Supporting Information

Cytotoxic Cycloartane Triterpenes of Traditional Chinese Medicine “Shengma” (*Cimicifuga dahurica*)

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Legends for Supporting Information Figures and Scheme

**Fig. 1S-8S** $^1$H, $^{13}$C, HSQC, HMBC, COSY and ROESY NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 1.

**Fig. 9S-14S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 2.

**Fig. 15S-20S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 3.

**Fig. 21S-26S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 4.

**Fig. 27S-32S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 5.

**Fig. 33S-38S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 6.

**Fig. 39S-44S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 7.

**Fig. 45S-50S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 8.

**Fig. 51S-56S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 9.

**Fig. 57S-62S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 10.

**Fig. 63S-68S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 11.

**Fig. 69S-74S** $^1$H, $^{13}$C, HSQC, and HMBC NMR spectra and ESIMS and HR-TOF-ESIMS experiments of compound 12.
Fig. 1S $^1$H NMR spectrum of compound 1 (C$_5$H$_5$N, 500 MHz).

Fig. 2S $^{13}$C NMR spectrum of compound 1 (C$_5$H$_5$N, 150 MHz).
Fig. 3S HSQC spectrum of compound 1
Fig. 4S HMBC spectrum of compound 1

Fig. 5S COSY spectrum of compound 1

Fig. 6S ROESY spectrum of compound 1
Fig. 7S ESI experiment of compound 1
Fig. 8S HR-TOF-ESI experiment of compound 1
Fig. 9S $^1$H NMR spectrum of compound 2 (C$_5$H$_5$N, 500 MHz).

Fig. 10S $^{13}$C NMR spectrum of compound 2 (C$_5$H$_5$N, 125 MHz).
Fig. 11S HSQC spectrum of compound 2.
Fig. 12S HMBC spectrum of compound 2.

Fig. 13S ESI experiment of compound 2.
Fig. 14S HR-TOF-ESI experiment of compound 2
Fig. 15S $^1$H NMR spectrum of compound 3 (C$_5$H$_5$N, 500 MHz).
Fig. 16 $^{13}$C NMR spectrum of compound 3 (C$_5$H$_5$N, 125 MHz).

Fig. 17 HSQC spectrum of compound 3.
Fig. 18S HMBC spectrum of compound 3.

Fig. 19S ESI experiment of compound 3
Fig. 20S HR-TOF-ESI experiment of compound 3
Fig. 21$^1$H NMR spectrum of compound 4 (C₅H₅N, 500 MHz).

Fig. 22$^1$C NMR spectrum of compound 4 (C₅H₅N, 125 MHz).
Fig. 23S HSQC spectrum of compound 4.

Fig. 24S HMBC spectrum of compound 4.
Fig. 25S ESI experiment of compound 4
Fig. 26S HR-TOF-ESI experiment of compound 4
Fig. 27S $^1$H NMR spectrum of compound 5 (C$_5$H$_5$N, 500 MHz).

Fig. 28S $^{13}$C NMR spectrum of compound 5 (C$_5$H$_5$N, 125 MHz).
Fig. 29S HSQC spectrum of compound 5.

Fig. 30S HMBC spectrum of compound 5.
Fig. 31S ESI experiment of compound 5
Fig. 32S HR-TOF-ESI experiment of compound 5
Fig. 33 $^1$H NMR spectrum of compound 6 (C$_5$H$_5$N, 500 MHz).

Fig. 34 $^{13}$C NMR spectrum of compound 6 (C$_5$H$_5$N, 150 MHz).
Fig. 35S. HSQC spectrum of compound 6

Fig. 36S. HMBC spectrum of compound 6
Fig. 37S ESI experiment of compound 6
Fig. 38S HR-TOF-ESI experiment of compound 6
**Fig. 39** $^1$H NMR spectrum of compound 7 (C$_5$H$_5$N, 500 MHz).

**Fig. 40** $^{13}$C NMR spectrum of compound 7 (C$_3$H$_5$N, 125 MHz).
Fig. 41S HSQC spectrum of compound 7.
Fig. 42S HMBC spectrum of compound 7.

Fig. 43S ESI experiment of compound 7
Fig. 44S HR-TOF-ESI experiment of compound 7
**Fig. 45** $^1$H NMR spectrum of compound 8 (C$_5$H$_5$N, 500 MHz).
Fig. 46S $^{13}$C NMR spectrum of compound 8 (C$_5$H$_5$N, 125 MHz).

Fig. 47S HSQC spectrum of compound 8.
Fig. 48S HMBC spectrum of compound 8.

Fig. 49S ESI experiment of compound 8.
Fig.50S HR-TOF-ESI experiment of compound 8
Fig. 51 \(^1\)H NMR spectrum of compound 9 (C\(_5\)H\(_5\)N, 500 MHz).

Fig. 52 \(^{13}\)C NMR spectrum of compound 9 (C\(_3\)H\(_5\)N, 150 MHz).
**Fig. 53S** HSQC spectrum of compound 9

**Fig. 54S** HMBC spectrum of compound 9
Fig.55S ESI experiment of compound 9
Fig. 56S HR-TOF-ESI experiment of compound 9
Fig. 57S ¹H NMR spectrum of compound 10 (C₅H₅N, 500 MHz).

Fig. 58S ¹³C NMR spectrum of compound 10 (C₅H₅N, 125 MHz).
Fig. 59S HSQC spectrum of compound 10.

Fig. 60S HMBC spectrum of compound 10.
Fig. 61S ESI experiment of compound 10
Fig. 62S HR-TOF-ESI experiment of compound 10
Fig. 63S $^1$H NMR spectrum of compound 11 (C$_5$H$_5$N, 500 MHz).

Fig. 64S $^{13}$C NMR spectrum of compound 11 (C$_5$H$_5$N, 125 MHz).
**Fig. 65S** HSQC spectrum of compound 11.
**Fig. 66S** HMBC spectrum of compound 11.

**Fig. 67S** ESI experiment of compound 11
Fig. 68S HR-TOF-ESI experiment of compound 11
Fig. 69S $^1$H NMR spectrum of compound 12 (C$_5$H$_5$N, 500 MHz).

Fig. 70S $^{13}$C NMR spectrum of compound 12 (C$_5$H$_5$N, 150 MHz).
Fig. 71S HSQC spectrum of compound 12.

Fig. 72S HMBC spectrum of compound 12.
Fig. 73S ESI experiment of compound 12
Fig. 74S HR-TOF-ESI experiment of compound 12