

Supporting information

Total Synthesis and Stereochemical Revision of Xiamenmycin A

Xiaozhen Jiao,^a Yangyang Yao,^a Beibei Yang,^a Xiaoyu Liu,^a Xiaoyu Li,^a Hongguang Yang,^a Li Li,^a Jun Xu,^b Minjuan Xu,^{c*} Ping Xie,^{a*}

^a State Key Laboratory of Bioactive Substances and Functions of Natural Medicines, Institute of Materia Medica, Beijing Key Laboratory of Active Substances Discovery and Drugability Evaluation, Peking Union Medical College and Chinese Academy of Medical Sciences, Beijing 100050, PR China. Fax: +86 10 63017757; Tel: +86 10 63165242; E-mail: xp@imm.ac.cn

^b Institute of Oceanology, Shanghai Jiao Tong University, Shanghai 200240, PR China.

^c Key Laboratory of Systems Biomedicine, Shanghai Center for Systems Biomedicine, Shanghai Jiao Tong University, Shanghai 200240, PR China. Fax: +86-21-34206866; Tel: +86-21-34206244; E-mail: minjuanxu@sjtu.edu.cn

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General Information

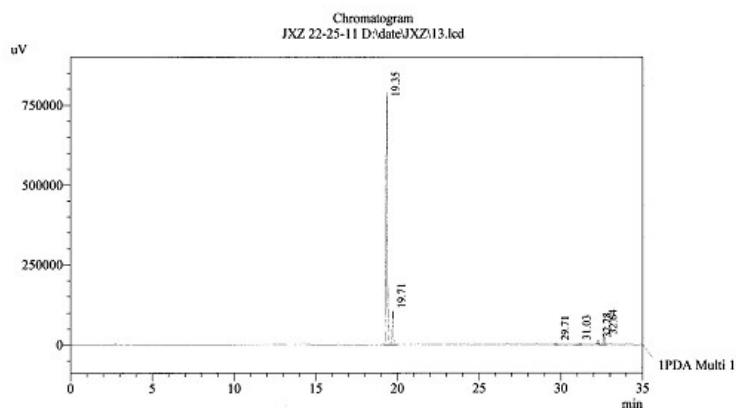
Solvents were dried according to standard procedures where needed. All reagents and solvents were purchased from commercial suppliers. Column chromatography was carried out on silica gel (160–200 mesh). Melting points were measured on microscope melting point apparatus. IR spectra were recorded on a Thermo Nicolet 5700 FT-IR microscope Centaur μ s spectrophotometer. NMR spectra were recorded on 400 or 600 MHz NMR spectrometer. Chemical shifts are referenced to the residual solvent peak and reported in ppm (δ scale) and all coupling constant (J) values are given in Hz. The following multiplicity abbreviations are used: (s) singlet, (d) doublet, (t) triplet, (q) quartet, (m) multiplet, and (br) broad. ESI-HRMS data were measured on orbitrap mass spectrometer.

HPLC analysis: Column: Pinnade II C18 Column size: 0.46 cm I.D. x 25 cm L x 5 μ m; column temperature: 35°C; injection volume: 20μL; mobile phase: CH₃CN/H₂O/0.1%HCOOH; flow rate: 1.0mL/min Wavelength : 272nm; a gradient program was used as follows:

Time(min)	CH ₃ CN(%)	H ₂ O(%)
0	5	95
5	5	95
35	90	10
40	90	10
50	5	95
55	5	95

Sample Information

Acquired by : Admin
Sample Name : JXZ 22-25-11
Tray# : 1
Vial# : 12
Injection Volume : 20 uL
Data Filename : 13.lcd
Method name : D:\方法\JXZ.lcm
Method Filename : JXZ-2.lcm
Batch Filename : JXZ.lcb
Report Filename : Default.lcr
Date Acquired : 2015-11-17 2:06:39
Data Processed : 2015-11-17 9:35:48



PeakTable

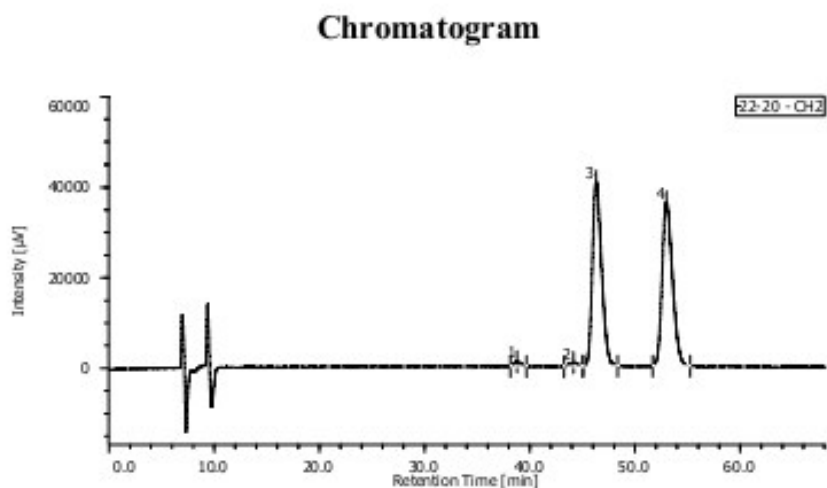
Peak#	Ret. Time	Area	Height	Area %
1	19.34	4080229	789568	82.389
2	19.70	554239	106634	11.191
3	29.71	23795	4479	0.480
4	31.03	39953	5912	0.807
5	32.28	74034	13252	1.495
6	32.64	138968	23930	2.806
7	36.98	41176	7852	0.831
Total		4952395	951628	100.000

PDA Ch1 272nm 4nm

HPLC spectra of compound 7 and 7' (entry 11 in Table 1)

HPLC ANALYSIS

Determination of the enantiomeric excess of compound **6** and **16**. column: CHIRALPAK OJ-H 0.46 cm I.D. x 25 cm L x 5 μ m; column temperature: 25°C; injection volume: 10 μ L; mobile phase: hexane/*i*-PrOH (9/1); flow rate: 0.3mL/min **Wavelength: 272 nm**



Chromatogram Information

User Name	Administrator
Date Modified	2015-10-29 16:24:52
Description	
HPLC System Name	HPLC
Injection Date	2015-10-29 15:12:14
Volume	10.00 [μ L]
Sample Number	1
Project Name	chiral drugs-sep
Acquisition Time	68.0 [min] + 10.0 [min]
Acquisition Sequence	JXZ-22-20-OJ-IPA1 (0.5-70-272)
Control Method	JXZ-OJ-IPA10 (0.5-70-272)
Peak ID Table	
Calibration Method	
Additional Information	

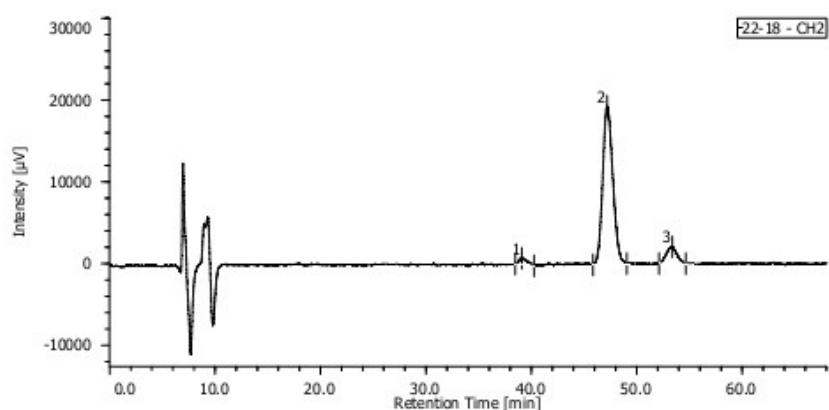
Channel & Peak Information Table

Chromatogram Name	22-20-CH2
Sample Name	CH2
Channel Name	CH2
Sampling Interval	500 [msec]
Peak Method	pcz-05-peak
Formula	

Decision										
#	Peak Name	CH	RT [min]	Area [μ V \cdot sec]	Height [μ V]	Area%	Height%	Resolution	Symmetry Factor	Capacity Factor
1	Unknown	2	38.767	51475	1064	1.019	1.340	3.855	1.195	N/A
2	Unknown	2	44.193	52500	933	1.040	1.180	1.590	N/A	N/A
3	Unknown	2	46.202	2480262	40840	49.056	51.663	3.948	1.296	N/A
4	Unknown	2	52.967	2471668	36215	48.885	45.811	N/A	1.277	N/A

HPLC spectra of rac-6

Chromatogram



Chromatogram Information

User Name Administrator
 Date Modified 2015-10-29 19:53:33
 Description
 HPLC System Name HPLC
 Injection Date 2015-10-29 18:45:31
 Volume 20.00 [µL]
 Sample Number 3
 Project Name chiral drugs-sep
 Acquisition Time 68.0 [min]
 Acquisition Sequence JX Z-22-18-OJ-IPA10(0.5-70-272)
 Control Method JX Z-OJ-IPA10(0.5-70-272)
 Peak ID Table
 Calibration Method
 Additional Information

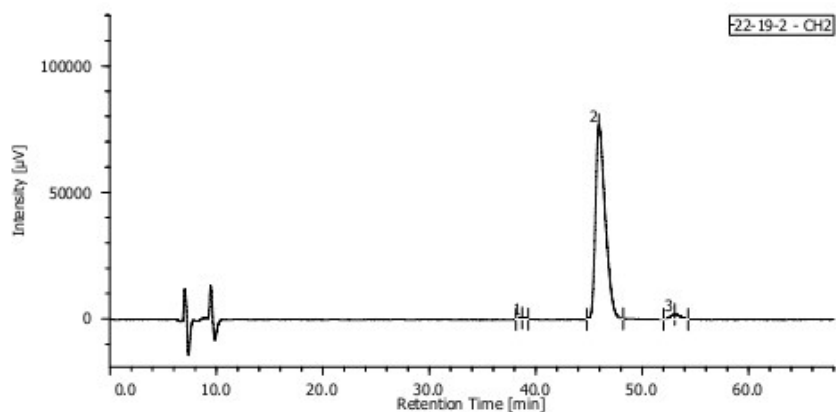
Channel & Peak Information Table

Chromatogram Name 22-18-CH2
 Sample Name
 Channel Name CH2
 Sampling Interval 500 [msac]
 Peak Method jxz-oj-peak
 Formula
 Decision

#	Peak Name	CH	TR [min]	Area [µV.sec]	Height [µV]	Area%	Height%	Resolution	Symmetry Factor	Capacity Factor
1	Unknown	2	39.083	45208	793	3.022	3.566	4.902	1.447	N/A
2	Unknown	2	47.192	1301437	89363	87.009	87.079	3.358	1.161	N/A
3	Unknown	2	53.350	149112	2080	9.969	9.355	N/A	1.029	N/A

HPLC spectra of 6

Chromatogram



Chromatogram Information

User Name Administrator
 Date Modified 2015-10-29 17:36:12
 Description
 HPLC System Name HPLC
 Injection Date 2015-10-29 16:28:09
 Volume 10.00 [μL]
 Sample Number 2
 Project Name chiral drugs-sep
 Acquisition Time 68.0 [min]
 Acquisition Sequence JXZ-22-19-2-OJ-IPA10(0.5-70-272)
 Control Method JXZ-OJ-IPA10(0.5-70-272)
 Peak ID Table
 Calibration Method
 Additional Information

Channel & Peak Information Table

Chromatogram Name 22-19-2-CH2
 Sample Name
 Channel Name CH2
 Sampling Interval 500 [msec]
 Peak Method jxz-oj-peak
 Formula
 Decision

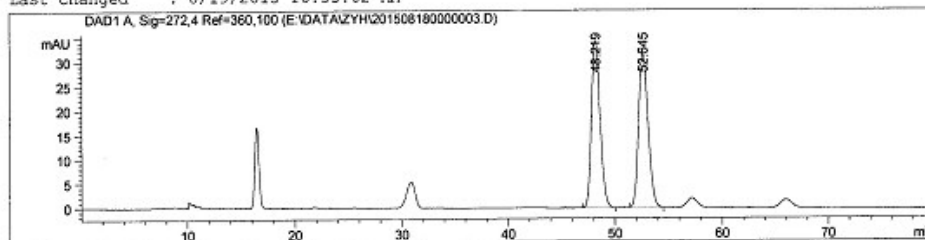
#	Peak Name	CH	IR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Resolution	Symmetry Factor	Capacity Factor
1	Unknown	2	38.708	18950	508	0.376	0.641	5.325	1.002	N/A
2	Unknown	2	45.913	4895067	76838	97.074	96.849	4.172	1.543	N/A
3	Unknown	2	53.058	128607	1992	2.550	2.510	N/A	1.084	N/A

HPLC spectra of 6 (After recrystallization)

Data File E:\DATA\ZYH\201508180000003.D
Sample Name: 21-6

=====

Acq. Operator : □ □	Seq. Line : 1
Acq. Instrument : Agilent 1260	Location : Vial 1
Injection Date : 8/18/2015 12:07:38 AM	Inj : 3
	Inj Volume : 10 µl
Acq. Method : C:\Chem32\1\DATA\ZYH\20150727 2015-08-18 12-24-45\20150818.M	
Last changed : 8/17/2015 9:24:45 PM by □ □	
Analysis Method : C:\CHEM32\2\METHODS\150818.M	
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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=272,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	48.219	BB	0.8650	1948.59386	34.39162	50.0452
2	52.645	BB	0.9428	1945.06433	31.56852	49.9548

Totals : 3893.64819 65.96015

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*** End of Report ***

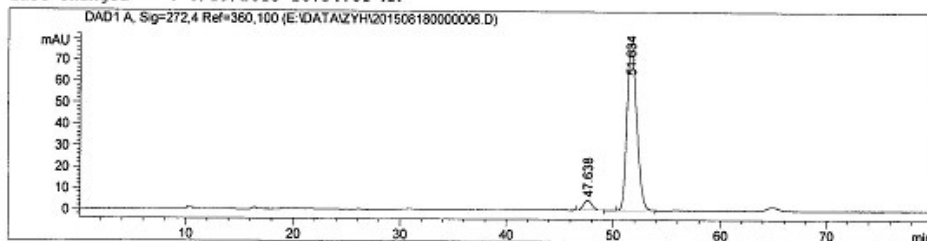
HPLC spectra of rac-16

Data File E:\DATA\ZYH\201508180000006.D
Sample Name: 22-9-BL

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Acq. Operator	: □ □	Seq. Line	: 3
Acq. Instrument	: Agilent 1260	Location	: Vial 3
Injection Date	: 8/18/2015 4:10:35 AM	Inj	: 1
		Inj Volume	: 10 µl
Acq. Method	: C:\Chem32\1\DATA\ZYH\20150727 2015-08-18 12-24-45\20150818.M		
Last changed	: 8/17/2015 9:24:45 PM by □ □		
Analysis Method	: C:\CHEM32\2\METHODS\150818.M		
Last changed	: 8/19/2015 10:34:01 AM		

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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=272,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	47.638	BB	0.6618	244.94620	4.49463	4.7715
2	51.634	BB	0.9497	4888.58838	78.16419	95.2285

Totals : 5133.53458 82.65883

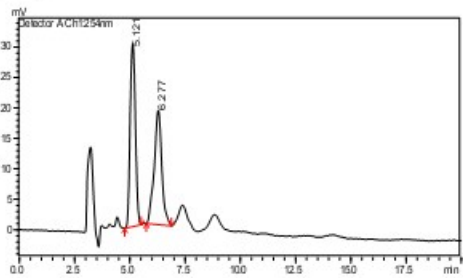
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*** End of Report ***

HPLC analysis for compound **1**, **24** and natural xiamenmycin A: CHIRALPAK OZ-H; Column size: 0.46 cm I.D. x 25 cm L x 5 μ m; column temperature: 35°C; injection volume: 5 μ L; mobile phase: n-Hexane/EtOH/TFA=80/20/0.1 (V/V/V); flow rate: 1.0 mL/min Wavelength: 254 nm

A) Mixture of synthetic samples

Column	: CHIRALCEL® OZ-H
Column size	: 0.46 cm I.D. x 25 cm L x 5 μ m
Injection	: 25 μ l
Mobile phase	: 烷烃和醇类
Flow rate	:
Wave length	:
Temperature	:
Sample solution	: 取 19-9 和 40-3 各 100UL 用 EtOH Hexane 稀释到 1ML
HPLC equipment	: Shimadzu LC 20 with UV detector SPD-20A
Sample structure	A150106X 19-9+40-3

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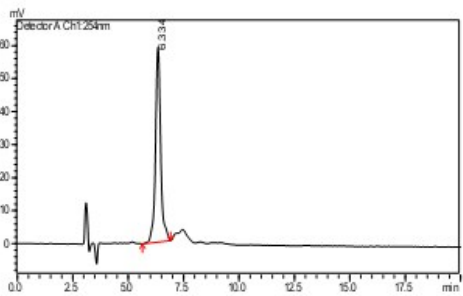
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Peak No.	Time	Area	Area %	Plate number	Tailing	Resolution
1	5.121	501812	52.6832	2002.330	1.123	--
2	6.277	450697	47.3168	1692.447	1.034	2.164

B) Compound 1 (synthetic sample)

Column	: CHIRALCEL® OZ-H
Column size	: 0.46 cm I.D. x 25 cm L x 5 μ m
Injection	: 5 μ l
Mobile phase	:
Flow rate	:
Wave length	:
Temperature	:
Sample solution	: 透样已配
HPLC equipment	: Shimadzu LC 20 with UV detector SPD-20A
Sample structure	A150106X 19-9

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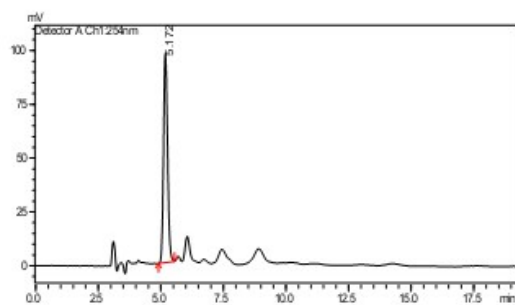
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Peak No.	Time	Area	Area %	Plate number	Tailing	Resolution
1	6.334	971074	100.0000	3647.273	1.156	--

C) Compound 24 (synthetic sample)

Column	: CHIRALCEL®	OZ-H
Column size	: 0.46 cm I.D. ×25 cm L×5 µm	
Injection	: 5 µl	
Mobile phase	:	
Flow rate	:	
Wave length	:	
Temperature	:	
Sample solution	: 送样已配	
HPLC equipment	: Shimadzu LC 20 with UV detector SPD-20A	
Sample structure	A150106X	40-3

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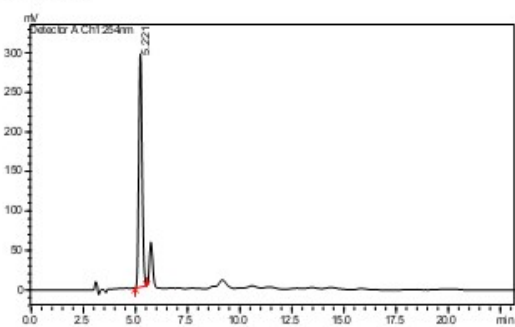
<Column Performance Report>

Peak No.	Time	Area	Area %	Plate number	Tailing	Resolution
1	5.172	1092709	100.0000	4120.876	1.227	--

D) Xiamenmycin sample (natural product)

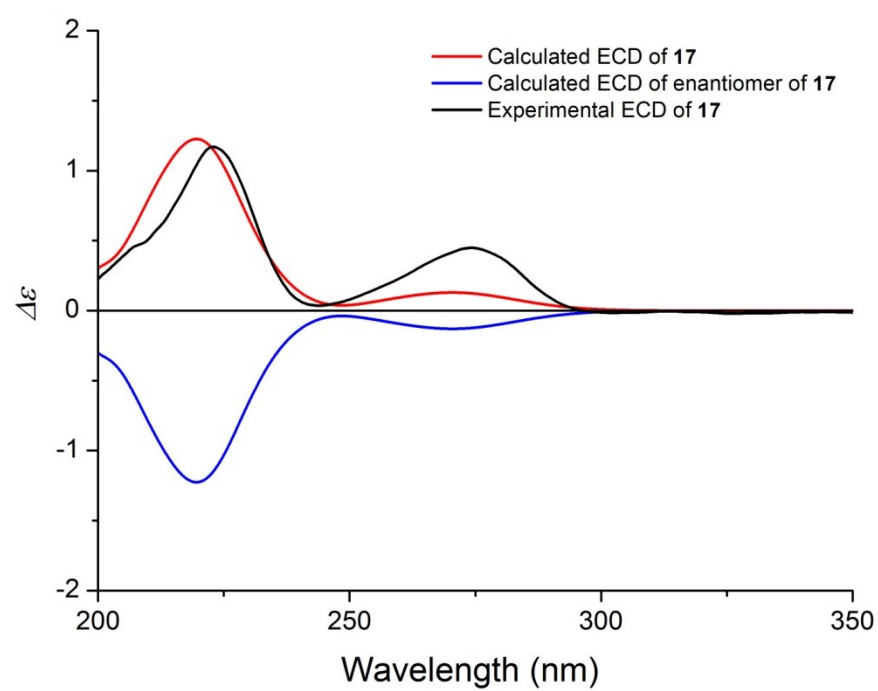
Column	: CHIRALCEL®	OZ-H
Column size	: 0.46 cm I.D. ×25 cm L×5 µm	
Injection	: 5 µl	
Mobile phase	:	
Flow rate	:	
Wave length	:	
Temperature	:	
Sample solution	: 送样已配	
HPLC equipment	: Shimadzu LC 20 with UV detector SPD-20A	
Sample structure	A150106X	Xia.A

< Chromatogram >



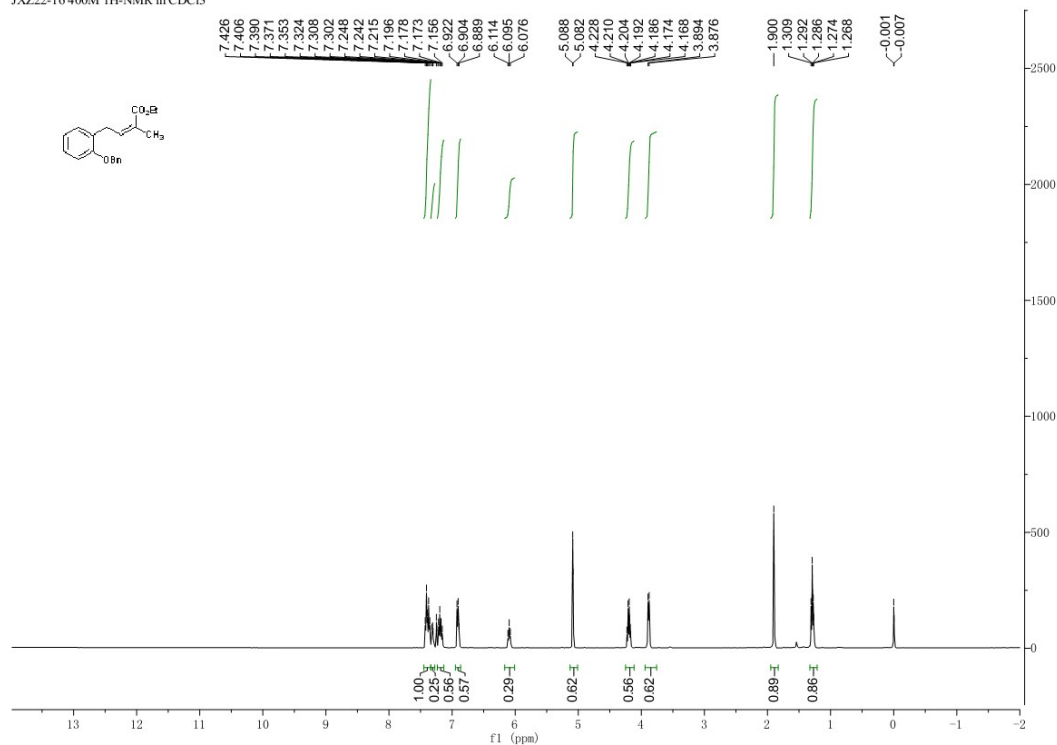
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Peak No.	Time	Area	Area %	Plate number	Tailing	Resolution
1	5.221	3311420	100.0000	4150.407	1.208	--



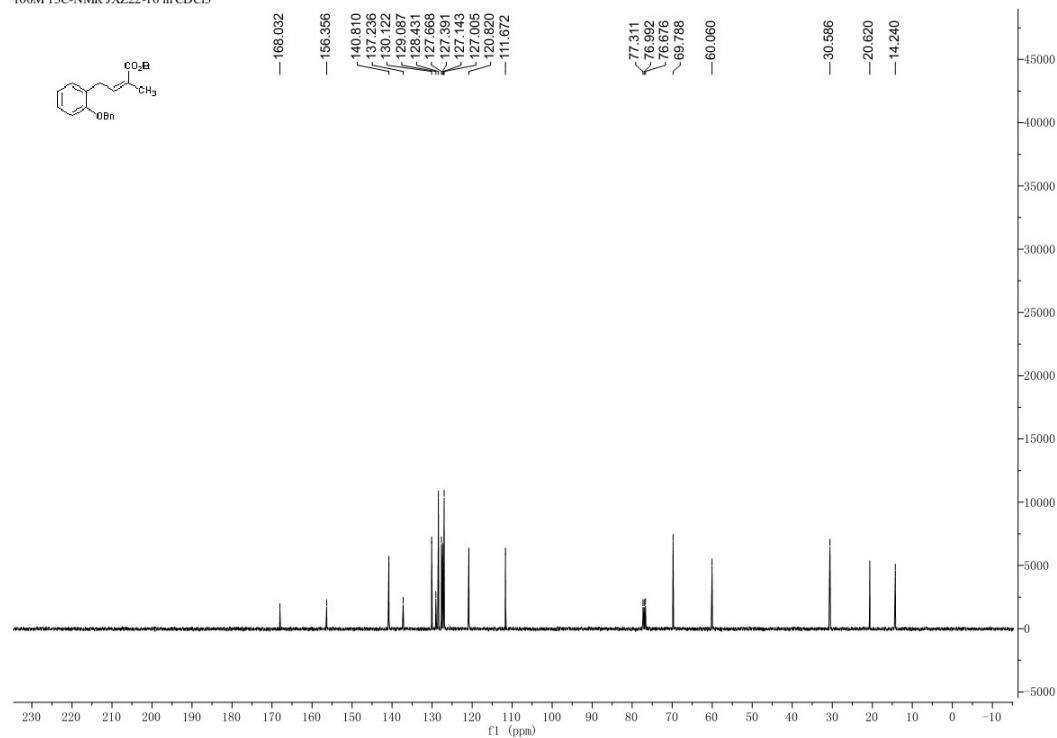
The theoretical CD spectrum and experimental CD spectrum of **17**

JXZ22-16 400M ¹H-NMR in CDCl₃



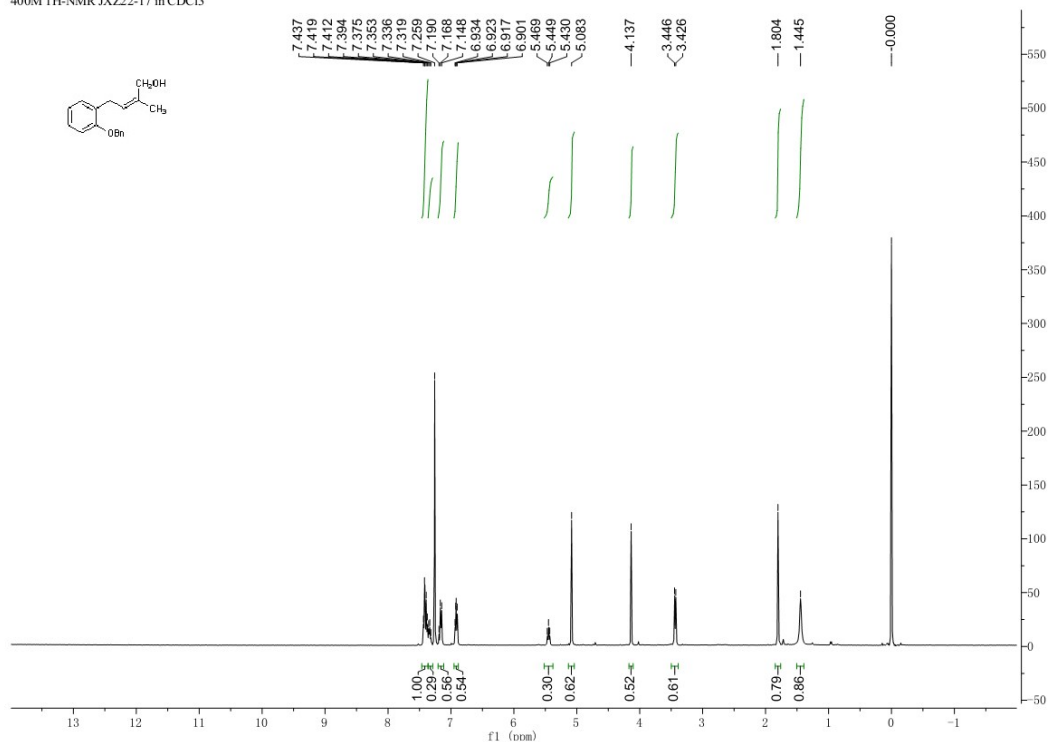
¹H NMR spectra of compound 4

100M ¹³C-NMR JXZ22-16 in CDCl₃



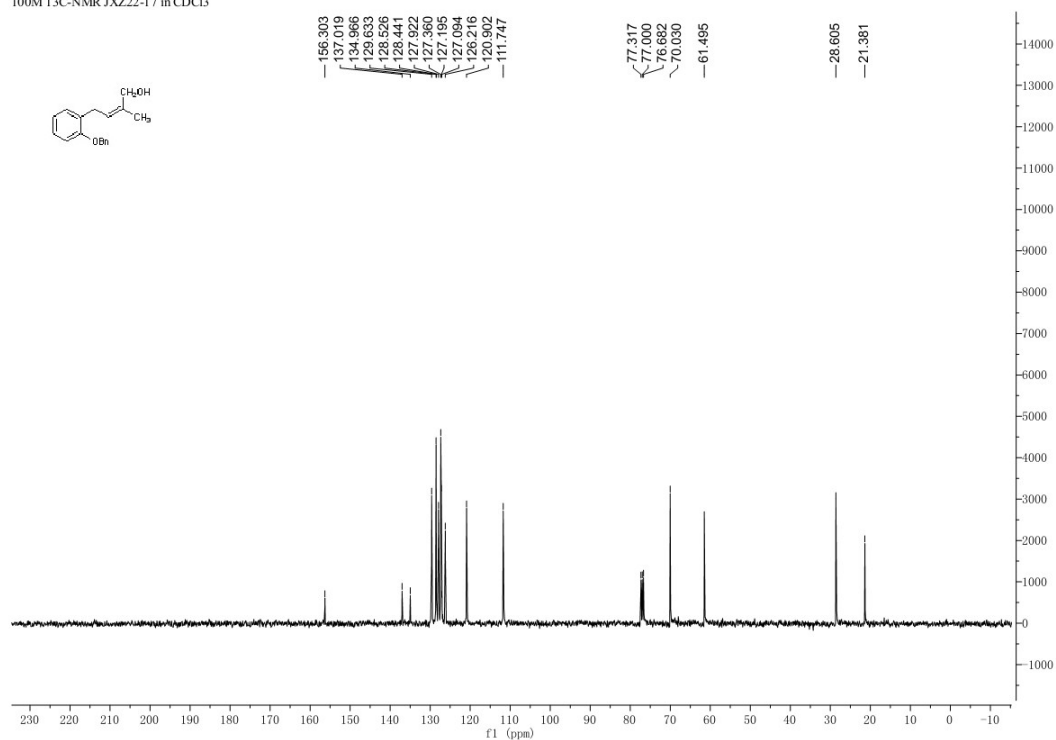
¹³C NMR spectra of compound 4

400M ¹H-NMR JXZ22-17 in CDCl₃



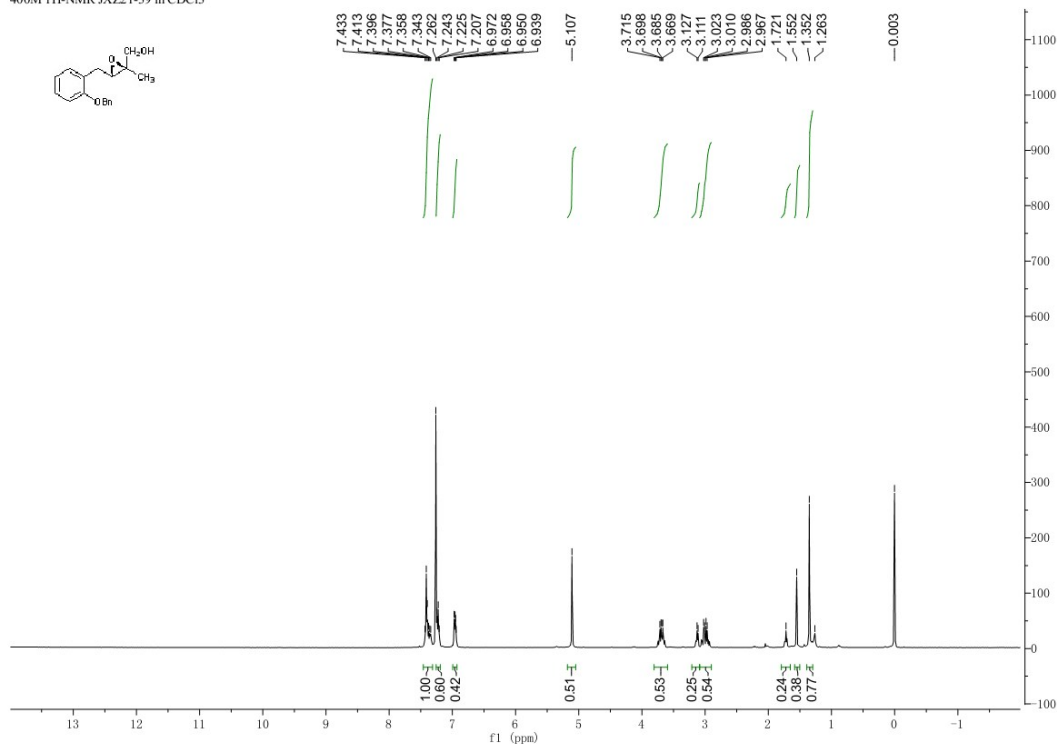
¹H NMR spectra of compound **5**

100M ¹³C-NMR JXZ22-17 in CDCl₃



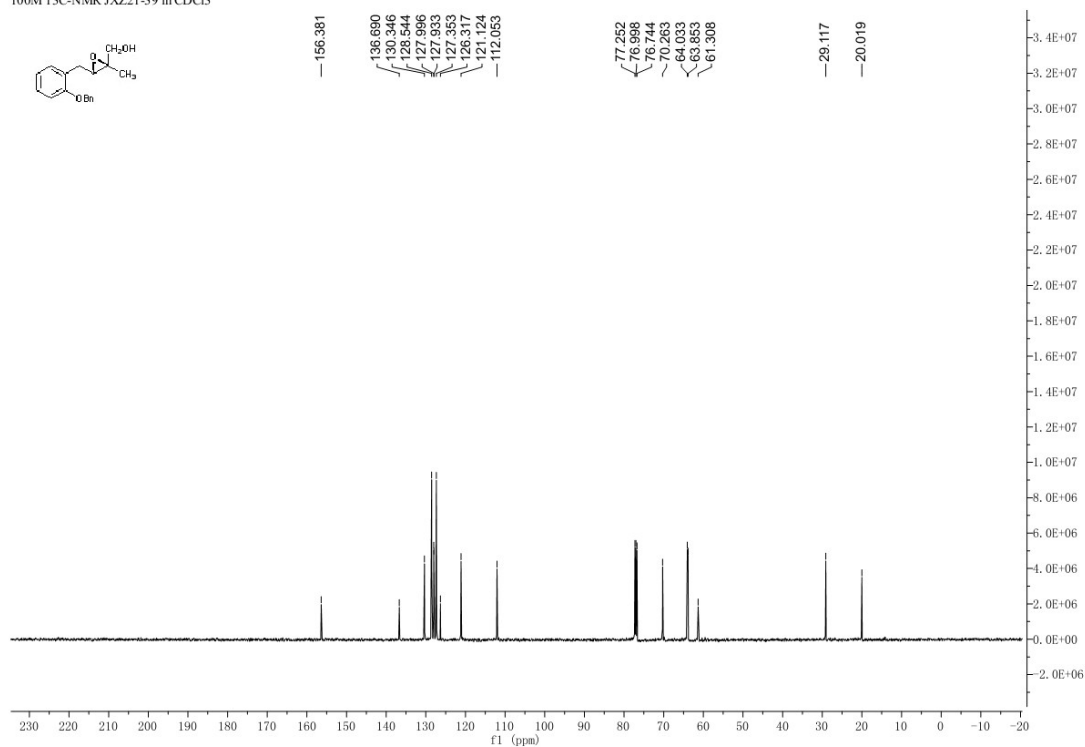
¹³C NMR spectra of compound **5**

400M ¹H-NMR JXZ21-39 in CDCl₃



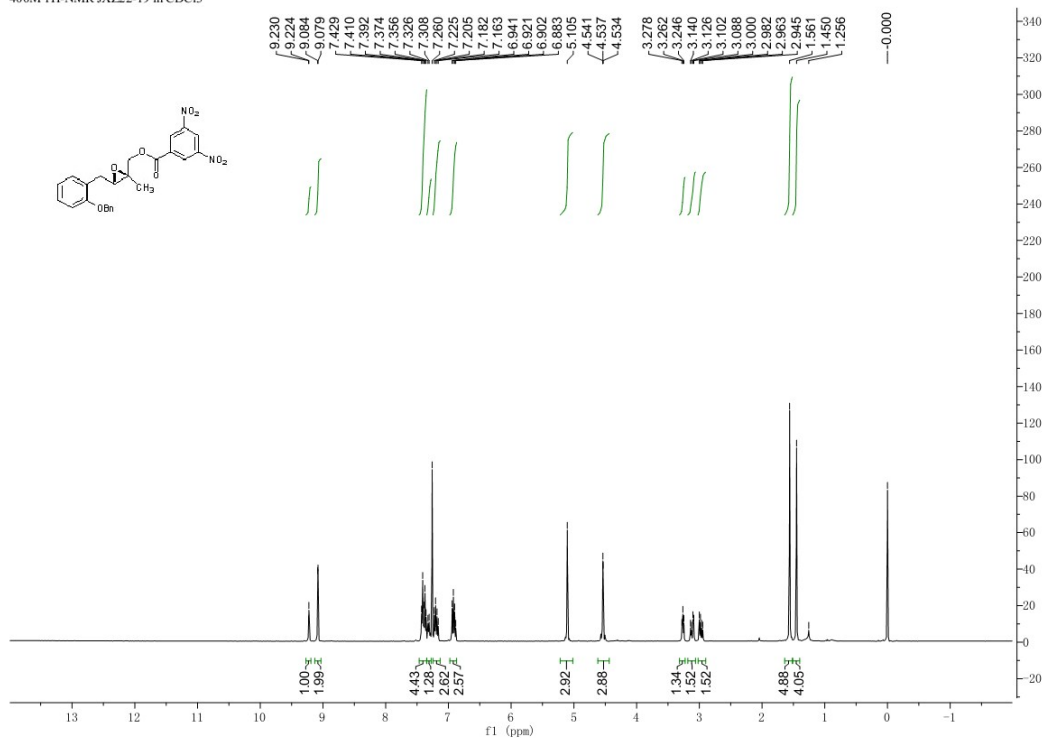
¹H NMR spectra of compound 6

100M ¹³C-NMR JXZ21-39 in CDCl₃



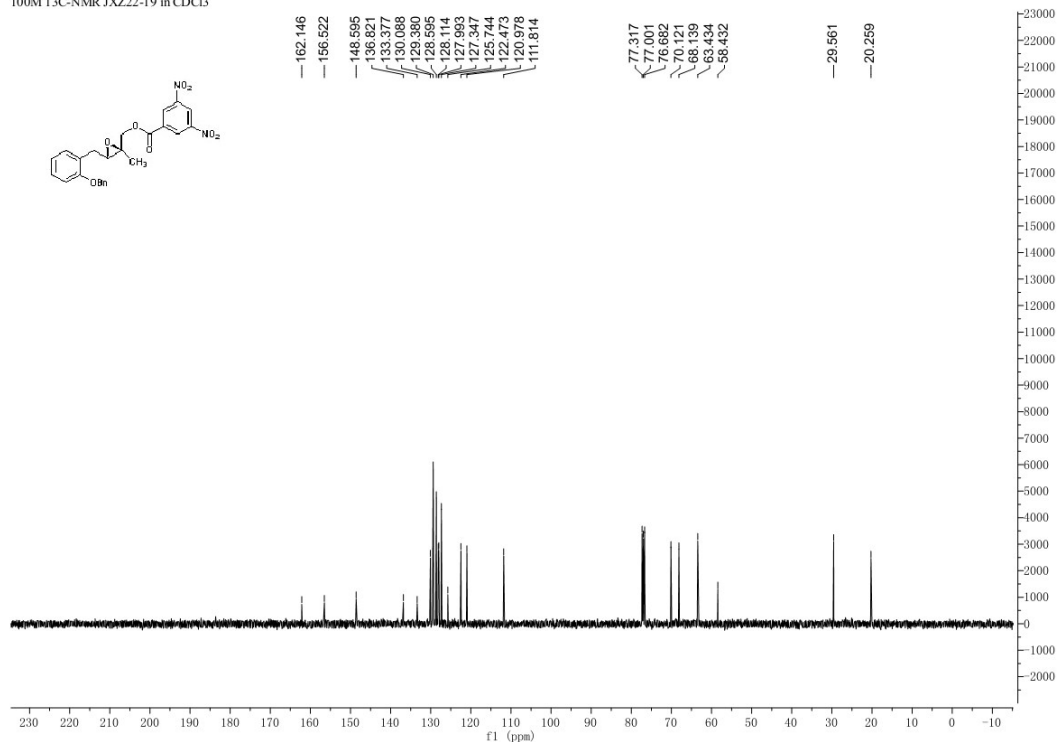
¹³C NMR spectra of compound 6

400M ¹H-NMR JXZ22-19 in CDCl₃

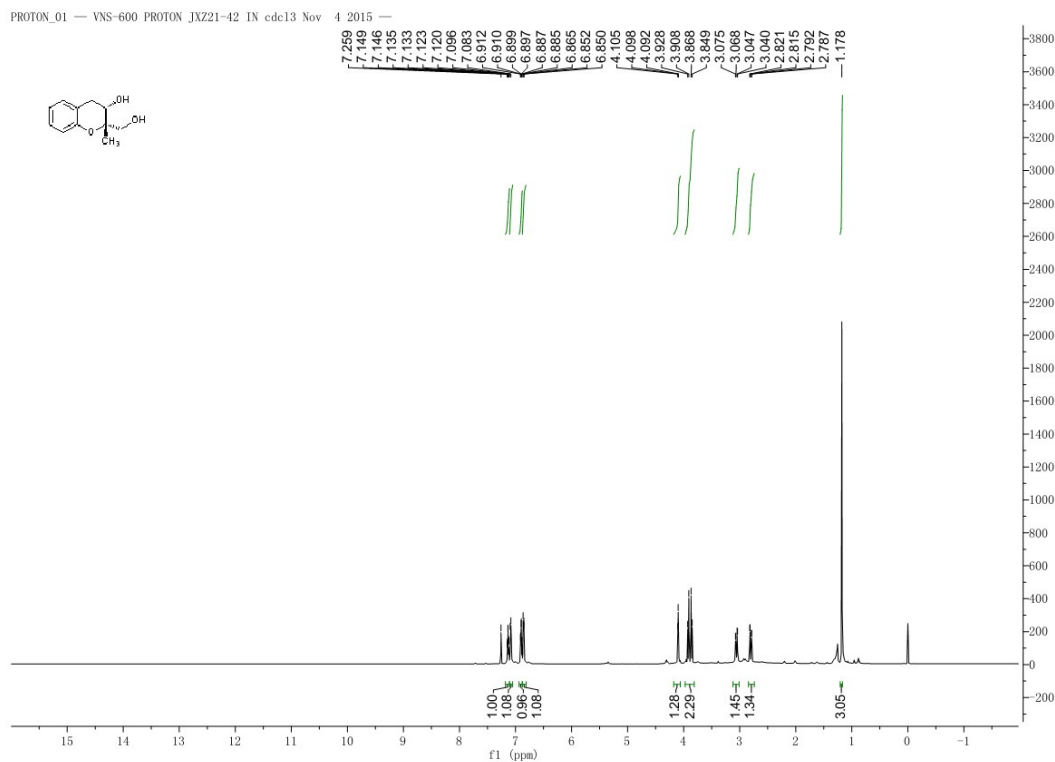


¹H NMR spectra of compound **6b**

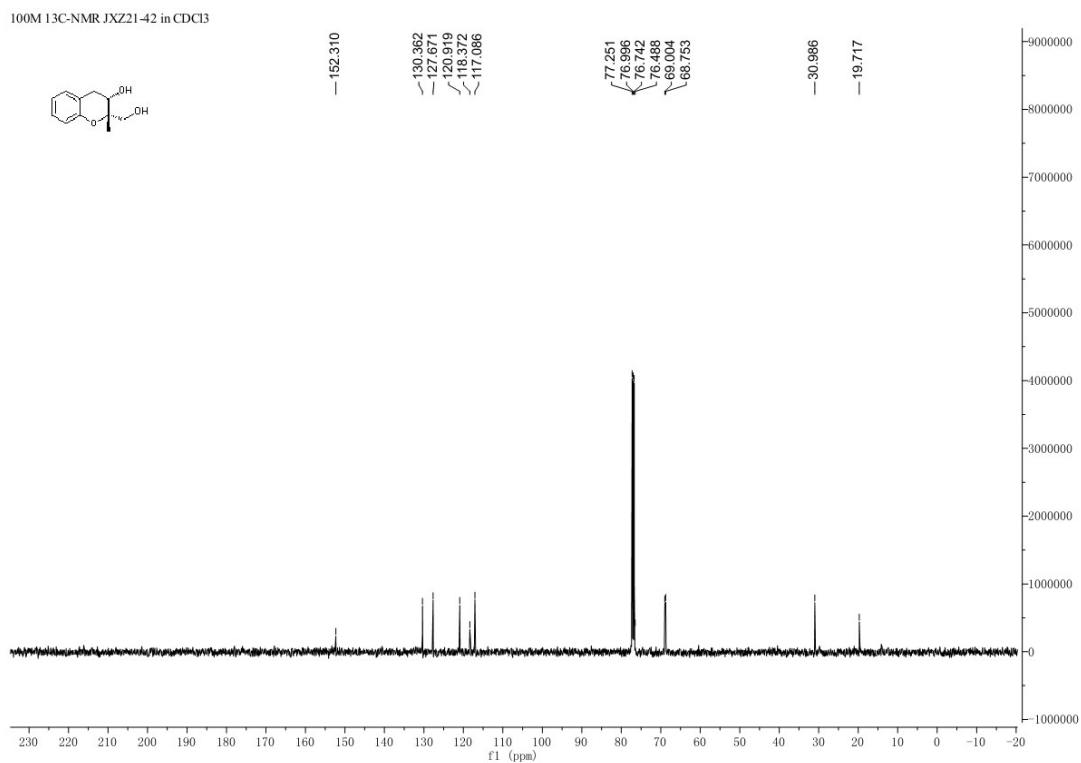
100M ¹³C-NMR JXZ22-19 in CDCl₃



¹³C NMR spectra of compound **6b**

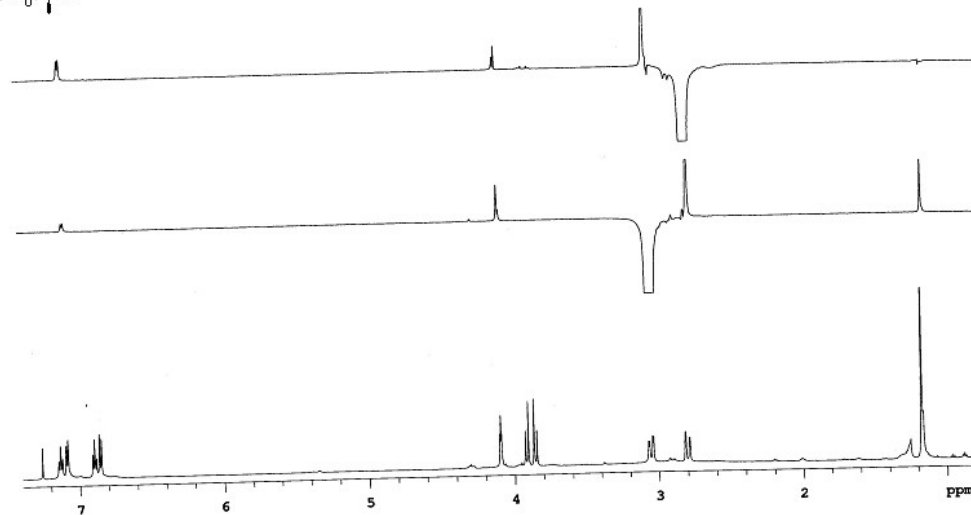
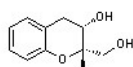


¹H NMR spectra of compound 7



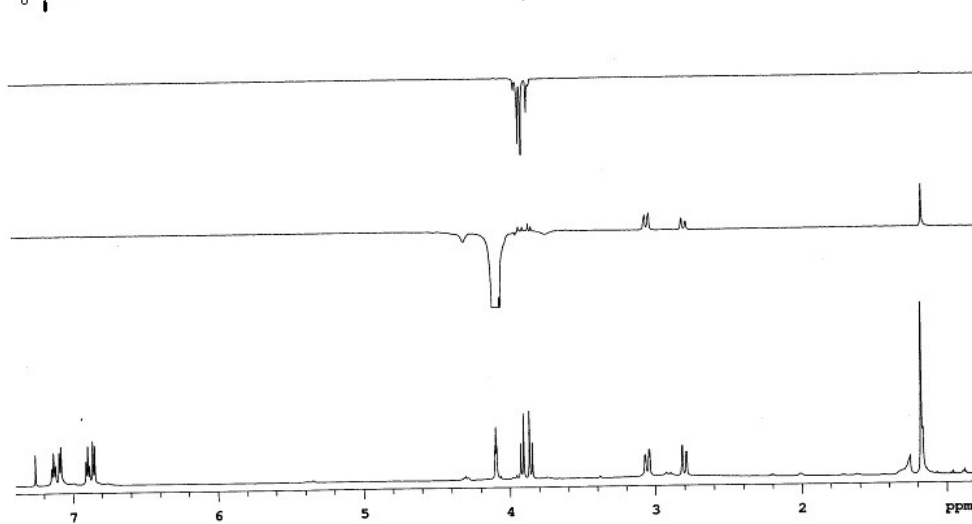
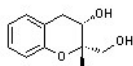
¹³C NMR spectra of compound 7

VNS-600 NOESY1D JXZ21-42 IN cdcl3 Nov 4 2015



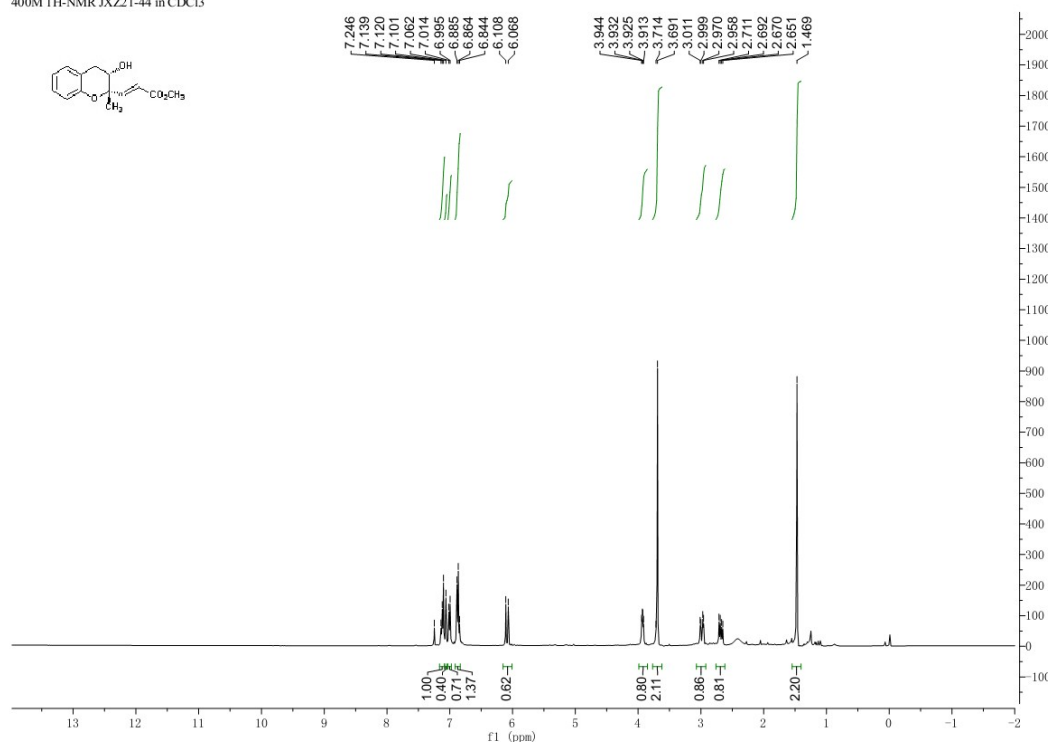
NOE spectra of compound 7

VNS-600 NOESY1D JXZ21-42 IN cdcl3 Nov 4 2015



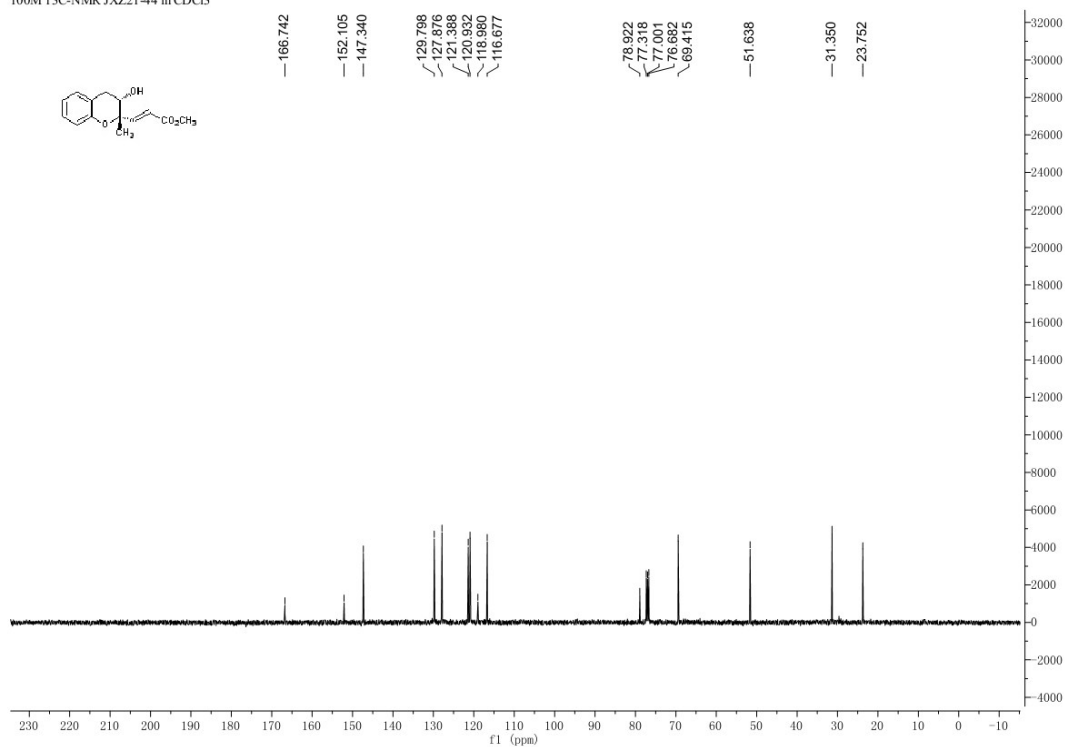
NOE spectra of compound 7

400M ¹H-NMR JXZ21-44 in CDCl₃

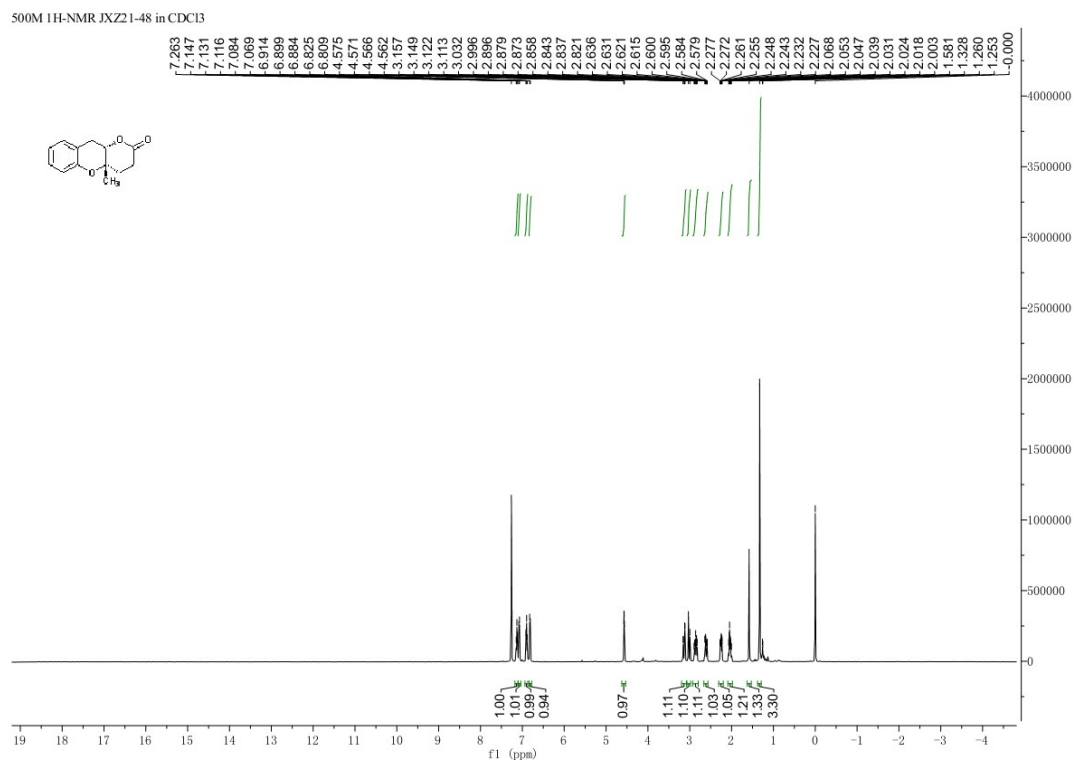


¹H NMR spectra of compound 8

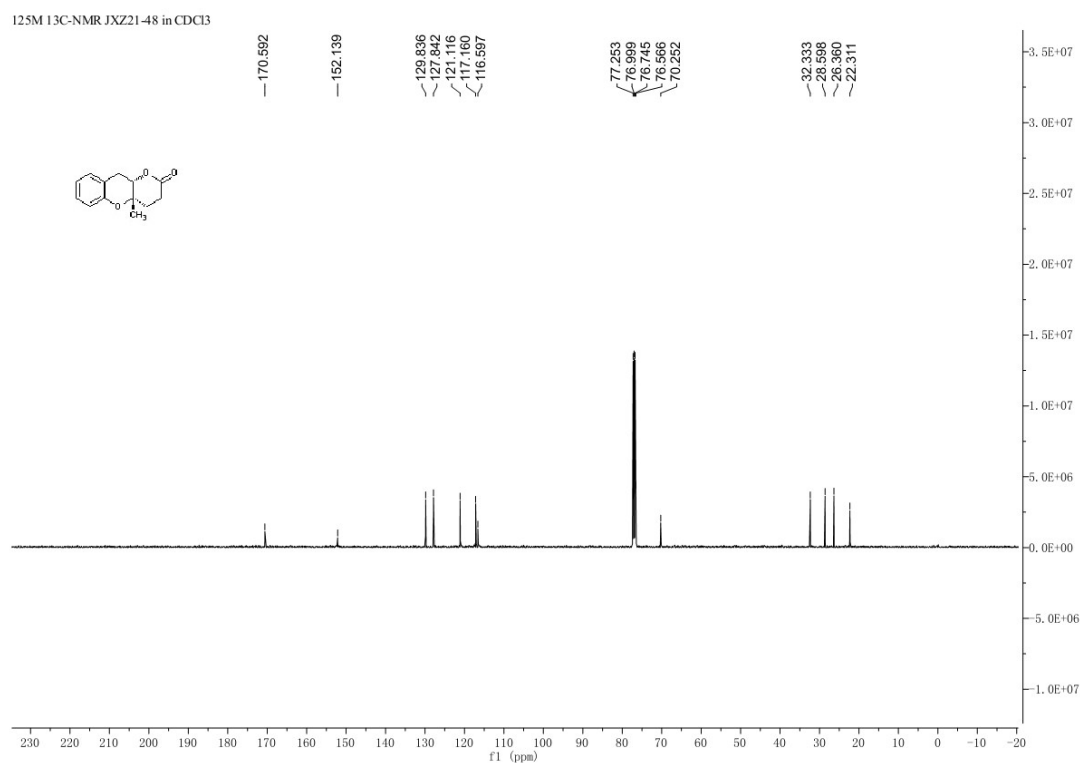
100M ¹³C-NMR JXZ21-44 in CDCl₃



¹³C NMR spectra of compound 8

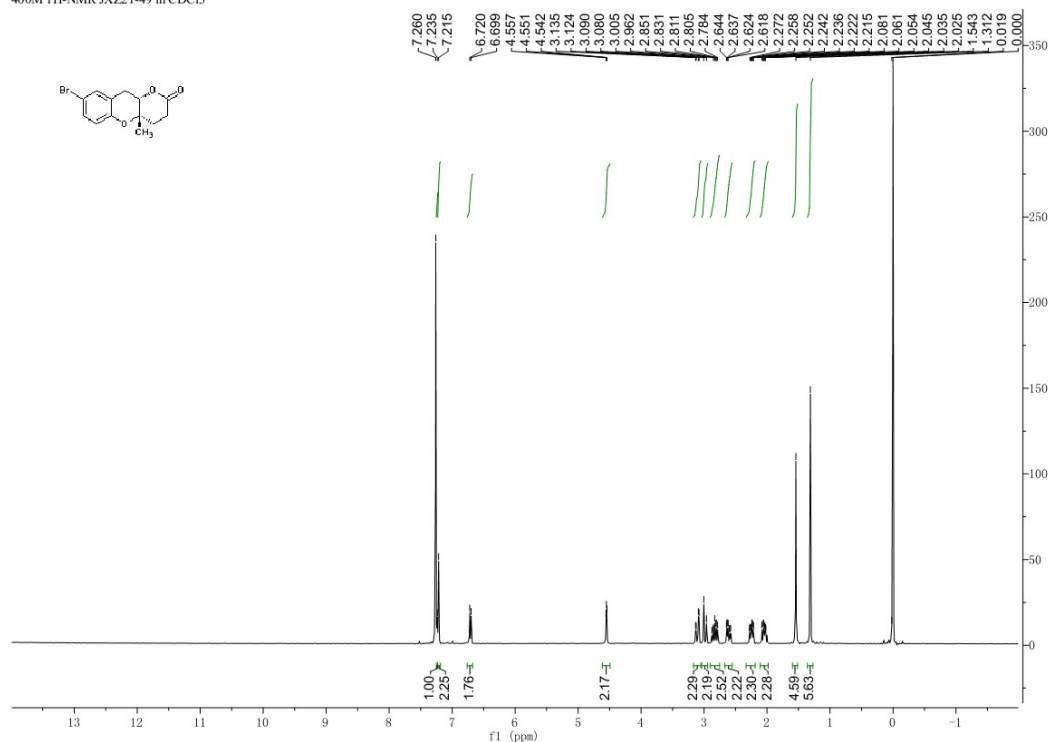


^1H NMR spectra of compound 9



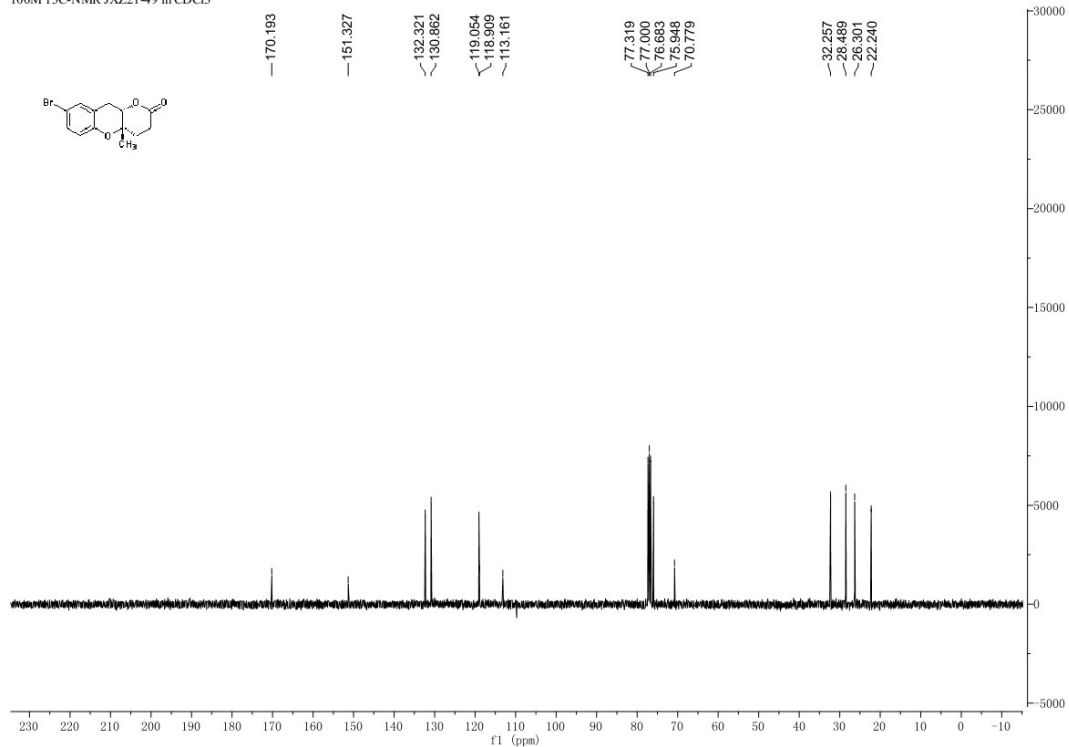
^{13}C NMR spectra of compound 9

400M ¹H-NMR JXZ21-49 in CDCl₃



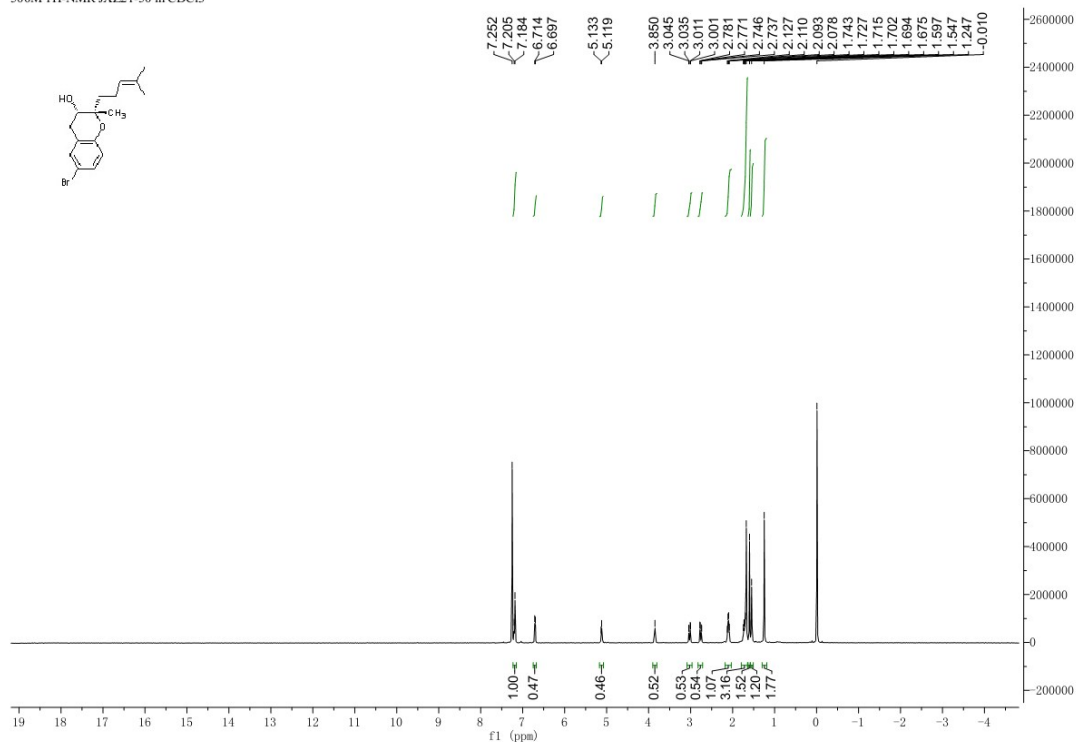
¹H NMR spectra of compound 10

100M ¹³C-NMR JXZ21-49 in CDCl₃



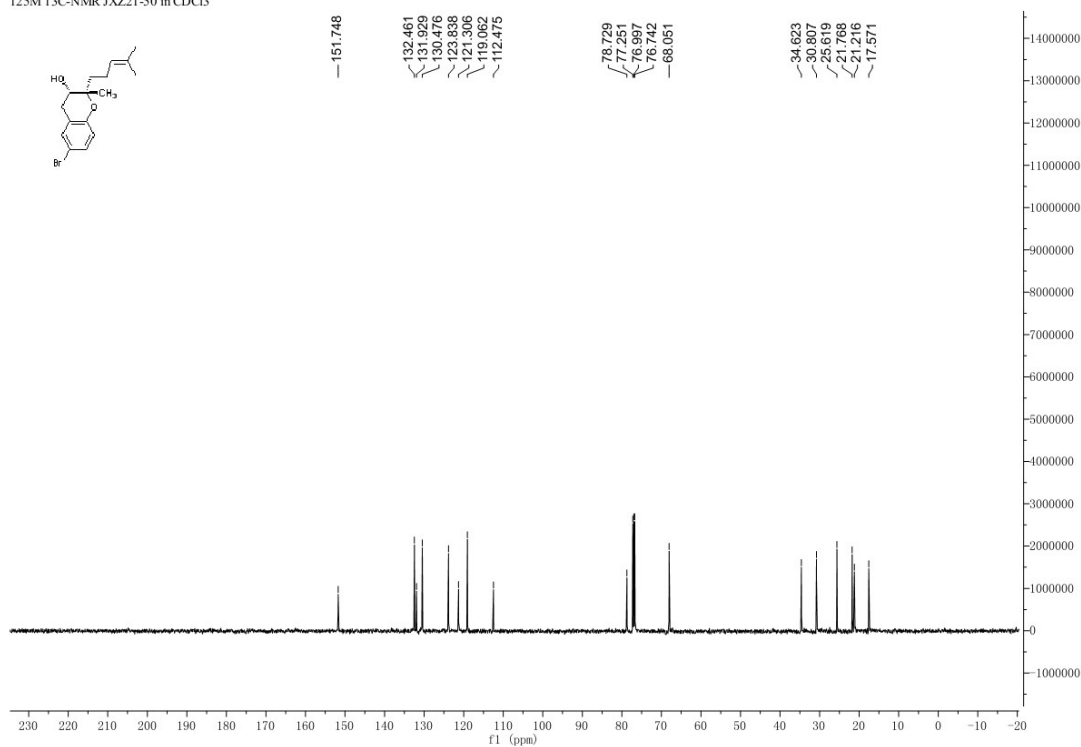
¹³C NMR spectra of compound 10

500M ^1H -NMR JXZ21-50 in CDCl_3



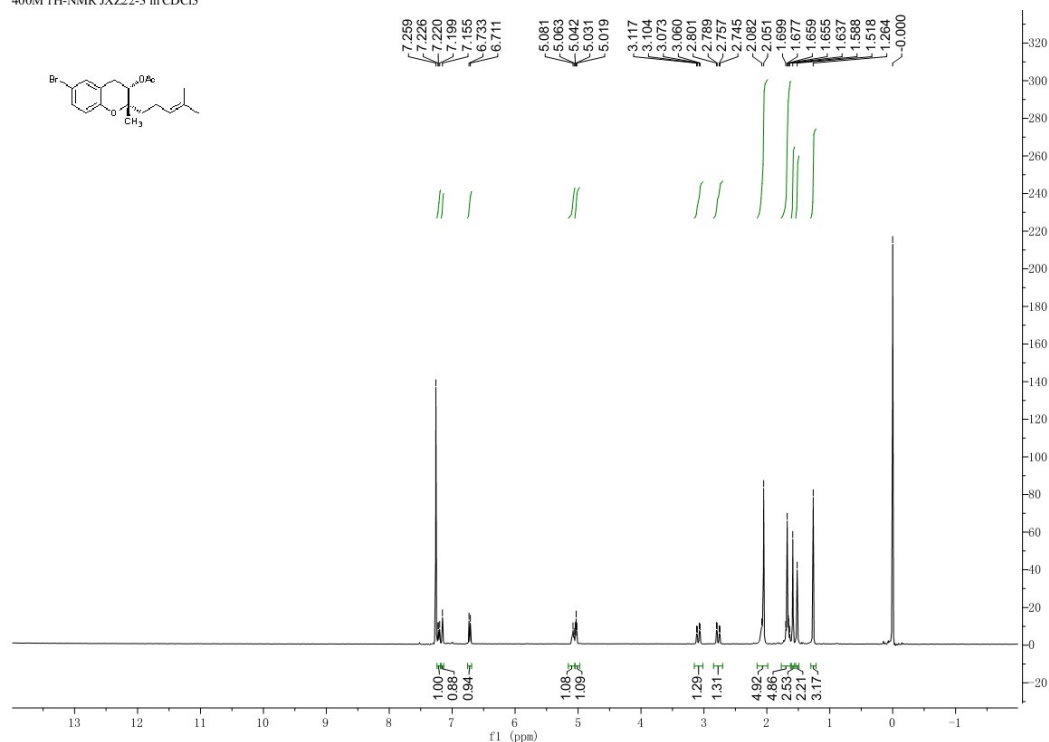
^1H NMR spectra of compound 11

125M ^{13}C -NMR JXZ21-50 in CDCl_3



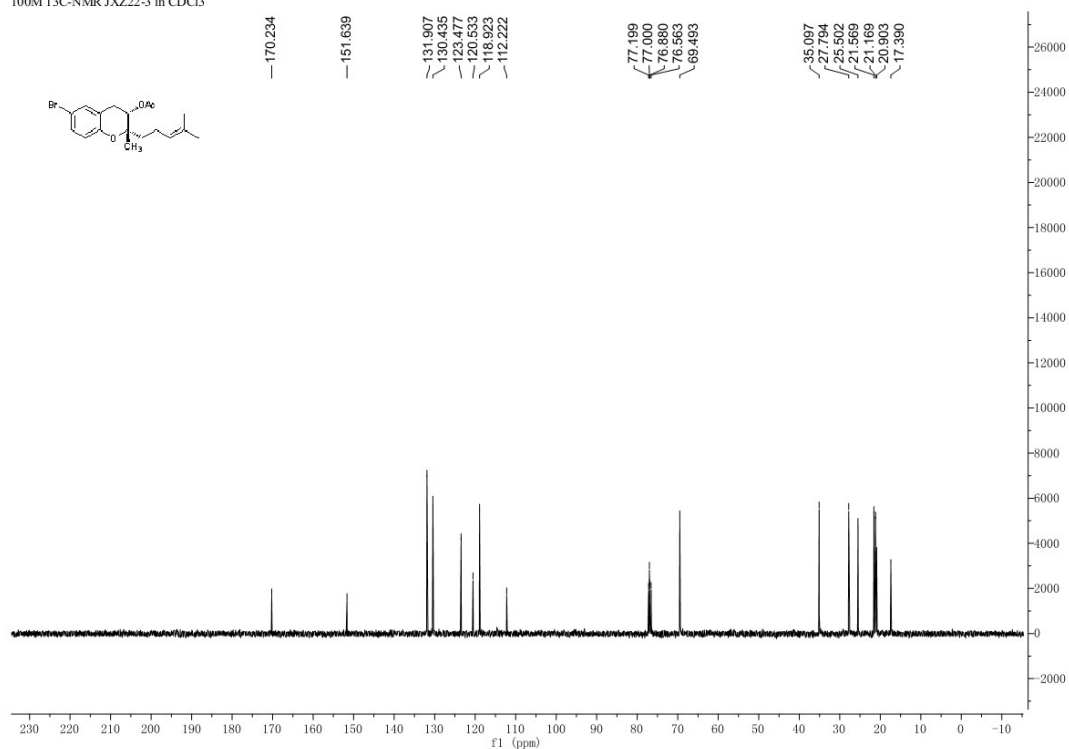
^{13}C NMR spectra of compound 11

400M ¹H-NMR JXZ22-3 in CDCl₃



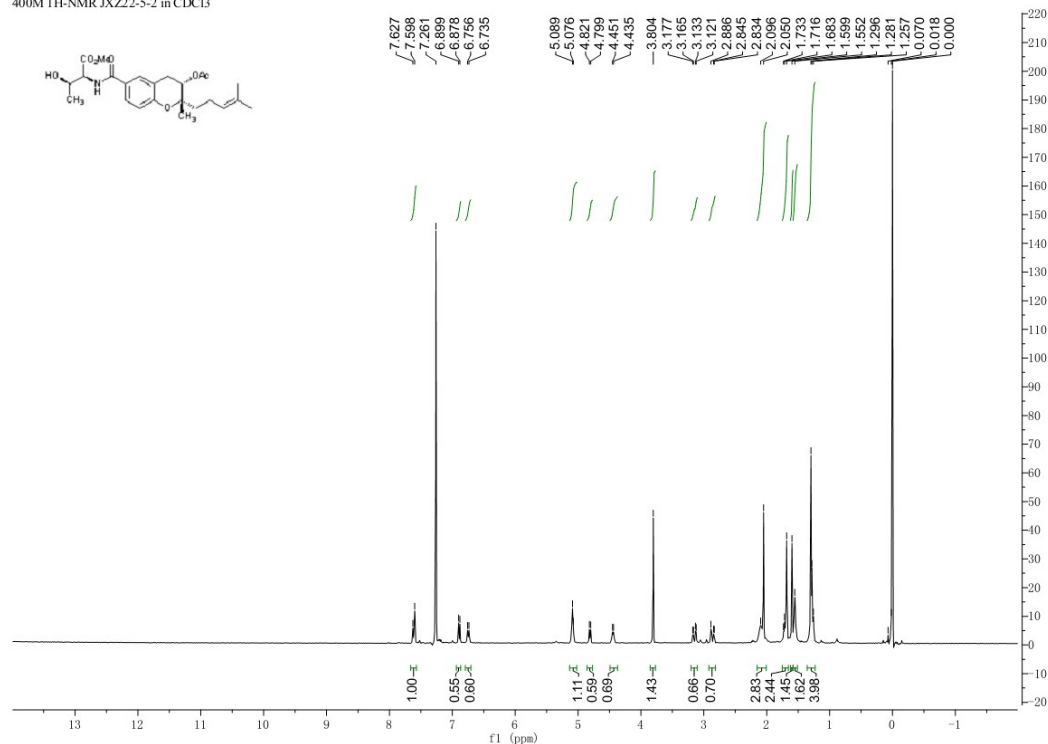
¹H NMR spectra of compound 12

100M ¹³C-NMR JXZ22-3 in CDCl₃



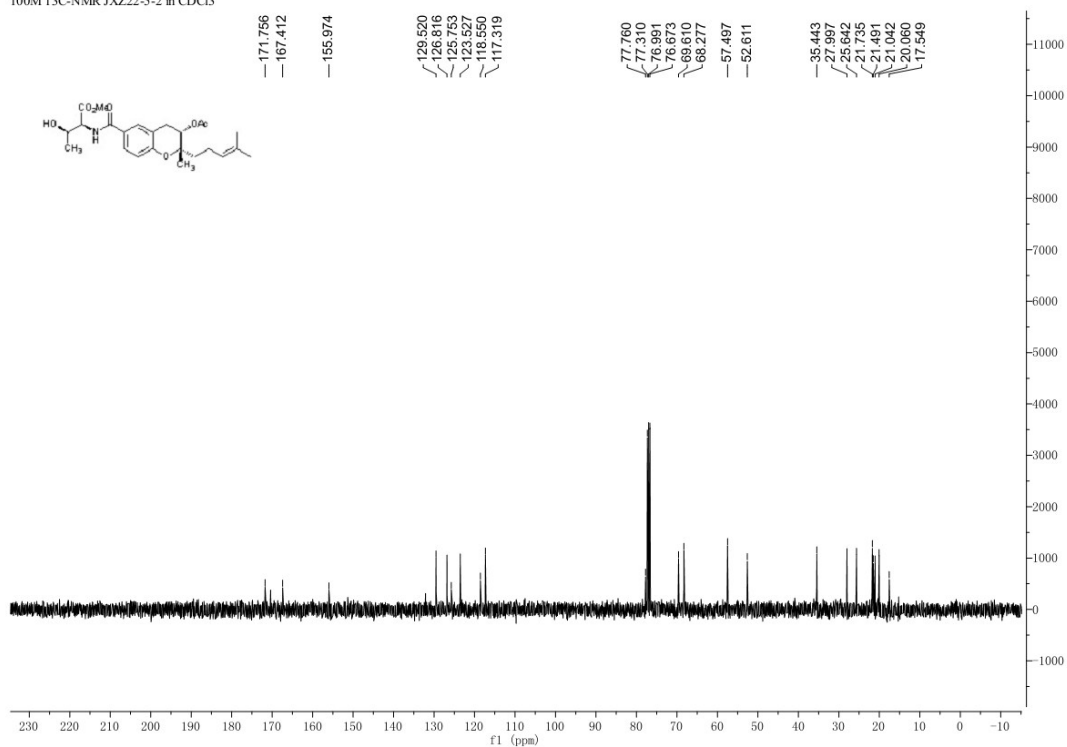
¹³C NMR spectra of compound 12

400M ¹H-NMR JXZ22-5-2 in CDCl₃

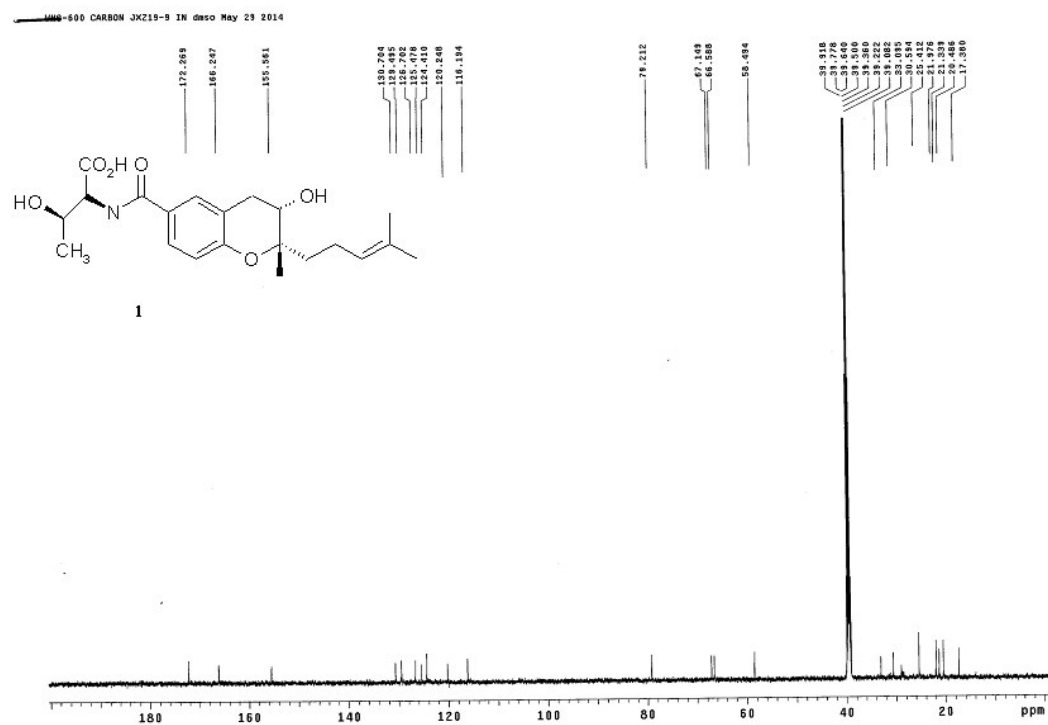
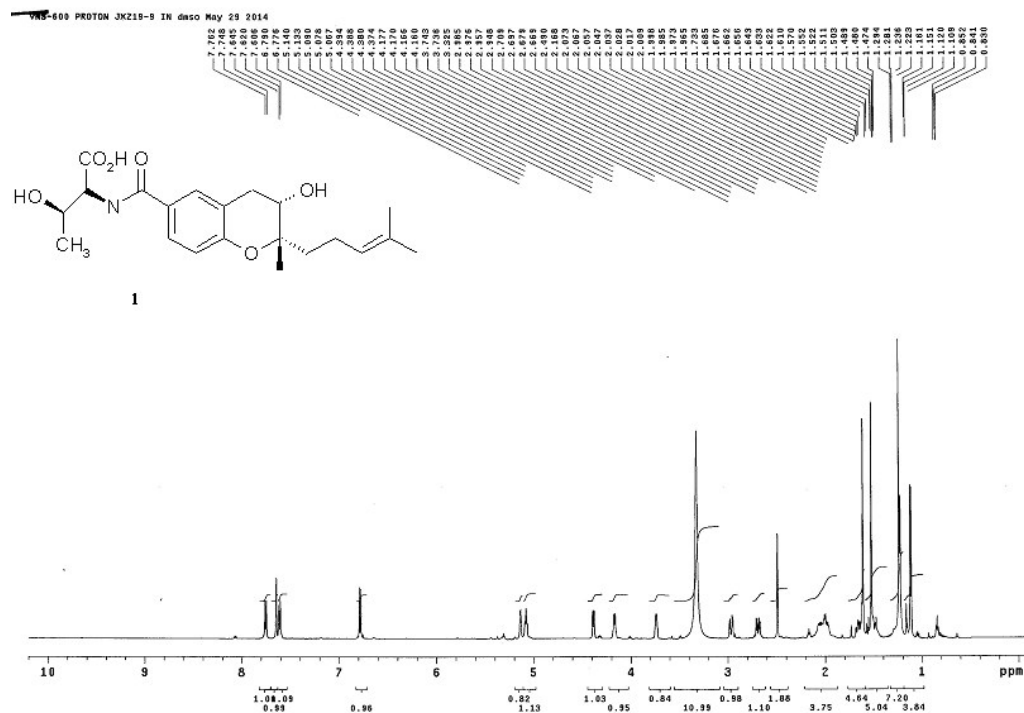


¹H NMR spectra of compound 13

100M ¹³C-NMR JXZ22-5-2 in CDCl₃



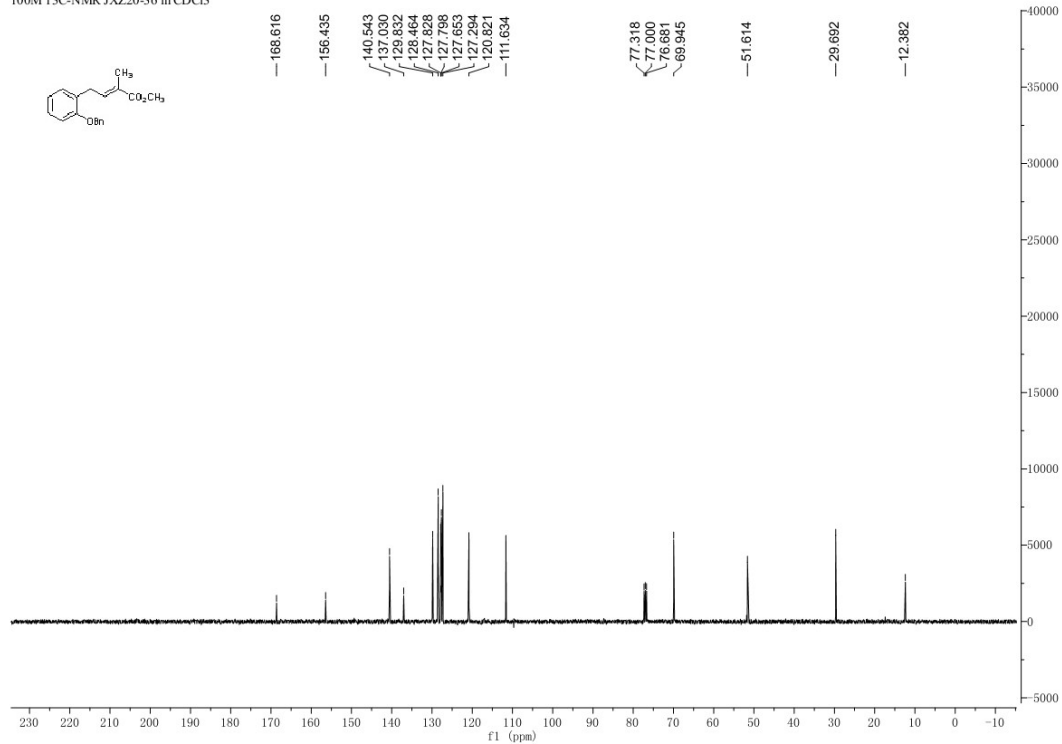
¹³C NMR spectra of compound 13



Chemical structure: CC(=C(C1=CC=C(C=C1)OC2=CC=CC=C2)C(=O)OCC

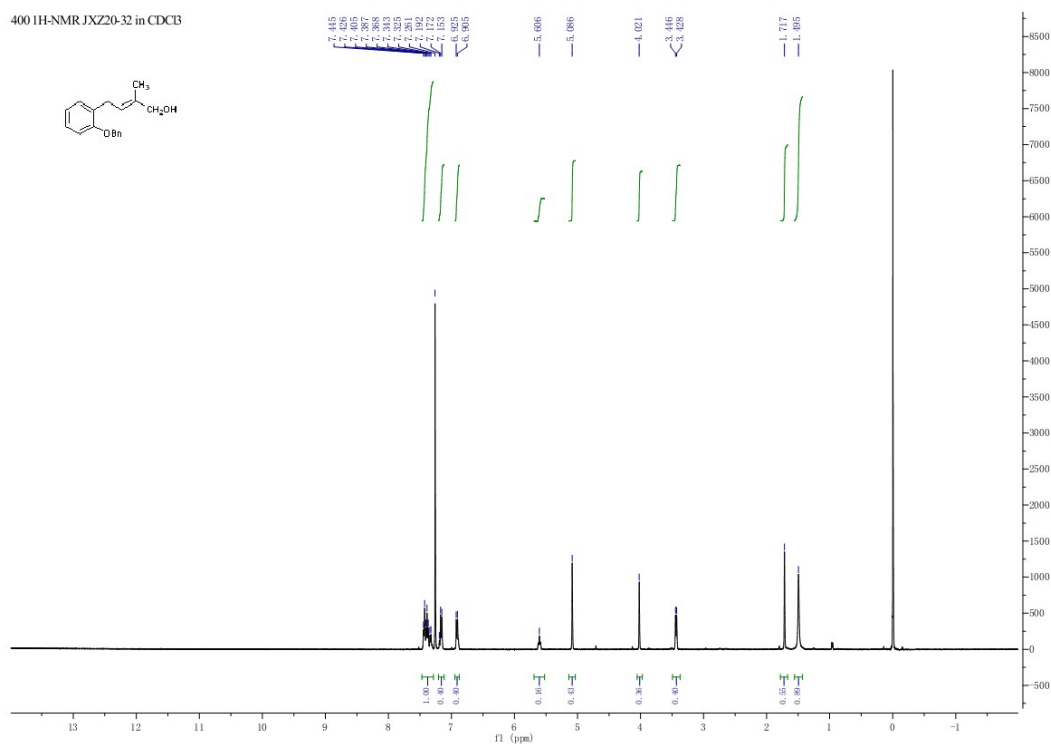
¹H NMR spectrum (CDCl₃) showing peaks and integration values:

Chemical Shift (ppm)	Integration
7.427, 7.408, 7.377, 7.375, 7.373, 7.371, 7.369, 7.367, 7.365, 7.363, 7.361, 7.359, 7.357, 7.355, 7.353, 7.351, 7.349, 7.347, 7.345, 7.343, 7.341, 7.339, 7.337, 7.335, 7.333, 7.331, 7.329, 7.327, 7.325, 7.323, 7.321, 7.319, 7.317, 7.315, 7.313, 7.311, 7.309, 7.307, 7.305, 7.303, 7.301, 7.299, 7.297, 7.295, 7.293, 7.291, 7.289, 7.287, 7.285, 7.283, 7.281, 7.279, 7.277, 7.275, 7.273, 7.271, 7.269, 7.267, 7.265, 7.263, 7.261, 7.259, 7.257, 7.255, 7.253, 7.251, 7.249, 7.247, 7.245, 7.243, 7.241, 7.239, 7.237, 7.235, 7.233, 7.231, 7.229, 7.227, 7.225, 7.223, 7.221, 7.219, 7.217, 7.215, 7.213, 7.211, 7.209, 7.207, 7.205, 7.203, 7.201, 7.199, 7.197, 7.195, 7.193, 7.191, 7.189, 7.187, 7.185, 7.183, 7.181, 7.179, 7.177, 7.175, 7.173, 7.171, 7.169, 7.167, 7.165, 7.163, 7.161, 7.159, 7.157, 7.155, 7.153, 7.151, 7.149, 7.147, 7.145, 7.143, 7.141, 7.139, 7.137, 7.135, 7.133, 7.131, 7.129, 7.127, 7.125, 7.123, 7.121, 7.119, 7.117, 7.115, 7.113, 7.111, 7.109, 7.107, 7.105, 7.103, 7.101, 7.099, 7.097, 7.095, 7.093, 7.091, 7.089, 7.087, 7.085, 7.083, 7.081, 7.079, 7.077, 7.075, 7.073, 7.071, 7.069, 7.067, 7.065, 7.063, 7.061, 7.059, 7.057, 7.055, 7.053, 7.051, 7.049, 7.047, 7.045, 7.043, 7.041, 7.039, 7.037, 7.035, 7.033, 7.031, 7.029, 7.027, 7.025, 7.023, 7.021, 7.019, 7.017, 7.015, 7.013, 7.011, 7.009, 7.007, 7.005, 7.003, 7.001, 6.999, 6.997, 6.995, 6.993, 6.991, 6.989, 6.987, 6.985, 6.983, 6.981, 6.979, 6.977, 6.975, 6.973, 6.971, 6.969, 6.967, 6.965, 6.963, 6.961, 6.959, 6.957, 6.955, 6.953, 6.951, 6.949, 6.947, 6.945, 6.943, 6.941, 6.939, 6.937, 6.935, 6.933, 6.931, 6.929, 6.927, 6.925, 6.923, 6.921, 6.919, 6.917, 6.915, 6.913, 6.911, 6.909, 6.907, 6.905, 6.903, 6.901, 6.899, 6.897, 6.895, 6.893, 6.891, 6.889, 6.887, 6.885, 6.883, 6.881, 6.879, 6.877, 6.875, 6.873, 6.871, 6.869, 6.867, 6.865, 6.863, 6.861, 6.859, 6.857, 6.855, 6.853, 6.851, 6.849, 6.847, 6.845, 6.843, 6.841, 6.839, 6.837, 6.835, 6.833, 6.831, 6.829, 6.827, 6.825, 6.823, 6.821, 6.819, 6.817, 6.815, 6.813, 6.811, 6.809, 6.807, 6.805, 6.803, 6.801, 6.799, 6.797, 6.795, 6.793, 6.791, 6.789, 6.787, 6.785, 6.783, 6.781, 6.779, 6.777, 6.775, 6.773, 6.771, 6.769, 6.767, 6.765, 6.763, 6.761, 6.759, 6.757, 6.755, 6.753, 6.751, 6.749, 6.747, 6.745, 6.743, 6.741, 6.739, 6.737, 6.735, 6.733, 6.731, 6.729, 6.727, 6.725, 6.723, 6.721, 6.719, 6.717, 6.715, 6.713, 6.711, 6.709, 6.707, 6.705, 6.703, 6.701, 6.699, 6.697, 6.695, 6.693, 6.691, 6.689, 6.687, 6.685, 6.683, 6.681, 6.679, 6.677, 6.675, 6.673, 6.671, 6.669, 6.667, 6.665, 6.663, 6.661, 6.659, 6.657, 6.655, 6.653, 6.651, 6.649, 6.647, 6.645, 6.643, 6.641, 6.639, 6.637, 6.635, 6.633, 6.631, 6.629, 6.627, 6.625, 6.623, 6.621, 6.619, 6.617, 6.615, 6.613, 6.611, 6.609, 6.607, 6.605, 6.603, 6.601, 6.599, 6.597, 6.595, 6.593, 6.591, 6.589, 6.587, 6.585, 6.583, 6.581, 6.579, 6.577, 6.575, 6.573, 6.571, 6.569, 6.567, 6.565, 6.563, 6.561, 6.559, 6.557, 6.555, 6.553, 6.551, 6.549, 6.547, 6.545, 6.543, 6.541, 6.539, 6.537, 6.535, 6.533, 6.531, 6.529, 6.527, 6.525, 6.523, 6.521, 6.519, 6.517, 6.515, 6.513, 6.511, 6.509, 6.507, 6.505, 6.503, 6.501, 6.499, 6.497, 6.495, 6.493, 6.491, 6.489, 6.487, 6.485, 6.483, 6.481, 6.479, 6.477, 6.475, 6.473, 6.471, 6.469, 6.467, 6.465, 6.463, 6.461, 6.459, 6.457, 6.455, 6.453, 6.451, 6.449, 6.447, 6.445, 6.443, 6.441, 6.439, 6.437, 6.435, 6.433, 6.431, 6.429, 6.427, 6.425, 6.423, 6.421, 6.419, 6.417, 6.415, 6.413, 6.411, 6.409, 6.407, 6.405, 6.403, 6.401, 6.399, 6.397, 6.395, 6.393, 6.391, 6.389, 6.387, 6.385, 6.383, 6.381, 6.379, 6.377, 6.375, 6.373, 6.371, 6.369, 6.367, 6.365, 6.363, 6.361, 6.359, 6.357, 6.355, 6.353, 6.351, 6.349, 6.347, 6.345, 6.343, 6.341, 6.339, 6.337, 6.335, 6.333, 6.331, 6.329, 6.327, 6.325, 6.323, 6.321, 6.319, 6.317, 6.315, 6.313, 6.311, 6.309, 6.307, 6.305, 6.303, 6.301, 6.299, 6.297, 6.295, 6.293, 6.291, 6.289, 6.287, 6.285, 6.283, 6.281, 6.279, 6.277, 6.275, 6.273, 6.271, 6.269, 6.267, 6.265, 6.263,	

100M ¹³C-NMR JXZ20-36 in CDCl₃

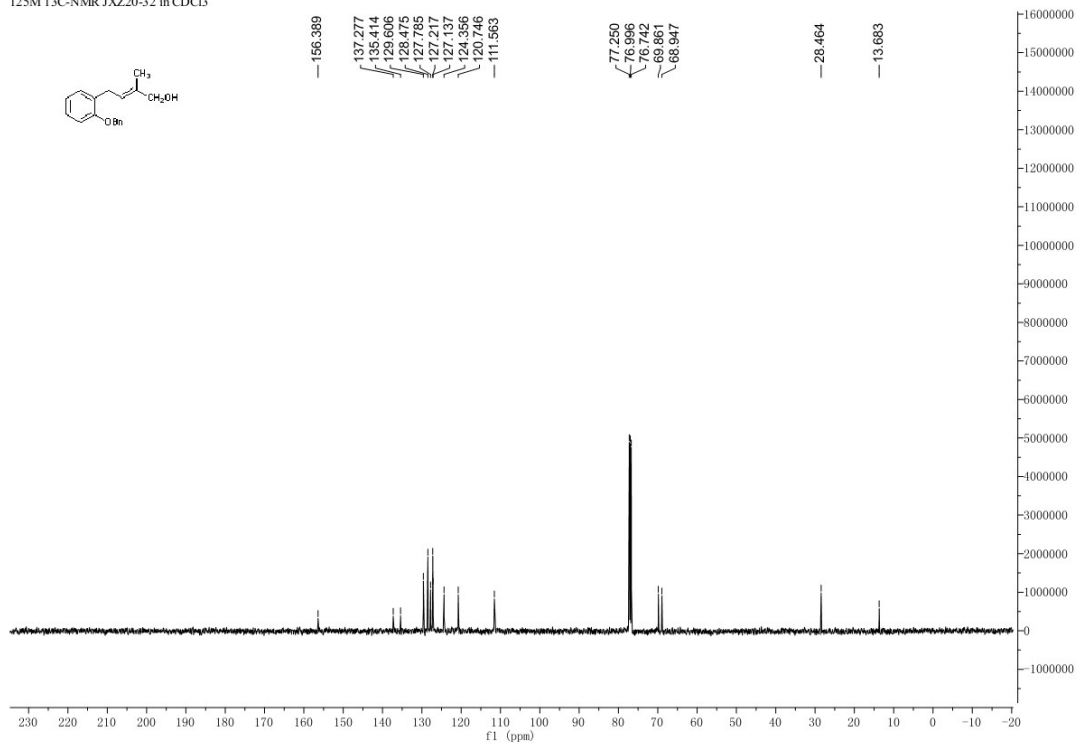
¹³C NMR spectra of compound **14**

400 1H-NMR JXZ20-32 in CDCl3



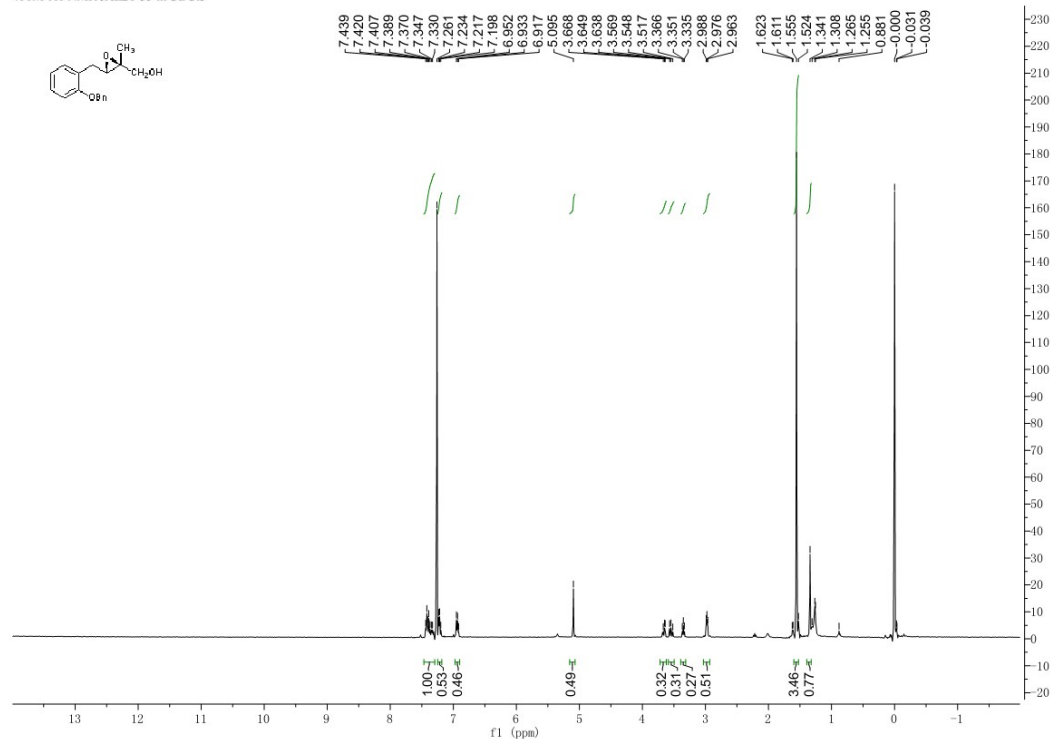
¹H NMR spectra of compound 15

125M 13C-NMR JXZ20-32 in CDCl3



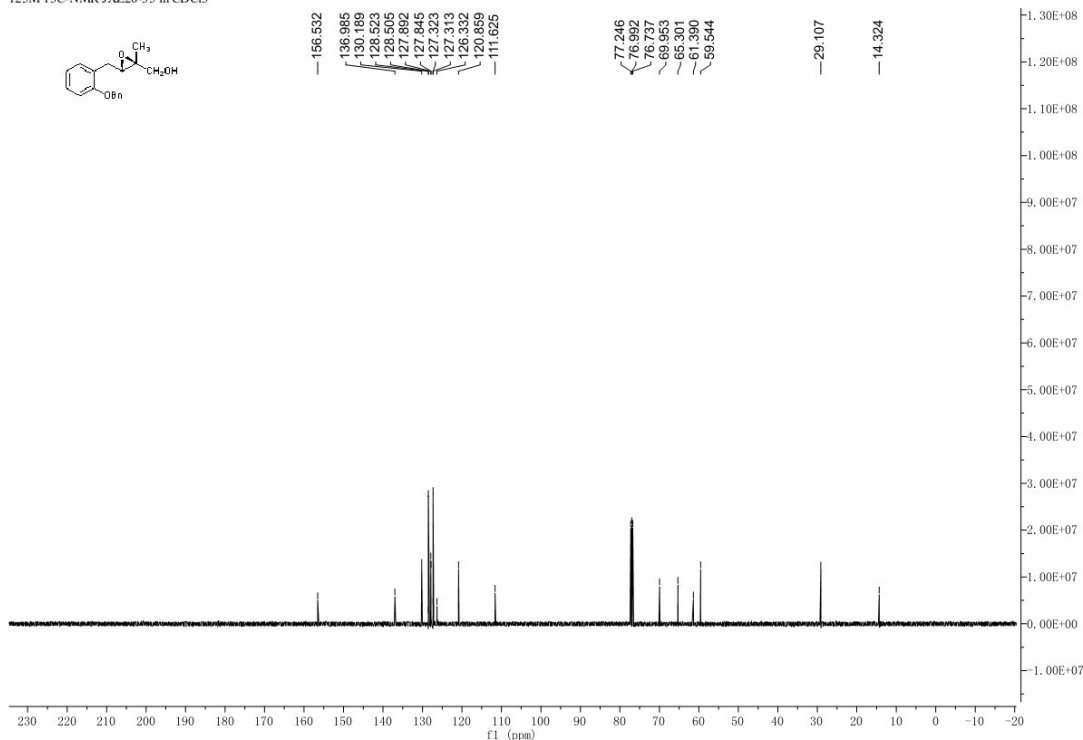
¹³C NMR spectra of compound 15

400M ¹H-NMR JXZ20-35 in CDCl₃

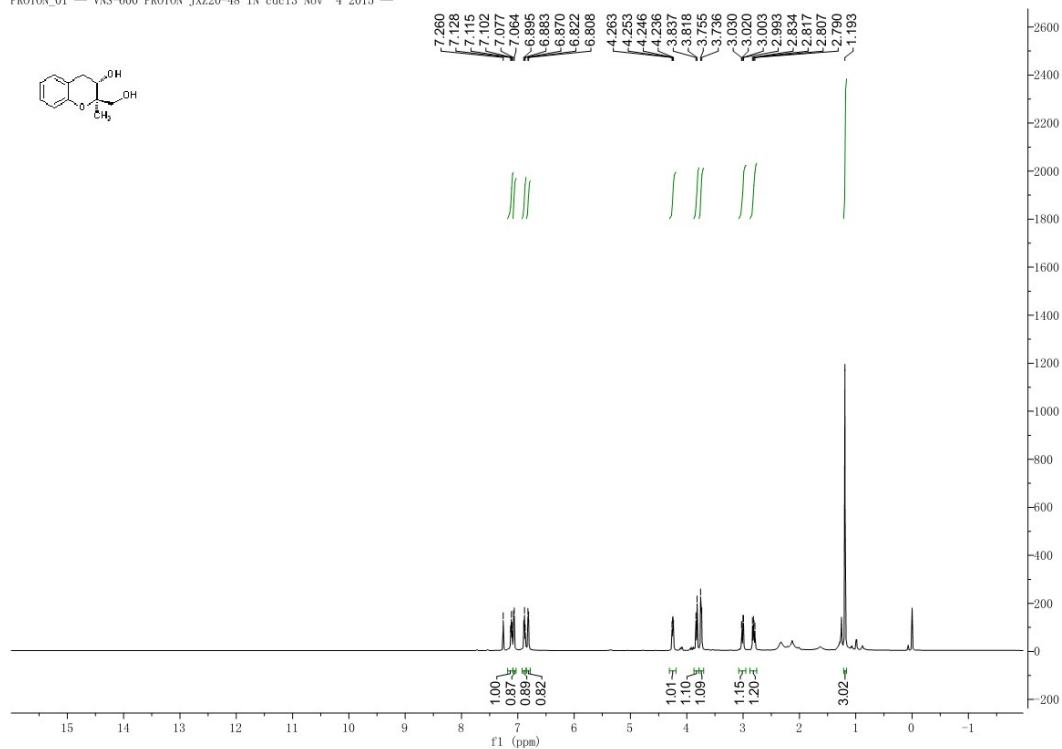


¹H NMR spectra of compound 16

125M ¹³C-NMR JXZ20-35 in CDCl₃



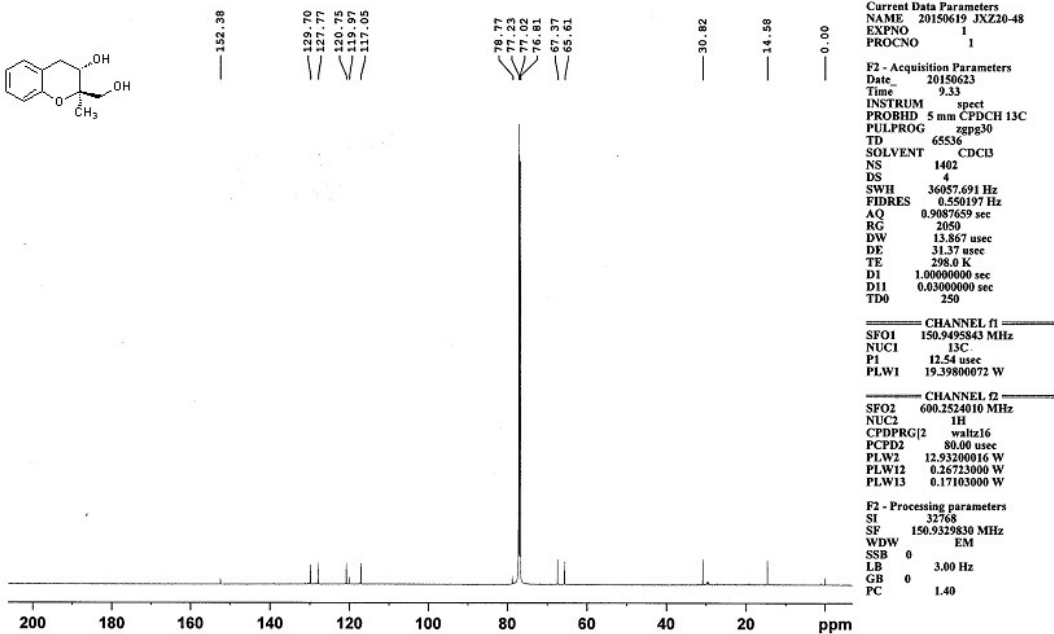
¹³C NMR spectra of compound 16



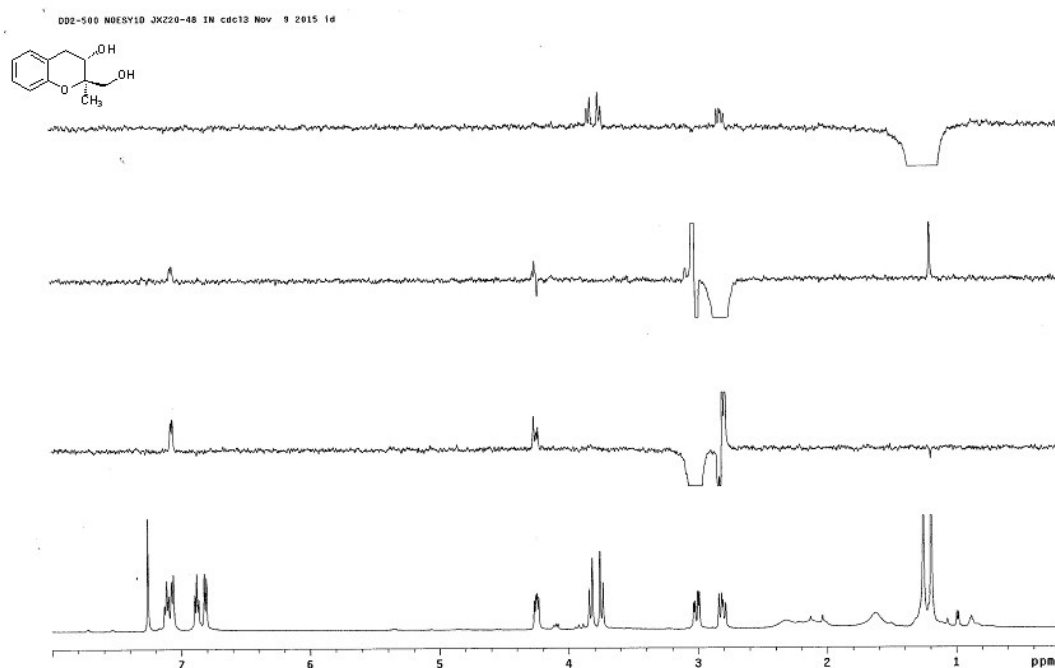
¹H NMR spectra of compound 17



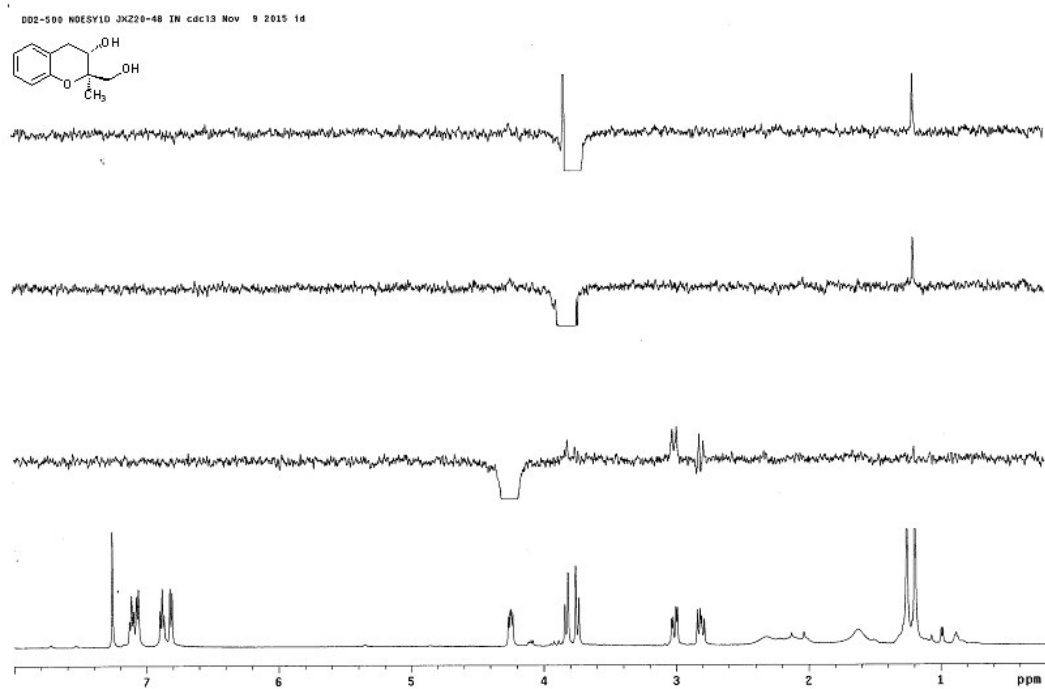
Bruker AVIIIHD 600 20150619
C13 CDC13 D:\DATA2015 32



¹³C NMR spectra of compound 17

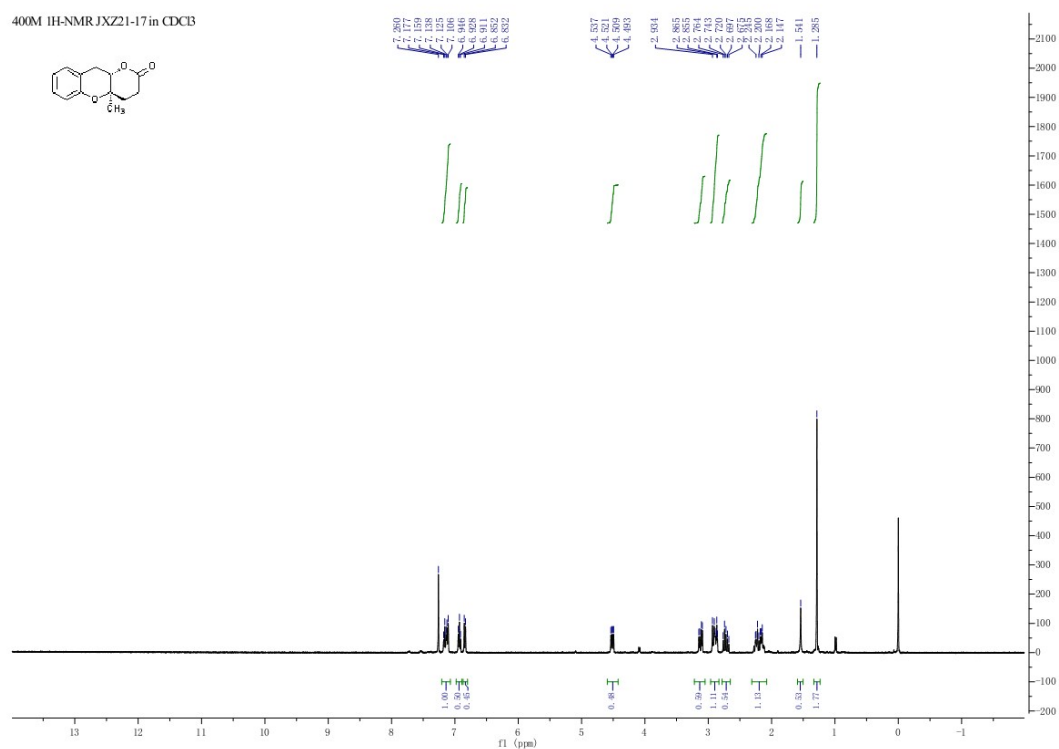


NOE spectra of compound 17

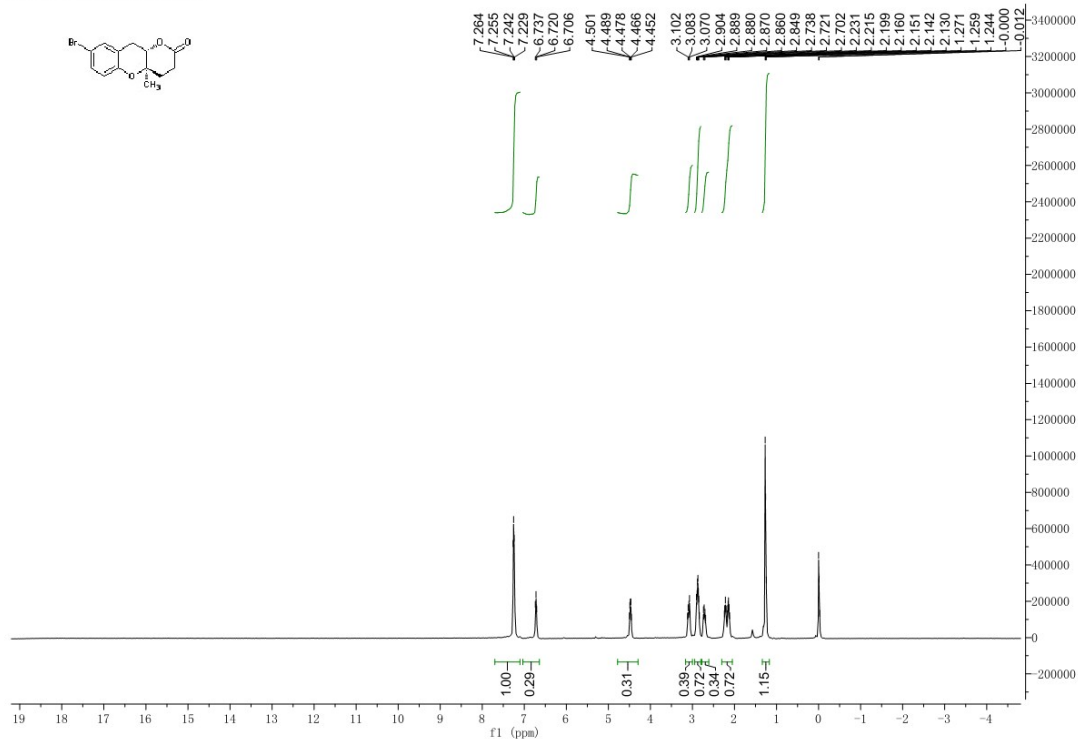


NOE spectra of compound 17

400M ¹H-NMR JXZ21-17 in CDCl₃

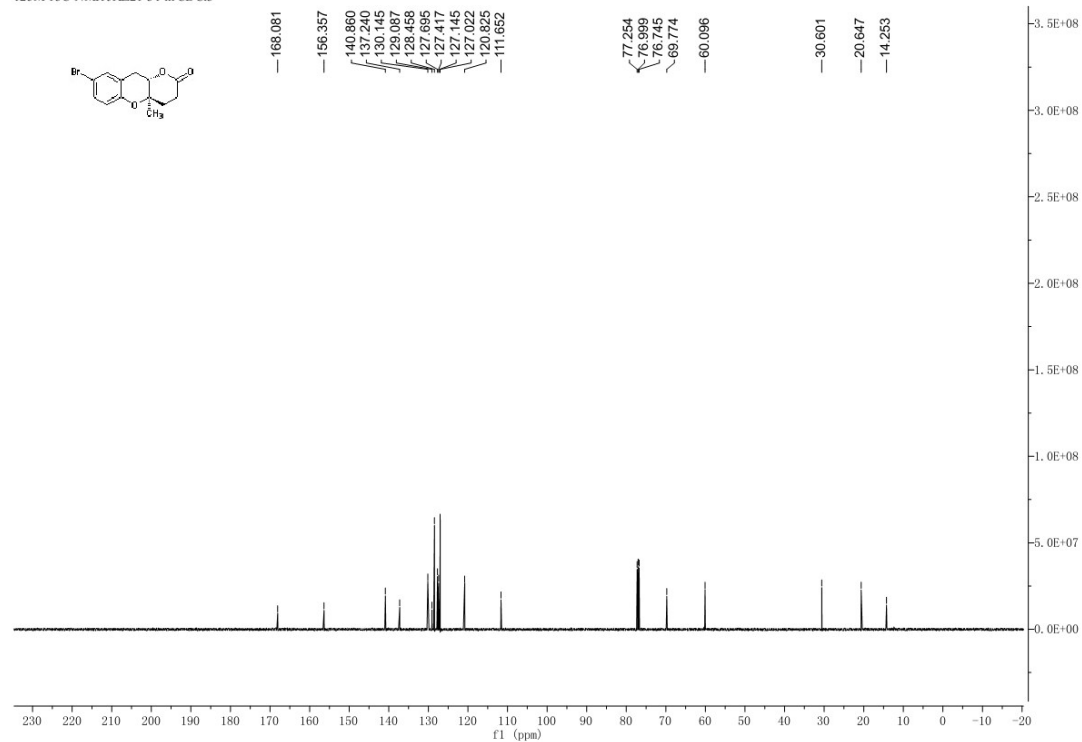


500M ¹H-NMR JXZ21-31 in CDCl₃



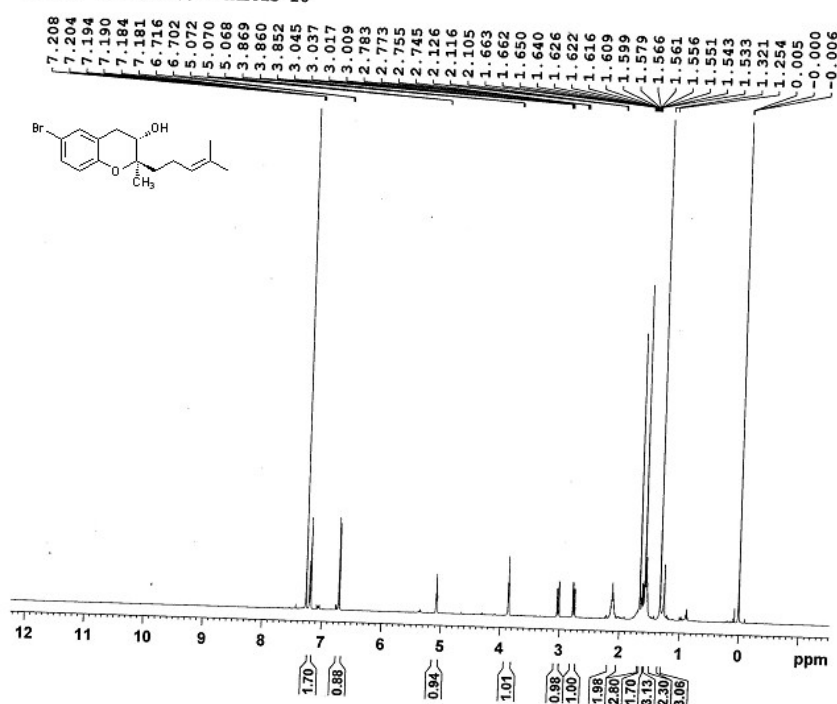
¹H NMR spectra of compound 20

125M ¹³C-NMR JXZ21-31 in CDCl₃



¹³C NMR spectra of compound 20

Bruker AVIIHHD 600 20150528
PROTON CDCl3 D:\DATA2015 16



Current Data Parameters
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EXPNO 1
PROCNO 1

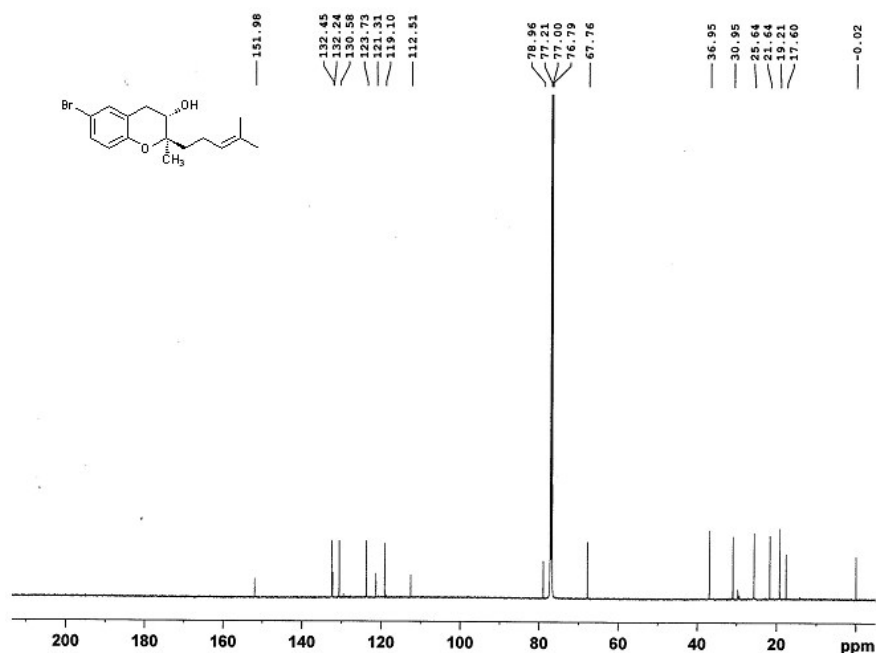
F2 - Acquisition Parameters
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Time 10.52
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TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.103399 Hz
AQ 2.7262976 sec
RG 64
EW 41.600 usec
DE 20.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

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NUC1 1H
P1 11.50 usec
PLW1 12.93200016 W
F2 - Processing parameters
SI 65536
SF 600.2500130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR spectra of compound 21



Bruker AVIIHHD 600 20150528
C13 CDCl3 D:\DATA2015 16



Current Data Parameters
NAME 20150528 jxx21-25-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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Time 10.55
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NS 442
DS 4
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FIDRES 0.550197 Hz
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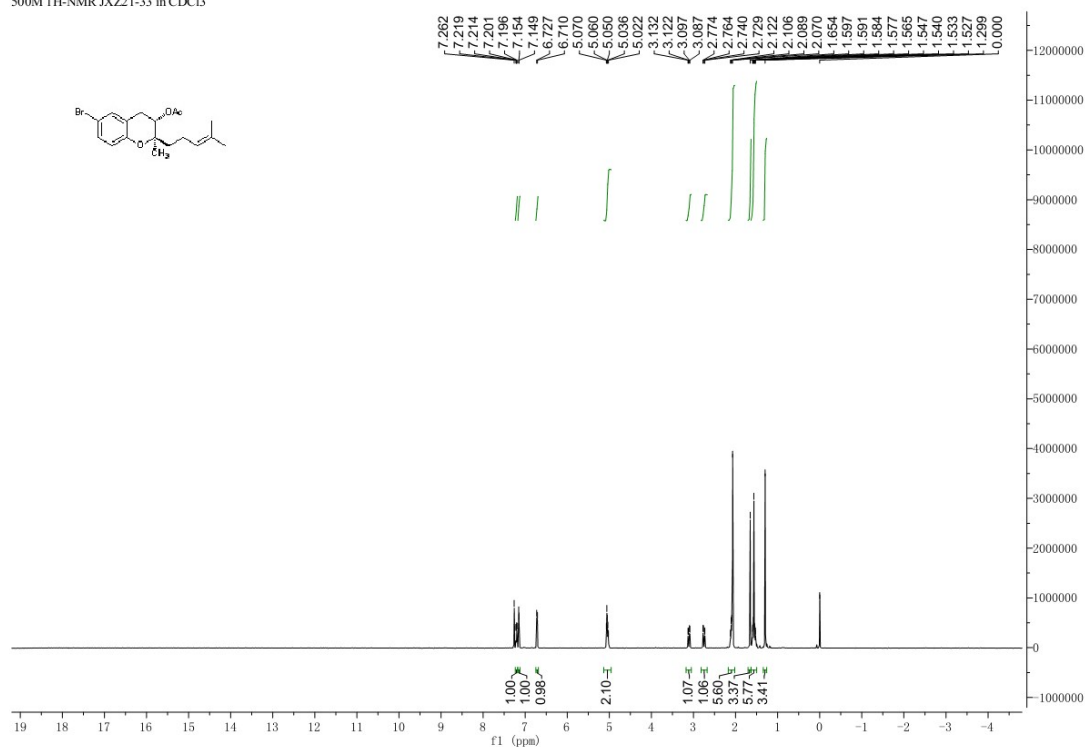
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PLW1 19.39800072 W

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NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 12.93200016 W
PLW12 0.26723000 W
PLW13 0.17103000 W

F2 - Processing parameters
SI 32768
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GB 0
PC 1.40

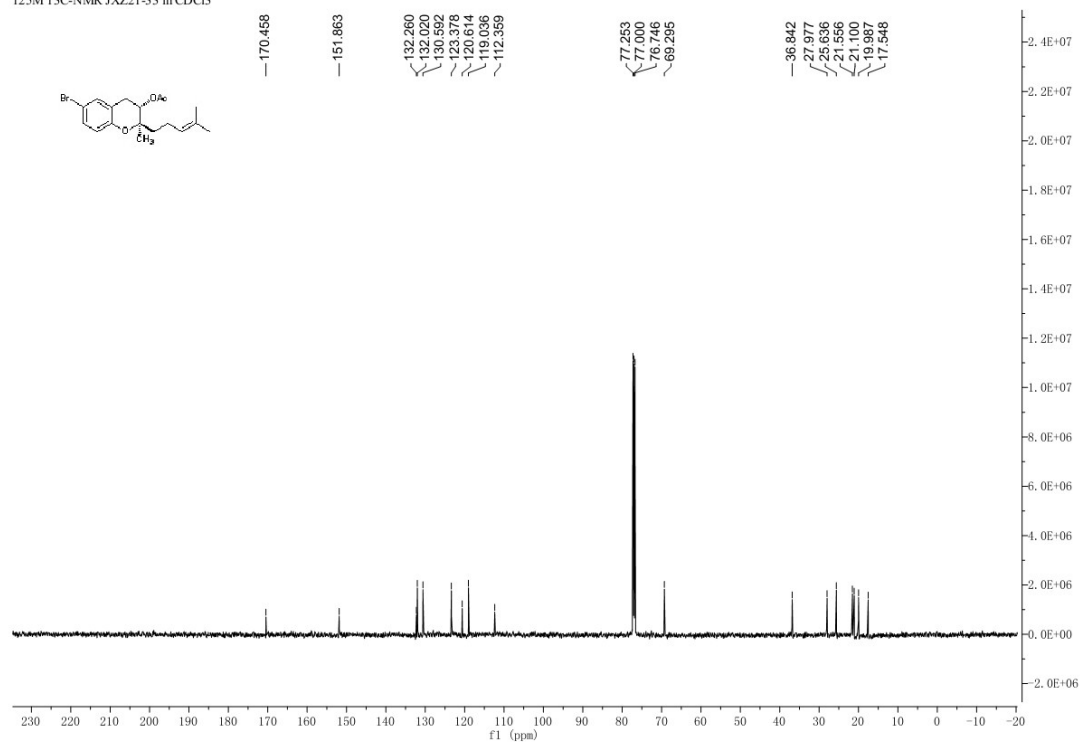
¹³C NMR spectra of compound 21

500M ¹H-NMR JXZ21-33 in CDCl₃

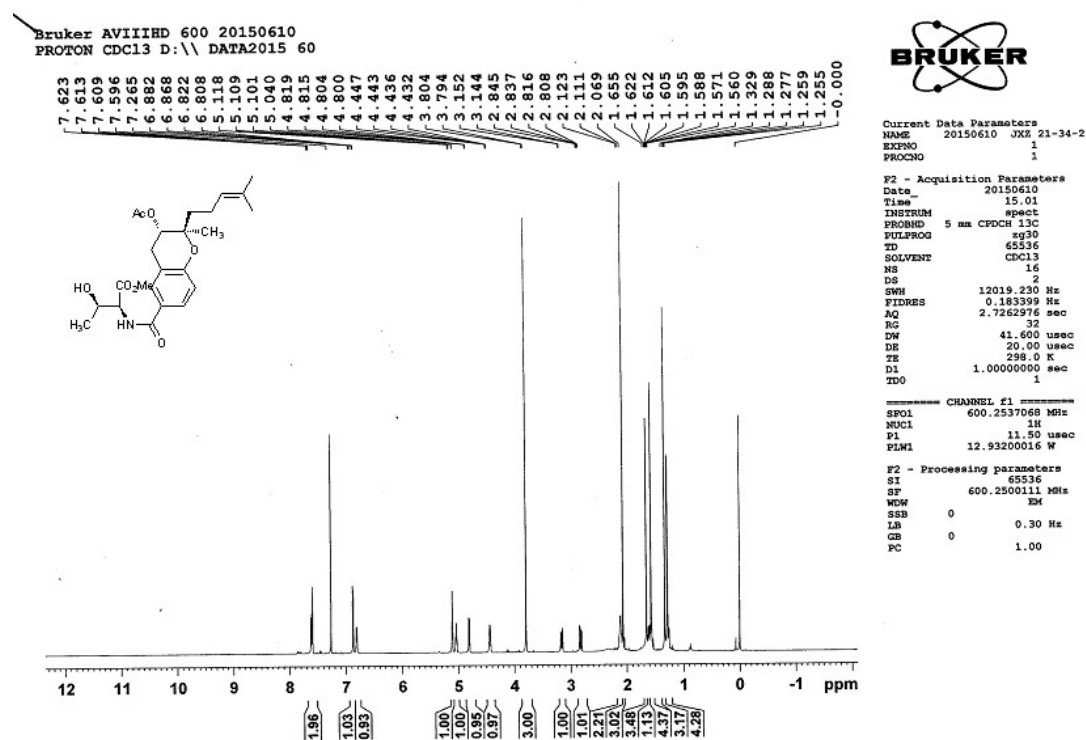


¹H NMR spectra of compound 22

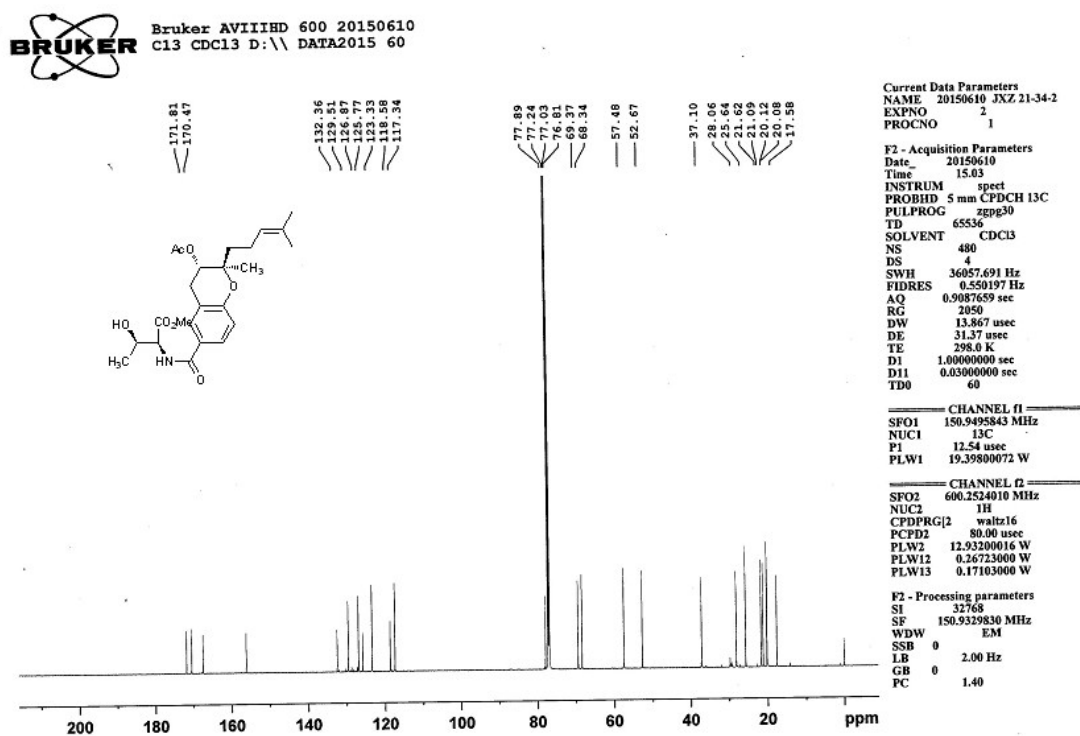
125M ¹³C-NMR JXZ21-33 in CDCl₃



¹³C NMR spectra of compound 22



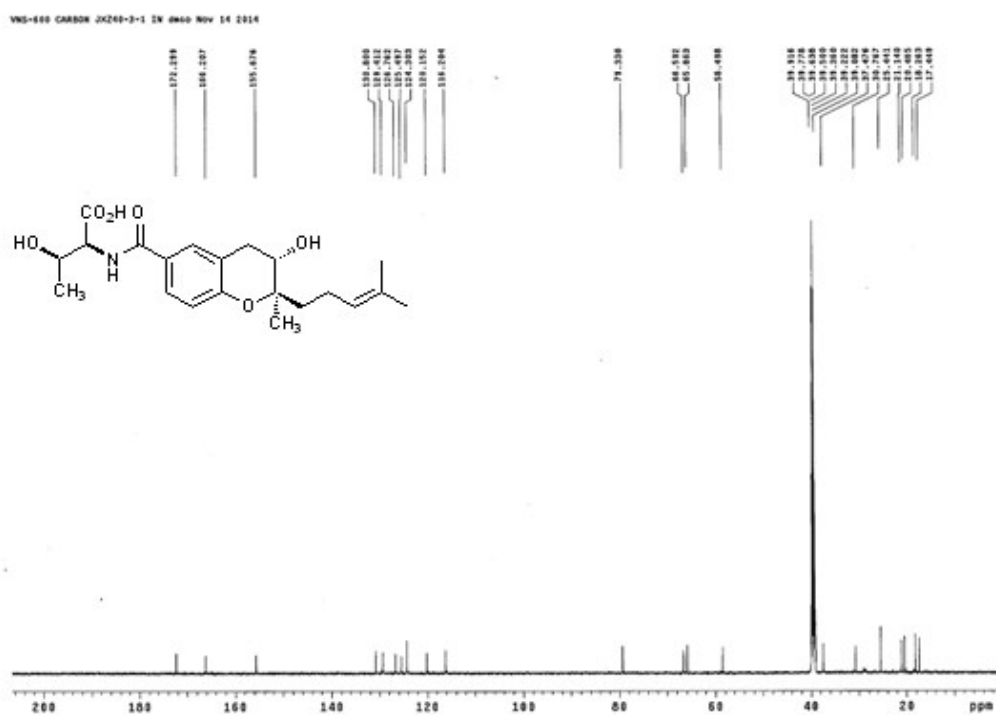
¹H NMR spectra of compound 23



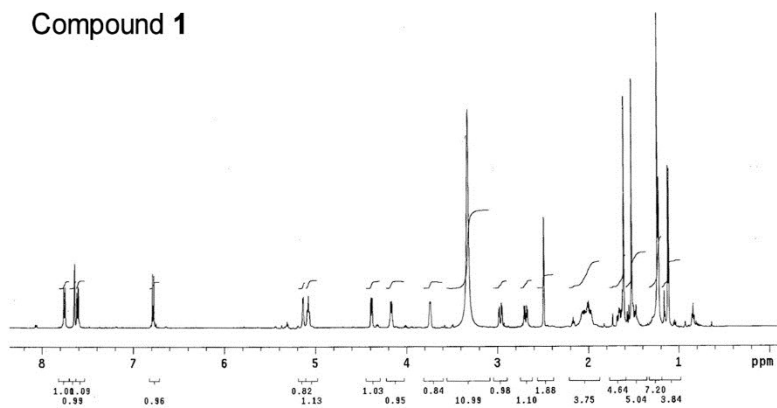
¹³C NMR spectra of compound 23



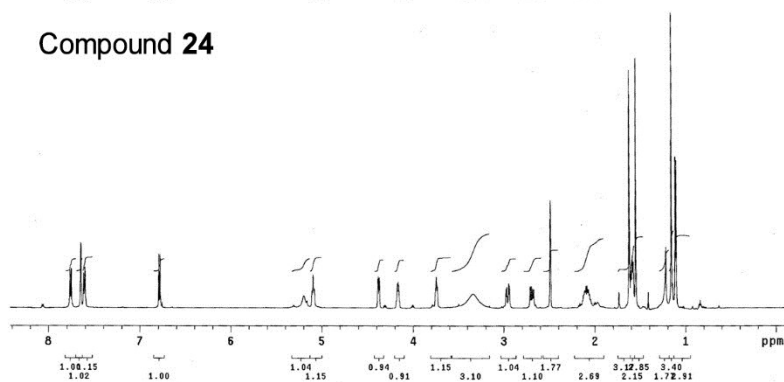
¹H NMR spectra of compound **24**

¹³C NMR spectra of compound **24**

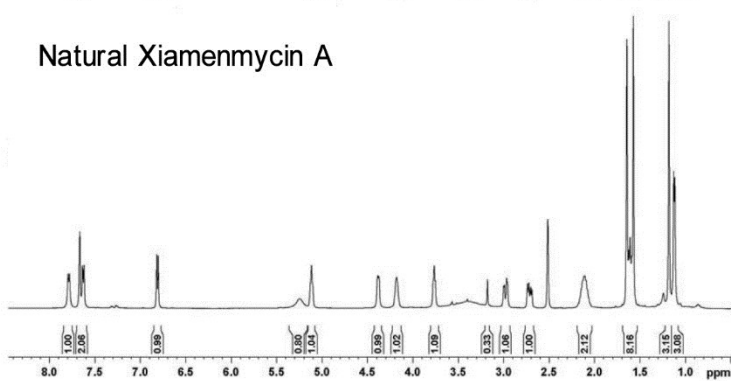
Compound **1**



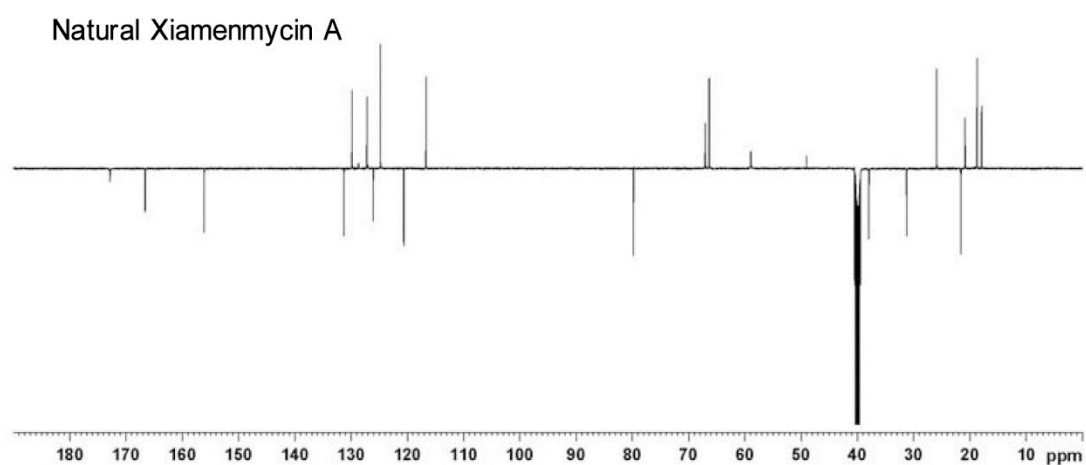
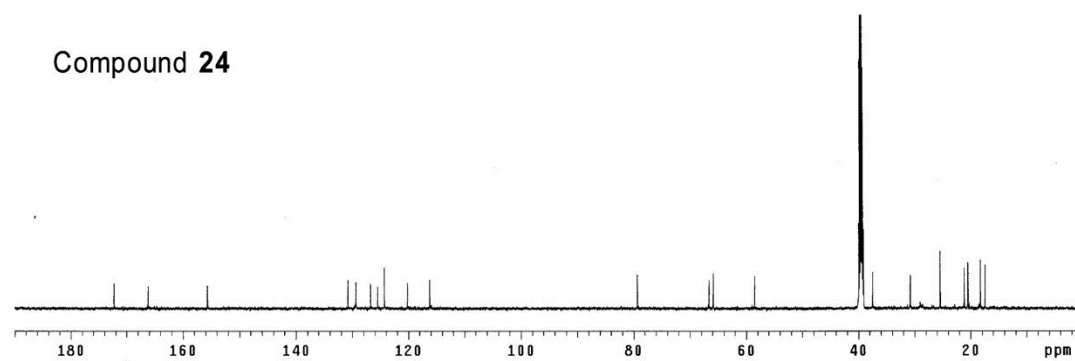
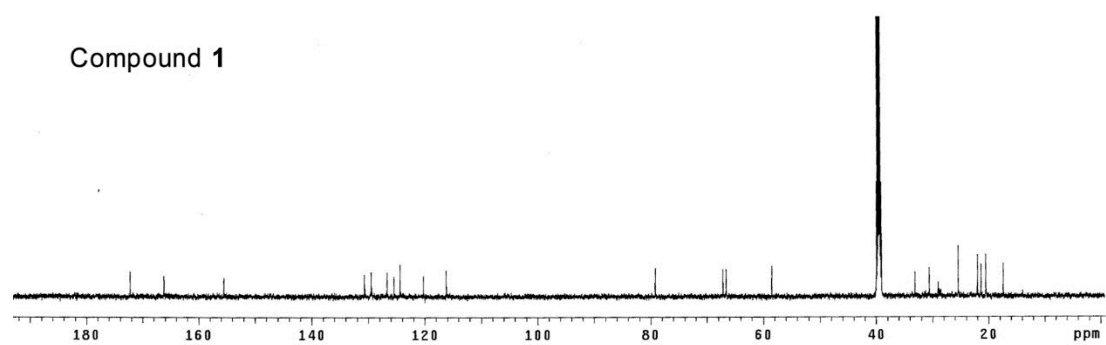
Compound **24**



Natural Xiamenmycin A



^1H NMR comparison of **1**, **24** and natural xiamenmycin A



^{13}C NMR comparison of **1**, **24** and natural xiamenmycin A

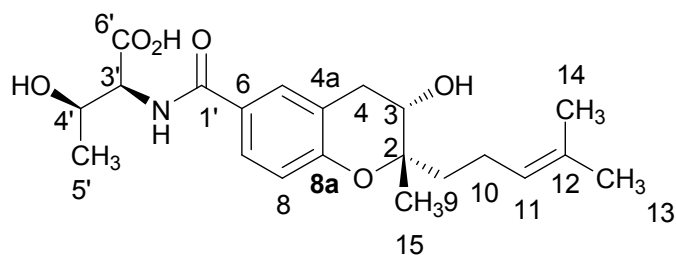


Table the comparison of ¹H and ¹³CNMR data of compound 1, 24 and reported natural xiamenmycin A

Position	δ_{H} (J in Hz)			δ_{C}		
	Natural Xiamenmycin A ¹	Compound 24	Compound 1	Natural Xiamenmycin A ¹	Compound 24	Compound 1
1	--	--	--	--	--	--
2	--	--	--	79.8	79.3	79.2
3	3.77, t	3.74,t(5.4)	3.74, br.	66.3	65.9	66.6
4	2.71,dd (17.3, 7.4)	2.69,dd (16.8,7.8)	2.69, dd (16.8, 7.2)	31.2	30.8	30.6
	2.98, dd (17.3, 5.2)	2.96,dd (16.8, 5.4)	2.96, dd (16.8, 5.4)			
4a	--	--	--	120.6	120.2	120.3
5	7.67, s	7.65, s	7.65, s	129.8	129.4	129.5
6	--	--	--	126.0	125.5	125.5
7	7.63, d (8.4)	7.61,d (8.4)	7.61, d (8.4)	127.2	126.8	126.7
8	6.81, d (8.4)	6.79, d (8.4)	6.78, d (8.4)	116.7	116.2	116.2
8a	--	--	--	156.1	155.7	155.6
9	1.60, m	1.59, m	1.69-1.61	38.0	37.5	33.1
10	2.10, m	2.09, m	2.05, m	21.6	21.1	21.3
11	5.12, dd(7.1,1.3)	5.10, t(6.6)	5.08,t (7.2)	124.8	124.3	124.4
12	--	--	--	131.3	130.8	130.7
13	1.57, s	1.55, s	1.52, s	17.9	17.4	17.4
14	1.65,s	1.62, s	1.62, s	25.9	25.4	25.4
15	1.18, s	1.16, s	1.23, s	18.7	18.3	22.0
1'	--	--	--	166.6	166.2	166.3
2'	7.78, d (7.8)	7.77,d (8.4)	7.75,d (8.4)	--	--	--
3'	4.38, brd	4.38,dd(3.6,8.4)	4.38,dd(3.6,8.4)	58.9	58.5	58.5
4'	4.18, brs	4.17,m	4.17, m	67.1	66.6	67.2
5'	1.12, d (6.0)	1.11,d(6.6)	1.11, d (6.6)	20.9	20.5	20.5
6'	--		--	172.8	172.3	172.3

1. M. J. Xu, X. J. Liu, Y. L. Zhao, D. Liu, Z. H. Xu, X. M. Lang, P. Ao, W. H. Lin, S. L. Yang, Z. G. Zhang and J. Xu, *Marine drugs*, 2012, **10**, 639-654.