

Novel flavan-3-ol-glutathione conjugates from degradation of proanthocyanidins as high bioactive antioxidants

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Table S1. Experimental domain for Box-Behnken design.

Variable	Factors levels		
	-1	0	1
Acidity (X_1 , M)	0.1	0.2	0.3
Temperature (X_2 , °C)	45	55	65
Time (X_3 , min)	20	30	40

Table S2. Analysis of variance (ANOVA) for surface quadratic models.

Responses	Source of variation	Sum of squares	Df	Mean Squares	F Value	P value
Y ₁	Model	1.99E+05	9	22141.61	757.01	< 0.0001
	X ₁	3202.4	1	3202.4	109.49	< 0.0001
	X ₂	15203.32	1	15203.32	519.79	< 0.0001
	X ₃	1005.54	1	1005.54	34.38	0.0006
	X ₁ X ₂	11927.92	1	11927.92	407.81	< 0.0001
	X ₁ X ₃	1922.38	1	1922.38	65.73	< 0.0001
	X ₂ X ₃	4120.36	1	4120.36	140.87	< 0.0001
	X ₁ ²	39406.38	1	39406.38	1347.28	< 0.0001
	X ₂ ²	76016.08	1	76016.08	2598.94	< 0.0001
	X ₃ ²	30274.14	1	30274.14	1035.05	< 0.0001
	Lack of Fit	151.11	3	50.37	3.76	0.1168
	C.V. %				0.67	

R²=0.9990, R² (adjusted) = 0.9977 and R² (predicted) = 0.9875.

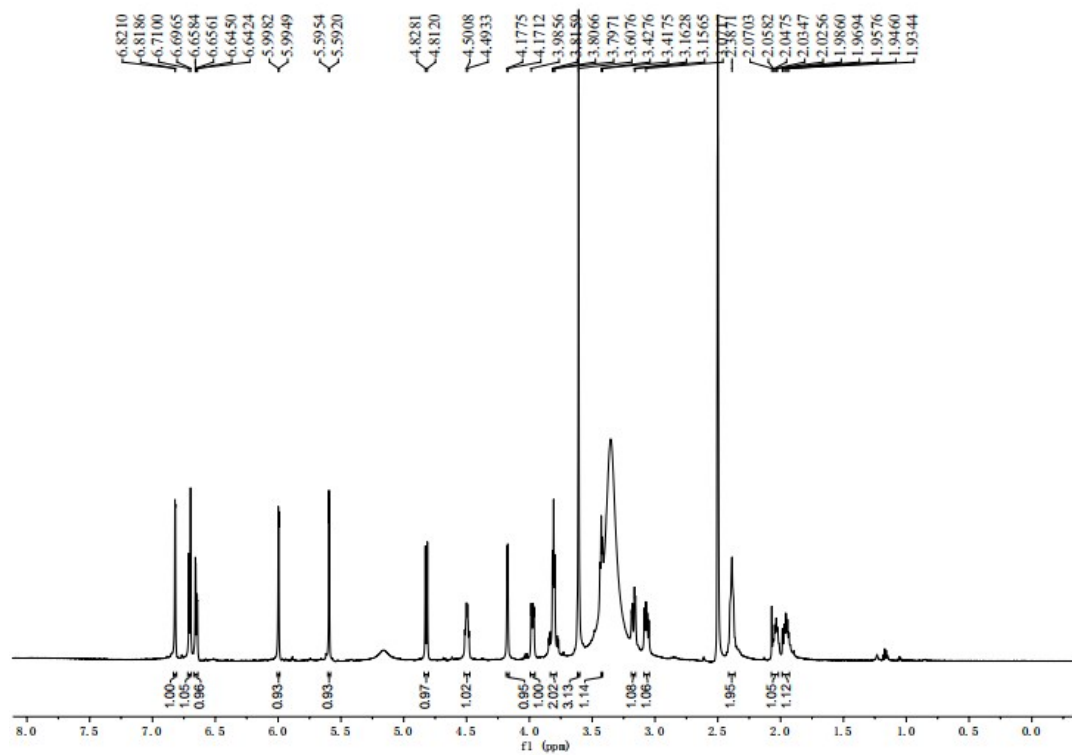


Figure S1. ¹H NMR spectrum (600 MHz, DMSO) of C-G-1.

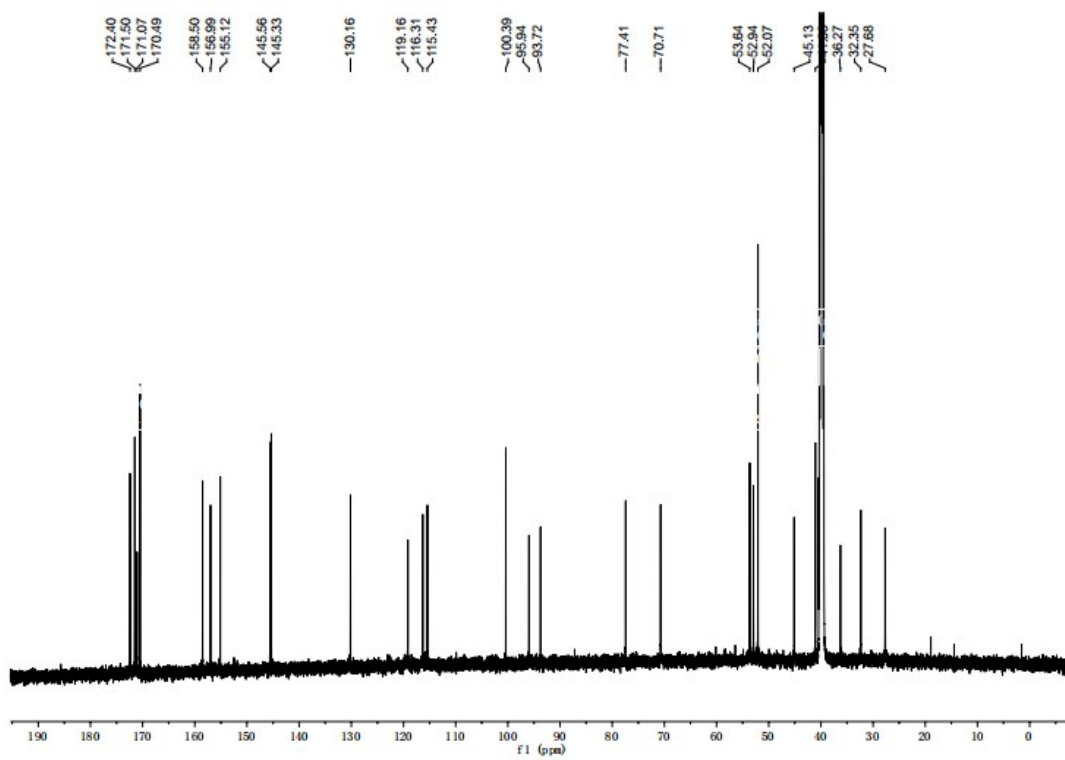


Figure S2. ^{13}C NMR spectrum (150 MHz, DMSO) of C-G-1.

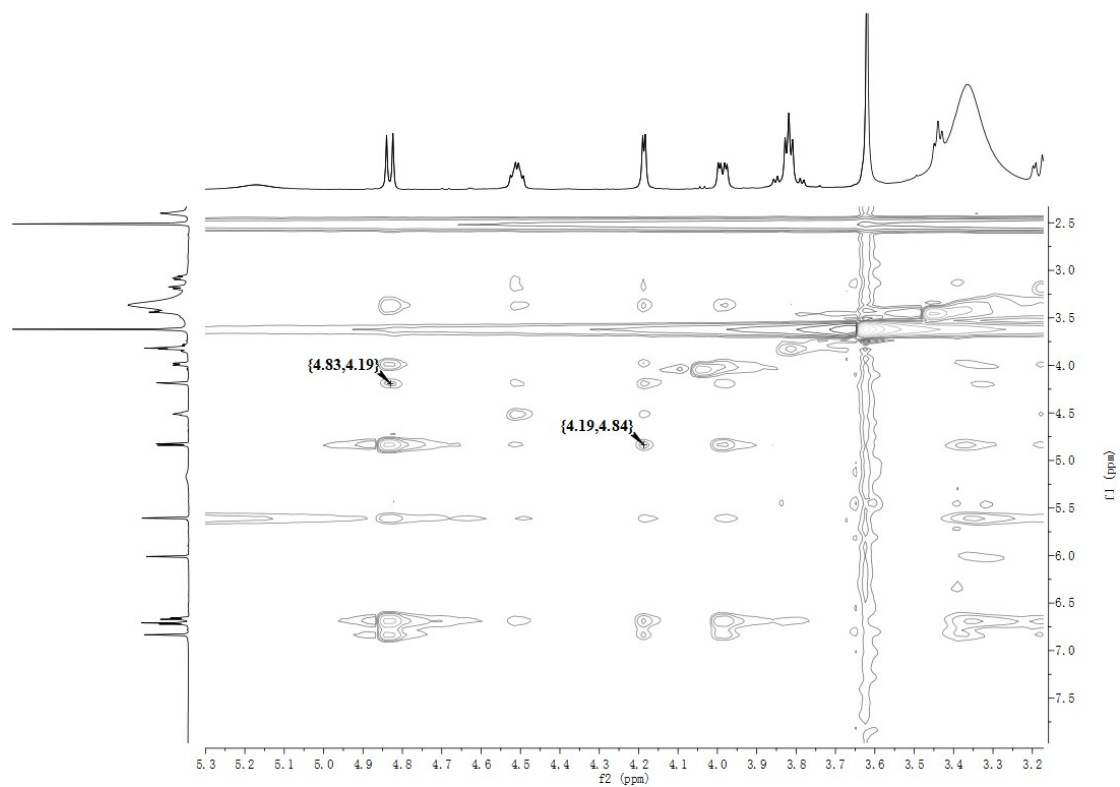


Figure S3. NOESY spectrum (600 MHz, DMSO) of C-G-1.

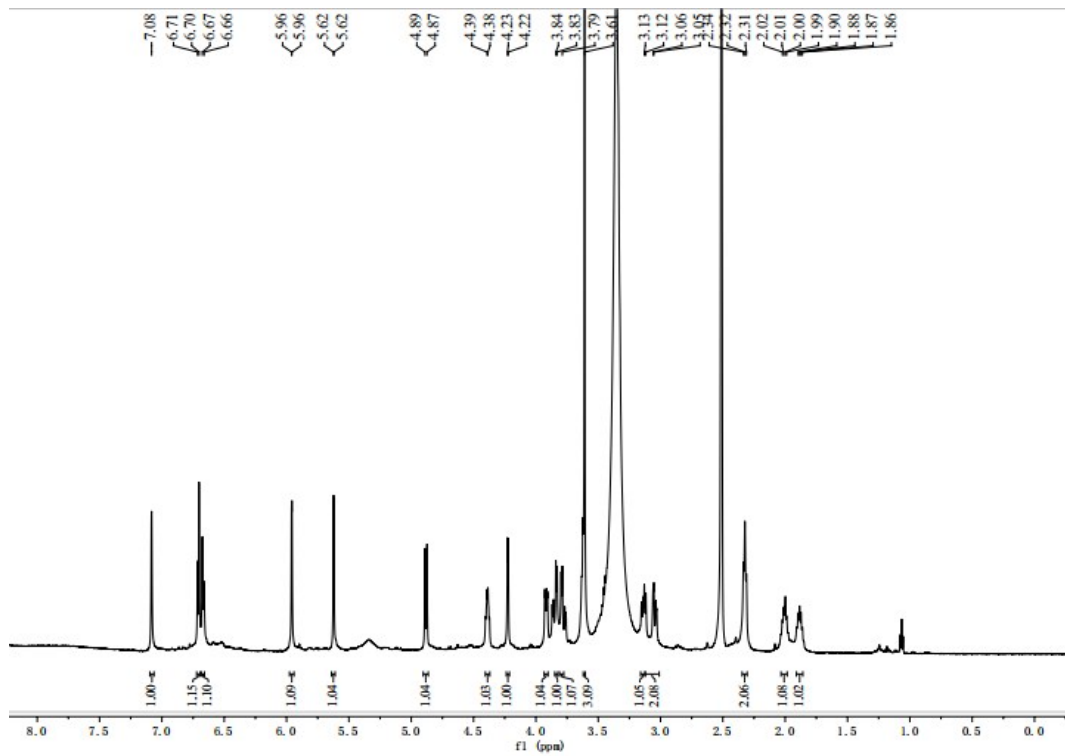


Figure S4. ¹H NMR spectrum (600 MHz, DMSO) of C-G-2.

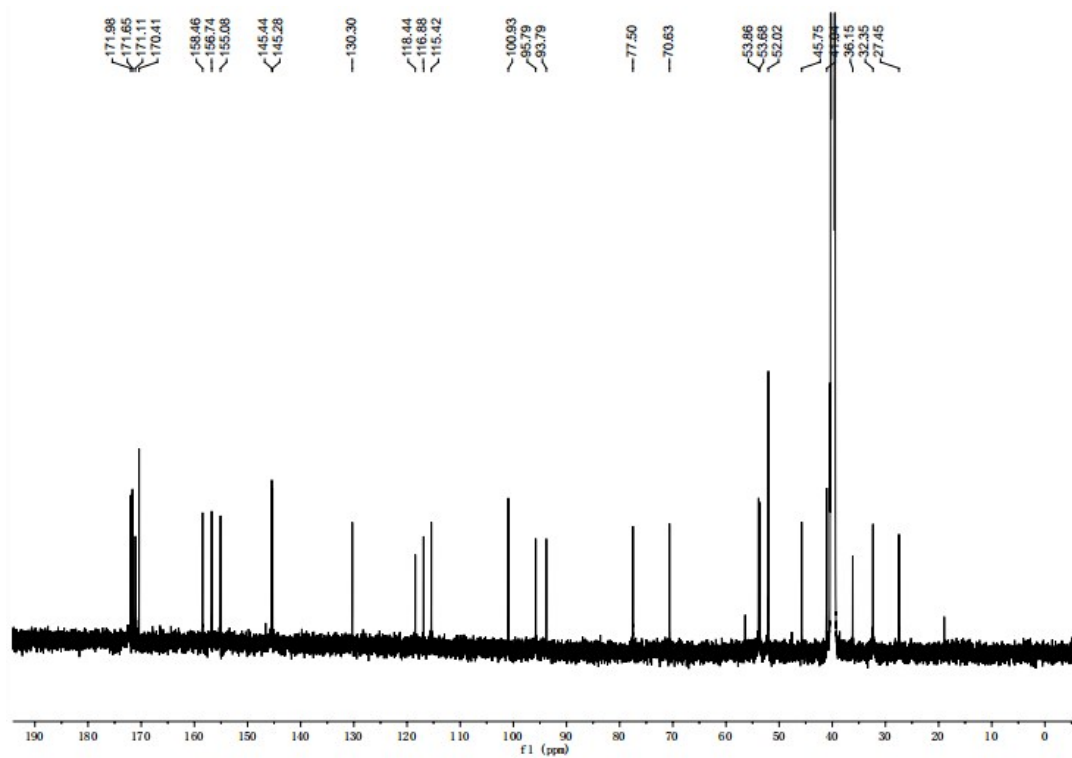


Figure S5. ^{13}C NMR spectrum (150 MHz, DMSO) of C-G-2.

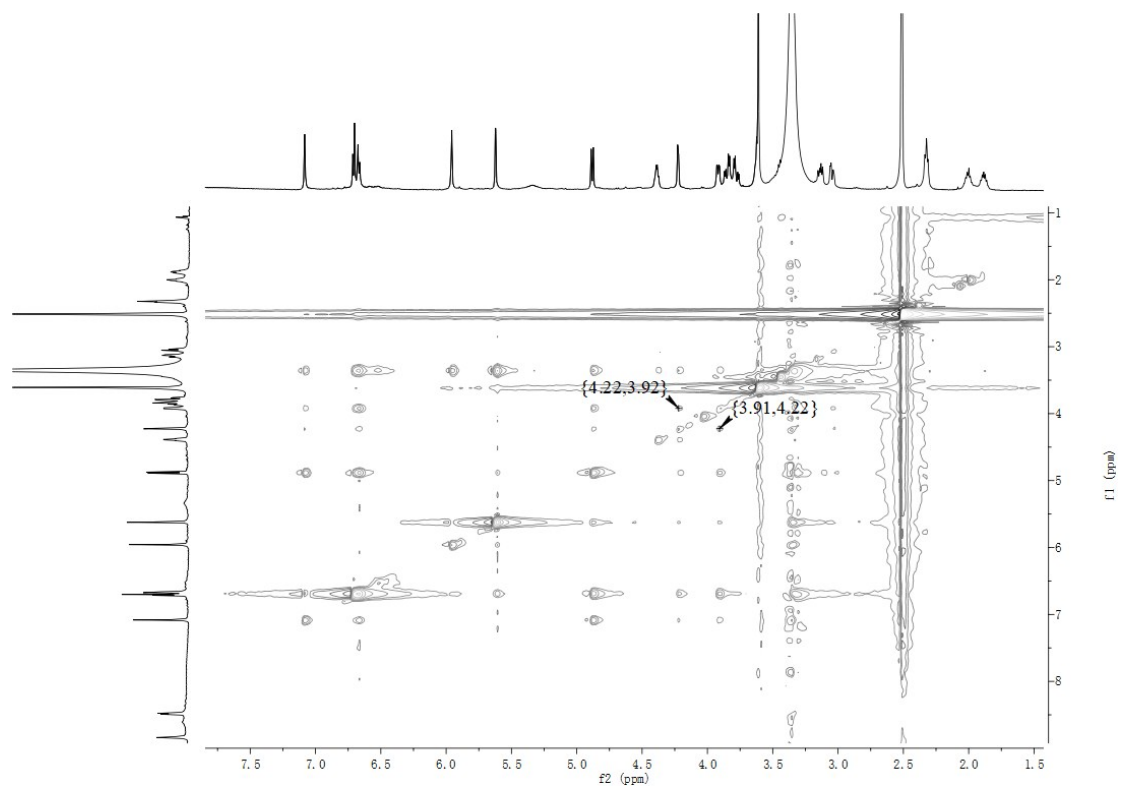


Figure S6. NOESY spectrum (600 MHz, DMSO) of C-G-2.

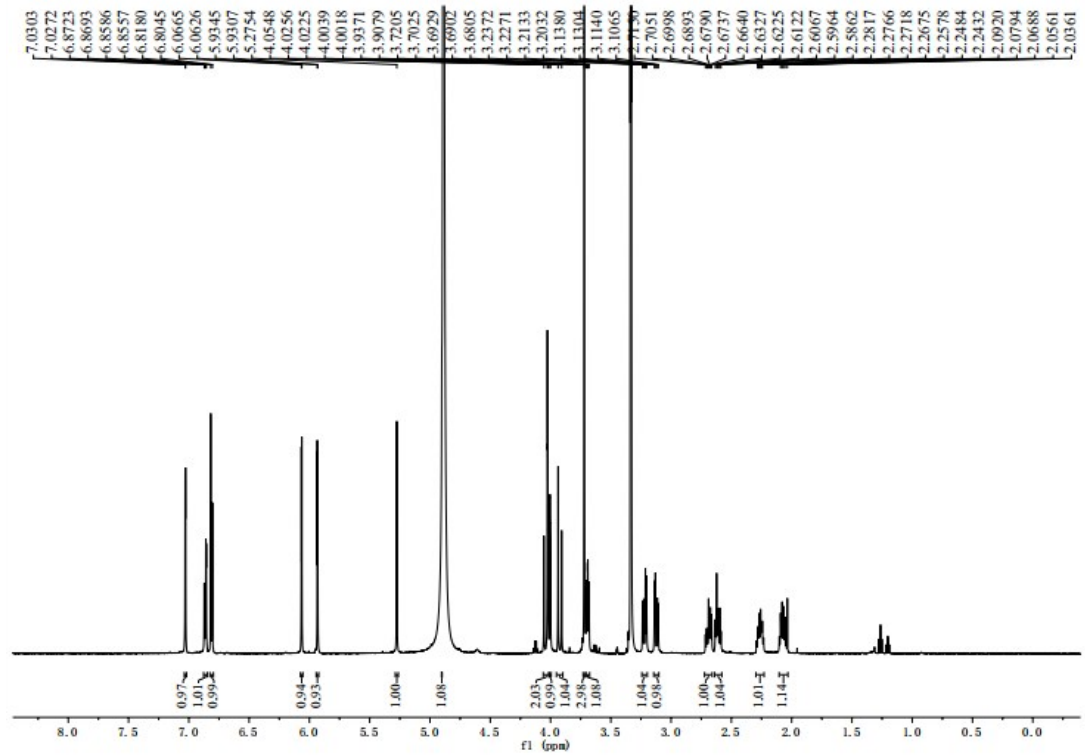


Figure S7. ¹H NMR spectrum (600 MHz, CD₃OD) of EC-G.

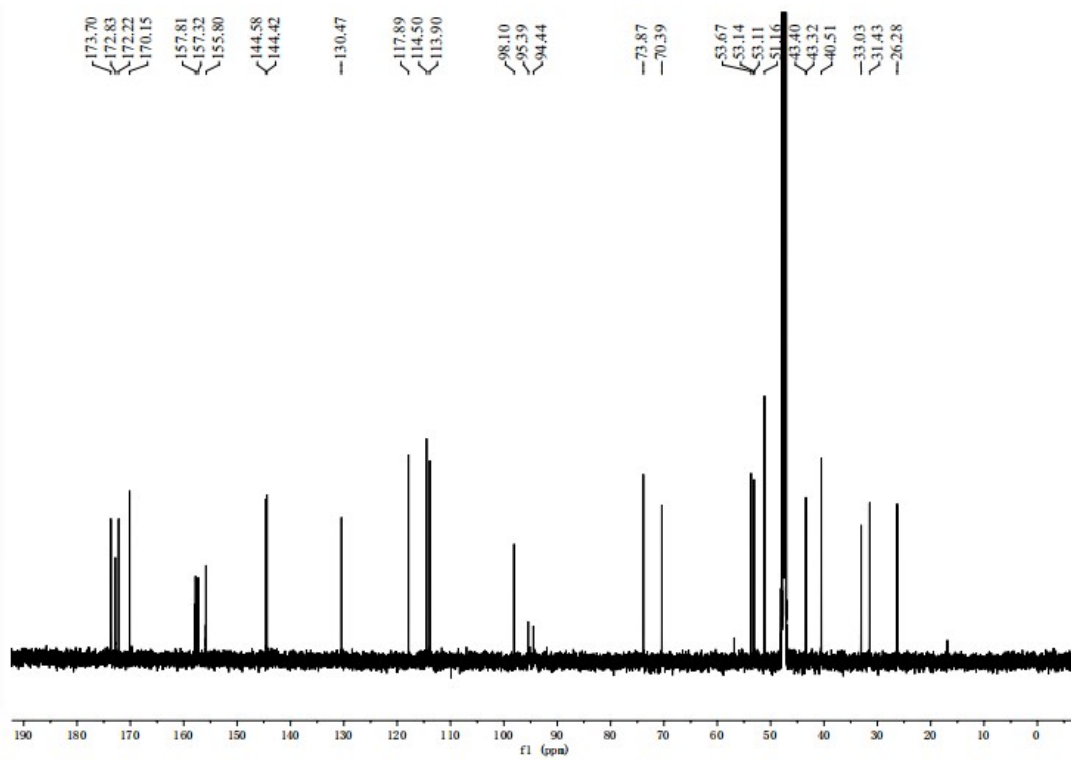


Figure S8. ^{13}C NMR spectrum (150 MHz, CD_3OD) of EC-G.

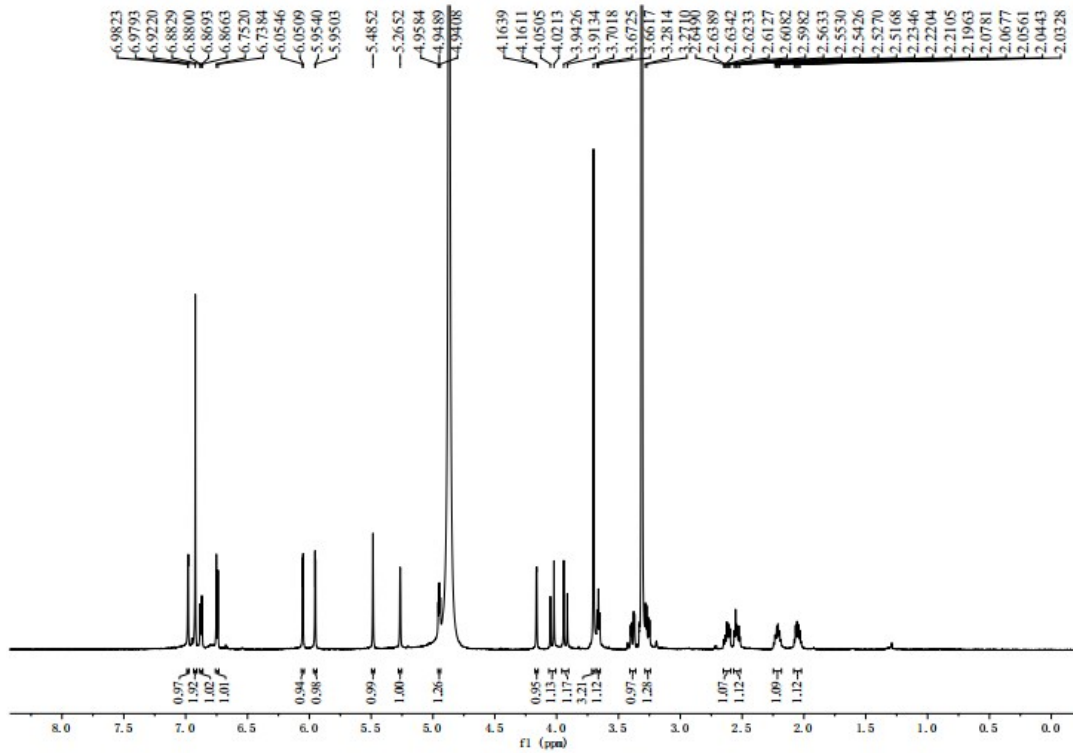


Figure S9. ¹H NMR spectrum (600 MHz, CD₃OD) of ECG-G.

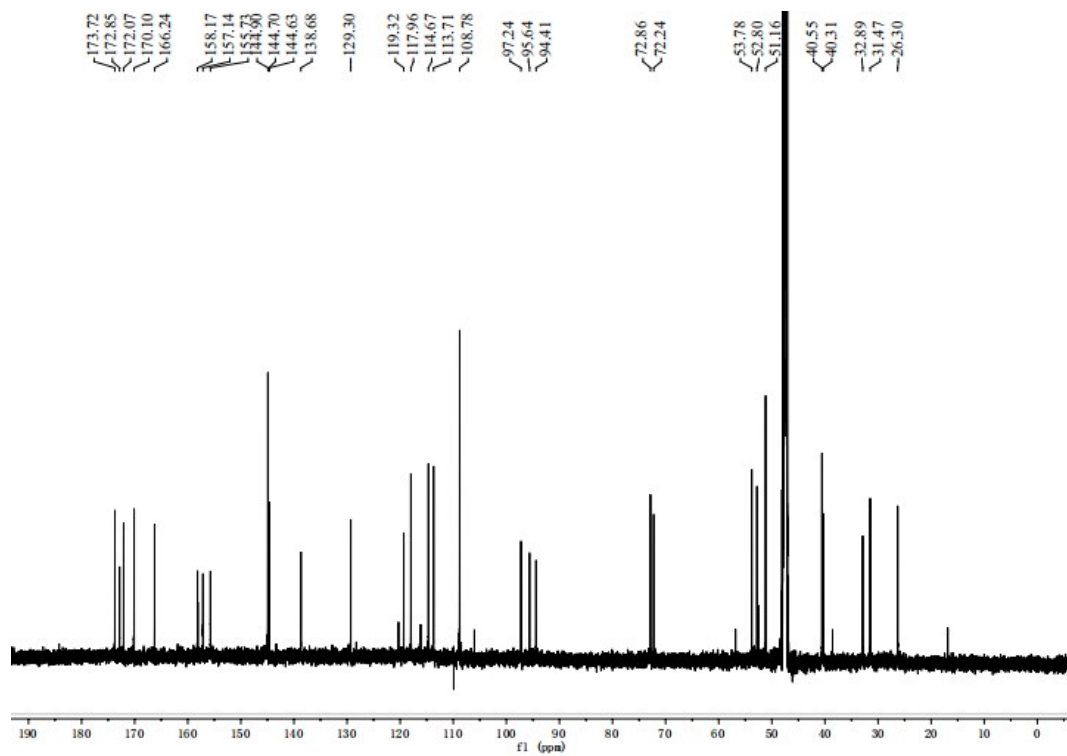


Figure S10. ^{13}C NMR spectrum (150 MHz, CD_3OD) of ECG-G.