

Synthesis of Trichodermin Derivatives and Their Antimicrobial and Cytotoxic Activities.

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








Part A: General conditions for the preparation of compounds 7–15.....S2

Part B: Antimicrobial and cytotoxic activities of compounds 1–16.....S3–S4

Part C: ¹H and ¹³C-NMR spectra for compounds 3–16.....S5–S18

PART A : PREPARATION OF COMPOUNDS 7–15

Table S1. Reaction condition data for preparation of 7–15.

Entry	acyl halide (mmol)	Trichodermol (mmol)	Pyridine (μ L)	CH ₂ Cl ₂ (mL)	time (h)	yield (%)
7	 0.14	0.04	100	4	15	85
8	 0.1	0.04	100	2	2	44.5
9	 0.2	0.08	200	4	2	91.7
10	 0.2	0.08	200	4	2	91.9
11	 0.2	0.08	200	4	2	81.8
12	 0.24	0.08	200	3	1	47.7
13	 0.1	0.04	100	2	2	62
14	 0.2	0.08	200	4	2	56.3
15	 0.2	0.08	200	4	2	94

PART B: BIOLOGICAL ACTIVITIES

Table S2. Antimicrobial activity of compounds 1-16. The results are expressed as MIC in µg/mL.

Entry	<i>A. baumannii</i> MB5973	<i>E.coli</i> MB2884	<i>E.coli</i> MB5746	<i>P. aeruginosa</i> MB5919	<i>S. aureus</i> EPI167	MRSA 5393	<i>C. albicans</i> MY1055	<i>B. subtilis</i> MB964
1	>64	>64	>64	>64	>64	>64	<4	no halo
2	>64	>64	>64	>64	>64	>64	8-16	no halo
3	>64	>64	>64	>64	>64	>64	>64	no halo
4	>64	>64	>64	>64	>64	>64	>64	no halo
5	>64	>64	>64	>64	>64	>64	>64	no halo
6	>64	>64	>64	>64	>64	>64	>64	no halo
7	>64	>64	>64	>64	>64	>64	16-32	no halo
8	>64	>64	nd	>64	>64	nd	nd	nd
9	>64	>64	64	>64	>64	>64	4-8	no halo
10	>64	>64	32	>64	>64	>64	8	no halo
11	>64	>64	32	>64	>64	>64	>64	no halo
12	>64	>64	>64	>64	>64	>64	4	no halo
13	>64	>64	>64	>64	>64	>64	4	no halo
14	>64	>64	>64	>64	>64	>64	8-16	no halo
15	>64	>64	>64	>64	>64	>64	8	no halo
16	>64	>64	>64	>64	>64	>64	>64	no halo

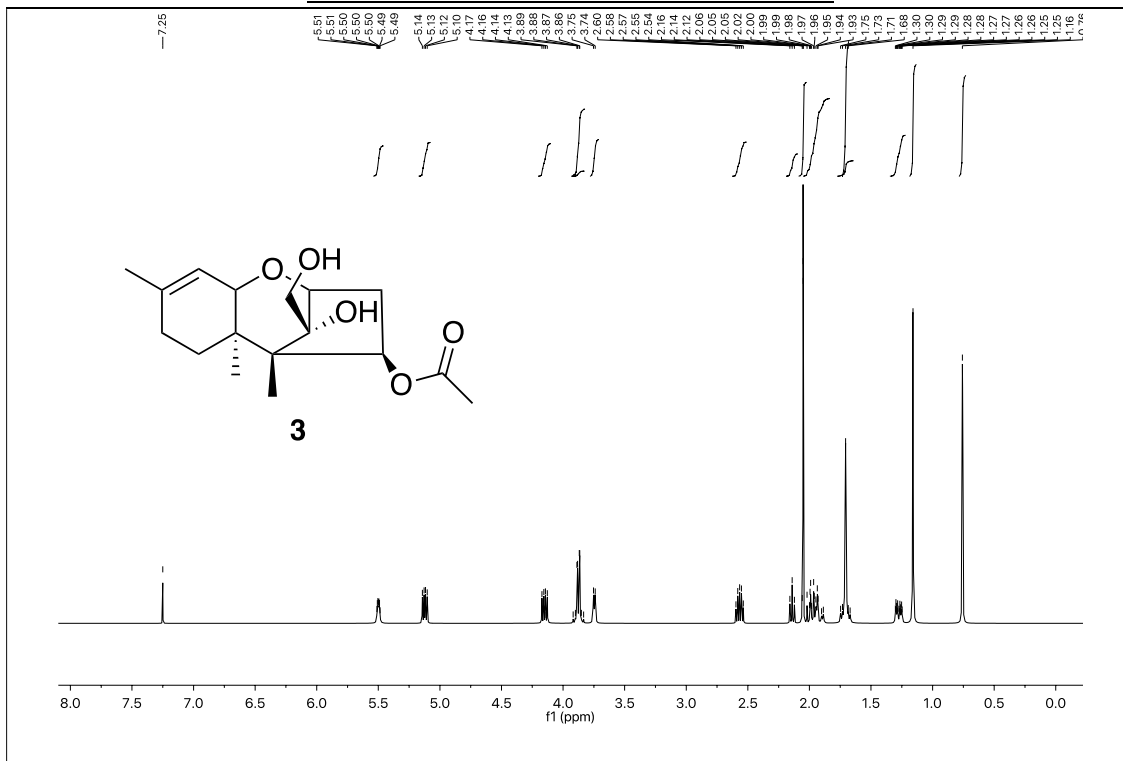
Nd = no data; MRSA= Methicillin-resistant *S. aureus*; MIC= minimal inhibitory concentration

Table S3. Cytotoxicity of compounds **1-16** in different human cell lines, measured at 24 hours of incubation. IC₅₀ (µg/mL).

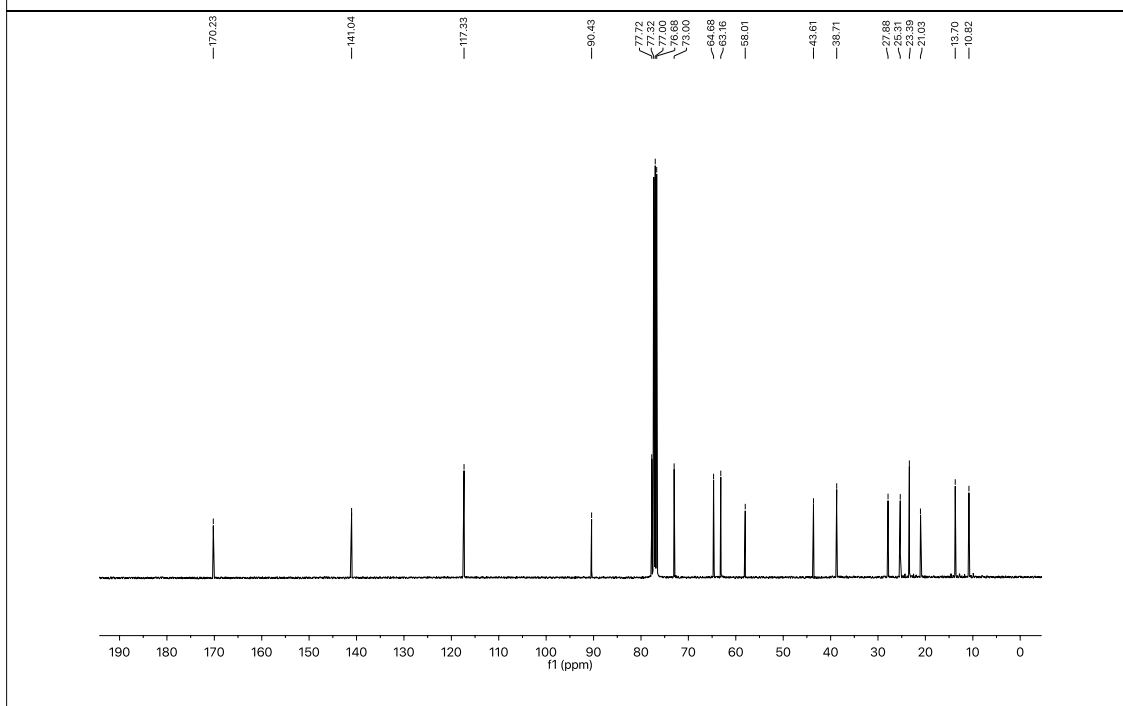
Entry	<i>A549</i>	<i>HepG2</i>	<i>HT29</i>	<i>MCF-7</i>	<i>RCC4-VA</i>	<i>RCC4-VHL</i>	<i>Fa2N4</i>
1	>20	>20	>20	<1.25	14.19	>20	12.09
2	>20	>20	>20	4.42	>20	>20	>20
3	>20	>20	>20	>20	>20	>20	>20
5	>20	>20	>20	>20	>20	>20	>20
6	>20	>20	>20	>20	>20	>20	>20
7	>20	>20	>20	13.52	>20	>20	>20
9	>20	>20	>20	1.93	>20	>20	>20
10	>20	14.20	>20	3.59	>20	>20	>20
11	>20	>20	>20	11.26	>20	>20	>20
12	>20	>20	>20	3.78	6.02	8.00	>20
13	>20	17.48	>20	2.15	>20	>20	>20
14	>20	>20	>20	5.22	>20	>20	>20
15	>20	>20	>20	2.03	17.14	>20	>20
16	>20	>20	>20	>20	>20	>20	>20

A549 = adenocarcinomic alveolar basal epithelial cells (CCL-185); HepG2= liver hepatocellular (CCL-8065); HT29= colorectal adenocarcinoma (HTB-38); MCF-7= breast carcinoma (HTB-22); RCC4-VA and RCC4-VHL = renal carcinoma; Fa2N4= immortalized human hepatocytes

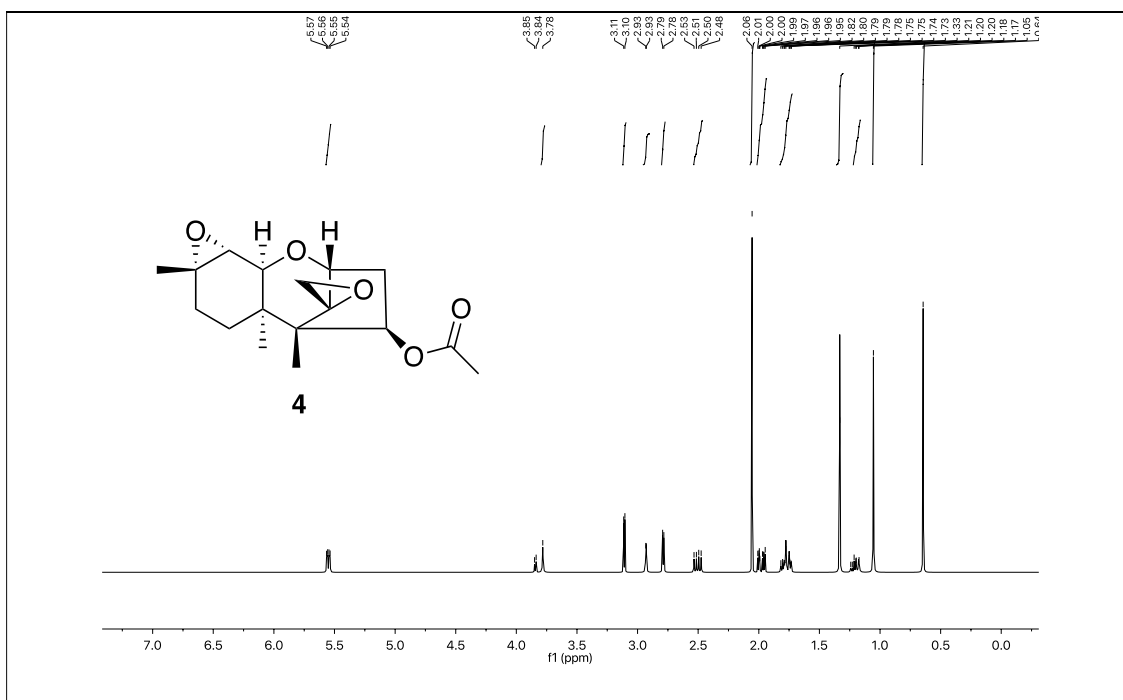
PART C: ¹H AND ¹³C-NMR SPECTRA



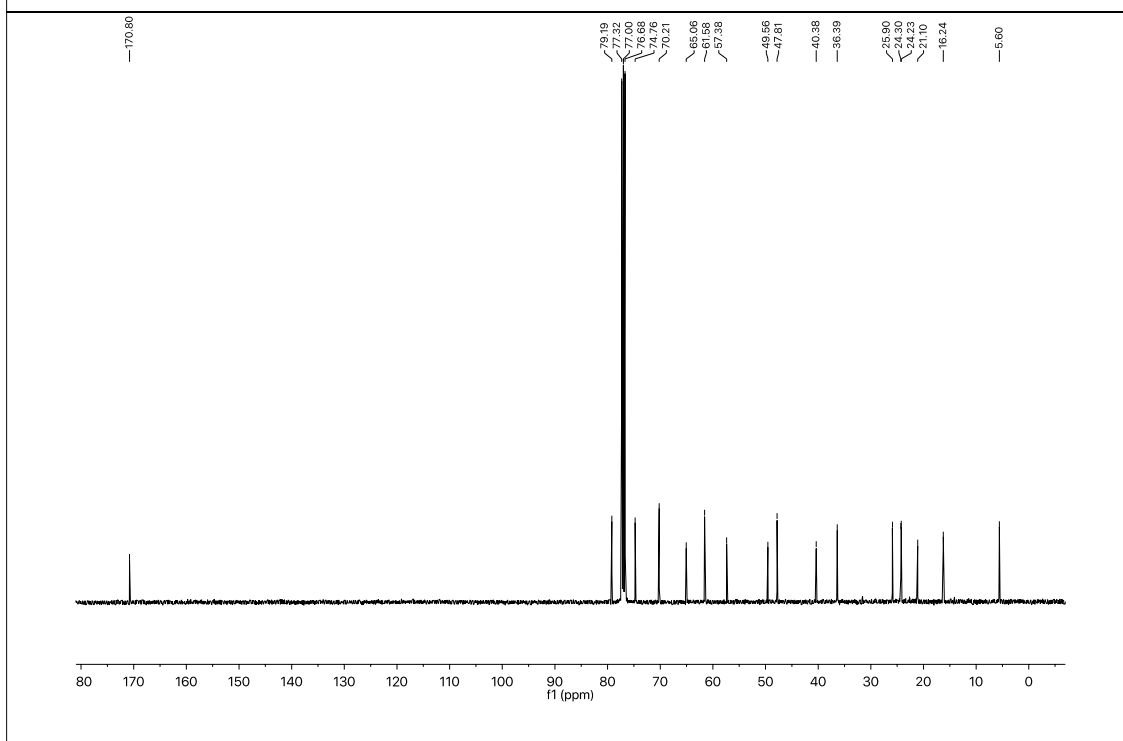
400 MHz ¹H NMR of compound 3 in CDCl₃



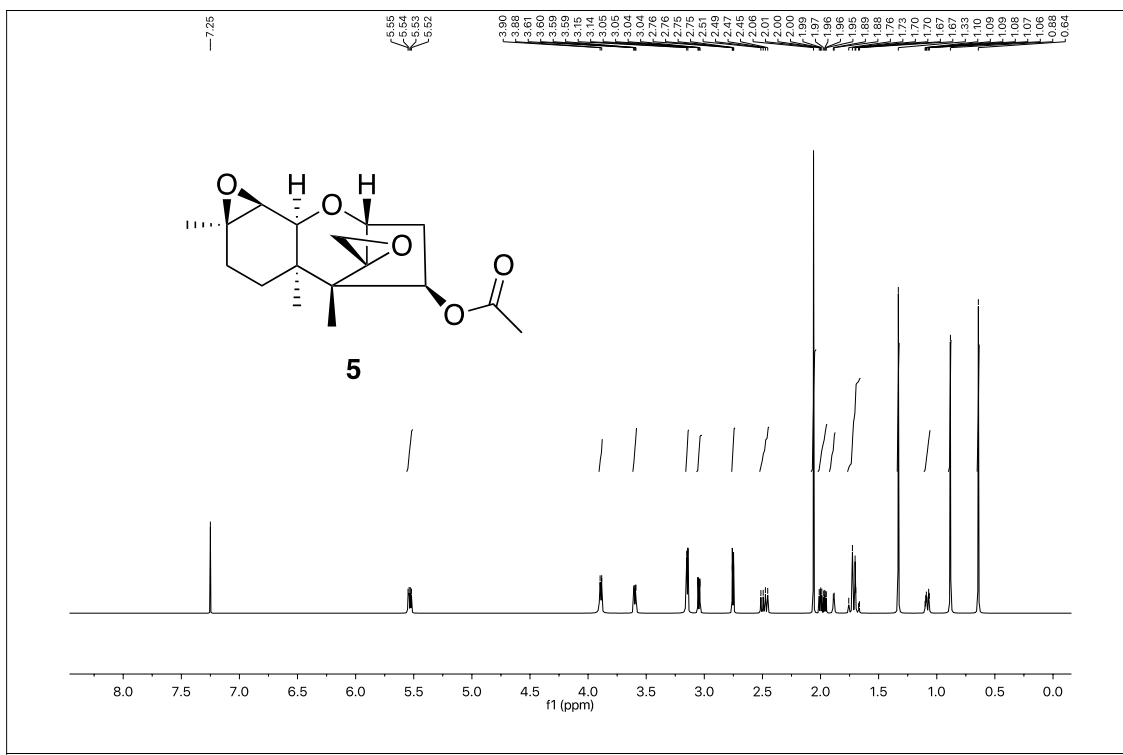
100 MHz ¹³C NMR of compound 3 in CDCl₃



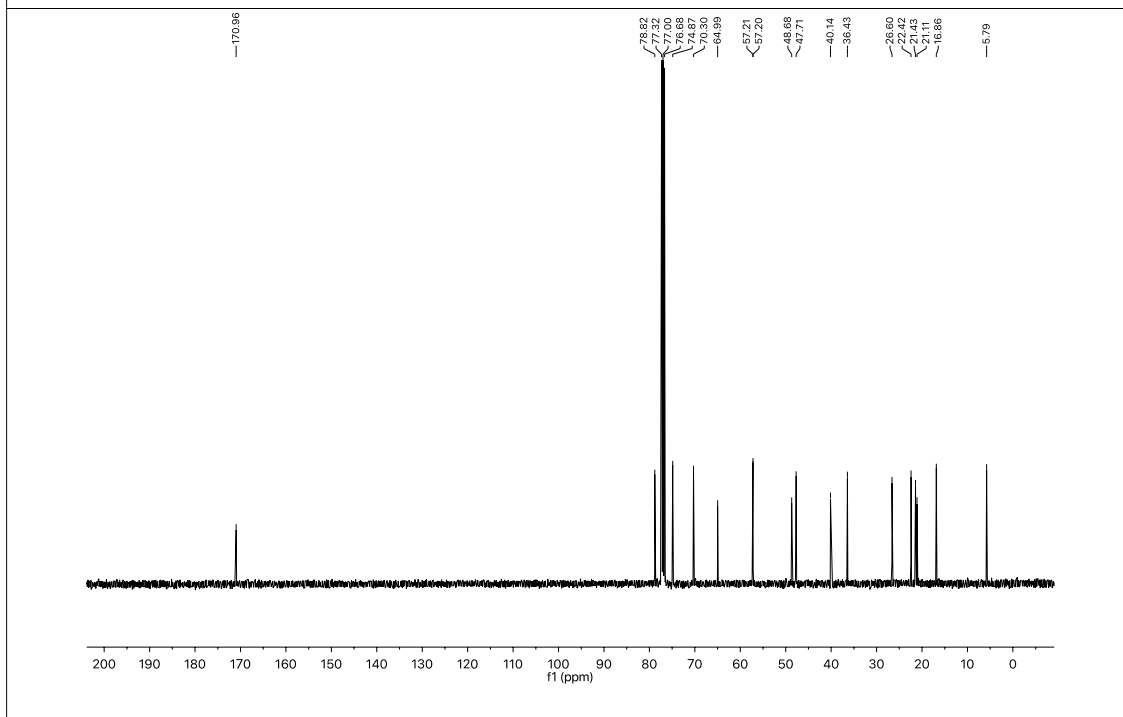
400 MHz ^1H NMR of compound **4** in CDCl_3



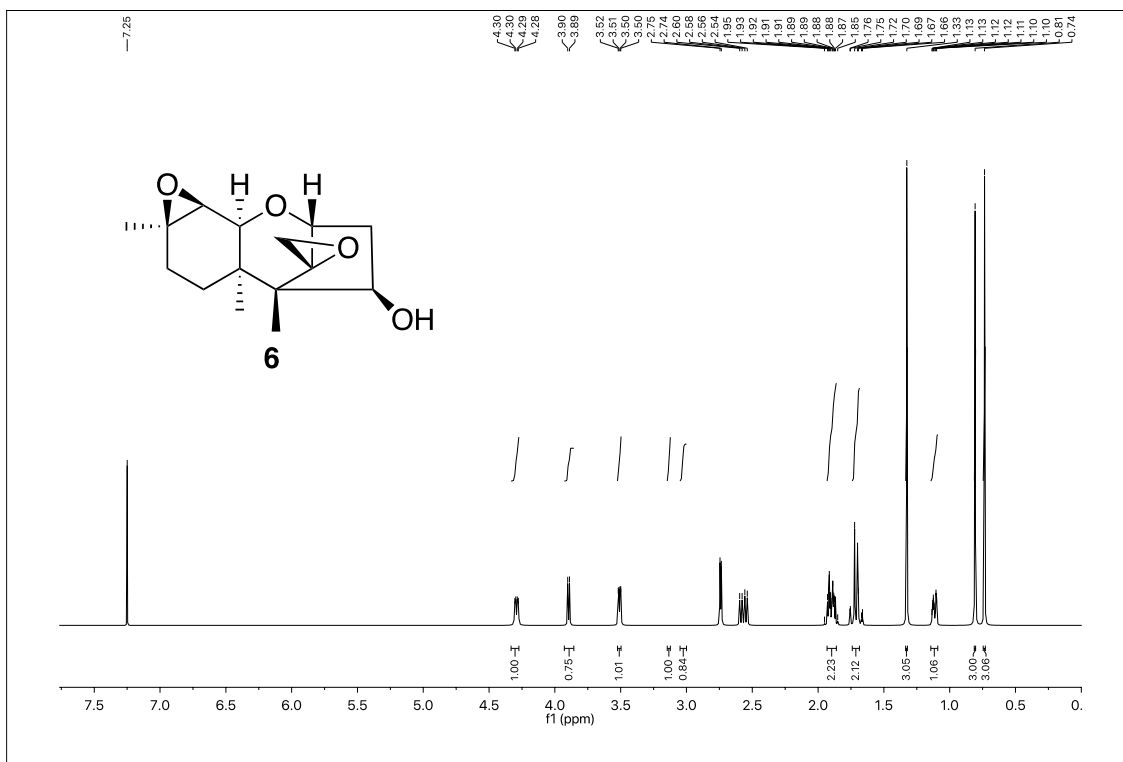
100 MHz ^{13}C NMR of compound **4** in CDCl_3



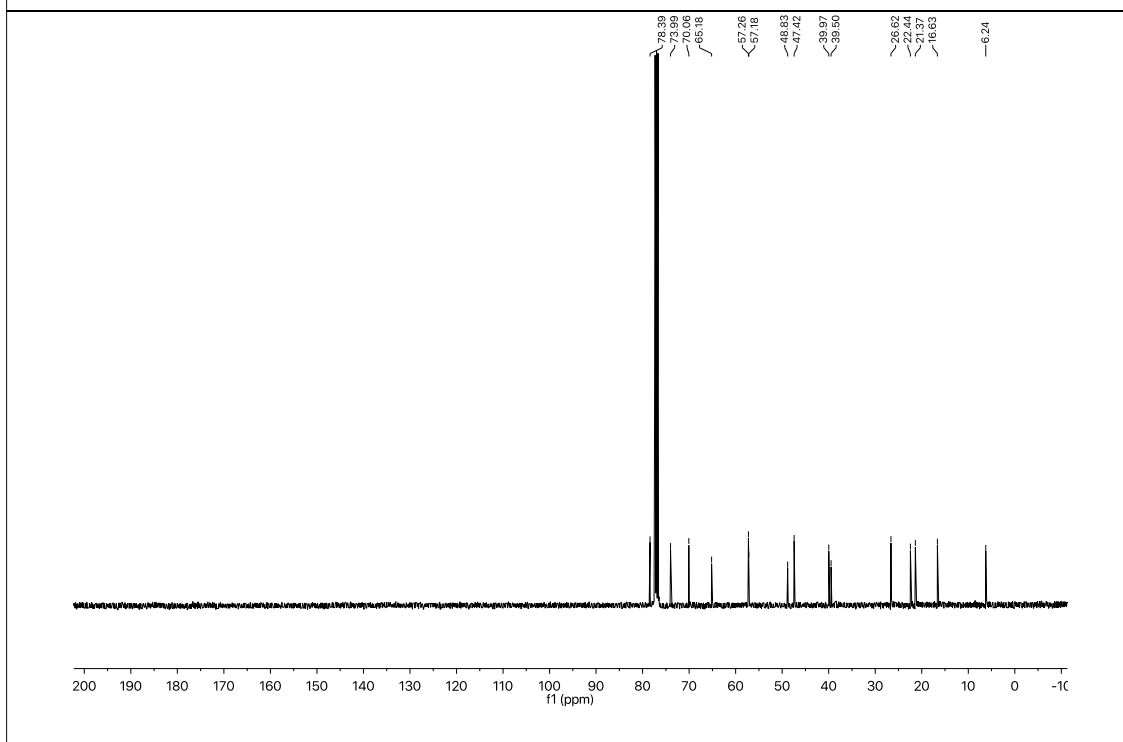
400 MHz ^1H NMR of compound 5 in CDCl_3



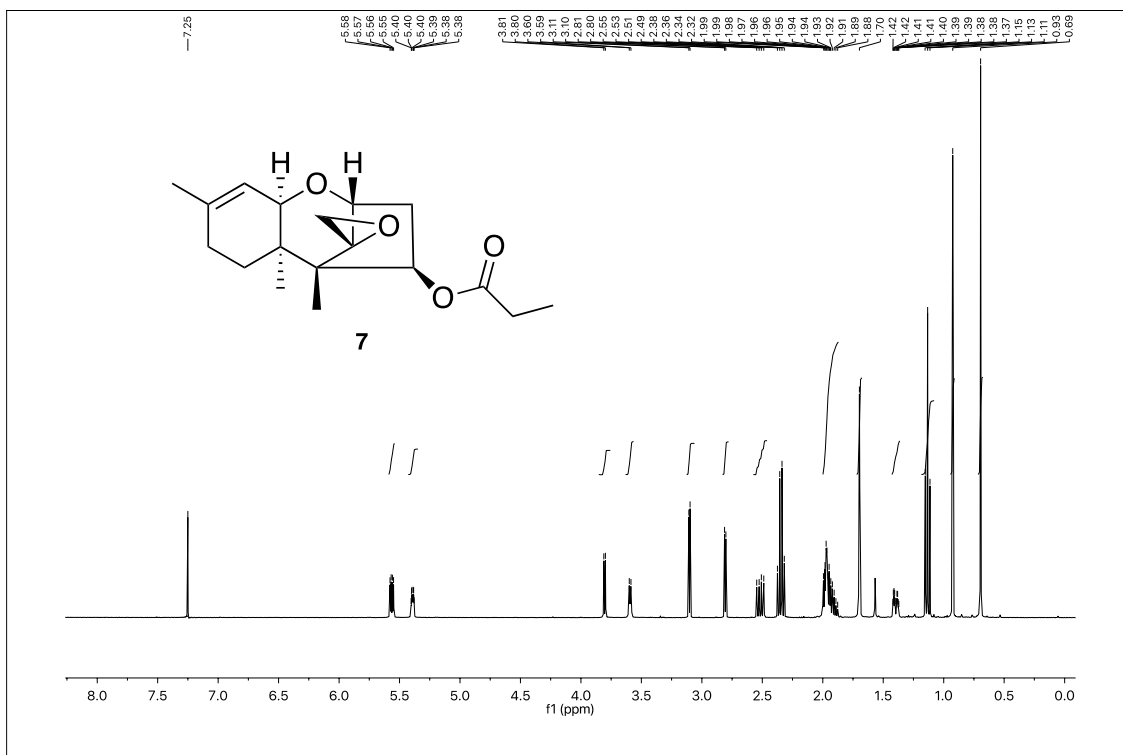
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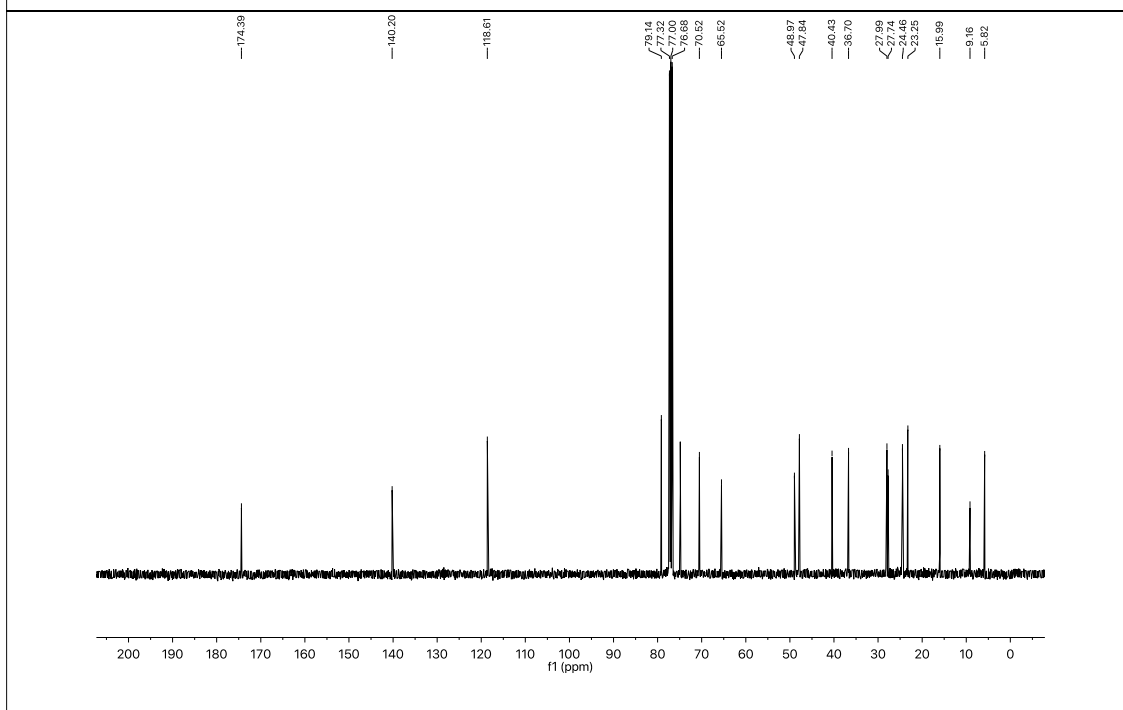
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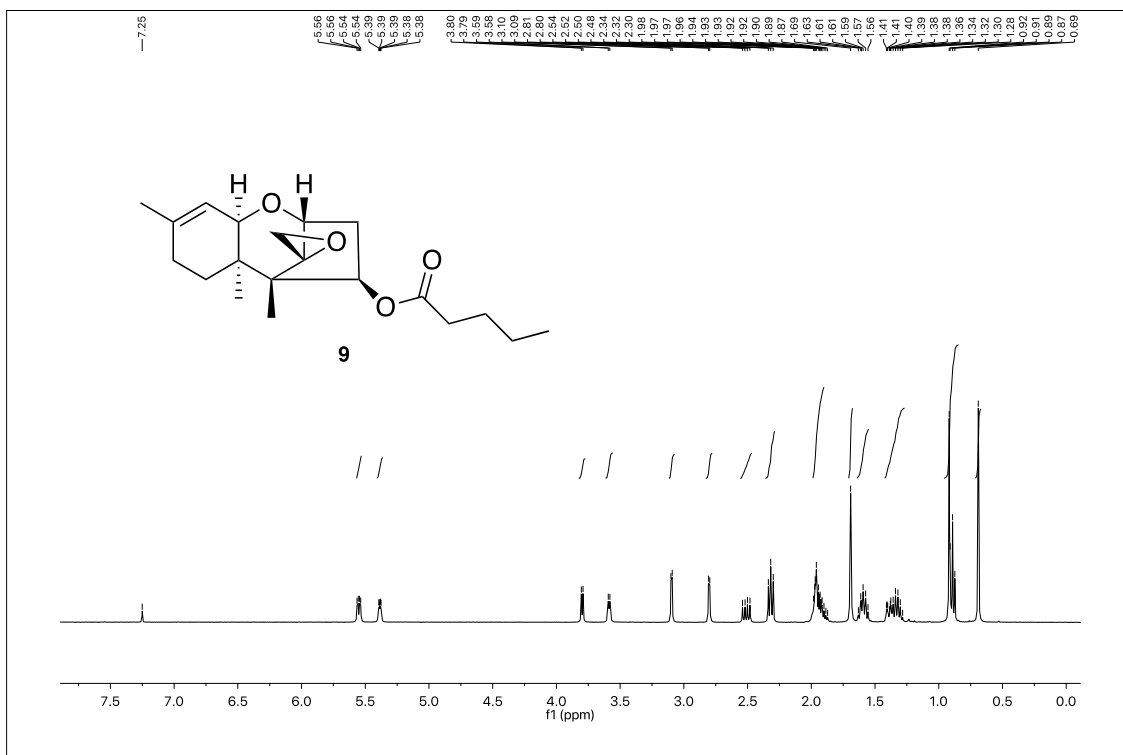
100 MHz ¹³C NMR of compound 6 in CDCl₃



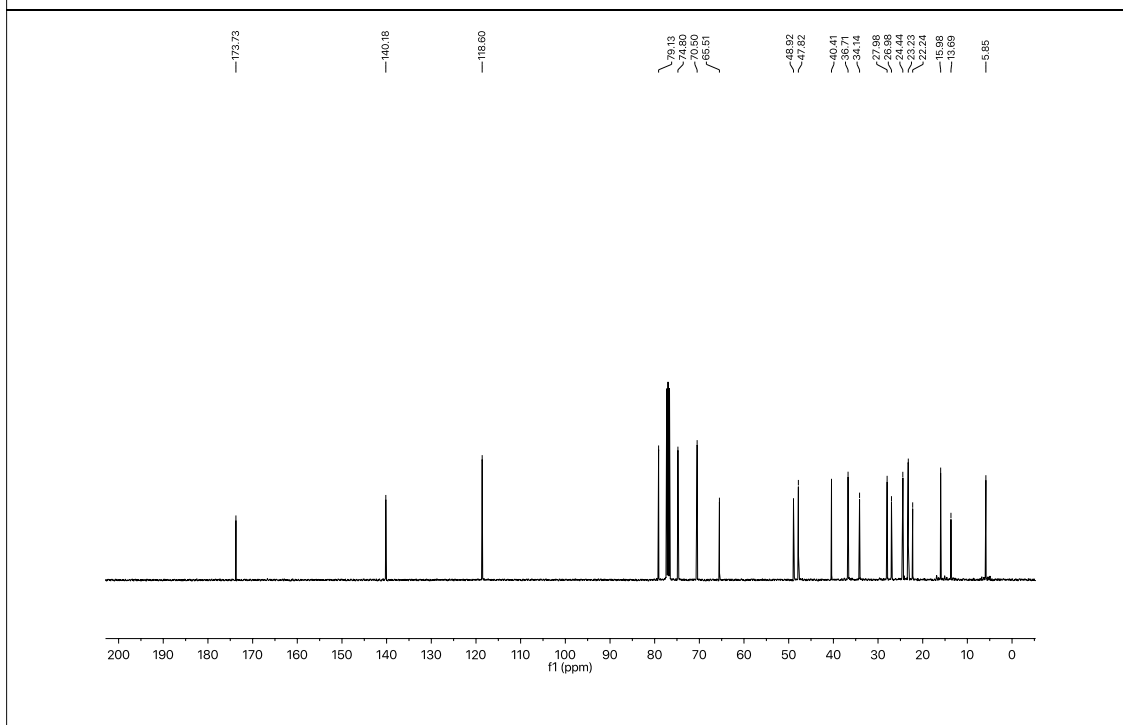
400 MHz ^1H NMR of compound 7 in CDCl_3



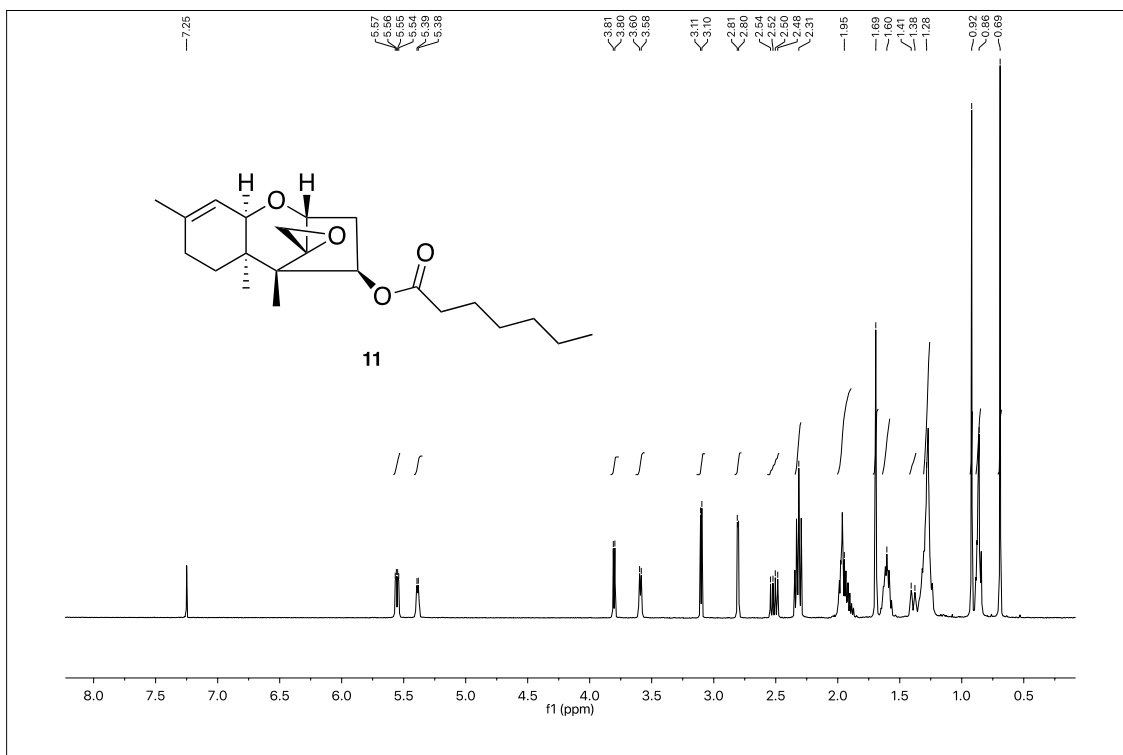
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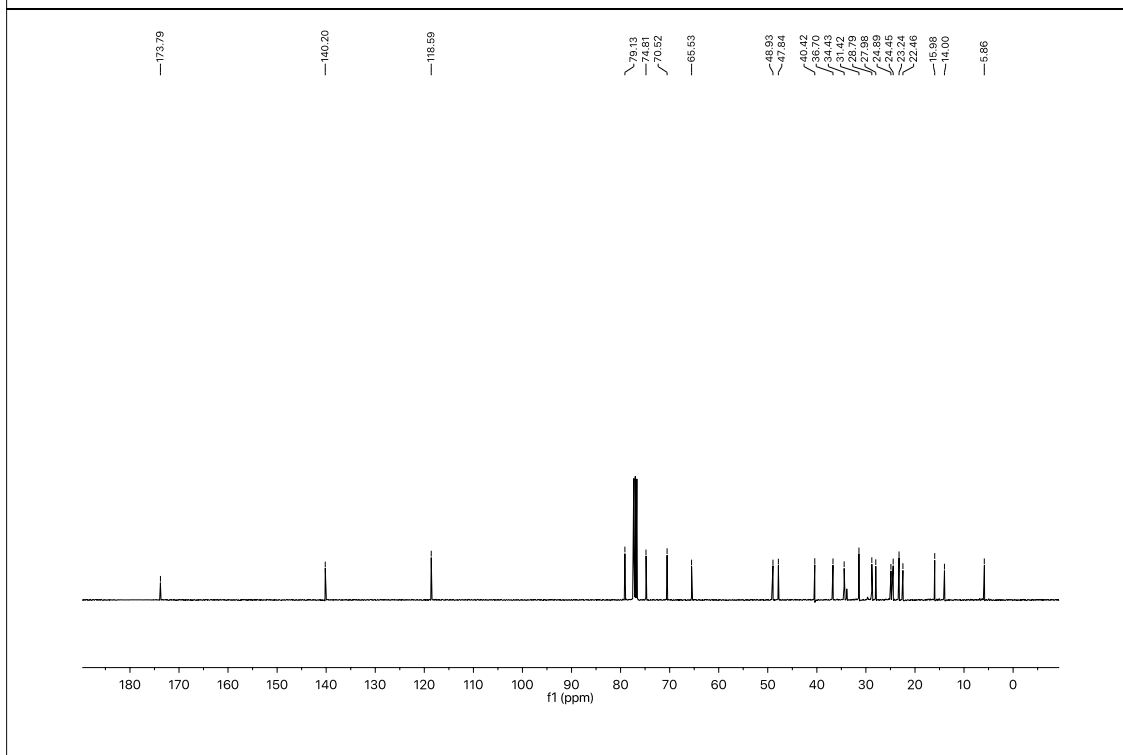
400 MHz ^1H NMR of compound **9** in CDCl_3



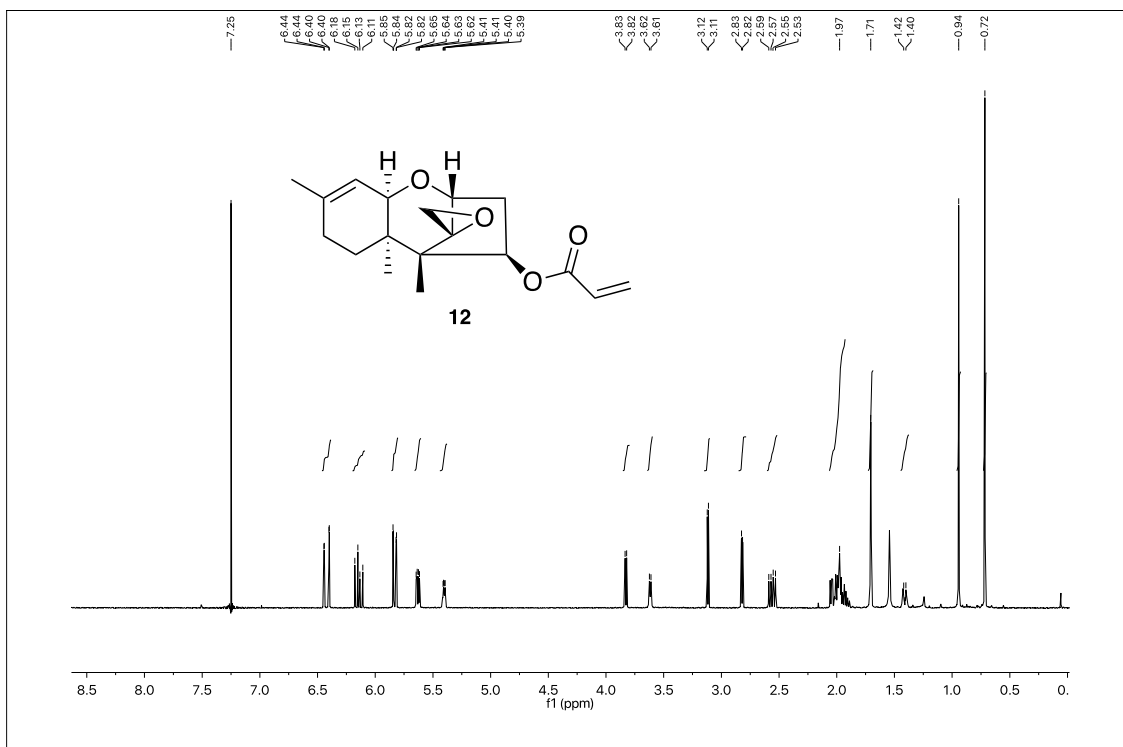
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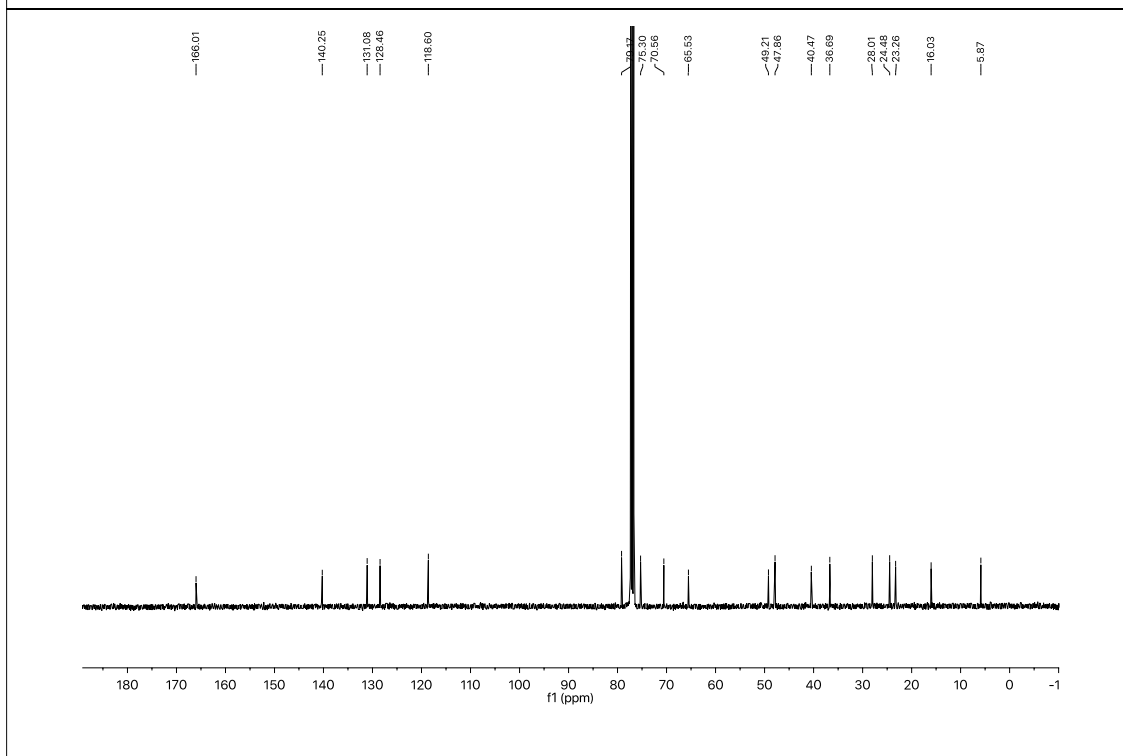
400 MHz ^1H NMR of compound **11** in CDCl_3



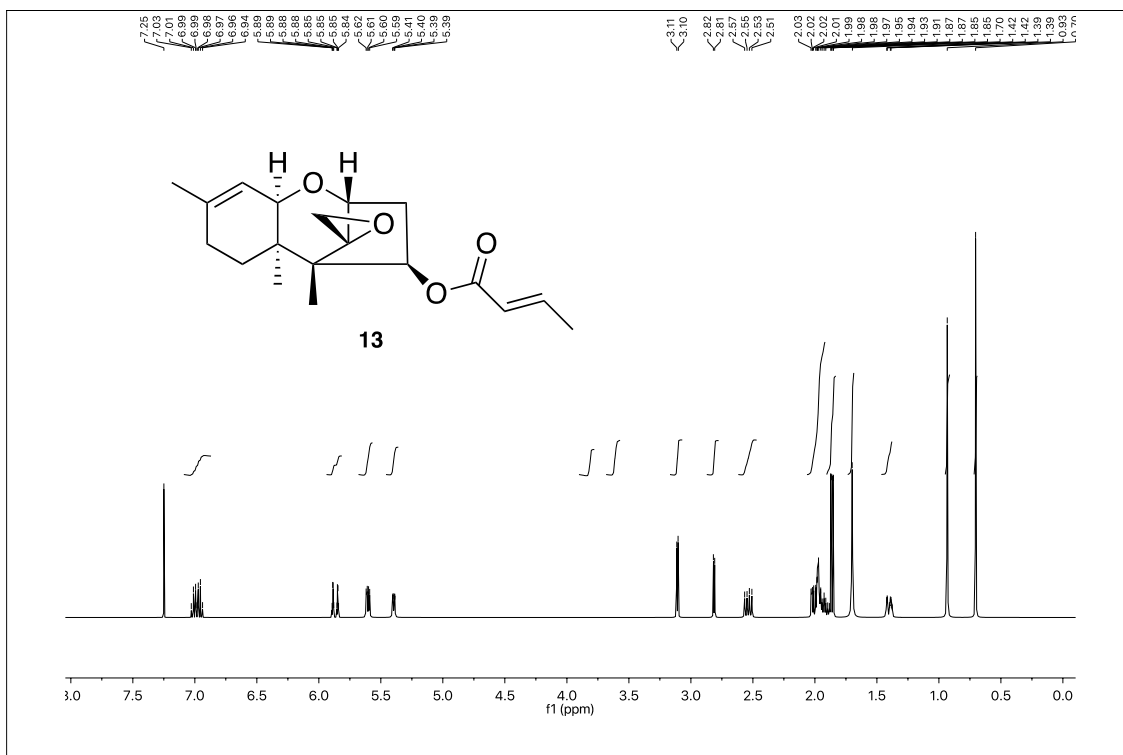
100 MHz ^{13}C NMR of compound **11** in CDCl_3



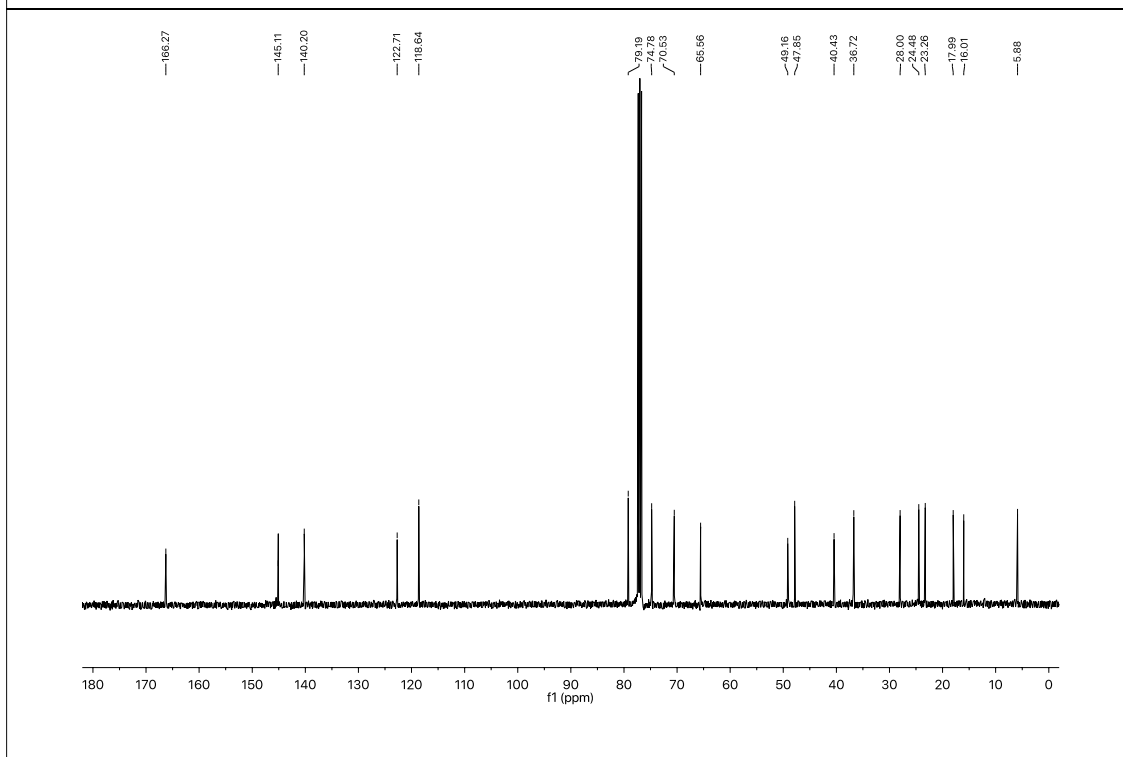
400 MHz ^1H NMR of compound **12** in CDCl_3



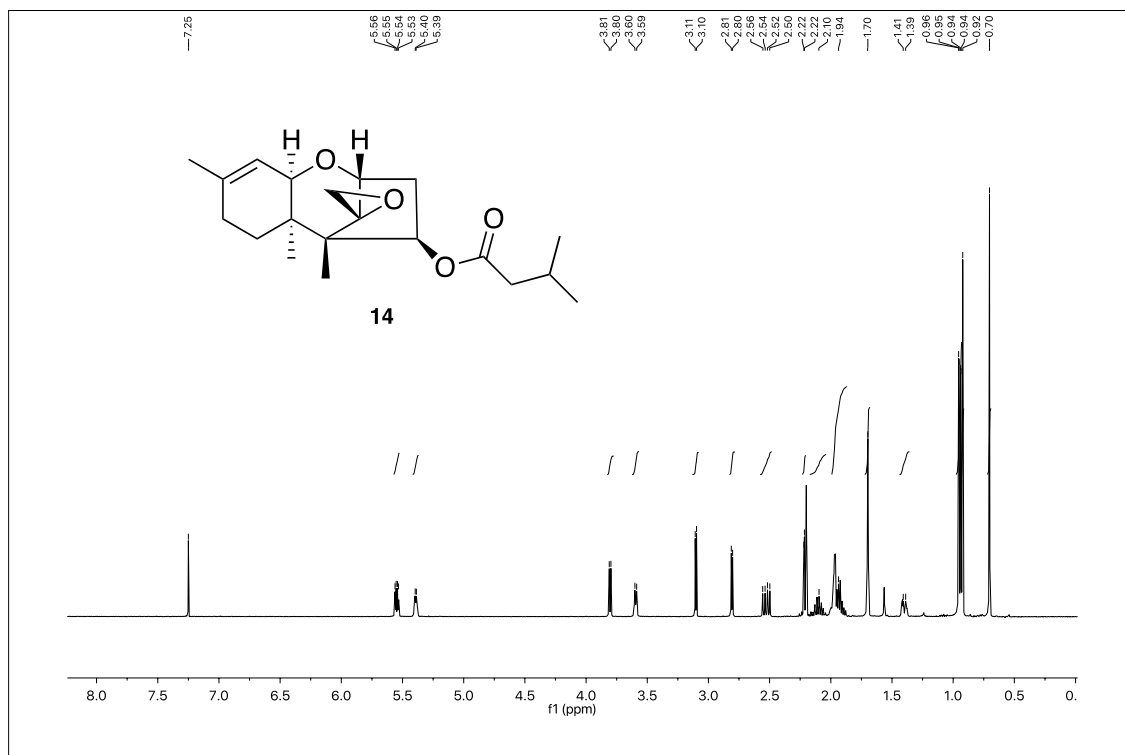
100 MHz ^{13}C NMR of compound **12** in CDCl_3



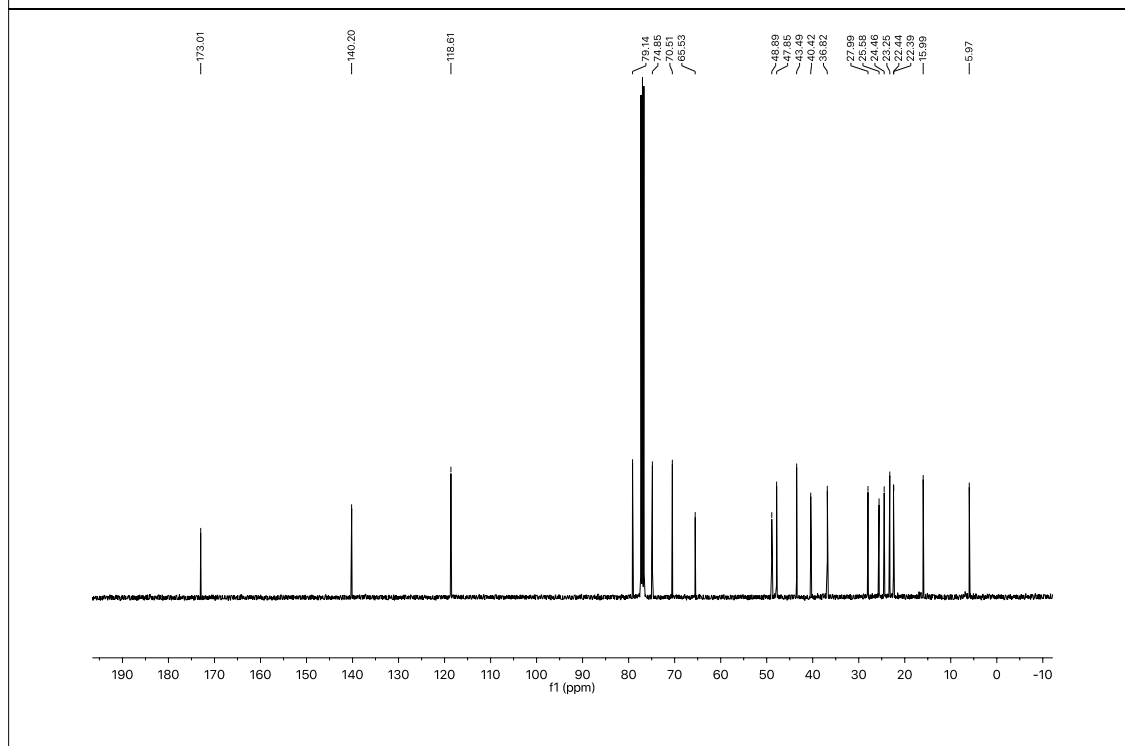
400 MHz ^1H NMR of compound **13** in CDCl_3



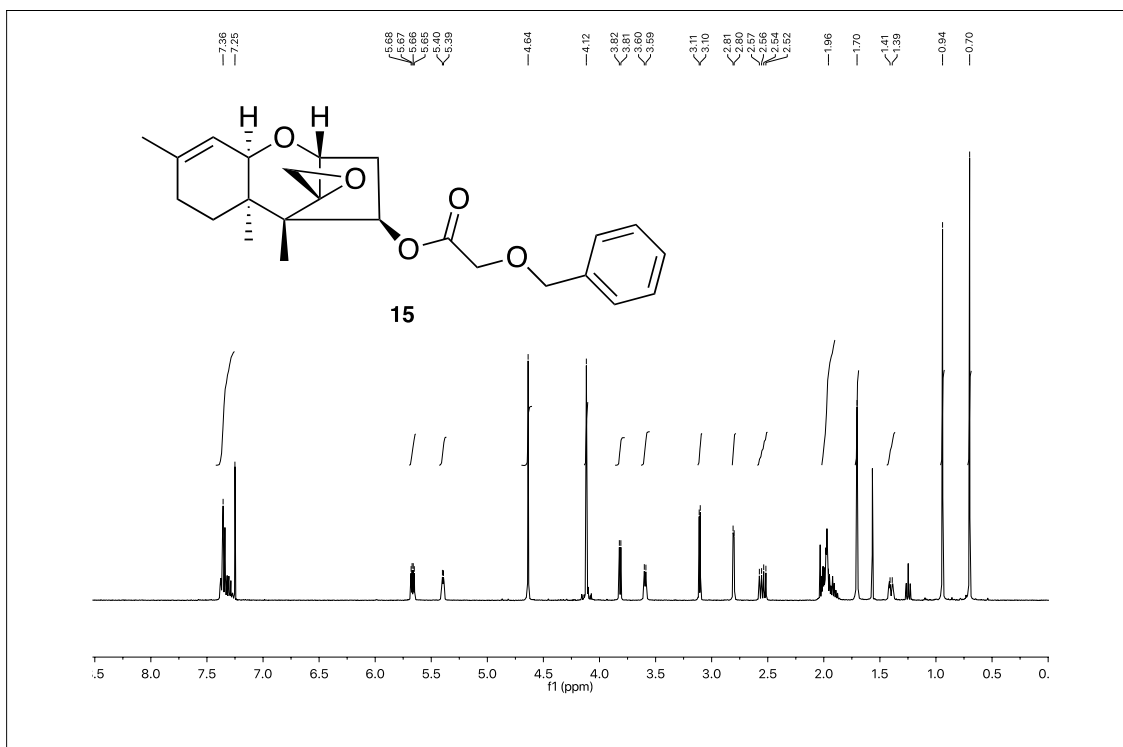
100 MHz ^{13}C NMR of compound **13** in CDCl_3



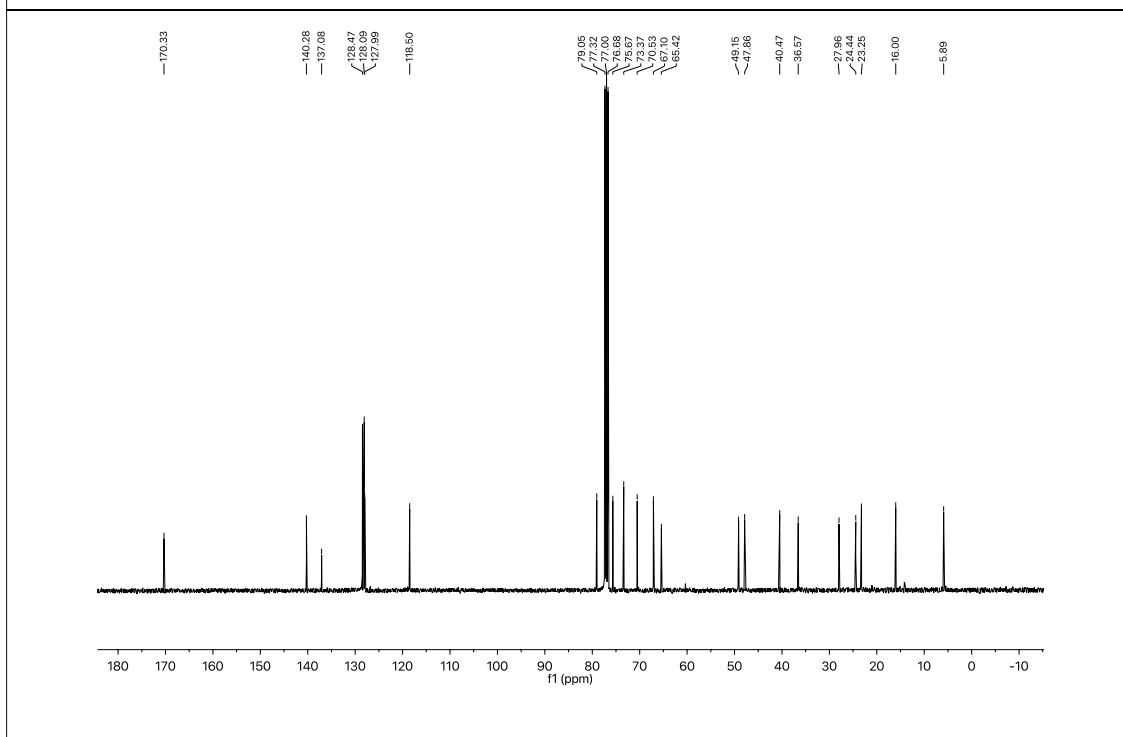
400 MHz ^1H NMR of compound **14** in CDCl_3



100 MHz ^{13}C NMR of compound **14** in CDCl_3



400 MHz ^1H NMR of compound **15** in CDCl_3



100 MHz ^{13}C NMR of compound **15** in CDCl_3

