

Antioxidant active phytochemicals in *Ternstroemia lineata* explained by aquaporin mechanisms

Nahim Salgado-Medrano ^{1,2}, César Millán-Pacheco ³, Verónica Rodríguez-López ³, Lucía Corona-Sánchez ³, François Mesnard ⁴, Roland Molinié ⁴, Eleazar León-Álvarez¹, María Luisa Villarreal ^{1,*} and Alexandre Toshirrico Cardoso-Taketa ^{1,*}

Supplementary Materials

Figures S1-S10

Tables S1 and S2

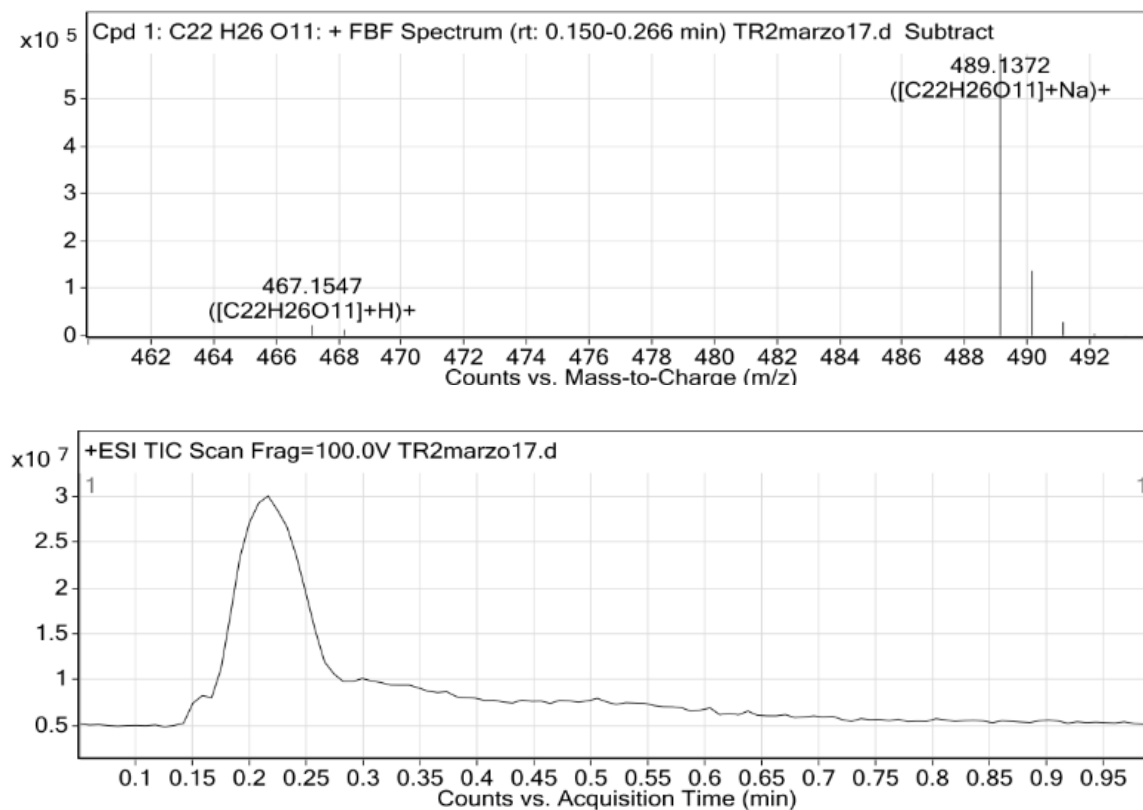


Figure S1. UHPLC-ESI-QTOF-MS analysis of **1**, showing the high-resolution mass spectra (above) and the UHPLC chromatogram (below). The molecular formula of **1** ($C_{22}O_{11}H_{26}$) was calculated through the molecular ion $[M+H]^+$ 467.1547 and the adduct $[M+Na]^+$ 489.1372.

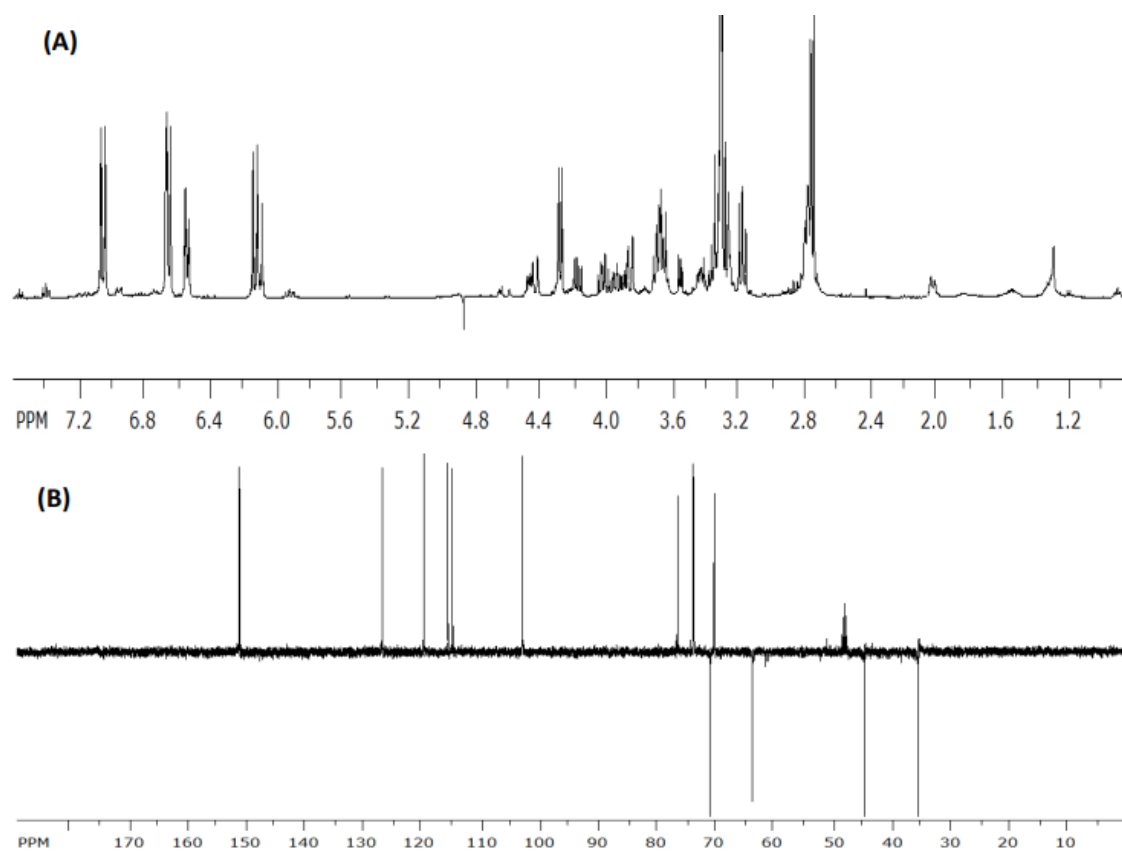


Figure S2. ¹H NMR (A) and ¹³C DEPT 135 (B) NMR spectra of **1** recorded at 400 MHz apparatus in CD₃OD.

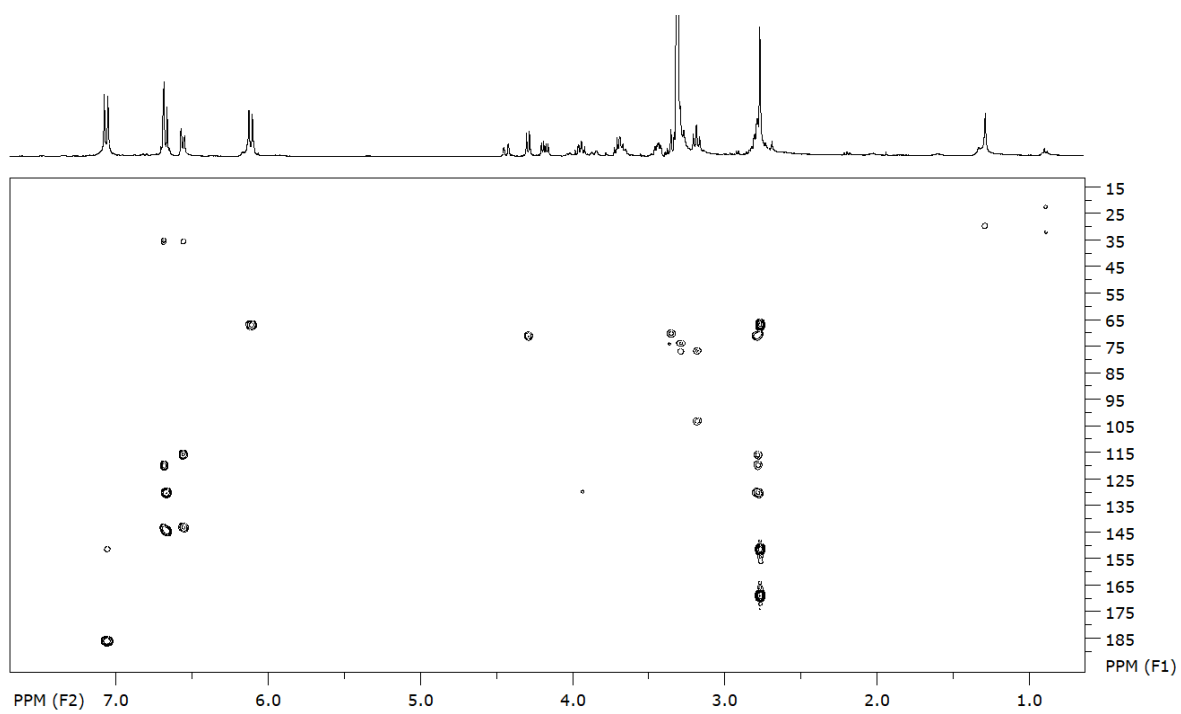
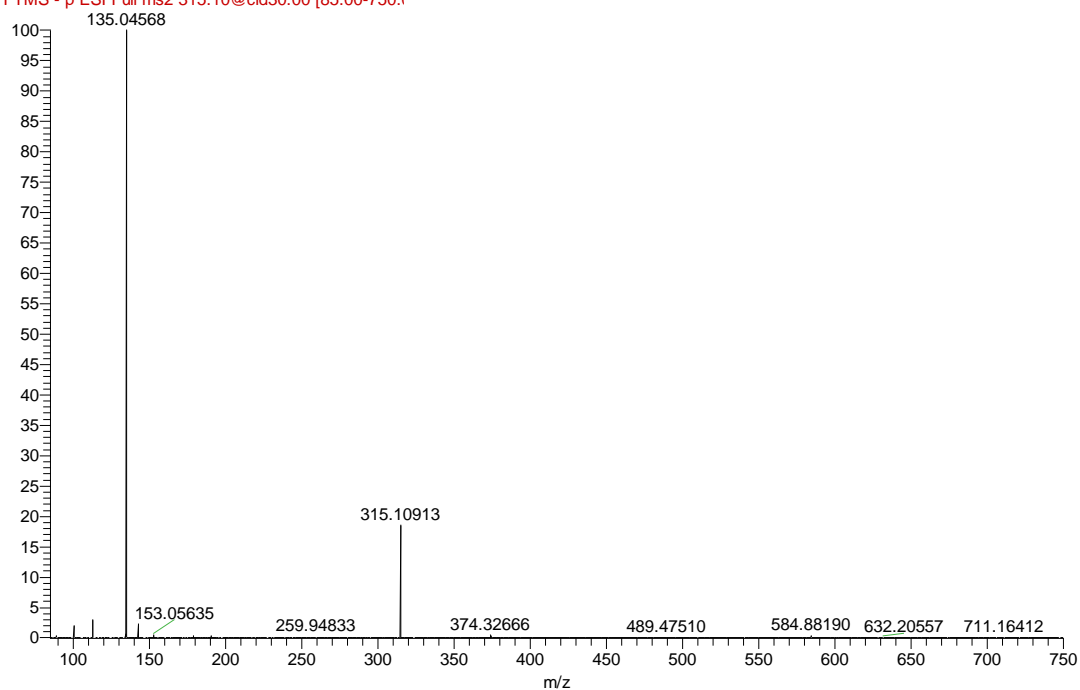


Figure S3. HMBC spectra of **1** recorded at 400 MHz apparatus in CD₃OD.

o140217_0028 #33 RT: 0.93 AV: 1 NL: 3.12E6
F: FTMS - p ESI Full ms2 315.10@cid30.00 [85.00-750.0]



o140217_0027 #17 RT: 0.48 AV: 1 NL: 5.25E6
F: FTMS + p ESI Full ms2 339.10@cid26.00 [90.00-500.0]

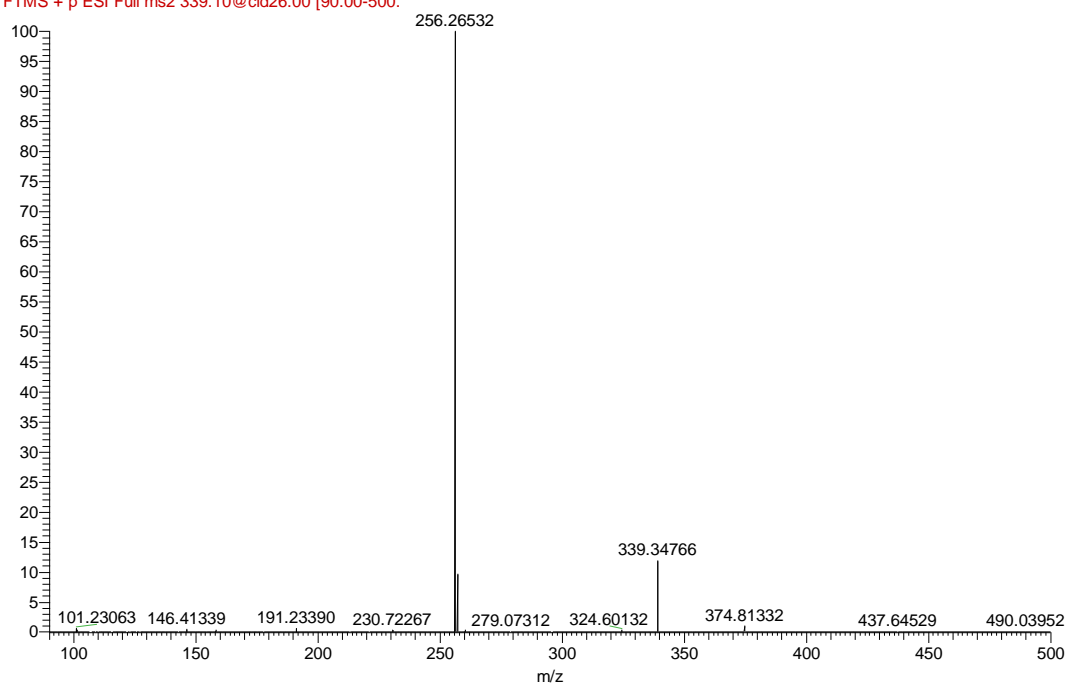


Figure S4. ESI-QTOF-MS analysis of **2**, showing the molecular ion $[M-H]^-$ of m/z 315.10913 (spectrum above) and the adduct $[M+Na]^+$ of m/z 339.34766 (spectrum below).

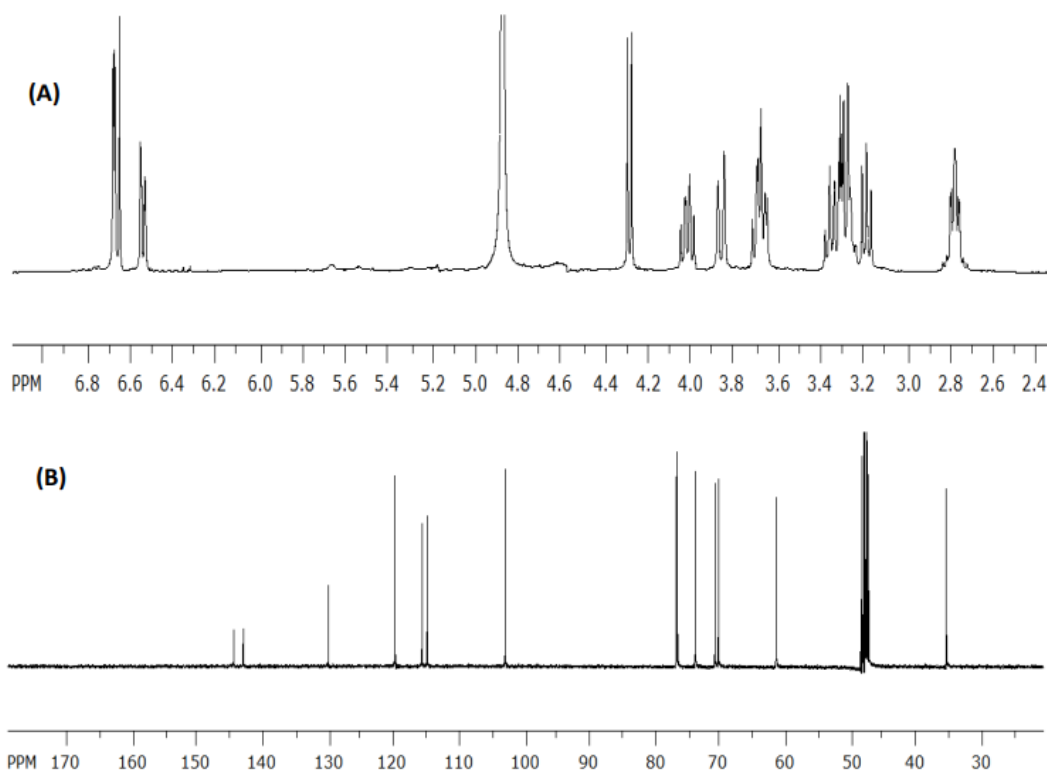


Figure S5. ¹H NMR (A) and ¹³C NMR (B) spectra of **2** recorded at 400 MHz apparatus in CD₃OD.

o140217_0031 #4 RT: 0.08 AV: 1 NL: 1.02E7
F: FTMS - p ESI Full ms [50.00-750.00]

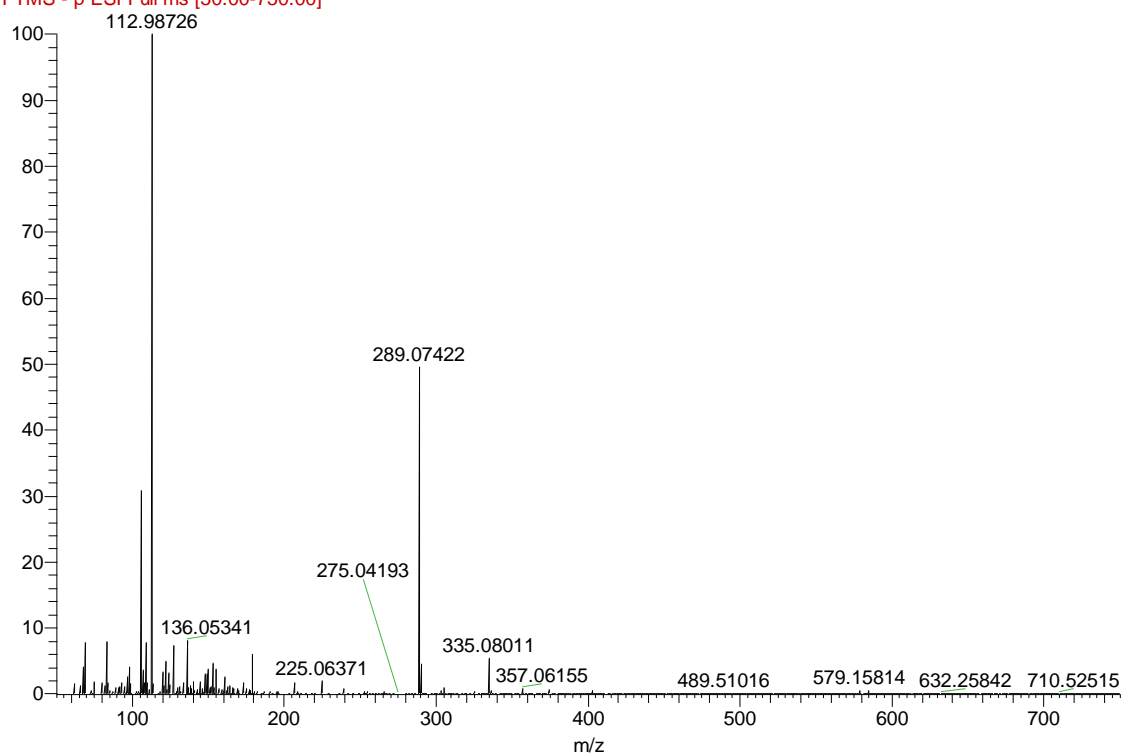


Figure S6. ESI-QTOF-MS analysis of **3**, showing the molecular ion $[M-H]^-$ of m/z 289.07422.

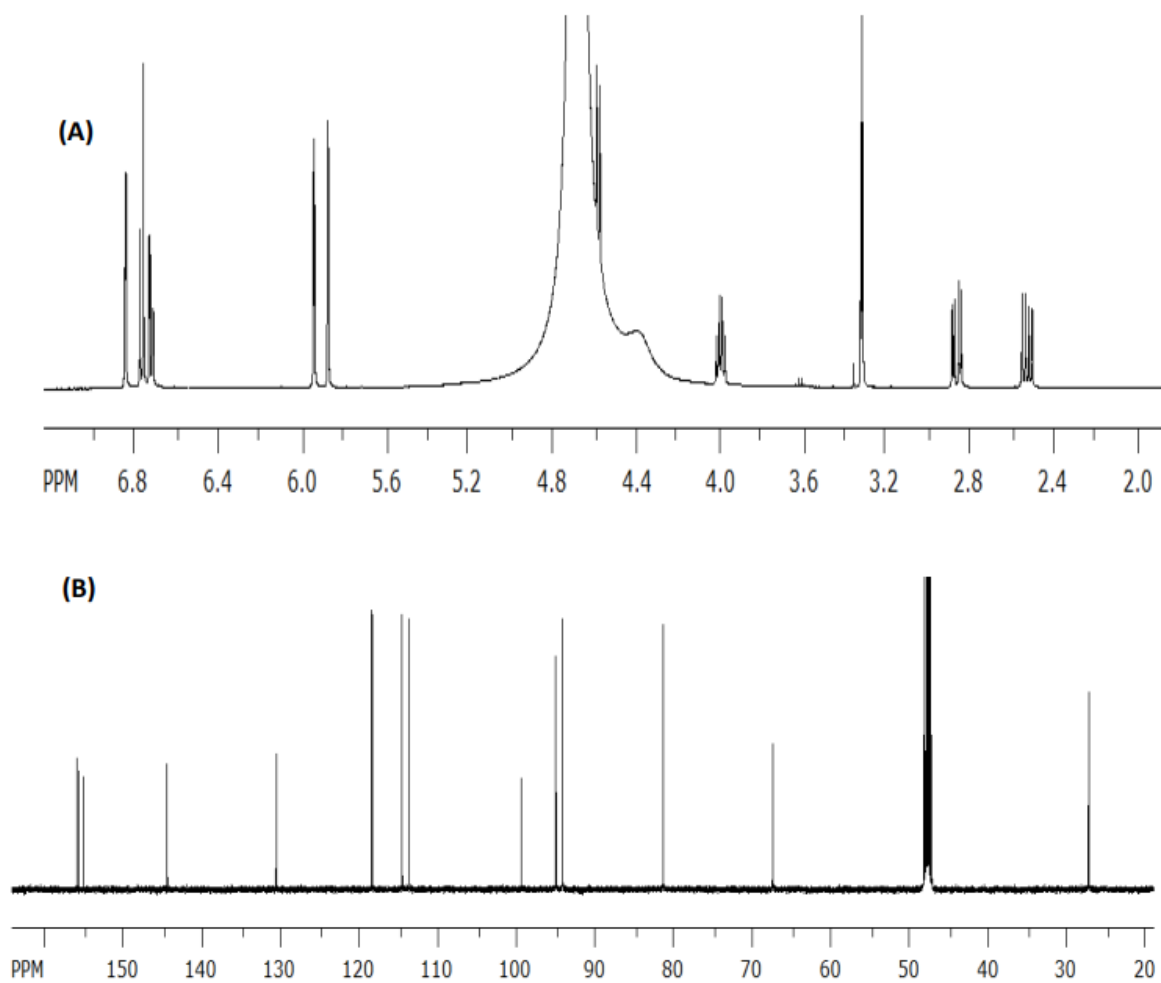


Figure S7. ¹H NMR (A) and ¹³C NMR (B) spectra of **3** recorded at 500 MHz apparatus in CD₃OD.

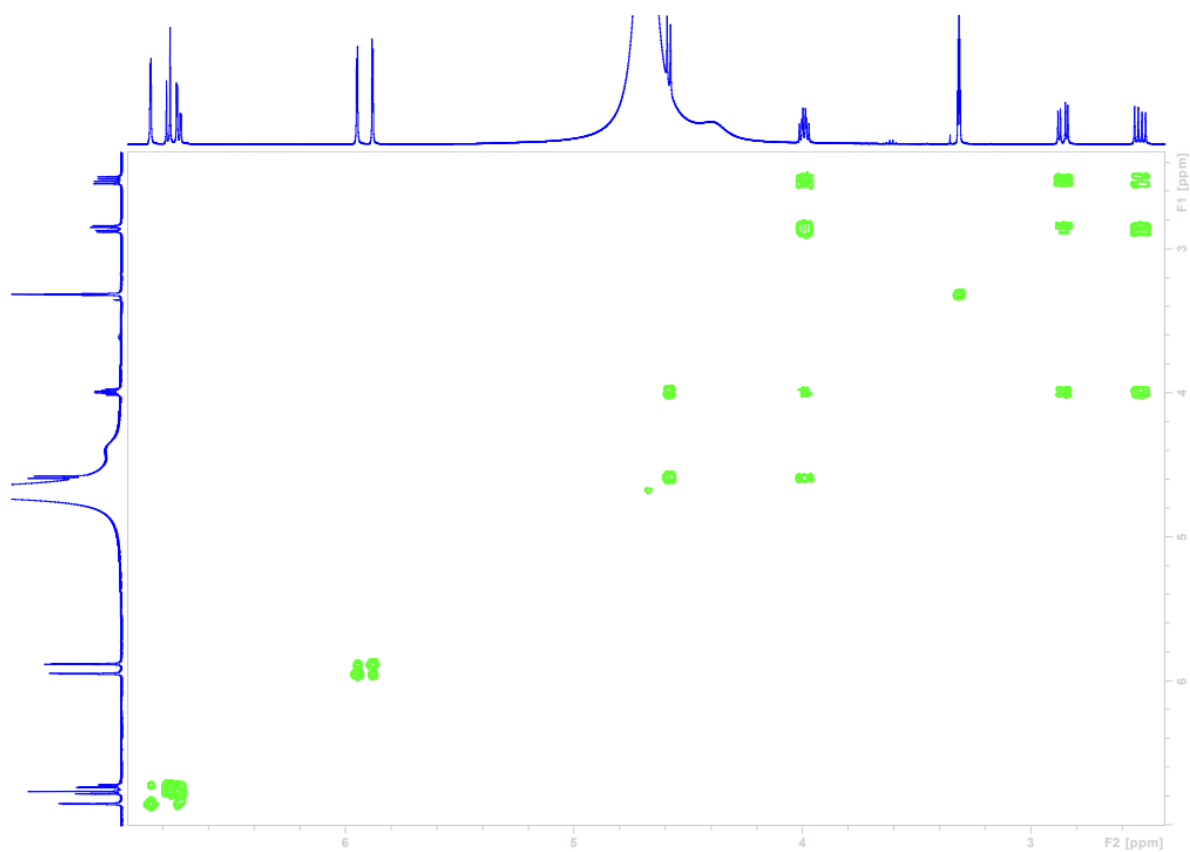


Figure S8. HHCOSY spectra of **3** recorded at 400 MHz apparatus in CD₃OD.

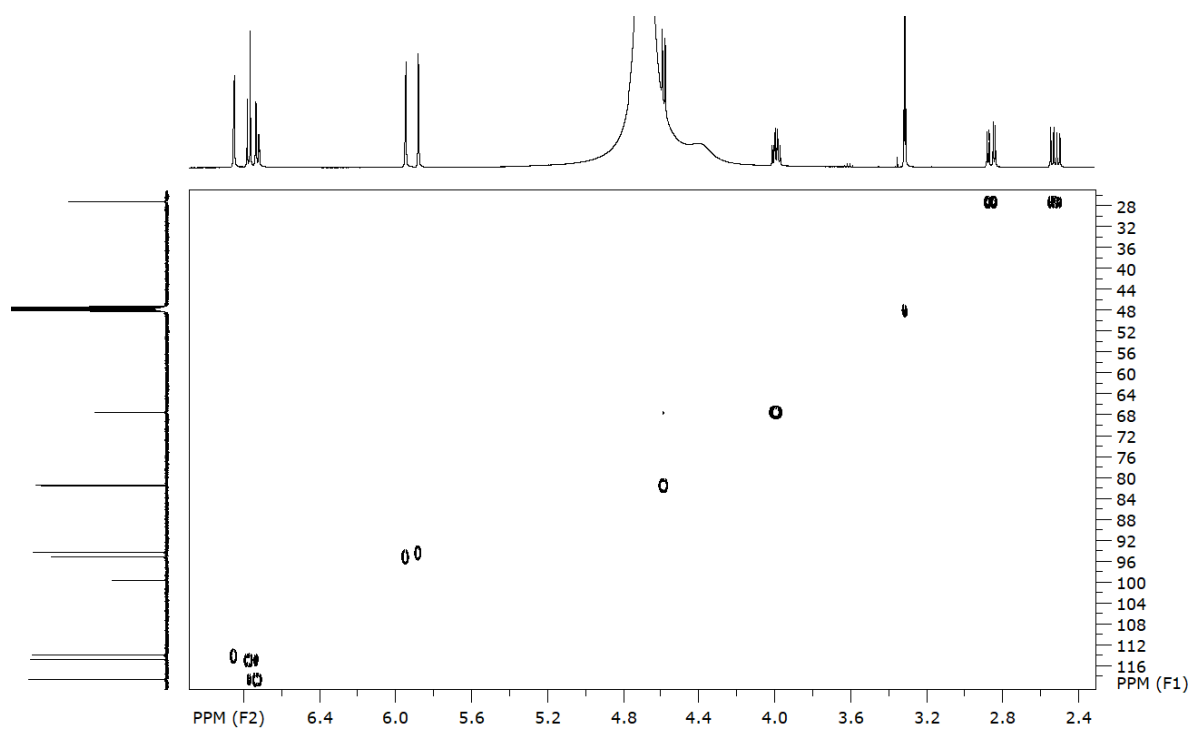


Figure S9. HSQC spectra of **3** recorded at 400 MHz apparatus in CD₃OD.

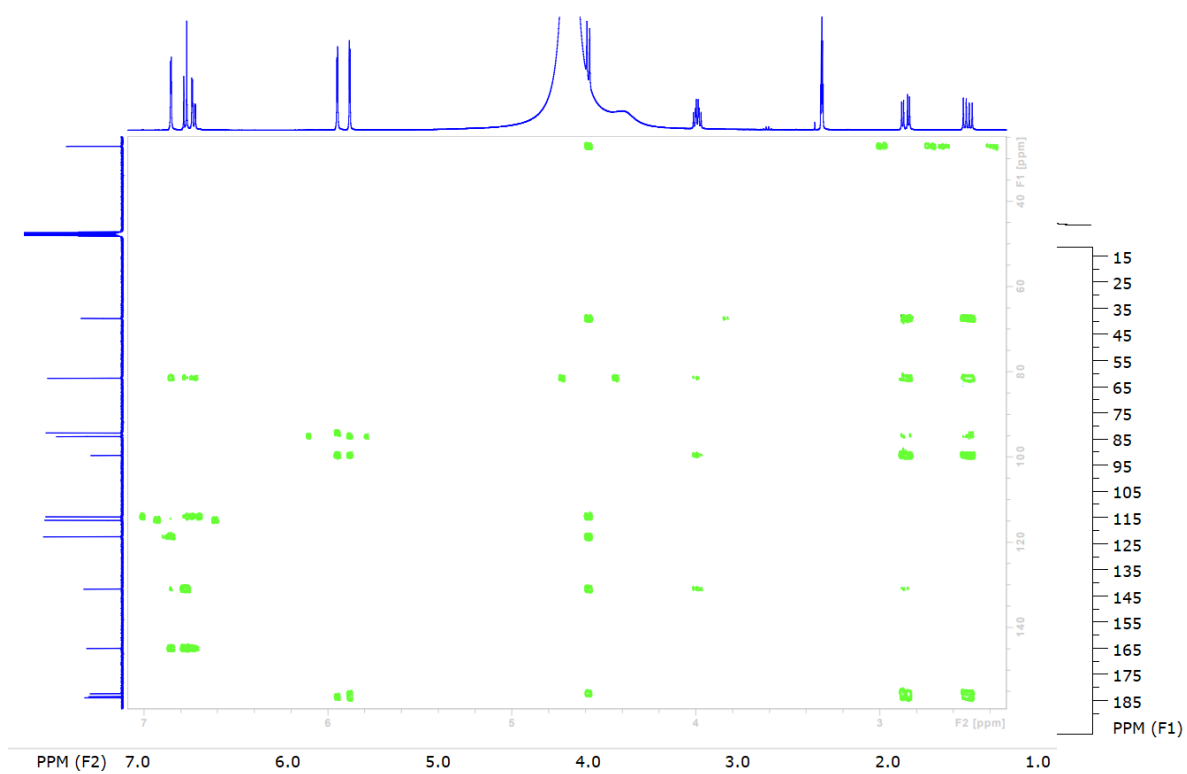


Figure S10. HMBC spectra of **3** recorded at 400 MHz apparatus in CD₃OD.

Table S1. NMR data of terngymnoside C (1)*, hydroxytyrosol 1-glucoside (2)*, and katsumandin (3)** at *400MHz (¹H) and **500 MHz (¹³C) in CD₃OD.

N°	1		2		N°	3	
	δ _H , mult, J = Hz	δ _C	δ _H , mult, J = Hz	δ _C		δ _H , mult, J = Hz	δ _C
1	4.29, d, 8.0	104.54	4.28, d, 8.0	104.41	1	4.58, d, 7.6	83.0
2	3.18, t, 8.0	75.29	3.18, t, 8.0	75.19	2	3.99, m	69.0
3	3.28, ov.	71.81	3.30, ov.	71.68	3	2.52, dd, 16.2, 8.0	28.6
4	3.34, t, 8.8	78.10	3.35, t, 8.4	78.19	1'		132.5
5	3.42, ov.	75.29	3.26, ov.	77.99	2'	6.85, d, 2.0	116.3
6	4.17, dd, 12.0, 6.0	65.19	3.64, ov.	62.80	3'		146.3
	4.43, dd, 12.0, 2.0		3.86, dd, 12.0, 2.0				
1'		131.68		131.59	4'		146.3
2'	6.68, d, 2.1	117.21	6.68, d, 2.1	117.21	5'	6.77, d, 8.2	115.5
3'		146.31		146.18	6'	6.73, dd, 8.2, 2.0	120.2
4'		144.80		144.72	1''		101.1
5'	6.66, d, 8.0	116.45	6.67, d, 8.0	116.41	2''		157.0
6'	6.54, dd, 8.0, 2.1	121.40	6.55, dd, 8.0, 2.1	121.37	3''		157.7
7'	2.77, m	36.74	2.80, m	36.64	4''	5.84, d, 2.3	95.8
						5.88, d, 2.3	
8'	3.68, m	72.25	3.66, m	72.20	5''		157.9
	4.02, m		4.02, m				
1''		68.24			6''	5.95, d, 2.3	96.7
2''	7.06, d, 10.1	152.90					
3''	6.14, d, 10.1	128.42					
4''		187.59					
5''	6.14, d, 10.1	128.42					

6''	7.06, d, 10.1	152.90
7''	2.74, m	45.90
8''		170.49

Table S2. Binding sites for each ligand herein tested. Amino acids were aligned previously. Docking studies were conducted on a single monomer. Those residues that belong to a contiguous monomer are shown with a *.

AQP3		1	2	3	Q	VC	AQP7		1	2	3	Q	VC
							LEU	52	*				*
ASN	32	*	*	*	*	*	VAL	55	*	*	*	*	*
GLN	34			*			HIS*	57		*			
ALA	35	*	*	*	*	*	MET	58	*	*	*	*	*
THR	36	*	*	*	*	*	VAL	59	*	*	*	*	
VAL	37	*											
THR	38			*									
LYS	39	*	*	*	*								
GLY	40	*	*	*	*								
SER*	41	*	*	*	*								
SER	41			*									
GLY*	42	*	*	*	*		TYR*	64	*	*	*	*	
GLY	43		*	*									
SER	44	*	*	*	*								
TYR	45	*	*	*	*	*	TYR	67	*	*		*	*
GLU	46				*								
LEU	48	*	*	*	*	*	VAL	70	*		*	*	*
							PHE	74	*		*	*	*
PHE	119	*					PHE	141				*	
							MET	147		*			
							VAL	148	*	*	*	*	
							THR	149	*	*	*	*	
THR	128	*					GLY	150	*				
ALA	129	*	*		*		ALA	153	*	*	*	*	
THR	130		*				THR	154		*	*	*	
							ALA	155		*	*	*	
							GLY	156	*	*	*	*	*

ALA	132	*	*	*	*	*	ILE	157	*	*	*	*	*
CYS	133	*	*	*	*	*	PHE	158	*				*
							ALA	159	*	*			*
PHE	135	*	*	*	*	*	THR	160	*	*	*	*	*
THR	136	*	*	*	*	*	TYR	161	*	*	*	*	*
ASP	137	*	*	*	*	*	LEU	162	*	*		*	
PRO	138	*					PRO	163	*	*	*	*	
LYS	139	*	*	*	*	*							
							GLY	214					*
GLY	194	*					GLY	218	*	*		*	*
TYR	195	*	*	*			MET	219	*	*		*	*
							ASN	220	*	*		*	
THR	197	*					THR	221	*	*	*	*	
SER	198	*	*	*	*	*	GLY	222	*	*	*	*	*
PHE	199	*	*	*			TYR	223	*	*	*	*	*
							ALA	224	*		*		
							ILE	225			*		
ARG	205	*	*	*	*		ARG	229	*		*	*	*
							ASP	230			*		
							ASN	249	*	*		*	

Residue's locations are based on sequence alignment (not shown). * Indicates residues on a chain contiguous to the original docked chain. Residues that are the same on both sequences are in bold.