Supplementary Materials: New Phragmalin-Type Limonoids from *Chukrasia tabularis* and Their α -Glucosidase Inhibitory Activity

Jun-Lin Peng, Jun Wang, Fan-Dong Kong, Zi-Qi Liu, Pei Wang, Bei Jiang, Cui-Juan Gai, Wen-Li Mei and Hao-Fu Dai

Contents

- Figure S1. ¹H-NMR (500 MHz) spectrum of the new compound 1 in CDCl₃.
- Figure S2. ¹³C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 1 in CDCl₃.
- Figure S3. HSQC spectrum of the new compound 1 in CDCl₃.
- Figure S4. 1H-1H COSY spectrum of the new compound 1 in CDCl3.
- Figure S5. HMBC spectrum of the new compound 1 in CDCl₃.
- Figure S6. ROESY spectrum of the new compound 1 in CDCl₃.
- Figure S7. Partial enlarged ROESY spectra of compound 1 in CDCl3.
- Figure S8. 1H -NMR (500 MHz) spectrum of the new compound 2 in CDCl3.
- Figure S9. ¹³C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 2 in CDCl₃.
- Figure S10. HSQC spectrum of the new compound 2 in CDCl₃.
- Figure S11. ¹H-¹H COSY spectrum of the new compound 2 in CDCl₃.
- Figure S12. HMBC spectrum of the new compound 2 in CDCl₃.
- Figure S13. ROESY spectrum of the new compound 2 in CDCl₃.
- Figure S14. Partial enlarged ROESY spectra of compound 2 in CDCl₃.
- Figure S15. 1H-NMR (500 MHz) spectrum of the new compound 3 in CDCl3.
- Figure S16. ¹³C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 3 in CDCl₃.
- Figure S17. HSQC spectrum of the new compound 3 in CDCl₃.
- Figure S18. ¹H-¹H COSY spectrum of the new compound 3 in CDCl₃.
- Figure S18. HMBC spectrum of the new compound 3 in CDCl₃.
- Figure S20. ROESY spectrum of the new compound 3 in CDCl3.
- Figure S21. Partial enlarged ROESY spectra of compound 3 in CDCl₃.
- Figure S22. 1H-NMR (500 MHz) spectrum of the new compound 4 in CDCl3.
- Figure S23. 13C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 4 in CDCl3.
- Figure S24. HSQC spectrum of the new compound 4 in CDCl₃.
- Figure S25. 1H-1H COSY spectrum of the new compound 4 in CDCl₃.
- Figure S26. HMBC spectrum of the new compound 4 in CDCl₃.
- Figure S27. ROESY spectrum of the new compound 4 in CDCl₃.
- Figure S28. Partial enlarged ROESY spectra of compound 4 in CDCl₃.

Figure S29. ¹H-NMR (500 MHz) spectrum of the new compound 5 in CDCl₃.

Figure S30. ¹³C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 5 in CDCl₃.

Figure S31. HSQC spectrum of the new compound 5 in CDCl₃.

Figure S32. ¹H-¹H COSY spectrum of the new compound 5 in CDCl₃.

Figure S33. HMBC spectrum of the new compound 5 in CDCl₃.

Figure S34. ROESY spectrum of the new compound 5 in CDCl₃.

Figure S35. Partial enlarged ROESY spectra of compound 5 in CDCl₃.

Figure S36. HR-ESI-MS spectrum of the new compound 1.

Figure S37. HR-ESI-MS spectrum of the new compound 2.

Figure S38. HR-ESI-MS spectrum of the new compound 3.

Figure S39. HR-ESI-MS spectrum of the new compound 4.

Figure S40. HR-ESI-MS spectrum of the new compound 5.

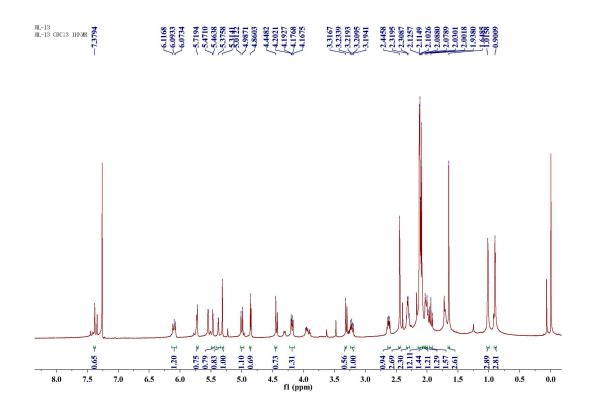


Figure S1. ¹H-NMR (500 MHz) spectrum of the new compound 1 in CDCl₃.

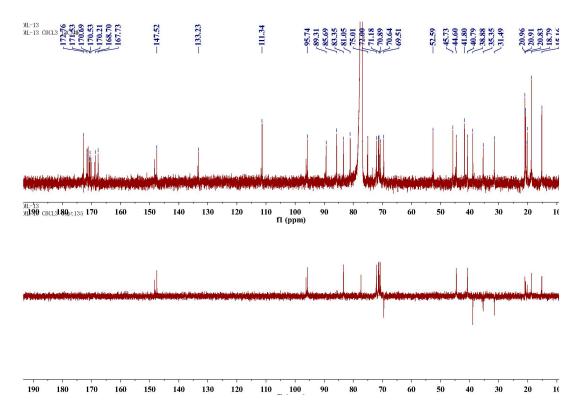
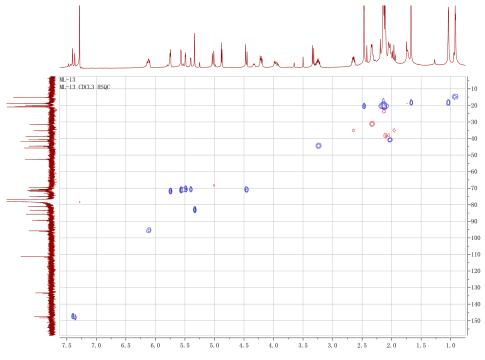
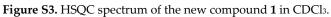


Figure S2. ¹³C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 1 in CDCl₃.





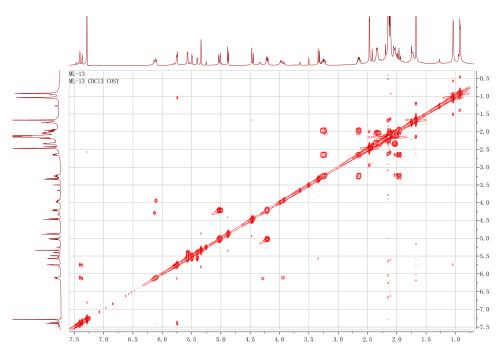
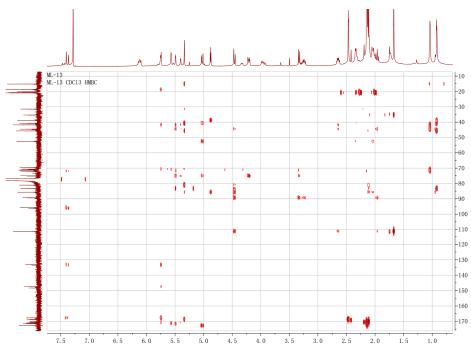
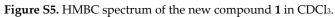
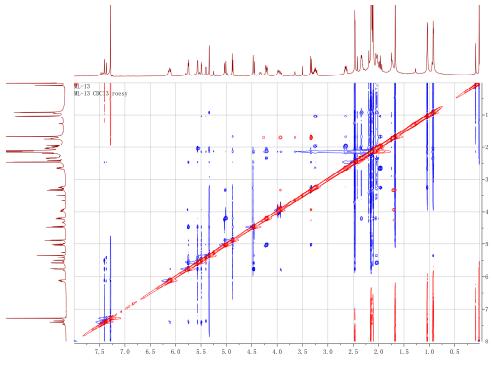


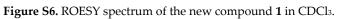
Figure S4. ¹H-¹H COSY spectrum of the new compound 1 in CDCl₃.











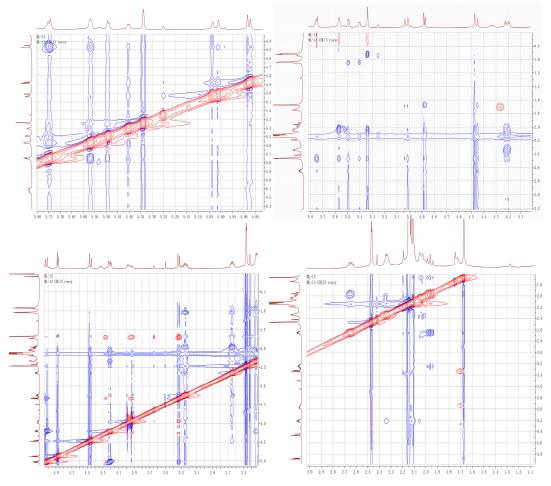


Figure S7. Cont.

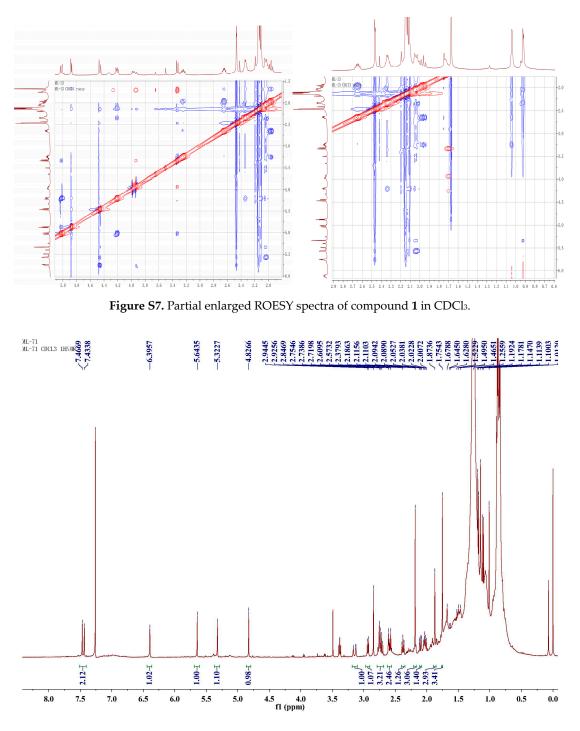


Figure S8. 1H-NMR (500 MHz) spectrum of the new compound 2 in CDCl3.

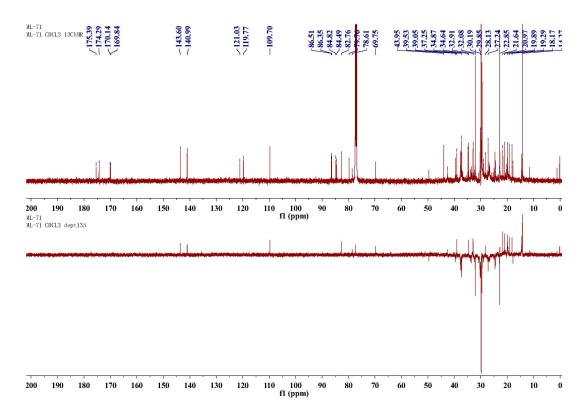
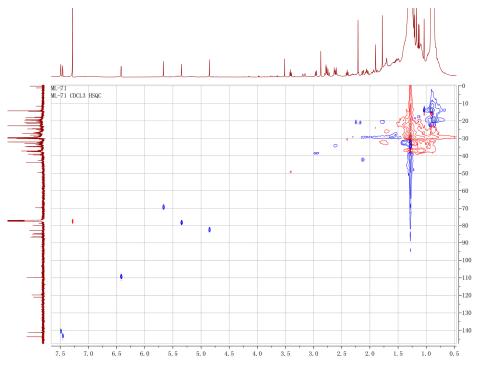
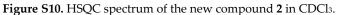


Figure S9. ¹³C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 2 in CDCl₃.





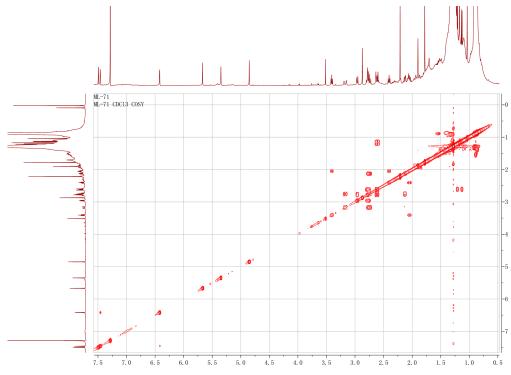
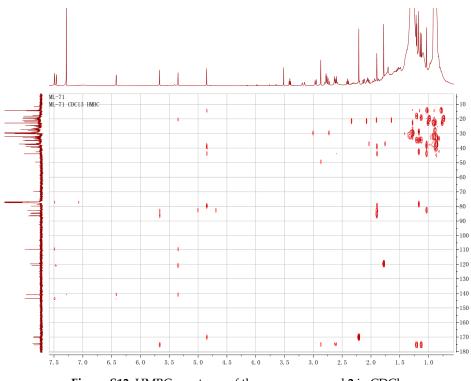
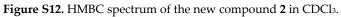


Figure S11. ¹H-¹H COSY spectrum of the new compound 2 in CDCl₃.





```
S9 of S26
```

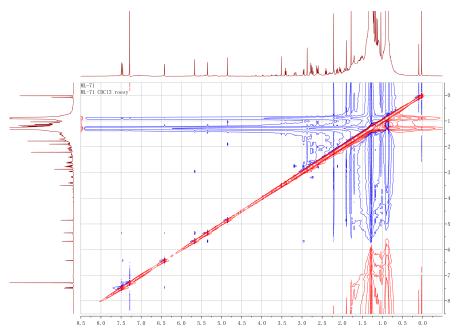


Figure S13. ROESY spectrum of the new compound 2 in CDCl₃.

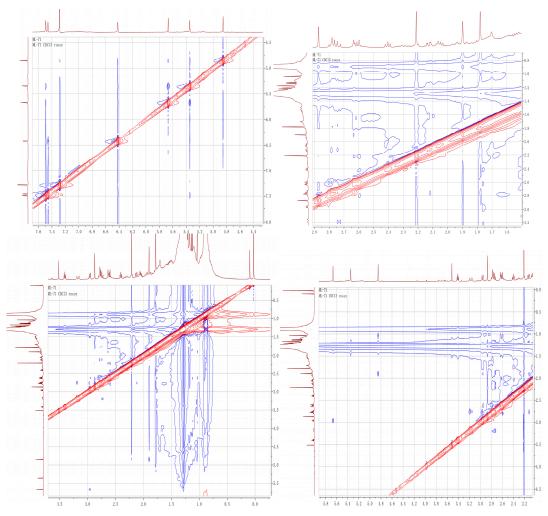


Figure S14. Partial enlarged ROESY spectra of compound 2 in CDCl₃.

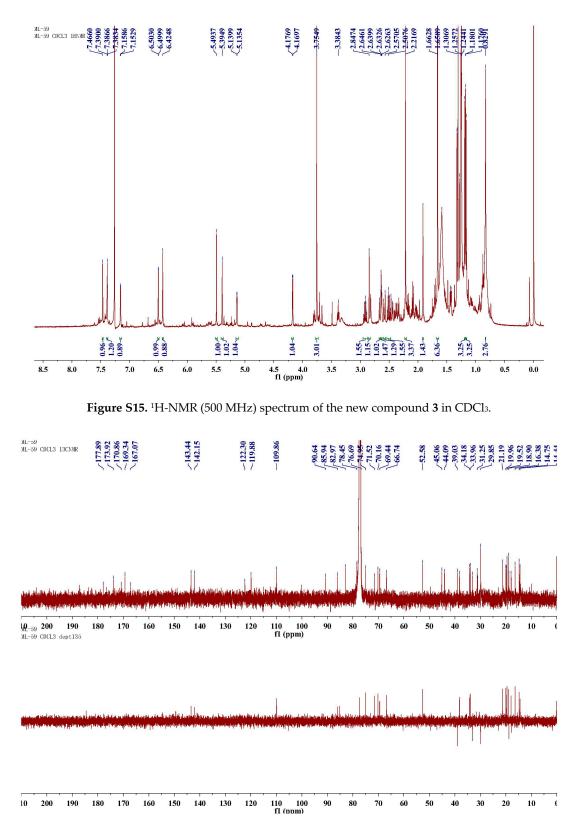


Figure S16. ¹³C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 3 in CDCl₃.

S11 of S26

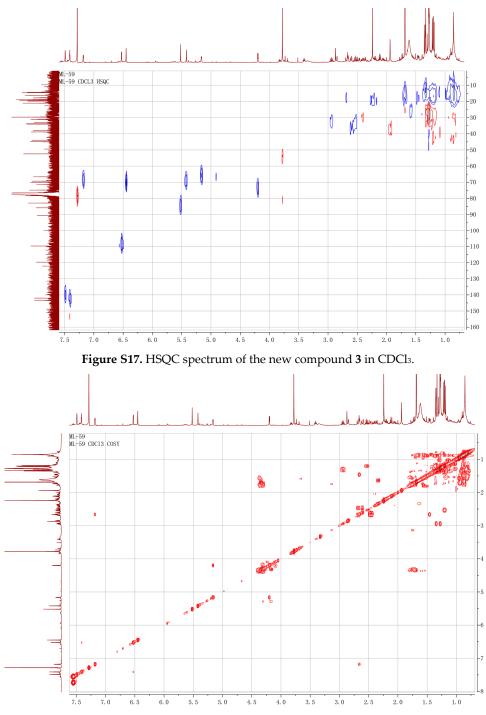


Figure S18. ¹H-¹H COSY spectrum of the new compound 3 in CDCl₃.

S12 of S26

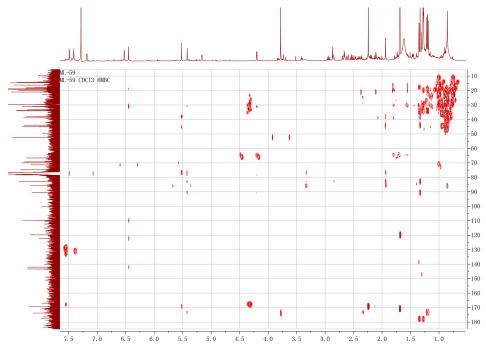
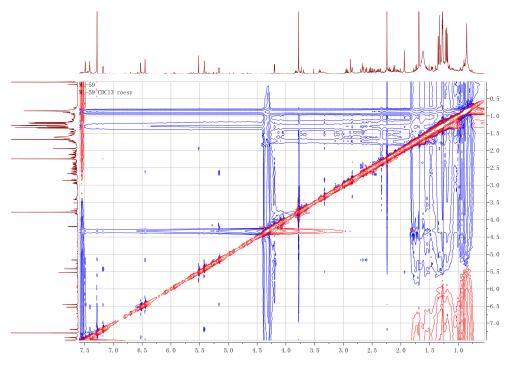
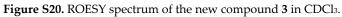


Figure S19. HMBC spectrum of the new compound 3 in CDCl₃.





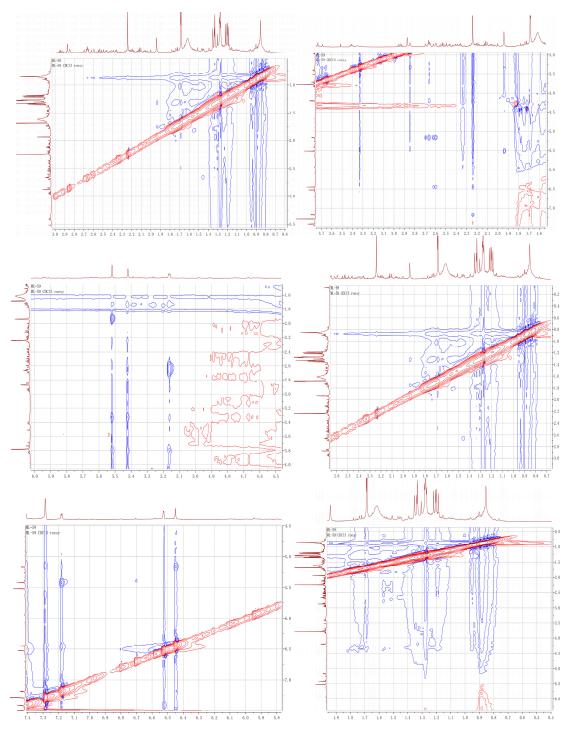


Figure S21. Partial enlarged ROESY spectra of compound 3 in CDCl₃.

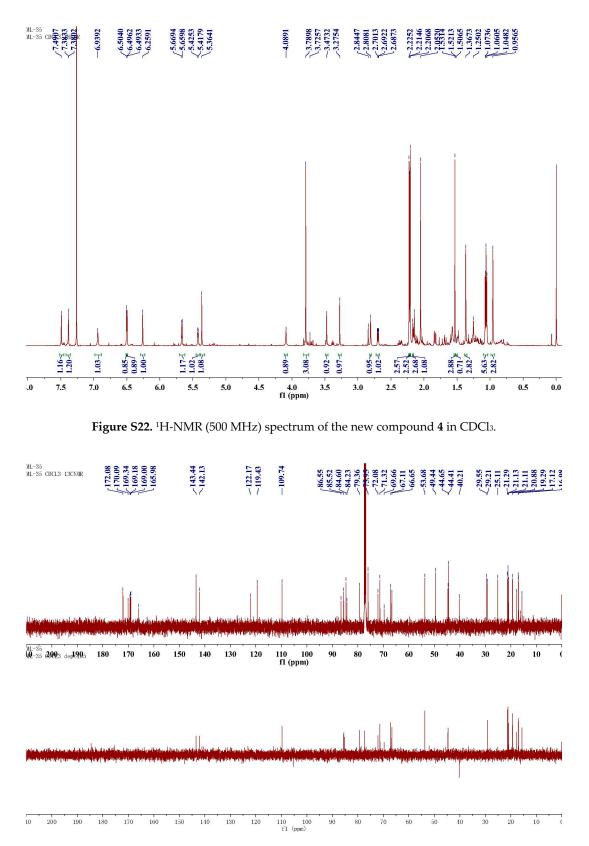


Figure S23. ¹³C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 4 in CDCl₃.

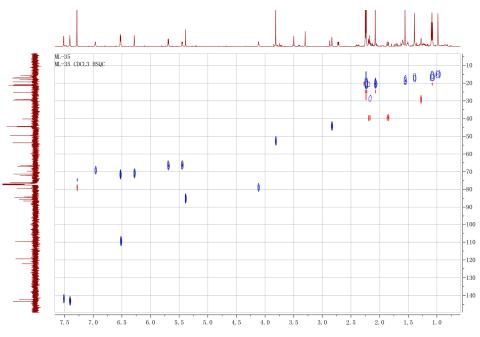


Figure S24. HSQC spectrum of the new compound 4 in CDCl₃.

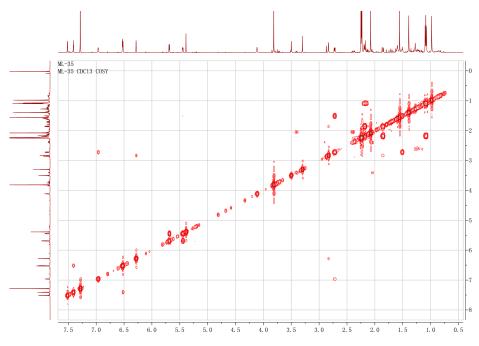
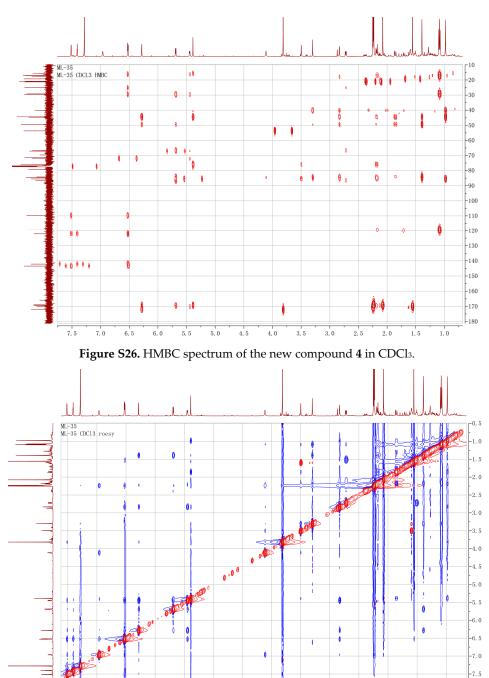
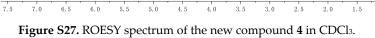


Figure S25. 1H-1H COSY spectrum of the new compound 4 in CDCl3.





1.0

7.0

6.5

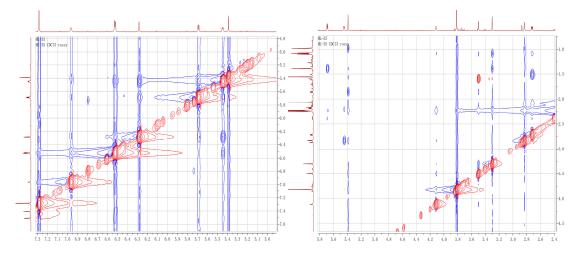


Figure S28. Partial enlarged ROESY spectra of compound 4 in CDCl3.

7.1.5 Ref 7.1.5 Ref 7.1.5 Ref 7.1.5 Ref 7.1.5 Ref 6.9843 6.9843 6.9843 6.9843 6.9843 6.9843 6.9843 6.9843 6.9843 6.9843 6.9843 6.9843 6.9843 6.5154 6.51542 7.51052

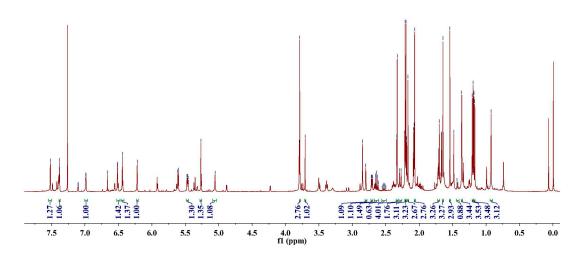


Figure S29. ¹H-NMR (500 MHz) spectrum of the new compound 5 in CDCl₃.

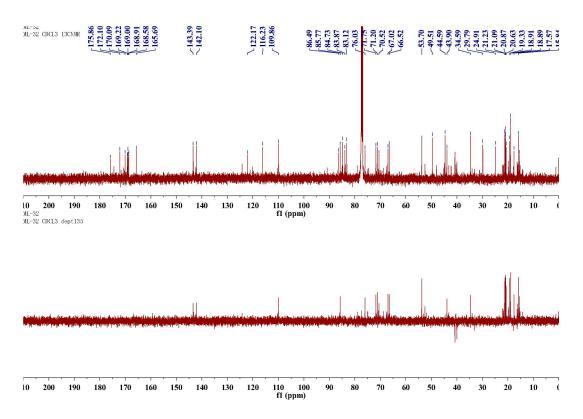
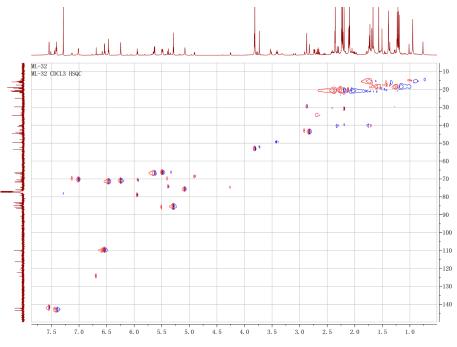
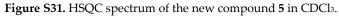


Figure S30. ¹³C-NMR (125 MHz) and DEPT NMR spectrum of the new compound 5 in CDCl₃.





S19 of S26

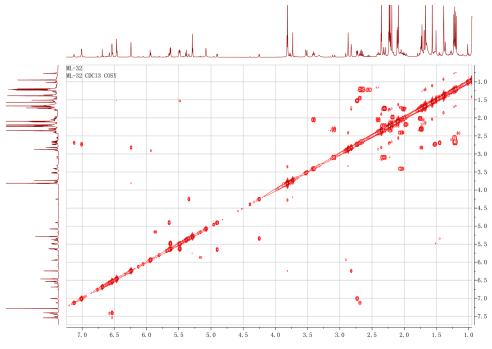


Figure S32. ¹H-¹H COSY spectrum of the new compound 5 in CDCl₃.

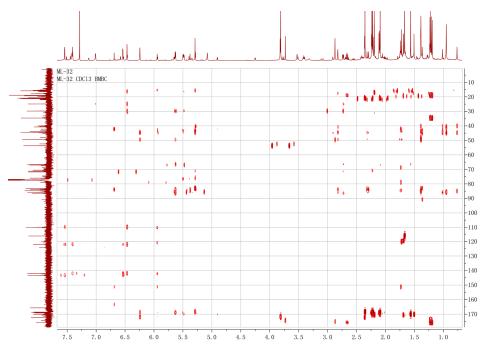


Figure S33. HMBC spectrum of the new compound 5 in CDCl₃.

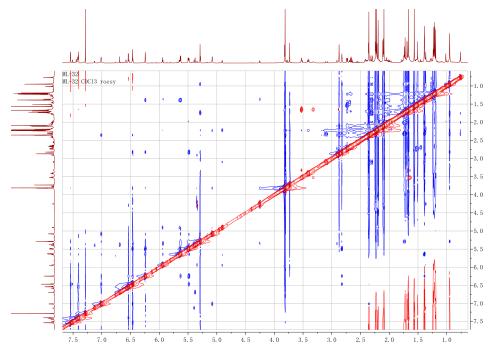


Figure S34. ROESY spectrum of the new compound 5 in CDCl₃.

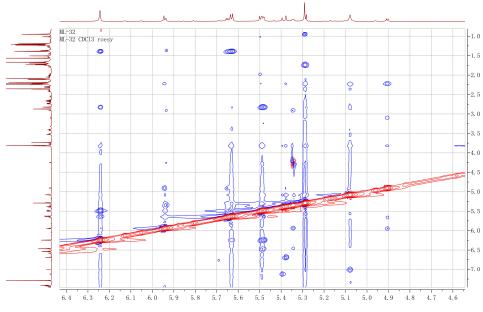


Figure S35. Cont.

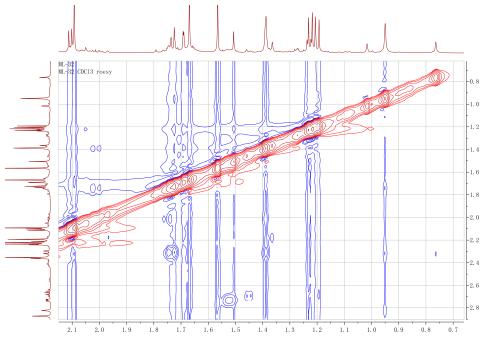


Figure S35. Partial enlarged ROESY spectra of compound 5 in CDCl₃.

Sample Group Info. Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2) User Spectra Fragmentor Voltage Collision Energy 0 Ionization Mode ESI x10 4 + Scan (0.213-0.229 min, 2 Scans) ML-13.d. Subtract (64)	
Fragmentor Voltage Collision Energy Ionization Mode 135 0 ESI	
135 0 ESI	
2- 810.2817 1.8- (M+NH4)+ 1.6- 1.4- 1.2-	
1- 0.8- 0.6- 0.4-	
0.2- 0 809.4 809.6 809.8 810 810.2 810.4 810.6 810.8 811 Counts vs. Mass-to-Charge (m/z) Peak List	811.2
m/z z Abund Formula Ion	
318.3011 16140.07	
453.1673 1 19408.77	
460.2691 1 21296.88	
810.2817 1 18257.66 C37 H44 O19 (M+NH4)+	
815.2368 1 38883.53	
816.2404 1 16098.89	
816.2404 1 16098.89 831.2107 1 15305.69	
816.2404 1 16098.89 831.2107 1 15305.69 861.3651 1 22889.48	
816.2404 1 16098.89 831.2107 1 15305.69	
816.2404 1 16098.89 831.2107 1 15305.69 861.3651 1 22889.48 Formula Calculator Element Limits	
816.2404 1 16098.89 831.2107 1 15305.69 861.3651 1 122889.48 Formula Calculator Element Limits Element Min	
816.2404 1 16098.89 831.2107 1 15305.69 861.3651 1 22889.48 Formula Calculator Element Limits Element Min Max C 3 H 0 0 30	
816.2404 1 16098.89 831.2107 1 15305.69 861.3651 1 122889.48 Formula Calculator Element Limits Element Min C 3 60 120 0 120 0 0 Formula Calculator Results	
816.2404 1 16098.89 831.2107 1 15305.69 861.3651 1 122889.48 Formula Calculator Element Limits Element Min C 3 60 120 0 120 0 0 Formula Calculator Results	Diff. (ppm) DBE -0.1 10

Agilent Technologies

Page 1 of 1

Printed at: 3:43 PM on: 7/30/2015

Figure S36. HR-ESI-MS spectrum of the new compound 1.

Sample Gro Acquisition Version User Spec	-		ries TOF/65								
Liser Sner			3.05.01 (B51	00 series	Info.						
user oper	ctra										
	ntor Volta	ige	Collision E	nergy	Ionizatio ESI						
		min) MI -71	d Subtract (4	.0)		-					
1.6		······) ME 71.		••)	643.2383						
1.4					(M+H)+						
1.2-											
1-											
0.8											
0.6											
0.4											
0.2											
0	642.4	642.6	642.8	643	643.2	643.4 643.6	643.8	644	,		
				Counts v	vs. Mass-to-Cha	arge (m/z)					
Peak List	ZA	bund	Formula		Ior	1					
318.3001		7773.34									
415.2115		5415.18									
432.238	1	5571.8									
437.1935	1 2	0423.27									
437.1935 453.1673		0423.27 4216.02									
	1 5										
453.1673 454.1704 460.2691	1 5 1 1 1 2	4216.02 3927.89 3567.01									
453.1673 454.1704 460.2691 643.2383	1 5 1 1 1 2 1 1	4216.02 3927.89 3567.01 4764.36	C33 H38	013	(M-	+H)+					
453.1673 454.1704 460.2691 643.2383 Formula Ca	1 5 1 1 1 2 1 1 Iculator	4216.02 3927.89 3567.01 4764.36 Element L		013	(M+	+H)+					
453.1673 454.1704 460.2691 643.2383	1 5 1 1 1 2 1 1	4216.02 3927.89 3567.01 4764.36		D13	(M+	+H)+					
453.1673 454.1704 460.2691 643.2383 Formula Cal Element	1 5 1 1 1 2 1 1 Iculator	4216.02 3927.89 3567.01 4764.36 Element L Max		013	(M-	+H)+					
453.1673 454.1704 460.2691 643.2383 Formula Cal Element C H O	1 5 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	4216.02 3927.89 3567.01 4764.36 Element L Max 3 60 0 120 0 30		013	(M+	+H)+					
453.1673 454.1704 460.2691 643.2383 Formula Cal Element C H O Formula Cal	1 5 1 1 1 2 1 1 Iculator	4216.02 3927.89 3567.01 4764.36 Element L 3 60 0 120 0 30 Results	imits								
453.1673 454.1704 460.2691 643.2383 Formula Cal Element C H O	1 5 1 1 1 2 1 1 Iculator	4216.02 3927.89 3567.01 4764.36 Element L Max 3 60 0 120 0 30	imits	D13		H)+	Diff. (mDa)		Diff. (ppm)	DI	3E

Agilent Technologies

Page 1 of 1

Printed at: 3:33 PM on: 8/27/2015

Figure S37. HR-ESI-MS spectrum of the new compound 2.

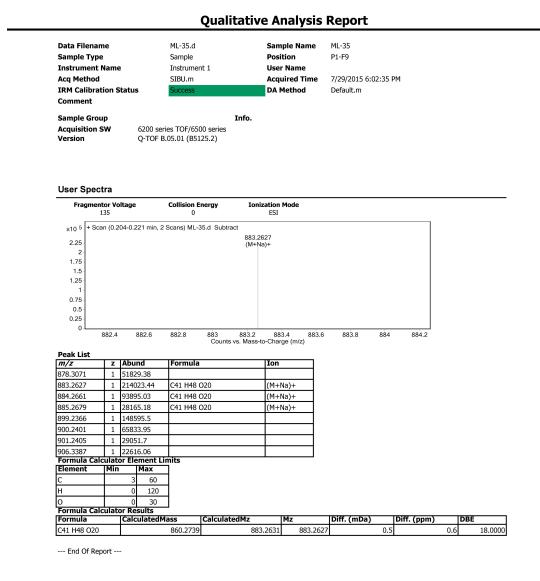
274.2734 1 24594.75 Image: constraint of the second seco	Acq Meti IRM Cali Commen	bratio		us	Sample Instrument 1 SIBU.m Success	Use Acc	sition er Name Juired Time Method	P1-B7 8/27/2015 3:22 Default.m	:12 PM		
Fragmentor Voltage 135 Collision Energy 0 Ionization Mode ESI x10 4 9 8 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 7 6 5 4 3 6 8 68.4 Collision Energy 8 8 69.2 8 69.4 8 69.6 Bob 8 6 8 6 8 69.6 Bob 8 6 8 6 8 6 8 6 8 6 8 6 8 6 8 6 8 6 8	Acquisiti										
135 0 ESI x10 4 87 6 4 37 6 4 32 1 * Scan (0.193 min) ML-59.d Subtract (2) 869.2623 (M+K)+ 869.2623 (M+K)+ 868.4 868.6 868.8 869.2 869.4 869.6 869.8 870 870.2 Peak List 774.2734 1 24594.75 Image: Counts vs. Mass-to-Charge (m/z) Status 849.3333 1 36407.78 Image: Counts vs. Mass-to-Charge (M+K)+ 453.167 1 20425.79 Image: Counts vs. Mass-to-Charge (M+K)+ 849.3333 1 36407.78 Image: Counts vs. Mass-to-Charge (M+K)+ State											
869.2623 (M+K)+ 868.4 868.6 868.8 869.2 869.4 869.6 869.8 870.2 Peak List m/z z Abund Formula Ion 274.2734 1 24594.75	Frag		Voltag	e							
853.2882 1 23147.75 Image: Constraint of the system	9- 8- 7- 6- 5- 4- 3- 2-	+ Scan (0.193 n	nin) ML-59.c	i Subtract (2)						
869.2623 1 80176.62 C41 H50 O18 (M+K)+ 870.2657 1 37090.45 C41 H50 O18 (M+K)+ Formula Calculator Element Limits Element Min Max C 3 60 H 0 120 O 0 30 Formula Calculator Results Formula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE	Peak List <i>m/z</i> 274.2734 318.2999 453.167	t	z Ab 1 24! 1 250 1 204	und 594.75 527.38 125.79	Cou	ints vs. Mass-to-Cha	irge (m/z)	\$ 869.8	870 870).2	
870.2657 1 37090.45 C41 H50 018 (M+K)+ Formula Calculator Element Limits Element Min Max C 3 60 H 0 120 O 0 30 Formula Calculator Results Formula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE	Peak Lisi <i>m/z</i> 274.2734 318.2999 453.167 848.3333	t	z Ab 1 24 1 250 1 20 1 36	und 594.75 527.38 425.79 407.78	Cou	ints vs. Mass-to-Cha	irge (m/z)	\$ 869.8	870 870		
Formula Calculator Element Limits Element Min Max C 3 60 H 0 120 O 0 30 Formula Calculator Results Formula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE	Peak Lisi m/z 274.2734 318.2999 453.167 848.3333 849.3373	t	z Ab 1 249 1 250 1 204 1 364 1 364	und 594.75 527.38 425.79 407.78 535.67	Cou	ints vs. Mass-to-Cha	irge (m/z)	5 869.8	870 870		
Element Min Max C 3 60 H 0 120 O 0 30 Formula Calculator Results Formula CalculatedMass Formula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE	Peak Lisi m/z 274.2734 318.2999 453.167 848.3333 849.3373 853.2882	t	z Ab 1 24! 1 256 1 204 1 364 1 176 1 23:	und 594.75 527.38 425.79 407.78 535.67 447.75	Cou	Ints vs. Mass-to-Cha	I	5 869.8	870 870	1.2	
C 3 60 H 0 120 O 0 30 Formula Calculator Results CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE	Peak List m/z 274.2734 318.2999 453.167 848.3333 849.3373 853.2882 869.2623 870.2657	t	z Ab 1 24! 1 256 1 204 1 364 1 176 1 233 1 803 1 370	und 594.75 527.38 425.79 407.78 535.67 147.75 176.62 090.45	Cou Formula	Ints vs. Mass-to-Cha	rrge (m/z)	5 869.8	870 870		
O 0 30 Formula Calculator Results Formula CalculatedMass (CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE	Peak List m/z 274.2734 318.2999 453.167 848.3333 849.3373 853.2882 869.2623 870.2657	t	z Ab 1 249 1 256 1 204 1 364 1 176 1 233 1 803 1 370 ator E 1	und 594.75 527.38 425.79 407.78 535.67 147.75 176.62 190.45 Iement Li	Cou Formula	Ints vs. Mass-to-Cha	rrge (m/z)	5 869.8	870 870		
Formula Calculator Results Formula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE	Peak Liss m/z 274.2734 318.2999 453.167 848.3333 849.3373 853.2882 869.2623 870.2657 Formula	t	z Ab 1 24! 1 256 1 204 1 264 1 264 1 264 1 364 1 176 1 233 1 803 1 370 ator E Inn	und 594.75 527.38 425.79 407.78 535.67 447.75 76.62 190.45 Iement Li Max	Cou Formula	Ints vs. Mass-to-Cha	rrge (m/z)	5 869.8	870 870		
Formula CalculatedMass CalculatedMz Mz Diff. (mDa) Diff. (ppm) DBE	Peak Liss m/z 274.2734 318.2999 453.167 848.3333 849.3373 853.2882 869.2623 870.2657 Formula Element	t	z Ab 1 24! 1 256 1 204 1 364 1 176 1 23: 1 80: 1 376 ator E	und 594.75 527.38 425.79 407.78 535.67 147.75 5090.45 166.62 190.45 167.62 1090.45 168 1090.45 10	Cou Formula	Ints vs. Mass-to-Cha	rrge (m/z)	5 869.8	870 870		
	Peak Lisi <i>m/z</i> 274.2734 318.2999 453.167 848.3333 849.3373 853.2882 869.2623 870.2657 Formula Element C H O	Calcul	z Ab 1 24! 1 256 1 200 1 360 1 176 1 231 1 370 ator E	und 594.75 527.38 125.79 107.78 135.67 147.75 176.62 1090.45 Iement Li Max 3 60 0 120 0 30	Cou Formula	Ints vs. Mass-to-Cha	rrge (m/z)	5 869.8	870 870	.1.2	
	Peak Lisi m/z 274.2734 318.2999 453.167 848.3333 849.3373 853.2882 869.2623 870.2657 Formula Element C H O Formula	t Calcul Calcul	z Ab 1 24! 1 256 1 204 1 364 1 176 1 23: 1 80: 1 370 ator E In	und 594.75 527.38 425.79 407.78 335.67 447.75 5090.45 Identify and Part Li Max 3 60 0 120 0 30 0 30	Cou	Ints vs. Mass-to-Che Ion (M+ (M+	-K)+ -K)+				IDBF
	Peak Lisi m/z 274.2734 318.2999 453.167 848.3333 849.3373 853.2882 869.2623 870.2657 Formula Element C H O Formula Formula	t Calcul Calcul	z Ab 1 24! 1 256 1 204 1 364 1 176 1 23: 1 80: 1 370 ator E In	und 594.75 527.38 425.79 407.78 335.67 447.75 5090.45 Identify and Part Li Max 3 60 0 120 0 30 0 30	Cou	Ints vs. Mass-to-Che Ion (M4 (M4 (M4	rrge (m/z)	Diff. (mDa)	Diff. (p	pm)	

Agilent Technologies

Page 1 of 1

Printed at: 8:55 AM on: 8/28/2015

Figure S38. HR-ESI-MS spectrum of the new compound 3.



🔆 Agilent Technologies

Page 1 of 1

Printed at: 3:46 PM on: 7/30/2015

Figure S39. HR-ESI-MS spectrum of the new compound 4.

Sample Gro Acquisition Version															
				es TOF/650 05.01 (B51)	00 series	Info.									
User Spe	stra														
Fragme	ntor Vol 135	tage		Collision E	nergy	Ionization ESI	Mode								
x10 5 + So	an (0.19	2-0.225	5 min. 3 §	Scans) ML-3	32.d Subtrac	t									
1.6				,		925.2737									
1.4						(M+Na)+									
1.2															
1-															
0.8															
0.6															
0.4															
0.4 - 0.2 -															
0.4	924.4	924	4.6	924.8		925.2 92	5.4 9	925.6	925.8	926	926.2	2			
0.4 - 0.2 - 0 -	924.4	924	4.6	924.8		925.2 92 s. Mass-to-Cha	5.4 g ge (m/z)	925.6	925.8	926	926.2	2			
0.4 0.2 0 Peak List					Counts v	s. Mass-to-Cha	5.4 g ge (m/z)	925.6	925.8	926	926.2	2			
0.4- 0.2- 0- Peak List <i>m/z</i>	z	Abunc	d	924.8 Formula	Counts v	925.2 92 s. Mass-to-Cha	5.4 9 ge (m/z)	925.6	925.8	926	926.2	2			
0.4 - 0.2 - 0 - Peak List <i>m/z</i> 899.2368	z	Abunc 67953.	d .05		Counts v	s. Mass-to-Cha	5.4 g ge (m/z)	925.6	925.8	926	926.2	2			
0.4- 0.2- 0 Peak List <i>m/z</i> 899.2368 900.2403	z 1	Abunc 67953. 31764.	d .05 .8		Counts v	s. Mass-to-Cha	5.4 \$ ge (m/z)	925.6	925.8	926	926.2	2			
0.4 - 0.2 - 0 - Peak List <i>m/z</i> 899.2368	z 1 1 1	Abunc 67953.	d .05 .8 .2		Counts v	s. Mass-to-Cha	5.4 \$ ge (m/z)	925.6	925.8	926	926.2	2			
0.4- 0.2- 0- Peak List <i>m/z</i> 899.2368 900.2403 920.3182	z 1 1 1 1	Abunc 67953. 31764. 63077.	d .05 .8 .2 .12		Counts v	s. Mass-to-Cha	5.4 s ge (m/z) Na)+	925.6	925.8	926	926.2	2			
0.4- 0.2- 0- Peak List <i>m/z</i> 899.2368 900.2403 920.3182 921.3218	z 1 1 1 1 1 1	Abunc 67953. 31764. 63077. 28484.	d .05 .8 .2 .12 2.28	Formula	Counts v	s. Mass-to-Cha	ge (m/z)	925.6	925.8	926	926.2	2			
0.4- 0.2- 0 Peak List <i>m/z</i> 899.2368 900.2403 920.3182 921.3218 925.2737	z 1 1 1 1 1 1 1 1 1	Abunc 67953. 31764. 63077. 28484. 152962	d .05 .8 .2 .12 2.28 .54	Formula C43 H50 C	Counts v	s. Mass-to-Cha	nge (m/z)	925.6	925.8	926	926.2	2			
0.4 0.2 0 Peak List 899.2368 900.2403 920.3182 925.2737 926.2772 941.2477 941.2477	z 1 1 1 1 1 1 1 1 1 1 1 1	Abunc 67953. 31764. 63077. 28484. 152962 67624. 106957 51154.	d .05 .8 .2 .12 2.28 .54 7.15 .05	Formula C43 H50 C C43 H50 C	Counts v	s. Mass-to-Cha	nge (m/z)	925.6	925.8	926	926.2	2			
0.4 0.2 0 Peak List <i>m/z</i> 899.2368 900.2403 920.3182 921.3218 925.2737 926.2772 941.2477 942.2508	z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Abunc 67953. 31764. 63077. 28484. 152962 67624. 106957 51154. r Elem	d .05 .8 .2 .12 2.28 .54 7.15 .05 ment Lin	Formula C43 H50 C C43 H50 C	Counts v	s. Mass-to-Cha	nge (m/z)	925.6	925.8	926	926.2	2			
0.4 0.2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	z 1 1 1 1 1 1 1 1 1 1 1 1	Abunc 67953. 31764. 63077. 28484. 152962 67624. 106957 51154. r Elem	d .05 .8 .2 .12 2.28 .54 7.15 .05 ment Lin fax	Formula C43 H50 C C43 H50 C	Counts v	s. Mass-to-Cha	nge (m/z)	925.6	925.8	926	926.2	2			
0.4 0.2 0 899.2368 900.2403 920.3182 921.3218 925.2737 941.2477 942.2508 Formula Ca Element C	z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Abund 67953. 31764. 63077. 28484. 152962 67624. 106957 51154. r Elem M 3	d .05 .8 .2 .12 2.28 .54 7.15 .05 ment Lin fax 60	Formula C43 H50 C C43 H50 C	Counts v	s. Mass-to-Cha	nge (m/z)	925.6	925.8	926	926.2	22			
0.4 0.2 0 899.2368 900.2403 920.3182 921.3218 925.2737 926.2772 926.2772 941.2477 942.2508 Formula Ca Element C H	z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Abund 67953. 31764. 63077. 28484. 152962 67624. 106957 51154. r Elern M 3 0	d .05 .8 .2 .12 2.28 .54 7.15 .05 nent Lin 4ax .60 .120	Formula C43 H50 C C43 H50 C	Counts v	s. Mass-to-Cha	nge (m/z)	925.6	925.8	926	926.2	22			
0.4 0.2 0 Peak List <i>m/z</i> 899.2368 900.2403 920.3182 921.3218 925.2737 921.2218 921.2477 941.2477 942.2508 Formula Ca Element C H O O	z 1 1 1 1 1 1 1 1 1 1 1 1 1	Abunc 67953. 31764. 63077. 28484. 152962 67624. 106957 51154. r Elem M 3 0 0	d .05 .8 .2 .12 2.28 .54 7.15 .05 ment Lir 4ax 60 120 30	Formula C43 H50 C C43 H50 C	Counts v	s. Mass-to-Cha	nge (m/z)	925.6	925.8	926	926.2	2			
0.4 0.2 0 899.2368 900.2403 920.3182 921.3218 925.2737 926.2772 9241.2477 942.2508 Formula Ca Element C H	z 1 1 1 1 1 1 1 1 1 1 1 1 1	Abunc 67953. 31764. 63077. 28484. 152962 67624. 106957 51154. r Elem 3 0 0 0	d .05 .8 .2 .12 2.28 .54 7.15 .05 ment Lir 4ax 60 120 30	Formula C43 H50 C C43 H50 C	Counts v	S. Mass-to-Cha	nge (m/z)		925.8	926	926.2 Diff. (pp		[D	BE	

Agilent Technologies

Page 1 of 1

Printed at: 3:45 PM on: 7/30/2015

Figure S40. HR-ESI-MS spectrum of the new compound 5.