

Supporting Information

Gossypitrin, A Naturally Occurring Flavonoid, Attenuates Iron-Induced Neuronal and Mitochondrial Damage

María Ángeles Bécquer-Viart ¹, Adonis Armentero-López ¹, Daniel Alvarez-Almiñanaque ¹, Roberto Fernández-Acosta ², Yasser Matos-Peralta ³, Richard F. D’Vries ⁴, Javier Marín-Prida ¹ and Gilberto L. Pardo-Andreu ^{1,*}

¹ Center for Research and Biological Evaluations, Institute of Pharmaceutical and Food Sciences, University of Havana, 222 St. #2317 b/ 23 and 31, La Coronela, La Lisa, CP 13600, La Habana, Cuba; mabecquer@ifal.uh.cu (M.A.B.-V.); adonis.armenteros@ifal.uh.cu (A.A.-L.); dani@ifal.uh.cu (D.A.-A.); javier.marin@ifal.uh.cu (J.M.-P.)

² Pharmacy Department, Institute of Pharmaceutical and Food Sciences, University of Havana, 222 St. #2317 b/ 23 and 31, La Coronela, La Lisa, CP 13600, La Habana, Cuba; roberto.fernandezac91@gmail.com

³ Bioinorganic Laboratory, Faculty of Chemistry, University of Havana, Zapata and G, Vedado, CP 10400, La Habana, Cuba; yasser.matos@fq.uh.cu

⁴ Facultad de Ciencias Básicas, Universidad Santiago de Cali, Calle 5 # 62-00, CP 76001, Cali, Valle del Cauca, Colombia; richard.dvries00@usc.edu.co

* Correspondence: gpardo@ifal.uh.cu; Tel.: +53-7271-8534

The ^1H -NMR, ^{13}C -NMR, and HSQC spectra of gossypitrin are shown in Figures S1, S2, and S3, respectively.

^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.07 (d, $J = 2.1$ Hz, 1H), 7.91 (dd, $J = 8.6, 2.1$ Hz, 1H), 6.99 (d, $J = 8.6$ Hz, 1H), 6.26 (s, 1H), 4.83 (d, $J = 7.3$ Hz, 1H), 3.75 (dd, $J = 9.6$ Hz, 1H), 3.59 (dd, $J = 12.4$ Hz, 1H), 3.46 – 3.25 (m, 38H).

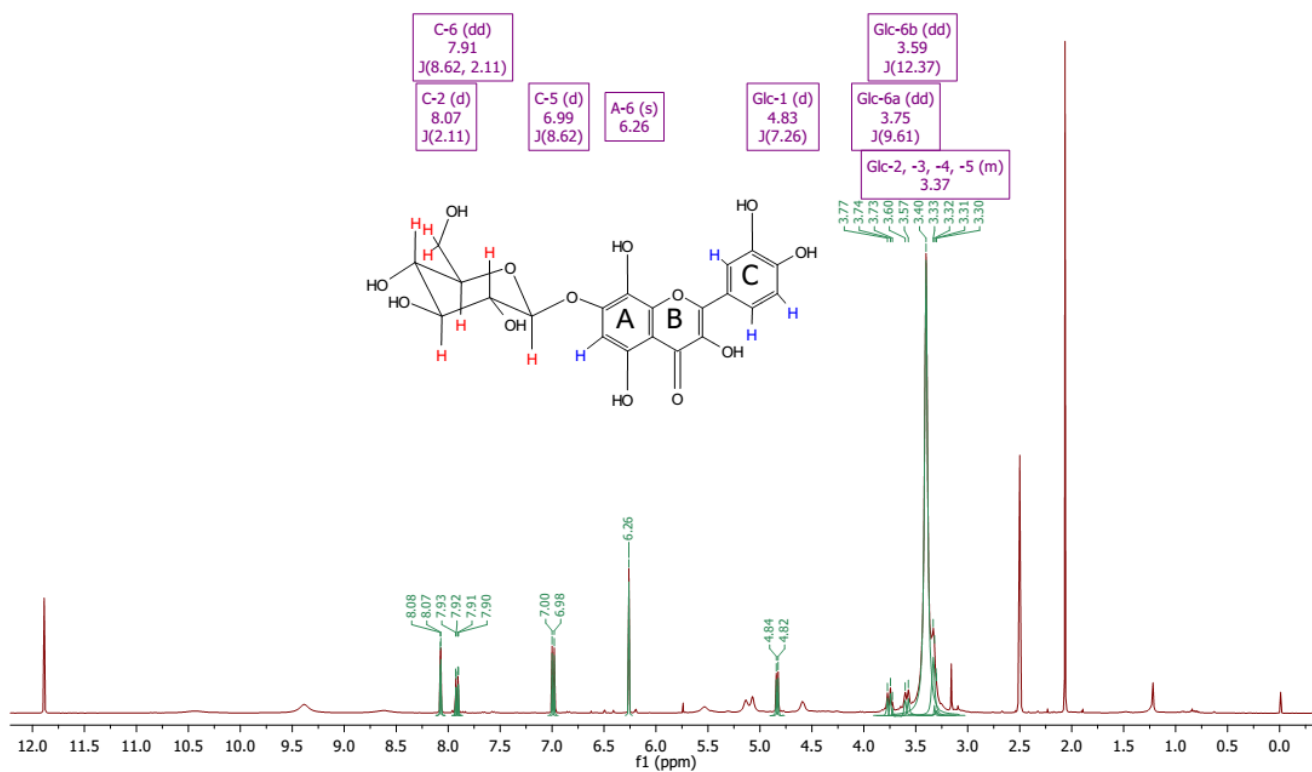


Figure S1. ^1H -NMR (400 MHz) spectrum of gossypitrin in $\text{DMSO}-d_6$.

^{13}C NMR (101 MHz, dms o) δ 176.23, 153.24, 152.50, 148.78, 146.07, 145.19, 145.11, 135.81, 124.52, 123.45, 122.54, 116.05, 115.95, 102.79, 102.00, 98.17, 76.88, 76.14, 73.29, 69.32, 60.34.

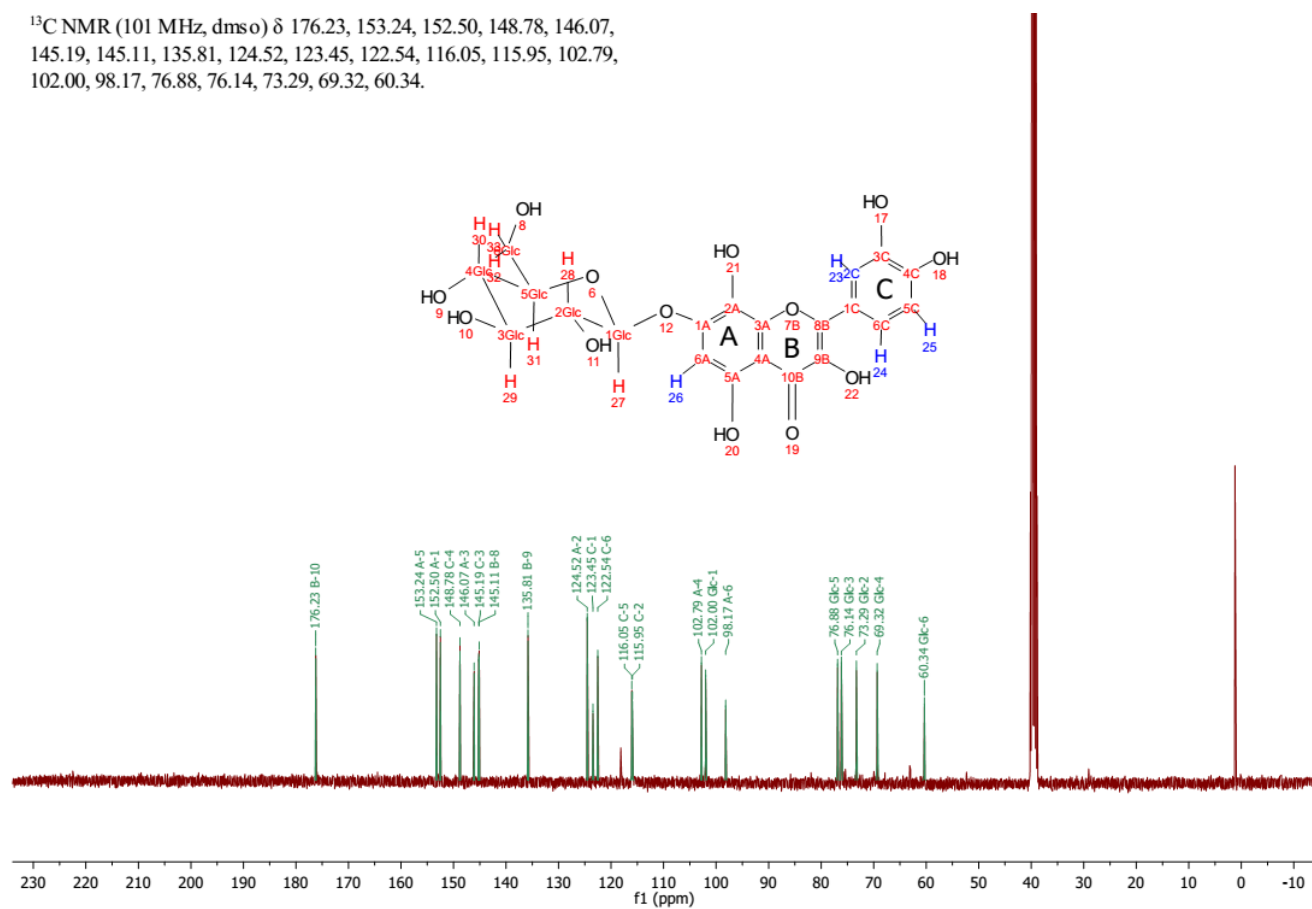


Figure S2. ^{13}C -NMR (101 MHz) spectrum of gossypitrin in $\text{DMSO-}d_6$.

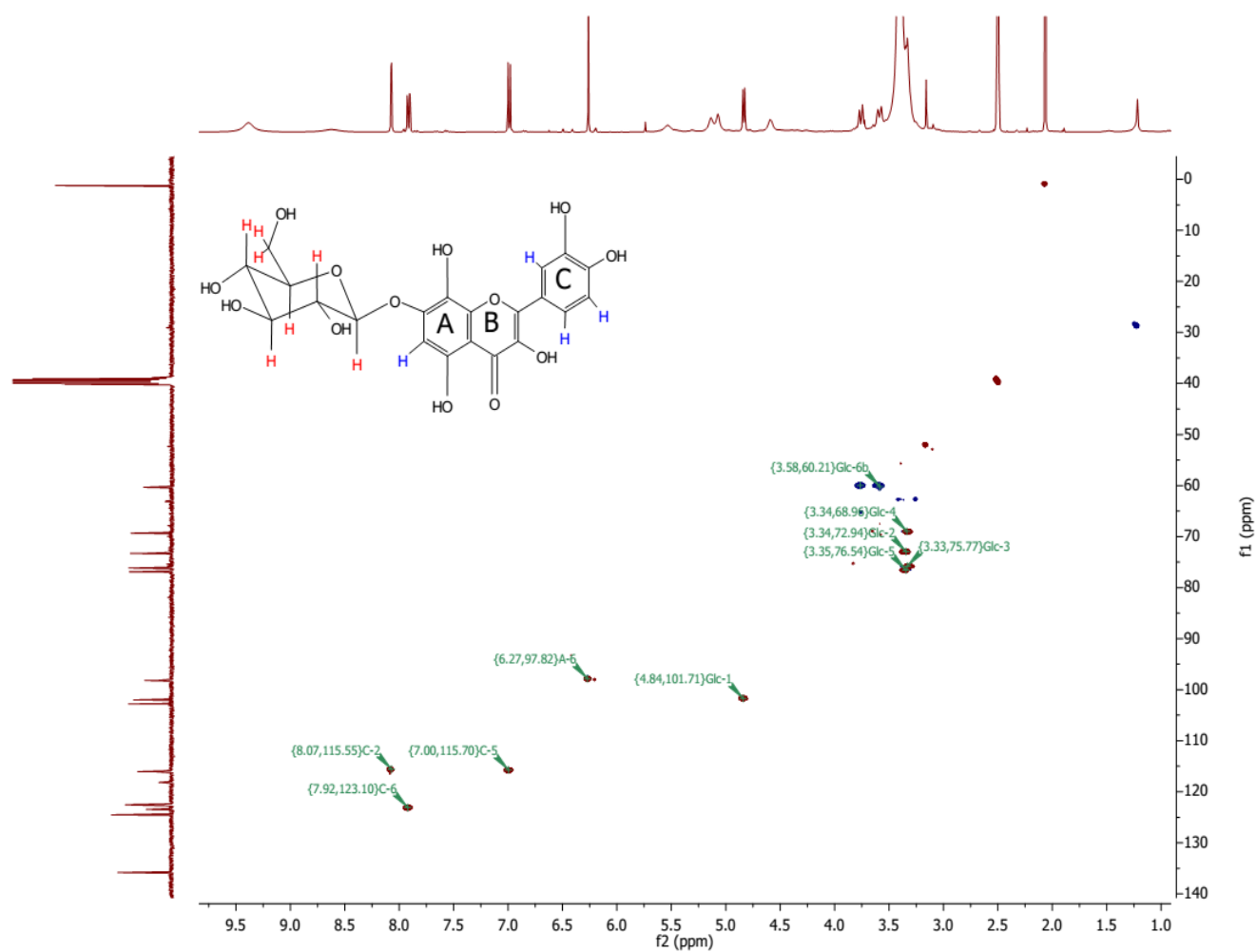


Figure S3. HSQC spectrum of gossypitrin in DMSO- d_6 .

In table 1, NMR data collected verified the structure of the gossypitrin molecule in comparison with previous report (Schliemann et al., 2006).

Table 1. ^1H (400 MHz) and ^{13}C (100 MHz) data of gossypitrin

No.	DMSO- d_6		Schliemann et al., 2006	
	δ , mult., J(Hz)	δ^a	δ (125 MHz)	
2		146.0	147.3	
3	9.41, s	135.7	135.6	
4		176.1	175.9	
5		153.1	151.0	
6	6.26, s	98.0	97.8	
7		152.4	150.0	
8		124.4	126.6	
9		145.0	143.1	
10		102.7	104.4	
1'		123.3	122.0	
2'	8.08, d	115.7	115.2	
3'		145.1	144.7	
4'		148.6	147.5	
5'	6.97, d	115.9	115.6	
6'	7.89, dd	122.4	120.3	
1''	4.84, d	101.8	101.4	
2''	3.74, m	73.2	73.2	
3''	3.76, m	76.0	75.3	
4''	3.14, m	69.2	69.6	
5''	3.32, m	76.7	77.3	
6''A		60.6	60.2	
6''B				

^a Chemical shift obtained from HSQC and HMBC spectra

Chemical shifts from the glycoside protons: $\delta = 5.56$ ppm, $\delta = 5.11$ ppm, $\delta = 4.82$ ppm and $\delta = 4.63$ ppm. Exchangeable phenolic signals of aglycone: $\delta = 11.89$ (s, 5-OH), $\delta = 10.5$ (s, 4'-OH), $\delta = 9.44$ (s, 3'-OH), $\delta = 8.66$ (s, 8-OH).

Reference

Schliemann, W.; Schneider, B.; Wray, V.; Schmidt, J.; Nimtz, M.; Porzel, A.; Böhm, H.,. Flavonols and an indole alkaloid skeleton bearing identical acylated glycosidic groups from yellow petals of *Papaver nudicaule*. *Phytochemistry* **2006**, 67, 191–201. DOI: 10.1016/j.phytochem.2005.11.002