SUPPLEMENTARY MATERIAL

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

Wei-sheng Feng^{a*}, Chun-Ge Li^a, Xiao-Ke Zheng^a, Ling-Ling Li^a, Wen-Jing Chen^a,
Yan-Li Zhang^a, Yan-Gang Cao^a, Jian-Hong Gong^{a,b} and Hai-Xue Kuang^b

^a*School of Pharmacy, Henan University of Traditional Chinese Medicine, Zhengzhou 450046, P.R. China ;* ^b*School 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 ^1H -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**

LCG-9-2 NOE
MEOD

Fig.S8 The NOESY spectrum of compound **1**

Thermo Scientific ~ VISIONpro SOFTWARE V4.41

Operator Name	(None Entered)	Date of Report	2015/3/16
Department	(None Entered)	Time of Report	16:29:31下午
Organization	(None Entered)		
Information	(None Entered)		

Scan Graph

Results Table - scan009, LCG-9-2, Cycle01

nm	A	Peak Pick Method
208.00	.843	Find 3 Peaks Above -3.0000 A
239.00	.153	Start Wavelength 200.00 nm
271.00	.029	Stop Wavelength 400.00 nm
		Sort By Wavelength

Sensitivity Very High

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 ^1H 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**

Thermo Scientific ~ VISIONpro SOFTWARE V4.41

Operator Name	(None Entered)	Date of Report	2015/3/16
Department	(None Entered)	Time of Report	16:10:41下午
Organization	(None Entered)		
Information	(None Entered)		

Scan Graph

Results Table - scan007.LCG-1.Cycle01

nm	A	Peak Pick Method
202.00	.679	Find 4 Peaks Above -3.0000 A
244.00	.406	Start Wavelength200.00 nm
339.00	.599	Stop Wavelength400.00 nm
		Sort By Wavelength

Sensitivity Very High

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 ^1H NMR spectrum of compound **3**

Fig. S21 The ^{13}C NMR spectrum of compound **3**

Fig. S22 The HSQC spectrum of compound **3**

Fig. S23 The HMBC spectrum of compound **3**

Thermo Scientific ~ VISIONpro SOFTWARE V4.41

Operator Name (None Entered)
 Department (None Entered)
 Organization (None Entered)
 Information (None Entered)

Date of Report 2015/3/16
 Time of Report 16:38:52下午

Scan Graph

Results Table - scan011, LCG-15, Cycle01

nm	A	Peak Pick Method
201.00	.532	Find 3 Peaks Above -3.0000 A
215.00	.638	Start Wavelength 200.00 nm
308.00	.429	Stop Wavelength 400.00 nm
		Sort By Wavelength

Sensitivity Very High

Fig. S24 The UV spectrum of compound 3

Fig. S25 The IR spectrum of compound 3

Display Report

Analysis Info

Analysis Name \\MQHD21303\Data\LCG\LCG-15-1-pos.d
Method tune_pos_mid_20141031.m
Sample Name Tunemix-Low
Comment

Acquisition Date 2015/2/4 16:21:38

Operator BDAL@DE
Instrument maXis HD 1820881.21303

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3600 V	Set Dry Heater	200 jnC
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 jnC

LCG-15-1-pos.d

Bruker Compass DataAnalysis 4.2

printed: 2015/2/4 21:47:33

by: ZMH

Page 1 of 1

Fig. S26 The HR-ESI-MS spectrum of compound **3**

Fig. S27 The ^1H NMR spectrum of compound **4**

Fig. S28 The ^{13}C NMR spectrum of compound **4**

LCG-9 NOE
MeOD

Fig. S29 The NOESY spectrum of compound 4

Display Report

Analysis Info

Analysis Name \\MQHD21303\Data\LCG\LCG-9-pos.d
Method tune_pos_mid_20141031.m
Sample Name Tunemix-Low
Comment

Acquisition Date 2015/2/4 11:54:20

Operator BDAL@DE
Instrument maXis HD 1820881.21303

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3600 V	Set Dry Heater	200 jnC
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 jnC

LCG-9-pos.d

Bruker Compass DataAnalysis 4.2

printed: 2015/2/4 21:37:17

by: ZMH

Page 1 of 1

Fig. S30 The HR-ESI-MS spectrum of compound 4