

BF₃-Et₂O Mediated Skeletal Rearrangements of Norbornyl Appended Cyclopentane-1,2-diols[†]

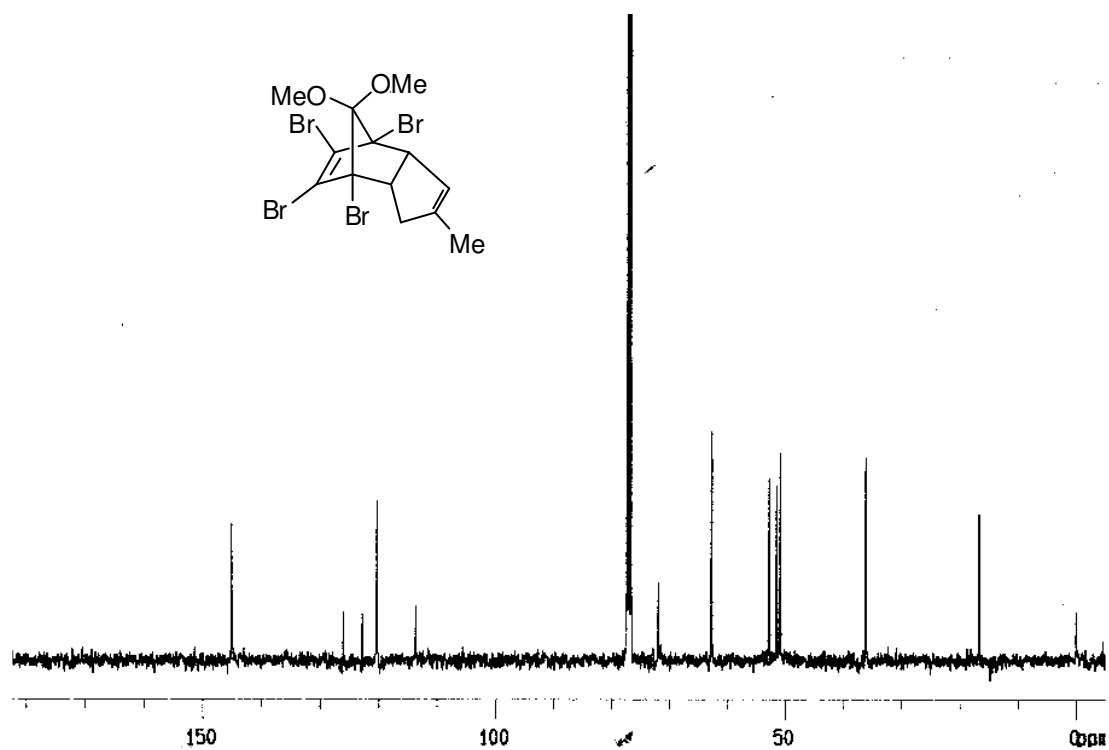
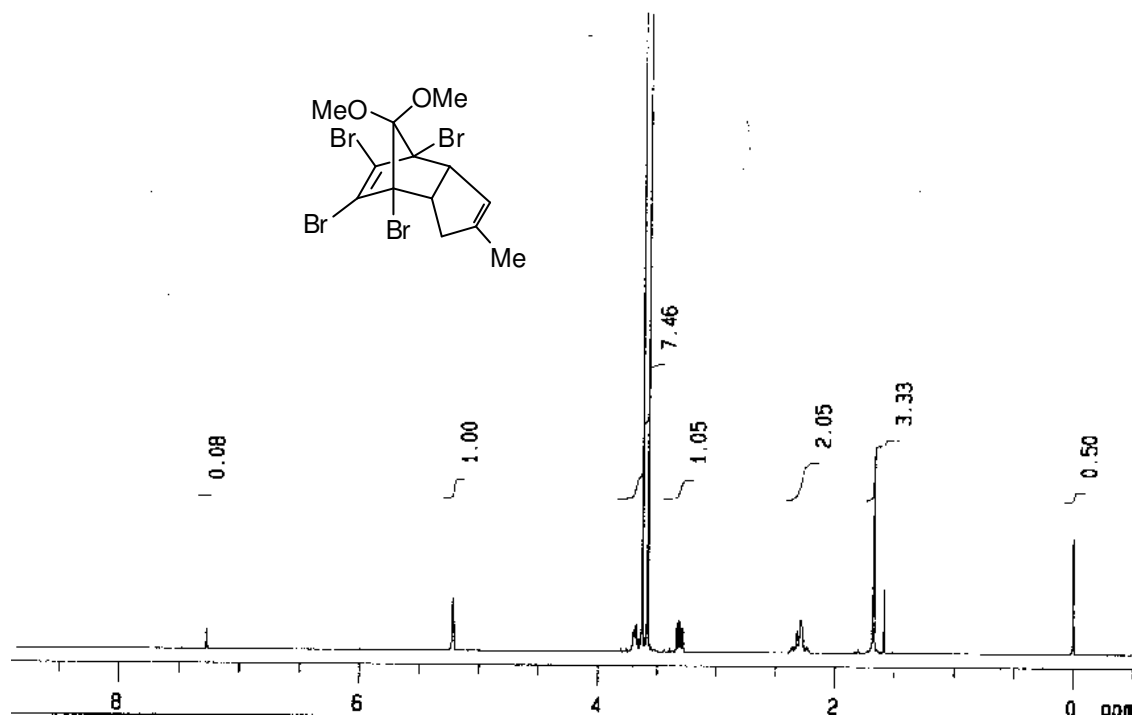
*Chintada Nageswara Rao^b and Faiz Ahmed Khan^{*a}*

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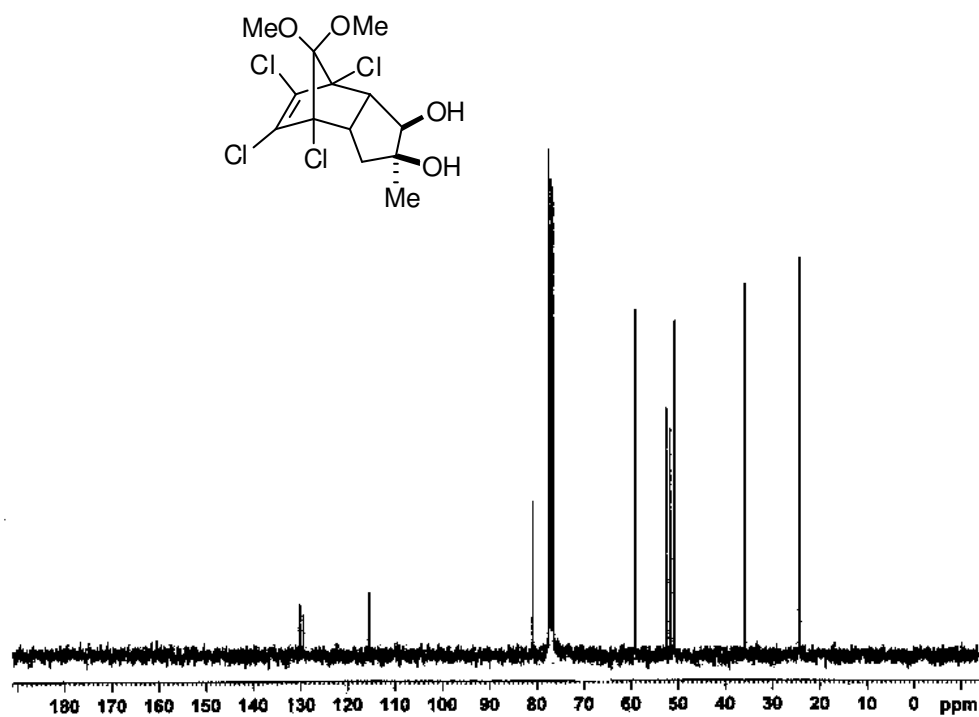
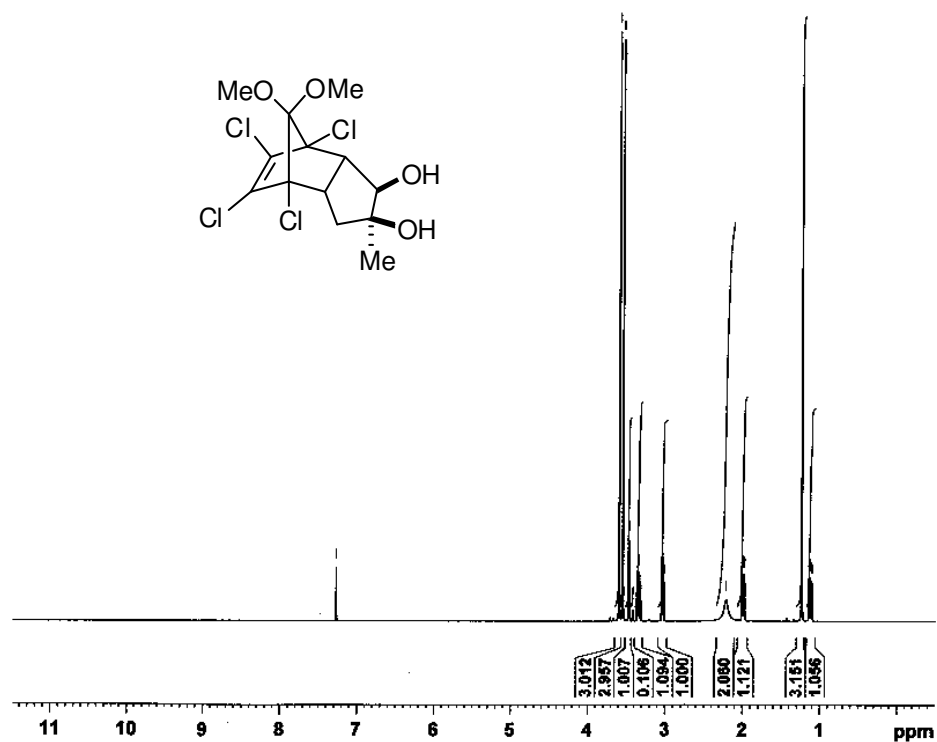
S2-S18	¹ H (400 MHz) & ¹³ C (100 MHz) NMR spectra of selected compounds
S19-S21	COSY, HMQC&HMBC (600 MHz) spectra of 8
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S35	X-ray Ortep diagram of 5

Selected Spectra

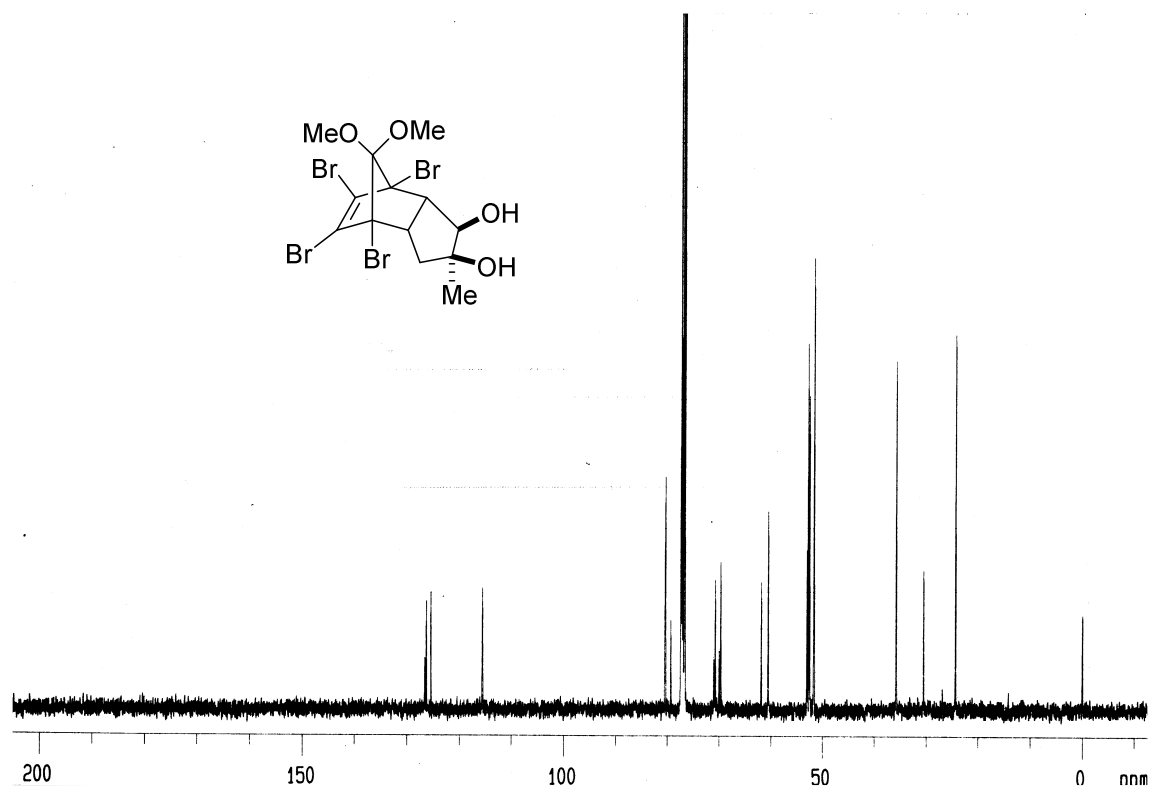
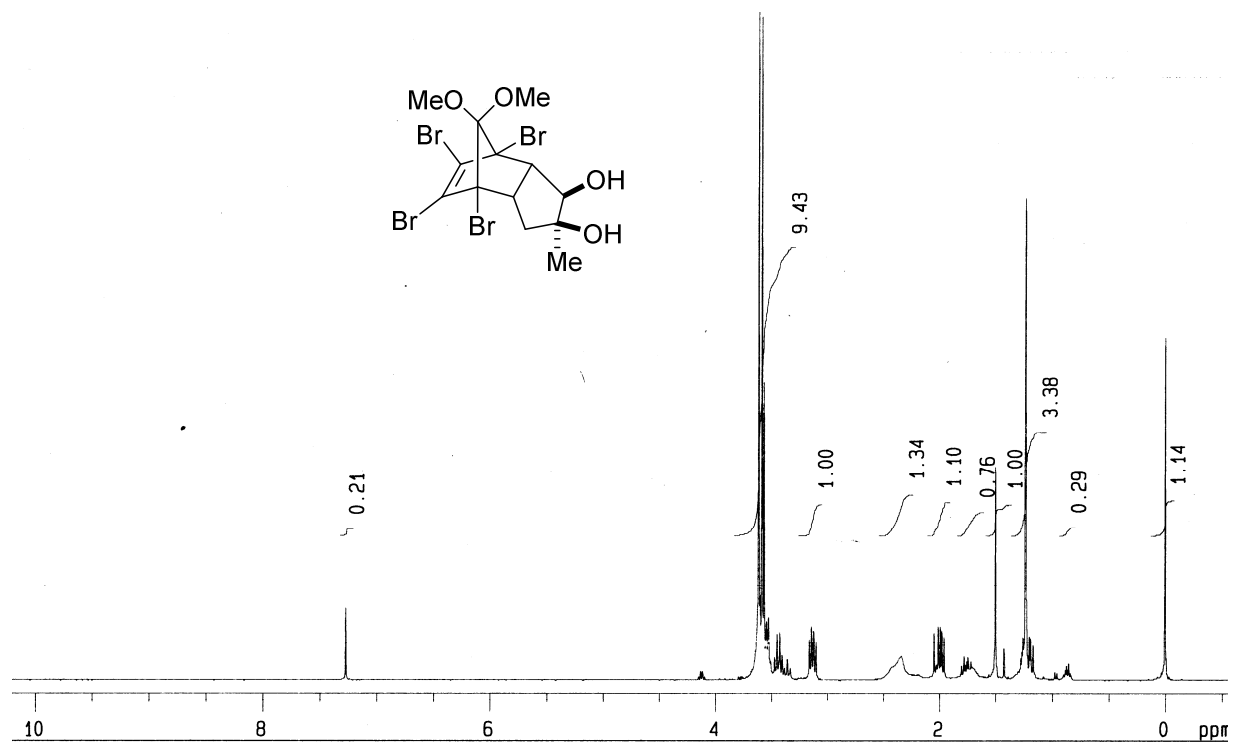
^1H & ^{13}C NMR (400 MHz, CDCl_3) of Compound 2



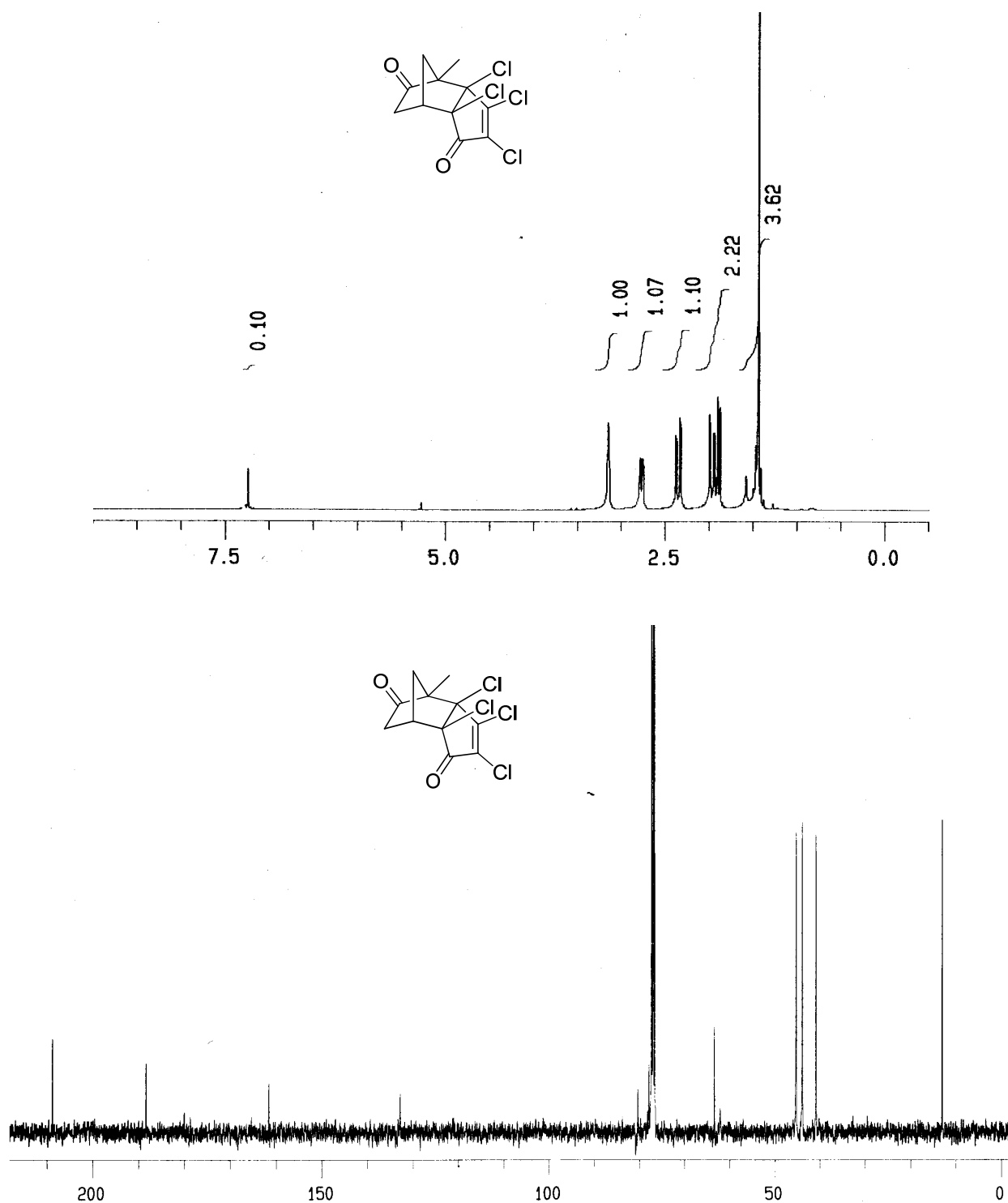
^1H (600 MHz, CDCl_3) & ^{13}C (75 MHz, CDCl_3) NMR of Compound 3



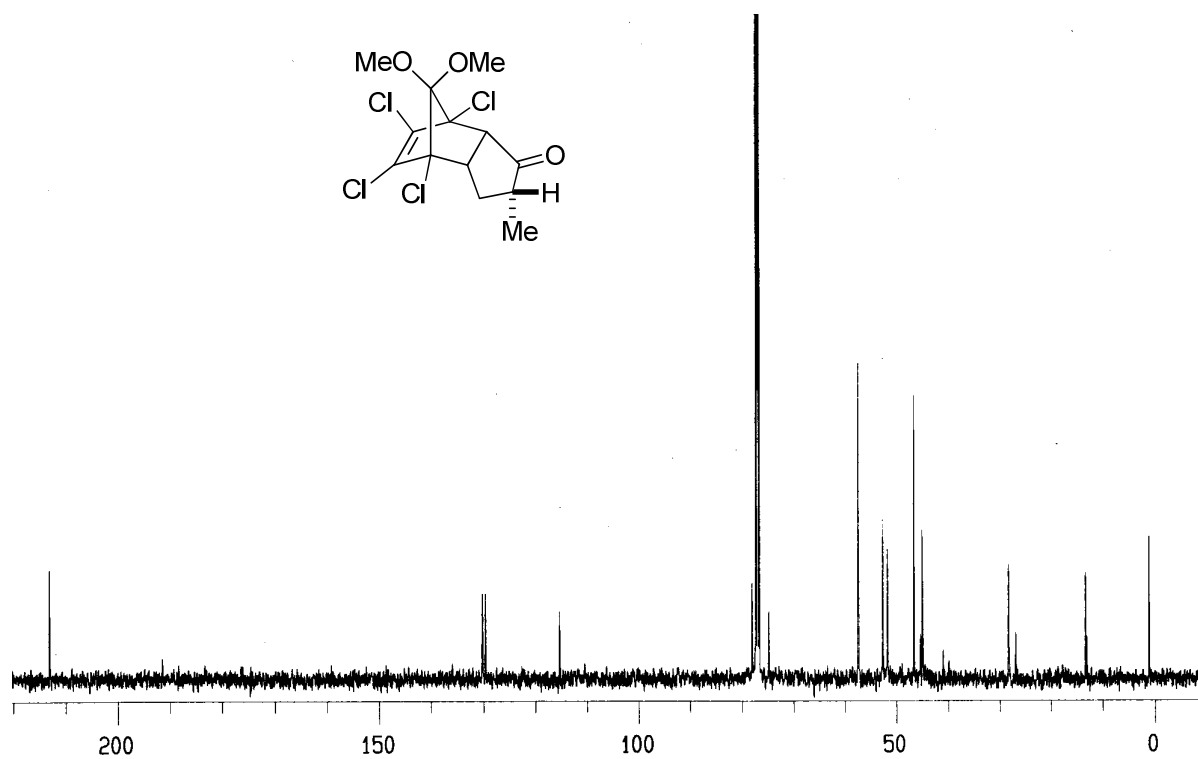
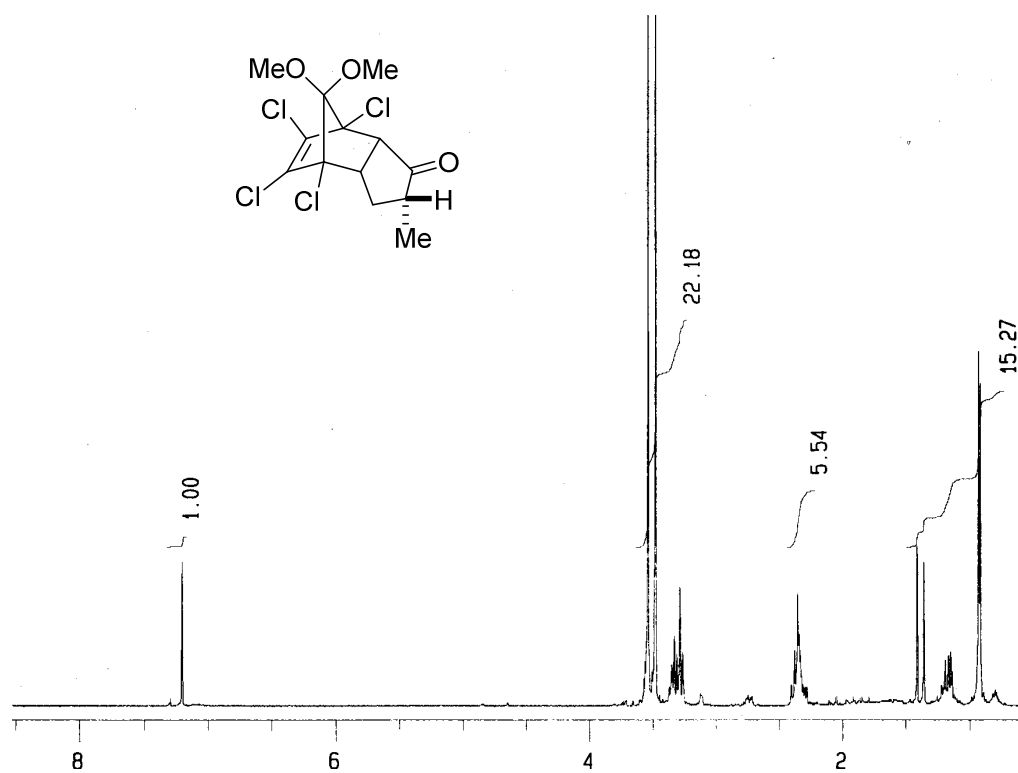
^1H (400 MHz, CDCl_3) & ^{13}C (100 MHz, CDCl_3) NMR of Compound 4



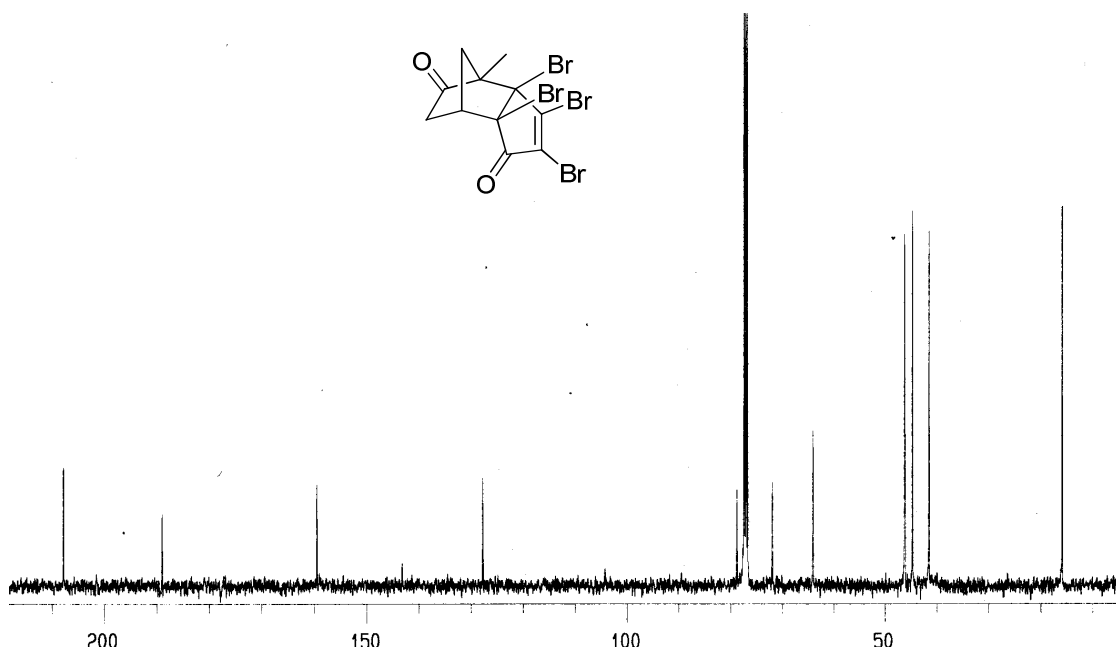
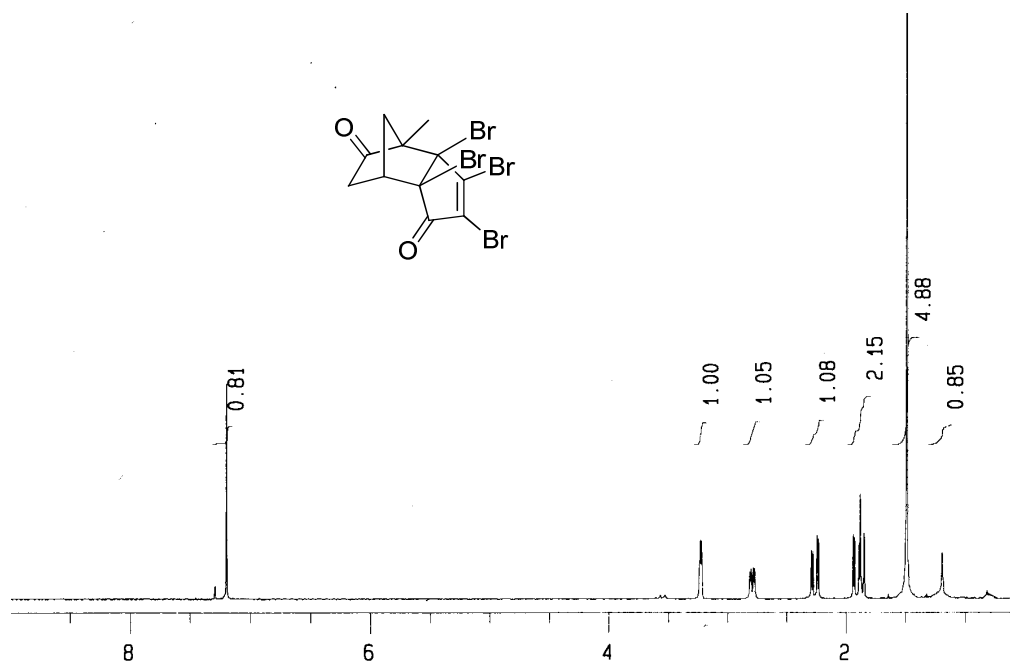
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of **5** in CDCl_3



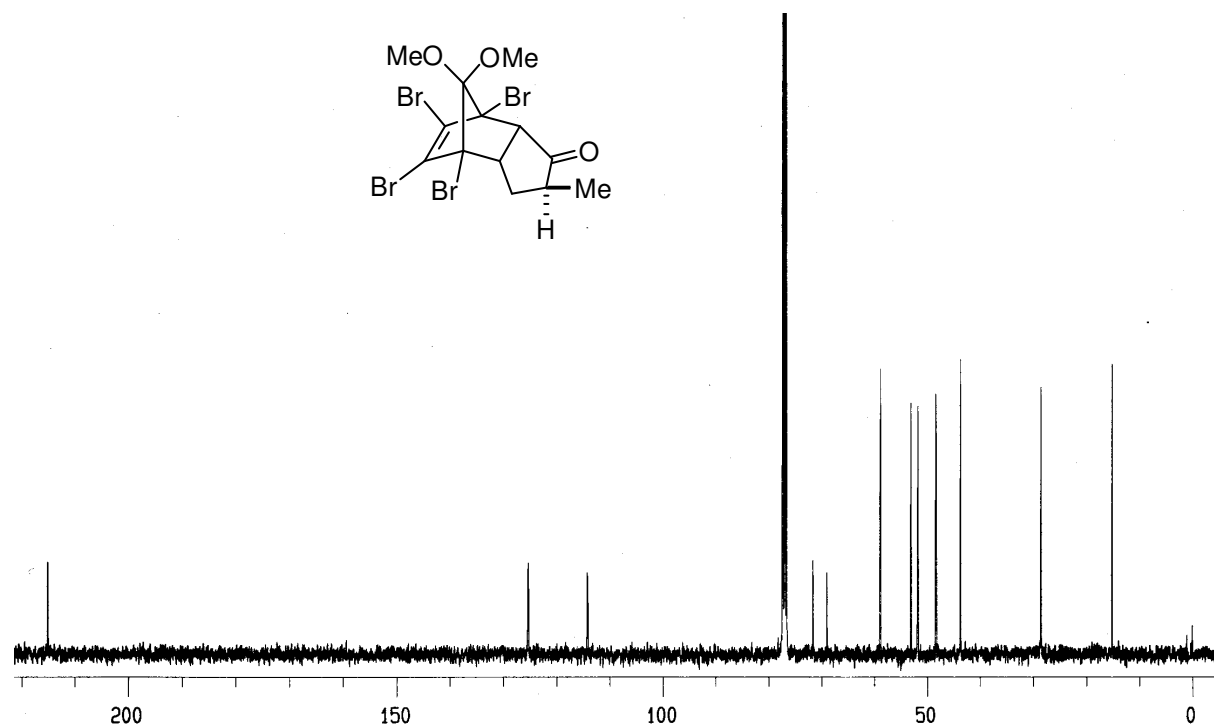
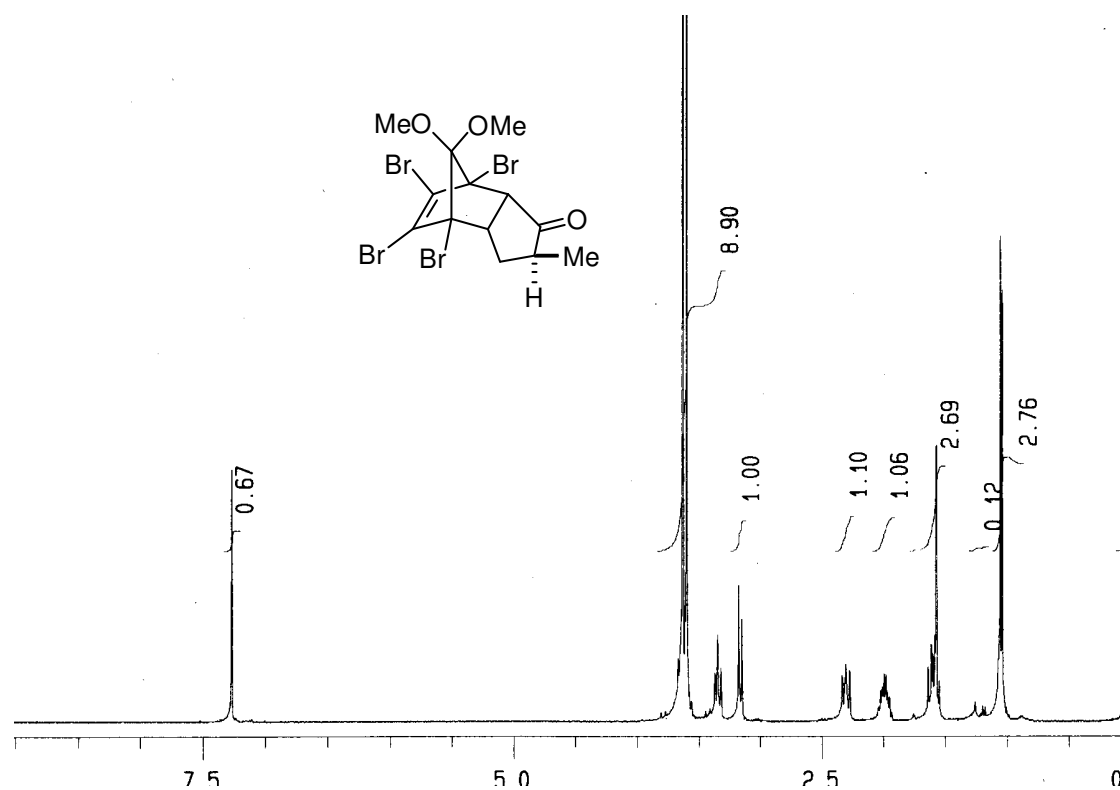
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 6 in CDCl_3



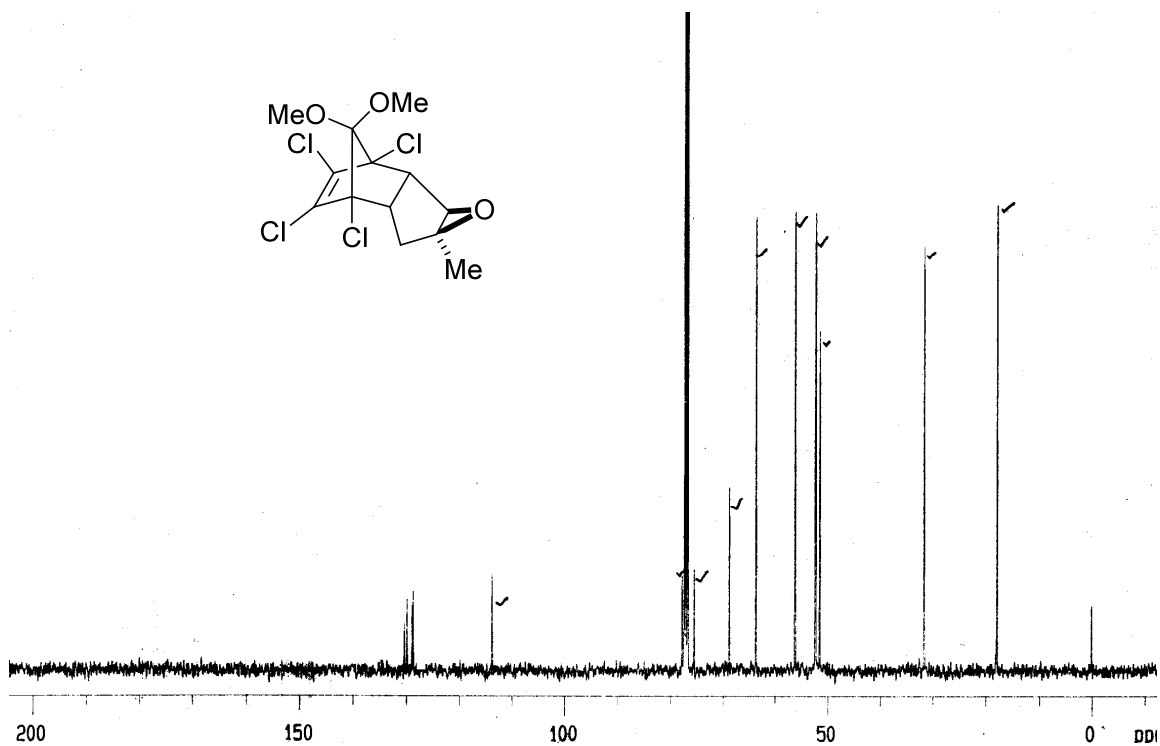
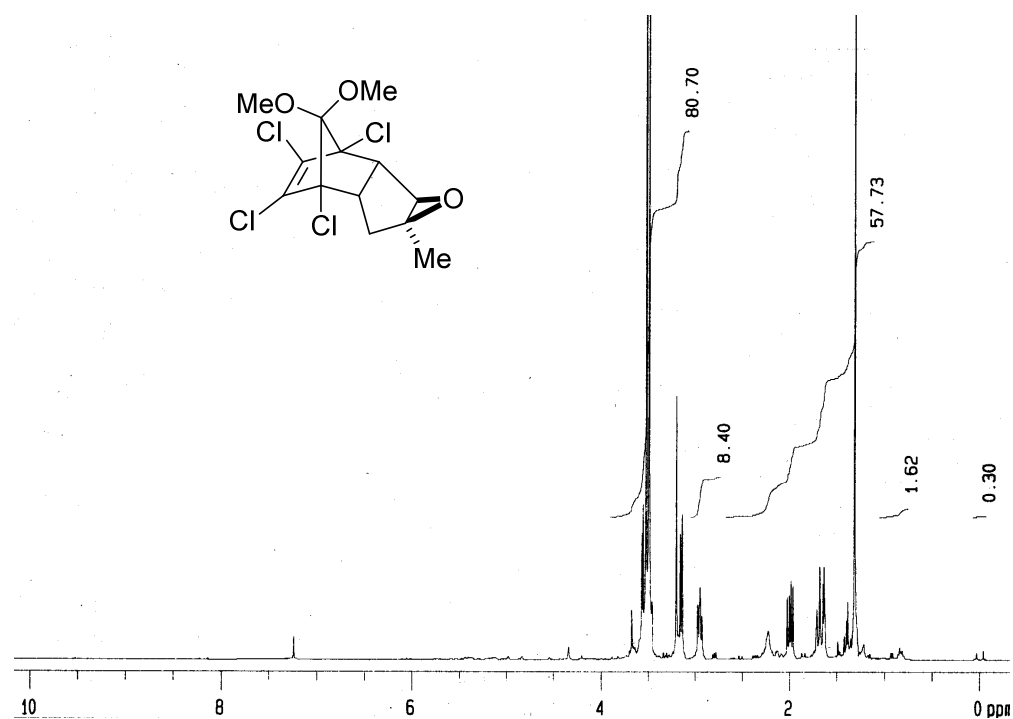
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of **7** in CDCl_3



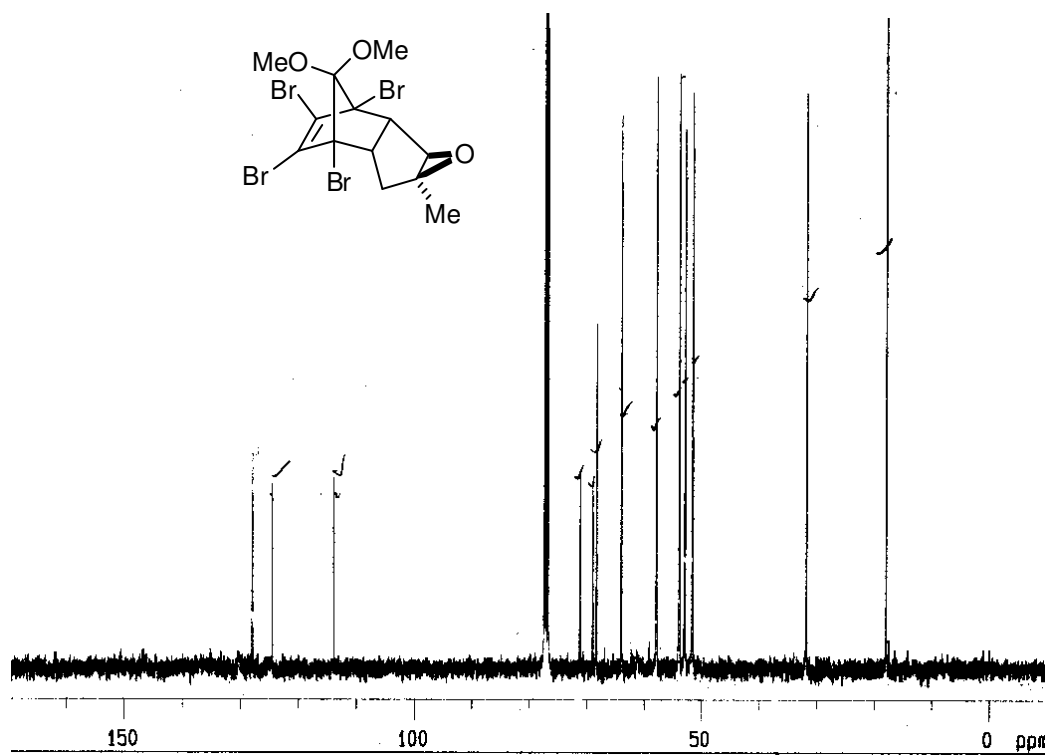
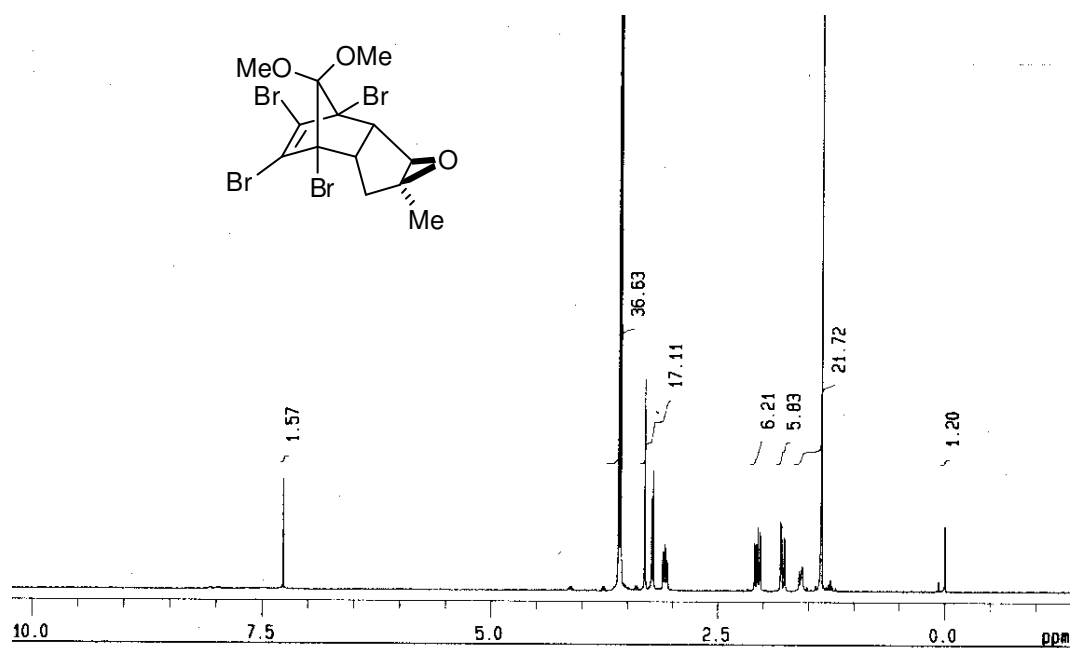
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 8 in CDCl_3



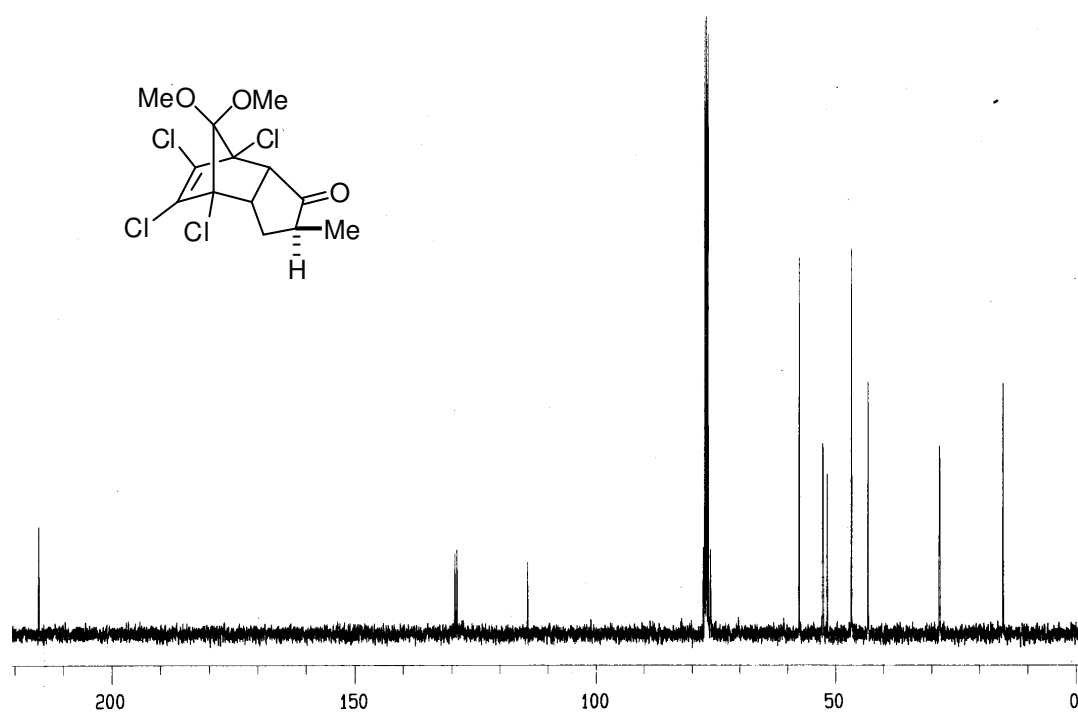
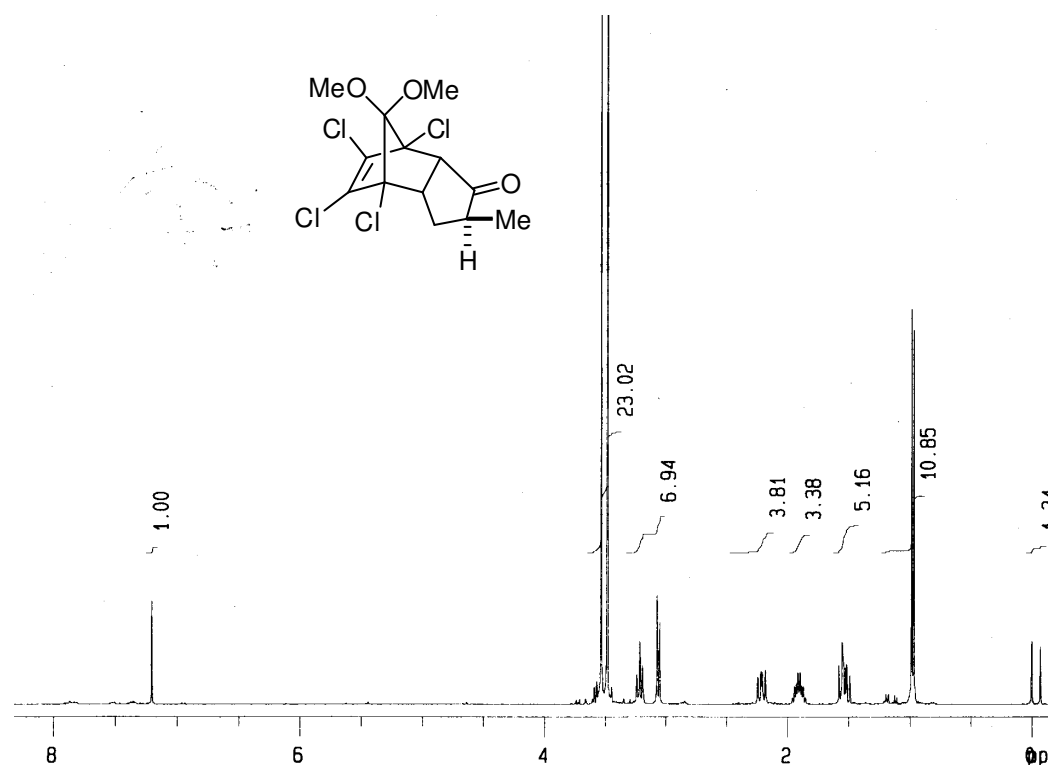
^1H NMR (400 MHz, CDCl_3) of Compound 9



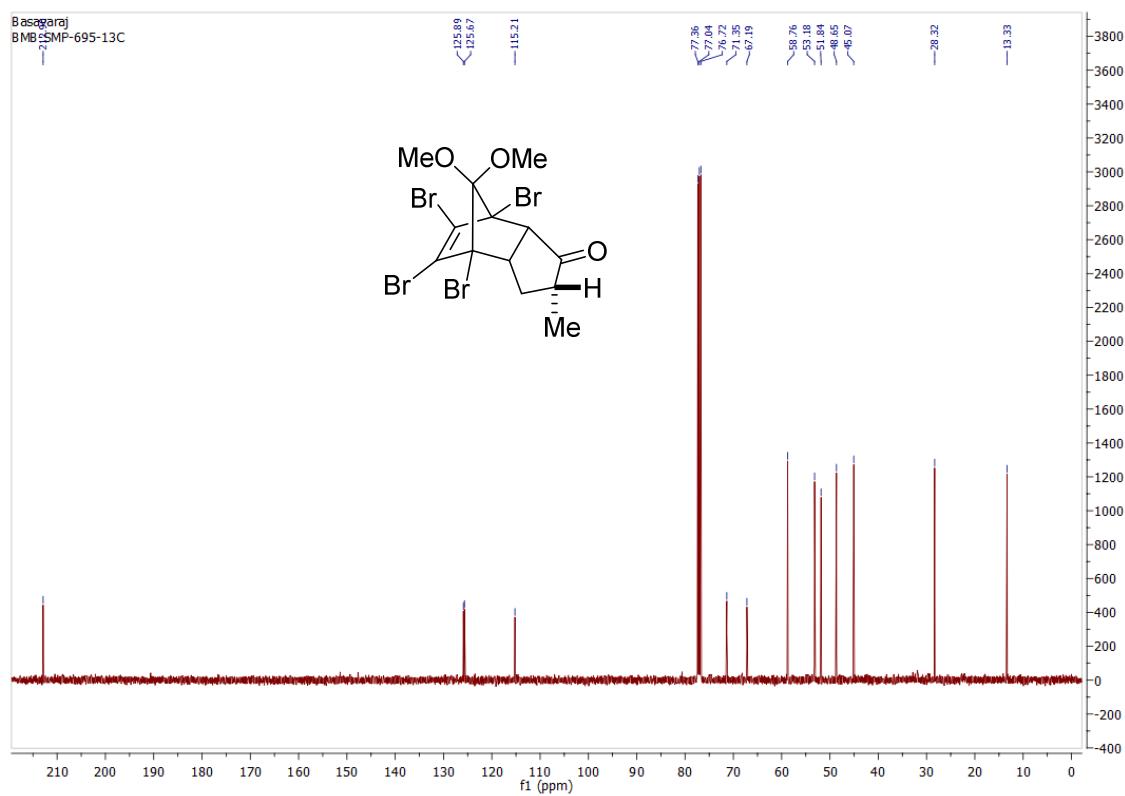
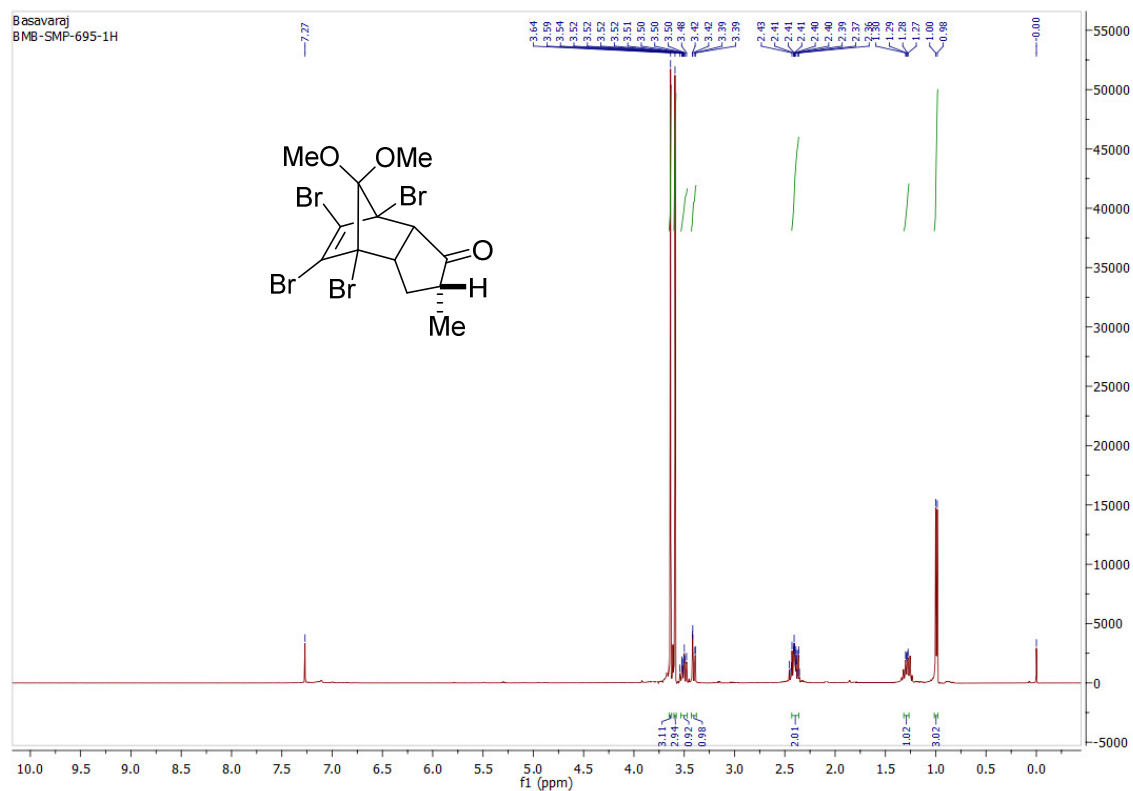
^1H NMR (400 MHz, CDCl_3) of Compound 10



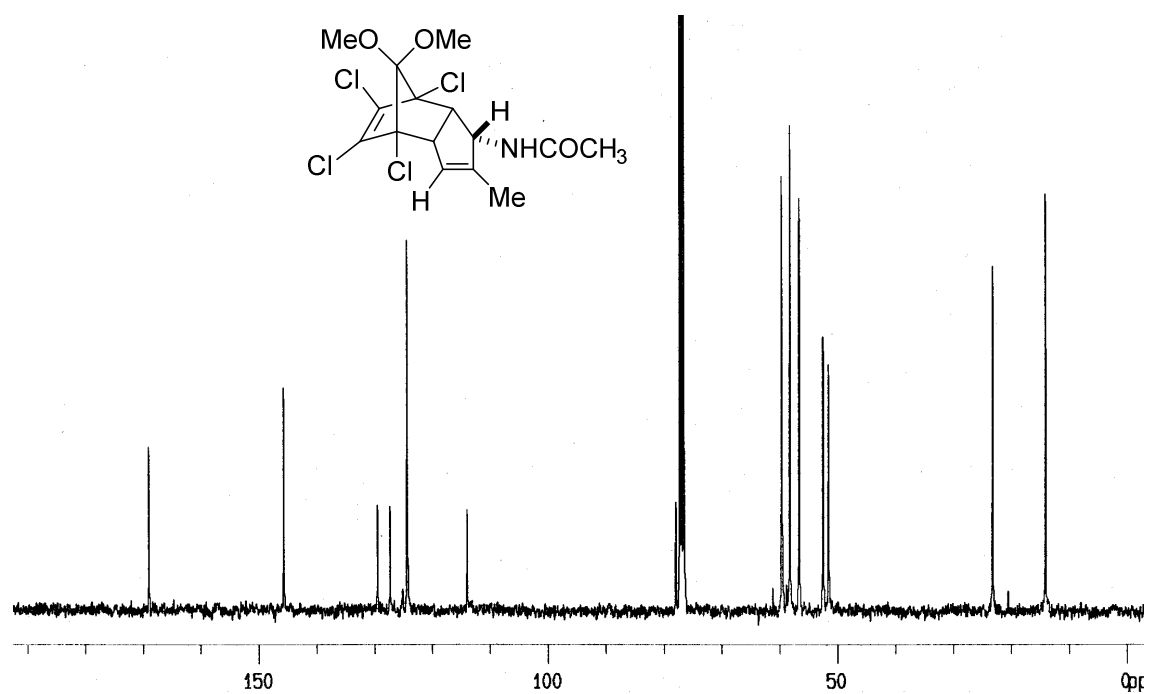
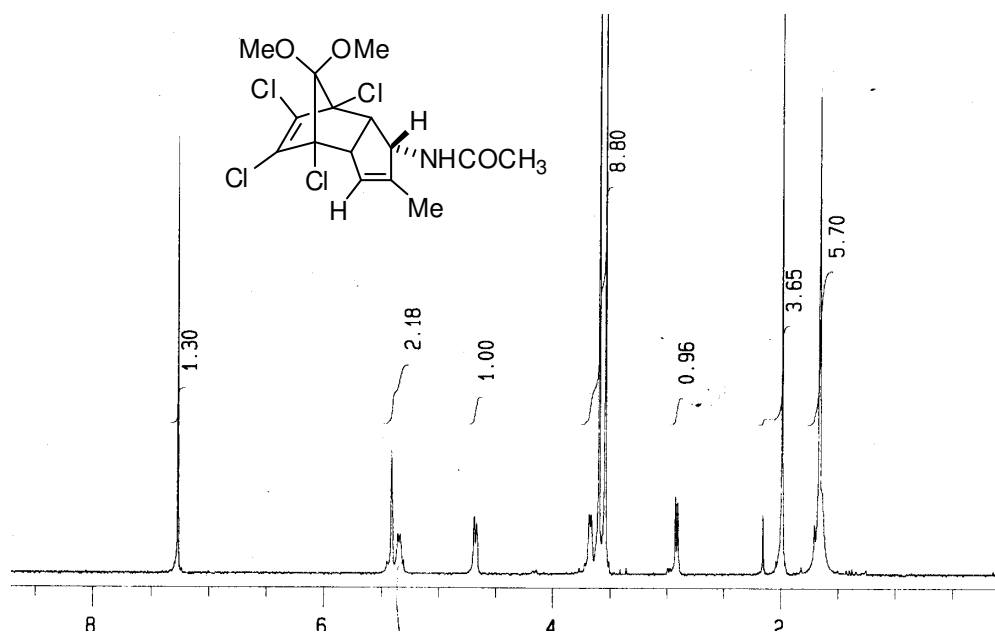
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 11 in CDCl_3



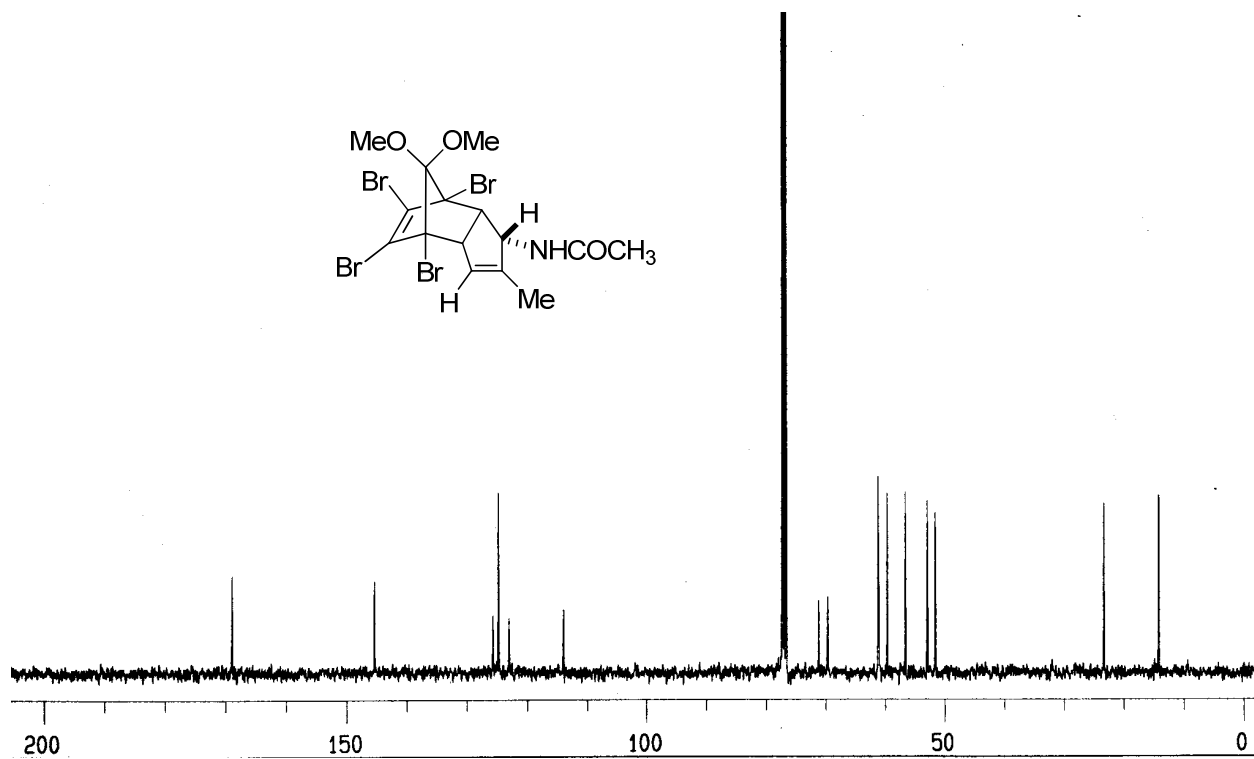
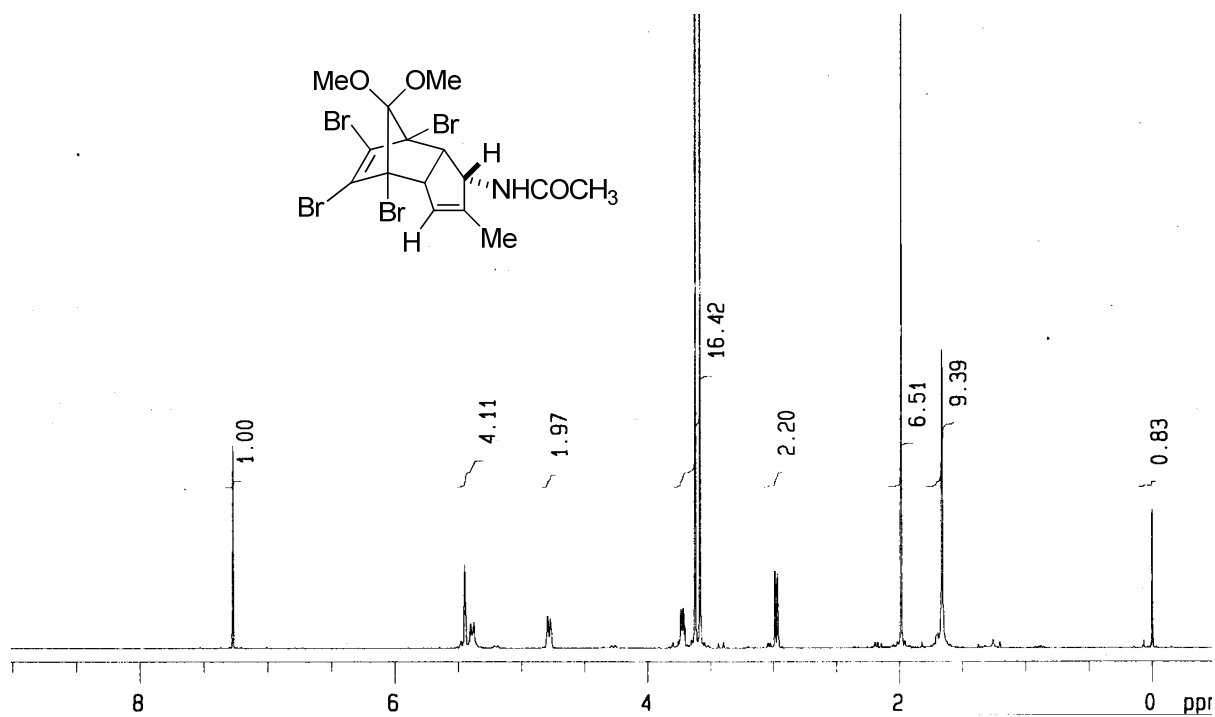
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 12 in CDCl_3



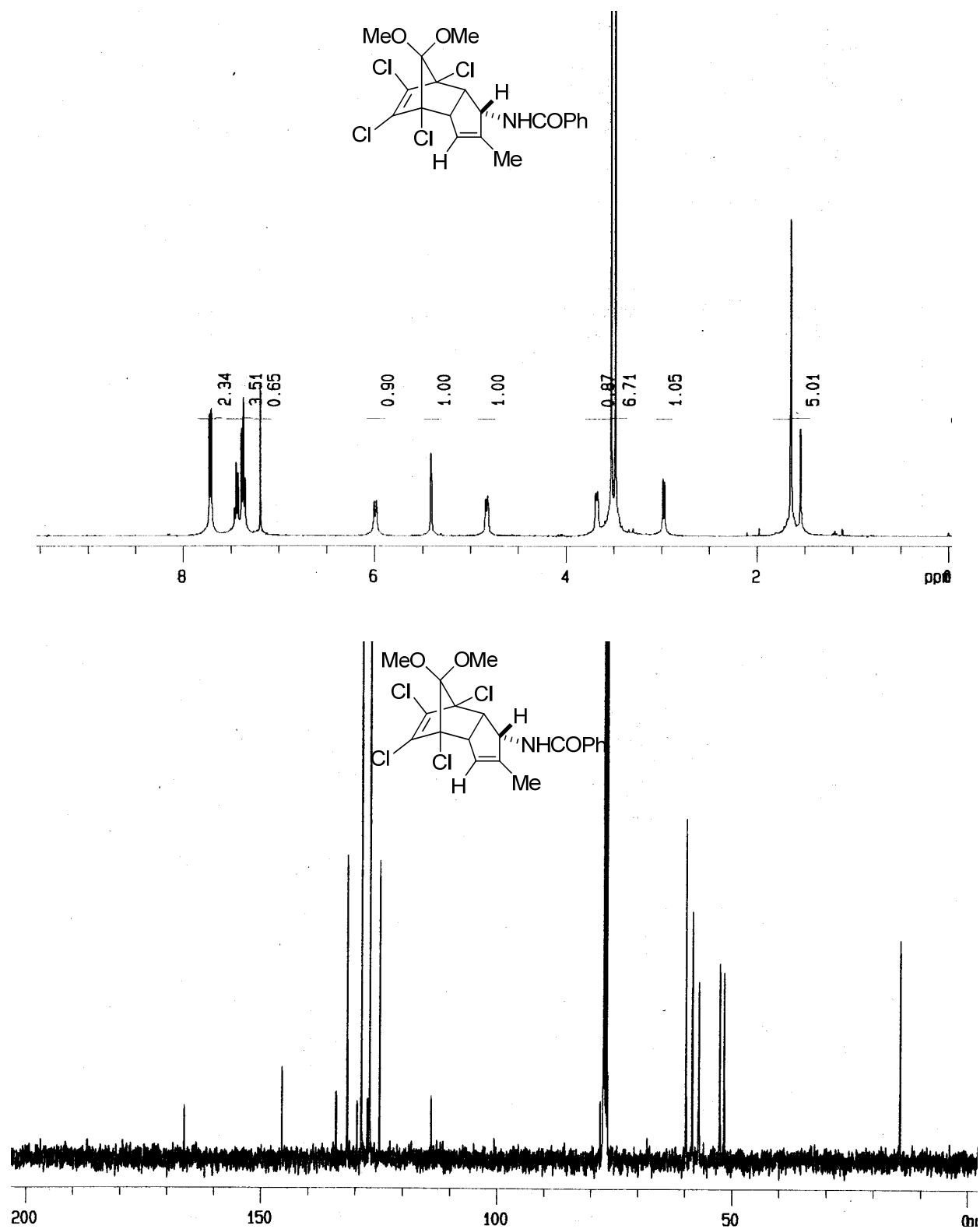
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 13 in CDCl_3



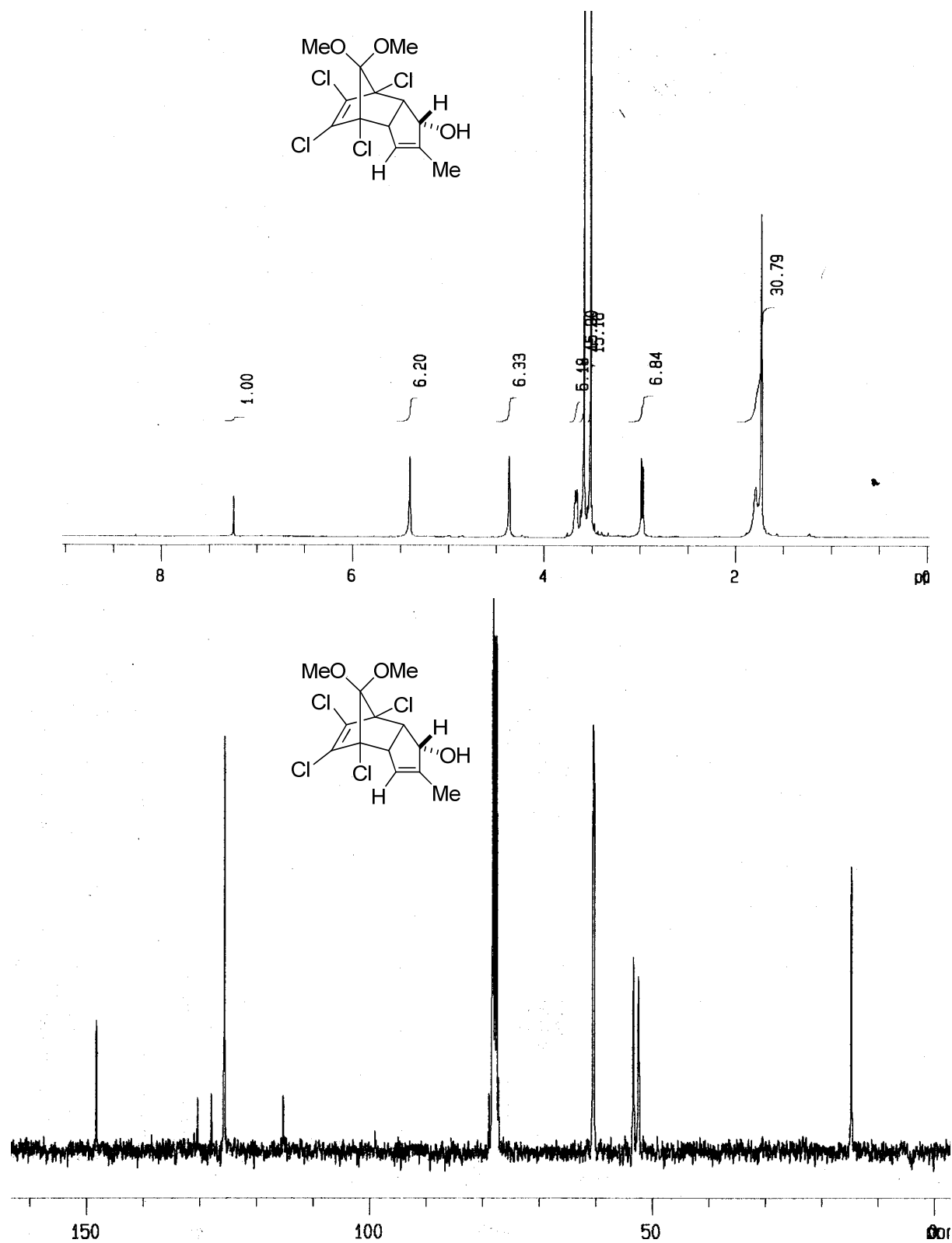
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 14 in CDCl_3



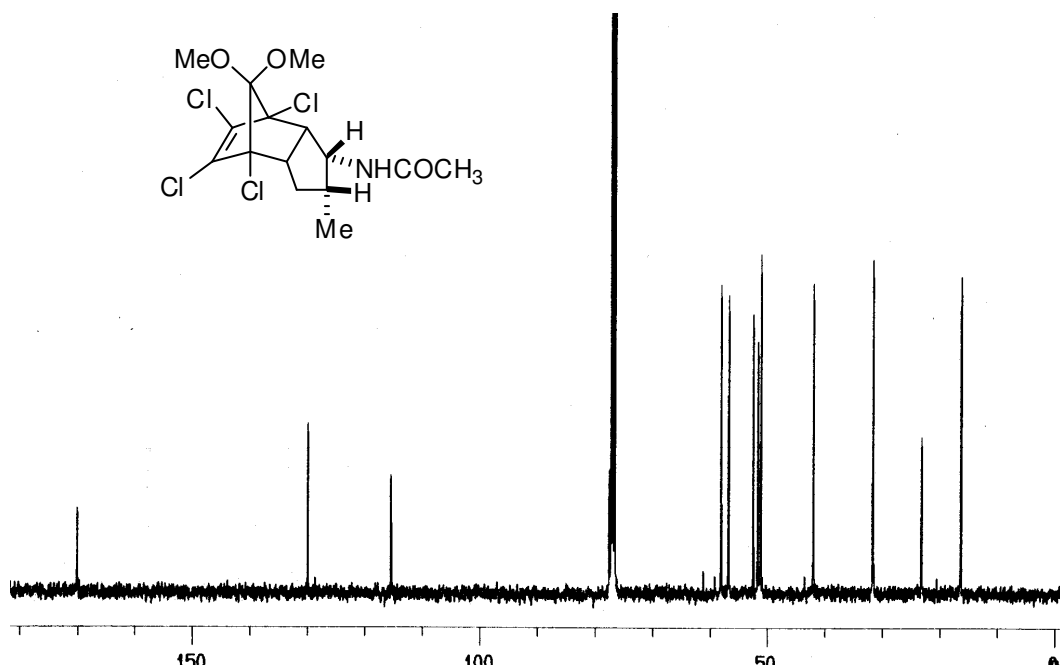
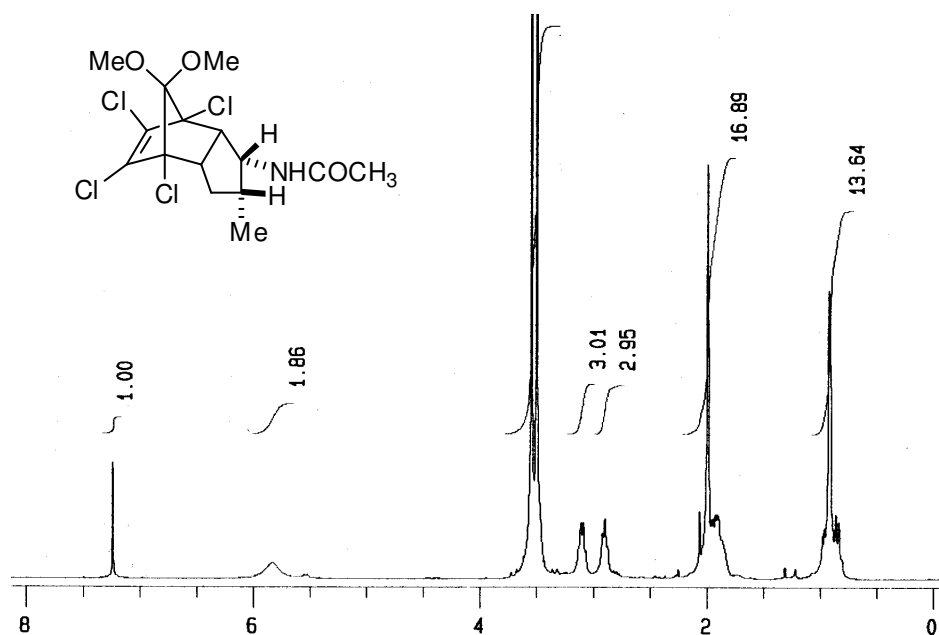
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 15 in CDCl_3



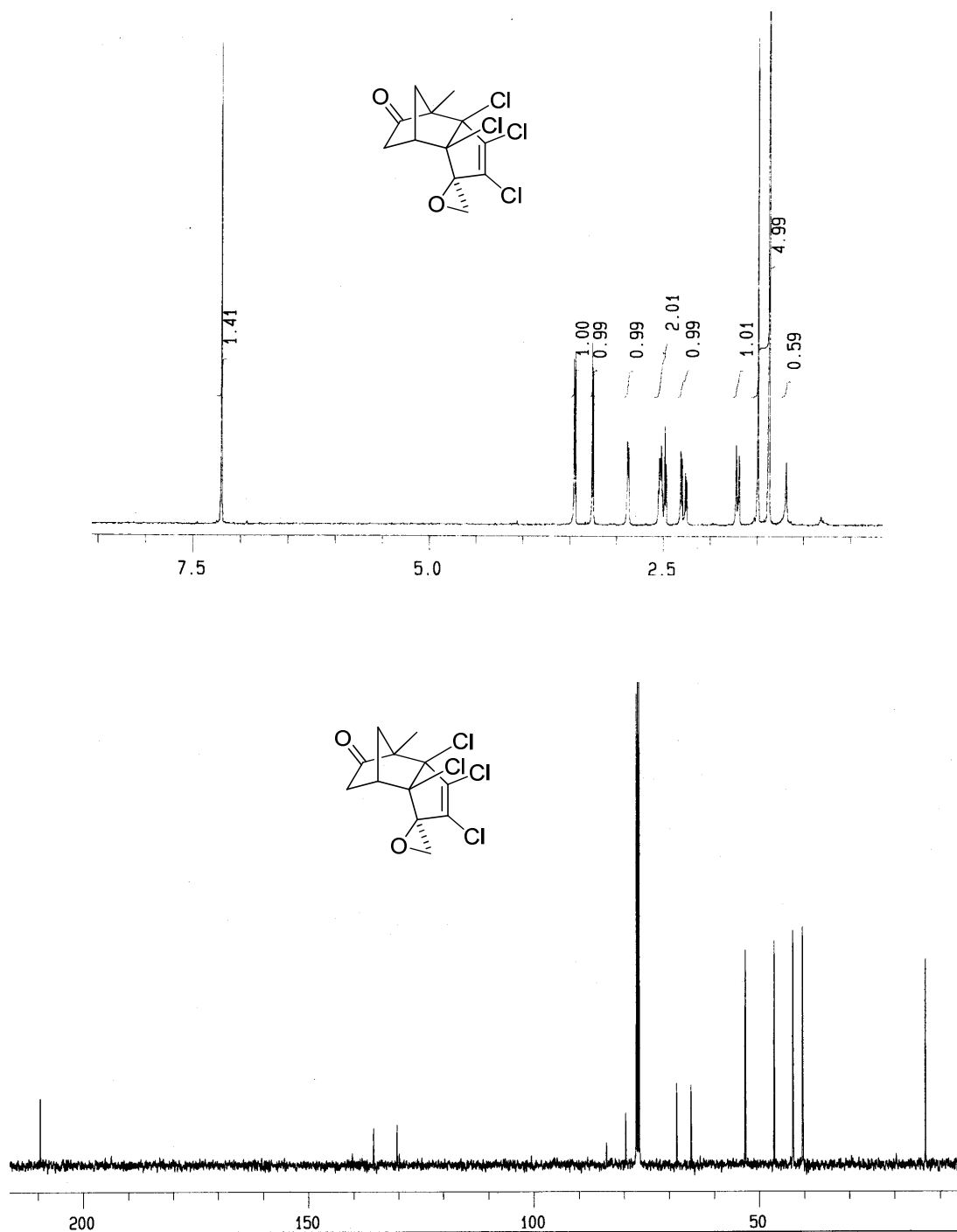
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 16 in CDCl_3



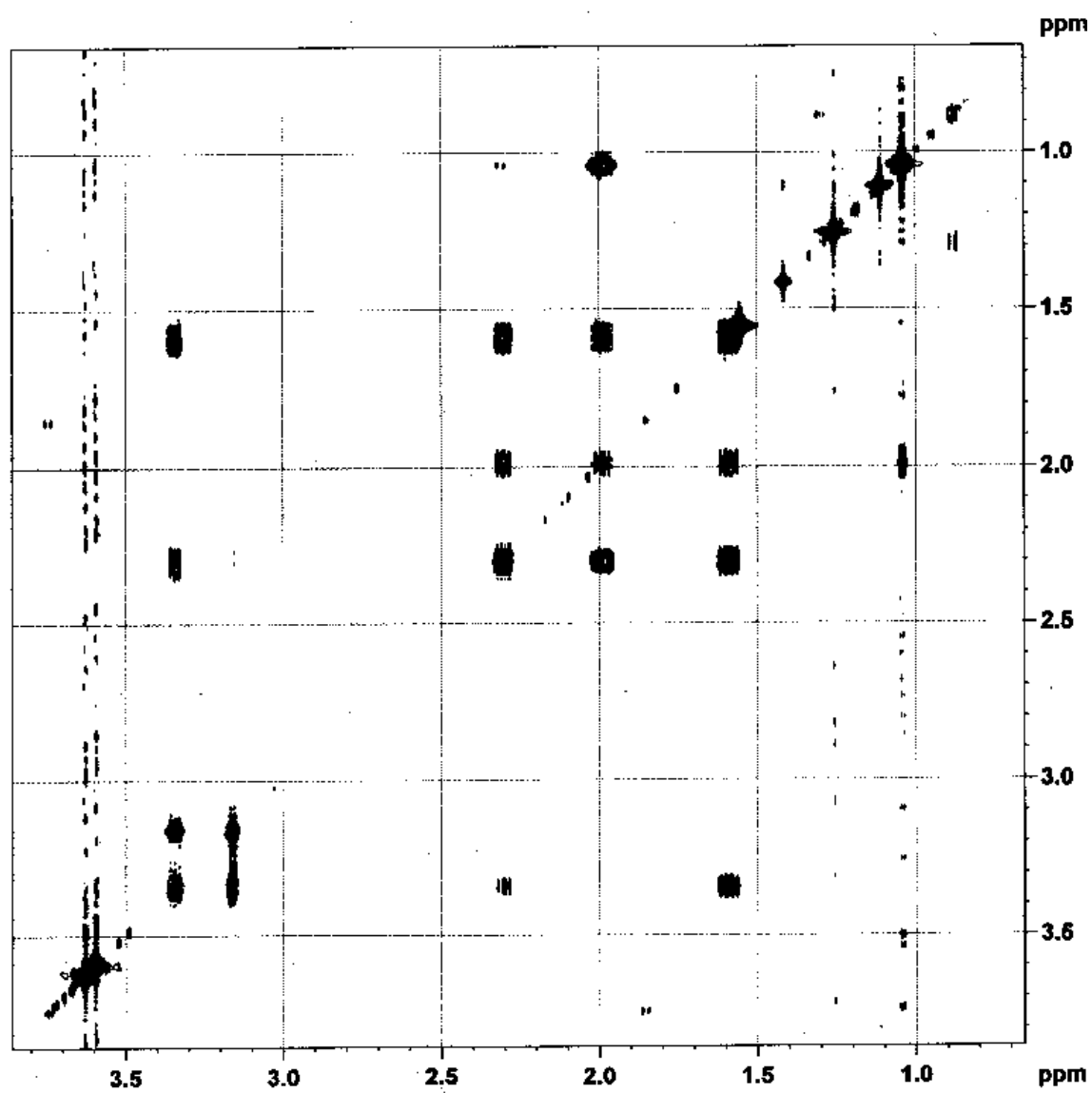
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 17 in CDCl_3



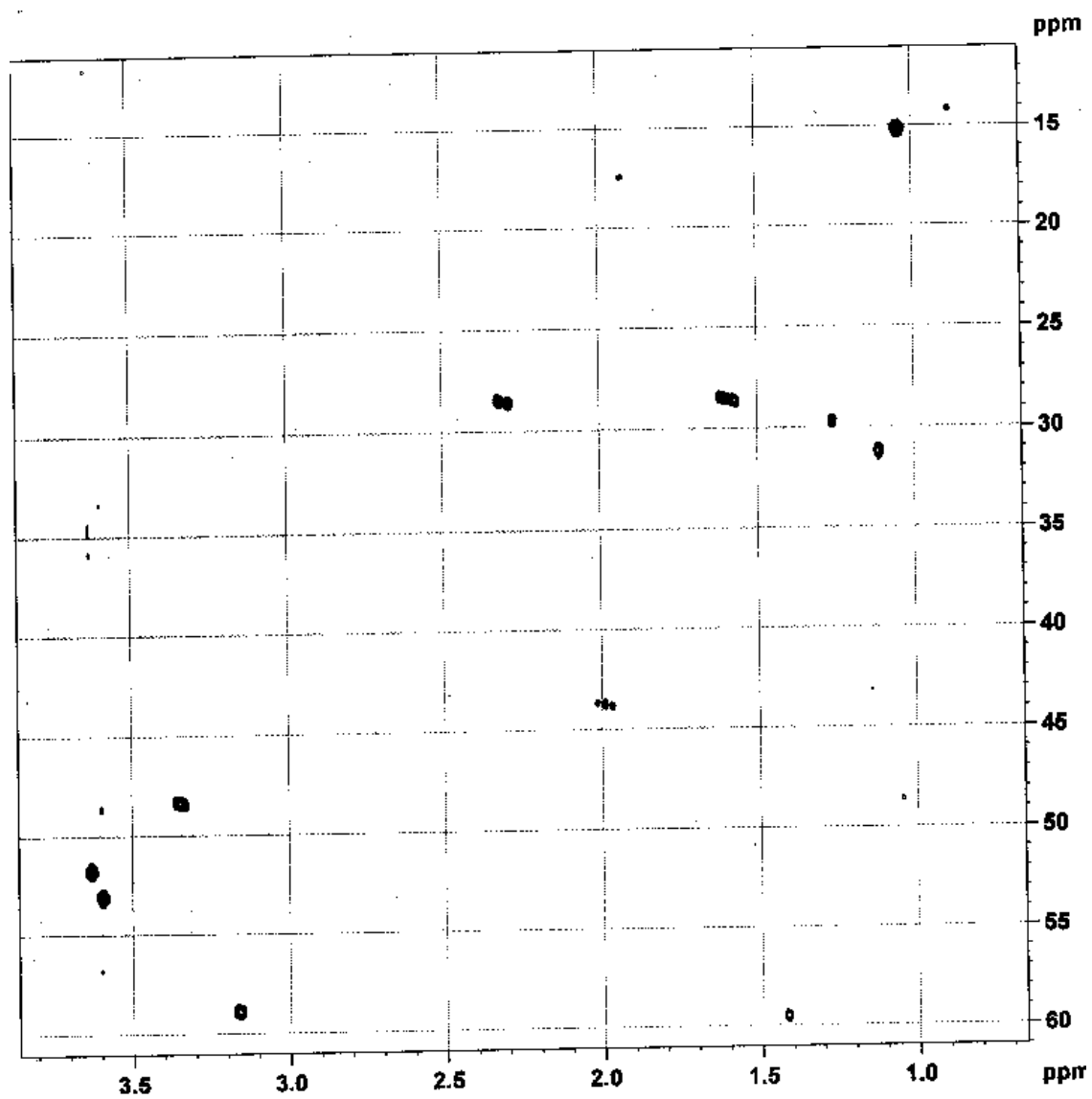
^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) of 18 in CDCl_3



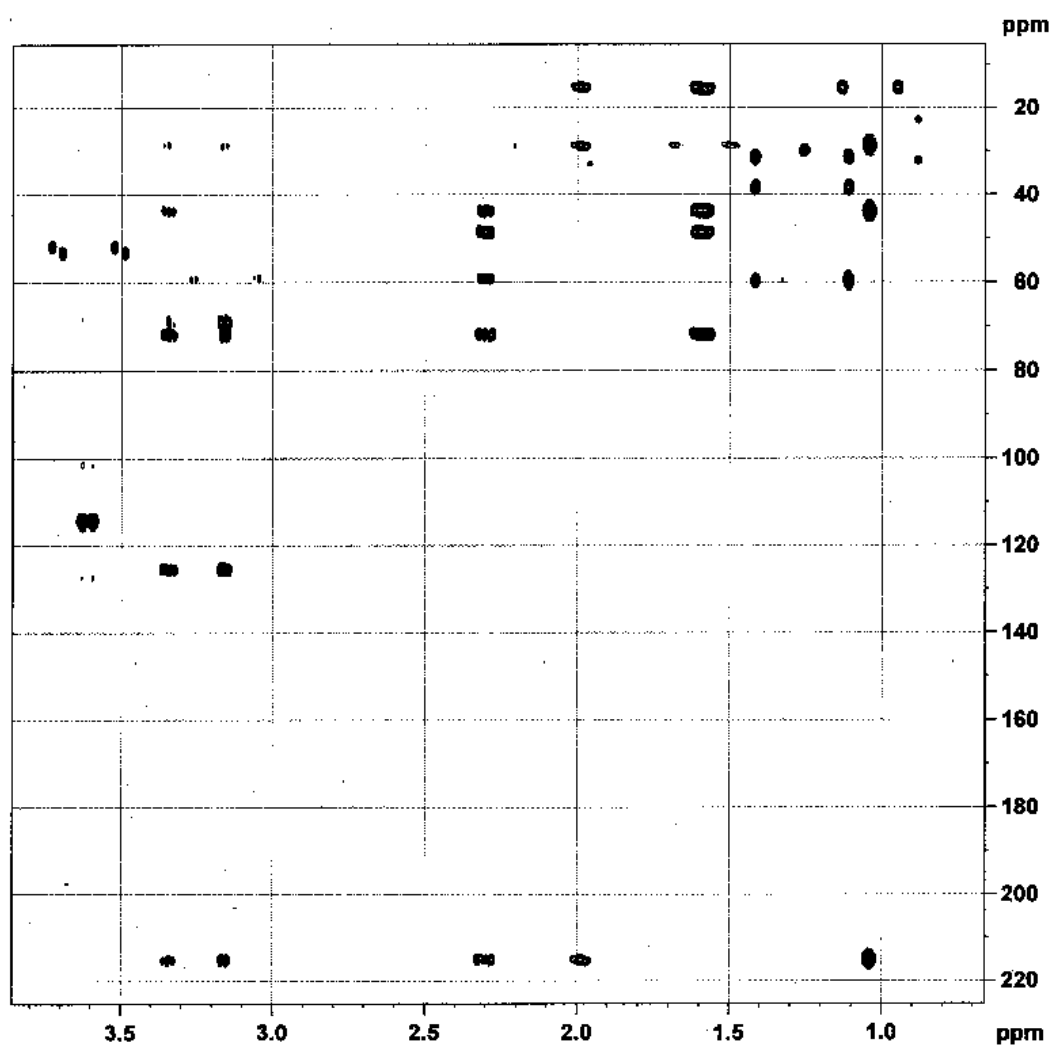
600 MHz $^1\text{H}/^1\text{H}$ COSY spectrum of 8 in CDCl_3 solution



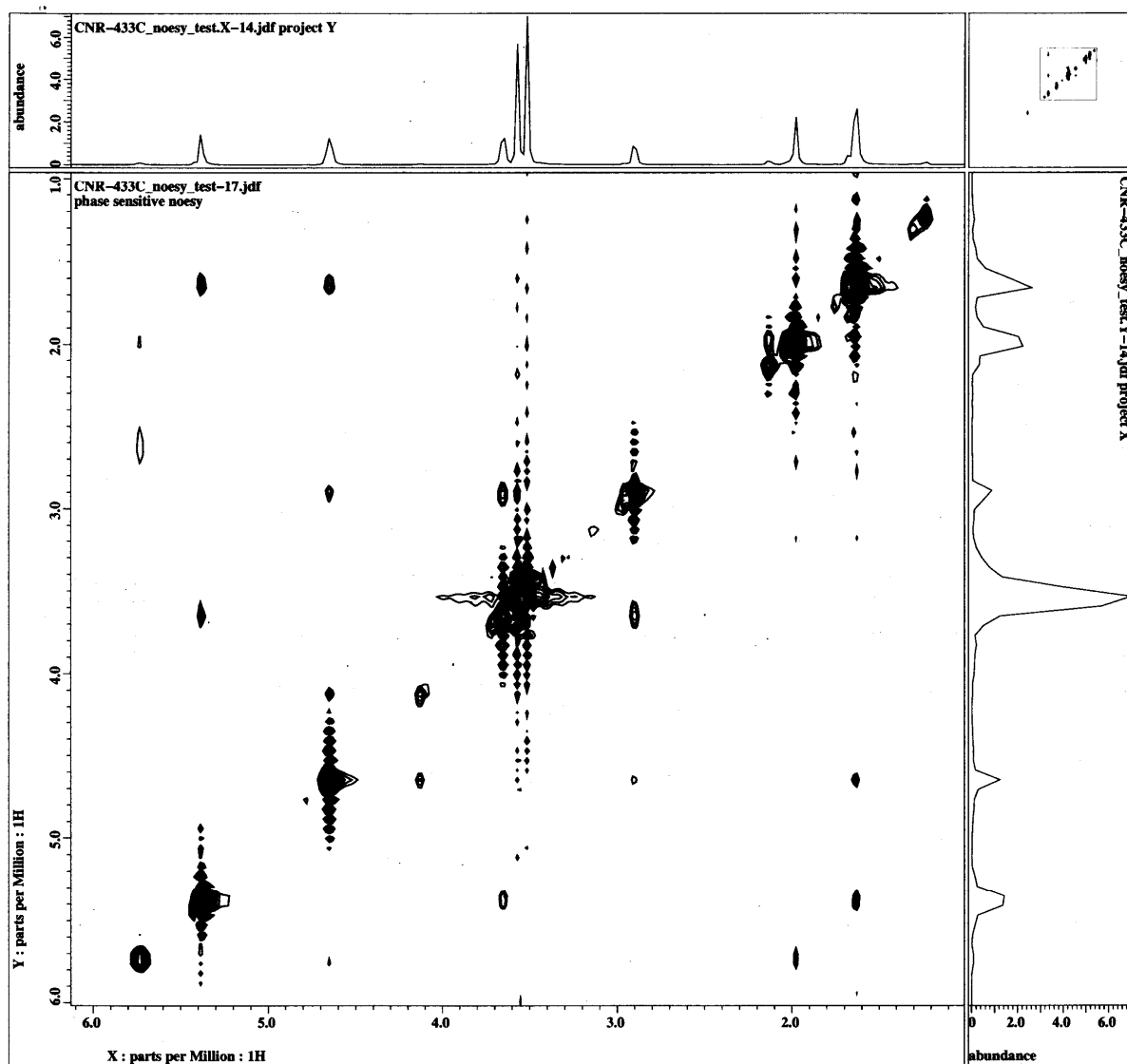
600 MHz HMQC spectrum of 8 in CDCl₃ solution



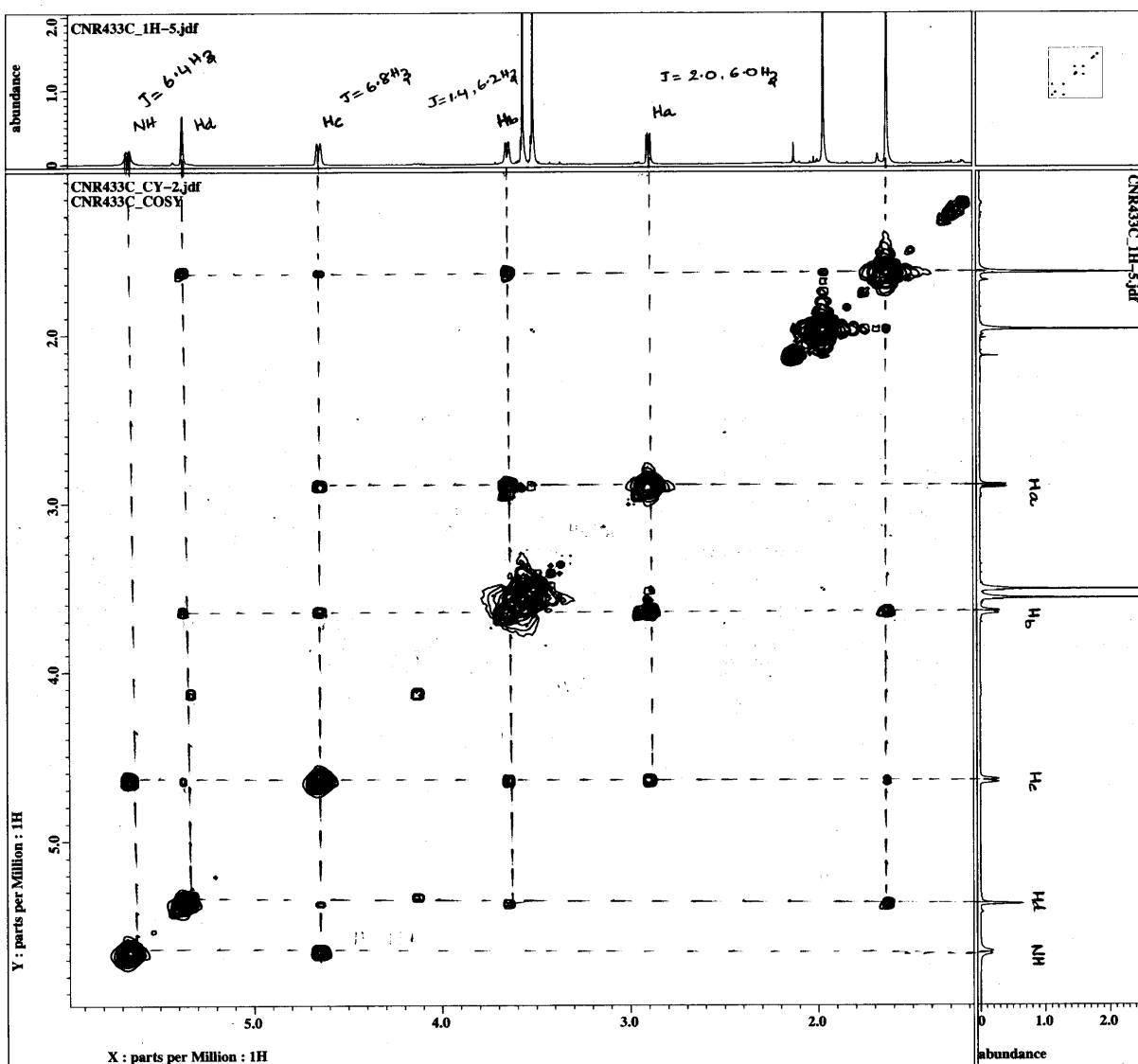
600 MHz HMBC spectrum of 8 in CDCl₃ solution



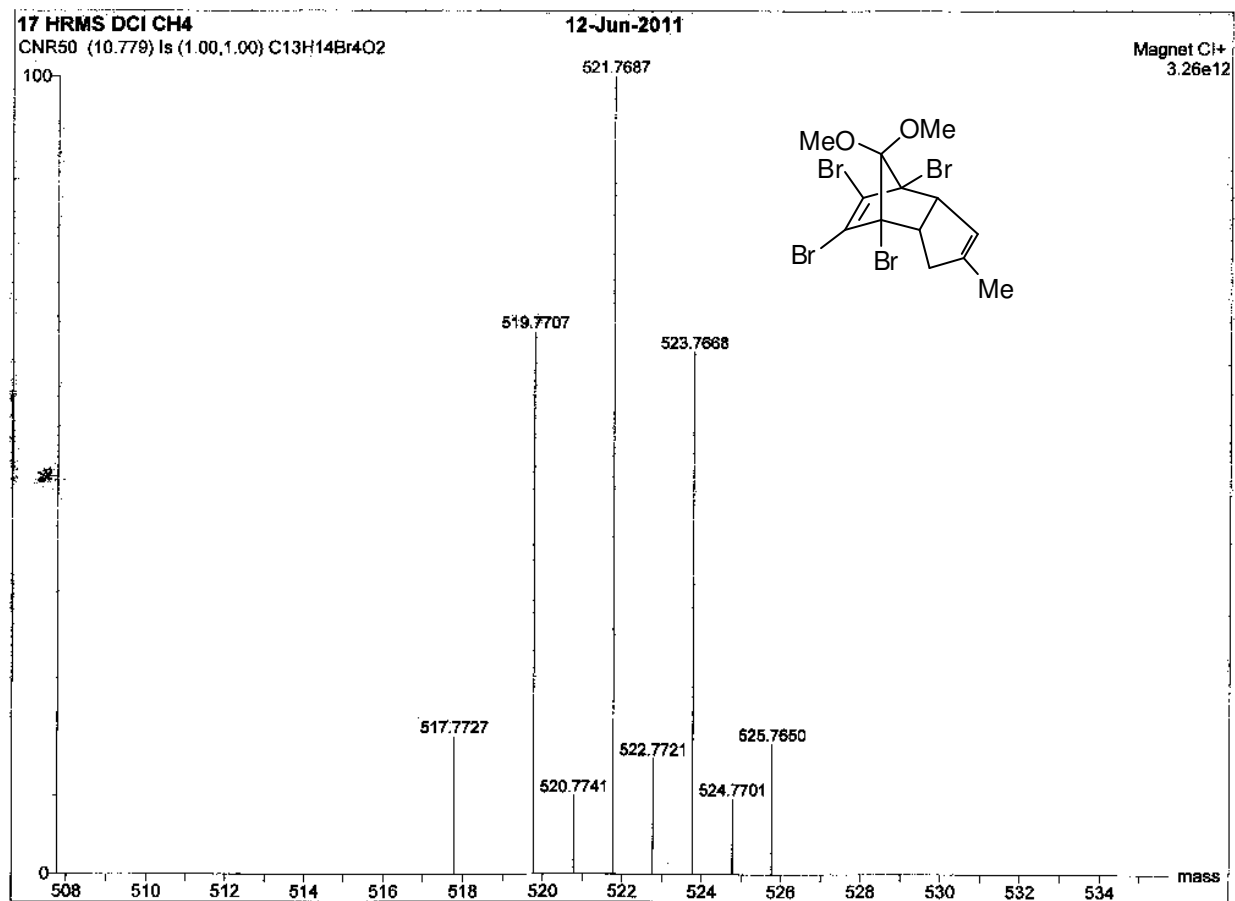
500 MHz $^1\text{H}/^1\text{H}$ NOESY spectrum of 13 in CDCl_3 solution



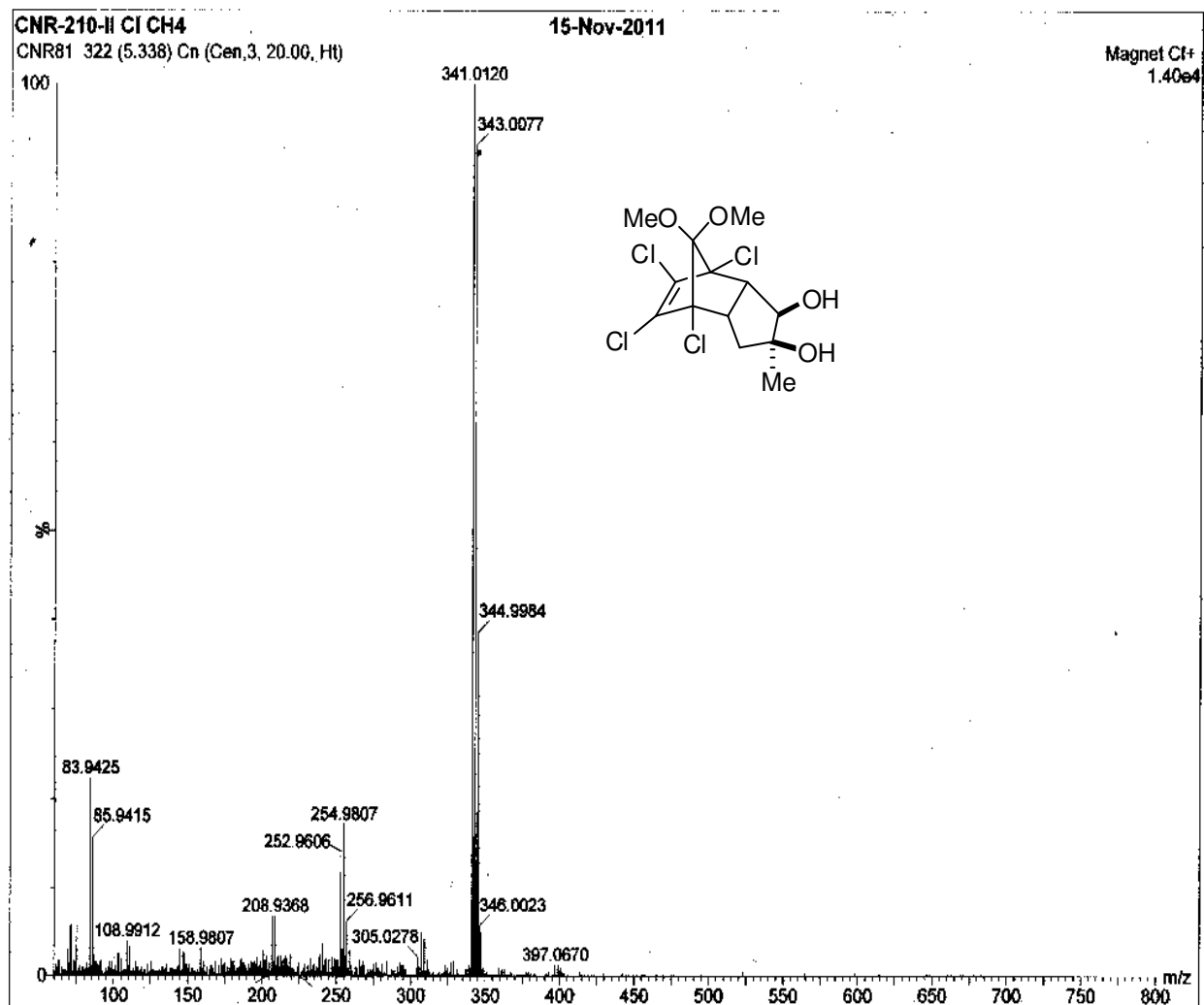
500 MHz $^1\text{H}/^1\text{H}$ COSY spectrum of 13 in CDCl_3 solution



HRMS (DCI) of Compound 2



HRMS (DCI) of Compound 3



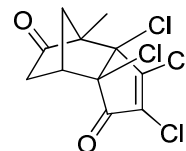
HRMS (EI) of Compound 5

Name : c:\mswin\data\massconv.mss
 Creation Date/Time : 25.10.04 at 9:13:50
 File Title : rei8ig / zimmer / khan
 Operator : franzus
 Instrument : CH7 A // EI
 AK : rei8ig
 Name : Zimmer / Khan
 Bezeichnung : CNR 22c
 MZ : 313.9
 Summenformel : C₁₁H₈O₂Cl₄
 Temp.°C : 80
 Job-Ms-Nr. : 2/25.685

Selected Isotopes:

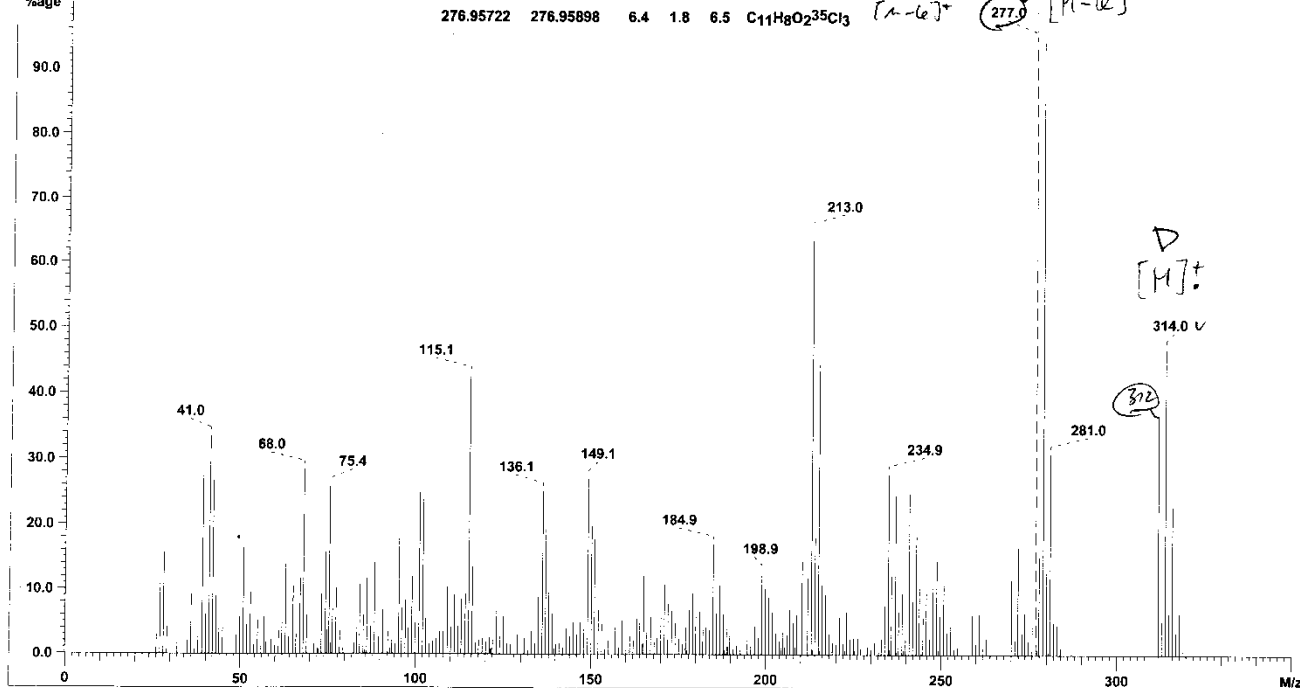
Symbol	Min	Max	Vcy	Name
C	0	40	4	Carbon-12
H	0	40	1	Hydrogen-1
O	2	2	2	Oxygen-16
[35Cl]	3	4	1	Chlorine-35

Allowable error = minimum of 20.0 ppm, 20.0 mmu.
 Ring/Double Bond limits = [-0.5 : 100.0]



SCAN GRAPH. Flagging=M/z.
 %age Scan 29-S:48. Entries=268. 100% Int.=12741.

Mass	Calculated	ppm	mmu	R/DB	Formula
311.92644	311.92783	4.4	1.4	6.0	C ₁₁ H ₈ O ₂ ³⁵ Cl ₄
276.95722	276.95898	6.4	1.8	6.5	C ₁₁ H ₈ O ₂ ³⁵ Cl ₃



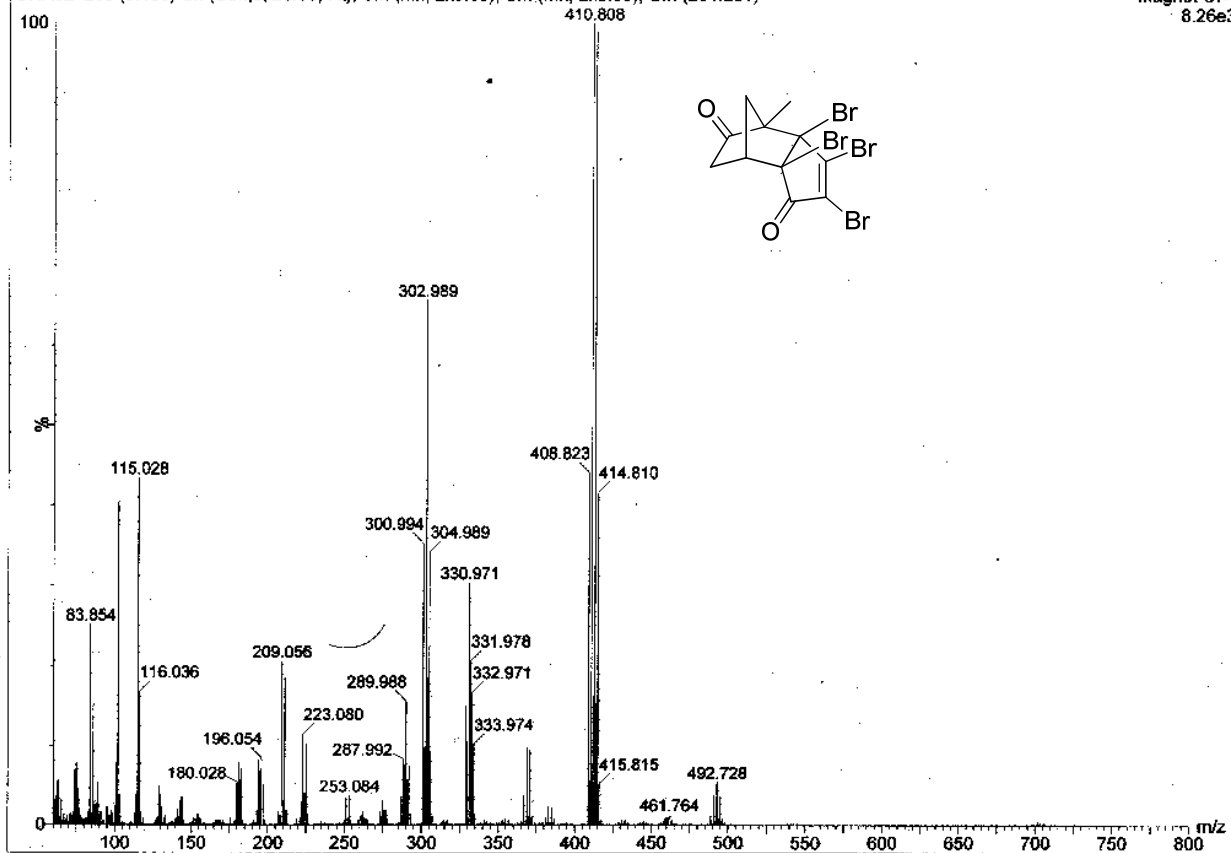
HRMS (DCI) of Compound 7

CNR-210-III Cl CH4

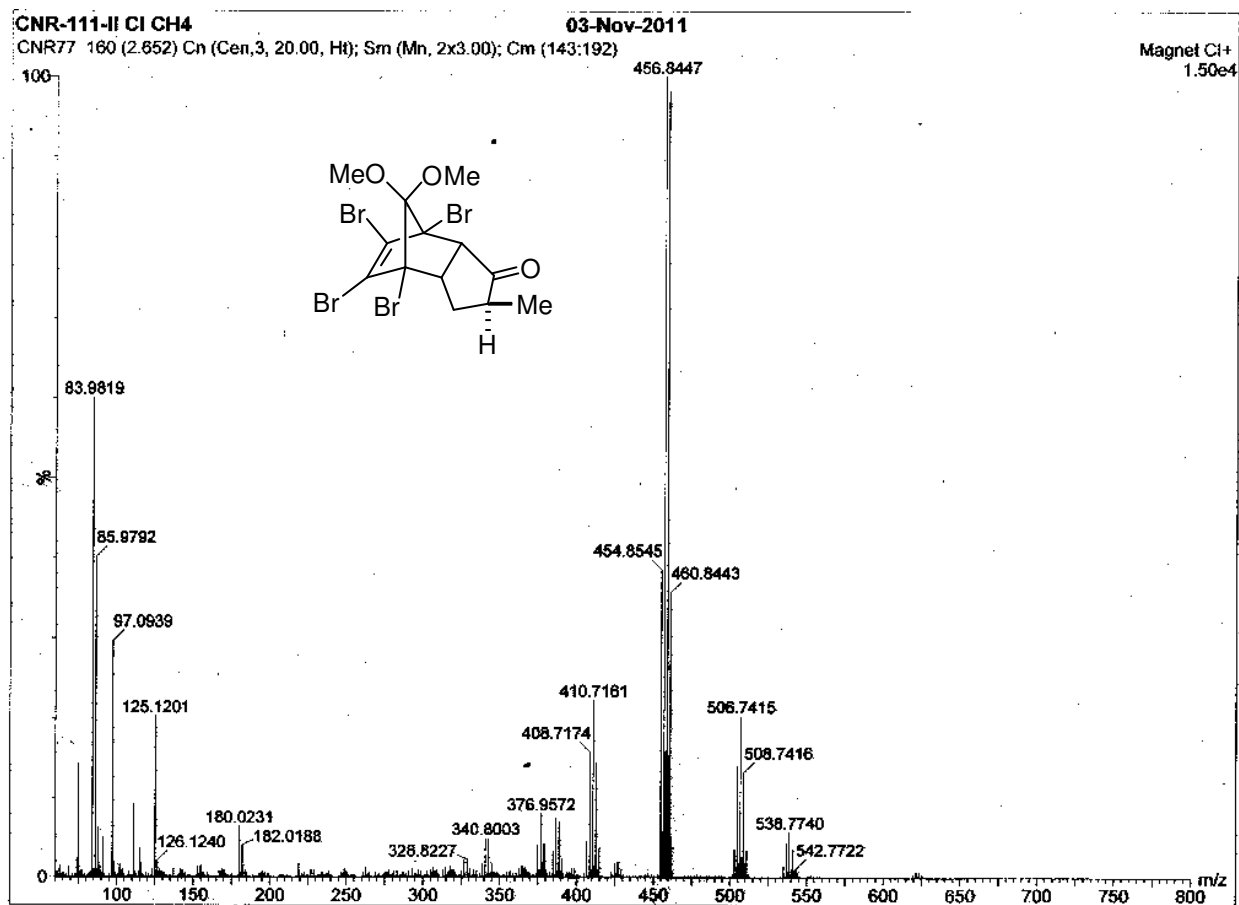
15-Nov-2011

CNR82 209 (3.465) Cn (Cen,3, 20.00, Ht); Sm (Mn, 2x3.00); Sm (Mn, 2x3.00); Cm (201:231)

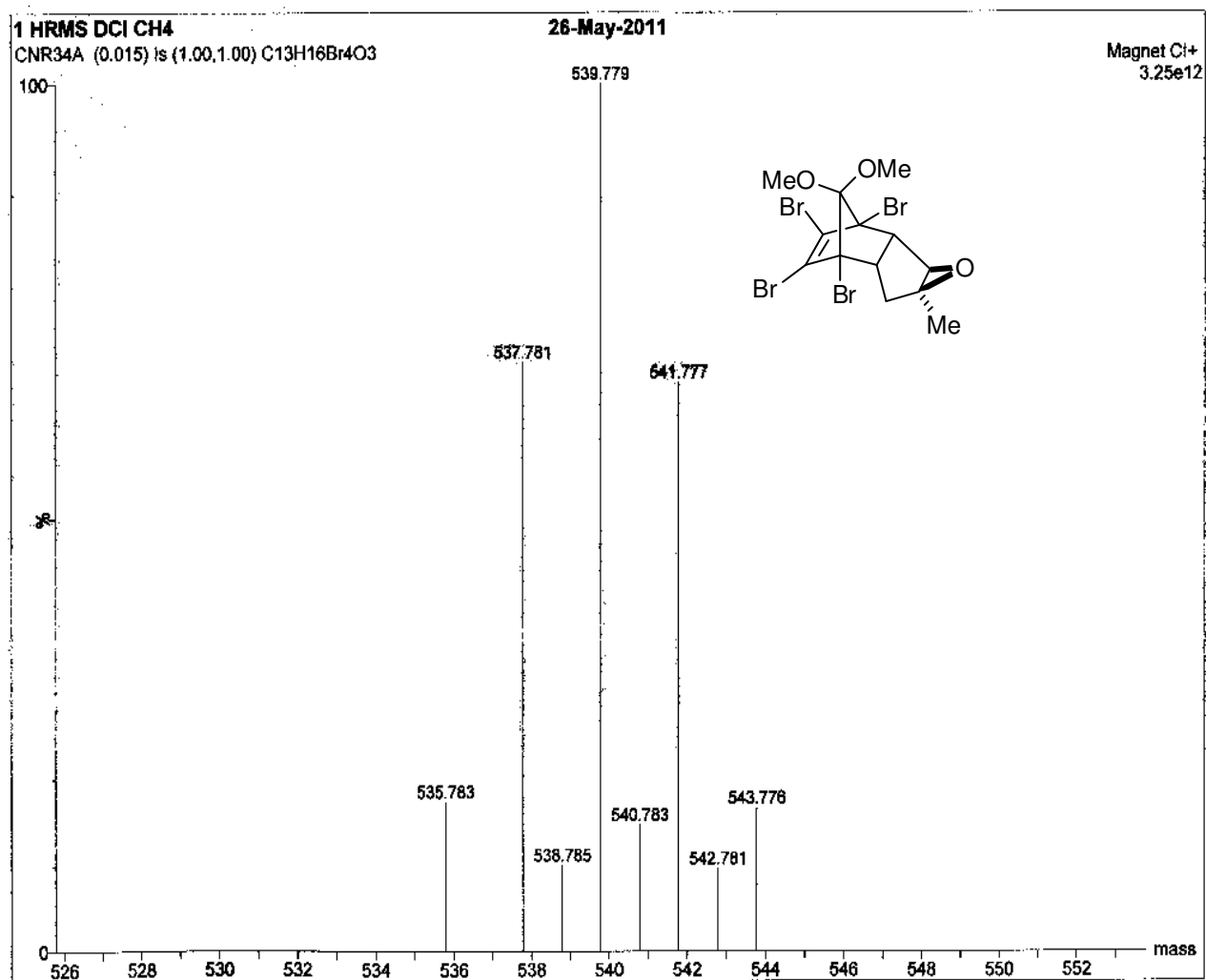
Magnet Cl+
8.26e3



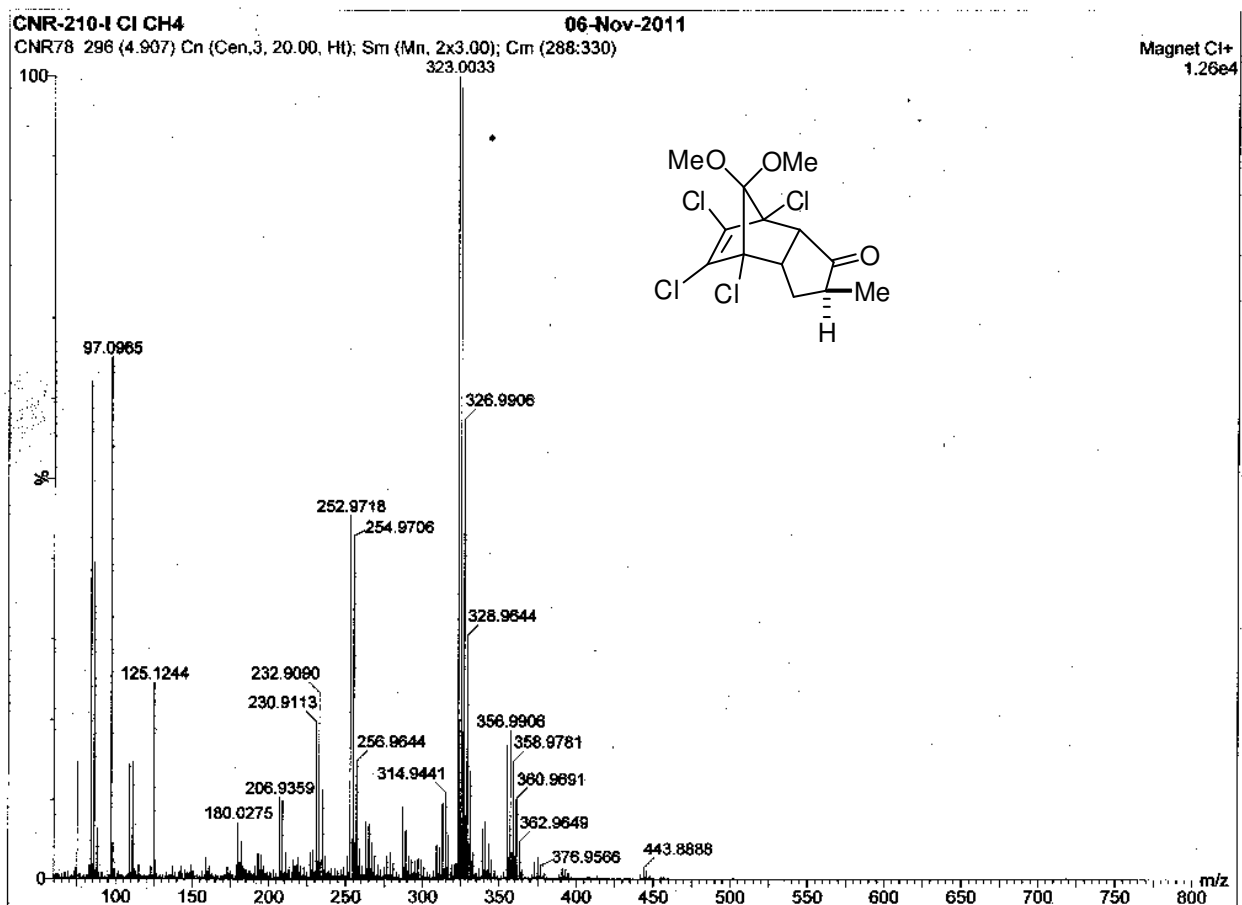
HRMS (DCI) of Compound 8



HRMS (DCI) of Compound 10



HRMS (DCI) of Compound 11



HRMS (ESI) of Compound 13

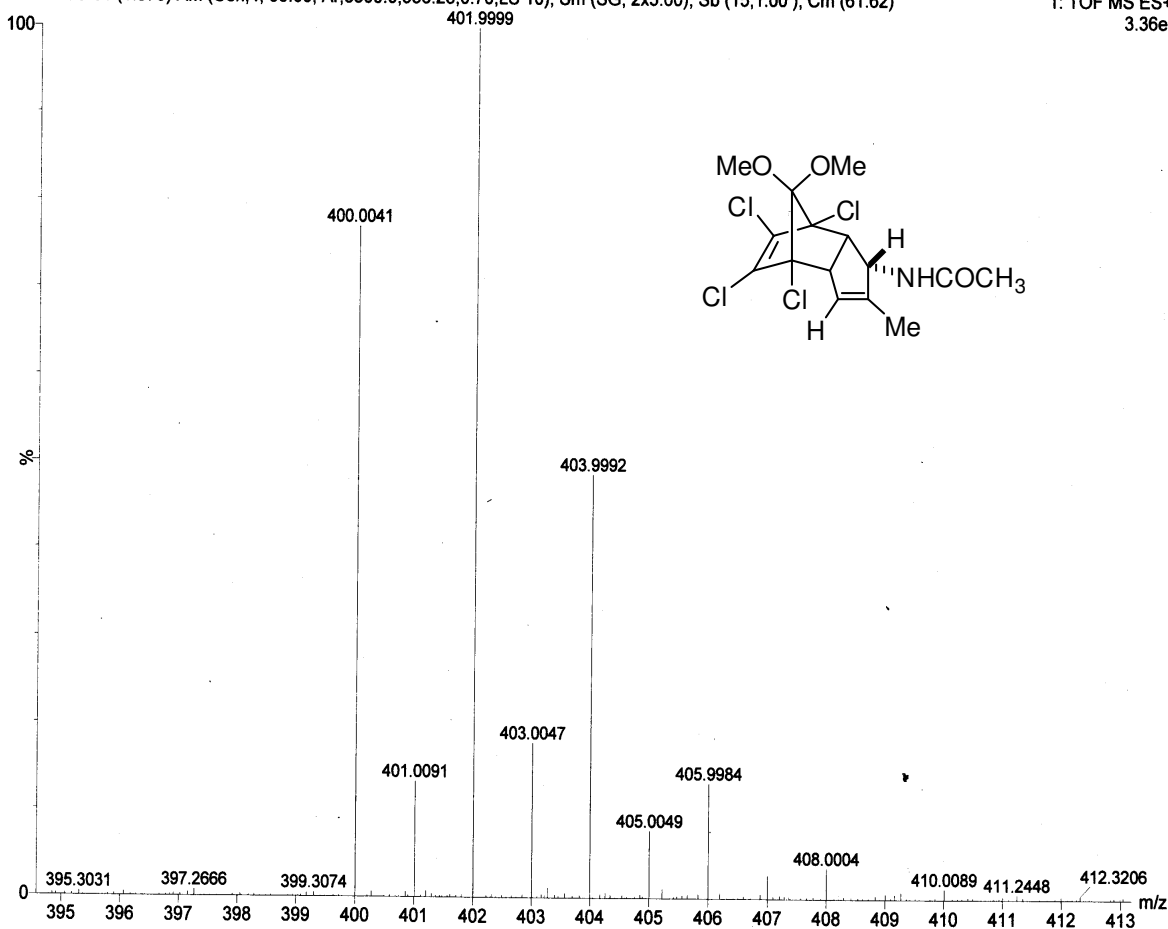
Electrospray ionisation-LC-MS

WATERS - HAB213

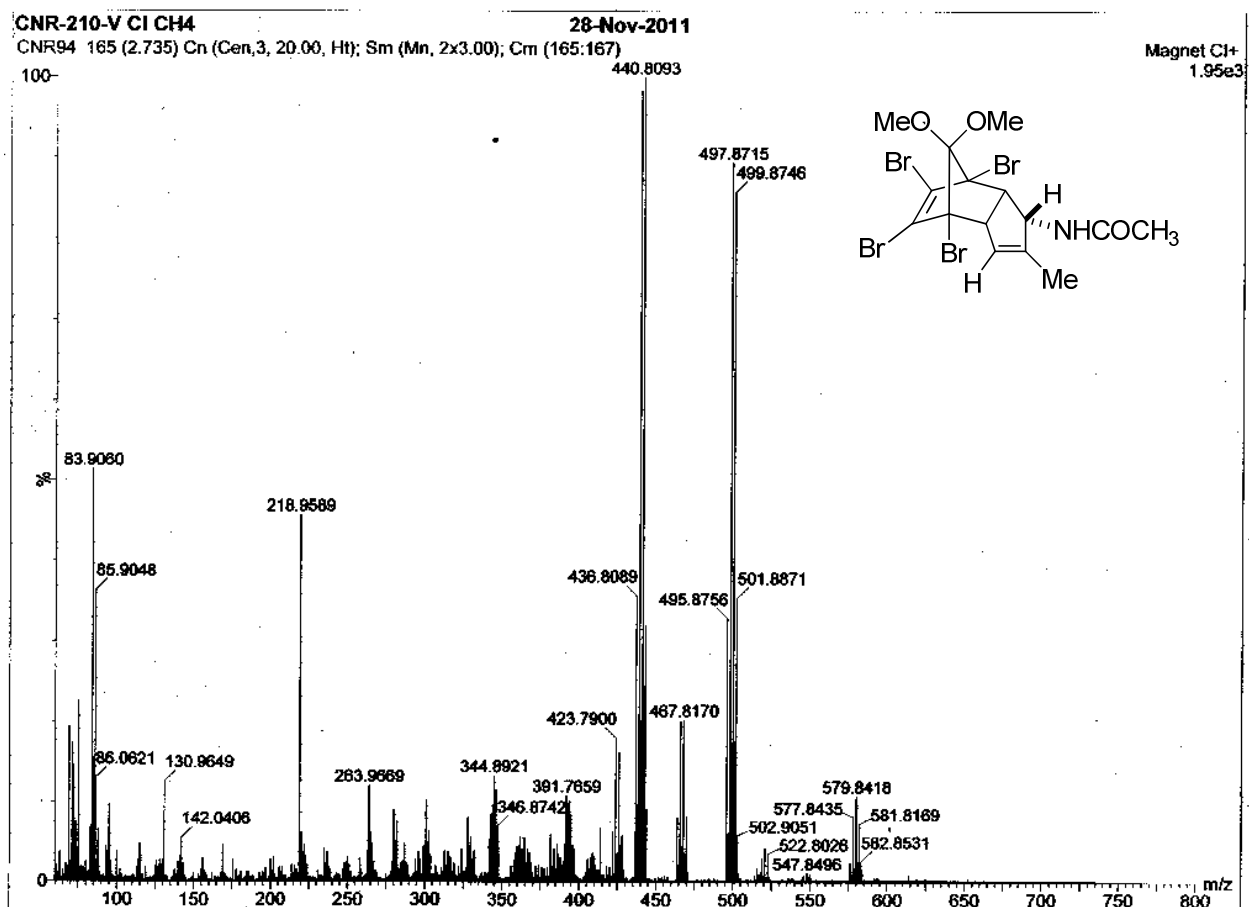
08-Apr-2008 12:15:09

CNR-433C 61 (1.379) AM (Cen, 4, 80.00, Ar, 8500.0, 556.28, 0.70, LS 10); Sm (SG, 2x5.00); Sb (15, 1.00); Cm (61:62)

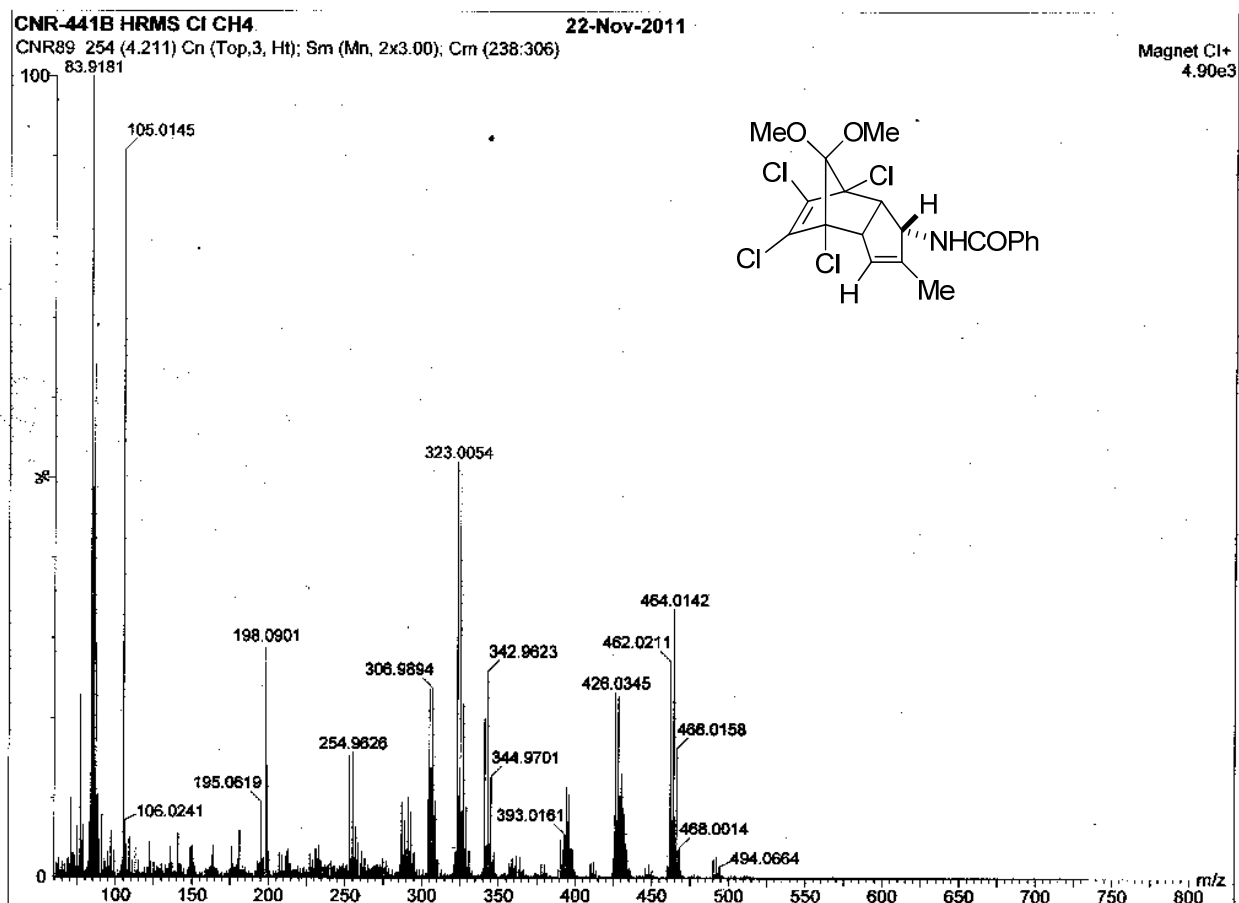
1: TOF MS ES+
3.36e3



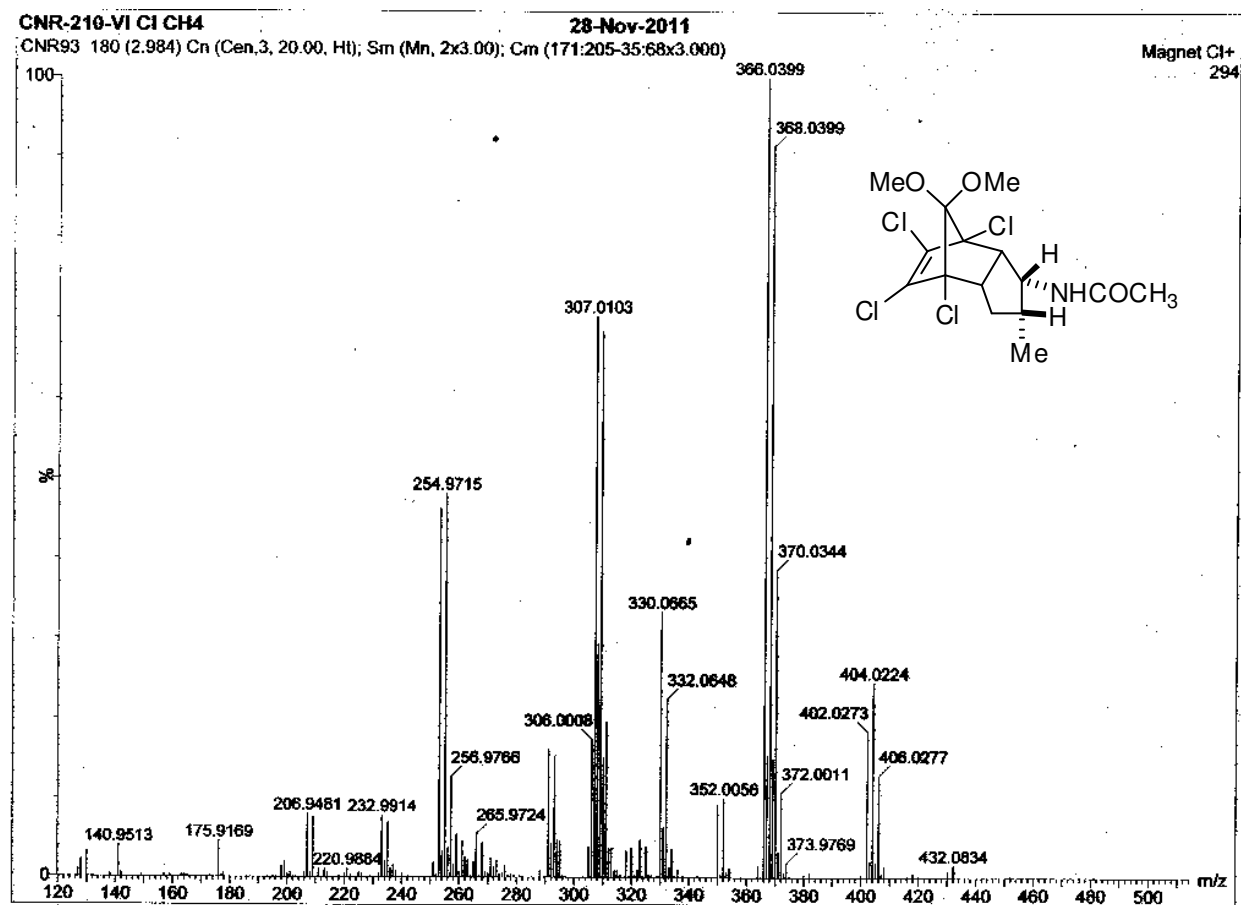
HRMS (DCI) of Compound 14



HRMS (DCI) of Compound 15



HRMS (DCI) of Compound 17



X-ray Ortep diagram of 5

