Supporting Information

Access to 6a-Alkylated Aporphines: Synthesis of (±)-*N*-Methylguattescidine

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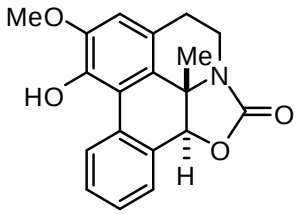
X-Ray crystal structure and data for compound 6 (CCDC-1495290)

***rel*-(3^1*S*,12b*S*)-8-Hydroxy-7-methoxy-3^1-methyl-3^1,4,5,12b-tetrahydro-2*H*-dibenzo[*de,g*]oxazolo[5,4,3-*ij*]quinolin-2-one (6)**



All measurements were made with a platform diffractometer equipped with a 4K CCD detector and a 30 Watt Cu microsource with compact multilayer optics. A hemisphere of data (2713 frames at 4 cm detector distance) was collected using a narrow-frame algorithm with scan widths of 0.50\% in omega and an exposure time of 20 s/frame. The data were integrated with the intensities corrected for Lorentz factor, polarization, air absorption, and absorption due to variation in the path length through the detector faceplate. The data were scaled, and an absorption correction was applied. Redundant reflections were averaged. Final cell constants were refined using 8154 reflections having I>10\s(I), and these, along with other information pertinent to data collection and refinement, are listed in Table S1. The Laue symmetry was determined to be mmm, and from the systematic absences noted the space group was shown to be either Pna2(1) or Pnma.

There is an alternate form of this material which can co-crystallize with the reported form. This forms as colorless blocks, in space group P2(1)/n, Z=4. Cell constants are a=9.9086(4), b=14.2352(6), c=10.6575(5), beta=91.707(2). This molecule has exactly the same geometry as the reported form, with the exception of a slightly different twist to the hydroxyl hydrogen group. This is caused by a completely different intermolecular hydrogen bonding pattern.

Figure S1. X-ray crystallographic structure of 6 showing the atom numbering scheme (The ellipsoid contour probability level is 70%)

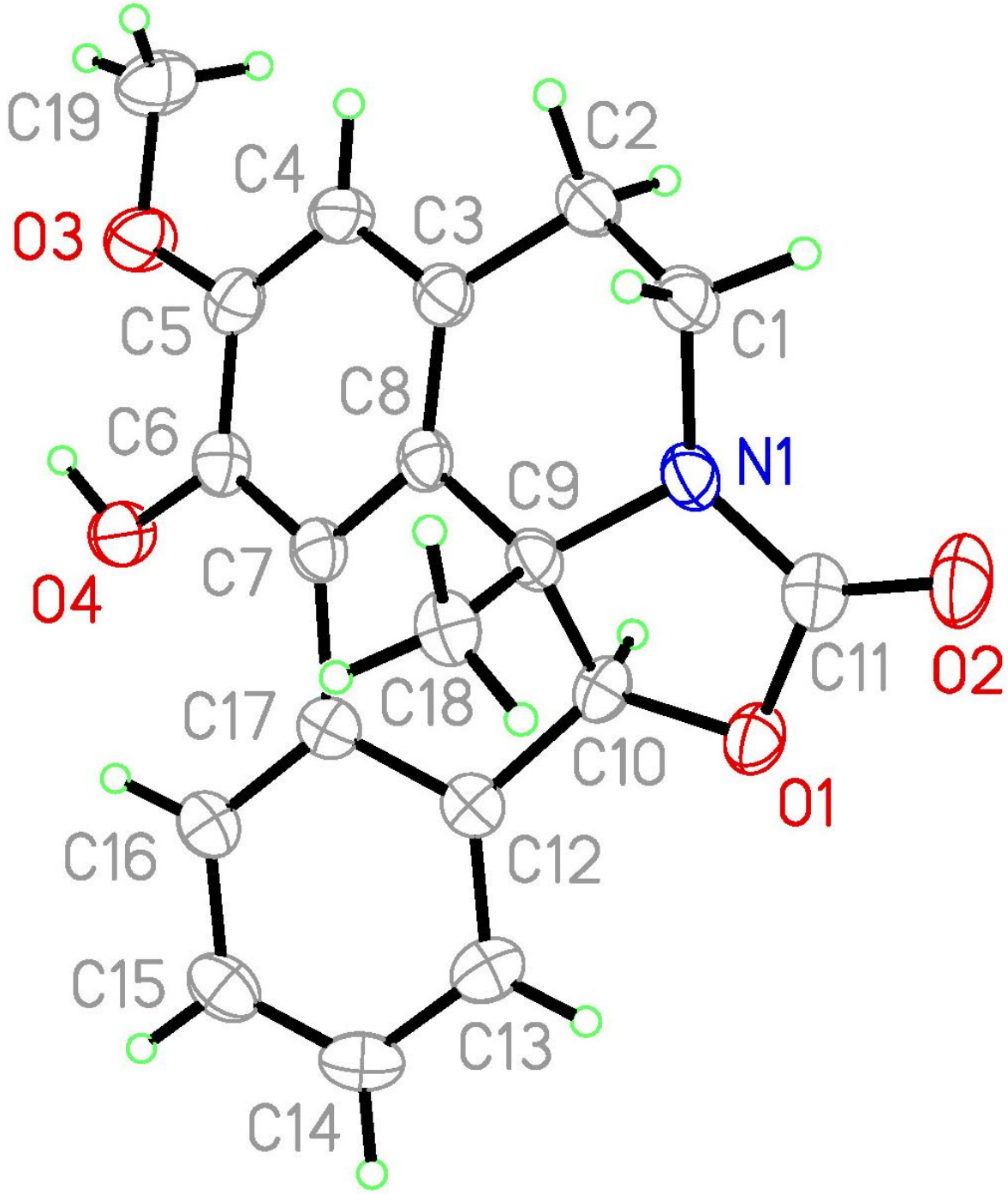


Table S1. Crystal data and structure refinement for 6

Identification code	**6**
Empirical formula	$C_{19}H_{17}NO_4$
Formula weight	323.34
Temperature	123(2) K
Wavelength	1.54178 Å
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 12.1383(2) Å alpha = 90 deg.
	b = 18.1897(4) Å beta = 90 deg.
	c = 7.0365(2) Å gamma = 90 deg.
Volume	1553.60(6) Å^3
Z, Calculated density	4, 1.382 Mg/m^3
Absorption coefficient	0.800 mm^-1
F(000)	680
Crystal color and shape	Colorless thin plate
Crystal size	0.40 x 0.20 x 0.10 mm
Theta range for data collection	4.38 to 66.55 deg.
Limiting indices	$0 \leq h \leq 14$, $0 \leq k \leq 21$, $-7 \leq l \leq 7$
Reflections collected / unique	10549 / 2550 [R(int) = 0.0199]
Completeness to theta = 66.55	97.7 %
Absorption correction	Empirical
Max. and min. transmission	0.7528 and 0.6535
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2364 / 2 / 221
Goodness-of-fit on F^2	1.061
Final R indices [I>4sigma(I)]	R1 = 0.0203, wR2 = 0.0537
R indices (all data)	R1 = 0.0205, wR2 = 0.0541
Absolute structure parameter	0.04(12)
Extinction coefficient	0.0060(3)
Largest diff. peak and hole	0.144 and -0.118 e.Å^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 6

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
O(1)	4633(1)	2786(1)	2492(1)	20(1)
O(2)	4318(1)	1961(1)	4863(2)	27(1)
O(3)	898(1)	6027(1)	3423(2)	25(1)
O(4)	2180(1)	5818(1)	482(1)	23(1)
N(1)	3041(1)	2854(1)	4075(2)	18(1)
C(1)	2103(1)	2760(1)	5334(2)	19(1)
C(2)	1681(1)	3523(1)	5916(2)	19(1)
C(3)	1703(1)	4100(1)	4352(2)	17(1)
C(4)	1186(1)	4784(1)	4623(2)	19(1)
C(5)	1348(1)	5336(1)	3296(2)	19(1)
C(6)	2032(1)	5244(1)	1696(2)	18(1)
C(7)	2572(1)	4573(1)	1413(2)	17(1)
C(8)	2337(1)	4013(1)	2757(2)	16(1)
C(9)	2904(1)	3301(1)	2396(2)	16(1)
C(10)	4096(1)	3483(1)	2051(2)	17(1)
C(11)	3998(1)	2482(1)	3947(2)	19(1)
C(12)	4201(1)	3848(1)	166(2)	17(1)
C(13)	4983(1)	3689(1)	-1194(2)	21(1)
C(14)	5025(1)	4091(1)	-2872(2)	24(1)
C(15)	4272(1)	4651(1)	-3174(2)	22(1)
C(16)	3478(1)	4817(1)	-1807(2)	19(1)
C(17)	3413(1)	4424(1)	-104(2)	17(1)
C(18)	2361(1)	2839(1)	819(2)	19(1)
C(19)	286(1)	6195(1)	5090(2)	28(1)

Table S3. Bond lengths for 6

Atom-Atom	Length [Å]	Atom-Atom	Length [Å]
O(1)-C(11)	1.3966(16)	C(5)-C(6)	1.4092(19)
O(1)-C(10)	1.4583(13)	C(6)-C(7)	1.3997(16)
O(2)-C(11)	1.2108(16)	C(7)-C(8)	1.4201(17)
O(3)-C(5)	1.3730(14)	C(7)-C(17)	1.5016(18)
O(3)-C(19)	1.4216(18)	C(8)-C(9)	1.4881(16)
O(4)-C(6)	1.3608(15)	C(9)-C(10)	1.5042(16)
N(1)-C(11)	1.3472(16)	C(9)-C(18)	1.5399(18)
N(1)-C(9)	1.4439(16)	C(10)-C(12)	1.4886(18)
N(1)-C(1)	1.4527(16)	C(12)-C(13)	1.3791(18)
C(1)-C(2)	1.5361(17)	C(12)-C(17)	1.4311(16)
C(2)-C(3)	1.5202(16)	C(13)-C(14)	1.3897(19)
C(3)-C(8)	1.3701(18)	C(14)-C(15)	1.3855(18)
C(3)-C(4)	1.4064(17)	C(15)-C(16)	1.3952(19)
C(4)-C(5)	1.3851(18)	C(16)-C(17)	1.3978(18)

Table S4. Bond angles for 6

Atom-Atom-Atom	Angle [deg]	Atom-Atom-Atom	Angle [deg]
C(11)-O(1)-C(10)	104.68(9)	N(1)-C(9)-C(8)	113.80(11)
C(5)-O(3)-C(19)	117.26(10)	N(1)-C(9)-C(10)	98.35(9)
C(11)-N(1)-C(9)	109.12(10)	C(8)-C(9)-C(10)	106.29(9)
C(11)-N(1)-C(1)	131.10(10)	N(1)-C(9)-C(18)	109.36(9)
C(9)-N(1)-C(1)	118.36(9)	C(8)-C(9)-C(18)	113.59(10)
N(1)-C(1)-C(2)	108.52(10)	C(10)-C(9)-C(18)	114.56(11)
C(3)-C(2)-C(1)	115.13(11)	O(1)-C(10)-C(12)	122.58(10)
C(8)-C(3)-C(4)	117.64(11)	O(1)-C(10)-C(9)	101.81(8)
C(8)-C(3)-C(2)	121.55(10)	C(12)-C(10)-C(9)	108.92(10)
C(4)-C(3)-C(2)	120.27(11)	O(2)-C(11)-N(1)	129.39(12)
C(5)-C(4)-C(3)	119.12(12)	O(2)-C(11)-O(1)	121.58(11)
O(3)-C(5)-C(4)	124.30(12)	N(1)-C(11)-O(1)	109.03(10)
O(3)-C(5)-C(6)	113.21(11)	C(13)-C(12)-C(17)	121.42(12)
C(4)-C(5)-C(6)	122.45(10)	C(13)-C(12)-C(10)	125.73(11)
O(4)-C(6)-C(7)	121.17(12)	C(17)-C(12)-C(10)	112.80(11)
O(4)-C(6)-C(5)	119.27(10)	C(12)-C(13)-C(14)	120.29(11)
C(7)-C(6)-C(5)	119.54(11)	C(15)-C(14)-C(13)	119.57(13)
C(6)-C(7)-C(8)	115.90(11)	C(14)-C(15)-C(16)	120.61(13)
C(6)-C(7)-C(17)	125.30(11)	C(15)-C(16)-C(17)	121.27(11)
C(8)-C(7)-C(17)	118.69(10)	C(16)-C(17)-C(12)	116.82(11)
C(3)-C(8)-C(7)	125.16(11)	C(16)-C(17)-C(7)	123.68(10)
C(3)-C(8)-C(9)	120.01(11)	C(12)-C(17)-C(7)	119.50(11)
C(7)-C(8)-C(9)	114.71(11)		

Table S5. Anisotropic displacement parameters (Å^2 x 10^3) for 6

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12].

Atom	U11	U22	U33	U23	U13	U12
O(1)	17(1)	18(1)	24(1)	5(1)	0(1)	2(1)
O(2)	22(1)	23(1)	35(1)	11(1)	-4(1)	2(1)
O(3)	30(1)	20(1)	26(1)	1(1)	6(1)	9(1)
O(4)	27(1)	17(1)	26(1)	7(1)	6(1)	5(1)
N(1)	19(1)	19(1)	16(1)	5(1)	-1(1)	0(1)
C(1)	19(1)	21(1)	18(1)	4(1)	1(1)	-2(1)
C(2)	19(1)	22(1)	15(1)	2(1)	-1(1)	-3(1)
C(3)	15(1)	20(1)	16(1)	1(1)	-2(1)	-2(1)
C(4)	18(1)	24(1)	16(1)	-2(1)	2(1)	1(1)
C(5)	18(1)	18(1)	22(1)	-1(1)	-1(1)	3(1)
C(6)	17(1)	17(1)	20(1)	2(1)	-2(1)	-1(1)
C(7)	17(1)	18(1)	17(1)	1(1)	-2(1)	-1(1)
C(8)	14(1)	18(1)	16(1)	0(1)	-3(1)	-1(1)
C(9)	17(1)	16(1)	14(1)	4(1)	0(1)	0(1)
C(10)	16(1)	14(1)	21(1)	0(1)	-1(1)	2(1)
C(11)	18(1)	17(1)	23(1)	2(1)	-3(1)	-2(1)
C(12)	17(1)	16(1)	17(1)	-1(1)	-1(1)	-3(1)
C(13)	19(1)	18(1)	26(1)	-2(1)	3(1)	0(1)
C(14)	24(1)	25(1)	22(1)	-3(1)	8(1)	-4(1)
C(15)	26(1)	22(1)	18(1)	2(1)	1(1)	-7(1)
C(16)	21(1)	17(1)	18(1)	1(1)	-1(1)	-3(1)
C(17)	17(1)	16(1)	17(1)	-2(1)	-1(1)	-3(1)
C(18)	21(1)	18(1)	19(1)	2(1)	-2(1)	-1(1)
C(19)	30(1)	23(1)	33(1)	-4(1)	8(1)	5(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 6

Atom	x	y	z	U(eq)
H(4X)	1661(11)	6170(7)	790(30)	35
H(1A)	2325	2478	6475	23
H(1B)	1512	2484	4676	23
H(2A)	914	3473	6377	22
H(2B)	2133	3703	6992	22
H(4)	731	4866	5701	23
H(10)	4326	3846	3041	21
H(13)	5495	3302	-984	25
H(14)	5567	3982	-3805	28
H(15)	4297	4925	-4324	26
H(16)	2972	5206	-2037	22
H(18A)	2856	2437	454	29
H(18B)	2217	3151	-289	29
H(18C)	1665	2635	1287	29
H(19A)	16	6702	5016	43
H(19B)	761	6141	6208	43
H(19C)	-341	5858	5194	43

Table S7. Torsion angles [deg] for 6

Atom-Atom-Atom-Atom	Angle [deg]	Atom-Atom-Atom-Atom	Angle [deg]
C(11)-N(1)-C(1)-C(2)	140.37(13)	C(7)-C(8)-C(9)-C(10)	48.65(14)
C(9)-N(1)-C(1)-C(2)	-54.84(14)	C(3)-C(8)-C(9)-C(18)	105.53(13)
N(1)-C(1)-C(2)-C(3)	38.58(14)	C(7)-C(8)-C(9)-C(18)	-78.23(13)
C(1)-C(2)-C(3)-C(8)	-18.36(16)	C(11)-O(1)-C(10)-C(12)	-155.37(11)
C(1)-C(2)-C(3)-C(4)	170.30(11)	C(11)-O(1)-C(10)-C(9)	-33.59(12)
C(8)-C(3)-C(4)-C(5)	-0.76(18)	N(1)-C(9)-C(10)-O(1)	39.75(11)
C(2)-C(3)-C(4)-C(5)	170.91(11)	C(8)-C(9)-C(10)-O(1)	157.64(10)
C(19)-O(3)-C(5)-C(4)	4.18(18)	C(18)-C(9)-C(10)-O(1)	-76.06(12)
C(19)-O(3)-C(5)-C(6)	-173.81(11)	N(1)-C(9)-C(10)-C(12)	170.53(9)
C(3)-C(4)-C(5)-O(3)	-179.12(12)	C(8)-C(9)-C(10)-C(12)	-71.57(12)
C(3)-C(4)-C(5)-C(6)	-1.32(19)	C(18)-C(9)-C(10)-C(12)	54.72(12)
O(3)-C(5)-C(6)-O(4)	0.05(16)	C(9)-N(1)-C(11)-O(2)	-165.19(13)
C(4)-C(5)-C(6)-O(4)	-177.97(12)	C(1)-N(1)-C(11)-O(2)	0.7(2)
O(3)-C(5)-C(6)-C(7)	178.17(11)	C(9)-N(1)-C(11)-O(1)	14.03(14)
C(4)-C(5)-C(6)-C(7)	0.15(19)	C(1)-N(1)-C(11)-O(1)	179.89(11)
O(4)-C(6)-C(7)-C(8)	-179.02(10)	C(10)-O(1)-C(11)-O(2)	-167.48(12)
C(5)-C(6)-C(7)-C(8)	2.90(17)	C(10)-O(1)-C(11)-N(1)	13.23(13)
O(4)-C(6)-C(7)-C(17)	4.83(19)	O(1)-C(10)-C(12)-C(13)	-16.11(17)
C(5)-C(6)-C(7)-C(17)	-173.25(11)	C(9)-C(10)-C(12)-C(13)	-134.53(12)
C(4)-C(3)-C(8)-C(7)	4.22(18)	O(1)-C(10)-C(12)-C(17)	166.19(10)
C(2)-C(3)-C(8)-C(7)	-167.34(11)	C(9)-C(10)-C(12)-C(17)	47.77(12)
C(4)-C(3)-C(8)-C(9)	-179.96(11)	C(17)-C(12)-C(13)-C(14)	0.28(18)
C(2)-C(3)-C(8)-C(9)	8.48(16)	C(10)-C(12)-C(13)-C(14)	-177.24(11)
C(6)-C(7)-C(8)-C(3)	-5.28(18)	C(12)-C(13)-C(14)-C(15)	-0.35(18)
C(17)-C(7)-C(8)-C(3)	171.14(11)	C(13)-C(14)-C(15)-C(16)	0.41(19)
C(6)-C(7)-C(8)-C(9)	178.70(10)	C(14)-C(15)-C(16)-C(17)	-0.40(18)
C(17)-C(7)-C(8)-C(9)	-4.88(16)	C(15)-C(16)-C(17)-C(12)	0.32(17)
C(11)-N(1)-C(9)-C(8)	-145.74(10)	C(15)-C(16)-C(17)-C(7)	-179.52(11)
C(1)-N(1)-C(9)-C(8)	46.34(14)	C(13)-C(12)-C(17)-C(16)	-0.26(17)
C(11)-N(1)-C(9)-C(10)	-33.74(12)	C(10)-C(12)-C(17)-C(16)	177.55(10)
C(1)-N(1)-C(9)-C(10)	158.34(10)	C(13)-C(12)-C(17)-C(7)	179.58(10)
C(11)-N(1)-C(9)-C(18)	86.05(12)	C(10)-C(12)-C(17)-C(7)	-2.60(14)
C(1)-N(1)-C(9)-C(18)	-81.87(13)	C(6)-C(7)-C(17)-C(16)	-24.40(18)
C(3)-C(8)-C(9)-N(1)	-20.48(15)	C(8)-C(7)-C(17)-C(16)	159.55(11)
C(7)-C(8)-C(9)-N(1)	155.76(10)	C(6)-C(7)-C(17)-C(12)	155.77(12)
C(3)-C(8)-C(9)-C(10)	-127.59(12)	C(8)-C(7)-C(17)-C(12)	-20.28(16)

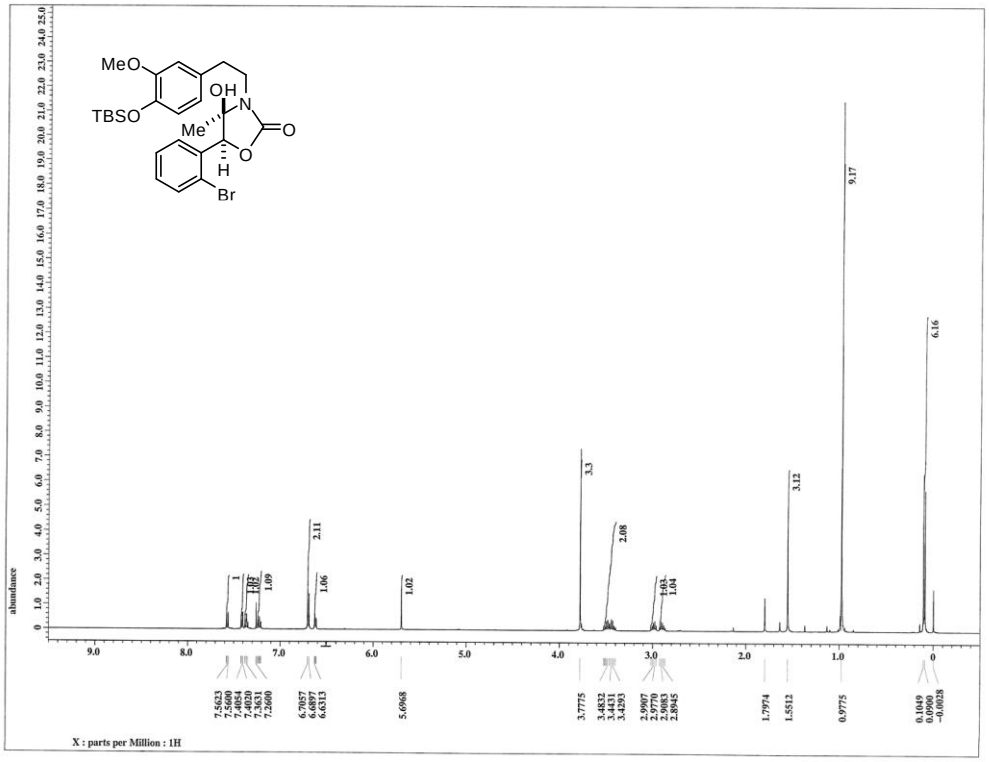
Table S8. Hydrogen bonds for 6 [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4X)...O(2)#1	0.924(9)	1.975(12)	2.7955(12)	147.0(16)

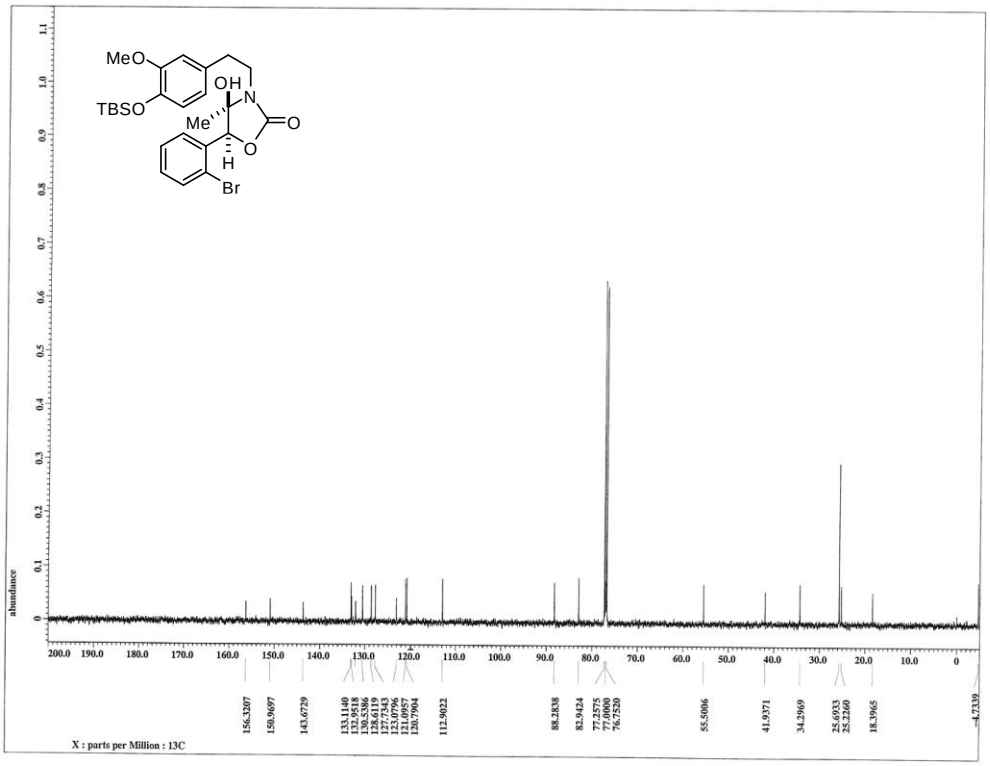
Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y+1/2,z-1/2

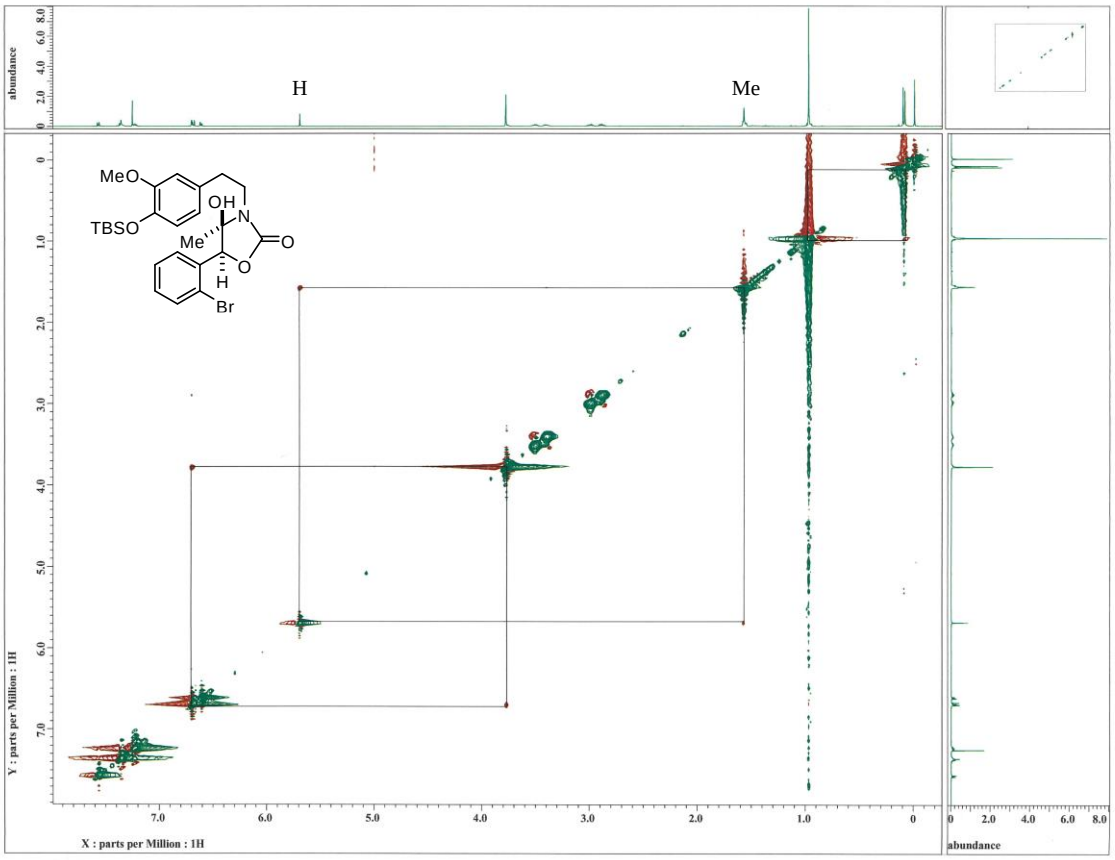
Copies of ^{1}H and ^{13}C NMR spectra



^{1}H NMR spectrum of compound **8** ($CDCl_3$, 500 MHz)

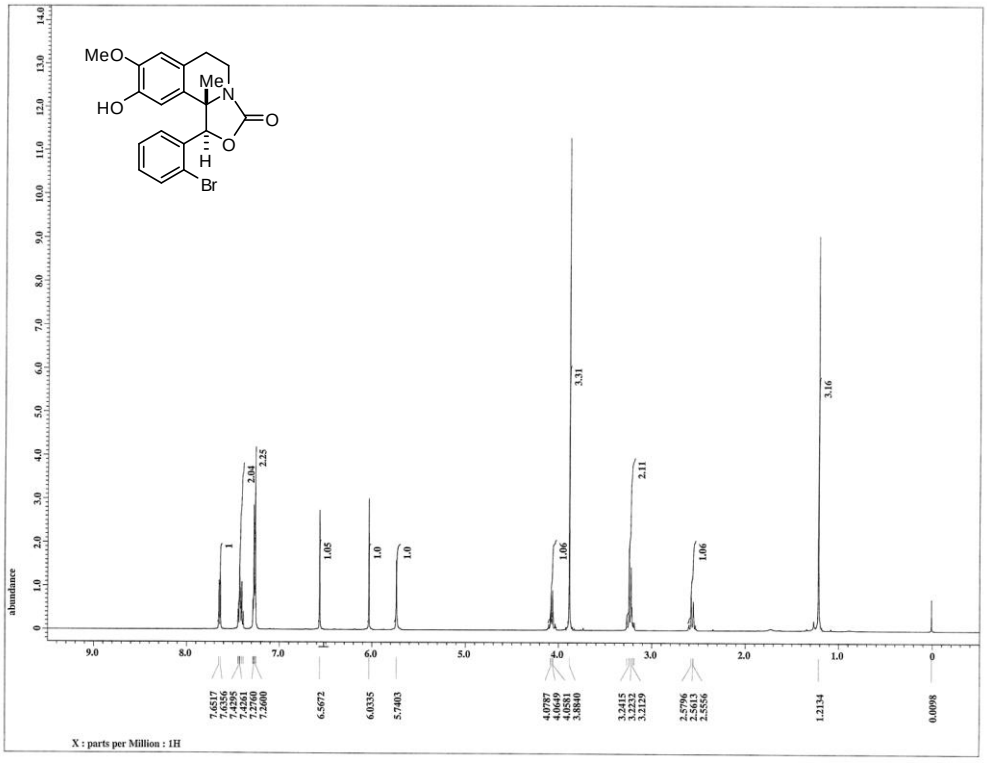


^{13}C NMR spectrum of compound **8** ($CDCl_3$, 125 MHz)

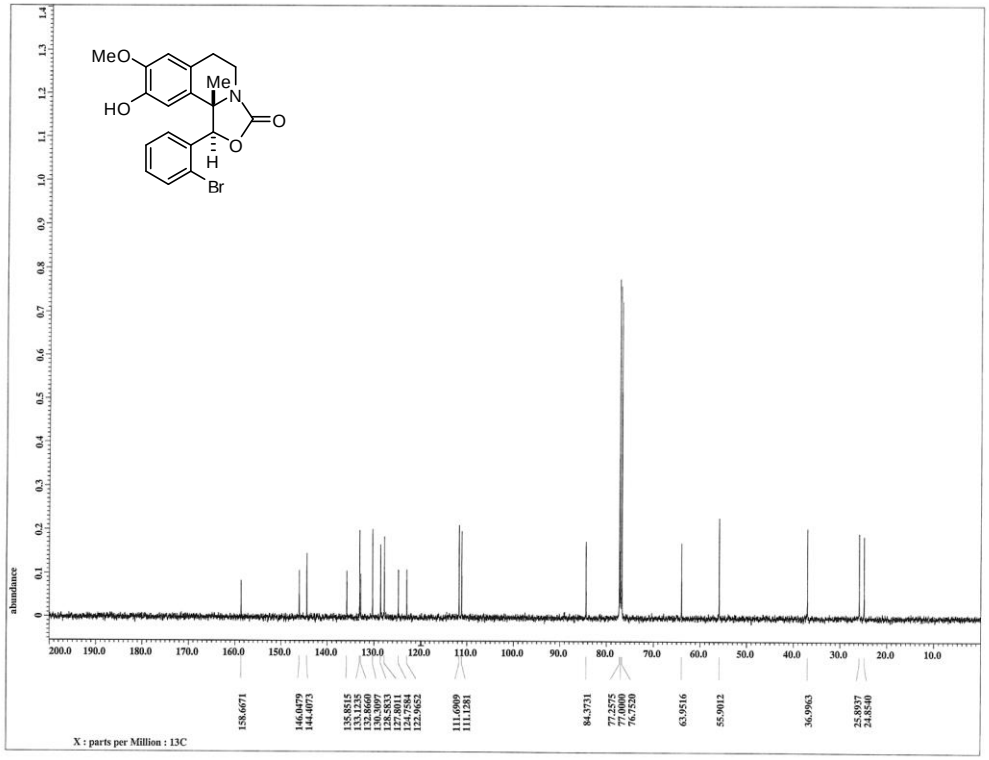


NOESY spectrum of compound **8** ($CDCl_3$, 500 MHz)

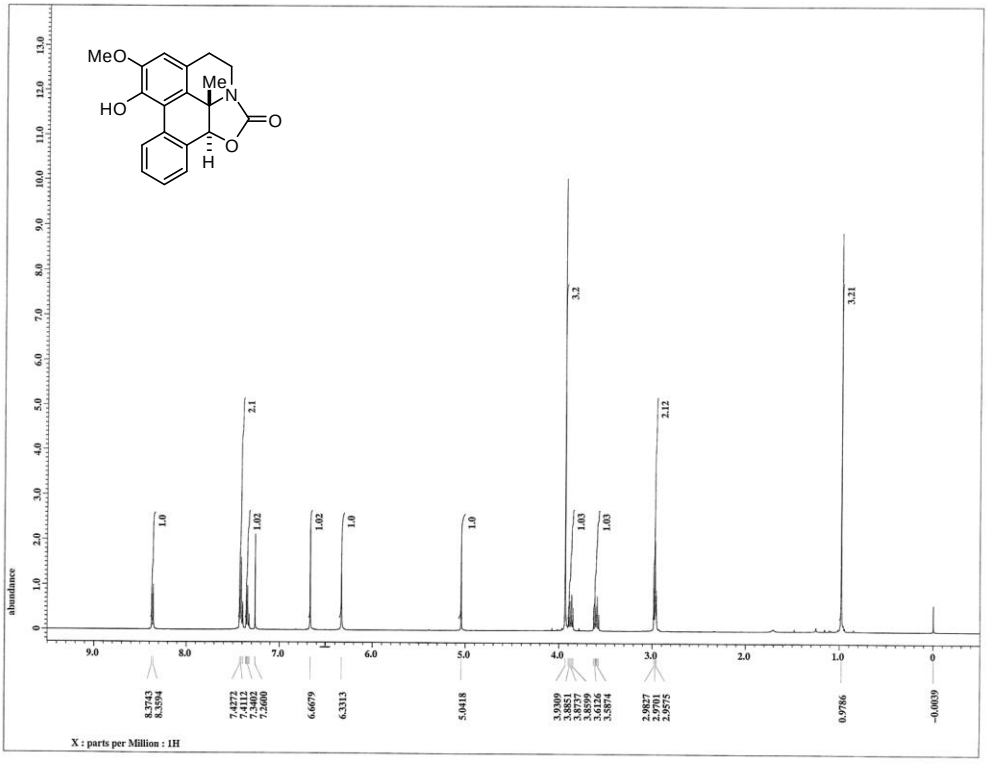
Correlations between the ether proton and the adjacent methyl group indicated both groups are on the same side.



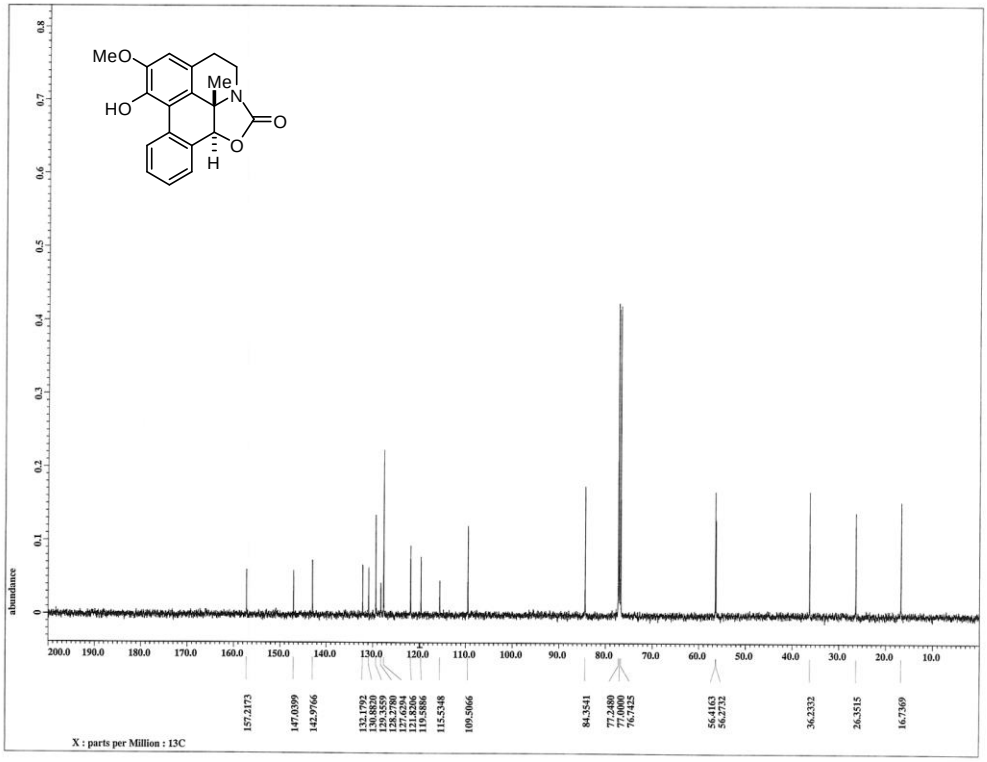
^{1}H NMR spectrum of compound **9** ($CDCl_3$, 500 MHz)



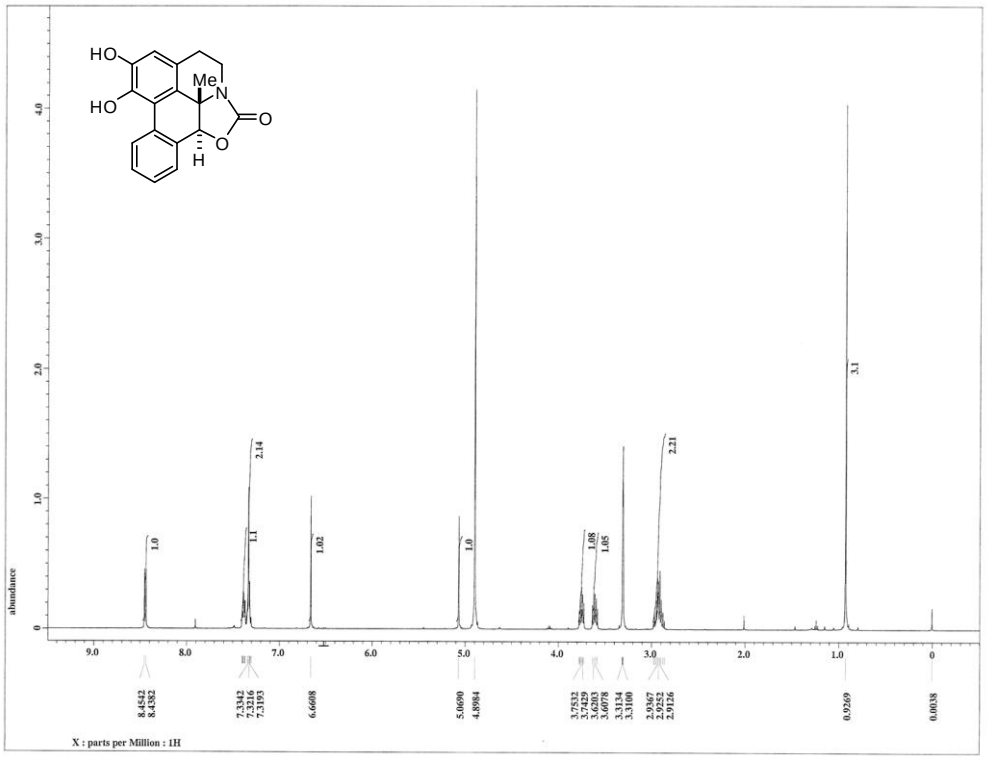
^{13}C NMR spectrum of compound **9** ($CDCl_3$, 125 MHz)



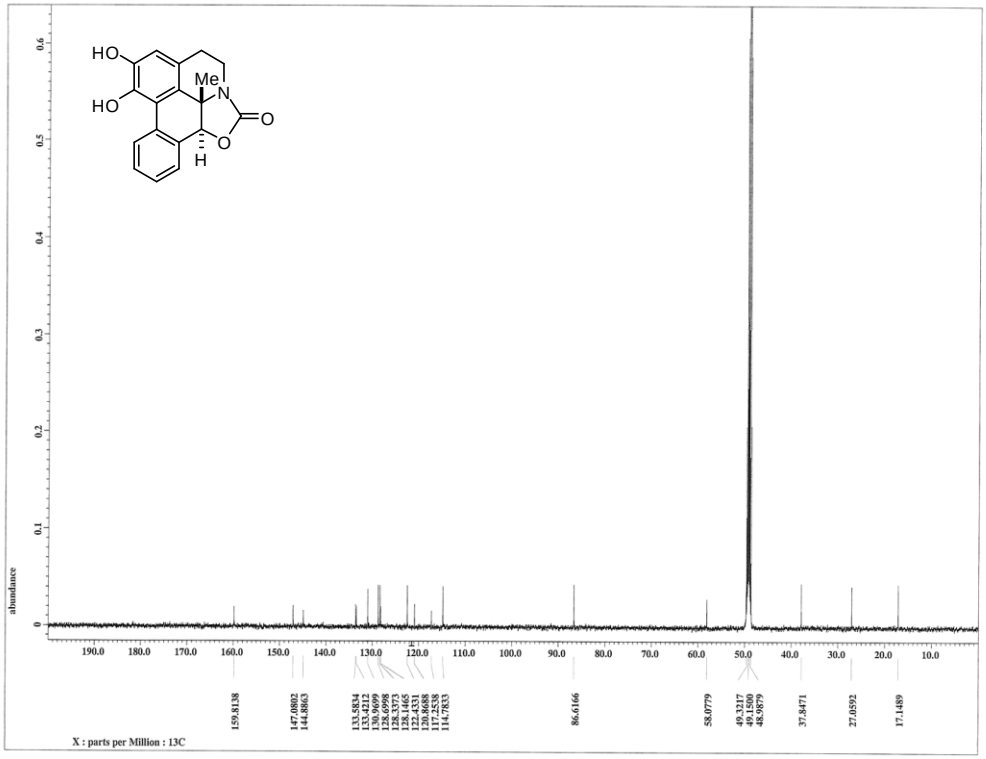
^{1}H NMR spectrum of compound **6** ($CDCl_3$, 500 MHz)



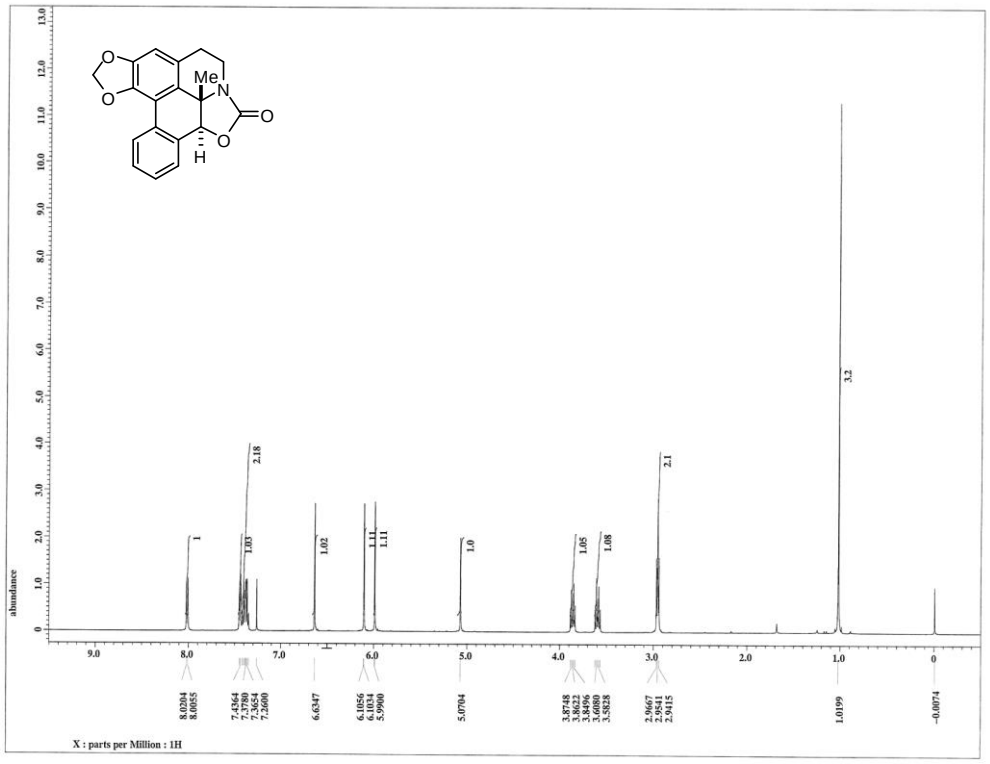
^{13}C NMR spectrum of compound **6** ($CDCl_3$, 125 MHz)



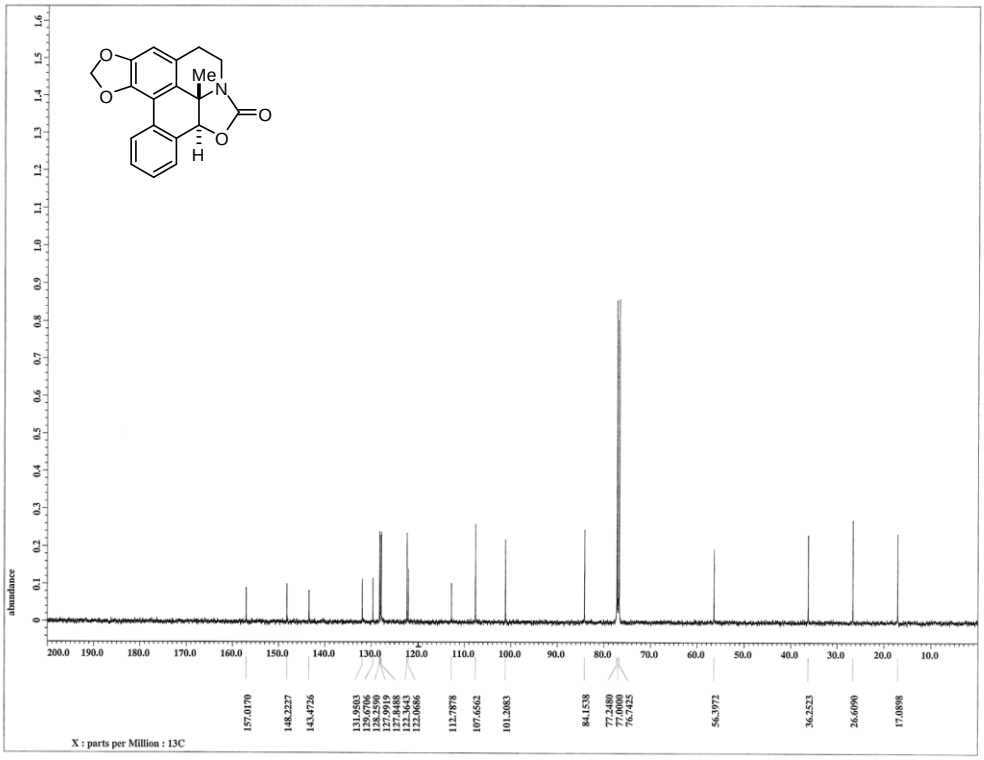
^{1}H NMR spectrum of compound **10** (CD_3OD_3, 500 MHz)



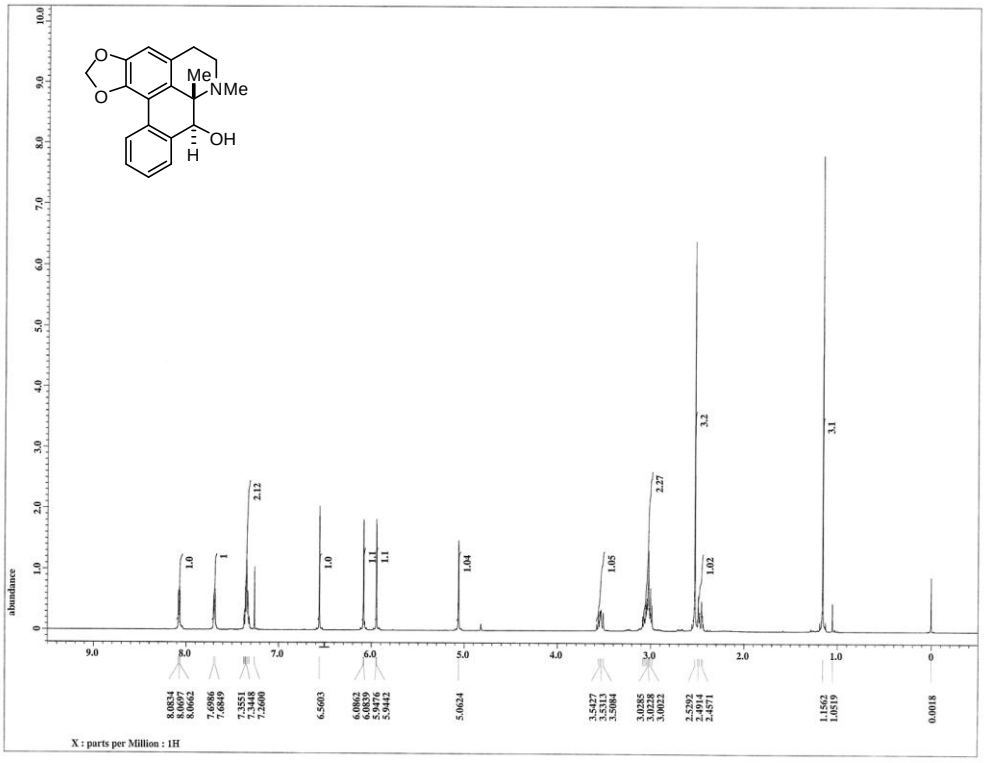
^{13}C NMR spectrum of compound **10** (CD_3OD_3, 125 MHz)



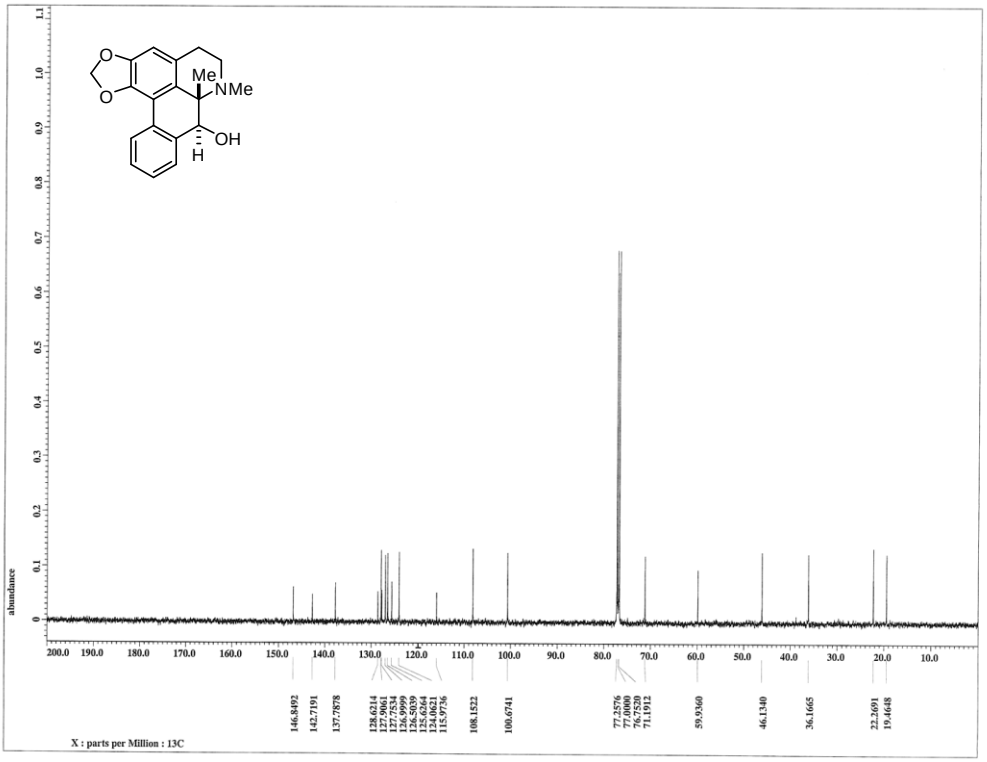
^{1}H NMR spectrum of compound **11** ($CDCl_3$, 500 MHz)



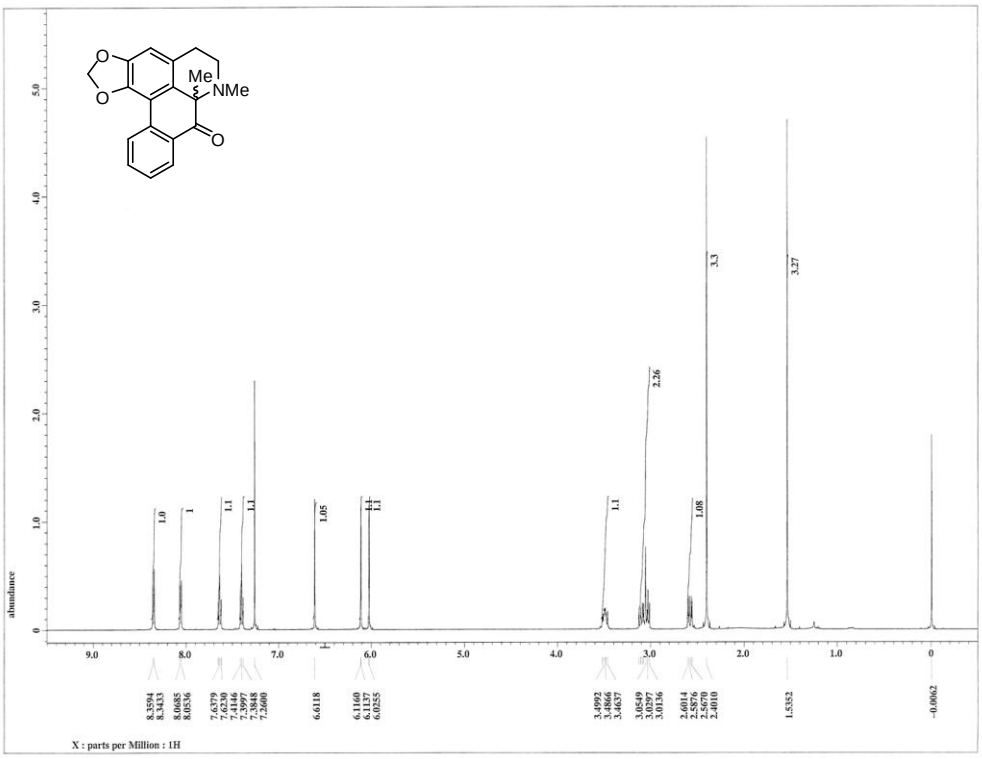
^{13}C NMR spectrum of compound **11** ($CDCl_3$, 125 MHz)



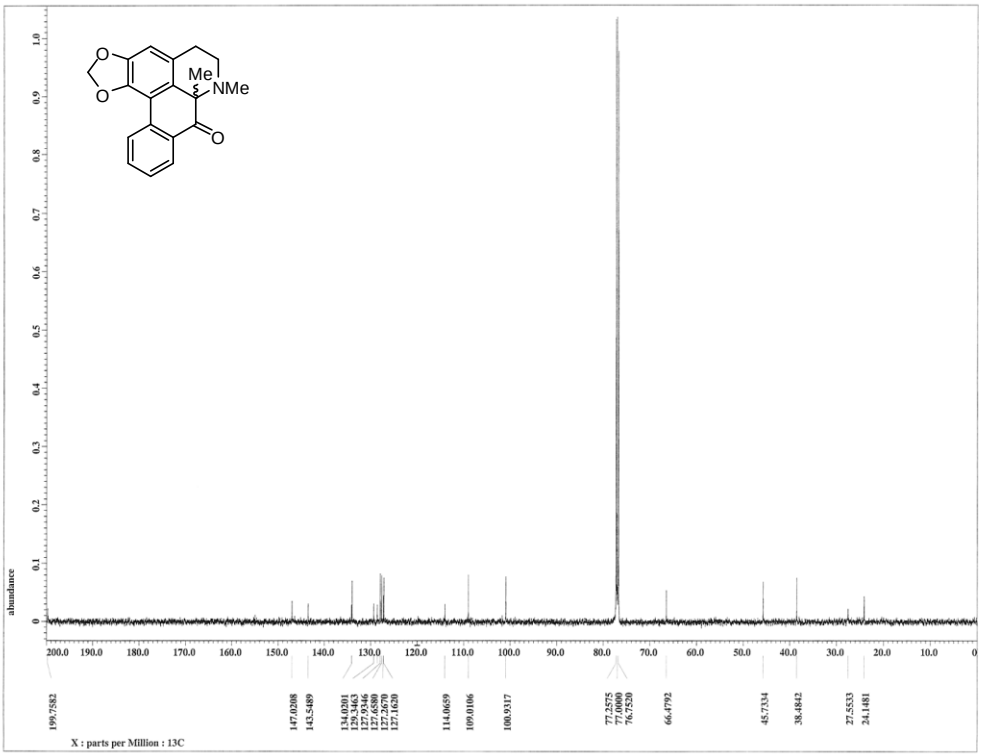
^{1}H NMR spectrum of compound **5** ($CDCl_3$, 500 MHz)



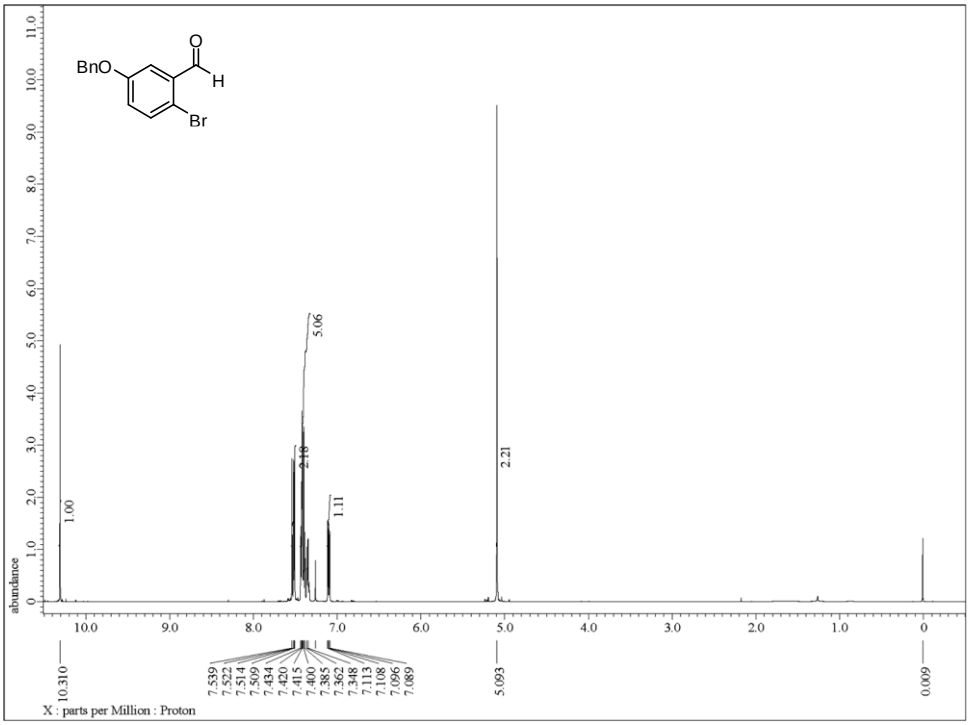
^{13}C NMR spectrum of compound **5** ($CDCl_3$, 125 MHz)



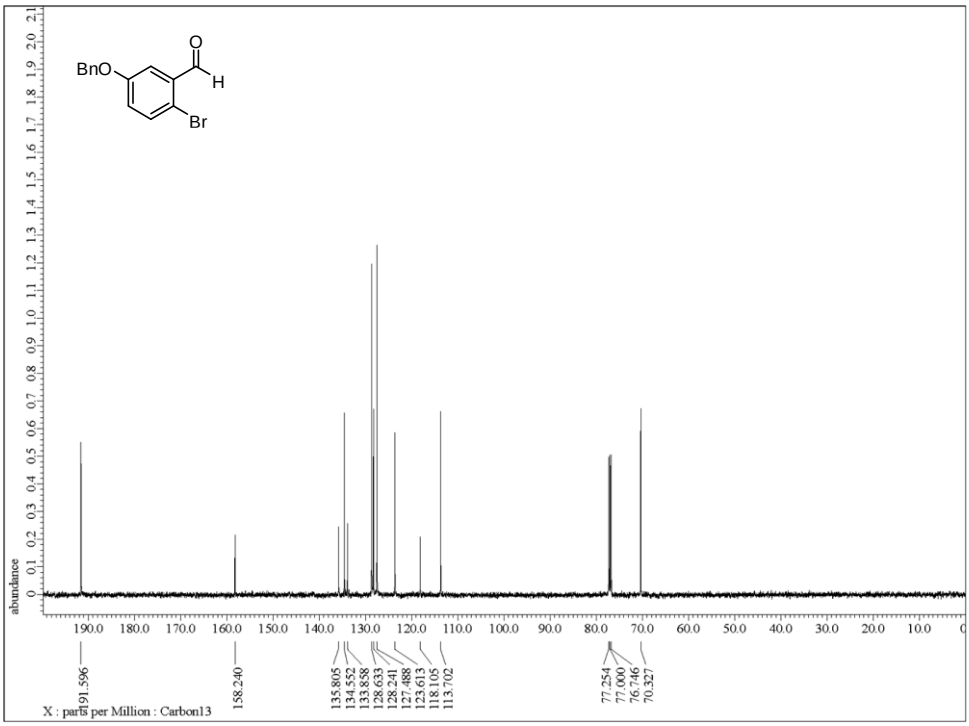
^{1}H NMR spectrum of compound **4** ($CDCl_3$, 500 MHz)



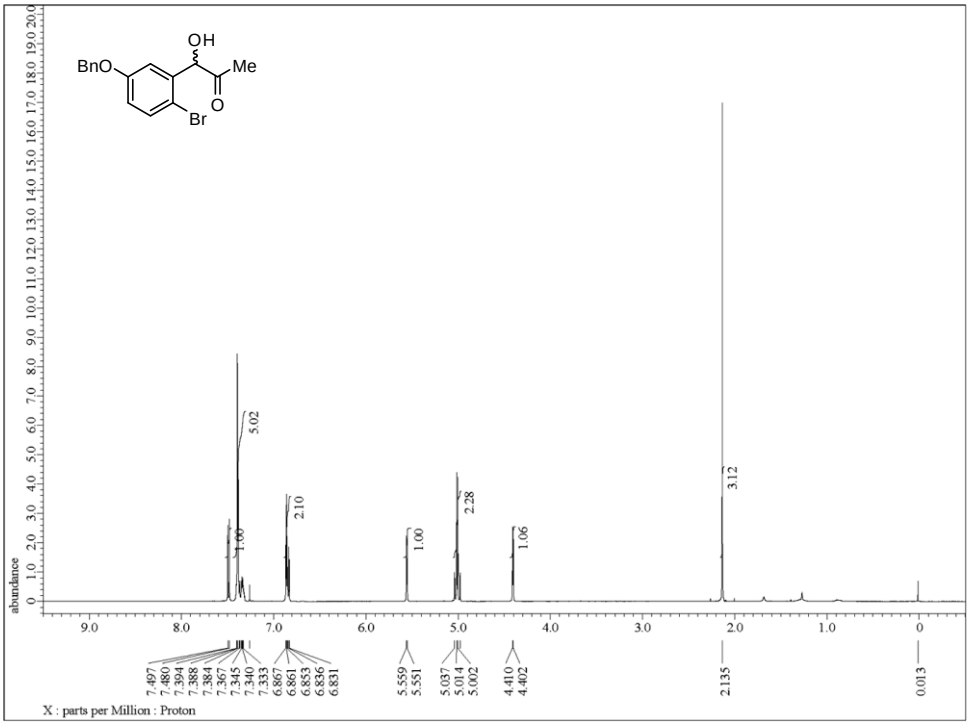
^{13}C NMR spectrum of compound **4** ($CDCl_3$, 125 MHz)



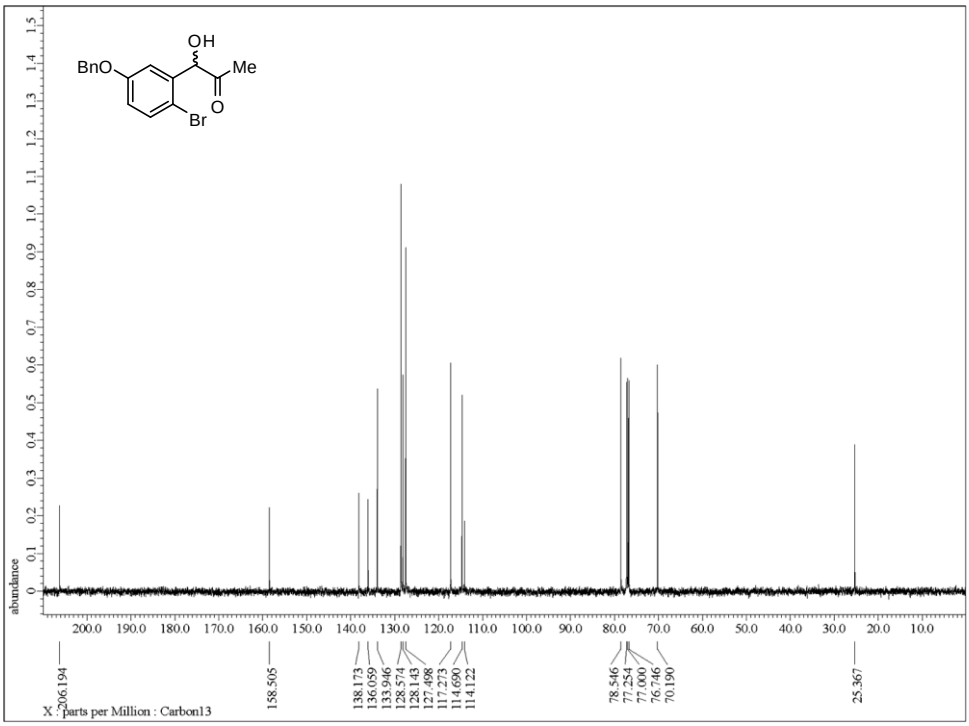
^{1}H NMR spectrum of compound **13a** ($CDCl_3$, 500 MHz)



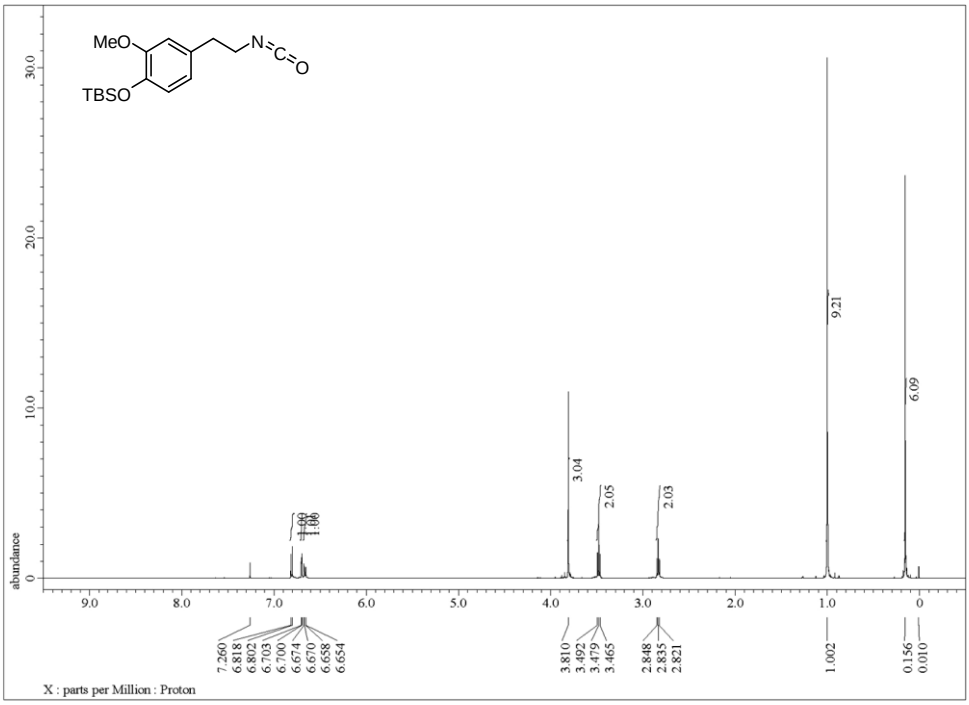
^{13}C NMR spectrum of compound **13a** ($CDCl_3$, 125 MHz)



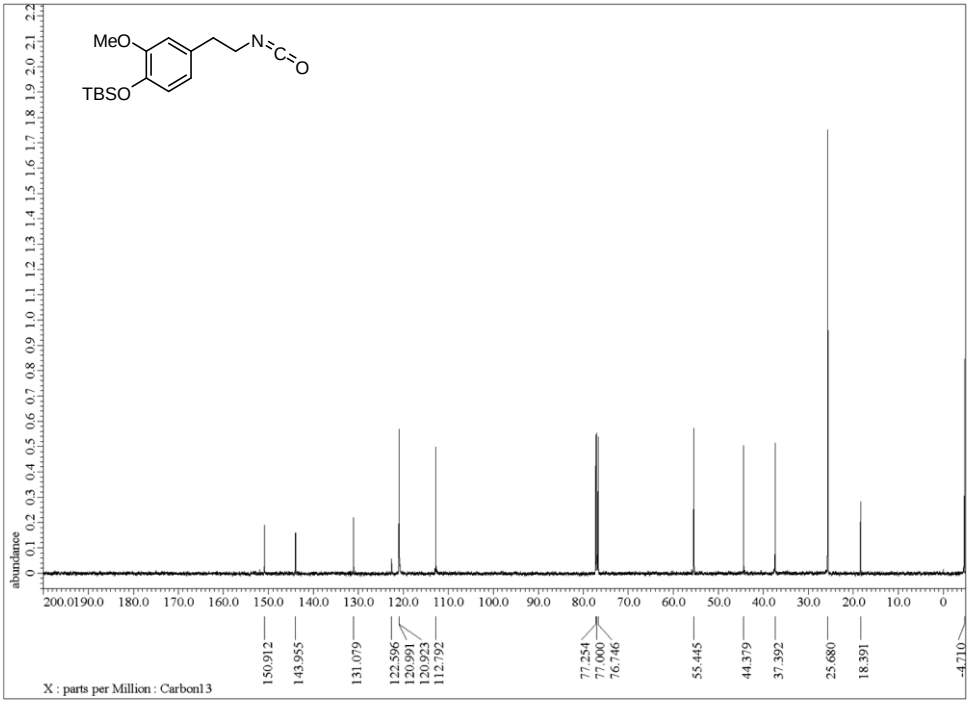
^{1}H NMR spectrum of compound **14a** ($CDCl_3$, 500 MHz)



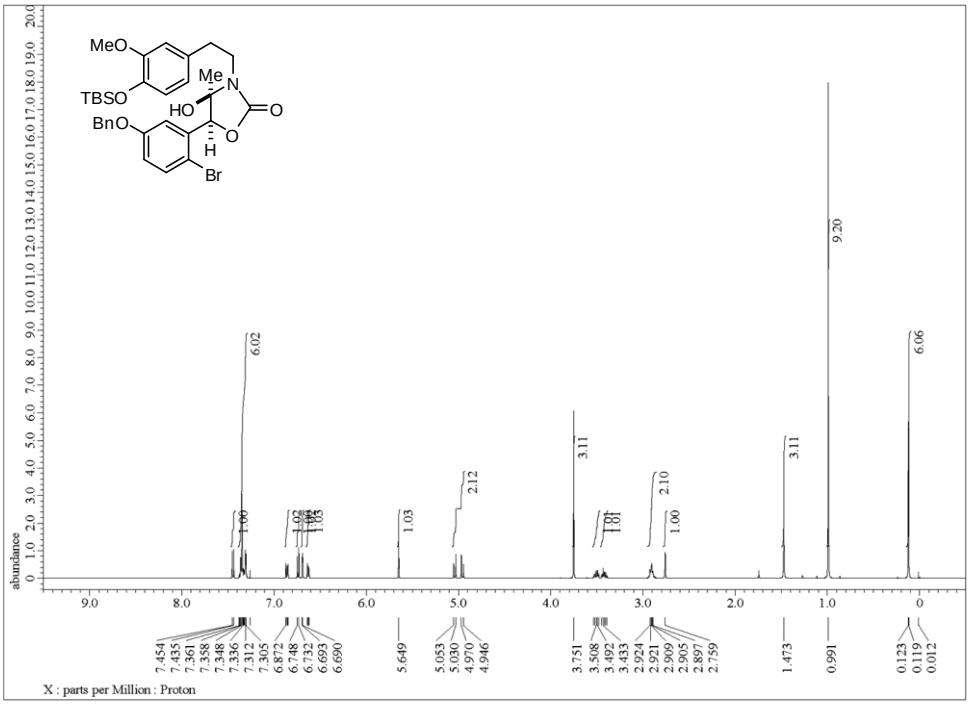
^{13}C NMR spectrum of compound **14a** ($CDCl_3$, 125 MHz)



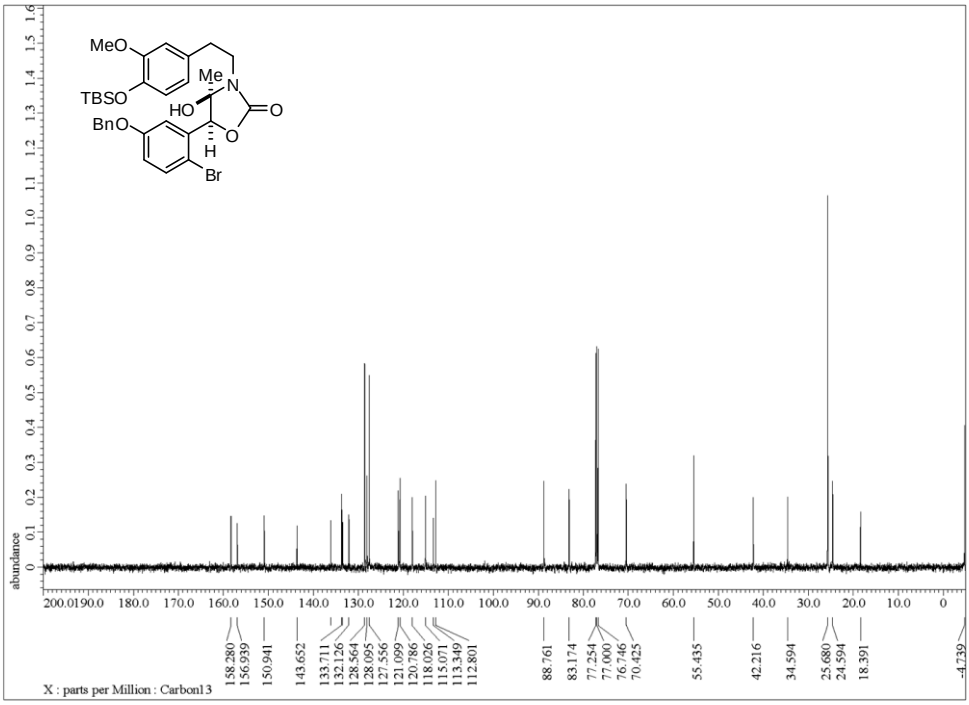
^{1}H NMR spectrum of compound **15** ($CDCl_3$, 500 MHz)



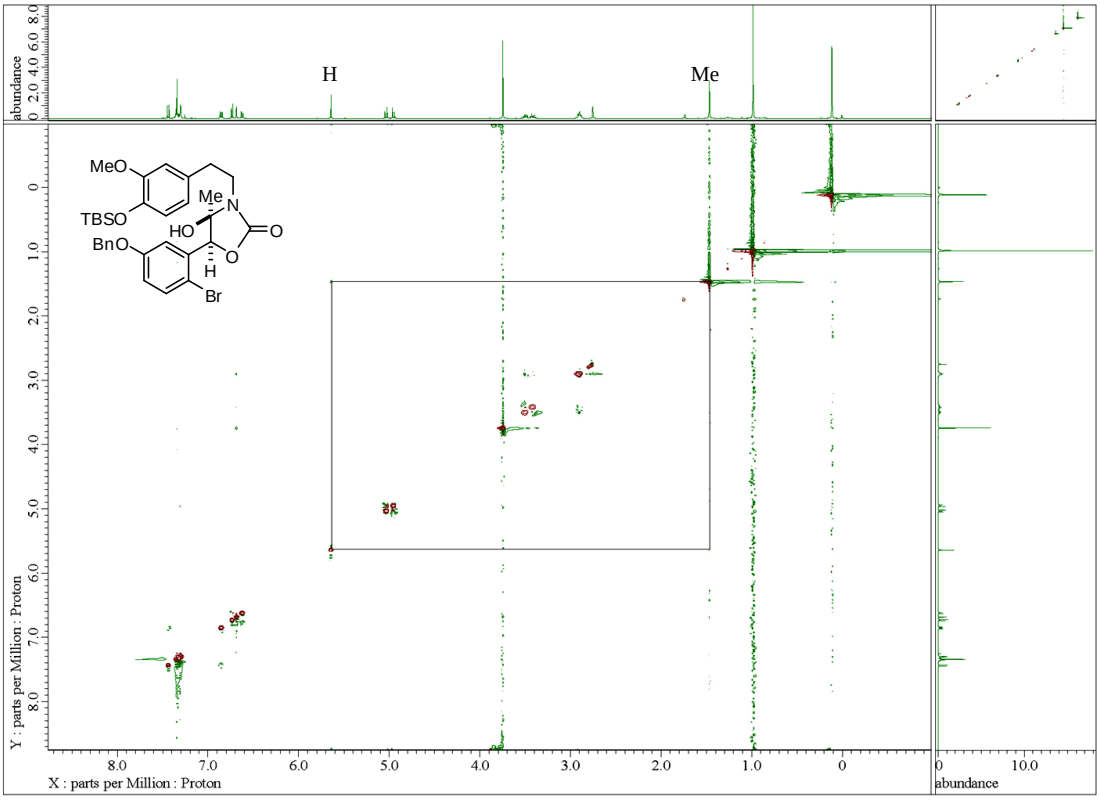
^{13}C NMR spectrum of compound **15** ($CDCl_3$, 125 MHz)



^{1}H NMR spectrum of compound ***rel*-(4*R*,5*S*)-16a** ($CDCl_3$, 500 MHz)

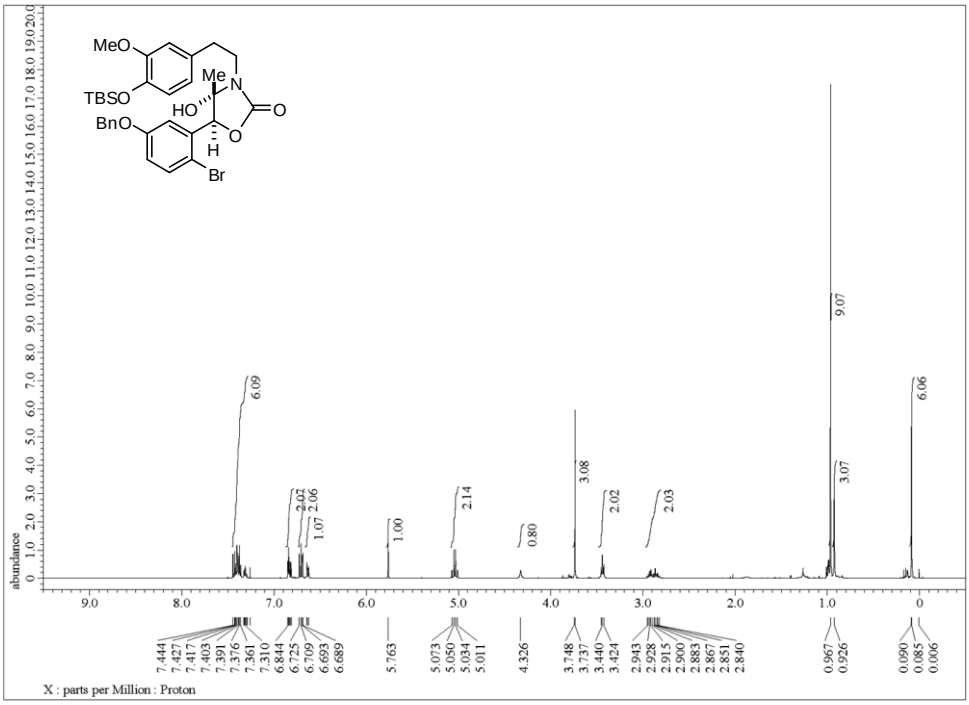


^{13}C NMR spectrum of compound ***rel*-(4*R*,5*S*)-16a** ($CDCl_3$, 125 MHz)

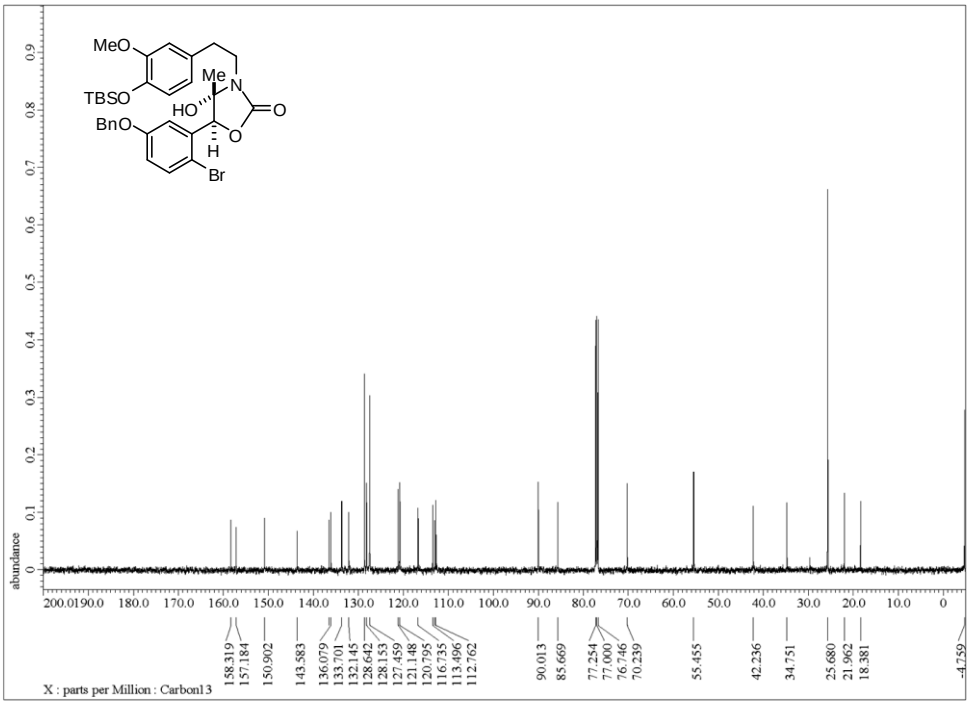


NOESY spectrum of compound ***rel*-(4*R*,5*S*)-16a** ($CDCl_3$, 500 MHz)

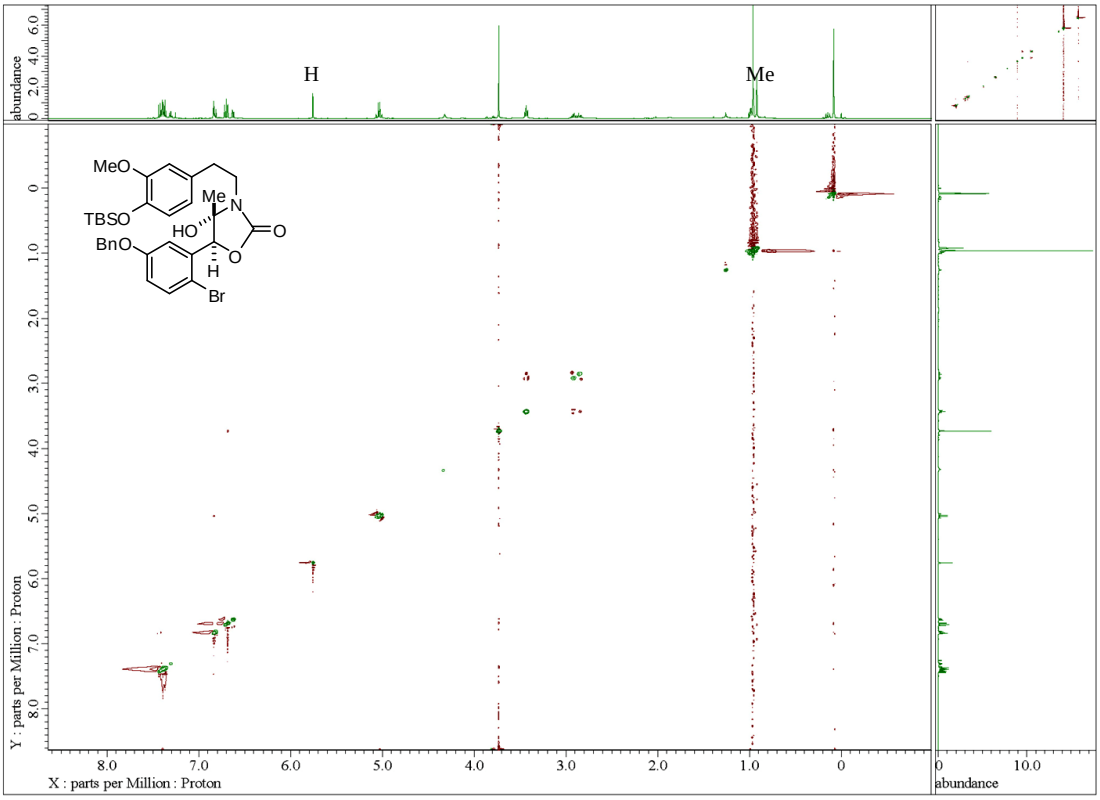
Correlations between the ether proton and the adjacent methyl group indicated both groups are on the same side.



^{1}H NMR spectrum of compound ***rel*-(4*S*,5*S*)-16a** ($CDCl_3$, 500 MHz)

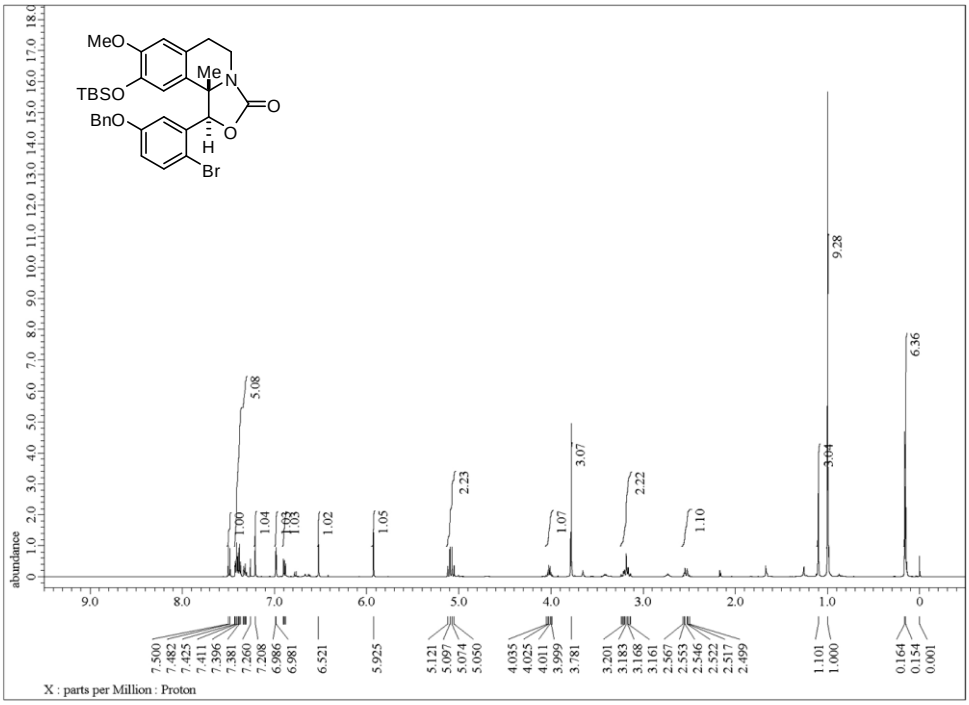


^{13}C NMR spectrum of compound ***rel*-(4*S*,5*S*)-16a** ($CDCl_3$, 125 MHz)

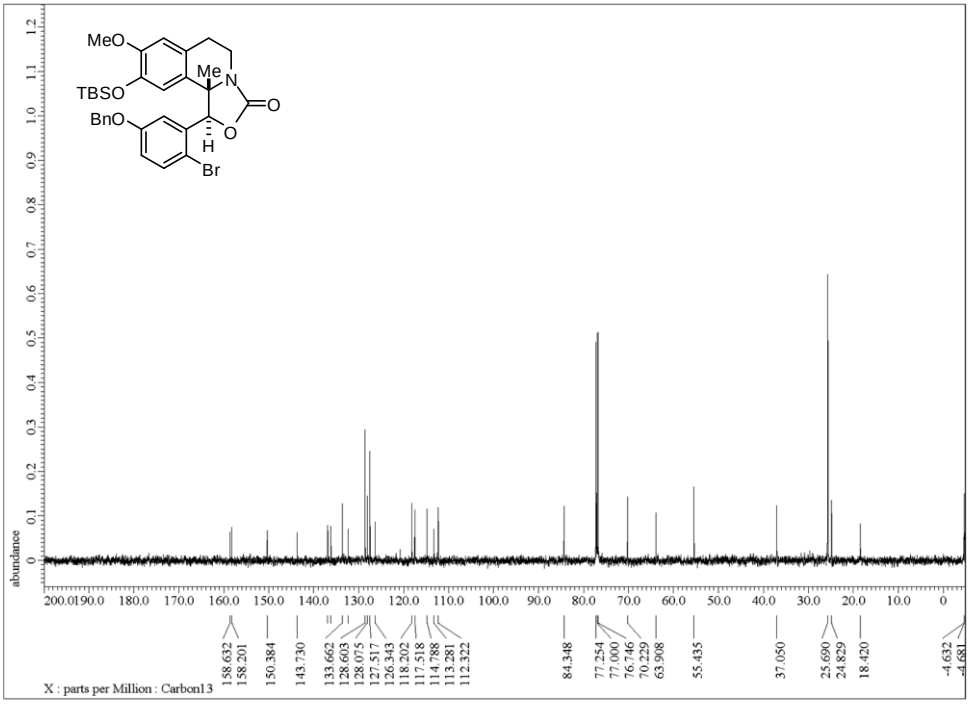


NOESY spectrum of compound ***rel*-(4*S*,5*S*)-16a** ($CDCl_3$, 500 MHz)

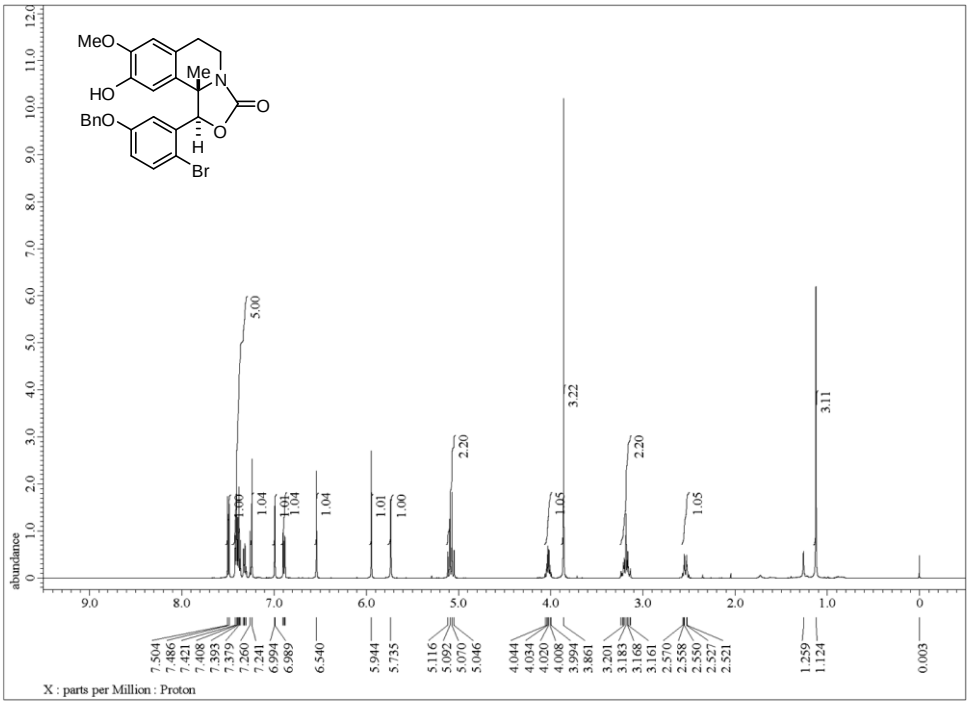
No correlations between the ether proton and the adjacent methyl group indicated both groups are on the opposite side.



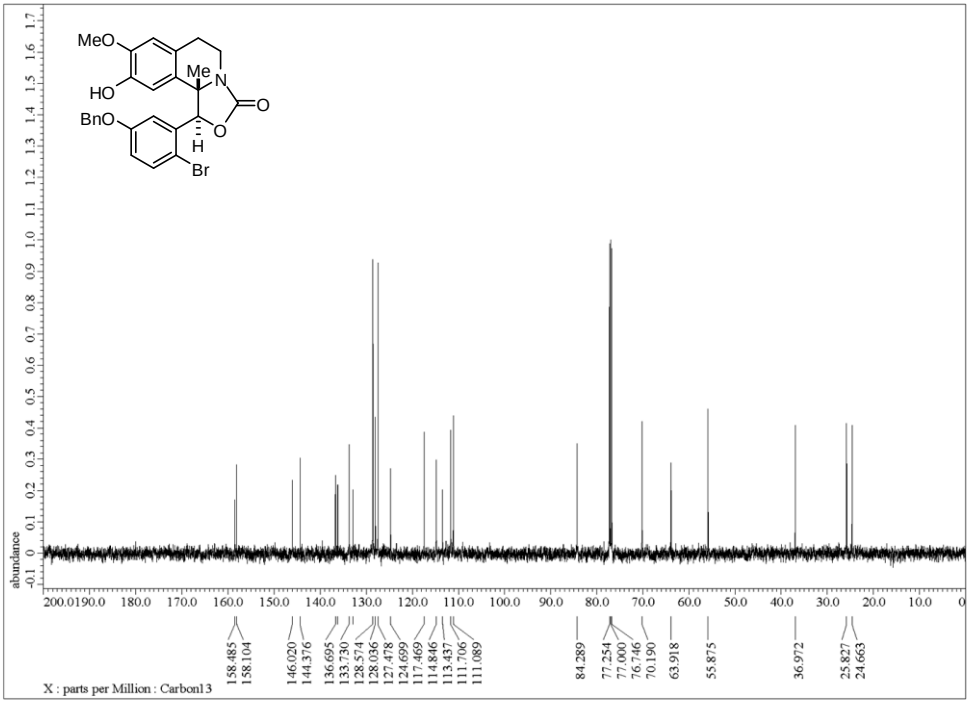
^{1}H NMR spectrum of compound **TBS-17a** ($CDCl_3$, 500 MHz)



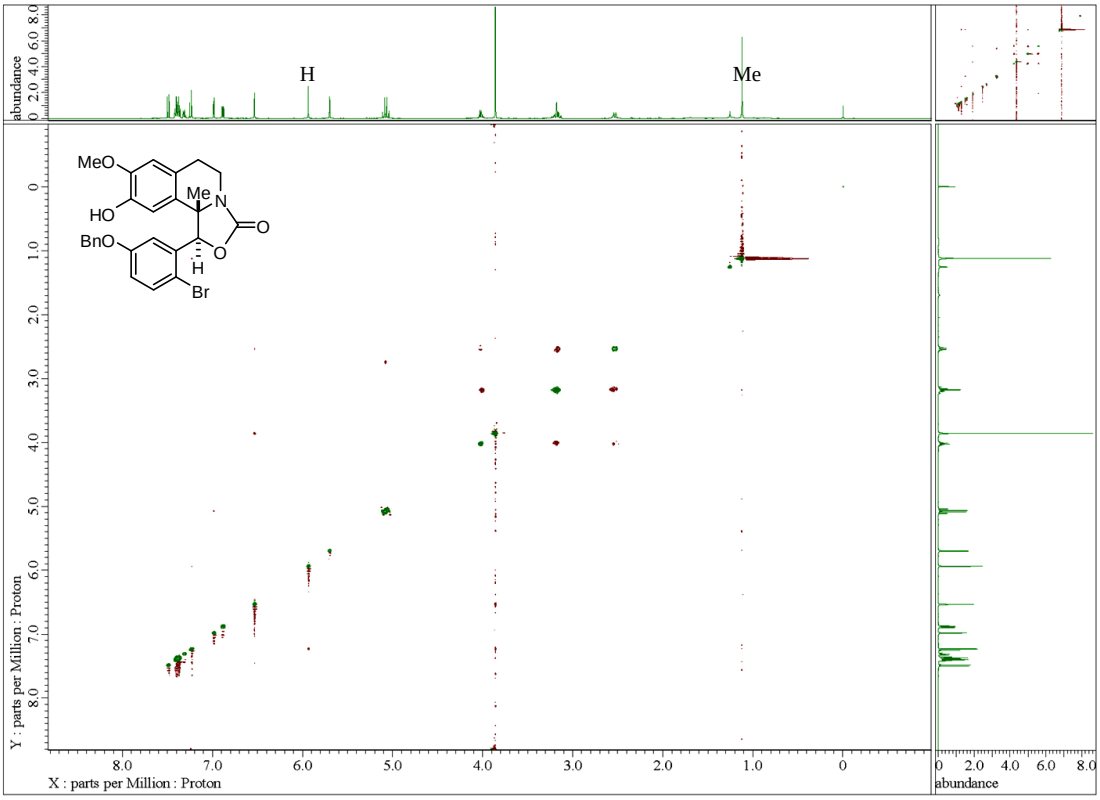
^{13}C NMR spectrum of compound **TBS-17a** ($CDCl_3$, 125 MHz)



^{1}H NMR spectrum of compound **17a** ($CDCl_3$, 500 MHz)

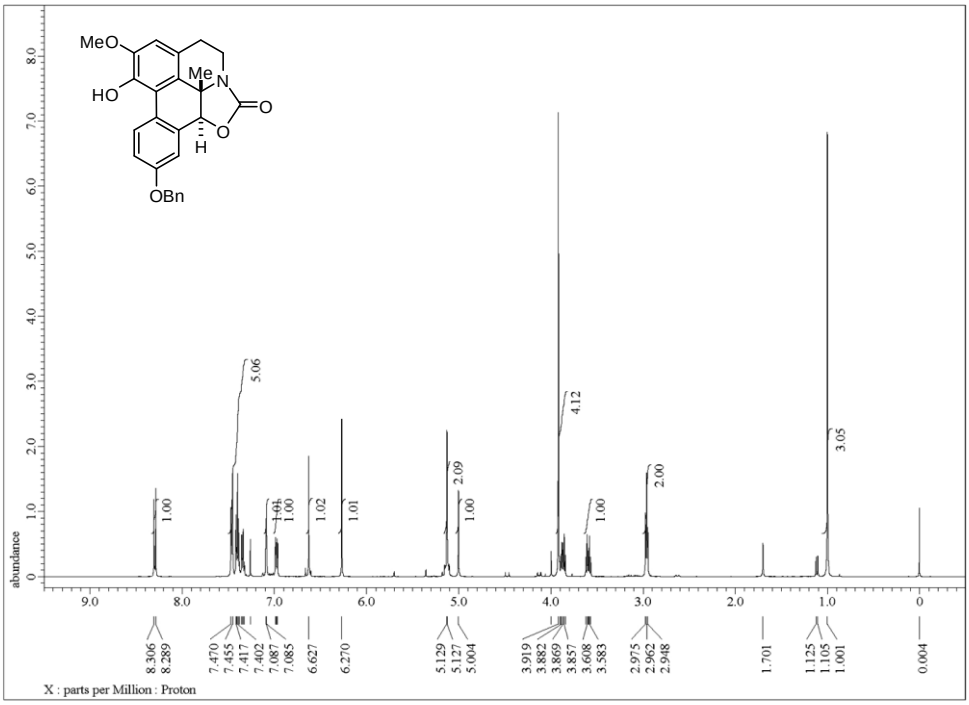


^{13}C NMR spectrum of compound **17a** ($CDCl_3$, 125 MHz)

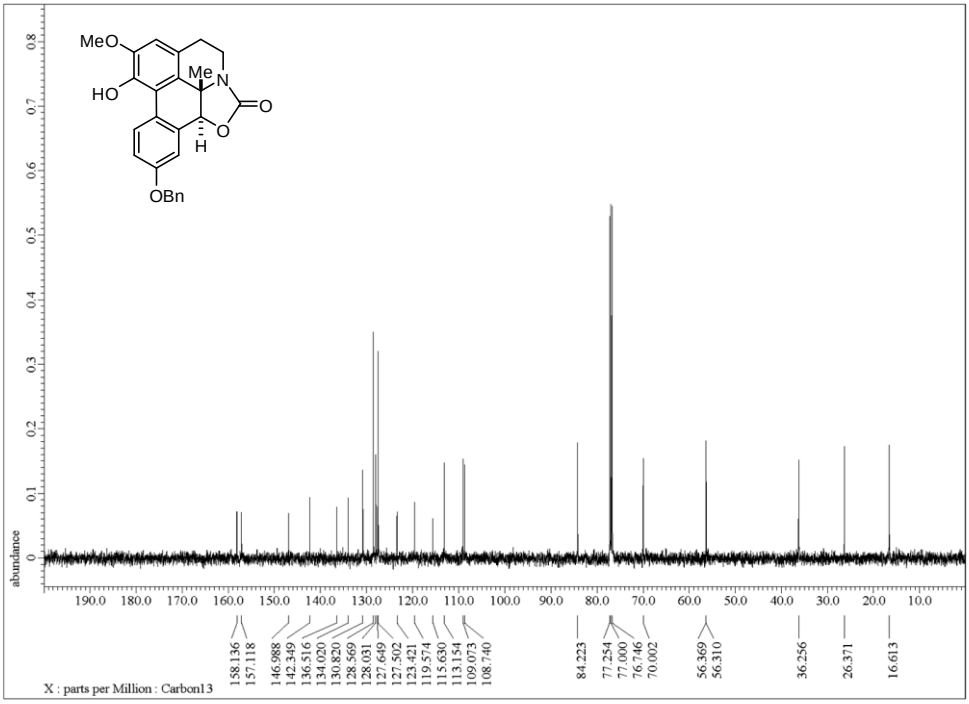


NOESY spectrum of compound **17a** ($CDCl_3$, 500 MHz)

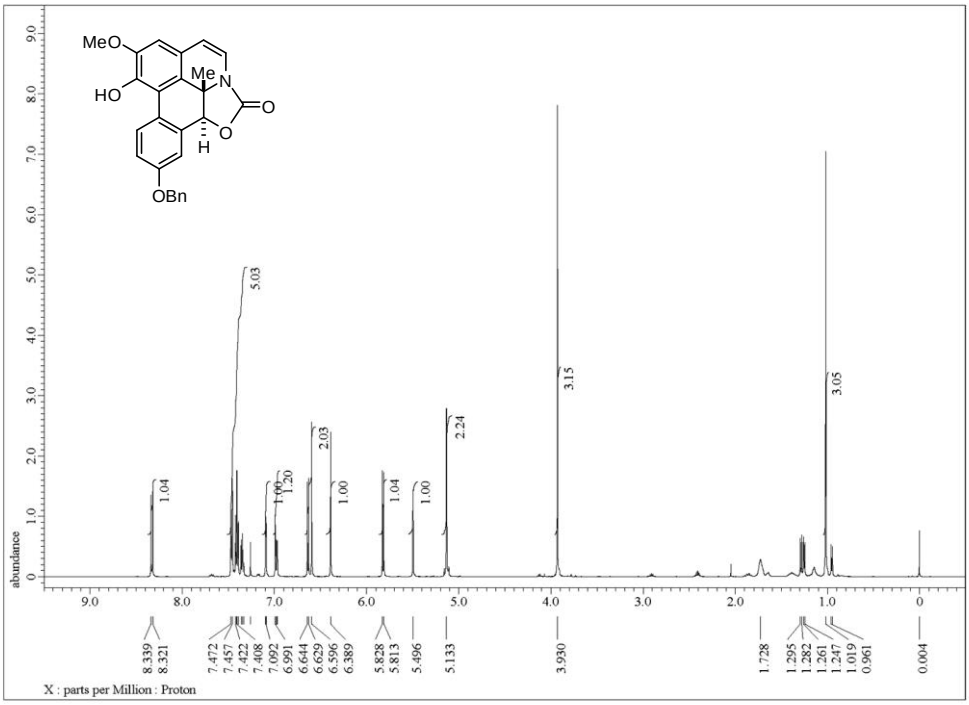
No correlations between the ether proton and the adjacent methyl group indicated an *anti*-configuration.



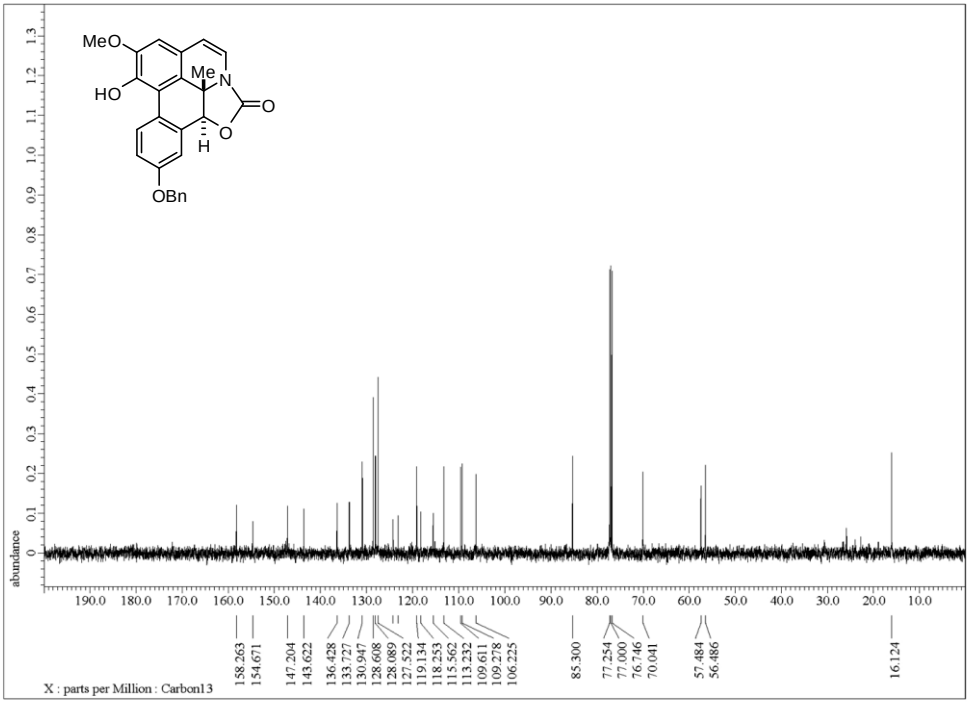
^{1}H NMR spectrum of compound **18a** ($CDCl_3$, 500 MHz)



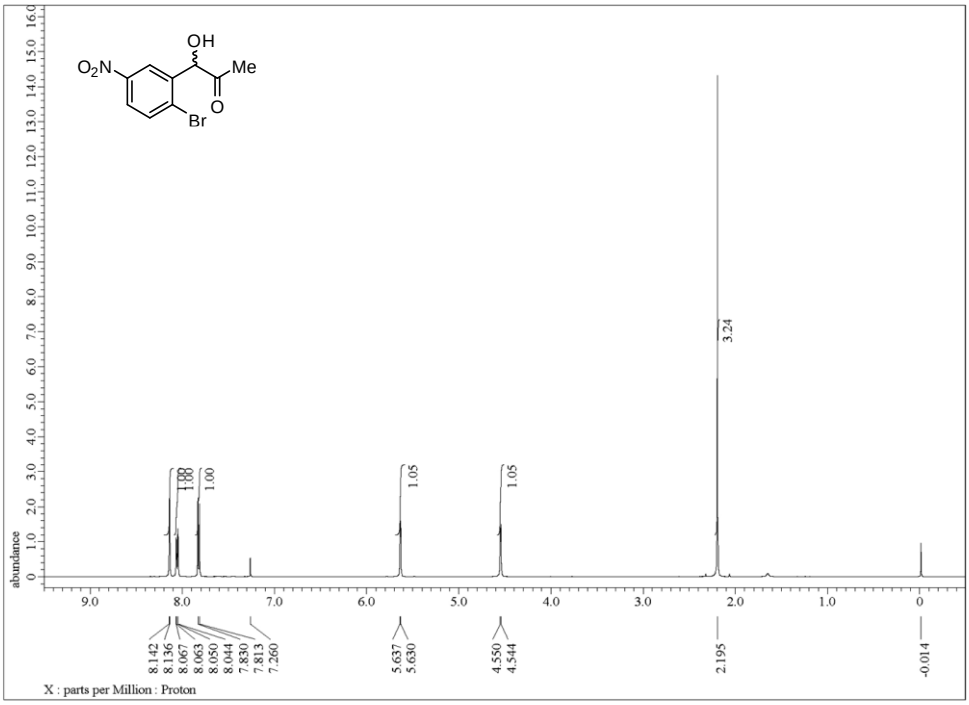
^{13}C NMR spectrum of compound **18a** ($CDCl_3$, 125 MHz)



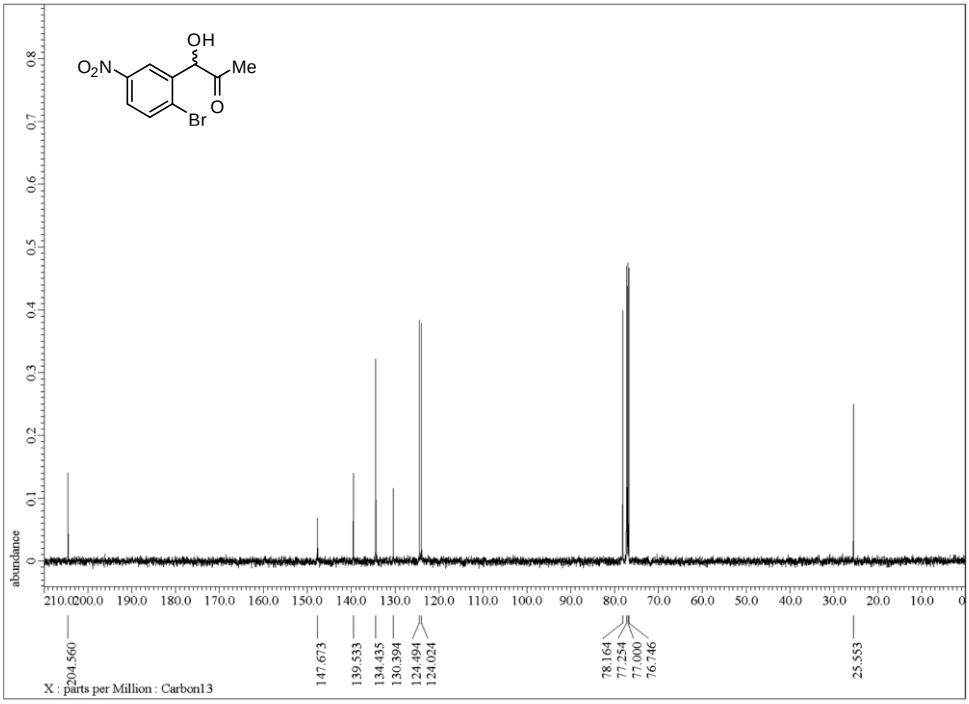
^{1}H NMR spectrum of compound **19a** ($CDCl_3$, 500 MHz)



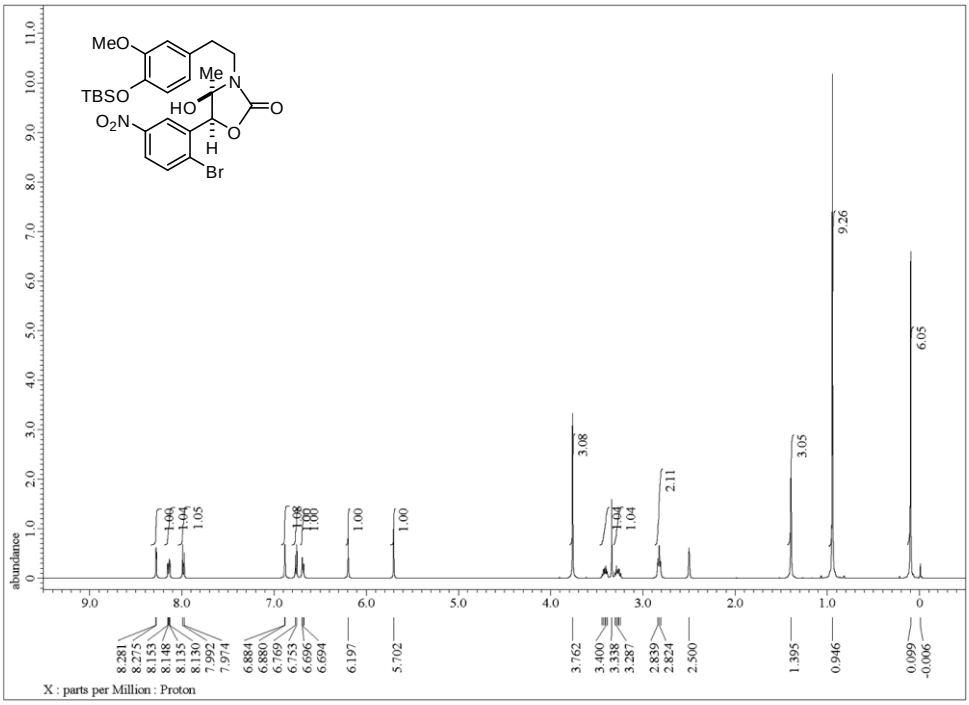
^{13}C NMR spectrum of compound **19a** ($CDCl_3$, 125 MHz)



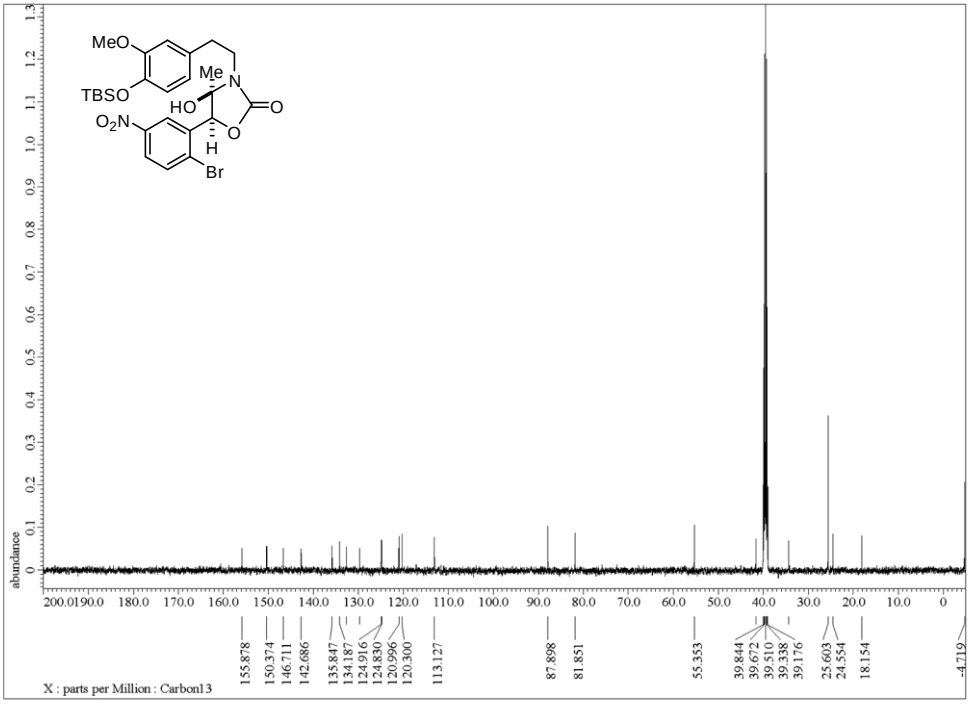
^{1}H NMR spectrum of compound **14b** ($CDCl_3$, 500 MHz)



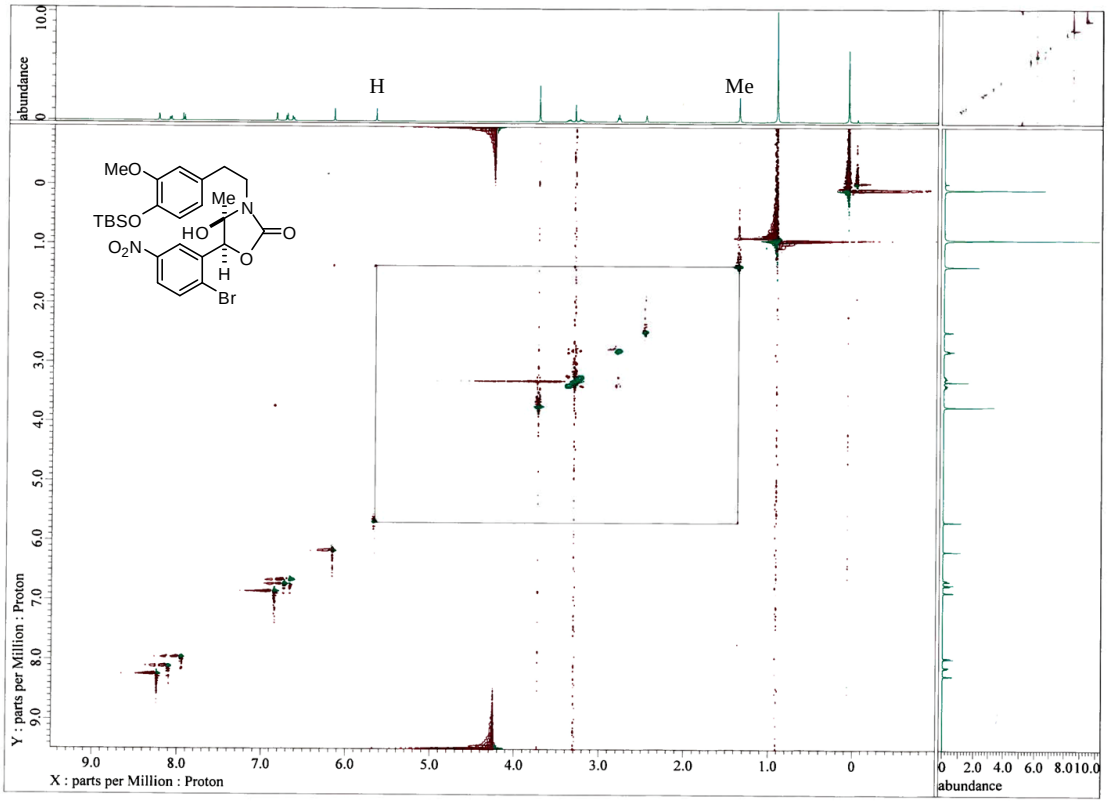
^{13}C NMR spectrum of compound **14b** ($CDCl_3$, 125 MHz)



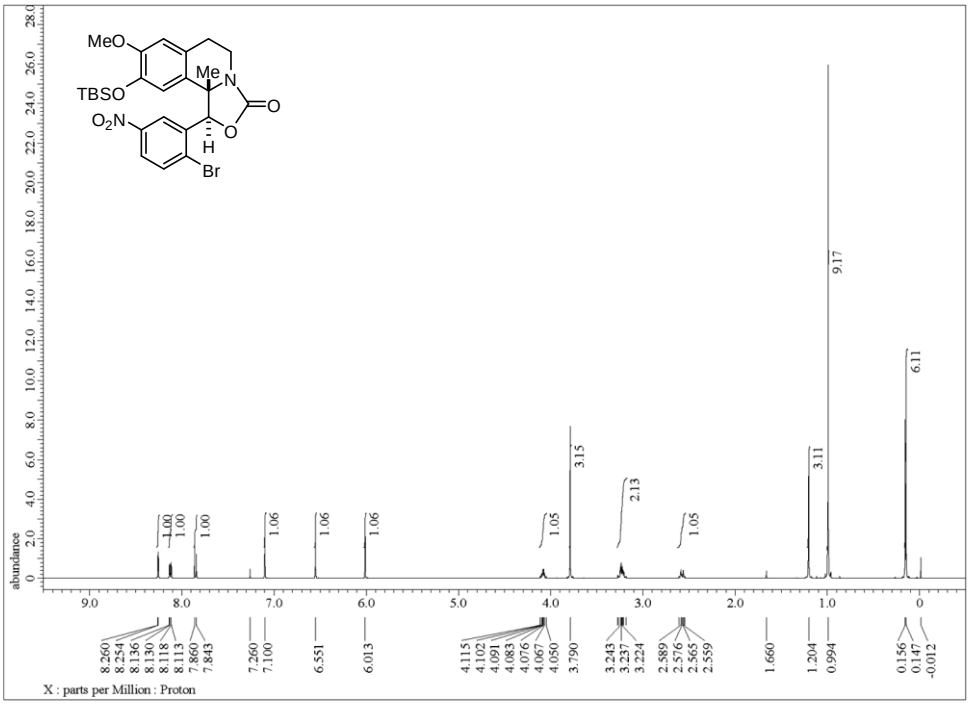
^{1}H NMR spectrum of compound ***rel*-(4*R*,5*S*)-16b** (DMSO-d_6, 500 MHz)



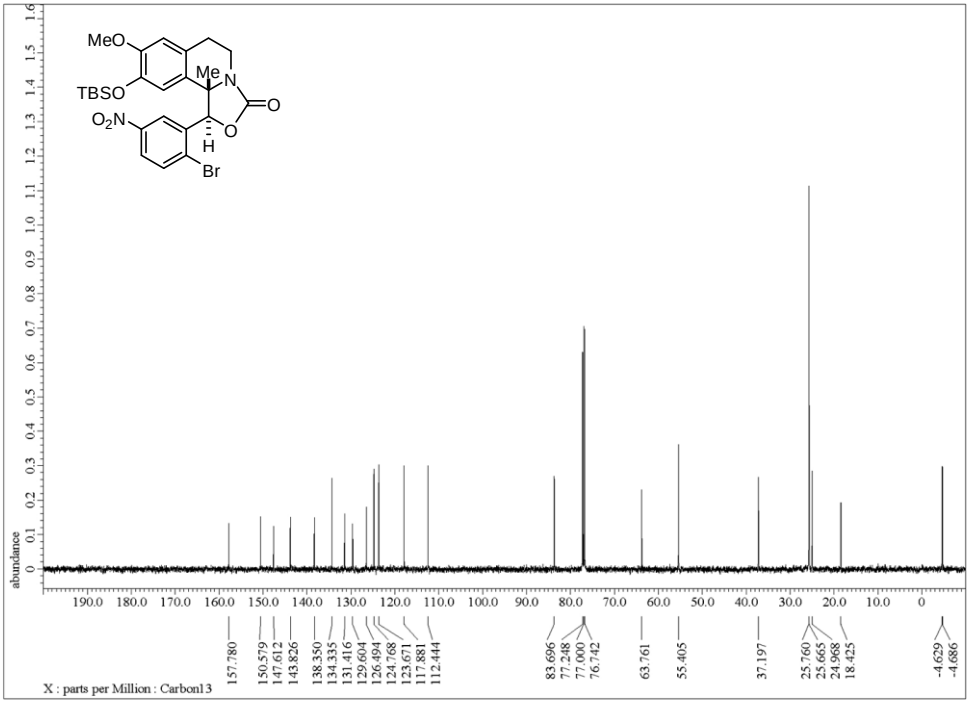
^{13}C NMR spectrum of compound ***rel*-(4*R*,5*S*)-16b** (DMSO-d_6, 125 MHz)



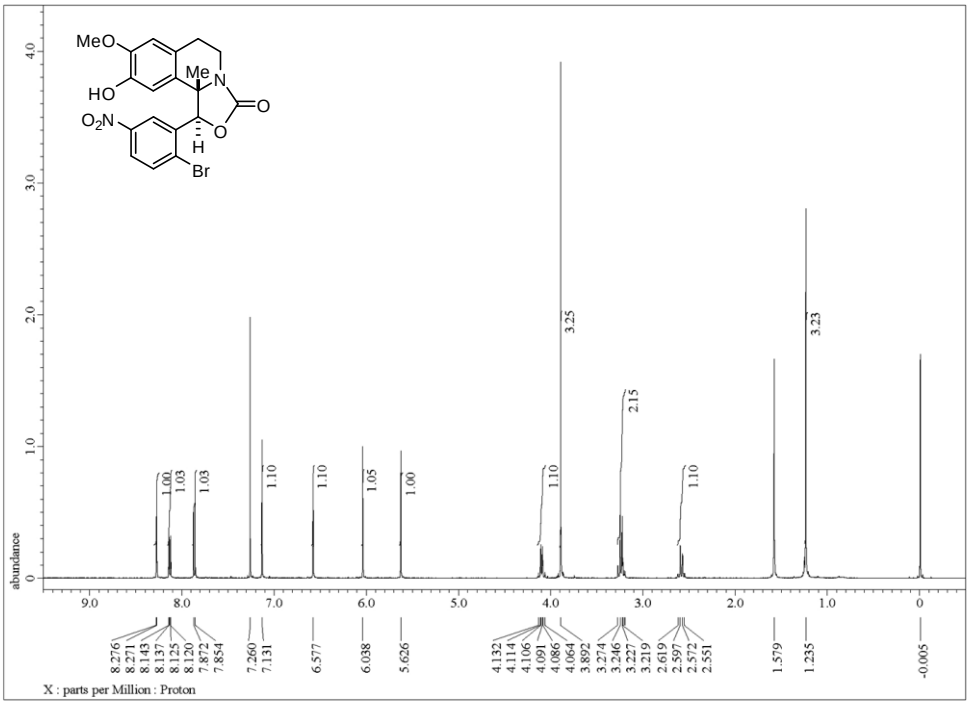
NOESY spectrum of compound ***rel*-(4*R*,5*S*)-16b** (DMSO-d_6, 125 MHz)
Correlations between the ether proton and the adjacent methyl group indicated both groups are on the same side.



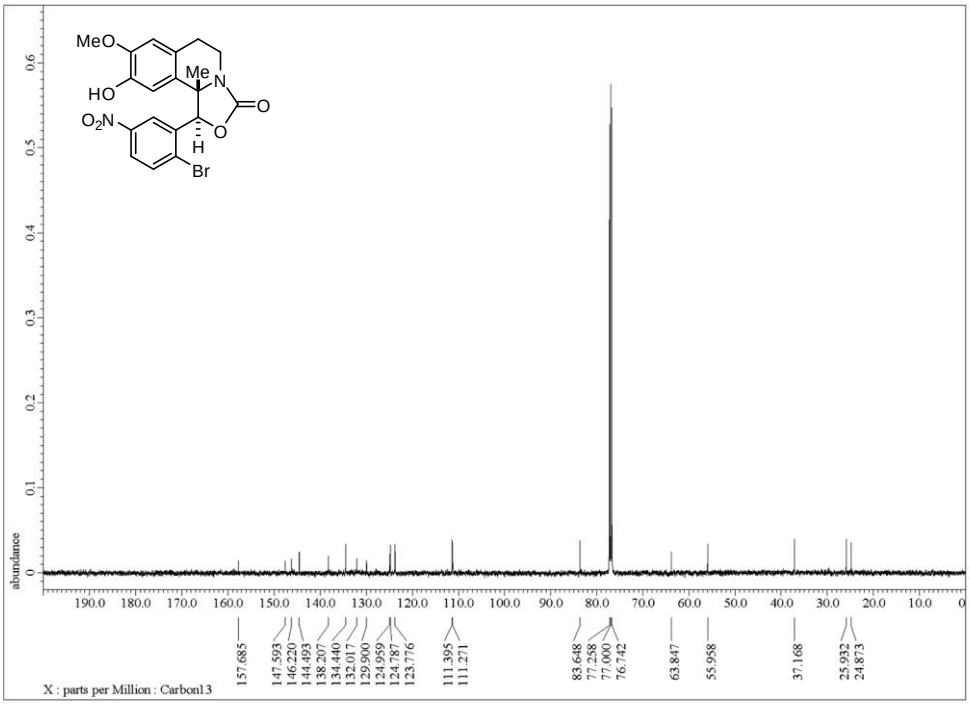
^{1}H NMR spectrum of compound **TBS-17b** ($CDCl_3$, 500 MHz)



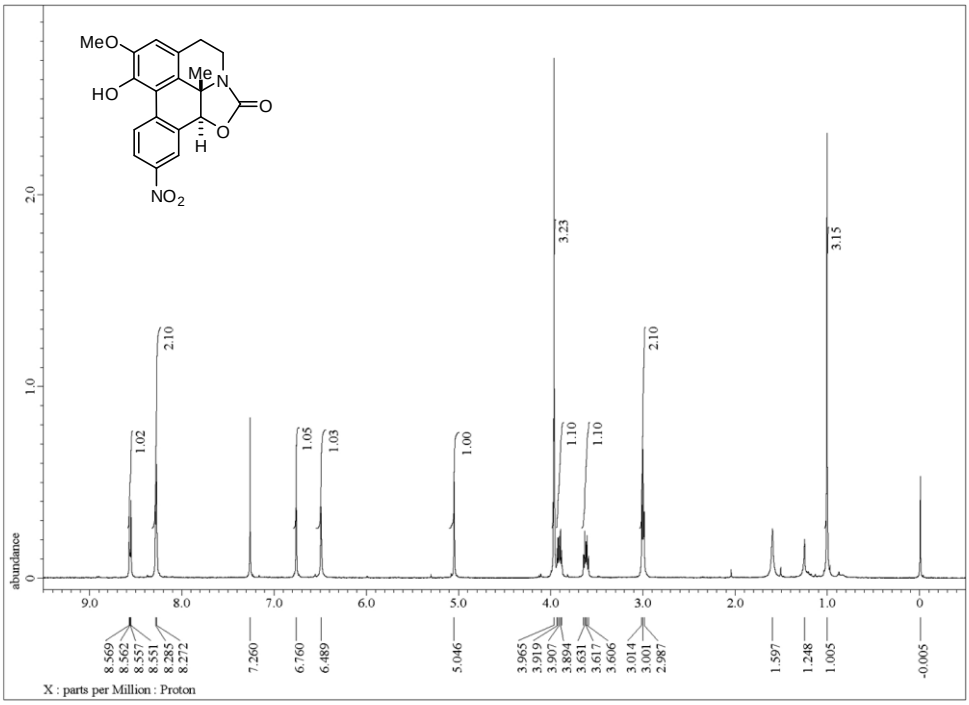
^{13}C NMR spectrum of compound **TBS-17b** ($CDCl_3$, 125 MHz)



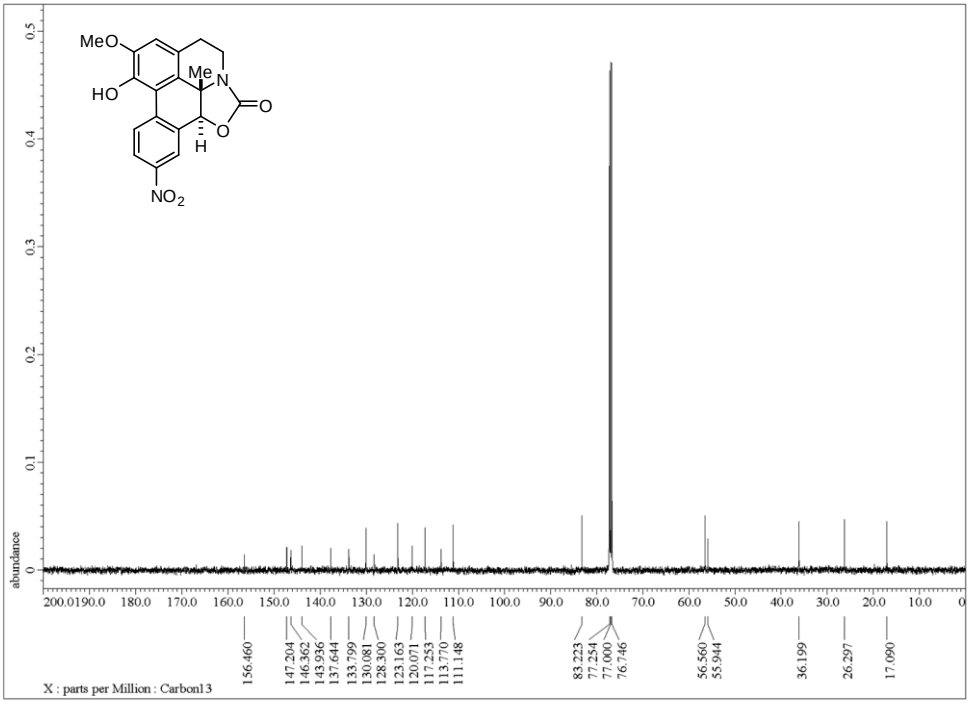
^{1}H NMR spectrum of compound **17b** ($CDCl_3$, 500 MHz)



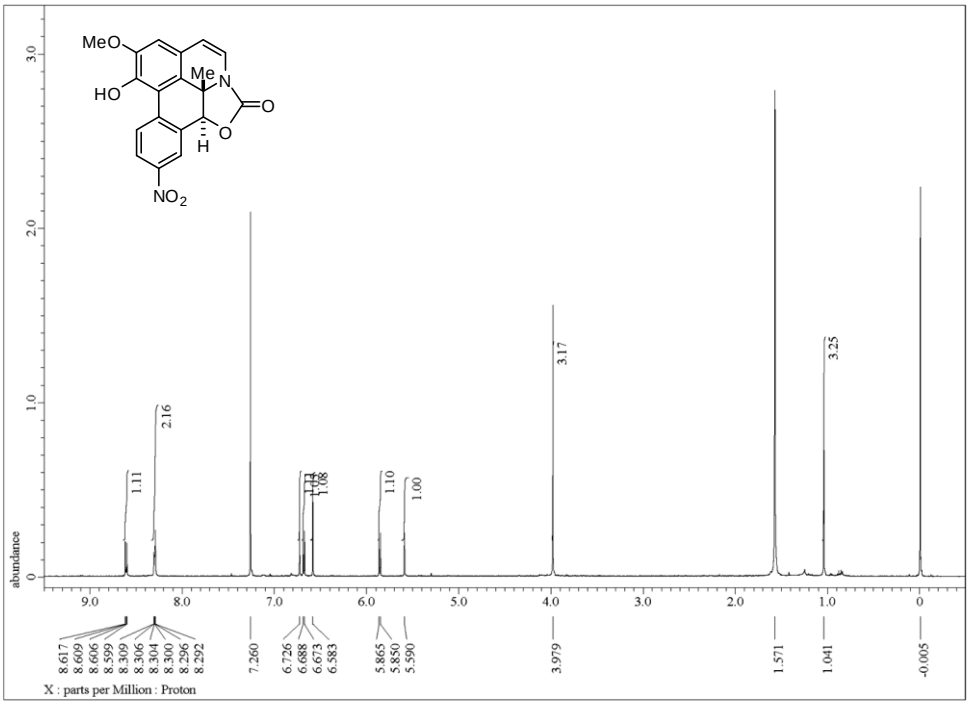
^{13}C NMR spectrum of compound **17b** ($CDCl_3$, 125 MHz)



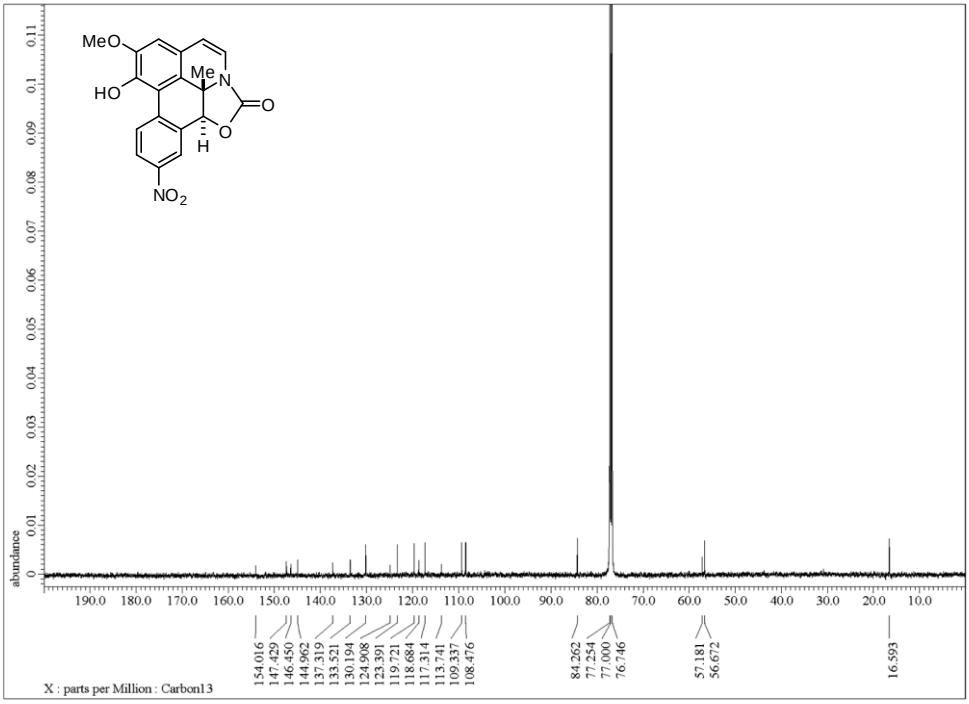
^{1}H NMR spectrum of compound **18b** ($CDCl_3$, 500 MHz)



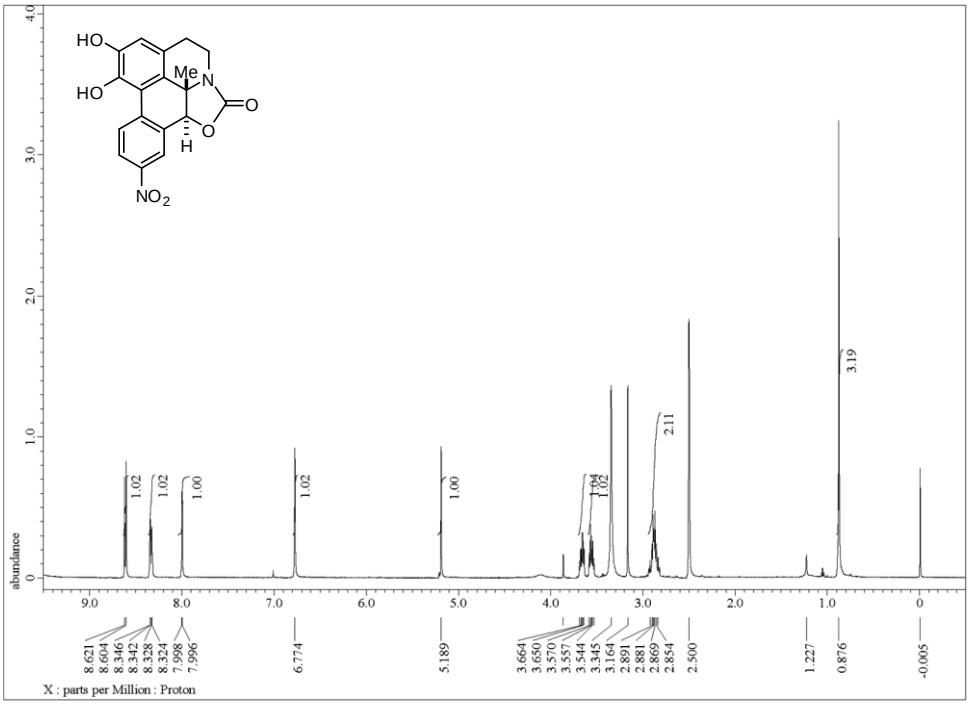
^{13}C NMR spectrum of compound **18b** ($CDCl_3$, 125 MHz)



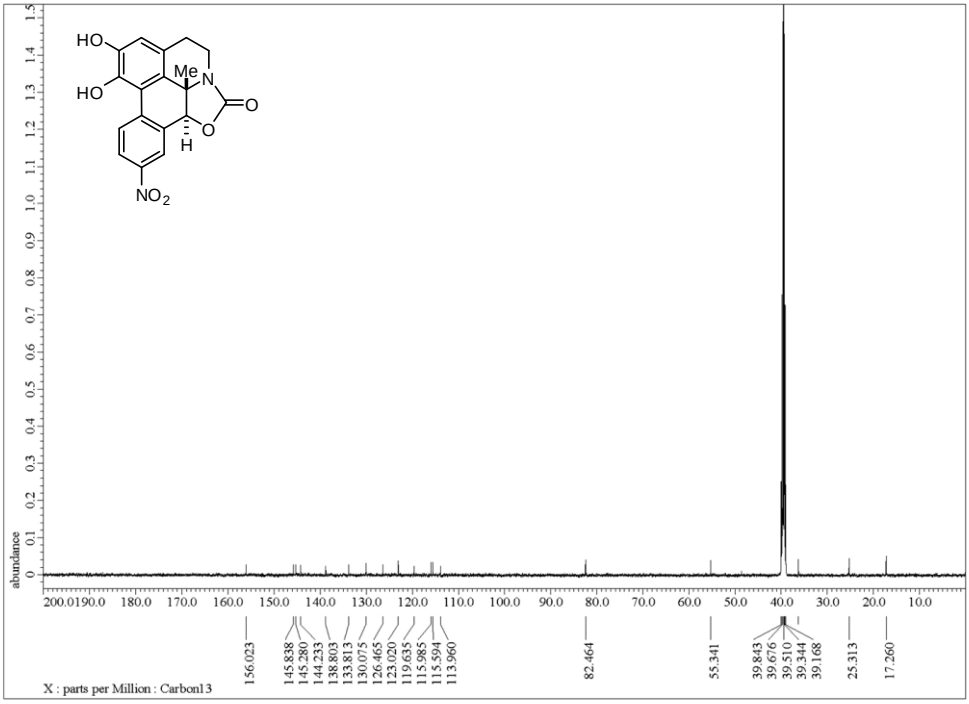
^{1}H NMR spectrum of compound **19b** ($CDCl_3$, 500 MHz)



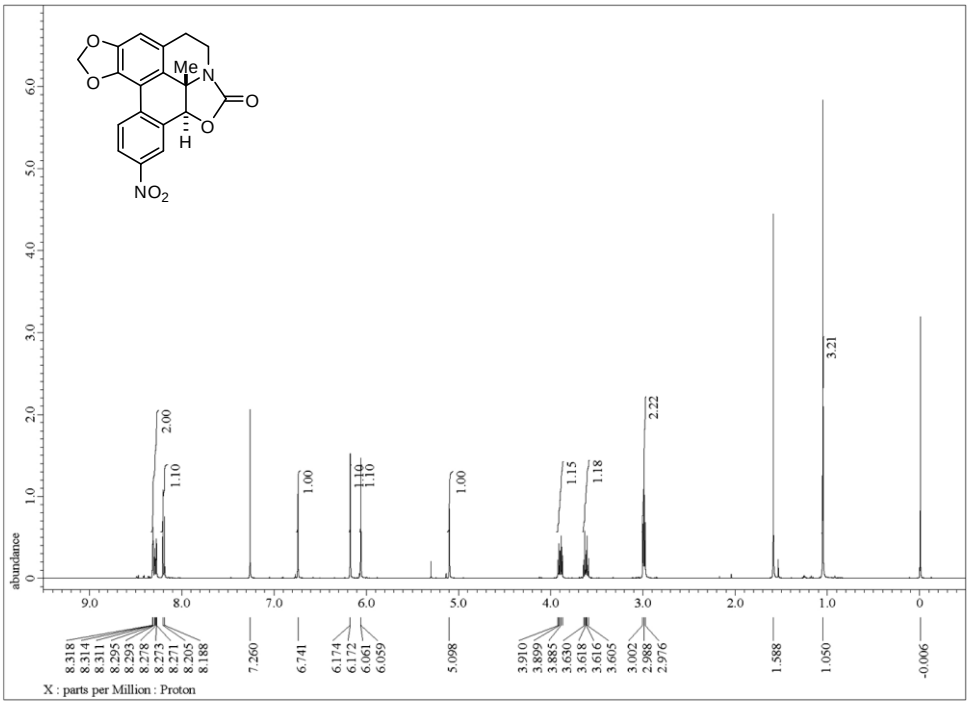
^{13}C NMR spectrum of compound **19b** ($CDCl_3$, 125 MHz)



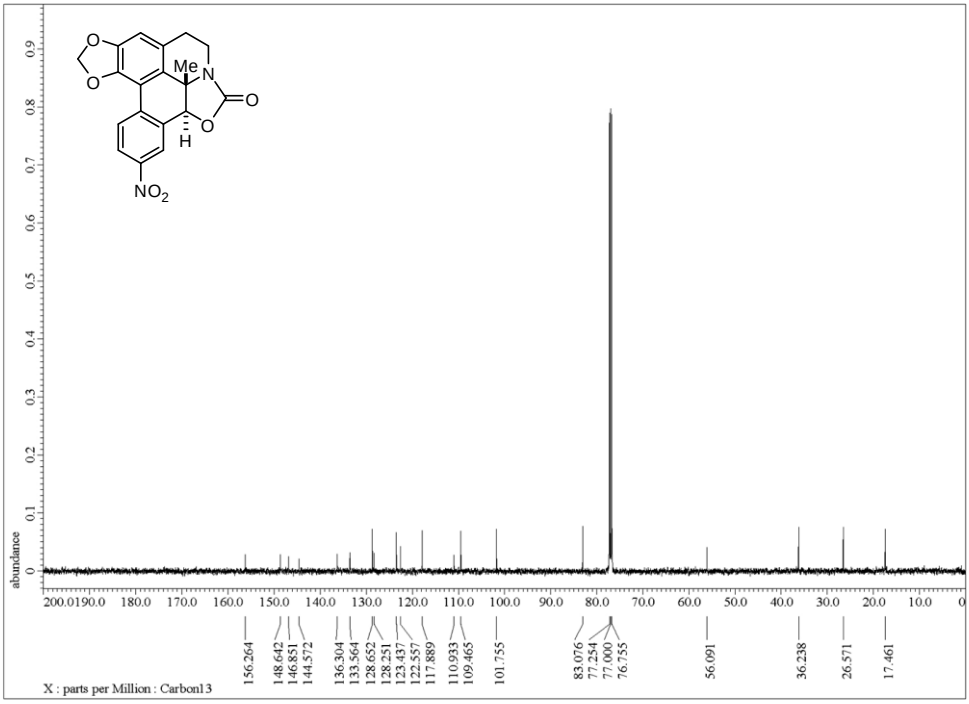
^{1}H NMR spectrum of compound **20** (DMSO-d_6, 500 MHz)



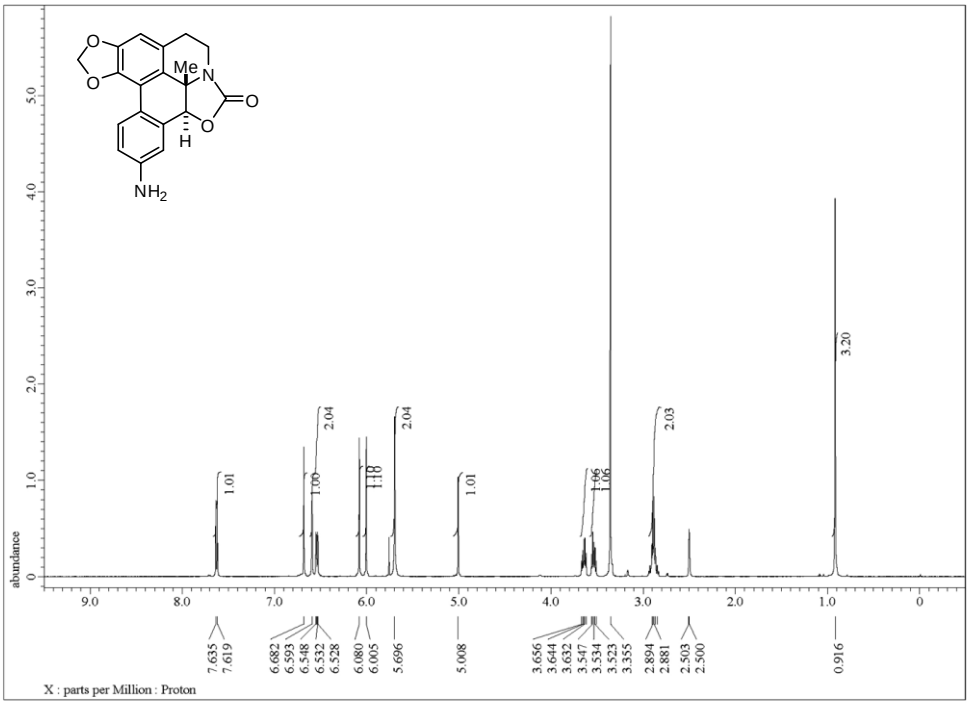
^{13}C NMR spectrum of compound **20** (DMSO-d_6, 125 MHz)



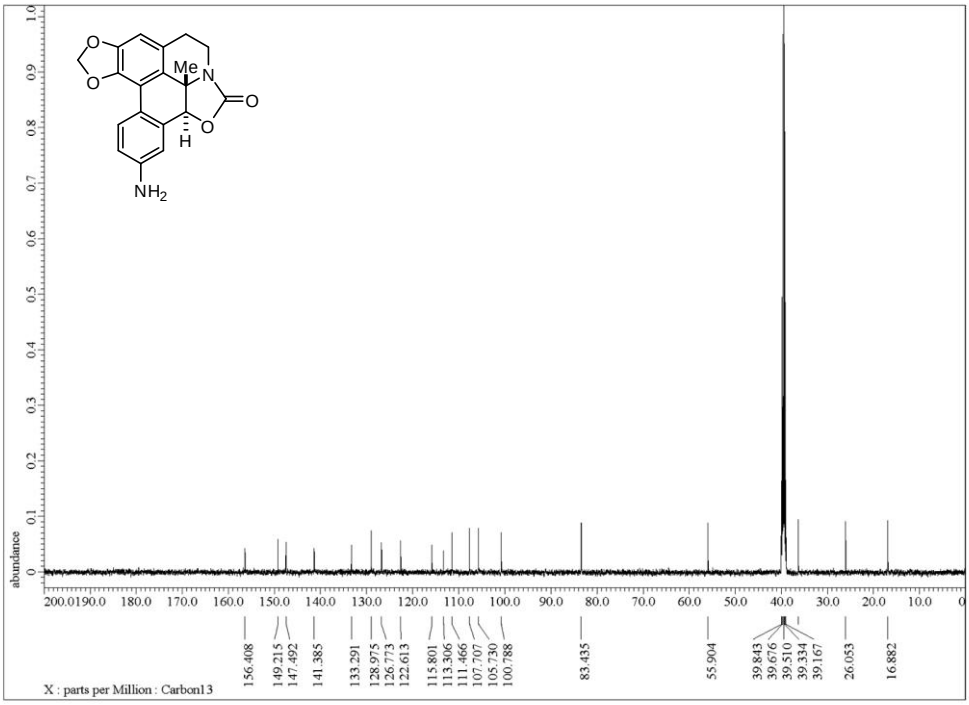
^{1}H NMR spectrum of compound **21** ($CDCl_3$, 500 MHz)



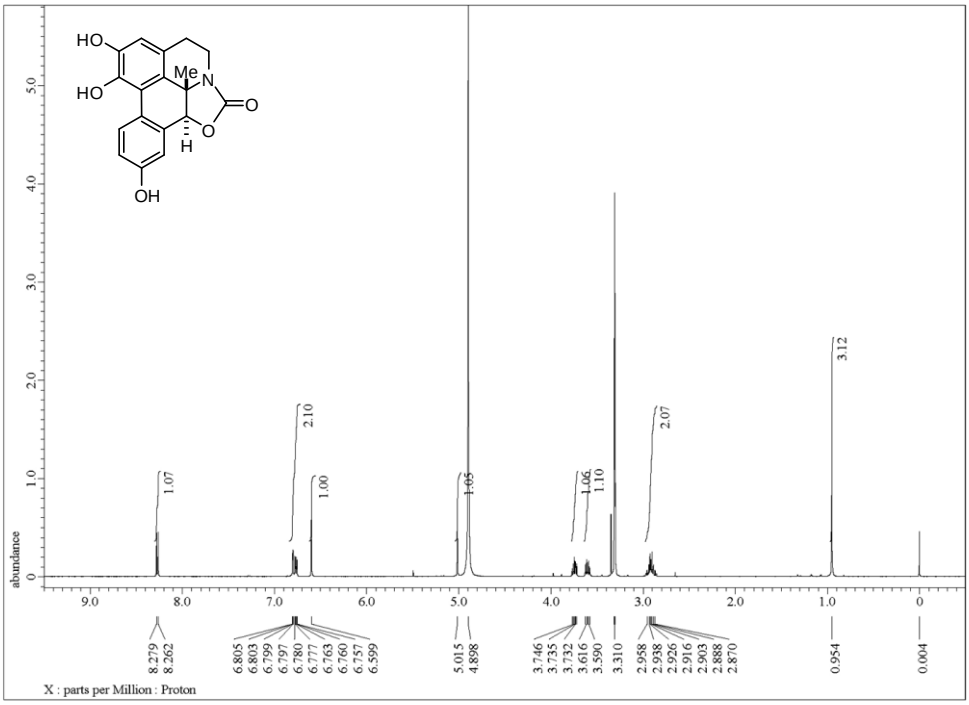
^{13}C NMR spectrum of compound **21** ($CDCl_3$, 125 MHz)



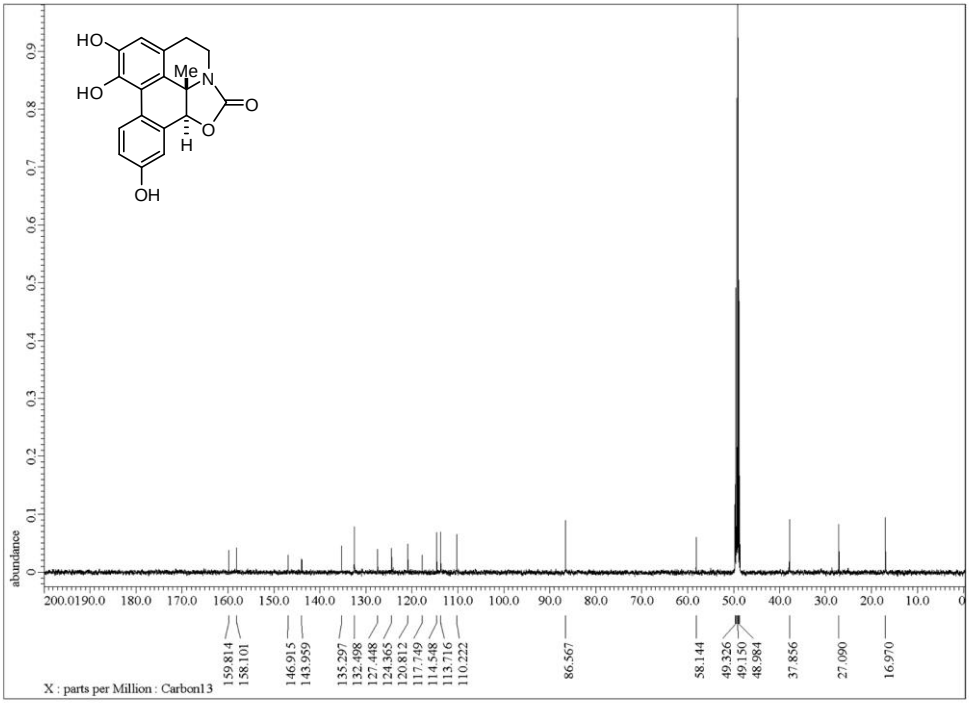
^{1}H NMR spectrum of compound **22** (DMSO-d_6, 500 MHz)



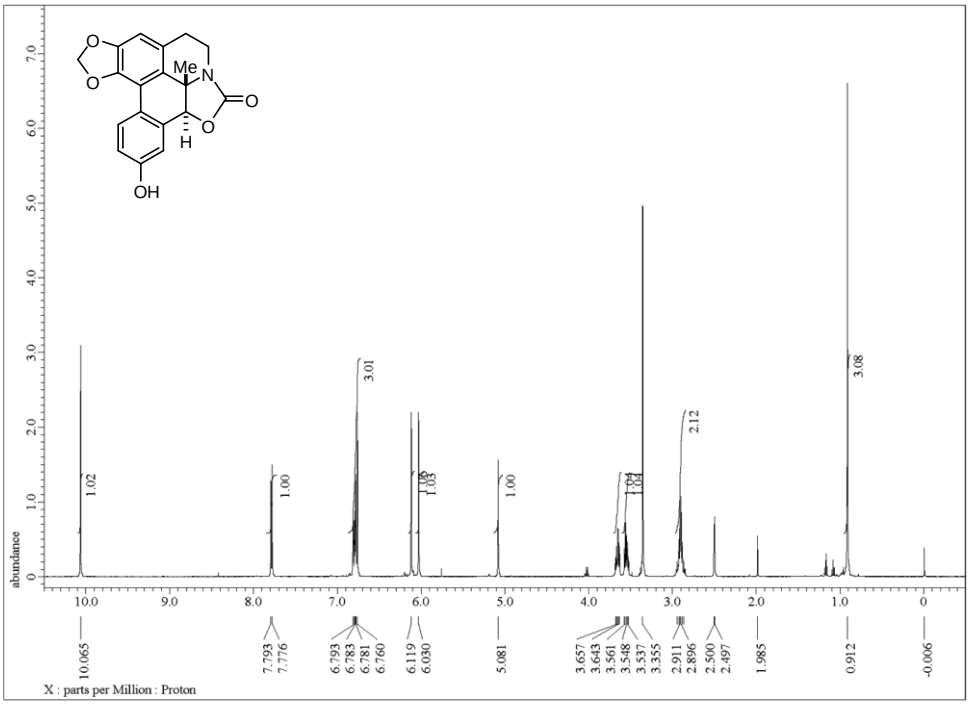
^{13}C NMR spectrum of compound **22** (DMSO-d_6, 125 MHz)



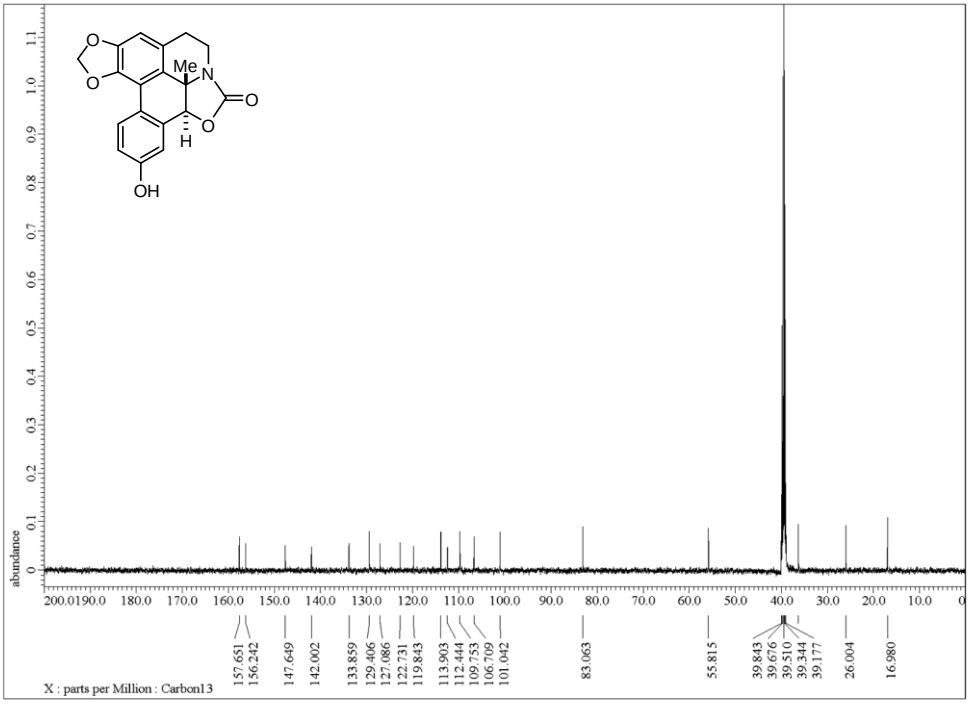
^{1}H NMR spectrum of compound **23** (CD_3OD, 500 MHz) prepared using Method A



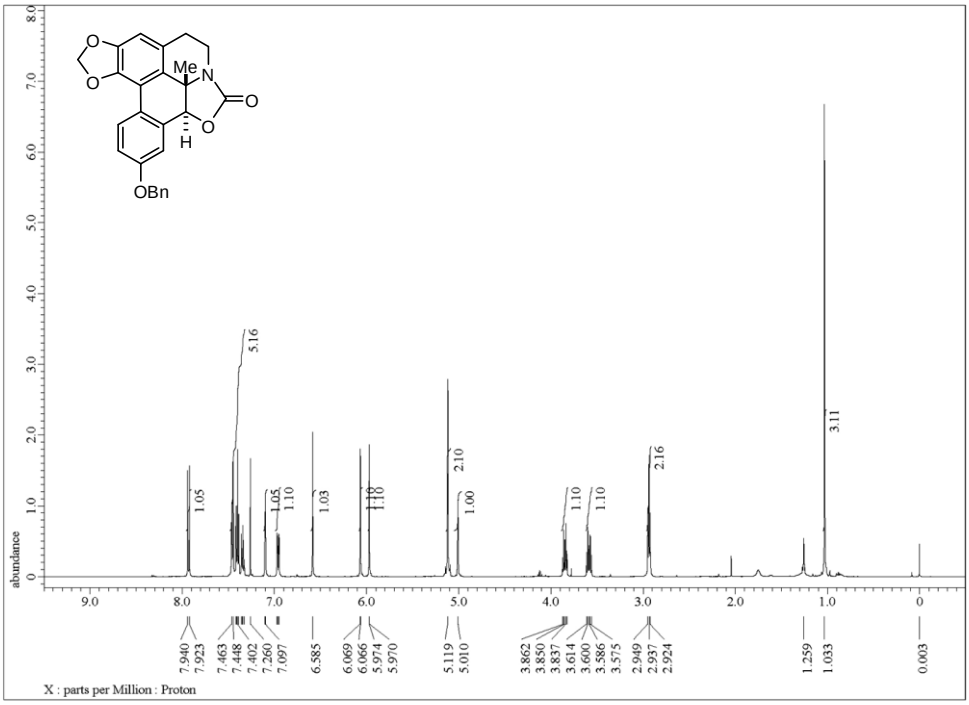
^{13}C NMR spectrum of compound **23** (CD_3OD, 125 MHz) prepared using Method A



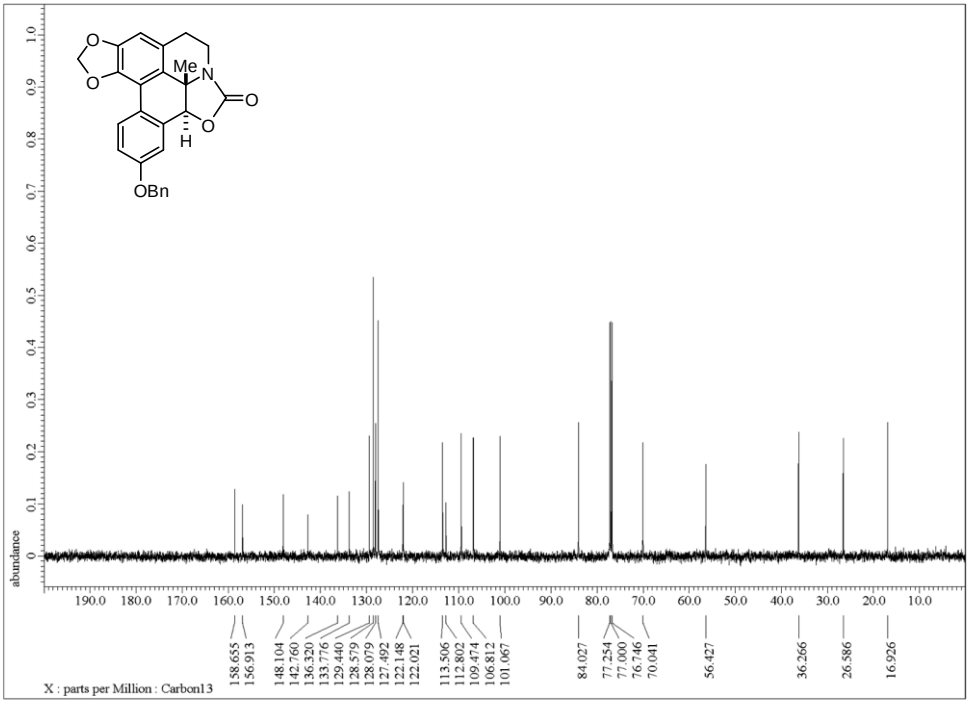
^{1}H NMR spectrum of compound **24** (DMSO-d_6, 500 MHz) prepared using Method A



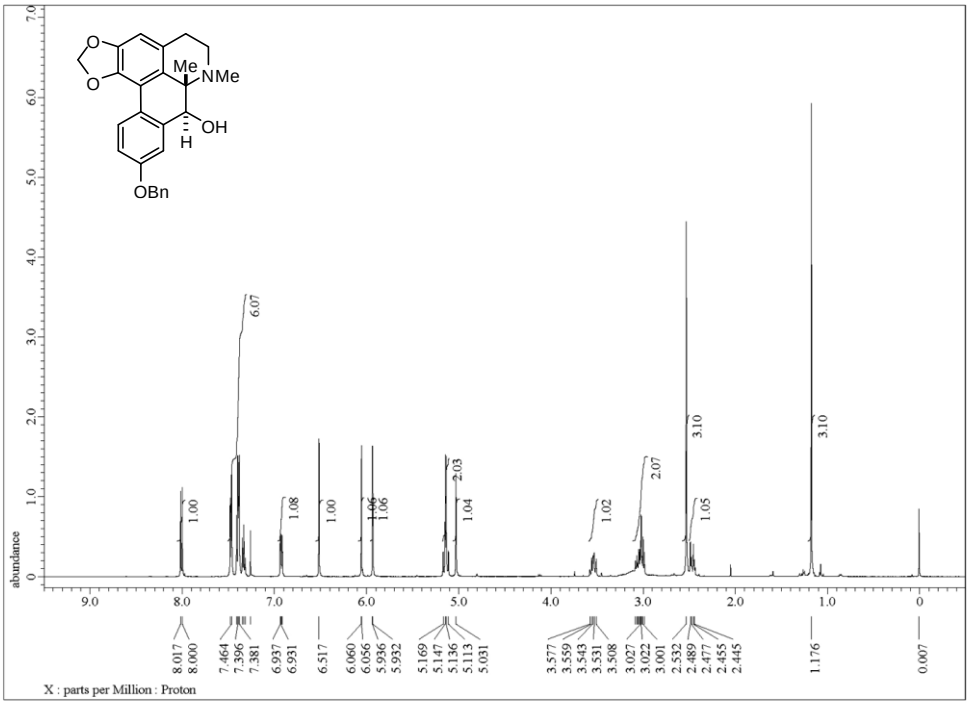
^{13}C NMR spectrum of compound **24** (DMSO-d_6, 125 MHz) prepared using Method A



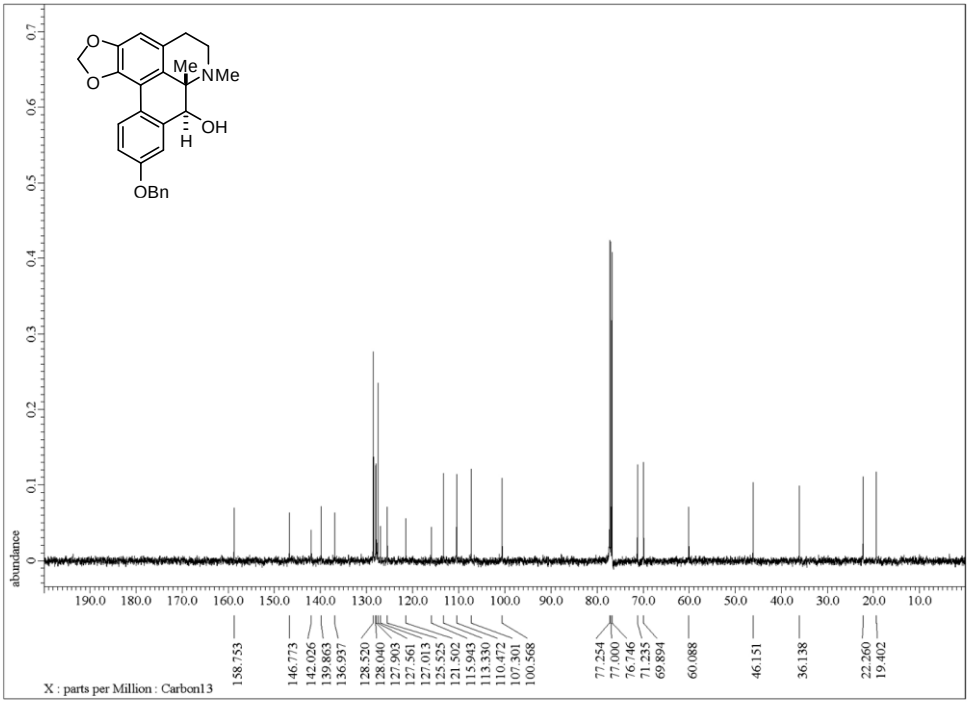
^{1}H NMR spectrum of compound **25** ($CDCl_3$, 500 MHz)



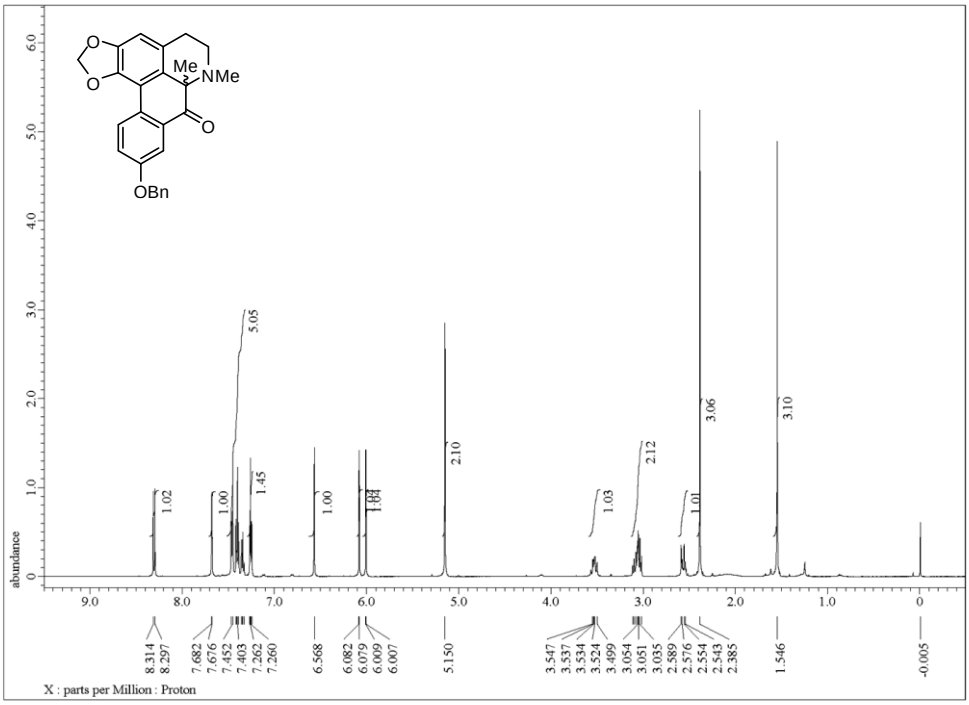
^{13}C NMR spectrum of compound **25** ($CDCl_3$, 125 MHz)



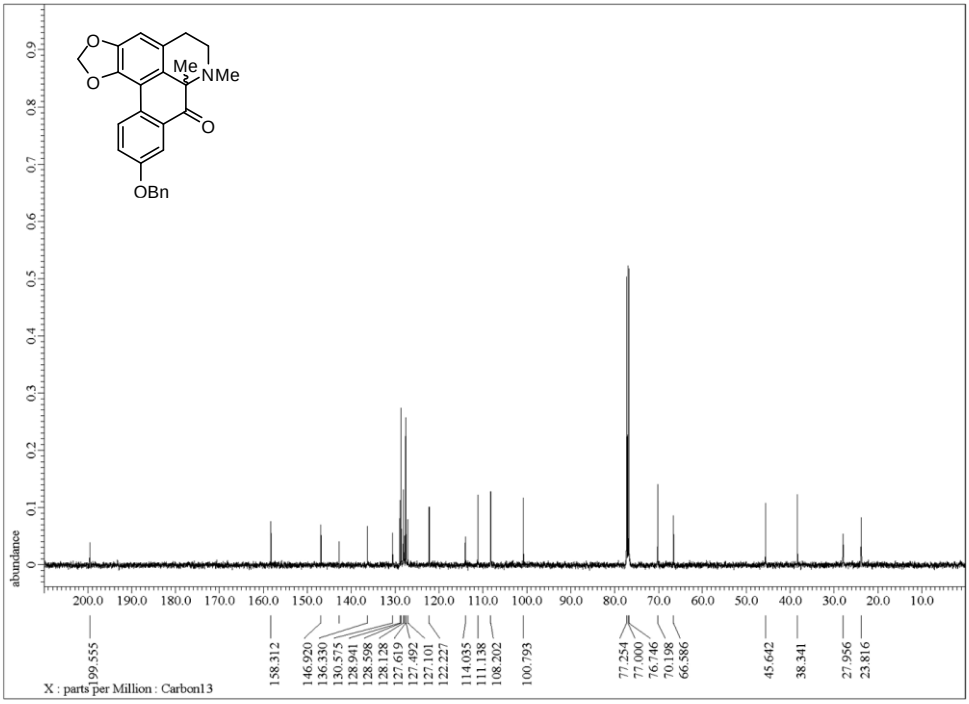
^{1}H NMR spectrum of compound **26** ($CDCl_3$, 500 MHz)



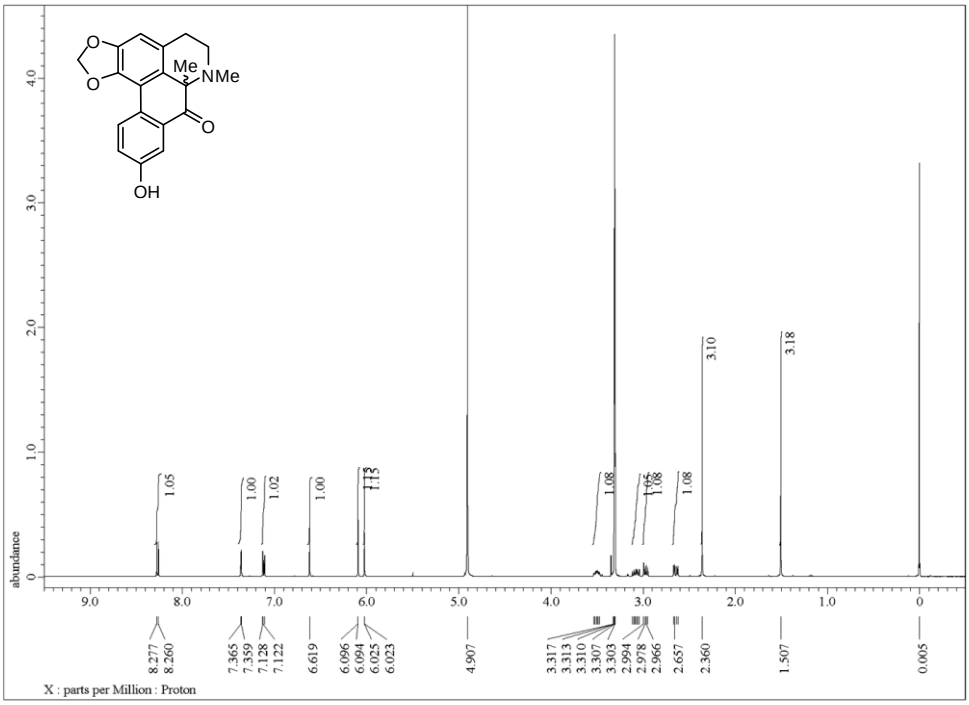
^{13}C NMR spectrum of compound **26** ($CDCl_3$, 125 MHz)



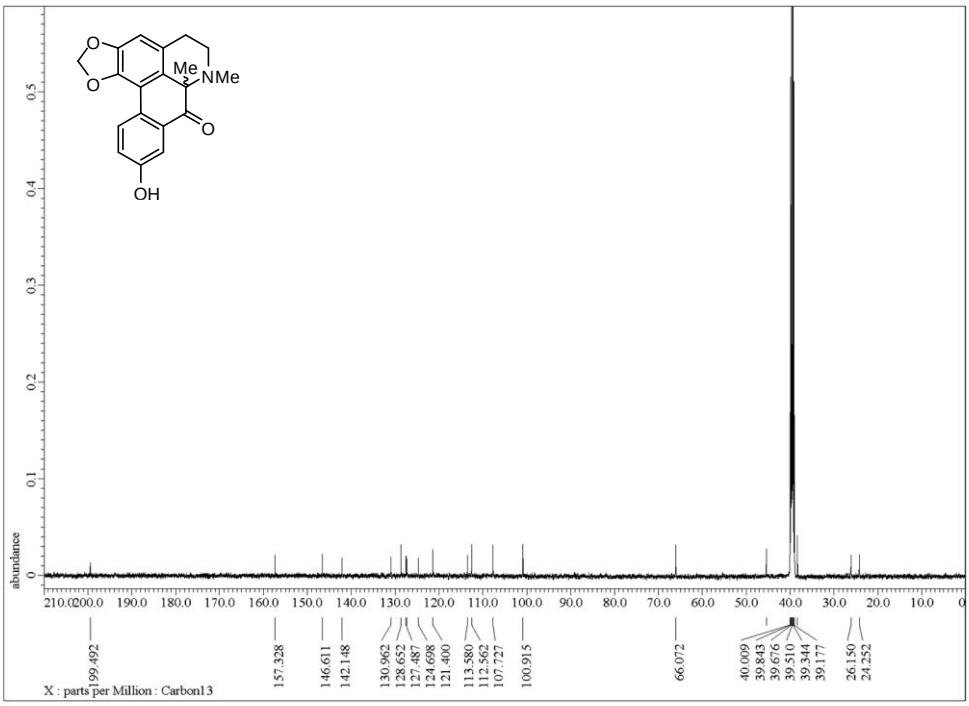
^{1}H NMR spectrum of compound **27** ($CDCl_3$, 500 MHz)



^{13}C NMR spectrum of compound **27** ($CDCl_3$, 125 MHz)



^{1}H NMR spectrum of compound (±)-**3** (CD_3OD, 500 MHz)



^{13}C NMR spectrum of compound (±)-**3** (DMSO-d_6, 125 MHz)