Supporting Information

Total synthesis of (-)-carinatine A and (+)-lycopladine A

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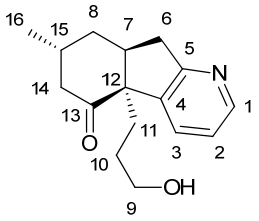
Table of contents

Comparison NMR data of (+)-lycopladine A and (-)-carinatine A

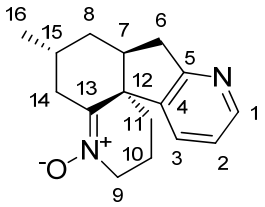


Comparison NMR data of synthetic (+)-2 with natural (+)-lycopladine A (Spectra in CD_3OD)

position	δ ^{1}H natural (ppm)	δ ^{1}H synthetic (ppm)[a]	Δ δ (ppm)	δ ^{13}C natural (ppm)	δ ^{13}C synthetic (ppm)[b]	Δ δ (ppm)
1	8.30 (1H, dd, 5.0, 1.4)	8.31 (1H, dd, 5.1, 1.4)	+0.01	148.8	148.8	--
3	7.67 (1H, dd, 7.7, 1.4)	7.67 (1H, dd, 7.7, 1.4)	--	136.1	136.2	+0.1
2	7.24 (1H, dd, 7.7, 5.0)	7.25 (1H, dd, 7.7, 5.1)	+0.01	123.0	123.1	+0.1
4	--	--	--	140.0	140.1	+0.1
5	--	--	--	164.3	164.3	--
9	3.53 (2H, m)	3.54 (2H, m)	+0.01	62.8	62.8	--
6a	3.09 (1H, dd, 16.5, 8.2)	3.09 (1H, dd, 16.4, 8.2)	--	38.6	38.6	--
6b	2.83 (1H, dd, 16.5, 9.1)	2.83 (1H, dd, 16.4, 9.0)	--	62.8	62.8	--
7	2.97 (1H, m)	2.97 (1H, m)	--	43.5	43.5	--
12	--	--	--	62.7	62.7	--
13	--	--	--	214.6	214.6	--
14	2.29 (2H, m)	2.29 (2H, dd, 5.3, 4.1)	--	47.7	47.7	--
15	2.12 (1H, m)	2.16-2.03 (2H, m)	--	29.5	29.6	+0.1
11a	2.06 (1H, ddd, 13.6, 13.6, 4.6)		--	43.5	43.5	--
11b	1.90, 1.88, 1.83 (3H, m)	1.92-1.79 (3H, m)	--			
8a			--	34.8	34.8	--
8b			--			
10a	1.56 (1H, m)	1.61-1.52 (1H, m)	--	29.1	29.1	--

10b	1.35 (1H, m)	1.39-1.32 (1H, m)	--			
16	1.08 (3H, d, 6.5)	1.09 (3H, d, 6.5)	+0.01	22.0	22.0	--

(a) Referenced relative to the center of the 3.31 ppm quintet resonance of CD_3OD. (b) Referenced relative to the center of the septet of CD_3OD at 49.0 ppm.



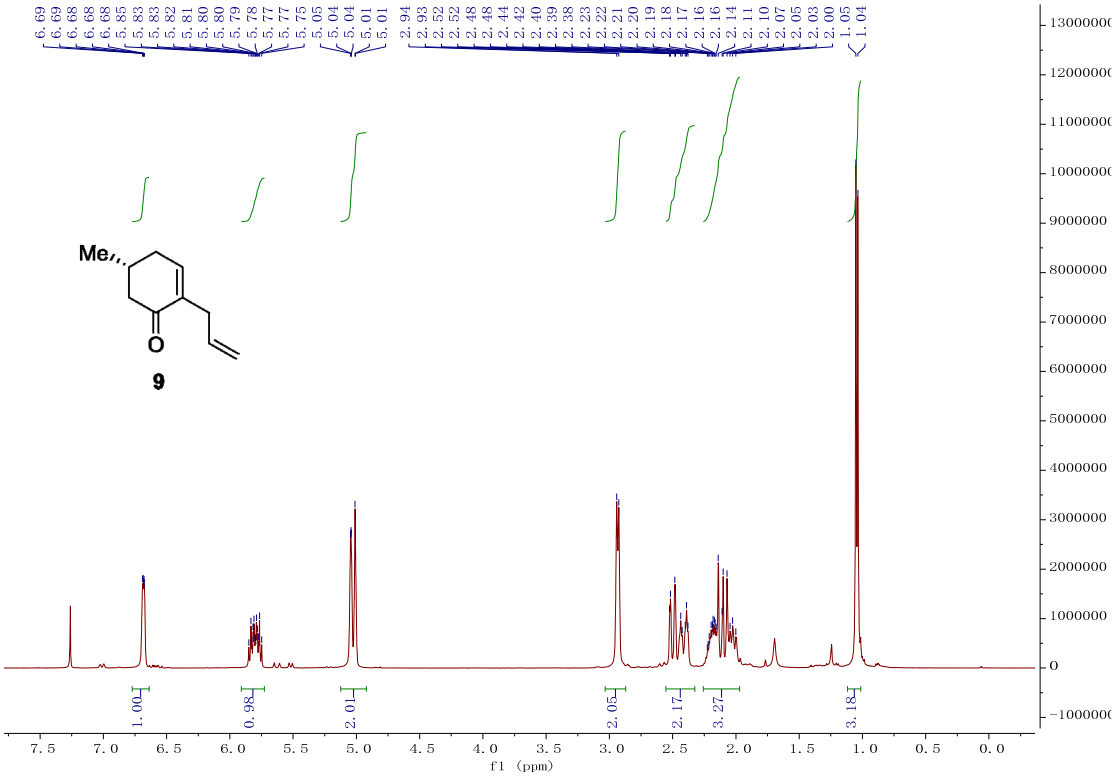
Comparison NMR data of synthetic (-)-1 with natural (-)-carinatine A (Spectra in CD_3OD)

position	δ ^{1}H natural (ppm)[(a)]	δ ^{1}H synthetic (ppm)[(b)]	Δ δ (ppm)	δ ^{13}C natural (ppm)	δ ^{13}C synthetic (ppm)[(d)]	Δ δ (ppm)
1	8.30 (1H, dd, 5.1, 1.3)	8.40 (1H, dd, 5.1, 1.4)	+0.10	149.5	149.5	--
2	7.18 (1H, dd, 7.7, 5.1)	7.28 (1H, dd, 7.7, 5.1)	+0.10	123.3	123.3	--
3	7.43 (1H, dd, 7.7, 1.3)	7.53 (1H, dd, 7.7, 1.4)	+0.10	134.2	134.1	-0.1
4	--	--	--	141.8	141.8	--
5	--	--	--	165.0	165.0	--
6a	3.48 (1H, dd, 17.3, 7.1)	3.58 (1H, dd, 17.2, 7.5)	+0.10	40.7	40.7	--
6b	2.60 (1H, d, 17.3)	2.70 (1H, d, 17.2)	+0.10			
7	2.66 (1H, q, 7.1)	2.77-2.73 (1H, m)	+0.09	45.3	45.3	--
8a	1.50 (1H, dt, 14.0, 7.1)	1.63-1.56 (1H, m)	+0.10	38.5	38.4	-0.1
8b	1.36 (1H, ddd, 14.0, 7.1, 3.1)	1.48-1.42 (1H, m)	+0.09			
9	3.90 (2H, m)[(c)]	4.00 (2H, m)	+0.10	59.1	59.0	-0.1
10	1.92, 1.91, 1.83, 1.75 (4H, m)	1.92-1.75 (4H, m)	+0.09 - 0.10	19.5	19.5	--
11				32.9	32.8	-0.1
12	--	--	--	52.6	52.5	-0.1
13	--	--	--	156.2	156.2	--
14a	2.94 (1H, dd, 17.1, 7.1)	3.04 (1H, dd, 16.8, 6.7)	+0.10	33.9	33.9	--

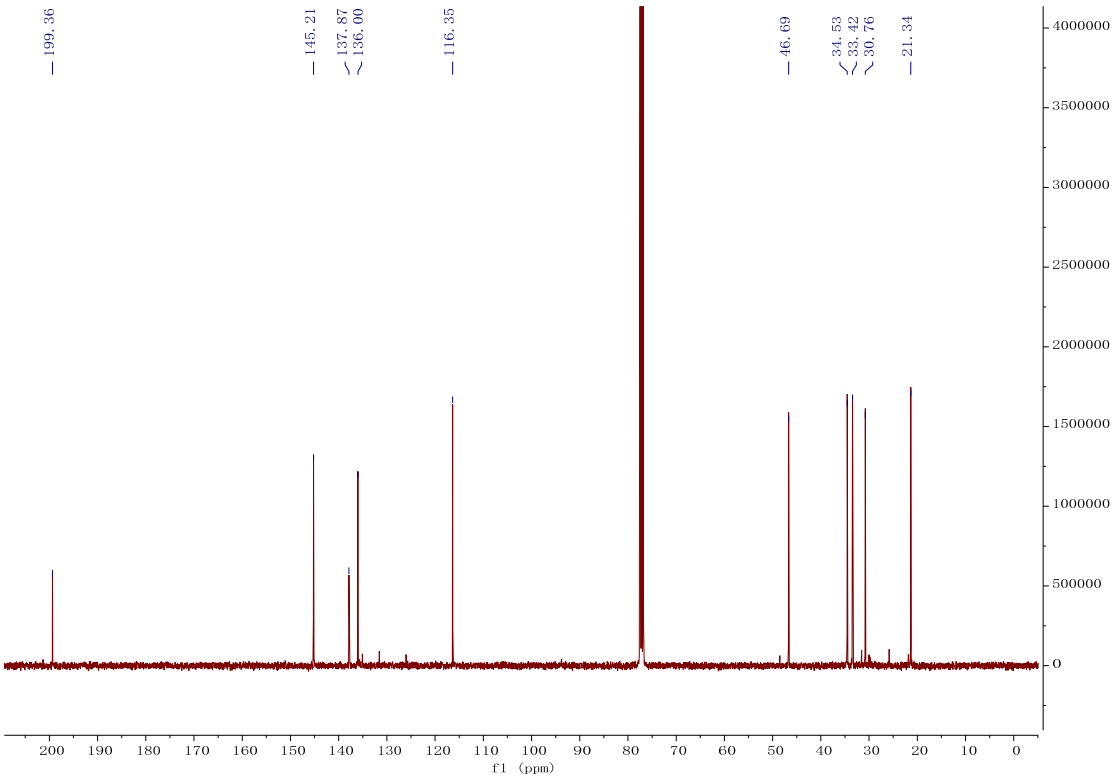
14b	2.01 (1H, m)	2.13-2.08 (1H, m)	+0.10			
15	1.60 (1H, m)	1.73-1.67 (1H, m)	+0.10	27.9	27.9	--
16	0.84 (3H, d, 6.8)	0.94 (3H, d, 6.8)	+0.10	20.1	20.1	--

(a) Referenced relative to 3.21 ppm quintet resonance of CD_3OD. (b) Referenced relative to the center of the 3.31 ppm. (c) Corrected number provided by Prof. Qin-shi Zhao and Fei Liu. (d) Referenced relative to the center of the septet of CD_3OD at 49.0 ppm.

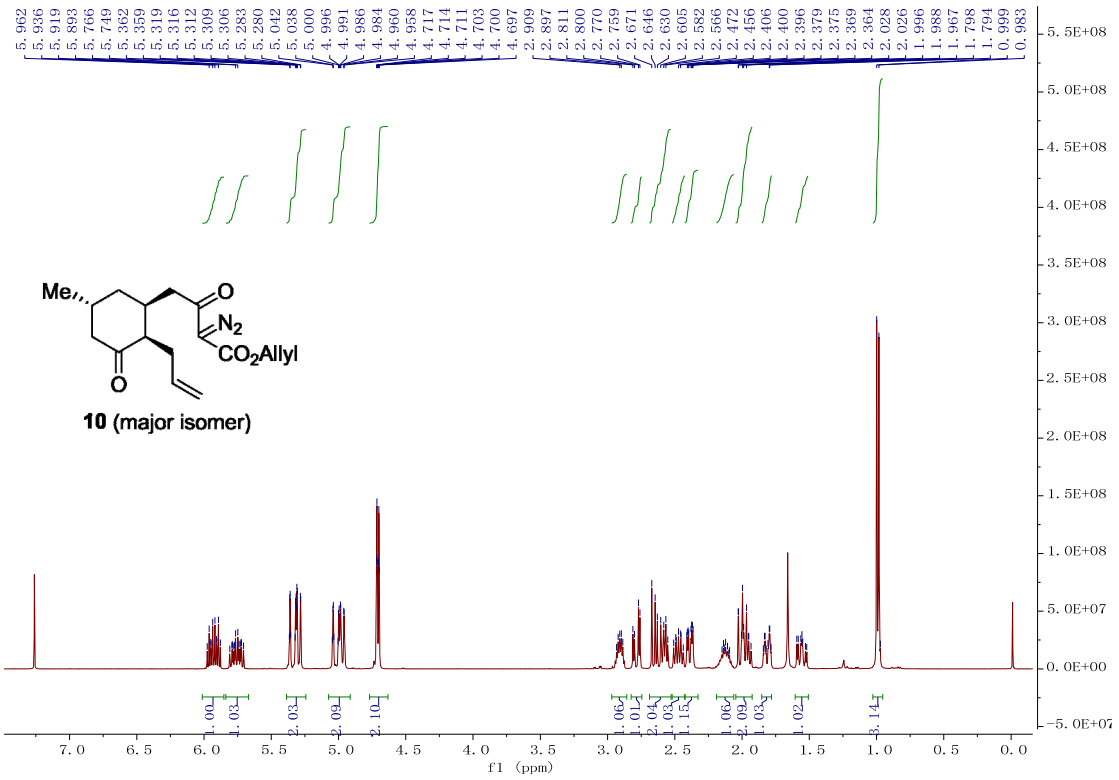
^{1}H and ^{13}C NMR spectrum of new compounds



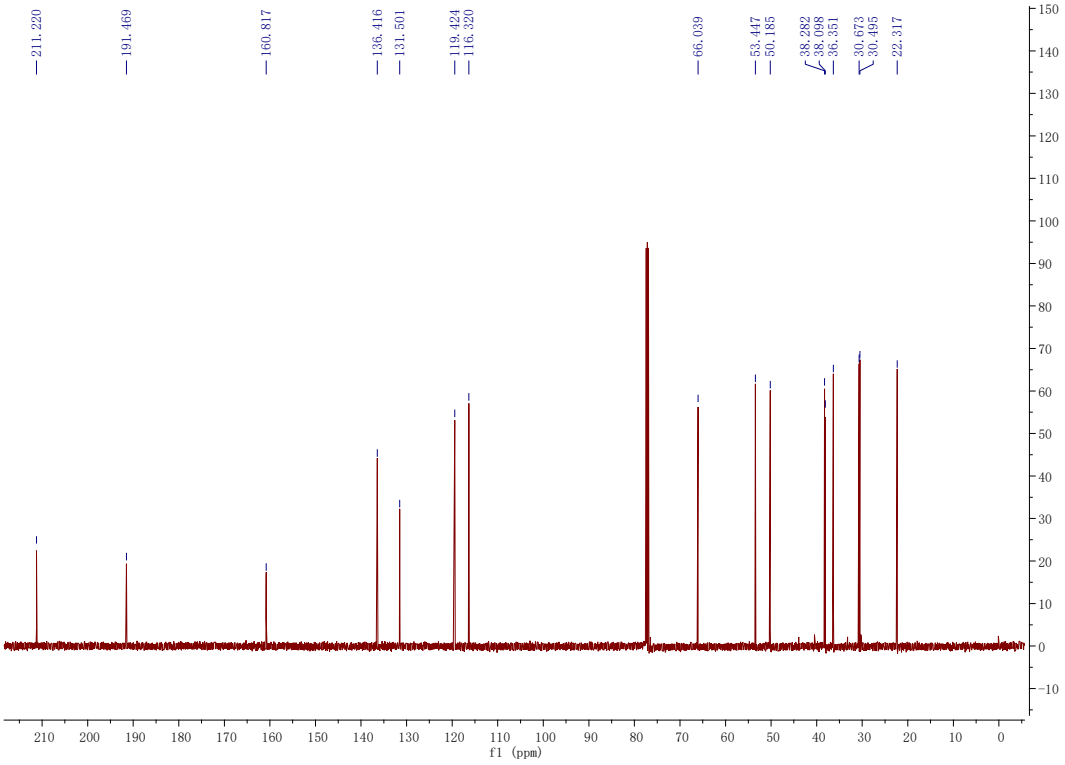
The ^{1}H NMR spectrum of **9**



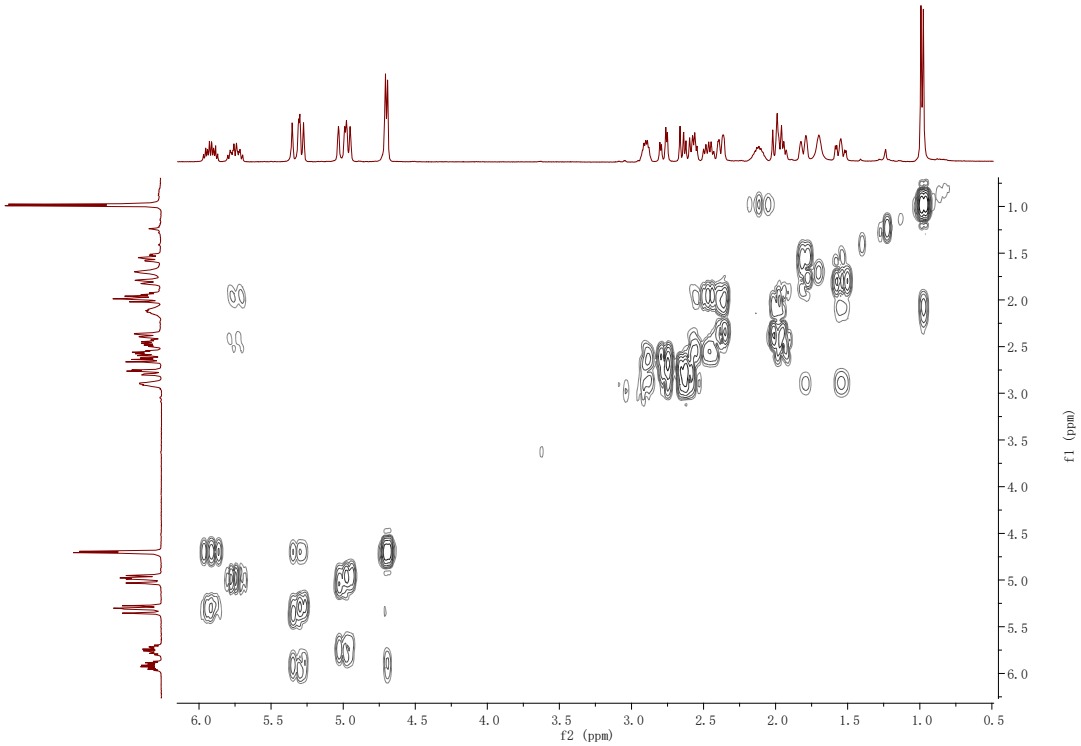
The ^{13}C NMR spectrum of **9**



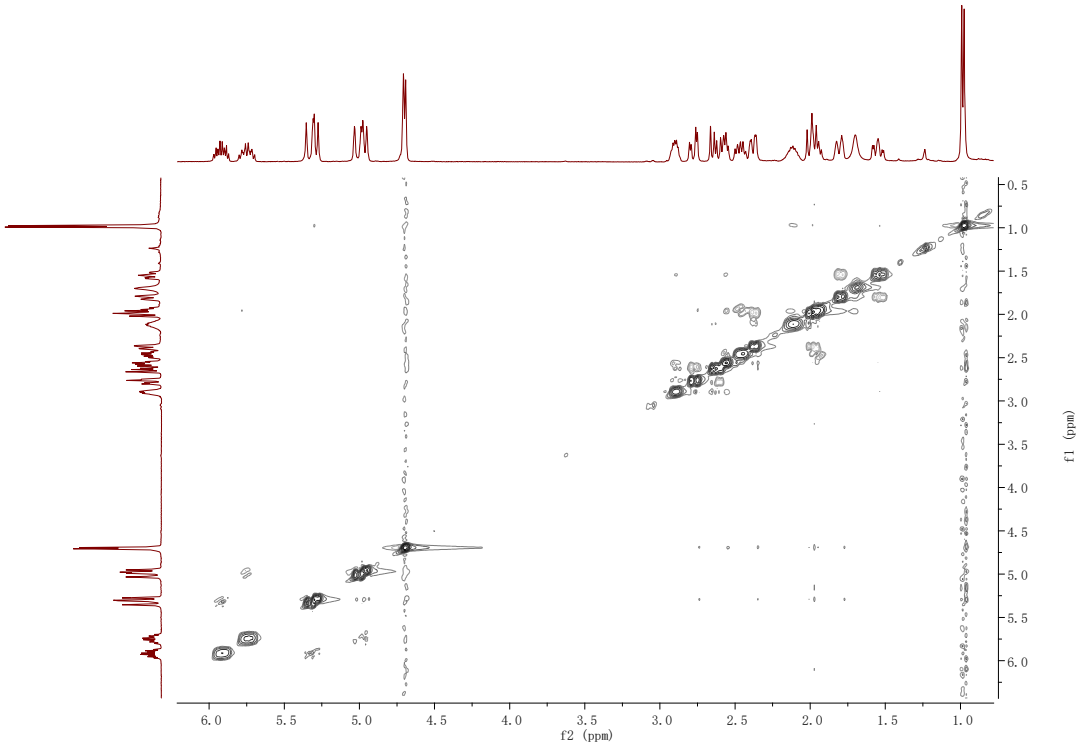
The ^{1}H NMR spectrum of **10** (major isomer)



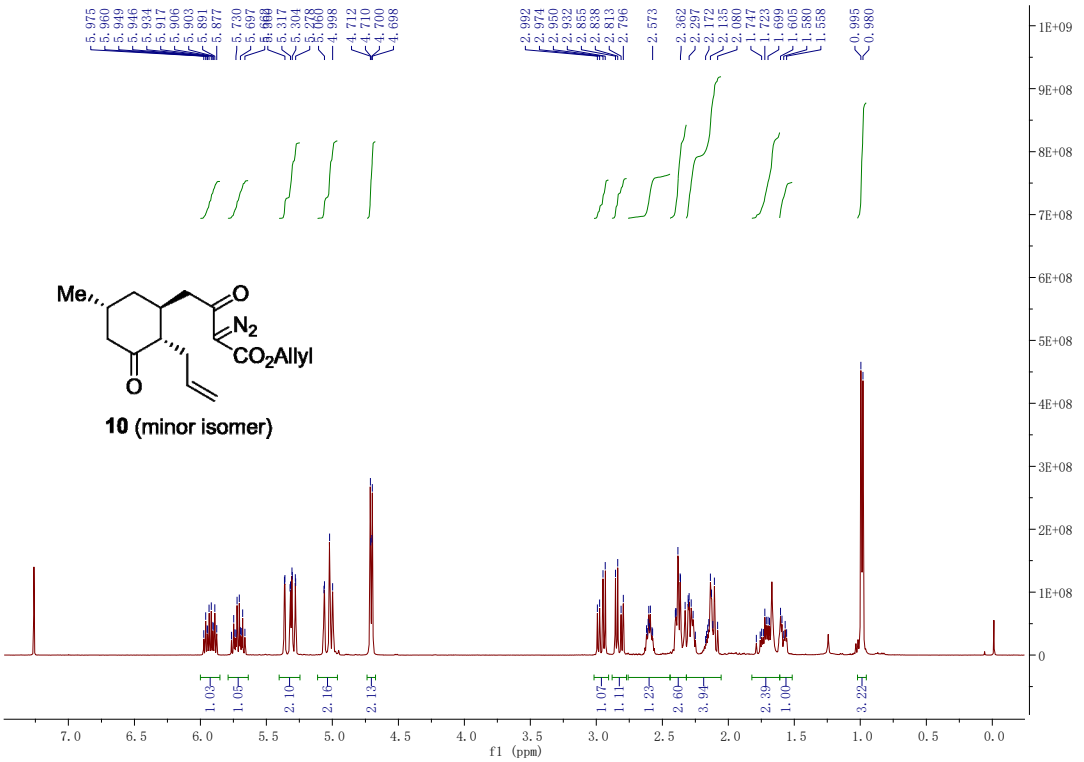
The ^{13}C NMR spetrum of **10** (major isomer)



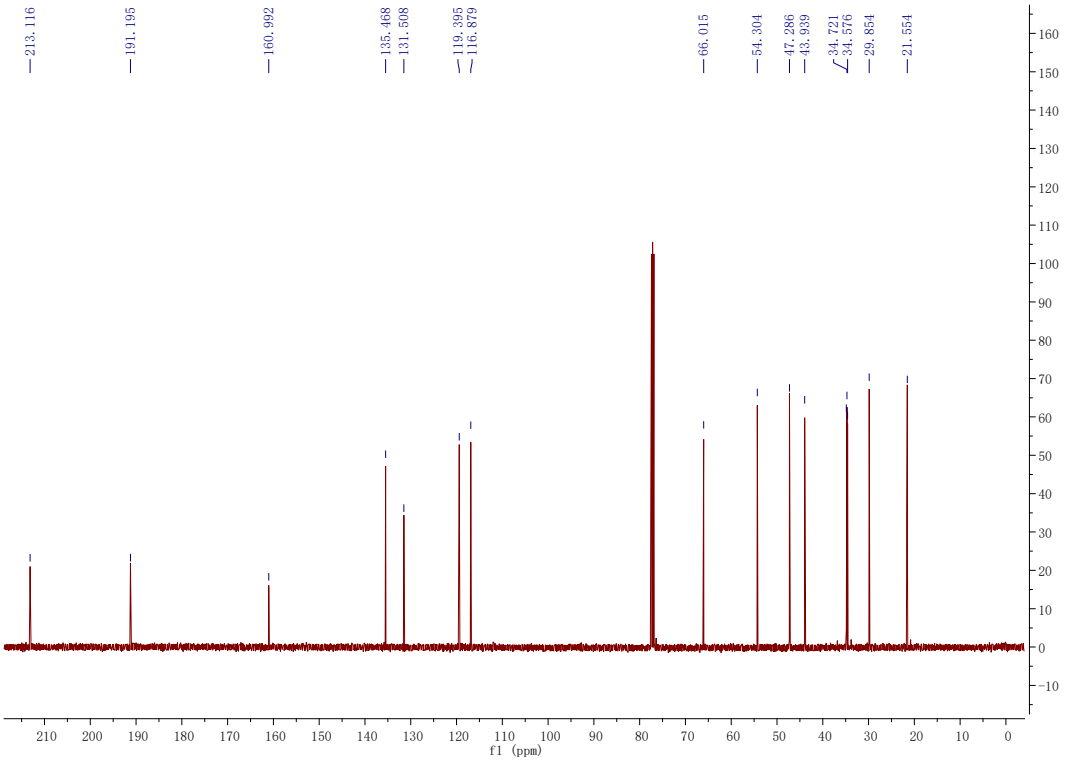
The COSY spectrum of **10** (major isomer)



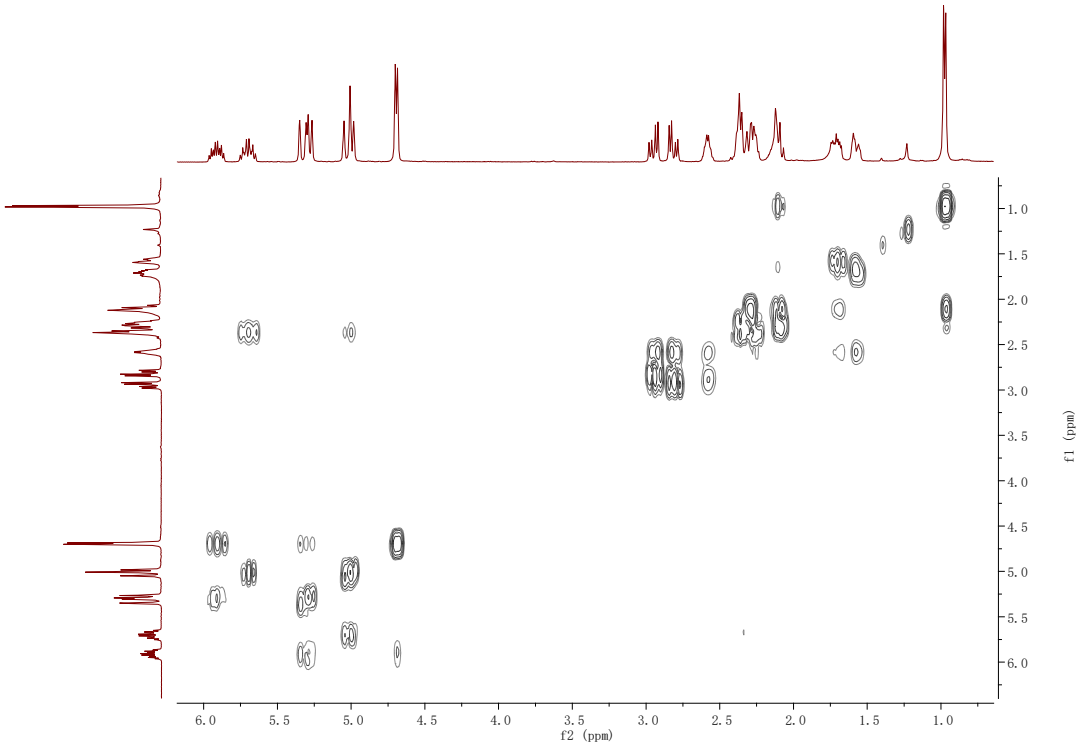
The NOE spectrum of **10** (major isomer)



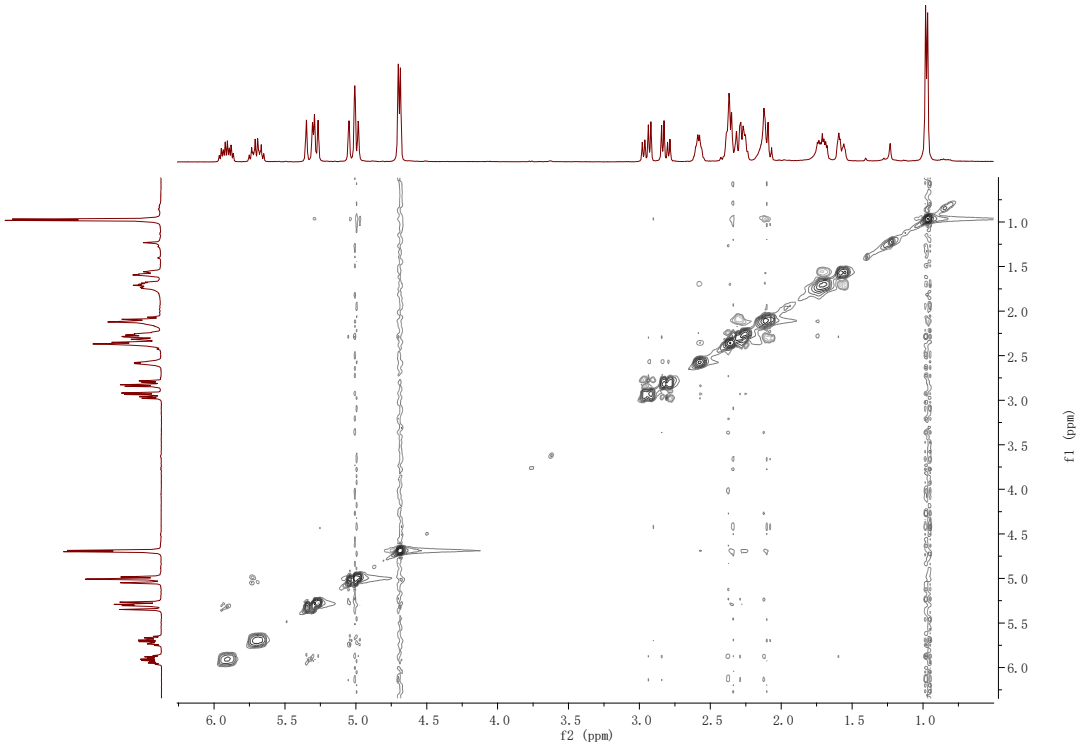
The ^{1}H NMR spectrum of **10** (minor isomer)



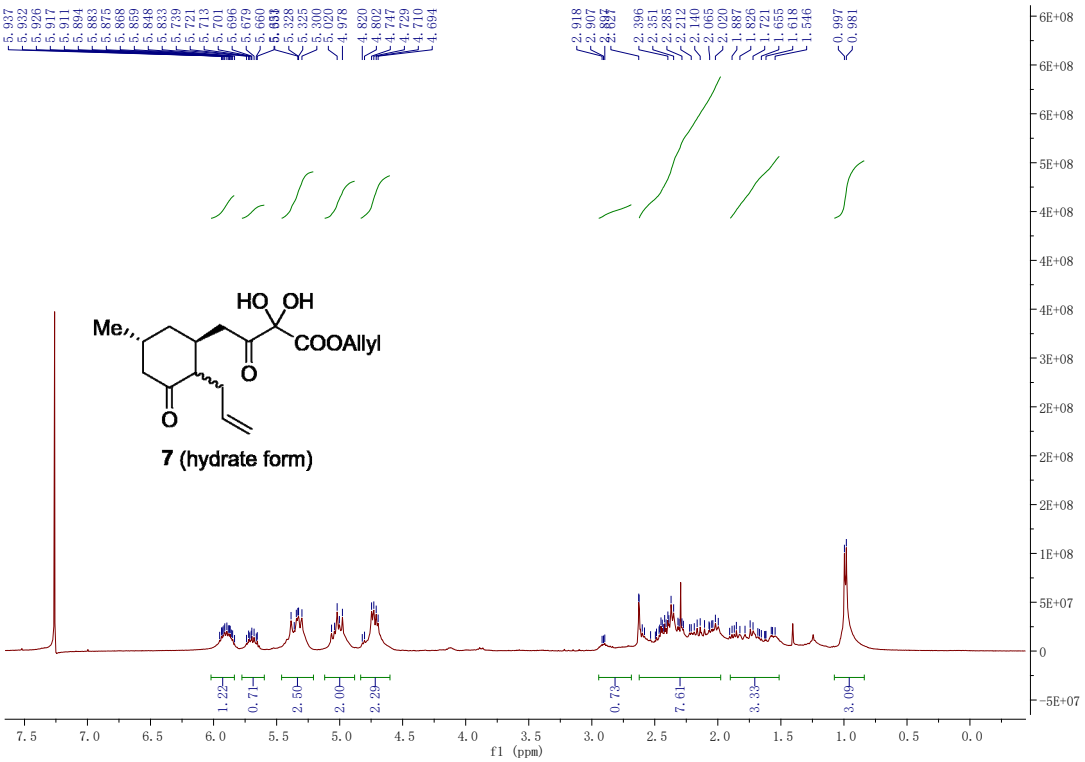
The ^{13}C NMR spectrum of **10** (minor isomer)



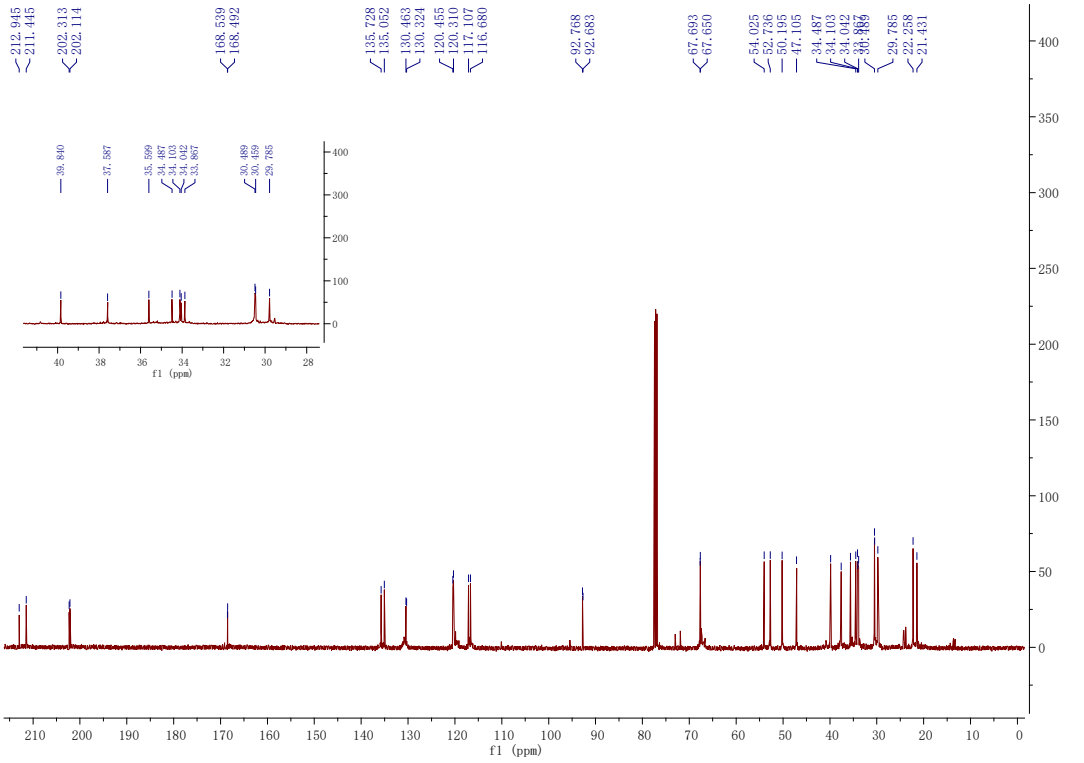
The COSY spectrum of **10** (minor isomer)



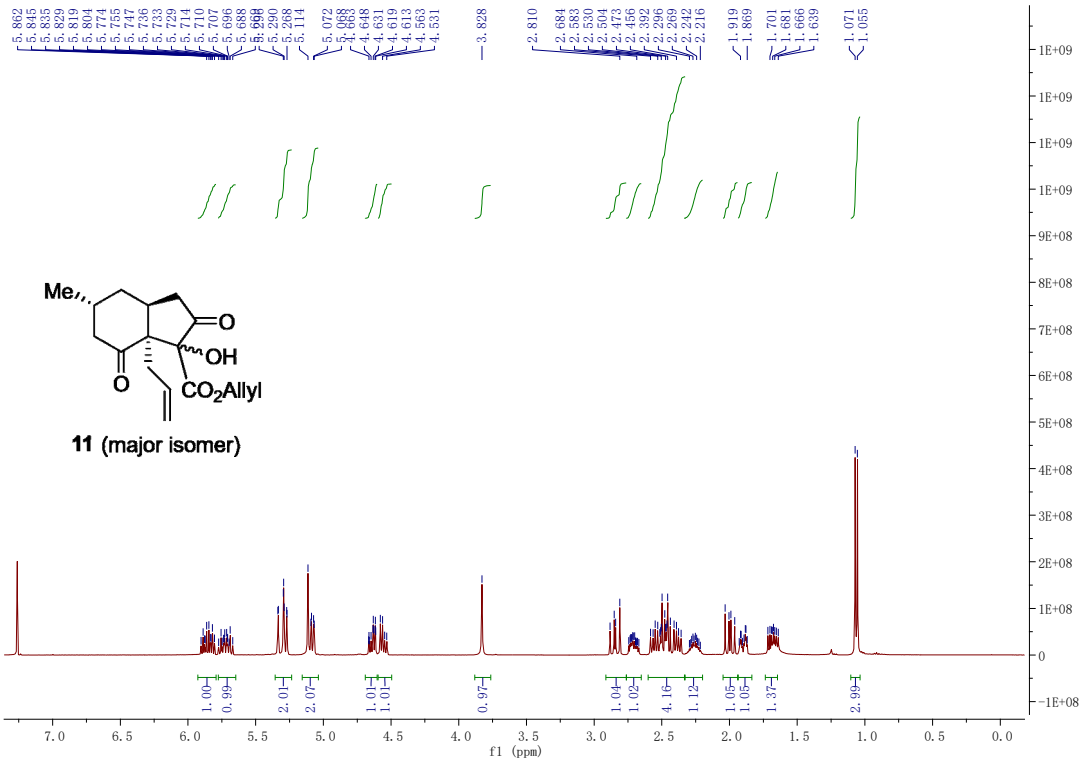
The NOE spectrum of **10** (minor isomer)



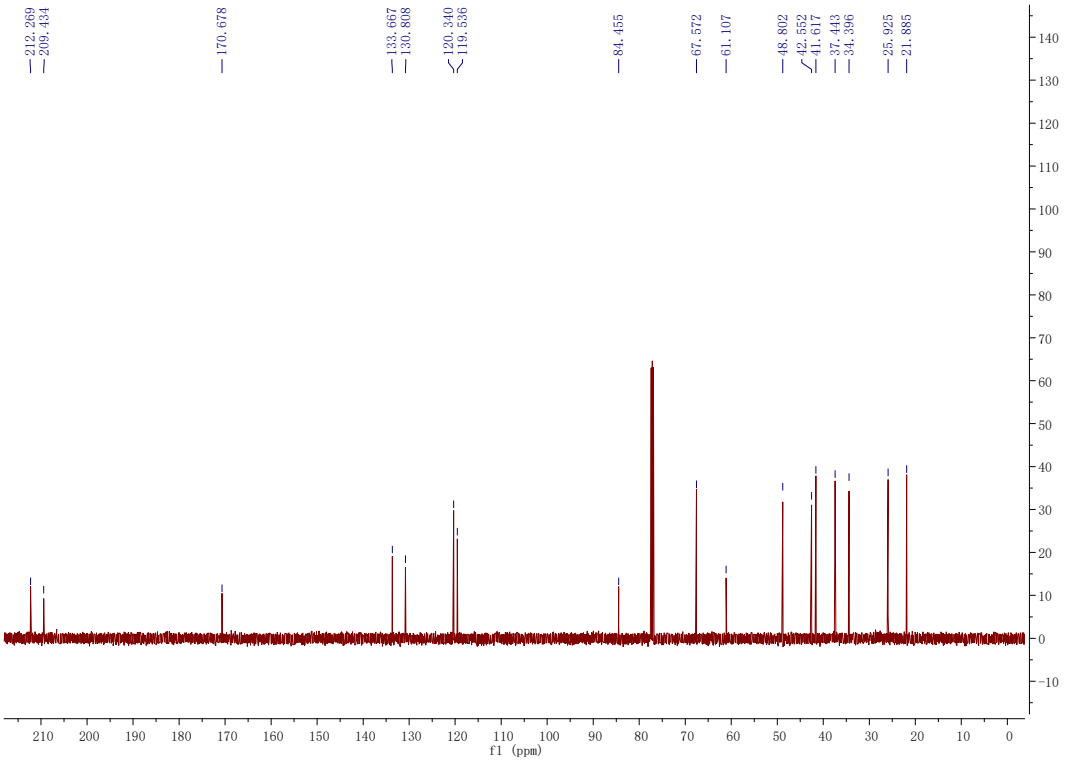
The ^{1}H NMR spectrum of **7** (hydrate form)



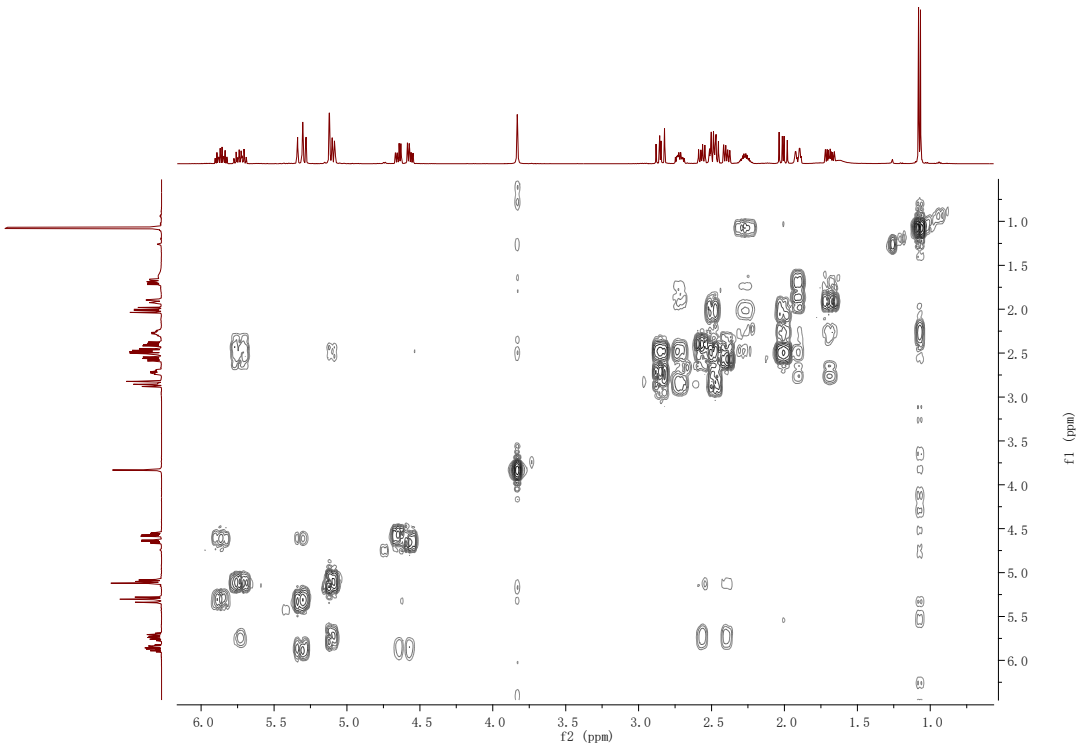
The ^{13}C NMR spectrum of **7** (hydrate form)



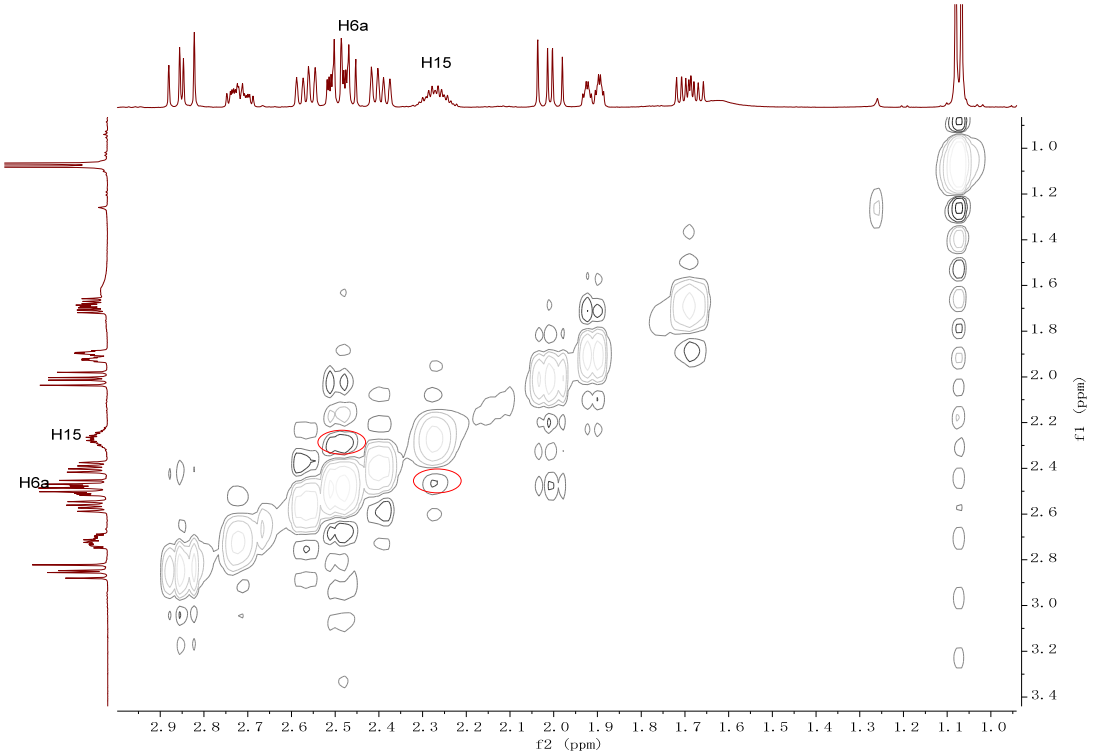
The ^{1}H NMR spectrum of **11** (major isomer)



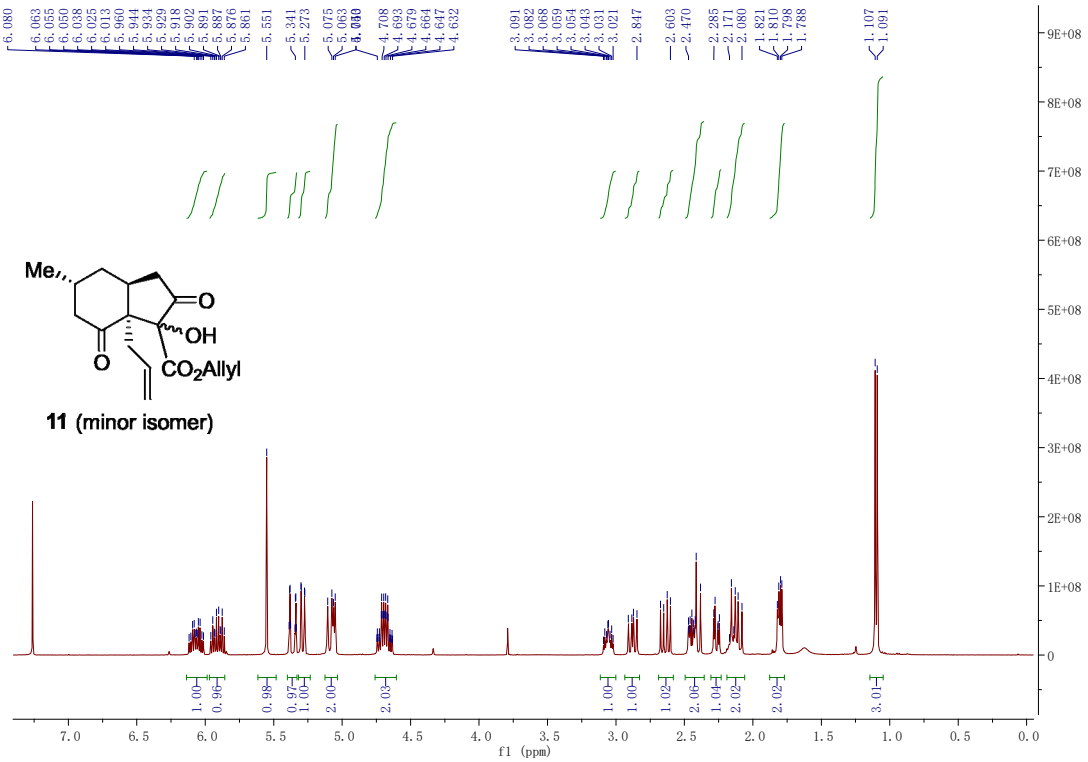
The ^{13}C NMR spectrum of **11** (major isomer)



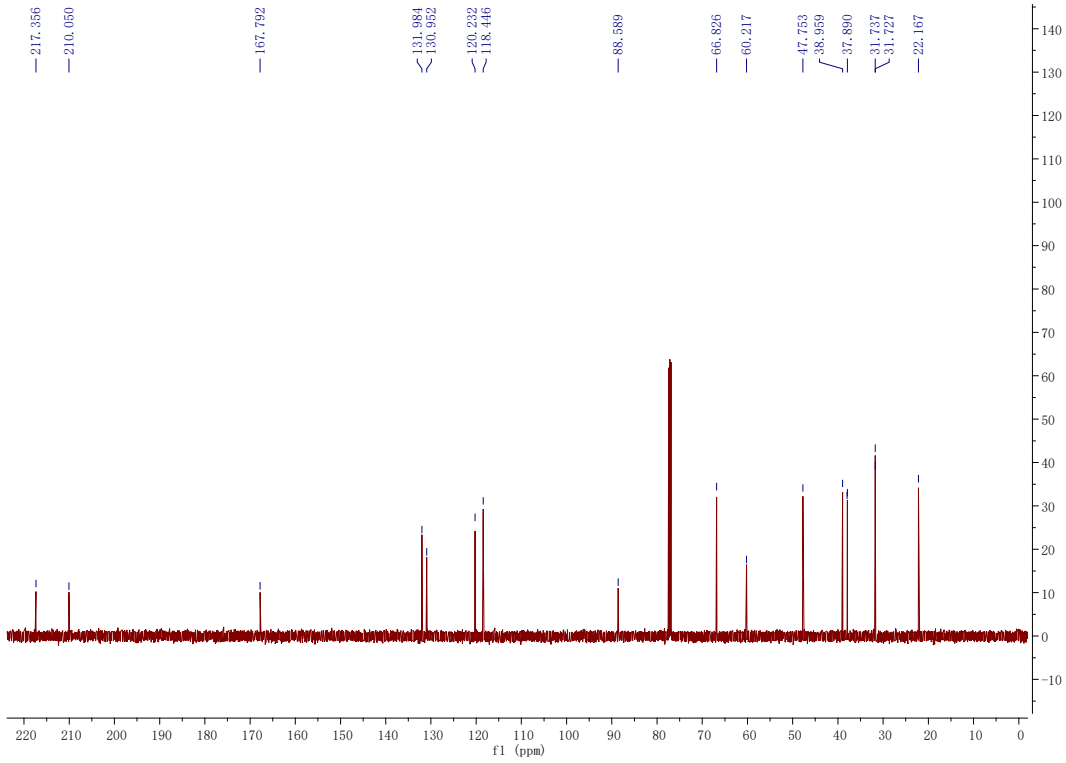
The COSY spectrum of **11** (major isomer)



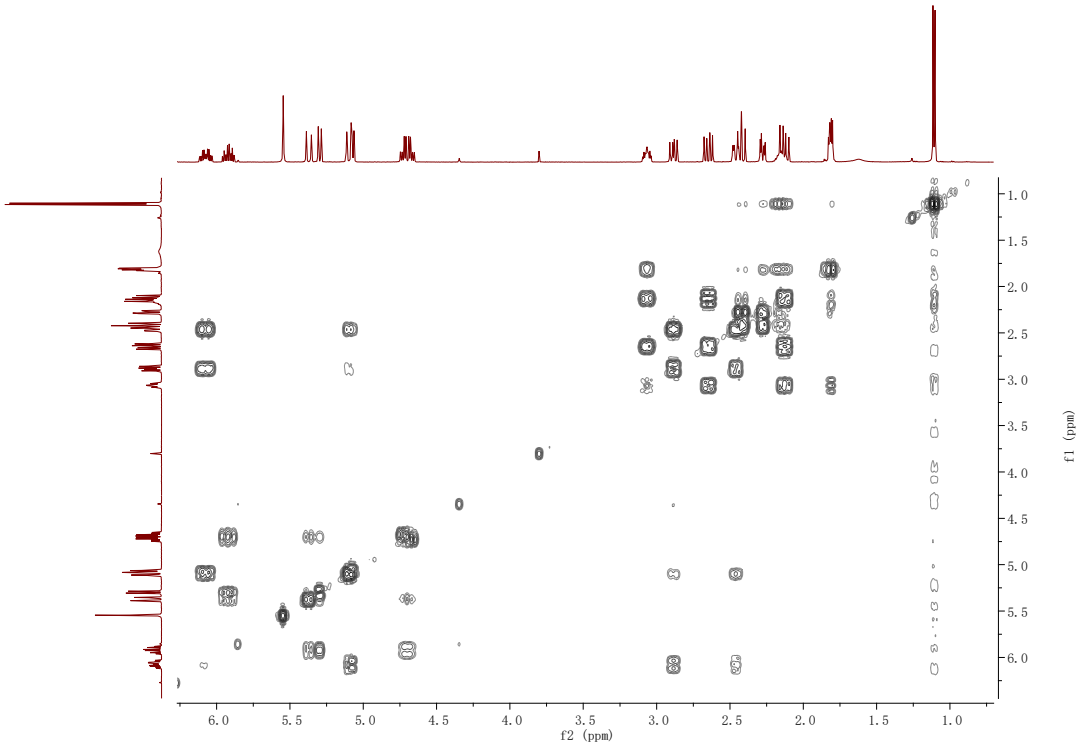
The NOE spectrum of **11** (major isomer)



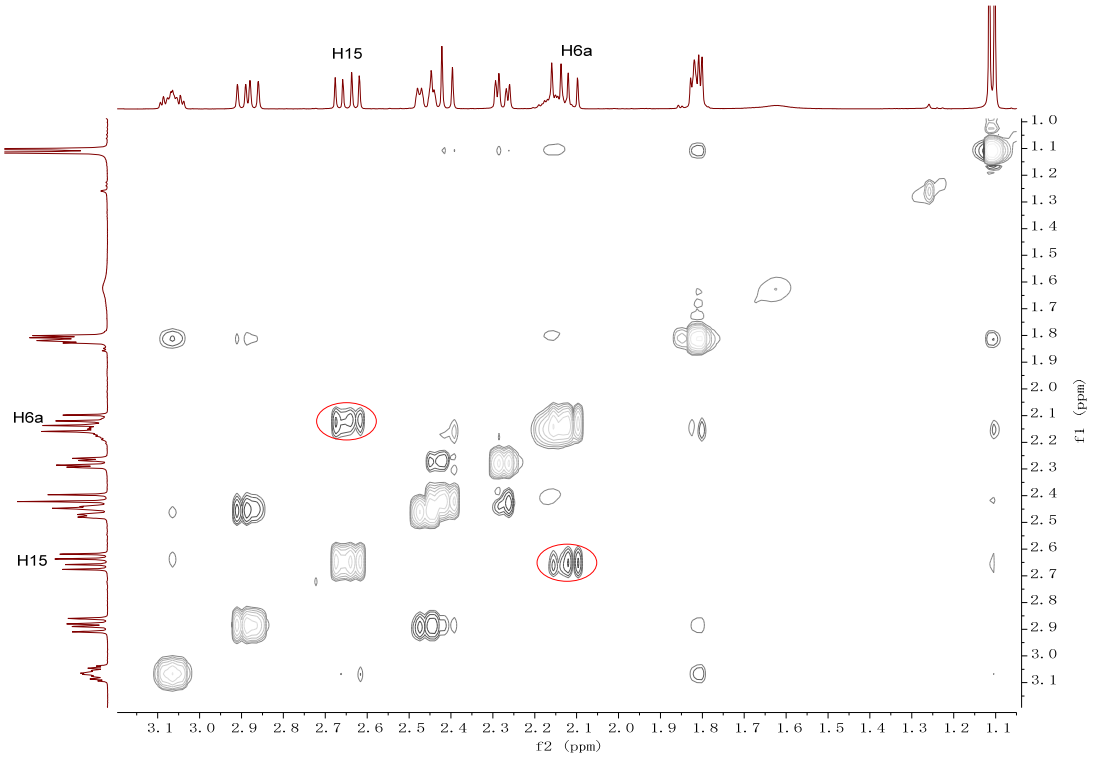
The ^{1}H NMR spectrum of **11** (minor isomer)



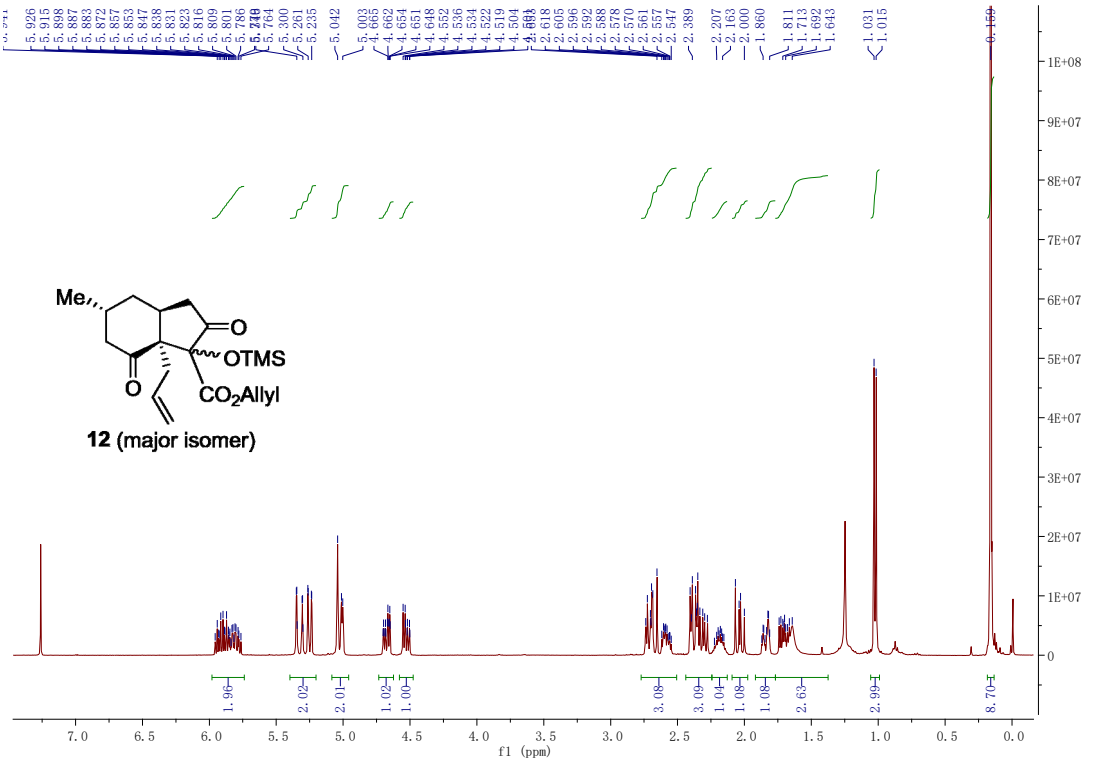
The ^{13}C NMR spectrum of **11** (minor isomer)



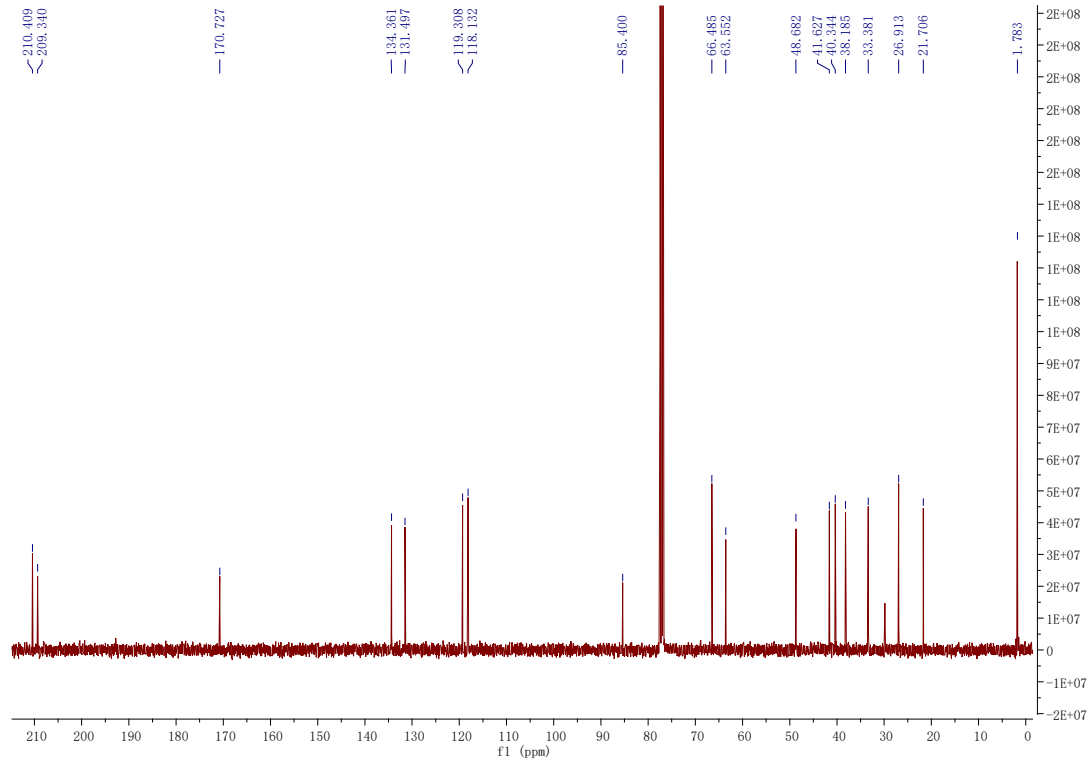
The COSY spectrum of **11** (minor isomer)



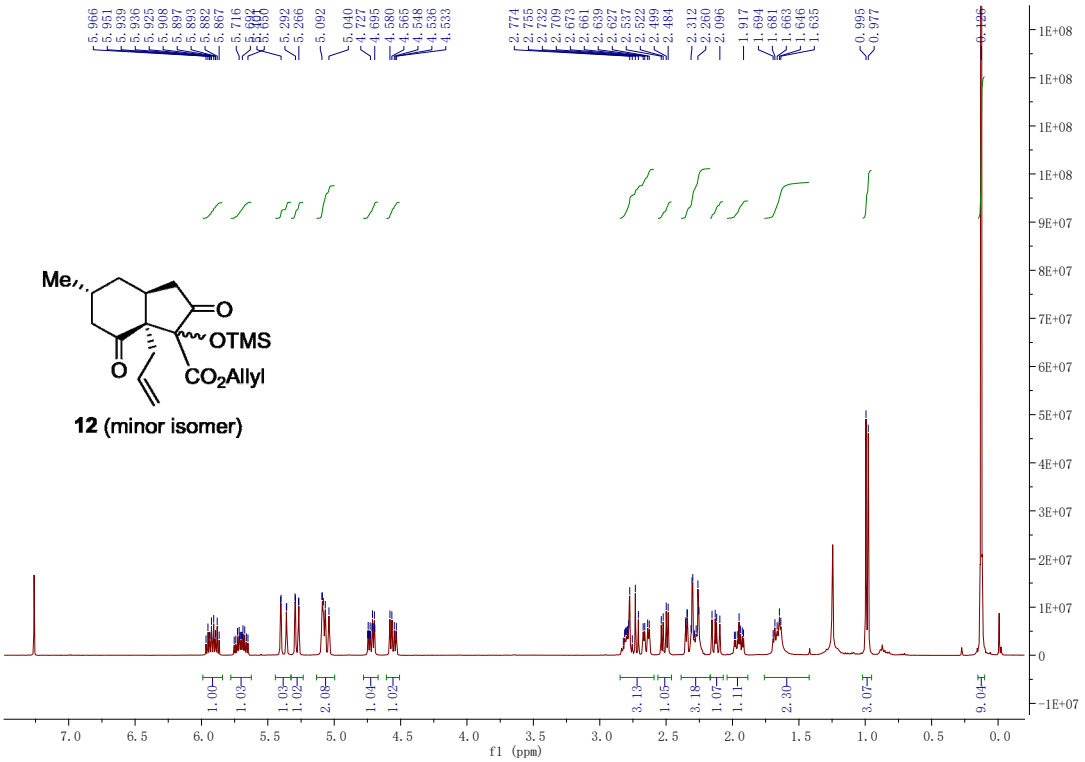
The NOE spectrum of **11** (minor isomer)



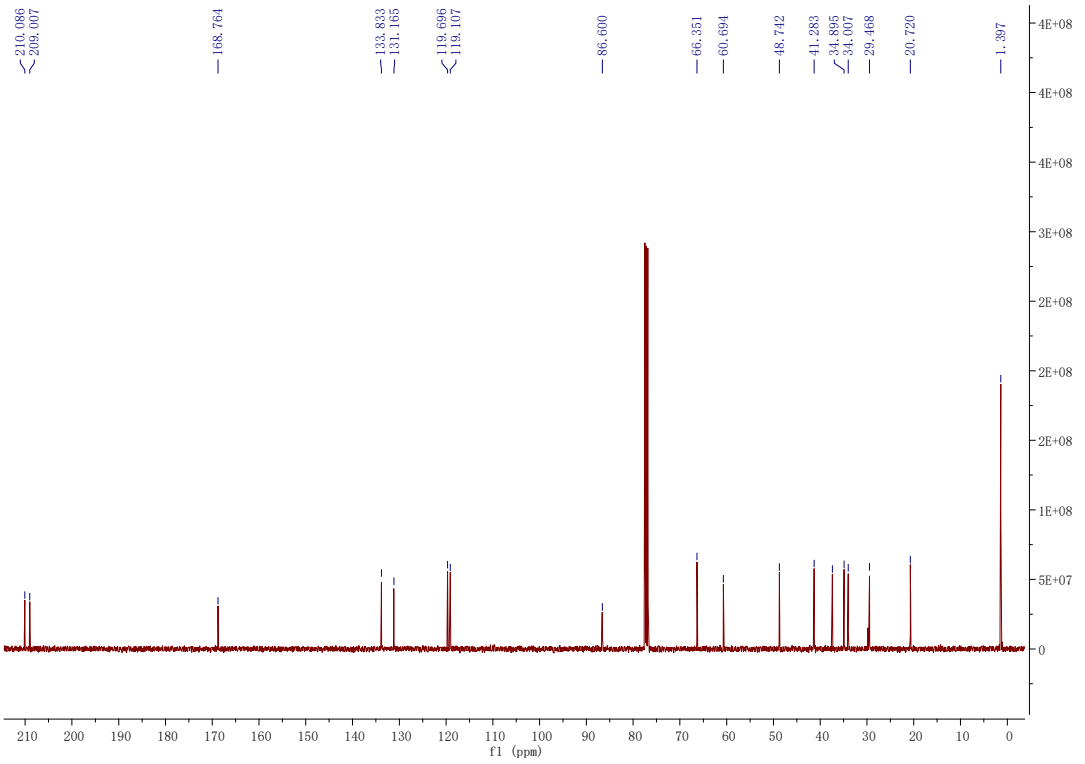
The ^{1}H NMR spectrum of **12** (major isomer)



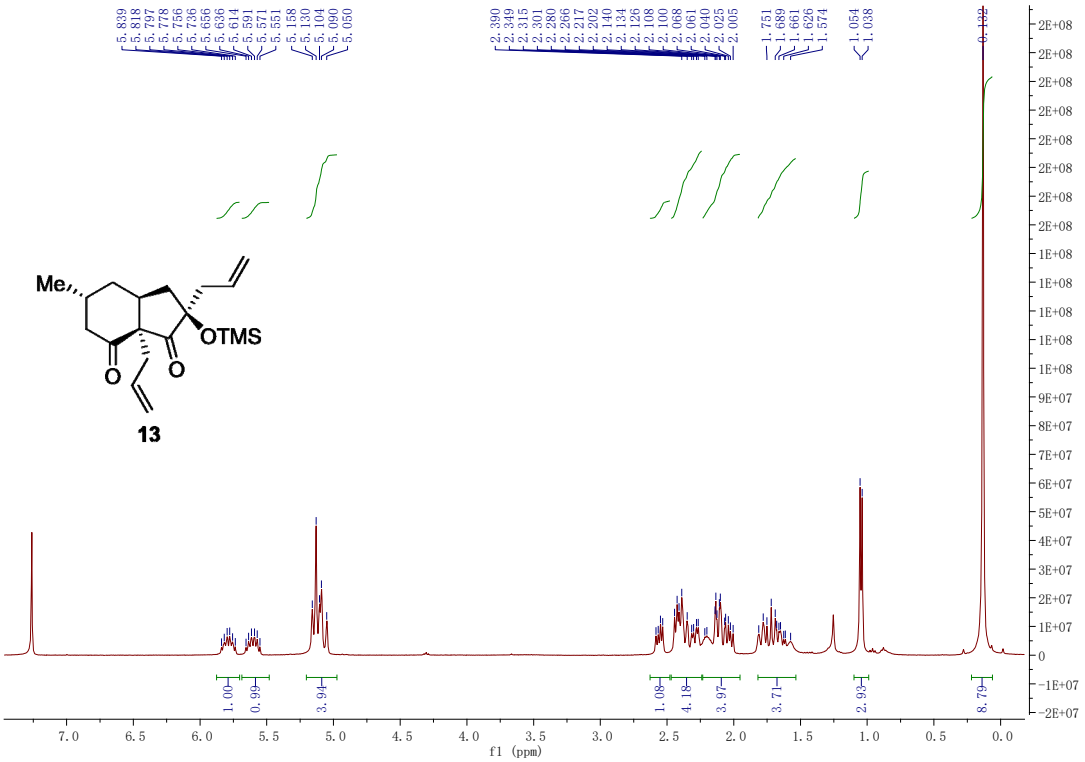
The ^{13}C NMR spectrum of **12** (major isomer)



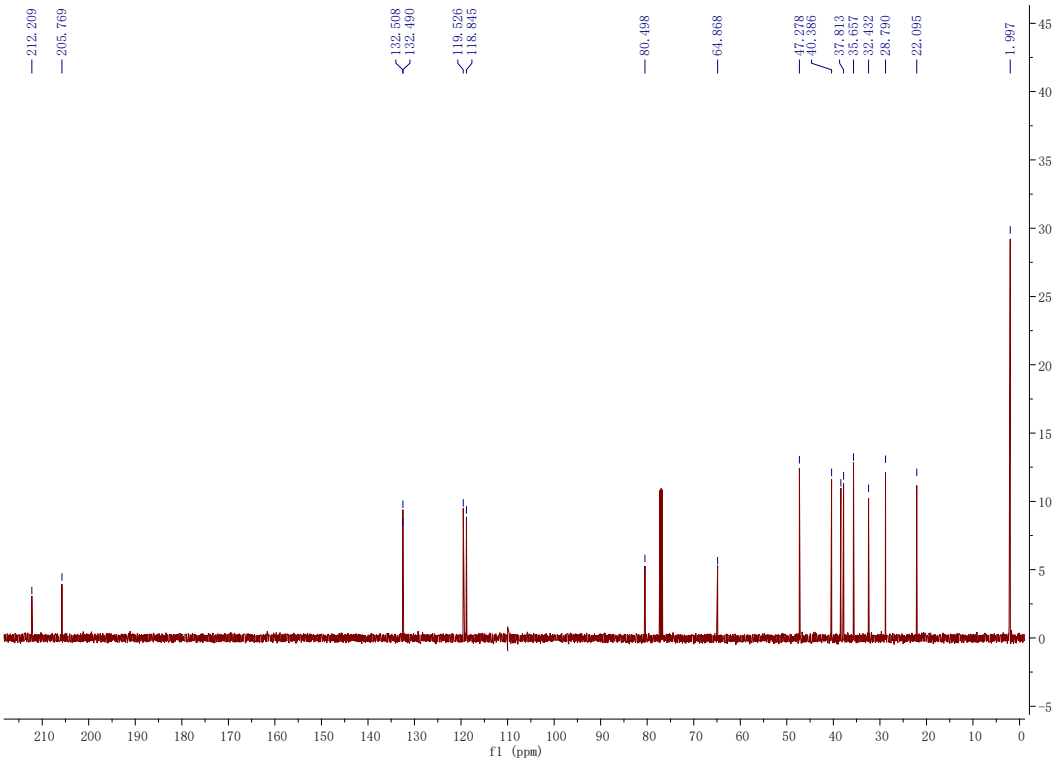
The ^{1}H NMR spectrum of **12** (minor isomer)



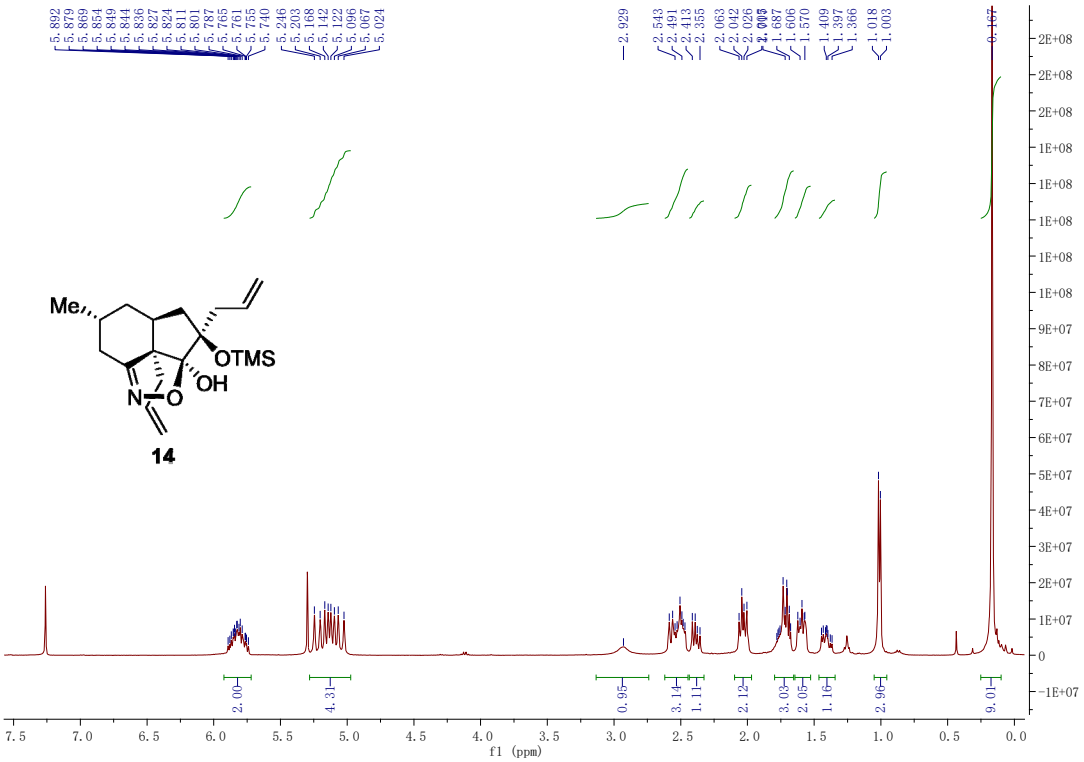
The ^{1}H NMR spectrum of **12** (minor isomer)



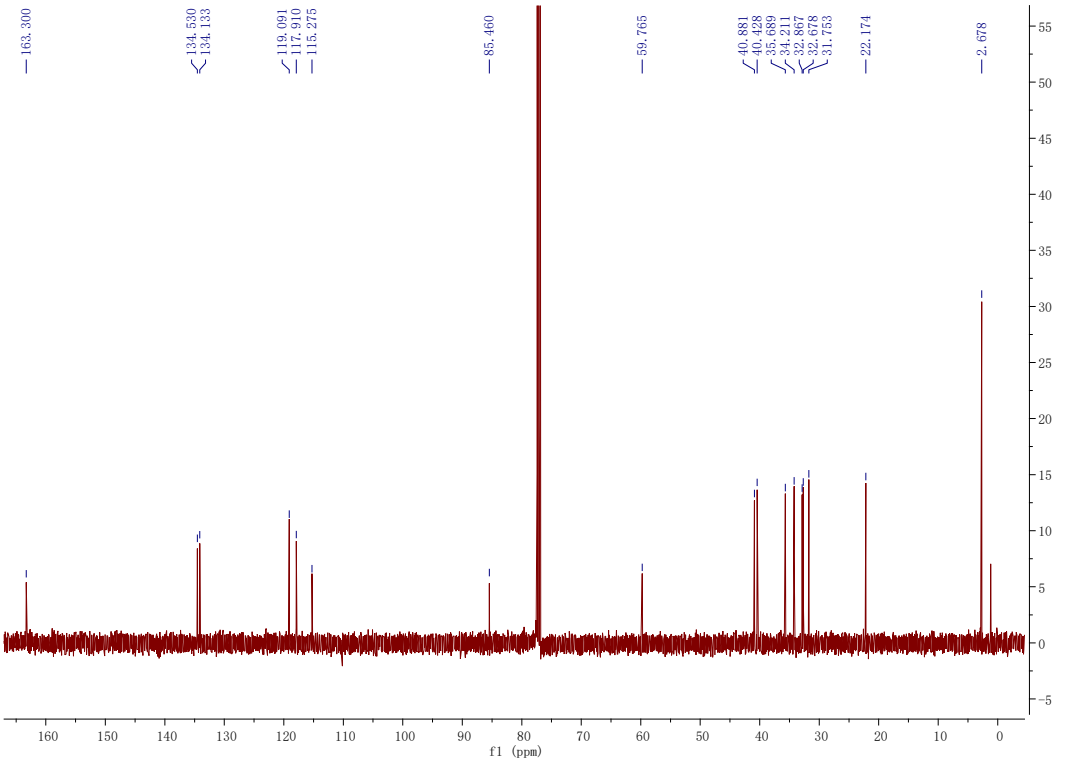
The ^{1}H NMR spectrum of **13**



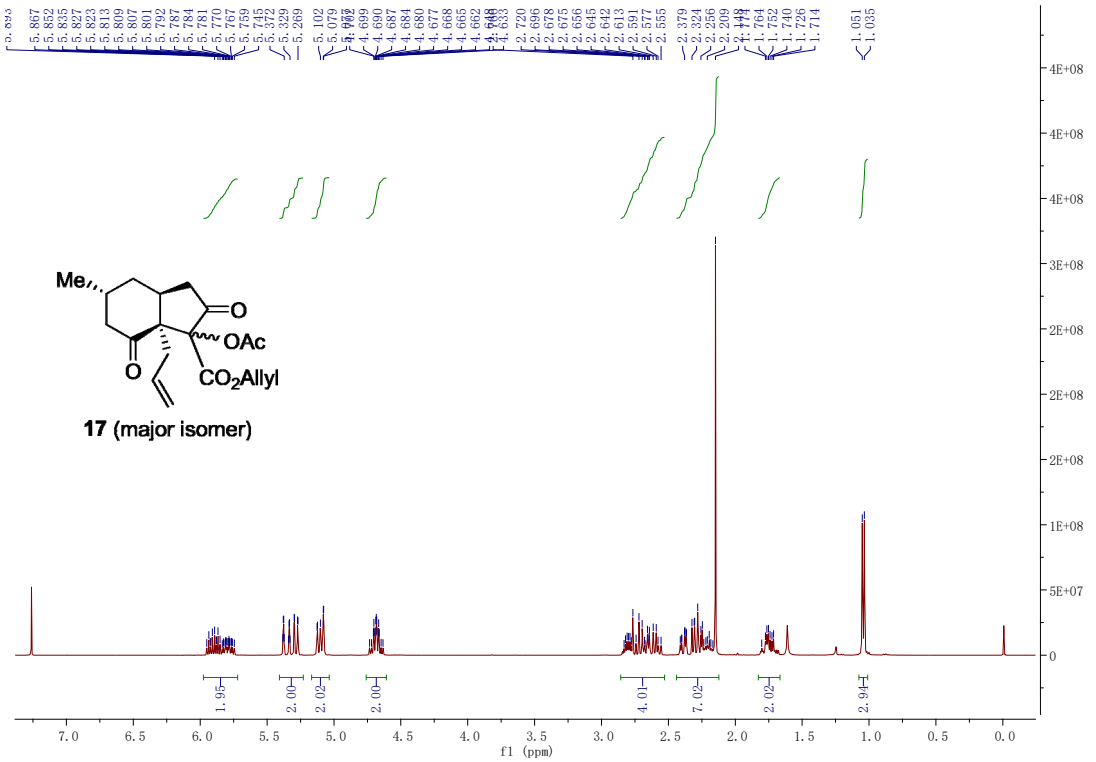
The ^{13}C NMR spectrum of **13**



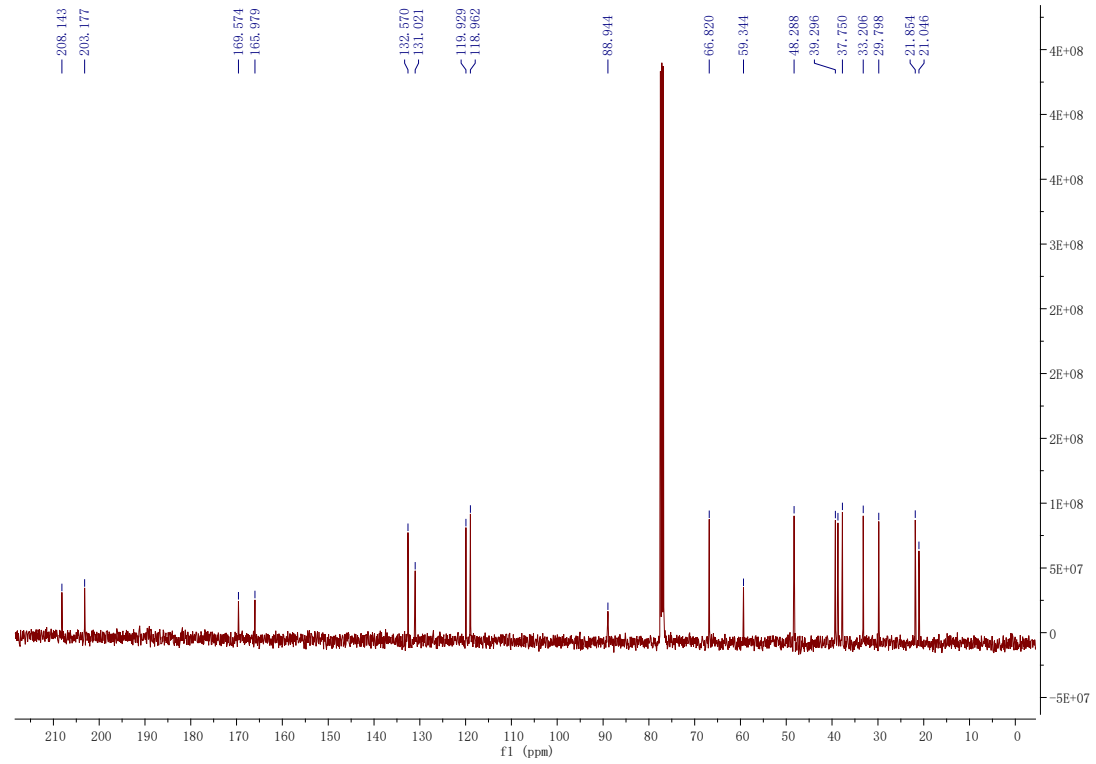
The ^{1}H NMR spectrum of **14**



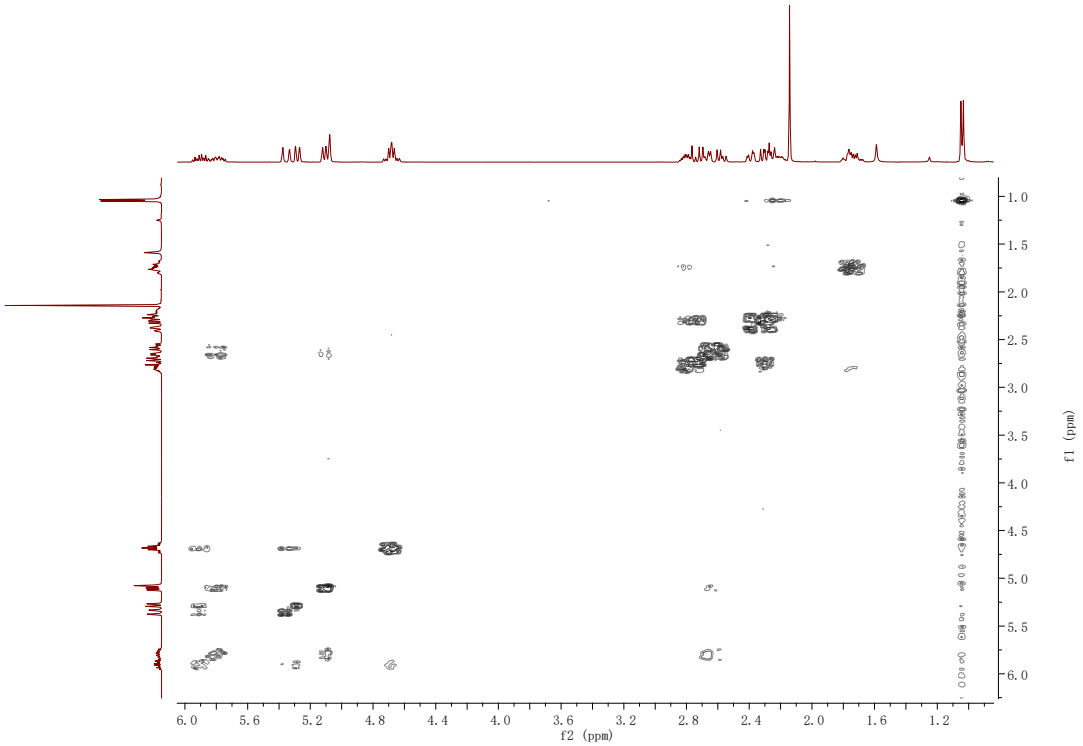
The ^{13}C NMR spectrum of **14**



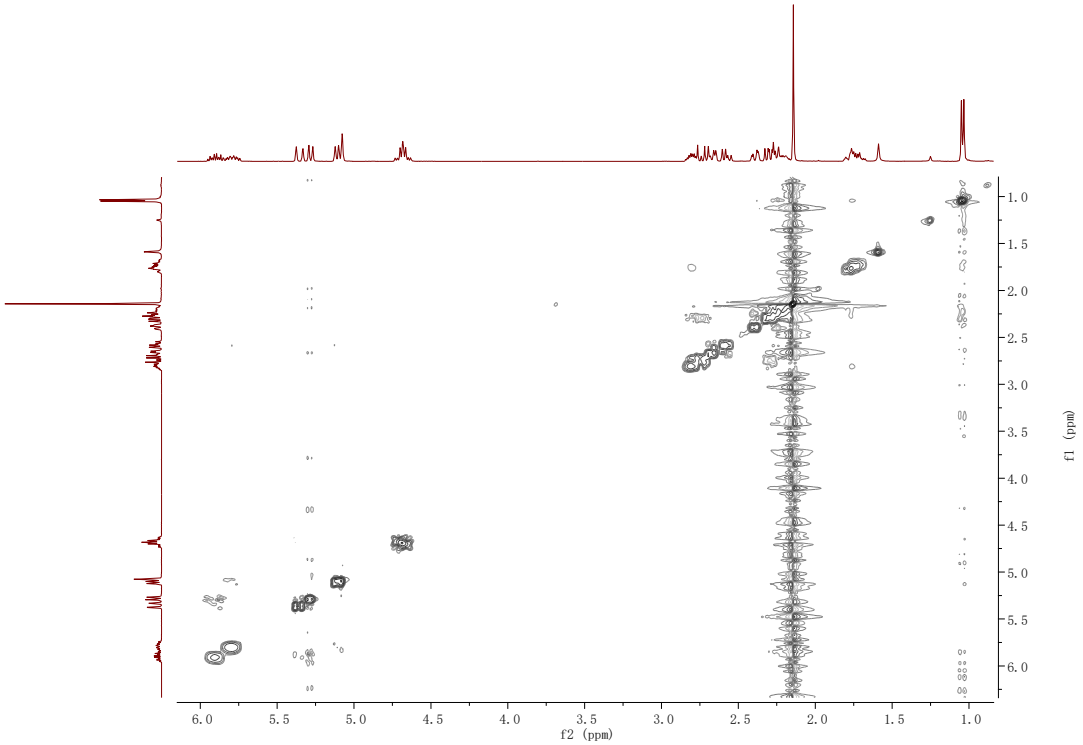
The ^{1}H NMR spectrum of **17** (major isomer)



The ^{13}C NMR spectrum of **17** (major isomer)

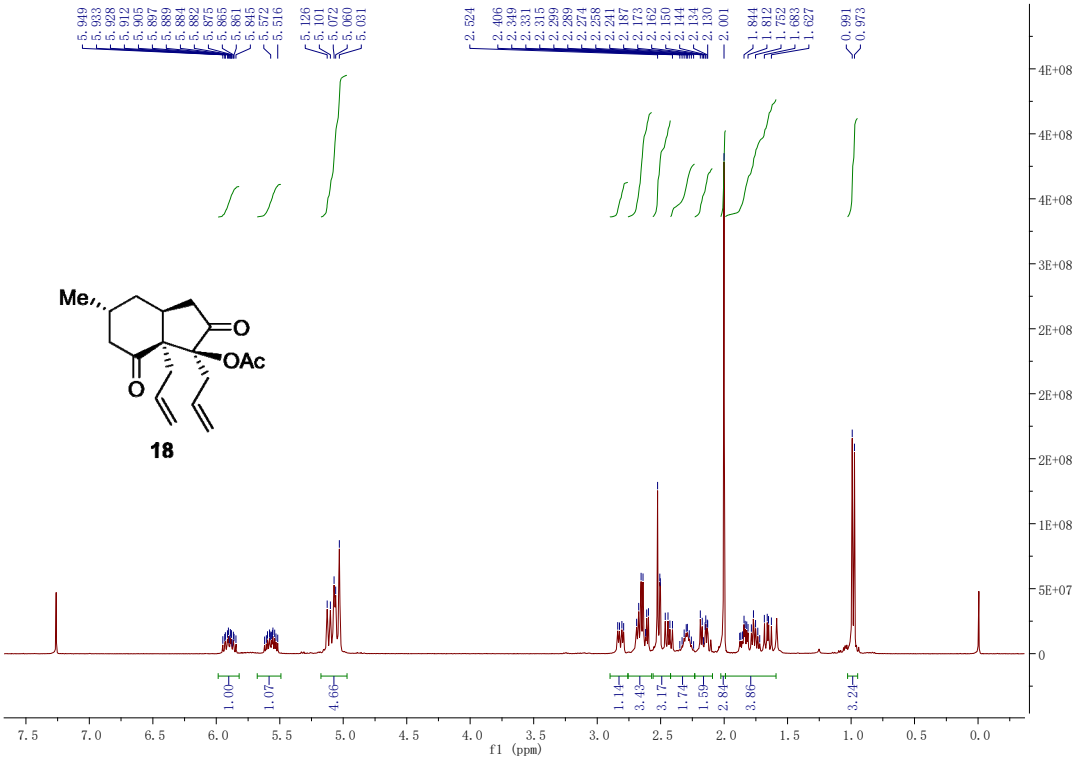


The COSY spectrum of **17** (major isomer)

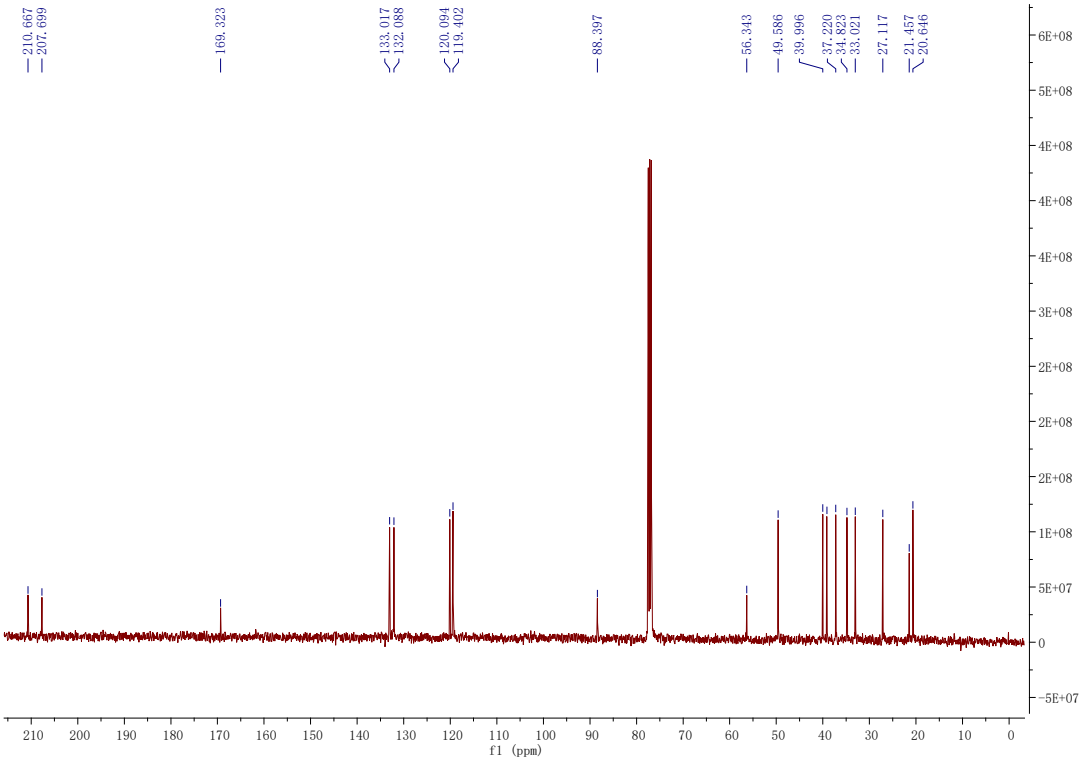


The NOE spectrum of **17** (major isomer)

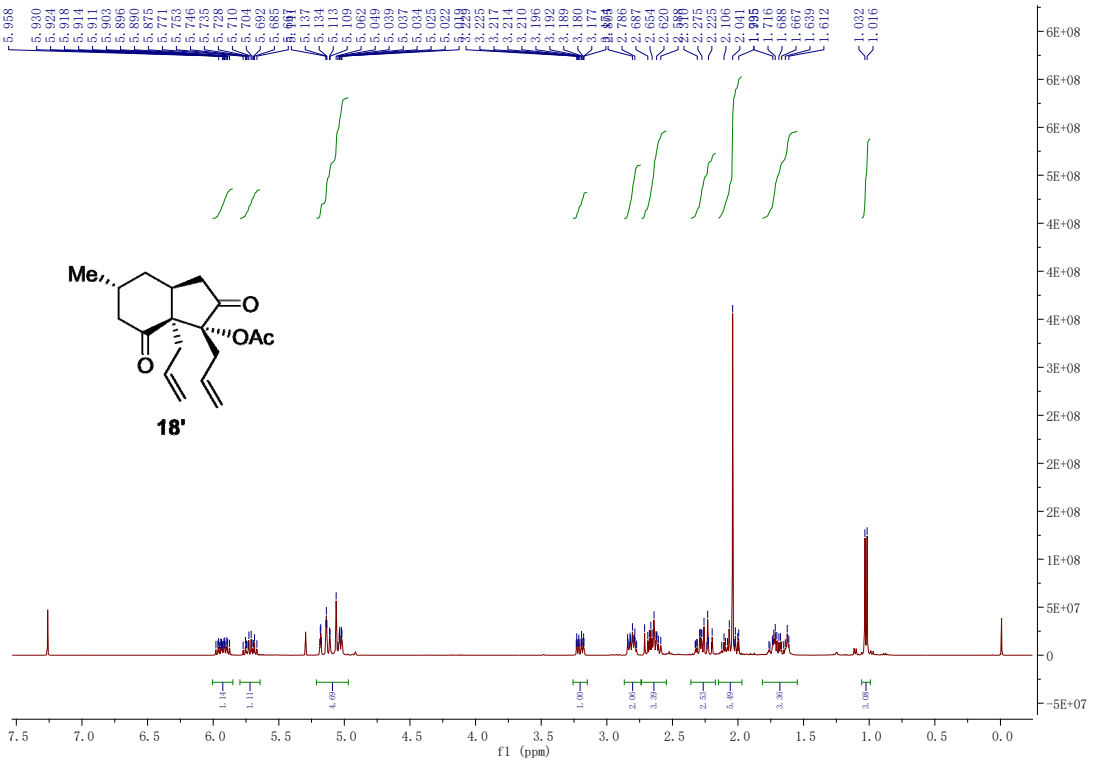
The minor isomer of **17** decomposed smoothly (acetyl removed) in column chromatography, preparative thin layer chromatography or HPLC so no clear NMR data were recorded



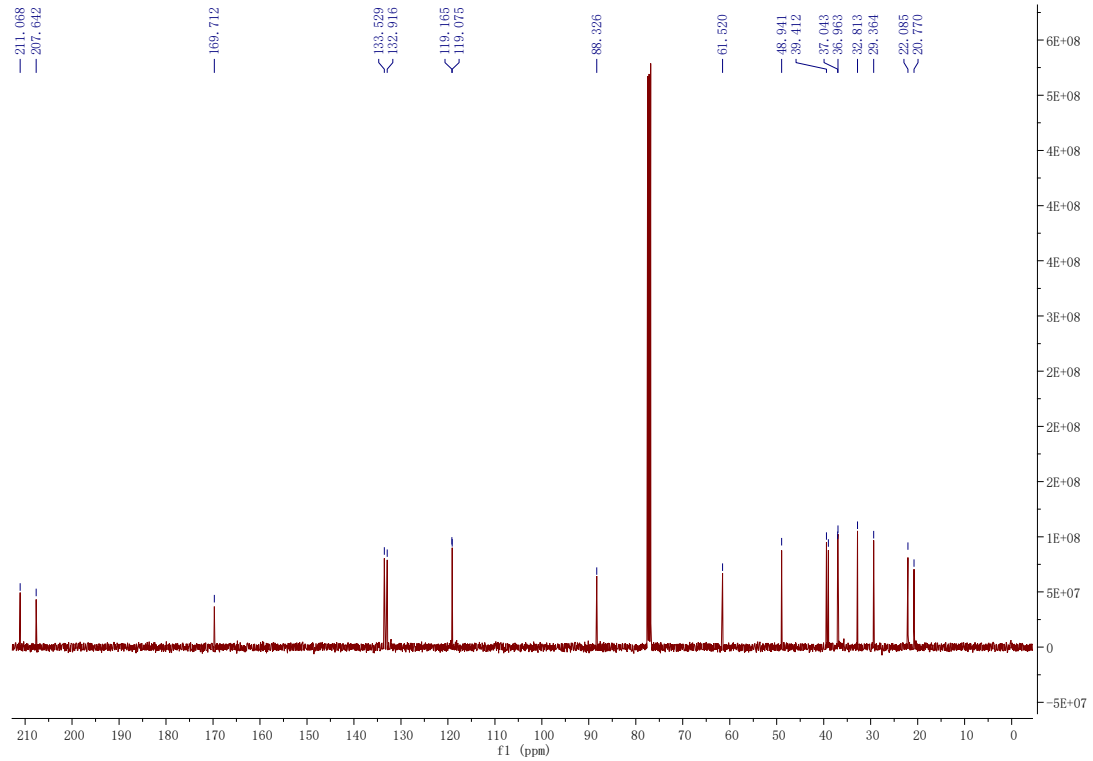
The ^{1}H NMR spectrum of **18**



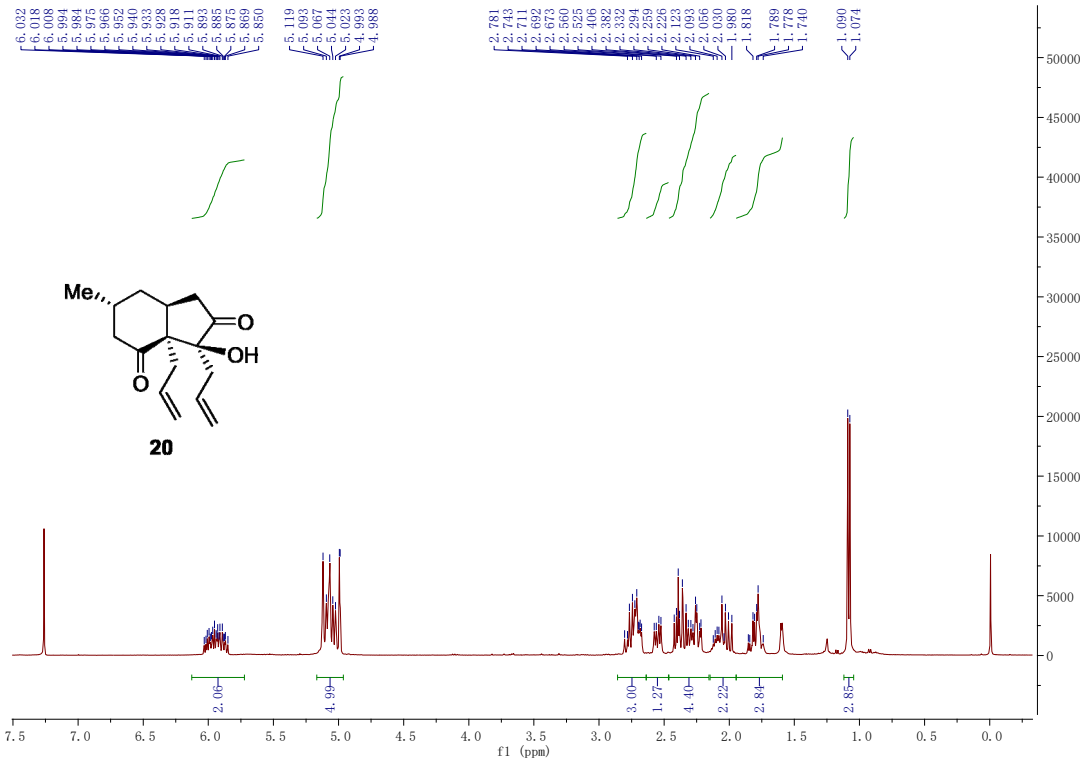
The ^{13}C NMR spectrum of **18**



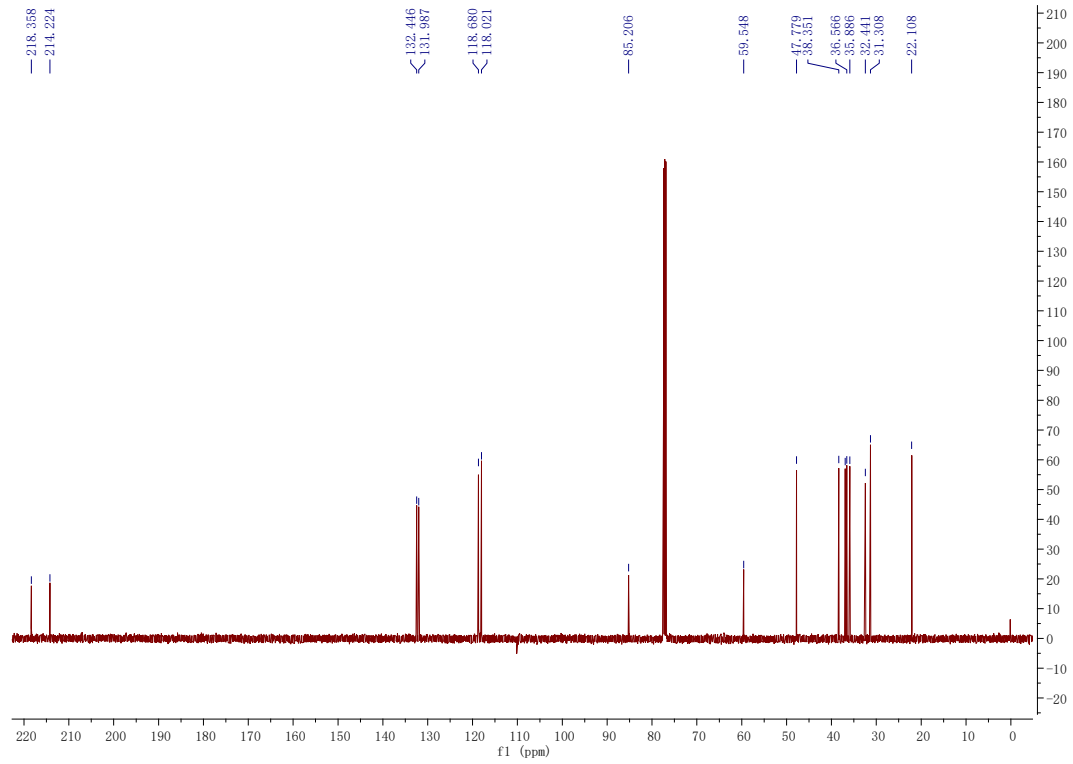
The ^{1}H NMR spectrum of **18'**



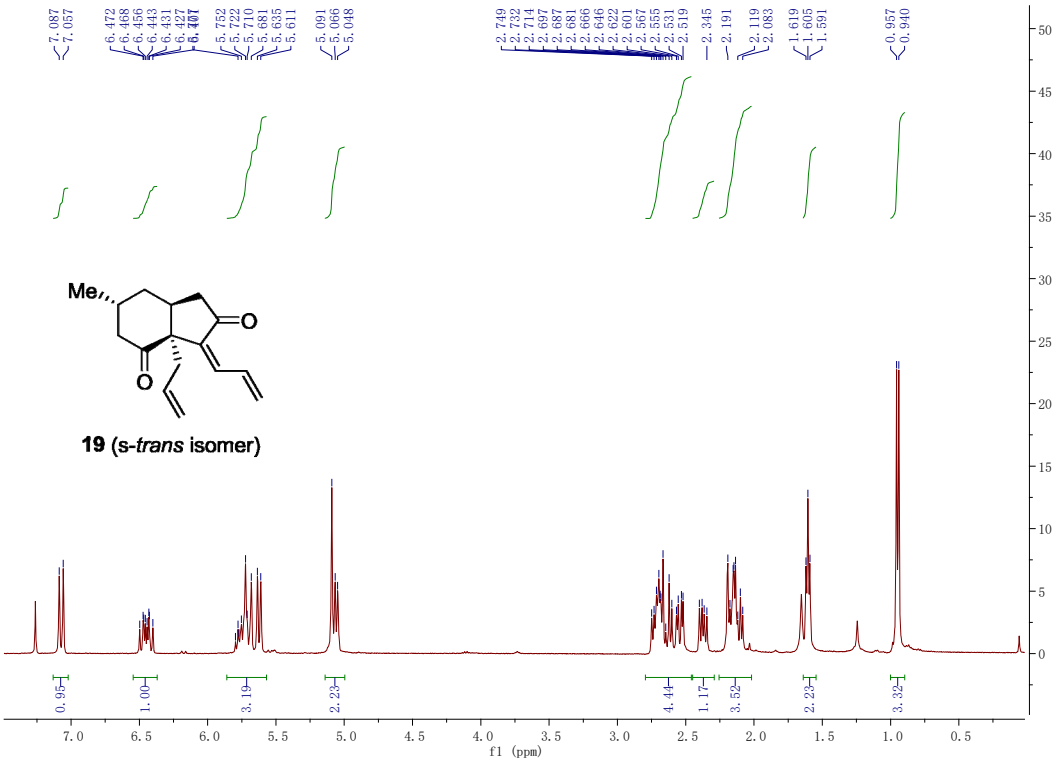
The ^{13}C NMR spectrum of **18'**



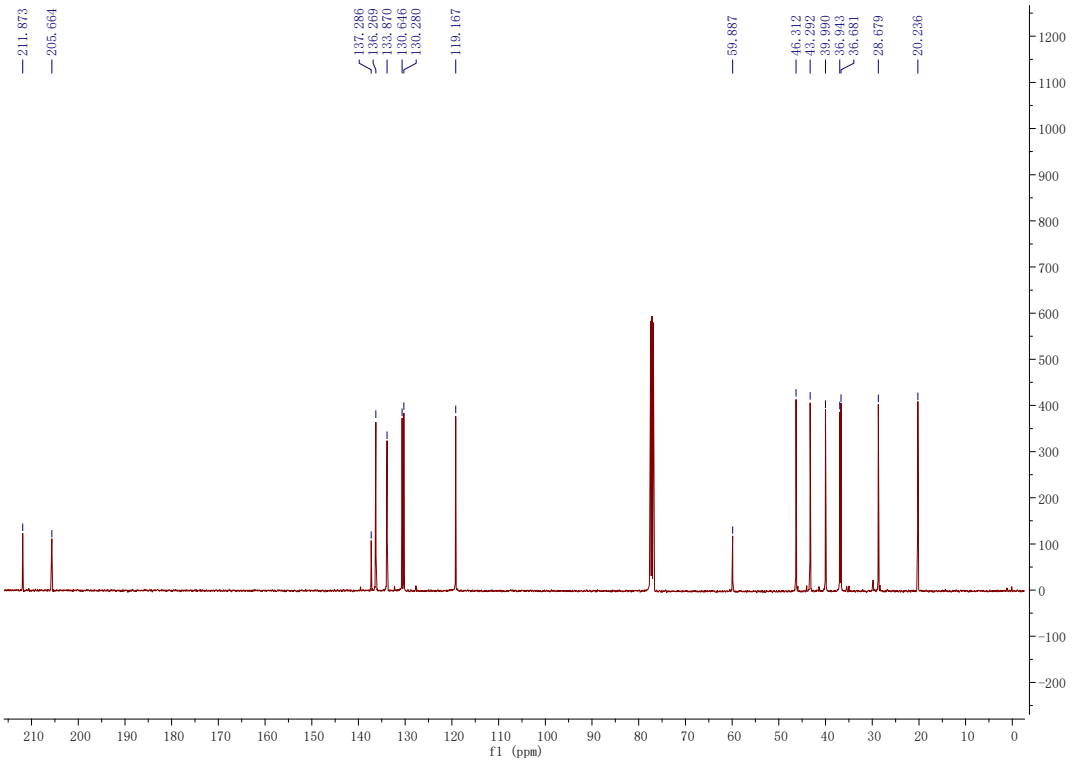
The ^{1}H NMR spectrum of **20**



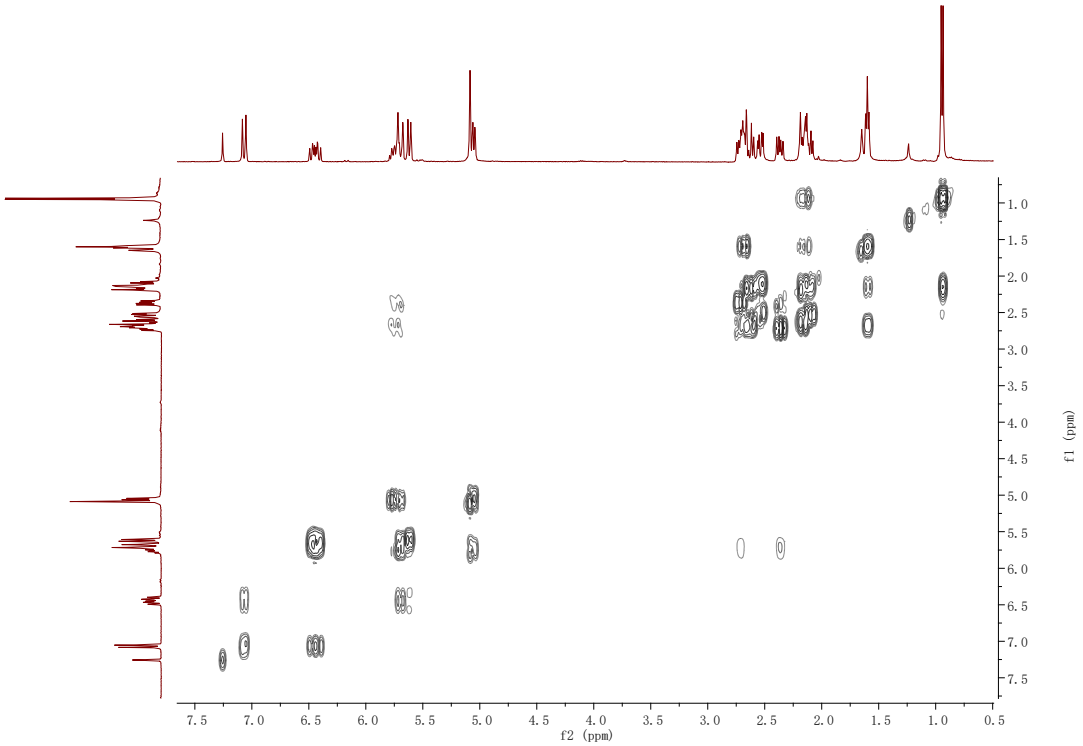
The ^{13}C NMR spectrum of **20**



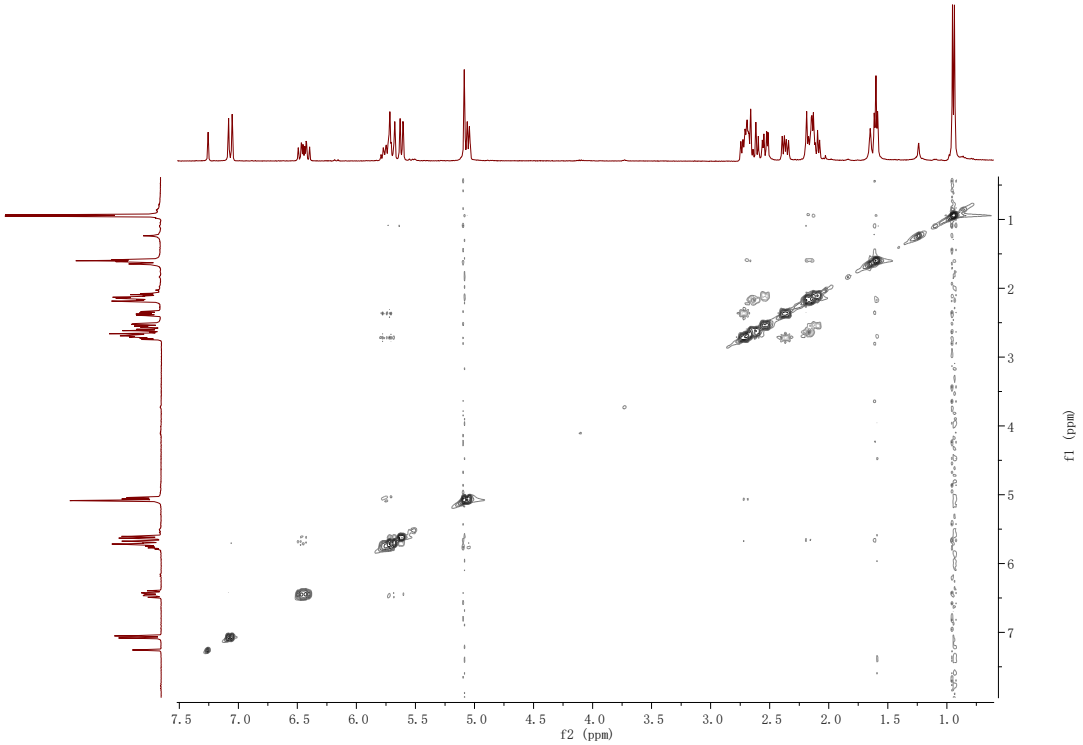
The ^{1}H NMR spectrum of **19** (s-*trans* isomer)



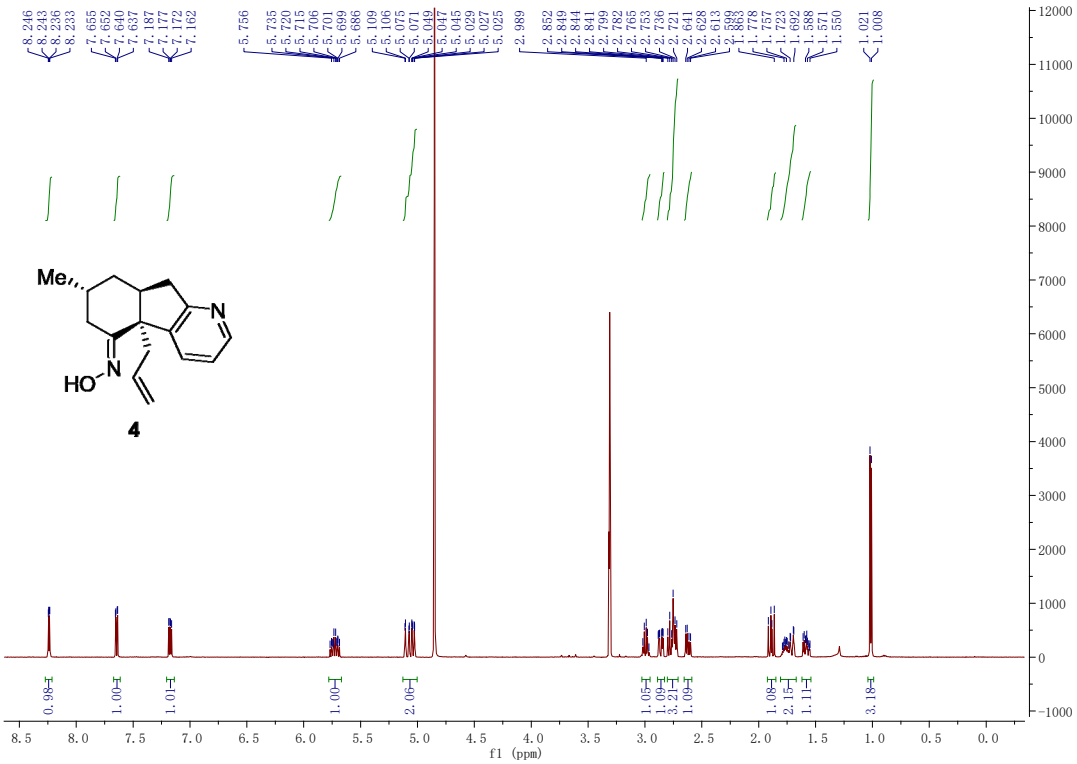
The ^{13}C NMR spectrum of **19** (s-*trans* isomer)



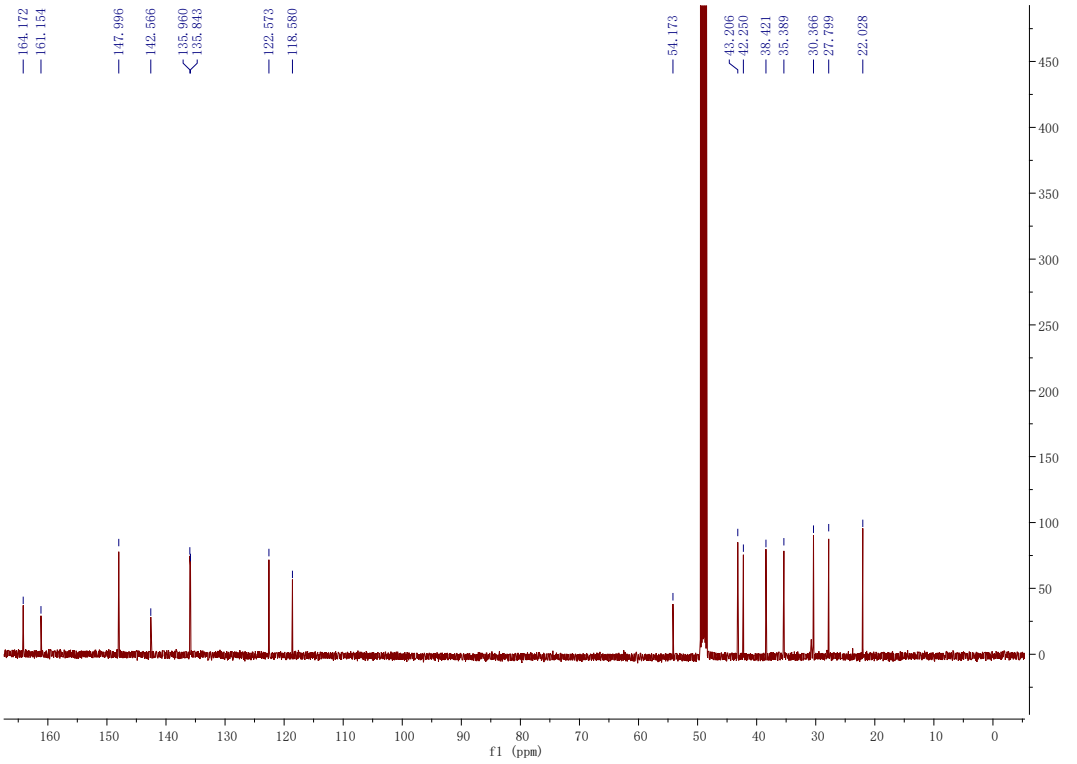
The COSY spectrum of **19** (s-*trans* isomer)



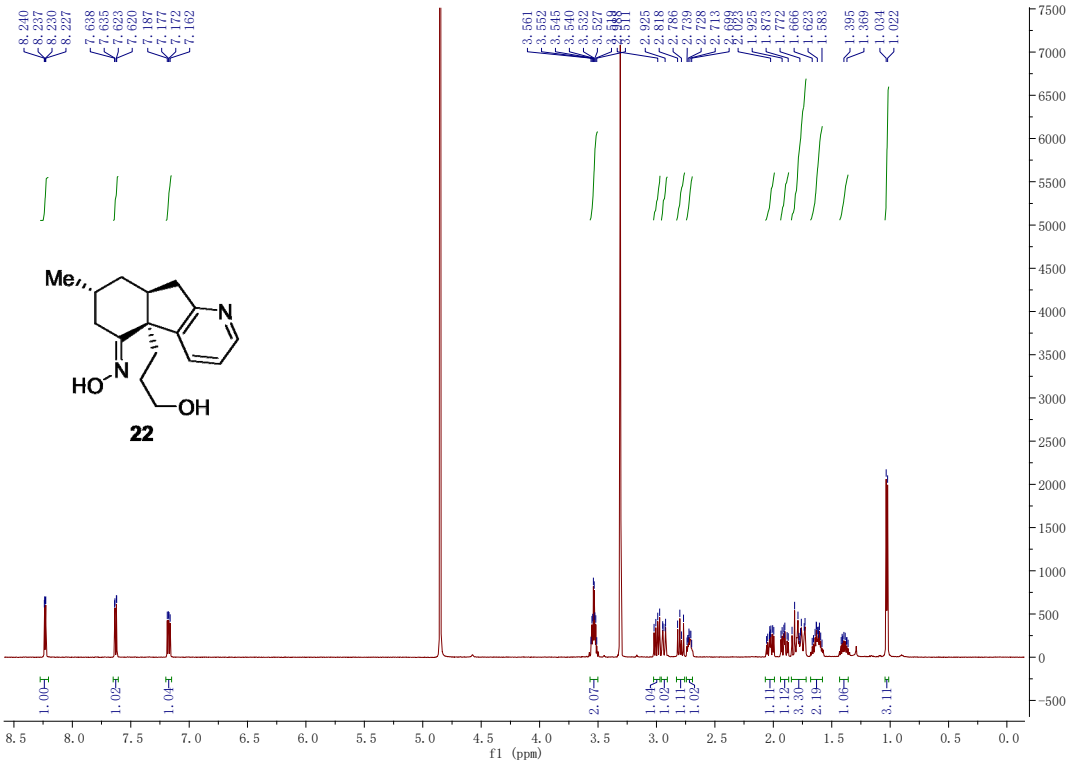
The NOE spectrum of **19** (s-*trans* isomer)



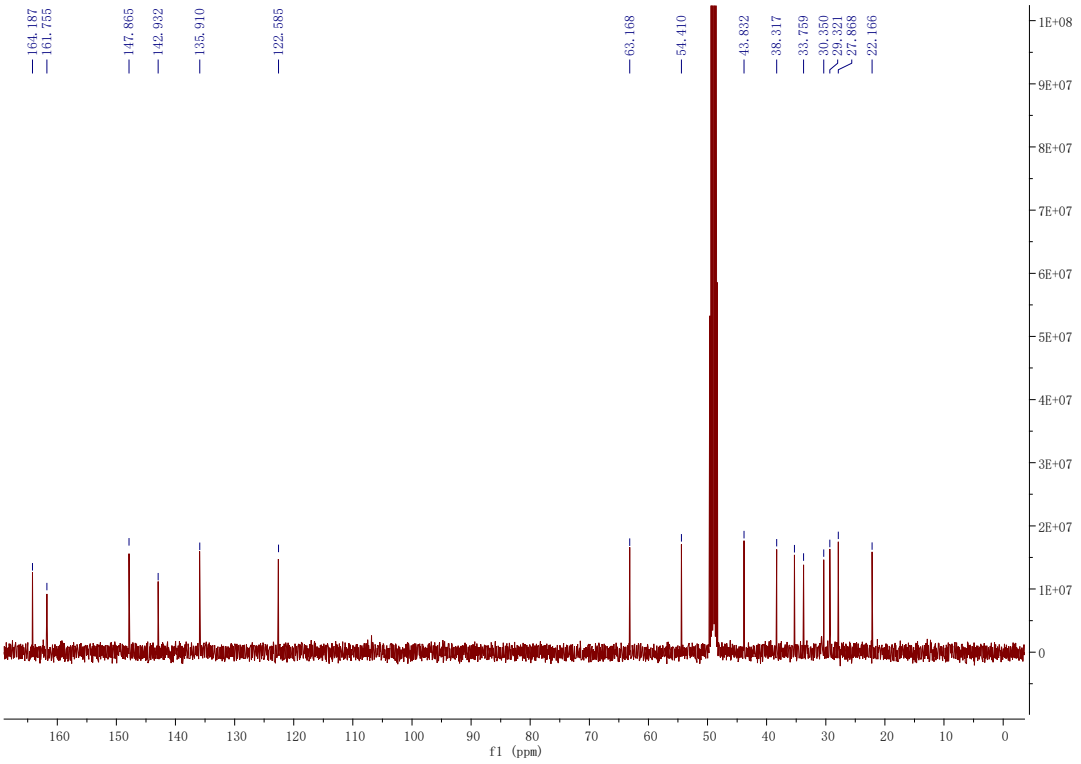
The ^{1}H NMR spectrum of **4**



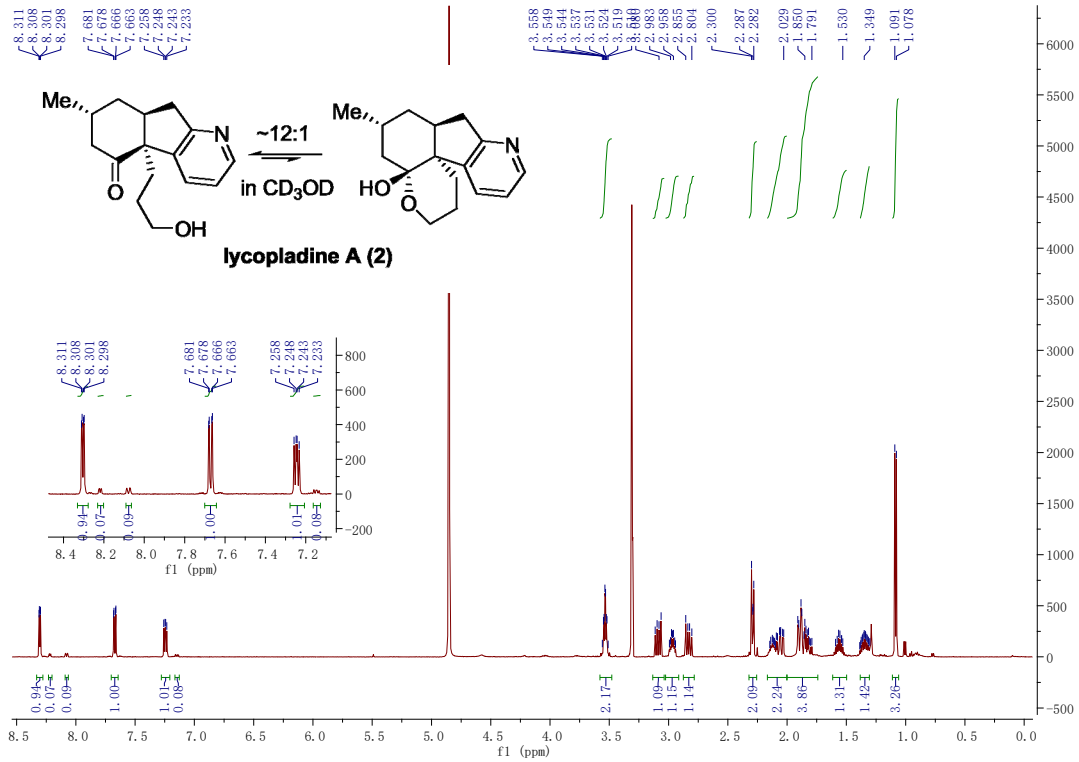
The ^{13}C NMR spectrum of **4**



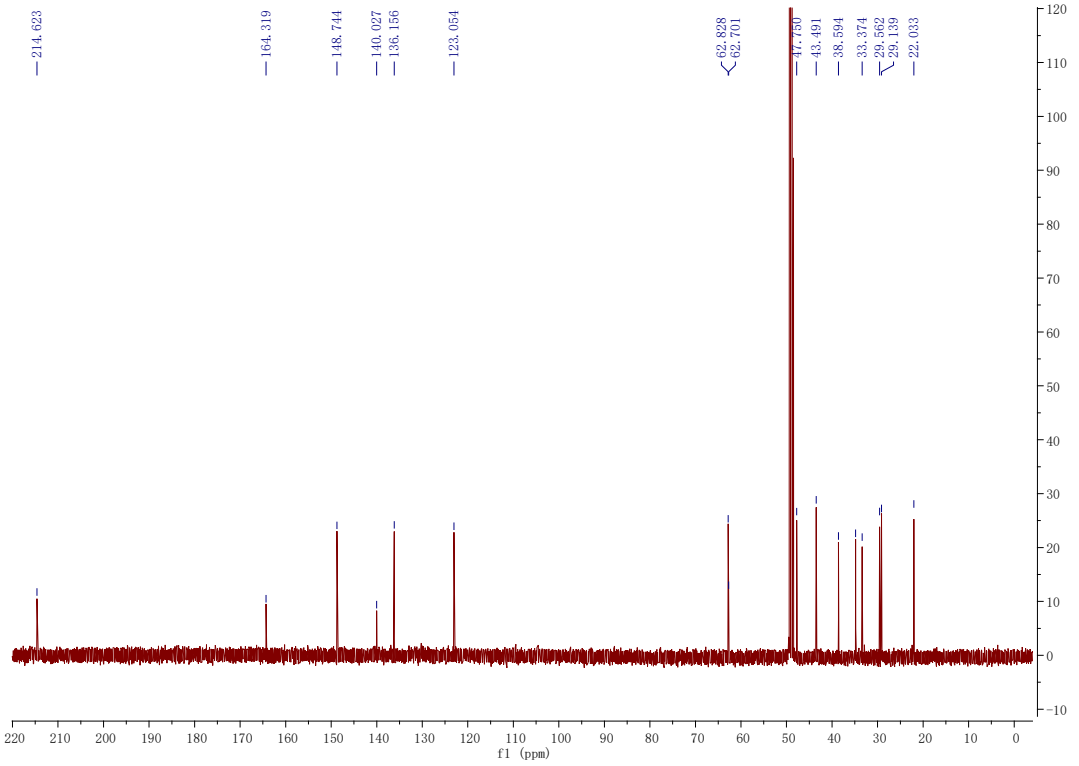
The ^{1}H NMR spectrum of **22**



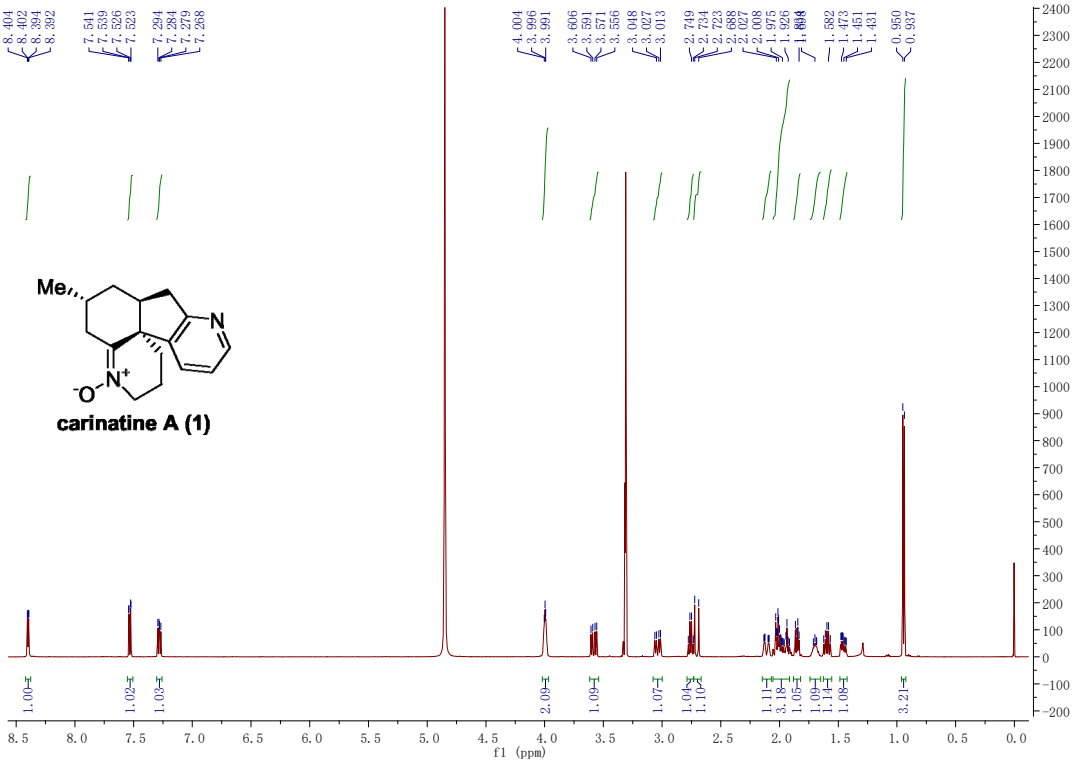
The ^{13}C NMR spectrum of **22**



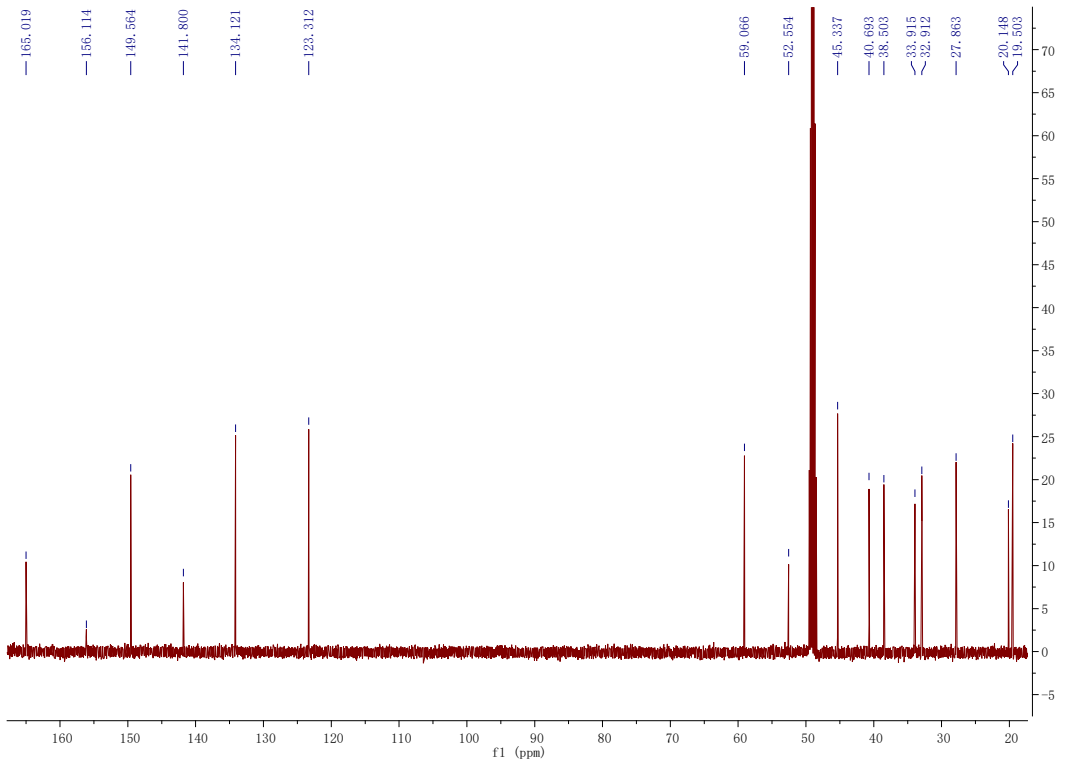
The ^{1}H NMR spectrum of lycopladine A (**2**)



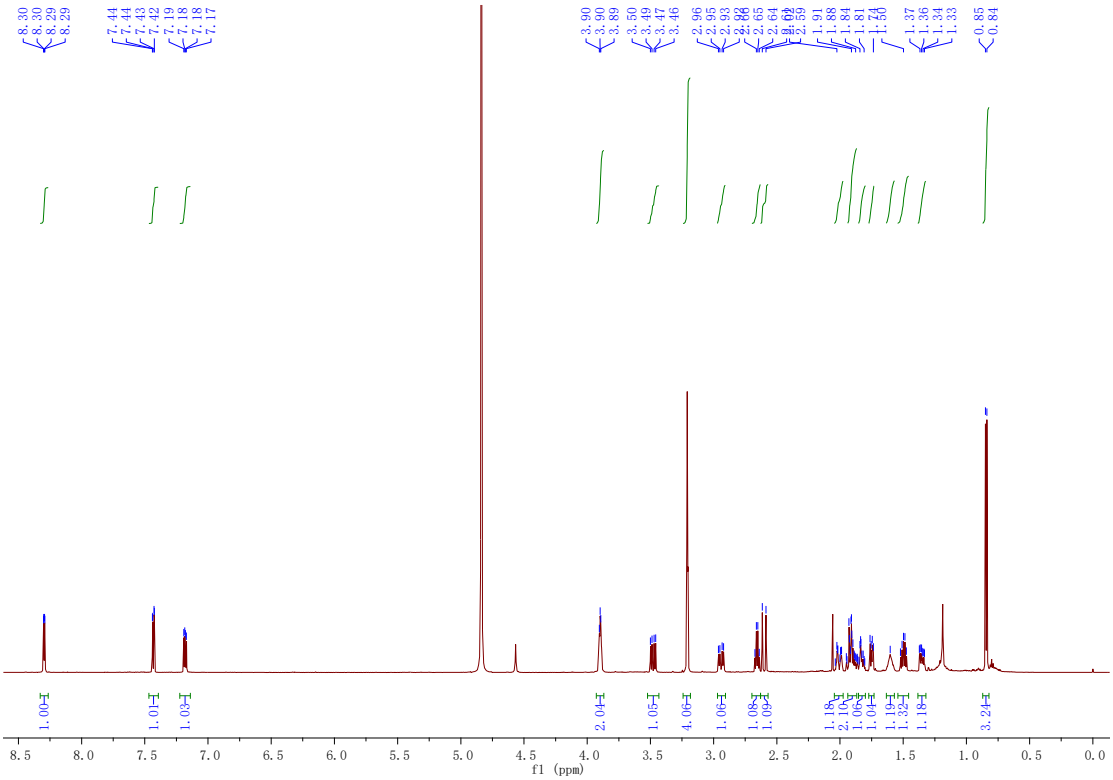
The ^{13}C NMR spectrum of lycopladine A (**2**)



The ^{1}H NMR spectrum of carinatine A (**1**)

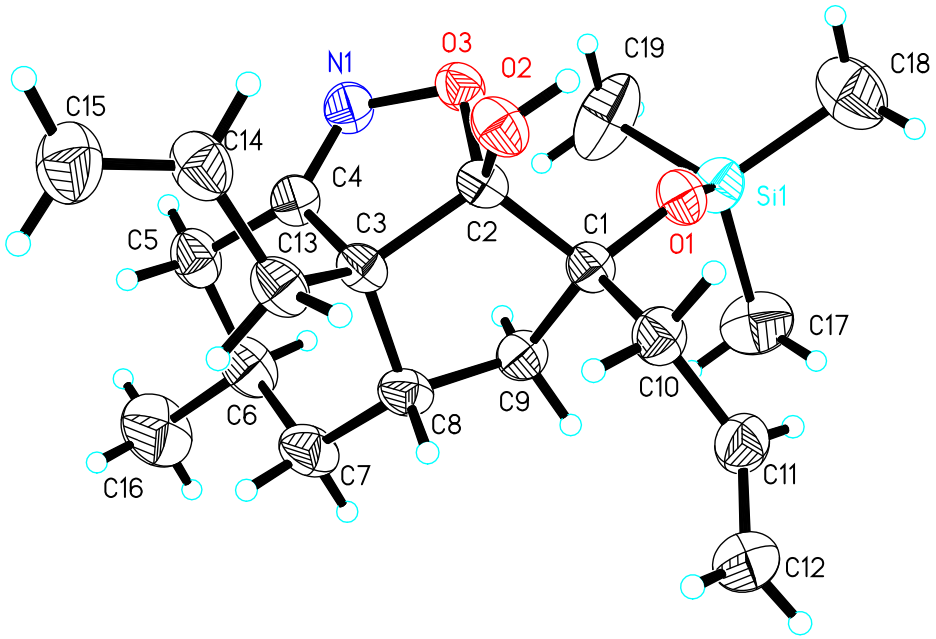


The ^{13}C NMR spectrum of carinatine A (**1**)



The original ^{1}H NMR data of carinatine A (from Prof. Qin-shi Zhao and Fei Liu)

X-ray crystal data of 14



(Ellipsoid contour probability at 30% level)

Table 1. Crystal data and structure refinement for 279.

Identification code	279
Empirical formula	C19 H31 N O3 Si
Formula weight	349.54
Temperature	296(2) K
Wavelength	1.54178 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 10.137(2) A alpha = 90 deg.
	b = 10.176(2) A beta = 90 deg.
	c = 40.850(8) A gamma = 90 deg.
Volume	4213.9(14) A^3
Z, Calculated density	8, 1.102 Mg/m^3
Absorption coefficient	1.098 mm^-1
F(000)	1520
Crystal size	0.41 x 0.36 x 0.10 mm
Theta range for data collection	4.33 to 65.99 deg.
Limiting indices	-11<=h<=11, -11<=k<=10, -44<=l<=48
Reflections collected / unique	19877 / 6947 [R(int) = 0.0307]
Completeness to theta = 65.99	95.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8981 and 0.6617
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	6947 / 0 / 433
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.1012
R indices (all data)	R1 = 0.0388, wR2 = 0.1032
Absolute structure parameter	0.02(2)
Largest diff. peak and hole	0.152 and -0.233 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 279.

		x	y	z	U(eq)
	Si(1)	8665(1)	3870(1)	2276(1)	62(1)
	Si(2)	3950(1)	6165(1)	239(1)	62(1)
O(1)	7702(1)	4665(1)	2535(1)	57(1)	
O(2)	4908(1)	5286(1)	2862(1)	56(1)	
O(3)	5321(1)	3442(1)	2551(1)	52(1)	
O(4)	4739(1)	5235(1)	-27(1)	56(1)	
O(5)	3562(1)	2836(1)	-51(1)	53(1)	
O(6)	5384(1)	2511(2)	-378(1)	58(1)	
	N(1)	4901(2)	2168(2)	2636(1)	55(1)
	N(2)	2278(2)	2390(2)	-128(1)	51(1)
	C(1)	7187(2)	4392(2)	2850(1)	48(1)
	C(2)	5673(2)	4172(2)	2845(1)	44(1)
	C(3)	5383(2)	3202(2)	3131(1)	46(1)
	C(4)	4920(2)	2031(2)	2945(1)	50(1)
	C(5)	4823(3)	723(2)	3105(1)	65(1)
	C(6)	6206(3)	376(2)	3225(1)	74(1)
	C(7)	6768(3)	1480(2)	3437(1)	70(1)
	C(8)	6729(2)	2857(2)	3286(1)	53(1)
	C(9)	7700(2)	3127(2)	3009(1)	54(1)
	C(10)	7470(2)	5623(2)	3060(1)	58(1)
	C(11)	8868(2)	5777(2)	3159(1)	68(1)
	C(12)	9259(3)	6062(3)	3455(1)	90(1)
	C(13)	4380(2)	3703(2)	3386(1)	57(1)
	C(14)	2984(2)	3760(3)	3275(1)	71(1)
	C(15)	1988(3)	3277(3)	3431(1)	91(1)
	C(16)	6198(5)	-930(3)	3413(1)	115(1)
	C(17)	10281(3)	3456(4)	2464(1)	100(1)
	C(18)	8976(4)	5087(4)	1945(1)	111(1)
	C(19)	7850(3)	2393(4)	2108(1)	119(1)
	C(20)	4430(2)	4755(2)	-345(1)	48(1)
	C(21)	4243(2)	3237(2)	-348(1)	46(1)

C(22)	3252(2)	2952(2)	-627(1)	46(1)
C(23)	2100(2)	2435(2)	-438(1)	48(1)
C(24)	774(2)	2325(2)	-588(1)	57(1)
C(25)	367(2)	3708(2)	-686(1)	61(1)
C(26)	1428(2)	4331(2)	-905(1)	61(1)
C(27)	2843(2)	4303(2)	-768(1)	51(1)
C(28)	3120(2)	5244(2)	-487(1)	52(1)
C(29)	5617(2)	5101(2)	-565(1)	58(1)
C(30)	5694(2)	6509(2)	-656(1)	67(1)
C(31)	5795(3)	6973(3)	-954(1)	84(1)
C(32)	3735(2)	1992(2)	-895(1)	57(1)
C(33)	3793(3)	597(2)	-795(1)	73(1)
C(34)	3203(4)	-365(3)	-946(1)	102(1)
C(35)	-979(2)	3725(3)	-855(1)	88(1)
C(36)	5191(4)	6473(4)	566(1)	103(1)
C(37)	3487(4)	7780(3)	63(1)	99(1)
C(38)	2495(3)	5323(3)	412(1)	104(1)
H(2A)	5087	5771	2708	84
H(6A)	5861	2645	-220	87
H(5A)	4513	69	2950	78
H(5B)	4212	757	3288	78
H(6B)	6777	274	3033	88
H(7A)	7678	1268	3488	83
H(7B)	6284	1499	3642	83
H(8A)	6901	3494	3461	64
H(9A)	7706	2409	2852	65
H(9B)	8586	3249	3093	65
H(10A)	7206	6396	2937	69
H(10B)	6929	5583	3255	69
H(11A)	9511	5661	3000	81
H(12A)	8642	6184	3621	107
H(12B)	10155	6144	3500	107
H(13A)	4427	3137	3577	69
H(13B)	4645	4577	3454	69
H(14A)	2815	4176	3077	86
H(15A)	2115	2853	3630	109
H(15B)	1144	3355	3344	109
H(16A)	5825	-1605	3277	172
H(16B)	5679	-838	3608	172
H(16C)	7086	-1164	3470	172
H(17A)	10153	2825	2635	150
H(17B)	10673	4237	2552	150
H(17C)	10853	3091	2300	150
H(18A)	8155	5321	1844	166

H(18B)	9554	4709	1785	166
H(18C)	9378	5858	2037	166
H(19A)	7694	1774	2281	179
H(19B)	8408	2001	1945	179
H(19C)	7025	2639	2010	179
H(24A)	150	1961	-432	68
H(24B)	803	1756	-778	68
H(25A)	300	4237	-486	73
H(26A)	1186	5239	-945	73
H(26B)	1425	3880	-1114	73
H(27A)	3448	4518	-947	61
H(28A)	2424	5207	-324	63
H(28B)	3200	6140	-566	63
H(29A)	6422	4858	-452	69
H(29B)	5566	4580	-764	69
H(30A)	5669	7117	-487	81
H(31A)	5823	6400	-1131	101
H(31B)	5837	7875	-988	101
H(32A)	3153	2067	-1083	69
H(32B)	4608	2263	-965	69
H(33A)	4289	391	-611	88
H(34A)	2698	-197	-1131	122
H(34B)	3286	-1220	-868	122
H(35A)	-1627	3337	-713	133
H(35B)	-932	3233	-1055	133
H(35C)	-1225	4616	-902	133
H(36A)	5447	5653	663	154
H(36B)	4815	7033	730	154
H(36C)	5951	6892	472	154
H(37A)	2843	7653	-107	148
H(37B)	4256	8193	-28	148
H(37C)	3123	8328	231	148
H(38A)	1859	5172	242	155
H(38B)	2109	5862	579	155
H(38C)	2760	4497	505	155

Table 3. Bond lengths [A] and angles [deg] for 279.

Si(1)-O(1)	1.6493(14)	Si(2)-O(4)	1.6492(14)
Si(1)-C(19)	1.848(3)	Si(2)-C(38)	1.846(3)
Si(1)-C(17)	1.856(3)	Si(2)-C(37)	1.855(3)
Si(1)-C(18)	1.861(3)	Si(2)-C(36)	1.860(3)

O(1)-C(1)	1.417(2)	C(14)-H(14A)	0.9300
O(2)-C(2)	1.375(2)	C(15)-H(15A)	0.9300
O(2)-H(2A)	0.8200	C(15)-H(15B)	0.9300
O(3)-N(1)	1.409(2)	C(16)-H(16A)	0.9600
O(3)-C(2)	1.459(2)	C(16)-H(16B)	0.9600
O(4)-C(20)	1.421(2)	C(16)-H(16C)	0.9600
O(5)-N(2)	1.414(2)	C(17)-H(17A)	0.9600
O(5)-C(21)	1.454(2)	C(17)-H(17B)	0.9600
O(6)-C(21)	1.378(2)	C(17)-H(17C)	0.9600
O(6)-H(6A)	0.8200	C(18)-H(18A)	0.9600
N(1)-C(4)	1.269(2)	C(18)-H(18B)	0.9600
N(2)-C(23)	1.278(2)	C(18)-H(18C)	0.9600
C(1)-C(9)	1.533(3)	C(19)-H(19A)	0.9600
C(1)-C(10)	1.545(3)	C(19)-H(19B)	0.9600
C(1)-C(2)	1.552(3)	C(19)-H(19C)	0.9600
C(2)-C(3)	1.555(2)	C(20)-C(28)	1.532(3)
C(3)-C(4)	1.489(3)	C(20)-C(29)	1.543(2)
C(3)-C(13)	1.544(2)	C(20)-C(21)	1.556(3)
C(3)-C(8)	1.545(3)	C(21)-C(22)	1.549(2)
C(4)-C(5)	1.486(3)	C(22)-C(23)	1.496(2)
C(5)-C(6)	1.526(4)	C(22)-C(27)	1.546(3)
C(5)-H(5A)	0.9700	C(22)-C(32)	1.546(3)
C(5)-H(5B)	0.9700	C(23)-C(24)	1.482(3)
C(6)-C(7)	1.528(4)	C(24)-C(25)	1.521(3)
C(6)-C(16)	1.534(3)	C(24)-H(24A)	0.9700
C(6)-H(6B)	0.9800	C(24)-H(24B)	0.9700
C(7)-C(8)	1.532(3)	C(25)-C(35)	1.530(3)
C(7)-H(7A)	0.9700	C(25)-C(26)	1.536(3)
C(7)-H(7B)	0.9700	C(25)-H(25A)	0.9800
C(8)-C(9)	1.526(3)	C(26)-C(27)	1.540(3)
C(8)-H(8A)	0.9800	C(26)-H(26A)	0.9700
C(9)-H(9A)	0.9700	C(26)-H(26B)	0.9700
C(9)-H(9B)	0.9700	C(27)-C(28)	1.519(3)
C(10)-C(11)	1.482(3)	C(27)-H(27A)	0.9800
C(10)-H(10A)	0.9700	C(28)-H(28A)	0.9700
C(10)-H(10B)	0.9700	C(28)-H(28B)	0.9700
C(11)-C(12)	1.305(3)	C(29)-C(30)	1.482(3)
C(11)-H(11A)	0.9300	C(29)-H(29A)	0.9700
C(12)-H(12A)	0.9300	C(29)-H(29B)	0.9700
C(12)-H(12B)	0.9300	C(30)-C(31)	1.308(3)
C(13)-C(14)	1.487(3)	C(30)-H(30A)	0.9300
C(13)-H(13A)	0.9700	C(31)-H(31A)	0.9300
C(13)-H(13B)	0.9700	C(31)-H(31B)	0.9300
C(14)-C(15)	1.291(4)	C(32)-C(33)	1.479(3)

C(32)-H(32A)	0.9700	C(36)-H(36A)	0.9600
C(32)-H(32B)	0.9700	C(36)-H(36B)	0.9600
C(33)-C(34)	1.302(4)	C(36)-H(36C)	0.9600
C(33)-H(33A)	0.9300	C(37)-H(37A)	0.9600
C(34)-H(34A)	0.9300	C(37)-H(37B)	0.9600
C(34)-H(34B)	0.9300	C(37)-H(37C)	0.9600
C(35)-H(35A)	0.9600	C(38)-H(38A)	0.9600
C(35)-H(35B)	0.9600	C(38)-H(38B)	0.9600
C(35)-H(35C)	0.9600	C(38)-H(38C)	0.9600

O(1)-Si(1)-C(19)	111.87(11)	C(13)-C(3)-C(8)	112.27(14)
O(1)-Si(1)-C(17)	111.76(11)	C(4)-C(3)-C(2)	100.71(13)
C(19)-Si(1)-C(17)	111.32(18)	C(13)-C(3)-C(2)	114.93(15)
O(1)-Si(1)-C(18)	103.77(12)	C(8)-C(3)-C(2)	106.58(15)
C(19)-Si(1)-C(18)	110.22(19)	N(1)-C(4)-C(5)	122.34(17)
C(17)-Si(1)-C(18)	107.54(17)	N(1)-C(4)-C(3)	115.03(17)
O(4)-Si(2)-C(38)	111.95(11)	C(5)-C(4)-C(3)	120.90(16)
O(4)-Si(2)-C(37)	111.97(11)	C(4)-C(5)-C(6)	106.69(18)
C(38)-Si(2)-C(37)	110.99(17)	C(4)-C(5)-H(5A)	110.4
O(4)-Si(2)-C(36)	103.99(12)	C(6)-C(5)-H(5A)	110.4
C(38)-Si(2)-C(36)	110.14(17)	C(4)-C(5)-H(5B)	110.4
C(37)-Si(2)-C(36)	107.48(17)	C(6)-C(5)-H(5B)	110.4
C(1)-O(1)-Si(1)	134.64(13)	H(5A)-C(5)-H(5B)	108.6
C(2)-O(2)-H(2A)	109.5	C(5)-C(6)-C(7)	110.79(19)
N(1)-O(3)-C(2)	109.72(12)	C(5)-C(6)-C(16)	110.9(3)
C(20)-O(4)-Si(2)	133.83(12)	C(7)-C(6)-C(16)	110.8(2)
N(2)-O(5)-C(21)	109.92(12)	C(5)-C(6)-H(6B)	108.1
C(21)-O(6)-H(6A)	109.5	C(7)-C(6)-H(6B)	108.1
C(4)-N(1)-O(3)	110.08(14)	C(16)-C(6)-H(6B)	108.1
C(23)-N(2)-O(5)	109.86(14)	C(6)-C(7)-C(8)	115.74(17)
O(1)-C(1)-C(9)	115.15(15)	C(6)-C(7)-H(7A)	108.3
O(1)-C(1)-C(10)	106.13(15)	C(8)-C(7)-H(7A)	108.3
C(9)-C(1)-C(10)	112.47(15)	C(6)-C(7)-H(7B)	108.3
O(1)-C(1)-C(2)	112.48(14)	C(8)-C(7)-H(7B)	108.3
C(9)-C(1)-C(2)	102.63(15)	H(7A)-C(7)-H(7B)	107.4
C(10)-C(1)-C(2)	107.90(15)	C(9)-C(8)-C(7)	116.53(18)
O(2)-C(2)-O(3)	108.87(14)	C(9)-C(8)-C(3)	102.95(14)
O(2)-C(2)-C(1)	115.97(15)	C(7)-C(8)-C(3)	113.36(18)
O(3)-C(2)-C(1)	108.96(13)	C(9)-C(8)-H(8A)	107.9
O(2)-C(2)-C(3)	112.27(14)	C(7)-C(8)-H(8A)	107.9
O(3)-C(2)-C(3)	104.45(14)	C(3)-C(8)-H(8A)	107.9
C(1)-C(2)-C(3)	105.66(14)	C(8)-C(9)-C(1)	104.31(15)
C(4)-C(3)-C(13)	113.64(16)	C(8)-C(9)-H(9A)	110.9
C(4)-C(3)-C(8)	107.81(15)	C(1)-C(9)-H(9A)	110.9

C(8)-C(9)-H(9B)	110.9	H(18B)-C(18)-H(18C)	109.5
C(1)-C(9)-H(9B)	110.9	Si(1)-C(19)-H(19A)	109.5
H(9A)-C(9)-H(9B)	108.9	Si(1)-C(19)-H(19B)	109.5
C(11)-C(10)-C(1)	114.54(18)	H(19A)-C(19)-H(19B)	109.5
C(11)-C(10)-H(10A)	108.6	Si(1)-C(19)-H(19C)	109.5
C(1)-C(10)-H(10A)	108.6	H(19A)-C(19)-H(19C)	109.5
C(11)-C(10)-H(10B)	108.6	H(19B)-C(19)-H(19C)	109.5
C(1)-C(10)-H(10B)	108.6	O(4)-C(20)-C(28)	115.19(15)
H(10A)-C(10)-H(10B)	107.6	O(4)-C(20)-C(29)	106.39(15)
C(12)-C(11)-C(10)	124.6(2)	C(28)-C(20)-C(29)	112.38(15)
C(12)-C(11)-H(11A)	117.7	O(4)-C(20)-C(21)	111.98(15)
C(10)-C(11)-H(11A)	117.7	C(28)-C(20)-C(21)	102.36(15)
C(11)-C(12)-H(12A)	120.0	C(29)-C(20)-C(21)	108.47(15)
C(11)-C(12)-H(12B)	120.0	O(6)-C(21)-O(5)	108.91(15)
H(12A)-C(12)-H(12B)	120.0	O(6)-C(21)-C(22)	112.13(15)
C(14)-C(13)-C(3)	115.66(16)	O(5)-C(21)-C(22)	104.74(14)
C(14)-C(13)-H(13A)	108.4	O(6)-C(21)-C(20)	115.52(16)
C(3)-C(13)-H(13A)	108.4	O(5)-C(21)-C(20)	109.30(14)
C(14)-C(13)-H(13B)	108.4	C(22)-C(21)-C(20)	105.67(14)
C(3)-C(13)-H(13B)	108.4	C(23)-C(22)-C(27)	107.15(14)
H(13A)-C(13)-H(13B)	107.4	C(23)-C(22)-C(32)	113.06(16)
C(15)-C(14)-C(13)	125.4(2)	C(27)-C(22)-C(32)	112.62(14)
C(15)-C(14)-H(14A)	117.3	C(23)-C(22)-C(21)	100.95(13)
C(13)-C(14)-H(14A)	117.3	C(27)-C(22)-C(21)	106.28(15)
C(14)-C(15)-H(15A)	120.0	C(32)-C(22)-C(21)	115.78(15)
C(14)-C(15)-H(15B)	120.0	N(2)-C(23)-C(24)	122.28(17)
H(15A)-C(15)-H(15B)	120.0	N(2)-C(23)-C(22)	114.50(16)
C(6)-C(16)-H(16A)	109.5	C(24)-C(23)-C(22)	121.38(15)
C(6)-C(16)-H(16B)	109.5	C(23)-C(24)-C(25)	106.51(16)
H(16A)-C(16)-H(16B)	109.5	C(23)-C(24)-H(24A)	110.4
C(6)-C(16)-H(16C)	109.5	C(25)-C(24)-H(24A)	110.4
H(16A)-C(16)-H(16C)	109.5	C(23)-C(24)-H(24B)	110.4
H(16B)-C(16)-H(16C)	109.5	C(25)-C(24)-H(24B)	110.4
Si(1)-C(17)-H(17A)	109.5	H(24A)-C(24)-H(24B)	108.6
Si(1)-C(17)-H(17B)	109.5	C(24)-C(25)-C(35)	111.8(2)
H(17A)-C(17)-H(17B)	109.5	C(24)-C(25)-C(26)	110.24(17)
Si(1)-C(17)-H(17C)	109.5	C(35)-C(25)-C(26)	110.93(19)
H(17A)-C(17)-H(17C)	109.5	C(24)-C(25)-H(25A)	107.9
H(17B)-C(17)-H(17C)	109.5	C(35)-C(25)-H(25A)	107.9
Si(1)-C(18)-H(18A)	109.5	C(26)-C(25)-H(25A)	107.9
Si(1)-C(18)-H(18B)	109.5	C(25)-C(26)-C(27)	115.57(15)
H(18A)-C(18)-H(18B)	109.5	C(25)-C(26)-H(26A)	108.4
Si(1)-C(18)-H(18C)	109.5	C(27)-C(26)-H(26A)	108.4
H(18A)-C(18)-H(18C)	109.5	C(25)-C(26)-H(26B)	108.4

C(27)-C(26)-H(26B)	108.4	Si(2)-C(36)-H(36A)	109.5
H(26A)-C(26)-H(26B)	107.4	Si(2)-C(36)-H(36B)	109.5
C(28)-C(27)-C(26)	115.81(17)	H(36A)-C(36)-H(36B)	109.5
C(28)-C(27)-C(22)	103.40(14)	Si(2)-C(36)-H(36C)	109.5
C(26)-C(27)-C(22)	113.66(16)	H(36A)-C(36)-H(36C)	109.5
C(28)-C(27)-H(27A)	107.9	H(36B)-C(36)-H(36C)	109.5
C(26)-C(27)-H(27A)	107.9	Si(2)-C(37)-H(37A)	109.5
C(22)-C(27)-H(27A)	107.9	Si(2)-C(37)-H(37B)	109.5
C(27)-C(28)-C(20)	103.98(16)	H(37A)-C(37)-H(37B)	109.5
C(27)-C(28)-H(28A)	111.0	Si(2)-C(37)-H(37C)	109.5
C(20)-C(28)-H(28A)	111.0	H(37A)-C(37)-H(37C)	109.5
C(27)-C(28)-H(28B)	111.0	H(37B)-C(37)-H(37C)	109.5
C(20)-C(28)-H(28B)	111.0	Si(2)-C(38)-H(38A)	109.5
H(28A)-C(28)-H(28B)	109.0	Si(2)-C(38)-H(38B)	109.5
C(30)-C(29)-C(20)	114.08(18)	H(38A)-C(38)-H(38B)	109.5
C(30)-C(29)-H(29A)	108.7	Si(2)-C(38)-H(38C)	109.5
C(20)-C(29)-H(29A)	108.7	H(38A)-C(38)-H(38C)	109.5
C(30)-C(29)-H(29B)	108.7	H(38B)-C(38)-H(38C)	109.5
C(20)-C(29)-H(29B)	108.7		
H(29A)-C(29)-H(29B)	107.6		
C(31)-C(30)-C(29)	125.9(2)		
C(31)-C(30)-H(30A)	117.0		
C(29)-C(30)-H(30A)	117.0		
C(30)-C(31)-H(31A)	120.0		
C(30)-C(31)-H(31B)	120.0		
H(31A)-C(31)-H(31B)	120.0		
C(33)-C(32)-C(22)	115.04(16)		
C(33)-C(32)-H(32A)	108.5		
C(22)-C(32)-H(32A)	108.5		
C(33)-C(32)-H(32B)	108.5		
C(22)-C(32)-H(32B)	108.5		
H(32A)-C(32)-H(32B)	107.5		
C(34)-C(33)-C(32)	125.0(3)		
C(34)-C(33)-H(33A)	117.5		
C(32)-C(33)-H(33A)	117.5		
C(33)-C(34)-H(34A)	120.0		
C(33)-C(34)-H(34B)	120.0		
H(34A)-C(34)-H(34B)	120.0		
C(25)-C(35)-H(35A)	109.5		
C(25)-C(35)-H(35B)	109.5		
H(35A)-C(35)-H(35B)	109.5		
C(25)-C(35)-H(35C)	109.5		
H(35A)-C(35)-H(35C)	109.5		
H(35B)-C(35)-H(35C)	109.5		

Table 4. Torsion angles [deg] for 279.

C(19)-Si(1)-O(1)-C(1)	68.0(2)	C(8)-C(3)-C(4)-C(5)	53.8(2)
C(17)-Si(1)-O(1)-C(1)	-57.6(2)	C(2)-C(3)-C(4)-C(5)	165.22(18)
C(18)-Si(1)-O(1)-C(1)	-173.2(2)	N(1)-C(4)-C(5)-C(6)	104.6(2)
C(38)-Si(2)-O(4)-C(20)	68.5(2)	C(3)-C(4)-C(5)-C(6)	-59.6(2)
C(37)-Si(2)-O(4)-C(20)	-56.9(2)	C(4)-C(5)-C(6)-C(7)	53.3(2)
C(36)-Si(2)-O(4)-C(20)	-172.6(2)	C(4)-C(5)-C(6)-C(16)	176.7(2)
C(2)-O(3)-N(1)-C(4)	1.5(2)	C(5)-C(6)-C(7)-C(8)	-52.0(3)
C(21)-O(5)-N(2)-C(23)	1.8(2)	C(16)-C(6)-C(7)-C(8)	-175.4(3)
Si(1)-O(1)-C(1)-C(9)	5.8(3)	C(6)-C(7)-C(8)-C(9)	-72.6(3)
Si(1)-O(1)-C(1)-C(10)	130.93(16)	C(6)-C(7)-C(8)-C(3)	46.7(3)
Si(1)-O(1)-C(1)-C(2)	-111.30(18)	C(4)-C(3)-C(8)-C(9)	83.89(17)
N(1)-O(3)-C(2)-O(2)	-121.59(15)	C(13)-C(3)-C(8)-C(9)	-150.19(16)
N(1)-O(3)-C(2)-C(1)	111.06(15)	C(2)-C(3)-C(8)-C(9)	-23.53(18)
N(1)-O(3)-C(2)-C(3)	-1.48(18)	C(4)-C(3)-C(8)-C(7)	-42.9(2)
O(1)-C(1)-C(2)-O(2)	-84.78(19)	C(13)-C(3)-C(8)-C(7)	83.0(2)
C(9)-C(1)-C(2)-O(2)	150.89(14)	C(2)-C(3)-C(8)-C(7)	-150.30(16)
C(10)-C(1)-C(2)-O(2)	31.9(2)	C(7)-C(8)-C(9)-C(1)	165.09(17)
O(1)-C(1)-C(2)-O(3)	38.44(19)	C(3)-C(8)-C(9)-C(1)	40.36(18)
C(9)-C(1)-C(2)-O(3)	-85.90(16)	O(1)-C(1)-C(9)-C(8)	-163.87(16)
C(10)-C(1)-C(2)-O(3)	155.16(14)	C(10)-C(1)-C(9)-C(8)	74.37(19)
O(1)-C(1)-C(2)-C(3)	150.17(14)	C(2)-C(1)-C(9)-C(8)	-41.32(18)
C(9)-C(1)-C(2)-C(3)	25.83(17)	O(1)-C(1)-C(10)-C(11)	-74.1(2)
C(10)-C(1)-C(2)-C(3)	-93.11(16)	C(9)-C(1)-C(10)-C(11)	52.6(2)
O(2)-C(2)-C(3)-C(4)	118.76(16)	C(2)-C(1)-C(10)-C(11)	165.11(17)
O(3)-C(2)-C(3)-C(4)	0.95(17)	C(1)-C(10)-C(11)-C(12)	-133.6(3)
C(1)-C(2)-C(3)-C(4)	-113.93(15)	C(4)-C(3)-C(13)-C(14)	-43.6(2)
O(2)-C(2)-C(3)-C(13)	-3.8(2)	C(8)-C(3)-C(13)-C(14)	-166.25(18)
O(3)-C(2)-C(3)-C(13)	-121.59(16)	C(2)-C(3)-C(13)-C(14)	71.7(2)
C(1)-C(2)-C(3)-C(13)	123.53(16)	C(3)-C(13)-C(14)-C(15)	130.0(3)
O(2)-C(2)-C(3)-C(8)	-128.84(16)	Si(2)-O(4)-C(20)-C(28)	3.9(3)
O(3)-C(2)-C(3)-C(8)	113.36(15)	Si(2)-O(4)-C(20)-C(29)	129.16(17)
C(1)-C(2)-C(3)-C(8)	-1.52(18)	Si(2)-O(4)-C(20)-C(21)	-112.49(18)
O(3)-N(1)-C(4)-C(5)	-165.93(18)	N(2)-O(5)-C(21)-O(6)	-121.87(16)
O(3)-N(1)-C(4)-C(3)	-0.8(2)	N(2)-O(5)-C(21)-C(22)	-1.75(18)
C(13)-C(3)-C(4)-N(1)	123.32(19)	N(2)-O(5)-C(21)-C(20)	111.08(16)
C(8)-C(3)-C(4)-N(1)	-111.57(19)	O(4)-C(20)-C(21)-O(6)	-84.58(18)
C(2)-C(3)-C(4)-N(1)	-0.1(2)	C(28)-C(20)-C(21)-O(6)	151.48(14)
C(13)-C(3)-C(4)-C(5)	-71.3(2)	C(29)-C(20)-C(21)-O(6)	32.5(2)

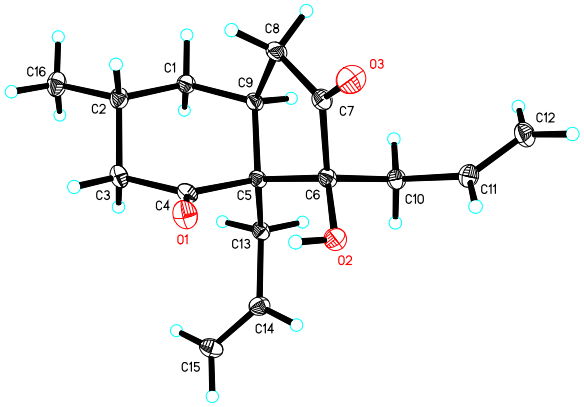
O(4)-C(20)-C(21)-O(5)	38.63(19)	C(23)-C(24)-C(25)-C(35)	178.23(18)
C(28)-C(20)-C(21)-O(5)	-85.31(16)	C(23)-C(24)-C(25)-C(26)	54.4(2)
C(29)-C(20)-C(21)-O(5)	155.74(14)	C(24)-C(25)-C(26)-C(27)	-52.5(2)
O(4)-C(20)-C(21)-C(22)	150.85(14)	C(35)-C(25)-C(26)-C(27)	-176.9(2)
C(28)-C(20)-C(21)-C(22)	26.91(17)	C(25)-C(26)-C(27)-C(28)	-73.0(2)
C(29)-C(20)-C(21)-C(22)	-92.04(16)	C(25)-C(26)-C(27)-C(22)	46.6(2)
O(6)-C(21)-C(22)-C(23)	119.07(16)	C(23)-C(22)-C(27)-C(28)	84.26(17)
O(5)-C(21)-C(22)-C(23)	1.12(18)	C(32)-C(22)-C(27)-C(28)	-150.81(16)
C(20)-C(21)-C(22)-C(23)	-114.27(15)	C(21)-C(22)-C(27)-C(28)	-23.03(18)
O(6)-C(21)-C(22)-C(27)	-129.26(16)	C(23)-C(22)-C(27)-C(26)	-42.1(2)
O(5)-C(21)-C(22)-C(27)	112.79(15)	C(32)-C(22)-C(27)-C(26)	82.8(2)
C(20)-C(21)-C(22)-C(27)	-2.60(18)	C(21)-C(22)-C(27)-C(26)	-149.40(15)
O(6)-C(21)-C(22)-C(32)	-3.4(2)	C(26)-C(27)-C(28)-C(20)	165.53(15)
O(5)-C(21)-C(22)-C(32)	-121.33(16)	C(22)-C(27)-C(28)-C(20)	40.54(17)
C(20)-C(21)-C(22)-C(32)	123.28(16)	O(4)-C(20)-C(28)-C(27)	-163.72(15)
O(5)-N(2)-C(23)-C(24)	-165.72(17)	C(29)-C(20)-C(28)-C(27)	74.22(19)
O(5)-N(2)-C(23)-C(22)	-1.0(2)	C(21)-C(20)-C(28)-C(27)	-41.95(17)
C(27)-C(22)-C(23)-N(2)	-111.13(18)	O(4)-C(20)-C(29)-C(30)	-74.8(2)
C(32)-C(22)-C(23)-N(2)	124.20(18)	C(28)-C(20)-C(29)-C(30)	52.1(2)
C(21)-C(22)-C(23)-N(2)	-0.1(2)	C(21)-C(20)-C(29)-C(30)	164.56(18)
C(27)-C(22)-C(23)-C(24)	53.8(2)	C(20)-C(29)-C(30)-C(31)	-127.1(3)
C(32)-C(22)-C(23)-C(24)	-70.9(2)	C(23)-C(22)-C(32)-C(33)	-42.4(2)
C(21)-C(22)-C(23)-C(24)	164.77(17)	C(27)-C(22)-C(32)-C(33)	-164.08(19)
N(2)-C(23)-C(24)-C(25)	102.8(2)	C(21)-C(22)-C(32)-C(33)	73.3(2)
C(22)-C(23)-C(24)-C(25)	-60.9(2)	C(22)-C(32)-C(33)-C(34)	124.6(3)

Table 5. Hydrogen bonds for 279 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2A)...N(1)#1	0.82	2.00	2.802(2)	165.7
O(6)-H(6A)...N(2)#2	0.82	2.02	2.825(2)	166.4

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y+1/2,-z+1/2 #2 x+1/2,-y+1/2,-z

X-ray crystal data of 20



(Ellipsoid contour probability at 30% level)

Table 1. Crystal data and structure refinement for mo_dm15450_0m.

Identification code	mo_dm15450_0m
Empirical formula	C16 H22 O3
Formula weight	262.33
Temperature	130 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 1 21 1
Unit cell dimensions	a = 7.946(2) Å a= 90°.
	b = 11.256(3) Å b= 101.141(4)°.
	c = 8.207(2) Å g = 90°.
Volume	720.3(3) Å3
Z	2
Density (calculated)	1.210 Mg/m3
Absorption coefficient	0.082 mm-1
F(000)	284
Crystal size	0.2 x 0.15 x 0.1 mm3
Theta range for data collection	2.529 to 30.441°.
Index ranges	-11<=h<=10, -16<=k<=14, -11<=l<=11
Reflections collected	7046
Independent reflections	4082 [R(int) = 0.0303]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.5518
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	4082 / 1 / 174
Goodness-of-fit on F2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.1148
R indices (all data)	R1 = 0.0584, wR2 = 0.1224

Absolute structure parameter -1.4(8)
Extinction coefficientn/a
Largest diff. peak and hole 0.482 and -0.169 e.Å-3

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103)
for mo_dm15450_0m. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	9540(2)	8496(2)	3942(2)	32(1)
O(2)	10541(2)	8372(2)	1058(2)	27(1)
O(3)	13009(2)	10110(2)	2455(3)	39(1)
C(1)	7586(3)	11766(2)	3269(3)	23(1)
C(2)	7647(3)	11065(2)	4867(3)	25(1)
C(3)	7297(3)	9743(2)	4463(3)	25(1)
C(4)	8526(3)	9285(2)	3432(3)	22(1)
C(5)	8494(3)	9912(2)	1767(3)	18(1)
C(6)	10120(3)	9593(2)	1047(3)	21(1)
C(7)	11503(3)	10351(2)	2143(3)	25(1)
C(8)	10670(3)	11409(2)	2798(3)	26(1)
C(9)	8730(3)	11272(2)	2134(3)	21(1)
C(10)	9974(3)	10006(2)	-766(3)	23(1)
C(11)	11553(3)	9740(2)	-1456(3)	28(1)
C(12)	12268(3)	10490(3)	-2361(3)	34(1)
C(13)	6761(3)	9651(2)	602(3)	21(1)
C(14)	6415(3)	8352(2)	300(3)	26(1)
C(15)	5091(3)	7794(2)	691(3)	30(1)
C(16)	6368(3)	11563(3)	5851(3)	33(1)

Table 3. Bond lengths [Å] and angles [°] for mo_dm15450_0m.

O(1)-C(4)	1.217(3)	C(2)-C(16)	1.522(3)
O(2)-H(2)	0.8400	C(3)-H(3A)	0.9900
O(2)-C(6)	1.415(3)	C(3)-H(3B)	0.9900
O(3)-C(7)	1.205(3)	C(3)-C(4)	1.502(3)
C(1)-H(1A)	0.9900	C(4)-C(5)	1.534(3)
C(1)-H(1B)	0.9900	C(5)-C(6)	1.562(3)
C(1)-C(2)	1.523(3)	C(5)-C(9)	1.565(3)
C(1)-C(9)	1.527(3)	C(5)-C(13)	1.546(3)
C(2)-H(2A)	1.0000	C(6)-C(7)	1.537(3)
C(2)-C(3)	1.538(3)	C(6)-C(10)	1.542(3)

C(7)-C(8) 1.511(3)
C(8)-H(8A) 0.9900
C(8)-H(8B) 0.9900
C(8)-C(9) 1.540(3)
C(9)-H(9) 1.0000
C(10)-H(10A) 0.9900
C(10)-H(10B) 0.9900
C(10)-C(11) 1.503(3)
C(11)-H(11) 0.9500
C(11)-C(12) 1.323(4)
C(12)-H(12A) 0.9500
C(12)-H(12B) 0.9500
C(13)-H(13A) 0.9900
C(13)-H(13B) 0.9900
C(13)-C(14) 1.499(3)
C(14)-H(14) 0.9500
C(14)-C(15) 1.317(3)
C(15)-H(15A) 0.9500
C(15)-H(15B) 0.9500
C(16)-H(16A) 0.9800
C(16)-H(16B) 0.9800
C(16)-H(16C) 0.9800

C(6)-O(2)-H(2) 109.5
H(1A)-C(1)-H(1B) 107.6
C(2)-C(1)-H(1A) 108.6
C(2)-C(1)-H(1B) 108.6
C(2)-C(1)-C(9) 114.44(19)
C(9)-C(1)-H(1A) 108.6
C(9)-C(1)-H(1B) 108.6
C(1)-C(2)-H(2A) 108.4
C(1)-C(2)-C(3) 109.93(19)
C(3)-C(2)-H(2A) 108.4
C(16)-C(2)-C(1) 110.7(2)
C(16)-C(2)-H(2A) 108.4
C(16)-C(2)-C(3) 111.0(2)
C(2)-C(3)-H(3A) 109.6
C(2)-C(3)-H(3B) 109.6
H(3A)-C(3)-H(3B) 108.2
C(4)-C(3)-C(2) 110.11(18)
C(4)-C(3)-H(3A) 109.6
C(4)-C(3)-H(3B) 109.6
O(1)-C(4)-C(3) 121.0(2)
O(1)-C(4)-C(5) 122.6(2)
C(3)-C(4)-C(5) 116.32(19)
C(4)-C(5)-C(6) 111.02(17)
C(4)-C(5)-C(9) 107.35(17)
C(4)-C(5)-C(13) 108.83(17)
C(6)-C(5)-C(9) 102.72(16)
C(13)-C(5)-C(6) 115.19(17)
C(13)-C(5)-C(9) 111.37(17)
O(2)-C(6)-C(5) 115.61(17)
O(2)-C(6)-C(7) 113.21(18)
O(2)-C(6)-C(10) 105.81(17)
C(7)-C(6)-C(5) 101.63(17)
C(7)-C(6)-C(10) 108.02(17)
C(10)-C(6)-C(5) 112.49(17)
O(3)-C(7)-C(6) 124.6(2)
O(3)-C(7)-C(8) 125.9(2)
C(8)-C(7)-C(6) 109.44(18)
C(7)-C(8)-H(8A) 110.6
C(7)-C(8)-H(8B) 110.6
C(7)-C(8)-C(9) 105.81(19)
H(8A)-C(8)-H(8B) 108.7
C(9)-C(8)-H(8A) 110.6
C(9)-C(8)-H(8B) 110.6
C(1)-C(9)-C(5) 114.21(17)
C(1)-C(9)-C(8) 114.91(19)
C(1)-C(9)-H(9) 107.8
C(5)-C(9)-H(9) 107.8
C(8)-C(9)-C(5) 103.91(17)
C(8)-C(9)-H(9) 107.8
C(6)-C(10)-H(10A) 109.0
C(6)-C(10)-H(10B) 109.0
H(10A)-C(10)-H(10B) 107.8
C(11)-C(10)-C(6) 113.06(18)
C(11)-C(10)-H(10A) 109.0
C(11)-C(10)-H(10B) 109.0
C(10)-C(11)-H(11) 117.8
C(12)-C(11)-C(10) 124.4(2)
C(12)-C(11)-H(11) 117.8
C(11)-C(12)-H(12A) 120.0
C(11)-C(12)-H(12B) 120.0
H(12A)-C(12)-H(12B) 120.0
C(5)-C(13)-H(13A) 108.8
C(5)-C(13)-H(13B) 108.8
H(13A)-C(13)-H(13B) 107.7
C(14)-C(13)-C(5) 113.62(18)

C(14)-C(13)-H(13A)	108.8	H(15A)-C(15)-H(15B)	120.0
C(14)-C(13)-H(13B)	108.8	C(2)-C(16)-H(16A)	109.5
C(13)-C(14)-H(14)	118.2	C(2)-C(16)-H(16B)	109.5
C(15)-C(14)-C(13)	123.6(2)	C(2)-C(16)-H(16C)	109.5
C(15)-C(14)-H(14)	118.2	H(16A)-C(16)-H(16B)	109.5
C(14)-C(15)-H(15A)	120.0	H(16A)-C(16)-H(16C)	109.5
C(14)-C(15)-H(15B)	120.0	H(16B)-C(16)-H(16C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103) for mo_dm15450_0m. The anisotropic displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	33(1)	30(1)	35(1)	10(1)	9(1)	11(1)
O(2)	26(1)	21(1)	34(1)	1(1)	10(1)	6(1)
O(3)	16(1)	52(1)	48(1)	-12(1)	3(1)	3(1)
C(1)	21(1)	21(1)	28(1)	-2(1)	9(1)	1(1)
C(2)	20(1)	32(1)	23(1)	-1(1)	6(1)	0(1)
C(3)	21(1)	30(1)	25(1)	6(1)	7(1)	0(1)
C(4)	19(1)	22(1)	27(1)	2(1)	4(1)	-3(1)
C(5)	15(1)	17(1)	23(1)	1(1)	6(1)	0(1)
C(6)	17(1)	20(1)	27(1)	0(1)	7(1)	1(1)
C(7)	19(1)	28(1)	27(1)	-2(1)	7(1)	-2(1)
C(8)	19(1)	27(1)	34(1)	-5(1)	10(1)	-5(1)
C(9)	20(1)	19(1)	25(1)	0(1)	8(1)	-1(1)
C(10)	19(1)	25(1)	26(1)	-1(1)	6(1)	1(1)
C(11)	26(1)	28(1)	31(1)	-3(1)	10(1)	3(1)
C(12)	25(1)	43(1)	37(1)	-2(1)	12(1)	-5(1)
C(13)	17(1)	23(1)	25(1)	1(1)	5(1)	1(1)
C(14)	21(1)	26(1)	30(1)	-4(1)	5(1)	-1(1)
C(15)	24(1)	27(1)	37(1)	0(1)	3(1)	-5(1)
C(16)	29(1)	43(2)	30(1)	-2(1)	13(1)	3(1)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for mo_dm15450_0m.

	x	y	z	U(eq)
H(2)	10635	8103	2026	40

H(1A)	7932	12596	3560	27
H(1B)	6387	11781	2648	27
H(2A)	8825	11141	5559	30
H(3A)	7429	9282	5508	30
H(3B)	6105	9642	3849	30
H(8A)	11098	12159	2395	31
H(8B)	10921	11414	4027	31
H(9)	8444	11704	1051	25
H(10A)	8977	9610	-1464	28
H(10B)	9761	10873	-826	28
H(11)	12071	8983	-1228	33
H(12A)	11782	11255	-2613	41
H(12B)	13268	10264	-2759	41
H(13A)	5826	9997	1092	26
H(13B)	6745	10049	-476	26
H(14)	7194	7907	-202	31
H(15A)	4291	8217	1194	36
H(15B)	4936	6969	470 36	
H(16A)	5202	11481	5200	50
H(16B)	6616	12404	6091	50
H(16C)	6461	11124	6896	50

Table 6. Torsion angles [°] for mo_dm15450_0m.

O(1)-C(4)-C(5)-C(6)	-11.6(3)
O(1)-C(4)-C(5)-C(9)	-123.2(2)
O(1)-C(4)-C(5)-C(13)	116.2(2)
O(2)-C(6)-C(7)-O(3)	28.0(3)
O(2)-C(6)-C(7)-C(8)	-150.20(19)
O(2)-C(6)-C(10)-C(11)	-54.7(2)
O(3)-C(7)-C(8)-C(9)	-176.4(2)
C(1)-C(2)-C(3)-C(4)	54.8(2)
C(2)-C(1)-C(9)-C(5)	50.5(3)
C(2)-C(1)-C(9)-C(8)	-69.4(3)
C(2)-C(3)-C(4)-O(1)	117.7(2)
C(2)-C(3)-C(4)-C(5)	-58.9(2)
C(3)-C(4)-C(5)-C(6)	164.94(18)
C(3)-C(4)-C(5)-C(9)	53.4(2)
C(3)-C(4)-C(5)-C(13)	-67.3(2)
C(4)-C(5)-C(6)-O(2)	47.3(2)
C(4)-C(5)-C(6)-C(7)	-75.76(19)
C(4)-C(5)-C(6)-C(10)	168.97(17)
C(4)-C(5)-C(9)-C(1)	-47.4(2)
C(4)-C(5)-C(9)-C(8)	78.6(2)
C(4)-C(5)-C(13)-C(14)	-58.0(2)
C(5)-C(6)-C(7)-O(3)	152.7(2)
C(5)-C(6)-C(7)-C(8)	-25.5(2)
C(5)-C(6)-C(10)-C(11)	178.16(18)
C(5)-C(13)-C(14)-C(15)	119.5(3)
C(6)-C(5)-C(9)-C(1)	-164.51(18)
C(6)-C(5)-C(9)-C(8)	-38.6(2)
C(6)-C(5)-C(13)-C(14)	67.4(2)
C(6)-C(7)-C(8)-C(9)	1.8(3)
C(6)-C(10)-C(11)-C(12)	-136.7(3)
C(7)-C(6)-C(10)-C(11)	66.8(2)
C(7)-C(8)-C(9)-C(1)	148.3(2)
C(7)-C(8)-C(9)-C(5)	22.8(2)
C(9)-C(1)-C(2)-C(3)	-52.6(2)
C(9)-C(1)-C(2)-C(16)	-175.58(19)
C(9)-C(5)-C(6)-O(2)	161.74(17)
C(9)-C(5)-C(6)-C(7)	38.7(2)
C(9)-C(5)-C(6)-C(10)	-76.6(2)
C(9)-C(5)-C(13)-C(14)	-176.14(18)
C(10)-C(6)-C(7)-O(3)	-88.8(3)
C(10)-C(6)-C(7)-C(8)	93.0(2)
C(13)-C(5)-C(6)-O(2)	-77.0(2)
C(13)-C(5)-C(6)-C(7)	159.99(18)
C(13)-C(5)-C(6)-C(10)	44.7(2)
C(13)-C(5)-C(9)-C(1)	71.6(2)
C(13)-C(5)-C(9)-C(8)	-162.41(18)
C(16)-C(2)-C(3)-C(4)	177.62(19)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mo_dm15450_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(1)	0.84	1.99	2.643(2)	134.1

Symmetry transformations used to generate equivalent atoms: