Isolation, Structure Elucidation, and Antiproliferative Activity of

Butanolides and Lignan Glycosides from the Fruit of

Hernandia nymphaeifolia

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Figure S1. ¹H NMR spectrum of **1** (600MHz, in CDCl₃).



Figure S2. ¹³C NMR spectrum of **1** (150MHz, in CDCl₃).

 $\mathbf{2}$



Figure S3. H-H COSY experiment of 1 (600MHz, in CDCl₃).



Figure S4. HMQC experiment of 1 (600MHz, in CDCl₃).



Figure S5. HMBC experiment of 1 (600MHz, in CDCl₃).

 $\mathbf{5}$



Figure S6. NOESY experiment of 1 (600MHz, in CDCl₃).



Figure S7. ¹H NMR spectrum of **2** (400MHz, in CDCl₃).

 $\mathbf{7}$



Figure S8. ¹³C NMR spectrum of **2** (100MHz, in CDCl₃).







Figure S10. HMQC experiment of 2 (400MHz, in CDCl₃).



Figure S11. HMBC experiment of 2 (400MHz, in CDCl₃).



Figure S12. NOESY experiment of 2 (400MHz, in CDCl₃).



Figure S13. ¹H NMR spectrum of **3** (400MHz, in CDCl₃).



Figure S14. ¹³C NMR spectrum of **3** (100MHz, in CDCl₃)



Figure S15. H-H COSY experiment of 3 (400MHz, in CDCl₃)



Figure S16. HMQC experiment of 3 (400MHz, in CDCl₃)



Figure S17. HMBC experiment of 3 (400MHz, in CDCl₃)



Figure S18. NOESY experiment of 3 (400MHz, in CDCl₃)



Figure S19. ¹H NMR spectrum of **4** (400MHz, in CDCl₃).



Figure S20.¹³C NMR spectrum of **4** (100MHz, in CDCl₃).



Figure S21. COSY experiment of 4 (400MHz, in CDCl₃).



Figure S22 HMQC experiment of 4 (400MHz, in CDCl₃).



Figure S23. HMBC experiment of 4 (400MHz, in CDCl₃).



Figure S24. NOESY experiment of 4 (400MHz, in CDCl₃).



Figure S25. ¹H NMR spectrum of **5** (400MHz, in CDCl₃).



Figure S26. ¹³C NMR spectrum of 5 (100MHz, in CDCl₃).



Figure S27. H-H COSY experiment of 5 (400MHz, in CDCl₃).



Figure S28. HMQC experiment of 5 (400MHz, in CDCl₃).



Figure S29. HMBC experiment of 5 (400MHz, in CDCl₃).



Figure S30. NOESY experiment of 5 (400MHz, in CDCl₃)



Figure S31. ¹H NMR spectrum of 6 (600MHz, in CDCl₃)



Figure S32. ¹³C NMR spectrum of 6 (150MHz, in CDCl₃)



Figure S33. H-H COSY experiment of 6 (600MHz, in CDCl₃)



Figure S34. HMQC experiment of 6 (600MHz, in CDCl₃)



Figure S35. HMBC experiment of 6 (600MHz, in CDCl₃)



Figure S36. NOESY experiment of 6 (600MHz, in CDCl₃).



Figure S37. ¹H NMR spectrum of 7 (400MHz, in CDCl₃).



Figure S38. ¹³C NMR spectrum of 7 (100MHz, in CDCl₃).



Figure S39. H-H COSY experiment of 7 (400MHz, in CDCl₃).



Figure S40. HMQC experiment of 7 (400MHz, in CDCl₃).



Figure S41. HMBC experiment of 7 (400MHz, in CDCl₃).



Figure S42. NOESY experiment of 7 (400MHz, in CDCl₃).

Figure S43. EIMS spectrum for 7





Figure S44. ¹H MNR spectrum of **8** (400MHz, in CD₃OD)



Figure S45. ¹³C MNR spectrum of 8 (100MHz, in CD₃OD)



Figure S46. H-H COSY experiment of 8 (400MHz, in CD₃OD)



Figure S47. HMQC experiment of 8 (400MHz, in CD₃OD)



Figure S48. HMBC experiment of 8 (400MHz, in CD₃OD)



Figure S49. NOESY experiment of 8 (400MHz, in CD₃OD)



Figure S50. ROESY experiment of 8 (400MHz, in CD₃OD)



Figure S51. ¹H MNR spectrum of 9 (400MHz, in CD₃OD)



Figure S52. ¹³C MNR spectrum of **9** (100MHz, in CD₃OD)



Figure S53. H-H COSY experiment of 9 (400MHz, in CD₃OD)



Figure S54. HMQC experiment of 9 (400MHz, in CD₃OD).



Figure S55. HMBC experiment of 9 (400MHz, in CD₃OD).



Figure S56. NOESY experiment of **9** (400MHz, in CD₃OD).



Figure S57. ¹H NMR spectrum of **9** (400MHz, in DMSO-*d*₆).

Figure S58. HRFABMS data of 1.

Data : EI-HR-2017-066 Date : 09-Mar-2018 15:59 Instrument : MStation Sample : 16SA-HPH-F13-e-1 Note : No.225 Inlet : Direct Ion Mode : EI+ RT : 2.50 min Scan # : 31 Elements : C 25/0, H 43/0, O 3/0 Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50 Unsaturation (U.S.) : -0.5 - 10.0

 Observed m/z
 Int%
 Err[ppm / mmu]
 U.S. Composition

 1
 390.3137
 21.80
 +0.8 / +0.3
 5.0
 C25 H42 O3

Figure S59. HRFABMS data of 2.

Data : EI-HR-2017-008 Date : 27-Jun-2017 11:33 Instrument : MStation Sample : 16SA-HPE-F3-b-4 Note : No.33 Inlet : Direct Ion Mode : EI+ RT : 1.50 min Scan# : 19 Elements : C 29/0, H 50/0, O 3/0 Mass Tolerance : 1000ppm, Spmu if m/z < 5, 50mmu if m/z > 50 Unsaturation (U.S.) : -0.5 - 10.0 Observed m/z Int% Err[nom / mmu] U.S. Composition

Obs	served m/z	Int%	Err[ppm /	mmu]	U.S.	Composition
1	446.3743	27.14	-3.8 /	-1.7	5.0	C29 H50 O3

~	6	٦
-	2	4
•••	L,	2
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Figure S60. HRFABMS data of 3.

Data : EI-HR-2017-065 Date : 09-Mar-2018 15:53 Instrument : MStation Sample : 16SA-HPE-F3-b-2-a Note : No.226 Inlet : Direct Ion Mode : EI+ RT : 2.25 min Scan# : 28 Elements : C 25/0, H 44/0, O 3/0 Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50 Unsaturation (U.S.) : -0.5 - 10.0 Dbserved m/z Int% Err[ppm / mmu] U.S. Composition

1 392.3302 26.64 +2.9 / +1.2 4.0 C25 H44 O3

Figure S61. HRFABMS data of **4**.

Data : 分子生薬学_20180117108 Date : 03-Sep-2018 11:22 Instrument : MStation Sample : 16SA_HPB_F1_e Note : Nacl Inlet : Direct Ion Mode : FAB+ RT : 6.61 min Scan # : 70 Elements : C 38/0, H 46/0, O 3/0, Na 1/0 Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50 Unsaturation (U.S.) : -0.5 - 5.0

Observed m/z	Int%	Encloom / umal	U.S.	Composition
1 441.3357	100.00	+2.8 / +1.2	4.5	C27 H46 O3 No

5	9

Figure S62. HRFABMS data of 5.

Data : EI-HR-2017-027 Date : 18-Oct-2017 13:51 Instrument : MStation Sample : 16SA-HPE-F4-d-1 Note : No.91 Inlet : Direct Ion Mode : EI+ RT : 14.33 min Scan# : 173 Elements : C 29/0, H 50/0, O 3/0 Mass Tolerance : 1000ppm, Smmu if m/z < 5, 500mmu if m/z > 500 Unsaturation (U.S.) : -0.5 - 20.0 Observed m/z Int% Err[ppm / mmu] U.S. Composition

1 446.3749 25.71 -2.5 / -1.1 5.0 C29 H50 O3

Figure S63. HRFABMS data of 6.

Data : EI-HR-2017-025 Date : 18-Oct-2017 10:28 Instrument : MStation Sample : 16SA-HP-LHe-F6-5-e-1 Note : No.93 Inlet : Direct Ion Mode : EI+ RT : 10.58 min Scan# : 128 Elements : C 25/0, H 44/0, O 4/0 Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 500mmu if m/z > 500 Unsaturation (U.S.) : -0.5 - 10.0

Ob	served m/z	Int%	Err[ppm /	mmu]	U.S.	Composition
1	408.3230	26.36	-2.4 /	-1.0	4.0	C25 H44 O4

0	n
h	sU)
~	~

Figure S64. HRFABMS data of 7.

Data : EI-HR-2017-064 Date : 09-Mar-2018 15:46 Instrument : MStation Sample : 16SA-HPE-F4-f-2-b Note : No.227 Inlet : Direct Ion Mode : EI+ RT : 3.84 min Scan# : 47 Elements : C 28/0, H 50/0, O 4/0 Mass Tolerance : 1000ppm, Smmu if m/z < 5, 50mmu if m/z > 50 Unsaturation (U.S.) : -0.5 - 10.0 Observed m/z Int% Err[ppm / mmu] U.S. Composit

 Observed m/z
 Int%
 Err[ppm / mmu]
 U.S. Composition

 1
 450.3702
 16.95
 -1.6 / -0.7
 4.0
 C28 H50 O4

Figure S65. HRFABMS data of 8.

Data : 分子生薬学_20180117330 Date : 23-Oct-2019 16:50 Instrument : MStation Sample : 16SA_HPB_F5_a_4_b Note : NBA+NaCl Inlet : Direct Ion Mode : FAB+ RT : 2.22 min Scan# : 20 Elements : C 27/0, H 36/0, O 13/0, Na 1/0 Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50 Unsaturation (U.S.) : -0.5 - 10.0

Ob	served m/z	Int%	Err[ppm	/ mmu]	U.S.	Composit	tion	
1	591.2022	34.41	-5.3 /	-3.2	9.5	C27 H36	013	Na

0	1
b	н
~	-

Figure S66. HRFABMS data of 9.

Data : 分子生薬学_20180117331 Date : 23-Oct-2019 17:12 Instrument : MStation Sample : 16SA_HPB_F5_d_1_c_1_b Note : NBA+NaCl Inlet : Direct Ion Mode : FAB+ RT : 2.69 min Scan # : 24 Elements : C 26/0, H 34/0, O 12/0, Na 1/0 Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50 Unsaturation (U.S.) : -0.5 - 10.0

 Observed m/z
 Int%
 Err[ppm / mmu]
 U.S. Composition

 1
 561.1958
 7.66
 +1.8 / +1.0
 9.5
 C26 H34 O12 Na