

Electronic Supplementary Information For:

**A Novel D-ring Modified Taxoid: Synthesis and Biological Evaluation
of a γ -Lactone Analogue of Docetaxel**

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Table 1. ^1H -NMR and ^{13}C -NMR Spectroscopic Data for Compounds **12** and **13**

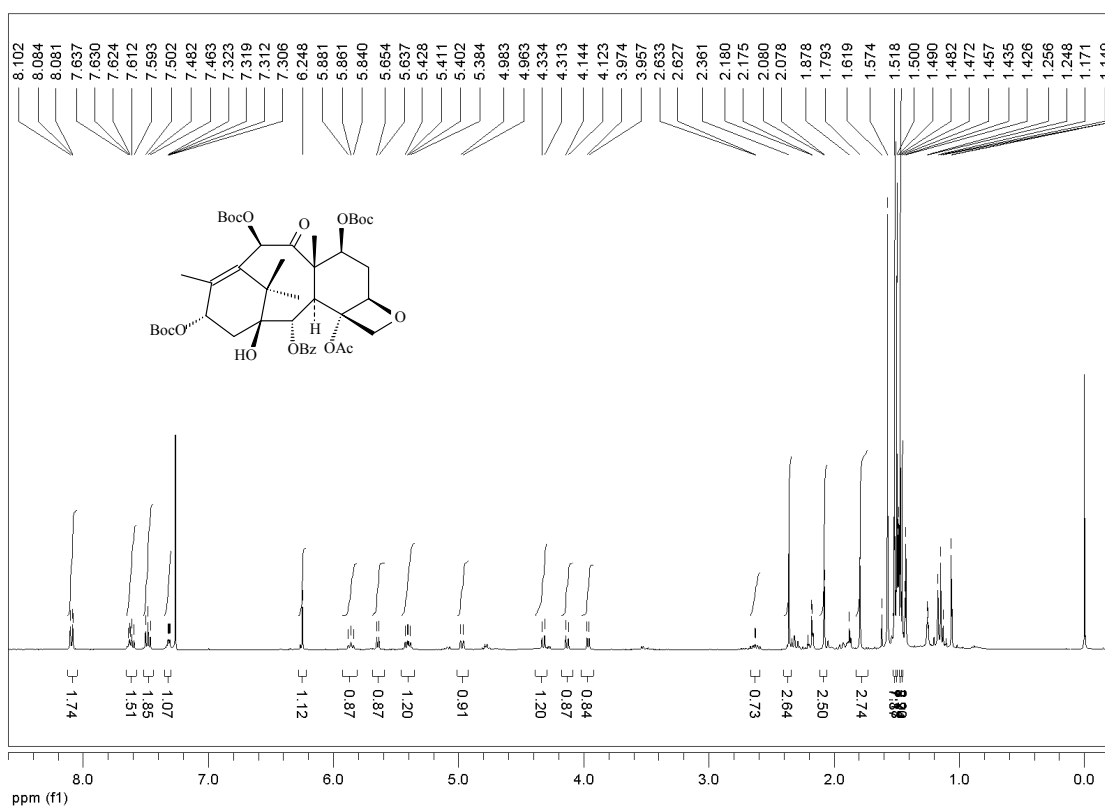
Position	12		13	
	^1H -NMR	^{13}C -NMR	^1H -NMR	^{13}C -NMR
1	—	90.1 s	—	90.2 s
2	4.24 d (4.8)	72.1 d	4.23 d (4.4)	72.1 d
3	3.50 d (4.8)	45.3 d	3.74 d (4.4)	43.4 d
4	—	74.0 s	—	75.4 s
5	5.32 t (2.8)	81.7 d	3.79 t (2.8)	81.1 d
6	2.00 m, 2.12 m	30.0 t	1.85 m, 2.24 m	30.6 t
7	5.20 dd (4.8, 11.6)	71.6 d	5.44 dd (4.4, 11.2)	71.4 d
8	—	59.0 s	—	59.1 s
9	—	201.9 s	—	202.0 s
10	6.44 s	78.0 d	6.48 s	78.3 d
11	—	132.0 s	—	132.0 s
12	—	143.8 s	—	144.2 s
13	5.82 dd (5.6, 8.4)	71.3 d	5.72 dd (2.4, 10.0)	69.8 d
14	3.13 dd (5.6, 15.2)	32.7 t	3.13 dd (4.0, 15.6)	32.5 t
	2.64 dd (10.0, 15.2)		2.64 dd (10.0, 15.6)	
15	—	41.1 s	—	40.6 s
16	1.15 s	19.5 q	1.15 s	18.8 q
17	1.28 s	26.0 q	1.22 s	27.1 q
18	2.31 s	16.1 q	2.29 s	16.6 q
19	1.29 s	12.7 a	1.35 s	12.7 q
20	4.08 ABq (9.2)	62.9 t	4.52 ABq (12.0)	64.7 t
	3.59 dABq(6.0, 9.2)		4.41 ABq (12.0)	
$\text{O}_2\text{C}=\text{O}$	—	151.9 s	—	151.8 s
$\begin{array}{c} (\text{CH}_3)_3 \\ \\ \text{C}-\text{O} \end{array}$	1.44, 1.47, 1.49, s	27.6 q	1.44, 1.47, 1.50, s	27.7 q
$\text{C}=\text{O}$	—	83.0 s	—	82.8 s
$\begin{array}{c} \text{C}=\text{O} \\ \\ \text{CH}_3 \end{array}$	—	171.0 s	—	170.5 s
	2.34 s	21.3 q	2.13 s	20.7 q

Table 2 NMR Data for Compound **15** (400 Mz for ^1H and 100 Mz for ^{13}C)

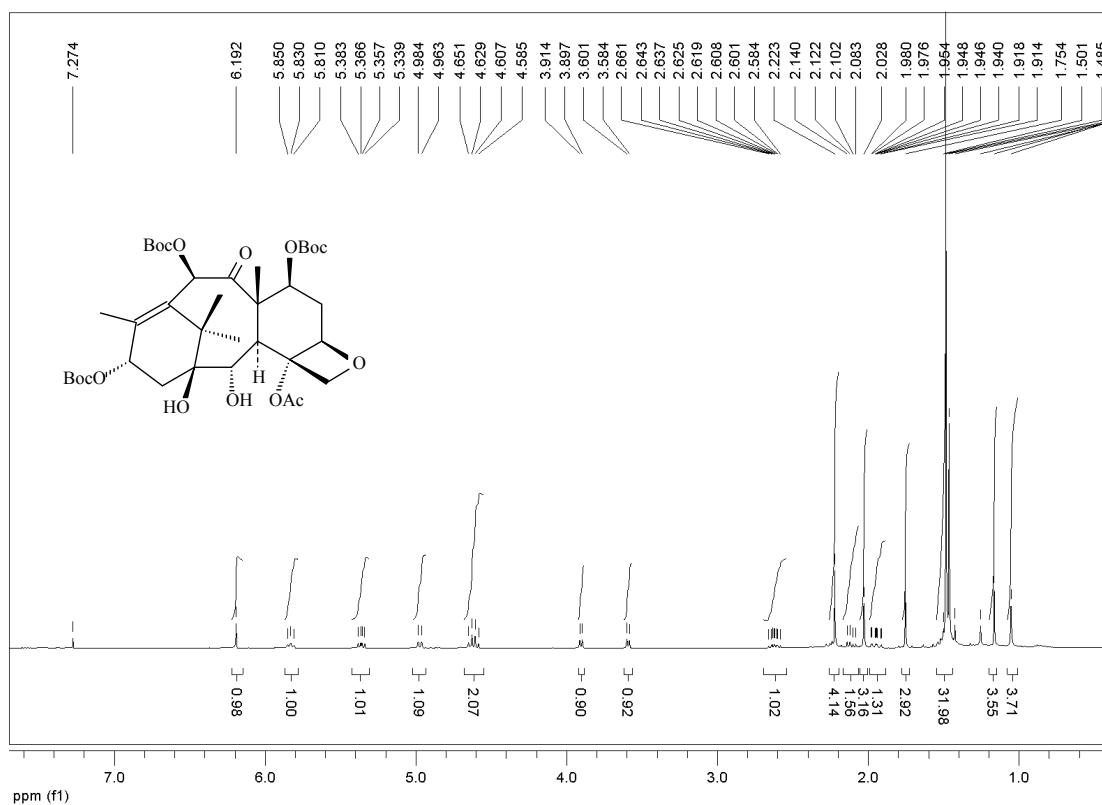
Position	δ_{H}	Mult ($J = \text{Hz}$)	δ_{C}	HMBC (H \rightarrow C)
1	—	—	90.6 s	—
2	4.46	d (6.8)	80.5 d	C-1, C-3, C-8, C-14, C-15
3	2.70	d (6.8)	46.4 d	C-1, C-2, C-4, C-7, C-8, C-20
4	—	—	77.1 s	—
5	4.61	t (5.2)	81.8 d	C-3, C-4, C-7
6	2.28	m (α)	29.2 t	C-4, C-5, C-7, C-8
	2.32	m (β)		C-4, C-5, C-7, C-8
7	5.15	dd (6.4, 8.0)	71.5 d	C-6, C-8, C-9, C-19, C-Boc
8	—	—	57.8 s	—
9	—	—	202.2 s	—
10	6.37	s	77.8 d	C-9, C-11, C-12, C-15, C-Boc
11	—	—	131.2 s	—
12	—	—	142.9 s	—
13	5.72	dd (3.6, 7.2)	70.7 s	C-11, C-12, C-Boc
14	2.21	m	34.1 t	C-1, C-2, C-13, C-15
	2.90	dd (9.6, 16.0)		C-1, C-2, C-12, C-13
15	—	—	40.4 s	—
16	1.20	s	19.0 q	C-1, C-11, C-15, C-17
17	1.23	s	26.7 q	C-1, C-11, C-15, C-16
18	2.19	s	16.4 q	C-1, C-11, C-12, C-13
19	1.53	s	13.5 q	C-3, C-7, C-8
20	2.79	ABq (12.0)	46.1 t	C-3, C-4, C-21
	3.03	ABq (12.0)		C-3, C-4, C-5, C-21
21	—	—	170.6 s	—
$\begin{array}{c} \text{O} \\ \\ \text{C}=\text{O} \\ \\ \text{O} \end{array}$	—	—	151.8	—
$\begin{array}{c} (\text{CH}_3)_3 \\ \\ \text{C}-\text{O} \end{array}$	1.48	s	27.6 q	C-Boc
$\begin{array}{c} (\text{CH}_3)_3 \\ \\ \text{C}-\text{O} \end{array}$	—	—	83.4 s	—

Table 3 NMR Data for Compound **16** (400 Mz for ^1H and 100 Mz for ^{13}C)

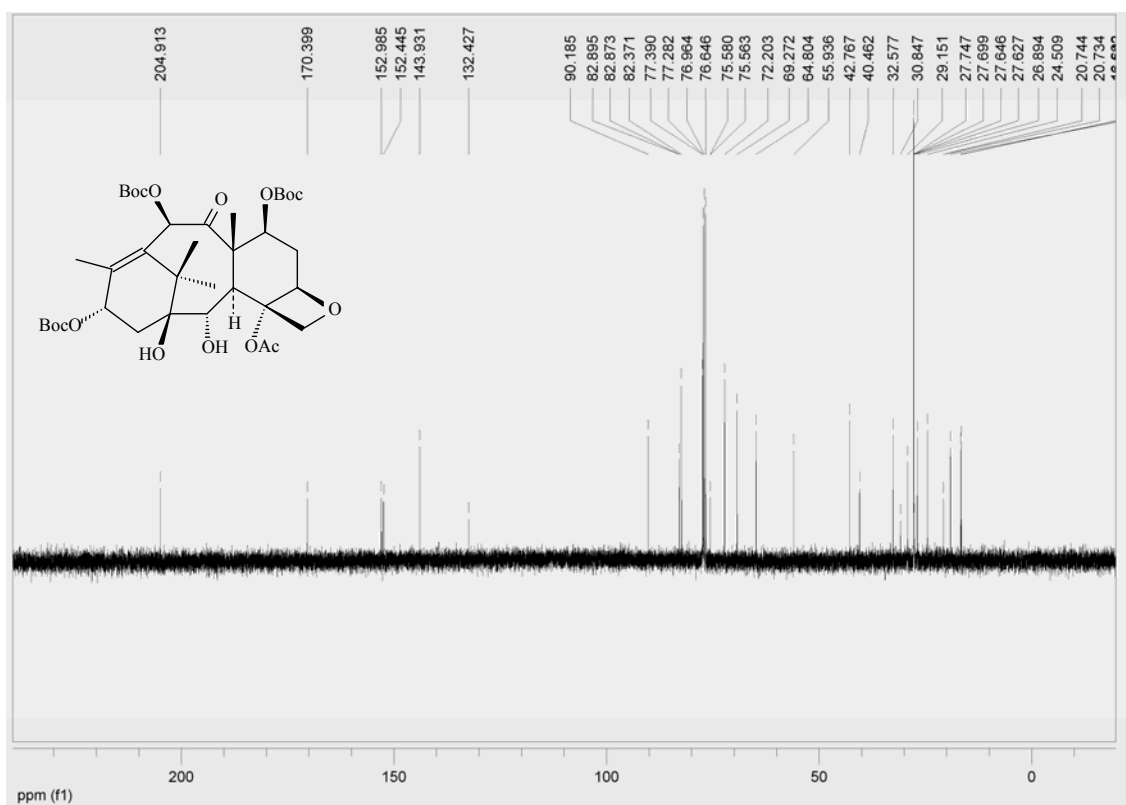
Position	δ_{H}	Mult ($J = \text{Hz}$)	δ_{C}	HMBC (H \rightarrow C)
1	—	—	78.6 s	—
2	4.05	d (6.4)	74.1 d	C-1, C-3, C-8, C-14
3	2.84	d (6.4)	48.0 d	C-1, C-2, C-4, C-7, C-8, C-20
4	—	—	76.9 s	—
5	4.61	t (3.6)	81.6 d	C-3, C-4, C-7
6	2.15	m (α)	27.3 t	C-7
	2.28	m (β)		C-7
7	5.00	dd (4.8, 10.8)	72.3d	C-6, C-8, C-9, C-19, C-Boc
8	—	—	57.0 s	—
9	—	—	202.5 s	—
10	6.30	s	77.1d	C-9, C-11, C-12, C-15, C-Boc
11	—	—	132.4 s	—
12	—	—	141.0 s	—
13	5.73	t (7.2)	71.5 s	C-11, C-12, C-Boc
14	2.31	m	35.6 t	C-1, C-2, C-12, C-13, C-15
	2.38	m		C-1, C-2, C-12, C-13, C-15
15	—	—	42.2 s	—
16	1.08	s	19.4 q	C-1, C-11, C-15, C-17
17	1.15	s	26.3 q	C-1, C-11, C-15, C-16
18	2.05	s	15.2 q	C-1, C-9, C-11, C-12, C-13
19	1.56	s	12.1 q	C-3, C-9, C-8, C-13
20	2.73	ABq (12.4)	48.3 t	C-3, C-4, C-21
	3.20	ABq (12.4)		C-3, C-4, C-5, C-21
21	—	—	172.4 s	—
(CH ₃) ₃ C—O	1.49	s	27.4 q	C-Boc
	—	—	82.9 s	—



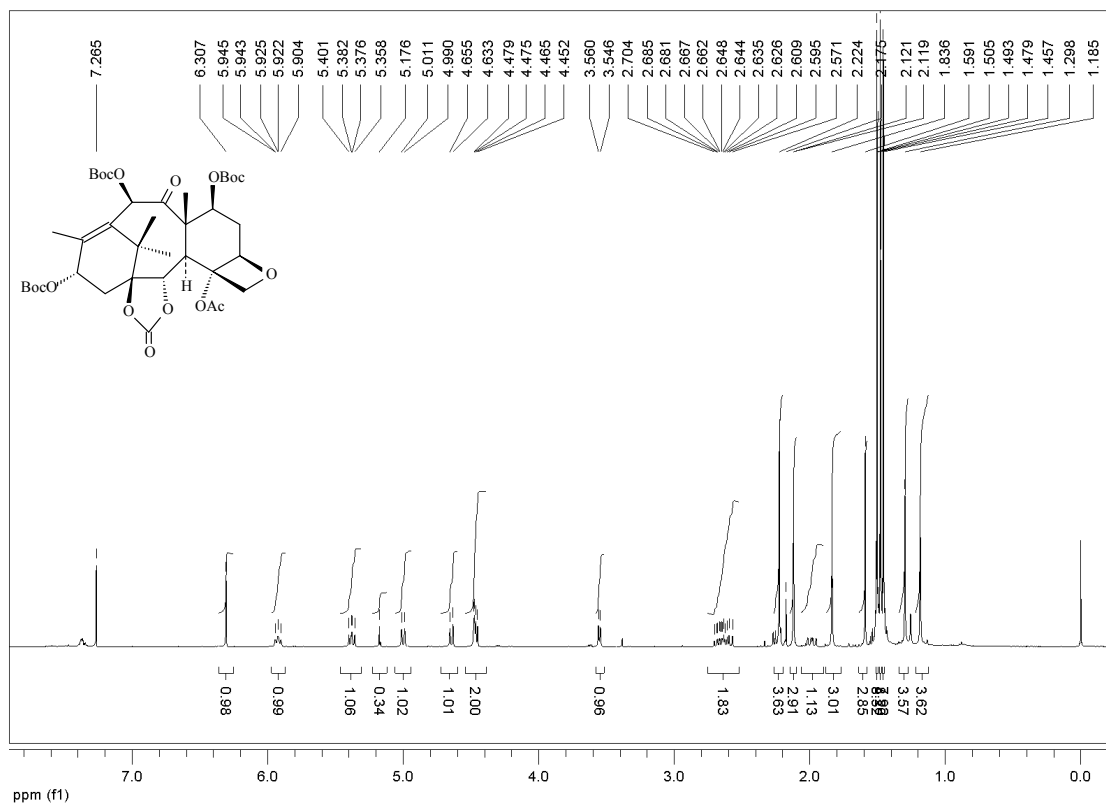
¹H NMR spectrum of 7,10,13-triBoc-10-DAB



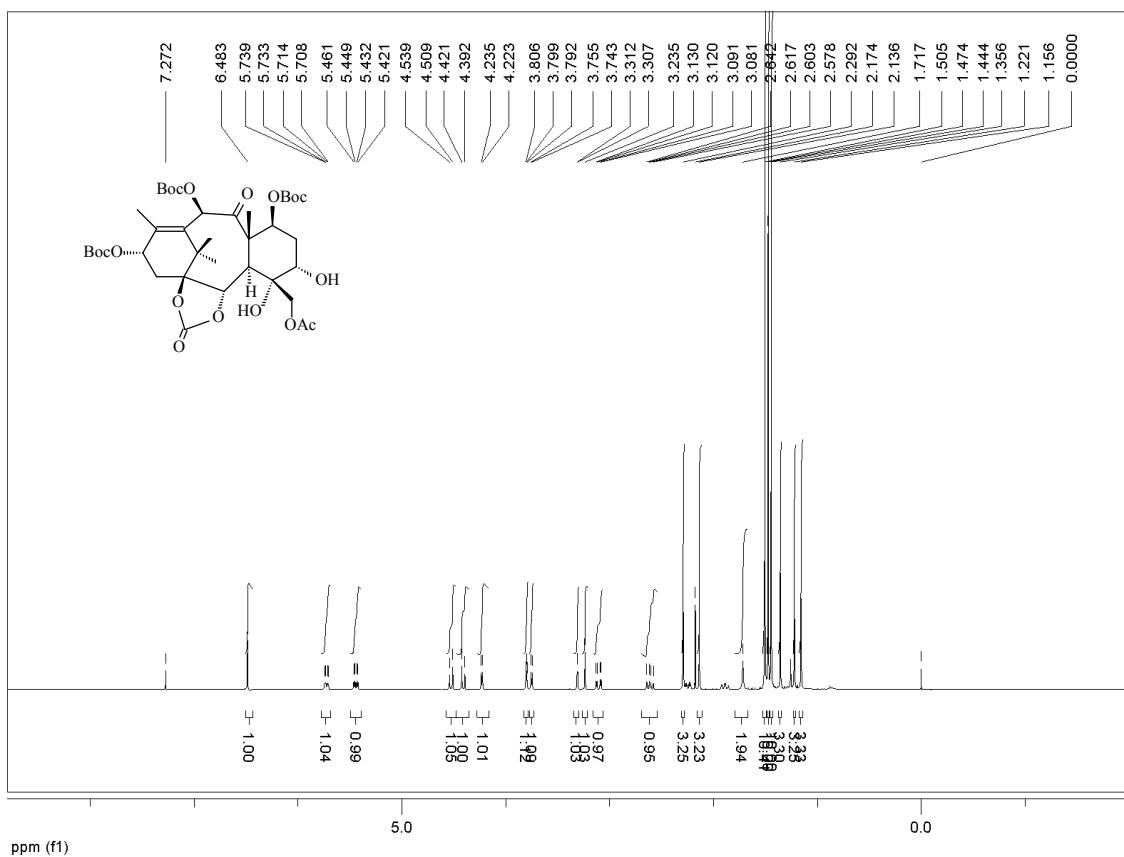
¹H NMR spectrum of 7,10,13-triBoc-2-debenzoate-10-DAB



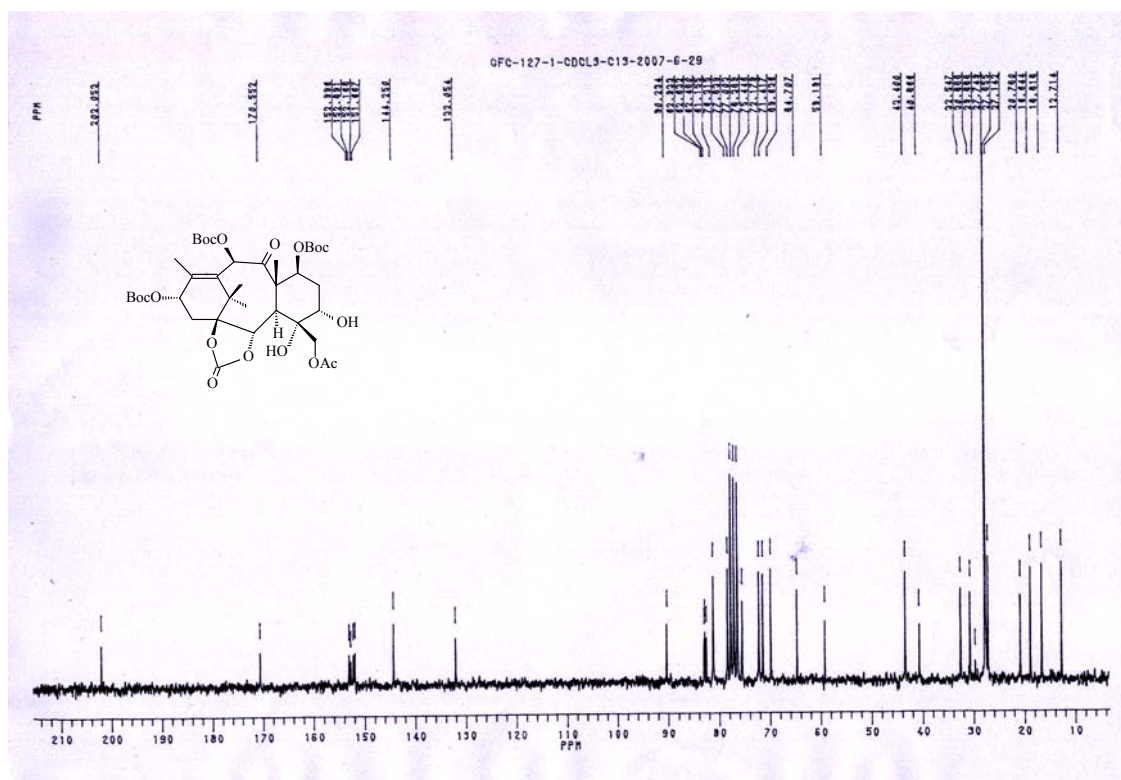
¹³C NMR spectrum of 7,10,13-triBoc-2-debenzoate-10-DAB



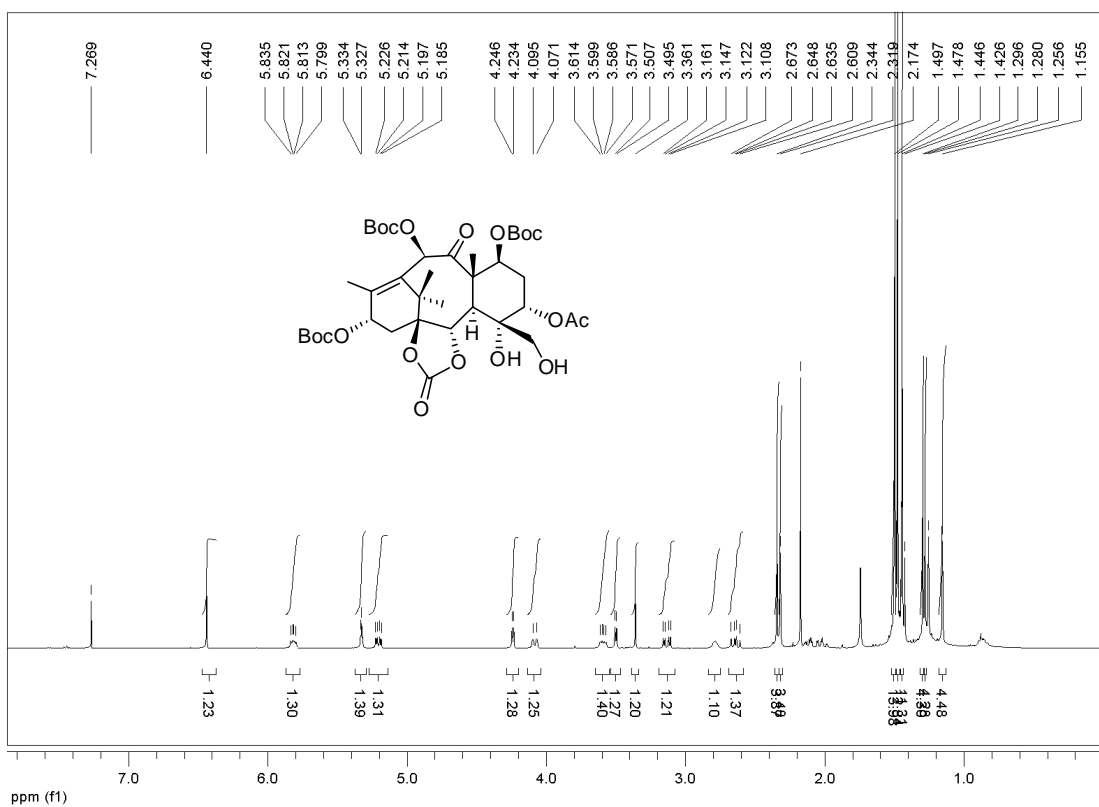
¹H NMR spectrum of compound **11**



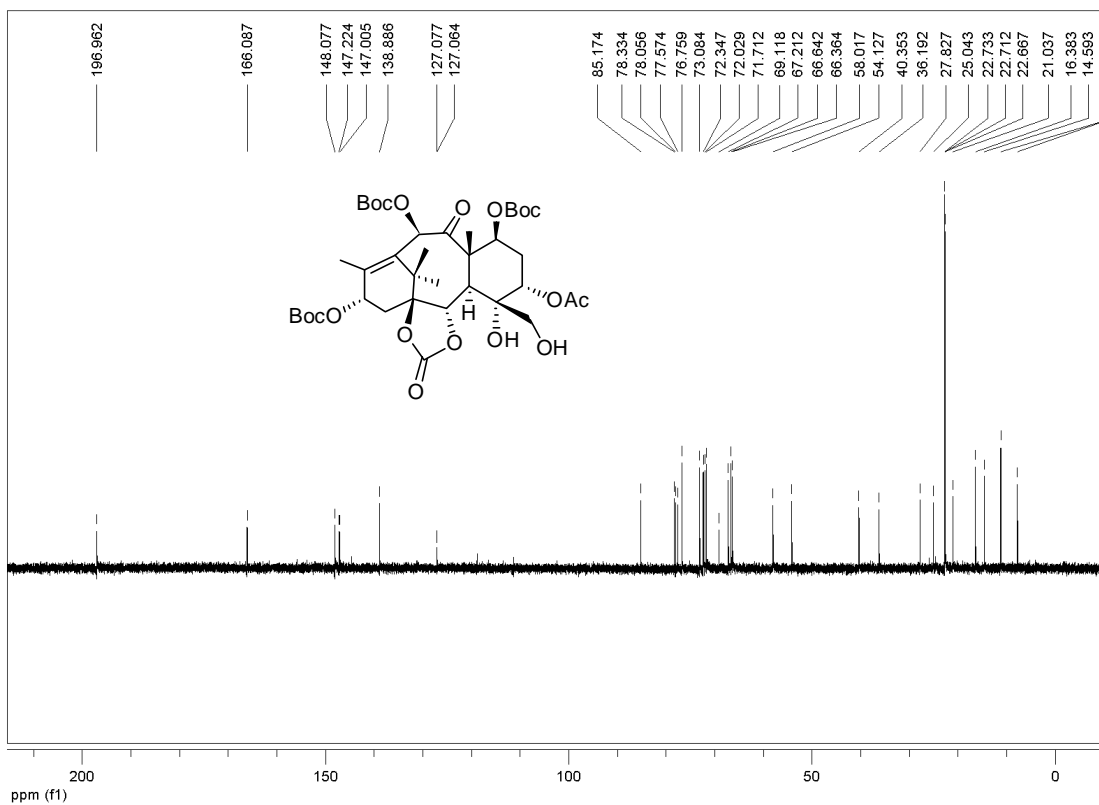
¹H NMR spectrum of compound **12**



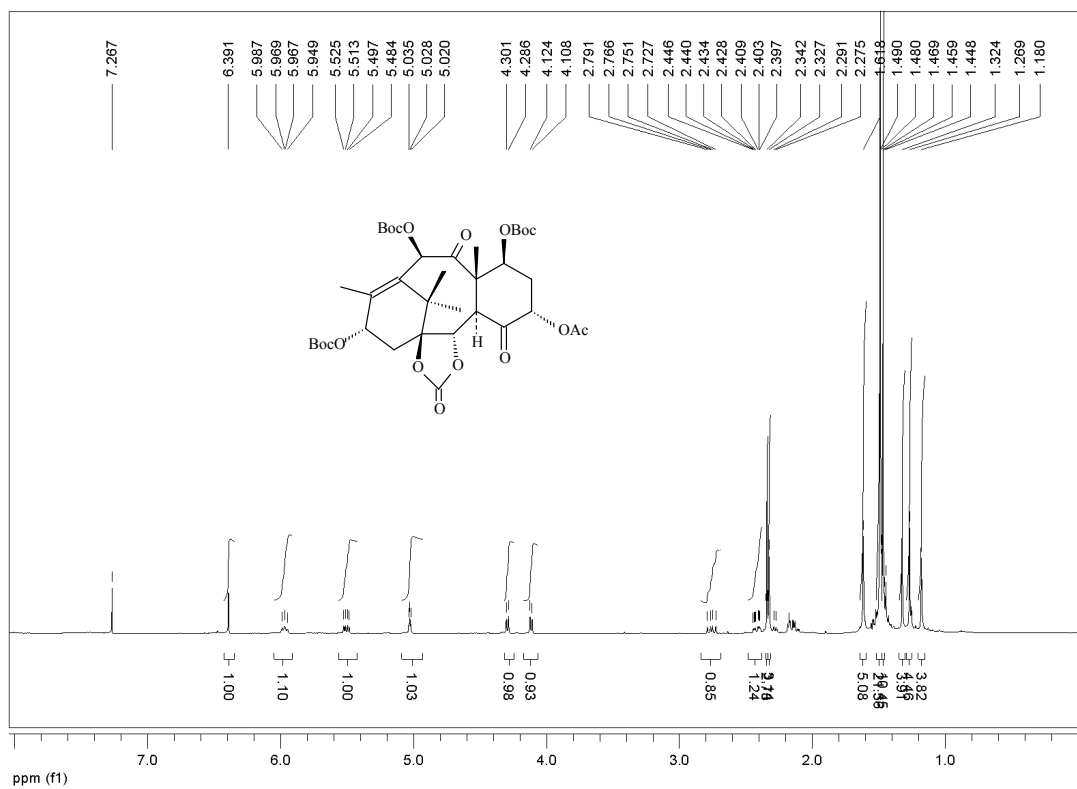
¹³C NMR spectrum of compound 12



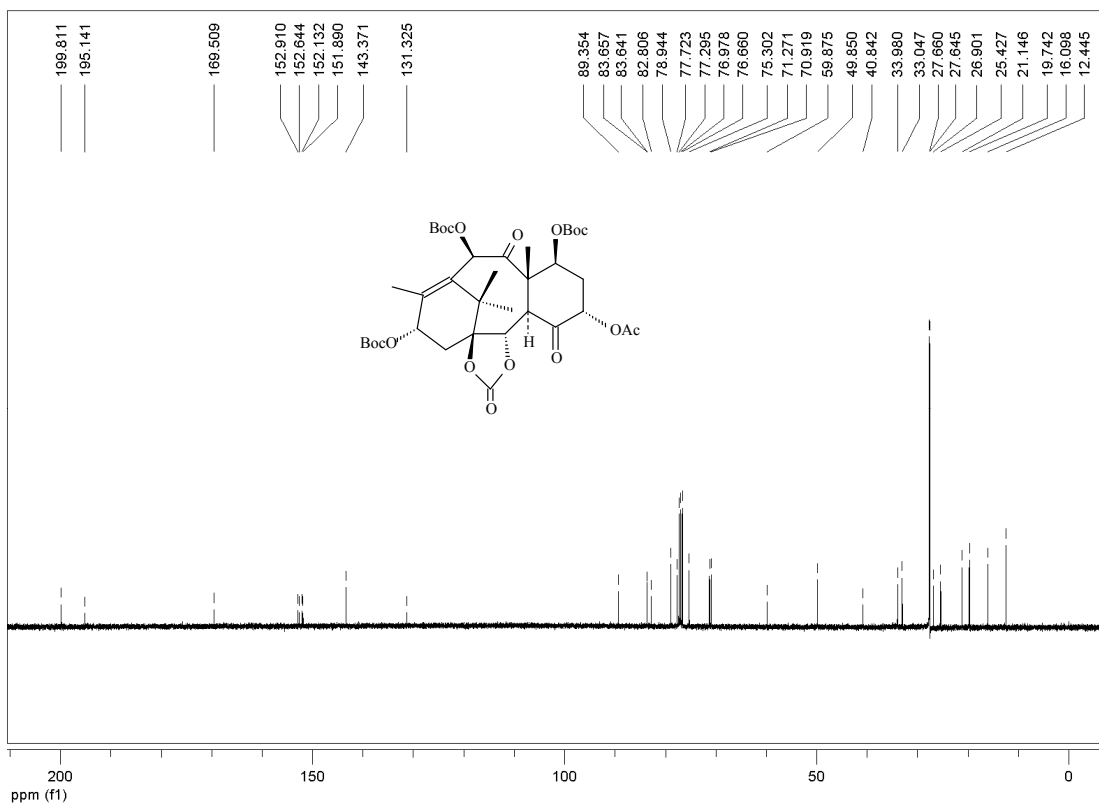
¹H NMR spectrum of compound 13



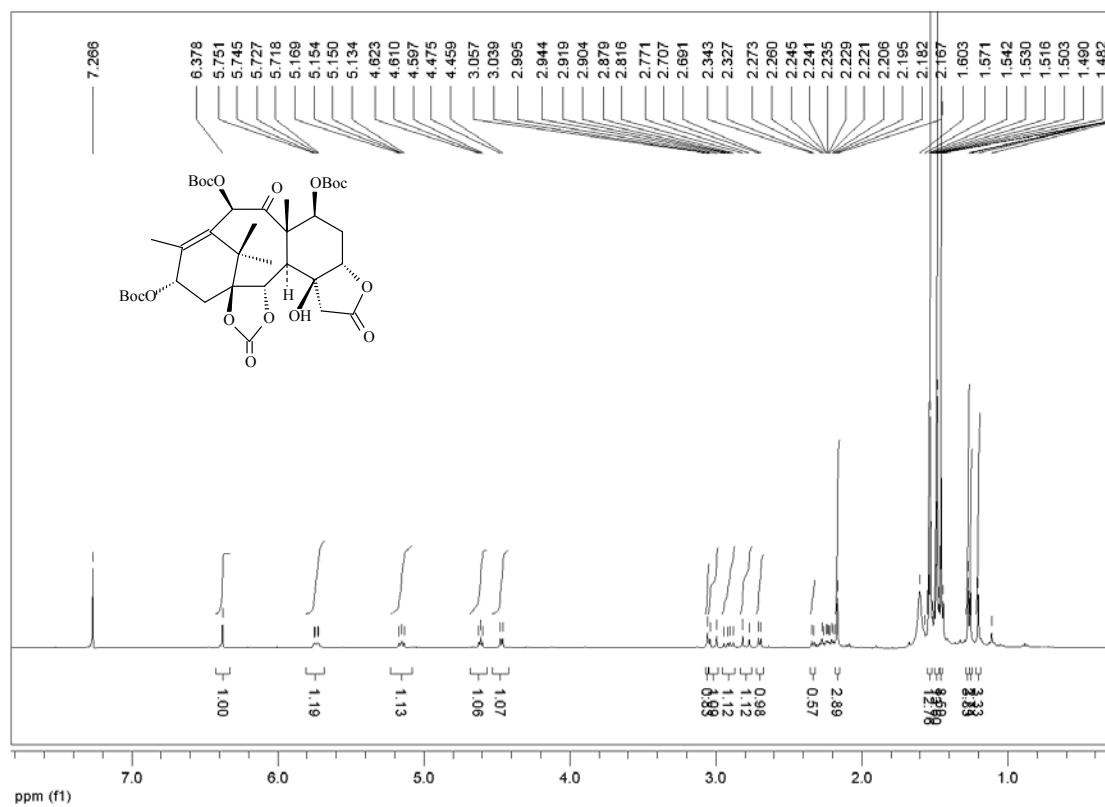
¹³C NMR spectrum of compound **13**



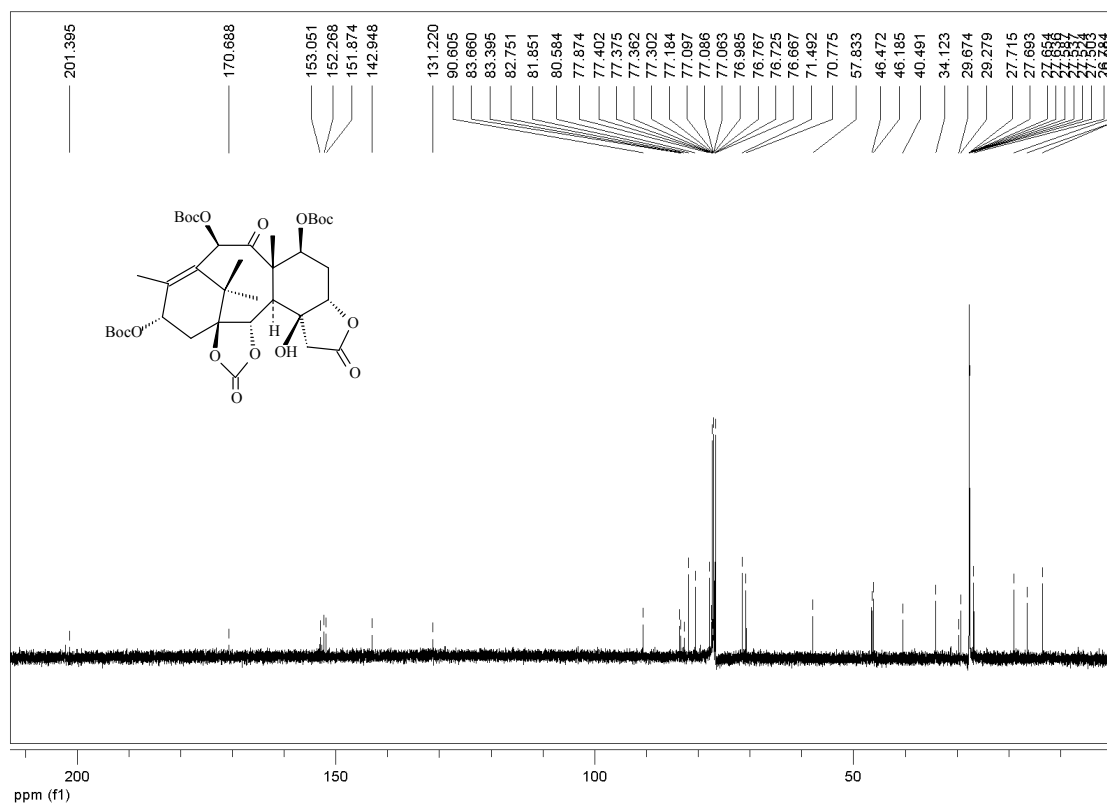
¹H NMR spectrum of compound **14**



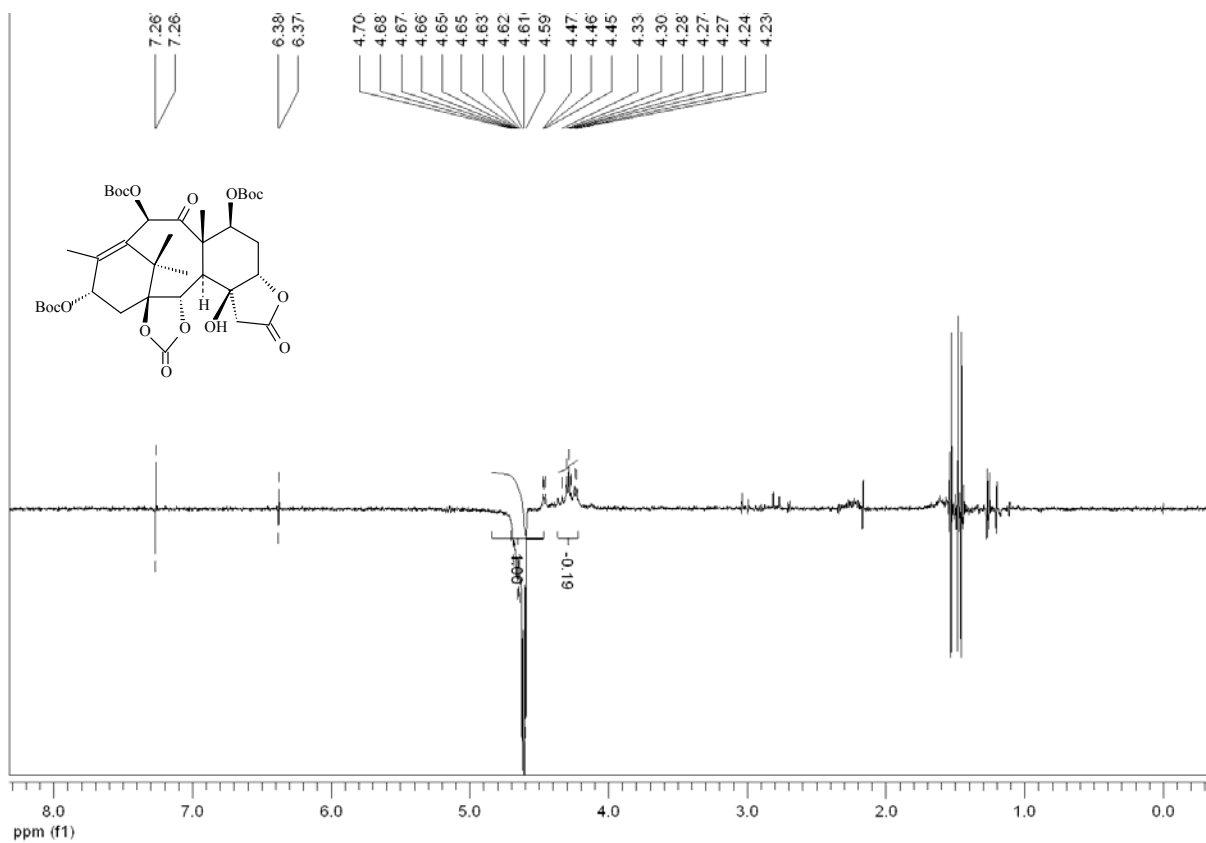
¹³C NMR spectrum of compound **14**



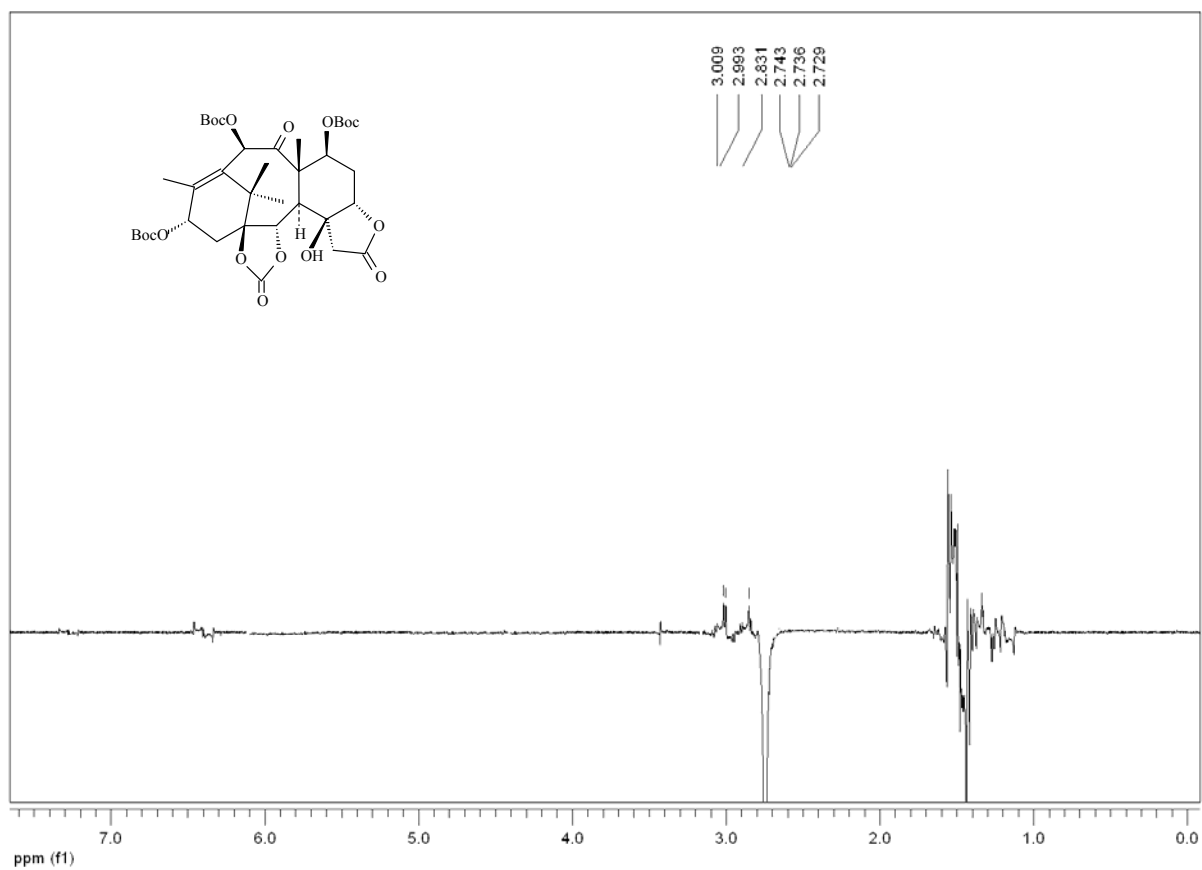
¹H NMR spectrum of compound **15**



¹³C NMR spectrum of compound **15**

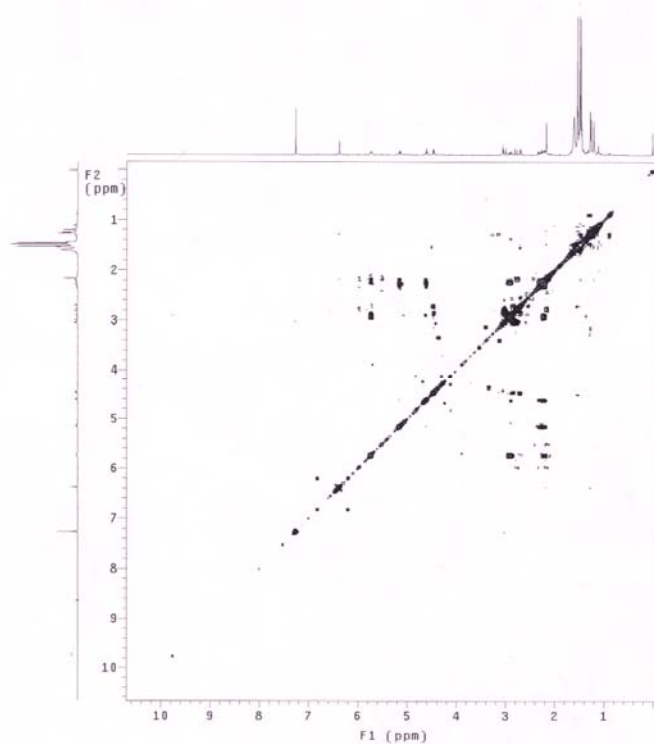
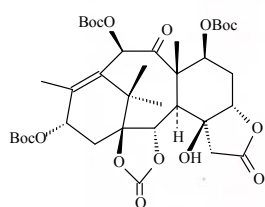


NOEds Spectrum of compound **15**

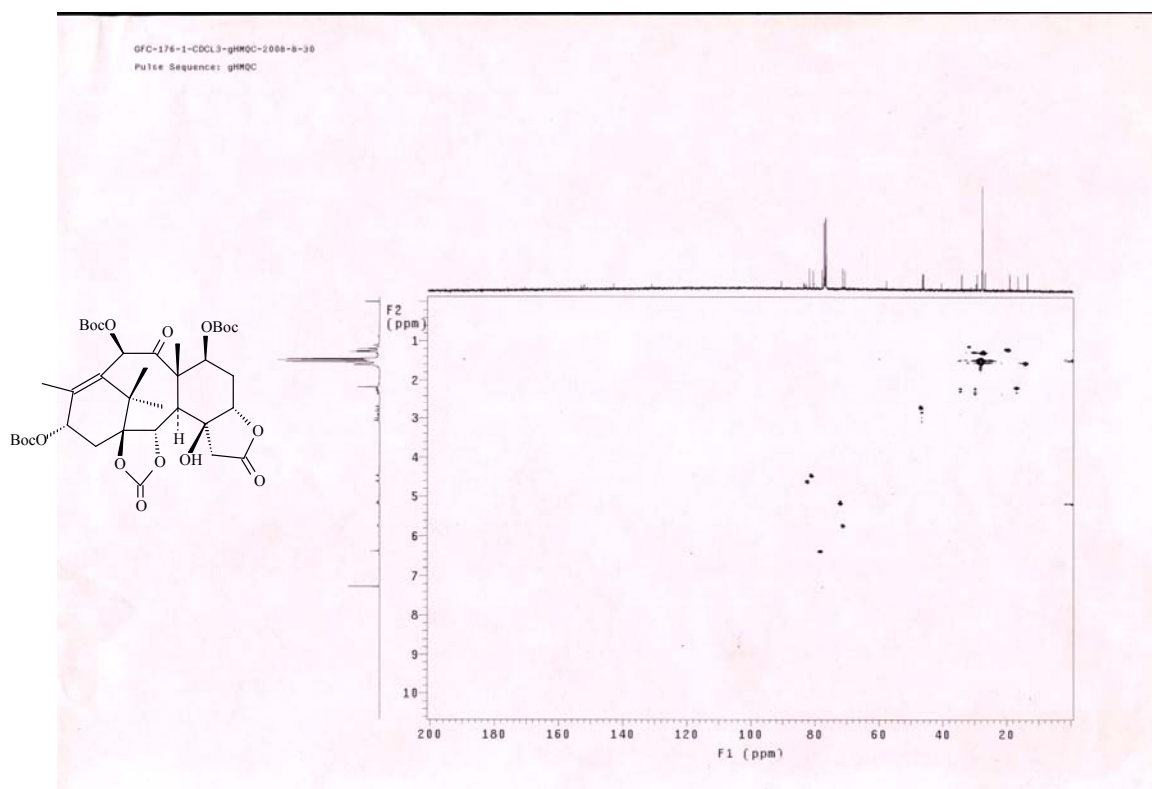


NOEds Spectrum of compound **15**

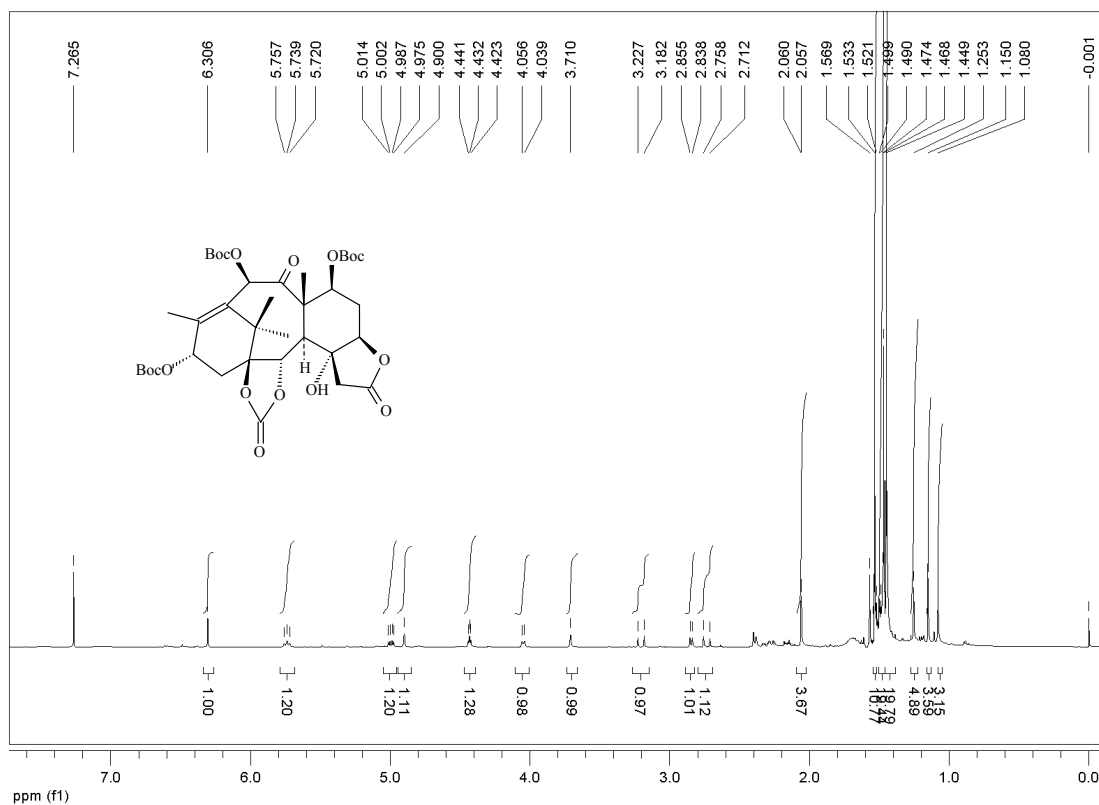
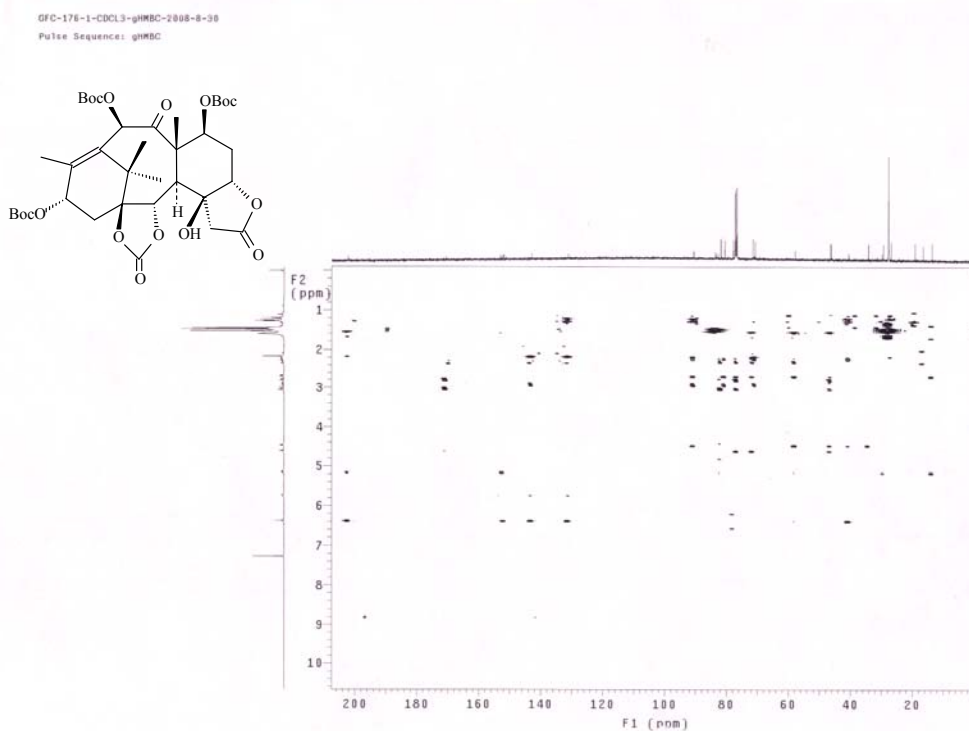
^1H - ^1H cosy



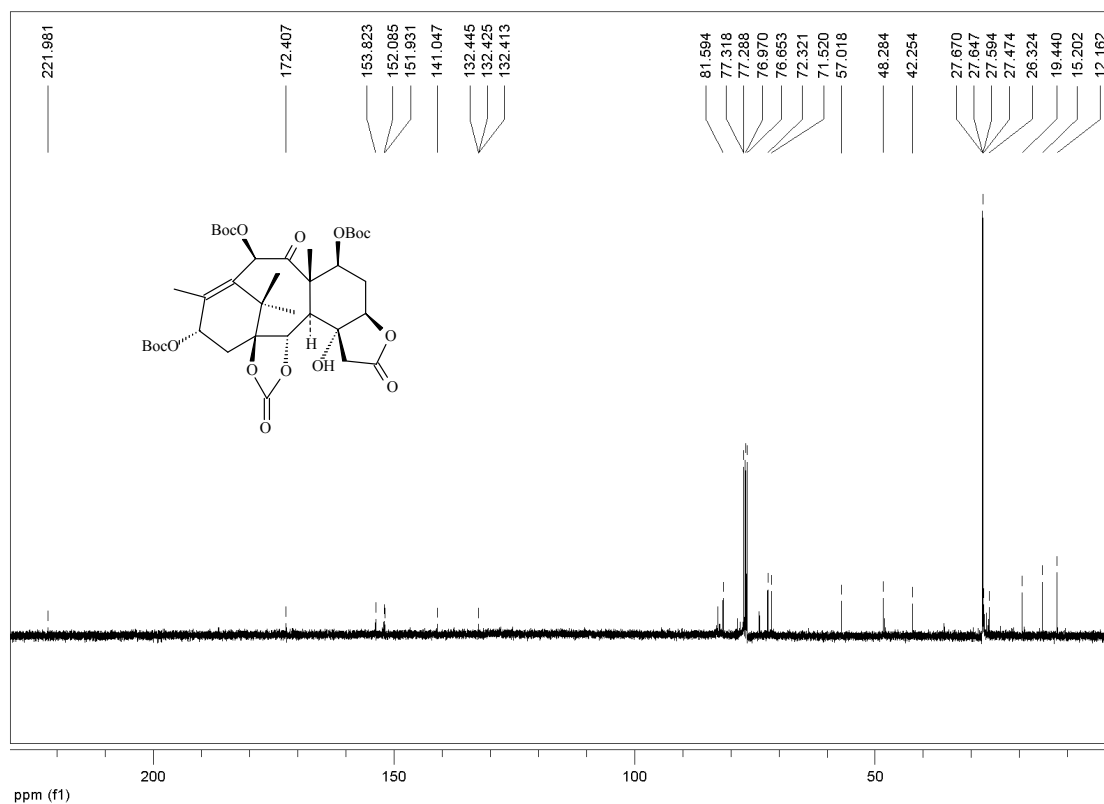
^1H - ^1H COSY spectrum of compound **15**



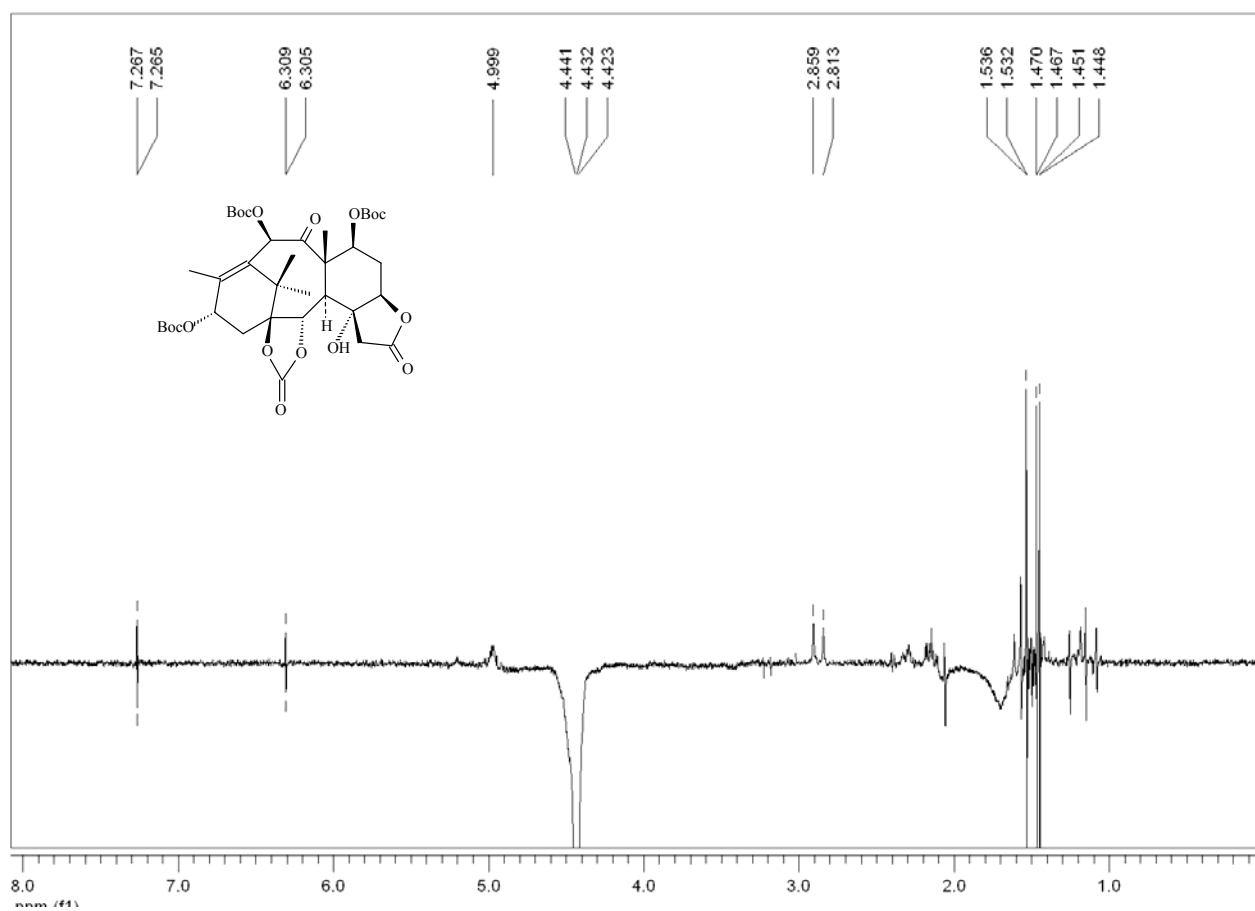
HMQC Spectrum of compound **15**



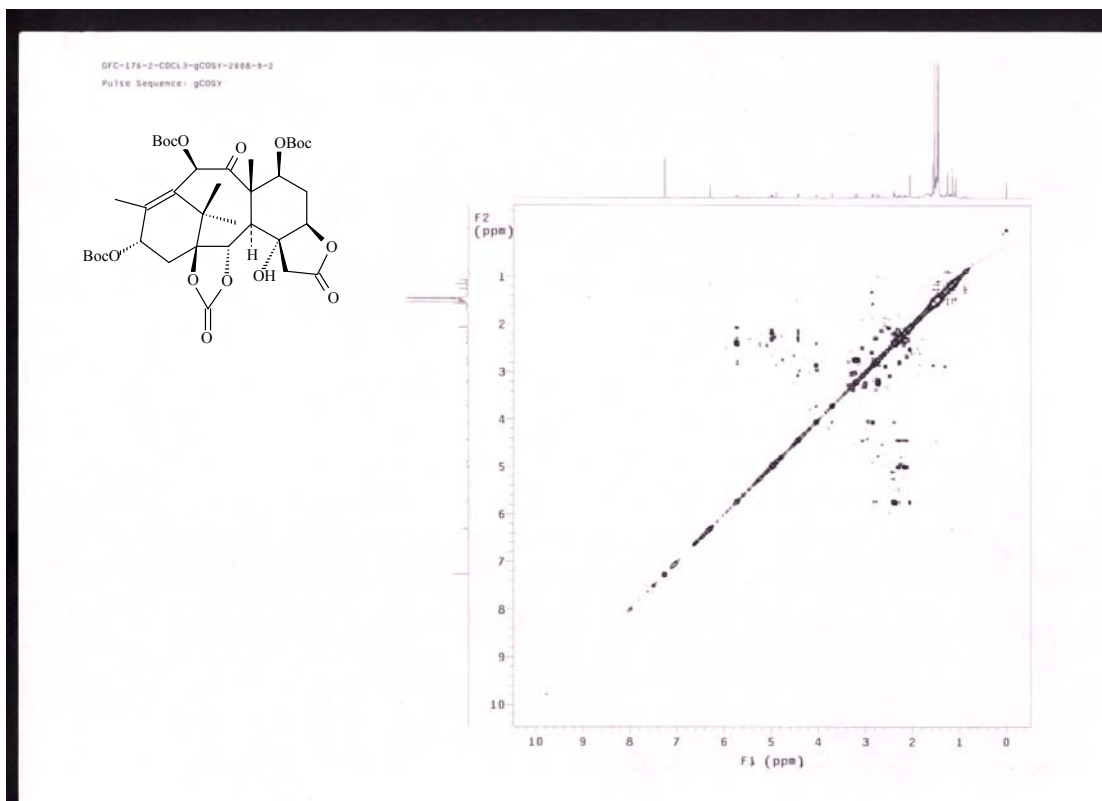
¹H NMR spectrum of compound 16



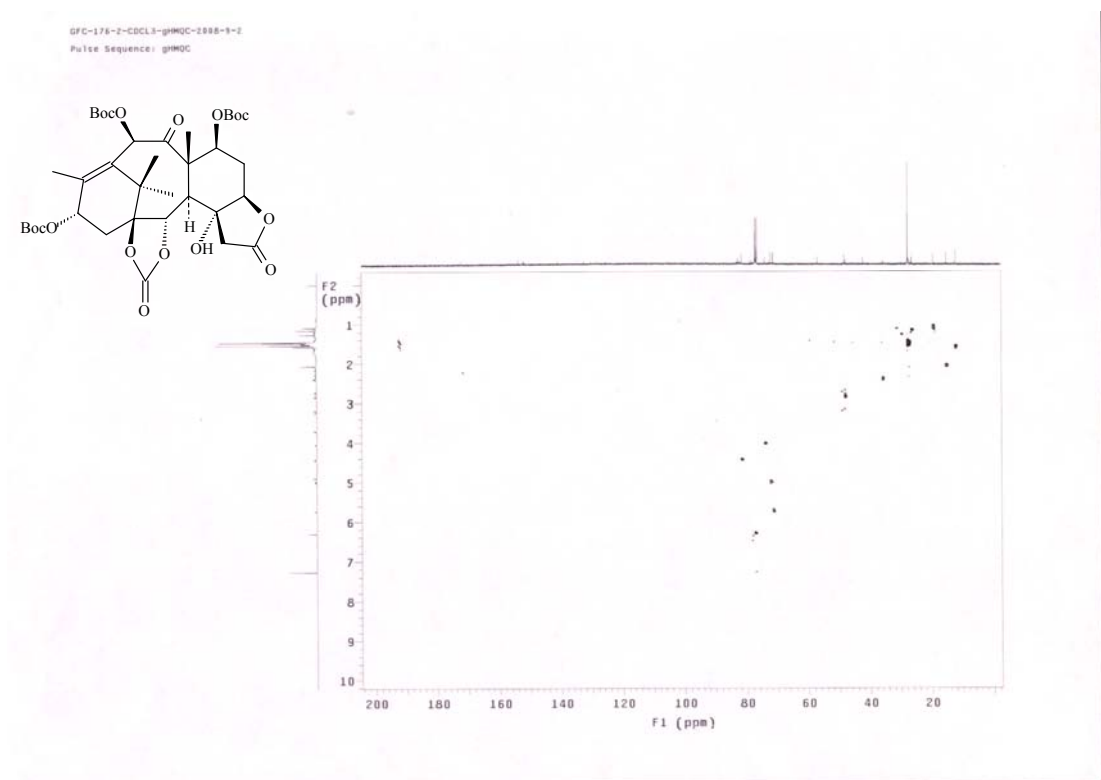
^{13}C NMR spectrum of compound **16**



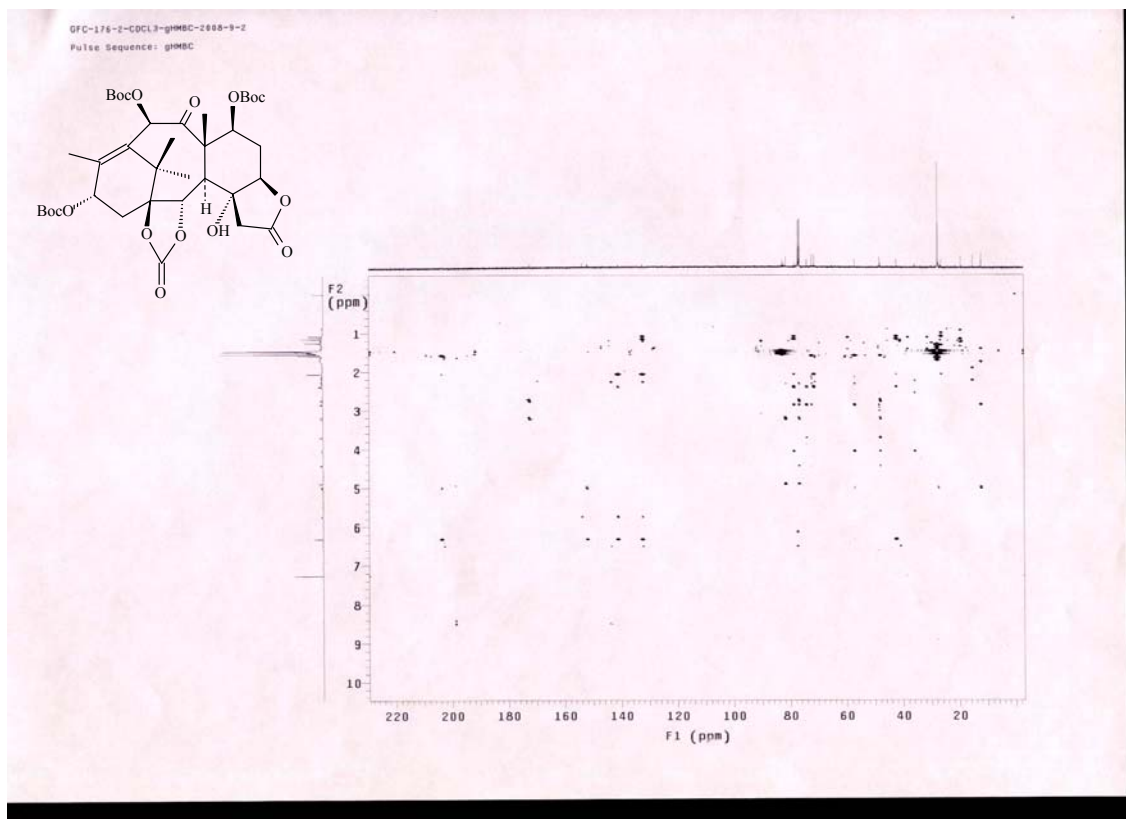
NOEs spectrum of compound **16**



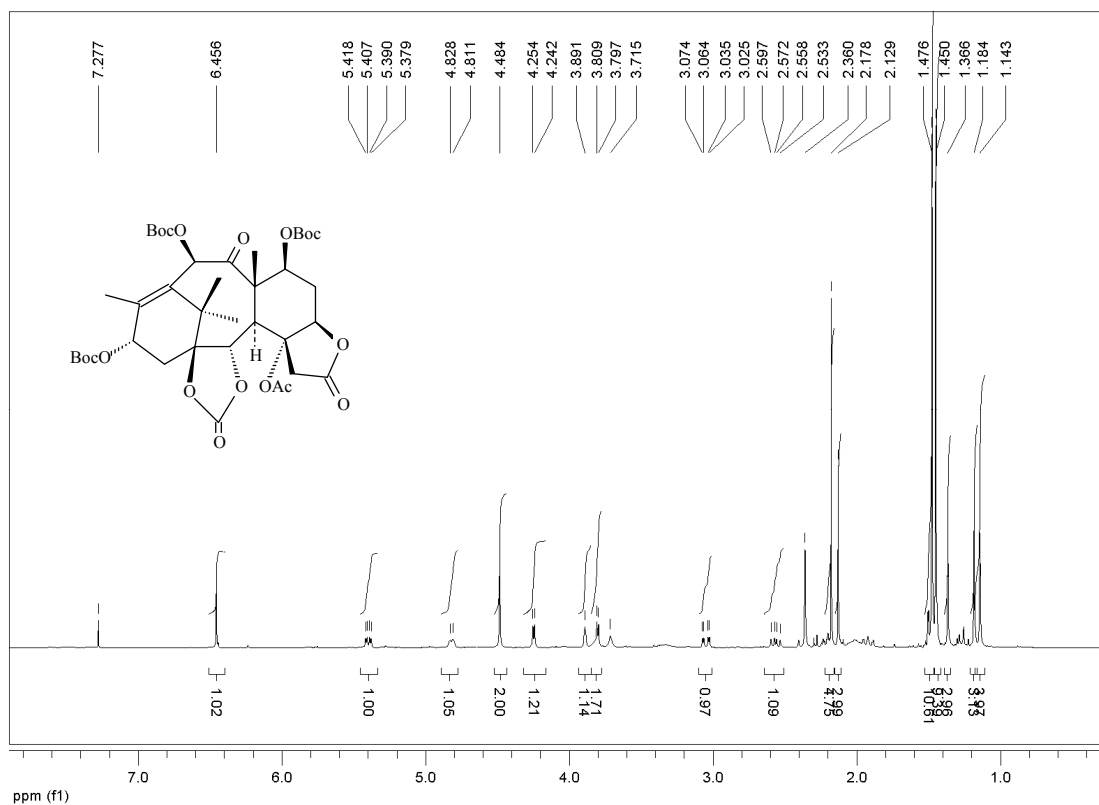
¹H-¹H COSY spectrum of compound 16



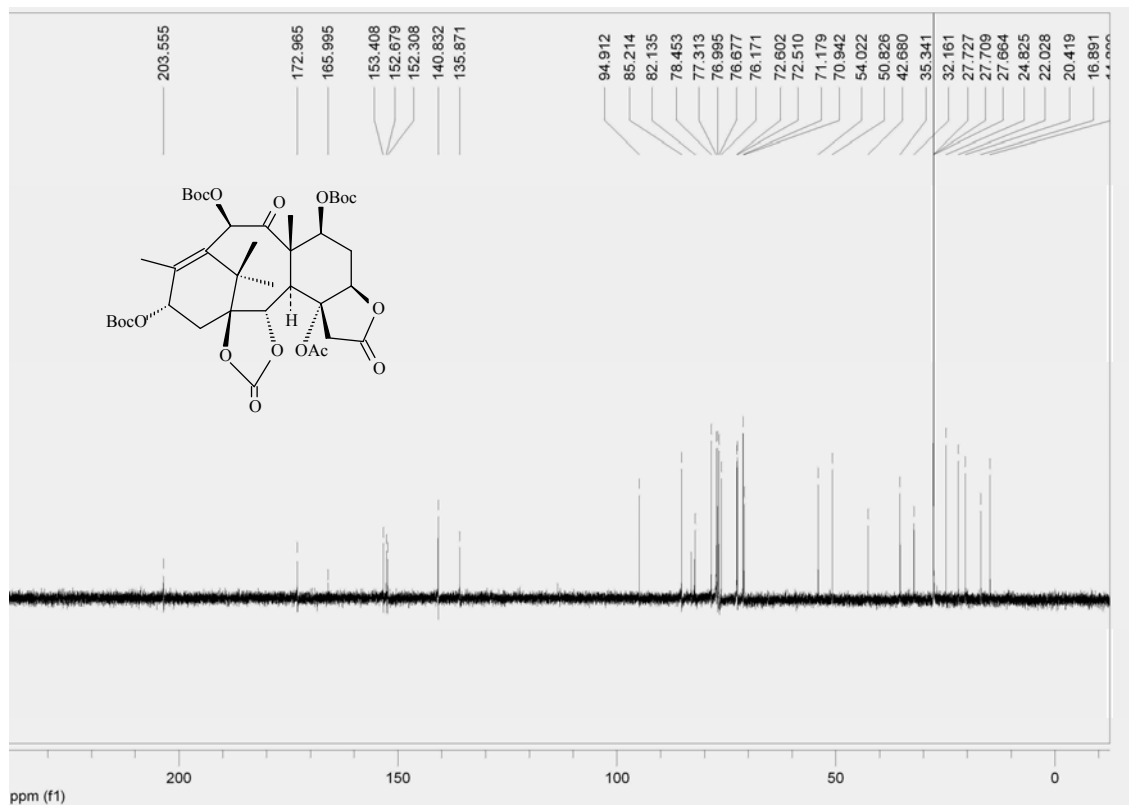
HMQC spectrum of compound 16



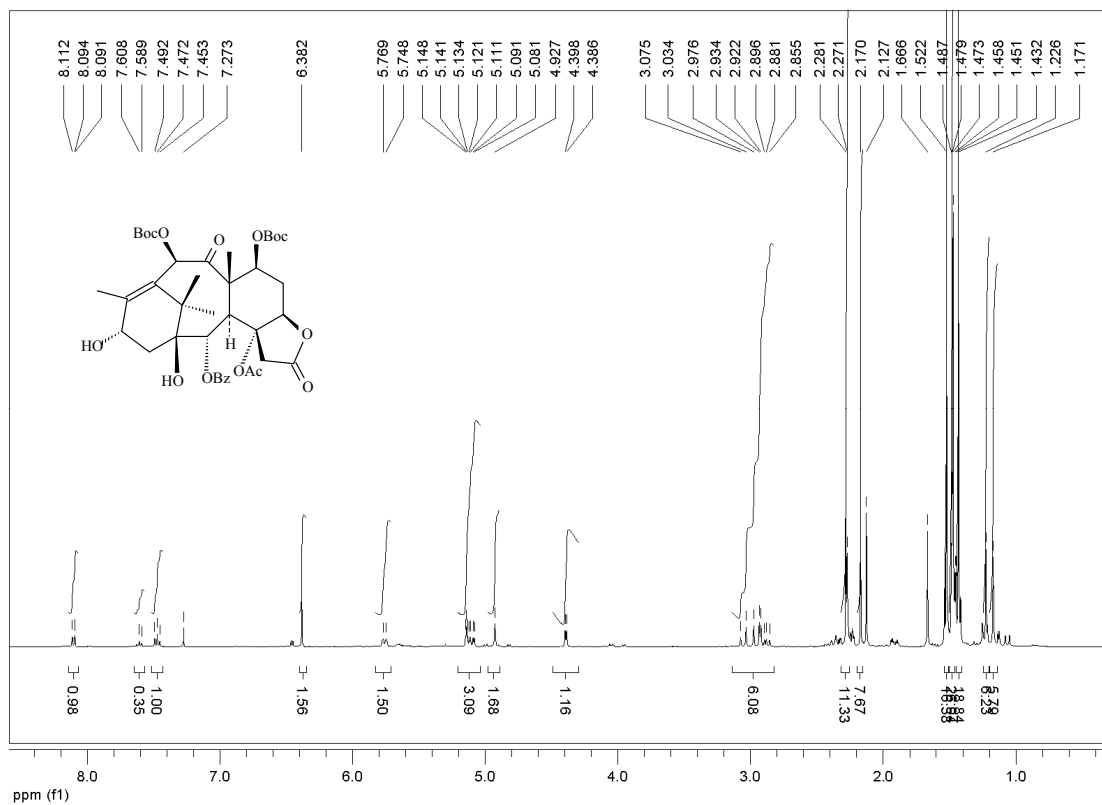
HMBC spectrum of compound 16



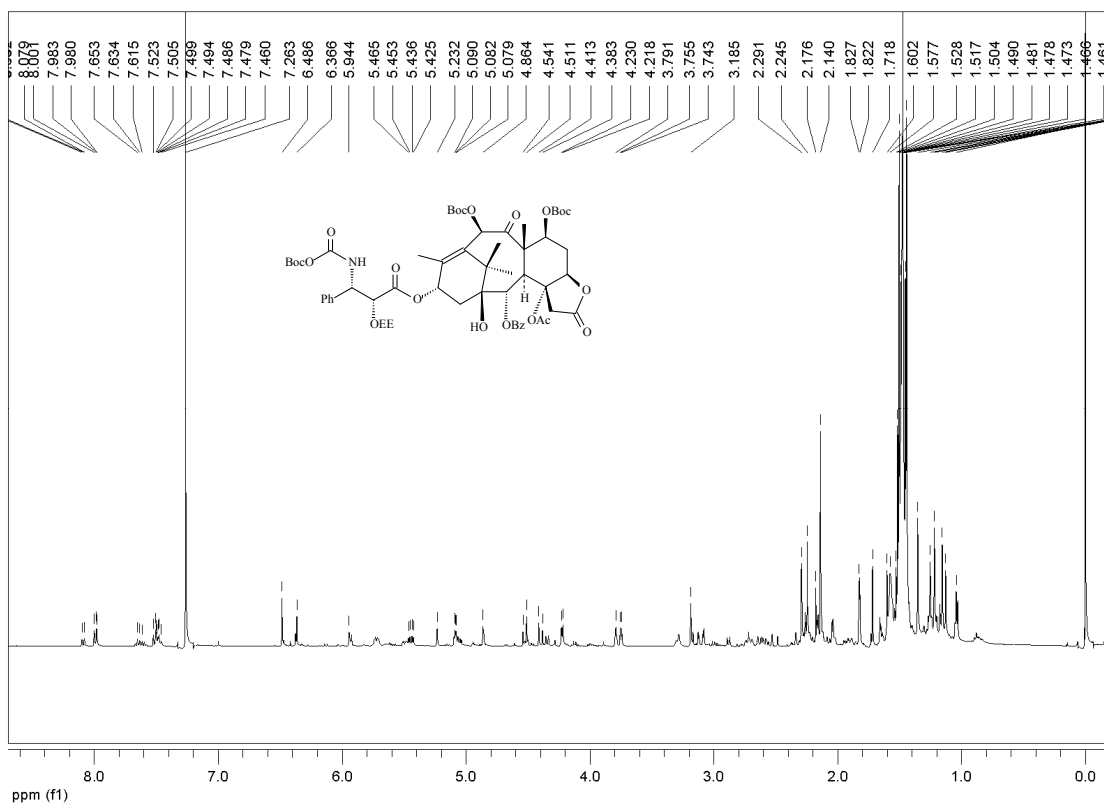
¹H NMR spectrum of compound 17



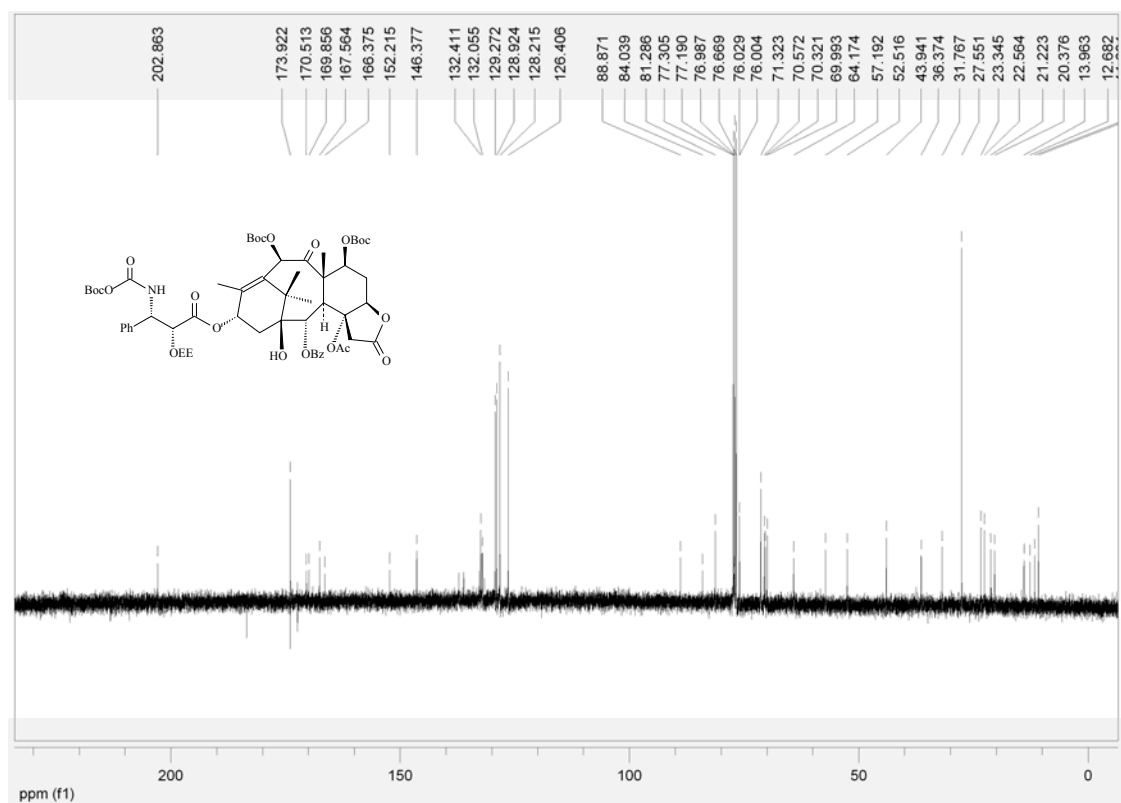
¹³C NMR spectrum of compound **17**



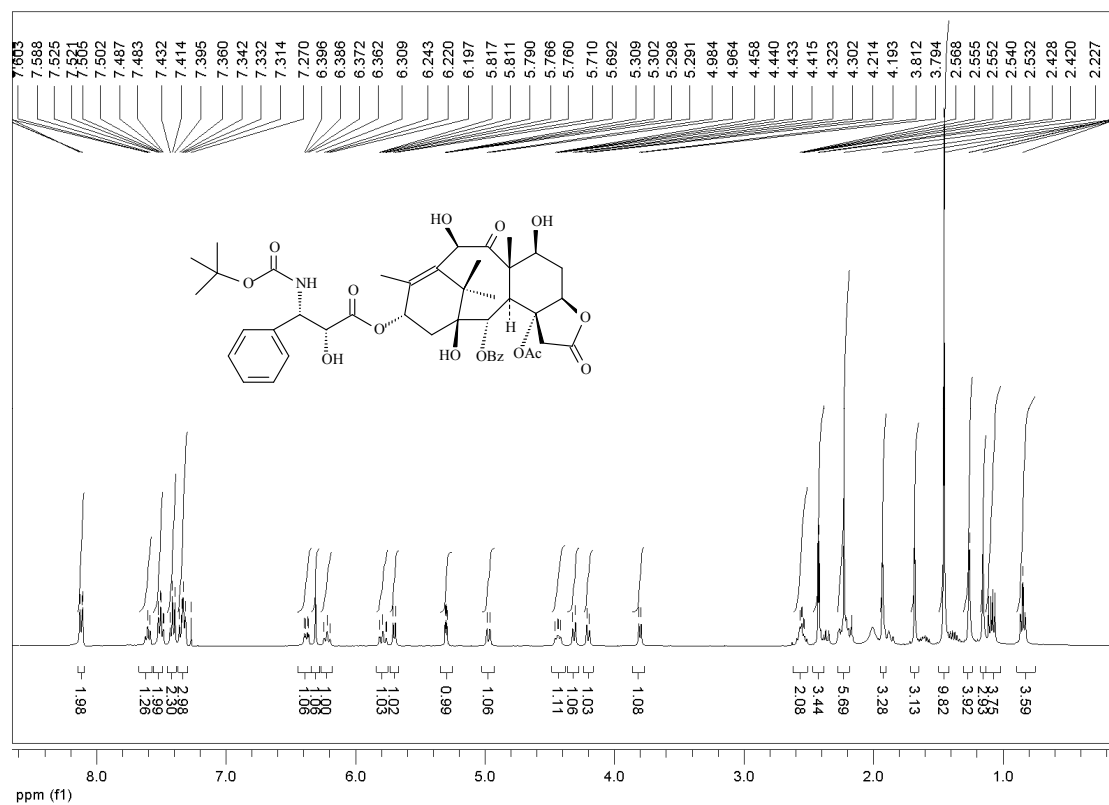
¹H NMR spectrum of compound **18**



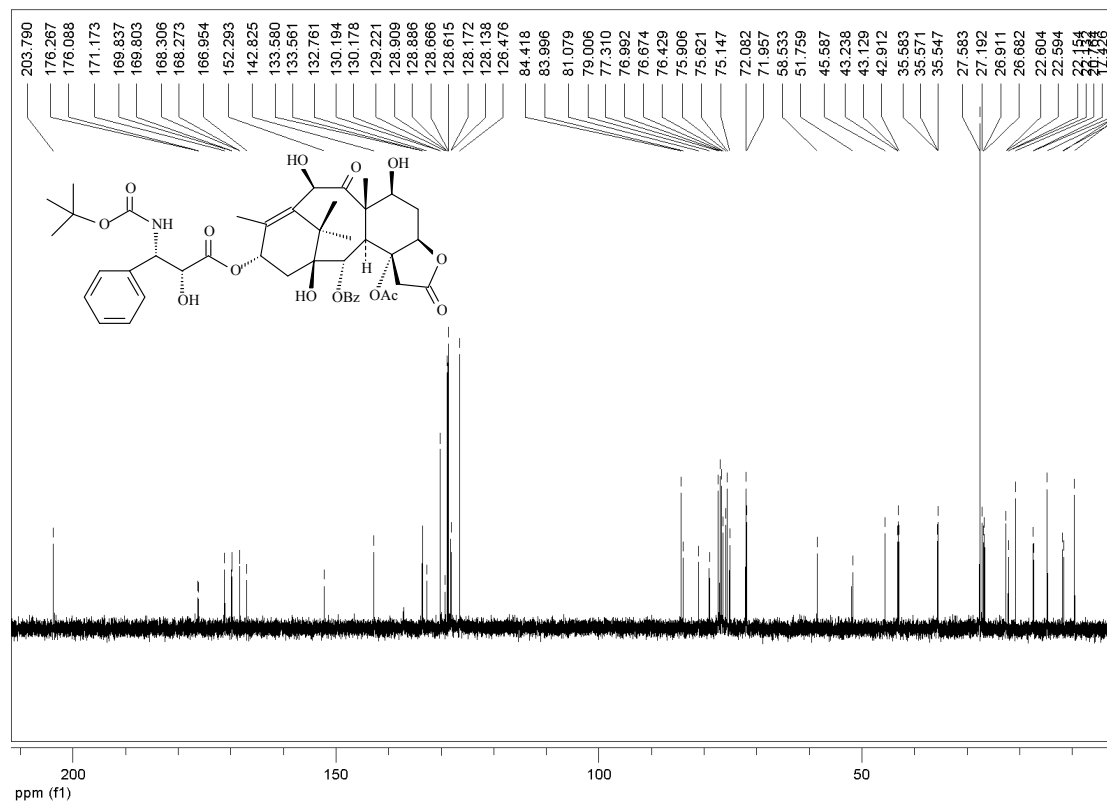
¹H NMR spectrum of side chain linked product of compound **18**



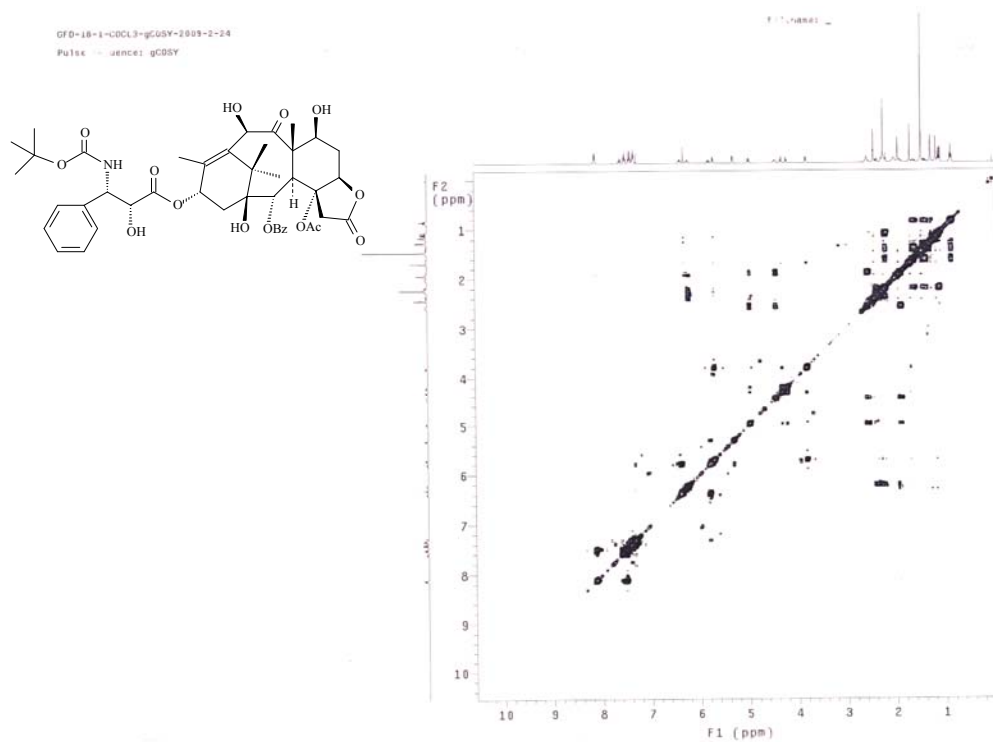
¹³C NMR spectrum of side chain linked product of compound **18**



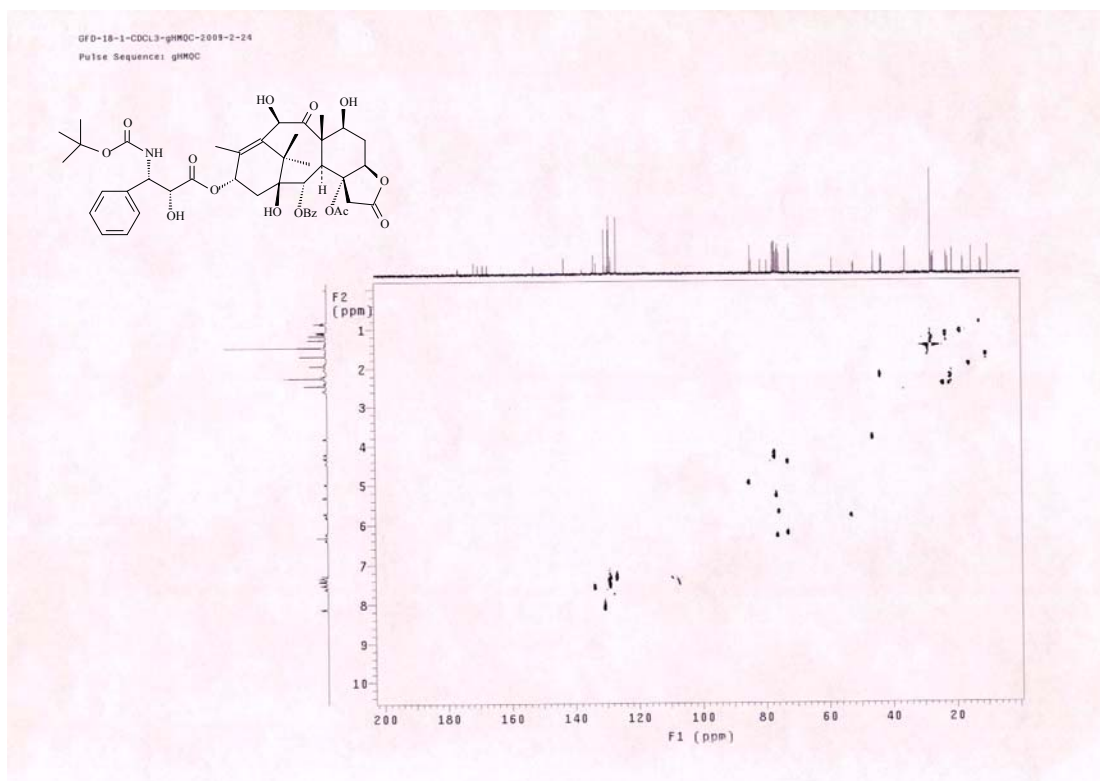
¹H NMR spectrum of compound 20



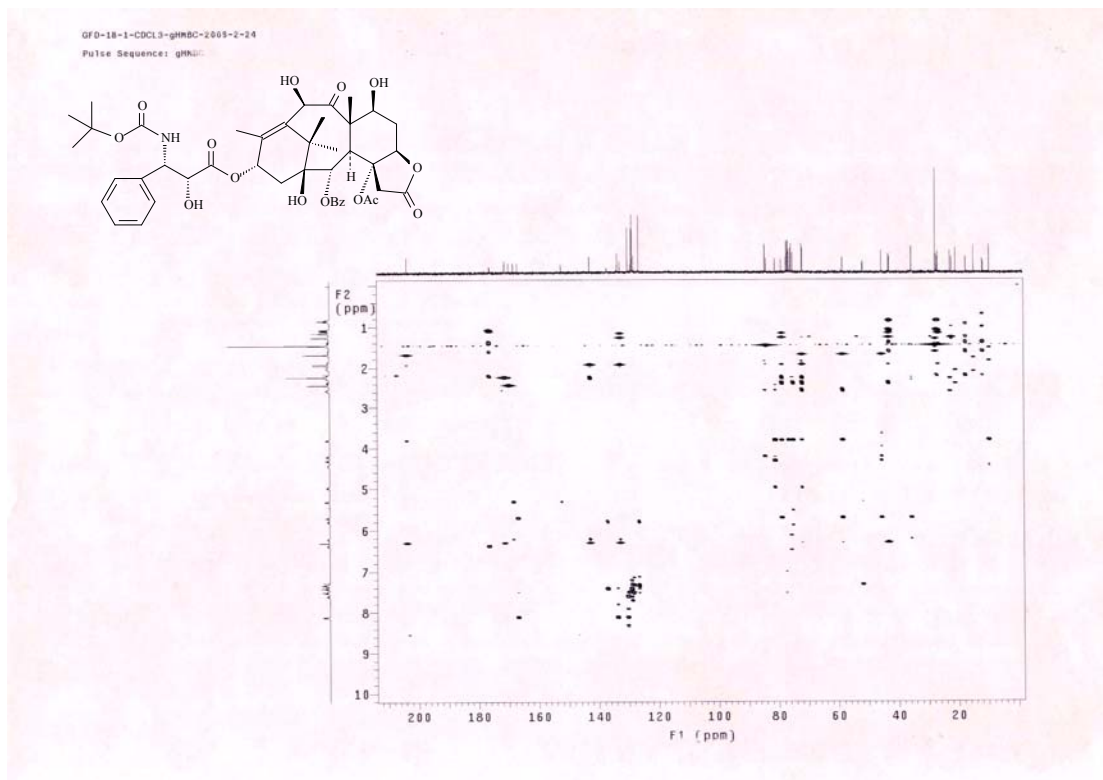
¹³C NMR spectrum of compound 20



¹H-¹H COSY spectrum of compound **20**

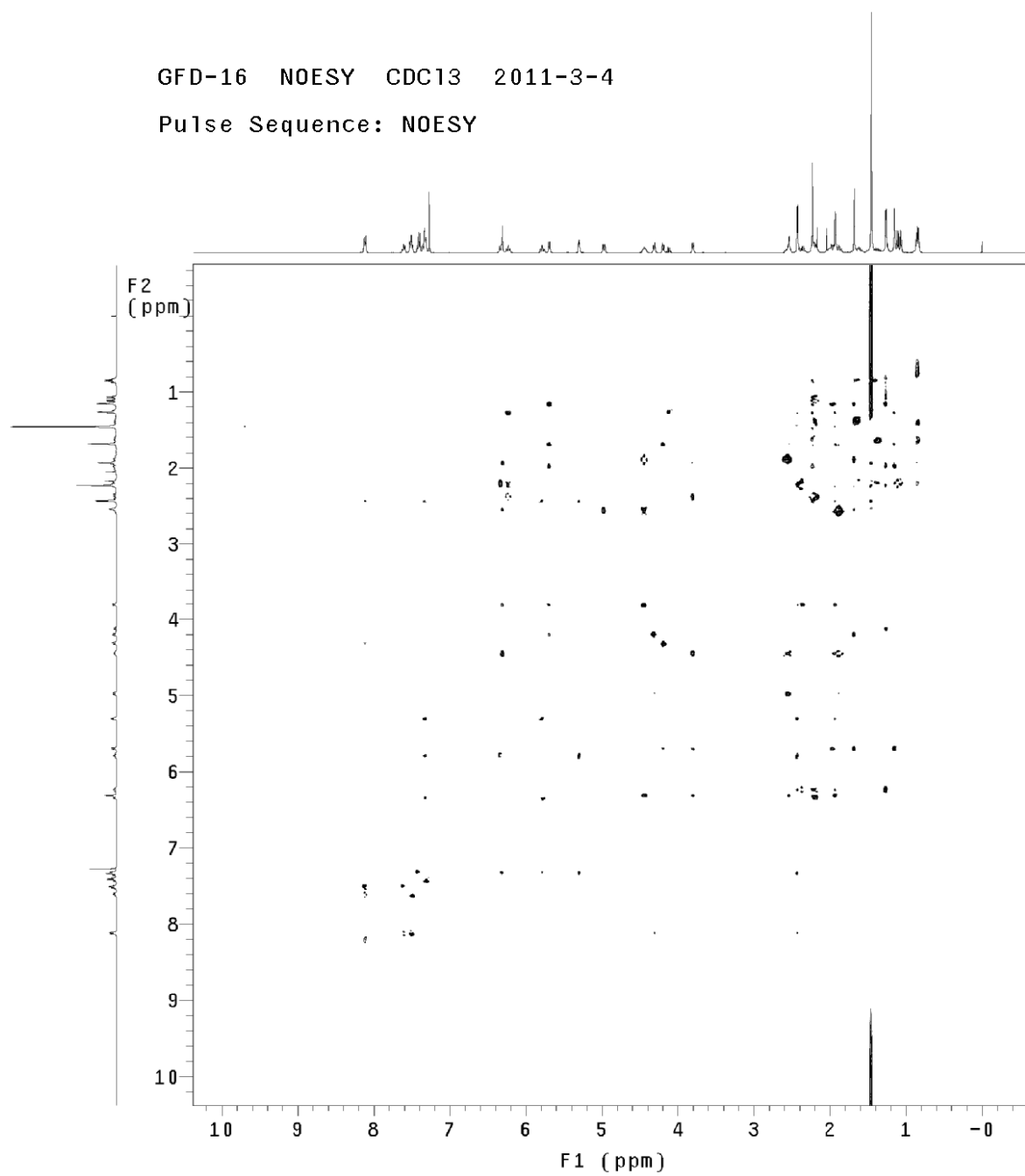


HMQC spectrum of compound **20**



GFD-16 NOESY CDC13 2011-3-4

Pulse Sequence: NOESY



NOESY spectrum of compound **20**