

Supplementary Materials: Enzymatic Synthesis of Novel and Highly-Soluble Puerarin

Glucoside by *Deinococcus geothermalis* Amylosucrase

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Table S1. ^1H and ^{13}C NMR assignments in DMSO- d_6 at 700 and 175 MHz for compounds (1).

position	δ_{C}	δ_{H} (J in HZ)
2	153.1	8.42, s
3	122.7	
4	174.8	
4a	116.6	
5	126.6	7.94, d, $J=8.8$ Hz
6	116.6	6.99, d, $J=8.8$ Hz
7	161.4	
8	112.7	
8a	156.9	
1'	125.6	
2'	129.9	7.52, d, $J=8.8$ Hz
3'	116.6	7.13, d, $J=8.8$ Hz
4'	156.9	
5'	116.6	7.13, d, $J=8.8$ Hz
6'	129.9	7.52, d, $J=8.8$ Hz
1''	73.4	4.81, d, $J=9.1$ Hz
2''	70.7	4.03, t, $J=9.1$ Hz
3''	78.8	3.26, t, $J=9.1$ Hz
4''	69.9	3.13, m
5''	81.9	3.24, m
6''	61.4	3.43, m
		3.72, m
1'''	98.0	5.42, d, $J=3.5$ Hz
2'''	71.6	3.35, m
3'''	73.1	3.64, m
4'''	69.9	3.13, m
5'''	73.8	3.48, m
6'''	60.7	3.47, m
		3.57, m

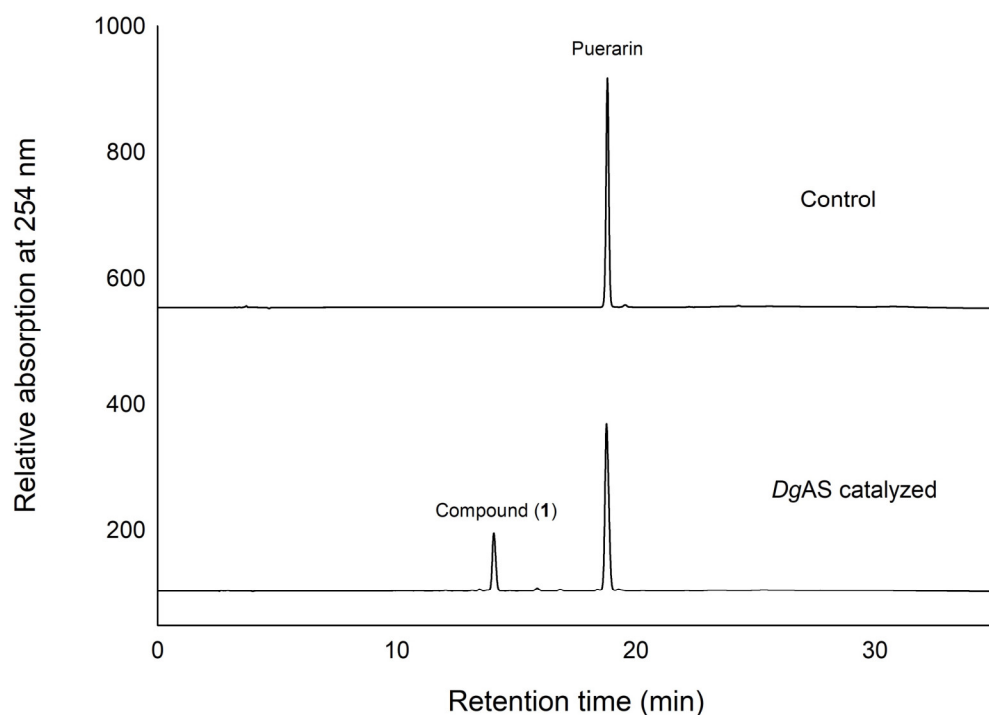


Figure S1. High-performance liquid chromatography (HPLC) analysis of the biotransformation products of puerarin using *Deinococcus geothermalis* amylosucrase (*DgAS*). The *DgAS* biotransformation mixture containing 25 μ g/mL of purified recombinant *DgAS* enzymes, 1 mg/mL of puerarin, 50% (w/v) sucrose, and 50 mM of phosphate buffer at pH 7 was incubated at 40°C for 24 h. After incubation, the biotransformation products were analyzed by HPLC. The HPLC operation procedure is described in the Materials and methods section.

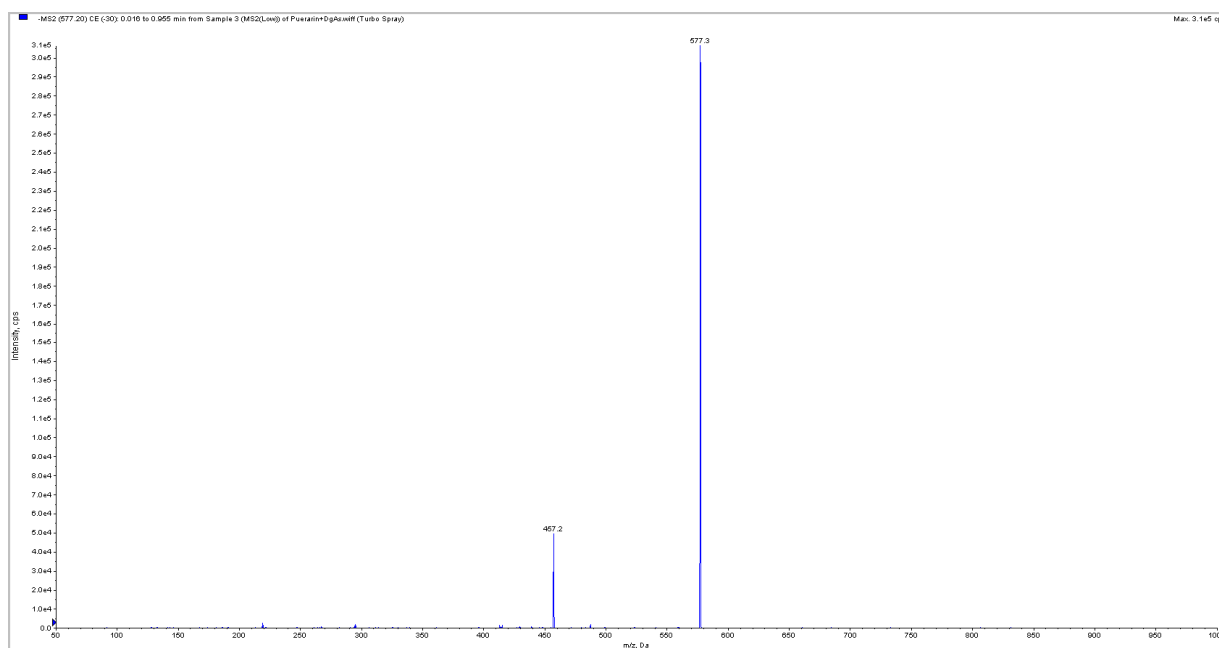


Figure S2. The mass-mass analysis of puerarin-4'-*O*- β -glucoside (**1**) at the negative mode. A significant signal at m/z 577.3 showed the corresponding m/z signal of molecular weight 416 of puerarin-4'-*O*- β -glucoside (**1**) ($416+180-18-1$) at the negative mode [puerarin -G - H].

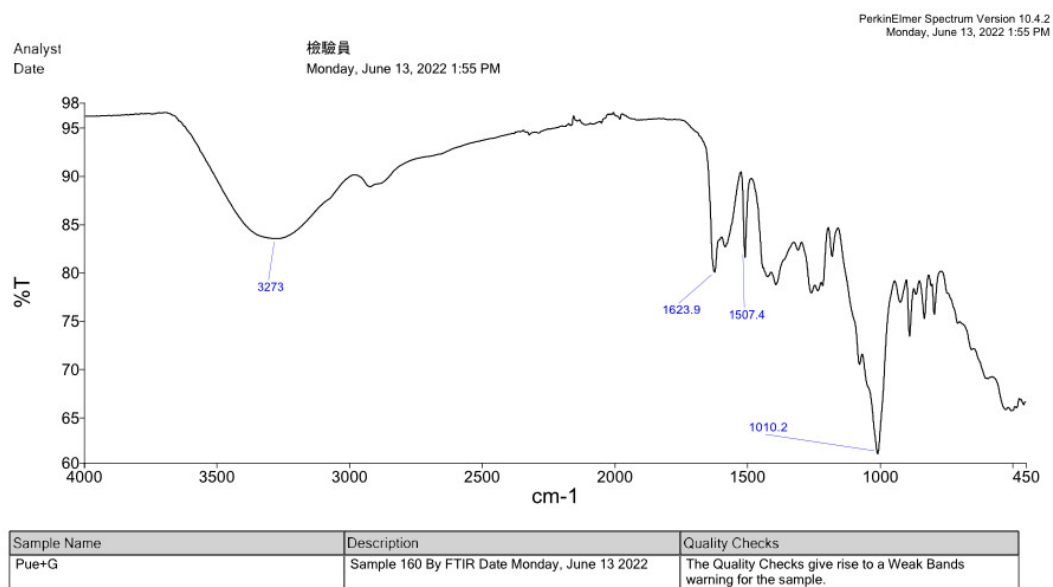


Figure 3. The infrared (IR) analysis of puerarin-4'-*O*- β -glucoside (**1**).

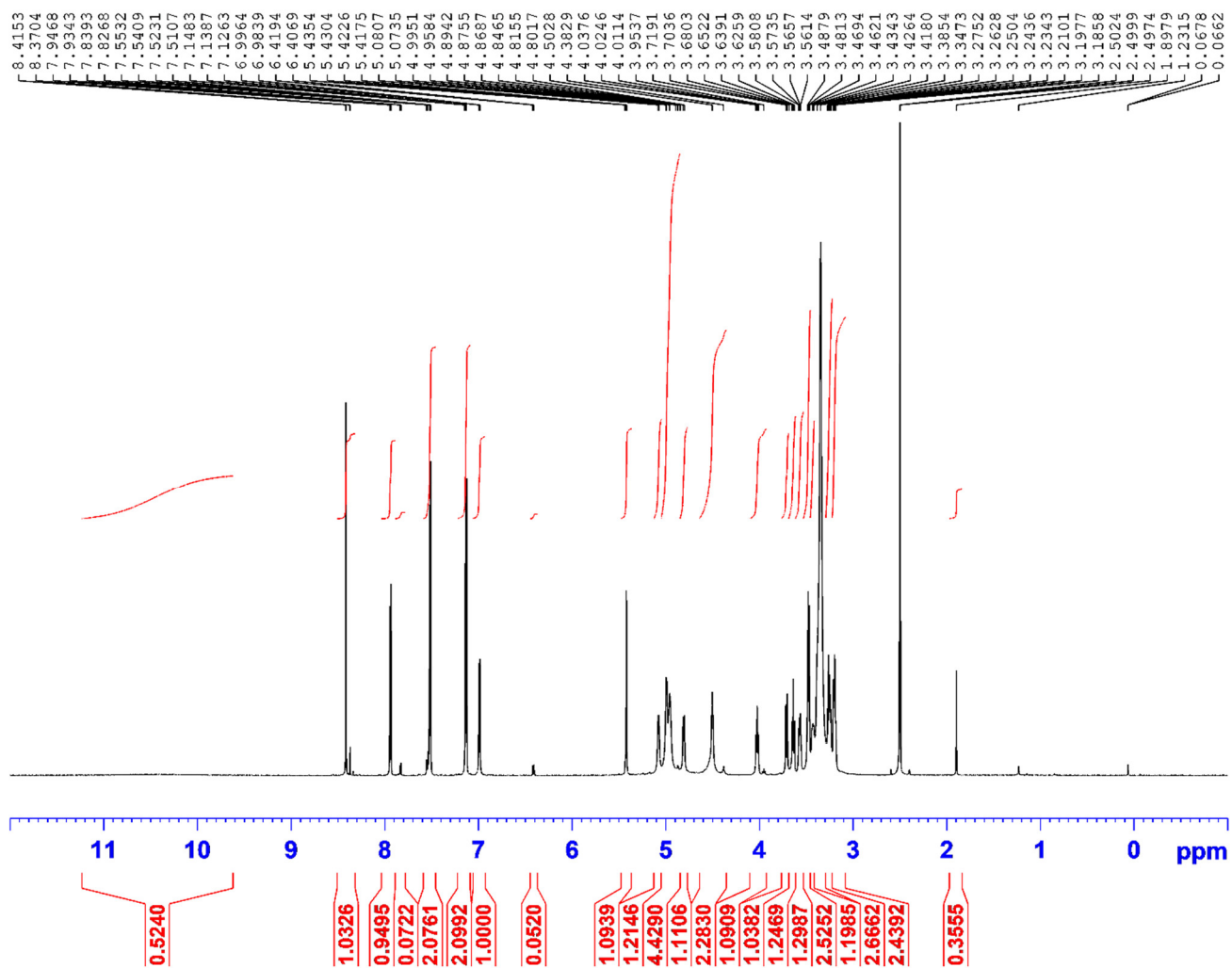


Figure S4. 1D NMR spectrum (¹H-NMR, 700 MHz, DMSO-*d*₆) of the puerarin-4'-O-β-glucoside (**1**).

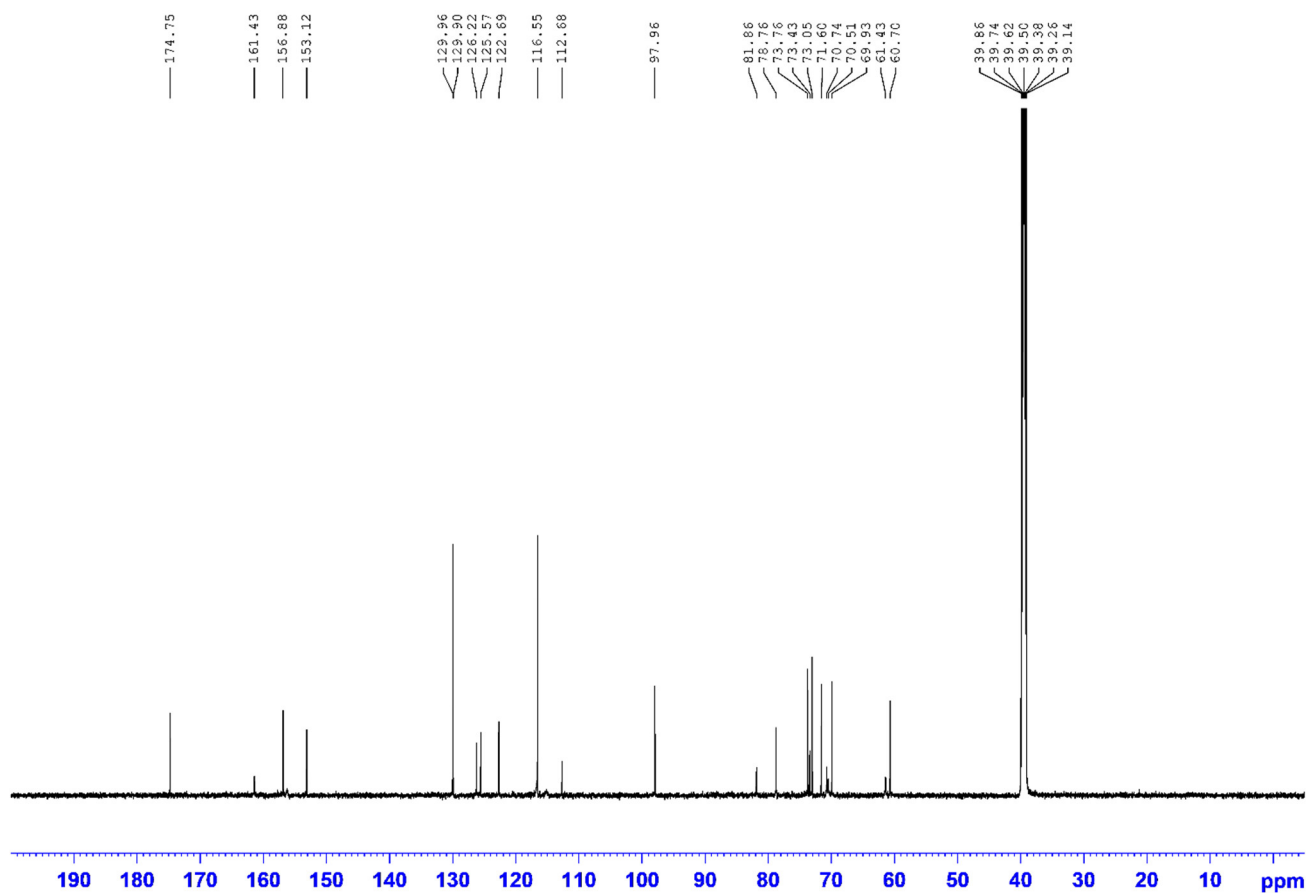


Figure S5. 1D NMR spectrum (^{13}C -NMR, 175 MHz, $\text{DMSO}-d_6$) of the puerarin-4'- O - β -D-glucoside (**1**).

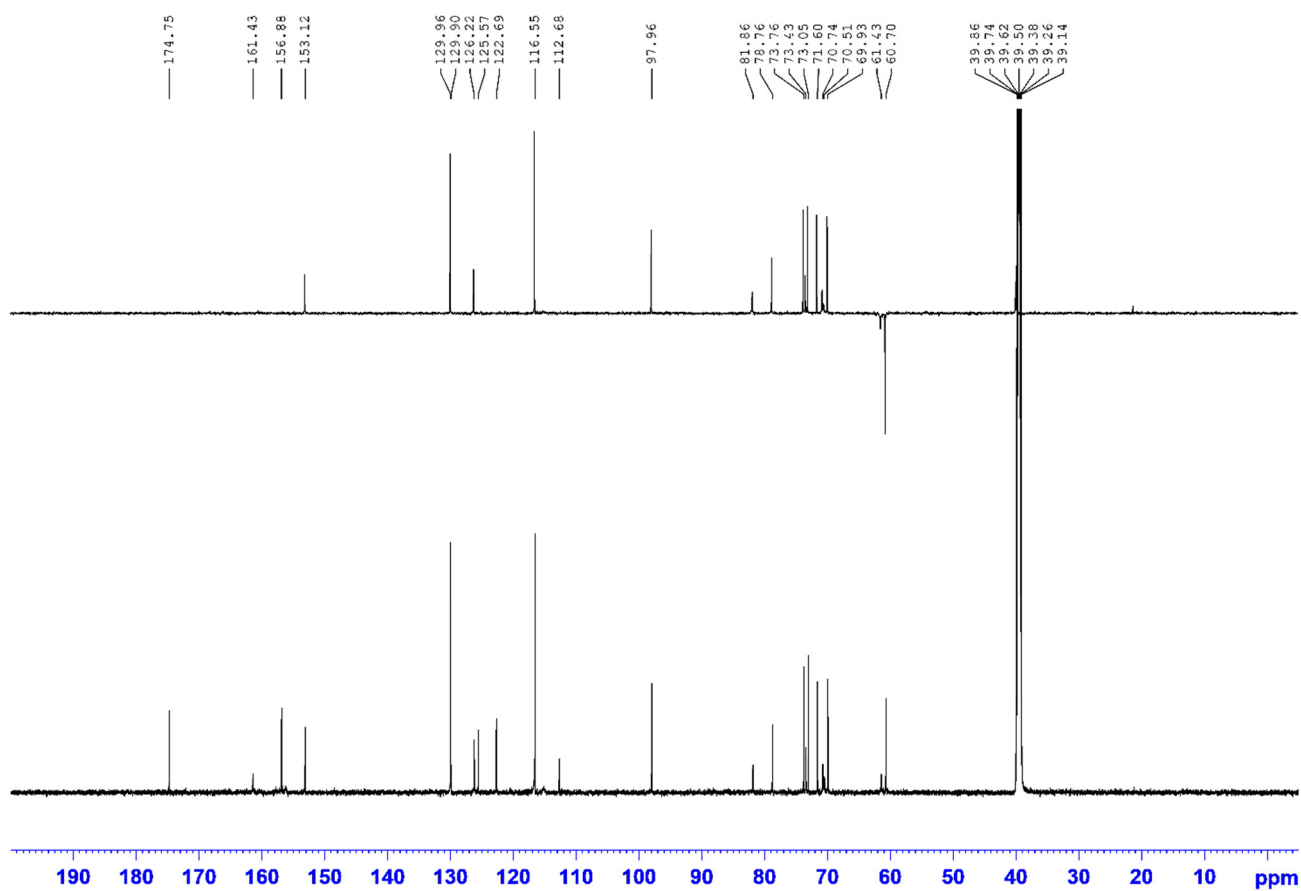


Figure S6. 1D NMR spectrum (DEPT-135, 175 MHz, DMSO-*d*₆) of the puerarin-4'-*O*-β-glucoside (1).

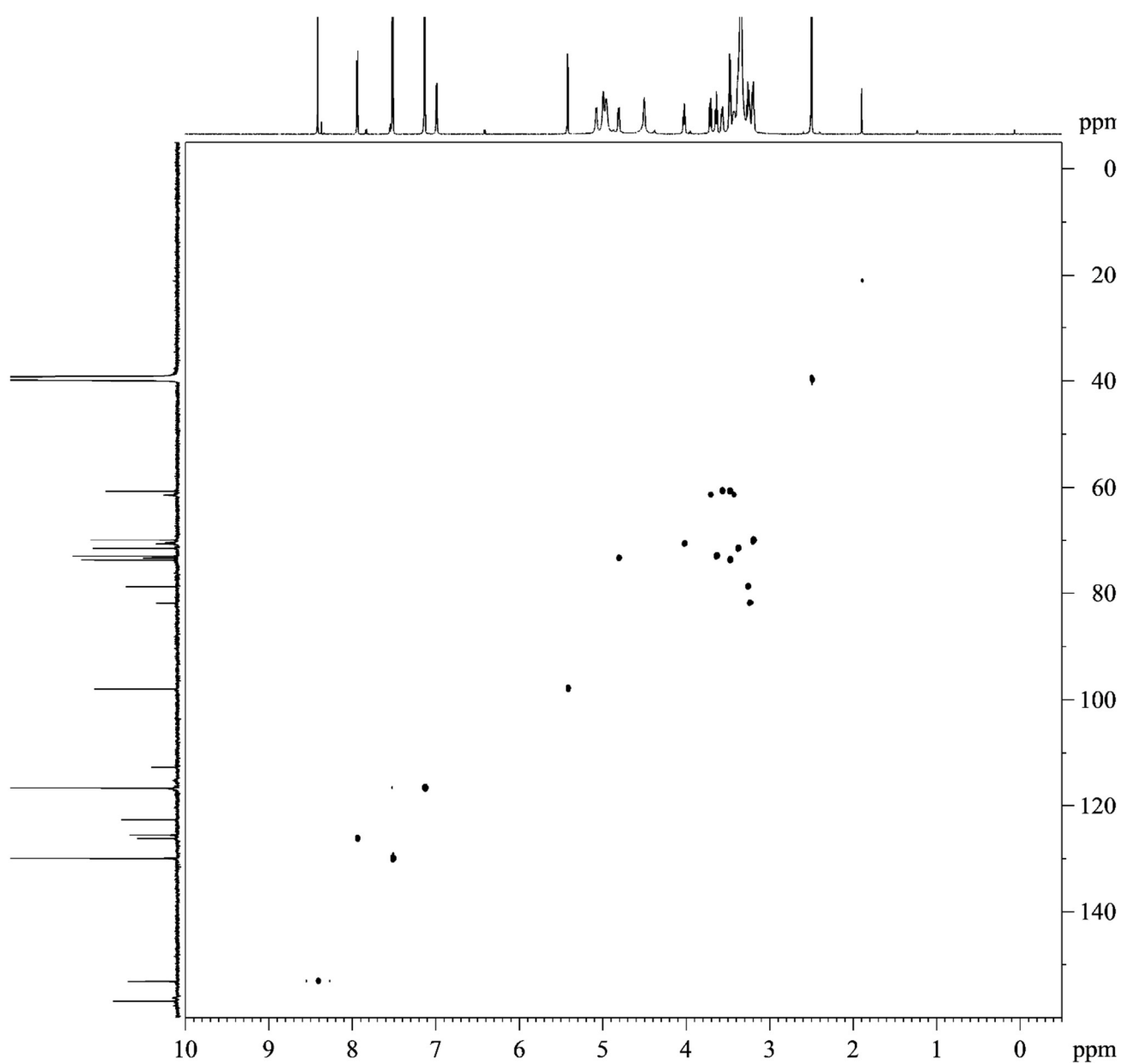


Figure S7. 2D NMR spectrum (^1H - ^{13}C HSQC, 700 MHz, $\text{DMSO}-d_6$) of the puerarin-4'- O - β -glucoside (1).

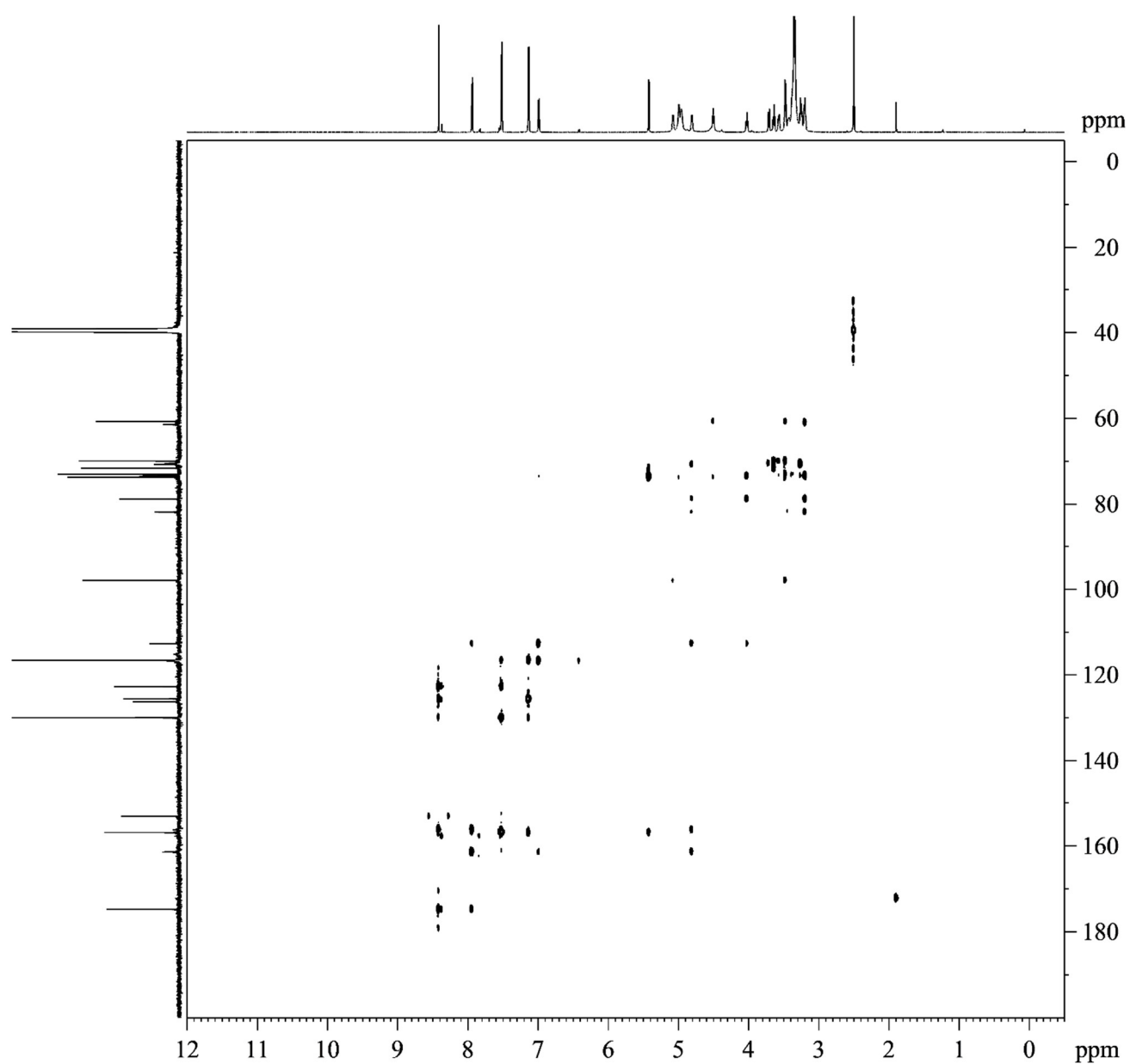


Figure S8. 2D NMR spectrum (^1H - ^{13}C HMBC, 700 MHz, $\text{DMSO}-d_6$) of the puerarin-4'- O - β -D-glucoside (**1**).

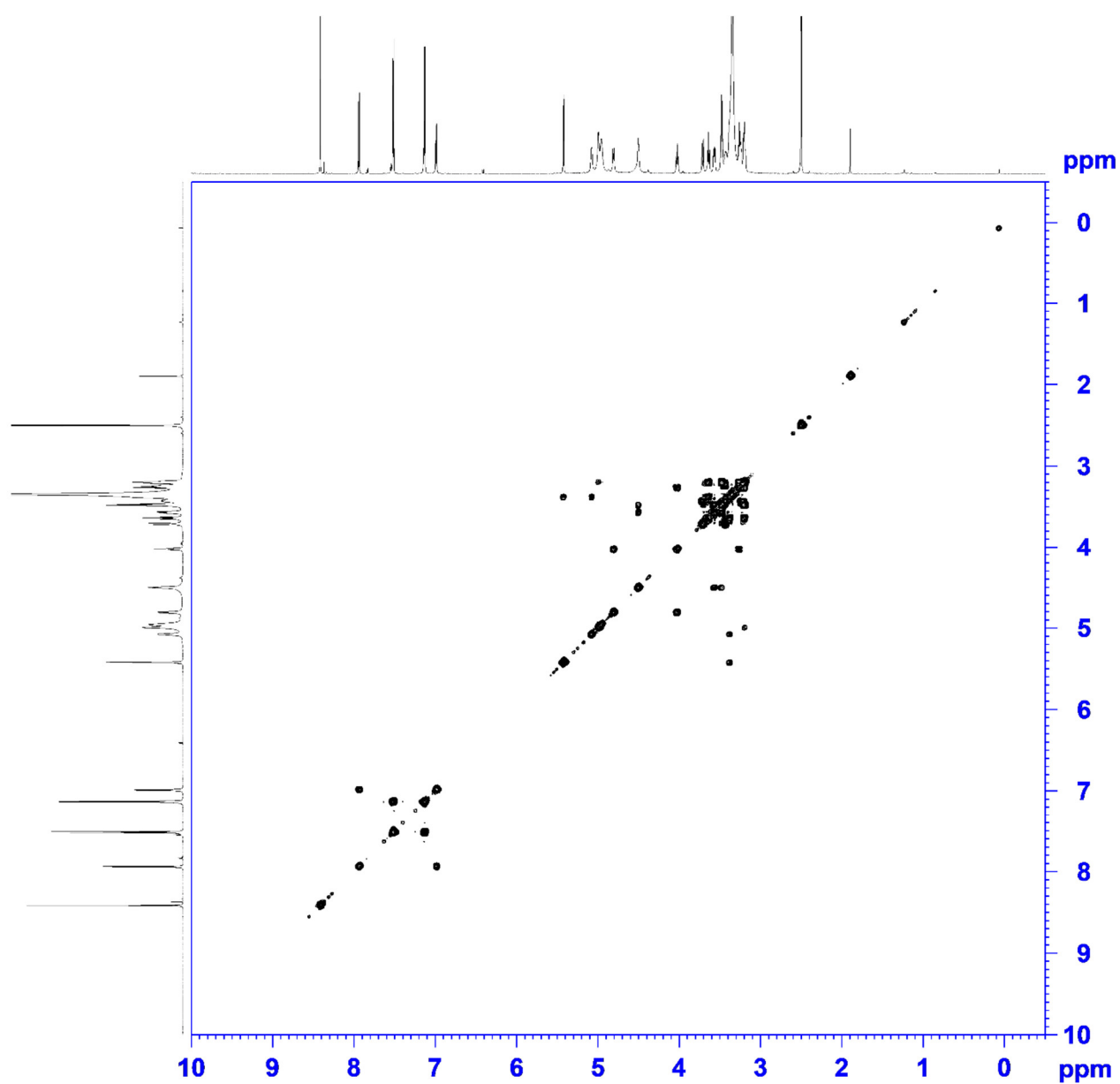


Figure S9. 2D NMR spectrum (^1H - ^1H COSY, 700 MHz, $\text{DMSO}-d_6$) of the puerarin-4'- O - β -D-glucoside (1).

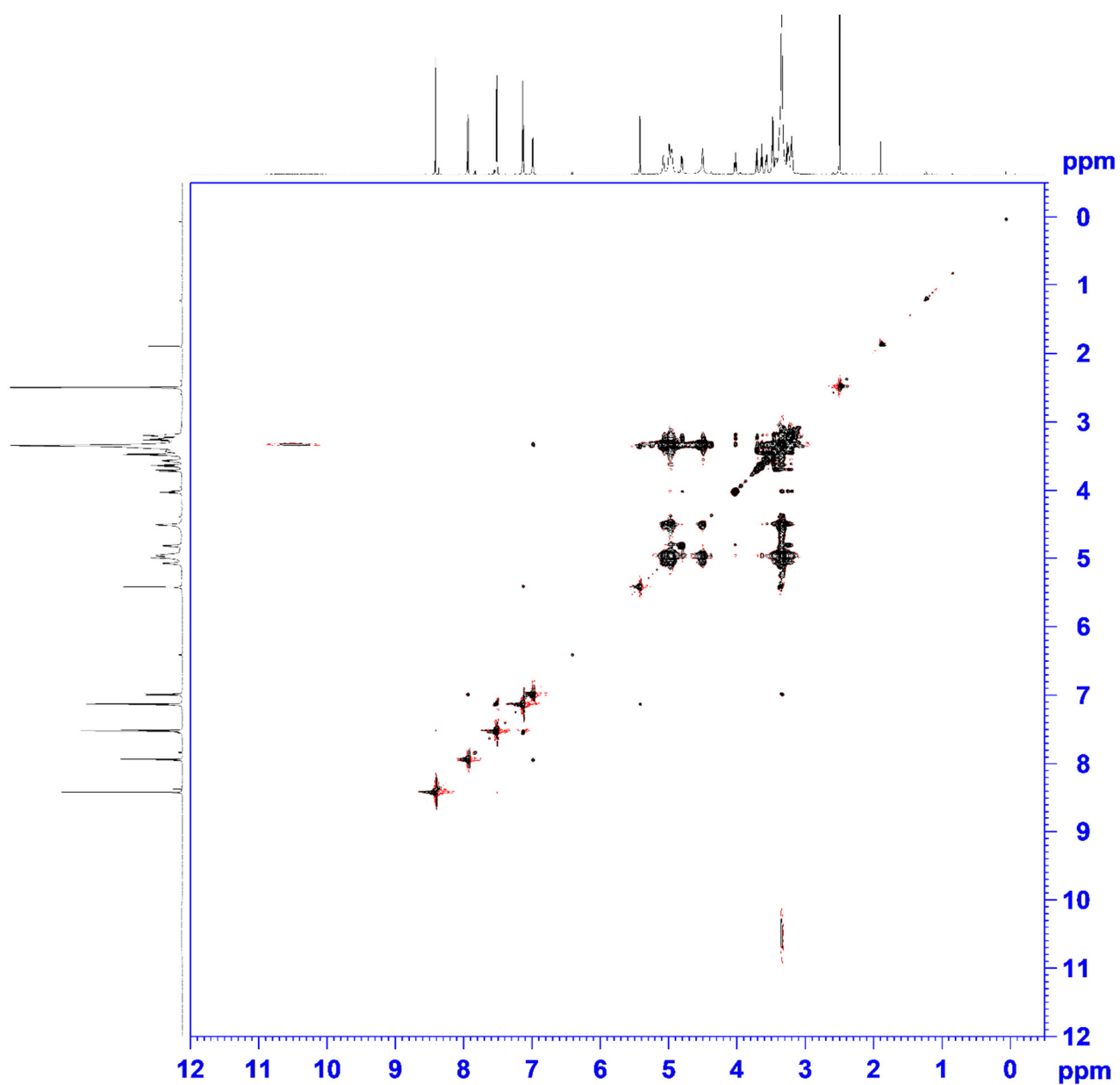


Figure S10. 2D NMR spectrum (^1H - ^1H NOESY, 700 MHz, $\text{DMSO}-d_6$) of the puerarin-4'-O- β -D-glucoside (1).