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Conformational Analysis of Phloroglucinols from *Hypericum Brasiliense* by using X-ray Diffraction and Molecular Modeling

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Table S1. Summary of the crystal structure data collection and refinement for japonicin A (**1**), uliginosin B (**2**) and isouliginosin B (**3**)

Identification code	Japonicin A (**1**)	Uliginosin B (**2**)	Isouliginosin B (**3**)
Empirical formula	$C_{25}H_{32}O_8$	$C_{28}H_{34}O_8$	$C_{28}H_{34}O_8$
Formula weight	460.51	498.55	498.55
Temperature	150(2) K	150(2) K	150(2) K
Wavelength	1.5418 Å	1.5418 Å	1.5418 Å
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	P 21/n	P 21/n	P -1
Unit cell dimensions	*a* = 9.2461(4) Å *b* = 17.8198(6) Å *c* = 28.8240(10) Å α = 90°. β = 90°. γ = 90°	*a* = 10.4085(4) Å *b* = 9.1035(3) Å *c* = 27.5920(10) Å α = 90.000(3)°. β = 99.070(3)°. γ = 90.000(3)°.	*a* = 10.4944(4) Å *b* = 10.7537(3) Å *c* = 12.3616(4) Å α = 103.610(3)°. β = 110.336(3)°. γ = 93.969(3)°
Volume	4749.1(3) Å^3	2581.76(16) Å^3	1253.80(8) Å^3
Z	8	4	2
Density (calculated)	1.288 Mg/m^3	1.283 Mg/m^3	1.321 Mg/m^3
Absorption coefficient	0.792 mm^{-1}	0.77 mm^{-1}	0.793 mm^{-1}
F(000)	1968	1064	532
Crystal size	0.39 x 0.11 x 0.06 mm^3	0.49 x 0.14 x 0.03 mm^3	0.38 x 0.22 x 0.09 mm^3
Theta range for data collection	3.07 to 62.48°.	3.24 to 62.68°	3.97 to 62.89°
Index ranges	-10<=h<=10, -20<=k<=20, -33<=l<=33	-11<=h<=11, -10<=k<=10, -31<=l<=31	-12<=h<=11, -12<=k<=12, -14<=l<=14
Reflections collected	39758	6833	32807

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Table S1. continuation

Identification code	Japonicin A (**1**)	Uliginosin B (**2**)	Isouliginosin B (**3**)
Independent reflections	3776 [R(int) = 0.0330]	6973 [R(int) = 0.0000]	3958 [R(int) = 0.0331]
Completeness to theta = 62.89°	99.8 %	98.5 %	98.0 %
Absorption correction	Analytical	Analytical	Semi-empirical from equivalents
Max. and min. transmission	0.962 and 0.829	0.937 and 0.552	0.9338 and 0.7521
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3776 / 0 / 309	6973 / 12 / 327	3958 / 0 / 342
Goodness-of-fit on F^2	1.060	1.059	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0510, wR2 = 0.1412	R1 = 0.0599, wR2 = 0.1644	R1 = 0.0381, wR2 = 0.1058
R indices (all data)	R1 = 0.0627, wR2 = 0.1490	R1 = 0.0902, wR2 = 0.1767	R1 = 0.0463, wR2 = 0.1131
Extinction coefficient	0.00008(4)	0.00009(7)	0.0009(3)
Largest diff. peak and hole	0.590 and -0.247 e.Å^{-3}	0.269 and -0.266 e.Å^{-3}	0.307 and -0.211 e.Å^{-3}

Uliginosin refinement performed on data obtained from a twinned sample. For japonicin A w=1/[\s^2 (F_o^2)+(0.0755P)^2+3.4186P] where P=(F_o^2+2F_c^2)/3, for uliginosin w=1/[\s^2(F_o^2)+(0.0574P)^2+0.2333P] where P=(F_o^2+2F_c^2)/3 and for isouliginosin w=1/[\s^2(F_o^2)+(0.0642P)^2^+0.4656P] where P=(F_o^2+2F_c^2)/3.