

Supporting Information

Biotransformation of geniposide into genipin by immobilized *Trichoderma reesei* and conformational study of genipin

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Figure S1: UV-VIS spectrum of genipin in MeOH.

Figure S2: FTIR spectrum of genipin.

Figure S3: EIMS spectrum of genipin.

Figure S4: ¹H-NMR spectrum of genipin in CDCl₃.

Figure S5: HPLC chromatograms of genipin using chiral columns under different conditions.

Figure S6: ¹H-NMR spectrum of acetylated genipin in C₅D₅N.

Figure S7: ¹H-NMR spectrum of geniposide in CDCl₃.

Figure S8: ¹H-NMR spectrum of genipin in DMCO-d₆.

Figure S9: ¹H-NMR spectrum of genipin in C₅D₅N.

Figure S10: ¹H-NMR spectrum of genipin in DMSO-d₆.

Table S1: Crystallographic data of genipin.

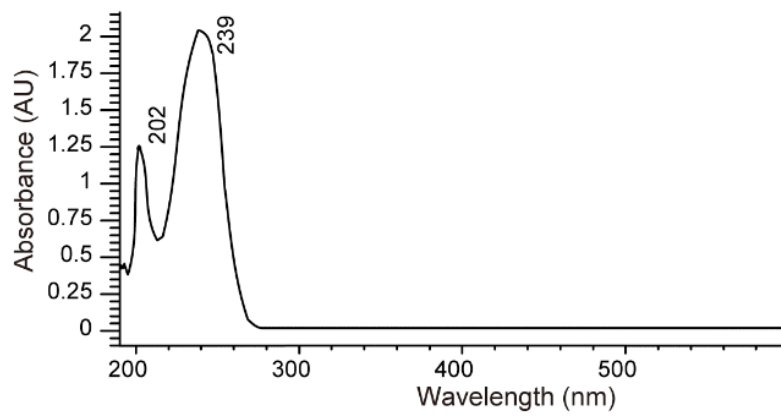


FIGURE S1: UV-VIS spectrum of genipin in MeOH.

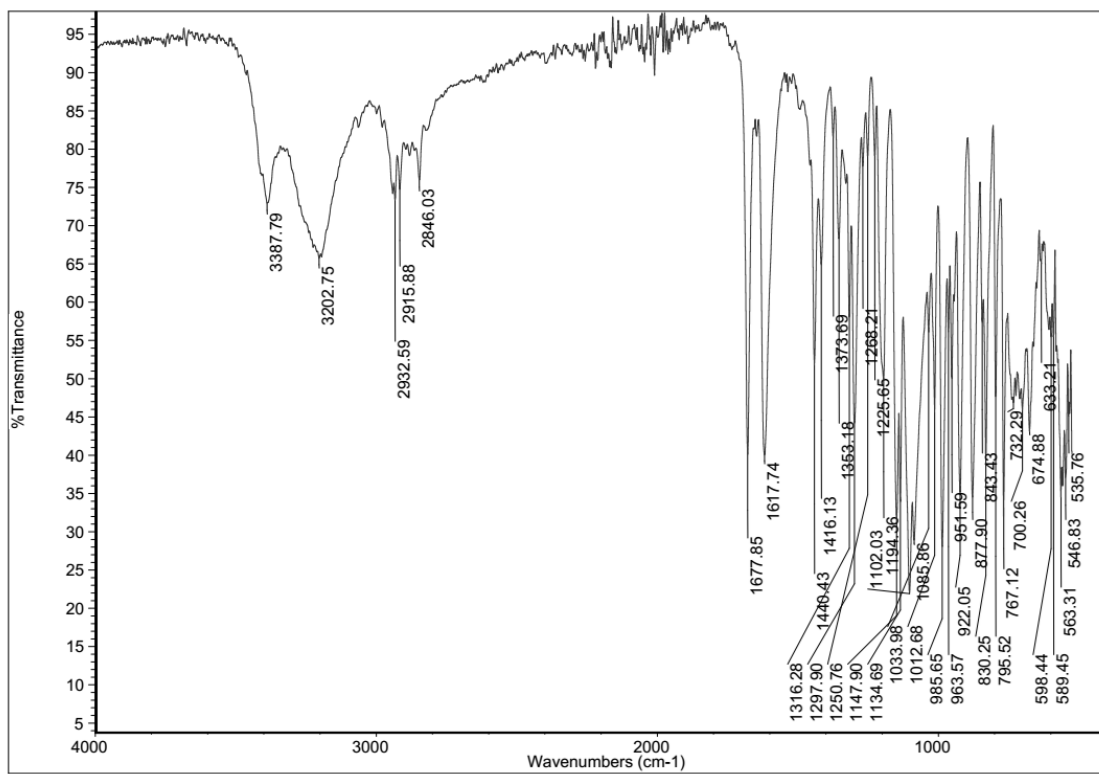


FIGURE S2: FTIR spectrum of genipin.

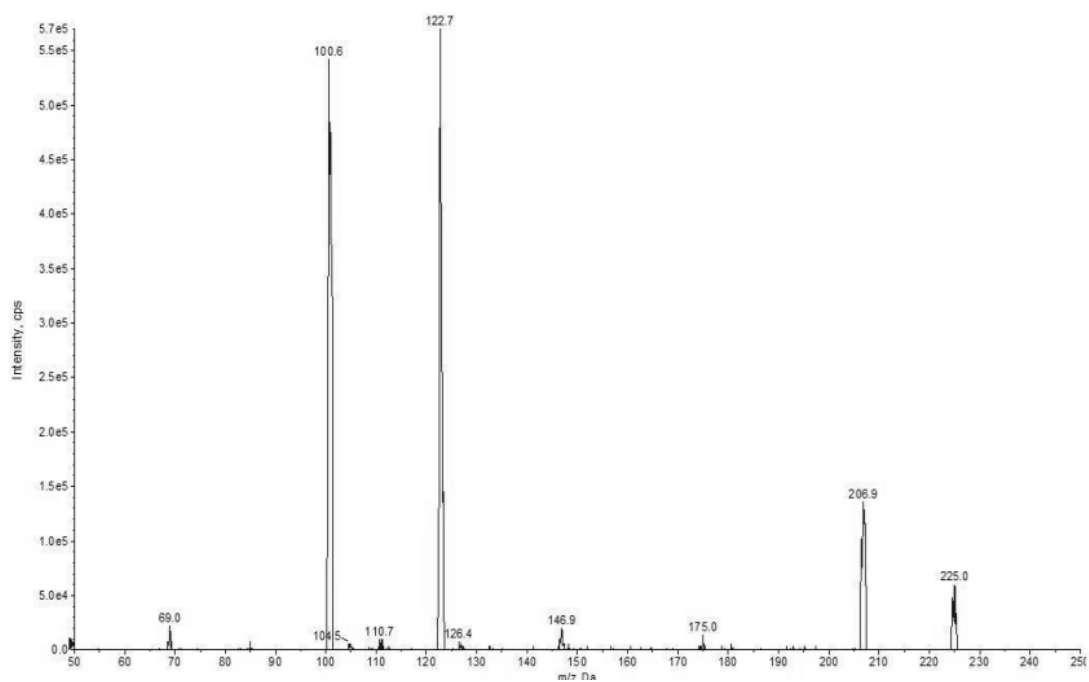


FIGURE S3: EIMS spectrum of genipin.

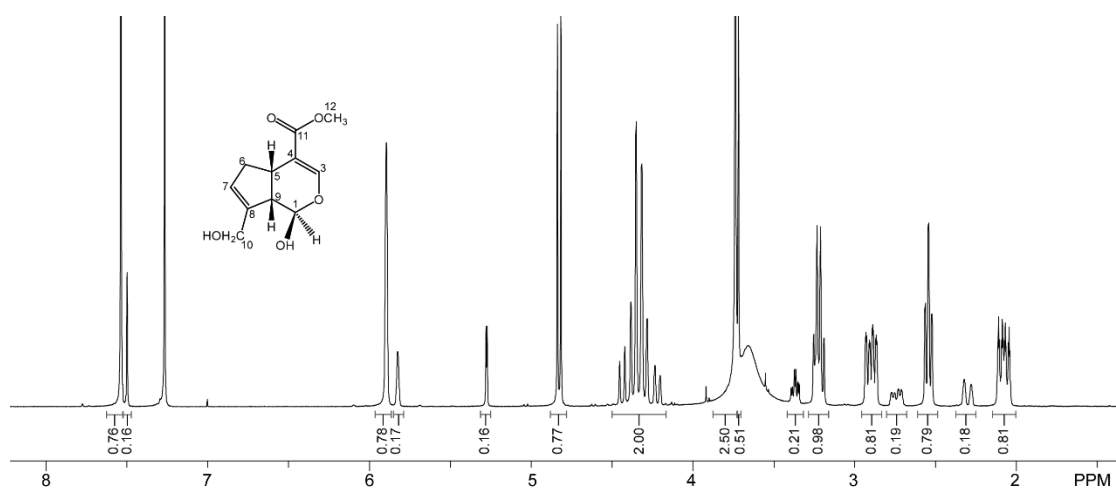


FIGURE S4: ¹H-NMR spectrum of genipin in CDCl₃.

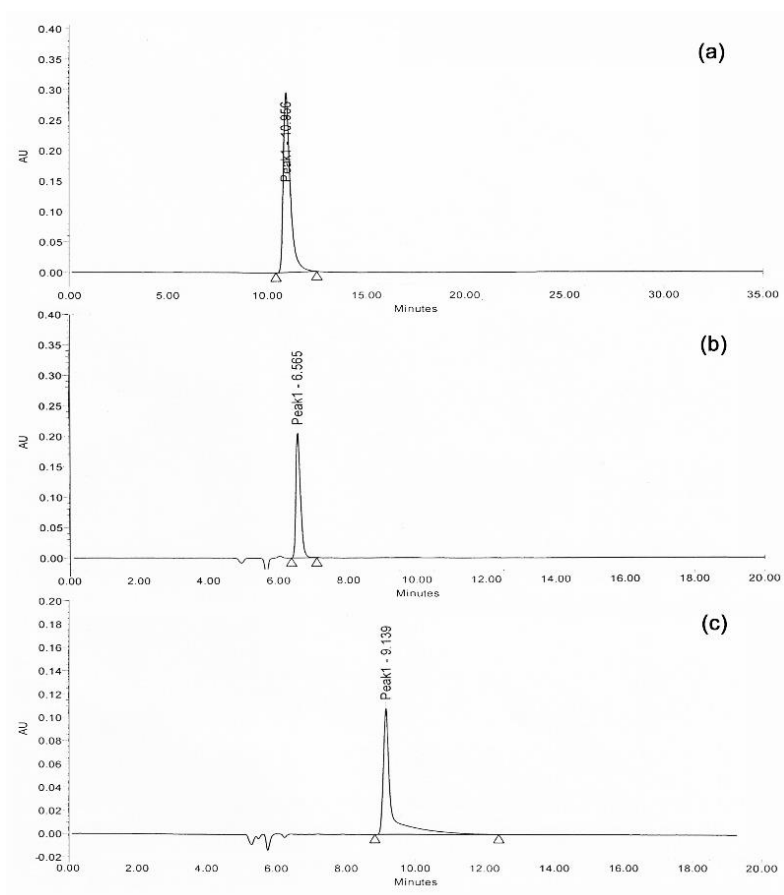


FIGURE S5: HPLC chromatograms of genipin using chiral columns under different conditions. (a) Entry 1; (b) Entry 2; (c) Entry 3.

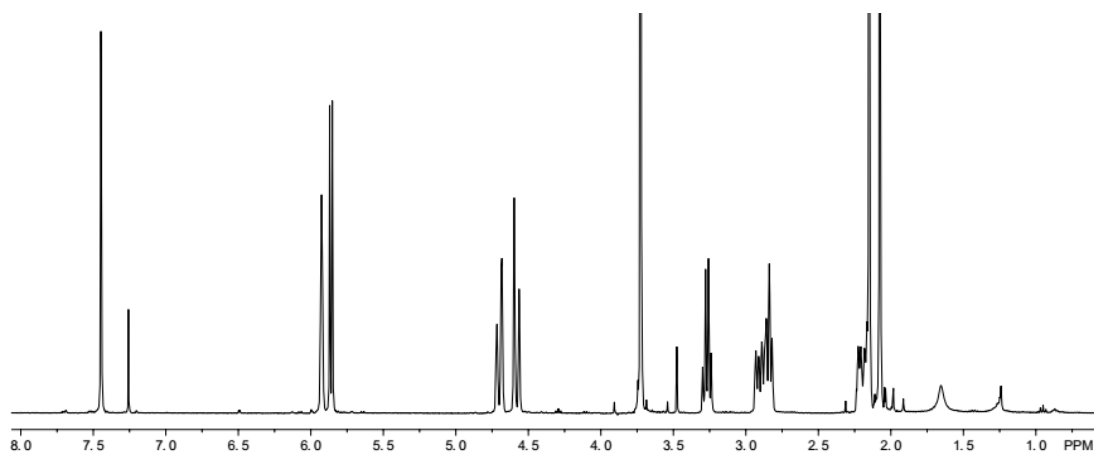


FIGURE S6: $^1\text{H-NMR}$ spectrum of acetylated genipin in $\text{C}_5\text{D}_5\text{N}$.

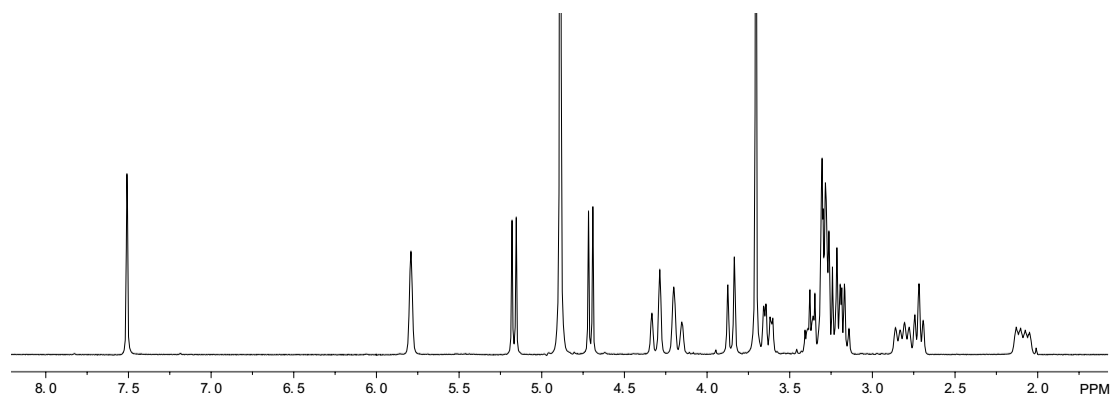


FIGURE S7: $^1\text{H-NMR}$ spectrum of geniposide in CDCl_3 .

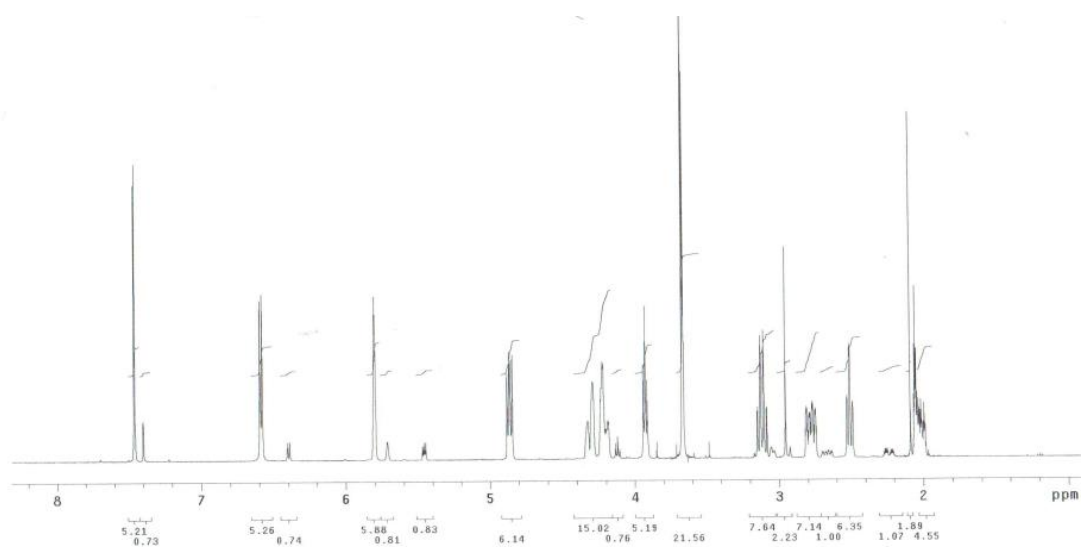


FIGURE S8: $^1\text{H-NMR}$ spectrum of genipin in DMCO-d_6 .

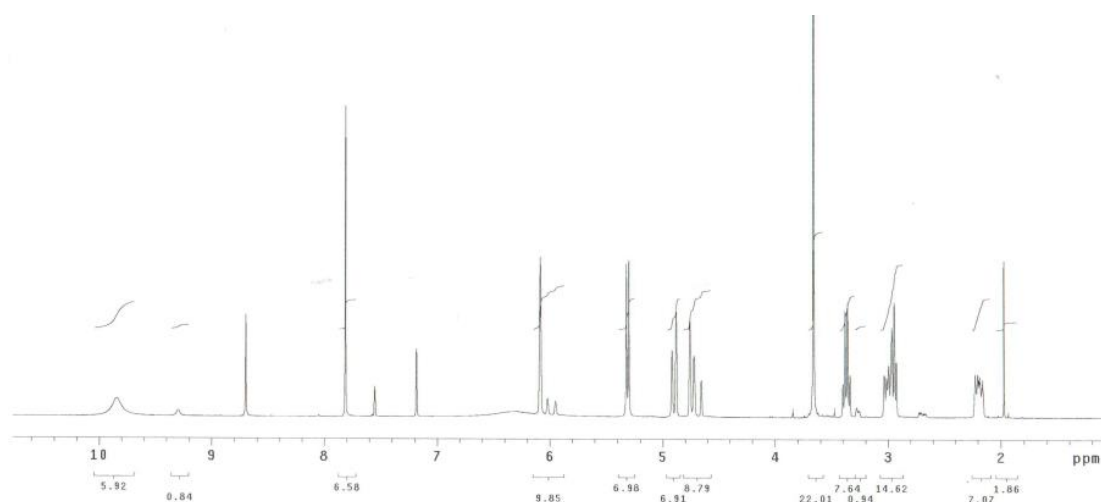


FIGURE S9: $^1\text{H-NMR}$ spectrum of genipin in $\text{C}_5\text{D}_5\text{N}$.

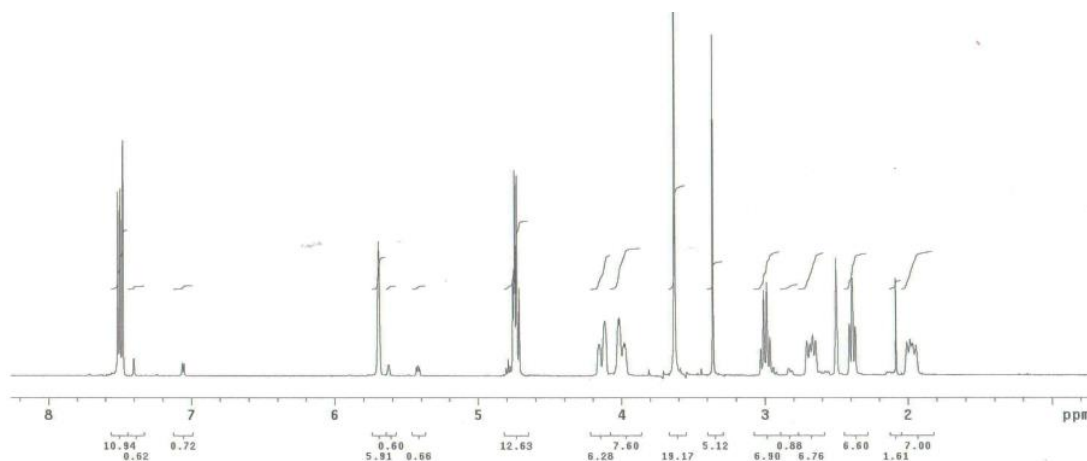


FIGURE S10: ^1H -NMR spectrum of genipin in DMSO-d_6 .

TABLE S1: Crystallographic data of genipin.

Empirical formula	$\text{C}_{11}\text{H}_{14}\text{O}_5$
Formula weight	226.22
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group (number)	P2 (1)
Unit cell dimensions	a=7.563(7) Å b=17.799(17) Å c=8.151(8) Å $\alpha=90^\circ$ $\beta=93.720(17)^\circ$ $\gamma=90^\circ$
Volume	1094.9(19) Å ³
Z	4
Calculated density	1.372 mg/m ³
Absorption coefficient	0.109 mm ⁻¹
F(000)	480
Crystal size	0.402 × 0.369 × 0.211 mm
θ range for data collection	2.29-25.50°
Limiting indices	$-9 \leq h \leq 9$, $-21 \leq k \leq 20$, $-6 \leq l \leq 9$
Reflections collected/ unique	5288/3614 [R(int)=0.0465]
Data/restrictions/parameters	3614/1/295
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.083
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0757; wR2 = 0.1930
R indices (all data)	R1 = 0.0882 wR2 = 0.2022
Largest diff. peak and hole	0.457 and -0.226 e ⁻ Å ⁻³