

Figure S1. ^1H -NMR spectrum (CD_3OD , 400 MHz) of aureusidin (**1**)

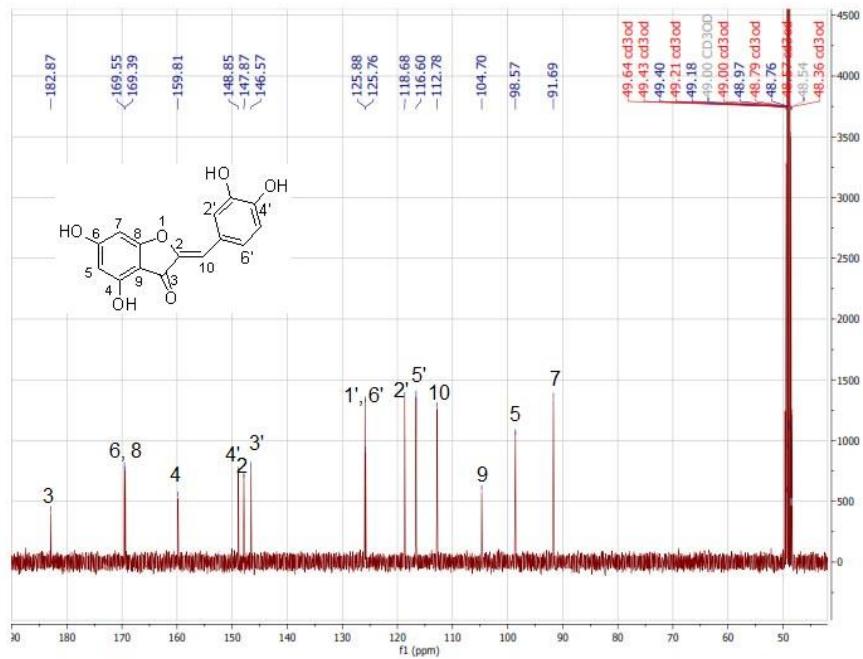


Figure S2. ^{13}C -NMR spectrum (CD_3OD , 101 MHz) of aureusidin (**1**)

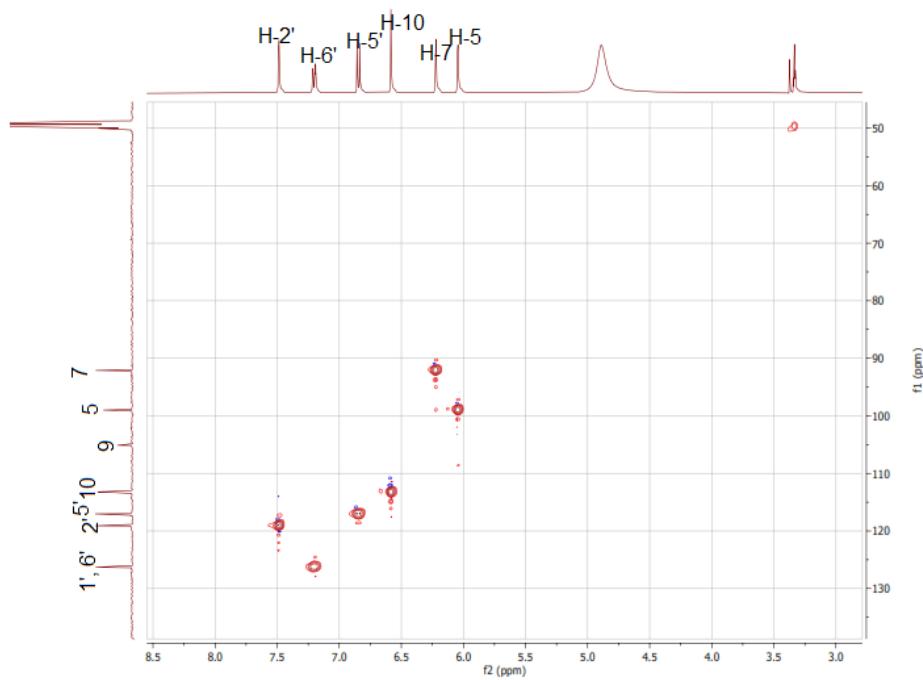


Figure S3. HSQC spectrum of aureusidin (**1**)

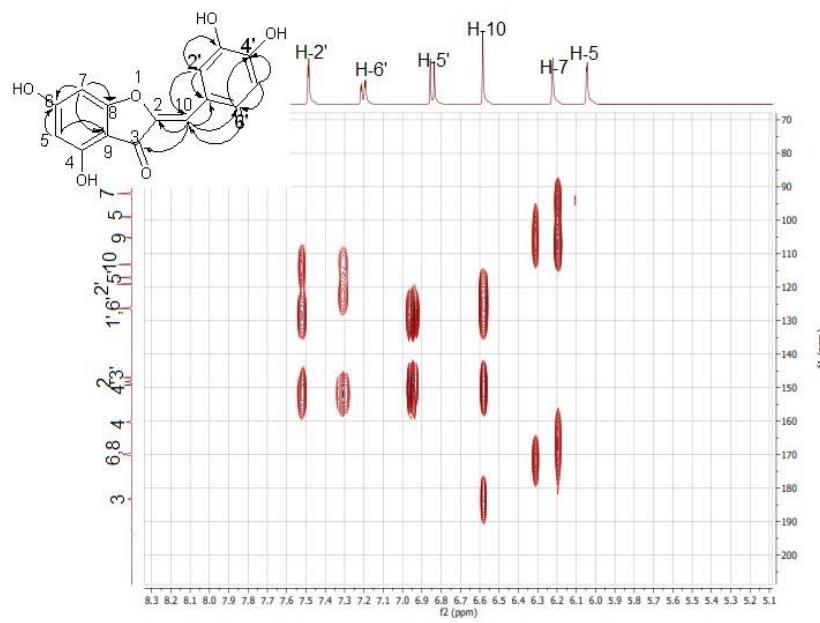


Figure S4. HMBC spectrum of aureusidin (**1**)

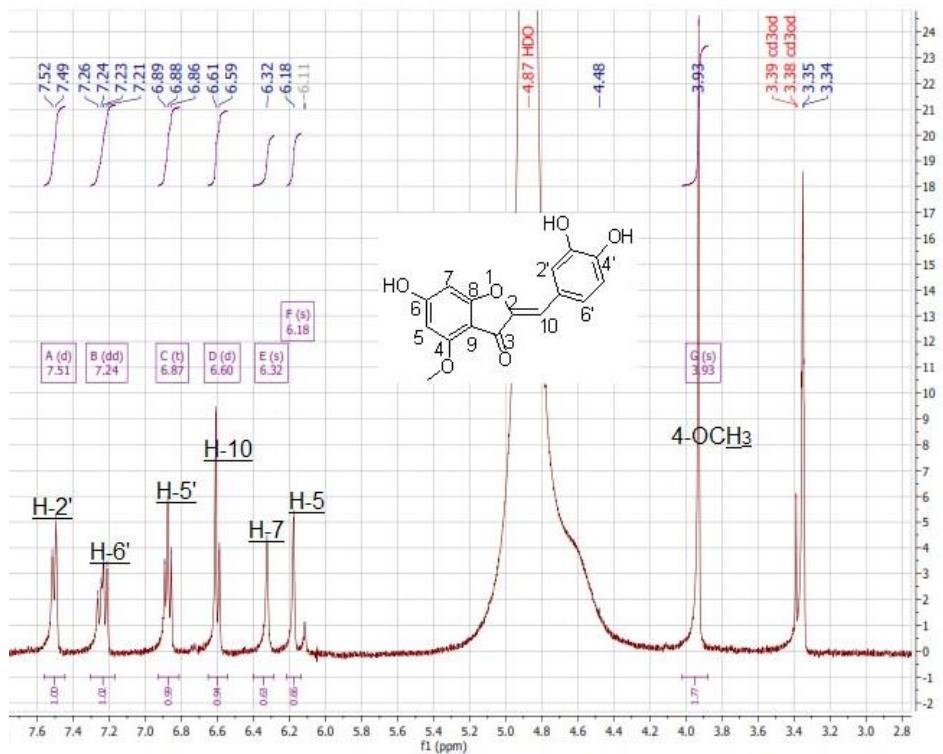


Figure S5. ^1H -NMR spectrum (CD₃OD, 400 MHz) of aureusidin-4-methyl ether (**2**)

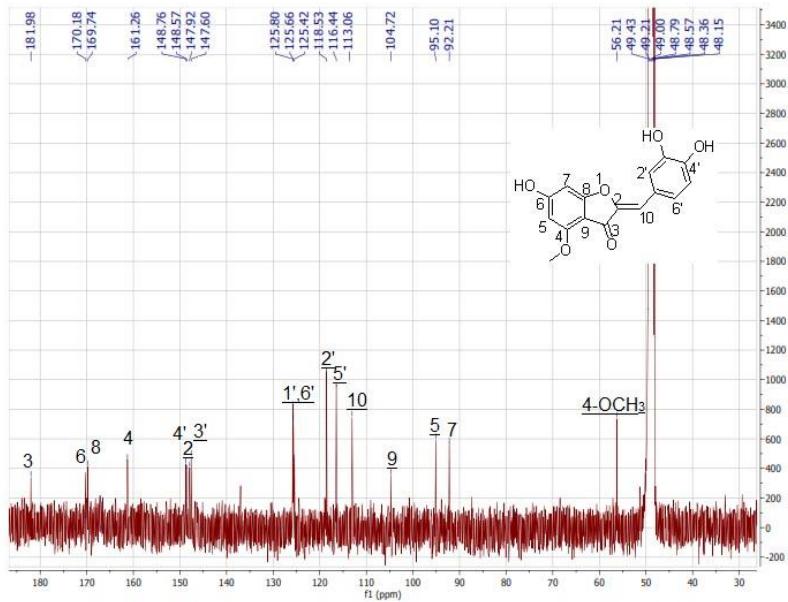


Figure S6. ^{13}C -NMR spectrum (CD₃OD, 101 MHz) of aureusidin-4-methyl ether (**2**)

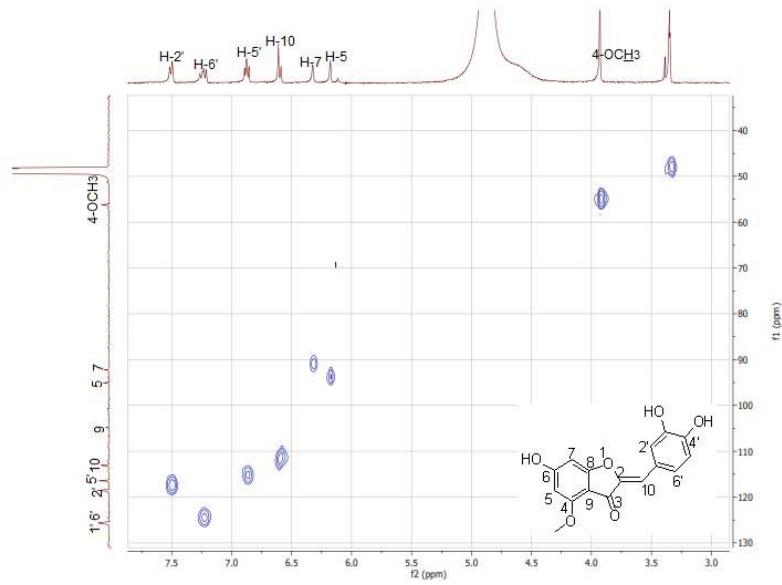


Figure S7. HSQC spectrum of aureusidin-4-methyl ether (**2**)

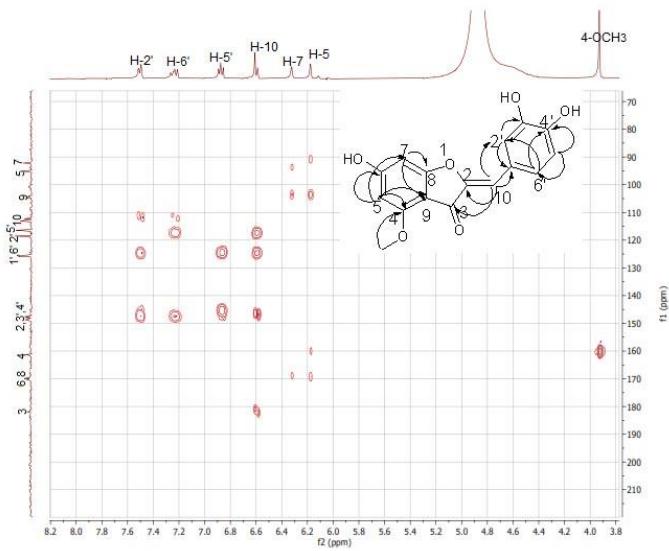


Figure S8. HMBC spectrum of aureusidin-4-methyl ether (**2**)

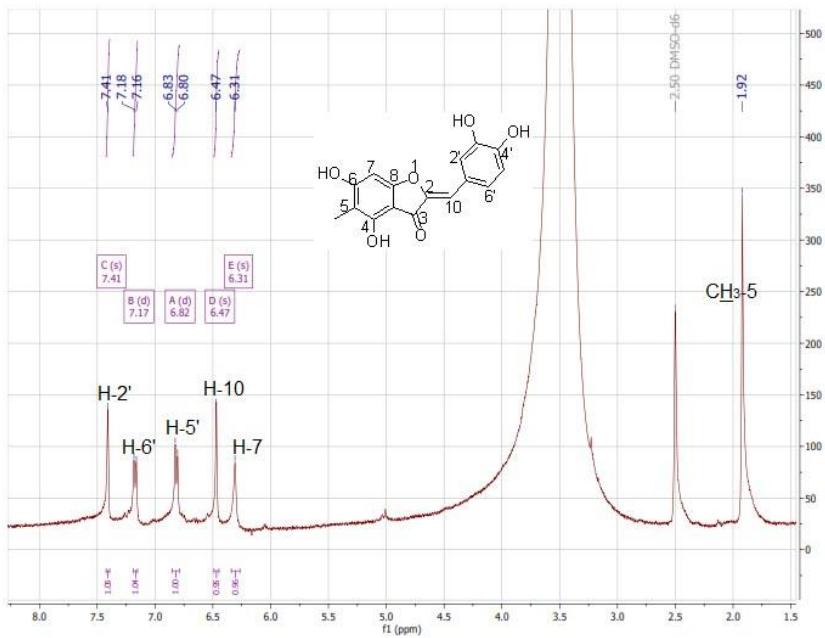


Figure S9. ¹H-NMR spectrum (DMSO-*d*₆, 400 MHz) of 5-methyl aureusidin (3)

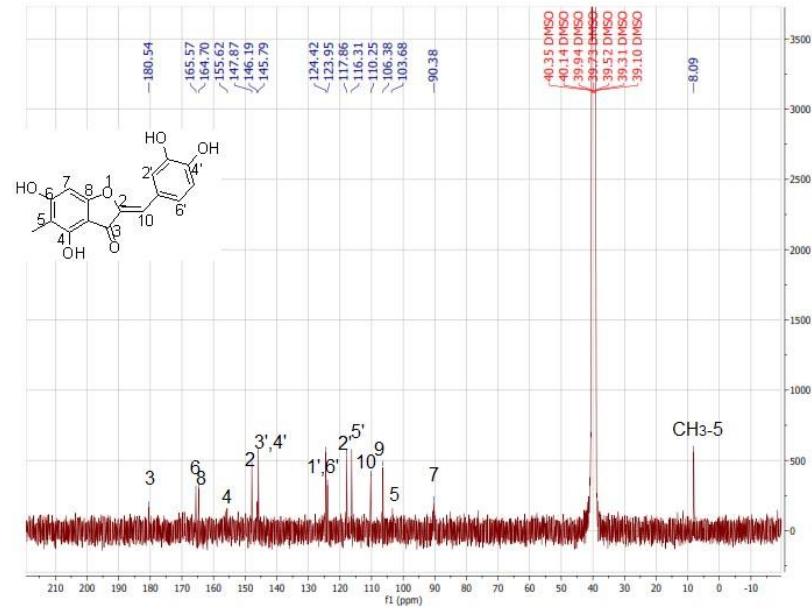


Figure S10. ¹³C-NMR spectrum (DMSO-*d*₆, 101 MHz) of 5-methyl aureusidin (3)

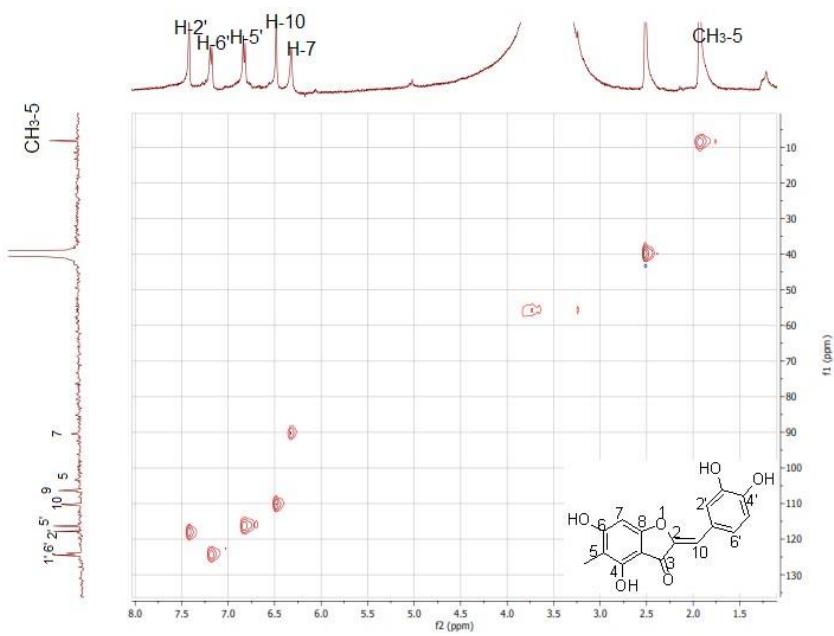


Figure S11. HSQC spectrum of 5-methyl aureusidin (**3**)

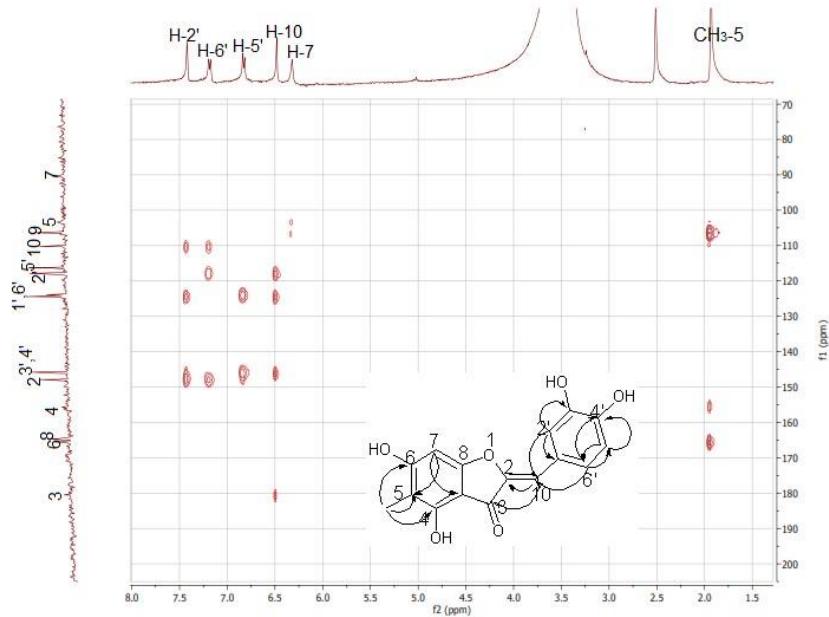


Figure S12. HMBC spectrum of 5-methyl aureusidin (**3**)

Table S1: Receptor interactions and binding energies of the tested compounds, and acarbose inside the binding pocket of α -amylase.

Tested compound	S Score Kcal/mole	RMSD_Refine	Amino acid bond	Distance Å
Acarbose	-22.09	1.82	Lys200/H-donor Lys200/H-donor His201/H-acceptor Gly306/H-acceptor Asp197/H-acceptor Asp300/H-acceptor	2.17 2.24 3.44 1.85 2.4 2.27
1	-17.55	2.00	Asp197/H-acceptor	2.04
3	-16.42	1.84	Asp197/H-acceptor	2.15
2	-15.21	1.46	Asp300/H-acceptor	2.74

Table S2: Receptor interactions and binding energies of the tested compounds, and acarbose inside the binding pocket of α -glucosidase.

Tested compound	S Score Kcal/mole	RMSD_Refine	Amino acid bond	Distance Å
Acarbose	-30.42	1.05	Asn258/H-acceptor Asp326/H-acceptor Asp326/H-acceptor Asp326/H-acceptor Arg411/H-donor Arg411/H-donor Ser 384/ H-acceptor His325/ H-acceptor	1.85 1.87 2.43 1.83 2.02 2.33 2.14 3.2
3	-21.61	2.10	Tyr63/ arene-arene Arg411/H-donor Asp382/H-acceptor	3.93 2.19 2.08
1	-20.64	2.54	Tyr63/ arene-arene Arg411/H-donor Asp382/H-acceptor	3.85 2.24 1.93
2	-20.47	1.36	Tyr63/ arene-arene	1.39

Table S3: Receptor interactions and binding energies of the tested compounds, and CP-91149 inside the binding pocket of glycogen phosphorylase.

Tested compound	S Score Kcal/mole	RMSD_Refine	Amino acid bond	Distance Å
CP-91149	-17.77	1.74	Lys191/ arene-cation Lys191/ arene-cation Arg193/ arene-cation Arg60/ H-donor	3.92 3.74 4.69 2.11
2	-13.42	1.41	Arg193/ arene-cation Arg60/arene-cation Lys191/ H-donor	2.09 3.11 3.55
1	-13.20	0.80	Arg60/ arene-cation	3.27
3	-12.84	1.72	Arg60/arene-cation Arg193/ arene-cation	3.92 3.96