Supporting Information

Prenylated phenolic compounds from licorice (*Glycyrrhiza uralensis*) and their anti-inflammatory activity against osteoarthritis

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List of Contents

Table S1 Extracted heats and weighting factors of the optimized conformers for compound **2**.

Conformer	Extracted heats	Boltzmann-calculated contribution (%)
2-1	-1375.6136983	2.36
2-2	-1375.6114524	0.22
2-3	-1375.6126285	0.76
2-4	-1375.6120171	0.40
2-5	-1375.612773	0.88
2-6	-1375.614953	8.92
2-7	-1375.6050163	0.00
2-8	-1375.6170954	86.46

Table S2 The sequences of the oligonucleotide primers used in this experiment.

	Forward primer	Reverse primer
iNOS	ATCCCG AAACGATACACTT	TCTGGCGAAGAACAATCC
COX-2	TCTACAAGACGCCACATCCC	ACGGGGTTGTTGATTTCGTCT
TNF-α	TCGTATGAAATGGCAAATCG	GGTCCCAACAAGGAGGAG
IL-6	TTAGCCACTCCTTCTGTGACTCC	ACCCCAATTTCCAATGCTCT
MMP3	GGAGGCAGCAGAGAACCTAC	TCCAACCCGAGGAACTTCTG
MMP13	CAGTGCTGCGGTTCACTTTG	TCATCATAACTCCACACGTGGTT
GAPDH	CCGTTGAATTTGCCGTGA	TGATGCCCTTTTGGCTCCC

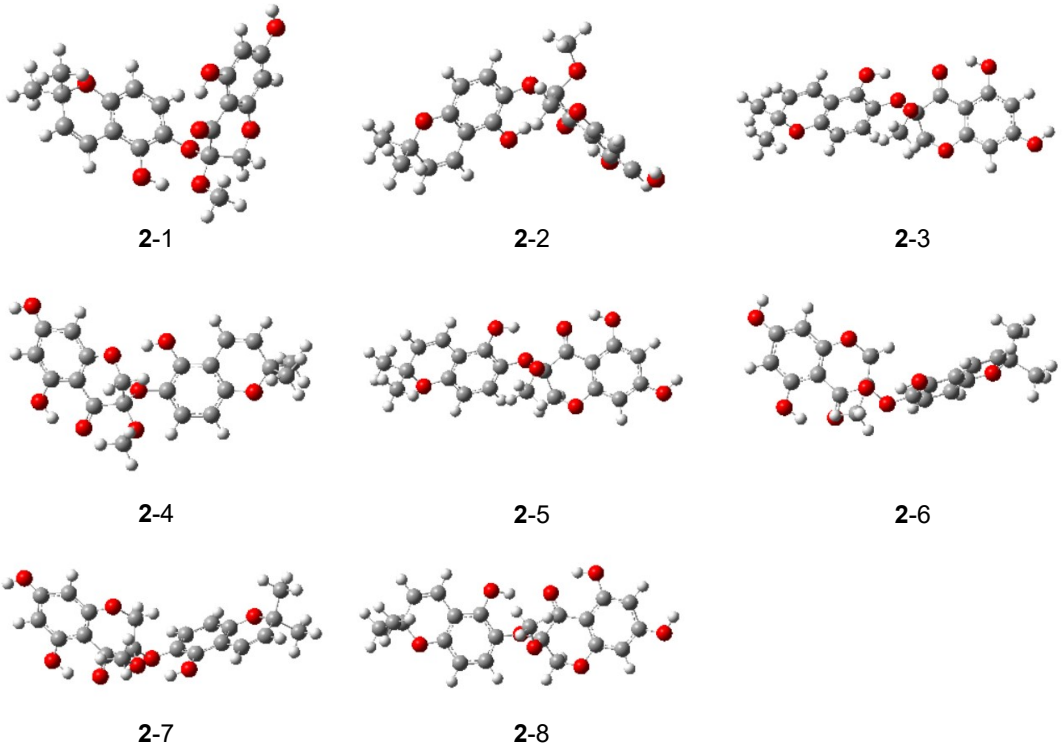

Fig. S1 Optimized geometries of predominant conformers for compound **2**.

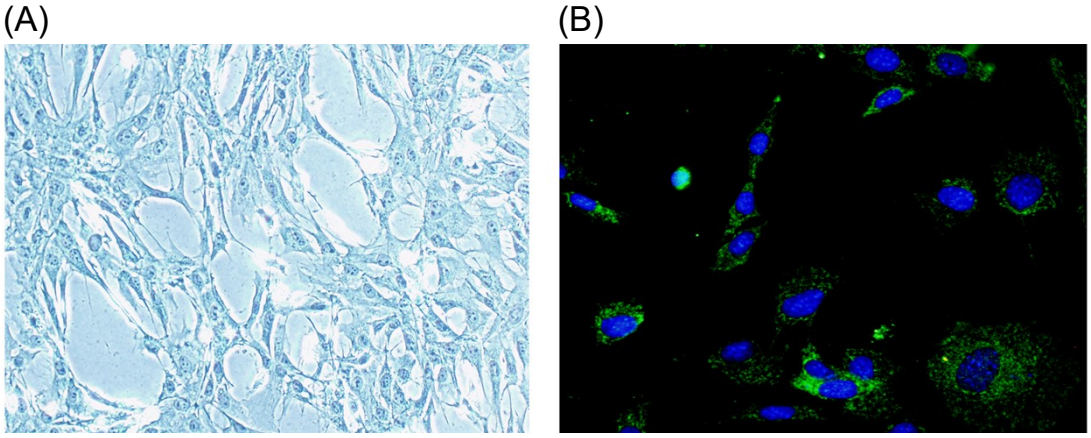

Fig. S2 Identification of mouse primary chondrocytes by Alcian blue staining (A) and type II collagen immunohistochemistry (B).

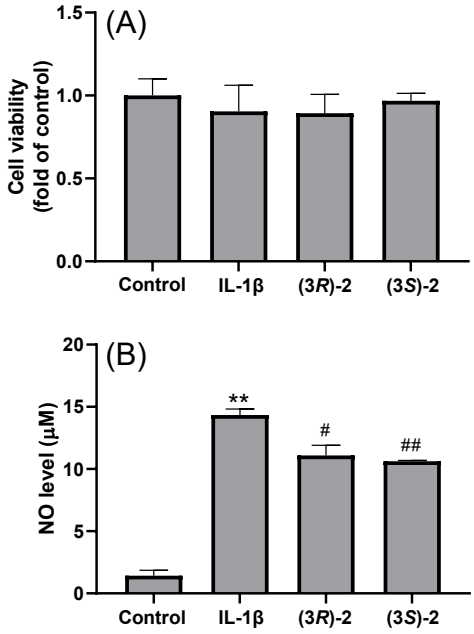

Fig. S3 (A) Cytotoxic effect of (3*R*)-**2** and (3*S*)-**2** at 10 μM: Primary mouse chondrocytes were treated with (3*R*)-**2** or (3*S*)-**2** for 36 h, and cell viability was evaluated using the MTT reagent. (B) NO inhibition effect of (3*R*)-**2** and (3*S*)-**2** at 10 μM: Chondrocytes were treated with (3*R*)-**2** or (3*S*)-**2** for 36 h after IL-1β stimulation, and NO level in culture media was determined using Griess assay. ** $p < 0.01$, vs. control group; $^{\#}p < 0.05$ and $^{\#\#}p < 0.01$, vs. IL-1β alone.

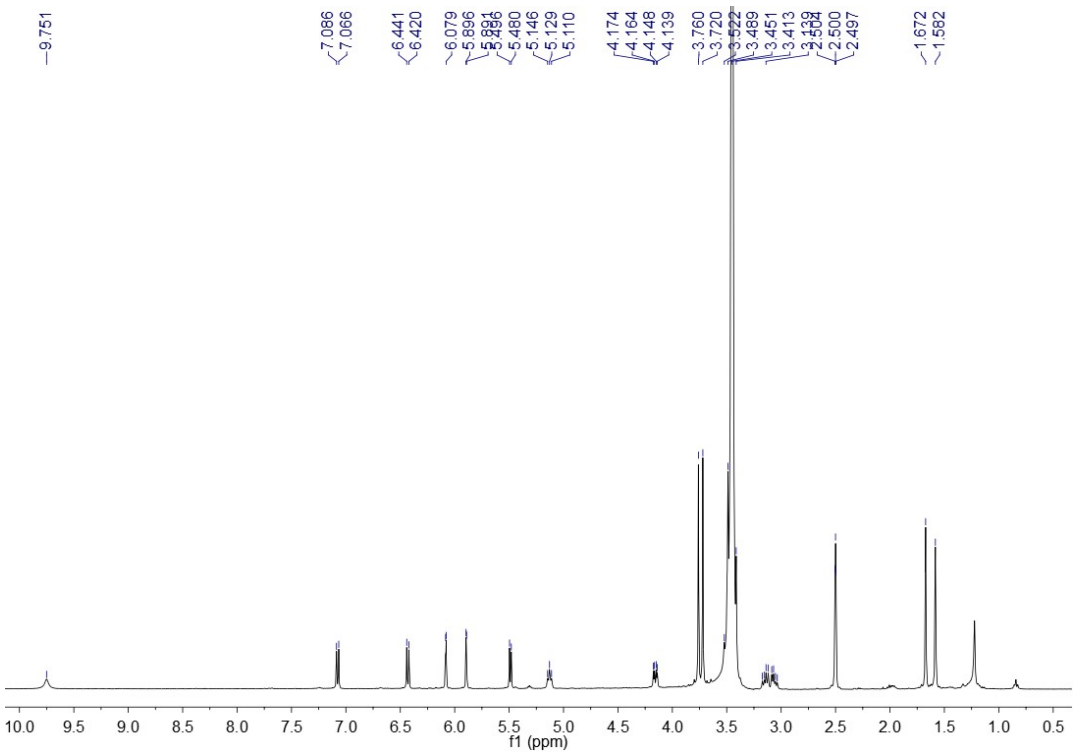

Fig. S4 ^{1}H NMR spectrum of glycyuralin Q (**1**) in DMSO-d_6 (400 MHz).

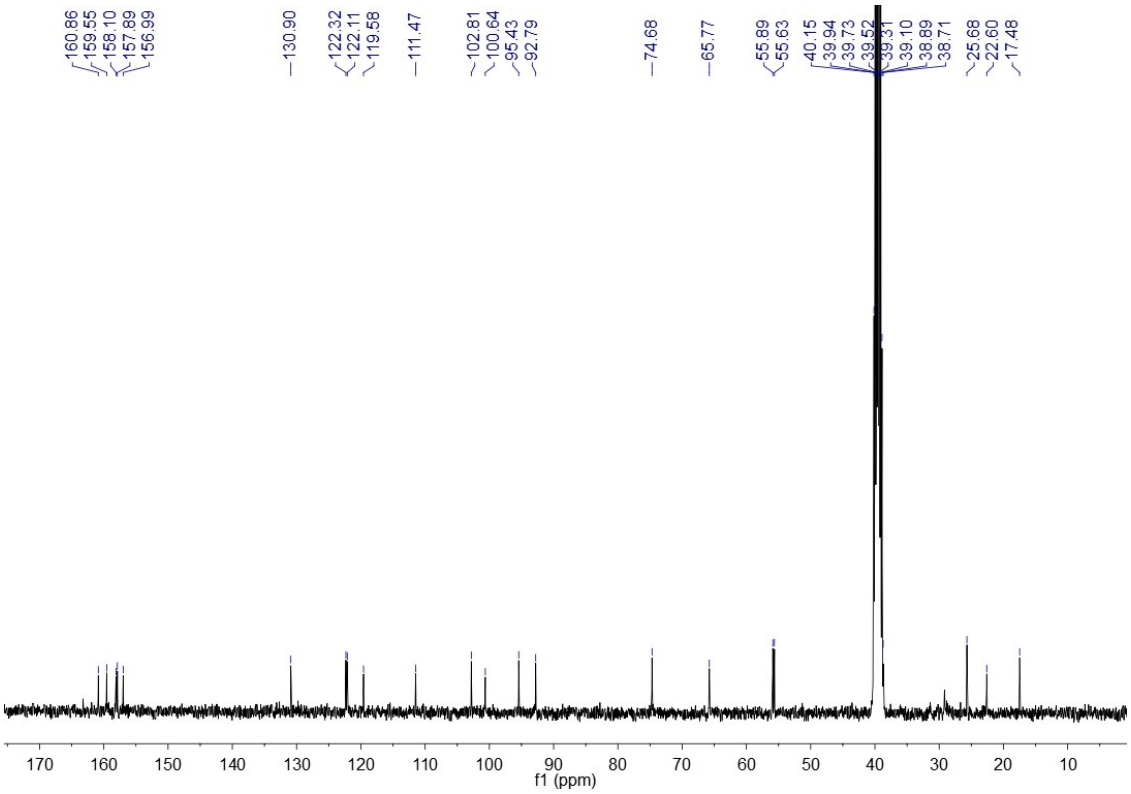

Fig. S5 ^{13}C NMR spectrum of glycyuralin Q (**1**) in DMSO-d_6 (100 MHz).

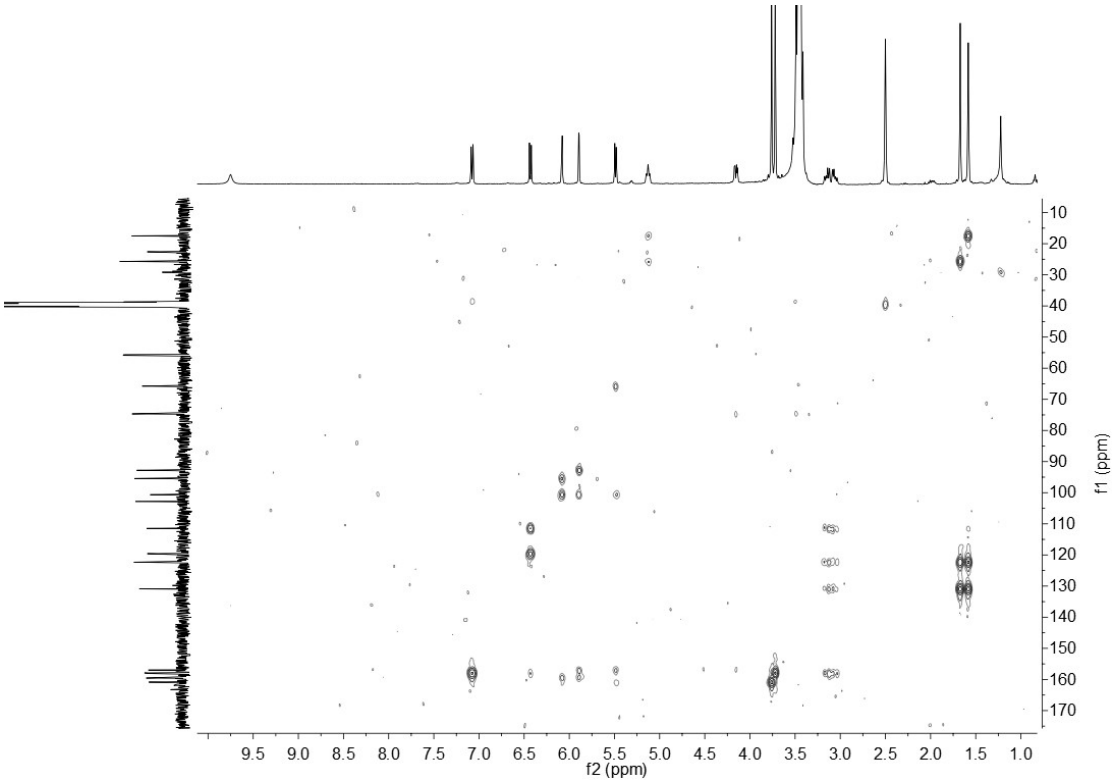

Fig. S6 HMBC spectrum of glycyuralin Q (**1**) in DMSO-d_6 (400 MHz).

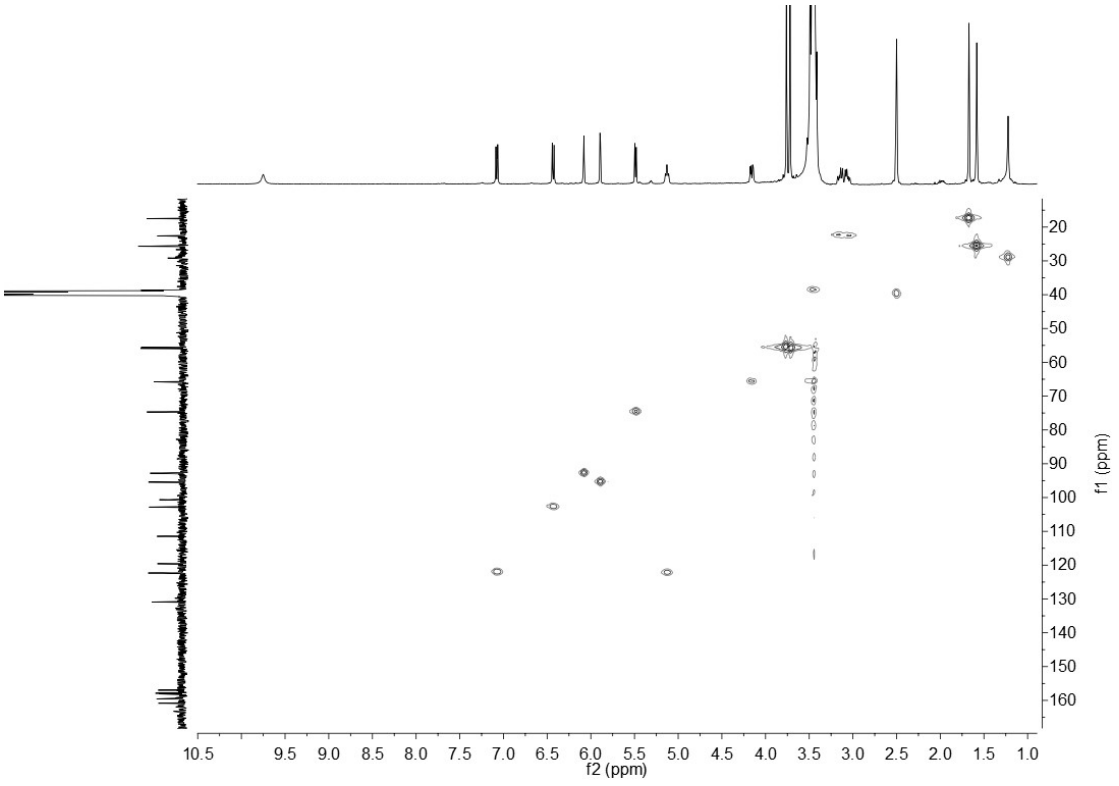

Fig. S7 HSQC spectrum of glycyuralin Q (**1**) in DMSO-d_6 (400 MHz).

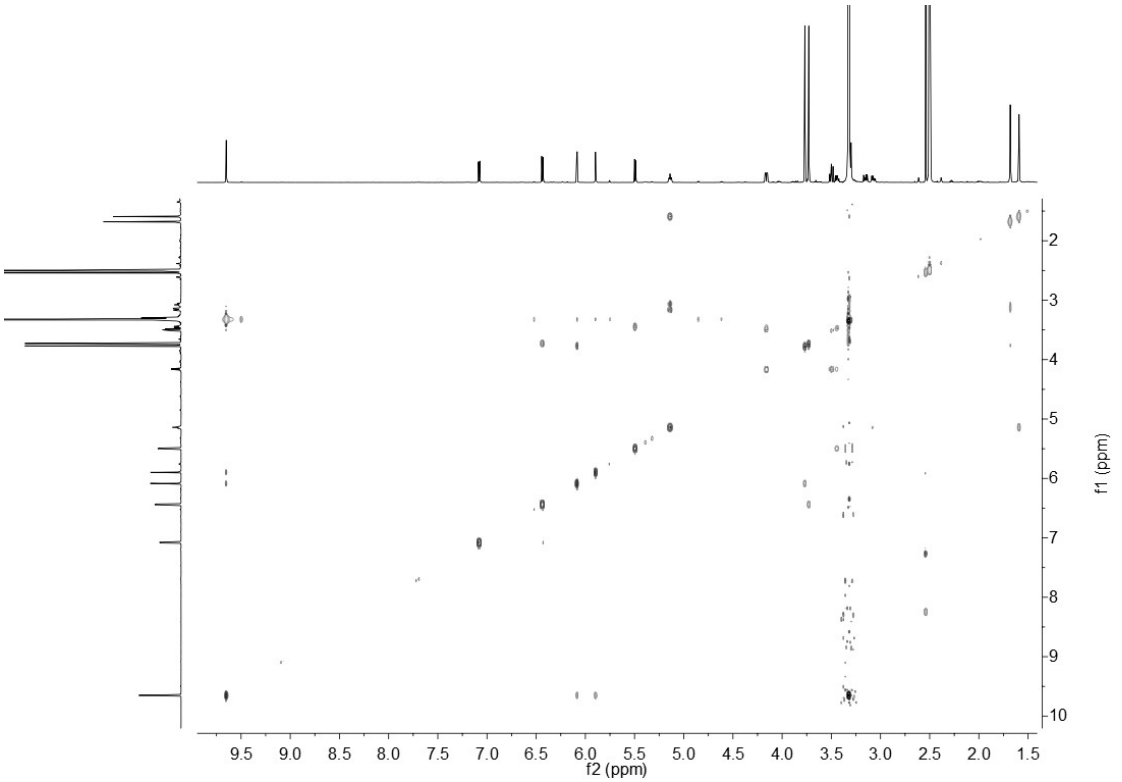

Fig. S8 NOESY spectrum of glycyuralin Q (**1**) in DMSO-d_6 (400 MHz).

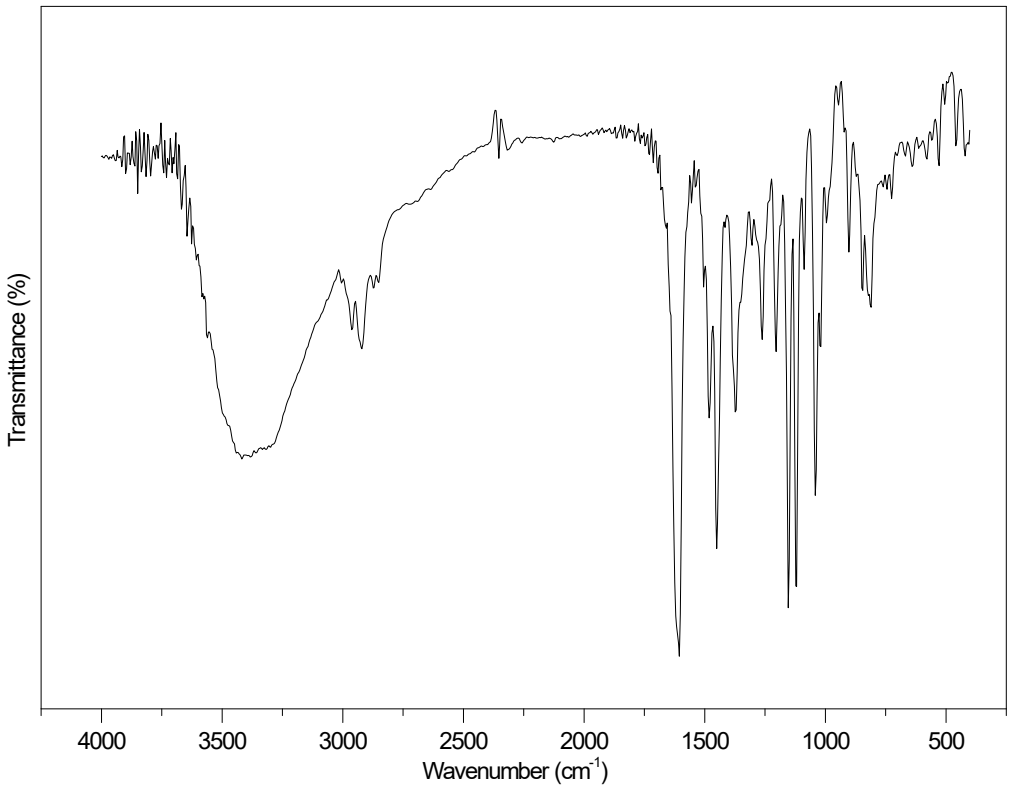

Fig S9 IR spectrum of glycyuralin Q (**1**).

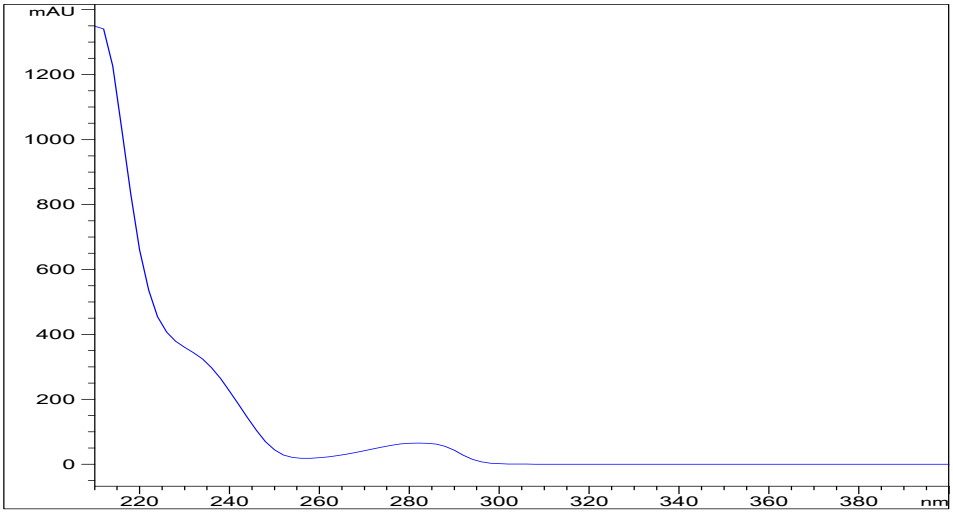

Fig. S10 UV spectrum of glycyuralin Q (**1**).

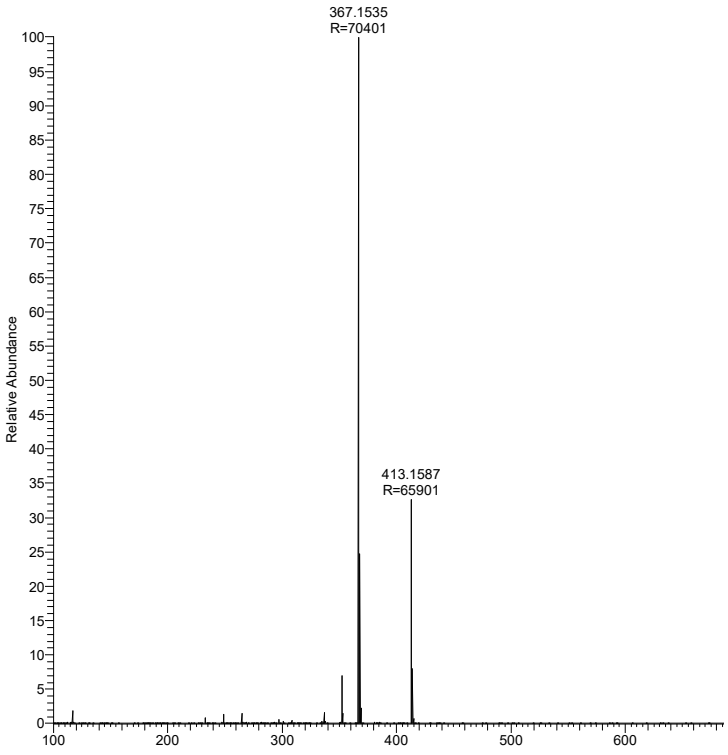

Fig. S11 HR-ESI-MS spectrum of glycyuralin Q (**1**).

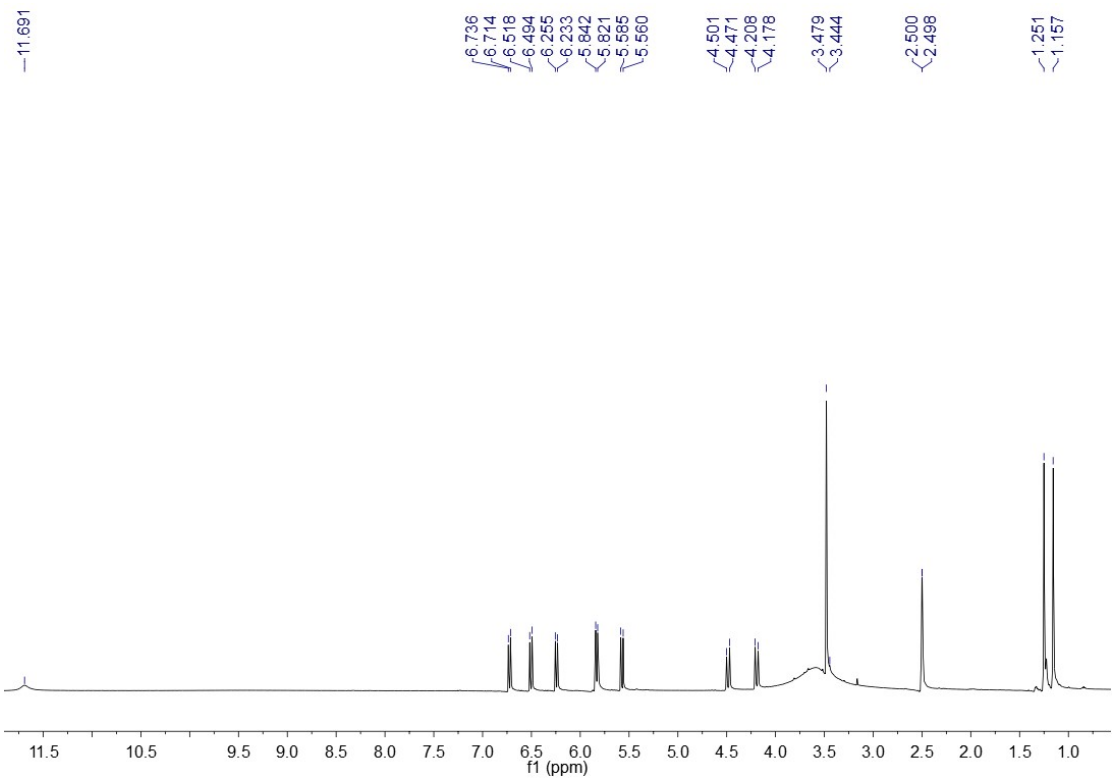

Fig. S12 ^{1}H NMR spectrum of glycyuralin R (**2**) in DMSO-d_6 (400 MHz).

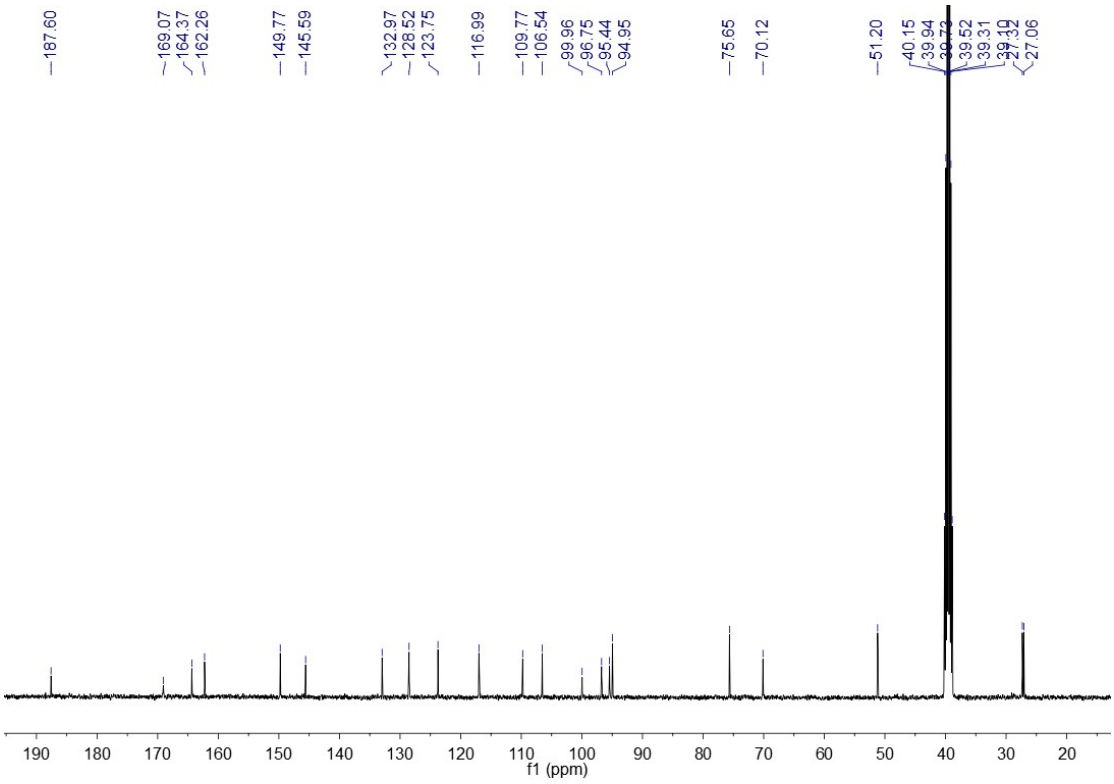

Fig. S13 ^{13}C NMR spectrum of glycyuralin R (**2**) in DMSO-d_6 (100 MHz).

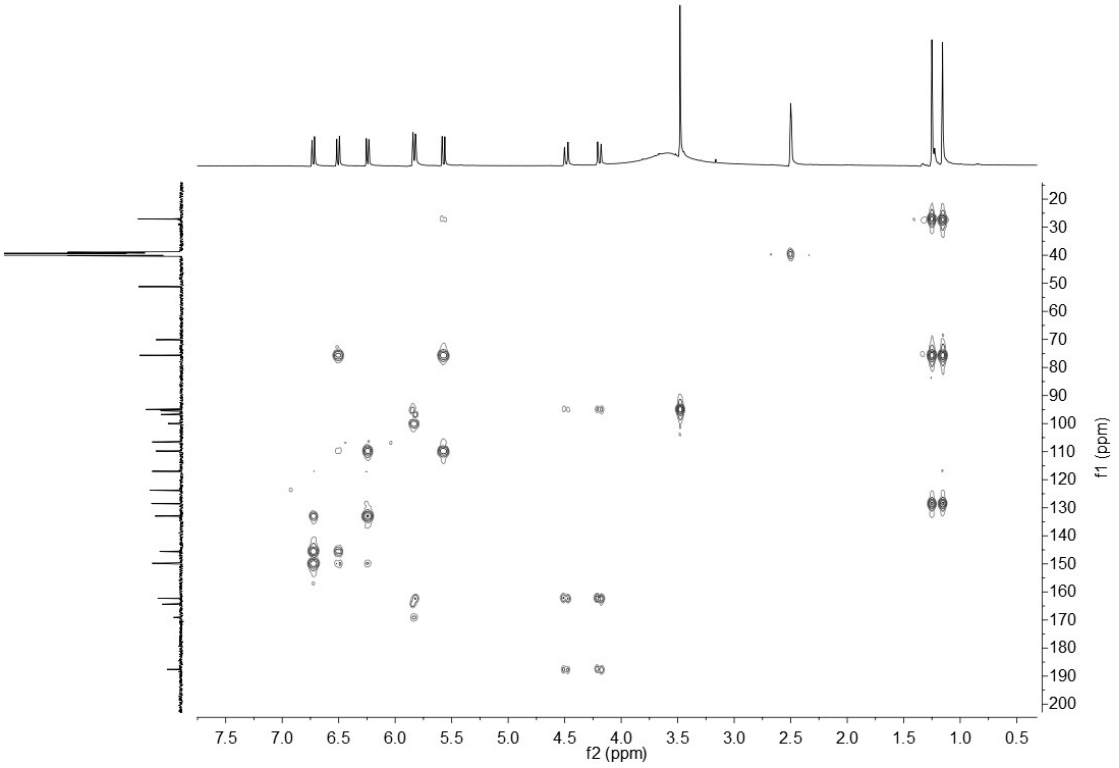

Fig. S14 HMBC spectrum of glycyuralin R (**2**) in DMSO-d_6 (400 MHz).

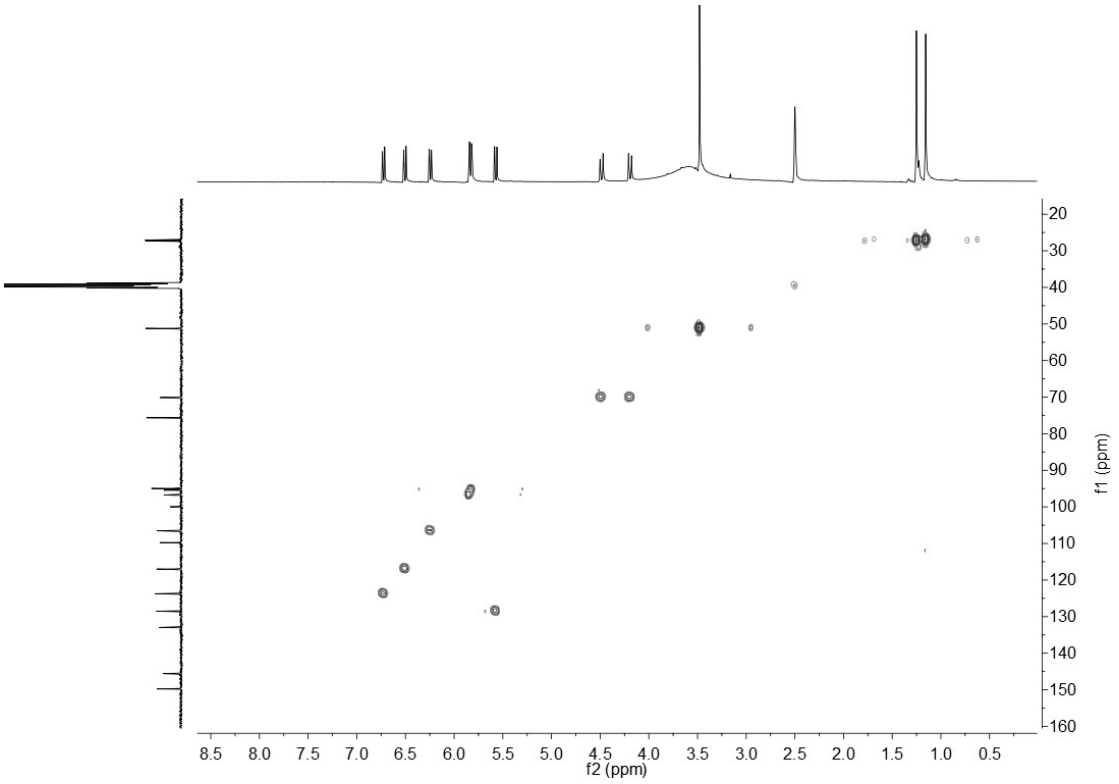

Fig. S15 HSQC spectrum of glycyuralin R (**2**) in DMSO-d_6 (400 MHz).

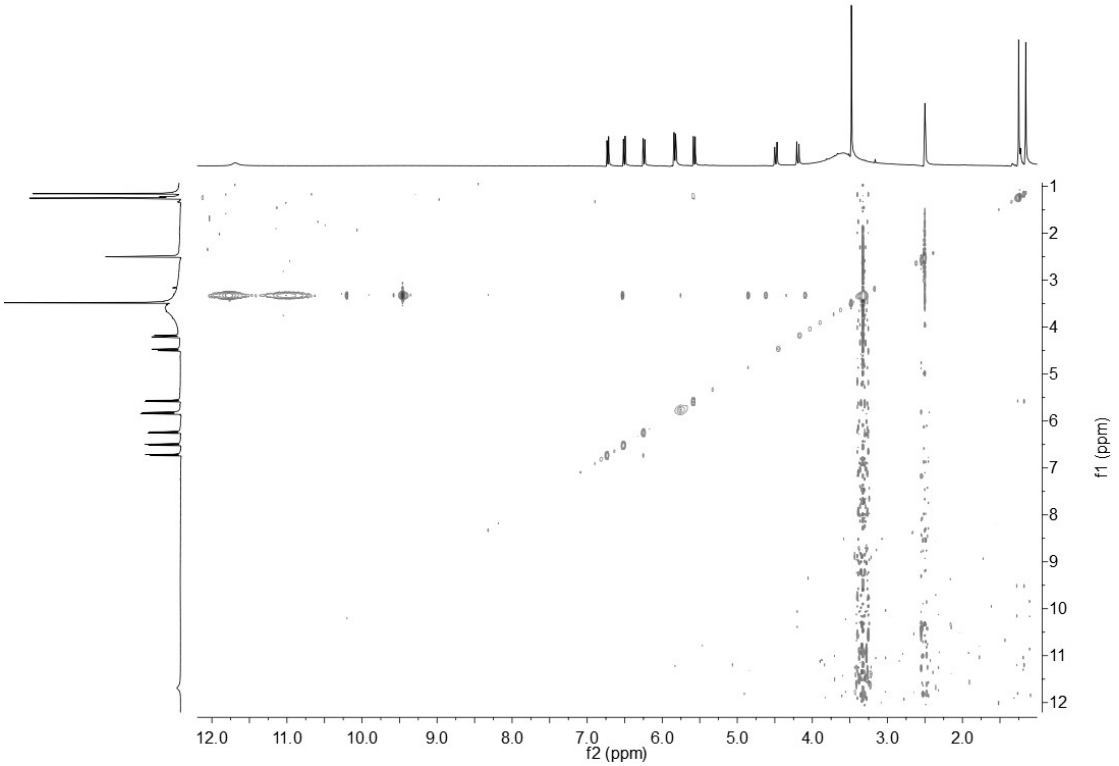

Fig. S16 NOESY spectrum of glycyuralin Q (**2**) in DMSO-d_6 (400 MHz).

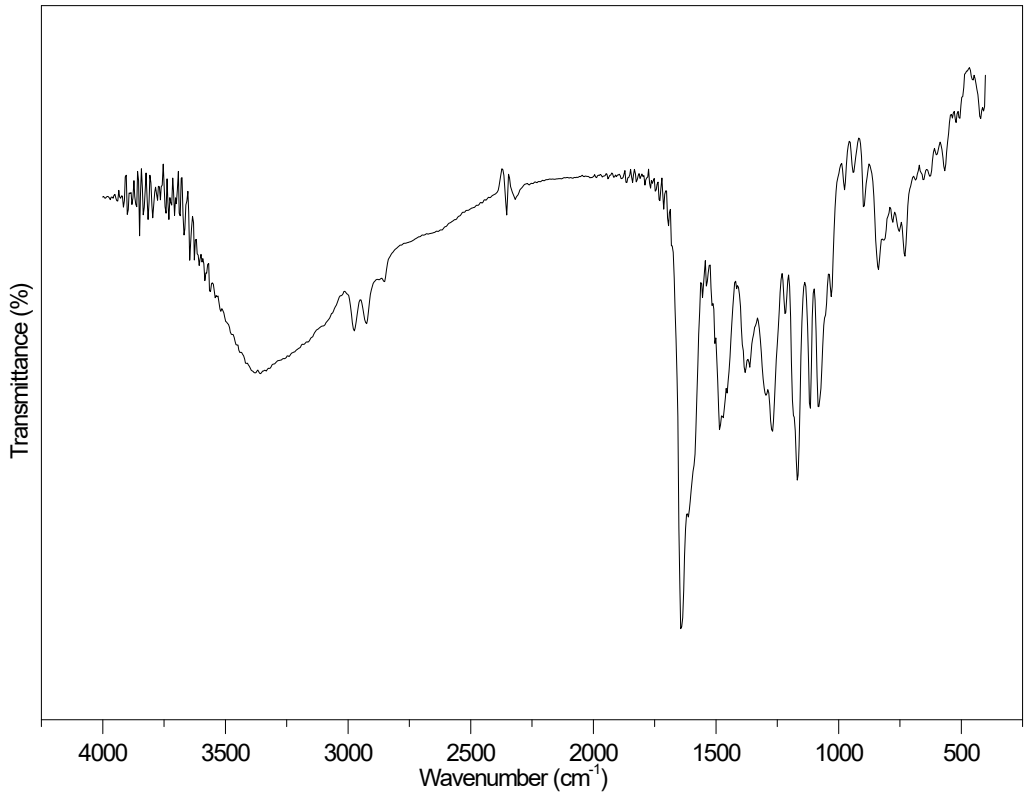

Fig. S17 IR spectrum of glycyuralin Q (**2**).

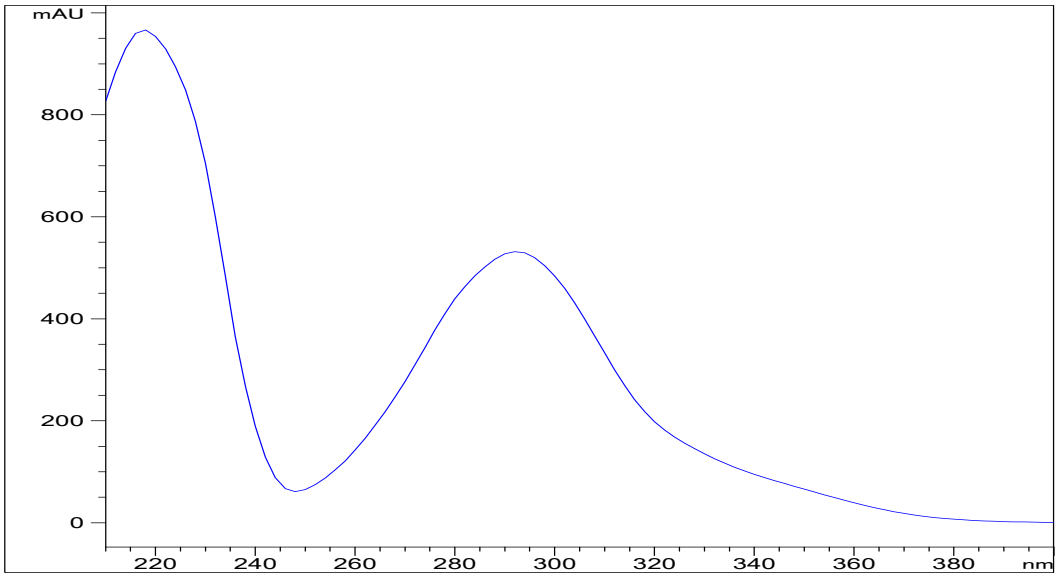

Fig. S18 UV spectrum of glycyuralin Q (**2**).

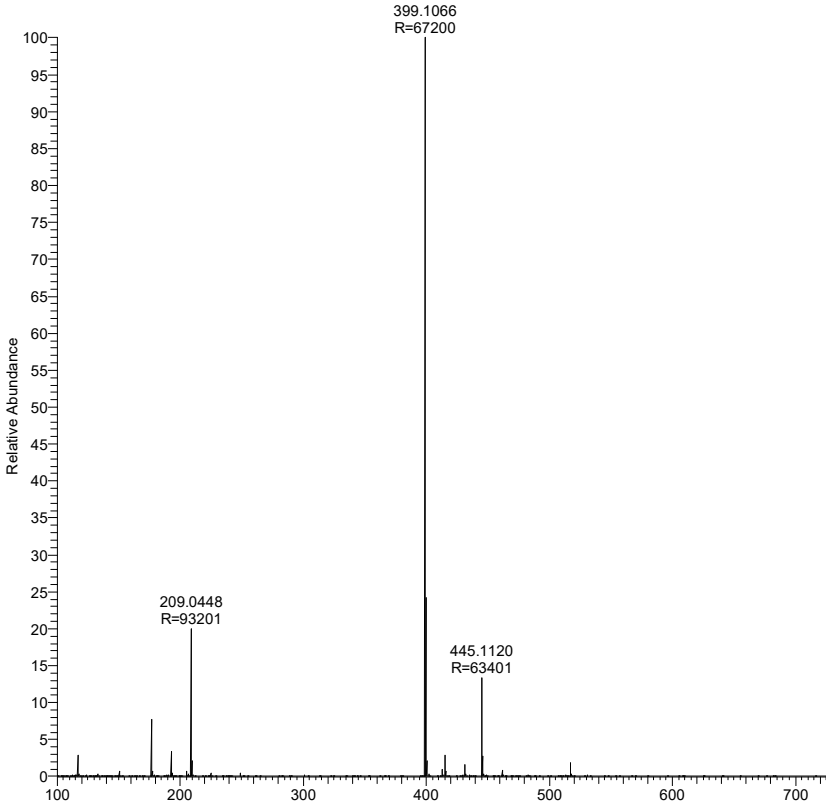

Fig. S19 HR-ESI-MS spectrum of glycyuralin R (**2**).

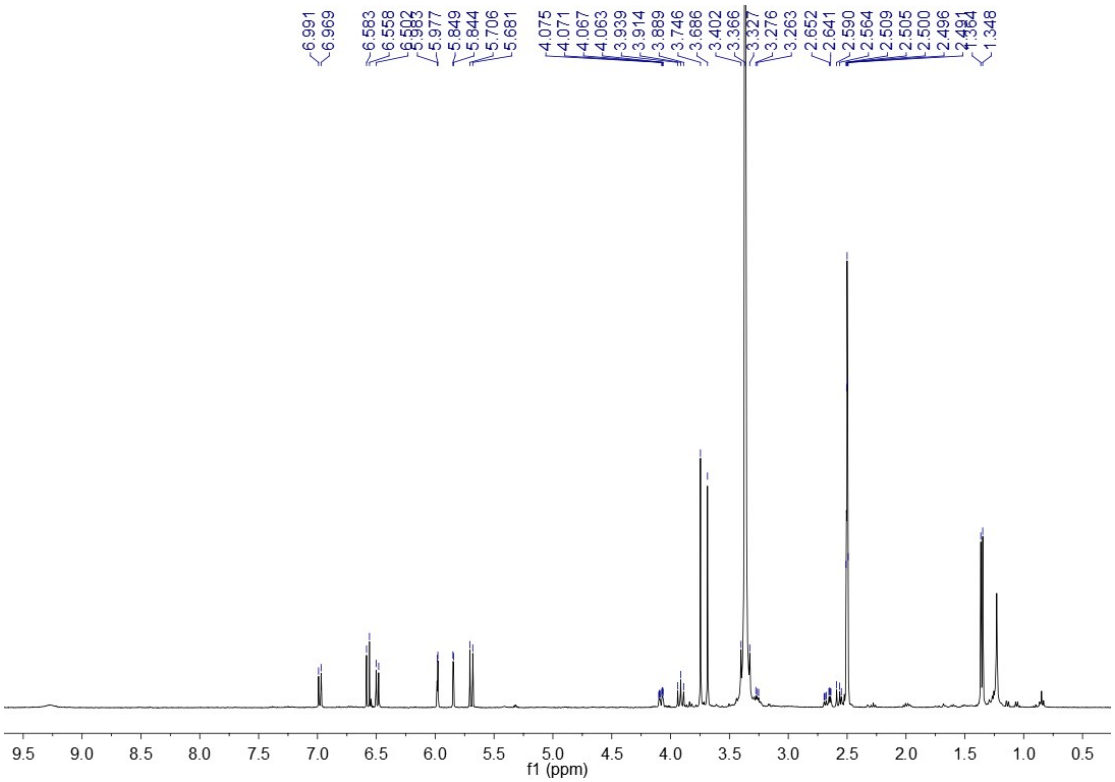

Fig. S20 ^{1}H NMR spectrum of glycyuralin S (**3**) in DMSO-d_6 (400 MHz).

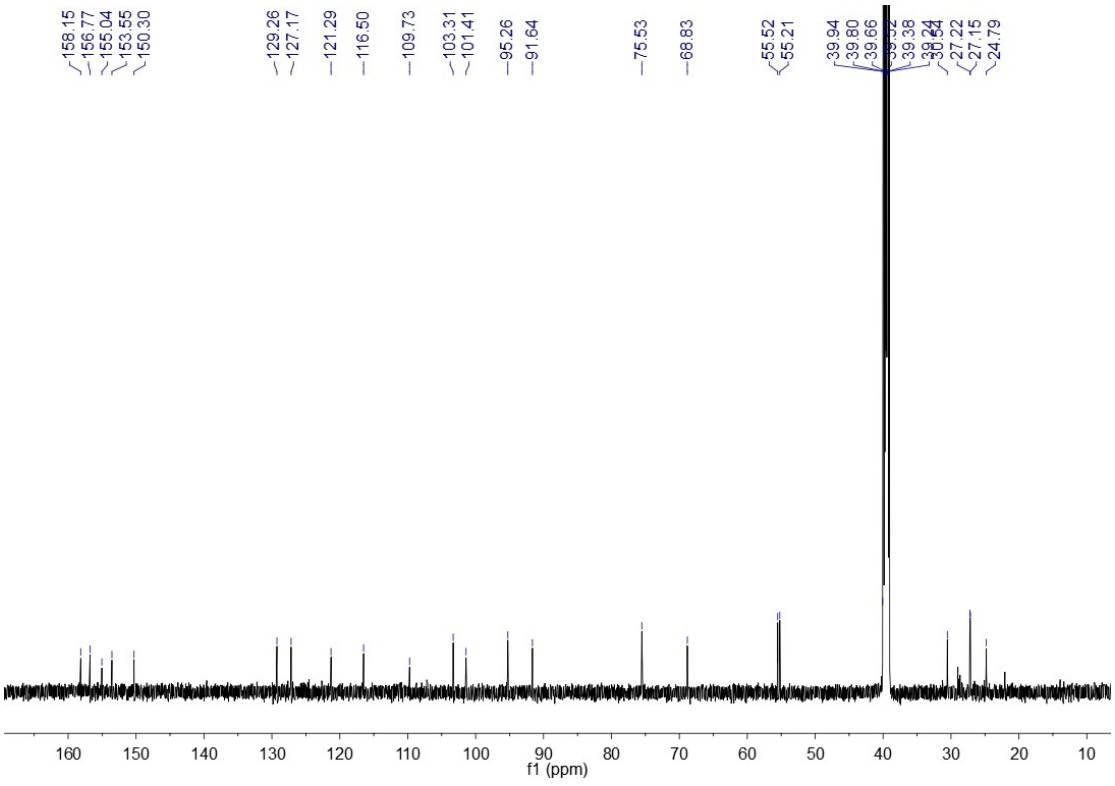

Fig. S21 ^{13}C NMR spectrum of glycyuralin S (**3**) in DMSO-d_6 (100 MHz).

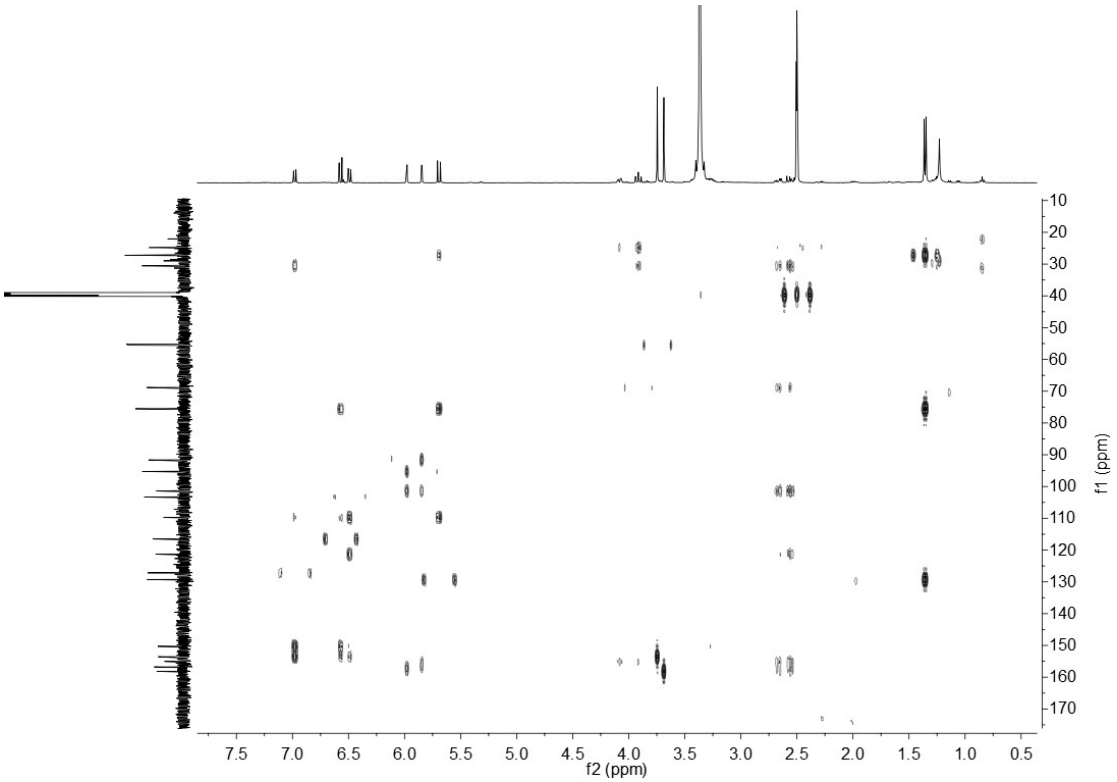

Fig. S22 HMBC spectrum of glycyuralin S (**3**) in DMSO-d_6 (400 MHz).

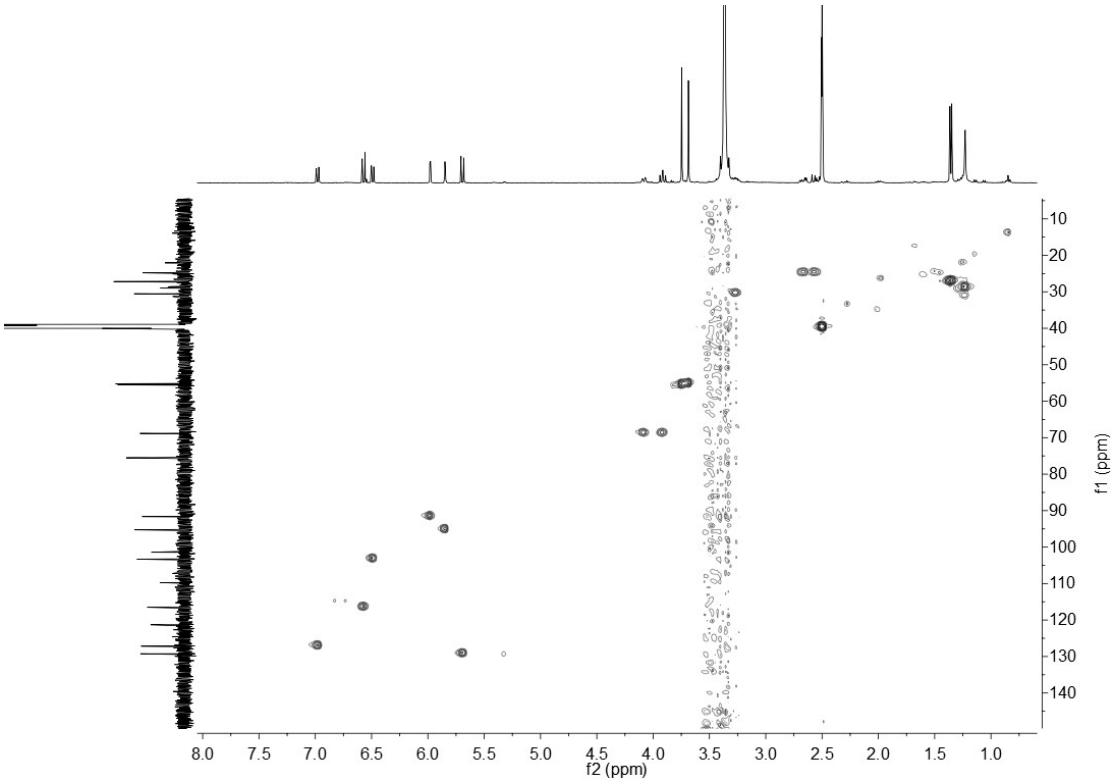

Fig. S23 HSQC spectrum of glycyuralin S (**3**) in DMSO-d_6 (400 MHz).

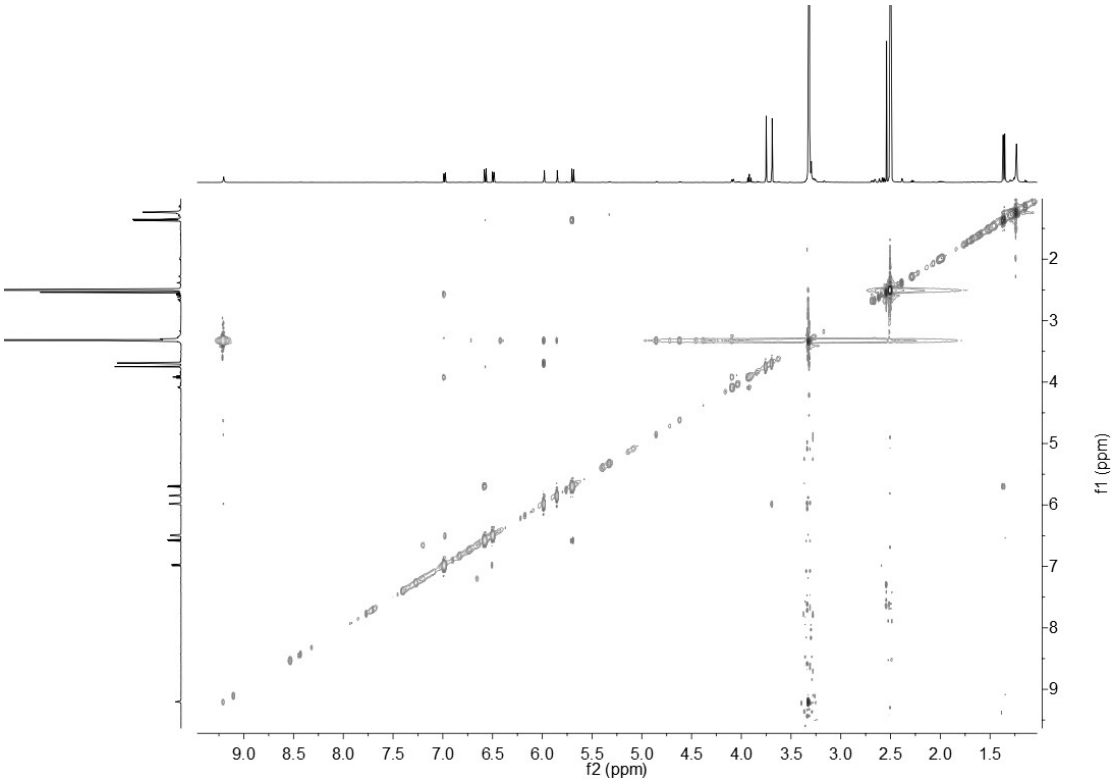

Fig. S24 NOESY spectrum of glycyuralin Q (**3**) in DMSO-d_6 (400 MHz).

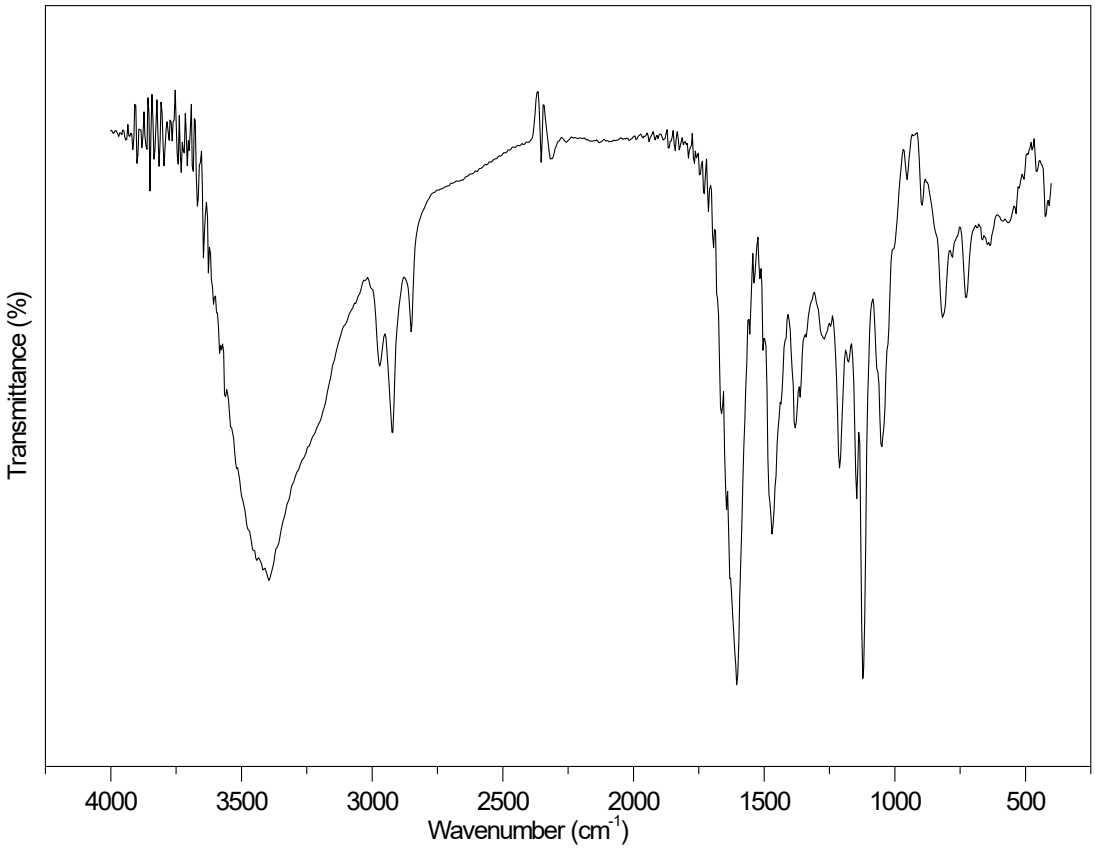

Fig. S25 IR spectrum of glycyuralin Q (**3**).

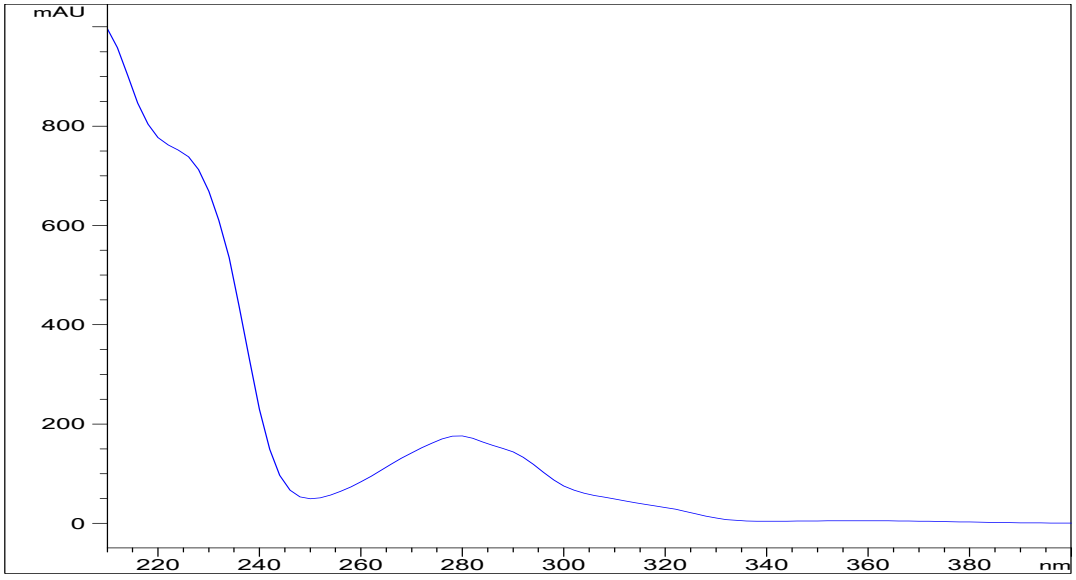

Fig. S26 UV spectrum of glycyuralin Q (**3**).

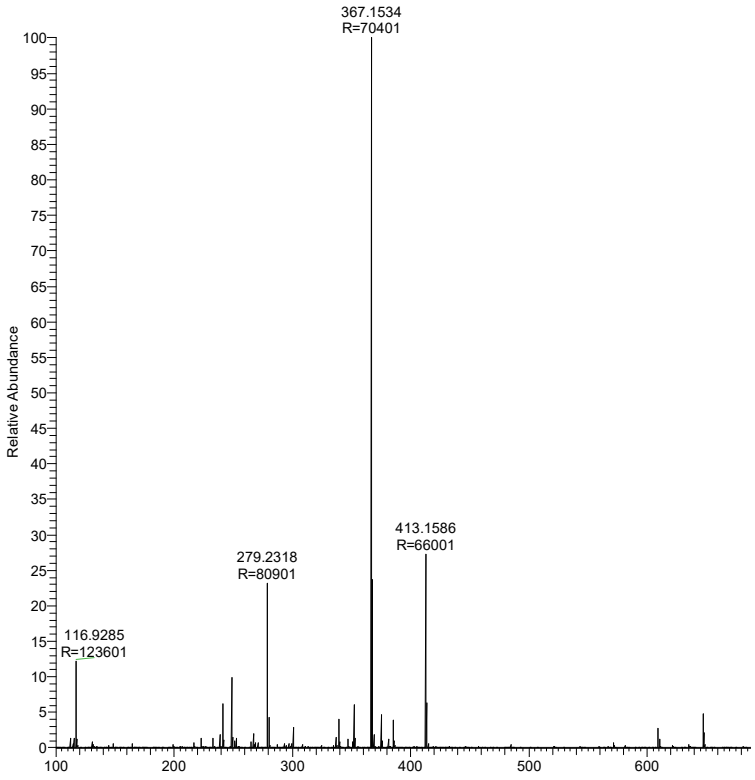

Fig. S27 HR-ESI-MS spectrum of glycyuralin S (**3**).