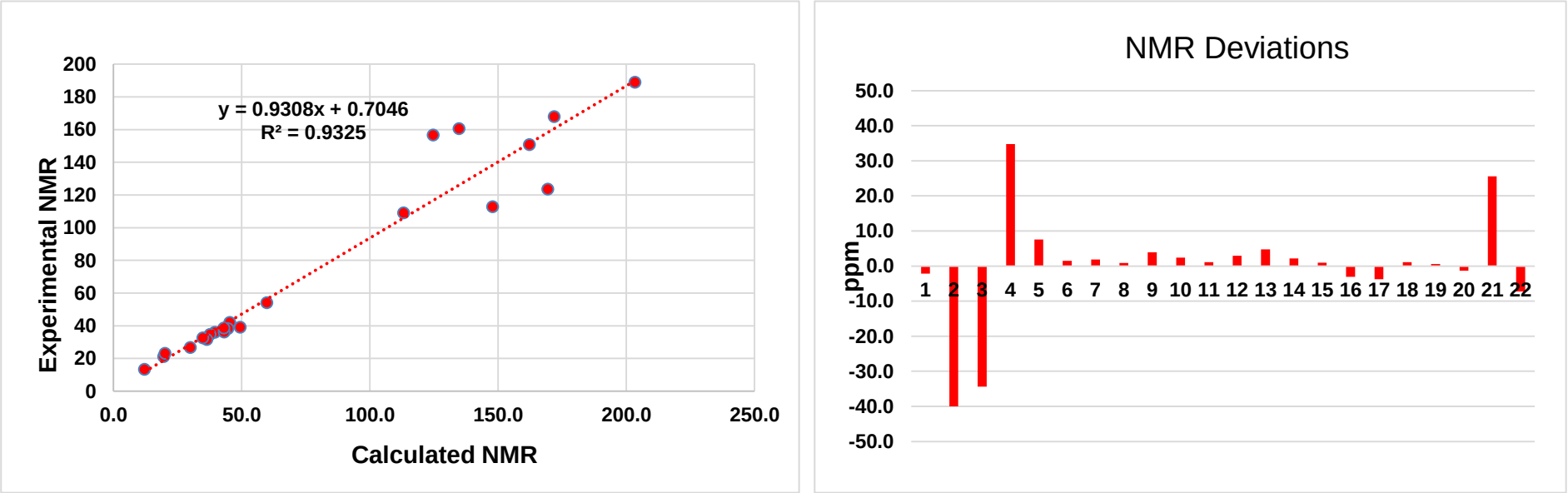


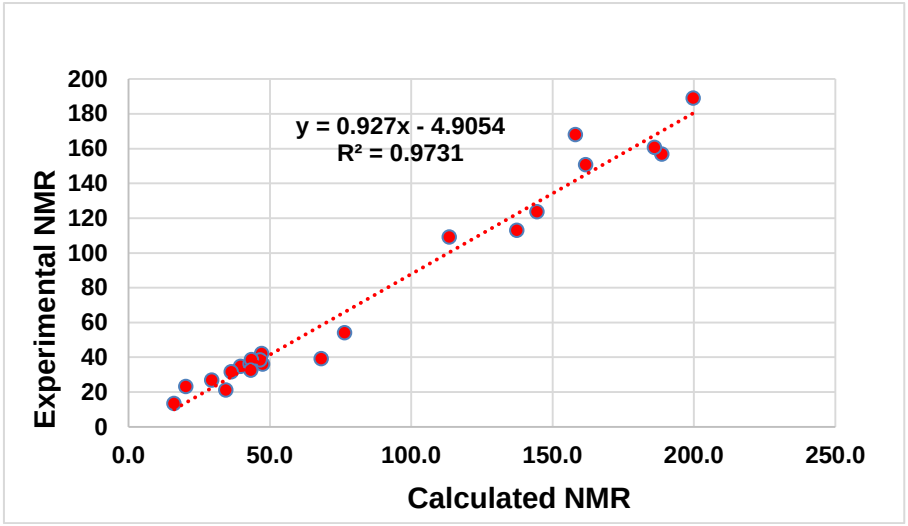
Figure S1. Four possible structures for compound **1**.

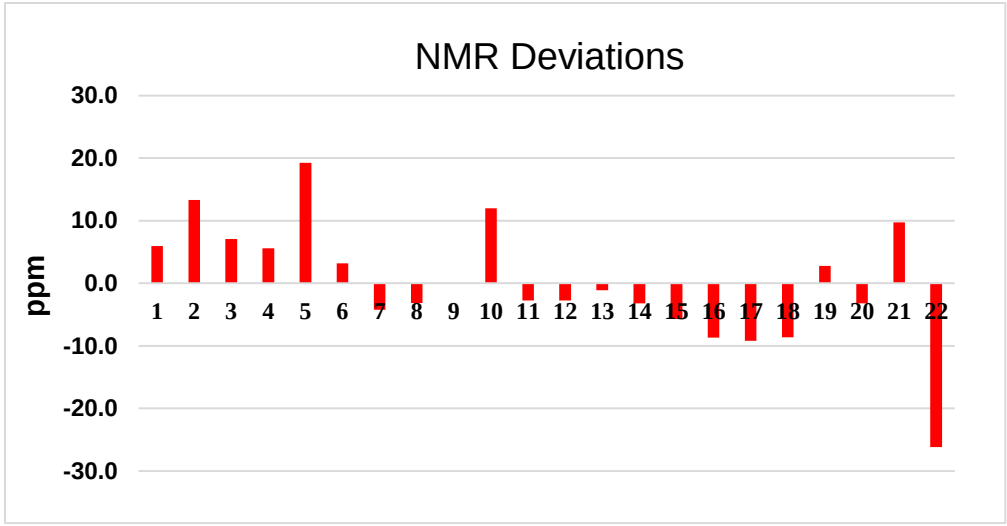


A **B**

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.

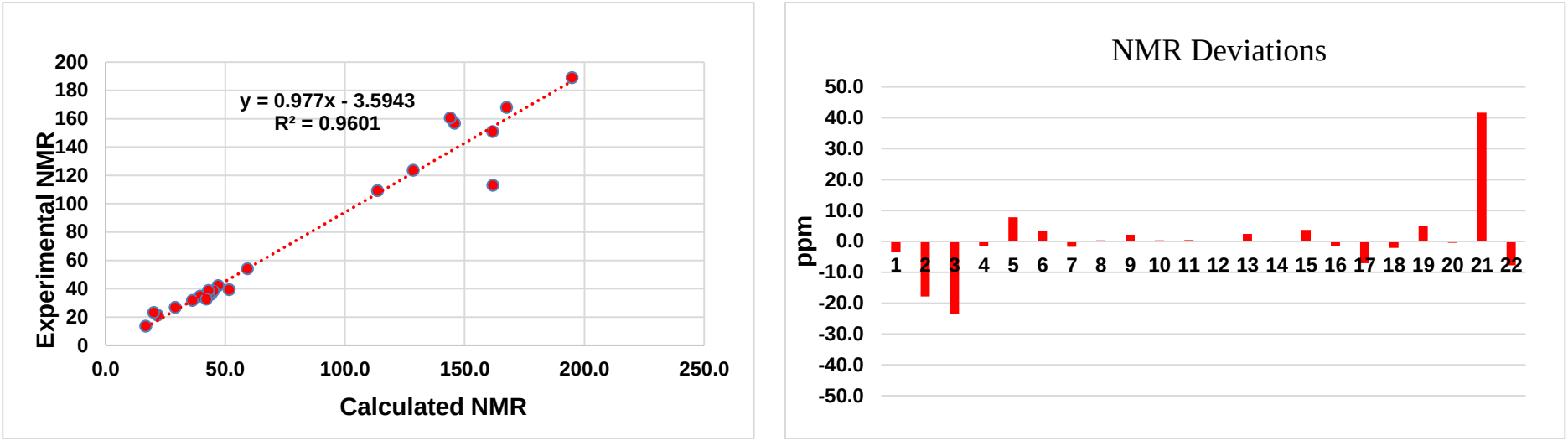




A **B**

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

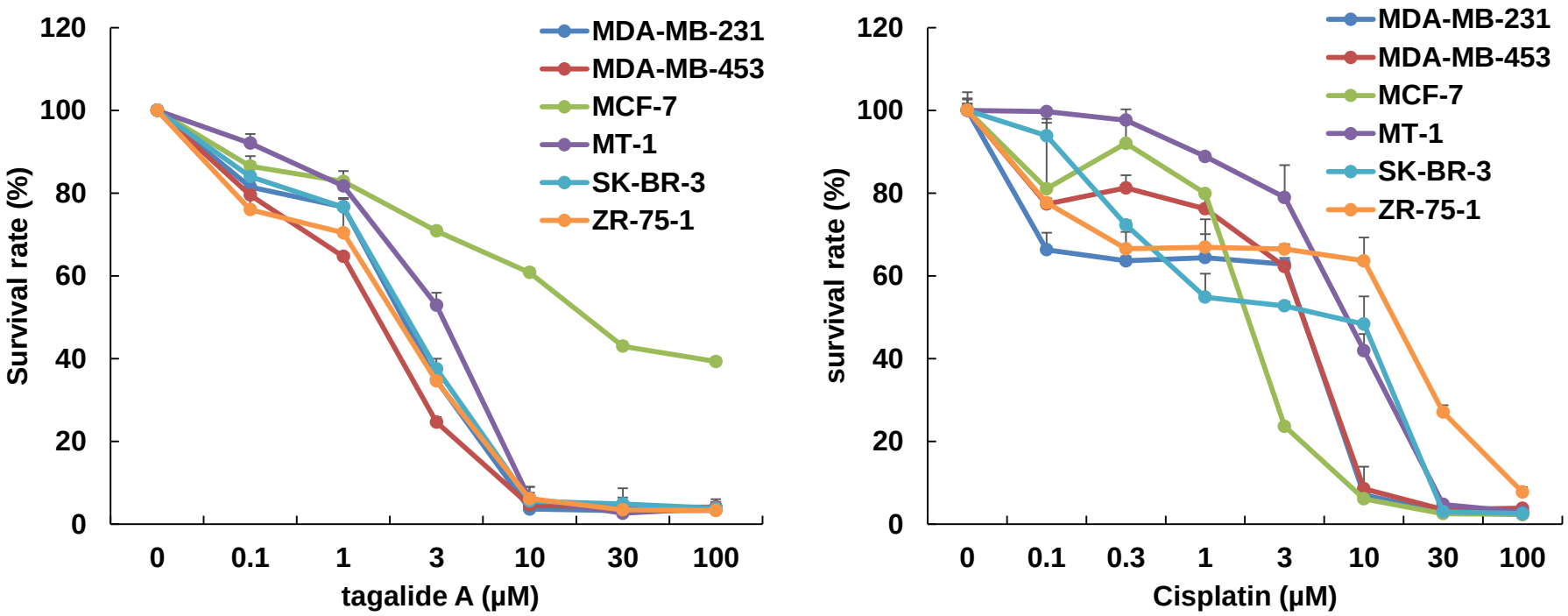


Figure S5. Tagalide A (**1**) inhibits the growth of six human breast cancer cell lines *in vitro*.

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.

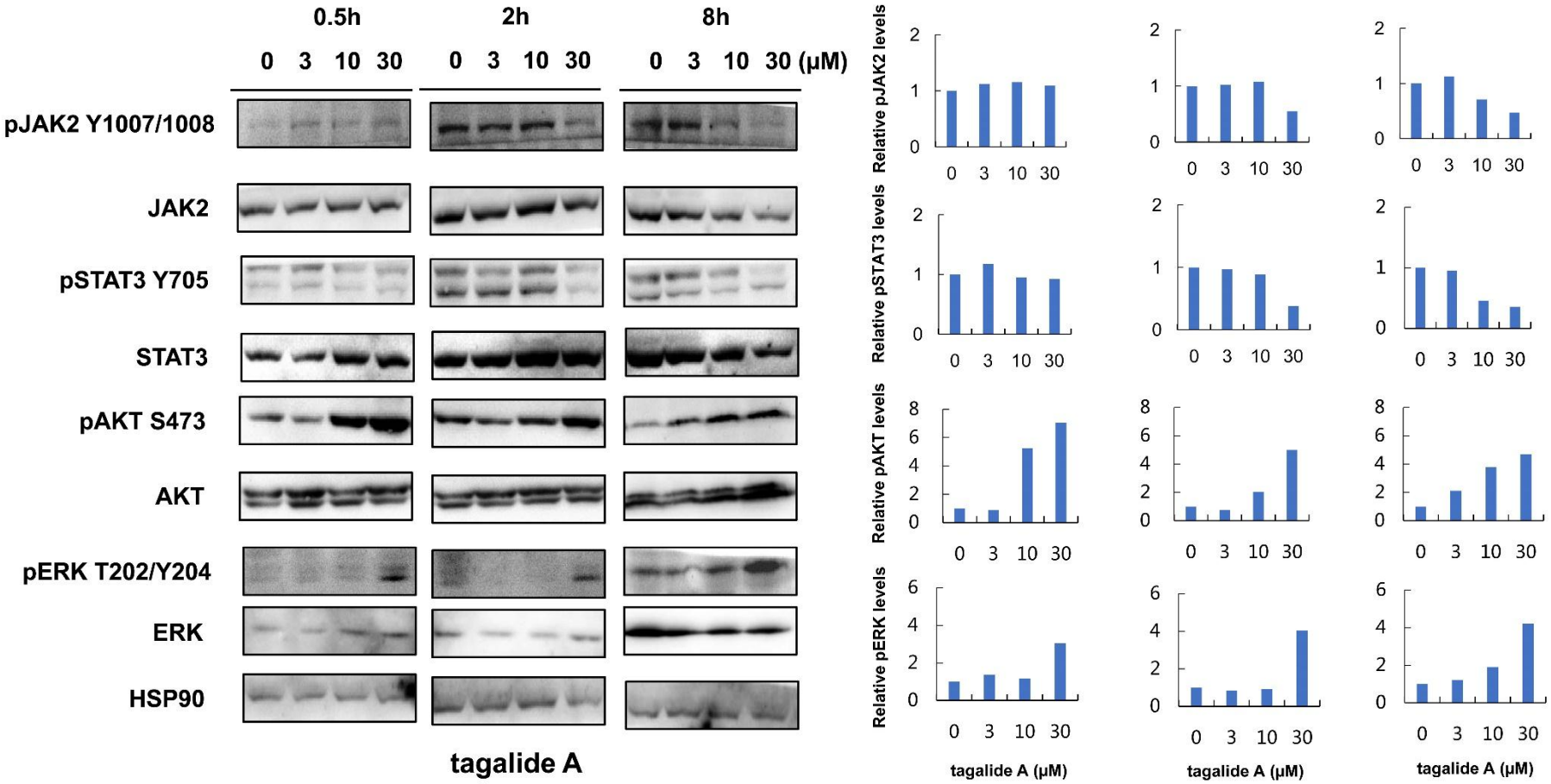


Figure S6. Tagalide A (**1**) inhibits phosphorylation of JAK2 and STAT3, but enhances that of AKT and ERK in MDA-MB-453 cells.

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

Analysis Info

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Sample Name	liwanshan_zxh-15_pos	Instrument / Ser#	maXis 29
Comment			

Acquisition Parameter

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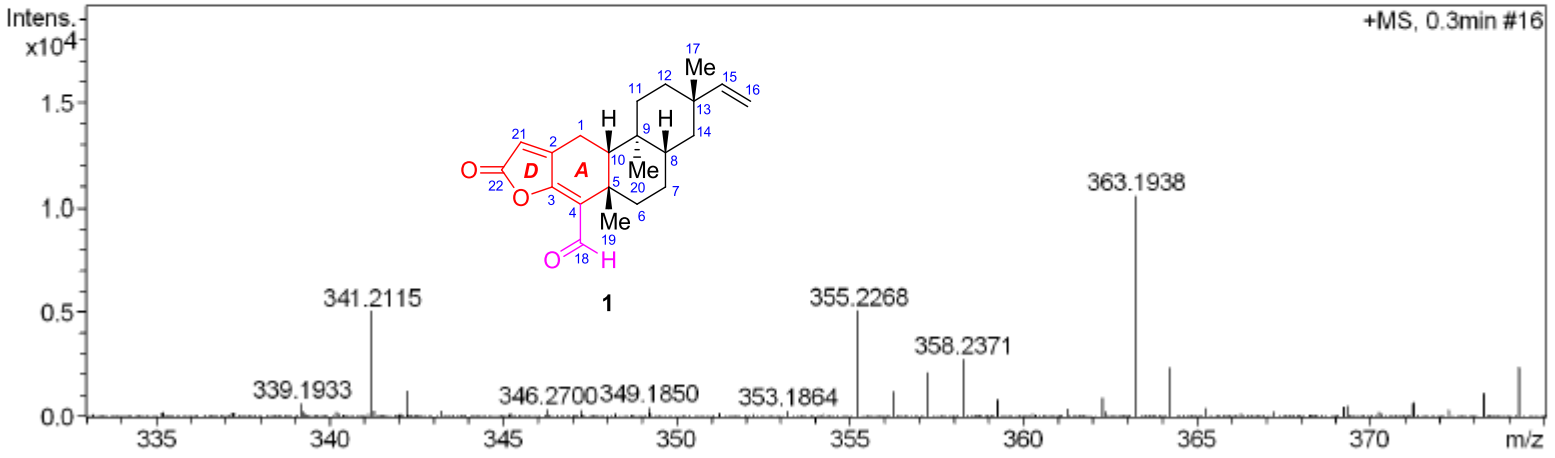

Meas. m/z	#	Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
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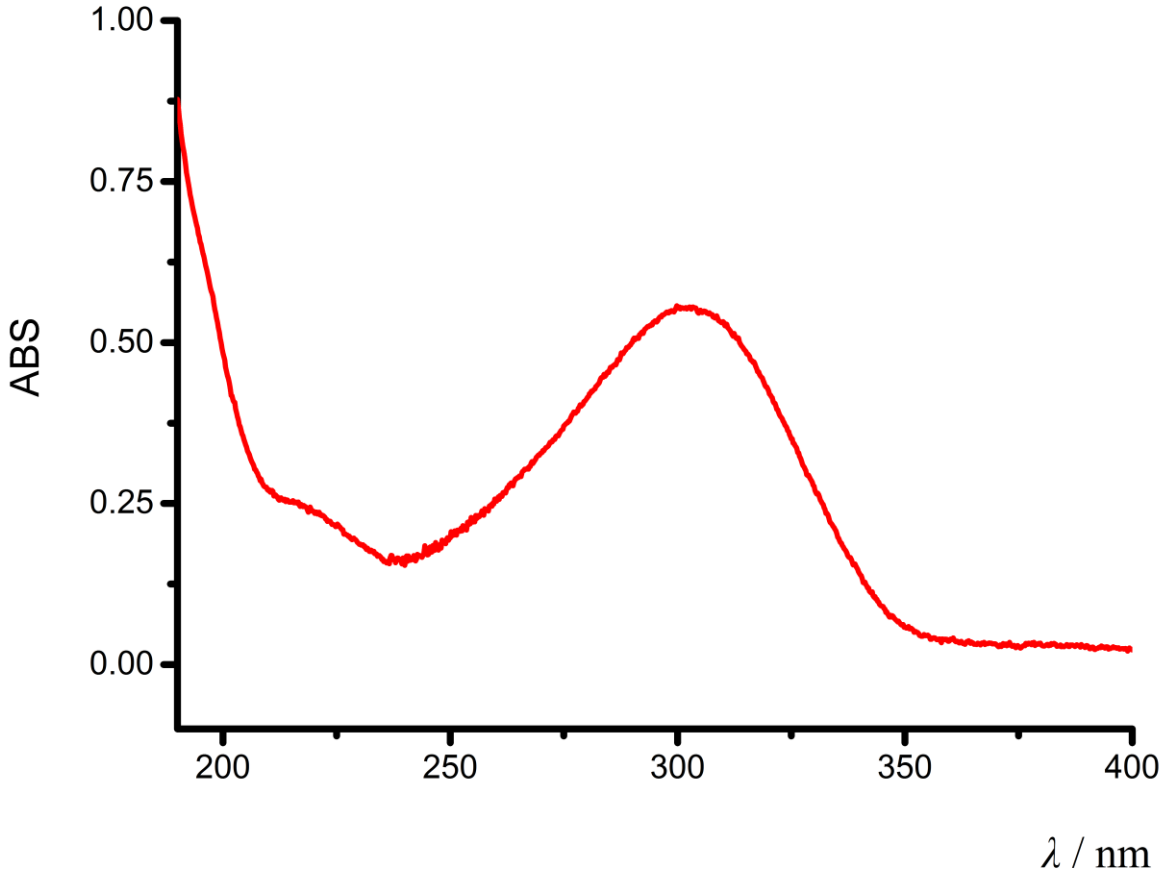
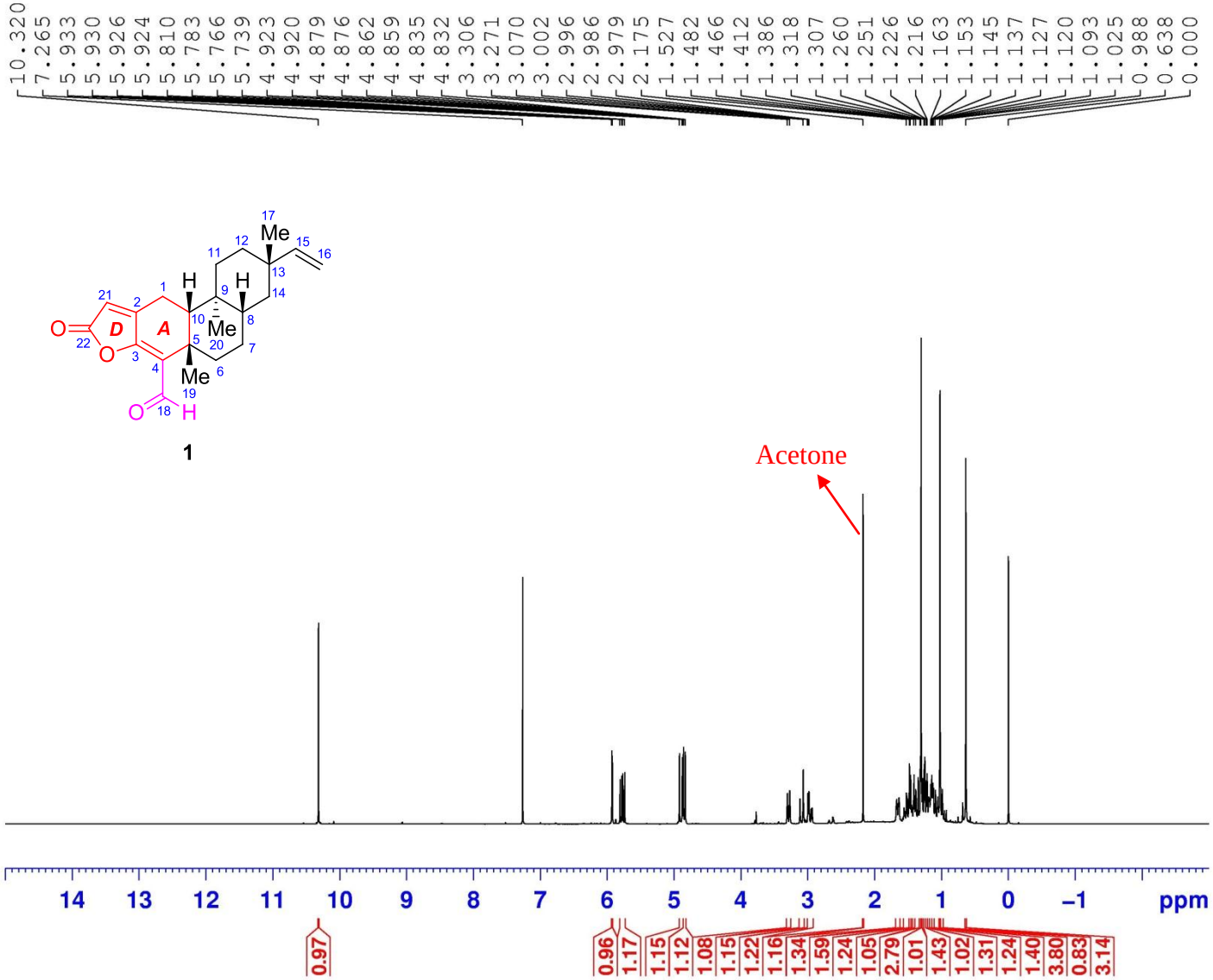
363.1938	1	C 22 H 28 Na O 3	100.00	363.1931	-2.0	-0.7	10.3	8.5	even	ok
703.3990	1	C 44 H 56 Na O 6	27.04	703.3969	-3.0	-2.1	41.9	16.5	even	ok

UV spectrum for tagalide A (1) (recorded in MeCN at 250 µg/mL)



^{1}H (400 MHz) NMR spectrum of tagalide A (1) in $CDCl_3$



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DE                10.00 usec
TE                297.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
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SF          400.1300079 MHz
WDW                   EM
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LB                0.30 Hz
GB                     0
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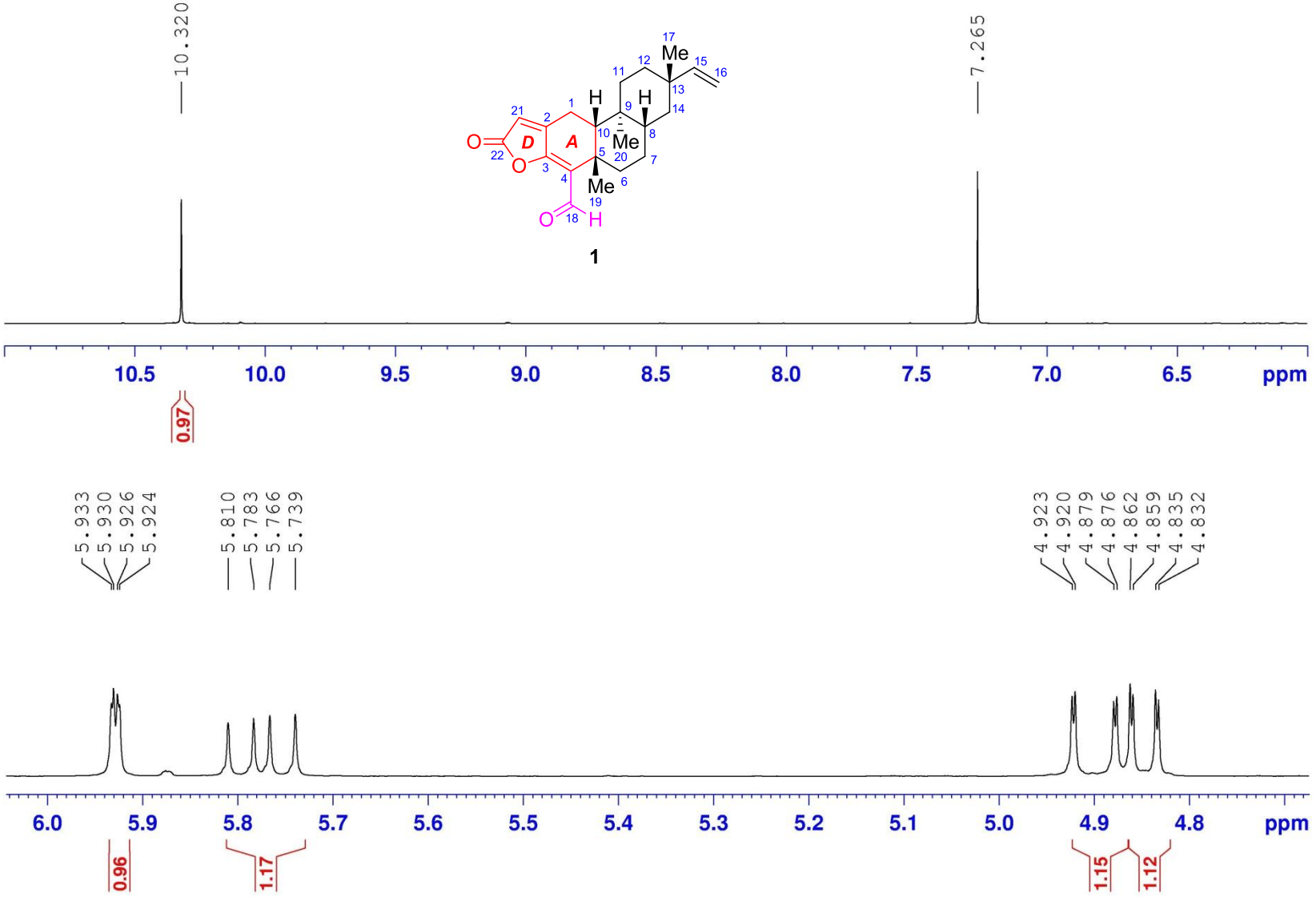
^{1}H (400 MHz) NMR spectrum of tagalide A (1) in $CDCl_3$



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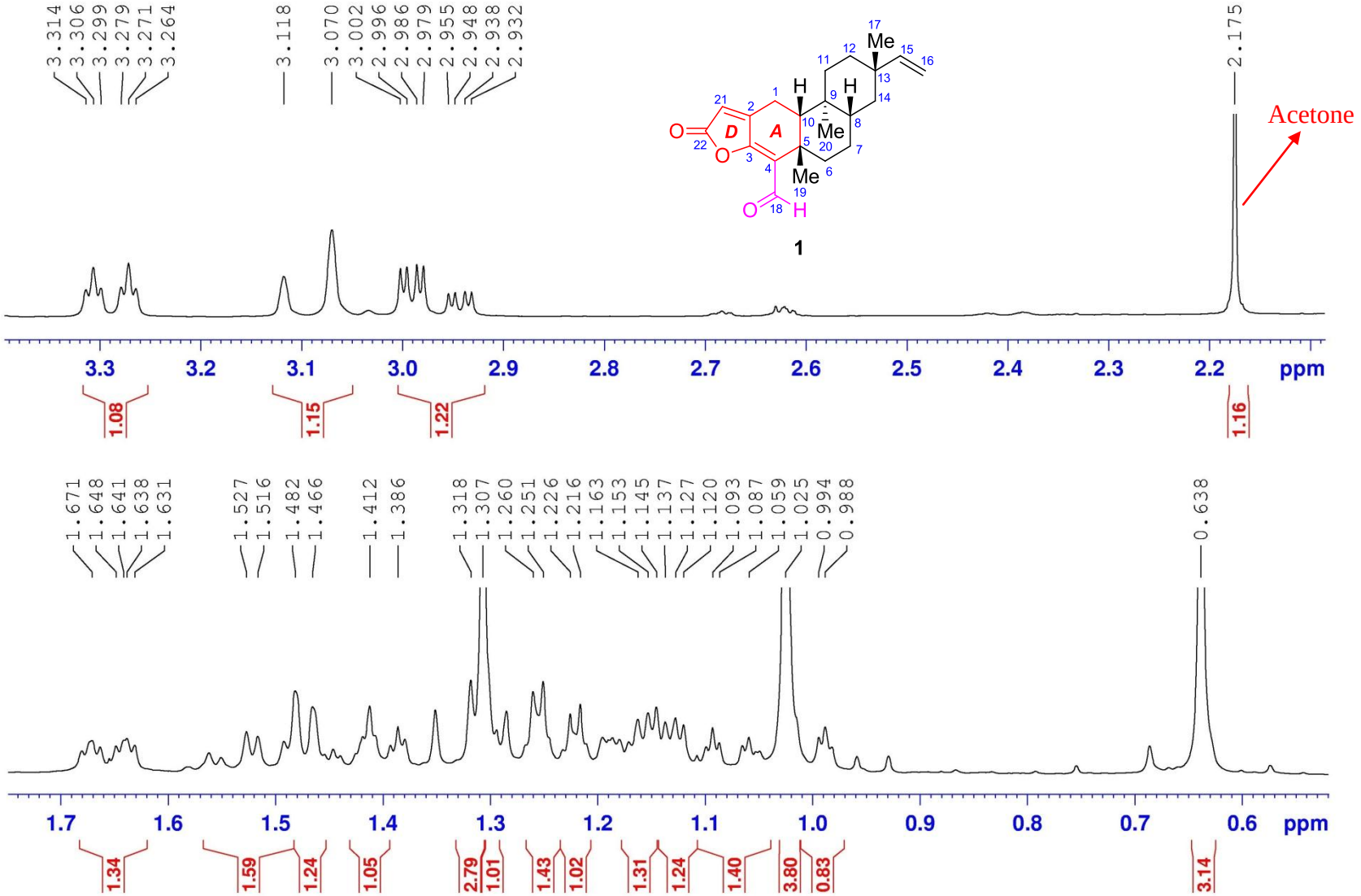
^{1}H (400 MHz) NMR spectrum of tagalide A (1) in $CDCl_3$



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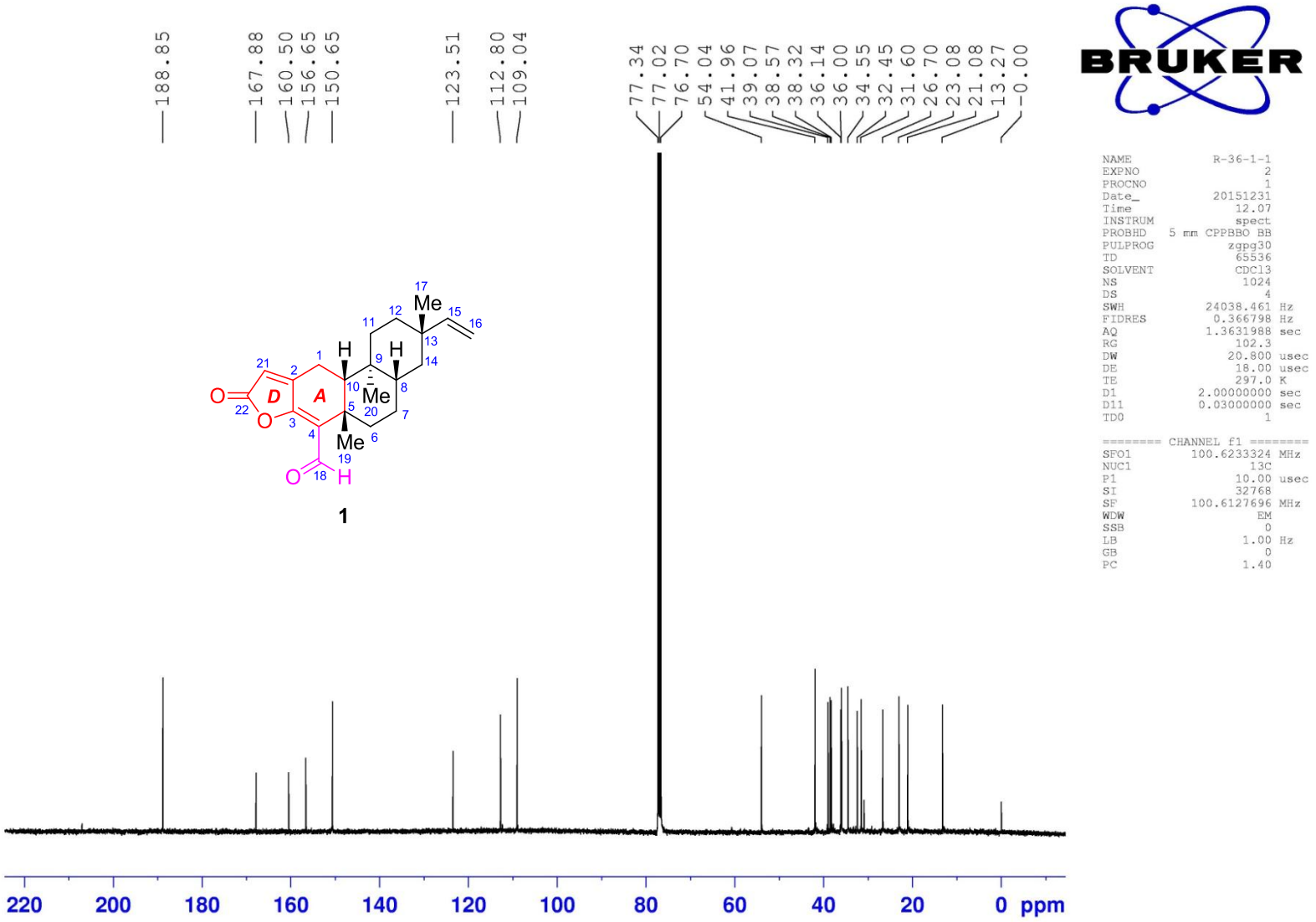

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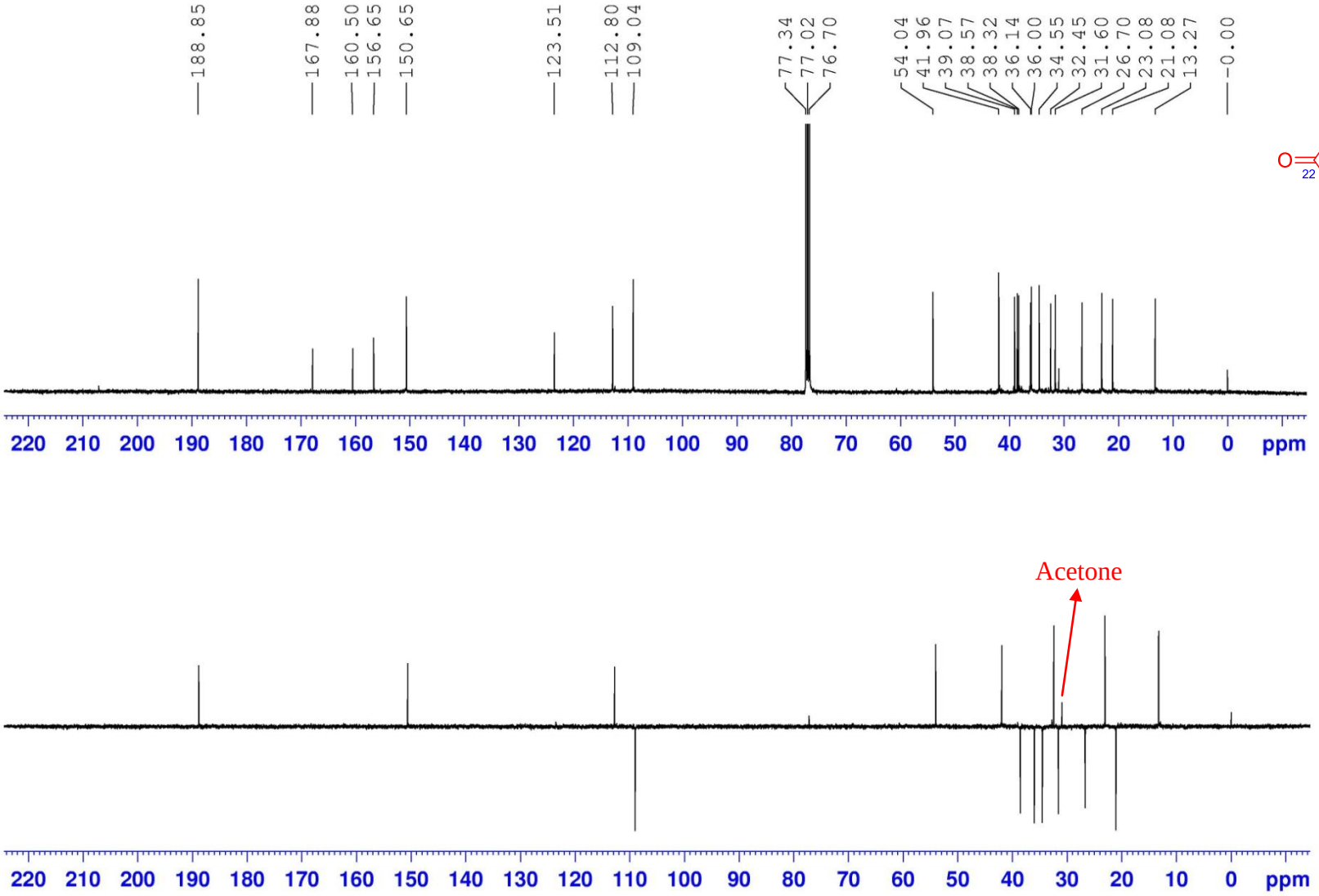
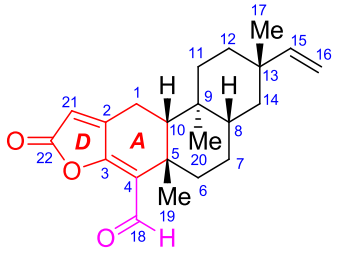
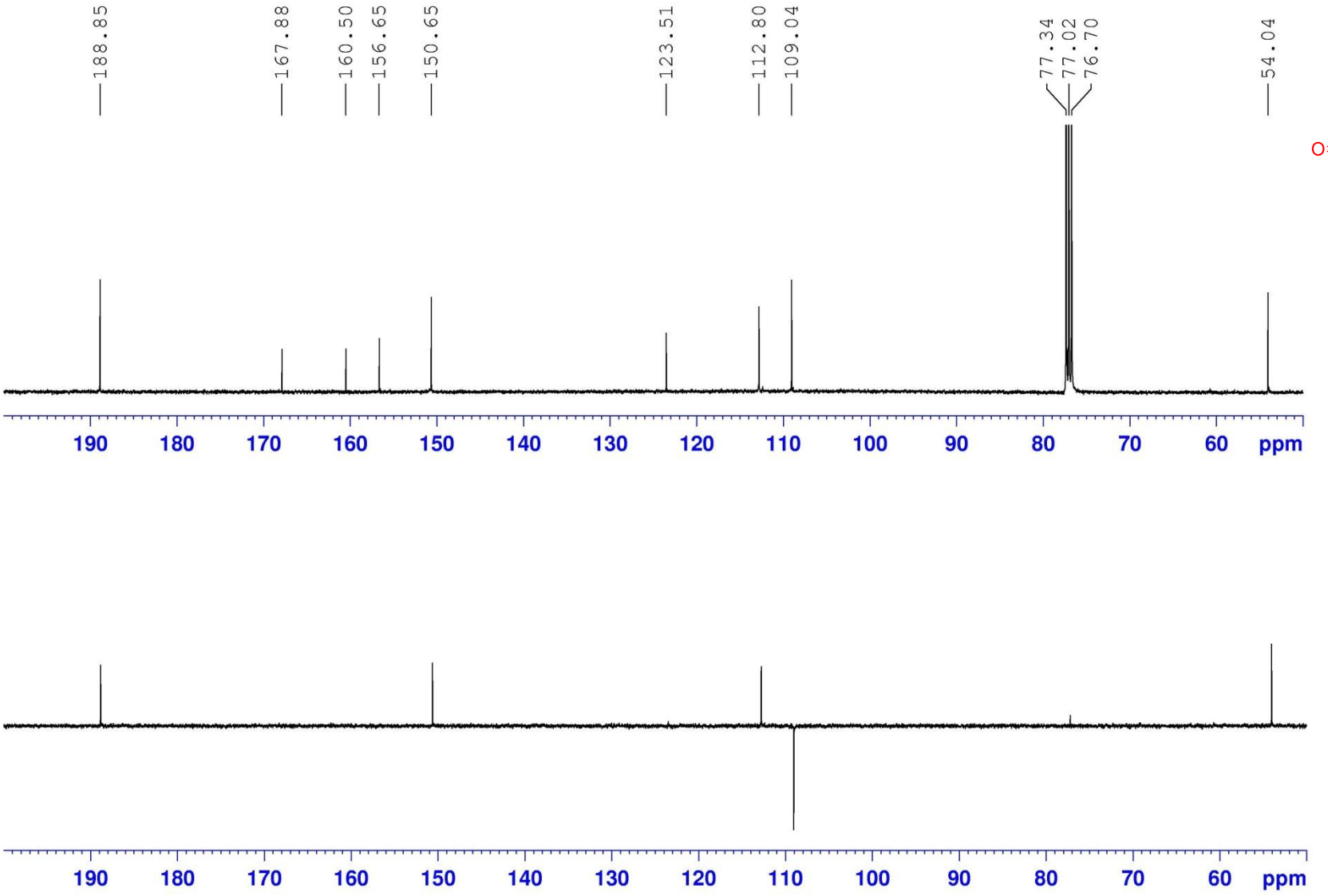
DEPT135 (100 MHz) spectrum of tagalide A (1) in $CDCl_3$

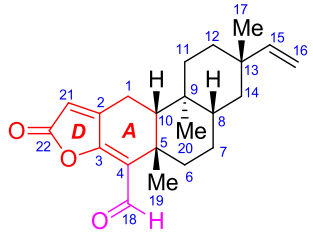




1

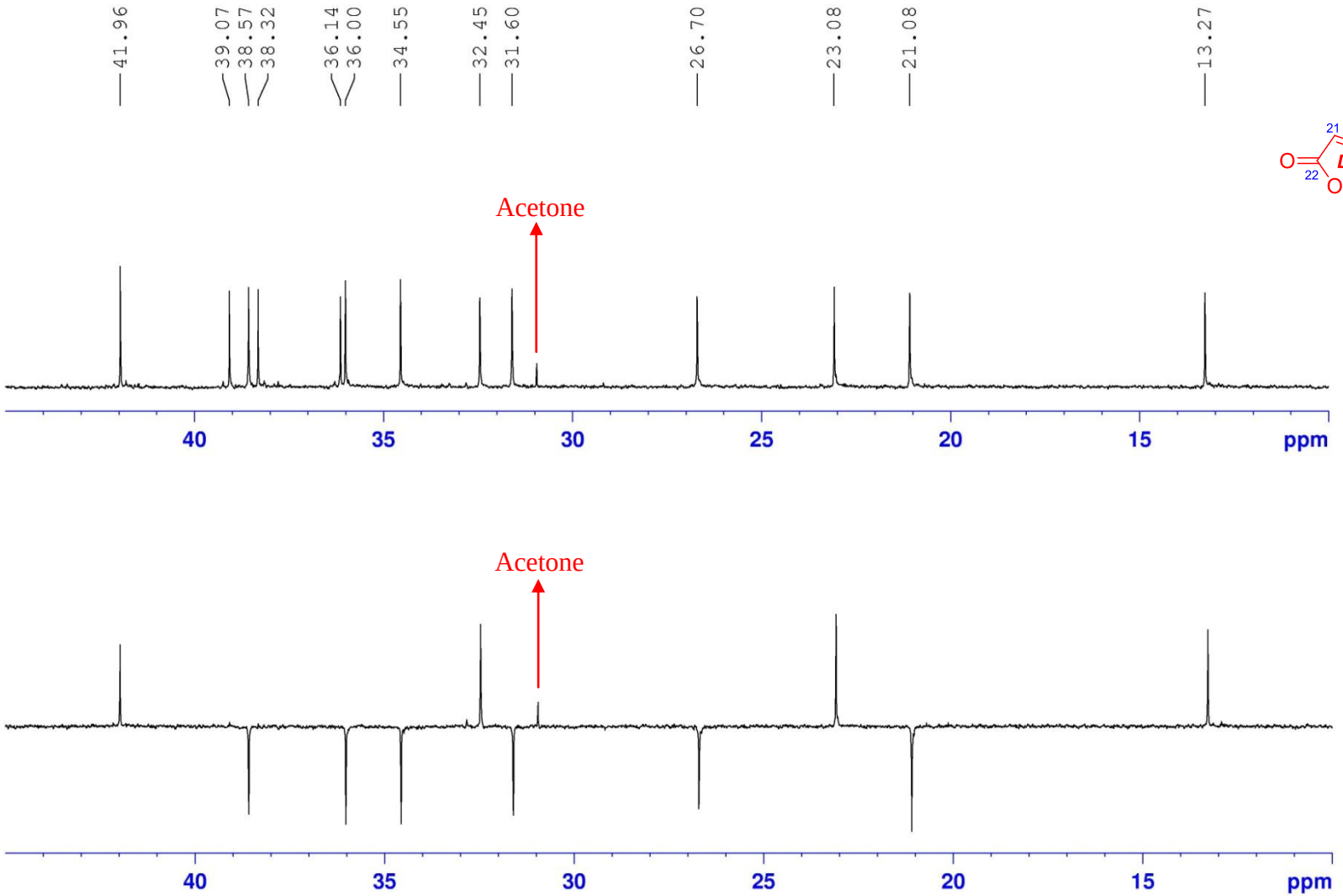
DEPT135 (100 MHz) experiment of tagalide A (1) in $CDCl_3$

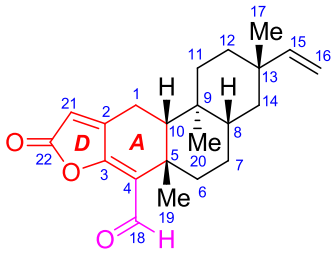




1

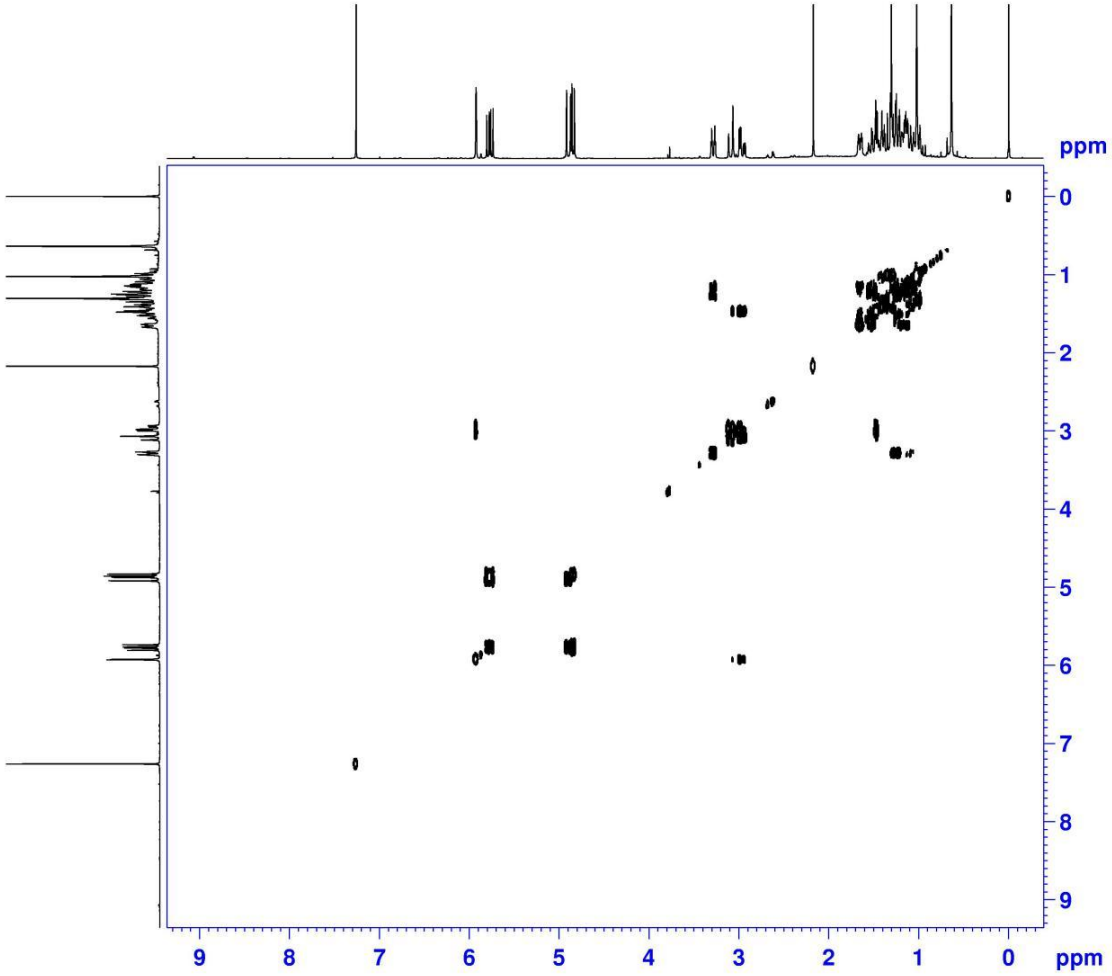
DEPT135 (100 MHz) experiment of tagalide A (1) in $CDCl_3$

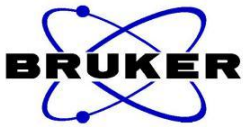




1

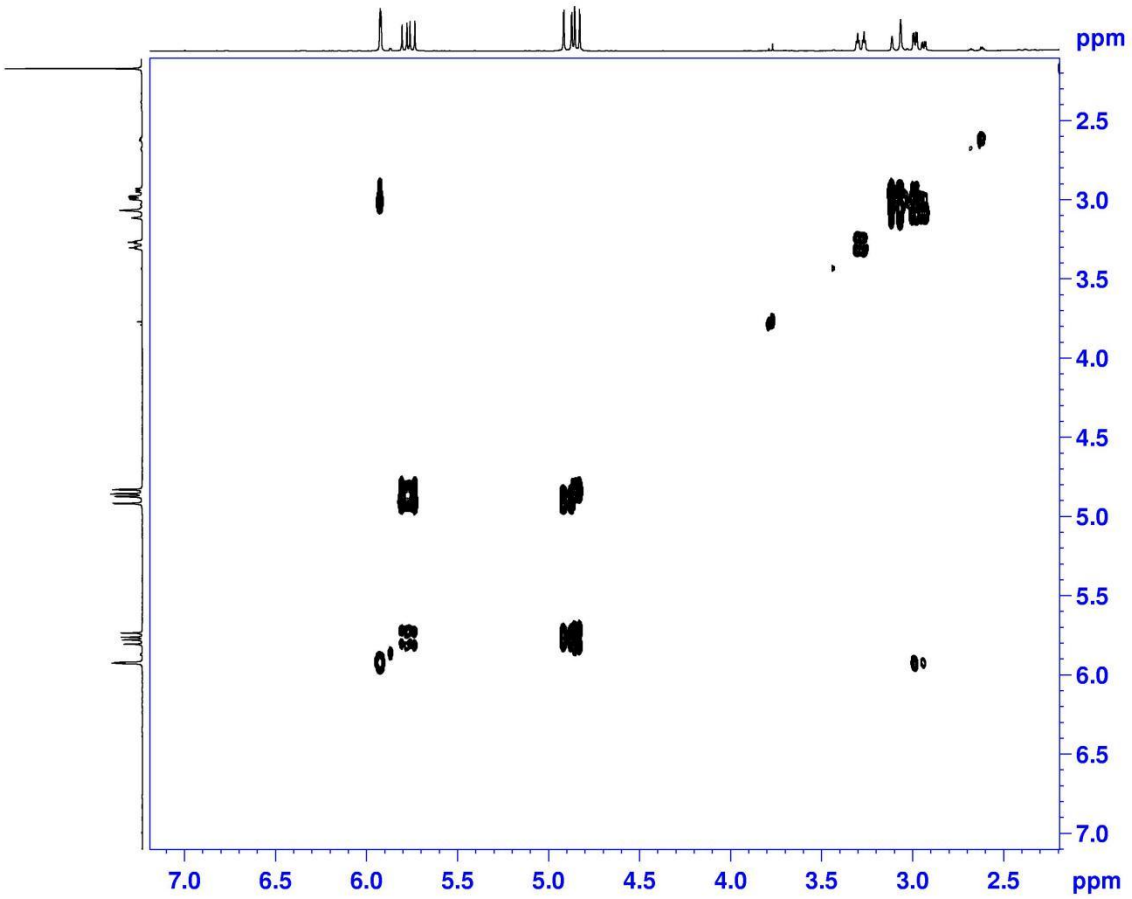
^{1}H-^{1}H COSY (400 MHz) spectrum of tagalide A (1) in $CDCl_3$





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	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	0.00000400	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	400.1300080	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	

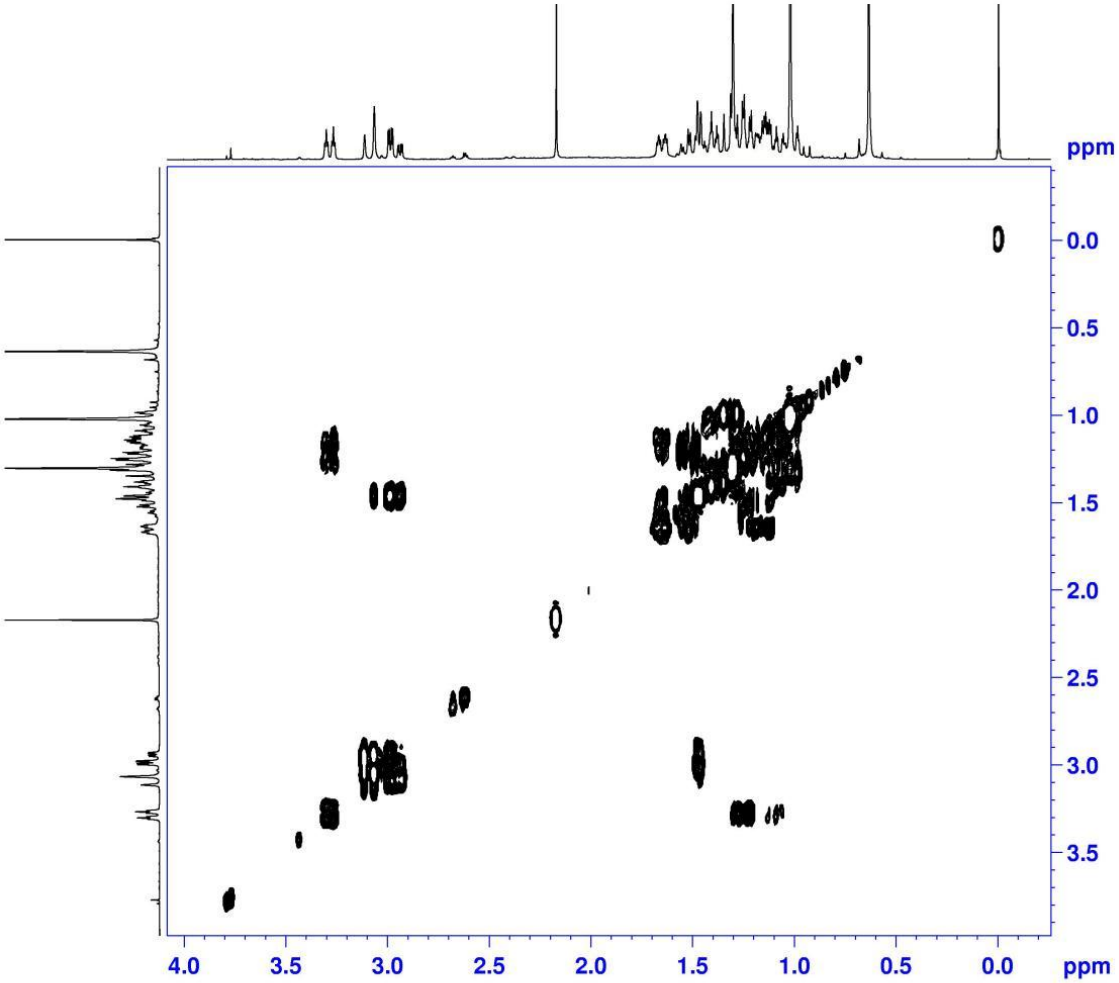
^{1}H-^{1}H COSY (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



BRUKER

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	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	0.00000400	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	400.1300080	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	

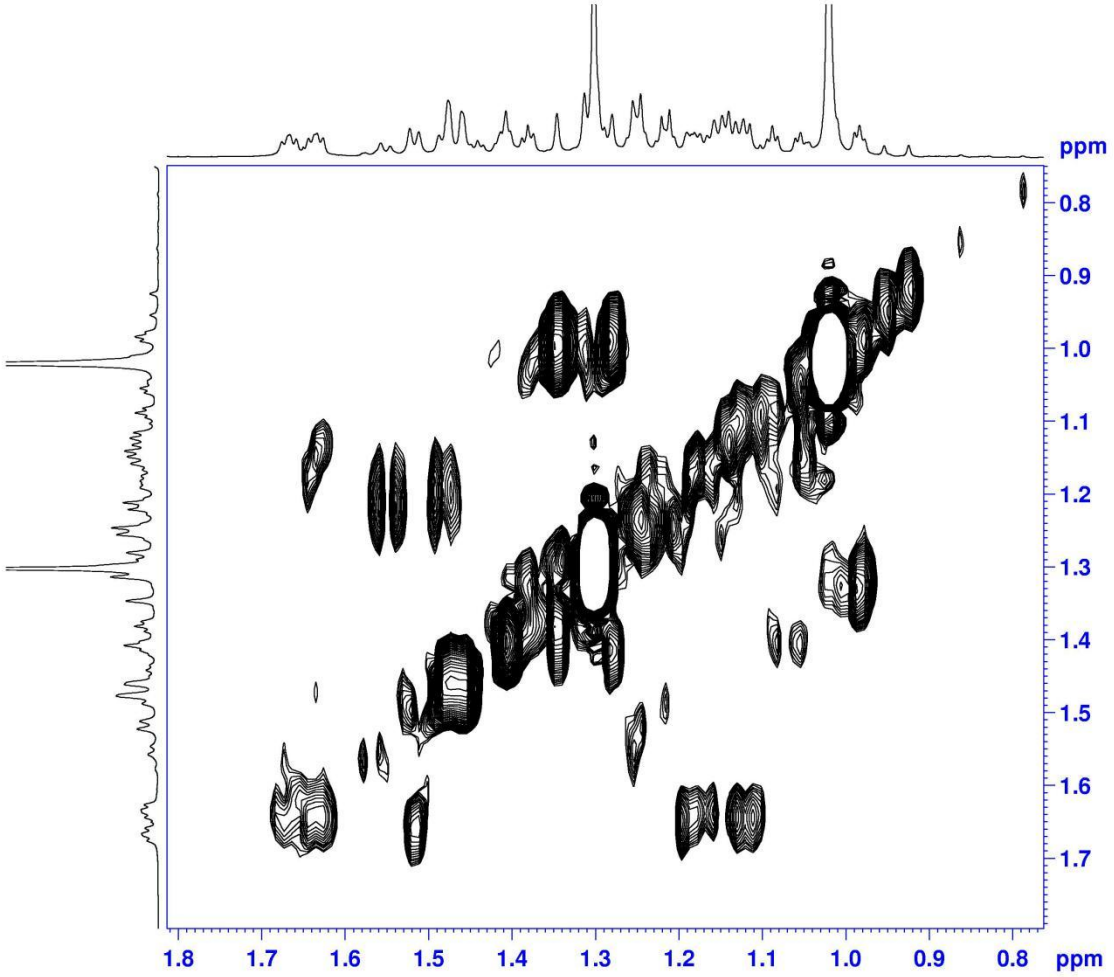
^{1}H-^{1}H COSY (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



BRUKER

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	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	0.00000400	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	400.1300080	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	

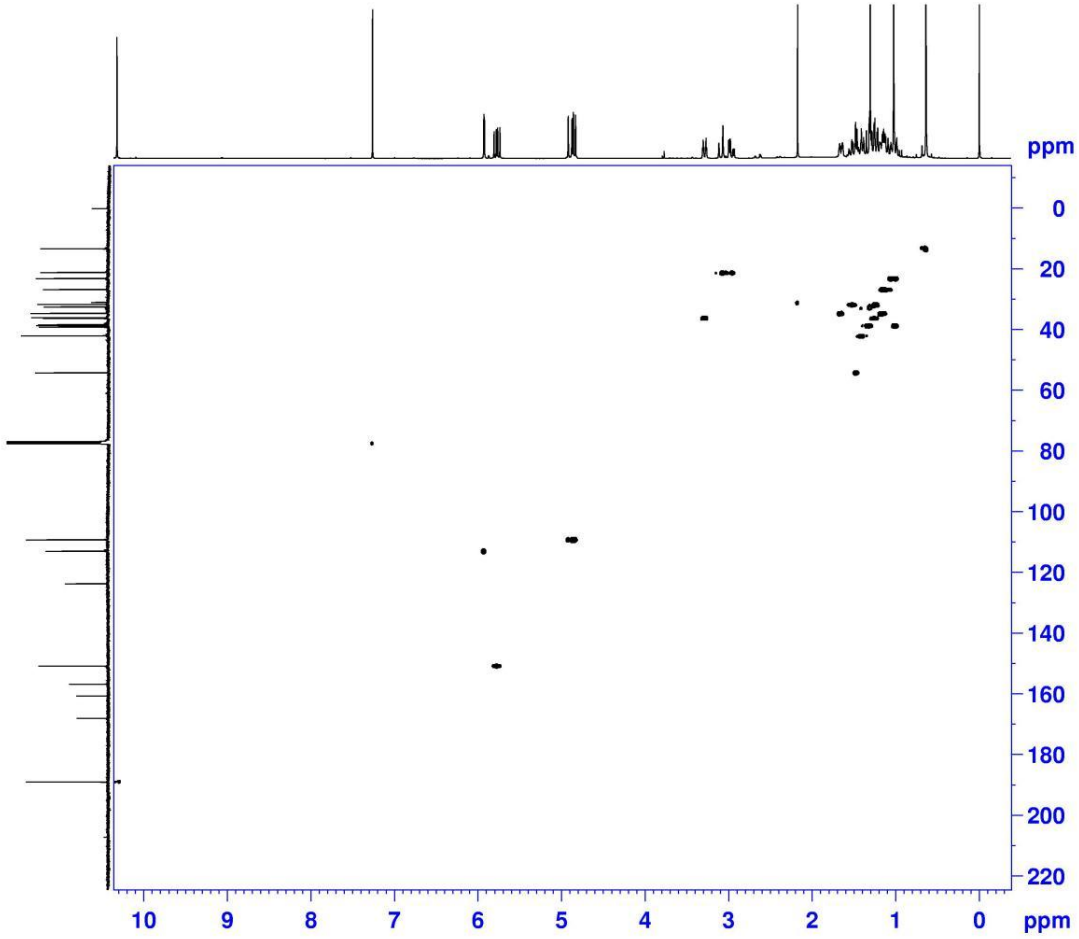
^{1}H-^{1}H COSY (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



BRUKER

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	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	0.00000400	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	400.1300080	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	

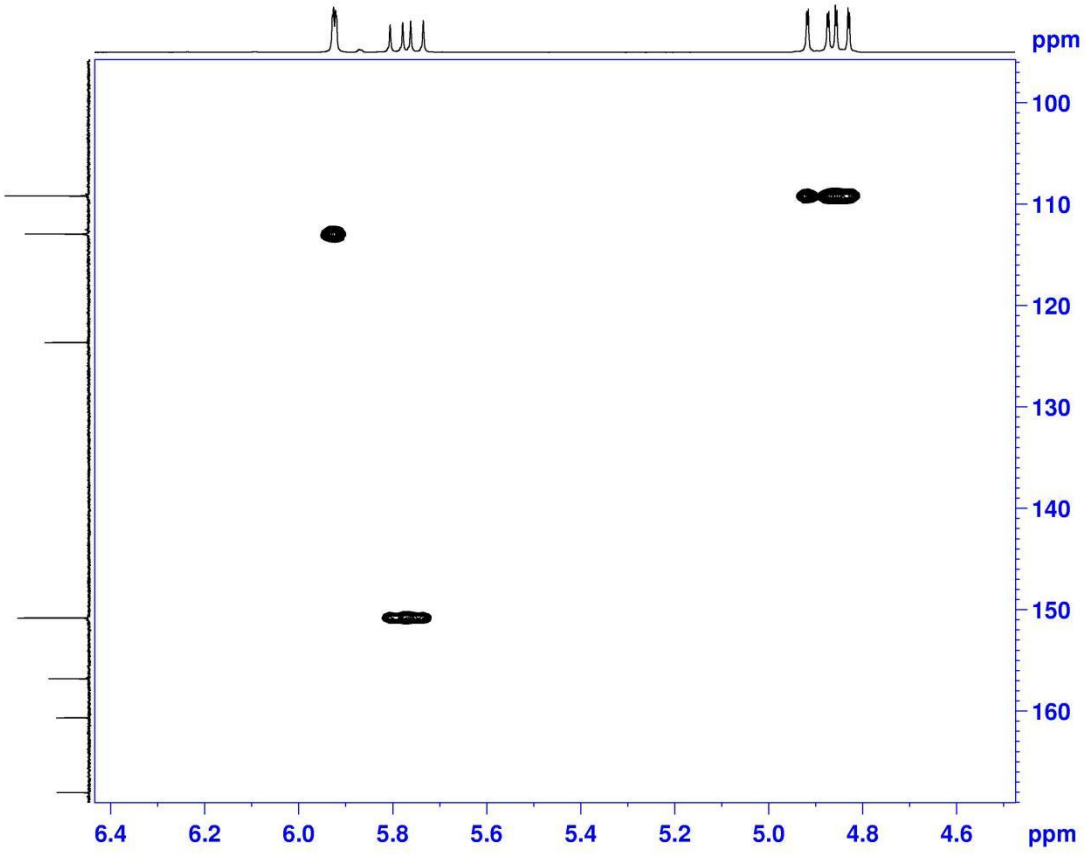
HSQC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



BRUKER

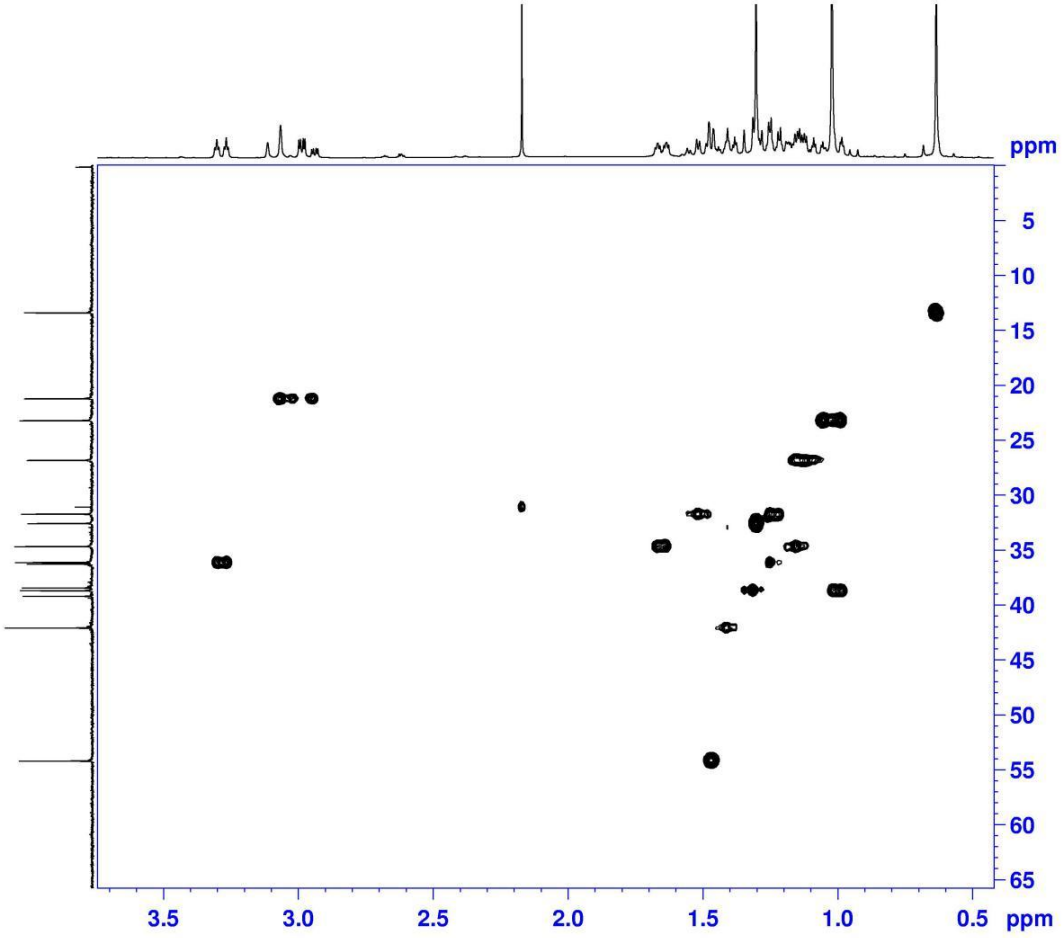
NAME	R-36-1-1	
EXPNO	5	
PROCNO	1	
Date_	20160203	
Time	21.47	
INSTRUM	spect	
PROBHD	5 mm CPPBBO BB	
PULPROG	hsqcetgpsi2	
TD	1024	
SOLVENT	CDCl3	
NS	16	
DS	16	
SWH	4302.926	Hz
FIDRES	4.202076	Hz
AQ	0.1190368	sec
RG	208.5	
DW	116.200	usec
DE	10.00	usec
TE	297.0	K
CNST2	145.0000000	
D0	0.00000300	sec
D1	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 ========		
SFO1	400.1320007	MHz
NUC1	1H	
P1	11.50	usec
P2	23.00	usec
P28	0.00	usec
ND0	2	
TD	256	
SFO1	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	

HSQC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



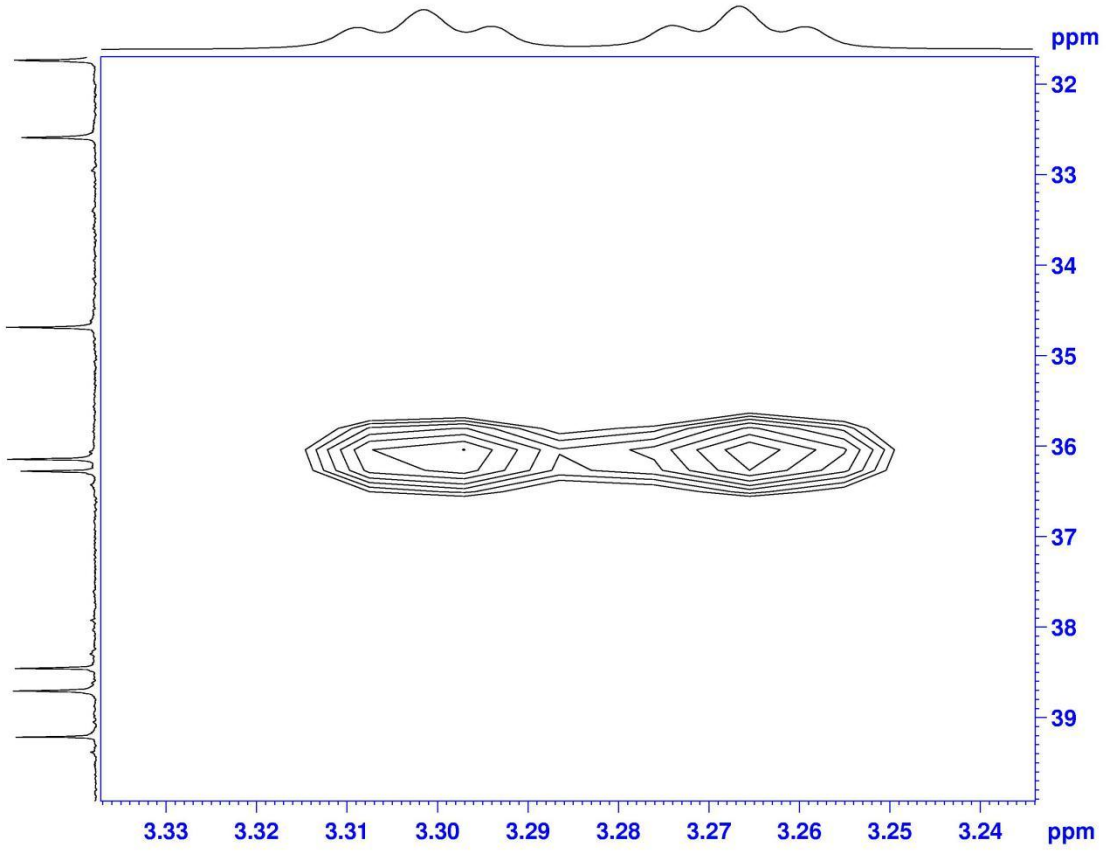

```
NAME                R-36-1-1
EXPNO                      5
PROCNO                     1
Date_               20160203
Time                   21.47
INSTRUM                spect
PROBHD     5 mm CPPBBO BB
PULPROG         hsqcetgpsi2
TD                      1024
SOLVENT               CDCl3
NS                       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 ========
SFO1            400.1320007 MHz
NUC1                      1H
P1                     11.50 usec
P2                     23.00 usec
P28                     0.00 usec
ND0                        2
TD                       256
SFO1             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
```

HSQC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



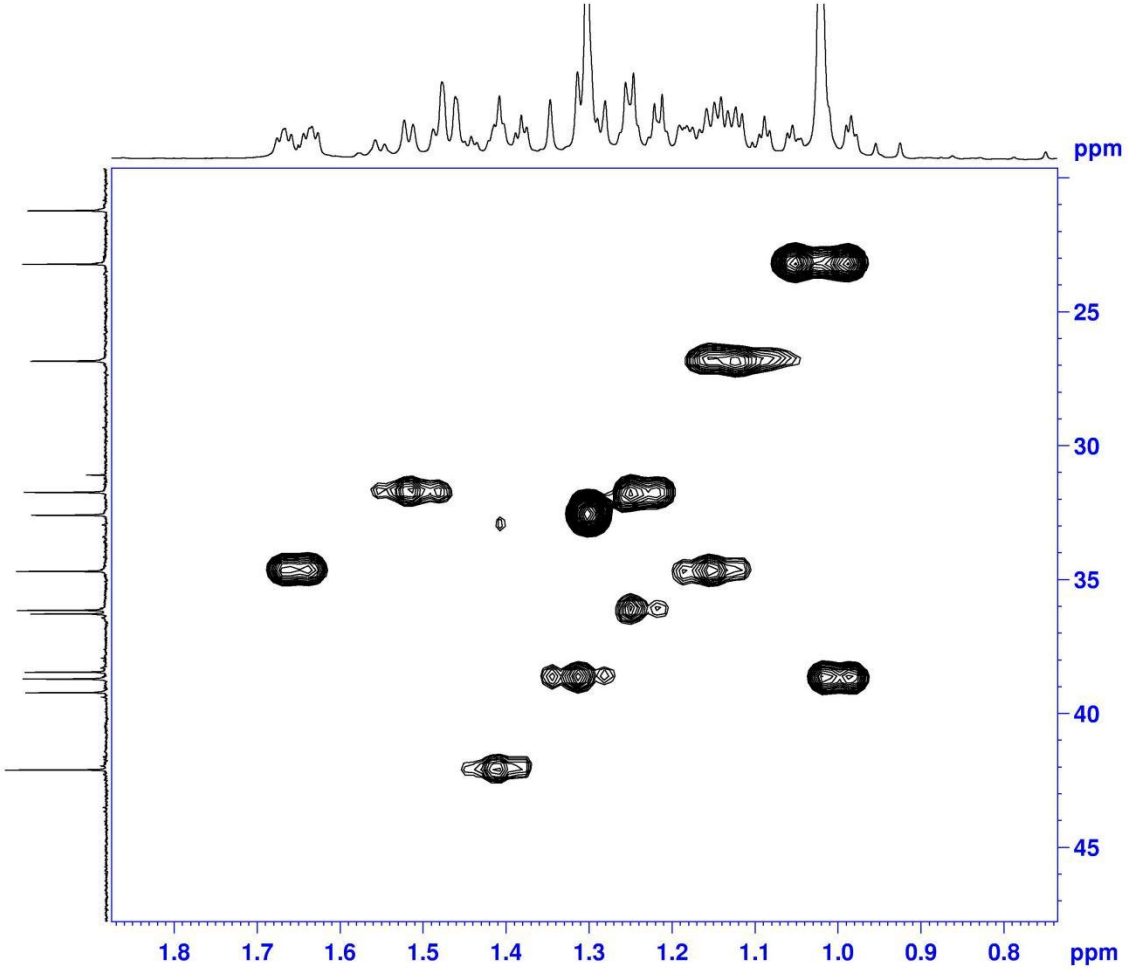

```
NAME                 R-36-1-1
EXPNO                       5
PROCNO                      1
Date_             20160203
Time                  21.47
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG        hsqcetgpsi2
TD                       1024
SOLVENT                CDCl3
NS                         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 ========
SFO1              400.1320007 MHz
NUC1                       1H
P1                      11.50 usec
P2                      23.00 usec
P28                      0.00 usec
ND0                         2
TD                        256
SFO1              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
```

HSQC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$




```
NAME                R-36-1-1
EXPNO                      5
PROCNO                     1
Date_               20160203
Time                   21.47
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG        hsqcetgpsi2
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 ========
SFO1             400.1320007 MHz
NUC1                      1H
P1                     11.50 usec
P2                     23.00 usec
P28                     0.00 usec
ND0                        2
TD                       256
SFO1               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
```

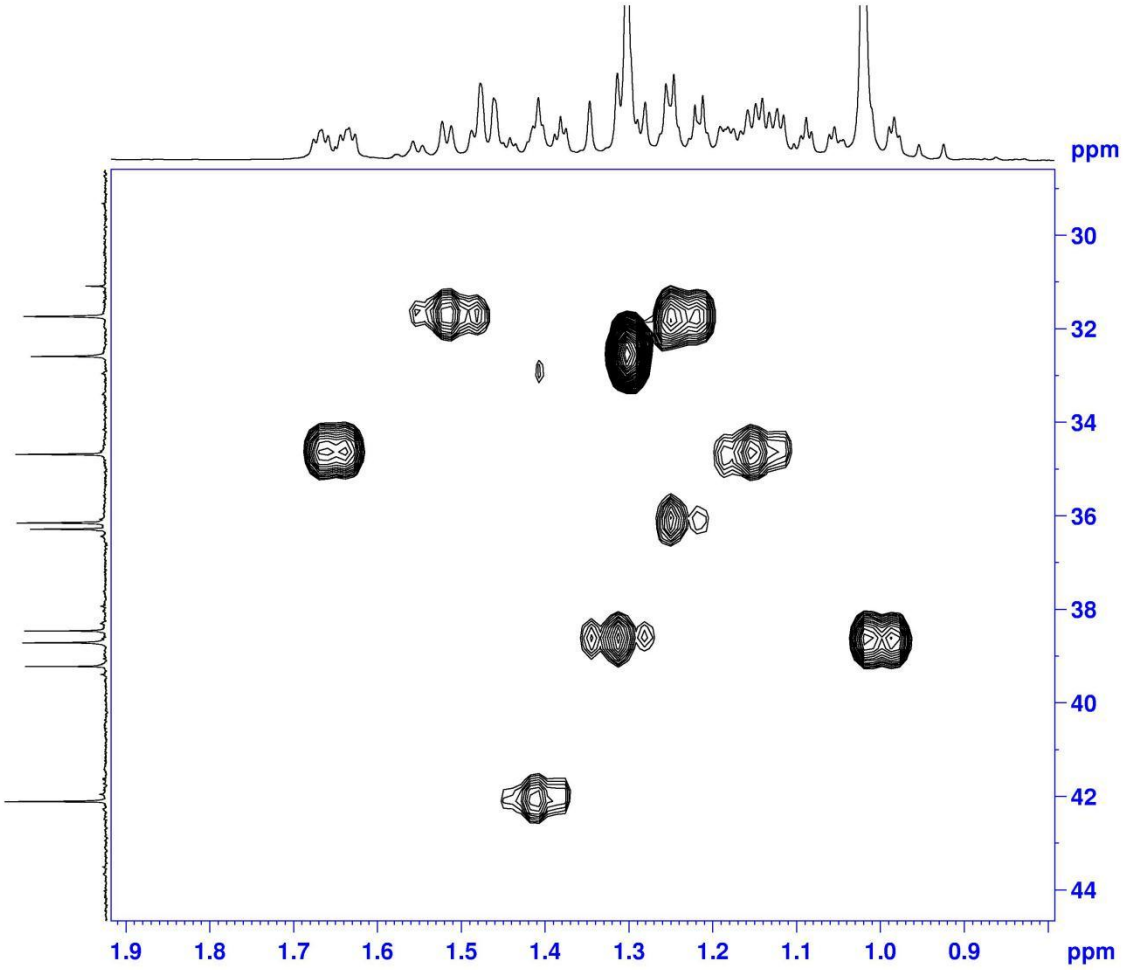
HSQC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



BRUKER

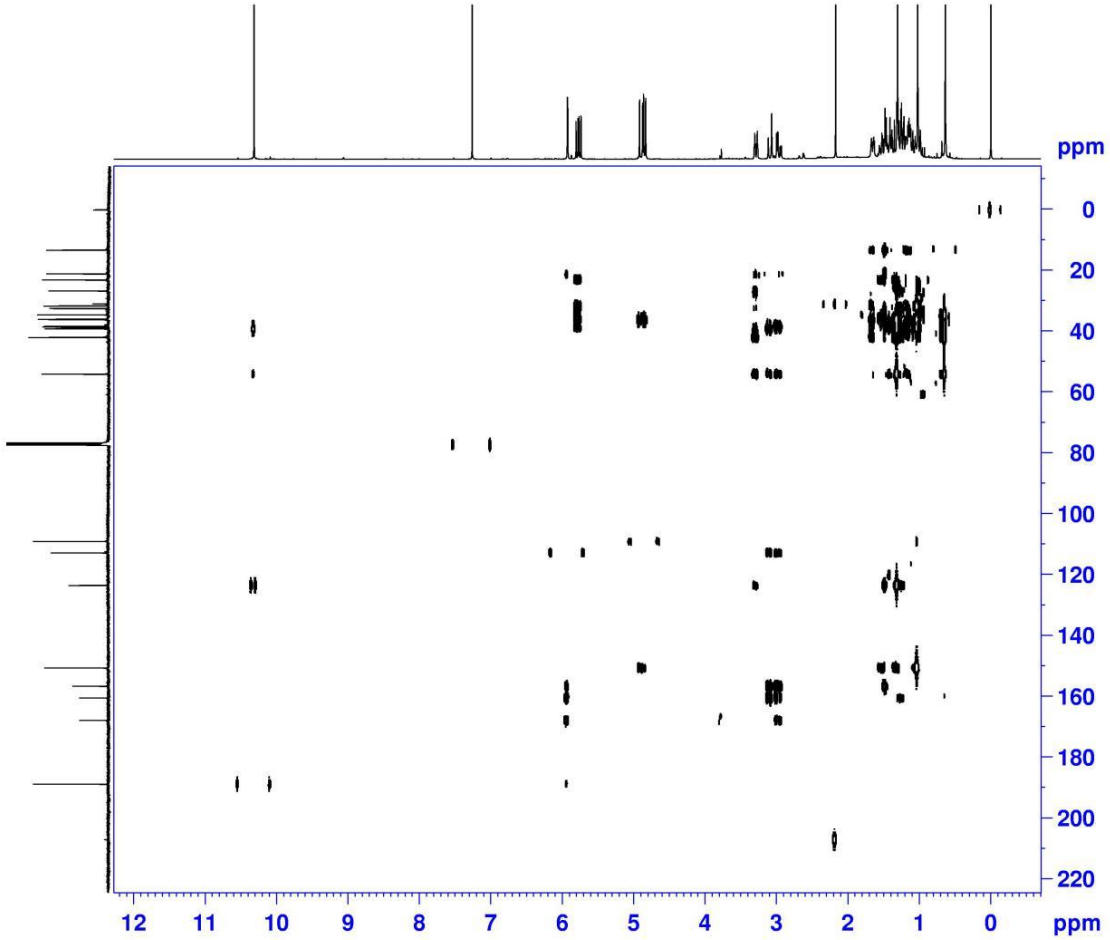
NAME	R-36-1-1
EXPNO	5
PROCNO	1
Date_	20160203
Time	21.47
INSTRUM	spect
PROBHD	5 mm CPPBBO BB
PULPROG	hsqcetgpsi2
TD	1024
SOLVENT	CDCl3
NS	16
DS	16
SWH	4302.926 Hz
FIDRES	4.202076 Hz
AQ	0.1190388 sec
RG	208.5
DW	116.200 usec
DE	10.00 usec
TE	297.0 K
CNST2	145.0000000
D0	0.00000300 sec
D1	1.46497905 sec
D4	0.00172414 sec
D11	0.03000000 sec
D16	0.00020000 sec
D24	0.00086207 sec
IN0	0.00002080 sec
ZGOPTNS	
========	CHANNEL f1 ========
SFO1	400.1320007 MHz
NUC1	1H
P1	11.50 usec
P2	23.00 usec
P28	0.00 usec
ND0	2
TD	256
SFO1	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

HSQC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



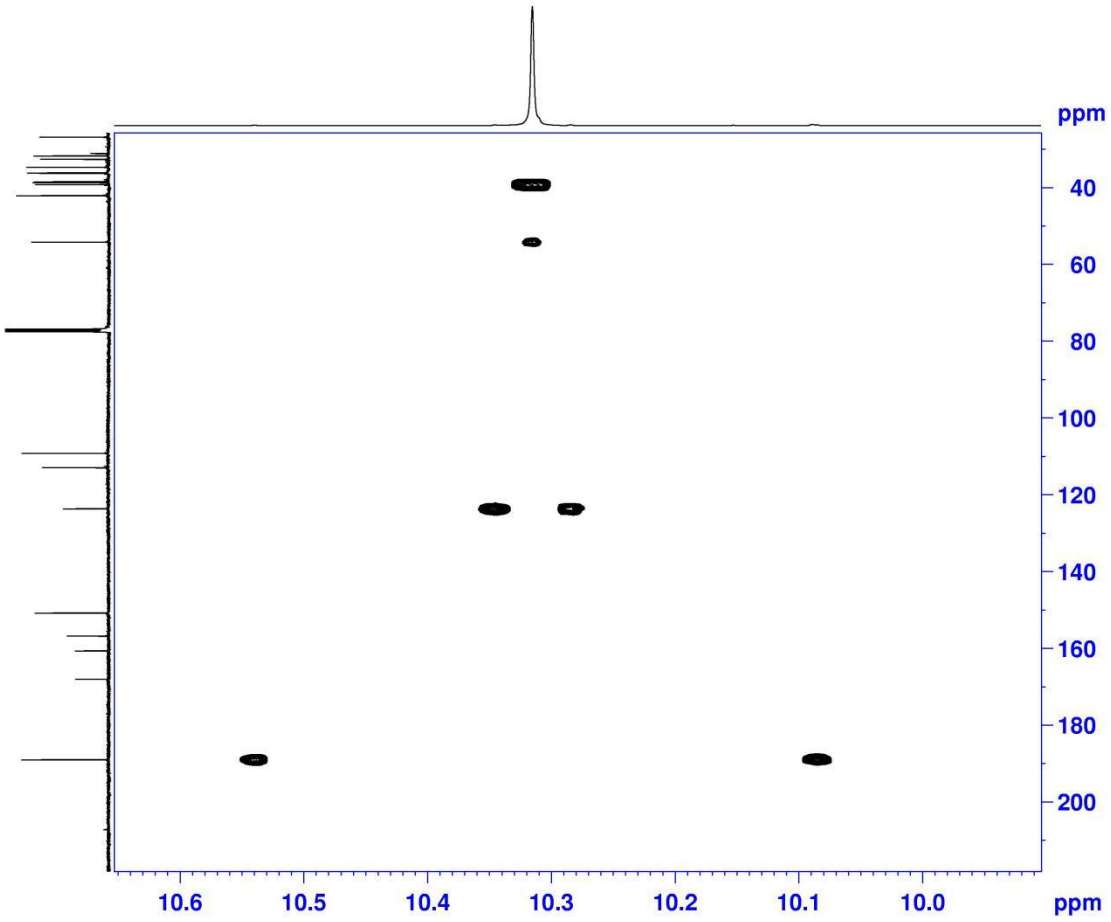

```
NAME              R-36-1-1
EXPNO                    5
PROCNO                   1
Date_             20160203
Time                 21.47
INSTRUM              spect
PROBHD    5 mm CPPBBO BB
PULPROG      hsqcetgpsi2
TD                    1024
SOLVENT             CDCl3
NS                      16
DS                      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 ========
SFO1           400.1320007 MHz
NUC1                     1H
P1                    11.50 usec
P2                    23.00 usec
P28                    0.00 usec
ND0                       2
TD                      256
SFO1            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 $CDCl_3$



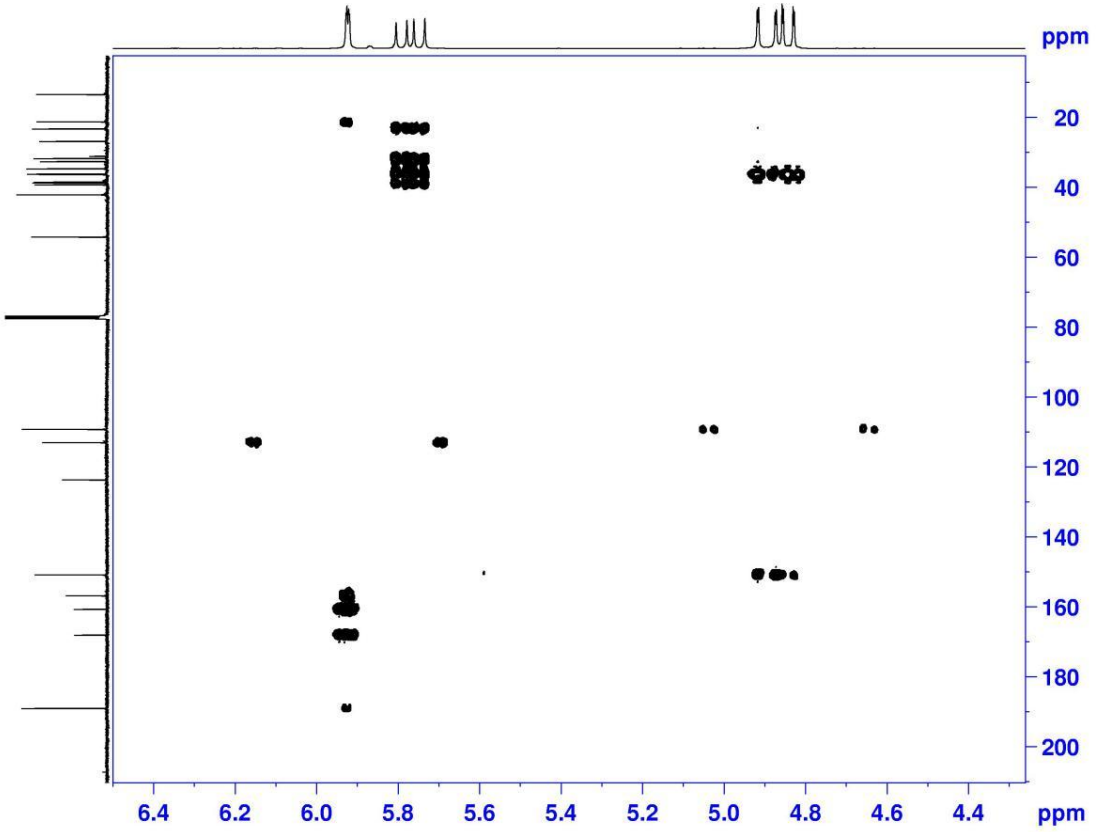

```
NAME                R-36-1-1
EXPNO                    106
PROCNO                     1
Date_               20160204
Time                   10.48
INSTRUM                spect
PROBHD   5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
TD                      4096
SOLVENT                CDCl3
NS                        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
FnMODE                     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 $CDCl_3$




```
NAME                R-36-1-1
EXPNO                    106
PROCNO                     1
Date_               20160204
Time                   10.48
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
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
FnMODE                     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
```

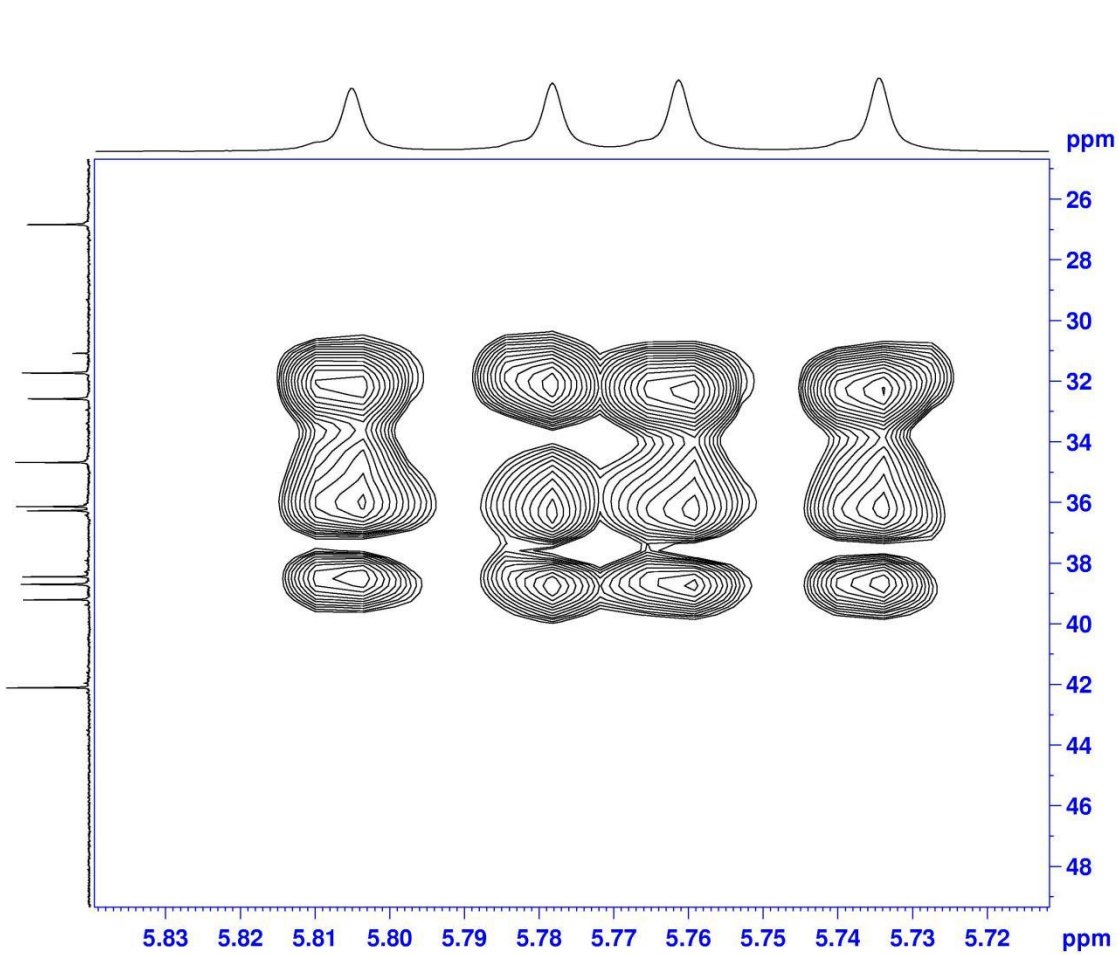
HMBC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



BRUKER

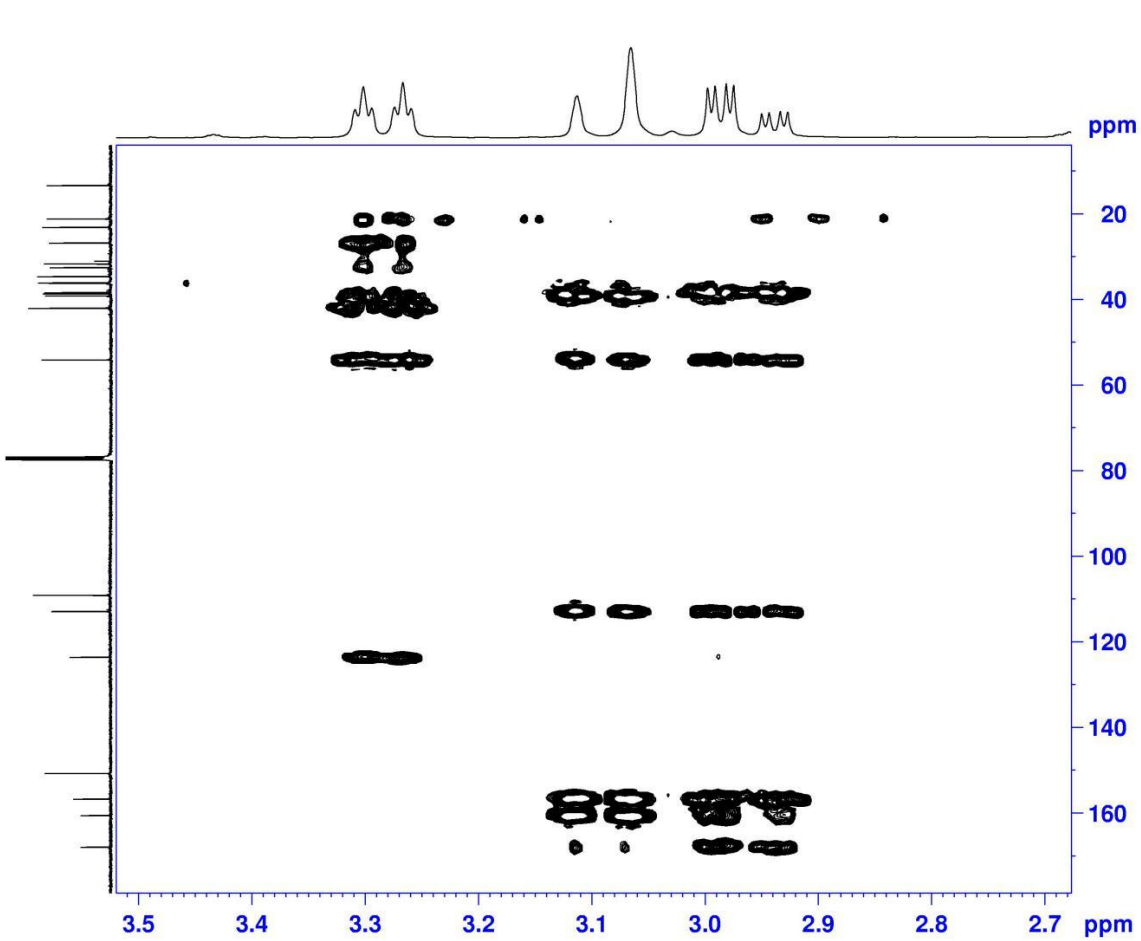
```
NAME              R-36-1-1
EXPNO                  106
PROCNO                   1
Date_             20160204
Time                 10.48
INSTRUM              spect
PROBHD    5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
TD                    4096
SOLVENT              CDCl3
NS                      32
DS                      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
FnMODE                 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 $CDCl_3$



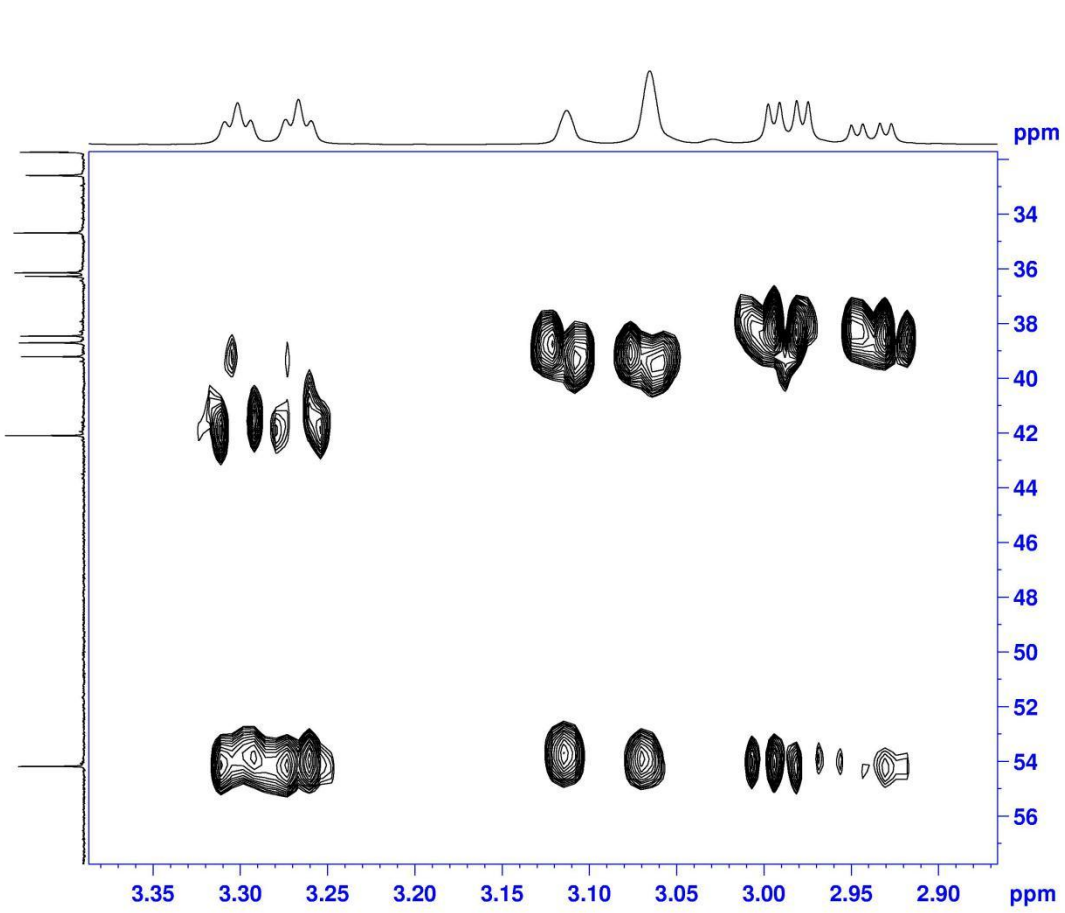

```
NAME                R-36-1-1
EXPNO                    106
PROCNO                     1
Date_               20160204
Time                   10.48
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
TD                      4096
SOLVENT              CDCl3
NS                        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
FnMODE                     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 $CDCl_3$



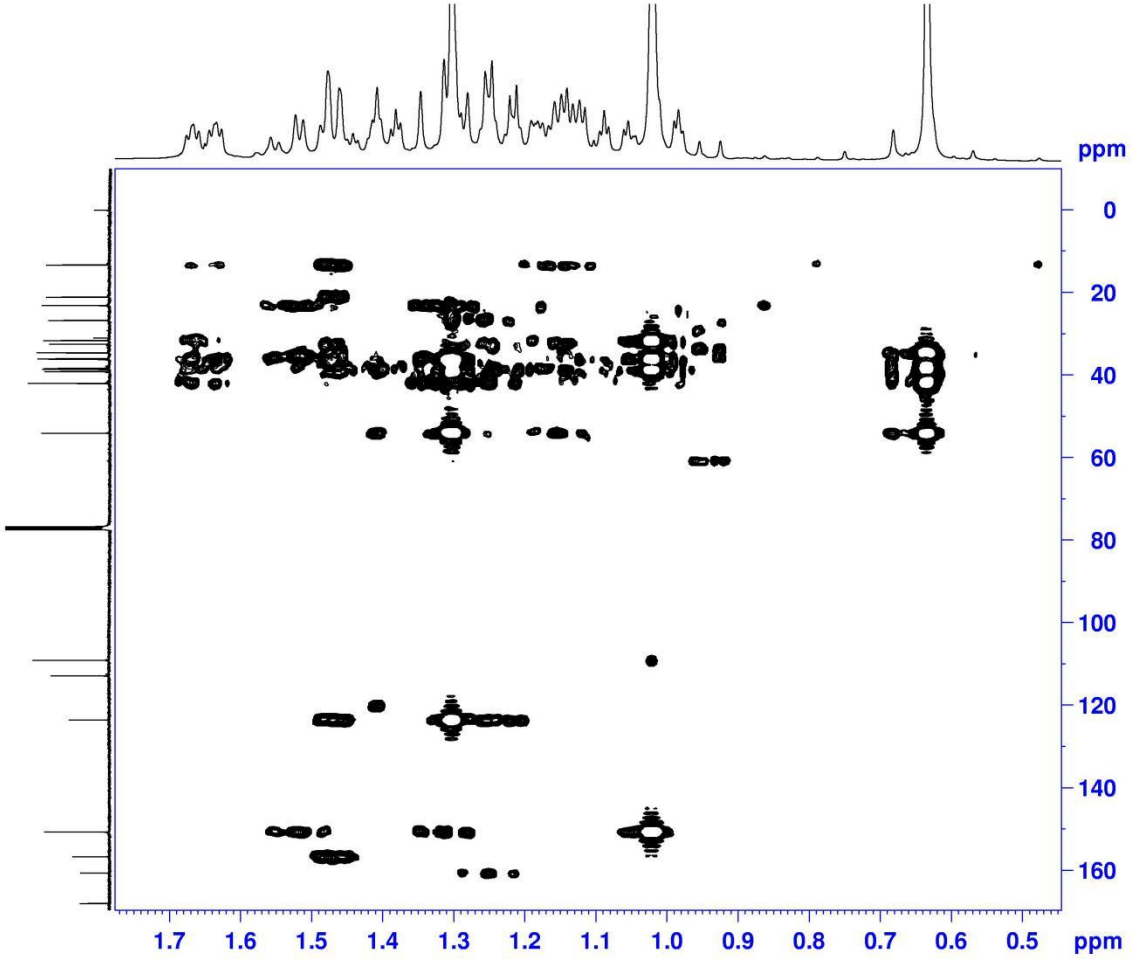

```
NAME                R-36-1-1
EXPNO                    106
PROCNO                     1
Date_               20160204
Time                   10.48
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
TD                      4096
SOLVENT              CDCl3
NS                        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
FnMODE                     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 $CDCl_3$




```
NAME                R-36-1-1
EXPNO                    106
PROCNO                     1
Date_             20160204
Time                   10.48
INSTRUM                spect
PROBHD     5 mm CPPBBO BB
PULPROG        hmbcgplpndqf
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
FnMODE                    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
```

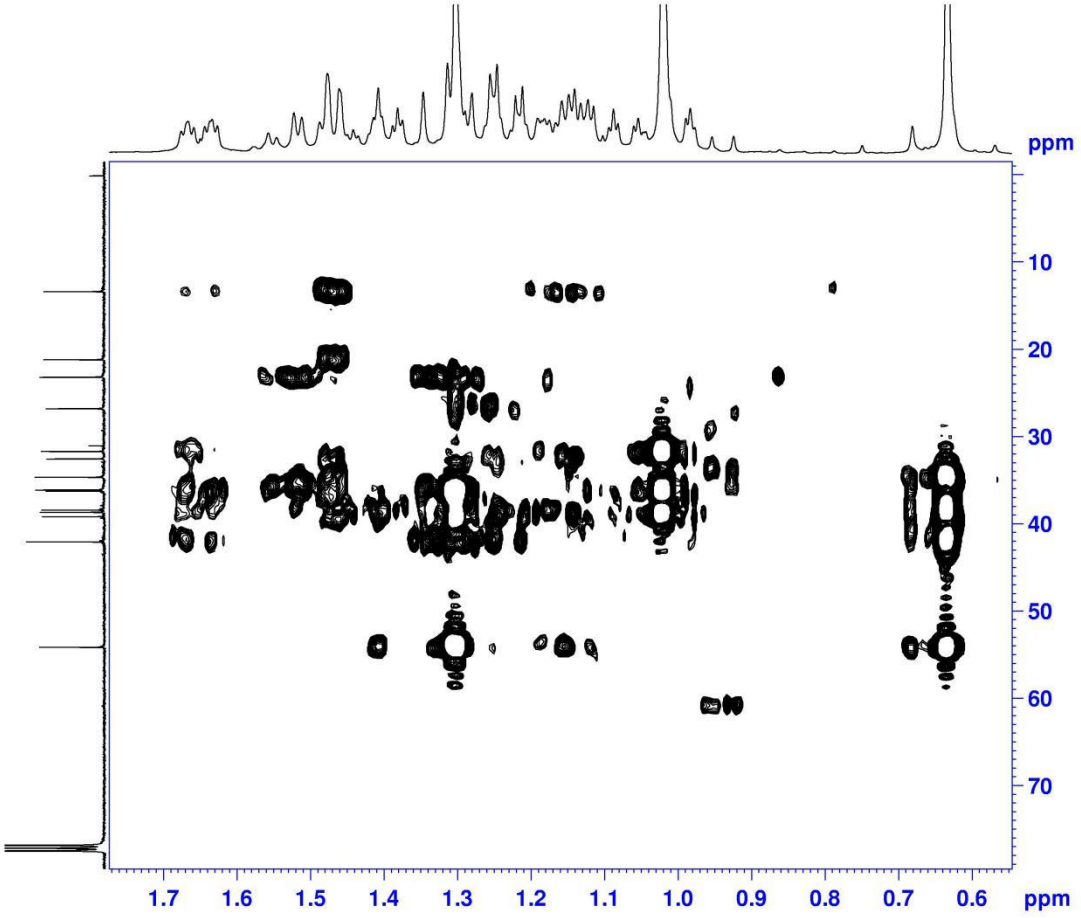
HMBC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



BRUKER

NAME	R-36-1-1
EXPNO	106
PROCNO	1
Date_	20160204
Time	10.48
INSTRUM	spect
PROBHD	5 mm CPPBBO BB
PULPROG	hmbcgplpndqf
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
FnMODE	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

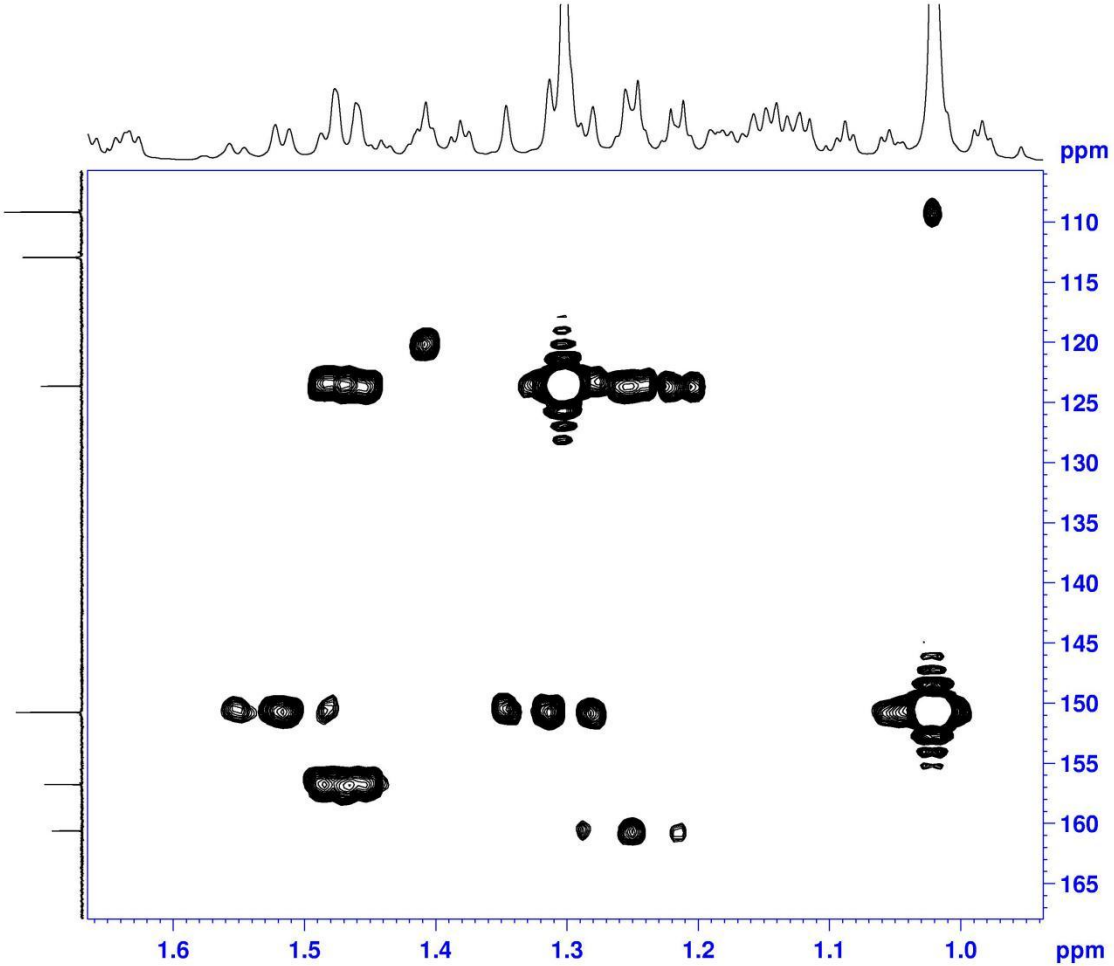
HMBC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



BRUKER

NAME	R-36-1-1
EXPNO	106
PROCNO	1
Date_	20160204
Time	10.48
INSTRUM	spect
PROBHD	5 mm CPPBBO BB
PULPROG	hmbcgplpndqf
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
FnMODE	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

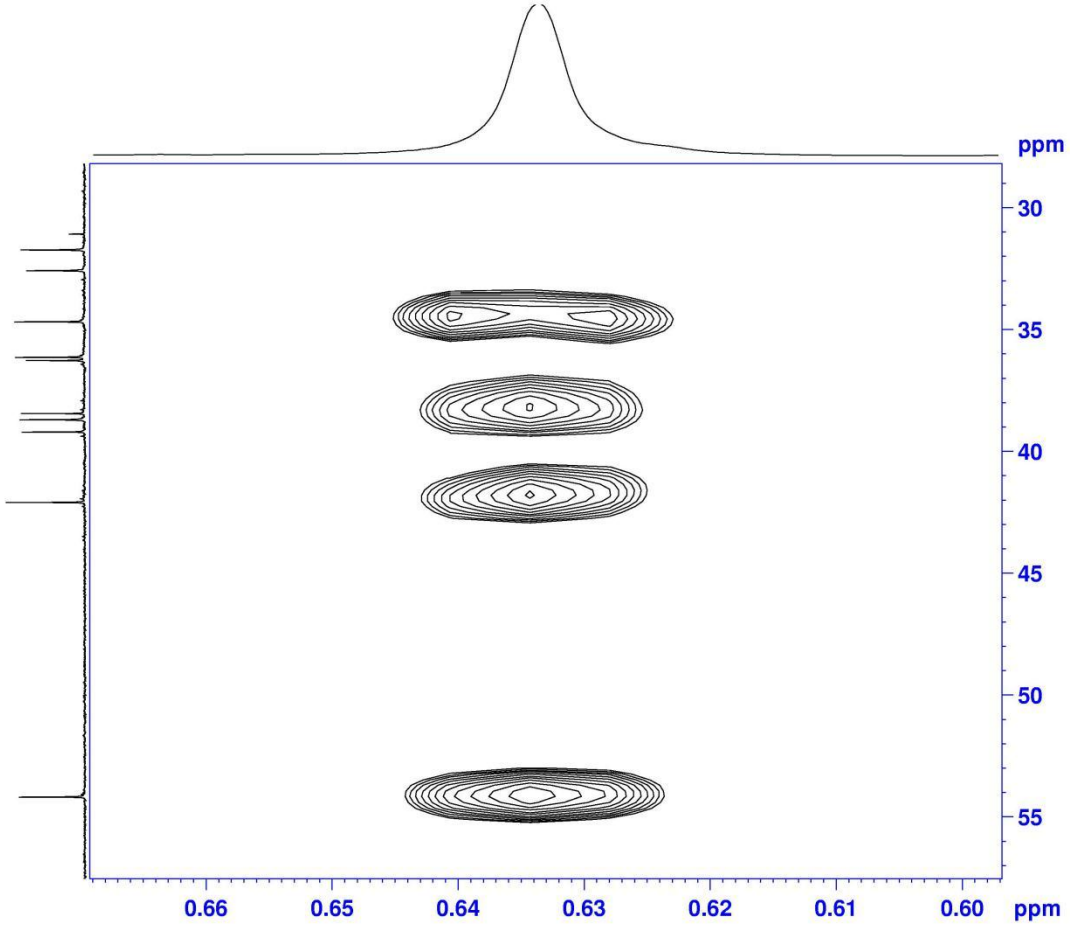
HMBC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$

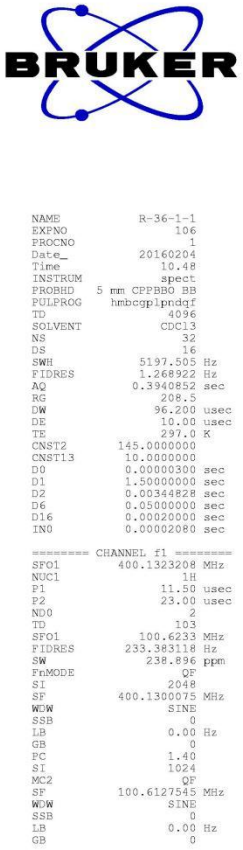


BRUKER

```
NAME                R-36-1-1
EXPNO                    106
PROCNO                     1
Date_               20160204
Time                   10.48
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
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              233.38318 Hz
SW                     238.896 ppm
FnMODE                     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
```

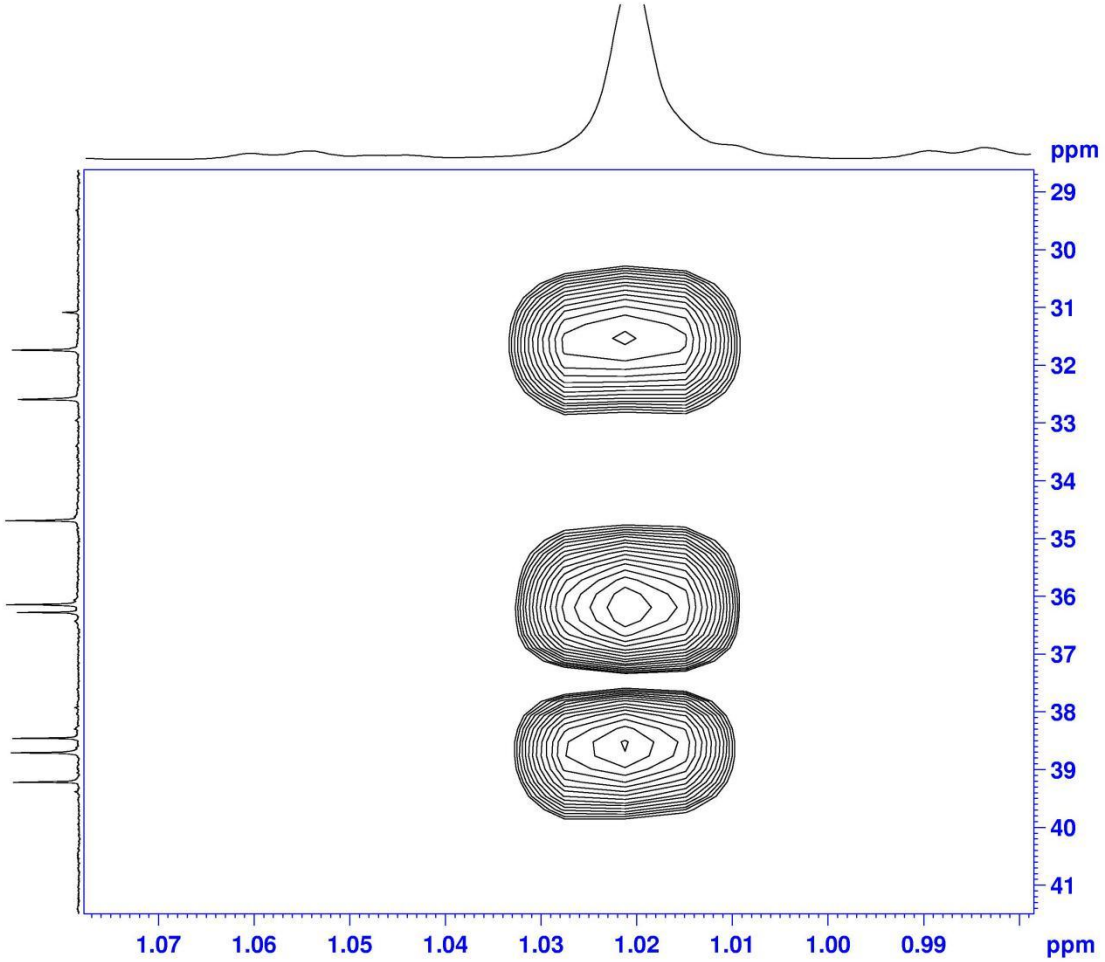
HMBC (400 MHz) spectrum of tagalide A (1) in $CDCl_3$





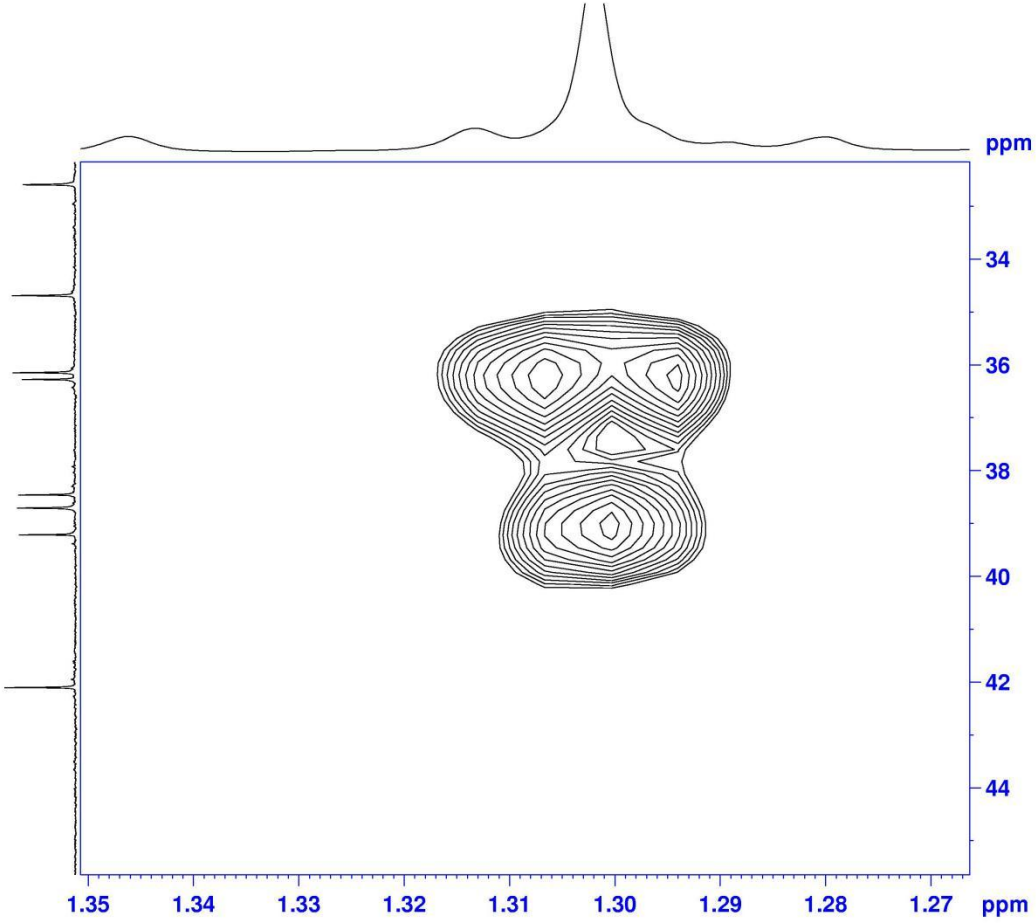
```
NAME                R-36-1-1
EXPNO                    106
PROCNO                     1
Date_               20160204
Time                   10.48
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
TD                      4096
SOLVENT              CDCl3
NS                        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
FnMODE                     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 $CDCl_3$



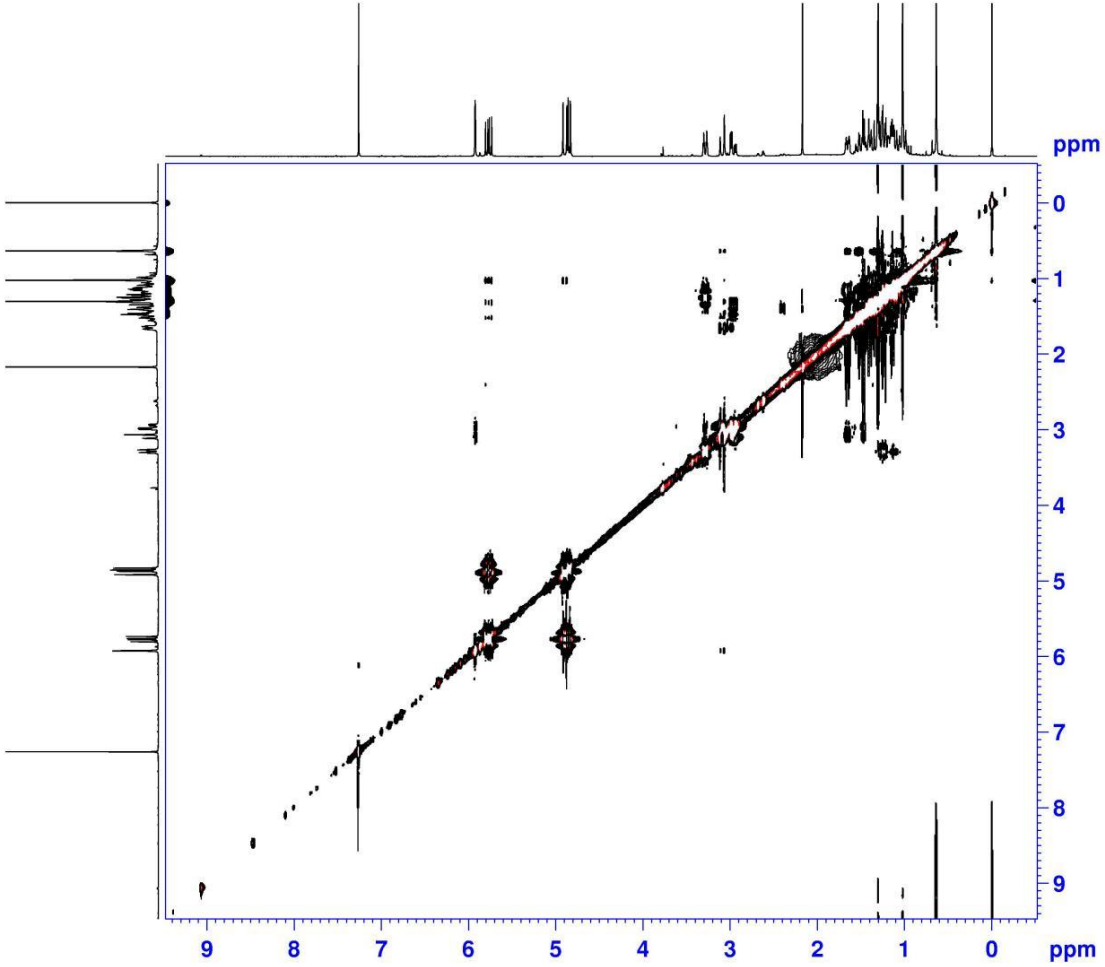

```
NAME                R-36-1-1
EXPNO                    106
PROCNO                     1
Date_               20160204
Time                   10.48
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG    hmbcgplpndqf
TD                      4096
SOLVENT              CDCl3
NS                        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
FnMODE                    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 $CDCl_3$



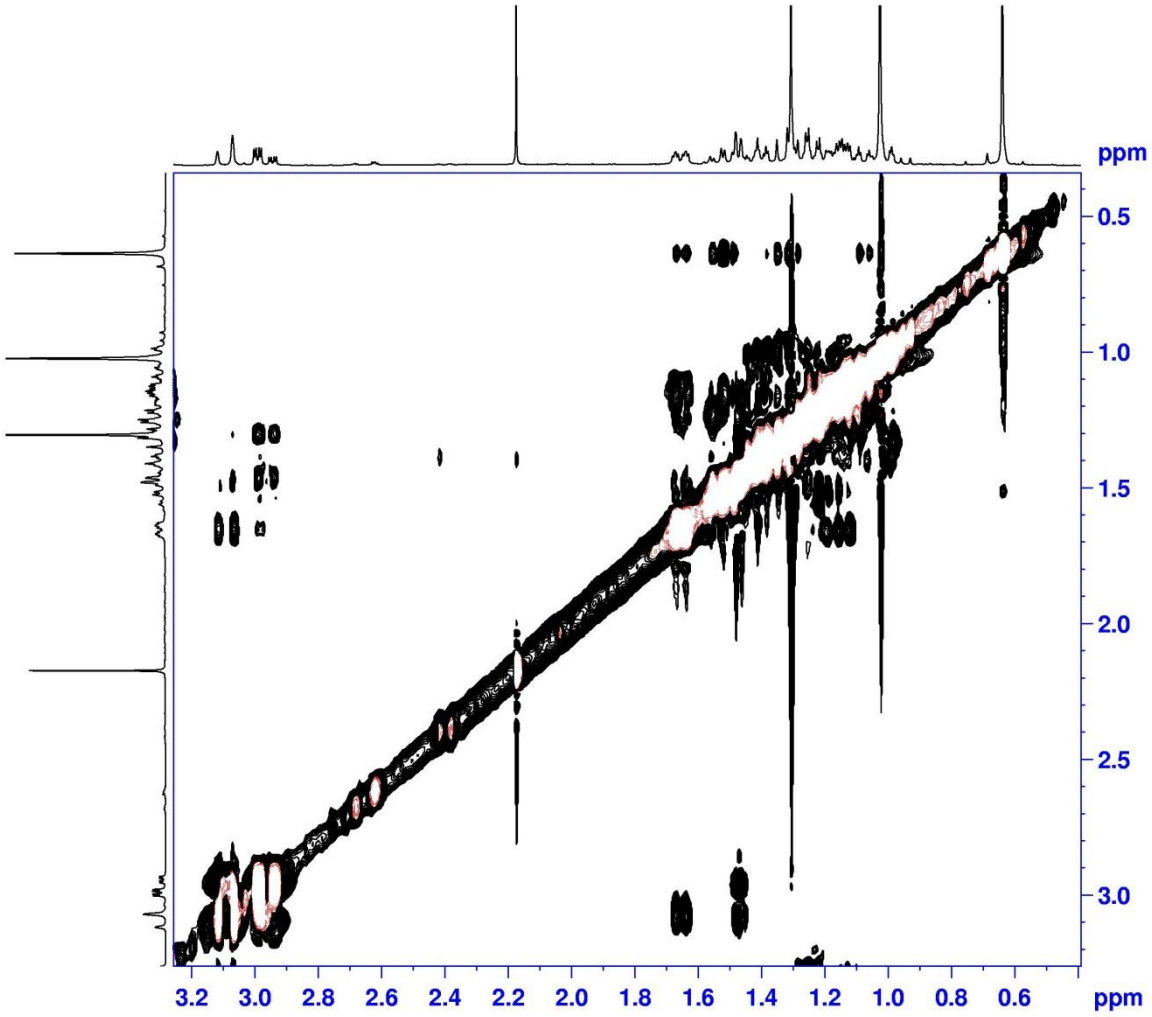
NAME	R-36-1-1
EXPNO	106
PROCNO	1
Date_	20160204
Time	10.48
INSTRUM	spect
PROBHD	5 mm CPPBBO BB
PULPROG	hmbcgplpndqf
TD	4096
SOLVENT	CDCl3
NS	32
DS	16
SWH	5197.505 Hz
FIDRES	1.268922 Hz
AQ	0.3940852 sec
RG	208.5
DW	96.200 usec
DE	10.00 usec
TE	297.0 K
CNST2	145.0000000
CNST13	10.0000000
D0	0.00000300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

NOESY (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



NAME	R-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	0.00002000	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	400.1300098	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	
PC	1.00	
SI	1024	
MC2	States-TPPI	
SF	400.1300098	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	

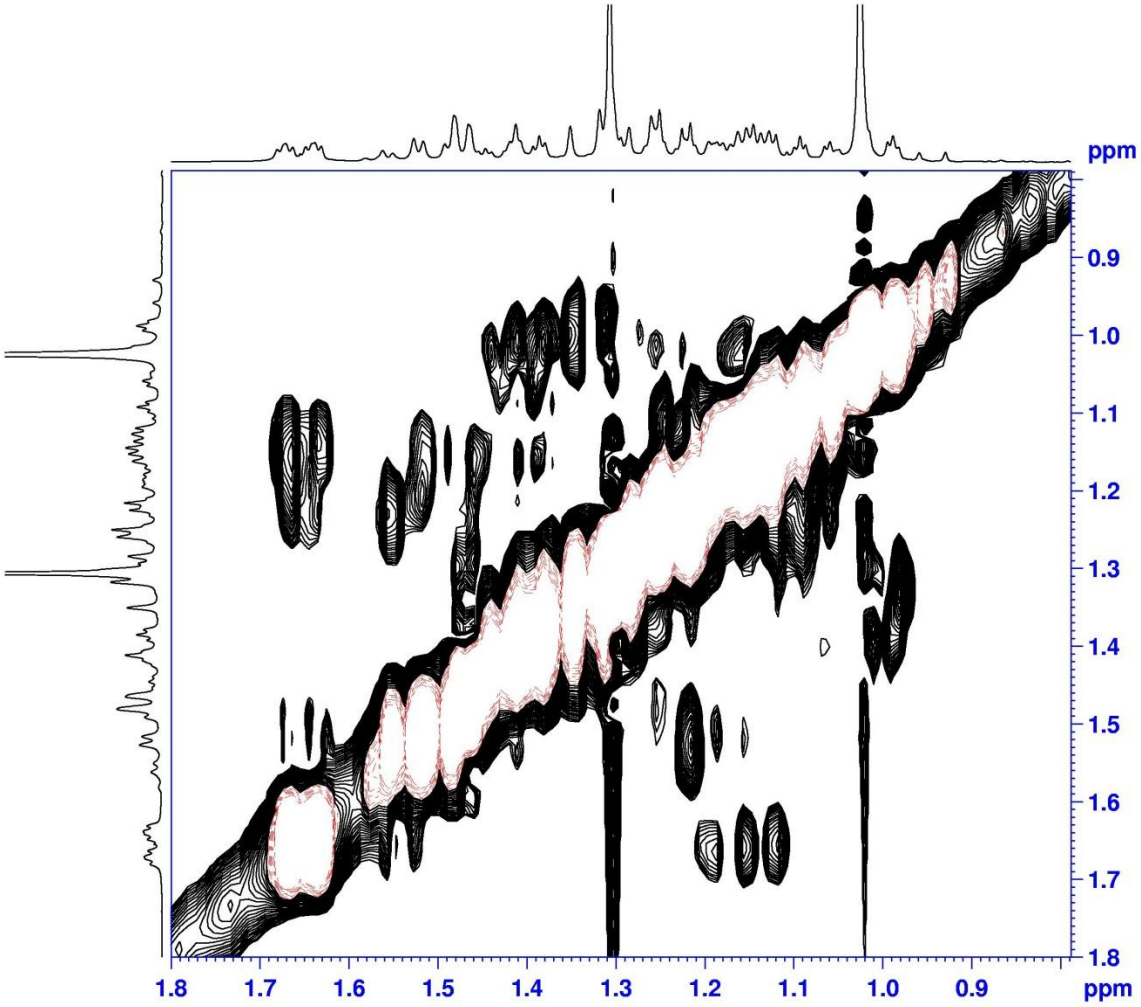
NOESY (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



BRUKER

NAME	EXH-15 R-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	0.00002000 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

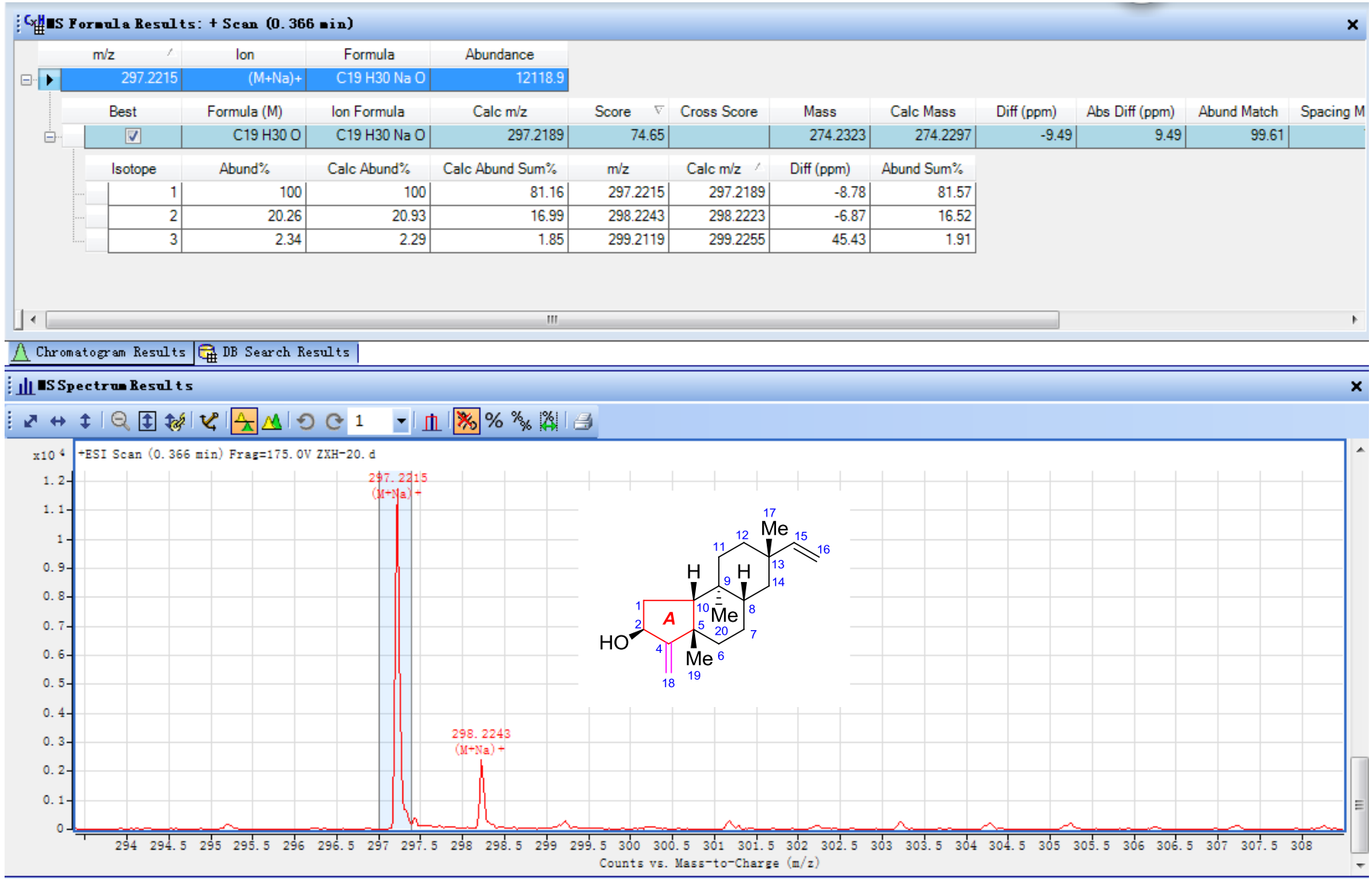
NOESY (400 MHz) spectrum of tagalide A (1) in $CDCl_3$



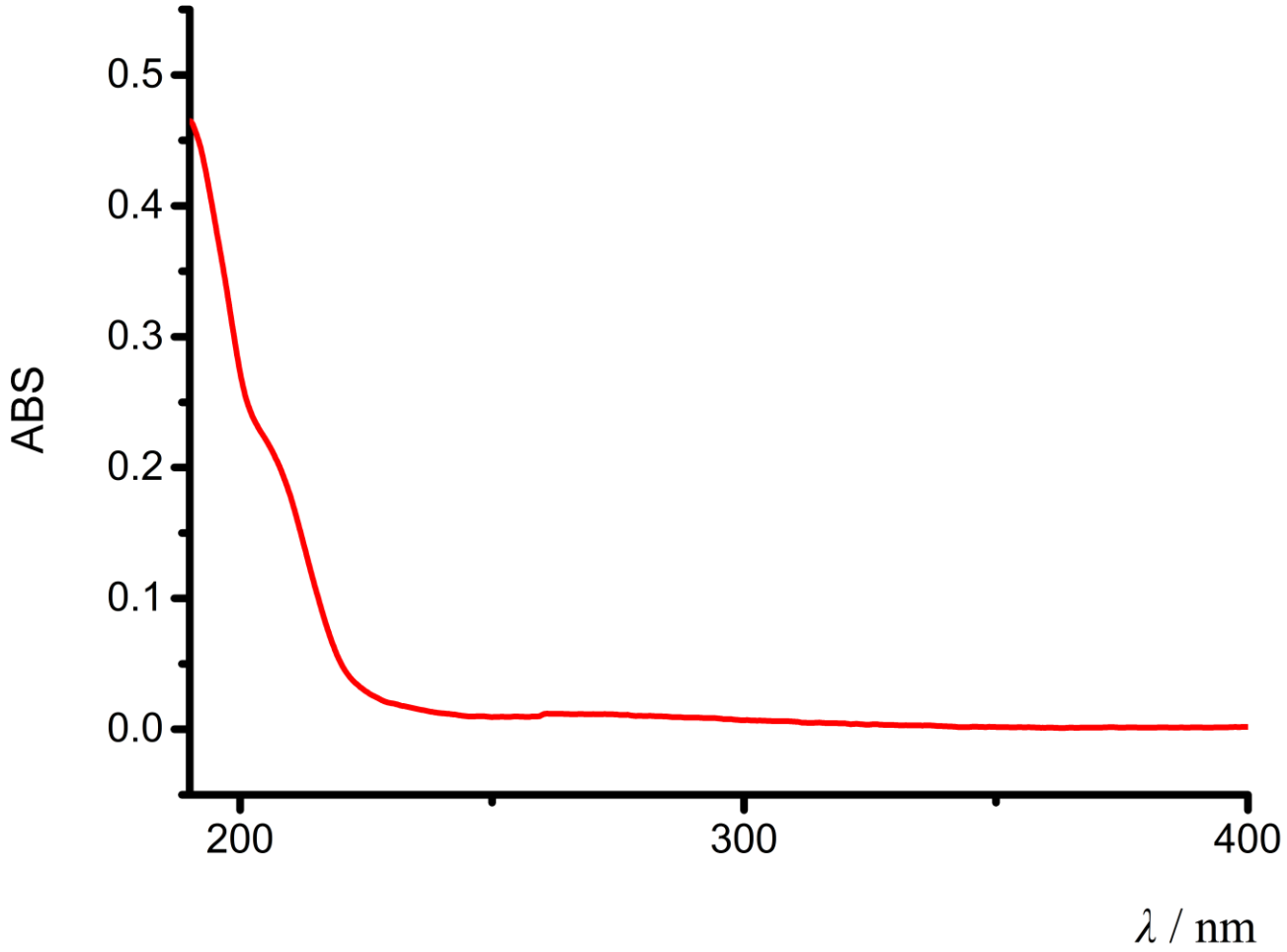
BRUKER

NAME	ZXH-15 R-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	0.00002000 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

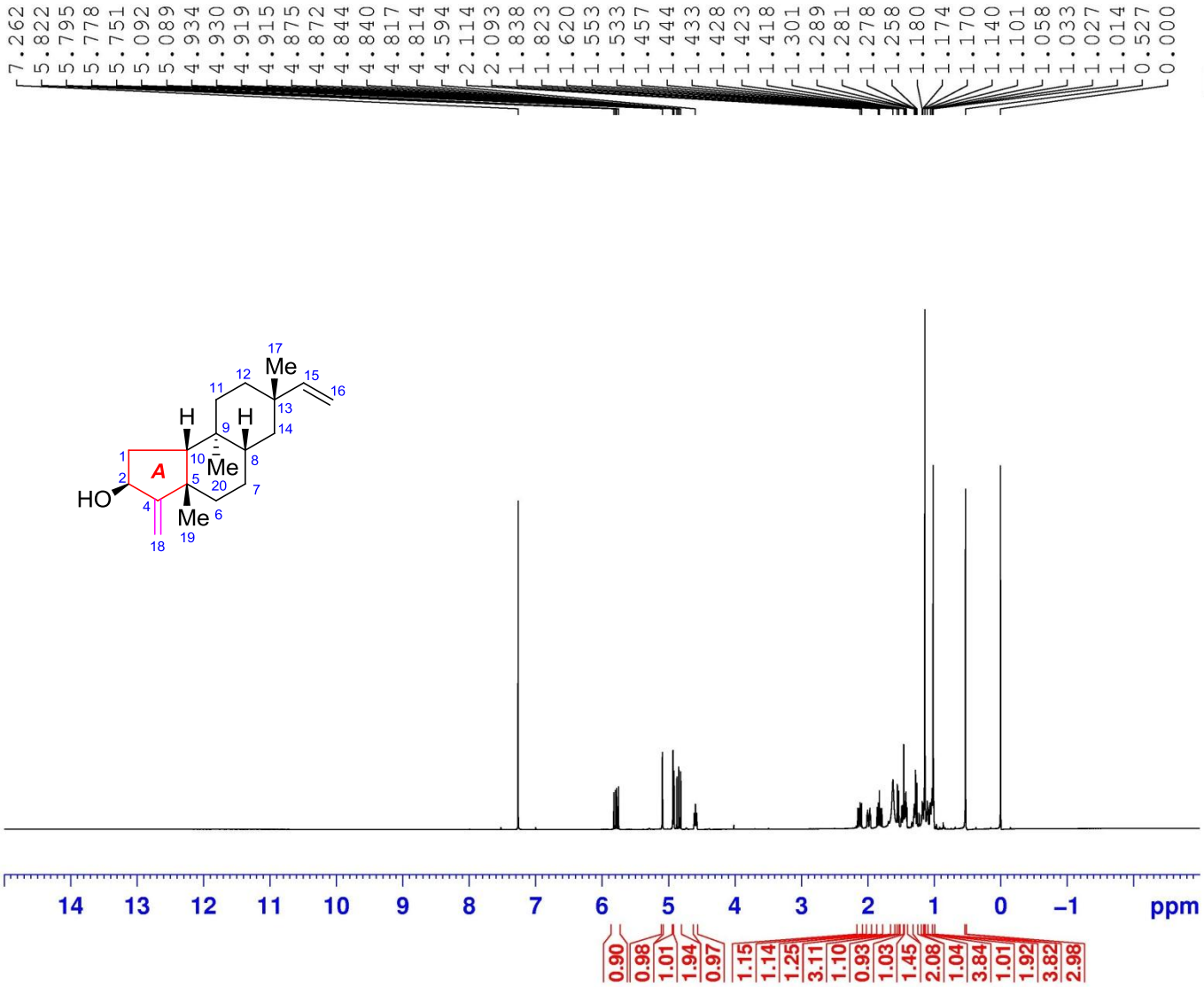
HRESIMS for tagalol A (2)



UV spectrum for tagalol A (2) (recorded in MeCN at 100 µg/mL)

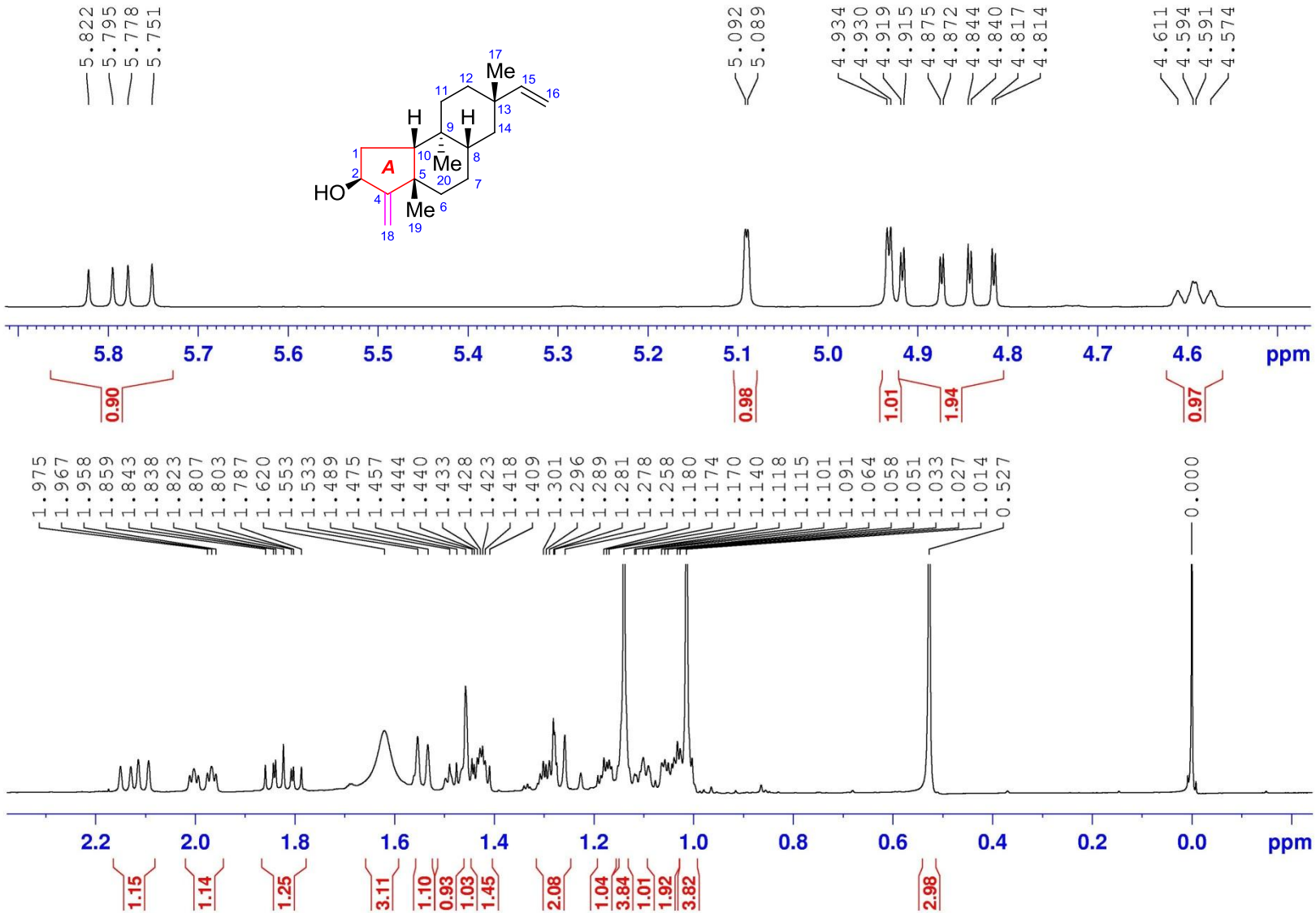


^{1}H (400 MHz) NMR spectrum of tagalol A (2) in $CDCl_3$

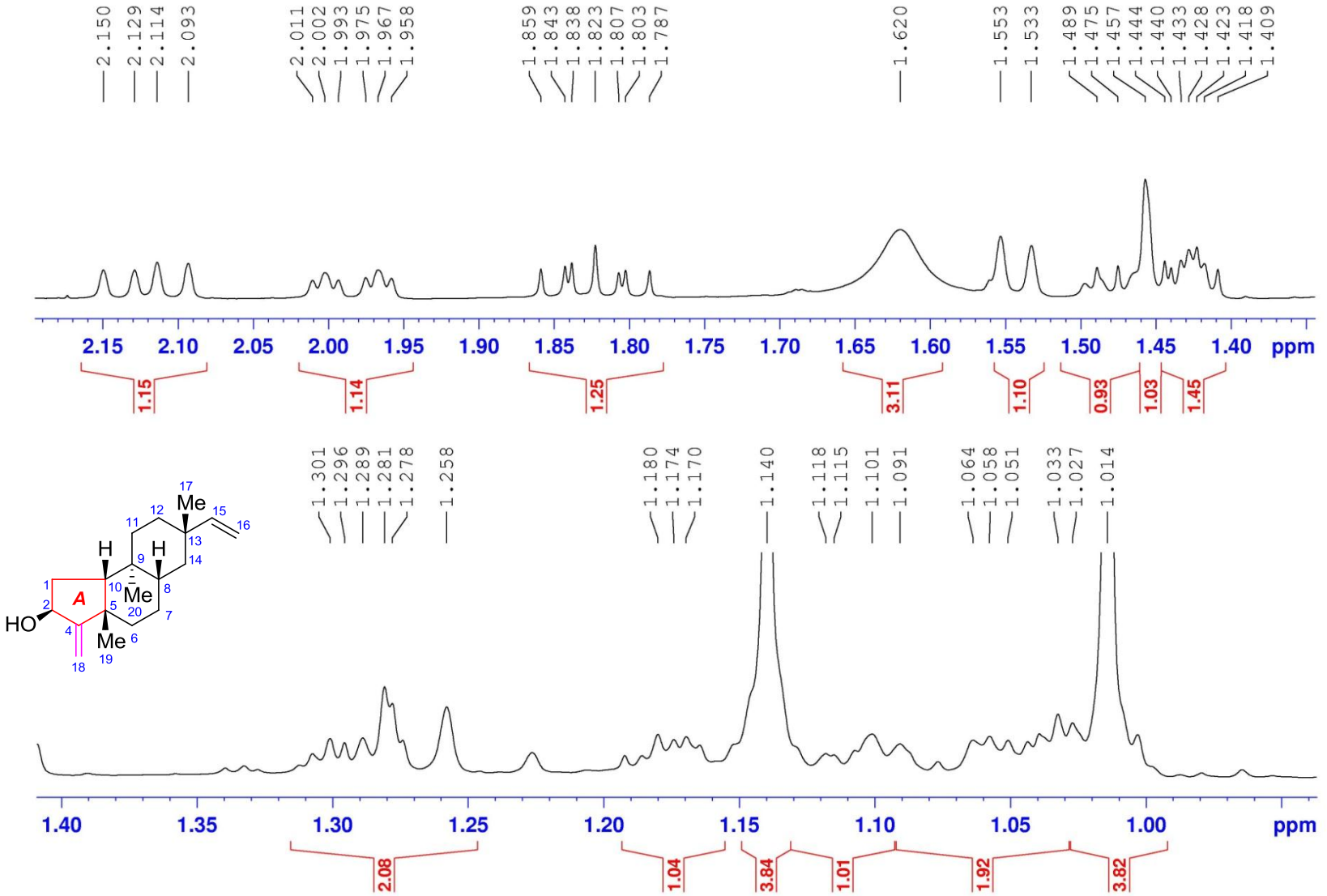



```
NAME            R-36-3-3
EXPNO                  1
PROCNO                 1
Date_           20160227
Time                3.35
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     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             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          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
```

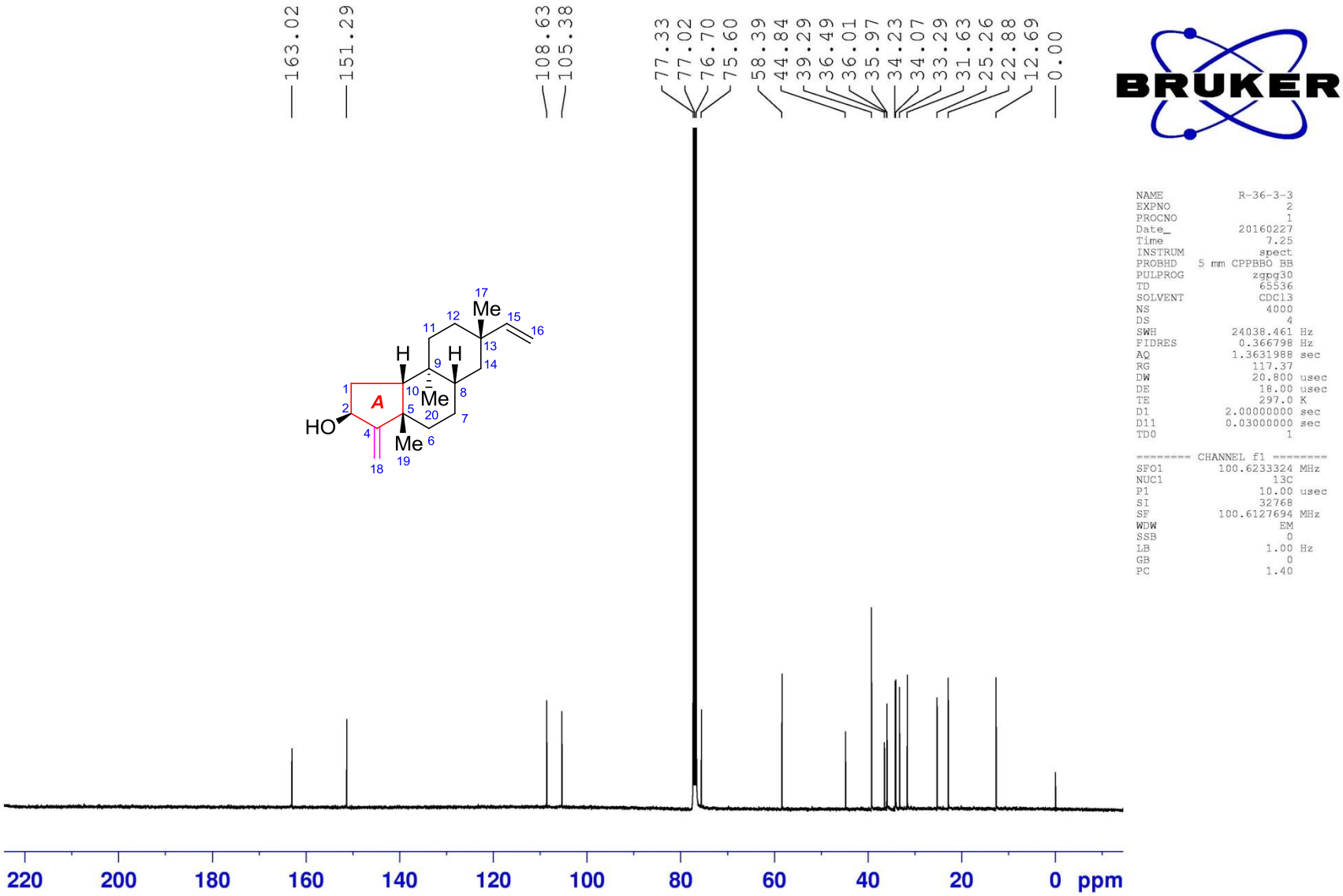
^{1}H (400 MHz) NMR spectrum of tagalol A (2) in $CDCl_3$



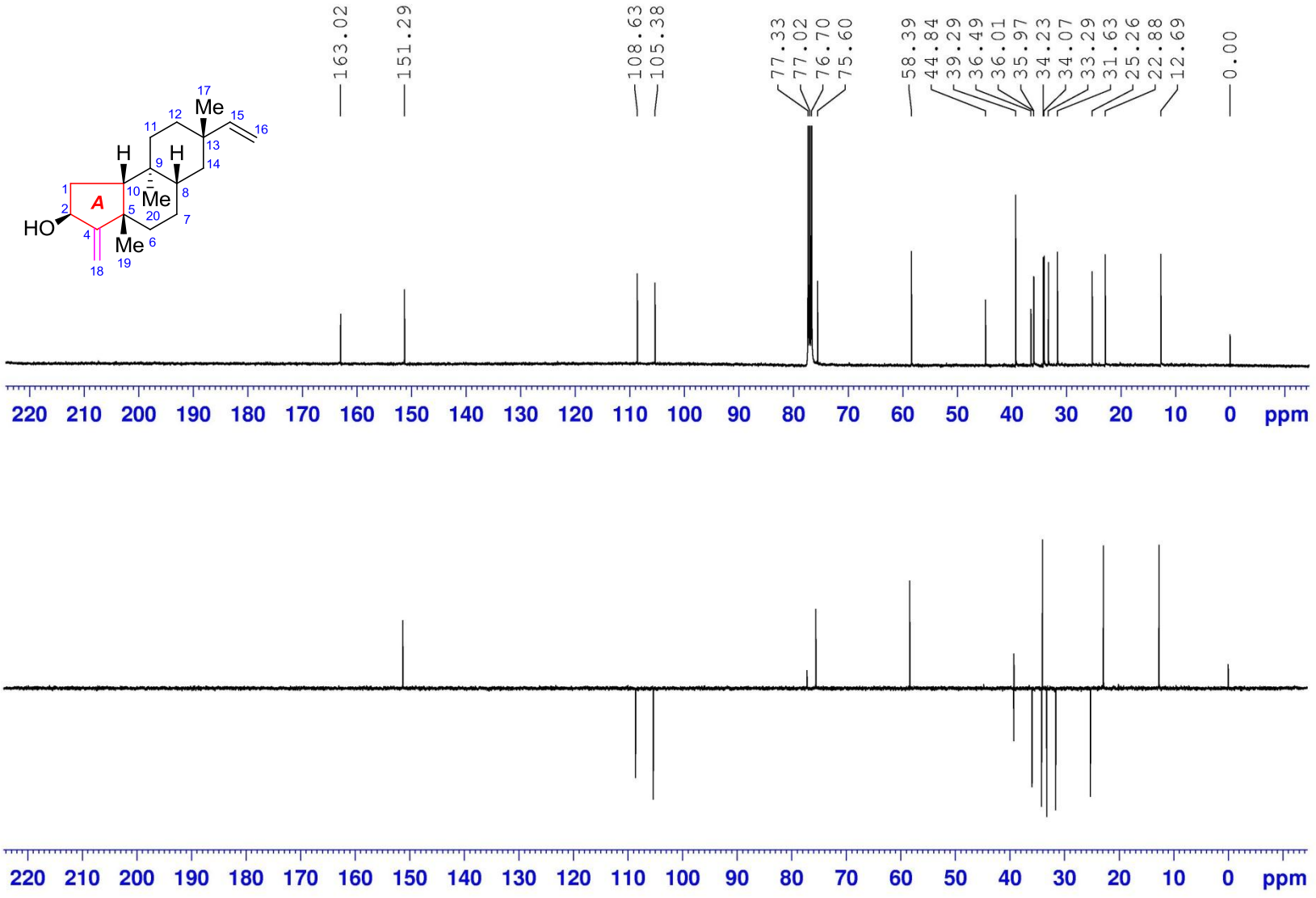
^{1}H (400 MHz) NMR spectrum of tagalol A (2) in $CDCl_3$



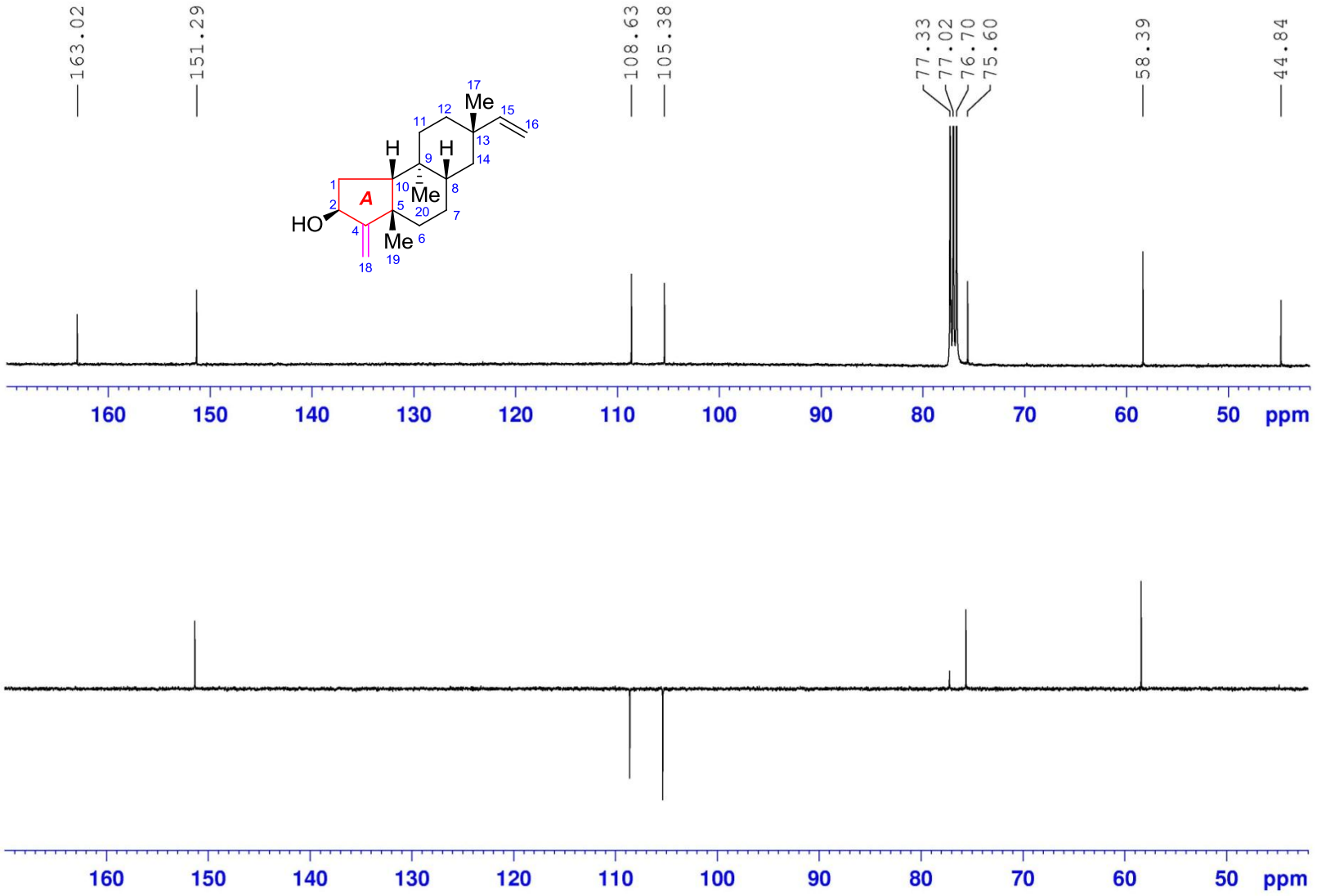
^{13}C (100 MHz) NMR spectrum of tagalol A (2) in $CDCl_3$



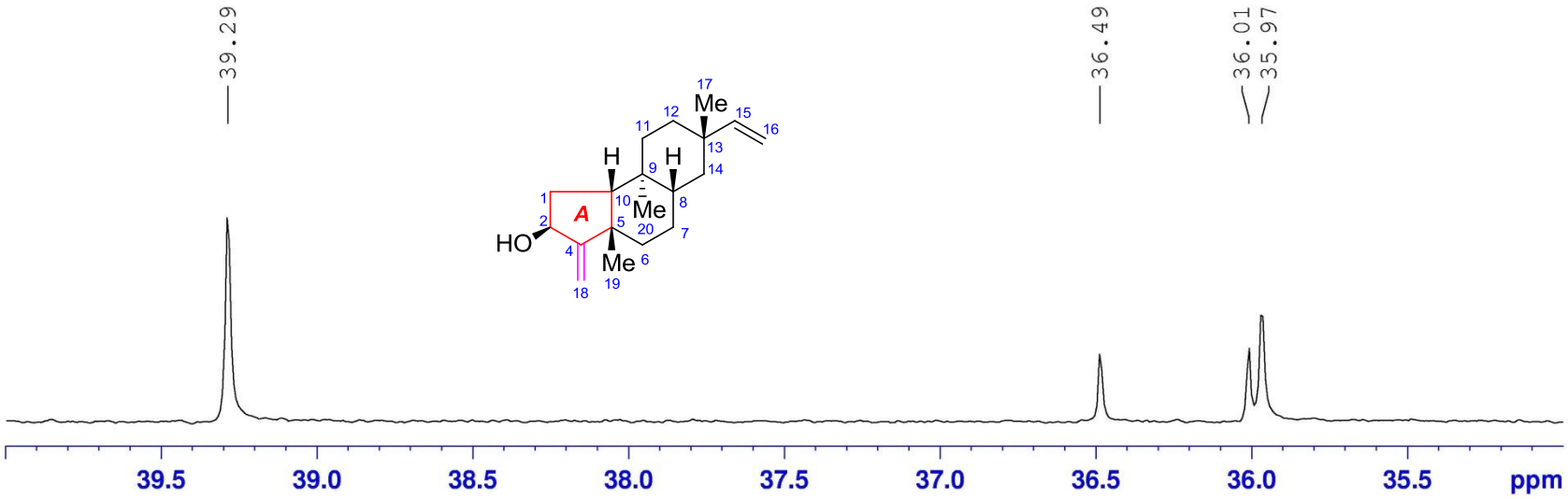
DEPT135 (100 MHz) experiment of tagalol A (2) in $CDCl_3$



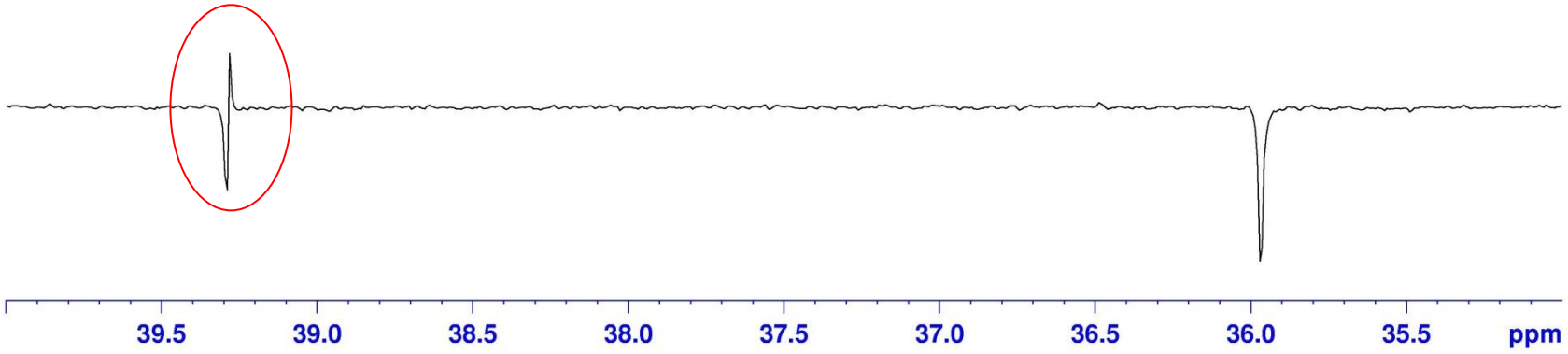
DEPT135 (100 MHz) experiment of tagalol A (2) in $CDCl_3$



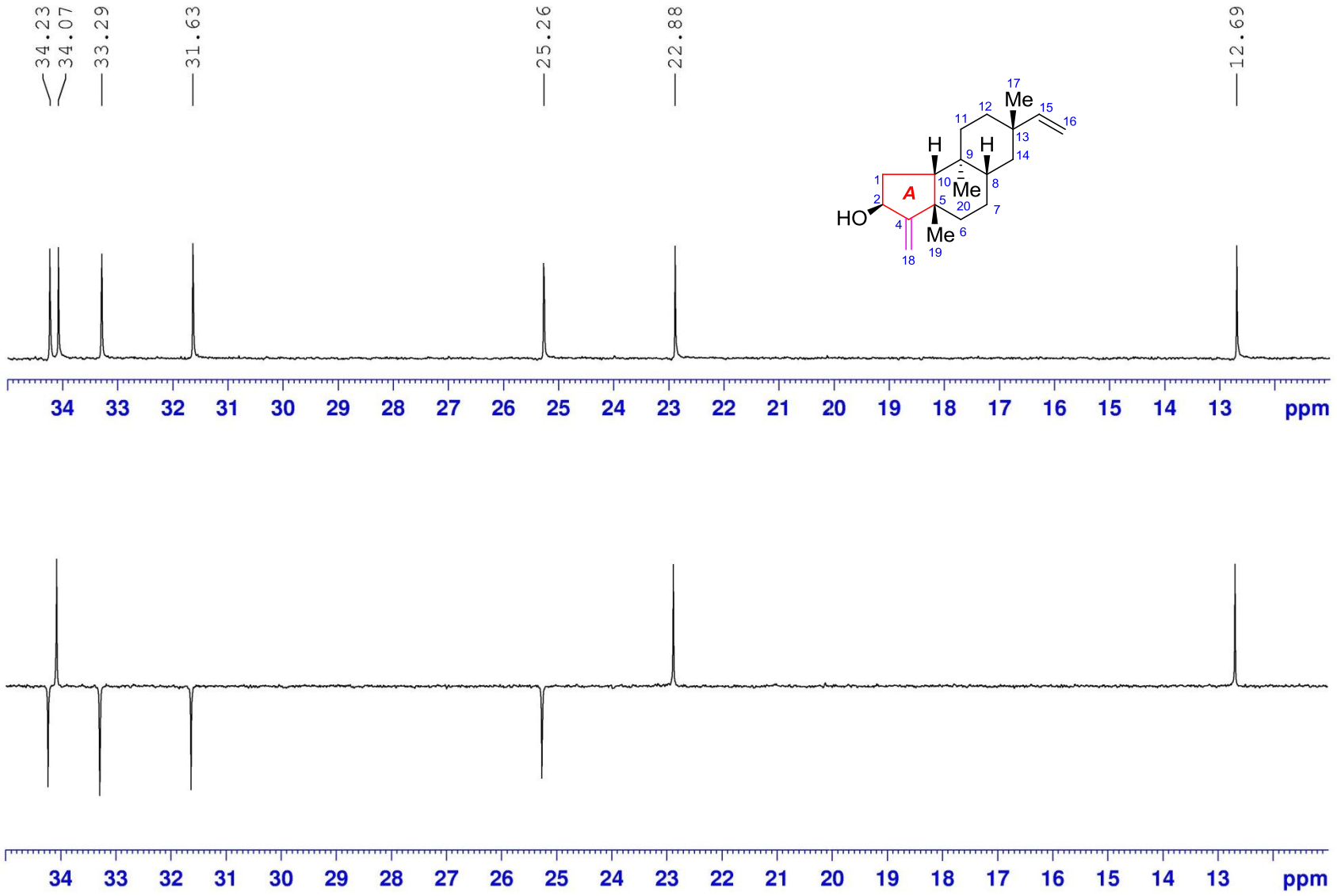
DEPT135 (100 MHz) experiment of tagalol A (2) in $CDCl_3$



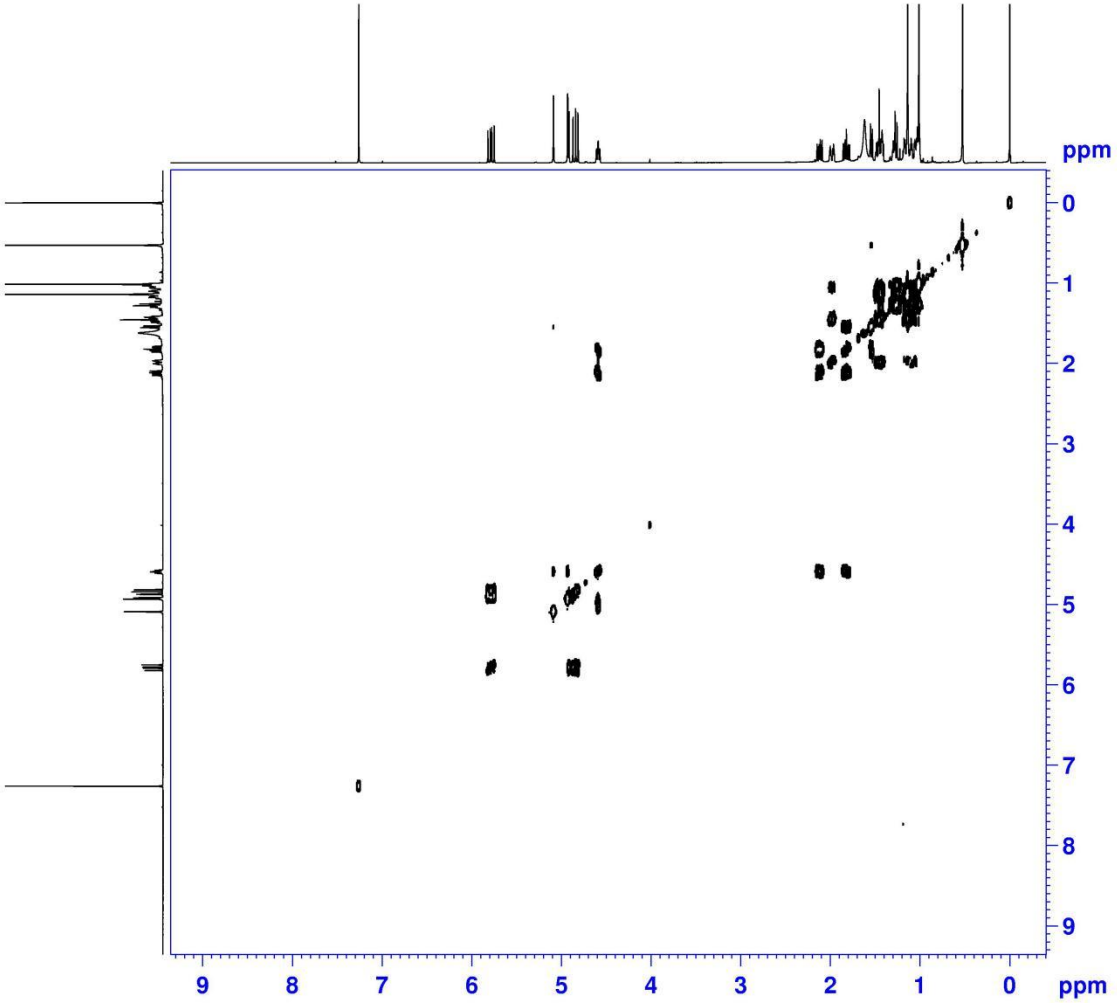
Overlapped ^{13}C signals



DEPT135 (100 MHz) experiment of tagalol A (2) in $CDCl_3$



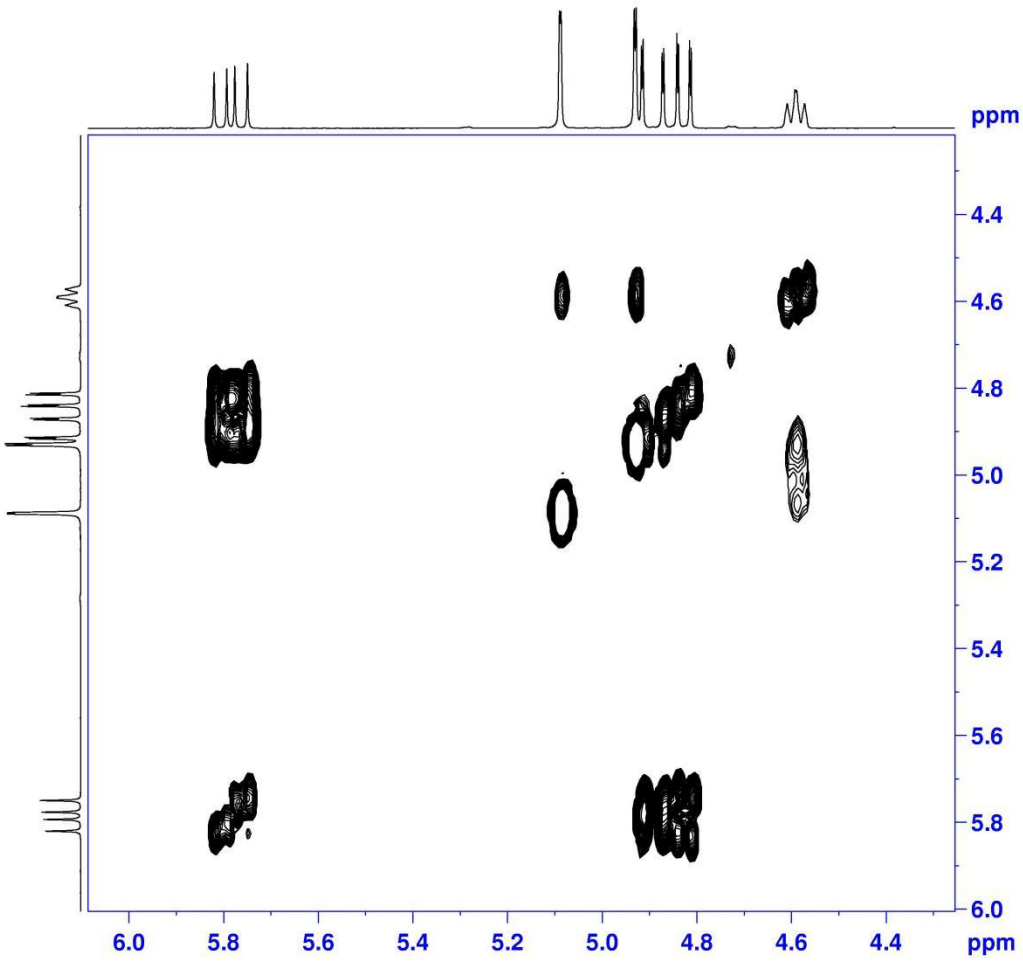
^{1}H-^{1}H COSY (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



BRUKER

```
NAME                R-36-3-3
EXPNO                      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                0.00000300 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
```

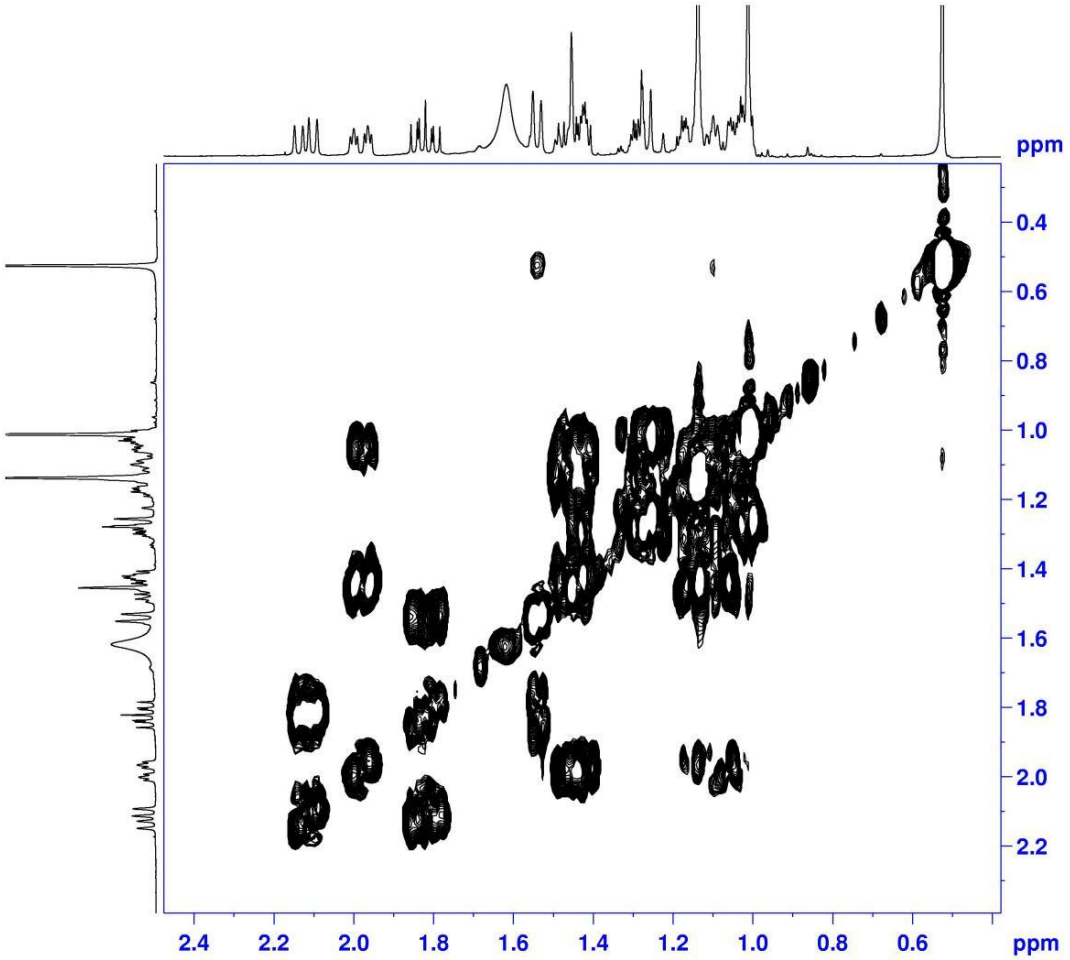
^{1}H-^{1}H COSY (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



BRUKER

```
NAME              R-36-3-3
EXPNO                    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                 0.00000300 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
```

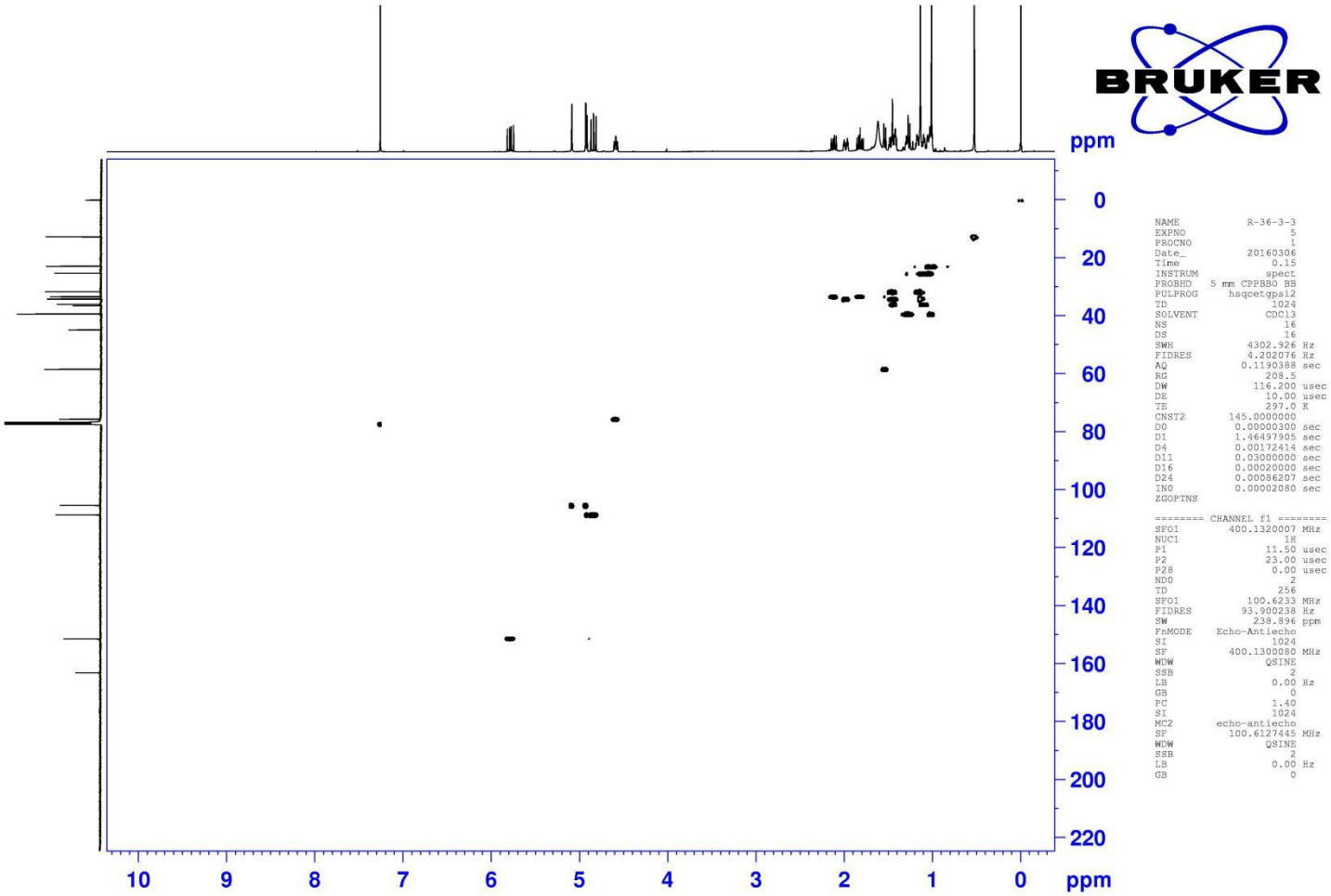
^{1}H-^{1}H COSY (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



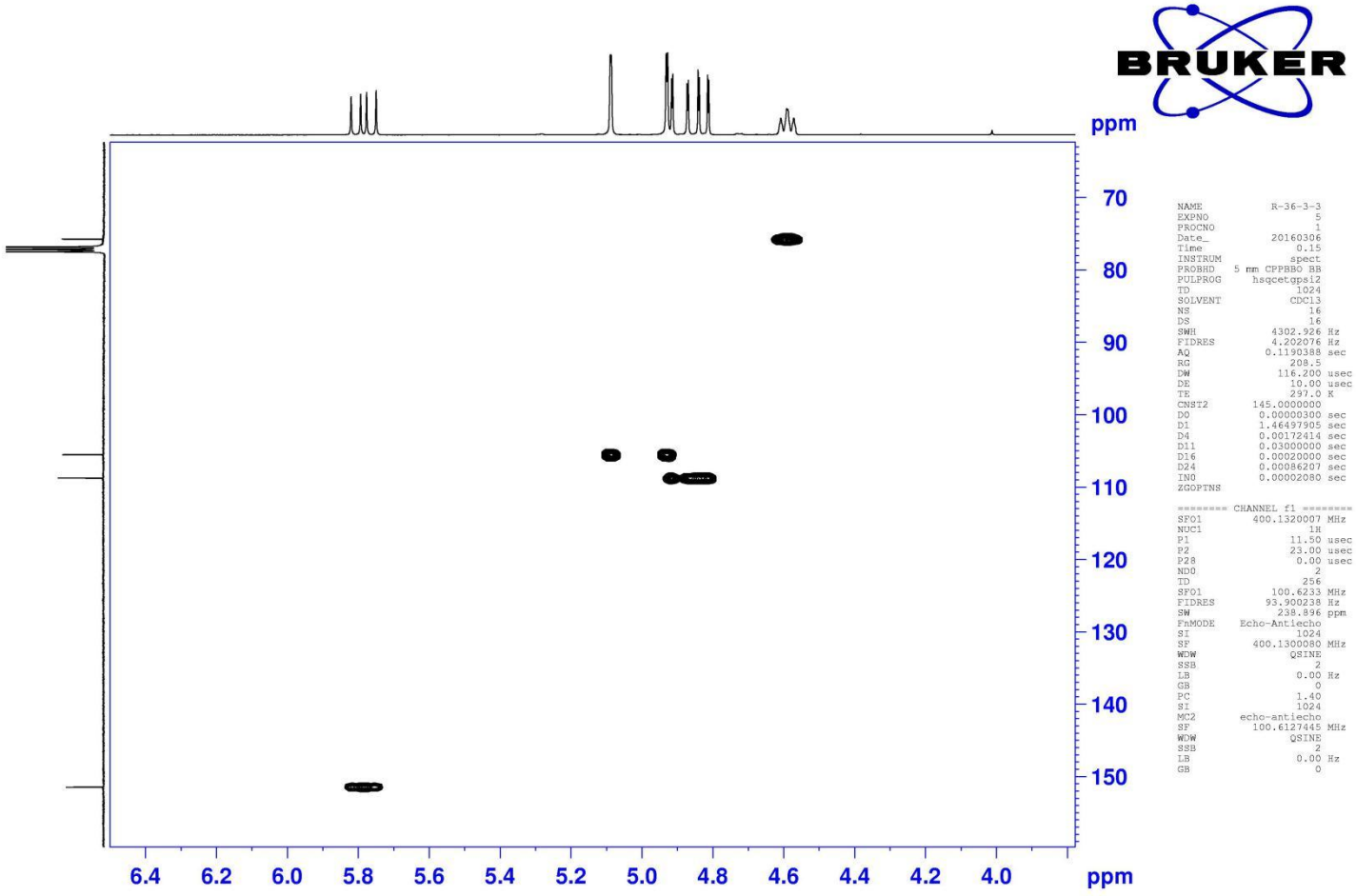
BRUKER

```
NAME                R-36-3-3
EXPNO                      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                 0.00000300 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
```

HSQC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$

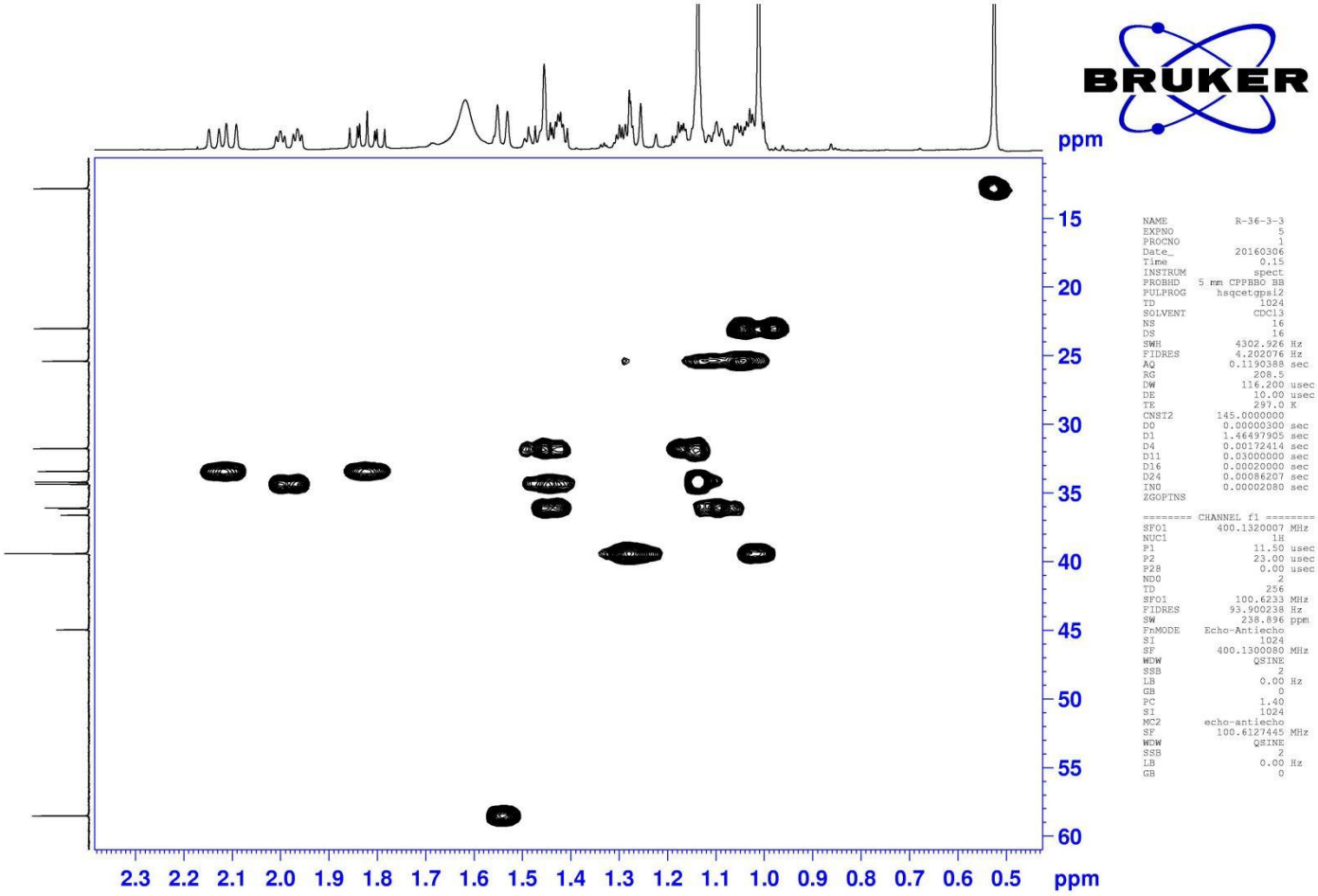


HSQC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



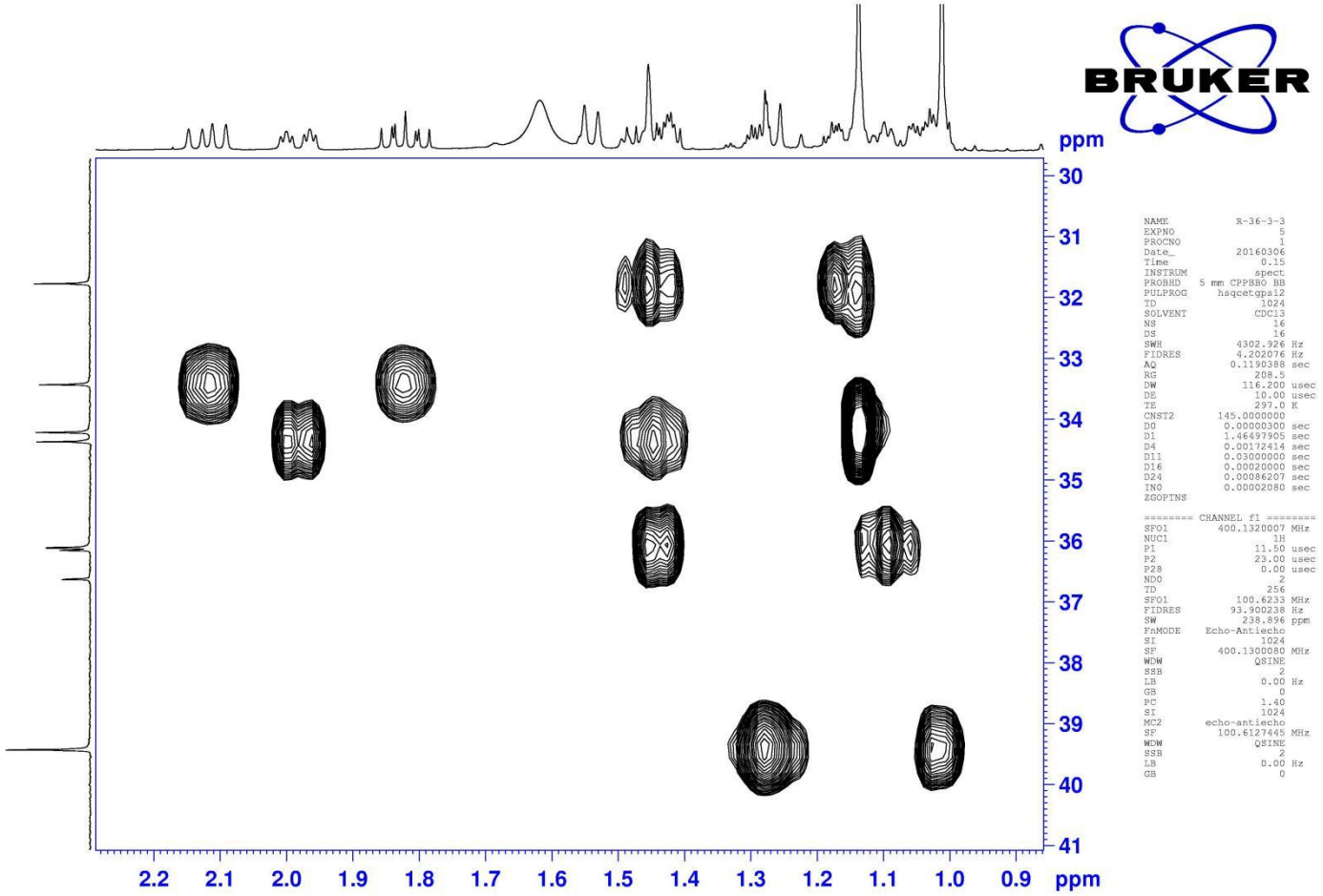

```
NAME                R-36-3-3
EXPNO                      5
PROCNO                     1
Date_               20160306
Time                   0.15
INSTRUM                spect
PROBHD     5 mm CPPBBO BB
PULPROG        hsqcetgpsi2
TD                      1024
SOLVENT                CDCl3
NS                        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 ========
SFO1               400.1320007 MHz
NUC1                        1H
P1                       11.50 usec
P2                       23.00 usec
P28                       0.00 usec
ND0                          2
TD                         256
SFO1               100.6233 MHz
FIDRES              93.900238 Hz
SW                    238.896 ppm
FnMODE        Echo-Antiecho
SI                        1024
SF                 400.1300080 MHz
WDW                      QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
PC                        1.40
SI                        1024
MC2               echo-antiecho
SF                 100.6127445 MHz
WDW                      QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
```

HSQC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



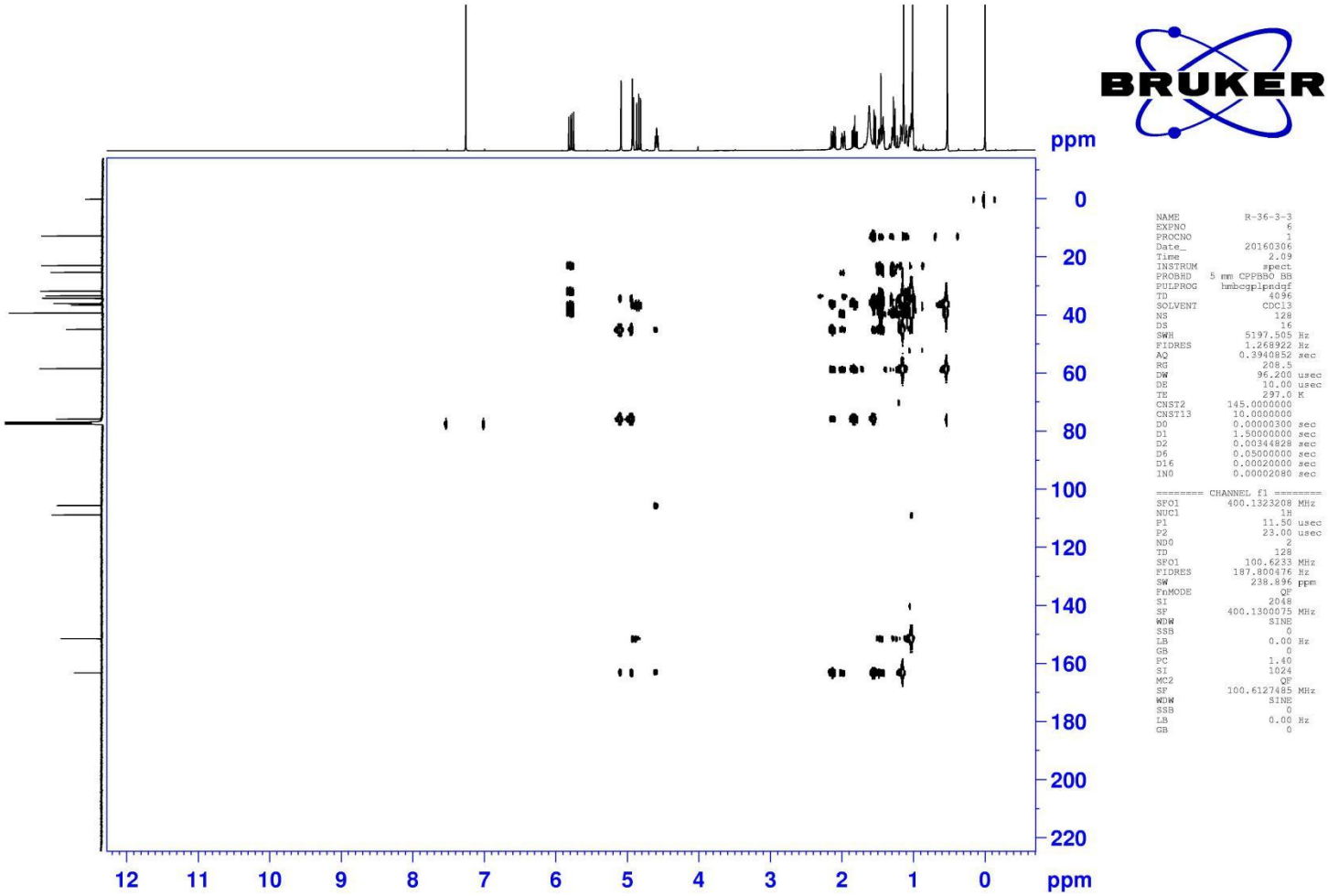

```
NAME                R-36-3-3
EXPNO                      5
PROCNO                     1
Date_               20160306
Time                    0.15
INSTRUM                spect
PROBHD    5 mm CPFBBO BB
PULPROG      hsqcetgpsi2
TD                      1024
SOLVENT              CDCl3
NS                        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
DZ4                0.00086207 sec
IN0                0.00002080 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1               400.1320007 MHz
NUC1                       1H
P1                    11.50 usec
P2                    23.00 usec
P28                    0.00 usec
ND0                        2
TD                       256
SFO1               100.6233 MHz
FIDRES             93.900238 Hz
SW                   238.896 ppm
FnMODE       Echo-Antiecho
SI                      1024
SF                 400.1300080 MHz
WDW                    QSINE
SSB                        2
LB                     0.00 Hz
GB                         0
PC                      1.40
SI                      1024
MC2             echo-antiecho
SF                 100.6127445 MHz
WDW                    QSINE
SSB                        2
LB                     0.00 Hz
GB                         0
```

HSQC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$




```
NAME                 R-36-3-3
EXPNO                       5
PROCNO                      1
Date_                20160306
Time                     0.15
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
IN0                  0.00002080 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1               400.1320007 MHz
NUC1                        1H
P1                      11.50 usec
P2                      23.00 usec
P28                      0.00 usec
ND0                         2
TD                        256
SFO1                100.6233 MHz
FIDRES               93.900238 Hz
SW                     238.896 ppm
FnMODE         Echo-Antiecho
SI                       1024
SF                 400.1300080 MHz
WDW                      QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
PC                       1.40
SI                       1024
MC2            echo-antiecho
SF                 100.6127445 MHz
WDW                      QSINE
SSB                         2
LB                       0.00 Hz
GB                          0
```

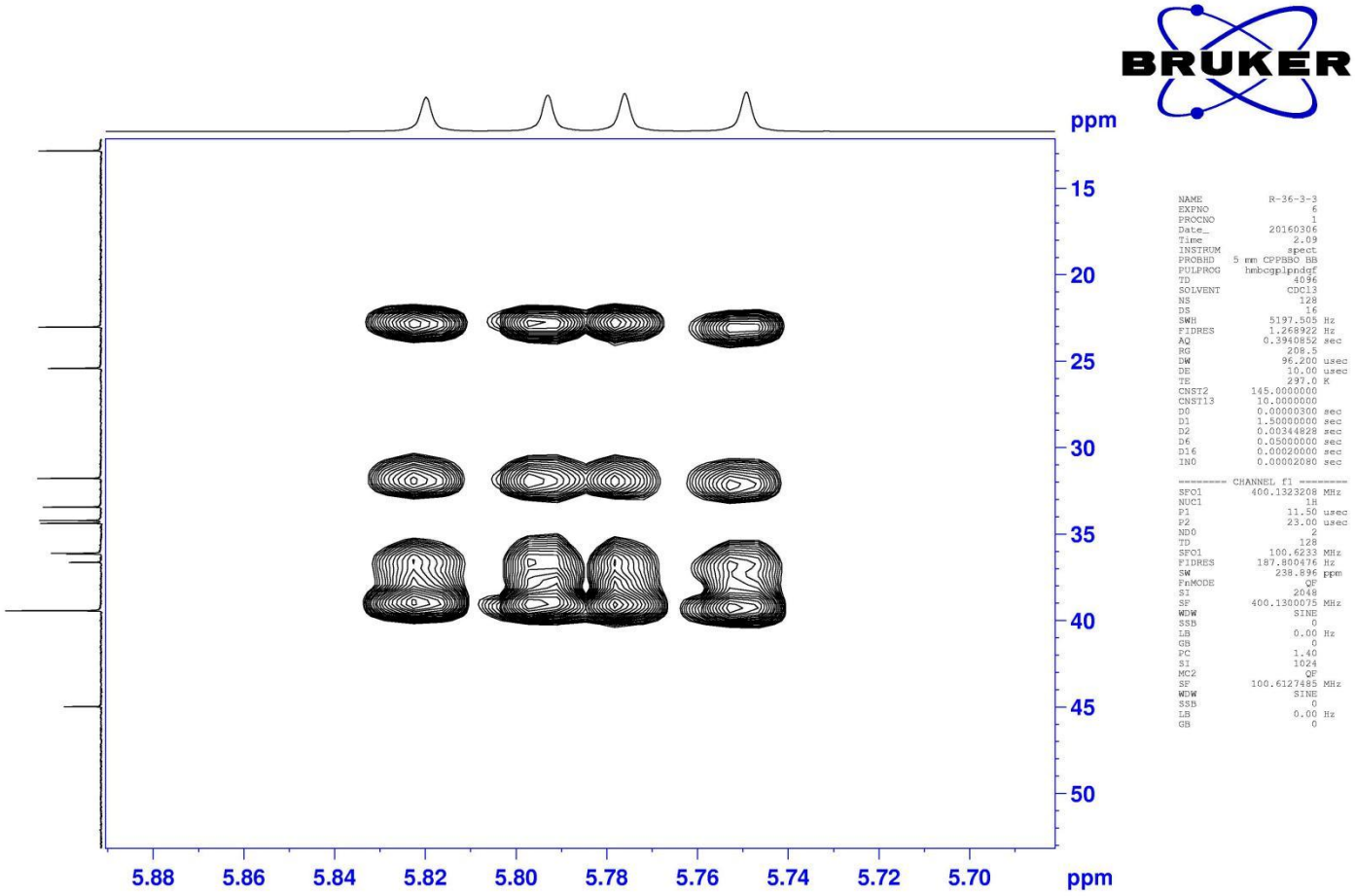
HMBC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



BRUKER

```
NAME              R-36-3-3
EXPNO                    6
PROCNO                   1
Date_             20160306
Time                 2.09
INSTRUM              spect
PROBHD  5 mm CPPBBO BB
PULPROG    hmbcgplpndqf
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           187.800476 Hz
SW                238.896 ppm
FnMODE                  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
```

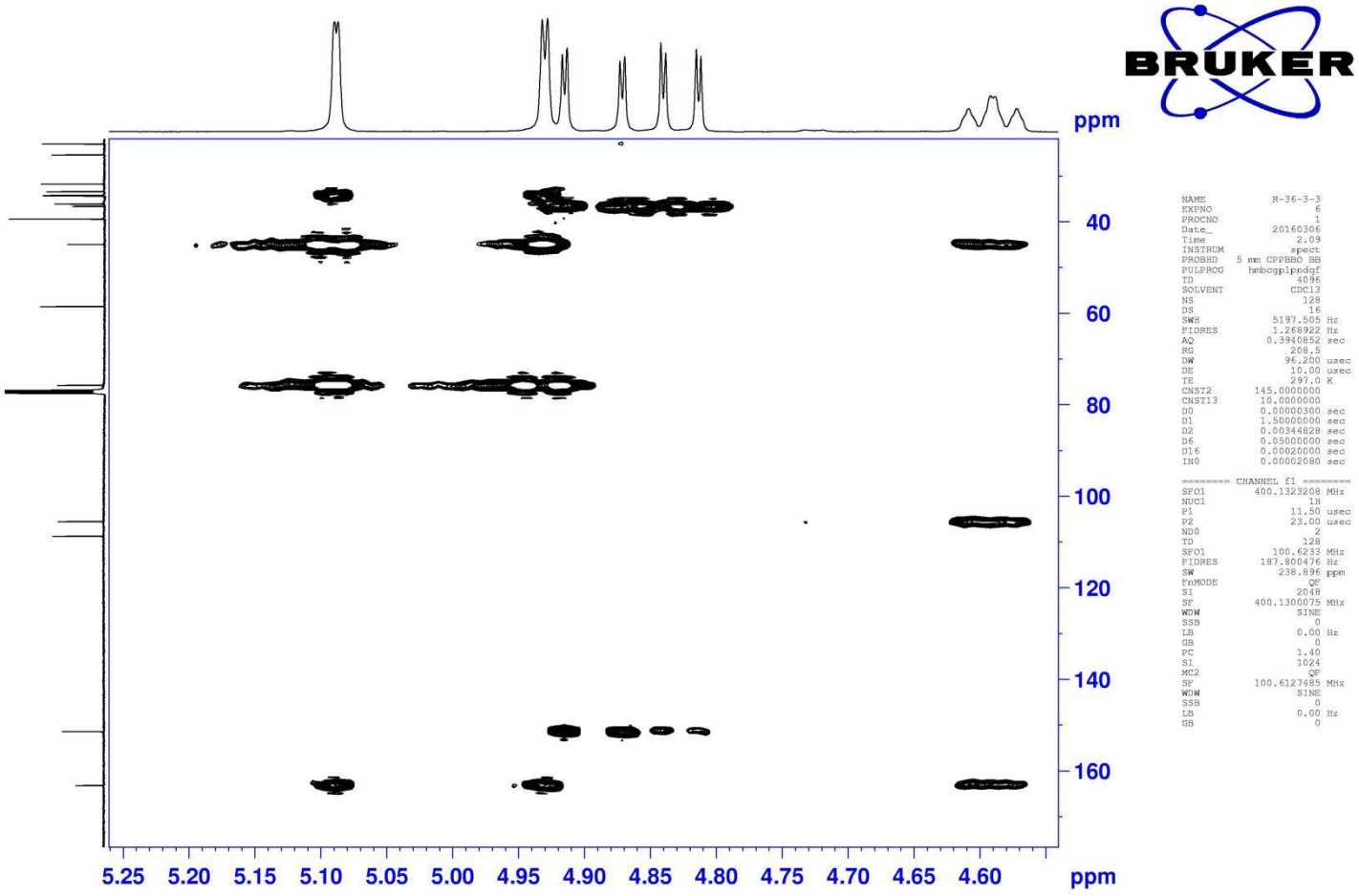
HMBC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



BRUKER

NAME	R-36-3-3
EXPNO	6
PROCNO	1
Date_	20160306
Time	2.09
INSTRUM	spect
PROBHD	5 mm CPPSBO BB
PULPROG	hmbcgplpndqf
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	187.800476 Hz
SW	238.896 ppm
FnMODE	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

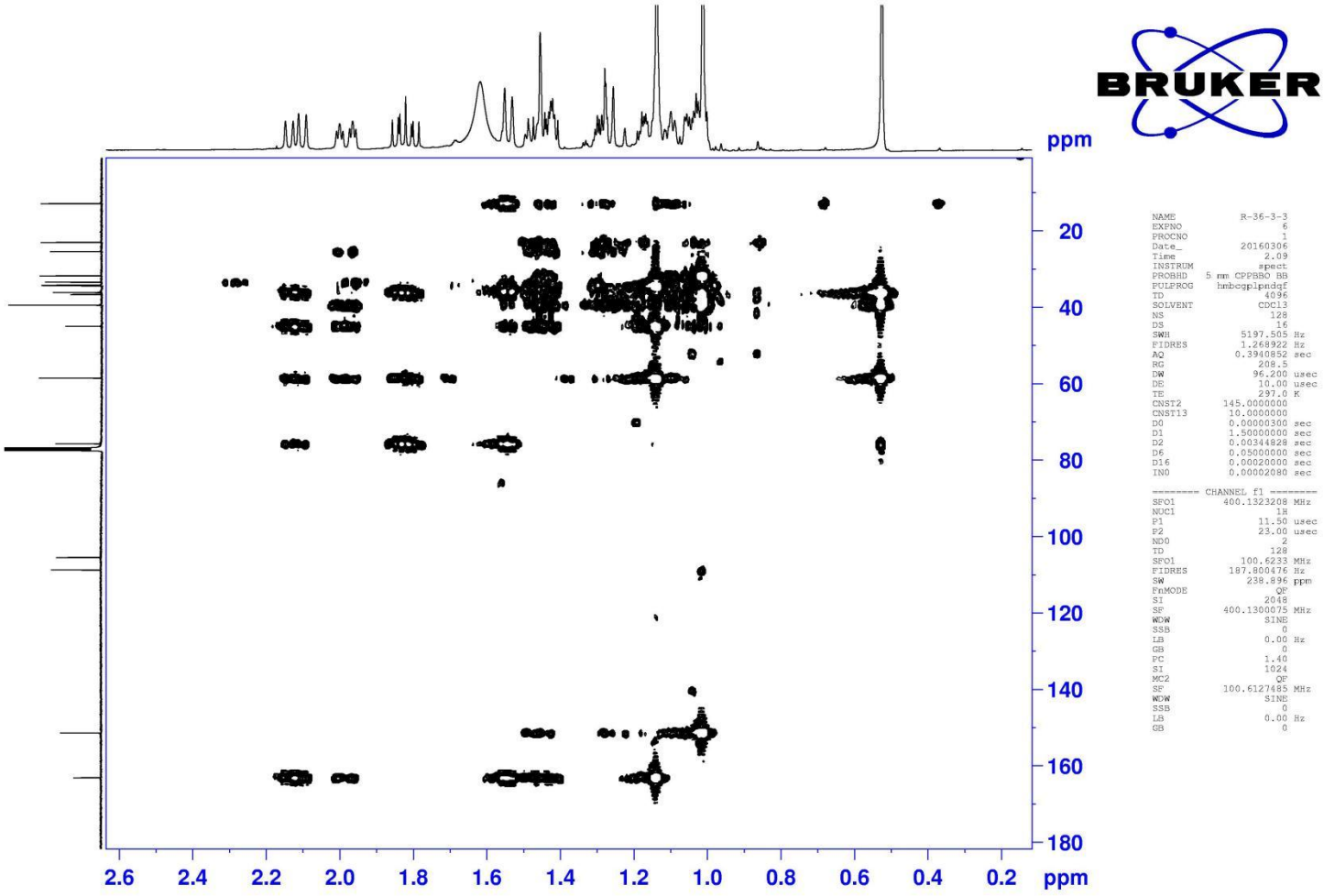
HMBC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



BRUKER

```
NAME                R-36-3-3
EXPNO                      6
PROCNO                     1
Date_               20160306
Time                    2.09
INSTRUM                 spect
PROBHD   5 mm CPPBBO BB
PULPROG         hmbcgplpndqf
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              187.800476 Hz
SW                    238.896 ppm
FnMODE                     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
```

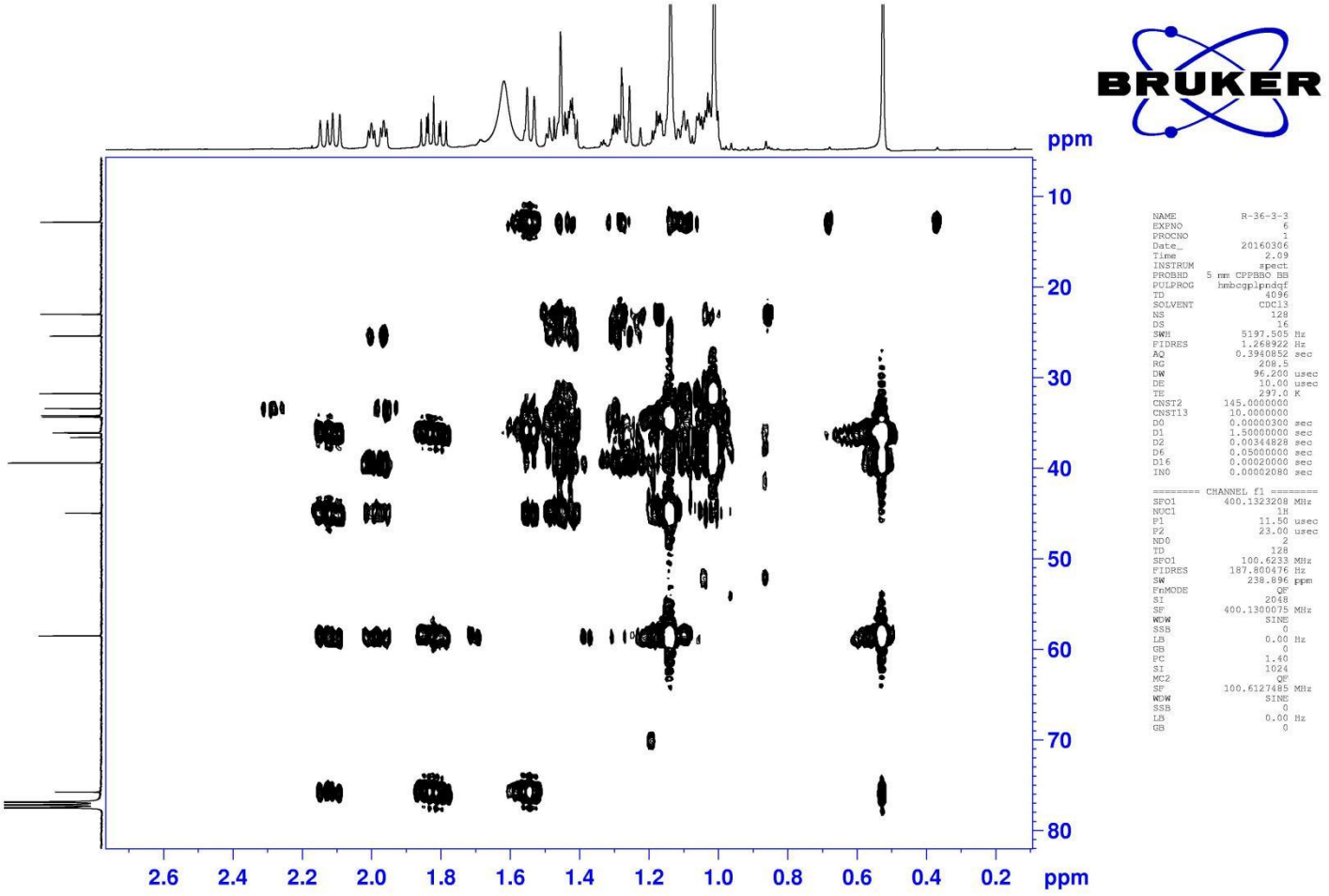
HMBC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



BRUKER

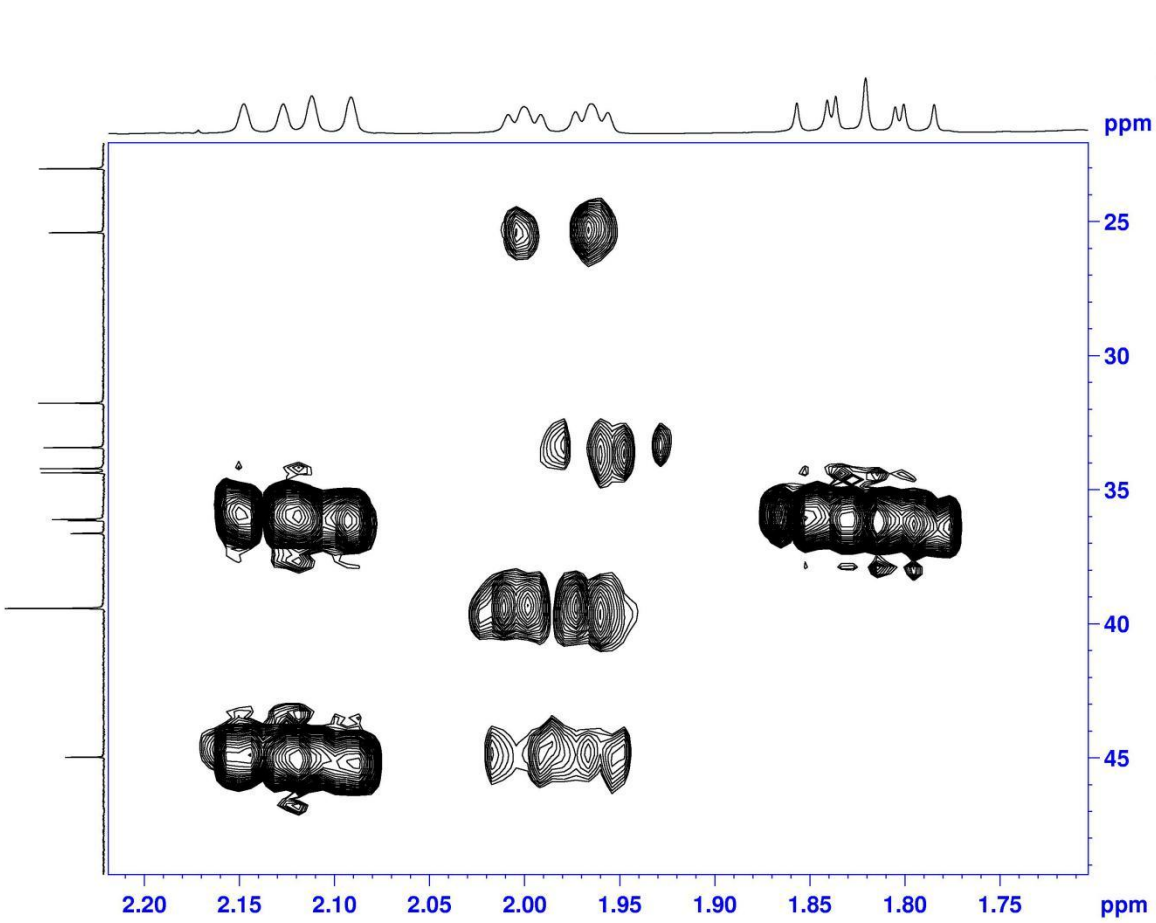
```
NAME                 R-36-3-3
EXPNO                       6
PROCNO                      1
Date_                20160306
Time                     2.09
INSTRUM                 spect
PROBHD    5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
TD                       4096
SOLVENT                 CDCl3
NS                        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               187.800476 Hz
SW                       238.896 ppm
FnMODE                      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 $CDCl_3$



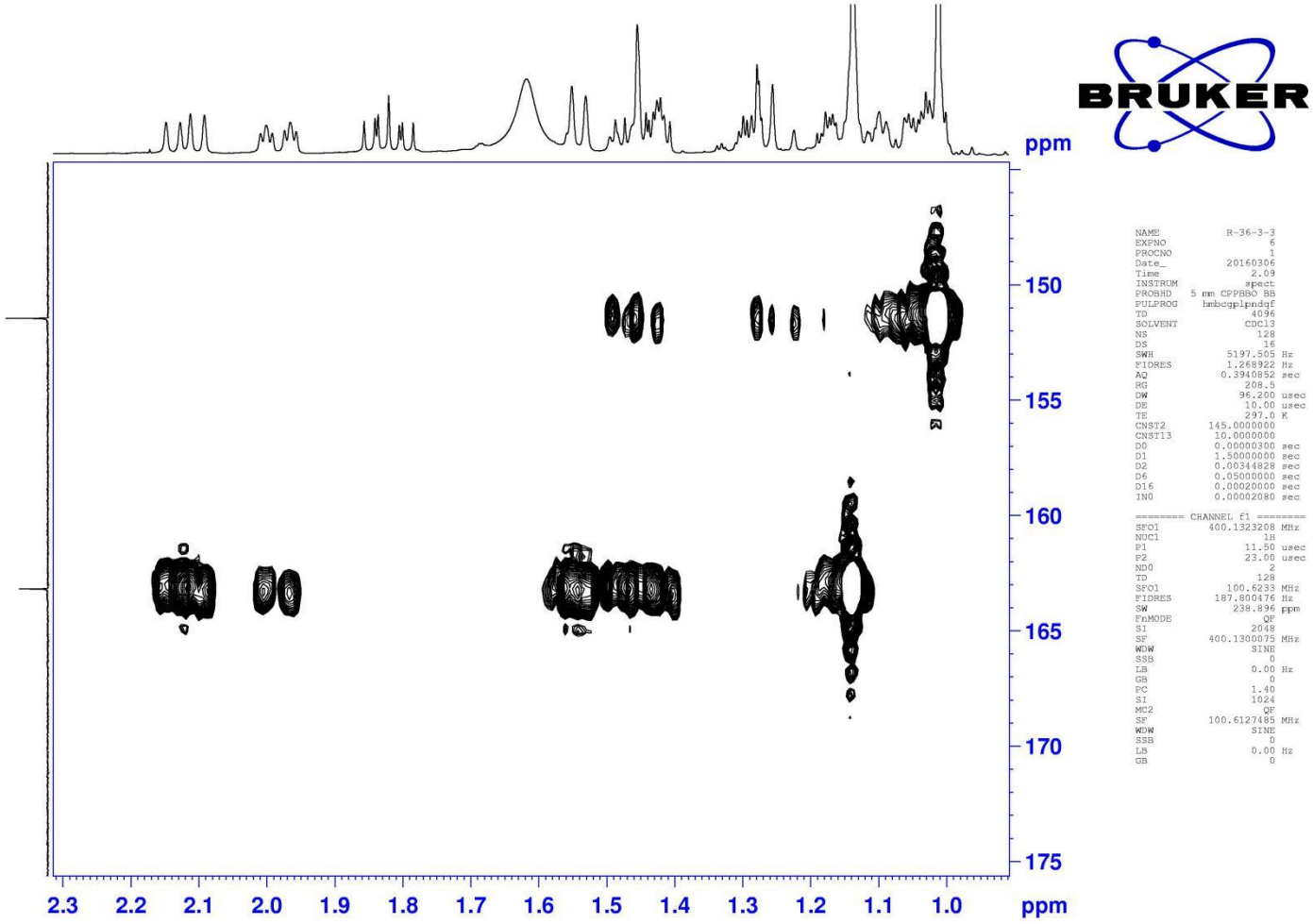

```
NAME                R-36-3-3
EXPNO                      6
PROCNO                     1
Date_               20160306
Time                    2.09
INSTRUM                 spect
PROBHD   5 mm CPPBBO BB
PULPROG    hmbcgplpndqf
TD                      4096
SOLVENT                 CDCl3
NS                       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              187.800476 Hz
SW                  238.896 ppm
FnMODE                     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 $CDCl_3$



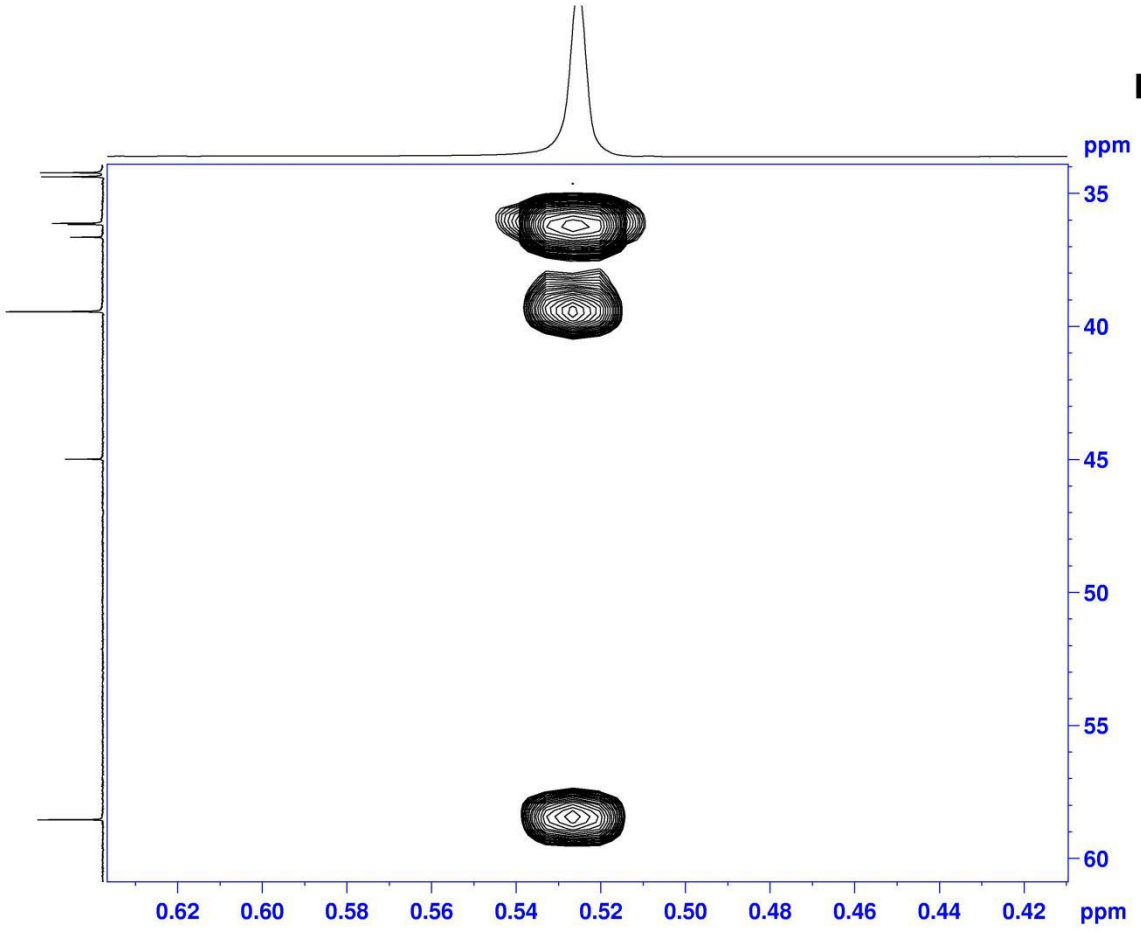

```
NAME                  R-36-3-3
EXPNO                        6
PROCNO                       1
Date_                 20160306
Time                      2.09
INSTRUM                  spect
PROBHD    5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
TD                        4096
SOLVENT                 CDCl3
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               187.800476 Hz
SW                       238.896 ppm
FnMODE                      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 $CDCl_3$




```
NAME                R-36-3-3
EXPNO                      6
PROCNO                     1
Date_               20160306
Time                    2.09
INSTRUM                 spect
PROBHD   5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
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              187.800476 Hz
SW                     238.896 ppm
FnMODE                      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
```

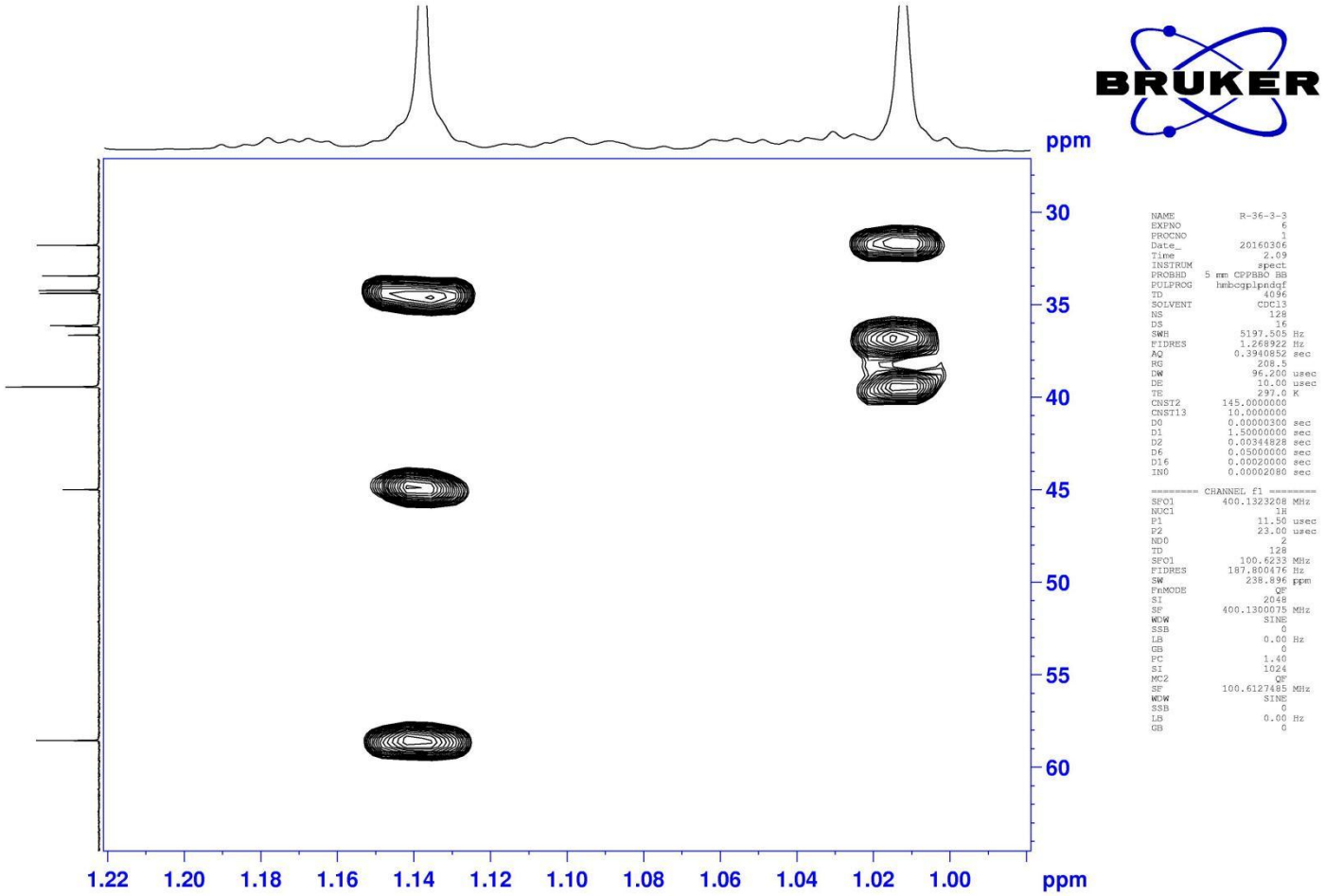
HMBC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



NAME R-36-3-3
EXPNO 6
PROCNO 1
Date_ 20160306
Time 2.09
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG hmbcgplpndqf
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

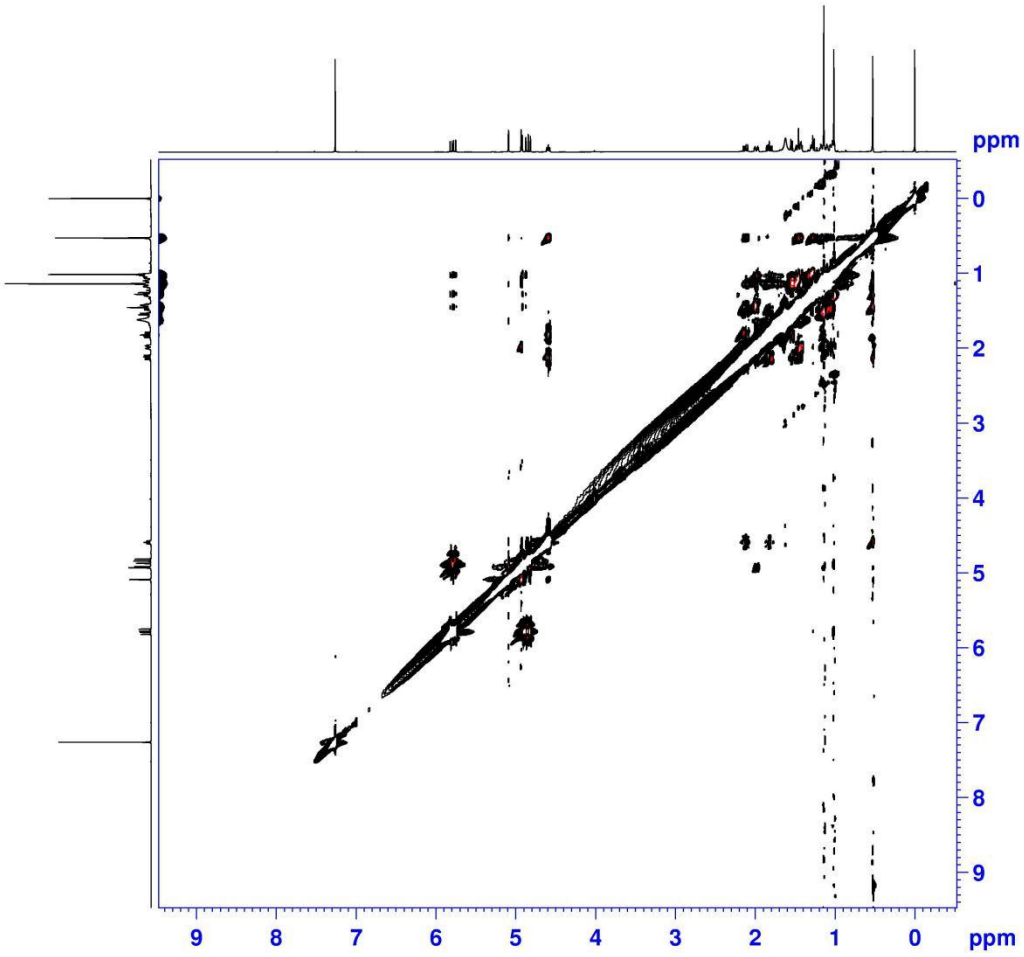
======== CHANNEL f1 ========
SFO1 400.1323208 MHz
NUC1 1H
P1 11.50 usec
P2 23.00 usec
ND0 2
TD 128
SFO1 100.6233 MHz
FIDRES 187.800476 Hz
SW 238.896 ppm
FnMODE QF
SI 2048
SF 400.1300075 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6127485 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

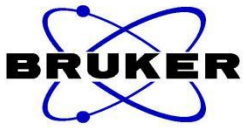
HMBC (400 MHz) spectrum of tagalol A (2) in $CDCl_3$




```
NAME                R-36-3-3
EXPNO                      6
PROCNO                     1
Date_               20160306
Time                    2.09
INSTRUM                 spect
PROBHD   5 mm CPPBBO BB
PULPROG     hmbcgplpndqf
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              187.800476 Hz
SW                  238.896 ppm
FnMODE                     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
```

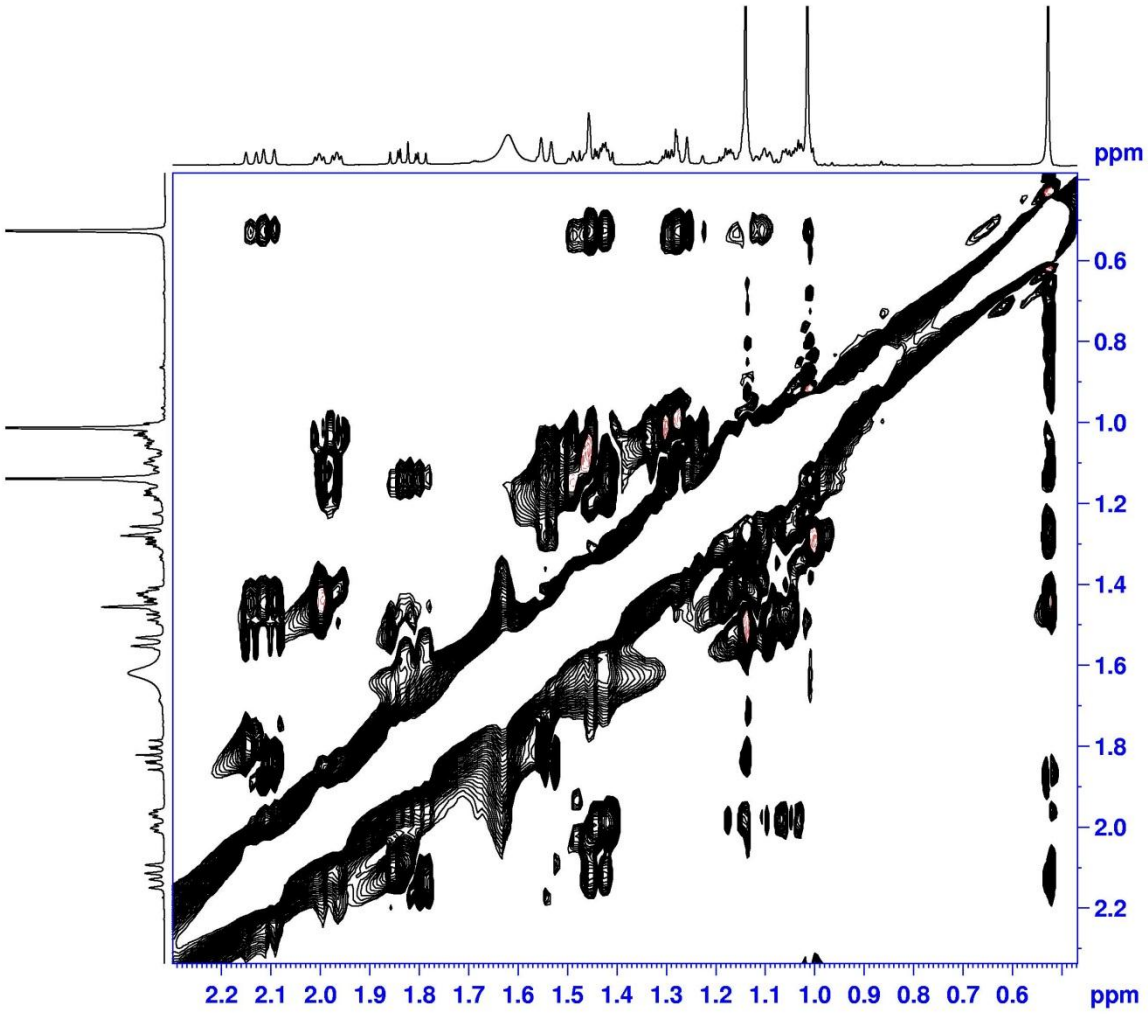
NOESY (400 MHz) spectrum of tagalol A (2) in $CDCl_3$





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
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	400.1300098 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	1024
MC2	States-TPPI
SF	400.1300098 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

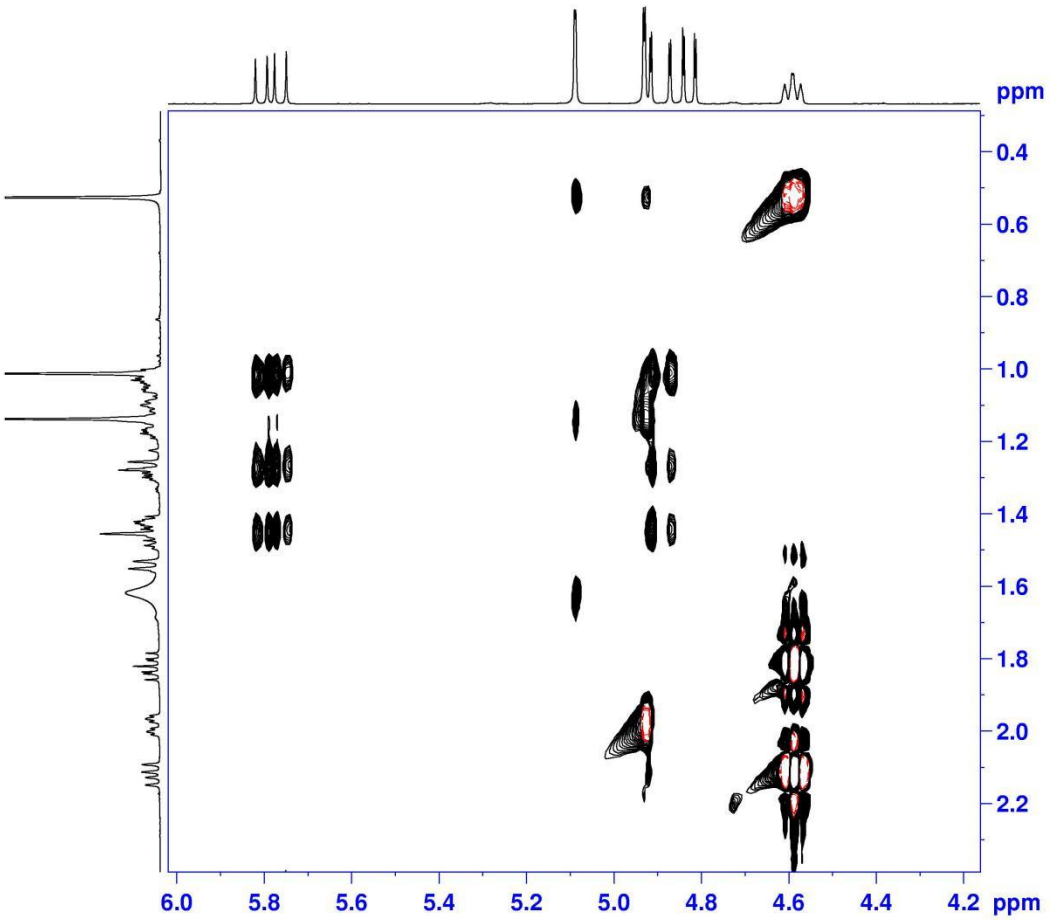
NOESY (400 MHz) spectrum of tagalol A (2) in $CDCl_3$



BRUKER

```
NAME          zxh-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 ========
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                400.1300089 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 $CDCl_3$




```
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
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              400.1300098 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
PC                      1.00
SI                      1024
MC2             States-TPPI
SF              400.1300098 MHz
WDW                    QSINE
SSB                        2
LB                      0.00 Hz
GB                         0
```