Electronic supplementary information for

# Ricinodols A-G: New Tetracyclic Triterpenoids as 11β-HSD1

## Inhibitors from Ricinodendron heudelotii

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Table S1. Preliminary assay results of tested compounds against human 11 $\beta$ -HSD1 at 10.0  $\mu$ M.

Table S2. Preliminary assay results of tested compounds against mouse 11 $\beta$ -HSD1 at 10.0  $\mu$ M.

**Figure S1.** Induced CD spectrum of the  $Mo_2^{4+}$  complex for **2** in DMSO **Figure S2.** Induced CD spectrum of the  $Mo_2^{4+}$  complex for **5** in DMSO

Figure S3. <sup>1</sup>H NMR spectrum of ricinodol A (1) in CDCl<sub>3</sub> Figure S4. <sup>13</sup>C NMR spectrum of ricinodol A (1) in CDCl<sub>3</sub> Figure S5. HSQC spectrum of ricinodol A (1) in CDCl<sub>3</sub> Figure S6. <sup>1</sup>H–<sup>1</sup>H COSY spectrum of ricinodol A (1) in CDCl<sub>3</sub> Figure S7. HMBC spectrum of ricinodol A (1) in CDCl<sub>3</sub> Figure S8. ROESY spectrum of ricinodol A (1) in CDCl<sub>3</sub> Figure S9. ESI(+)MS spectrum of ricinodol A (1) Figure S10. ESI(-)MS spectrum of ricinodol A (1) Figure S11. HRESI(-)MS spectrum of ricinodol A (1) Figure S12. IR spectrum of ricinodol A (1)

**Figure S13.** <sup>1</sup>H NMR spectrum of ricinodol B (**2**) in CDCl<sub>3</sub> **Figure S14.** <sup>13</sup>C NMR spectrum of ricinodol B (**2**) in CDCl<sub>3</sub>

Figure S15. HSQC spectrum of ricinodol B (2) in CDCl<sub>3</sub>

Figure S16. HMBC spectrum of ricinodol B (2) in CDCl<sub>3</sub>

Figure S17. ROESY spectrum of ricinodol B (2) in CDCl<sub>3</sub>

Figure S18. ESI(+)MS spectrum of ricinodol B (2)

Figure S19. ESI(–)MS spectrum of ricinodol B (2)

Figure S20. HRESI(+)MS spectrum of ricinodol B (2)

Figure S21. IR spectrum of ricinodol B (2)

Figure S22. <sup>1</sup>H NMR spectrum of ricinodol C (3) in CDCl<sub>3</sub>

Figure S23. <sup>13</sup>C NMR spectrum of ricinodol C (3) in CDCl<sub>3</sub>
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Figure S31. IR spectrum of ricinodol C (3)

Figure S32. <sup>1</sup>H NMR spectrum of ricinodol D (4) in CDCl<sub>3</sub> Figure S33. <sup>13</sup>C NMR spectrum of ricinodol D (4) in CDCl<sub>3</sub> Figure S34. HSQC spectrum of ricinodol D (4) in CDCl<sub>3</sub> Figure S35. HMBC spectrum of ricinodol D (4) in CDCl<sub>3</sub> Figure S36. ROESY spectrum of ricinodol C (4) in CDCl<sub>3</sub> Figure S37. ESI(+)MS spectrum of ricinodol D (4) Figure S38. ESI(-)MS spectrum of ricinodol D (4) Figure S39. HRESI(+)MS spectrum of ricinodol D (4) Figure S40. IR spectrum of ricinodol D (4)

Figure S41. <sup>1</sup>H NMR spectrum of ricinodol E (5) in CDCl<sub>3</sub> Figure S42. <sup>13</sup>C NMR spectrum of ricinodol E (5) in CDCl<sub>3</sub> Figure S43. HSQC spectrum of ricinodol E (5) in CDCl<sub>3</sub> Figure S44. HMBC spectrum of ricinodol E (5) in CDCl<sub>3</sub> Figure S45. ROESY spectrum of ricinodol E (5) in CDCl<sub>3</sub> Figure S46. ESI(+)MS spectrum of ricinodol E (5) Figure S47. ESI(-)MS spectrum of ricinodol E (5) Figure S48. HRESI(-)MS spectrum of ricinodol E (5) Figure S49. IR spectrum of ricinodol E (5)

Figure S50. <sup>1</sup>H NMR spectrum of ricinodol F (6) in CDCl<sub>3</sub>

Figure S51. <sup>13</sup>C NMR spectrum of ricinodol F (6) in CDCl<sub>3</sub>

Figure S52. HSQC spectrum of ricinodol F (6) in CDCl<sub>3</sub>

Figure S53. HMBC spectrum of ricinodol F (6) in CDCl<sub>3</sub>

Figure S54. ROESY spectrum of ricinodol F (6) in CDCl<sub>3</sub>

Figure S55. ESI(+)MS spectrum of ricinodol F (6)

**Figure S56.** ESI(–)MS spectrum of ricinodol F (6)

Figure S57. HRESI(–)MS spectrum of ricinodol F (6)

Figure S58. IR spectrum of ricinodol F (6)

**Figure S59.** <sup>1</sup>H NMR spectrum of ricinodol G (**7**) in CDCl<sub>3</sub> **Figure S60.** <sup>13</sup>C NMR spectrum of ricinodol G (**7**) in CDCl<sub>3</sub> **Figure S61.** HSQC spectrum of ricinodol G (**7**) in CDCl<sub>3</sub> **Figure S62.** HMBC spectrum of ricinodol G (**7**) in CDCl<sub>3</sub> Figure S63. ROESY spectrum of ricinodol G (7) in CDCl<sub>3</sub>
Figure S64. ESI(+)MS spectrum of ricinodol G (7)
Figure S65. ESI(-)MS spectrum of ricinodol G (7)
Figure S66. HRESI(-)MS spectrum of ricinodol G (7)
Figure S67. IR spectrum of ricinodol G (7)

μΜ.					
Compds no.	Exp. 1	Exp. 2	Exp. 3	Average	SD
1	63.0%	51.3%	61.6%	58.6%	6.4%
2	21.0%	17.4%	15.8%	18.1%	2.6%
3	64.3%	58.5%	59.8%	60.8%	3.0%
4	62.2%	58.5%	54.3%	58.4%	4.0%
5	98.8%	94.3%	95.4%	96.2%	2.4%
6	56.9%	53.0%	53.4%	54.4%	2.1%
7	55.2%	56.1%	56.5%	56.0%	0.6%
8	28.5%	28.8%	37.0%	31.4%	4.8%
9	12.1%	14.6%	19.6%	15.4%	3.8%
10	35.6%	27.8%	34.6%	32.7%	4.2%
Glycyrrhetinic acid 1 nM	27.6%	21.0%	19.1%	22.6%	4.4%
Glycyrrhetinic acid 10 nM	61.1%	67.6%	69.7%	66.1%	4.5%
Glycyrrhetinic acid 100 nM	95.8%	98.1%	94.7%	96.2%	1.8%

Table S1. Preliminary assay results of tested compounds against human 11β-HSD1 at 10.0

μΜ.					
Compds no.	Exp. 1	Exp. 2	Exp. 3	Average	SD
1	39.3%	40.2%	35.6%	38.4%	2.5%
2	41.6%	40.8%	33.4%	38.6%	4.5%
3	44.9%	47.9%	40.2%	44.3%	3.9%
4	35.8%	39.0%	32.1%	35.6%	3.5%
5	95.6%	96.4%	91.5%	94.5%	2.6%
6	74.2%	78.5%	73.9%	75.5%	2.6%
7	67.8%	64.1%	59.9%	63.9%	3.9%
8	28.2%	25.9%	25.6%	26.6%	1.4%
9	38.7%	44.0%	36.7%	39.8%	3.8%
10	38.8%	42.0%	35.9%	38.9%	3.1%
Glycyrrhetinic acid 1 nM	21.8%	17.4%	15.3%	18.2%	3.3%
Glycyrrhetinic acid 10 nM	55.9%	52.7%	51.5%	53.4%	2.3%
Glycyrrhetinic acid 100 nM	93.3%	95.5%	95.9%	94.9%	1.4%

Table S2. Preliminary assay results of tested compounds against mouse  $11\beta$ -HSD1 at 10.0



**Figure S1.** Induced CD spectrum of the  $Mo_2^{4+}$  complex for **2** in DMSO



**Figure S2.** Induced CD spectrum of the  $Mo_2^{4+}$  complex for **5** in DMSO



Figure S3. <sup>1</sup>H NMR spectrum of ricinodol A (1) in CDCl<sub>3</sub>



Figure S4. <sup>13</sup>C NMR spectrum of ricinodol A (1) in CDCl<sub>3</sub>



Figure S5. HSQC spectrum of ricinodol A (1) in CDCl<sub>3</sub>



**Figure S6.** <sup>1</sup>H–<sup>1</sup>H COSY spectrum of ricinodol A (1) in CDCl<sub>3</sub>



Figure S7. HMBC spectrum of ricinodol A (1) in CDCl<sub>3</sub>





## Figure S9. ESI(+)MS spectrum of ricinodol A (1)



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## Figure S10. ESI(–)MS spectrum of ricinodol A (1)



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## Figure S11. HRESI(-)MS spectrum of ricinodol A (1)

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 121 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass) Elements Used: C: 10-60 H: 1-110 O: 0-30 YJH LCT PXE KE324

01-Jun-2012 14:26:51 1: TOF MS ES-2:25e+004 RHA3-5212 20 (0.422) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (14:48) 519.3677 100-983.7170 % 509.3400 520.3720 537.3618 295.2272 341.2309 369.2248 187.0965 573.3312 739.5198 769.5985 799.5562 937.6590 ,∔L| m/z 1000 200 300 400 500 600 700 800 900 Minimum: -1.5 50.0 Maximum: 3.0 3.0 Mass Calc. Mass mDa PPM DBE i-FIT i-FIT (Norm) Formula 519.3677 519.3686 -0.9 -1.7 6.5 102.3 0.0 C31 H51 O6



Figure S12. IR spectrum of ricinodol A (1)



Figure S13. <sup>1</sup>H NMR spectrum of ricinodol B (2) in CDCl<sub>3</sub>



Figure S14. <sup>13</sup>C NMR spectrum of ricinodol B (2) in CDCl<sub>3</sub>



Figure S15. HSQC spectrum of ricinodol B (2) in CDCl<sub>3</sub>



Figure S16. HMBC spectrum of ricinodol B (2) in CDCl<sub>3</sub>



## Figure S18. ESI(+)MS spectrum of ricinodol B (2)





## Figure S19. ESI(-)MS spectrum of ricinodol B (2)



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# Figure S20. HRESI(+)MS spectrum of ricinodol B (2)

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			4	95.3439						967.	3.25+00 7043 968.7081
			41	95.3439	91				064	967.	3.25e+00 7043 968.7081 969.7128
105.042	<sup>25</sup> 192.0821	317,8959 <sup>41</sup>	49 1.2686 490.38	95.3439 496.344 79	91  _547.4539 <sup>6</sup>	<b>64</b> .3705	721.0234	885.6288	965	967. 5.1921	3.258+00 7043 968.708 969.7125 970.7165
105.042	25 192.0821 200	317.8959 <sup>41°</sup> 300	490.38 490.38	95.3439 496.344 79	91 547.4539 6 600	<b>64.3705</b>	721.0234	885.6288	965 3	967. 5.1921	3.25e+00 7043 968.7081 969.7125 970.7165
105.042	25 192.0821 200	317.6959 <sup>41</sup> 300	4) 1.2686 490.38 400	95.3439 496.344 79 500	91 547.4539 6 600	<b>54.3705</b>	721.0234	885.6288	965 3 900	967. 5.1921	3.25e+00 7043 968.7081 969.7125 970.7168 1000
105.042 1000	25 192.0621 200	317,8959 <sup>411</sup> 300	41 1.2686 490.38 400	95.3439 496.34 79 500 -1.5	91 547.4539 6 600	64.3705	721.0234	885.6288	965	967. 5.1921	3.25e+00 7043 968.7081 969.7125 970.7165 970.7165
105.042 100 1mum : imum :	25 192.0821 200	<b>317.6959<sup>41</sup></b> <b>300</b> 3.0	490.38 1.2686 490.38 400 3.0	95.3439 496.34 79 500 -1.5 50.0	91 547.4539 6 600	64.3705 700	721.0234 	885.6288	965	967. 5.1921	3.25e+00 7043 968.7081 969.7125 970.7165 
105.042 1000 imum: imum:	25 192.0621 200 Calc. Mas	317,6959 <sup>41</sup> 300 3.0 :5 mDa	41 1.2686 490.38 400 3.0 PPM	496.3439 496.344 79 500 -1.5 50.0 DBE	91 547.4539 6 600 i-FIT	64.3705 7 700 i−i	721.0234 800 FIT (Norm)	885.6288	965 3 900	967. 5.1921	3.25e+00 7043 968.7081 969.7125 970.7165 970.7166 1000



Figure S21. IR spectrum of ricinodol B (2)



Figure S22. <sup>1</sup>H NMR spectrum of ricinodol C (3) in CDCl<sub>3</sub>



Figure S23. <sup>13</sup>C NMR spectrum of ricinodol C (3) in CDCl<sub>3</sub>



Figure S24. HSQC spectrum of ricinodol C (3) in CDCl<sub>3</sub>



**Figure S25.** <sup>1</sup>H–<sup>1</sup>H COSY spectrum of ricinodol C (**3**) in CDCl<sub>3</sub>



Figure S26. HMBC spectrum of ricinodol C (3) in CDCl<sub>3</sub>



Figure S27. ROESY spectrum of ricinodol C (3) in CDCl<sub>3</sub>

## Figure S28. ESI(+)MS spectrum of ricinodol C (3)



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## Figure S29. ESI(-)MS spectrum of ricinodol C (3)



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## Figure S30. HRESI(-)MS spectrum of ricinodol C (3)

## **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 121 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass) Elements Used: C: 10-60 H: 1-110 O: 0-30 YJH LCT PXE KE324

YJH				LCT PXE	KE324				18-May-2012
RHA3-61 16	(0.351) AM2 (Ar,10	000.0,0.00,1.00	); ABS; Cm (	5:30)					14:18:18 1: TOF MS ES- 8 17e+004
100 %			50	519.3673 9.3386 55	8.3577				983.7148
107.99	18 265.14	79 347.1974	462.2	2979	605.312	21 739.5170	787.6093	813.5702 936	3.6733
100	200	300	400	500	600	700	800	900	1000
Minimum: Maximum:		3.0	3.0	-1.5 50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Formula	
519.3673	519.3686	-1.3	-2.5	6.5	123.9	0.0		СЗ1 Н51	06

Figure S31. IR spectrum of ricinodol C (3)




Figure S32. <sup>1</sup>H NMR spectrum of ricinodol D (4) in CDCl<sub>3</sub>



Figure S33. <sup>13</sup>C NMR spectrum of ricinodol D (4) in CDCl<sub>3</sub>



Figure S34. HSQC spectrum of ricinodol D (4) in CDCl<sub>3</sub>



Figure S35. HMBC spectrum of ricinodol D (4) in CDCl<sub>3</sub>



### Figure S37. ESI(+)MS spectrum of ricinodol D (4)



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### Figure S38. ESI(-)MS spectrum of ricinodol D (4)



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### Figure S39. HRESI(+)MS spectrum of ricinodol D (4)

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 Ions 191 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 RHA3-62 LCT PXE KE324 LCT PXE KE324

					LCT	PXE KE324						03-Sen-2012
RHA3-	-62_0903 27 (0	).582) AM2	? (Ar,10000.0	,0.00,1.00); AB	S; Cm (26:	38)					1: <sup>-</sup> 94	15:56:34 FOF MS ES+ 1.97e+004 37.7023
%-					495.3440	I						<b>968.705</b> 1
0	118.4756 118.9673	2	0.1758	455.3 437.3426	536	53704 537.3734	611.4272	731.5151	787.2943  788.2	2972	965.68	969.7096 1 970.7137
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Minim Maxim	um: um;		3.0	4.0	-1. 50.	5 0						1000
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495.34	440 495.	3450	-1.0	-2.0	6.5	60.	. 8	0.0	(	C30	H48 04	Na

Figure S40. IR spectrum of ricinodol D (4)





Figure S41. <sup>1</sup>H NMR spectrum of ricinodol E (5) in CDCl<sub>3</sub>



Figure S42. <sup>13</sup>C NMR spectrum of ricinodol E (5) in CDCl<sub>3</sub>



Figure S43. HSQC spectrum of ricinodol E (5) in CDCl<sub>3</sub>



Figure S44. HMBC spectrum of ricinodol E (5) in CDCl<sub>3</sub>



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Figure S45. ROESY spectrum of ricinodol E (5) in CDCl<sub>3</sub>

### Figure S46. ESI(+)MS spectrum of ricinodol E (5)



# Figure S47. ESI(–)MS spectrum of ricinodol E (5)

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Analysis Info Analysis Name Method Sample Name Comment	014-2601.D Copy of DSOP! yjm-RHA2-3114 W	WS2N.M 1-2		Acquisition Dat Operator Instrument	e 04/26/ Admin esquin	12 22:48 istrator s3000plu	16 Ja
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### Figure S48. HRESI(-)MS spectrum of ricinodol E (5)

**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 179 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 RHA3-3114-2 LCT PXE KE324

RHA3-3114-2					LCT PX	E KE324		27-Aug-201				
RHA3-3114-2_0827 42 (0.934) AM2 (Ar,10000.0,0.00,1.00); ABS; Cm (42:56) 1: TO									1: TOF	09:41:12 MS ES-		
100					471.3	9471			2.:	27e+004		
%						472.3507		485.3	260			
	457.3072 461.016		465.1799		469.3308	473.3541 477	.1670 479.2555 48	479.2555 483.3086				
45	55.0	460.0	465.	0	470.0	475.0	480.0	485.	0 0	· m/z		
Minimum: Maximum:	:		5.0	3.0	-1.5 50.0							
Mass	Calc. N	lass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formul	a			
471.3471	471.343	4	-0.3	-0.6	7.5	161.7	0.0	сзо н	147 04			



Figure S49. IR spectrum of ricinodol E (5)



## Figure S50. <sup>1</sup>H NMR spectrum of ricinodol F (6) in CDCl<sub>3</sub>



Figure S51. <sup>13</sup>C NMR spectrum of ricinodol F (6) in CDCl<sub>3</sub>



Figure S52. HSQC spectrum of ricinodol F (6) in CDCl<sub>3</sub>



Figure S53. HMBC spectrum of ricinodol F (6) in CDCl<sub>3</sub>





### Figure S55. ESI(+)MS spectrum of ricinodol F (6)



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### Figure S56. ESI(-)MS spectrum of ricinodol F (6)



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#### Figure S57. HRESI(-)MS spectrum of ricinodol 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 121 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass) Elements Used: C: 10-80 H: 1-110 O: 0-30 04-May-2012 18:19:21 1: TOF MS ES-3.70e+004 963.7169 yjh LCT PXE KE324 RHA2-3112-3 17 (0.335) AM2 (Ar, 10000.0,0.00,1.00); ABS; Cm (4:21) 100-% 519.3685 509.3397 536.3598 981.7021 445.2827<sup>507.3245</sup> 537.3609 600.3743 739.5179 265.1489 145.9368 325.1814 799.5566 873.6517 979.7134 0 J m/z 700 750 800 550 600 100 150 200 250 300 350 400 450 500 650 850 900 950 Minimum: Maximum: -1.5 5.0 3.0 50.0 Mass Calc. Mass DBE mDa PPM i-FIT i-FIT (Norm) Formula 519.3685 519.3686 -0.1 114.6 -0.2 6.5 0.0 C31 H51 O6







Figure S59. <sup>1</sup>H NMR spectrum of ricinodol G (7) in CDCl<sub>3</sub>



Figure S60. <sup>13</sup>C NMR spectrum of ricinodol G (7) in CDCl<sub>3</sub>



Figure S61. HSQC spectrum of ricinodol G (7) in CDCl<sub>3</sub>



Figure S62. HMBC spectrum of ricinodol G (7) in CDCl<sub>3</sub>



### Figure S64. ESI(+)MS spectrum of ricinodol G (7)



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### Figure S65. ESI(-)MS spectrum of ricinodol G (7)



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### Figure S66. HRESI(-)MS spectrum of ricinodol G (7)

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 121 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass) Elements Used: C: 10-80 H: 1-110 O: 0-30 yih LCT PXE KE324

LCT PXE KE324 04-May-2012 16:24:53 1: TOF MS ES-4.20a+004 983.7165 RHA2-3112-4 36 (0.759) AM2 (Ar, 10000.0,0.00, 1.00); ABS; Cm (23:42) 100 % 519.3675 536.3580 509.3391 537.3618 381.2194 507.3226 571.3291 645.4368 716.5317 739.5122 981.7002 799.5560815.5739 907.7100 ĻĻ<sub>im/z</sub> 1000 400 500 450 550 600 650 700 750 800 850 900 950 Minimum: Maximum: -1.5 50.0 5.0 3.0 Mass Calc. Mass mDa PPM D8E i-FIT i-FIT (Norm) Formula 519.3675 519.3686 -1.1 -2.1 6.5 106.5 0.0 C31 H51 O6

Figure S67. IR spectrum of ricinodol G (7)

