Supporting Information

SYNTHESIS, CONFORMATION, AND BIOLOGICAL ACTIVITIES OF A DES-A-RING ANALOG OF 18-DEOXY-APLOG-1, A SIMPLIFIED ANALOG OF DEBROMOAPLYSIATOXIN.

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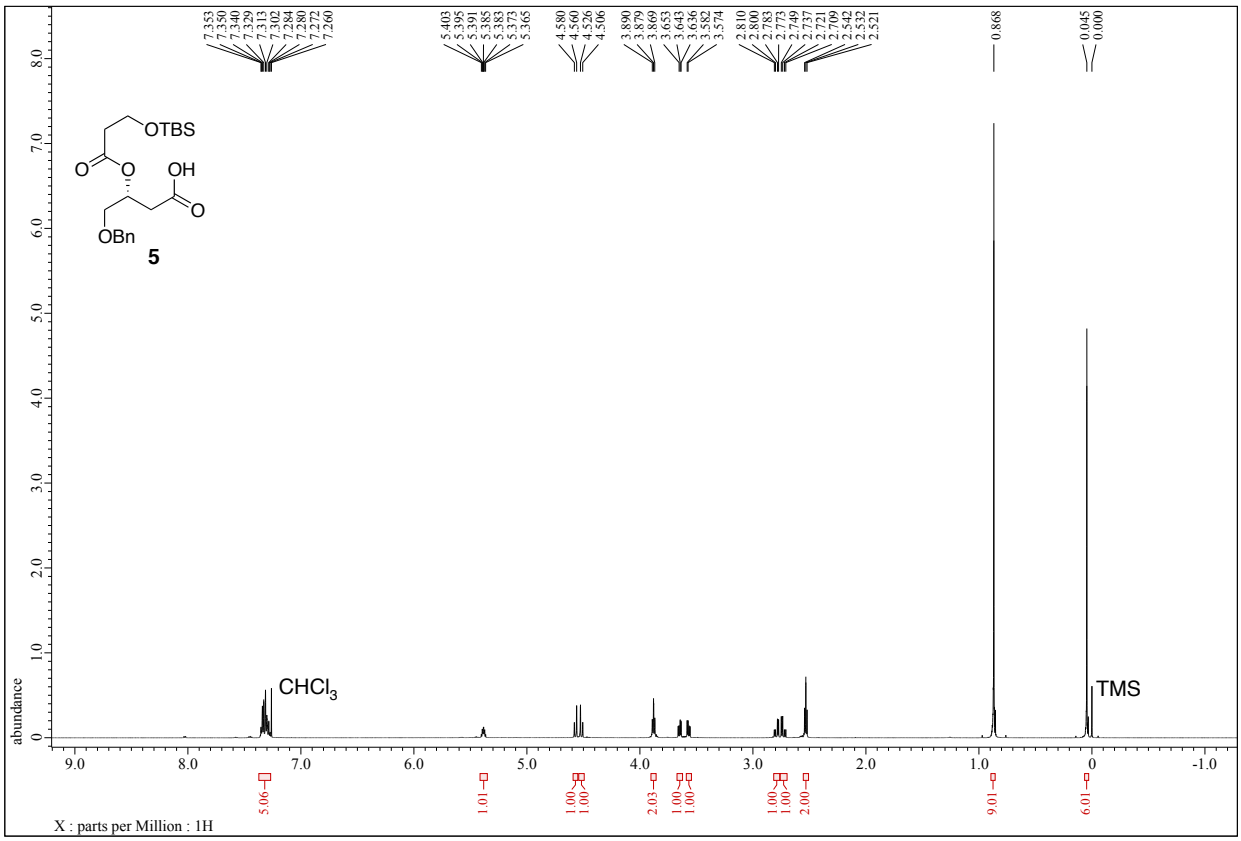
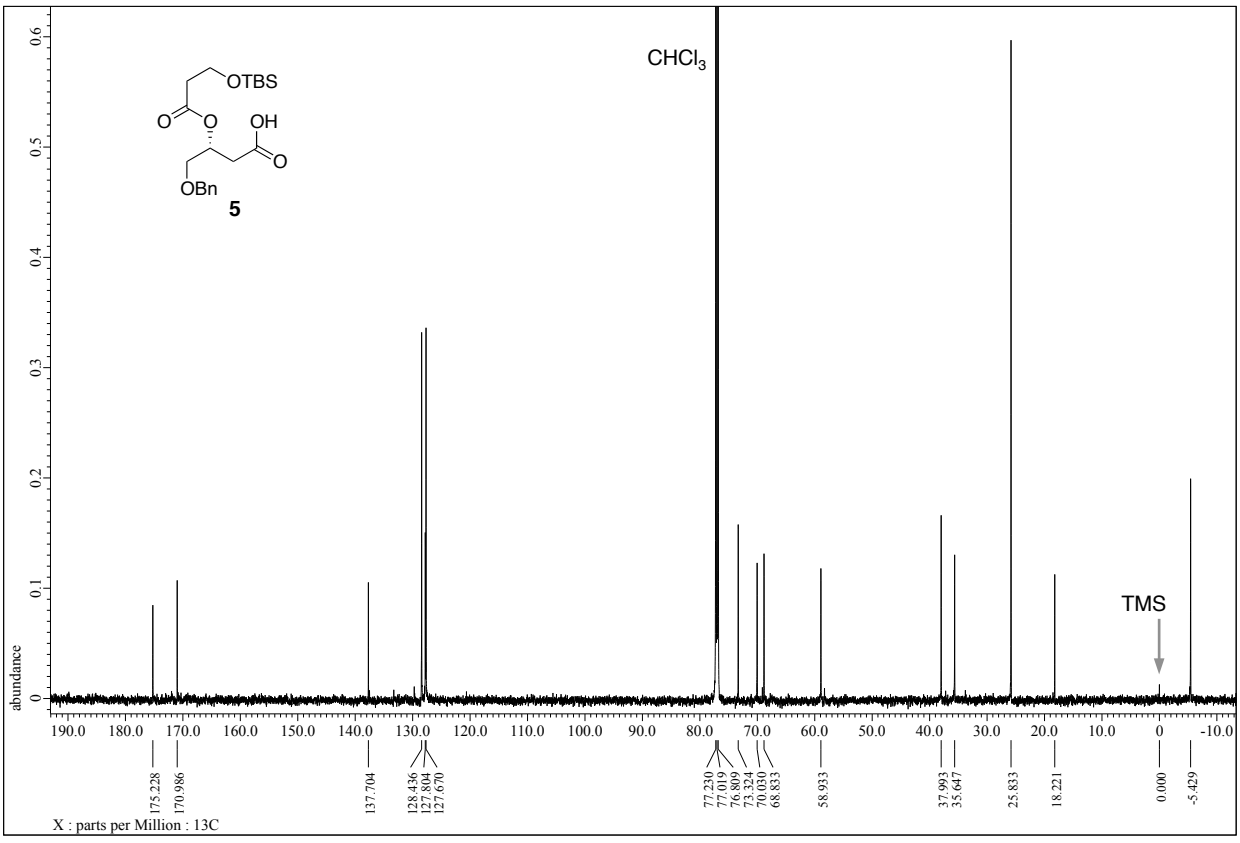
I. ^{1}H-1D and ^{13}C-1D NMR Spectra of 5, 6, 12, and 13

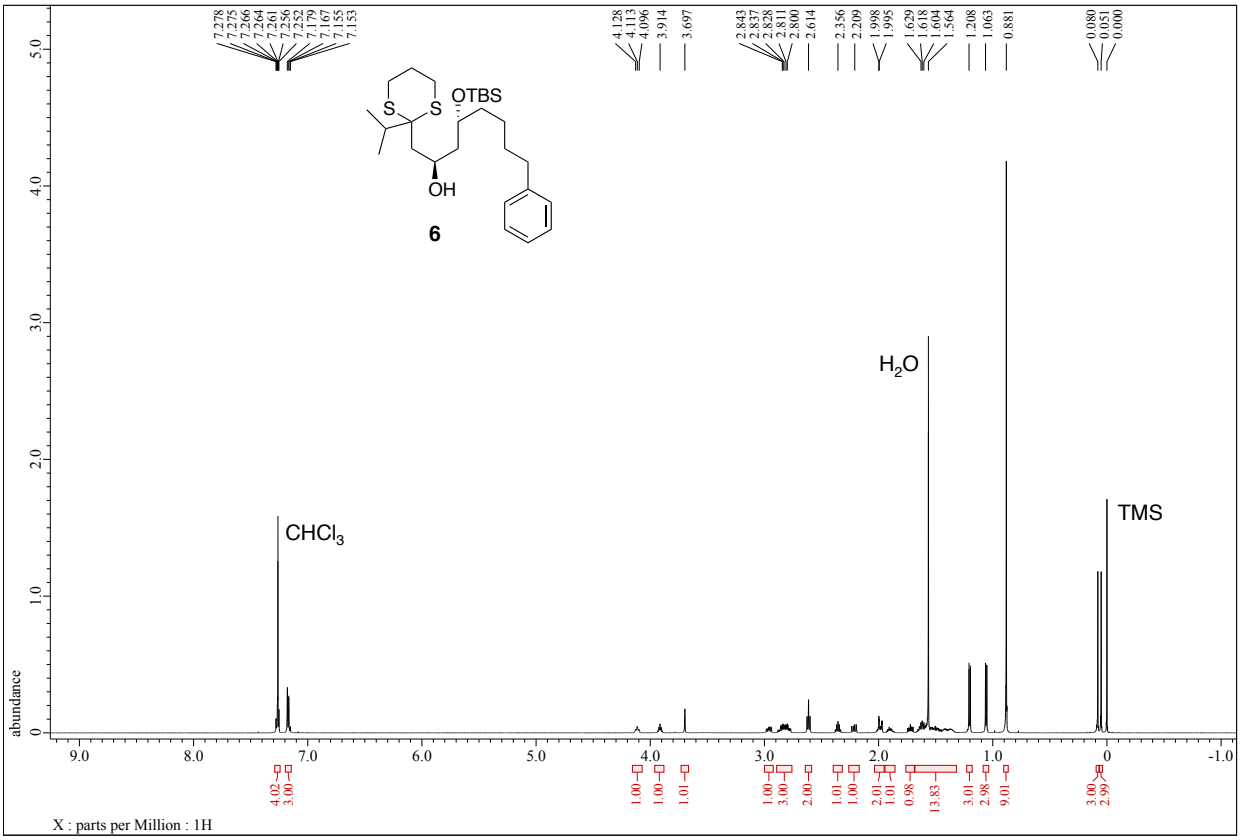
^{1}H-1D NMR spectrum of **5** (600 MHz, 297 K, CDC_3, 0.0484 M)



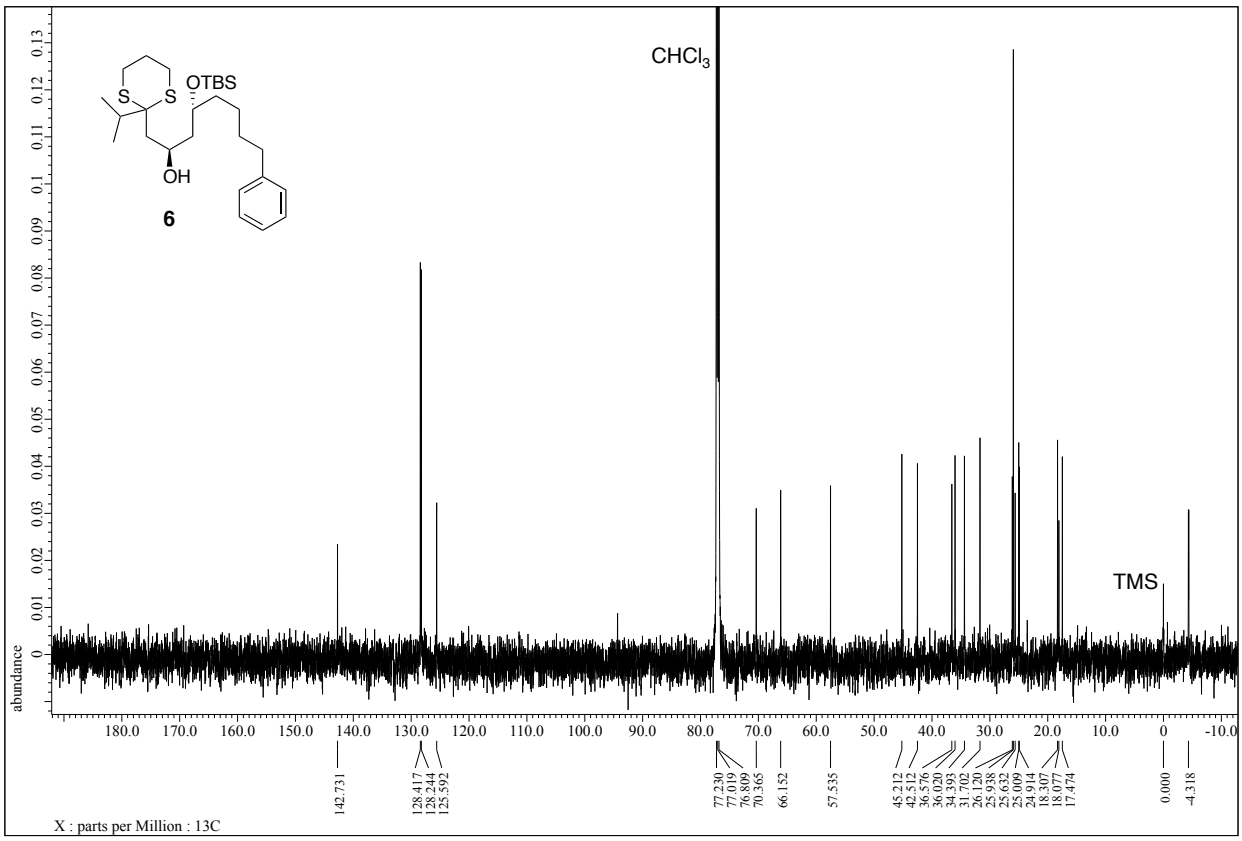
^{13}C-1D NMR spectrum of **5** ($CDCl_3$, 150 MHz, 298 K, 0.0484 M)



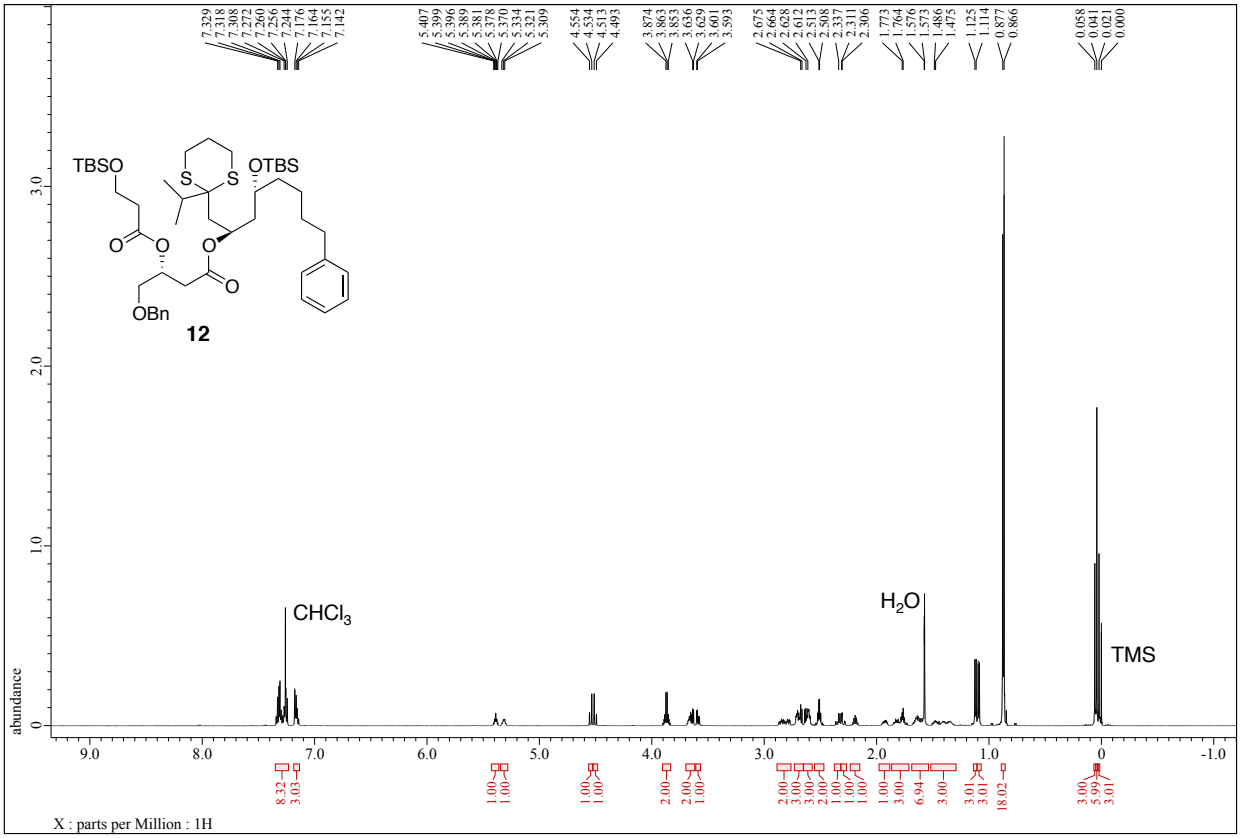
^{1}H-1D NMR spectrum of **6** (600 MHz, 297 K, $CDCl_3$, 0.0109 M)



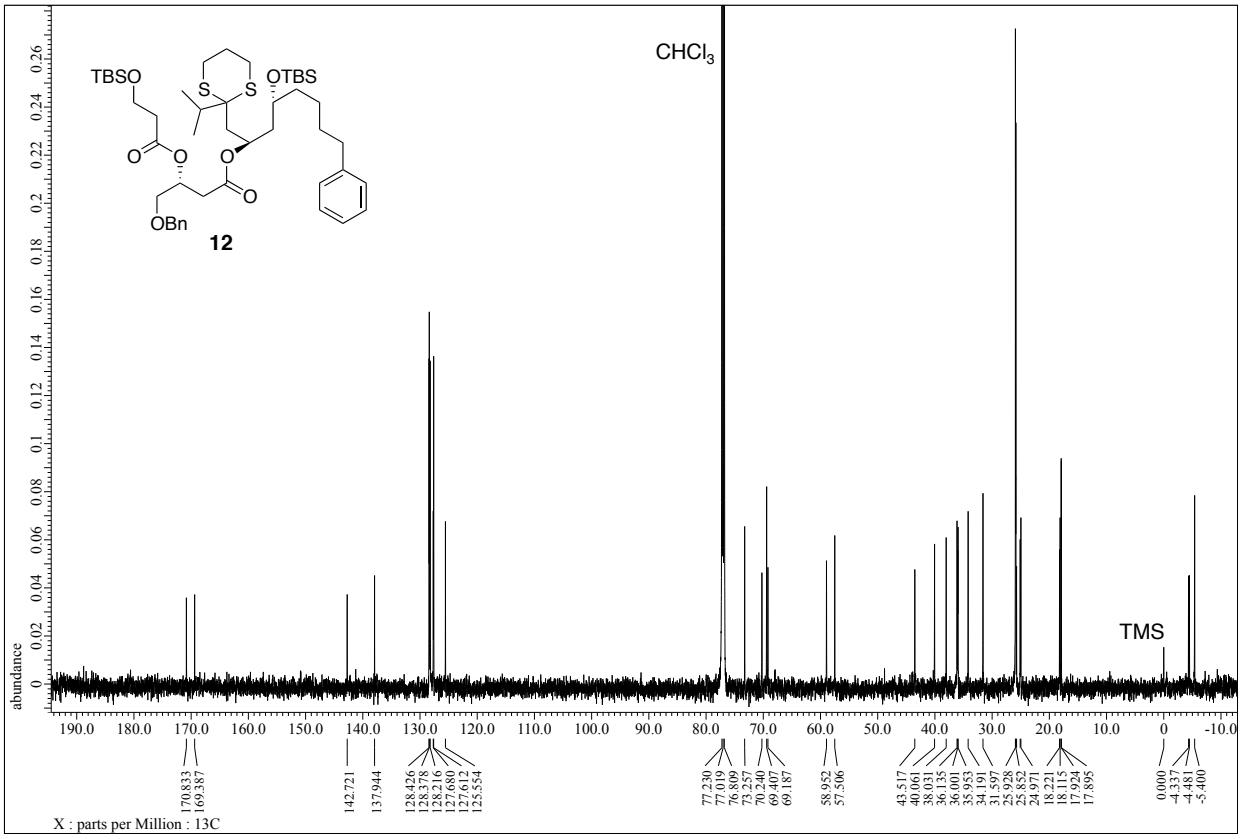
^{13}C-1D NMR spectrum of **6** (150 MHz, 298 K, $CDCl_3$, 0.0109 M)



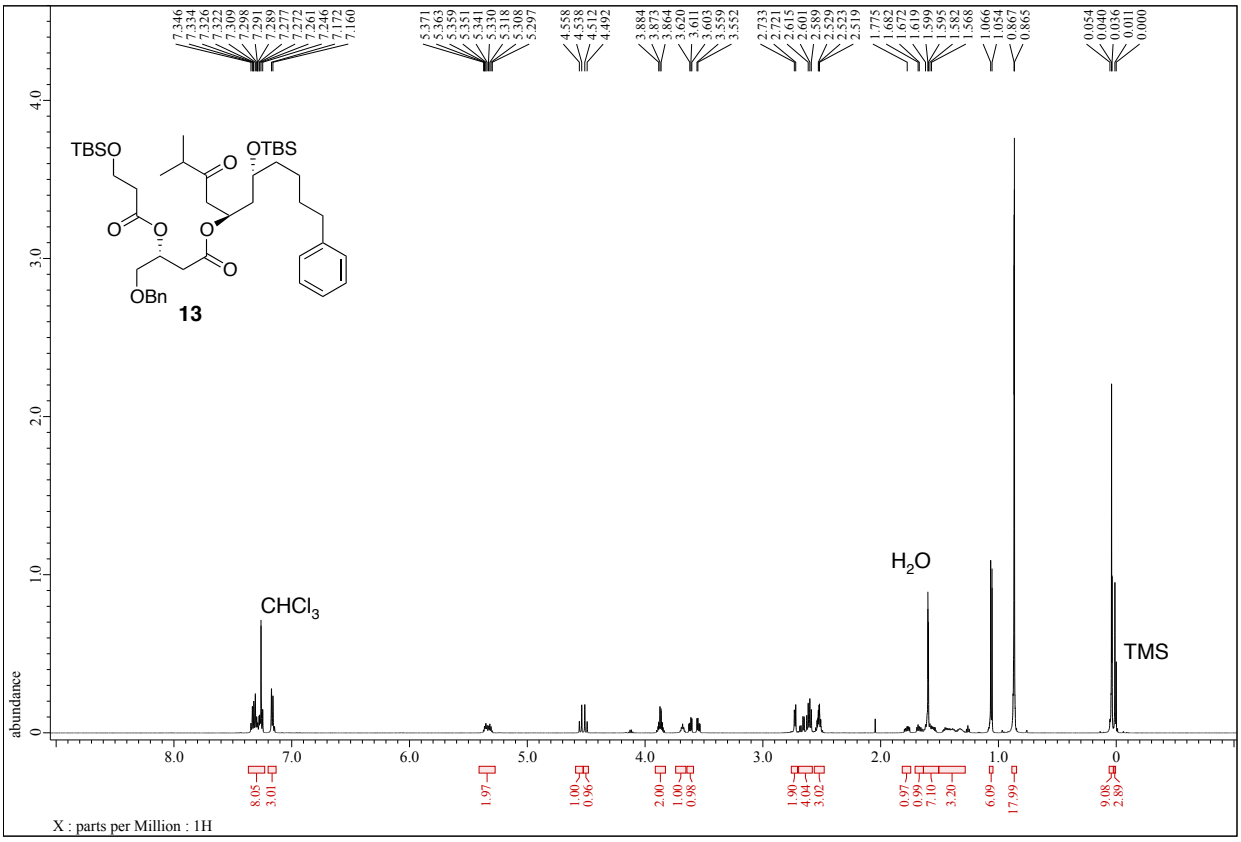
^{1}H-1D NMR spectrum of **12** (600 MHz, 297 K, $CDCl_3$, 0.0192 M)



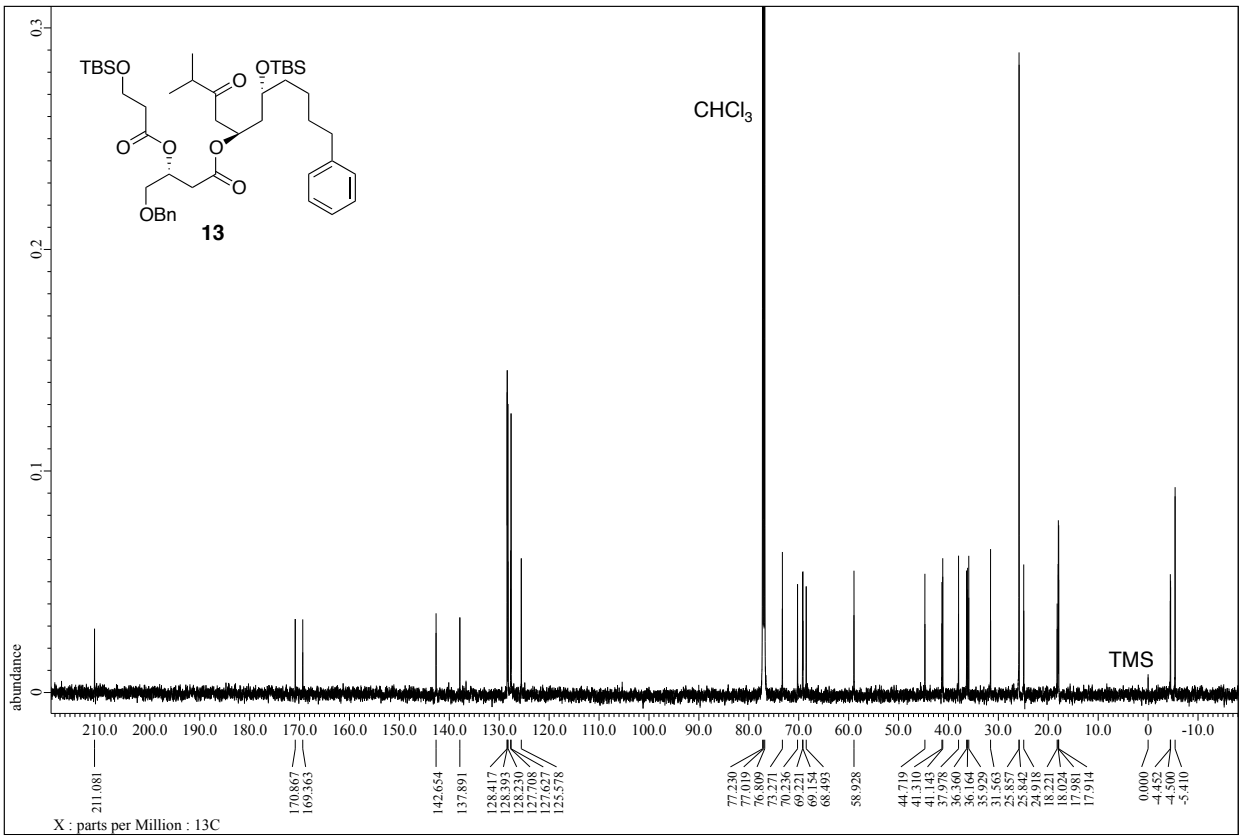
^{13}C-1D NMR spectrum of **12** (150 MHz, 298 K, $CDCl_3$, 0.0192 M)



^{1}H-1D NMR spectrum of **13** (600 MHz, 296 K, $CDCl_3$, 0.0229 M)

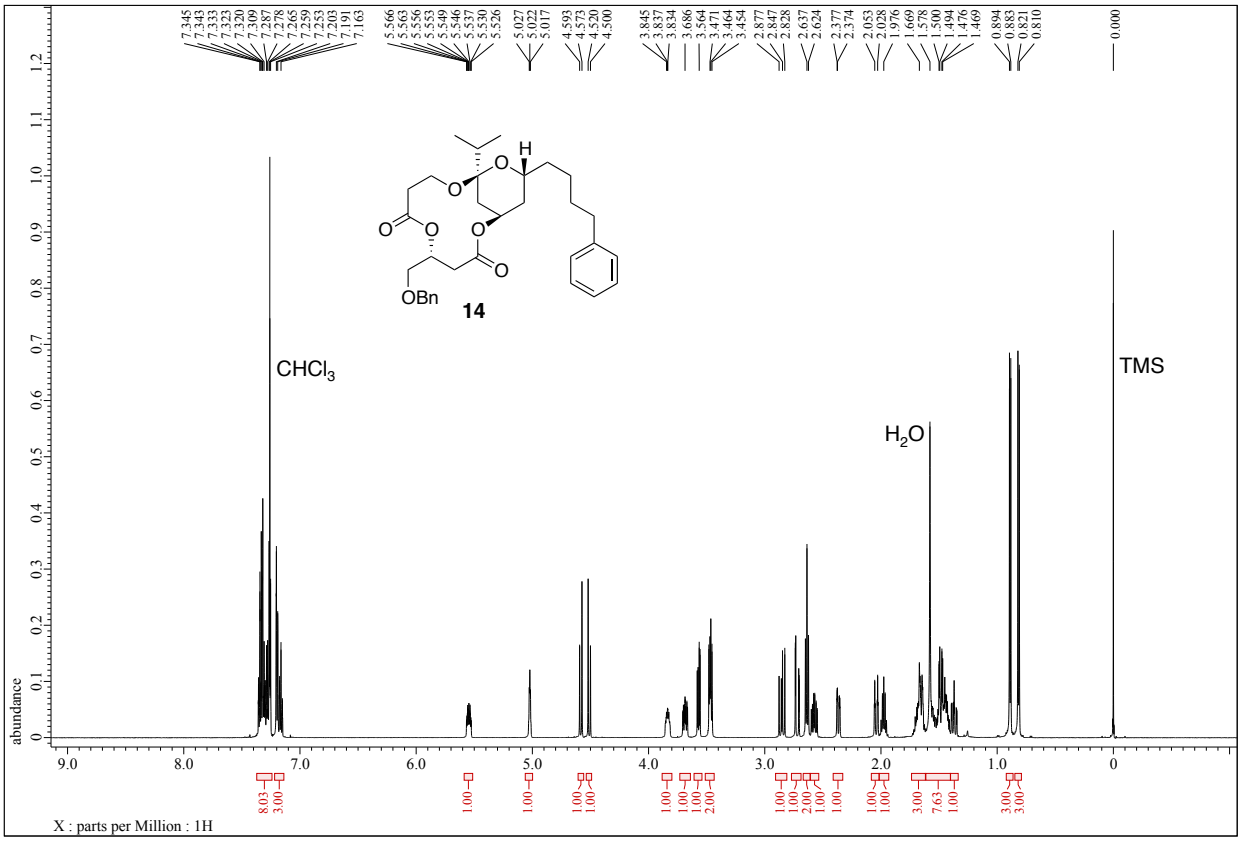


^{13}C-1D NMR spectrum of **13** (150 MHz, 297 K, $CDCl_3$, 0.0229 M)

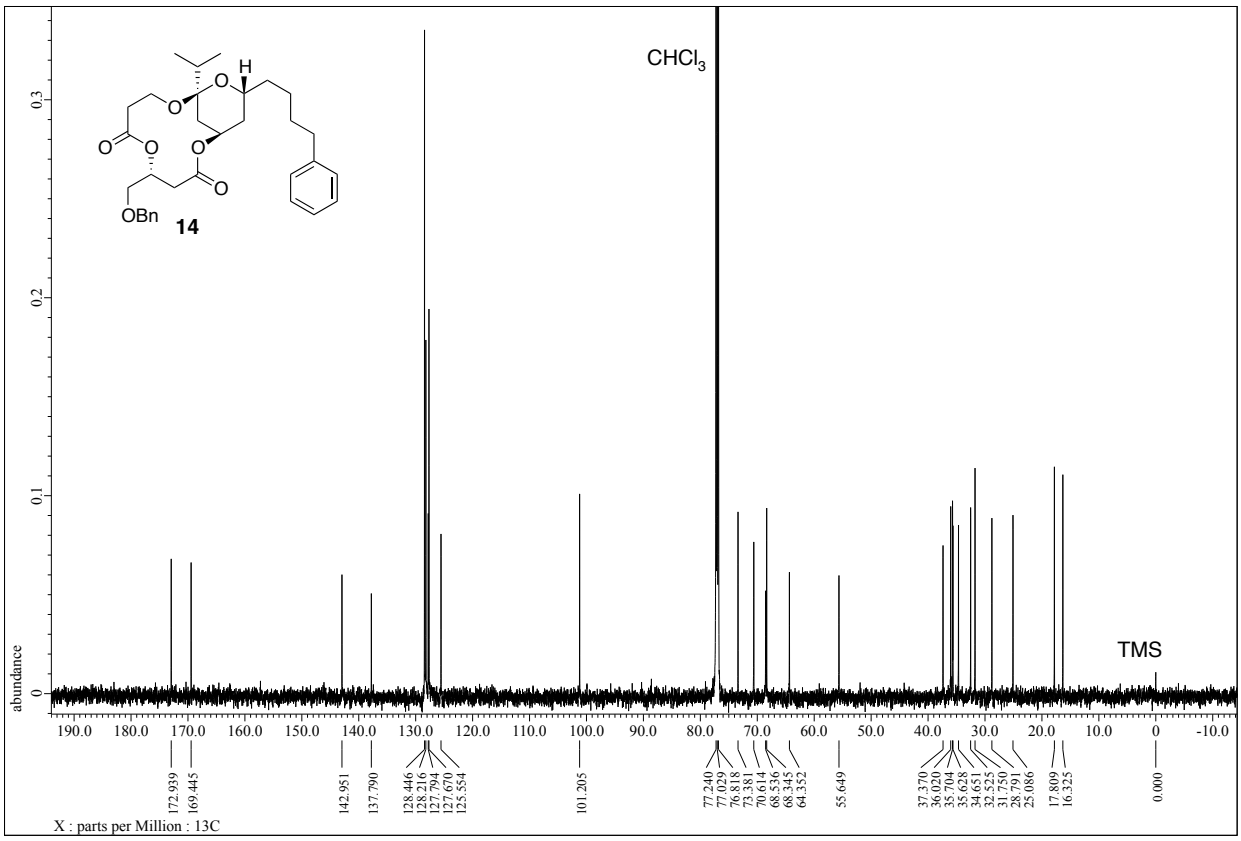


II. ^{1}H-1D, ^{13}C-1D, COSY, and NOESY Spectrum of 14 and 4

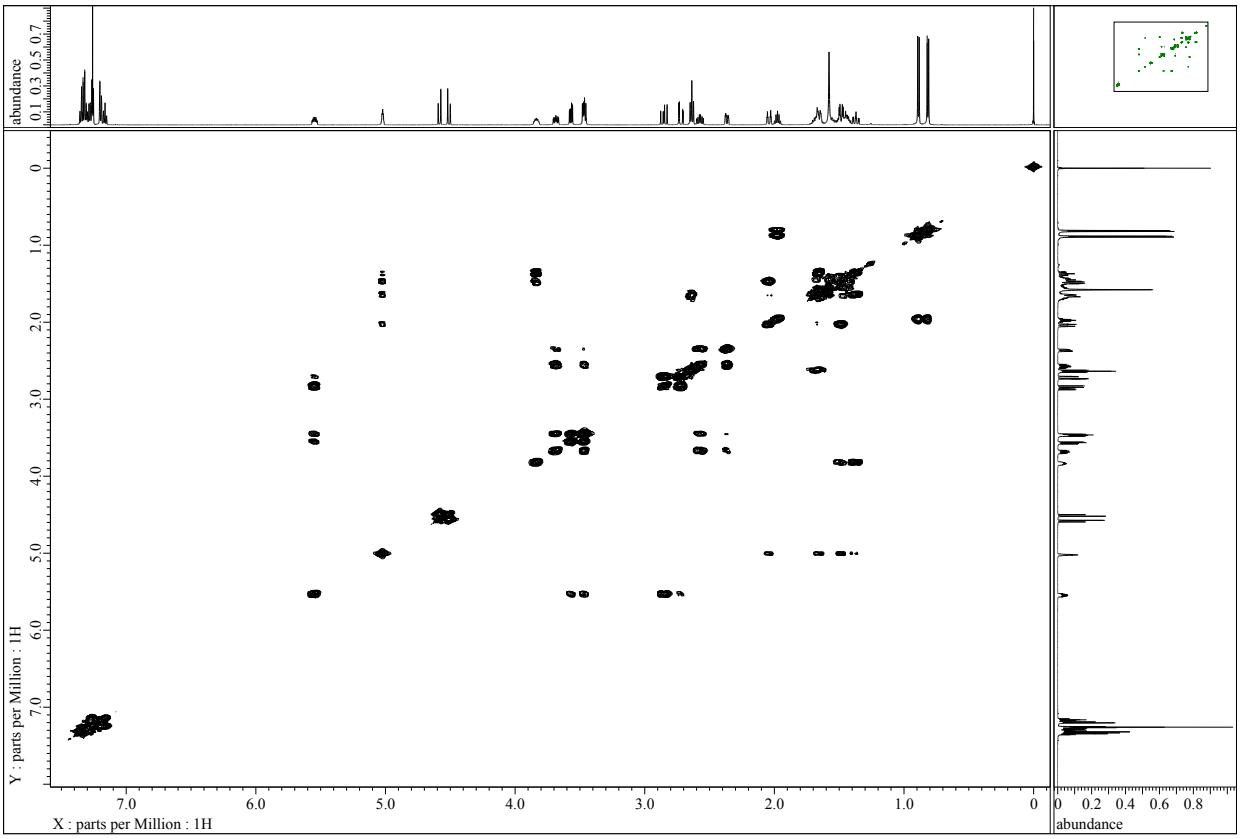
^{1}H-1D NMR spectrum of **14** (600 MHz, 297 K, $CDCl_3$, 0.0249 M)



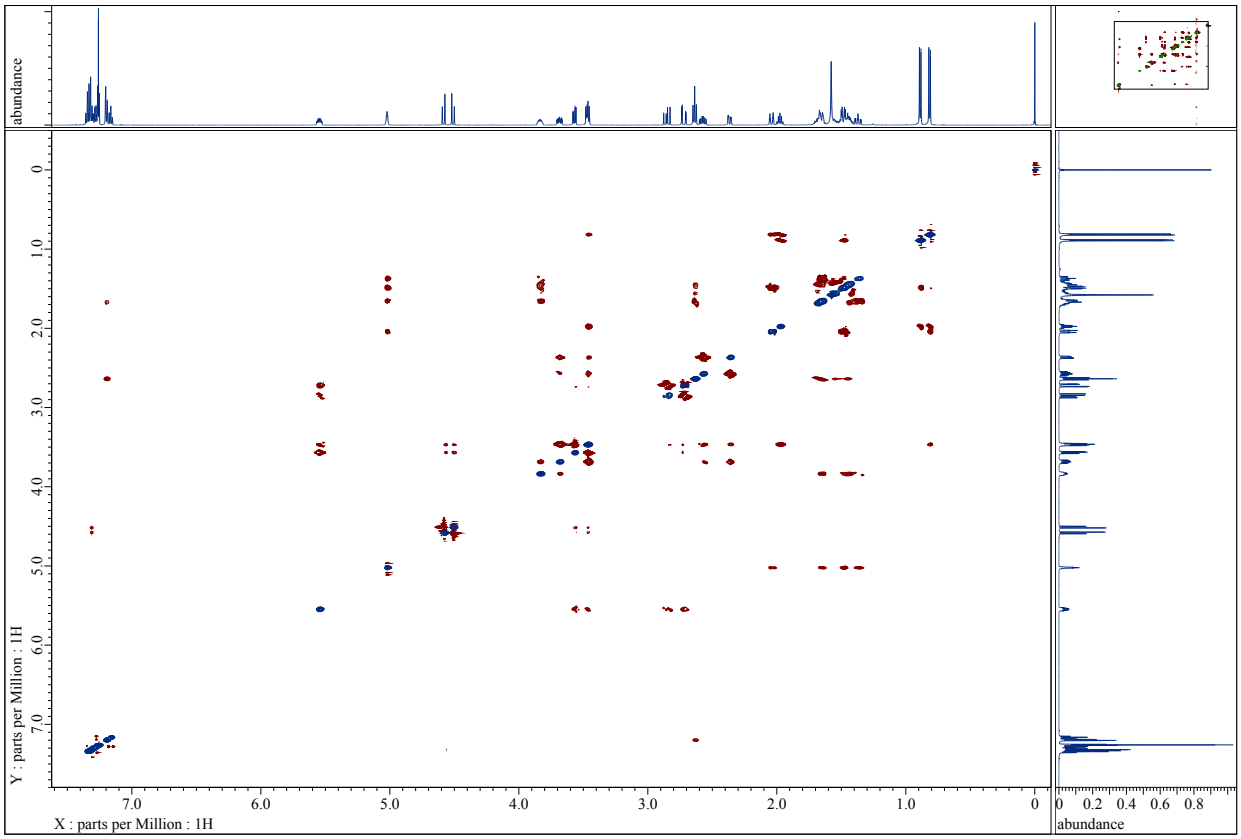
^{13}C-1D NMR spectrum of **14** (150 MHz, 298 K, $CDCl_3$, 0.0249 M)



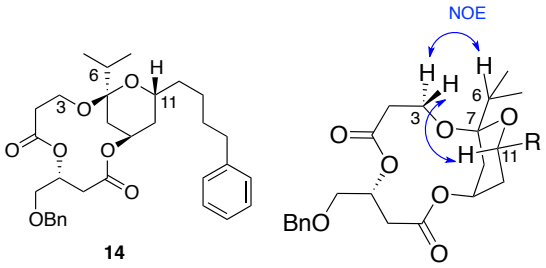
COSY spectrum of **14** (600 MHz, 297 K, $CDCl_3$, 0.0249 M)

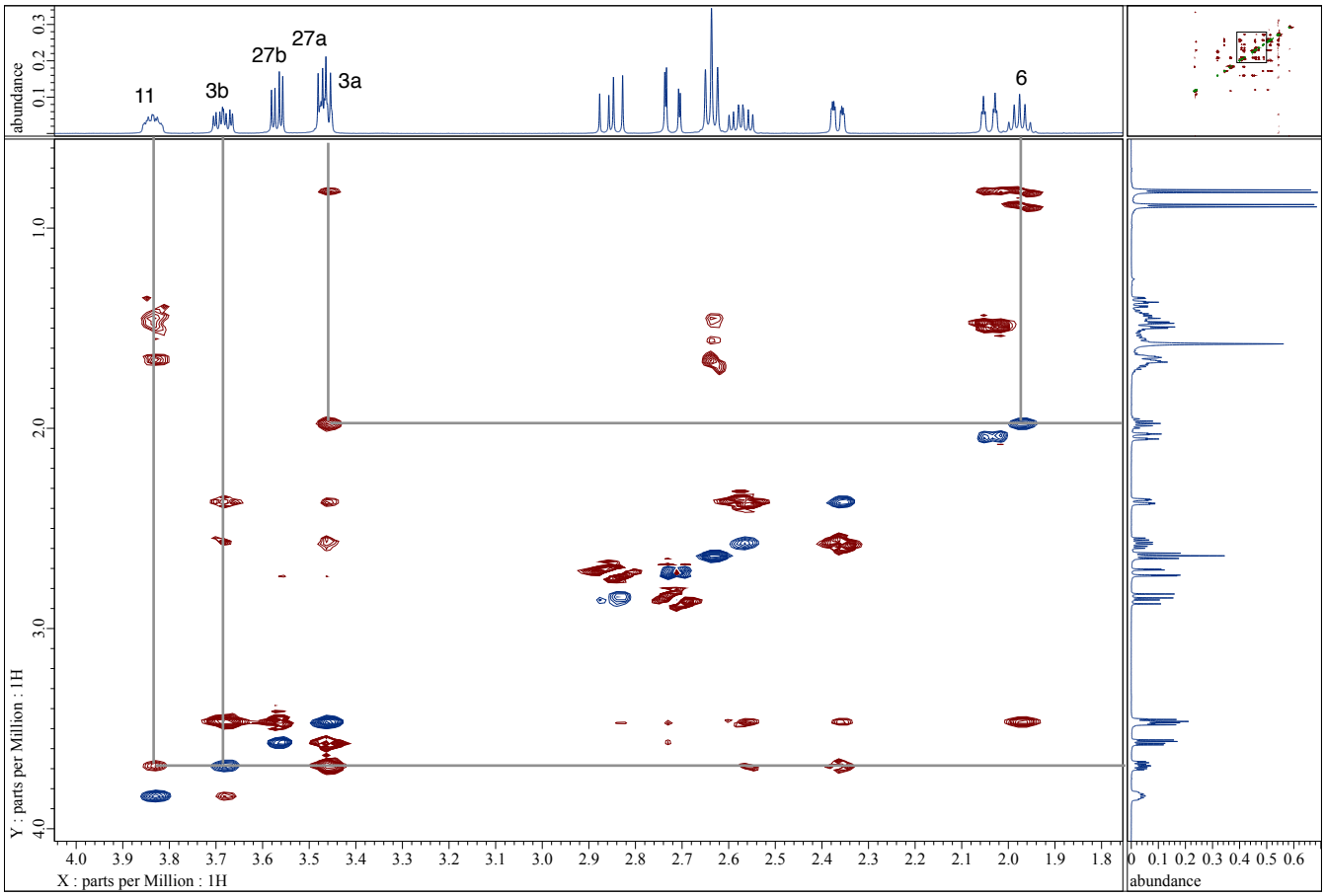


NOESY spectrum of **14** (600 MHz, 297 K, $CDCl_3$, 0.0249 M, mixing time: 0.5 s)

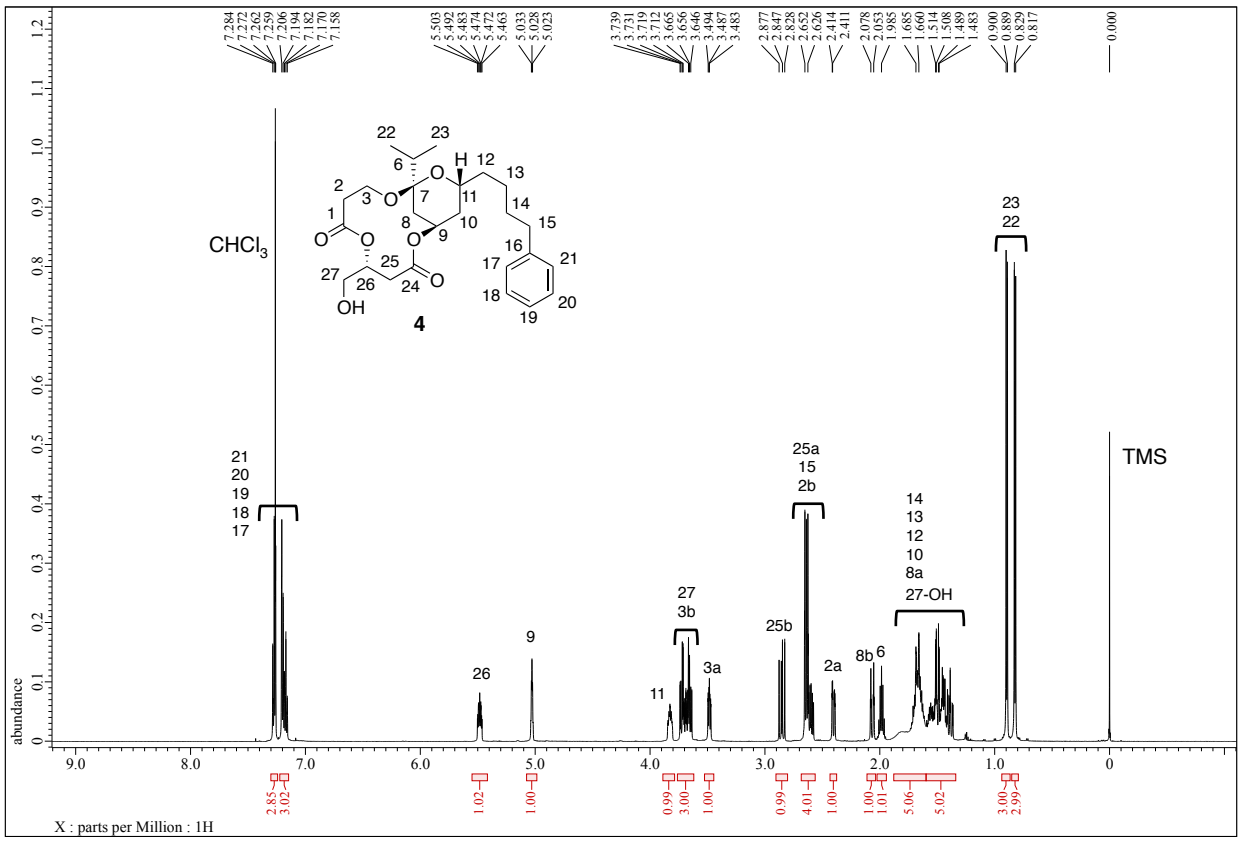


NOESY spectrum of **14** (600 MHz, 297 K, $CDCl_3$, 0.0249 M) (expanded)

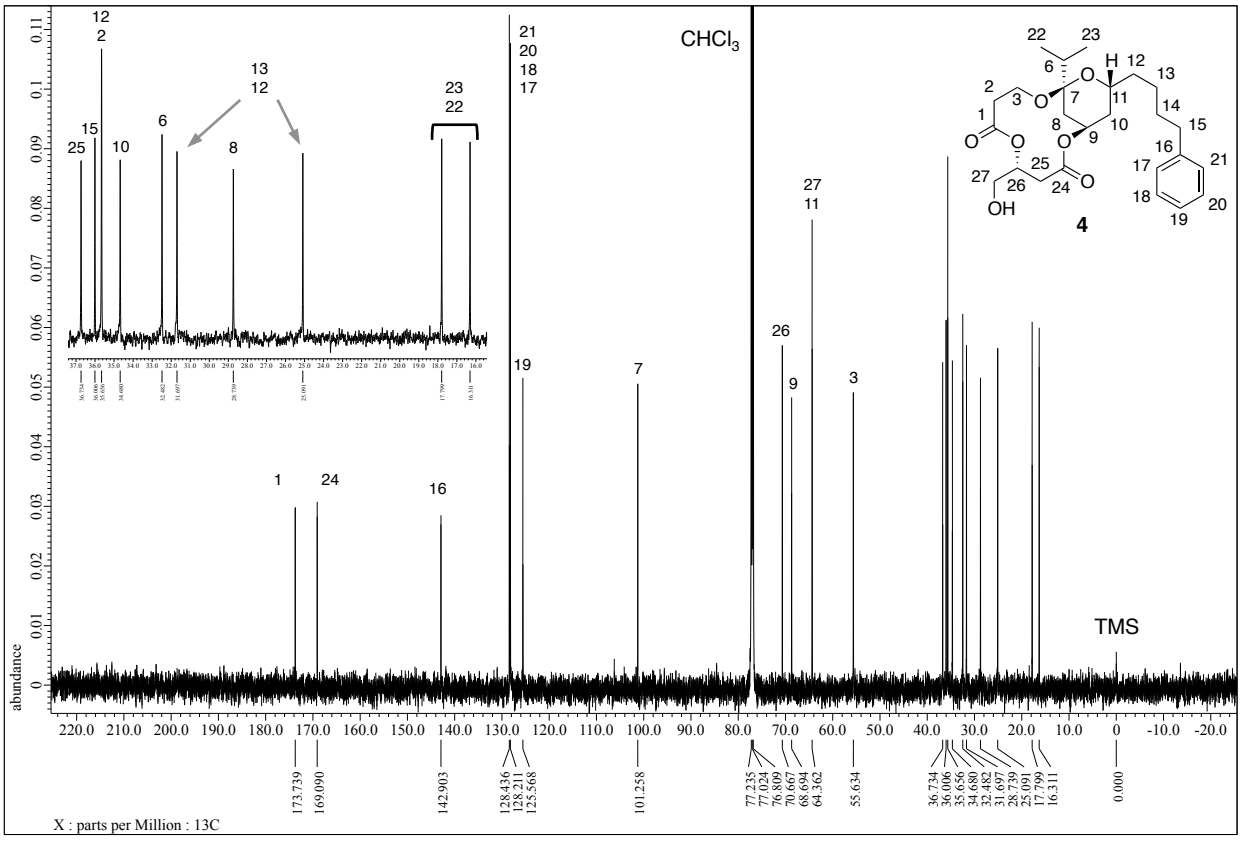




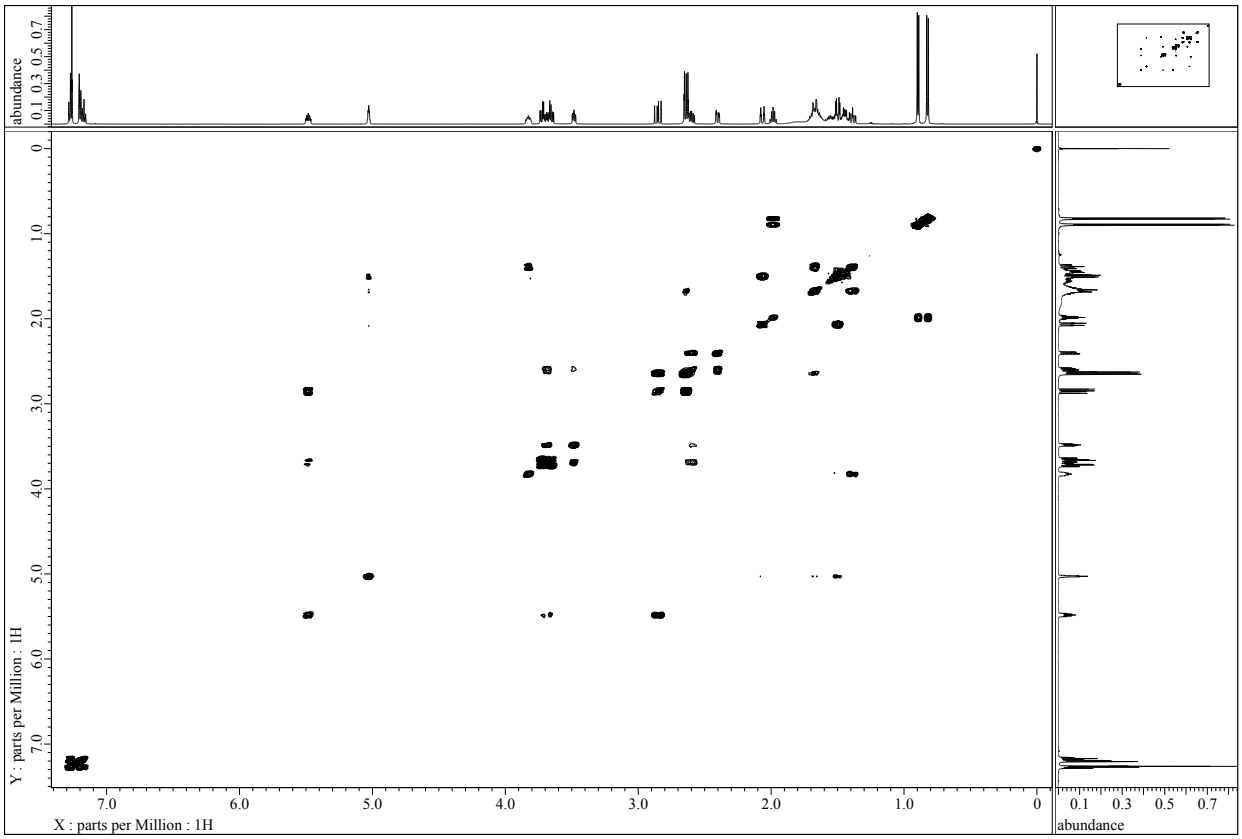
^{1}H-1D NMR spectrum of **4** (600 MHz, 296 K, $CDCl_3$, 0.0268 M)



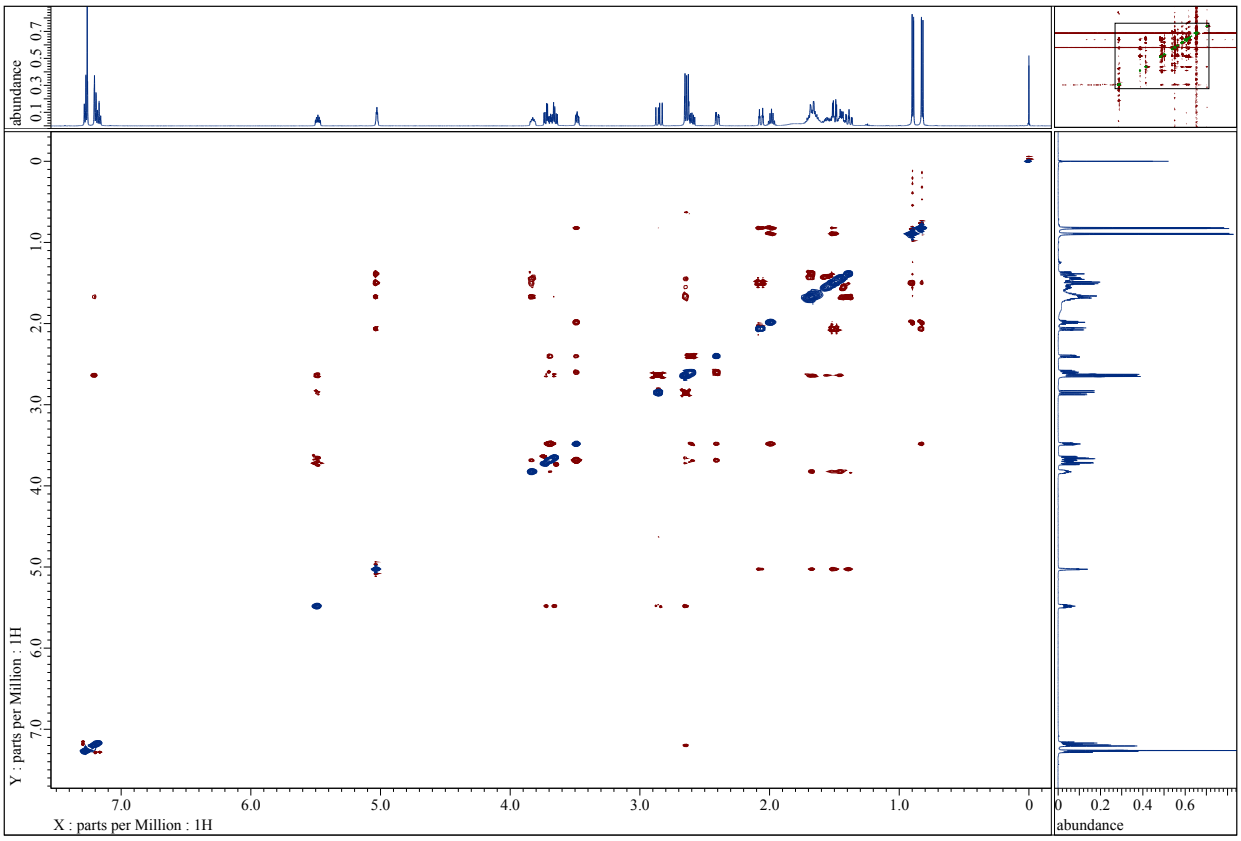
^{13}C-1D NMR spectrum of **4** (150 MHz, 297 K, $CDCl_3$, 0.0268 M)



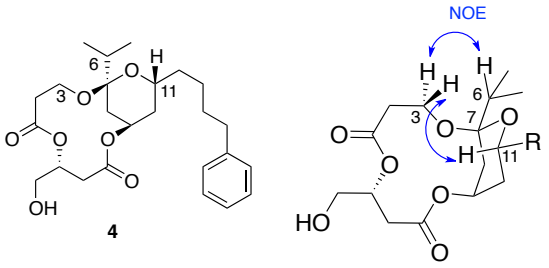
COSY spectrum of **4** (600 MHz, 296 K, $CDCl_3$, 0.0268 M)



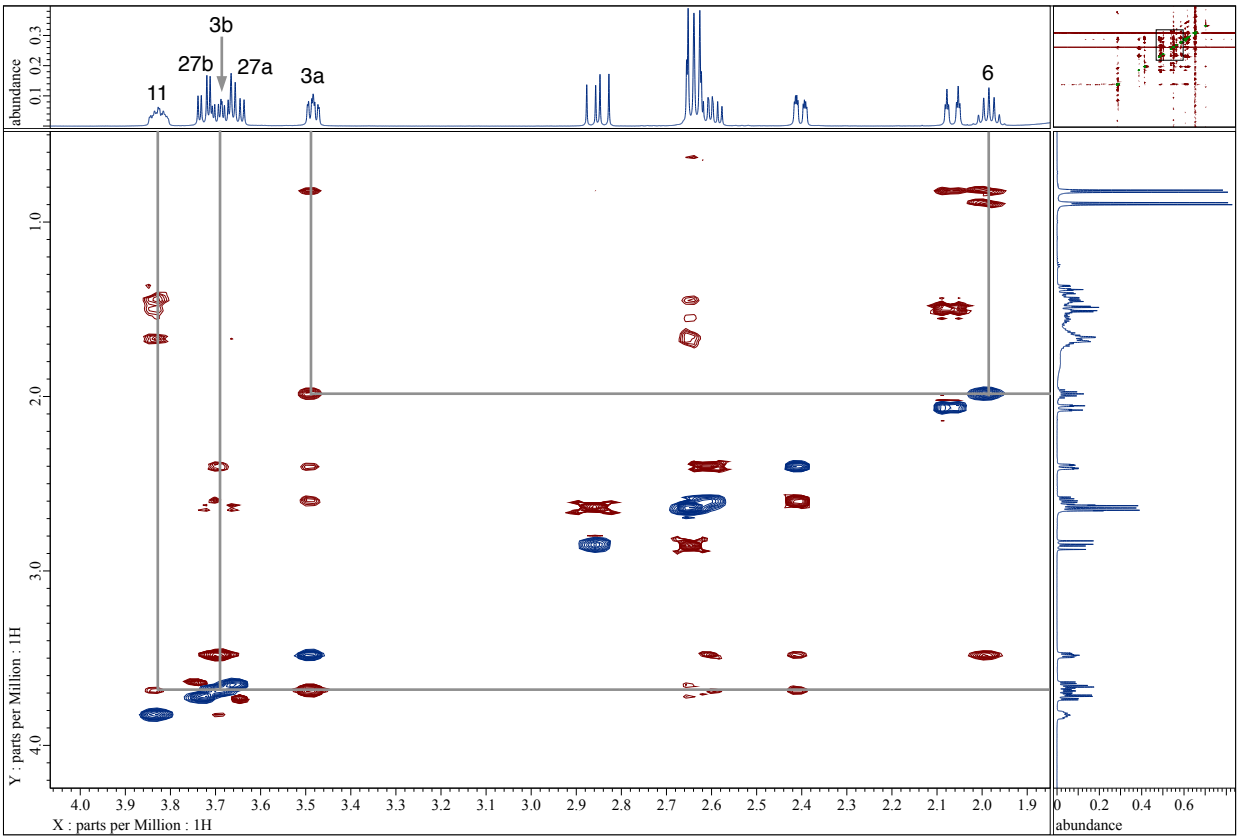
NOESY spectrum of **4** (600 MHz, 296 K, $CDCl_3$, 0.0268 M, mixing time: 0.5 s)



NOESY spectrum of **4** (600 MHz, 296 K, $CDCl_3$, 0.0268 M) (expanded)



4



III. Growth Inhibitory Activity of 4 and 18-deoxy-aplog-1 for 39 human cancer cell lines

		GI_{50} (M)	
Cancer type	Cell line	**4**	18-Deoxy-aplog-1[a]
Breast	HBC-4	−4.98	−6.28
	BSY-1	−4.78	−5.17
	HBC-5	−4.75	−4.81
	MCF-7	−4.72	−4.79
	MDA-MB-231	−4.90	−5.67
CNS	U251	−4.72	−4.91
	SF-268	−4.74	−4.89
	SF-295	−4.94	−5.14
	SF-539	−4.87	−4.98
	SNB-75	−4.81	−4.92
	SNB-78	−4.70	−4.80
Colon	HCC2998	−4.86	−5.53
	KM-12	−4.72	−5.04
	HT-29	−4.77	−4.95
	HCT-15	−4.69	−4.78
	HCT-116	−4.73	−4.91
Lung	NCI-H23	−4.83	−4.95
	NCI-H226	−4.77	−4.94
	NCI-H522	−4.73	−4.88
	NCI-H460	−5.53	−5.83
	A549	−4.92	−5.49
	DMS273	−4.89	−4.98
	DMS114	−4.77	−4.85
Melanoma	LOX-IMVI	−4.99	−5.17
Ovarian	OVCAR-3	−4.67	−4.87
	OVCAR-4	−4.68	−4.82
	OVCAR-5	−4.75	−4.96
	OVCAR-8	−4.69	−4.75
	SK-OV-3	−4.78	−4.77
Renal	RXF-631L	−4.72	−4.86
	ACHN	−4.78	−5.00
Stomach	St-4	−4.87	−6.05
	MKN1	−4.81	−4.90
	MKN7	−4.74	−4.94
	MKN28	−4.76	−4.78
	MKN45	−5.21	−6.09
	MKN74	−4.79	−4.83
Prostate	DU-145	−4.78	−4.92
	PC-3	−4.85	−5.26
MG-MID[b]		−4.82	−5.09

[a] R. C. Yanagita, H. Kamachi, K. Tanaka, A. Murakami, Y. Nakagawa, H. Tokuda, H. Nagai, and K. Irie, *Bioorg. Med. Chem. Lett.*, 2010, **20**, 6064.

[b] Full panel mean-graph midpoint