

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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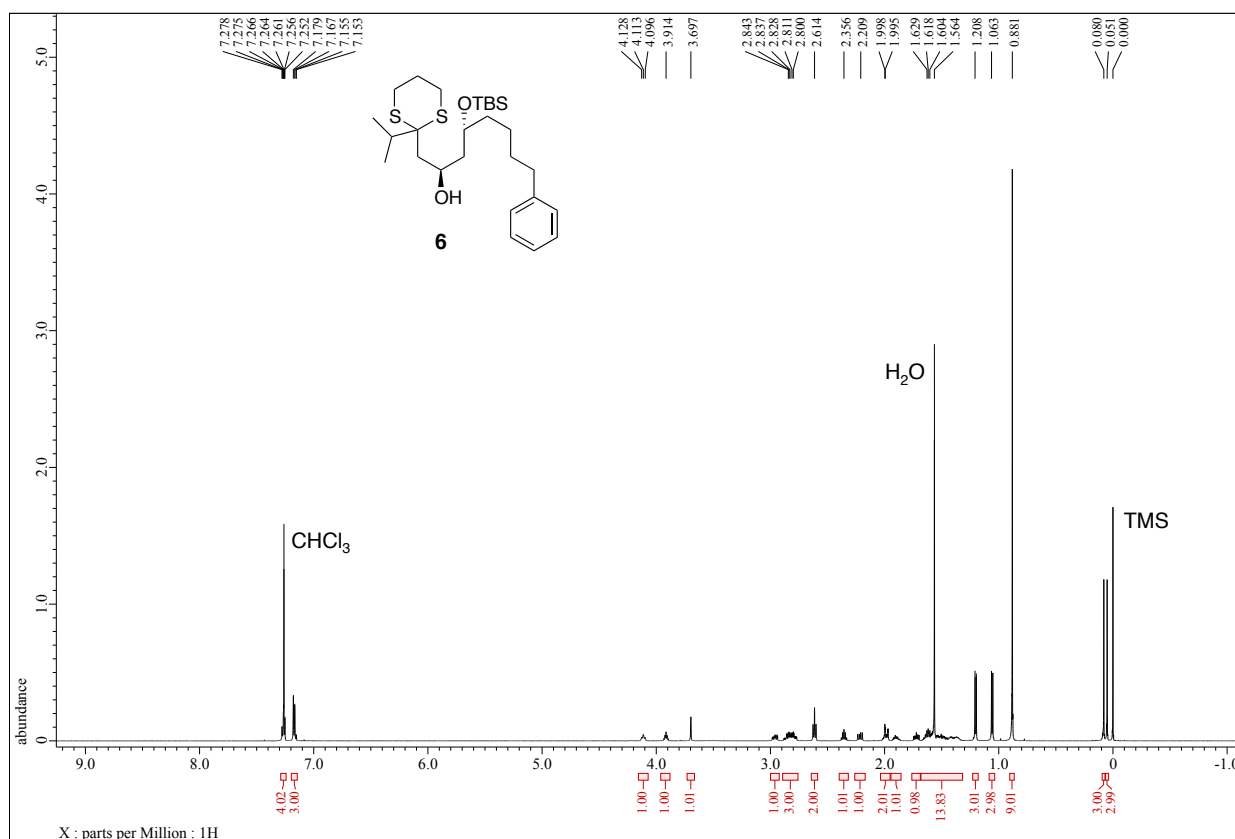
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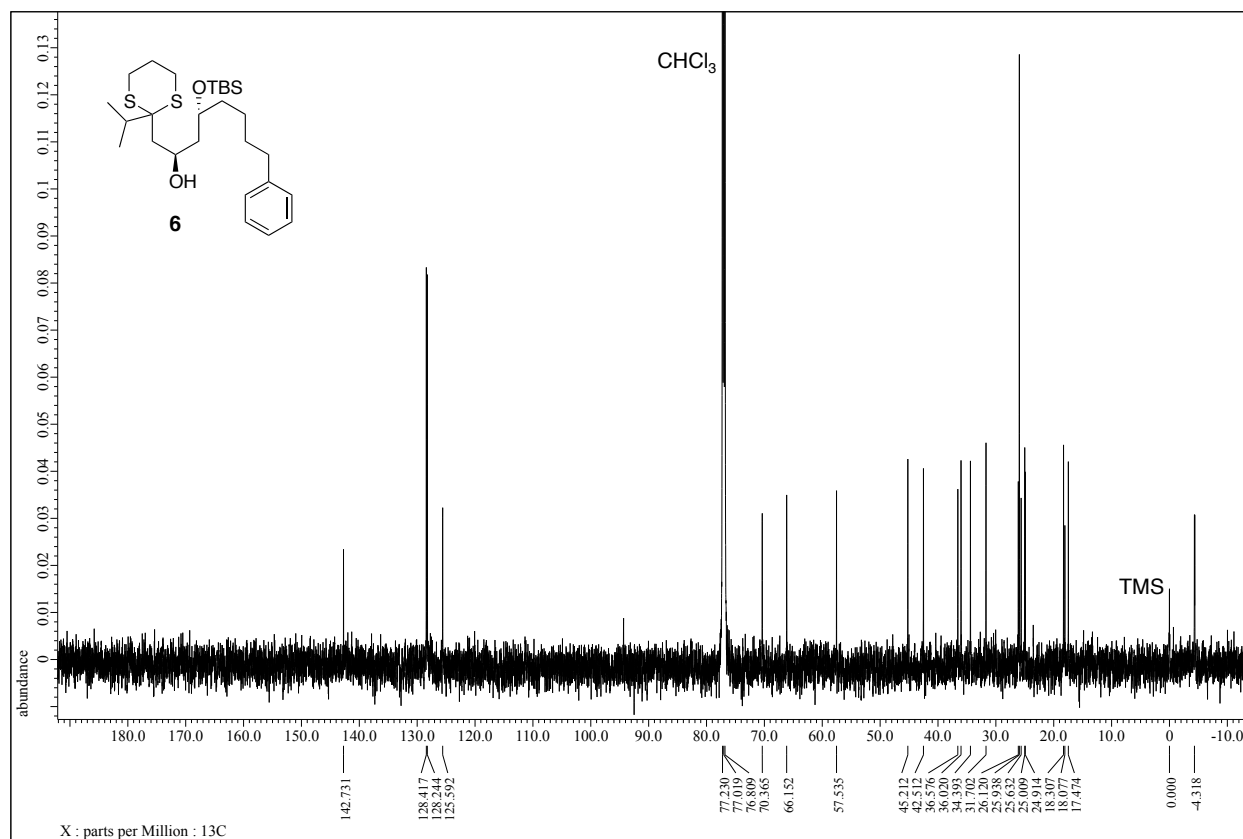
Contents

- I. ¹H-1D and ¹³C-1D NMR spectra of **5**, **6**, **12**, and **13**
- II. ¹H-1D, ¹³C-1D, COSY, and NOESY spectra of **14** and **4**
- III. Growth Inhibitory Activity of **4** and 18-Deoxy-aplog-1 for 39 Human Cancer Cell Lines

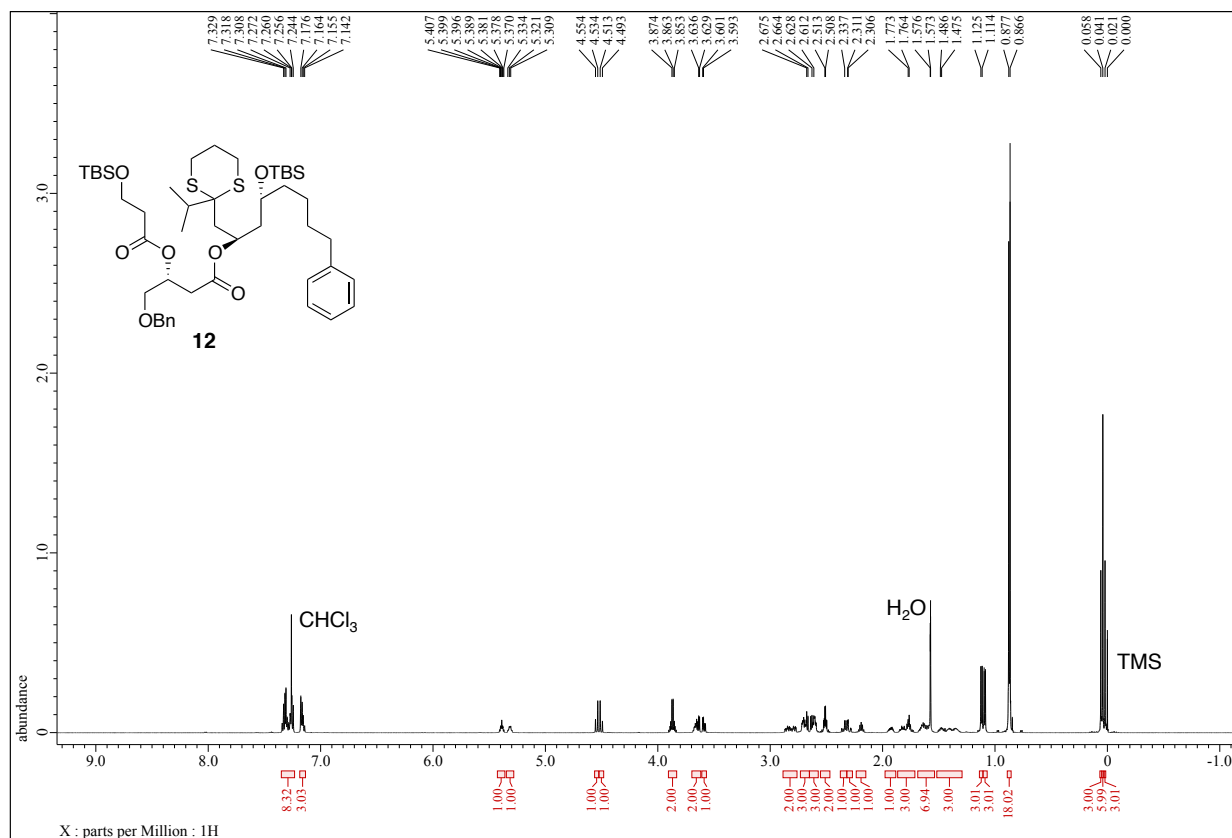
¹H-1D NMR spectrum of **6** (600 MHz, 297 K, CDCl₃, 0.0109 M)



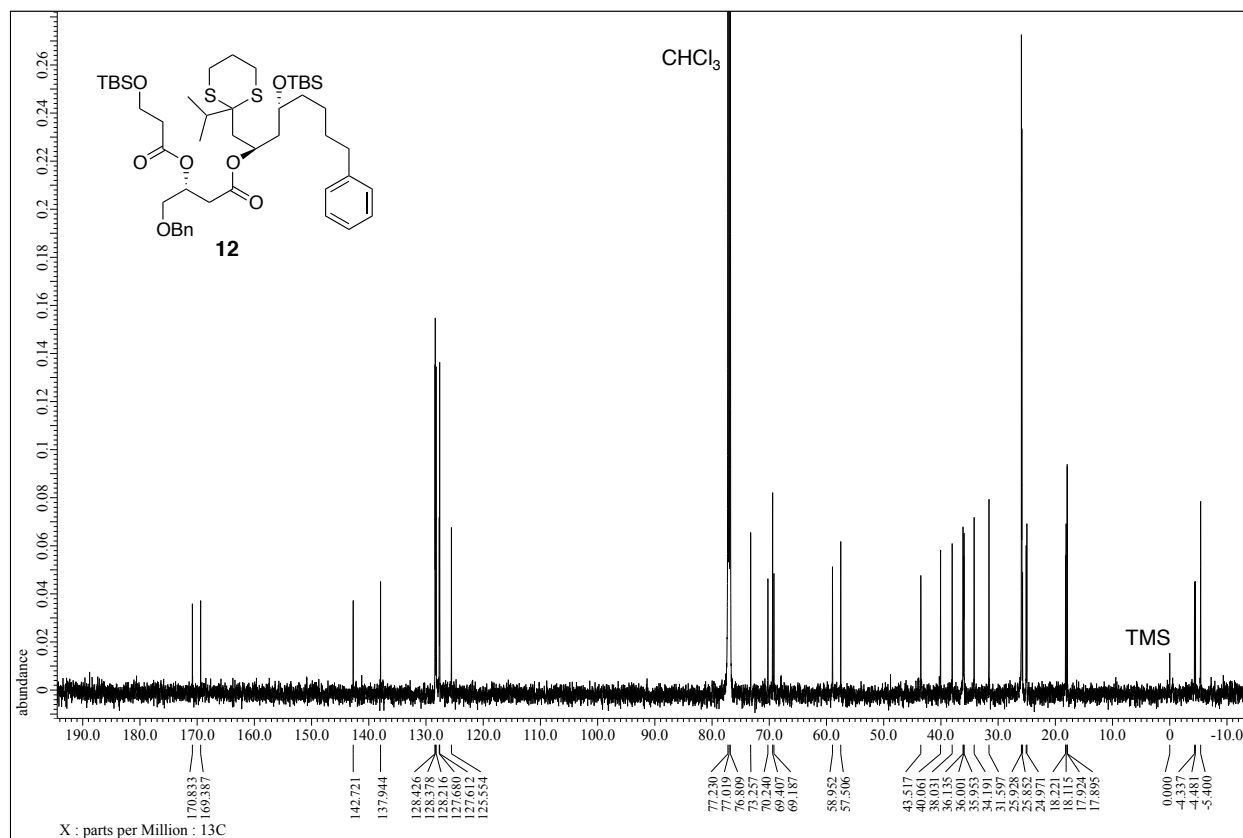
¹³C-1D NMR spectrum of **6** (150 MHz, 298 K, CDCl₃, 0.0109 M)



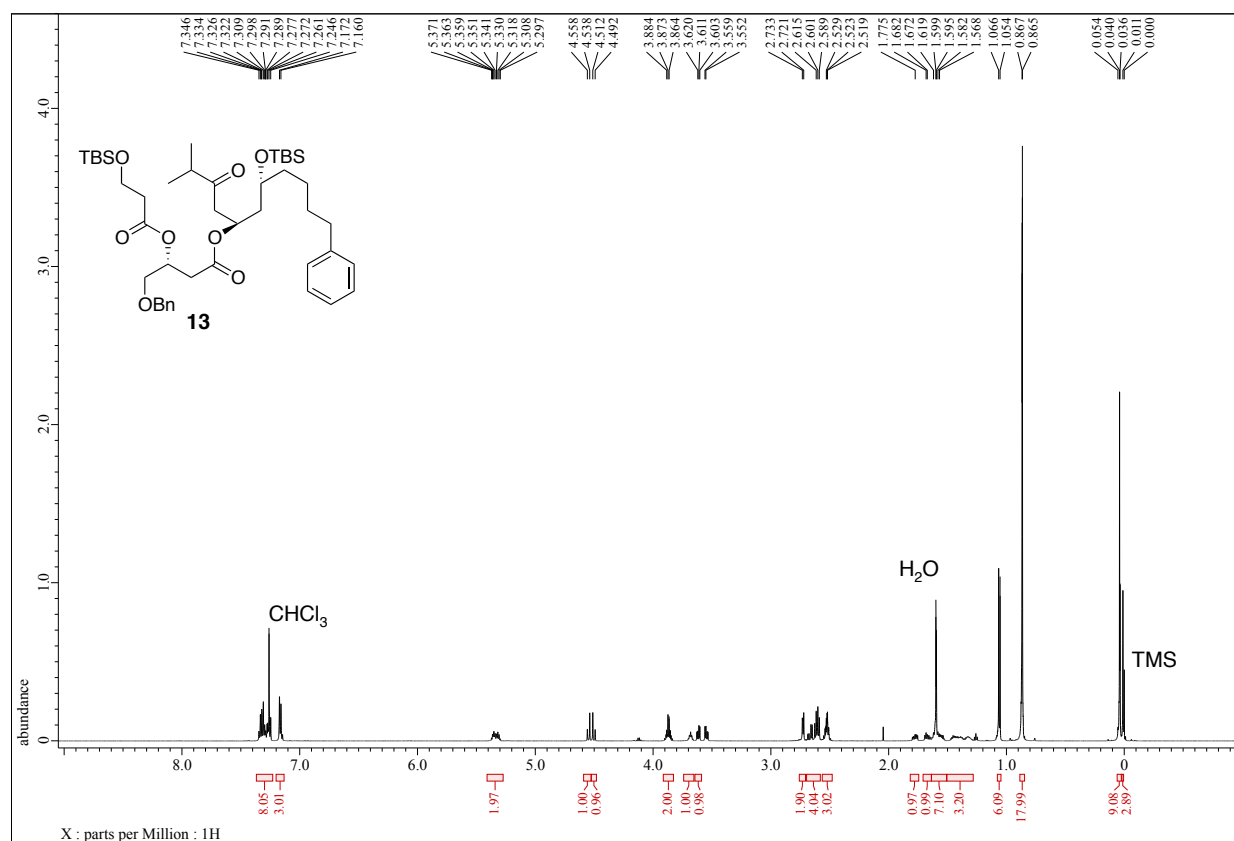
^1H -1D NMR spectrum of **12** (600 MHz, 297 K, CDCl_3 , 0.0192 M)



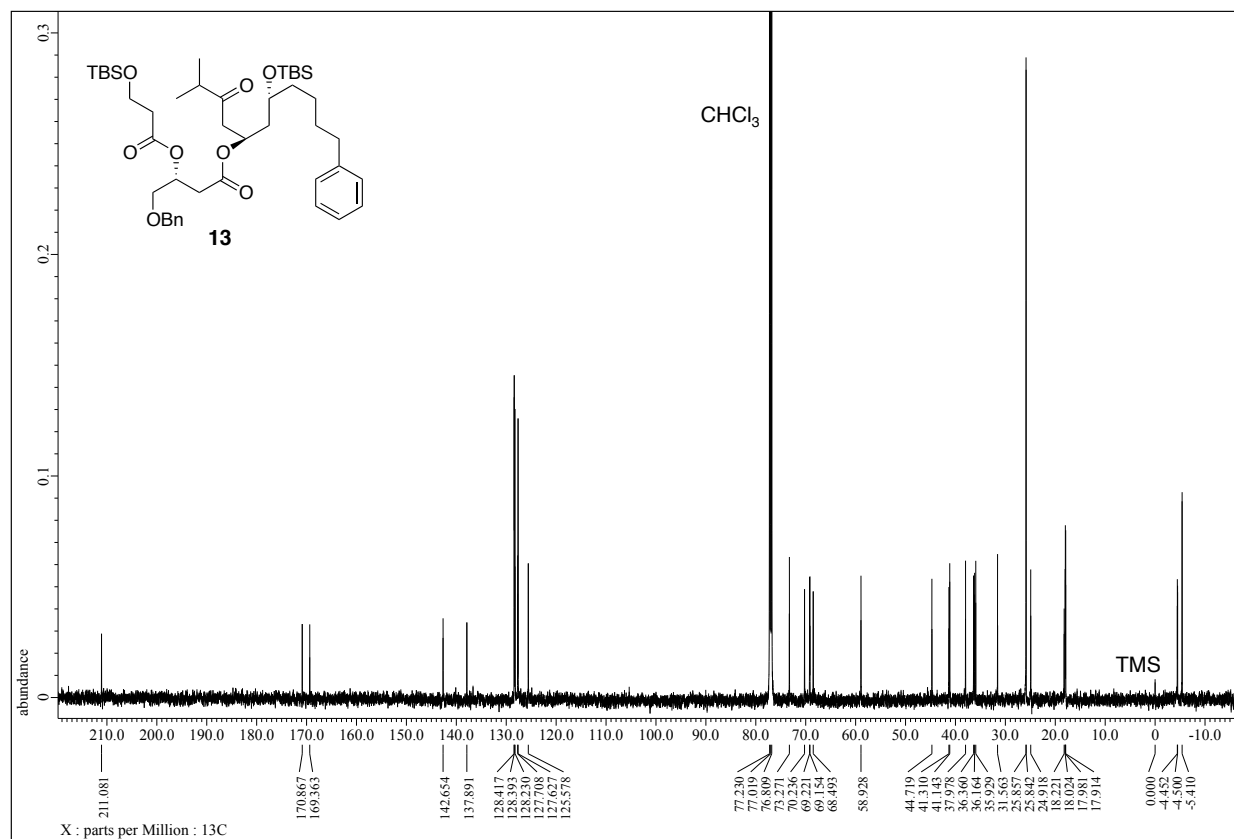
^{13}C -1D NMR spectrum of **12** (150 MHz, 298 K, CDCl_3 , 0.0192 M)



¹H-1D NMR spectrum of **13** (600 MHz, 296 K, CDCl₃, 0.0229 M)

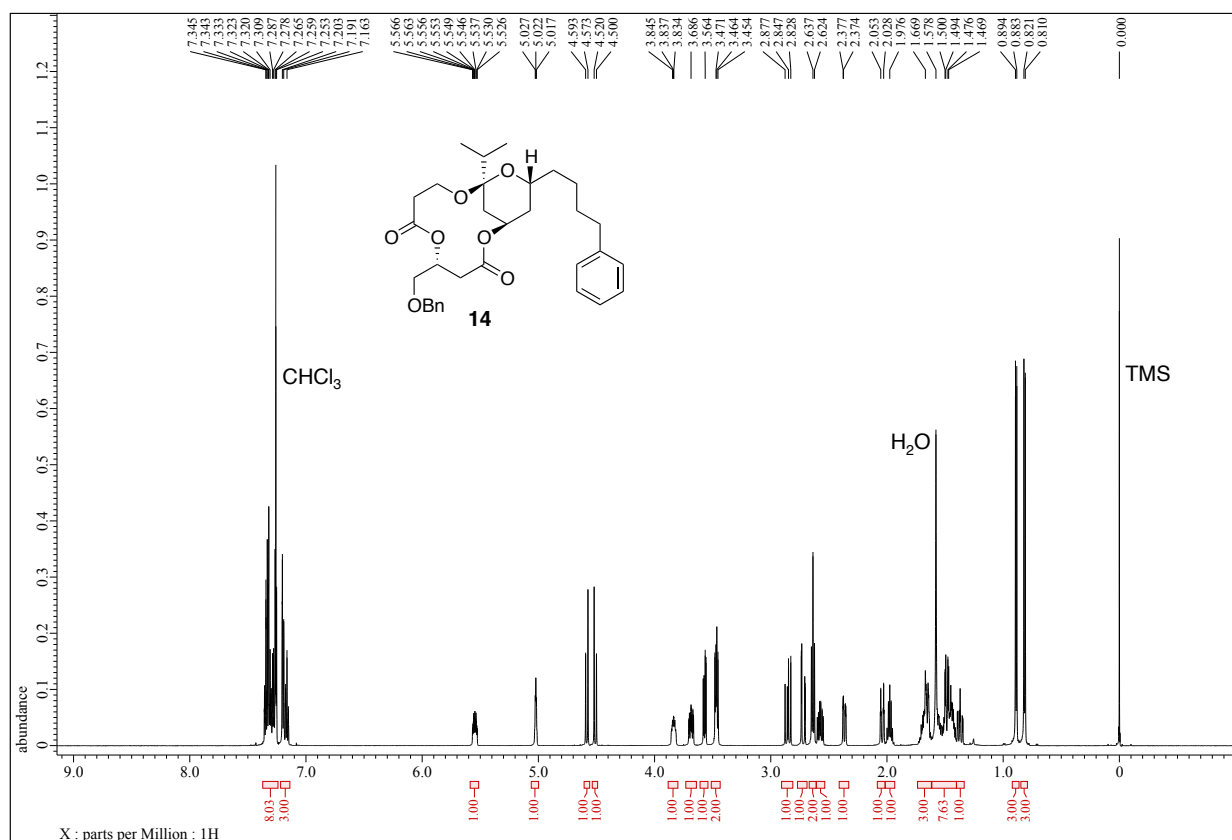


¹³C-1D NMR spectrum of **13** (150 MHz, 297 K, CDCl₃, 0.0229 M)

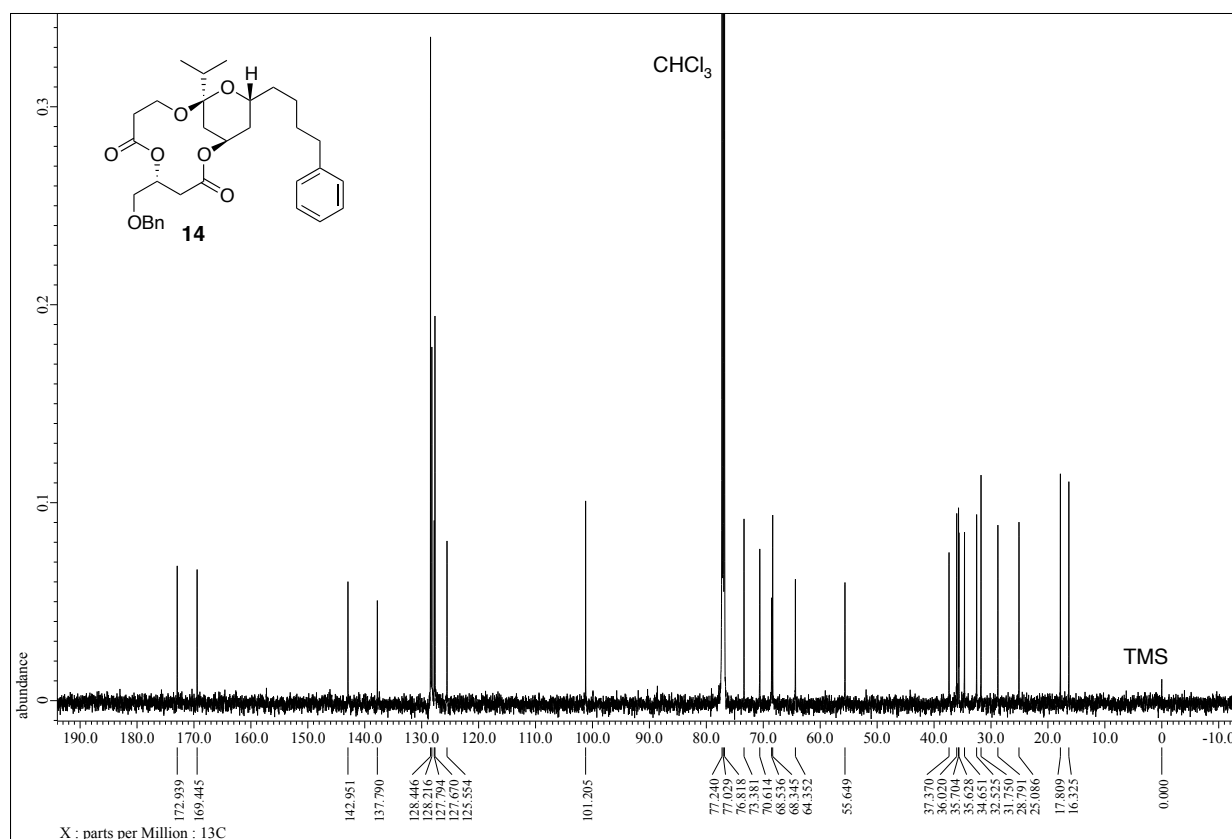


II. ¹H-1D, ¹³C-1D, COSY, and NOESY Spectrum of **14** and **4**

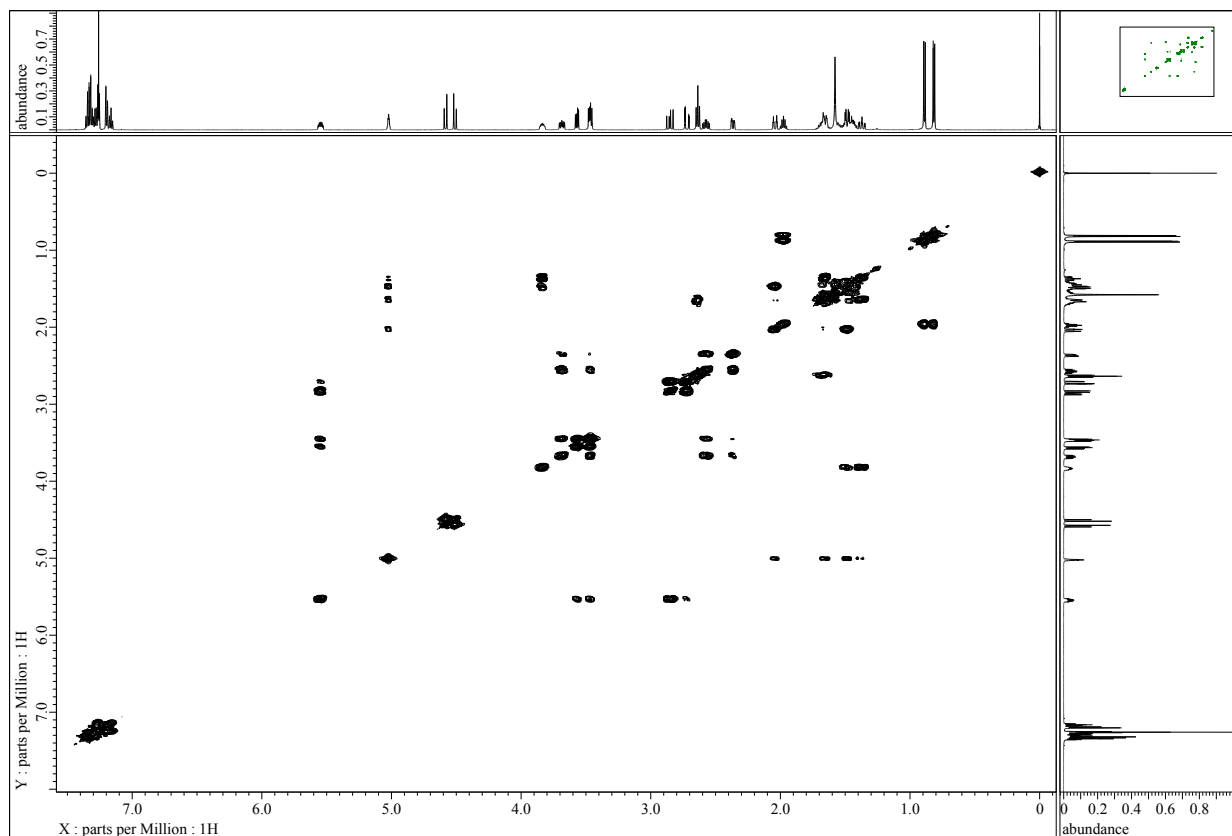
¹H-1D NMR spectrum of **14** (600 MHz, 297 K, CDCl₃, 0.0249 M)



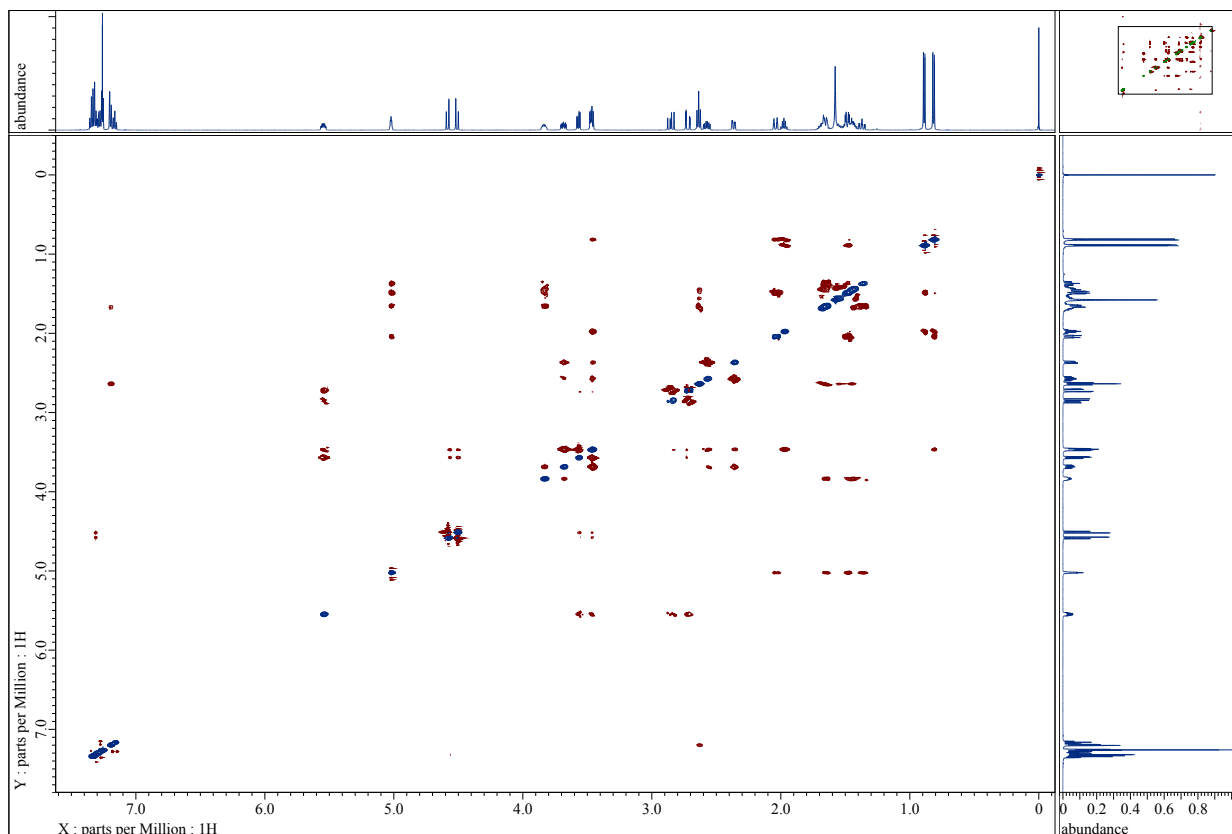
¹³C-1D NMR spectrum of **14** (150 MHz, 298 K, CDCl₃, 0.0249 M)



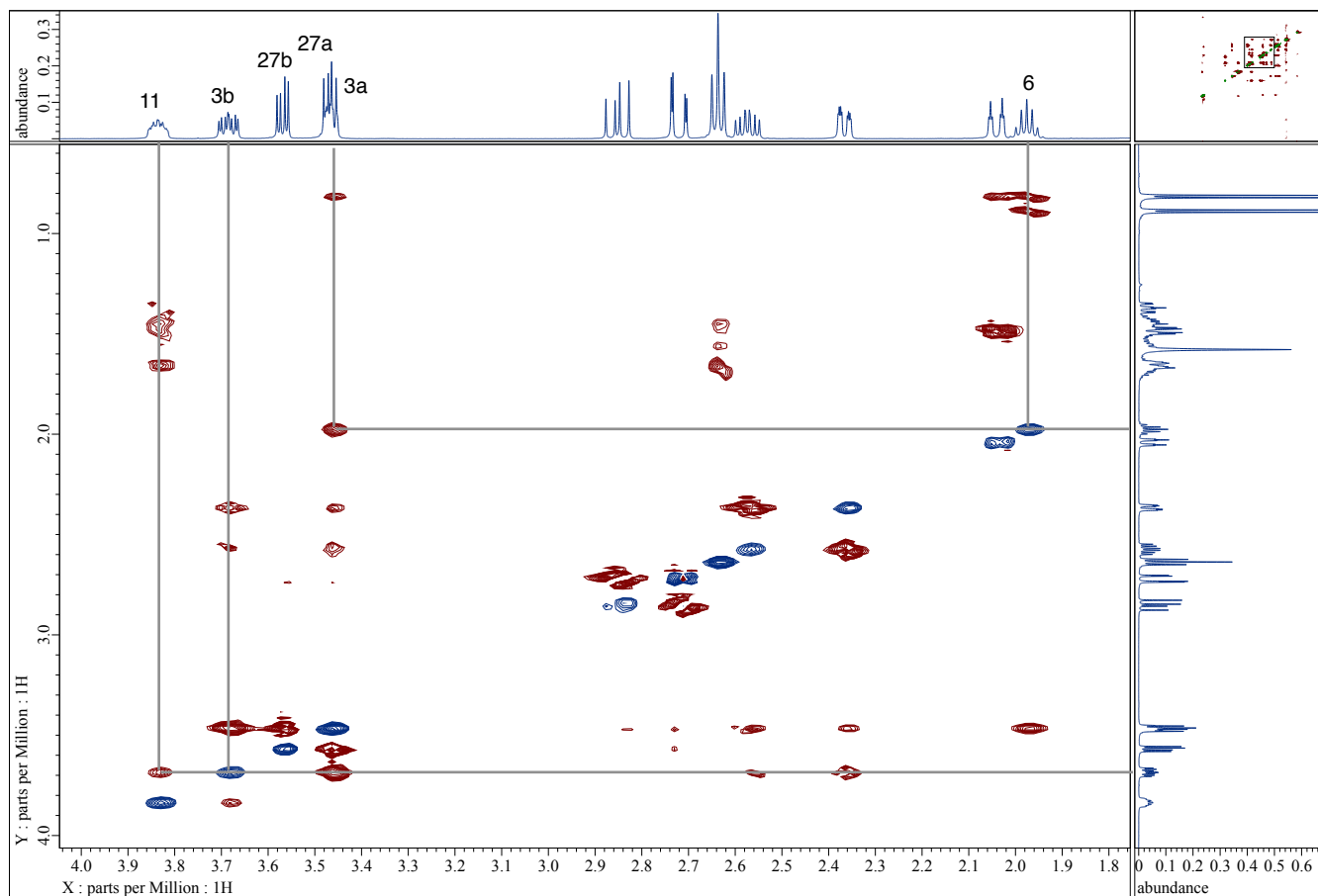
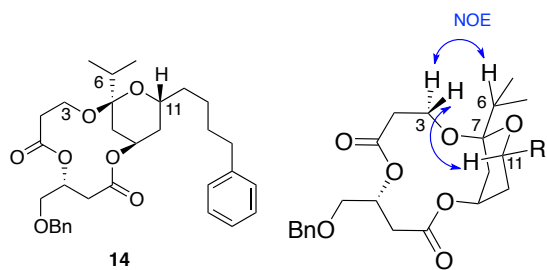
COSY spectrum of **14** (600 MHz, 297 K, CDCl₃, 0.0249 M)



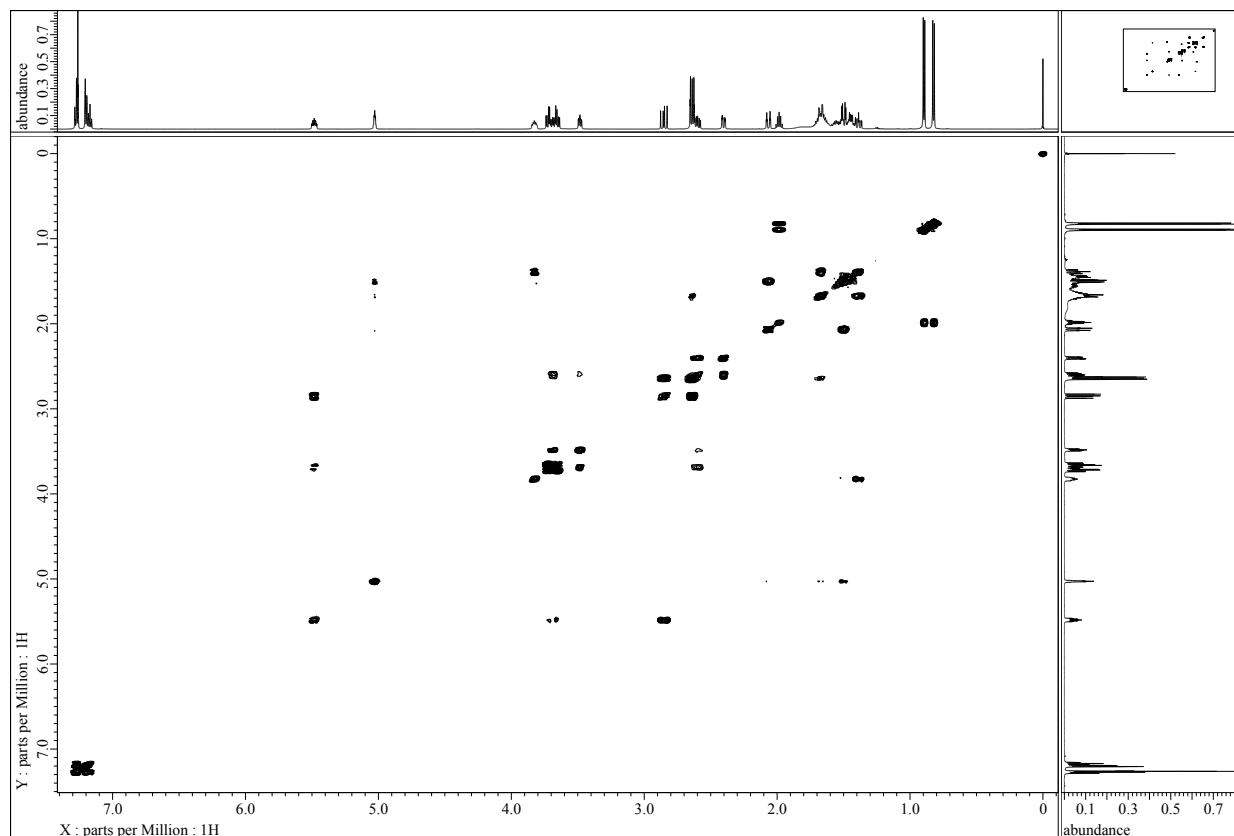
NOESY spectrum of **14** (600 MHz, 297 K, CDCl₃, 0.0249 M, mixing time: 0.5 s)



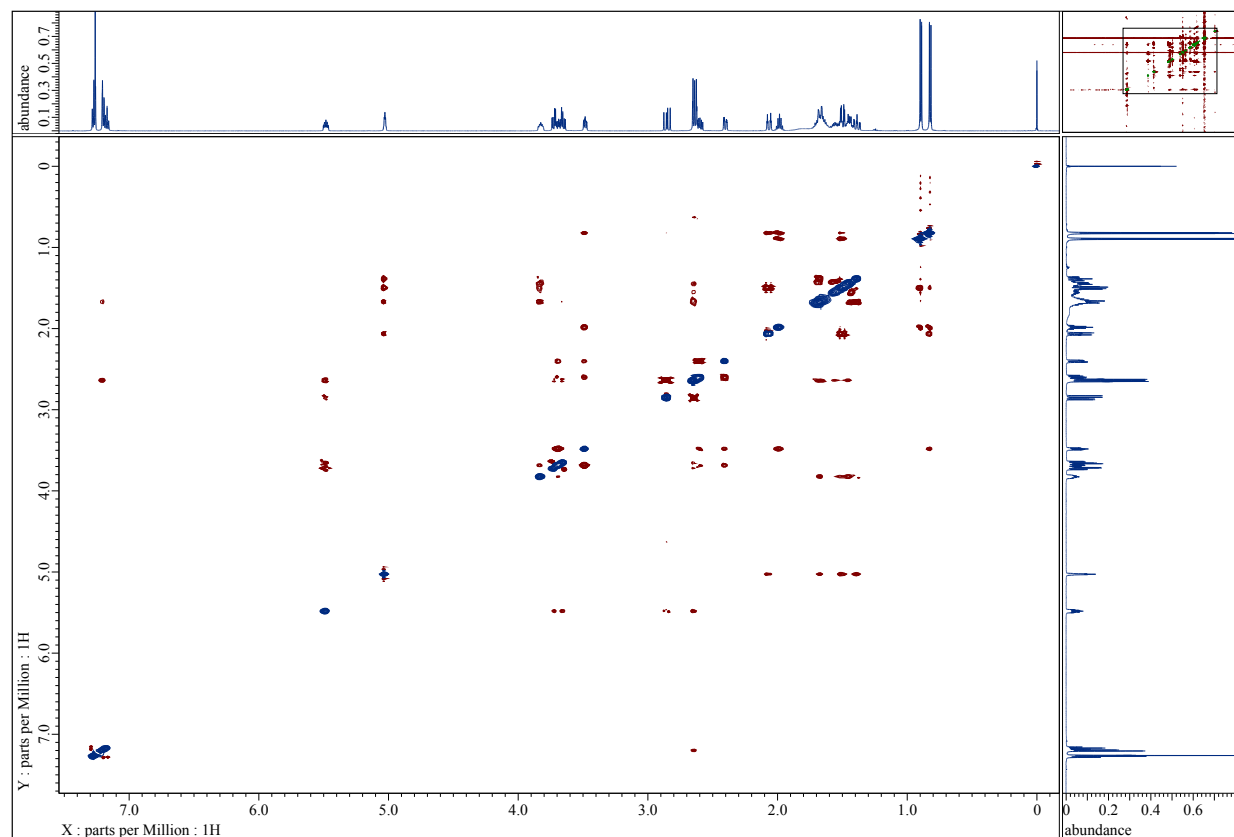
NOESY spectrum of **14** (600 MHz, 297 K, CDCl₃, 0.0249 M) (expanded)



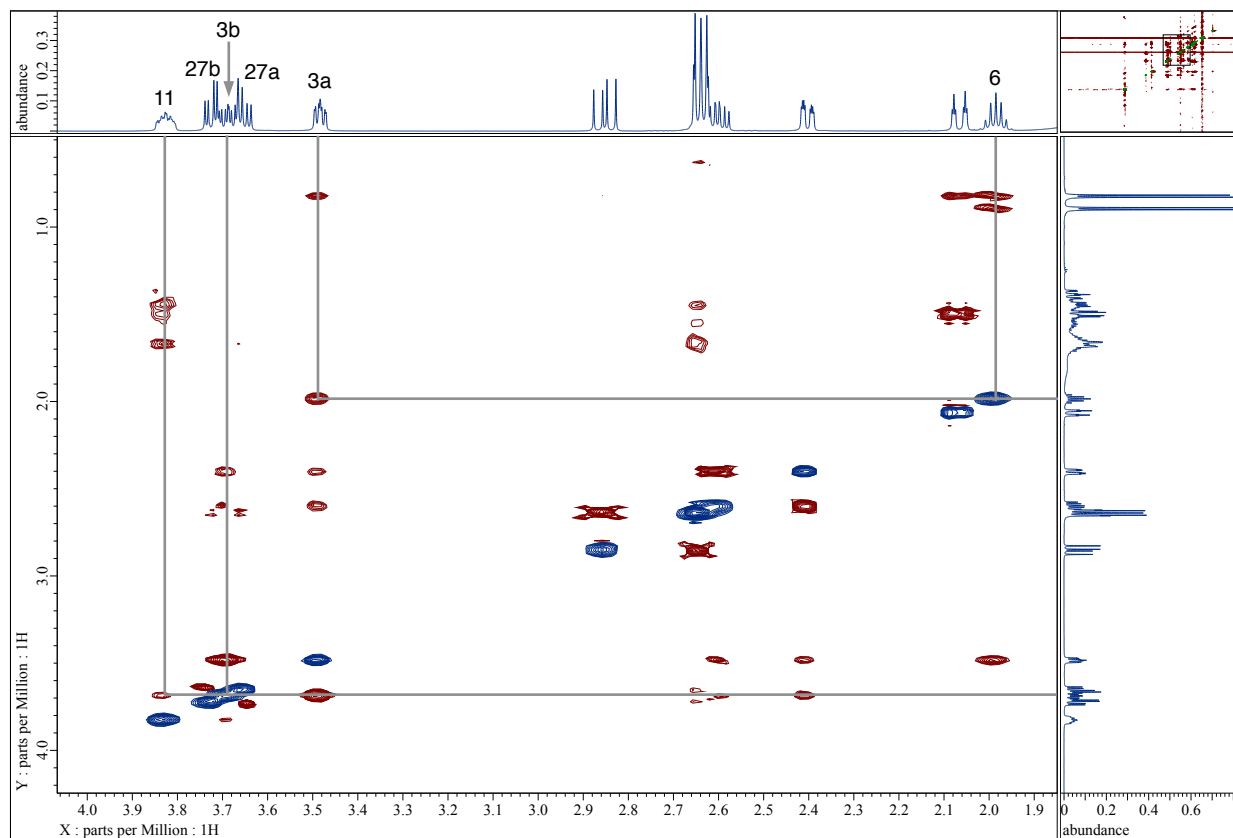
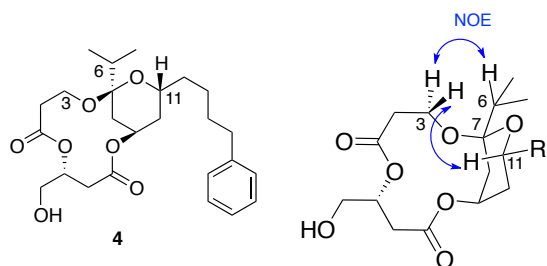
COSY spectrum of **4** (600 MHz, 296 K, CDCl₃, 0.0268 M)



NOESY spectrum of **4** (600 MHz, 296 K, CDCl₃, 0.0268 M, mixing time: 0.5 s)



NOESY spectrum of **4** (600 MHz, 296 K, CDCl₃, 0.0268 M) (expanded)



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

Cancer type	Cell line	GI ₅₀ (M)	
		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

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

^bFull panel mean-graph midpoint