

Supplementary Information

Simultaneous, Simple and Rapid Determination of Five Bioactive Free Anthraquinones in Radix et Rhizoma Rhei by Quantitative ^1H NMR

Jian-Wei Dong, Le Cai,* Yun-Shan Fang, Wei-He Duan, Zhen-Jie Li and Zhong-Tao Ding*

Key Laboratory of Medicinal Chemistry for Natural Resource, Ministry of Education, School of Chemical Science and Technology, Yunnan University, 650091 Kunming, P. R. China

Table S1. LODs and LOQs for the quantitation of rhein, physcion, chrysophanol, aloe-emodin, and emodin by q-HNMR

	LOD / ($\mu\text{g mL}^{-1}$)	LOQ / ($\mu\text{g mL}^{-1}$)
Rhein	2.02	6.73
Physcion	1.80	6.00
Chrysophanol	1.60	5.33
Aloe-emodin	0.98	3.27
Emodin	1.95	6.50

LOD: limit of detection; LOQ: limit of quantitation.

Table S2. Regression equation and linear range for the quantitation of rhein, physcion, chrysophanol, aloe-emodin, and emodin by HPLC

	Regression equation	Linear range / μg
Rhein	$A = 1378.3m - 22.245$ ($r^2 = 0.9997$)	0.04-2.0
Physcion	$A = 1632.9m - 37.554$ ($r^2 = 0.9999$)	0.2-2.8
Chrysophanol	$A = 6100.4m - 18.268$ ($r^2 = 0.9999$)	0.2-3.6
Aloe-emodin	$A = 4805.5m - 187.58$ ($r^2 = 0.9994$)	0.2-2.4
Emodin	$A = 2804.7m + 24.714$ ($r^2 = 0.9995$)	0.02-2.0

A: area; m: mass; r^2 : coefficient of determination.

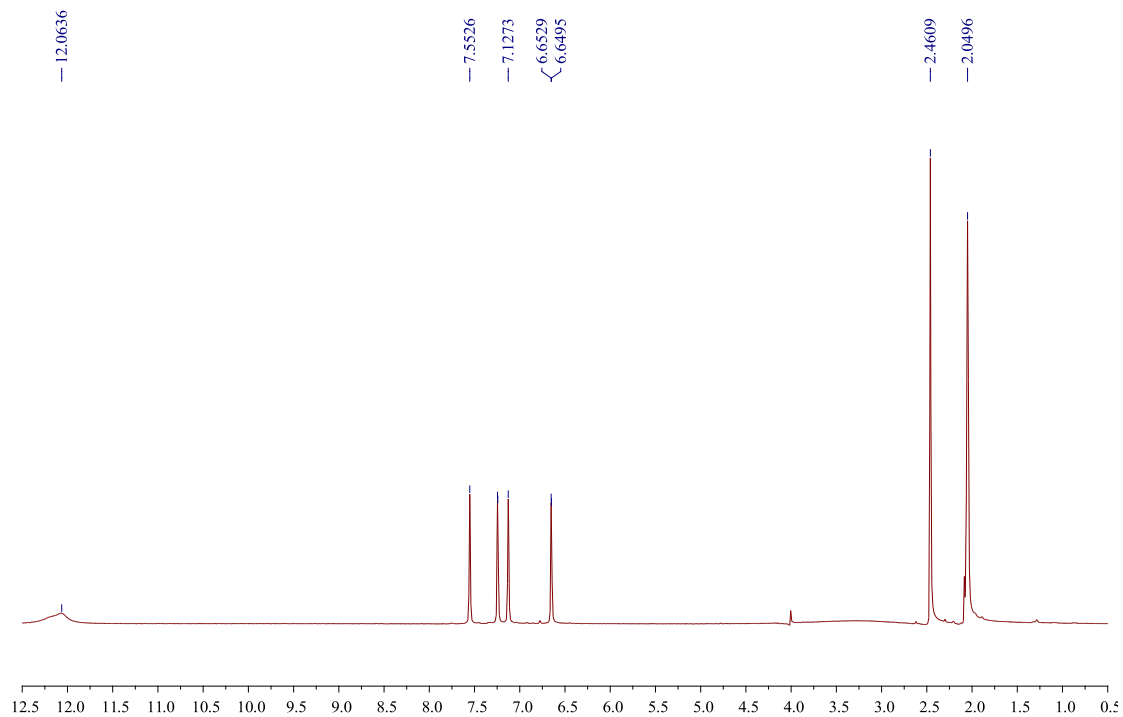


Figure S1. ^1H NMR spectrum (400 MHz, acetone- d_6) of emodin.

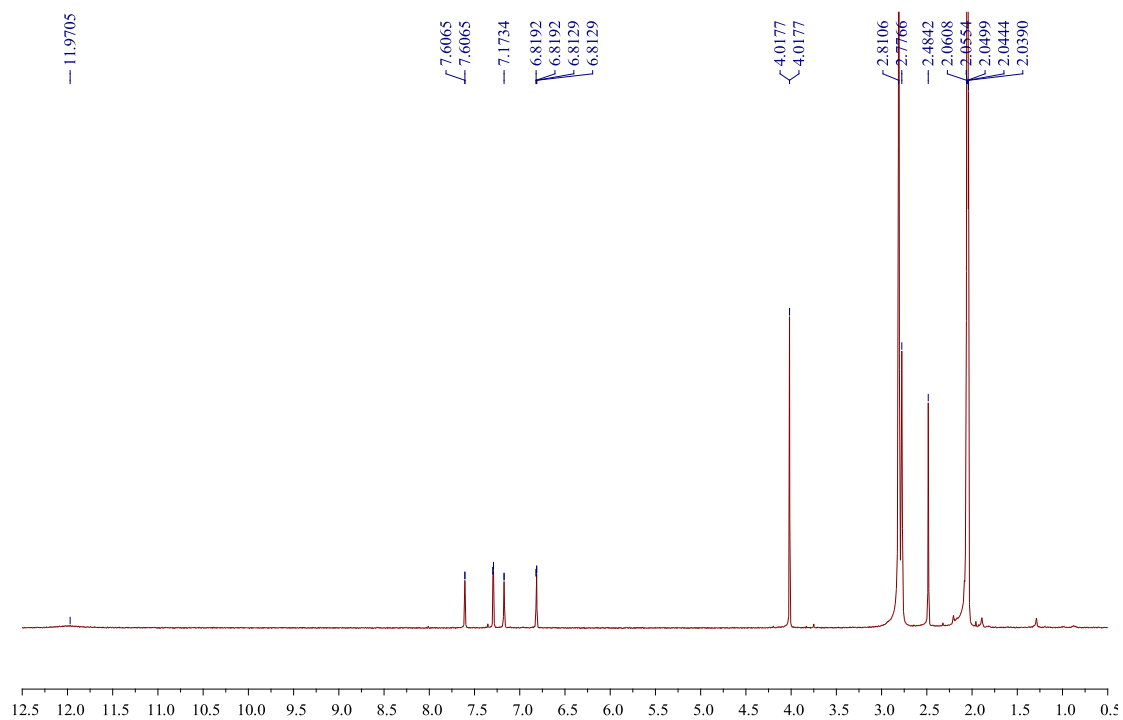


Figure S2. ^1H NMR spectrum (400 MHz, acetone- d_6) of physion.

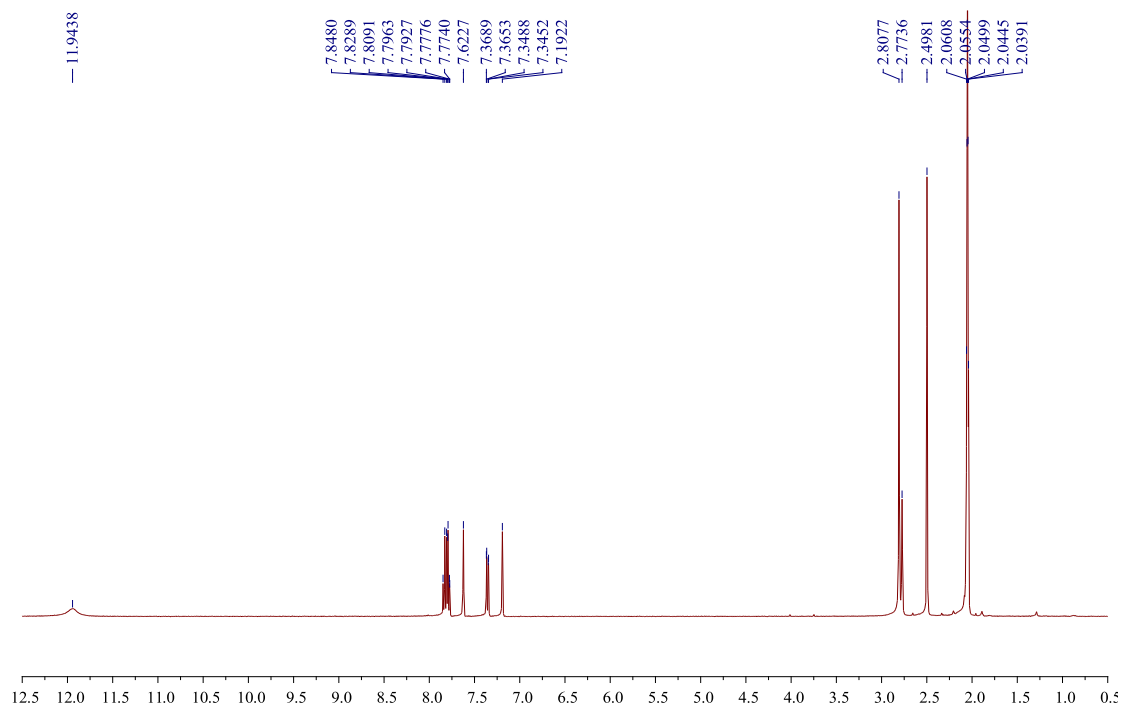


Figure S3. ^1H NMR spectrum (400 MHz, acetone- d_6) of chrysophanol.

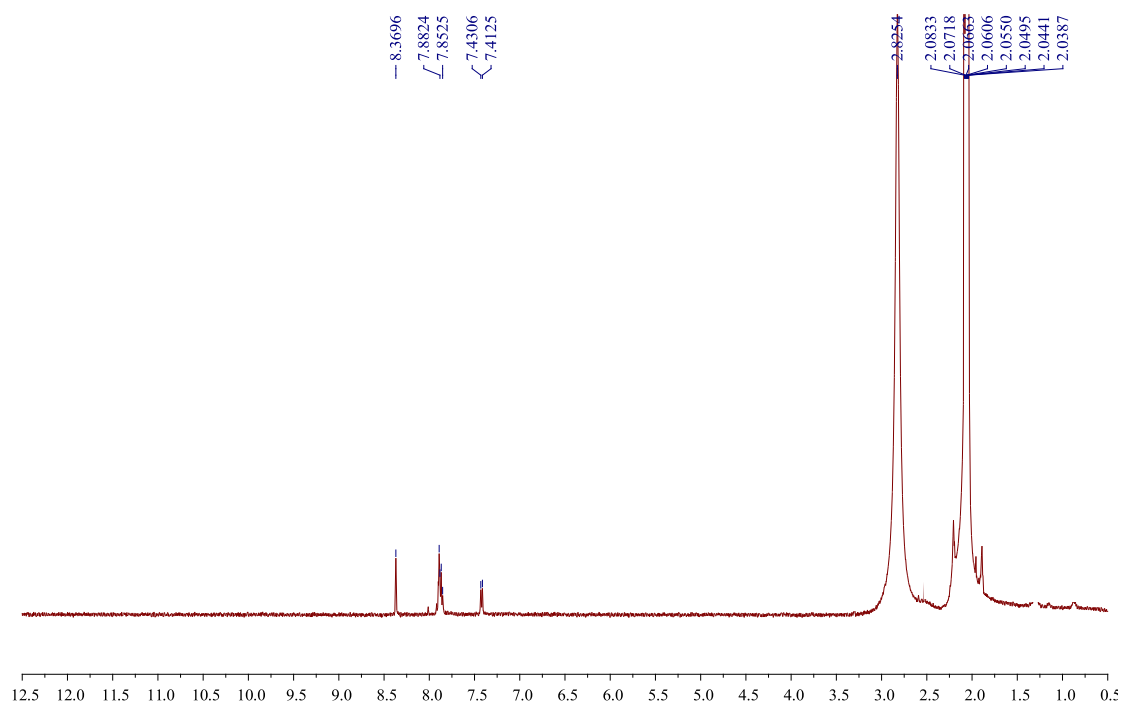


Figure S4. ^1H NMR spectrum (400 MHz, acetone- d_6) of rhein.

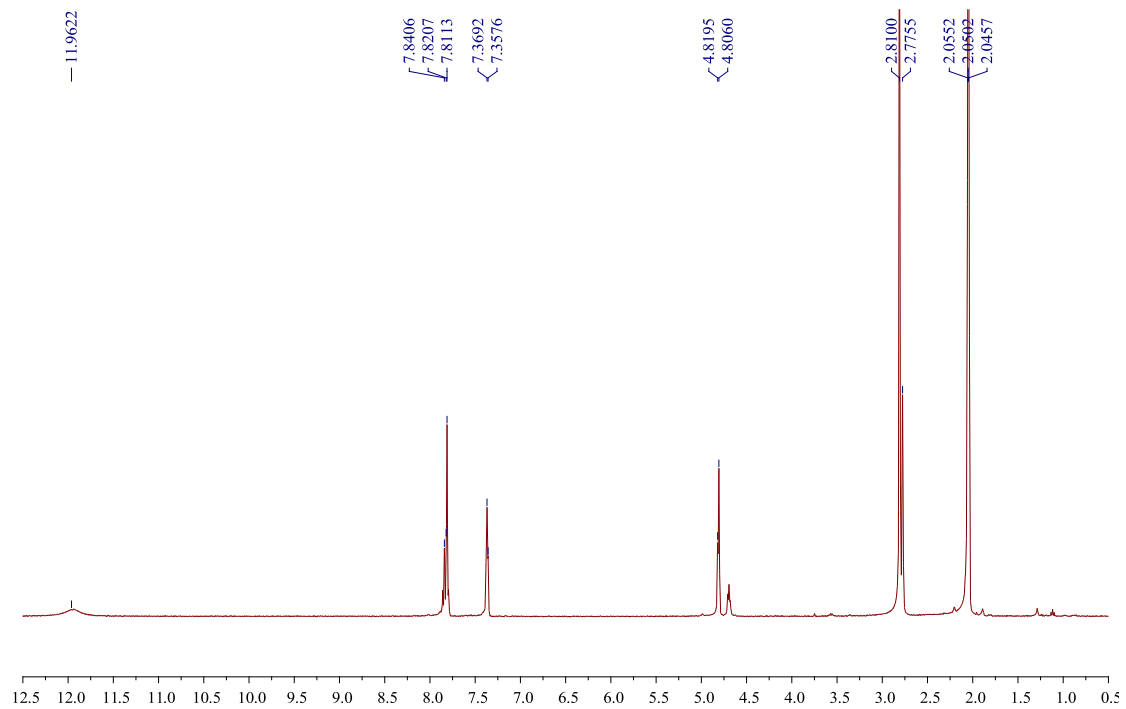


Figure S5. ^1H NMR spectrum (400 MHz, acetone- d_6) of aloë-emodin.

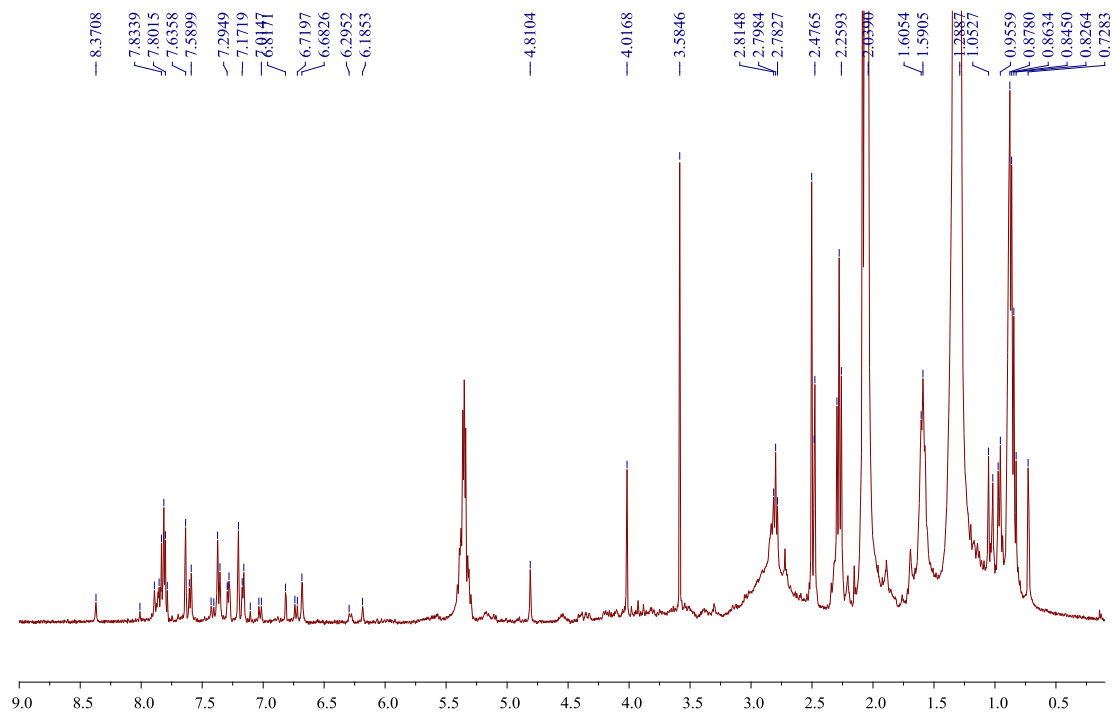


Figure S6. ^1H NMR spectrum (400 MHz, acetone- d_6) of *R. palmatum* extract.

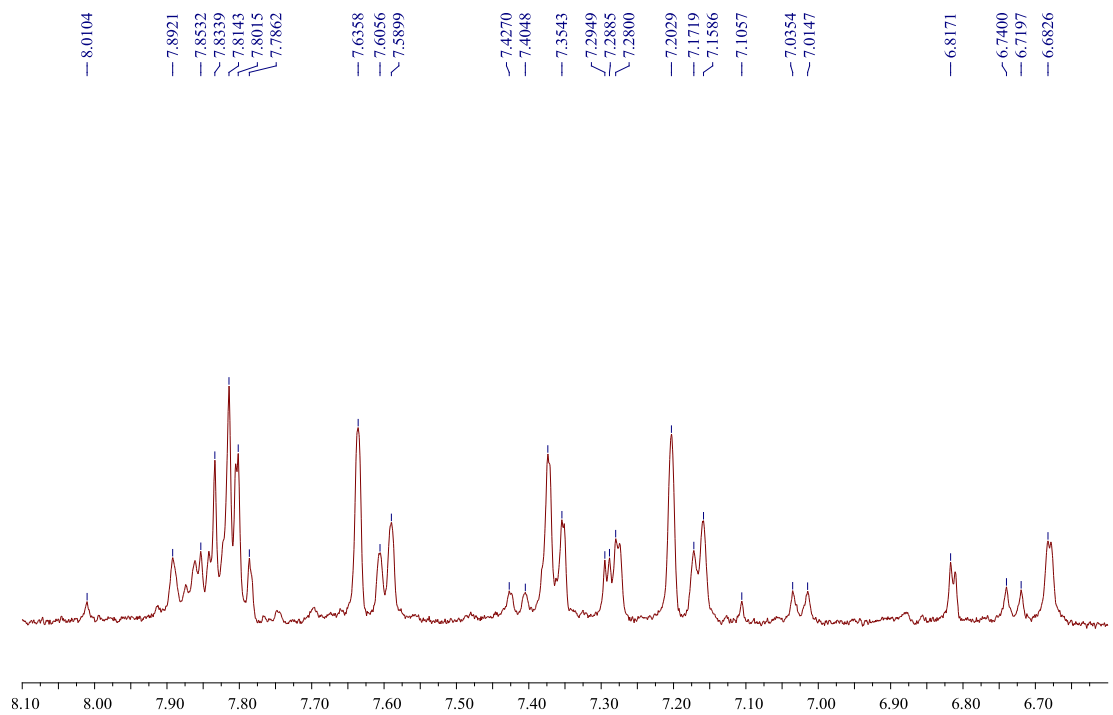


Figure S7. Detailed ^1H NMR spectrum (400 MHz, acetone- d_6) of *R. palmatum* extract.

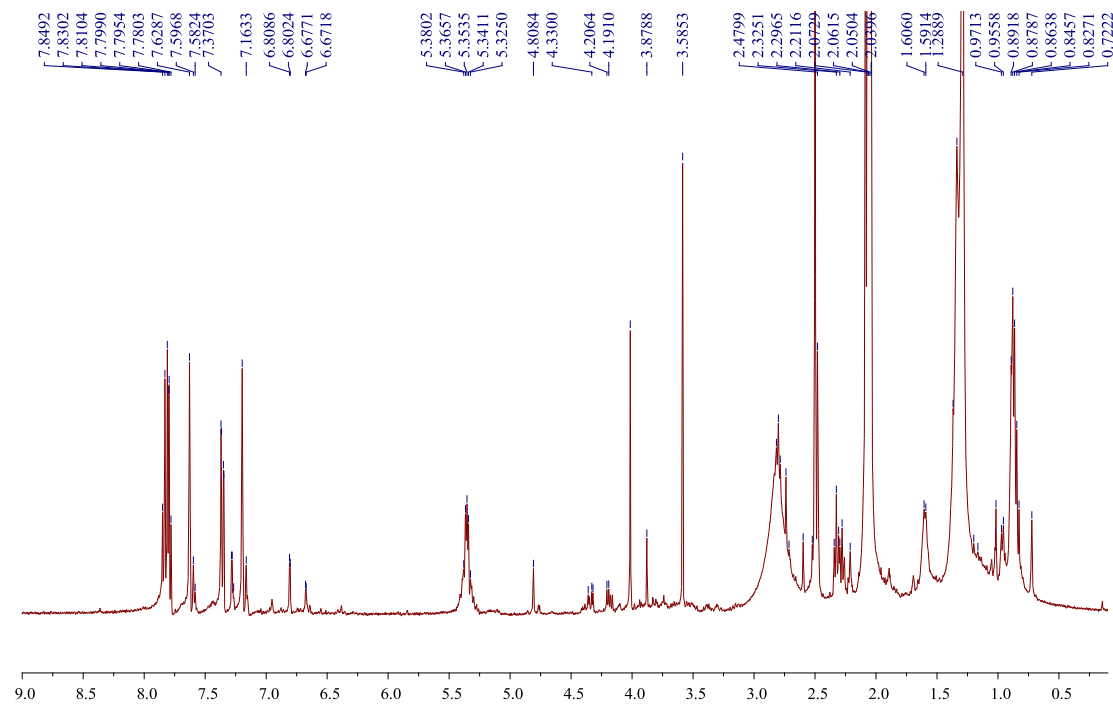


Figure S8. ^1H NMR spectrum (400 MHz, acetone- d_6) of *Rheum officinale* extract.

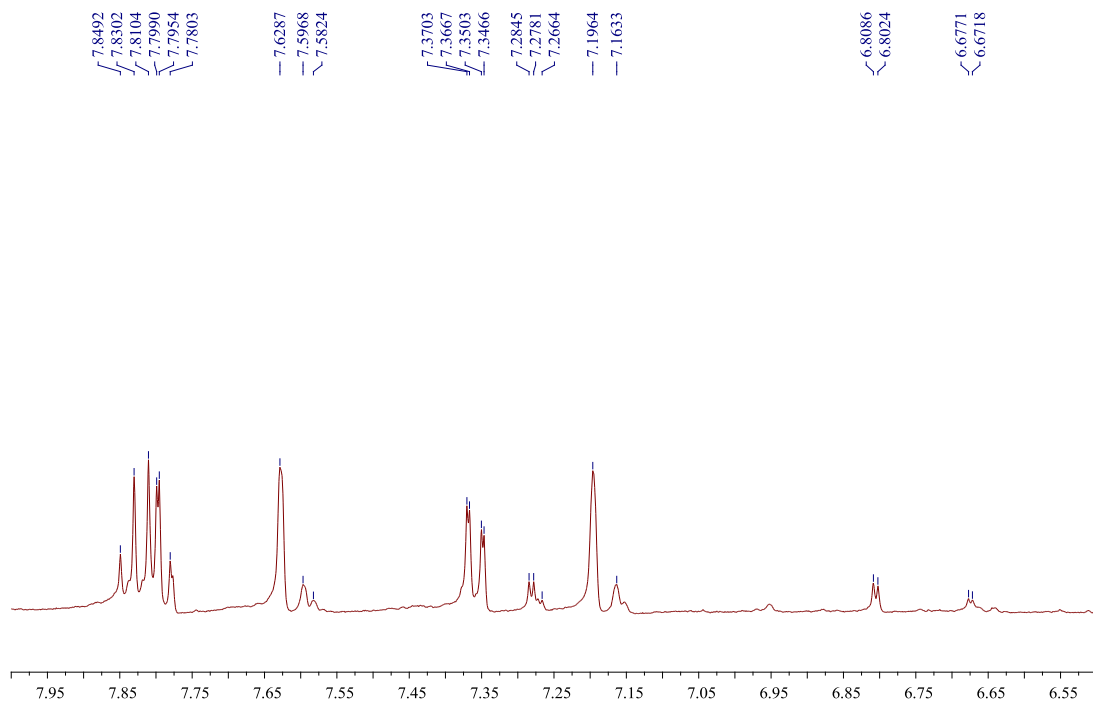


Figure S9. Detailed ^1H NMR spectrum (400 MHz, acetone- d_6) of *Rheum officinale* extract.

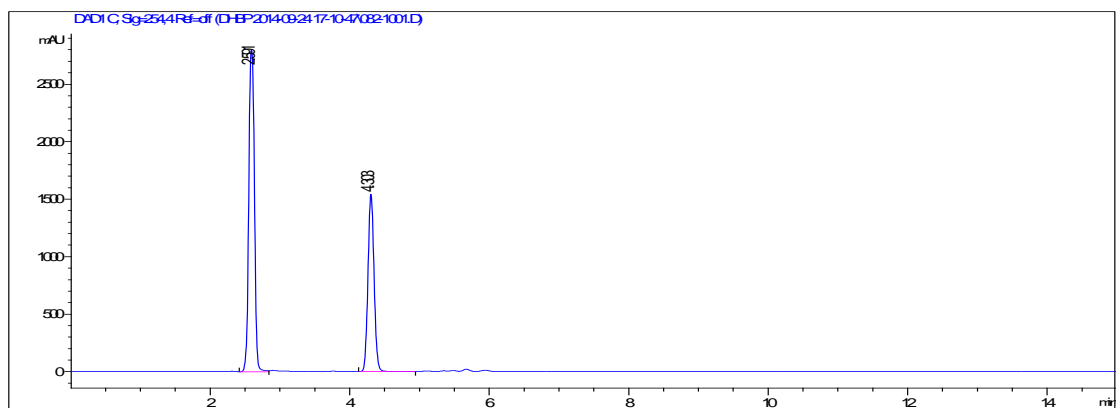


Figure S10. HPLC chromatogram of aloemodin (t_R 2.59 min is signal of solvents).

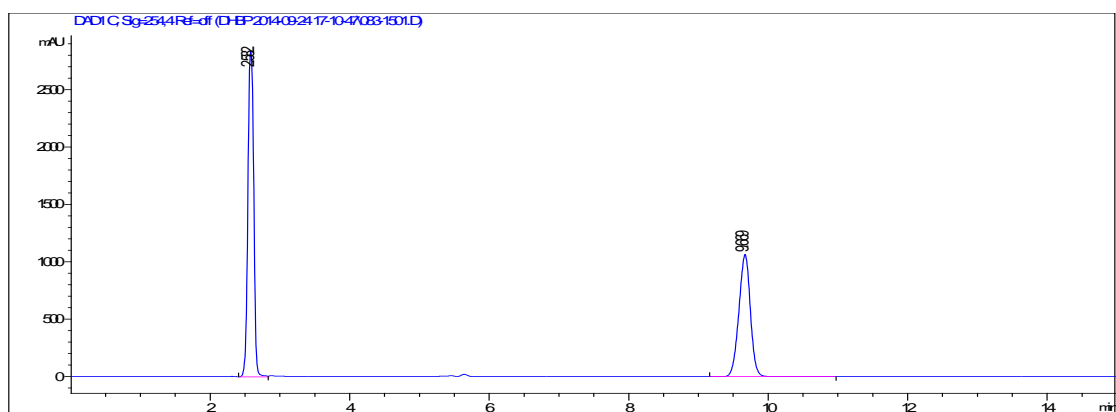


Figure S11. HPLC chromatogram of chrysophanol (t_R 2.58 min is signal of solvents).

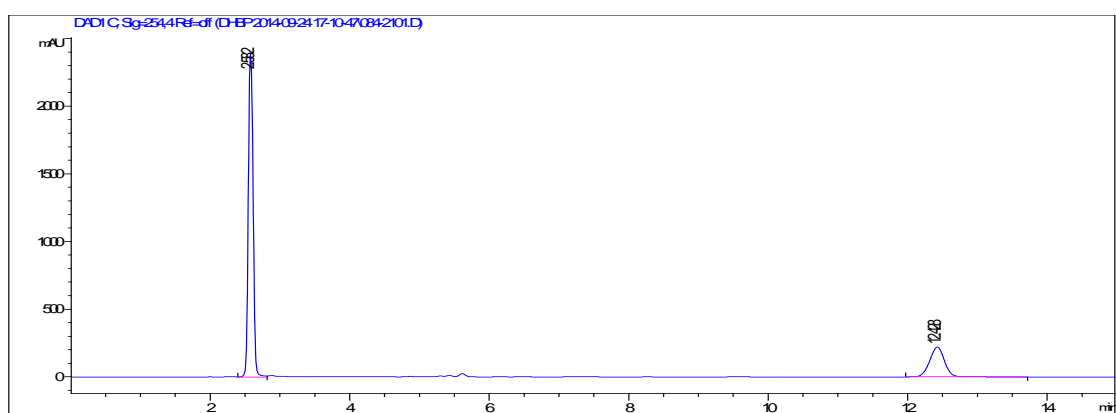


Figure S12. HPLC chromatogram of physcion (t_R 2.58 min is signal of solvents).

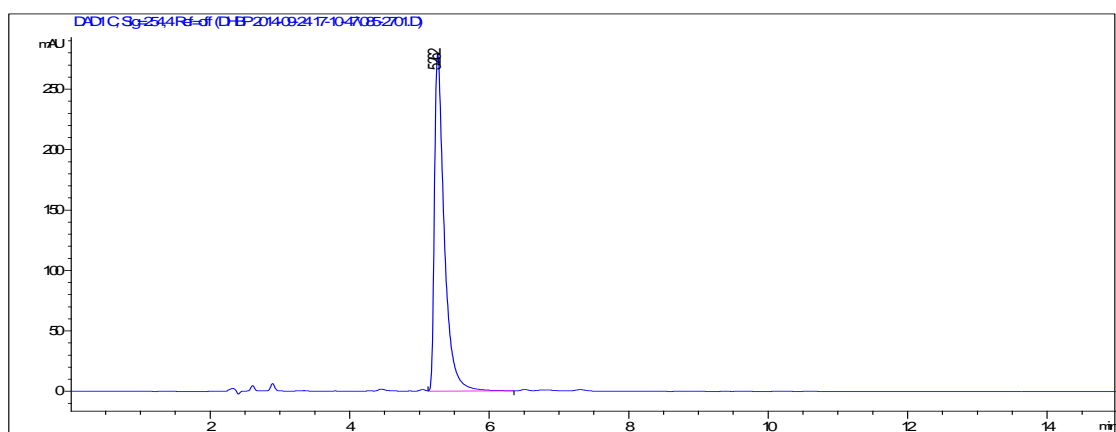


Figure S13. HPLC chromatogram of rhein.

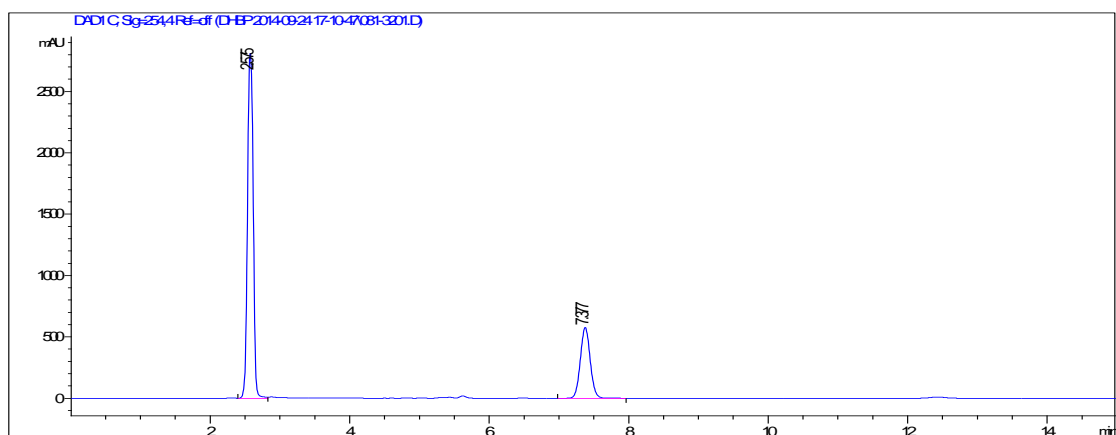


Figure S14. HPLC chromatogram of emodin (t_R 2.58 min is signal of solvents).

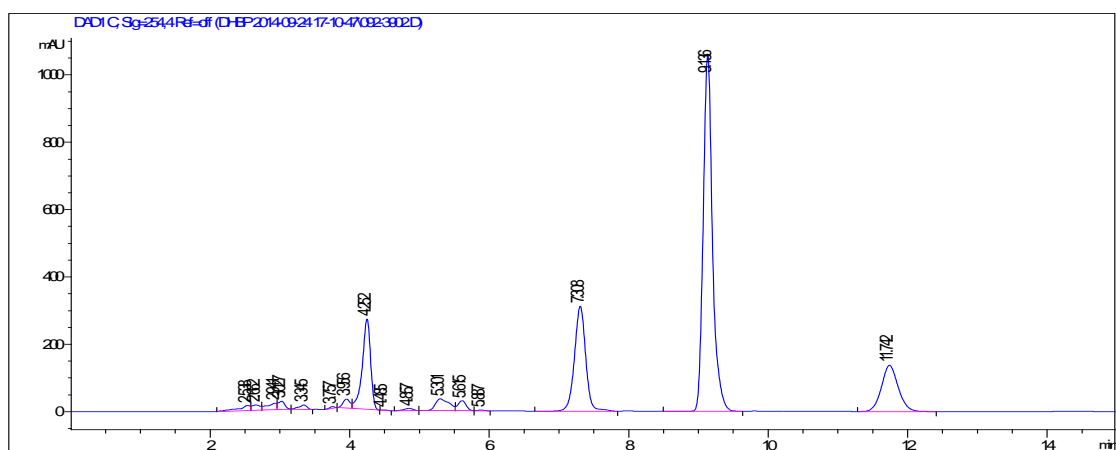


Figure S15. HPLC chromatogram of extract of *Rheum palmatum*.

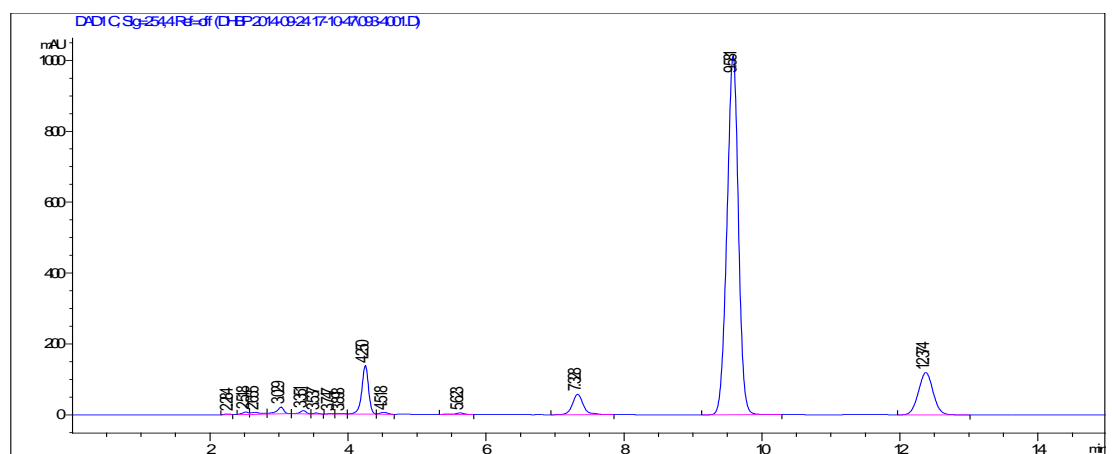


Figure S16. HPLC chromatogram of extract of *Rheum officinale*.