

Supplementary data

## Terpenoids and Phenylpropanoids in *Ligularia duciformis*, *L. kongkalingensis*, *L. nelumbifolia*, and *L. limprichtii*

Chiaki Kuroda <sup>1,\*</sup>, Ryohei Kobayashi <sup>1</sup>, Ayumi Nagata <sup>1</sup>, Yumi Nakadozono <sup>1</sup>, Taketo Itoh <sup>1</sup>, Yasuko Okamoto <sup>2</sup>, Motoo Tori <sup>2</sup>, Ryo Hanai <sup>3</sup>, and Xun Gong <sup>4</sup>

<sup>1</sup> Department of Chemistry, Rikkyo University, Nishi-Ikebukuro, Toshima-ku, Tokyo 171-8501, Japan

<sup>2</sup> Faculty of Pharmaceutical Sciences, Tokushima Bunri University, Yamashiro-cho, Tokushima 770-8514, Japan

<sup>3</sup> Department of Life Science, Rikkyo University, Nishi-Ikebukuro, Toshima-ku, Tokyo 171-8501, Japan

<sup>4</sup> Kunming Institute of Botany, Chinese Academy of Science, Kunming 650201, China

Table S1: Differences in the sequence of the rDNA ITS1-5.8S-ITS2 region.

Figure S1: <sup>1</sup>H NMR spectrum of **2**.

Figure S2: <sup>13</sup>C NMR spectrum of **2**.

Figure S3: <sup>1</sup>H NMR spectrum of **8**.

Figure S4: <sup>13</sup>C NMR spectrum of **8**.

Figure S5: LCMS profile (total ion chromatogram) of samples 1-6 and 9.

**Table S1.** Differences in the sequence of the rDNA ITS1-5.8S-ITS2 region.<sup>1</sup>

Sample no.	ITS1	5.8S	ITS2
		1 1 1 1 1 1 2 2 2 2 1	1 1 1 1 1 1 1 2 2
	1 6 6 6 7 0 1 1 3 8 8 0 0 2 2 3	2 2 2 3 4 4 6 7 7 9 0 0 0 5 5 6 9 1 2	
	8 3 4 5 8 4 8 0 7 2 4 8 4 5 3 4 8	6 7 8 3 1 4 9 0 2 9 1 4 7 1 6 8 9 7 1	
1	C K G G C C R T T Y Y C A S <sup>6</sup> <sup>6</sup> G	T C R G G T Y C A C C C C Y S A C Y C	
2	C T G G C C A T T T C C A C G C G	T C G A G T C C A C C C C T G A Y C C	
3	C T G G C T A T T T C C A C <sup>6</sup> <sup>6</sup> G	<sup>5</sup> C G A G T C C A C C Y C T G A T C Y	
4	Y T G G C C A T T T C C A C G C G	T C G A G T C Y A Y C C Y Y G A C C C	
5	C G G G Y C G T T C T C A C - - G	T C A G G T C C A C C C C C G A C T C	
6 <sup>2</sup>	C T G G C C A T T T C C A C G C G	T C G A G Y C Y A C C C C Y G W Y C C	
7	C K R K C C R Y W Y Y C R C <sup>6</sup> <sup>6</sup> G	T C R R G T C C A C Y C C Y G A C C C	
8	C T G G C C A T T T C Y A C G C G	<sup>5</sup> Y G A G T Y C A C C C C T G A T C C	
9 <sup>3</sup>	C T G G C C A T T T C Y A C G C G	T C R A G T C C A C C C C T G A T C C	
Ref <sup>4</sup>	C T G G C C A T T T C C A C G C K	T C G G K T Y C W C C Y C T G A C C C	

1 K=C+T; R=A+G; S=C+G; W=A+T; Y=C+T; -, deletion.

2 A sequence with A inserted between positions 22 and 23 in ITS2 was also present.

3 Accession no. LC333008 (*L. limprichtii*).

4 *A. L. duciformis* sequence in the GenBank/EMBL/DDBJ database (ID=LC128585).

5 A sequence with TT in place of T was also present.

6 Two sequences with and without GC were present.

Figure S1.  $^1\text{H}$  NMR spectrum of **2**.

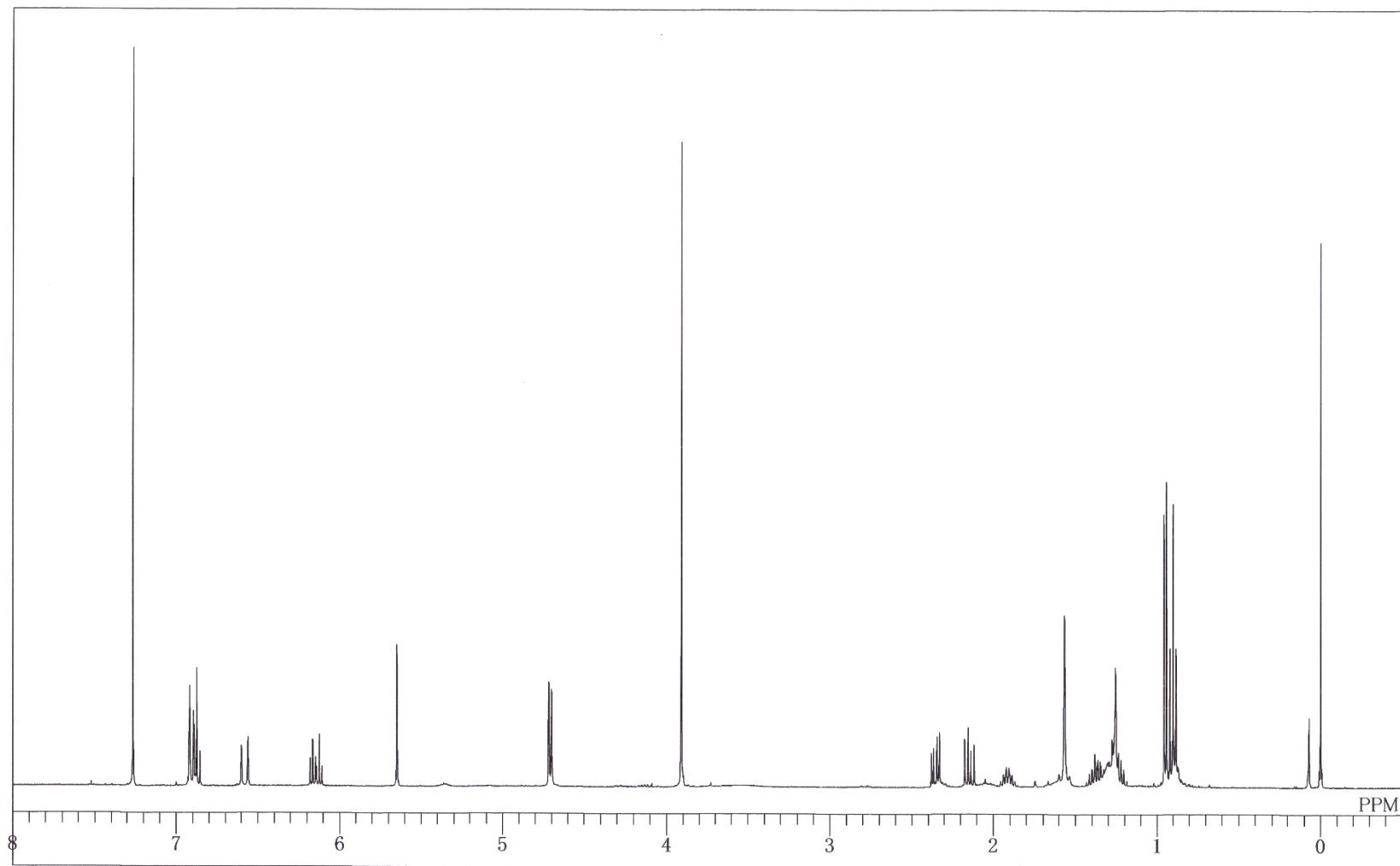


Figure S2.  $^{13}\text{C}$  NMR spectrum of **2**.

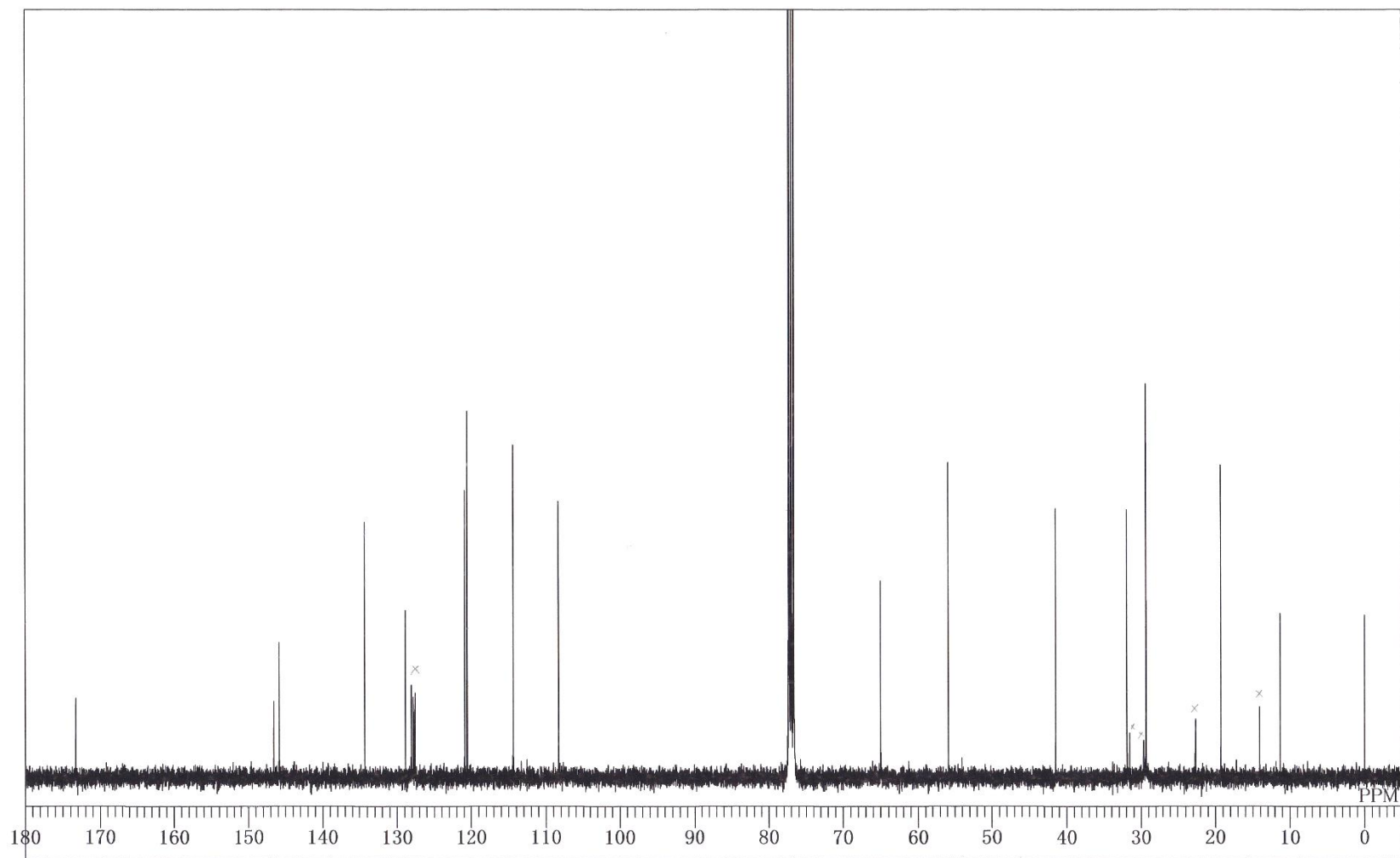


Figure S3.  $^1\text{H}$  NMR spectrum of **8**.

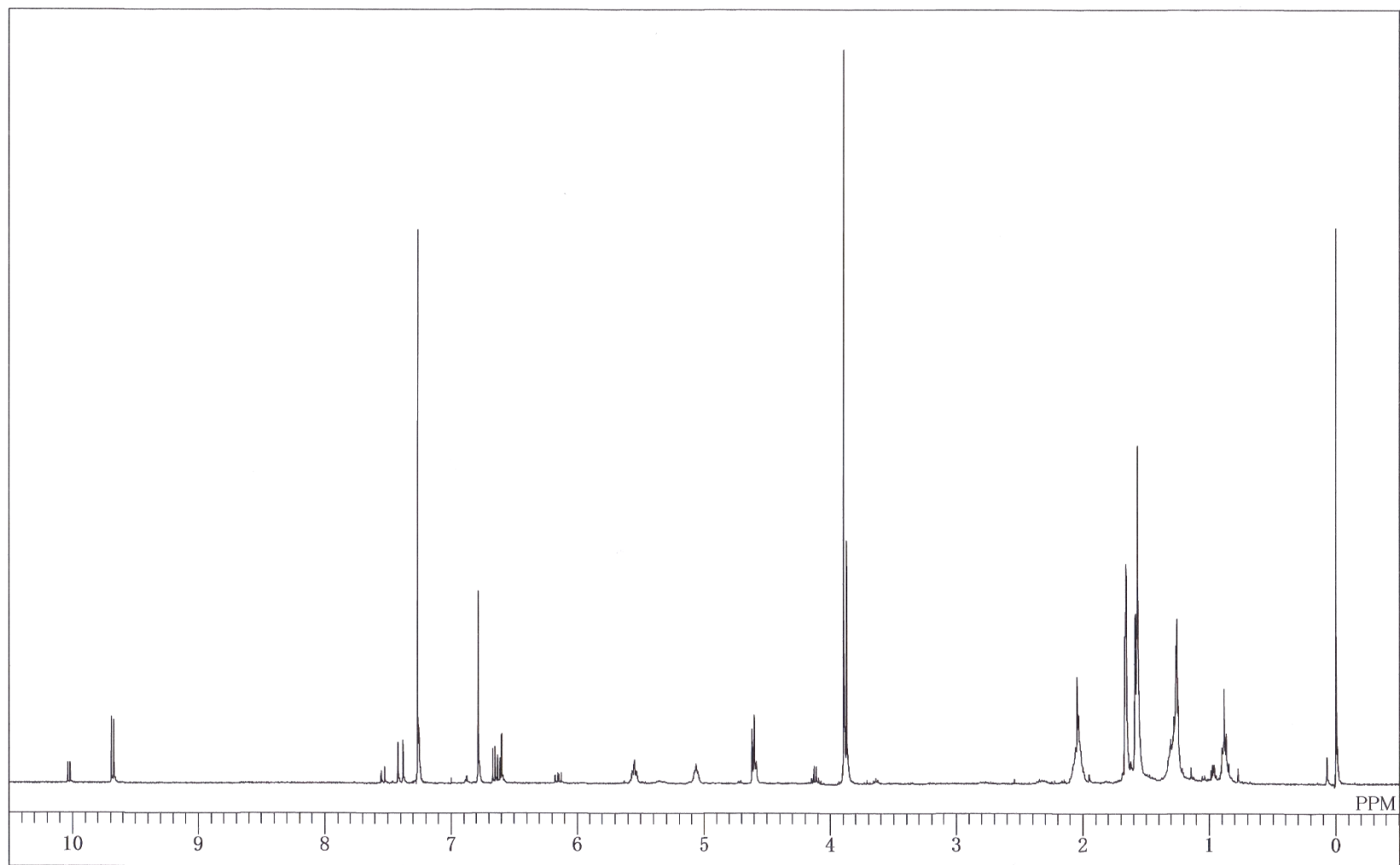


Figure S4.  $^{13}\text{C}$  NMR spectrum of **8**.

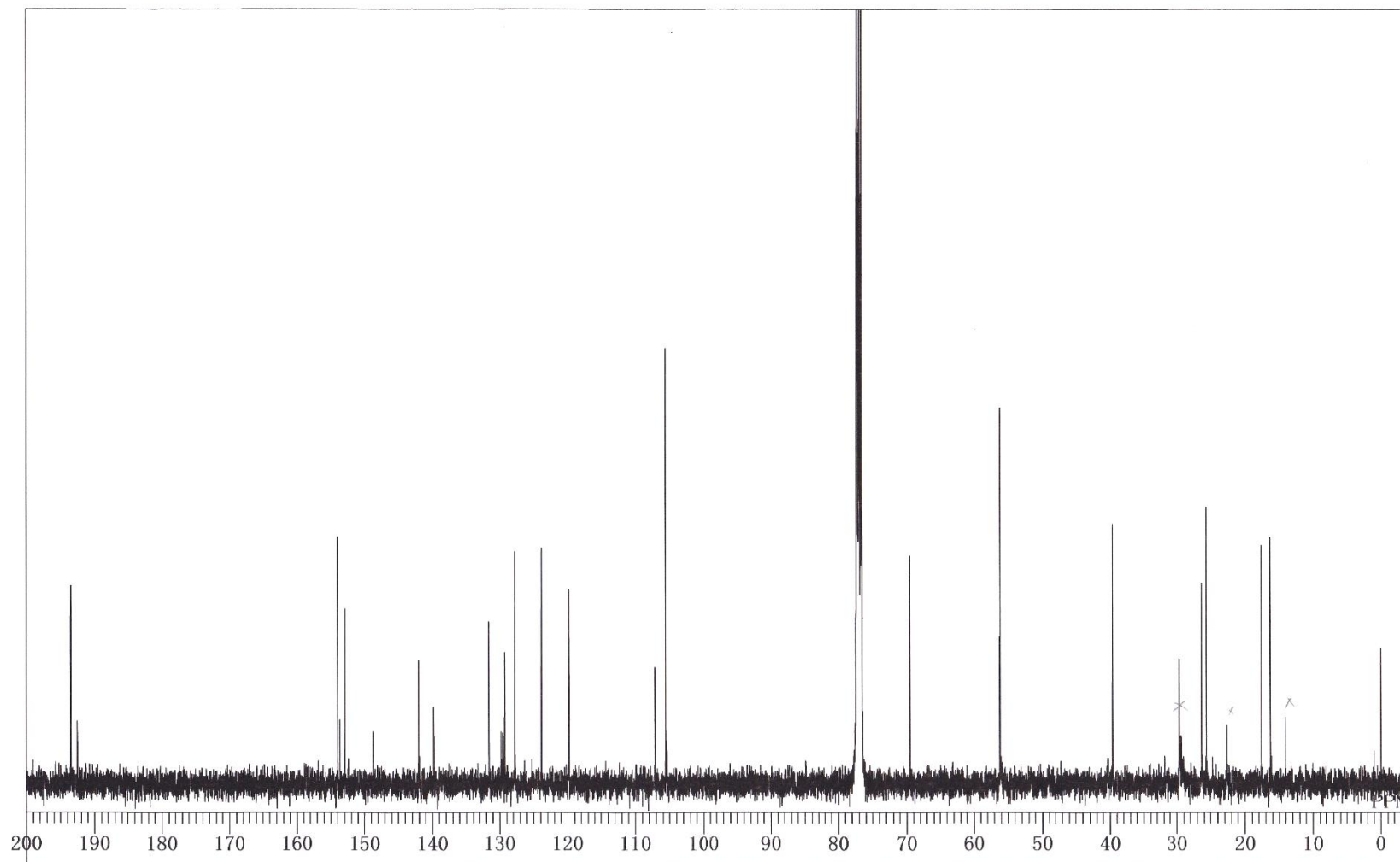
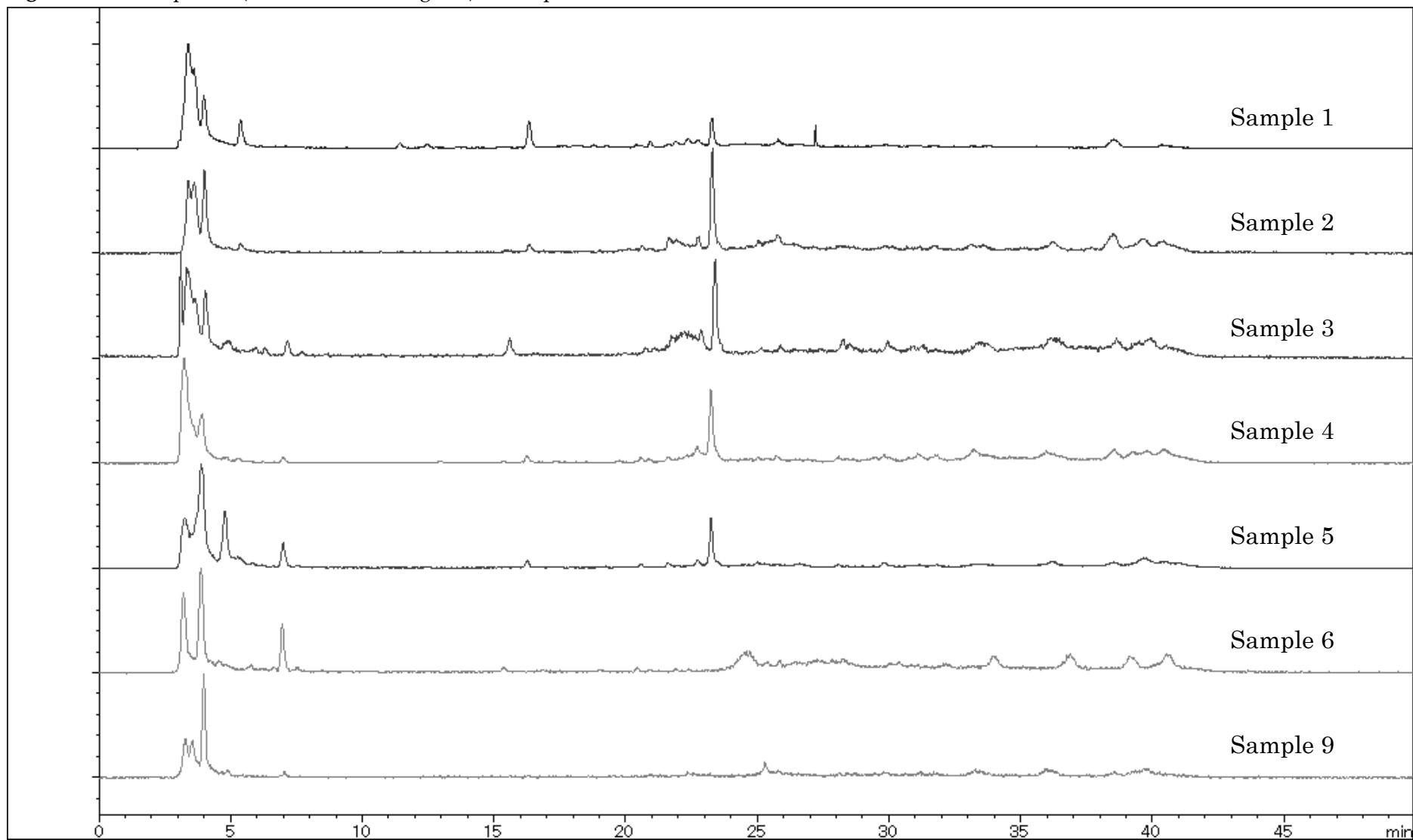


Figure S5. LCMS profile (total ion chromatogram) of samples 1-6 and 9.<sup>1</sup>



1 A peak at  $t_r = 23.3$  min is an impurity contaminated during sampling procedure.