

Supporting Information

Rec. Nat. Prod. 9:4 (2015) 484-495

Bioassay-guided isolation and characterization of wound healer compounds from *Morus nigra* L. (Moraceae)

**Esra Küpeli Akkol^a*, Ipek Süntar^a, Hikmet Keleş^b,
Ekrem Sezik^a and Gülnur Gürler^c**

^a*Department of Pharmacognosy, Faculty of Pharmacy, Gazi University, Etiler 06330, Ankara*

^b*Department of Pathology, Faculty of Veterinary Medicine, Afyon Kocatepe University, 03200, Afyonkarahisar-Türkiye*

^c*The Republic of Turkey, Ministry of Health, Altındağ Health Center, 06430, Ankara, Türkiye*

Table of Contents	Page
S1: General Considerations	2
S2: $^1\text{H-NMR}$ (400 MHz, CD_3OD) and $^{13}\text{C-NMR}$ (100 MHz, CD_3OD) data of Quercetin-3- <i>O</i> -rutinoside	2
S3: $^1\text{H-NMR}$ (400 MHz, CD_3OD) Spectrum of Quercetin-3- <i>O</i> -rutinoside (1)	3
S4: $^{13}\text{C-NMR}$ (100 MHz, CD_3OD) Spectrum of Quercetin-3- <i>O</i> -rutinoside (1)	4
S5: $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) and $^{13}\text{C-NMR}$ (100 MHz, $\text{DMSO-}d_6$) data of Kaempferol-3- <i>O</i> -rutinoside	5
S6: $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$) Spectrum Kaempferol-3- <i>O</i> -rutinoside (2)	6
S7: $^{13}\text{C-NMR}$ (100 MHz, $\text{DMSO-}d_6$) Spectrum Kaempferol-3- <i>O</i> -rutinoside (2)	7
S8: References	8

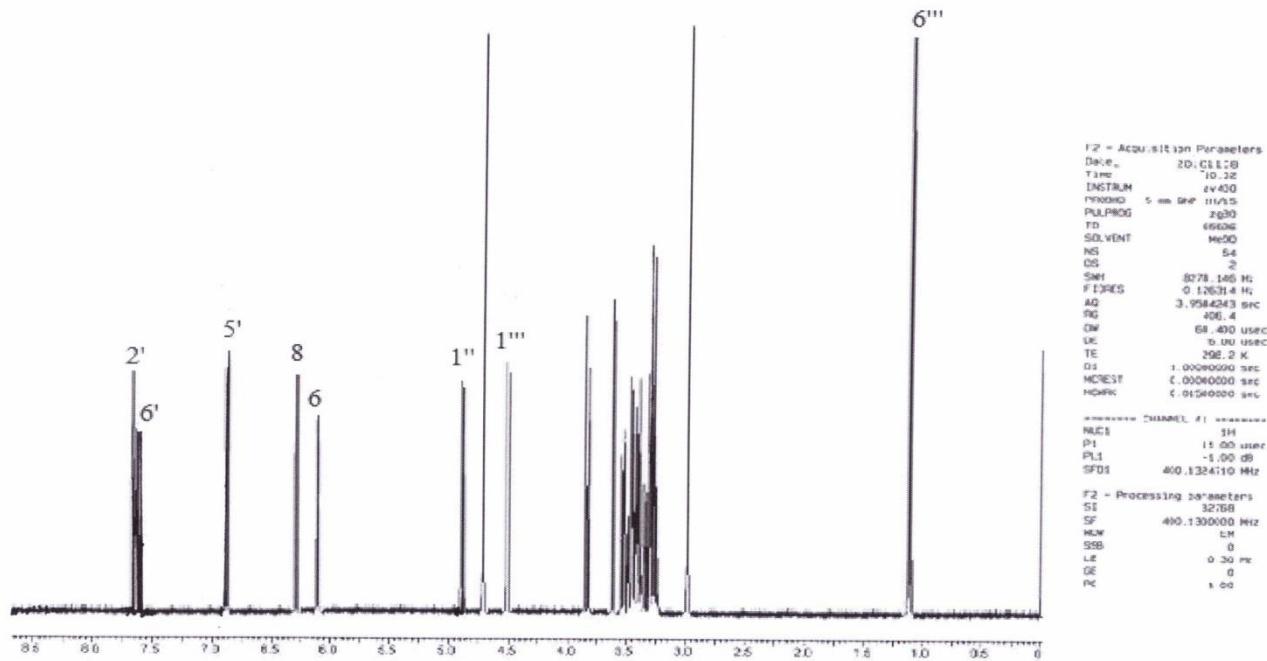
S1: General Considerations

For the identification of the active constituents Nuclear Magnetic Resonance (¹H and ¹³C NMR) and Mass Spectral (MS) techniques were employed. NMR spectra were recorded on a Bruker spectrometer (400 MHz for ¹H NMR and 100 MHz for ¹³C NMR) instrument, using CD₃OD and DMSO-*d*6 as solvent. A Finnigan spectrometer was used for FT-MS analyses. The isolated compounds were elucidated as quercetin-3-*O*-rutinoside (**1**) and kaempferol-3-*O*-rutinoside (**2**) respectively, by comparing their spectroscopic data with those of published literatures [1-3].

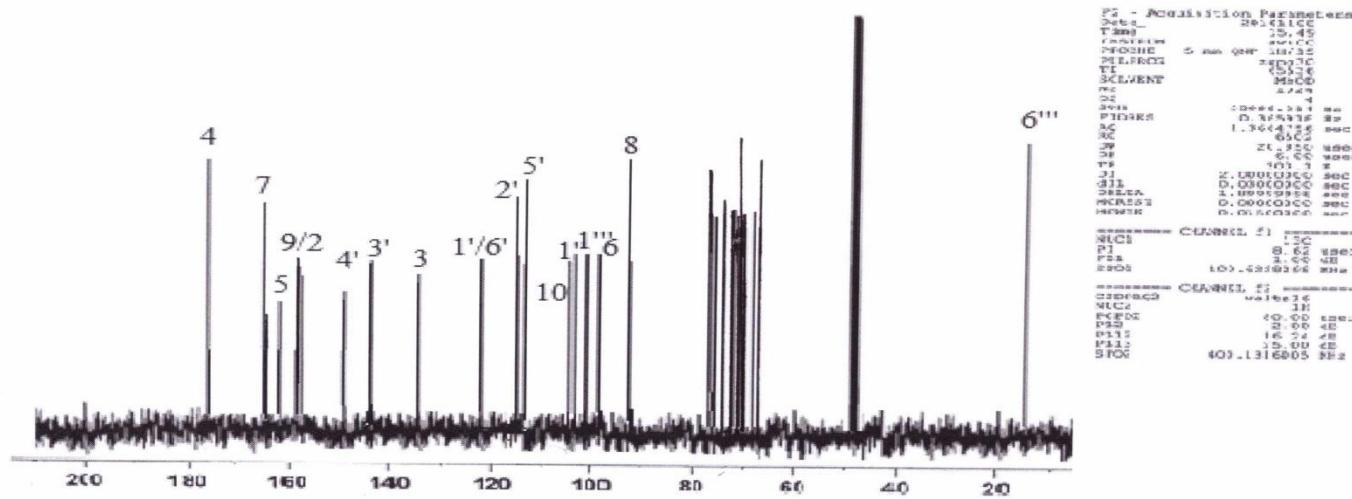
Quercetin-3-*O*-rutinoside (1); FABMS *m/z* (+ve ion mode): 611 [M+H]⁺ C₂₇H₃₀O₁₆, UV (MeOH, λ_{max} , nm): 361; 258

S2: ¹H-NMR (400 MHz, CD₃OD) and ¹³C-NMR (100 MHz, CD₃OD) data of Quercetin-3-*O*-rutinoside

Position	δ_{H} , ppm (J, Hz)	δ_{C} , ppm
2	-	158.22
3	-	134.52
4	-	178.39
5	-	162.48
6	6.10 s	99.72
7	-	166.58
8	6.28 s	94.90
9	-	158.91
10	-	105.32
1'	-	122.77
2'	7.64 s	117.37
3'	-	144.32
4'	-	150.23
5'	6.85 d (8.6)	115.46
6'	7.63 d (8.6)	122.47
1''	4.96 d (7.3)	103.63
2''		74.64
3''		77.81
4''	3.20-3.90 m	71.12
5''		78.09
6''		68.37
1'''	4.50 d (1.8)	101.92
2'''		71.32
3'''		72.13
4'''	3.20-3.90 m	73.73
5'''		68.91
6'''	1.12 d (6.0)	18.84



S3: ^1H -NMR (400 MHz, CD_3OD) Spectrum of Quercetin-3-*O*-rutinoside (**1**)

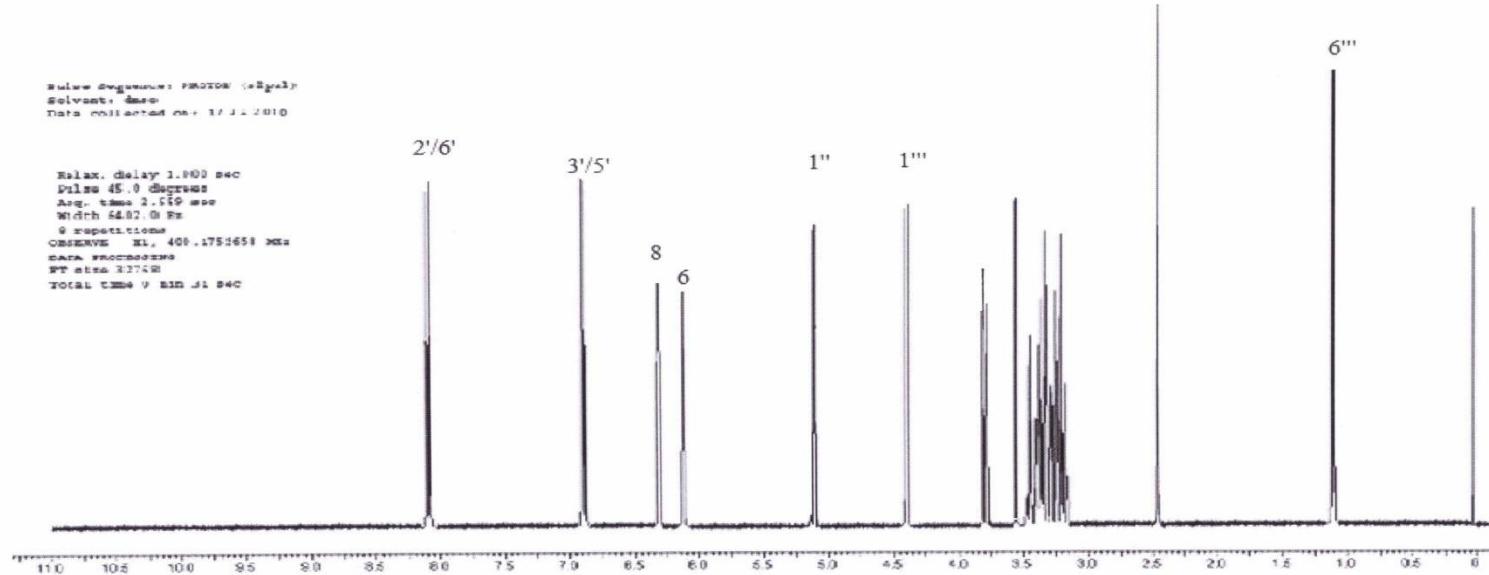


S4: ^{13}C -NMR (100 MHz, CD_3OD) Spectrum of Quercetin-3-*O*-rutinoside (**1**)

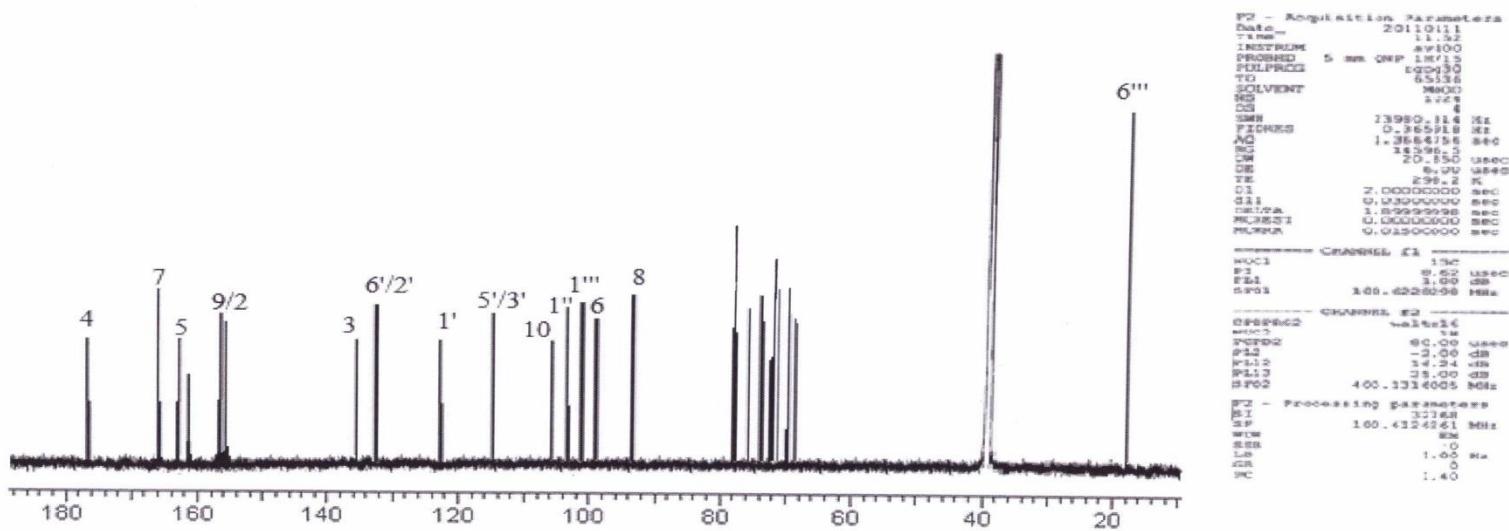
Kaempferol-3-O-rutinoside (2); FABMS *m/z* (+ve ion mode): 595 [M+H]⁺ C₂₇H₃₀O₁₅, UV (MeOH, λ_{max}, nm): 349.2; 266.

S5: ¹H-NMR (400 MHz, DMSO-*d*6) and ¹³C-NMR (100 MHz, DMSO-*d*6) data of Kaempferol-3-*O*-rutinoside

Position	δ_H, ppm (J, Hz)	δ_C, ppm
2	-	155.98
3	-	134.58
4	-	177.23
5	-	162.04
6	6.22 d (2.1)	98.88
7	-	163.31
8	6.33 d (2.1)	93.98
9	-	156.82
10	-	104.79
1'	-	121.39
2'	8.19 d (8.7)	130.76
3'	6.92 d (8.7)	113.40
4'	-	160.92
5'	6.92 (8.7)	114.87
6'	8.19 d (8.7)	131.03
1"	5.02 d (7.8)	102.11
2"		74.83
3"		75.48
4"	3.15-3.90 m	69.23
5"		77.65
6"		67.08
1'''	4.45 d (1.8)	100.10
2'''		70.89
3'''	3.15-3.90 m	72.23
4'''		73.46
5'''		67.88
6'''	1.09 d (6.1)	18.12



S6: ¹H-NMR (400 MHz, DMSO-*d*6) Spectrum Kaempferol-3-*O*-rutinoside (**2**)



S3: References

- [1] T. J. Mabry, K. R. Markham and M. B. Thomas (1970). The systematic identification of flavonoids. Springer-Verlag, New York Inc.
- [2] F. Fathiazar, A. Delazar, R. Amiri and S. D. Sarker, (2006). Extraction of flavonoids and quantification of rutin from waste tobacco leaves. *Iran J. Pharm. Res.* **3**, 222-227.
- [3] D. Deliorman Orhan, F. Ergun, E. Yeşilada, K. Tsuchiya, Y. Takaishi and K. Kawazoe (2007) Antioxidant activity of two flavonol glycosides from *Cirsium hypoleucum* DC. through bioassay-guided fractionation. *Turkish J. Pharm. Sci.* **4**, 1-14.