Supporting Information for

Nanomolar Antimalarial Agents against Chloroquine-Resistant *Plasmodium falciparum* from Medicinal Plants and their Structure-Activity Relationships

Bin Zhou,[†] Yan Wu,[†] Seema Dalal,[‡] Emilio F. Merino,[‡] Qun-Fang Liu,[†] Cheng-Hui Xu,[†] Tao Yuan,[†] Jian Ding,[†] David G. I. Kingston, [§] Maria B. Cassera,[‡] and Jian-Min Yue^{*, †}

[†]State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zuchongzhi Road, Shanghai 201203; University of Chinese Academy of Sciences, No.19A Yuquan Road, Beijing 100049, People's Republic of China

[‡]Department of Biochemistry, [§]Department of Chemistry and the Virginia Tech Center for Drug Discovery, MC 0308/0212, Virginia Tech, Blacksburg, Virginia 24061, United States

* E-mail: jmyue@simm.ac.cn

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Comounds	Method	Retention Time (min)	Purity (%)
1	А	12.27	95.65
2	А	17.35	98.00
3	А	16.97	98.10
4	А	12.54	96.99
5	А	12.28	98.98
6	А	18.74	94.77
7	А	7.16	94.79
8	А	14.89	95.61
9	А	10.35	97.98
10	А	8.99	94.56
11	А	19.49	98.75
12	А	19.19	98.06
13	А	5.23	97.74
14	А	14.35	98.84
15	В	18.84	99.28
16	А	13.06	97.36
17	А	15.94	98.96
18	А	16.35	98.79
19	А	17.35	96.33
20	А	10.77	98.27
21	А	10.76	97.87
22	А	12.65	98.91
23	В	18.99	96.84
24	А	14.08	98.15
25	А	19.01	99.06
26	А	12.14	97.87
27	А	15.24	98.38
28	А	16.34	96.49
29	А	16.46	98.30
30	А	18.25	99.78
31	А	13.15	97.98
32	A	17.09	96.89
33	A	17.05	99.02
34	A	17.04	99.53
35	A	11.71	95.45
36	A	12.23	99.51
37	A	9.20	99.39
58 20	A	1/.06	98.29
39	A	9.83	99.36
40	A	11.84	97.32
41	A	10.15	95.18
42	A	8.36	96.68
43	В	18.30	96.15
44	А	15.46	96.62

Table S1 The purities of compounds 1–44

The purities of compounds 1–44 were checked by reversed-phase HPLC, which was performed on an Aglient 1100 binary pump system with an Aglient 1100 detector (210 nm) using a YMC-Pack ODS-A (150×4.6 nm, *S*-5 μ m).

Methods: A: 30–80% CH₃CN in H₂O for 20 min, 0.5 ml/min; B: 30–90% CH₃CN in H₂O for 20 min, 0.5 ml/min



Figure S1. ¹H NMR spectrum of fortunilide A (1) in CDCl₃

Figure S2. ¹³C NMR spectrum of fortunilide A (1) in CDCl₃



3





fl (ppm)





fl (ppm)



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Figure S6. (+)-ESIMS of fortunilide A (1)



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100

Figure S7. (-)-ESIMS of fortunilide A (1)



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Figure S8. (+)-HRESIMS of fortunilide (1)

Elemental Composition Report

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Single Mass Analysis Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 336 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass) Elements Used: C: 5-80 H: 2-120 O: 0-20 Na: 0-1 CFS-17C LCT PXE KE324

CFS-	17C	11. 24	120	0, 0	-20	INC.	0-1			L	.СТ РХ	E KE	324								13	-Sep-2	013
CFS-	17C_0	913 4	3 (0.93	35) AM	2 (Ar,	0000.	0,0.00	0,1.00)	; ABS	; Cm	(27:45))									1: TO	FMSE 2.20e+	24 S+ 004
100]																785.2	781					
%																		8	17.303 	6			
0	467.1	950	•	53	7.337	57	9.293 5	94 80.296	50 613	4052	² 669.	689. 4199	2587 713	.4452		780.32	231		818 8	3.3072 19.300	⁵ 854.39	39	- /
Ŭ	460	480	500	520	540	560	580	600	620	640	660	680	700	720	740	760	780	800	820	840	860 8	80 80	INZ
Mini Maxi	mum: mum:					3.0	•	5.	.0		-1.5 50.0												
Mass		С	alc.	Mass	3	mDa	ı	PI	PM		DBE		i-FI	т	:	i-FIT	(Nc	rm)	Form	ula			
785.	2781	ד ד ד	85.2 85.2 85.2	785 809 751		-0. -2. 3.0	4 8	-0 -3 3 -	0.5 3.6 .8		18.5 21.5 30.5		78.4 78.8 78.3		(1.0 1.5 0.9			C41 C43 C50	H46 H45 H41	014 014 09	Na	



Figure S9. IR spectrum of fortunilide A (1)



Figure S10. ¹H NMR spectrum of fortunilide B (2) in CDCl₃

Figure S11. ¹³C NMR spectrum of fortunilide B (2) in CDCl₃



Figure S12. HSQC spectrum of fortunilide B (2) in CDCl₃



fl (ppm)



Figure S13. HMBC spectrum of fortunilide B (2) in CDCl₃



Figure S15. (+)-ESIMS of fortunilide B (2)



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Figure S16. (–)-ESIMS of fortunilide B (2)



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Figure S17. (+)-HRESIMS of fortunilide B (2)

Elemental Composition Report

Single Mass Analysis Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 337 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass) Elements Used: C: 5-80 H: 2-120 O: 0-20 Na: 0-1 CFS-13C-1 LCT PXE KE324

0.0 /00-1				LCT PXE K	E324		03-Sen-2013
CFS-13C-1_0	903 38 (0.831) AN	//2 (Ar,10000.0,0	0.00,1.00); ABS	; Cm (22:38)			15:27:14 1: TOF MS ES+
100						7 87.296 4 ! !	1.15e+004
%						784.2867 824	.3860
122.9	428 -	02 1380	422.6442			765.3124	839.4043
0	232 7302	402.1	297 423.14	⁶² 512.2380	647.2164	733.2854	840.4011 906 3199
100 150	200 250	300 350	400 450	500 550	600 650	700 750 800	850 900 950 m/z
Minimum: Maximum:		3.0	3.0	-1.5 50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
787.2964	787.2966 787.2977 787.2942	-0.2 -1.3 2.2	-0.3 -1.7 2.8	20.5 39.5 17.5	50.3 56.5 49.4	1.3 7.5 0.3	C43 H47 O14 C59 H40 O Na C41 H48 O14 Na

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Figure S18. IR spectrum of fortunilide B (2)



Figure S19. ¹H NMR spectrum of fortunilide C (3) in CDCl₃





Figure S21. HSQC spectrum of fortunilide C (3) in CDCl₃









Figure S24. (+)-ESIMS spectrum of fortunilide C (3)



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Figure S25. (–)-ESIMS spectrum of fortunilide C (3)



26

- AGA-

Figure S26. (+)-HRESIMS spectrum of fortunilide C (3)

Elemental Composition Report

Single Mass Analysis Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

657.2672 657.2676 -0.4 -0.6 15.5

Monoisotopic Mass, Even Electron Ions 272 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass) Elements Used: C: 5-80 H: 2-120 O: 0-20 Na: 0-1 CET PXE KE324 LCT PXE KE324 19-Nov-2013 15:55:04 1: TOF MS ES+ 6.72e+003 CFS-35B_1119 63 (1.378) AM2 (Ar,10500.0,0.00,0.70); ABS; Cm (56:80) 100 657,2672 %-658.2711
 581.3427
 588.4475
 603.2487
 617.2765
 625.4161
 635.2833
 646.2473
 1/
 680.3414
 m/z

 580
 585
 590
 595
 600
 605
 610
 615
 620
 625
 630
 635
 640
 645
 650
 655
 660
 665
 670
 675
 680
 685
٥٢ Minimum: -1.5 50.0 Maximum: 5.0 3.0 Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula

36.2

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0.0 C36 H42 O10 Na



Figure S27. IR spectrum of fortunilide C (3)



Figure S28. ¹H NMR spectrum of fortunilide D (4) in CDCl₃

Figure S29. ¹³C NMR spectrum of fortunilide D (4) in CDCl₃











fl (ppm)


1

1. C. A. *

Figure S33. (+)-ESIMS spectrum of fortunilide D (4)



Figure S34. (–)-ESIMS spectrum of fortunilide D (4)



Figure S35. (+)-HRESIMS spectrum of fortunilide D (4)

Elemental Composition Report

Single Mass Analysis Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 352 formula(e) evaluated with 3 results within limits (up to 50 closest results for each mass) Elements Used: C: 5-80 H: 2-120 O: 0-20 Na: 0-1 CFS-15B LCT PXE KE324 LCT PXE KE324

CFS-15B				LCT PXE KI	E324				13-Sep-2013
CFS-15B_0913	3 4 (0.070) AM2	(Ar,10000.0,0.	00,1.00); ABS; C	m (4:21)					13:42:58 1: TOF MS ES+
100							819.2851	I	1.558+004
%							820	2869	
						801.273	821	2914	
0	438.6412 ⁵	13.1754 55	631.	2389 687.239	8 705 2523	728.2675	82	2.2875 870.396	⁵ .909.8015
400	450	500	550 600	650	700	750 E	300	850 90) <u>950</u>
Minimum: Maximum:		3.0	4.0	-1.5 50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Formula	
819.2851	819.2840 819.2864 819.2875	1.1 -1.3 -2.4	1.3 -1.6 -2.9	17.5 20.5 39.5	61.4 65.7 73.4	0.0 4.3 11.9		C41 H48 C43 H47 C59 H40	016 Na 016 03 Na

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Figure S36. IR spectrum of fortunilide D (4)



Figure S37. ¹H NMR spectrum of fortunilide E (5) in CDCl₃









fl (ppm)



Figure S40. HMBC spectrum of fortunilide E (5) in CDCl₃



Figure S42. (+)-ESIMS spectrum of fortunilide E (5)



Figure S43. (–)-ESIMS spectrum of fortunilide E (5)



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Figure S44. (+)-HRESIMS spectrum of fortunilide E (5)

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Elemental Composition Report Page 1 Single Mass Analysis Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron lons 352 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass) Elements Used: C: 5-80 H: 2-120 O: 0-20 Na: 0-1 CFS-15A 13-Sep-2013 13:38:06 1: TOF MS ES+ 1.11e+004 LCT PXE KE324 CFS-15A_0913 4 (0.070) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (2:19) 819.2842 100 820.2875 % 819.0630 821.2885 803.2880 687.2364 705.2512 822.2861 867.2386 550.2474 627.2092 953.2844967.2779 m/z 472.6518 ۵ ل -600 450 500 550 650 700 750 850 800 900 950 1000 Minimum: -1.5 50.0 Maximum: 3.0 4.0 Mass Calc. Mass mDa РРМ DBE i-FIT i-FIT (Norm) Formula 0.2 -2.2 819.2840 819.2864 819.2842 0.2 -2.7 17.5 20.5 61.1 65.5 C41, H48 O16 Na C43 H47 O16 0.0

4.4



Figure S45. IR spectrum of fortunilide E (5)



Figure S46. ¹H NMR spectrum of fortunilide F (6) in CD₃OD

Figure S47. ¹³C NMR spectrum of fortunilide F (6) in CD₃OD













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Figure S51. (+)-ESIMS spectrum of fortunilide F (6)



Figure S52. (–)-ESIMS spectrum of fortunilide F (6)



Figure S53. (+)-HRESIMS spectrum of fortunilide F (6)

Elemental Composition Report Page 1 Single Mass Analysis Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3 Monoisotopic Mass, Even Electron Ions 239 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass) Elements Used: C: 5-80 H: 2-120 O: 0-20 Na: 0-1 CFS-34A LCT PXE KE324 31-Oct-2013 14:40:52 1: TOF MS ES+ 2.01e+004 CFS-34A_1031 37 (0.776) AM2 (Ar;10500.0,0.00,0.70); ABS; Cm (30:51) 591.2211 100-575.2262 618.2336 %ιİ 633.2524 143.0603 569.2408 806.3688 879.3139 957.3749 m/z 900 900 1000 180.0453 208.0407 365.6355 485.1973 521.2182 704.1678 0 년--100 · · · · · · ----------200 400 300 500 700 600 Minimum: -1.5 50.0 Maximum: 5.0 3.0 Mass Calc. Mass mDa i-FIT . i-FIT (Norm) Formula PPM DBE 591.2211 591.2206 0.5 0.8 13.5 108.9 0.0 C31 H36 O10 Na



Figure S54. IR spectrum of fortunilide F (6)





Figure S56. ¹³C NMR spectrum of fortunilide G (7) in CDCl₃







fl (ppm)





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Figure S60. (+)-ESIMS spectrum of fortunilide G (7)



Figure S61. (–)-ESIMS spectrum of fortunilide G (7)



Figure S62. (+)-HRESIMS spectrum of fortunilide G (7)

Elemental Composition Report

Single Mass Analysis Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

 Monoisotopic Mass, Even Electron Ions

 321 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

 Elements Used:

 C: 5-80
 H: 2-120

 CFS-17B_0913 42 (0.902) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (26:44)

 100

%	600 290.1	⁷⁵⁶ 342.1685	462.3127	537.3396	585.2471 625.3	940	756.2714 787. 788.2	2930 970	
0 L.,,i. 100	200	300	400	500	، ، . ، السينية السينية	ا	800 8	900	45.5933 m/z 1000
Minímum: Maximum:		3.0	3.0	-1.5 50.0					
Mass	Calc. Mas:	s mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Formula	
755.2683	755.2680 755.2704	0.3 -2.1	0.4 -2.8	18.5 21.5	80.6 86.9	0.0 6.3		C40 H44 C42 H43	013 Na 013

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13-Sep-2013 14:07:16 1: TOF MS ES+ 2.84e+004



Figure S63. IR spectrum of fortunilide G (7)



Figure S64. ¹H NMR spectrum of fortunilide H (8) in CDCl₃

Figure S65. ¹³C NMR spectrum of fortunilide H (8) in CDCl₃









fl (ppm)


Figure S69. (+)-ESIMS spectrum of fortunilide H (8)



Figure S70. (–)-ESIMS spectrum of fortunilide H (8)



Figure S71. (+)-HRESIMS spectrum of fortunilide H (8)

Elemental Composition Report

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Single Mass Analysis Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

CFS-21D	H: 2-120 - O: 0	-20 Na: 0-1		LCT PX	E KE324						31-Oct-2
CFS-21D_1	031 45 (0.989) AM2	2 (Ar,10500.0,0.0	00,0.70); ABS; (Cm (27:46)	I					1: 1	14:4 OF MS E
100				771.26	325						2.25e+
				i I							
%											
{				173	72.2658						
616	.2379 632.2472	73.2589 691.41	189 75	5.2674	801.2848 801.2848 87.2582	853.3672	869.3	755	919	4753 9	35.4672
616 0 500	.2379 632.2472	73.2589 691.41 680 700	189 75 720 740	5.2674 760 7	801.2848 87.2582 80 800 820	853.3672 	869.3 860	755 880	919 900 9	4753 ⁹ 20 9	35.4672
616 0 600 1inimum: 1aximum:	.2379 632.2472 63 620 640 660	73.2589 691.41 680 700 5.0	189 75 720 740 4.0	5.2674 7 760 7 -1.5 50.0	801.2848 87.2582 87.2582 80 800 820	853.3672 	869.37 860	755 880	919 900 g	. 4 753 ^g 20 g	35.4672
616 0 500 4inimum: 1aximum: 1ass	2379 632.2472 632.2472 620 640 660 Calc. Mass	73.2589 691.43 680 700 5.0 mDa	189 75 720 740 4.0 PPM	5.2674 7 760 7 -1.5 50.0 DBE	22.2658 601.2848 87.2682 j 80 800 820 i-FIT	853.3672 	869.33	755 880 rm) Fe	919 900 9	4753 ⁹ 20 9	35.4672 r 40



Figure S72. IR spectrum of fortunilide H (8)



Figure S73. ¹H NMR spectrum of fortunilide I (9) in CD₃OD

Figure S74. ¹³C NMR spectrum of fortunilide I (9) in CD₃OD















78

Figure S78. (+)-ESIMS spectrum of fortunilide I (9)



79

Figure S79. (–)-ESIMS spectrum of fortunilide I (9)



80

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Figure S80. (+)-HRESIMS spectrum of fortunilide I (9)

Elemental Composition Report

Page 1

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron lons 32 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

SIMM-Mass Spec	Q-Tof Ultima	23-Oct-201314:53:44		
CFS-30B 130938-2 146 (2.747) AM (Cen,5, 80.00, Ht,90	00.0,656.16,0.70); Sm (Mn, 2x0.00); Cm (133:147)	TOF MS ES+		
100- 805.2659		1.18 e 3		

%-

					806.26	79	807.313				
80	05.40 8	05.60	805.80	806.00	806.20	806.40	806.60	806.80	807.00		11112
Minimum: Maximum:	50.00 100.00			200.0	10.0	-1.5 50.0					
Mass	RA	Calc.	Mass	mDa	PPM	DBE	Score	Formu	la		
805,2659	100.00	805.20	684	-2.5	-3.0	17.5	1	C40	H46 016	Na	



Figure S81. IR spectrum of fortunilide I (9)



Figure S82. ¹H NMR spectrum of fortunilide J (10) in CD₃OD

Figure S83. ¹³C NMR spectrum of fortunilide J (10) in CD₃OD











Figure S87. (+)-ESIMS spectrum of fortunilide J (10)



Figure S88. (-)-ESIMS spectrum of fortunilide J (10)



89

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Figure S89. (-)-HRESIMS spectrum of fortunilide J (10)

Elemental Composition Report

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron lons 135 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass) Elements Used: C: 5-80 H: 2-120 O: 0-20 CFS-24C LCT PXE KE324

27-Sep-2013 10:42:02 1: TOF MS ES-1.92e+004 CFS-24C_0927 31 (0.687) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (19:35) 635.2475 100 -% 636.2513 637.2534 698.2390761.2459 117.2998 205.5604 309.3707 551.2212 597.2202 929.2774 964.8428 900 1000 366.9742 0 L 100 200 300 400 500 600 700 800 Marinum: -1.5 50.0 Maximum: 3.0 10.0 Mass Calc. Mass mDa i-FIT (Norm) Formula PPM DBE i-FIT 635.2492 635.2434 635.2475 -1.7 4.1 -2.7 6.5 16.5 25.5 56.3 63.5 0.0 7.3 C35 H39 O11 C42 H35 O6

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Figure S90. IR spectrum of fortunilide J (10)



Figure S91. ¹H NMR spectrum of fortunilide K (11) in CDCl₃

Figure S92. ¹³C NMR spectrum of fortunilide K (11) in CDCl₃







fl (ppm)





fl (ppm)



Figure S95. HMBC spectrum of fortunilid K (11) in CDCl₃

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Figure S97. (+)-ESIMS spectrum of fortunilide K (11)



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Figure S98. (–)-ESIMS spectrum of fortunilide K (11)



Figure S99. (+)-HRESIMS spectrum of fortunilide K (11)

Elemental Composition Report

Page 1

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron lons 130 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass) Elements Used: C: 5-80 H: 2-120 O: 0-20 CFS-250 LCT PXE KE324

CFS-25D_0927 24 (0.528) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (18:32)

27-Sep-2013 10:26:44 1: TOF MS ES-1.28e+004 661.2637 100 662.2689 % 615.2588 693.2565 113.8716 303.4586 3<u>37.1587</u> 455.2269 742.2632 807.2411909.4182941.4576 515.2067 4 0 — 100 300 200 400 500 800 600 700 900 Minimum: -1.5 50.0 3.0 Maximum: 10.0 DBE Mass Calc. Mass mDa PPM i-FIT (Norm) Formula i-FIT 615.2588 615.2594 17.5 26.5 -0.6 5.3 -1.0 8.6 50.6 52.4 0.2 C36 H39 O9 C43 H35 O4 615.2535



Figure S100. IR spectrum of fortunilide K (11)



Figure S101. ¹H NMR spectrum of fortunilide L (12) in CDCl₃










fl (ppm)



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Figure S106. (+)-ESIMS spectrum of fortunilide L (12)



107

Figure S107. (–)-ESIMS spectrum of fortunilide L (12)



108

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Figure S108. (+)-HRESIMS spectrum of fortunilide L (12)

Elemental Composition Report

Page 1

Single Mass Analysis Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3





Figure S109. IR spectrum of fortunilide L (12)