Supplementary Materials: 2-(2-Phenylethyl)chromone Derivatives of Agarwood Originating from *Gyrinops* salicifolia

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Figure S32. HRESI(+)MS spectrum of compound 4.

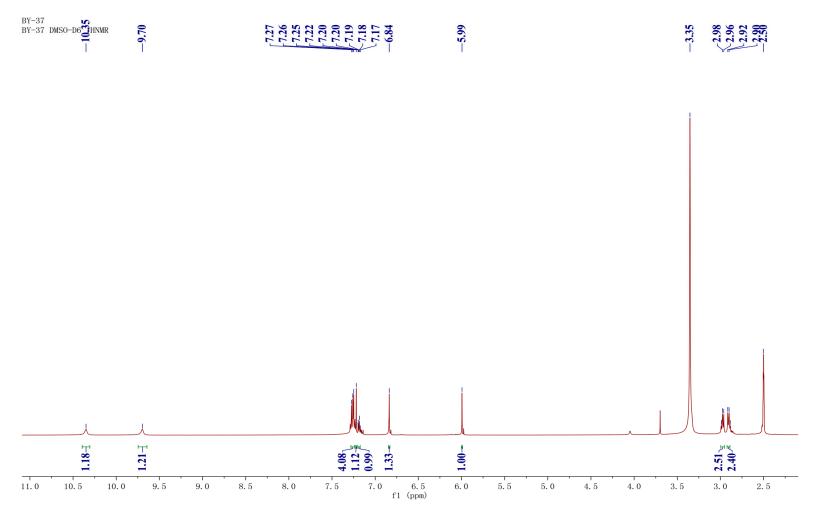


Figure S1. ¹H-NMR spectrum (500 MHz) of compound **1** in DMSO.

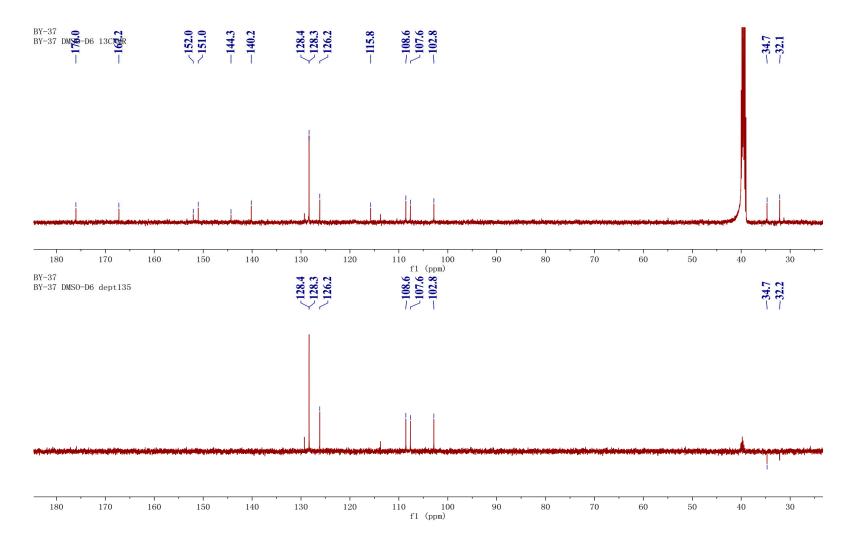


Figure S2. ¹³C-NMR spectrum (125 MHz) of compound 1 in DMSO.

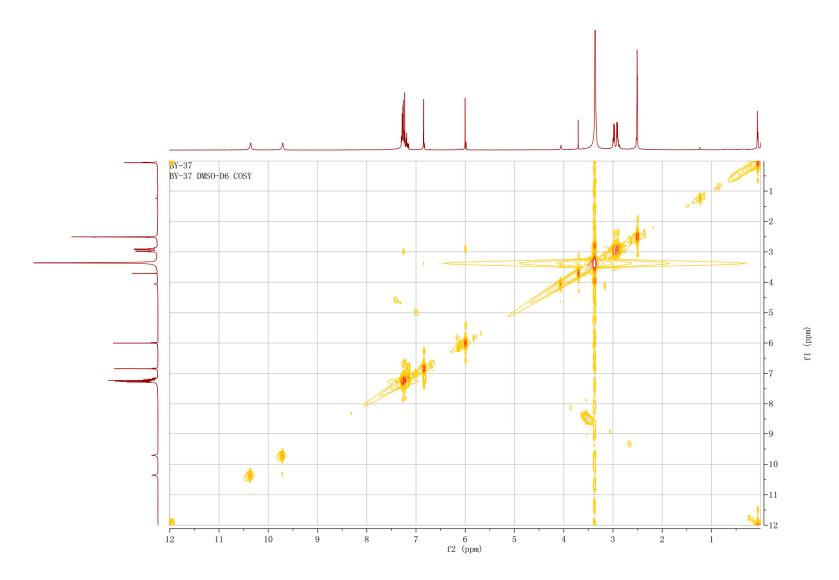


Figure S3. ¹H-¹H COSY spectrum (500 MHz) of compound **1** in DMSO.

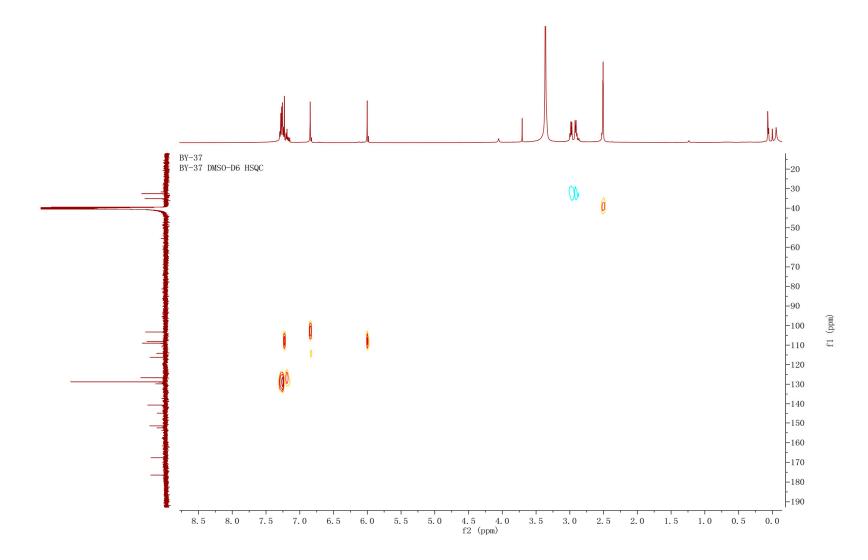


Figure S4. HSQC spectrum (500 MHz) of compound 1 in DMSO.

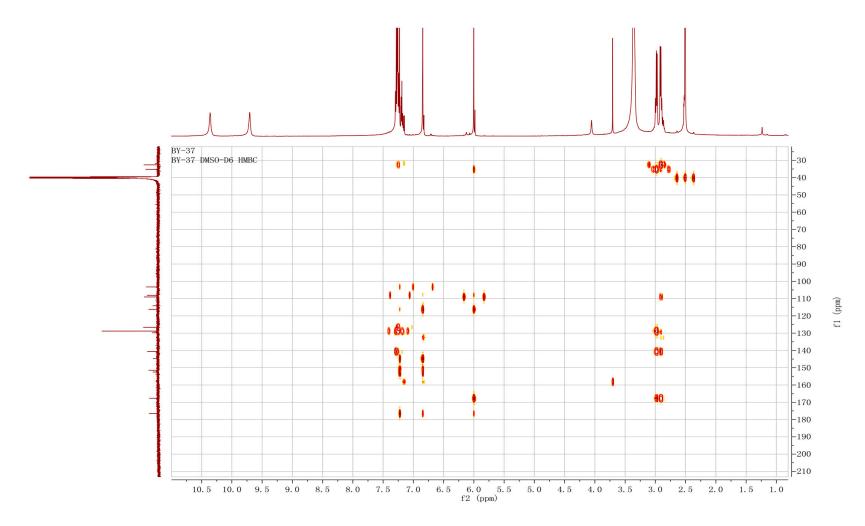


Figure S5. HMBC spectrum (500 MHz) of compound 1 in DMSO.

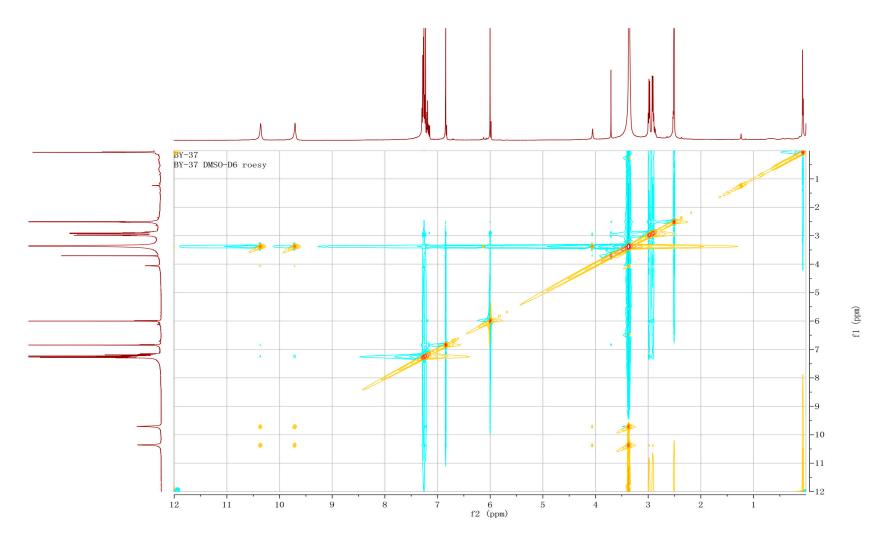


Figure S6. ROESY spectrum (400 MHz) of compound **1** in DMSO.

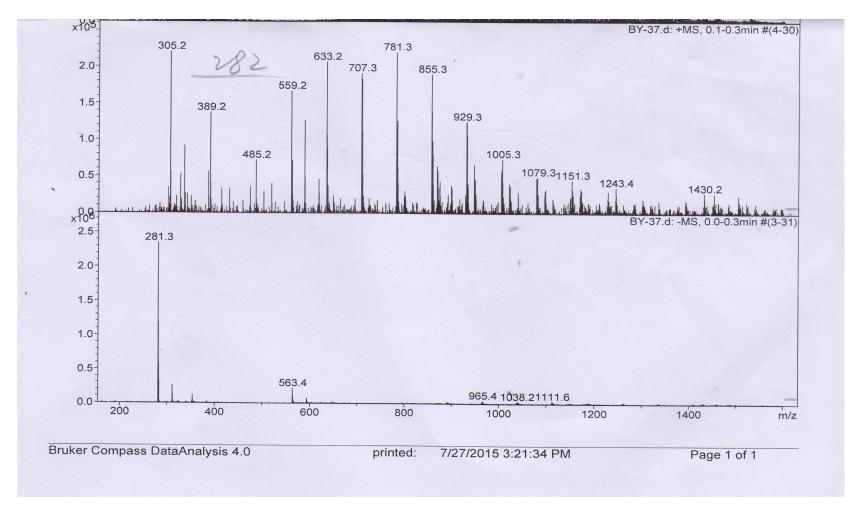


Figure S7. ESI(+)MS spectrum of compound **1**.

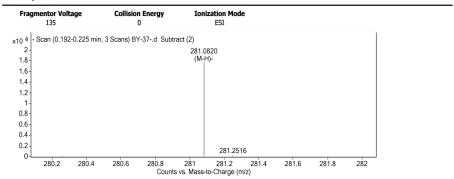
Qualitative Analysis Report

Data Filename BY-37-.d Sample Name Sample Type Sample Position P1-C1 **Instrument Name** Instrument 1 **User Name** Acq Method SIBU-ESI-i.m **Acquired Time** 10/22/2015 3:18:42 PM **IRM Calibration Status** DA Method ESI+.m Comment Sample Group Info.

 Acquisition SW
 6200 series TOF/6500 series

 Version
 Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund	Formula	Ion		
281.082	1	17761.73	C17 H14 O4	(M-H)-		
282.0851	1	3844.94	C17 H14 O4	(M-H)-		
311.0921	1	4198.39				
395.0744	1	31143.69				
396.0783	1	6990.37				
397.0799	1	1059.28				
425.0846	1	10681.58				
426.0884	1	2398.21				
Formula Calculator Floment Limits						

Formula Calculator Element Lin					
Element	Min	Max			
С	3	60			
Н	0	120			
0	0	30			
N	0	5			

N 0 5 Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C17 H14 O4	282.0892	281.0819	281.0820	0.0	-0.1	11.0000

⁻⁻⁻ End Of Report ---

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Figure S8. HRESI(+)MS spectrum of compound 1.

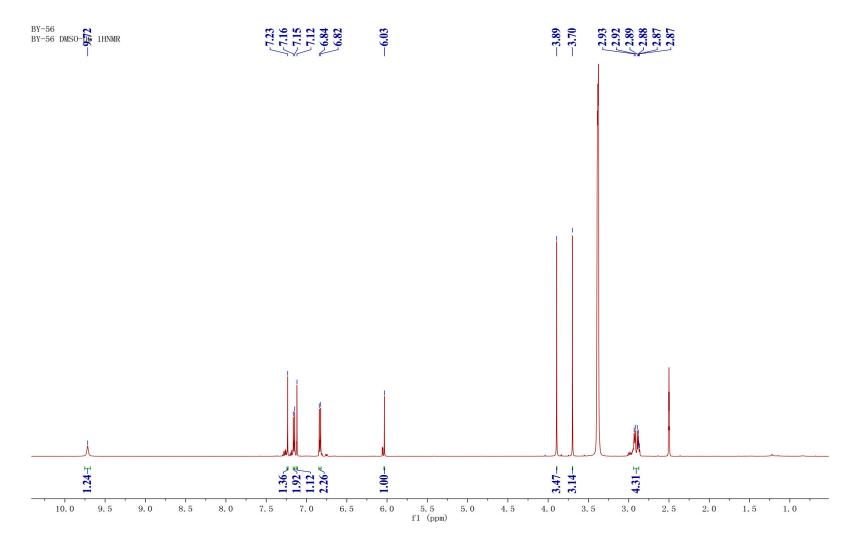


Figure S9. ¹H-NMR spectrum (500 MHz) of compound **2** in DMSO.

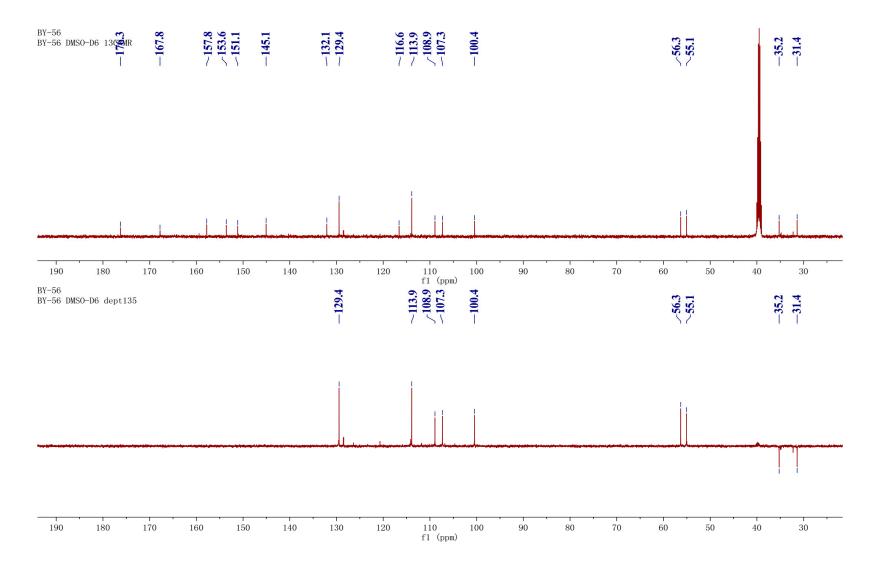


Figure S10. ¹³C-NMR spectrum (125 MHz) of compound 2 in DMSO.

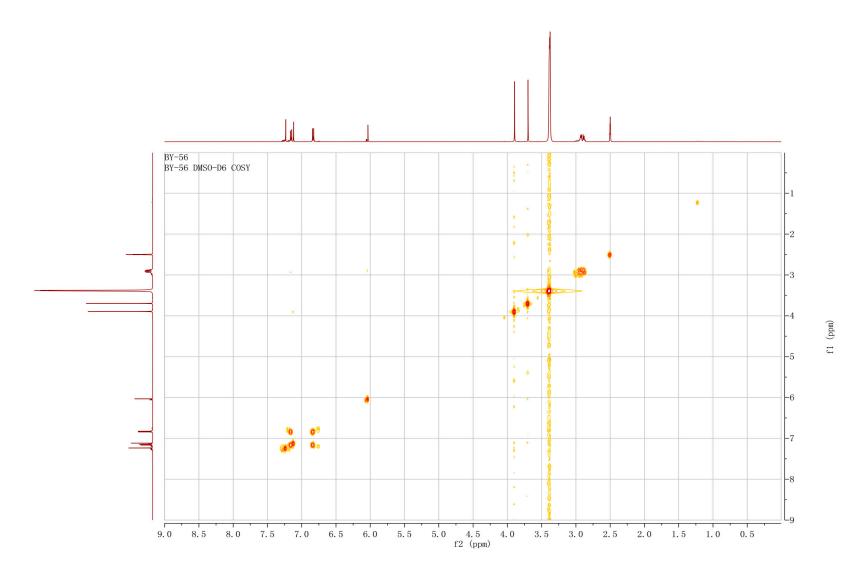


Figure S11. ¹H-¹H COSY spectrum (500 MHz) of compound **2** in DMSO.

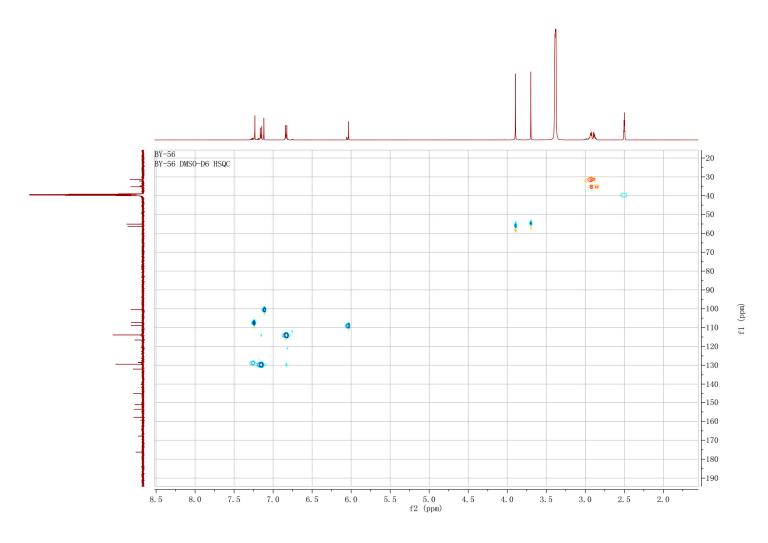


Figure S12. HSQC spectrum (500 MHz) of compound 2 in DMSO.

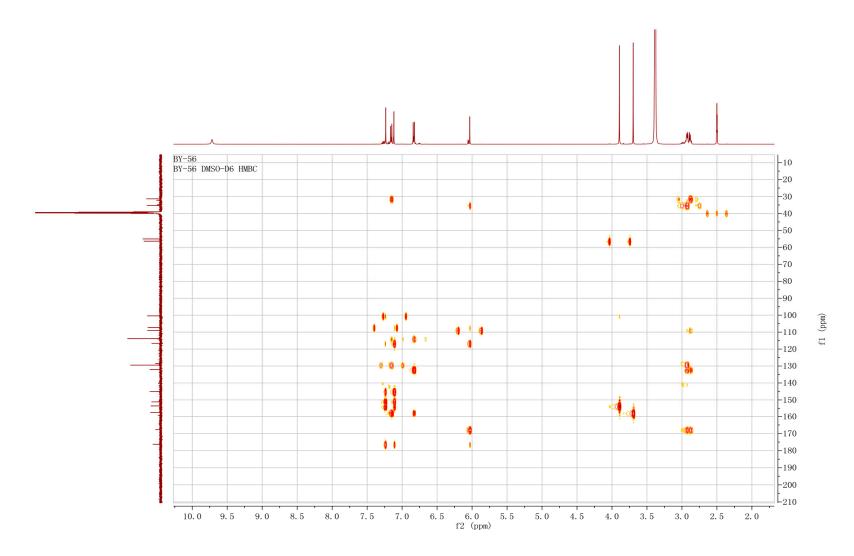


Figure S13. HMBC spectrum (500 MHz) of compound 2 in DMSO.

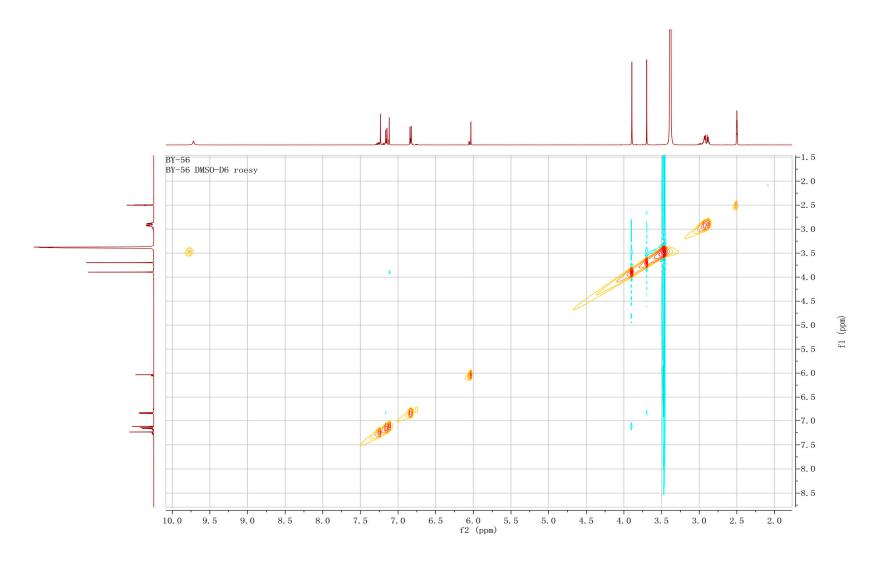


Figure S14. ROESY spectrum (400 MHz) of compound 2 in DMSO.

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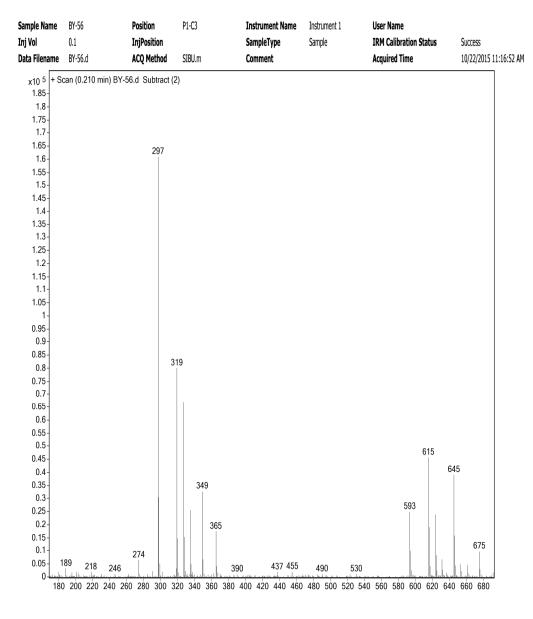


Figure S15. ESI(+)MS spectrum of compound **2**.

Qualitative Analysis Report

Data Filename BY-56.d BY-56 **Sample Name** Sample Type Sample Position P1-C3 **Instrument Name** Instrument 1 **User Name Acq Method** SIBU.m **Acquired Time** 10/22/2015 11:16:52 AM **IRM Calibration Status** DA Method ESI+.m Comment

 Sample Group
 Info.

 Acquisition SW
 6200 series TOF/6500 series

 Version
 Q-TOF B.05.01 (B5125.2)

User Spectra

Fra	gmentor Voltage 135	Collision Energy 0	Ionization Mode ESI		
x10 ⁵	+ Scan (0.210-0.227	min, 2 Scans) BY-56.d Subtra	act (2)		
1 - 0.9 -			327.1224 (M+H)+		
0.8-					
0.7-					
0.6-					
0.5-					
0.4-					
0.3-					
0.2-					
0.1-					
0-					
	326.2 326.4		327 327.2 327.4 vs. Mass-to-Charge (m/z)	327.6 327.8	328

Peak List

m/z	Z	Abund	Formula	Ion
297.1121	1	218337.25		
319.094	1	102590.45		
327.1224	1	90408.25	C19 H18 O5	(M+H)+
349.1047	1	43308.2		
593.2171	1	49472.85		
615.1992	1	108167.98		
623.2275	1	45127.51		
645.2098	1	93037.04		

Formula Calculator Element Limits

Licilicit	141111	riax			
С	3	60			
Н	0	120			
0	0	30			
N	0	30			
Francisco Calandata Baradta					

i oi iiiuia	Calculator	results	
Formula	- (Calculated	Ma

Formula	CalculatedMass	CalculatedMZ	MZ	DIπ. (MDa)	DIIT. (ppm)	DRE
C19 H18 O5	326.1154	327.1227	327.1224	0.3	1.0	11.0000

⁻⁻⁻ End Of Report ---

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Figure S16. HRESI(+)MS spectrum of compound **2**.

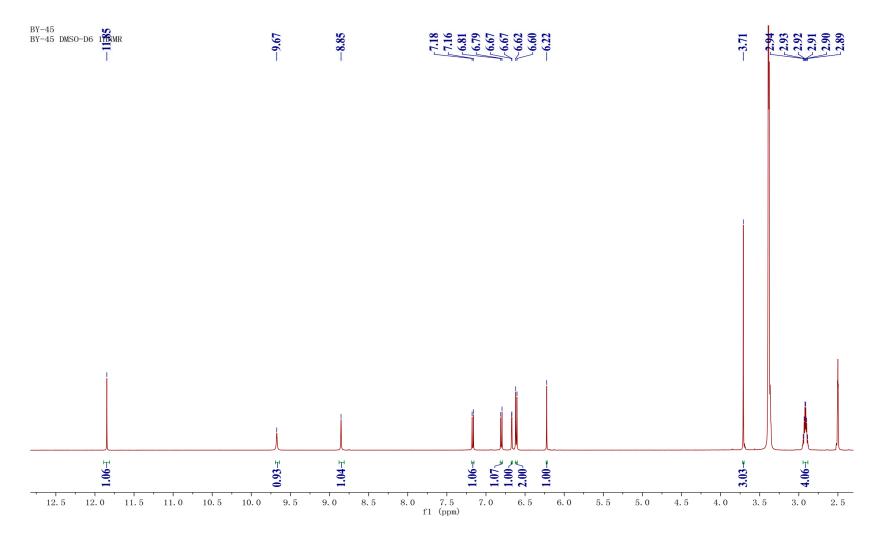


Figure S17. ¹H-NMR spectrum (500 MHz) of compound 3 in DMSO.

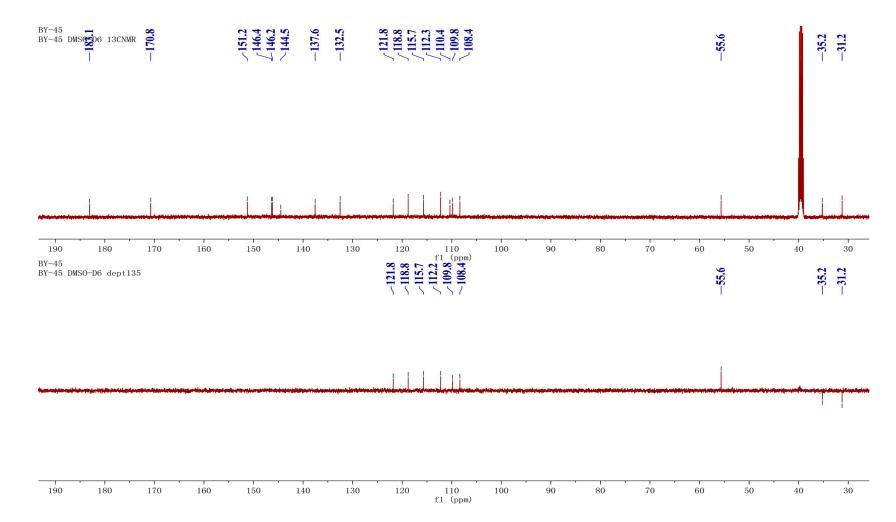


Figure S18. ¹³C-NMR spectrum (125 MHz) of compound 3 in DMSO.

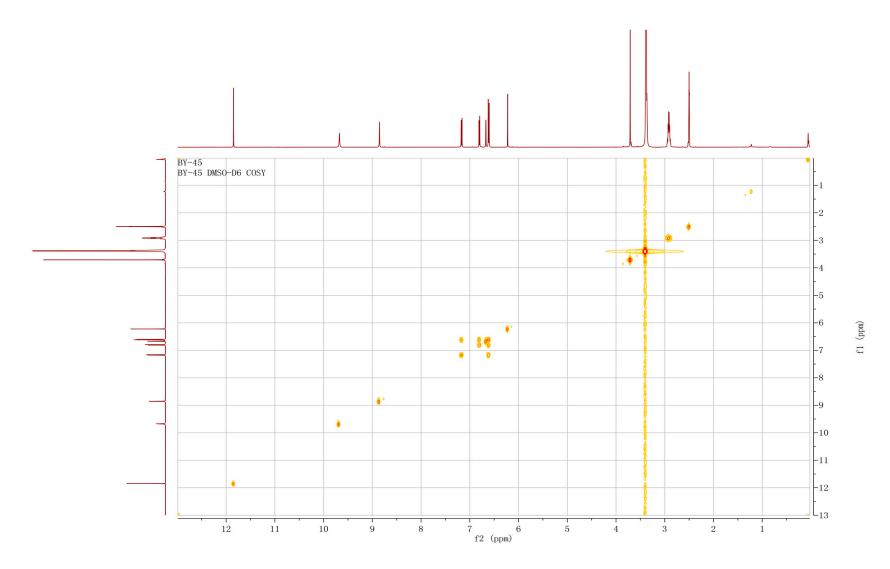


Figure S19. ¹H-¹H COSY spectrum (500 MHz) of compound **3** in DMSO.

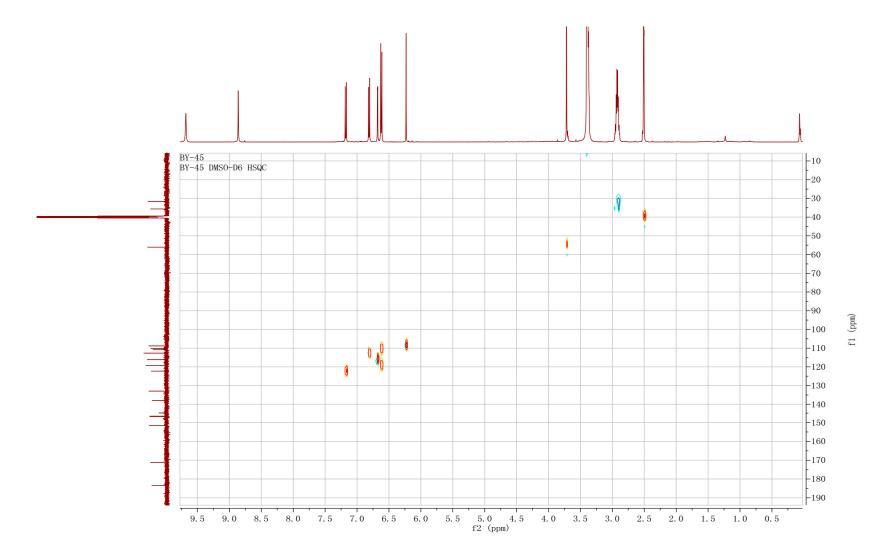


Figure S20. HSQC spectrum (500 MHz) of compound 3 in DMSO.

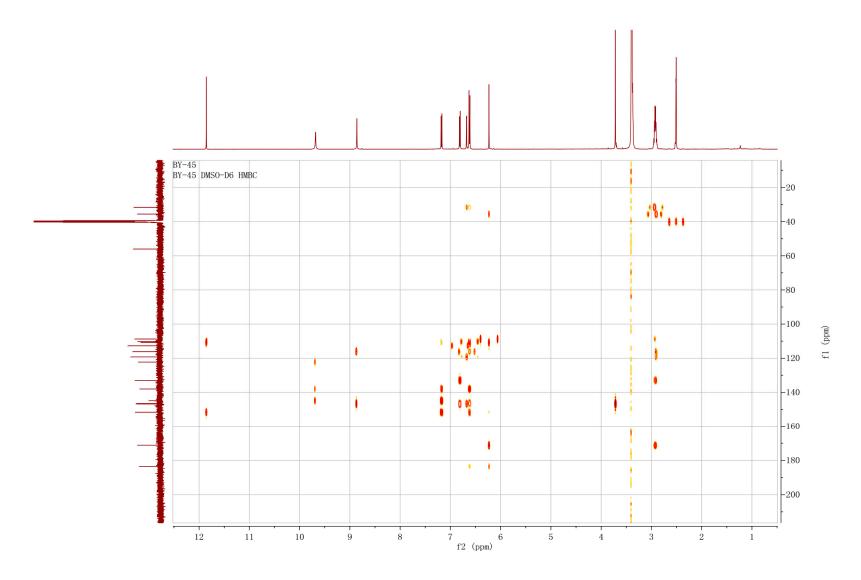


Figure S21. HMBC spectrum (500 MHz) of compound 3 in DMSO.

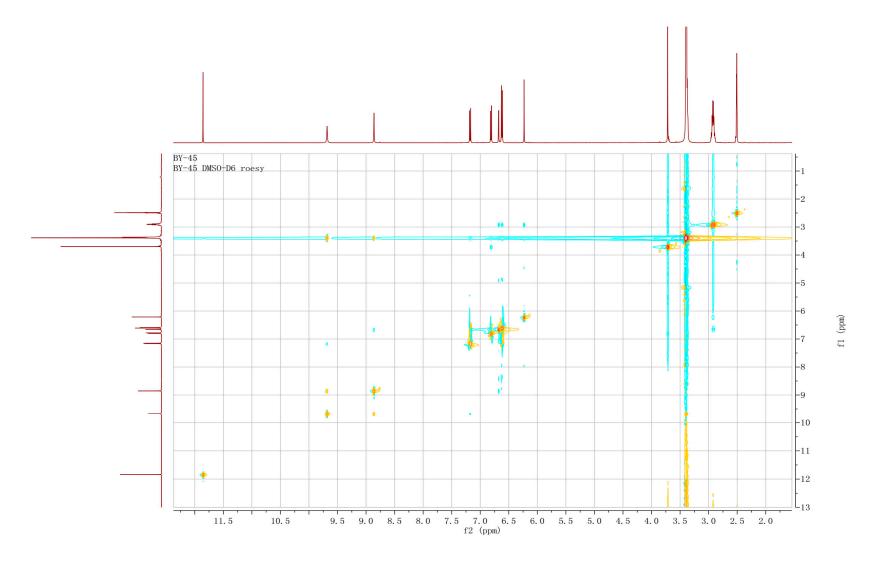


Figure S22. ROESY spectrum (400 MHz) of compound 3 in DMSO.

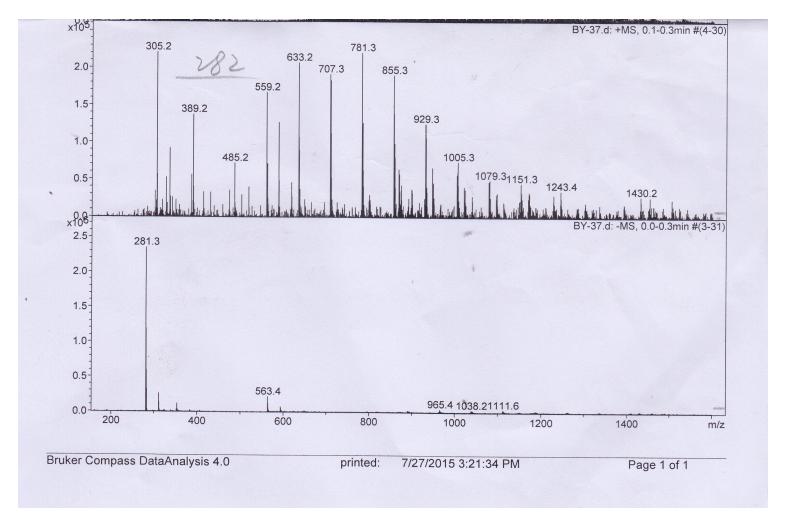
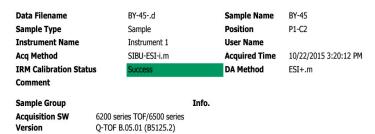


Figure S23. ESI(+)MS spectrum of compound **3**.

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Qualitative Analysis Report



User Spectra

Fragmentor Voltage 135	Collision Energy 0	Ionization Mod ESI	е			
3 - Scan (0.171-0.354 m	in, 12 Scans) BY-45d Subt	tract (2)				
9-		327.0873				
8-		(M-H)- 				
7-						
6-						
5-						
4-						
3-						
2-						
1						
326.2 326.4	326.6 326.8	327 327.2 vs. Mass-to-Charge (n	327.4	327.6	327.8	328

Peak List

m/z	Z	Abund	Formula	Ion
89.0246		1365.38		
327.0873	1	8401.06	C18 H16 O6	(M-H)-
328.0908	1	1529.88	C18 H16 O6	(M-H)-
390.0831	1	1013.56		
411.0692	1	706.99		
441.08	1	19259.49		
442.0848	1	3664.01		
443.0859	1	724.34		

Formula Calculator Element Limits

Element	Min	мах
С	3	60
Н	0	120
0	0	30
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMZ	MZ	DIIT. (MDa)	Diff. (ppm)	DRE
C18 H16 O6	328.0947	327.0874	327.0873	-0.1	-0.3	11.0000

⁻⁻⁻ End Of Report ---

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Figure S24. HRESI(+)MS spectrum of compound 3.

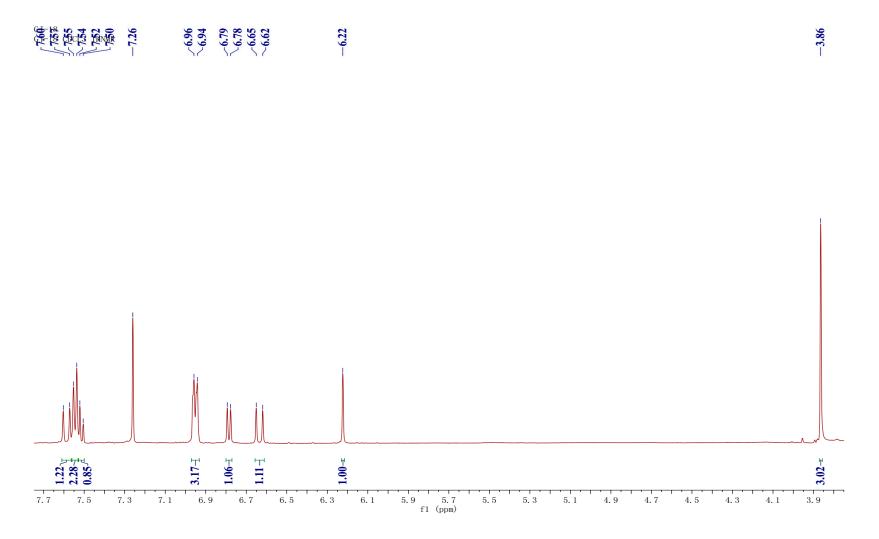
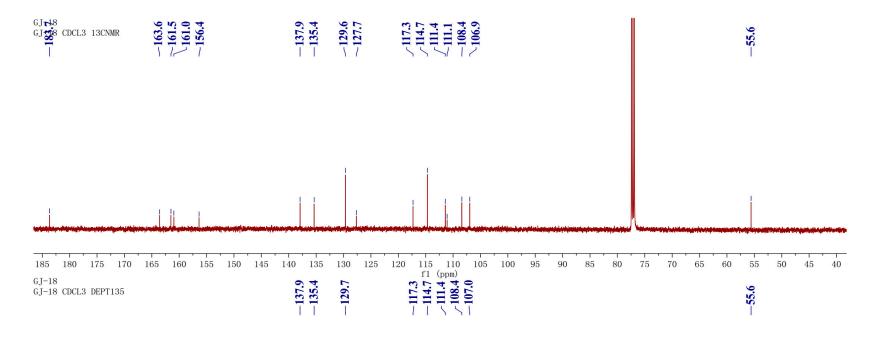


Figure S25. ¹H-NMR spectrum (500 MHz) of compound 4 in CDCl₃.



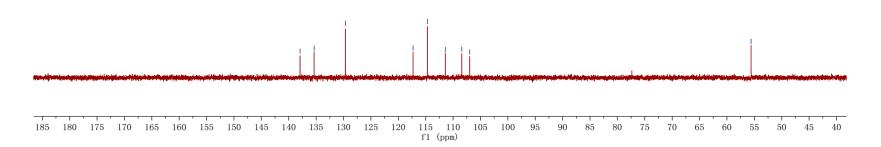


Figure S26. ¹³C-NMR spectrum (125 MHz) of compound 4 in CDCl₃.

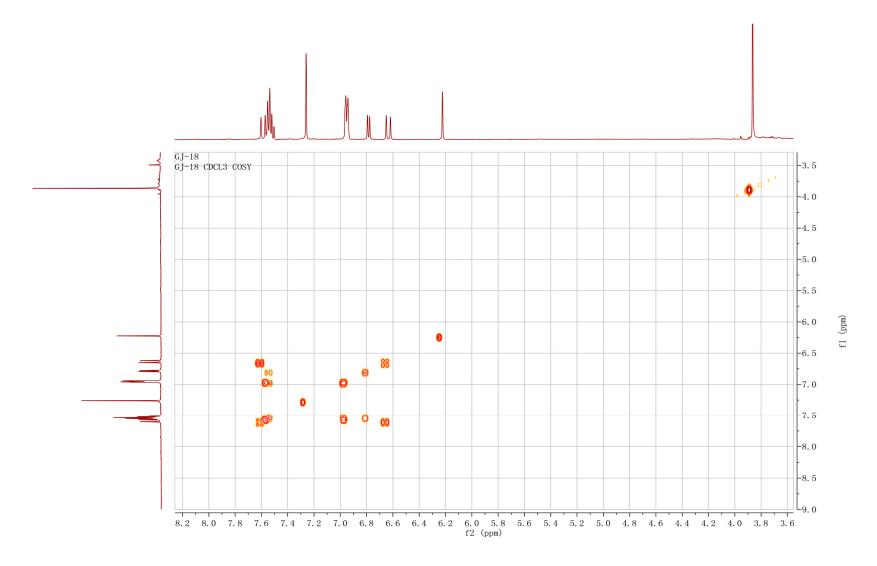


Figure S27. ¹H-¹H COSY spectrum (500 MHz) of compound 4 in CDCl₃.

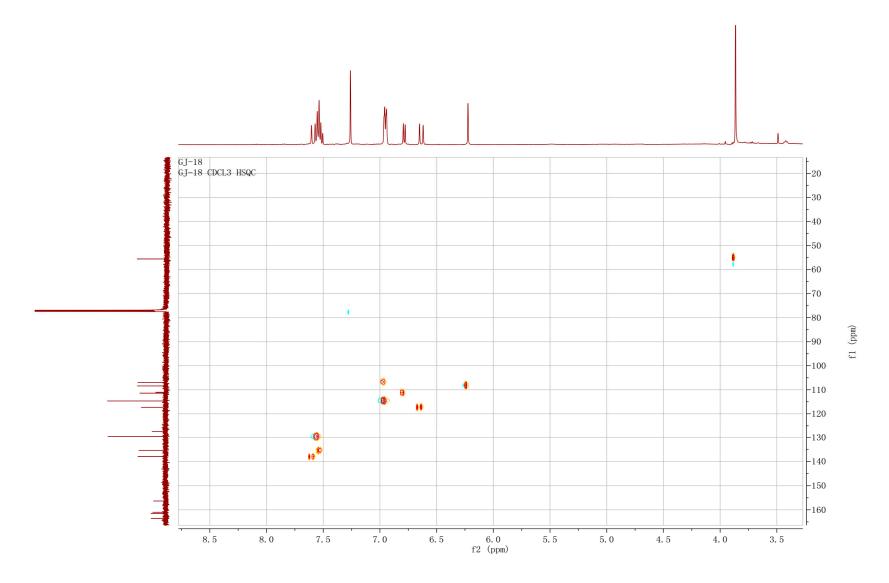


Figure S28. HSQC spectrum (500 MHz) of compound 4 in CDCl₃.

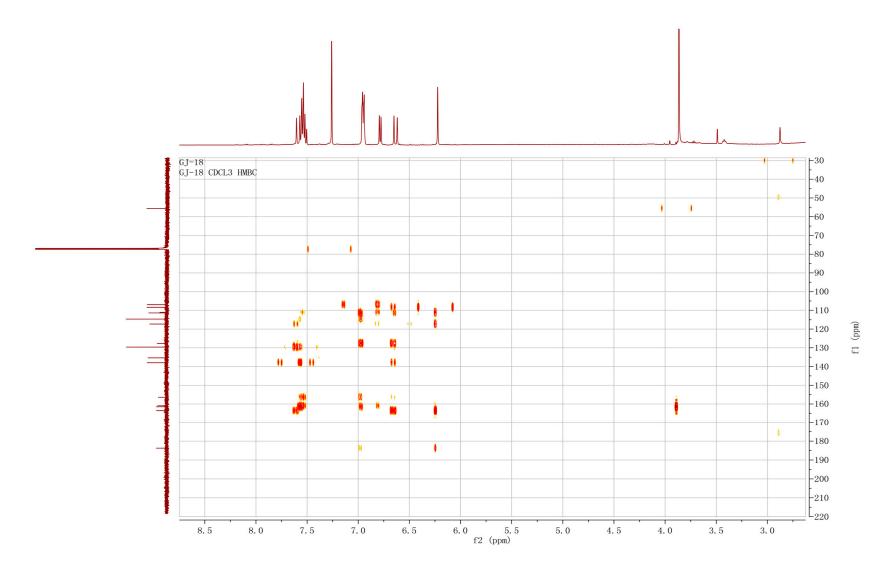


Figure S29. HMBC spectrum (500 MHz) of compound 4 in CDCl₃.

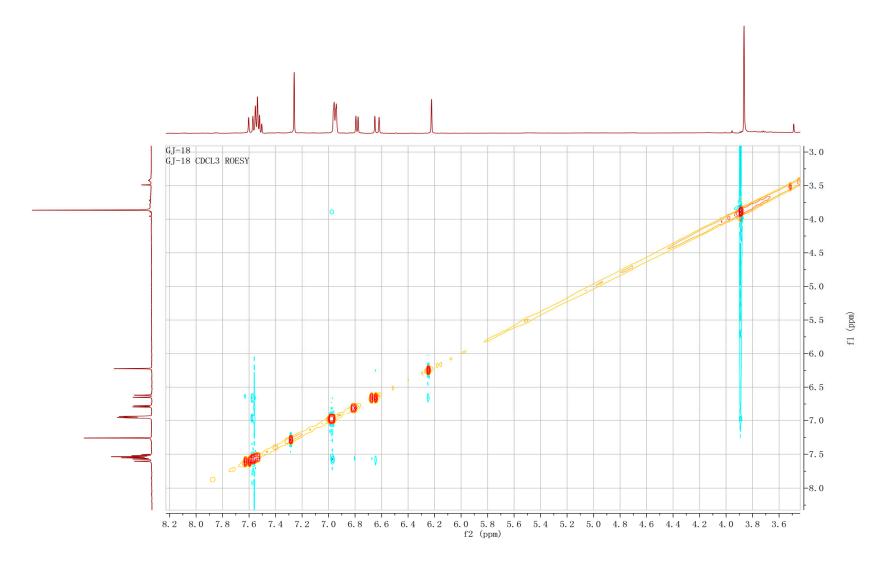


Figure S30. ROESY spectrum (400 MHz) of compound 4 in CDCl₃.

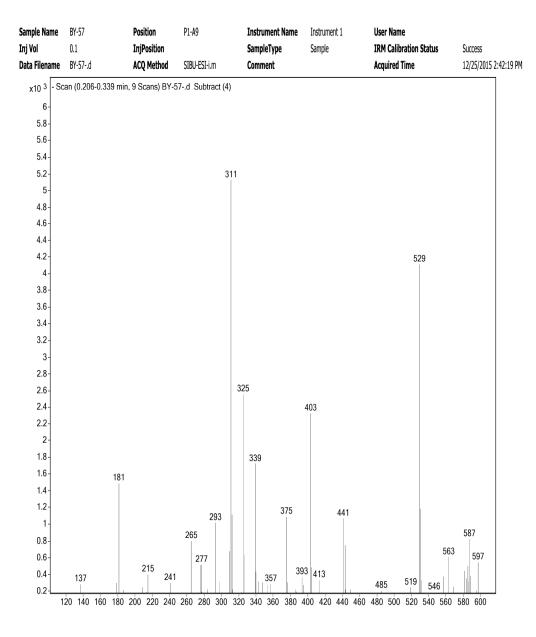
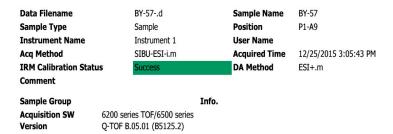


Figure S31. ESI(+)MS spectrum of compound 4.

Qualitative Analysis Report



User Spectra

x10 ³ - Scan (0.175-0.225 min, 4 Scans) BY-57d Subtract (3) 293.1787 (M-H)-
Z-5-1 (M-11)-
2-
1.5-
1-
0.5-
292.4 292.6 292.8 293 293.2 293.4 293.6 293.8 294

Peak List				
m/z	Z	Abu	nd]
311.1687	1	5084	1.09	
325.1844	1	6385	5.03]
339.2001	1	4304	1.08	1
375.2752	1	4148	3.44	1
403.3066	1	6881	.47	1
441.2495	1	3392	2.89	
529.2812	1	1260	9.48]
530.2839	1	4065	5.03	1
Formula Ca		or Ele		nii
Element	Min		Max]
С		3	120	
Н		0	240	
0		0	60	
N		0	10]
Formula Ca	lculate	or Re	sults	-

i oriniala Calculate	Titula Calculator Results								
Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE			
C20 H24 N O	294.1858	293.1785	293.1787	0.0	-0.1	9.5000			

⁻⁻⁻ End Of Report ---

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Figure S32. HRESI(+)MS spectrum of compound 4.