SUPPLEMENTARY MATERIAL

Three new sulphur glycosides from the seeds of *Descurainia sophia*

Wei-sheng Feng*¹*, Chun-Ge Li², Xiao-Ke Zheng¹, Ling-Ling Li³, Wen-Jing Chen¹,
Yan-Li Zhang¹, Yan-Gang Cao¹, Jian-Hong Gong¹✉ and Hai-Xue Kuang²

¹School of Pharmacy, Henan University of Traditional Chinese Medicine, Zhengzhou
450046, P.R. China ; ²School of Pharmacy, Heilongjiang University of Chinese
Medicine, Harbin 150040, P.R. China

Abstract:

Three new sulphur glycosides, raphanuside B-D (1-3), together with a known sulphur glycoside, raphanuside (4) were isolated from the decoction of the seeds of *Descurainia sophia* (L.) Webb ex Prantl, and the compound 4 was reported for the first time from this plant. Their structures were identified by means of UV, IR, 1D, 2D NMR (HSQC, HMBC and NOESY), and HR-ESI-MS spectroscopic data.

Keywords: Seeds; *Descurainia sophia*; Cruciferae; sulphur glycosides
Fig. S1 Key NOESY correlations of 1 and 4

Fig. S2 Key HMBC and NOESY correlations of 2

Fig. S3 Key HMBC correlations of 3
Fig. S4 The $^1$H-NMR spectrum of compound 1

Fig. S5 The $^{13}$C-NMR spectrum of compound 1
Fig. S6 The HSQC spectrum of compound 1

Fig. S7 The HMBC spectrum of compound 1
Fig. S8 The NOESY spectrum of compound 1

Fig. S9 The UV spectrum of compound 1
Fig. S10 The IR spectrum of compound 1

Fig. S11 The HR-ESI-MS spectrum of compound 1
Fig. S12 The $^1$H NMR spectrum of compound 2

Fig. S13 The $^{13}$C NMR spectrum of compound 2
Fig.S14 The HSQC spectrum of compound 2

Fig.S15 The HMBC spectrum of compound 2
Fig. S16 The NOESY spectrum of compound 2

Fig. S17 The UV spectrum of compound 2
Fig. S18 The IR spectrum of compound 2

Fig. S19 The HR-ESI-MS spectrum of compound 2
Fig. S20 The \textsuperscript{1}H NMR spectrum of compound 3

Fig. S21 The \textsuperscript{13}C NMR spectrum of compound 3
Fig. S22 The HSQC spectrum of compound 3

Fig. S23 The HMBC spectrum of compound 3
Fig. S24 The UV spectrum of compound 3

Fig. S25 The IR spectrum of compound 3
Fig. S26 The HR-ESI-MS spectrum of compound 3
Fig. S27 The $^1$H NMR spectrum of compound 4

Fig. S28 The $^{13}$C NMR spectrum of compound 4
Fig. S29 The NOESY spectrum of compound 4
Fig. S30 The HR-ESI-MS spectrum of compound 4