Electronic Supplementary Material (ESI) for RSC Advances.

Mexicanolide limonoids with in vitro neuroprotective activities from seeds of *Khaya senegalensis*

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Table of Contents

S33: HR-ESI-MS Spectrum of Compound **6** (Khasenegasin F)

S34: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **6** (Khasenegasin F)

S35: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **6** (Khasenegasin F)

S36: HSQC Spectrum of Compound **6** (Khasenegasin F)

S37: HMBC Spectrum of Compound **6** (Khasenegasin F)

S38: ROESY Spectrum of Compound **6** (Khasenegasin F)

S39: HR-ESI-MS Spectrum of Compound **7** (Khasenegasin G)

S40: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **7** (Khasenegasin G)

S41: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **7** (Khasenegasin G)

S42: HSQC Spectrum of Compound **7** (Khasenegasin G)

S43: HMBC Spectrum of Compound **7** (Khasenegasin G)

S44: ROESY Spectrum of Compound **7** (Khasenegasin G)

S45: HR-ESI-MS Spectrum of Compound **8** (Khasenegasin H)

S46: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **8** (Khasenegasin H)

S47: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **8** (Khasenegasin H)

S48: HSQC Spectrum of Compound **8** (Khasenegasin H)

S49: HMBC Spectrum of Compound **8** (Khasenegasin H)

S50: ROESY Spectrum of Compound **8** (Khasenegasin H)

S51: HR-ESI-MS Spectrum of Compound **9** (Khasenegasin I)

S52: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **9** (Khasenegasin I)

S53: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **9** (Khasenegasin I)

S54: HSQC Spectrum of Compound **9** (Khasenegasin I)

S55: HMBC Spectrum of Compound **9** (Khasenegasin I)

S56: ROESY Spectrum of Compound **9** (Khasenegasin I)

S57: HR-ESI-MS Spectrum of Compound **10** (Khasenegasin J)

S58: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **10** (Khasenegasin J)

S59: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **10** (Khasenegasin J)

S60: HSQC Spectrum of Compound **10** (Khasenegasin J)

S61: HMBC Spectrum of Compound **10** (Khasenegasin J)

S62: ROESY Spectrum of Compound **10** (Khasenegasin J)

S63: HR-ESI-MS Spectrum of Compound **11** (Khasenegasin K)

S64: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **11** (Khasenegasin K)

S65: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **11** (Khasenegasin K)

S66: HSQC Spectrum of Compound **11** (Khasenegasin K)

S67: HMBC Spectrum of Compound **11** (Khasenegasin K)

S68: ROESY Spectrum of Compound **11** (Khasenegasin K)

S69: HR-ESI-MS Spectrum of Compound **12** (Khasenegasin L)

S70: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **12** (Khasenegasin L)

S71: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **12** (Khasenegasin L)

S72: HSQC Spectrum of Compound **12** (Khasenegasin L)

S73: HMBC Spectrum of Compound **12** (Khasenegasin L)

S74: ROESY Spectrum of Compound **12** (Khasenegasin L)

S75: HR-ESI-MS Spectrum of Compound **13** (Khasenegasin M)

S76: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **13** (Khasenegasin M)

S77: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **13** (Khasenegasin M)

S78: HSQC Spectrum of Compound **13** (Khasenegasin M)

S79: HMBC Spectrum of Compound **13** (Khasenegasin M)

S80: ROESY Spectrum of Compound **13** (Khasenegasin M)

S81: HR-ESI-MS Spectrum of Compound **14** (Khasenegasin N)

S82: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **14** (Khasenegasin N)

S83: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **14** (Khasenegasin N)

S84: HSQC Spectrum of Compound **14** (Khasenegasin N)

S85: HMBC Spectrum of Compound **14** (Khasenegasin N)

S86: ROESY Spectrum of Compound **14** (Khasenegasin N)

S87: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **15** (fissinolide)

S88: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **15** (fissinolide)

S89: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **16** (swietmanin F)

S90: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **16** (swietmanin F)

S91: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **17** (seneganolide A)

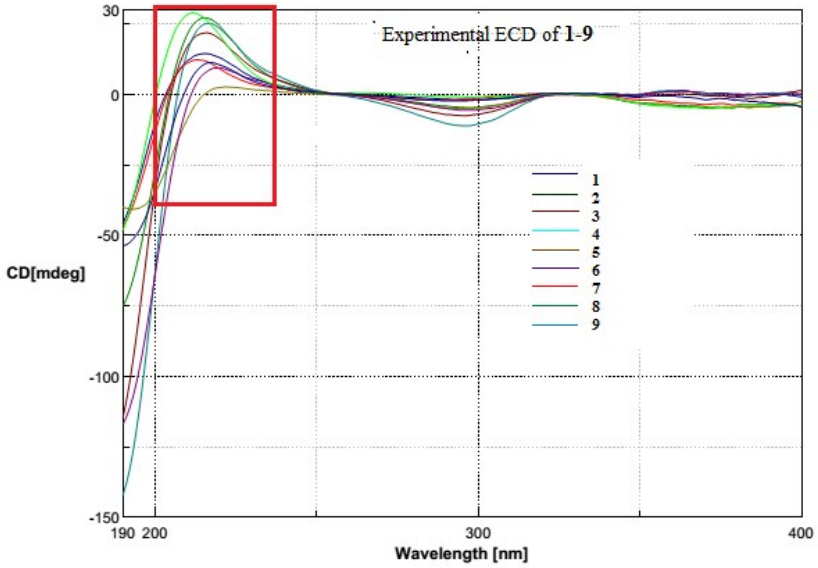
S92: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **17** (seneganolide A)

S93: NMR data comparing compound **15** with published NMR data (fissinolide)

S94: NMR data comparing compound **16** with published NMR data (swietmanin F)

S95: NMR data comparing compound **17** with published NMR data (seneganolide A)

S1: Experimental ECD of **1-9**



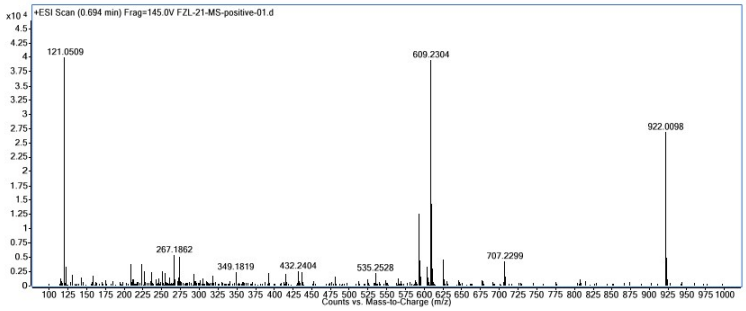
S2: The values of cell viabilities of compounds **2-10**, **12-15** and **17**

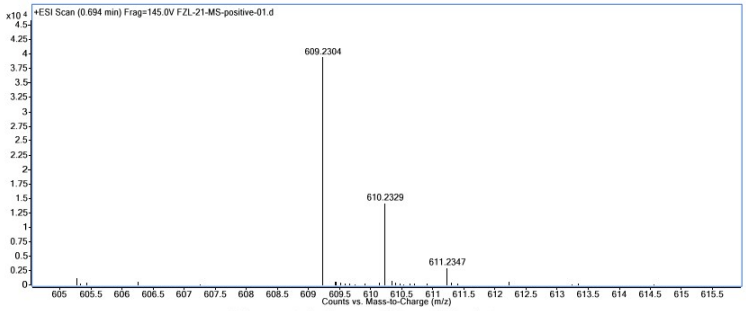
Compound	in vitro cytotoxicities (% of Control at 10 μM)	in vitro neuroprotective activities (% of Control at 10 μM)	in vitro neuroprotective activities (% of Control at 1 μM)
2	78.0 ± 3.3	53.2 ± 2.5	ND
3	107.0 ± 6.4	73.3 ± 3.9	ND
4	100.6 ± 10.2	68.3 ± 3.9	ND
5	85.2 ± 1.7	58.4 ± 3.1	ND
6	100.8 ± 9.8	88.5 ± 6.4***	87.6 ± 1.2%***
7	108.3 ± 7.0	52.5 ± 2.0	ND
8	104.0 ± 10.1	71.1 ± 1.2	ND
9	102.0 ± 5.9	60.2 ± 3.6	ND
10	100.7 ± 9.9	54.1 ± 3.6	ND
12	96.2 ± 5.3	56.0 ± 3.9	ND
13	83.6 ± 5.6	61.3 ± 3.7	ND
14	110.7 ± 1.8	66.3 ± 3.7	ND
15	109.2 ± 3.5	64.2 ± 3.9	ND
17	107.0 ± 10.4	78.4 ± 5.7*	76.5 ± 2.0%*
Edaravone	ND	86.7 ± 5.6***(50 μM)	

Cell viabilities were evaluated by MTT assay and the cell viability in control was taken as 100%, and the average value of cell viability under glutamate exposure was 53.6 ± 4.7%. Glutamate-injured cells differ significantly from the control at a level of $P<0.001$. The values expressed as mean ± SD of triplicate experiments. ND = not determined. (*$P<0.05$, ***$P<0.001$)

Khasenegasin A (**1**)

S3 HR-ESI-MS of Khasenegasin A (**1**)

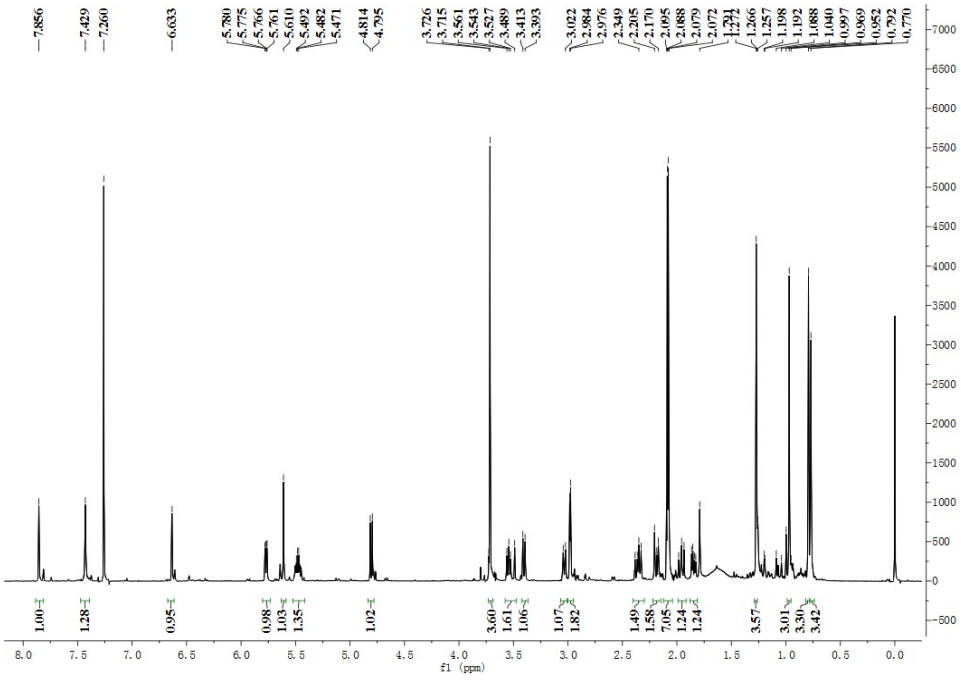




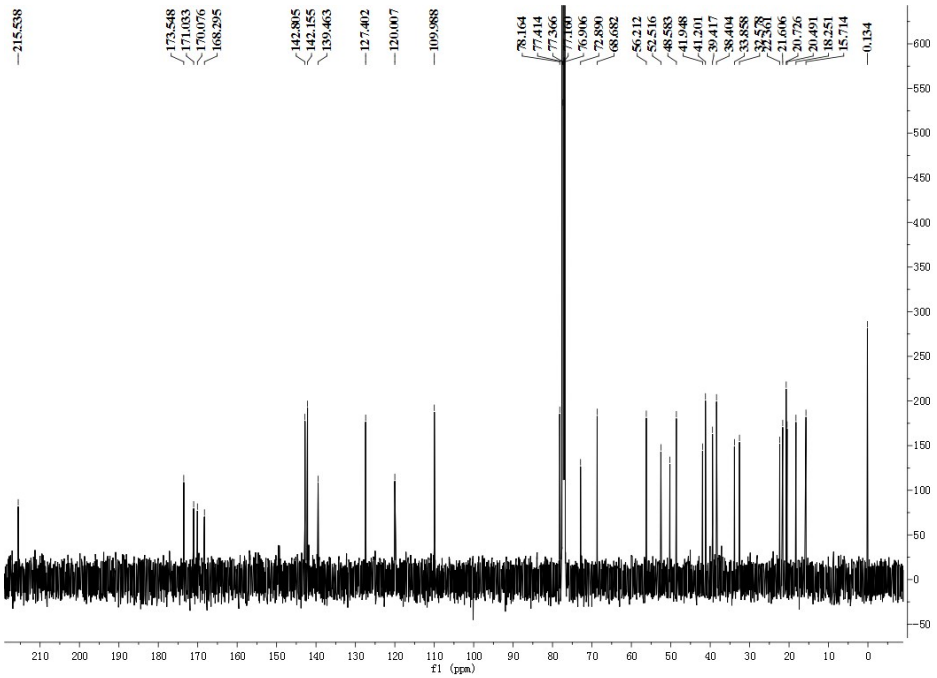
Elemental Composition Calculator

Target m/z:	609.2304	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C31H38NaO11		609.2306		0.4	

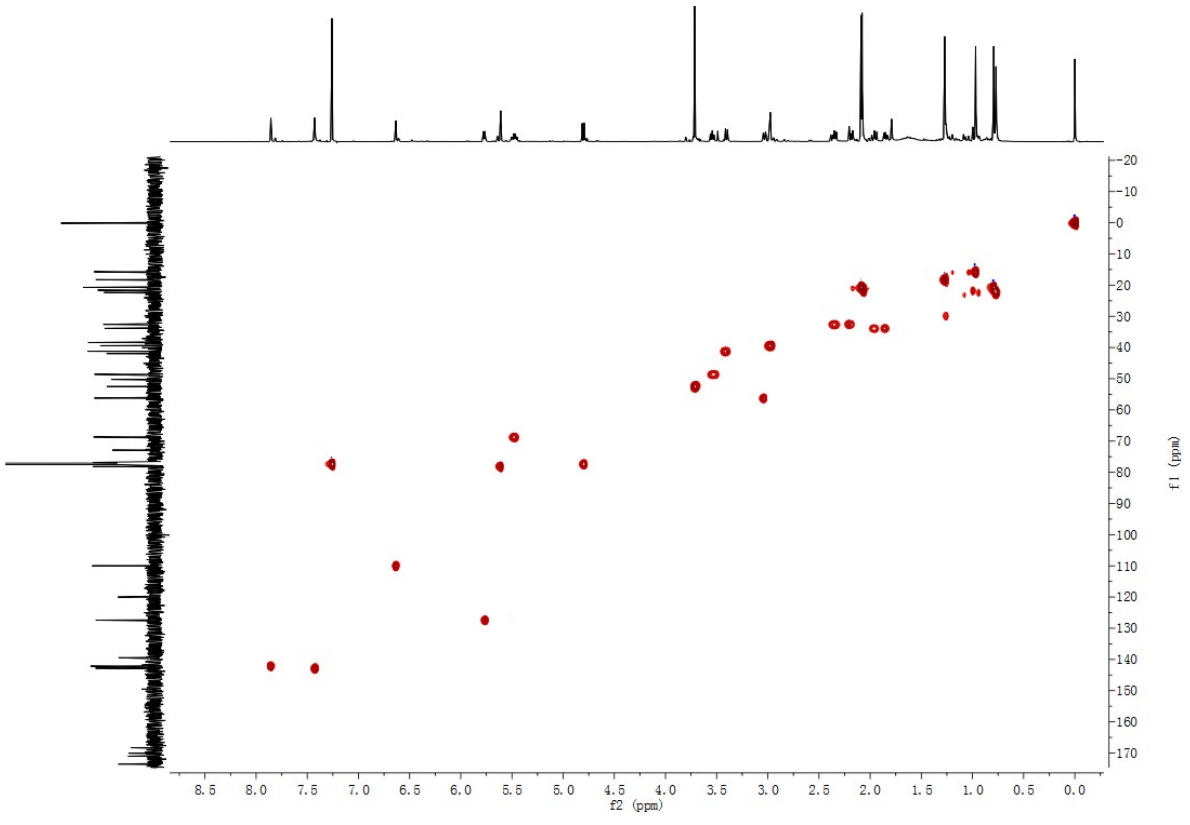
S4 ^{1}H NMR of Khasenegasin A (**1**)



S5 ^{13}C NMR of Khasenegasin A (**1**)

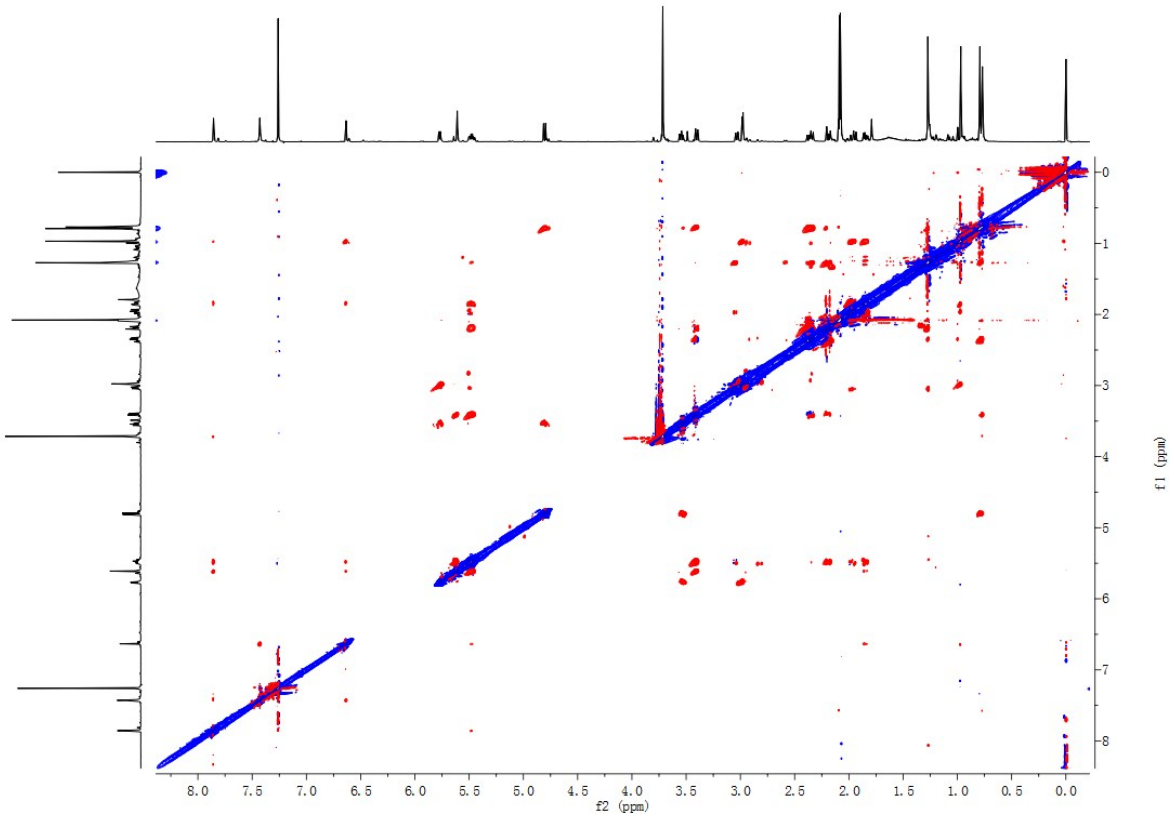


S6 HSQC of Khasenegasin A (**1**)



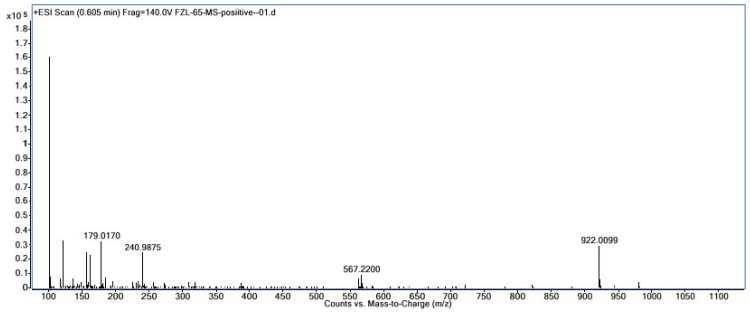
S7 HMBC of Khasenegasin A (**1**)

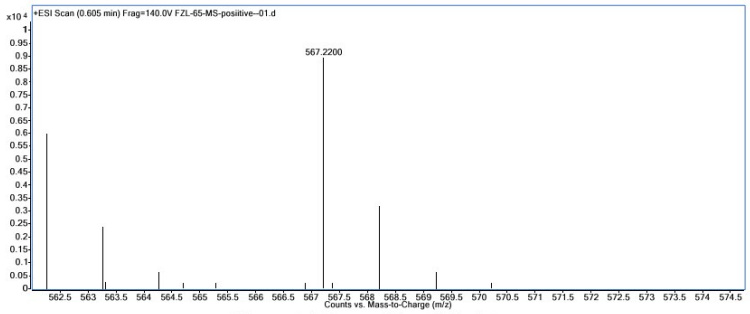
S8 ROSEY of Khasenegasin A (**1**)



Khasenegasin B (**2**)

S9 HR-ESI-MS of Khasenegasin B (**2**)

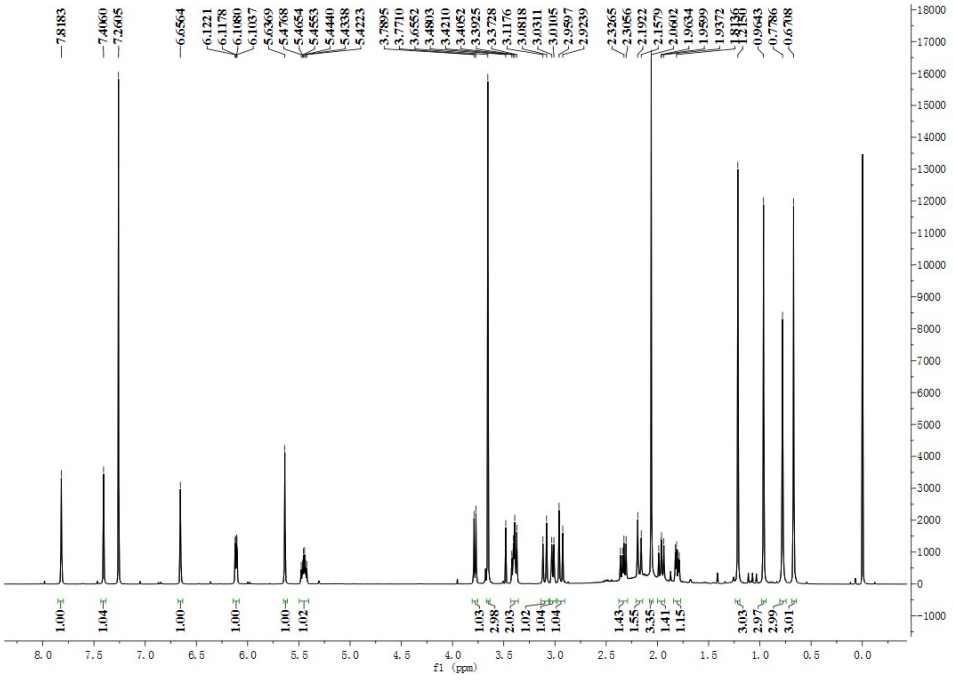




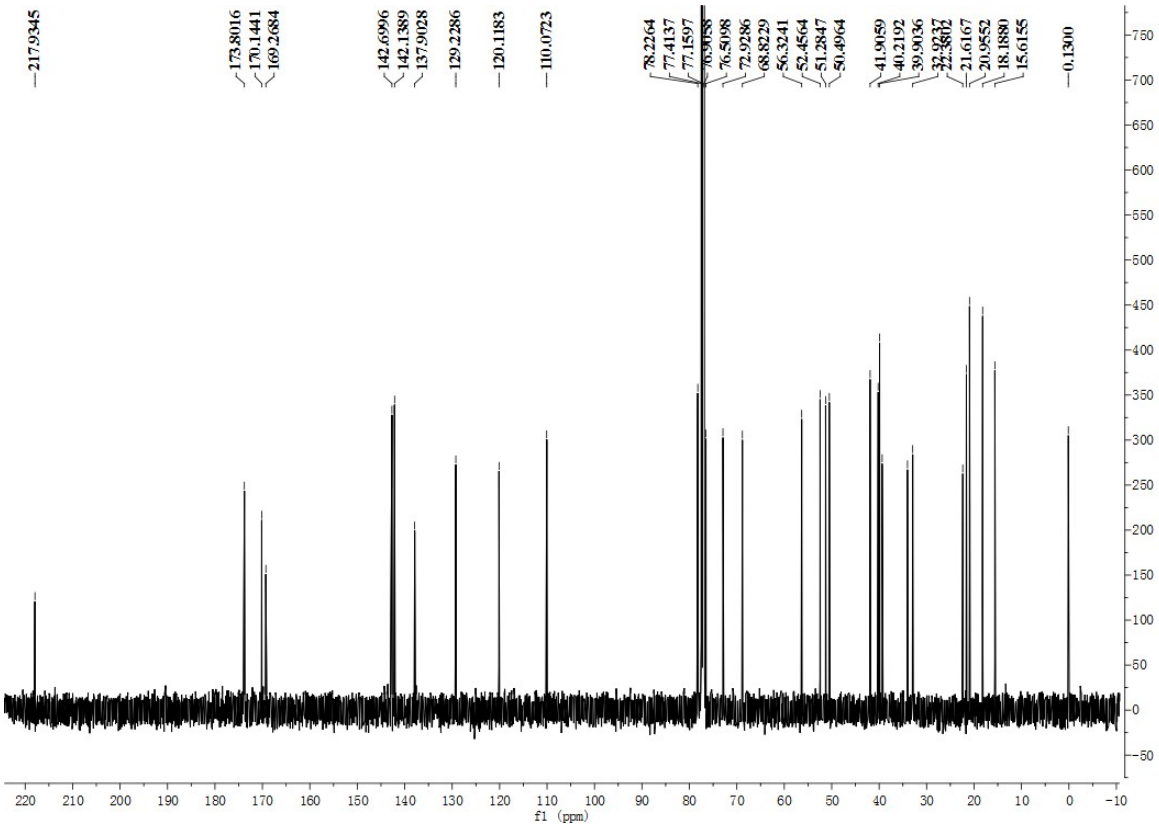
Elemental Composition Calculator

Target m/z:	567.2200	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C29H36NaO10		567.2201		0.15	

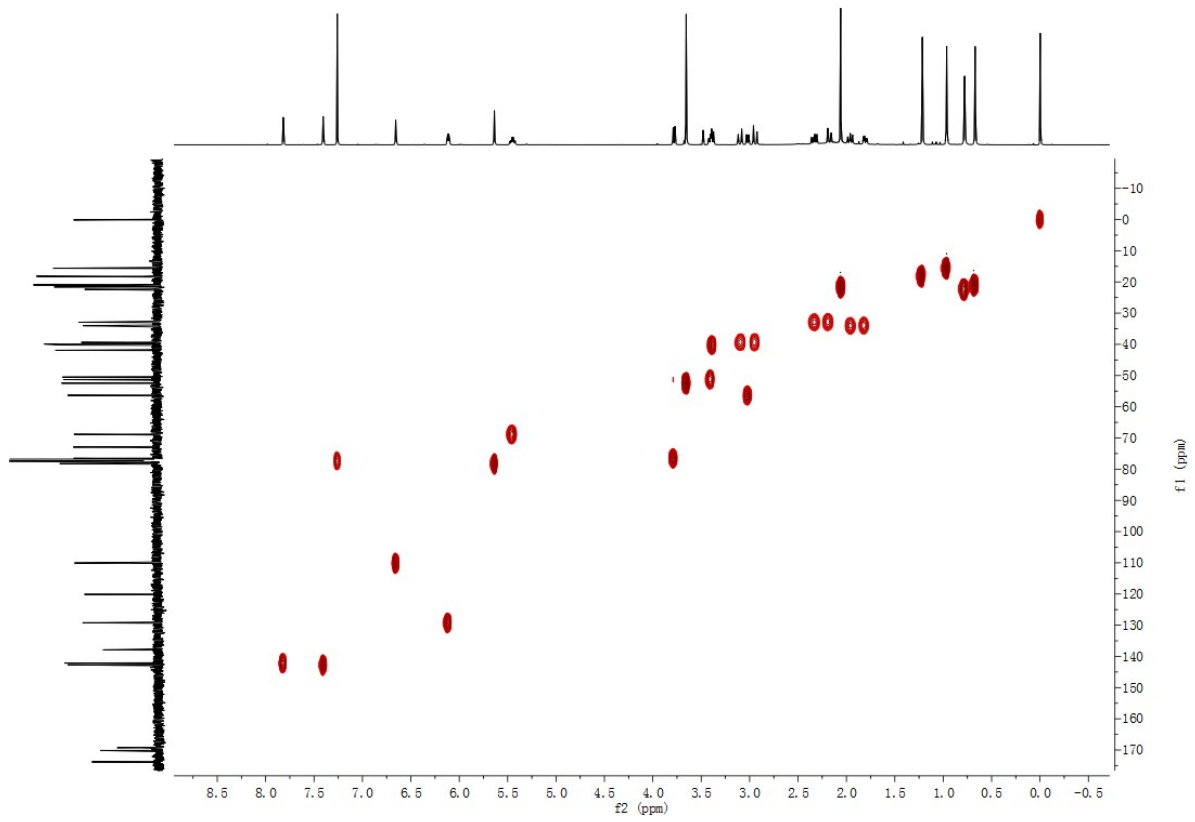
S10 ^{1}H NMR of Khasenegasin B (**2**)



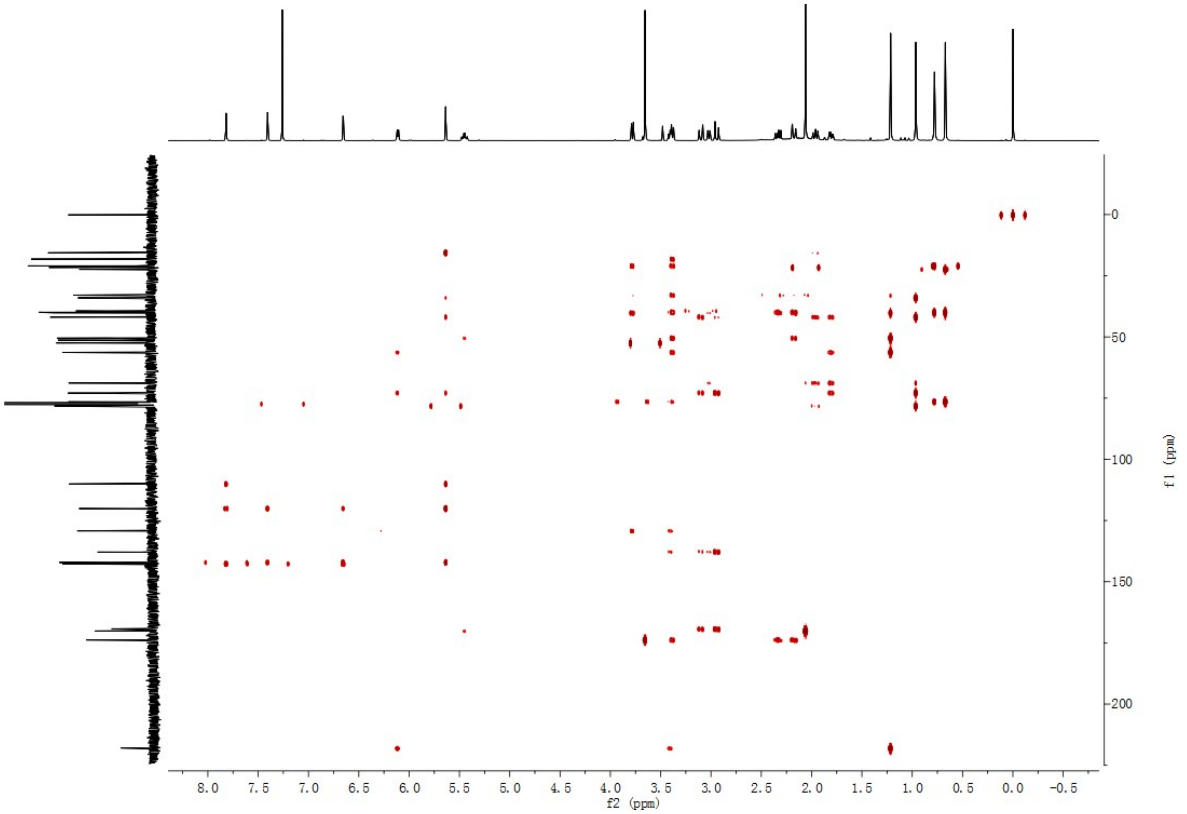
S11 ^{13}C NMR of Khasenegasin B (**2**)



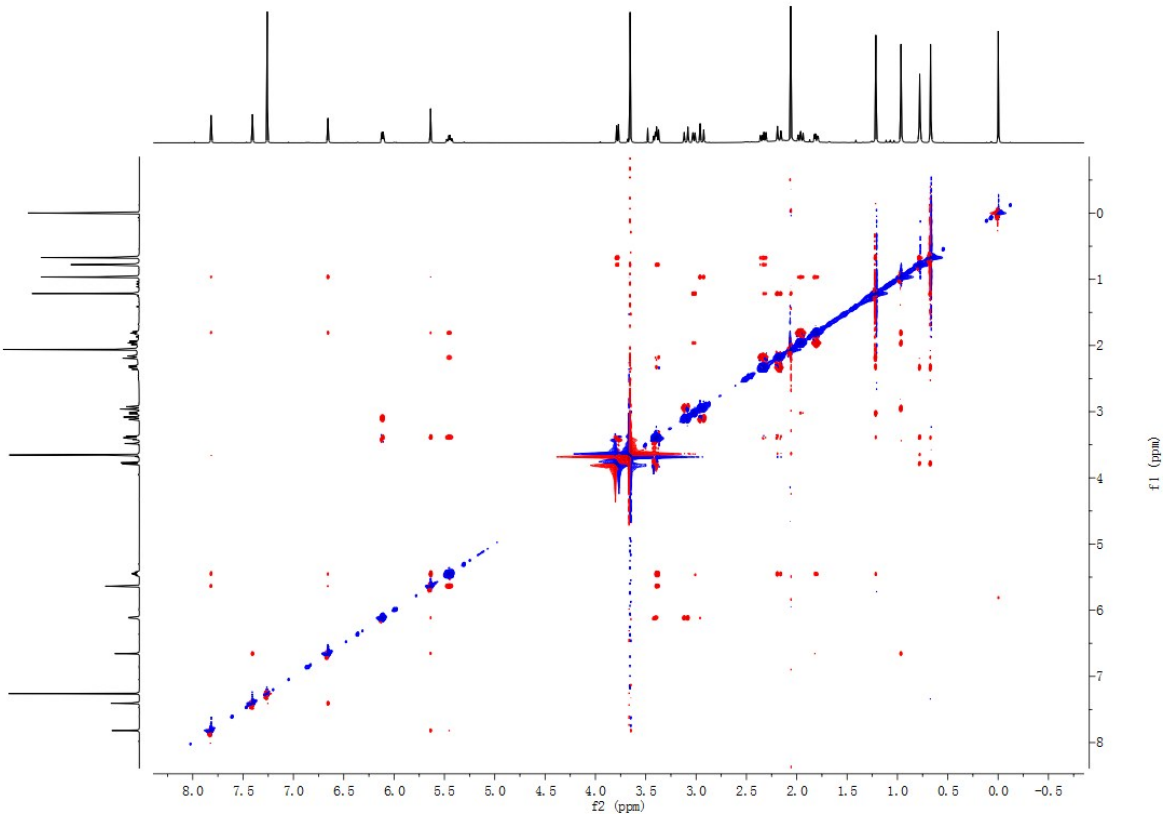
S12 HSQC of Khasenegasin B (**2**)



S13 HMBC of Khasenegasin B (**2**)

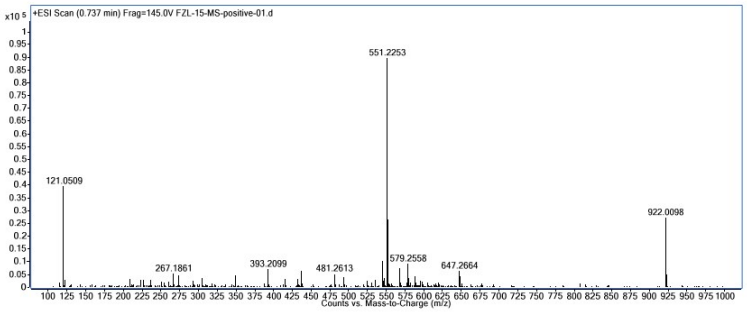


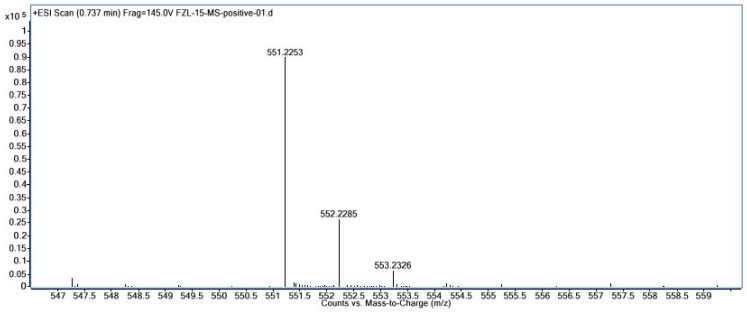
S14 ROSEY of Khasenegasin B (**2**)



Khasenegasin C (**3**)

S15 HR-ESI-MS of Khasenegasin C (**3**)

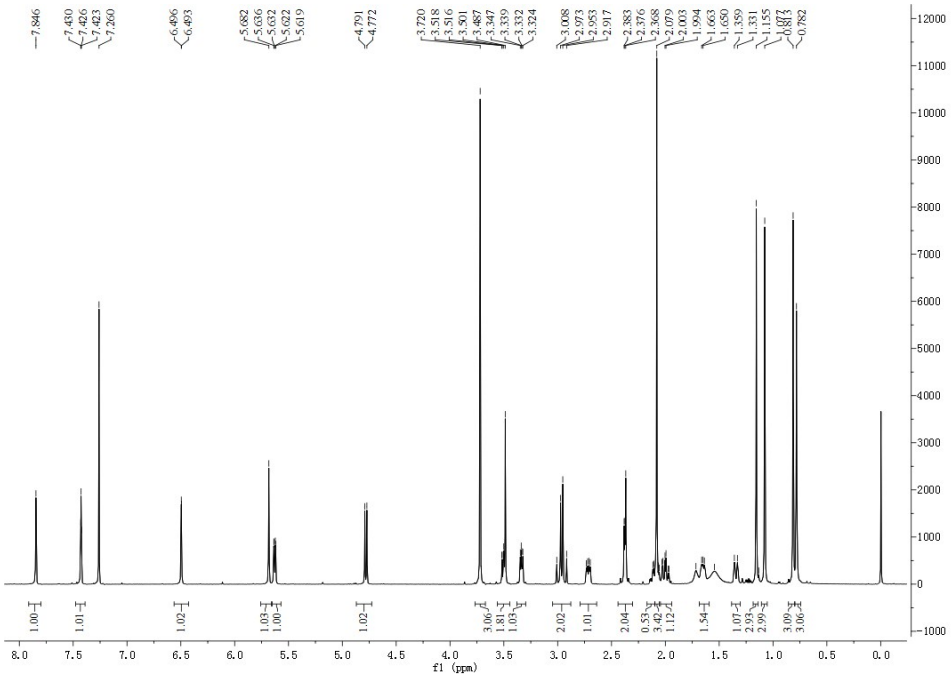




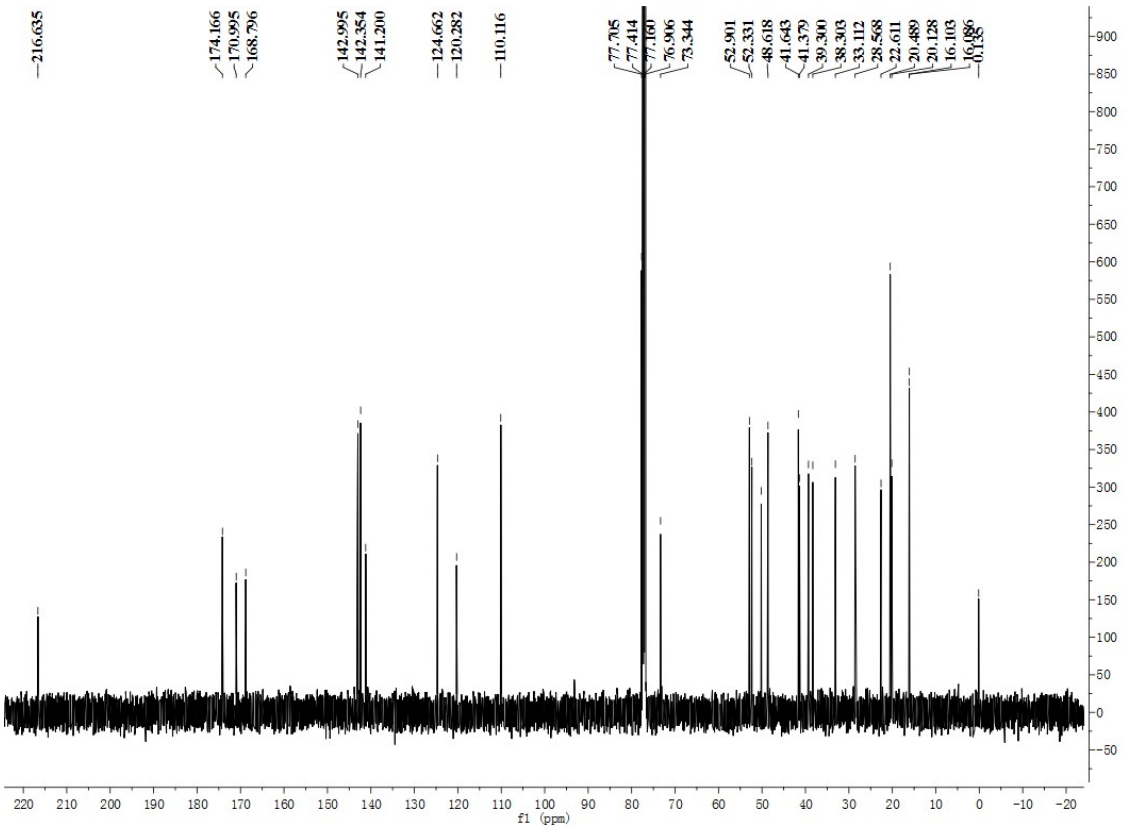
Elemental Composition Calculator

Target m/z:	551.2253	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C29H36NaO9		551.2252		-0.25	

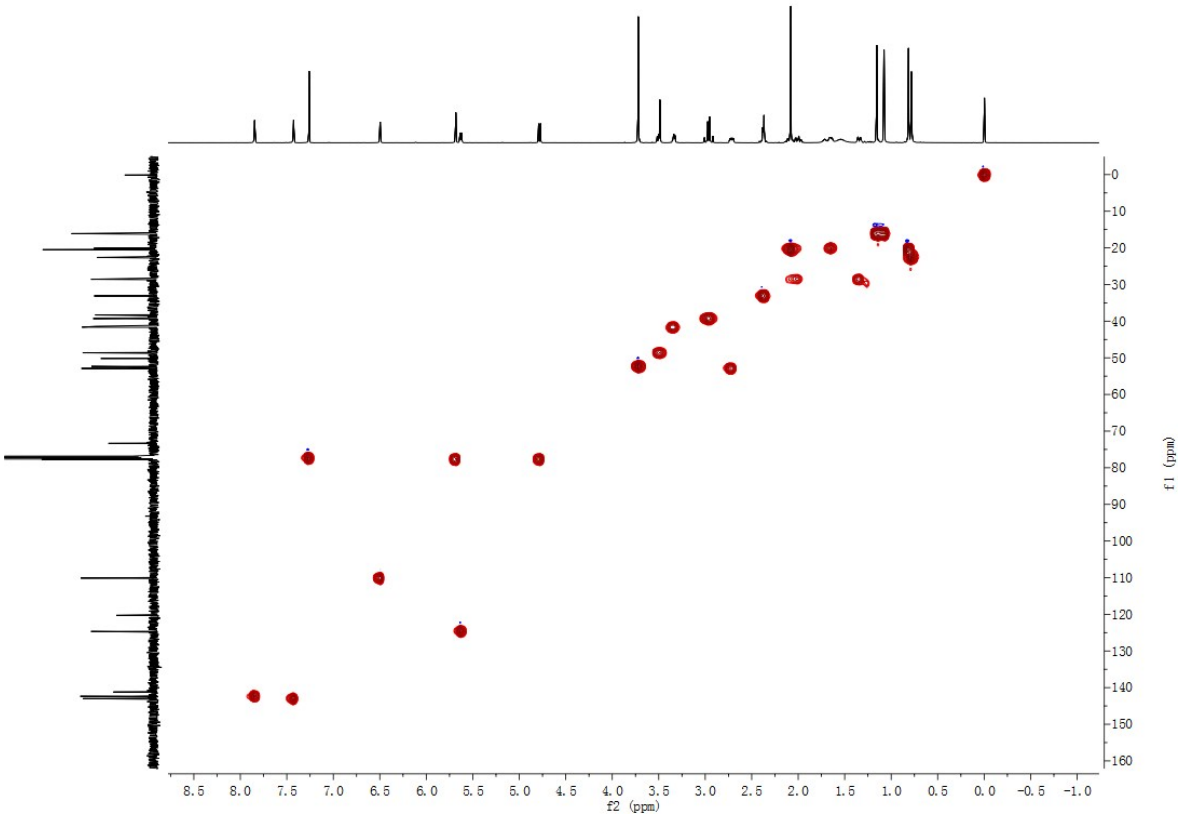
S16 ^{1}H NMR of Khasenegasin C (**3**)



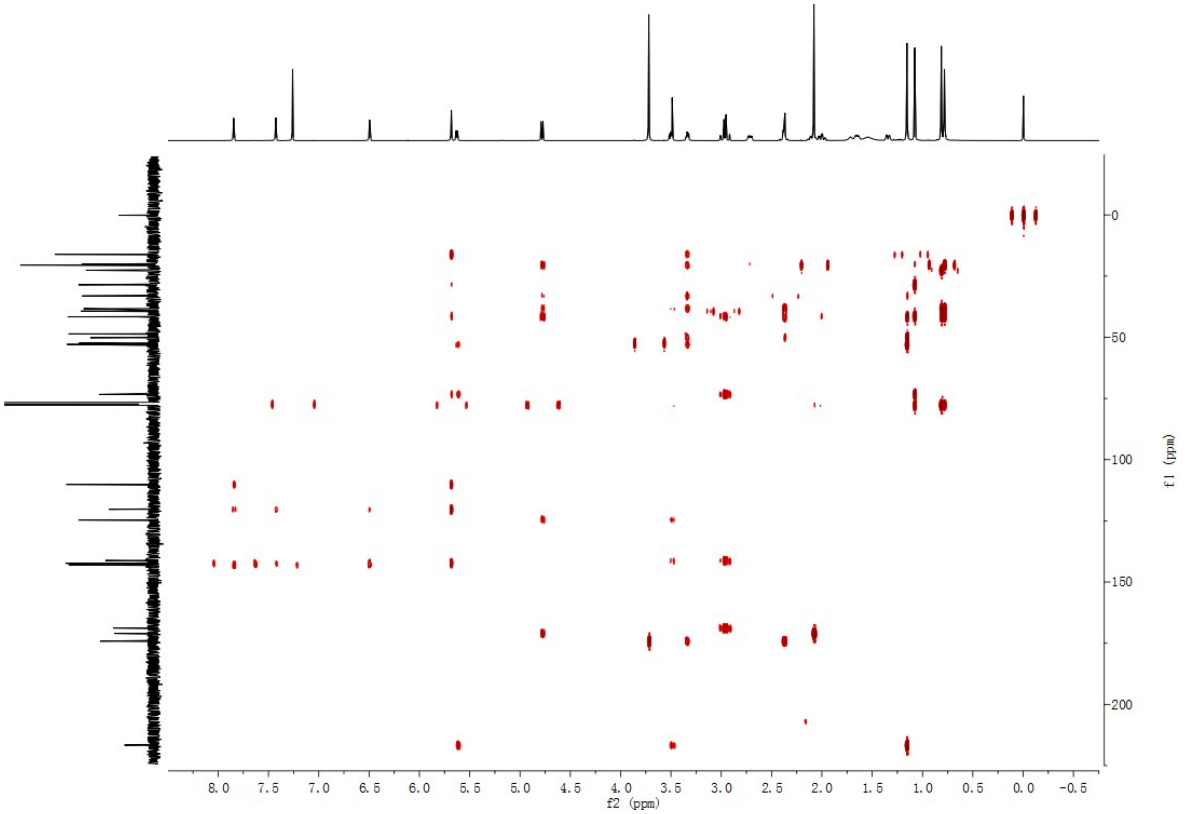
S17 ^{13}C NMR of Khasenegasin C (**3**)



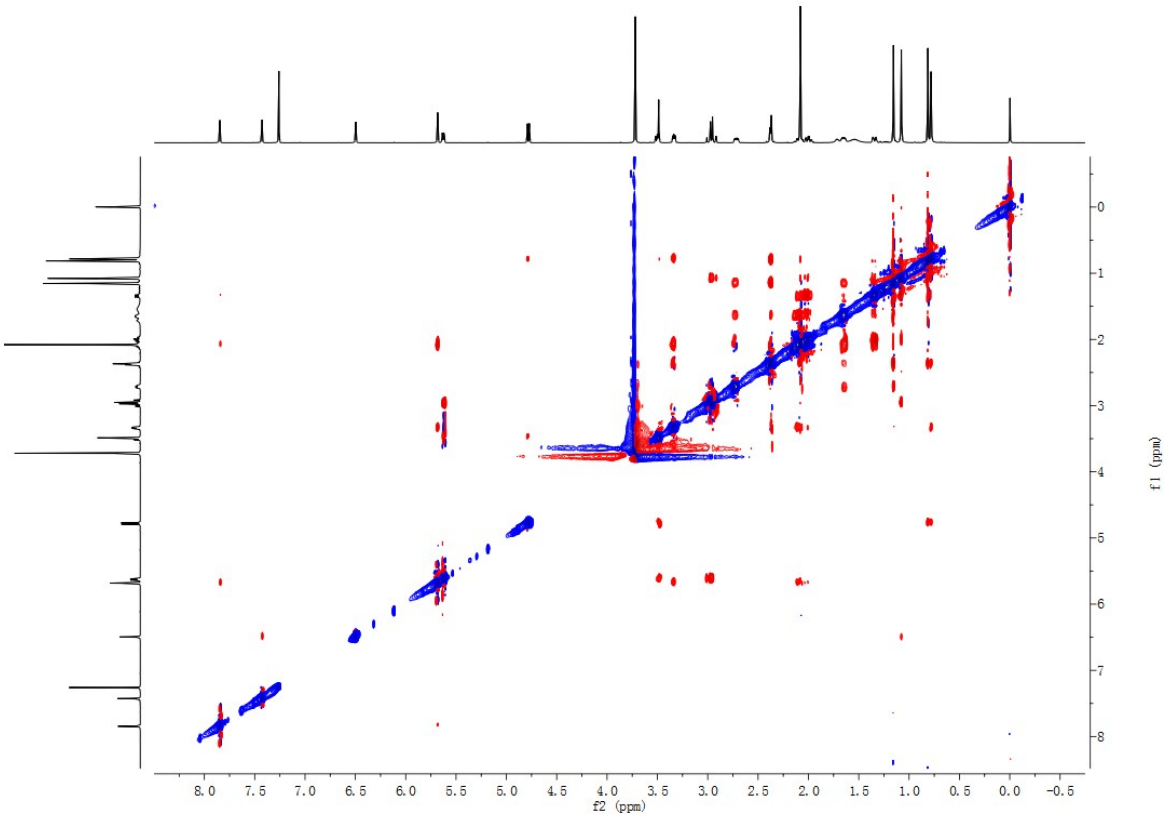
S18 HSQC of Khasenegasin C (**3**)



S19 HMBC of Khasenegasin C (**3**)

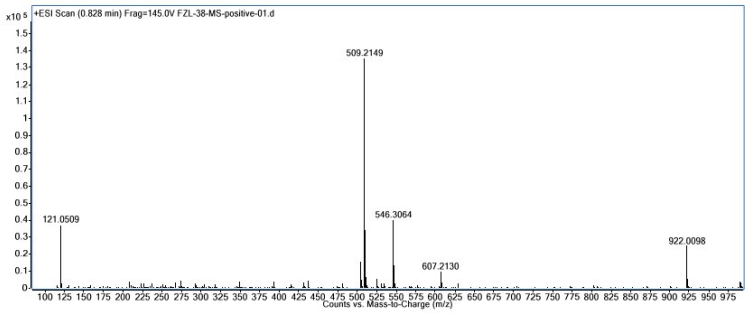


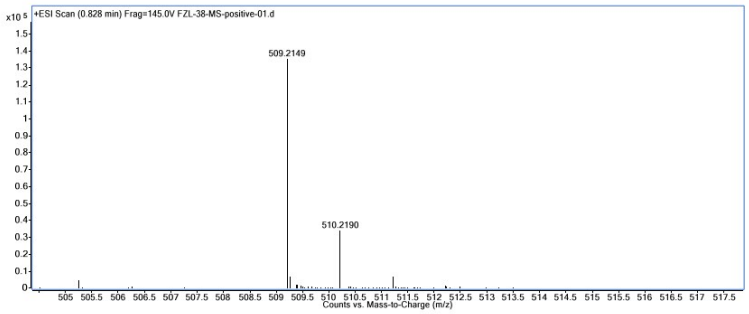
S20 ROSEY of Khasenegasin C (**3**)



Khasenegasin D (**4**)

S21 HR-ESI-MS of Khasenegasin D (**4**)

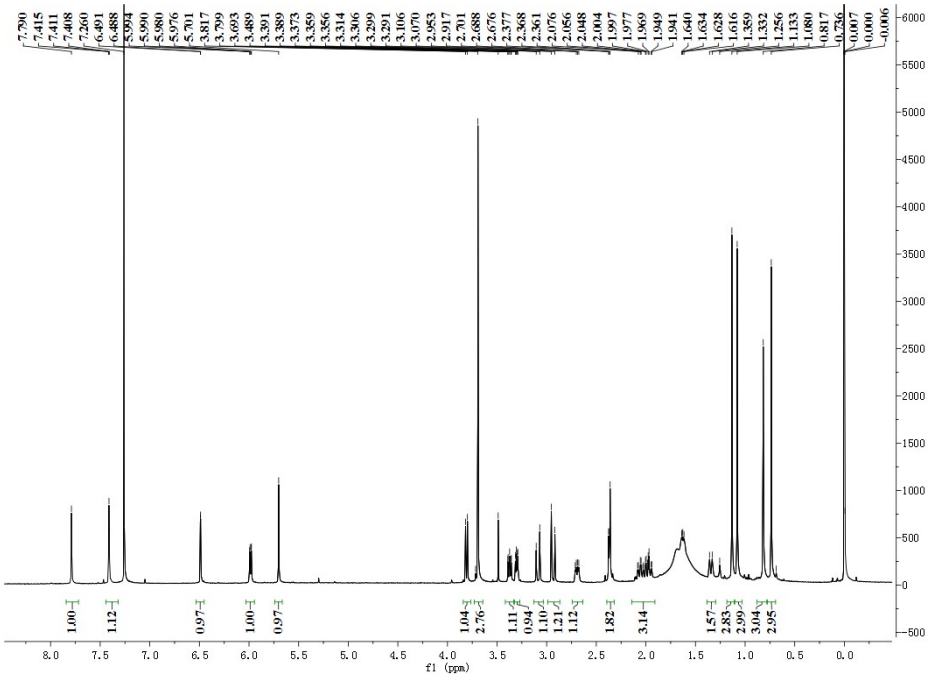




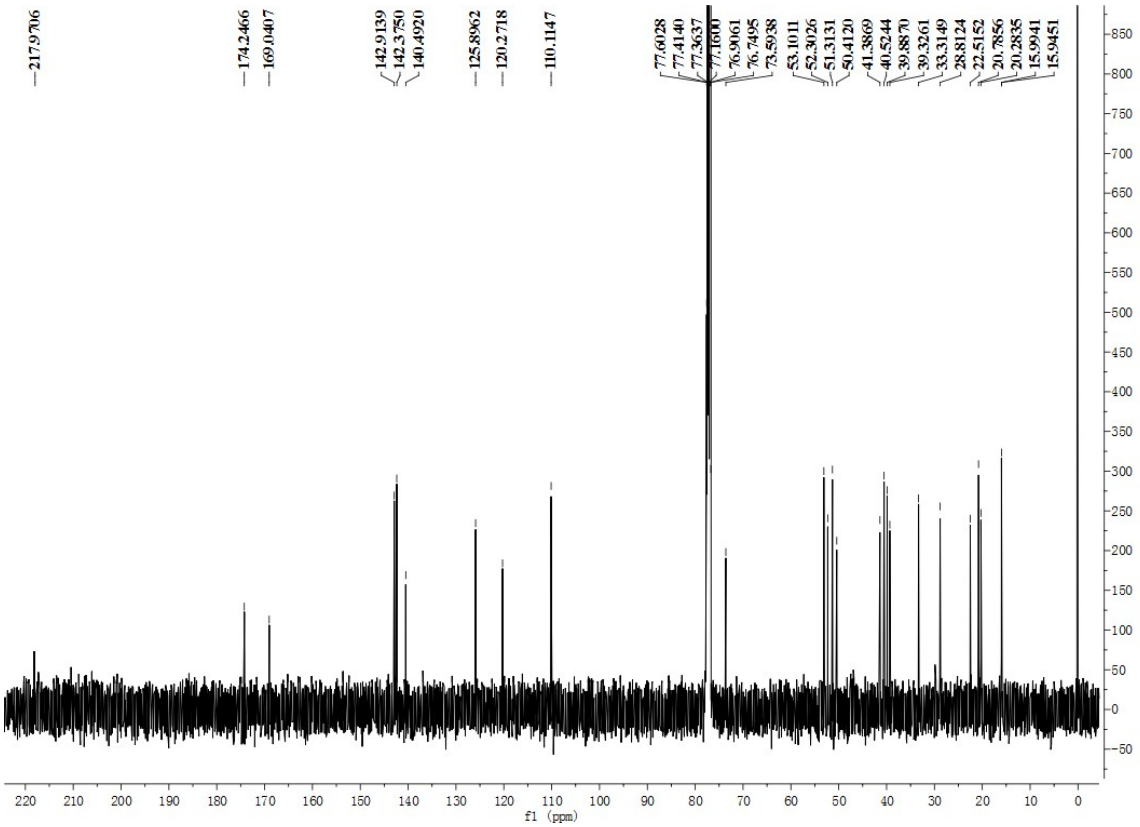
Elemental Composition Calculator

Target m/z:	509.2149	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C27H34NaO8		509.2146		-0.64	

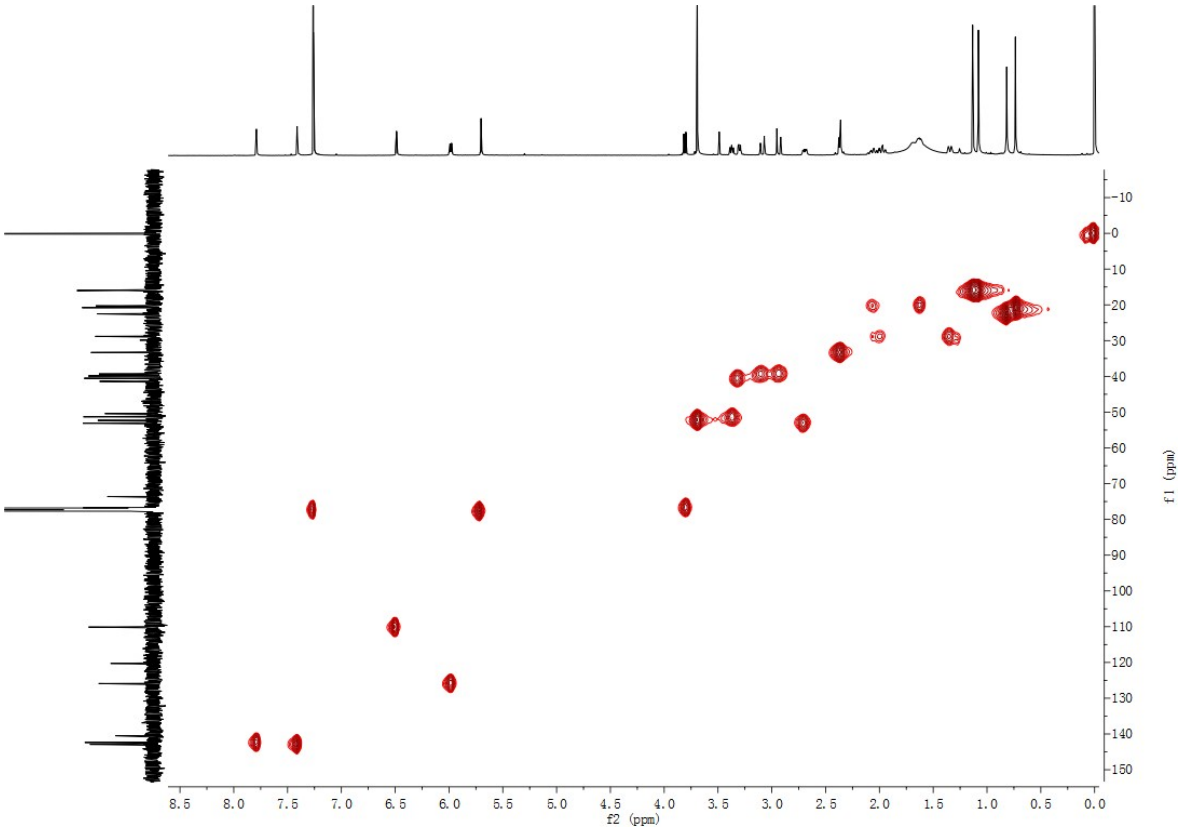
S22 ^{1}H NMR of Khasenegasin D (**4**)



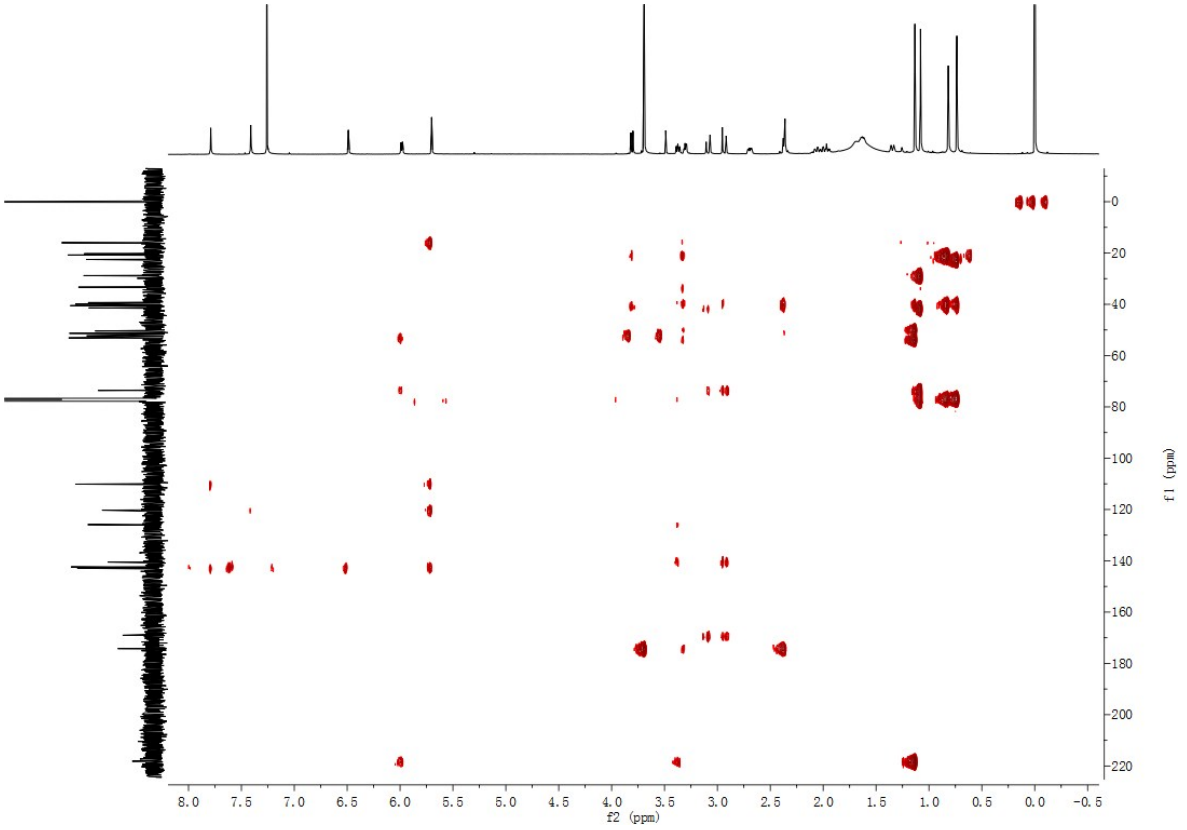
S23 ^{13}C NMR of Khasenegasin D (**4**)



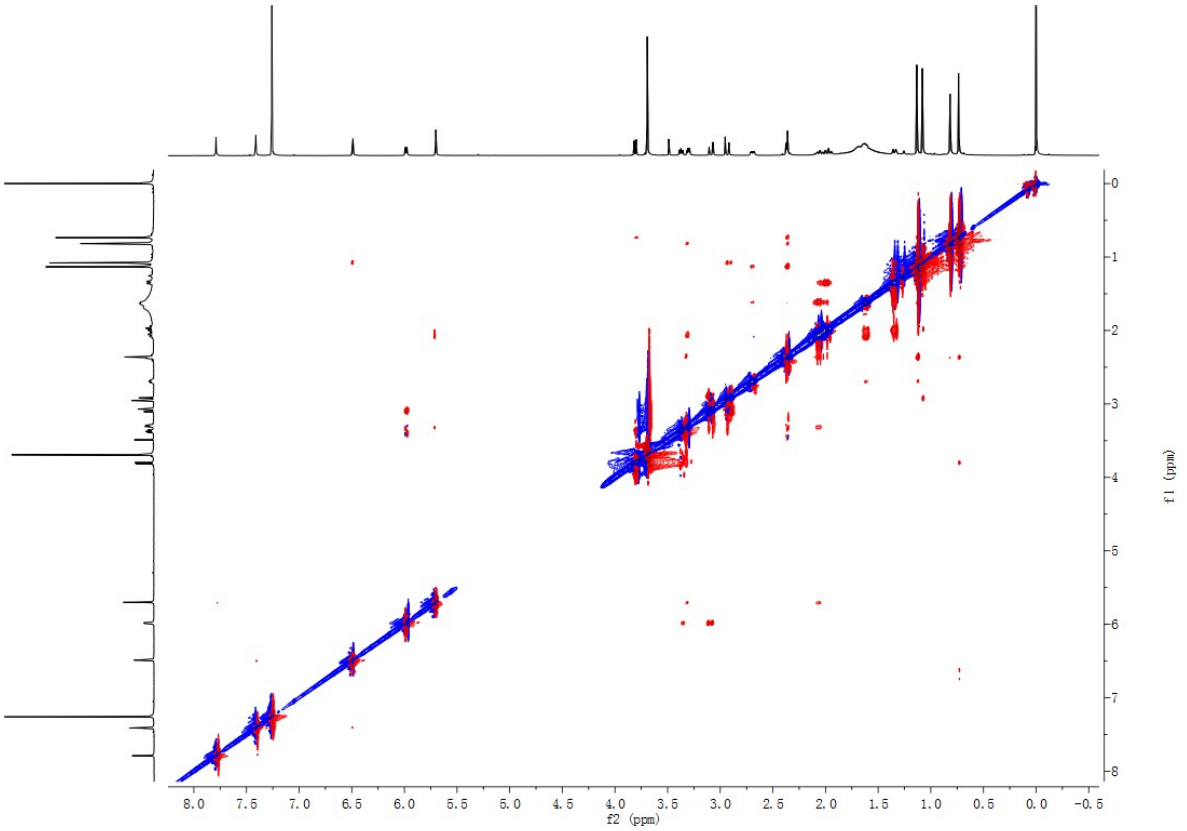
S24 HSQC of Khasenegasin D (**4**)



S25 HMBC of Khasenegasin D (**4**)

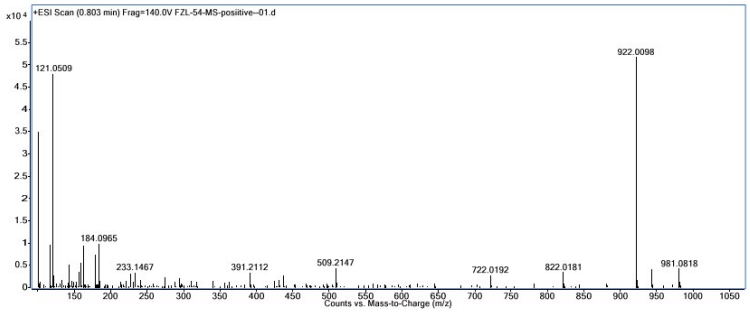


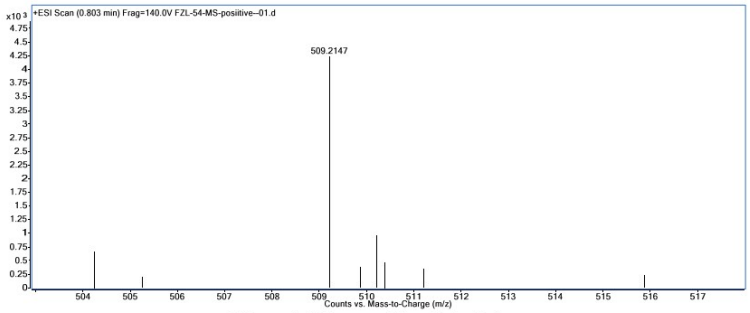
S26 ROSEY of Khasenegasin D (**4**)



Khasenegasin E (**5**)

S27 HR-ESI-MS of Khasenegasin E (**5**)

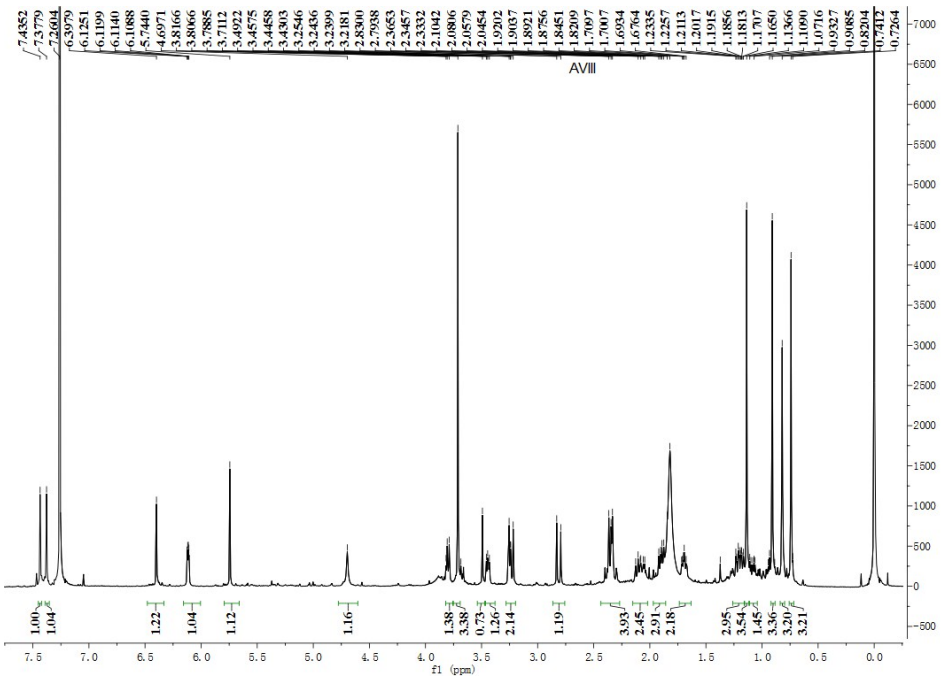




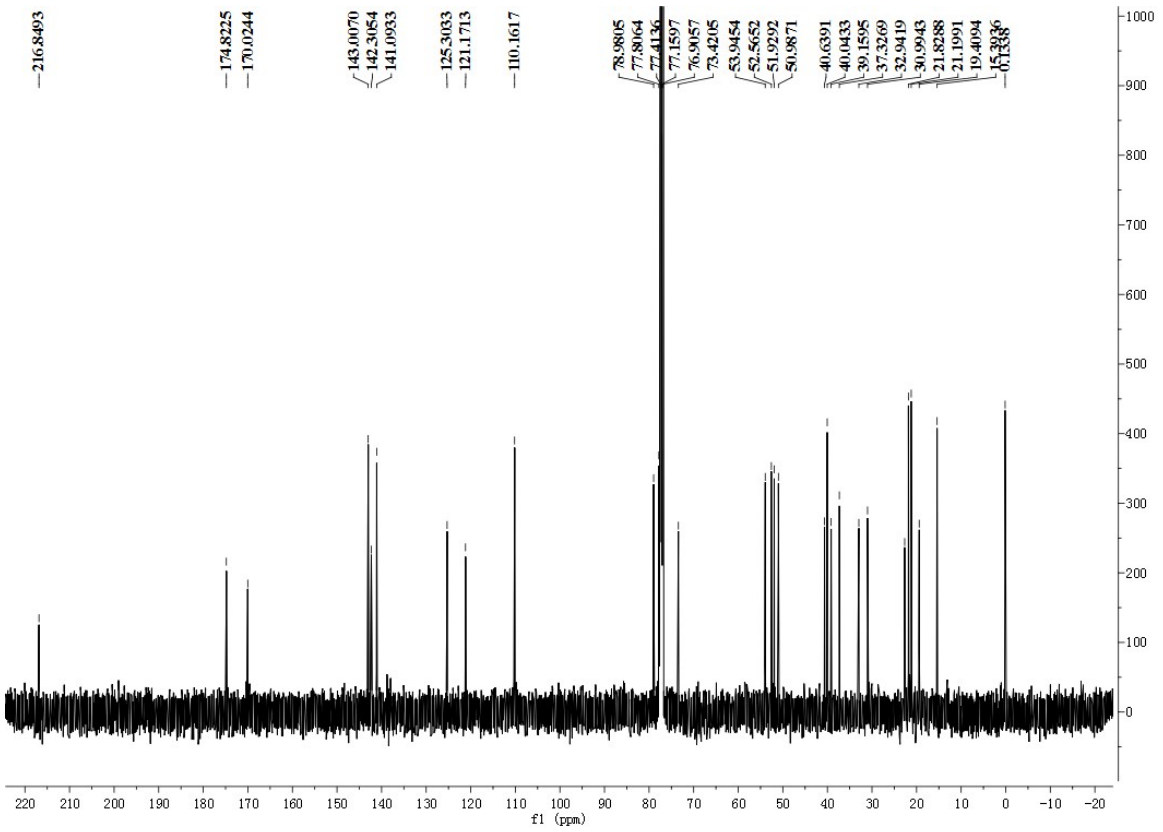
Elemental Composition Calculator

Target m/z:	509.2147	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C27H34NaO8		509.2146		-0.27	

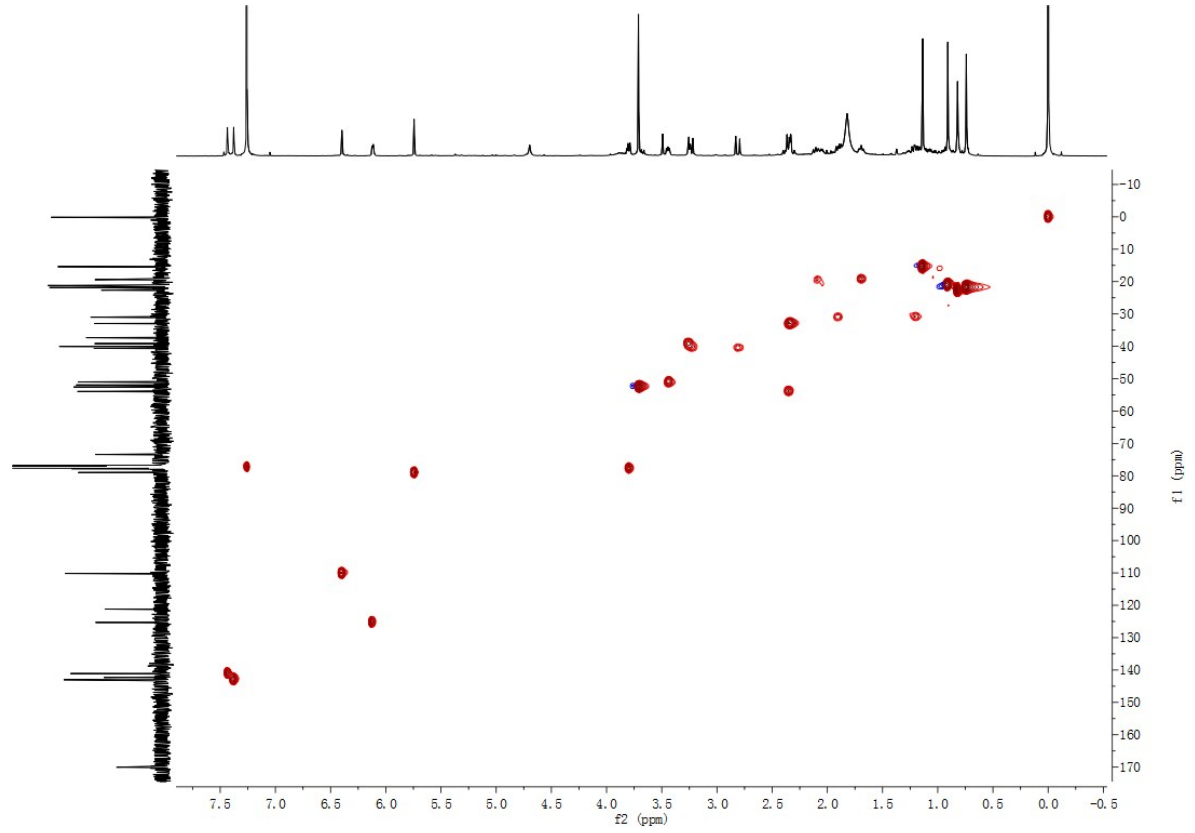
S28 ^{1}H NMR of Khasenegasin E (**5**)



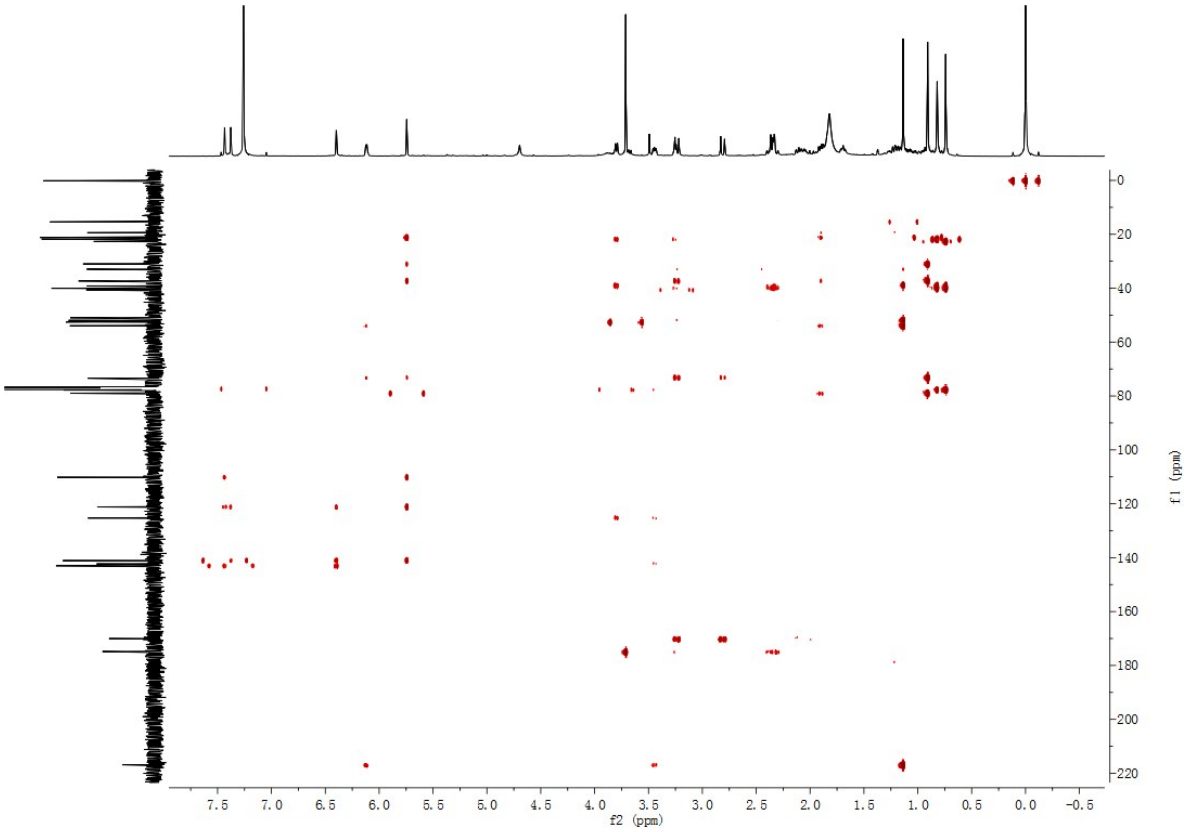
S29 ^{13}C NMR of Khasenegasin E (**5**)



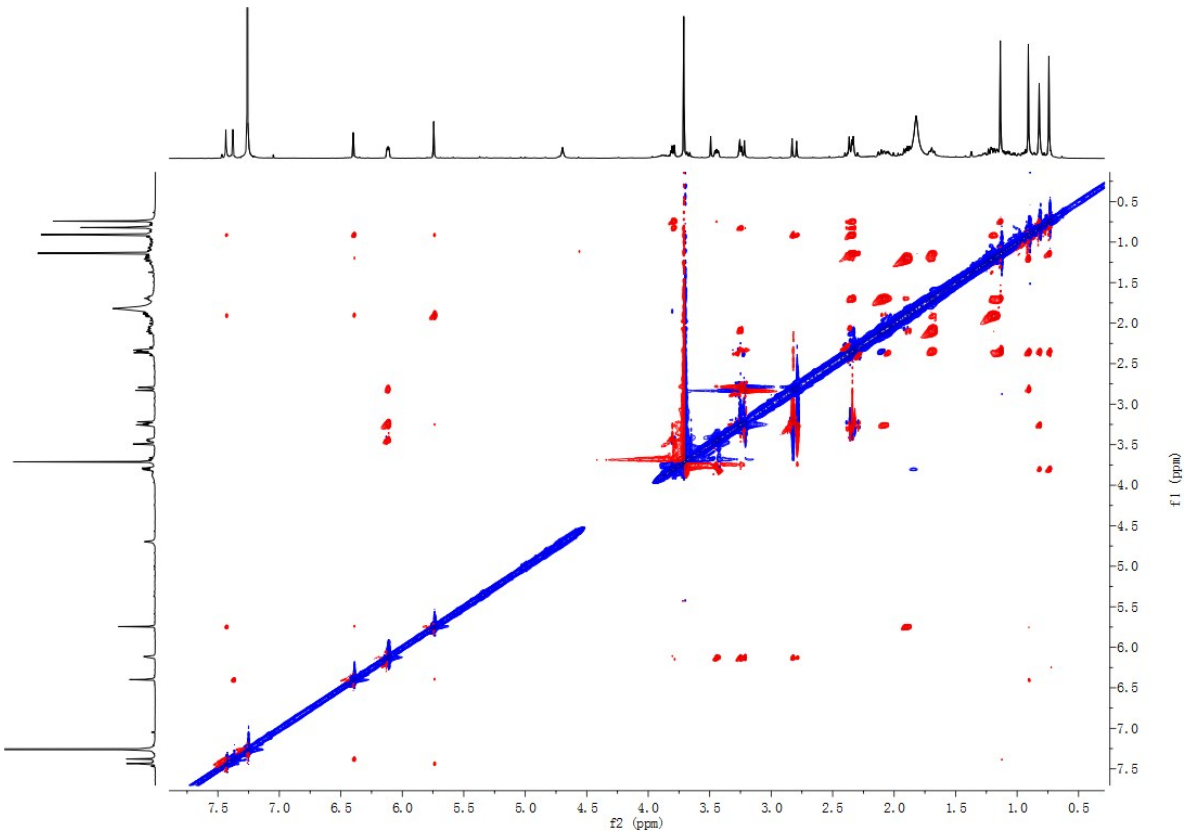
S30 HSQC of Khasenegasin E (**5**)



S31 HMBC of Khasenegasin E (**5**)

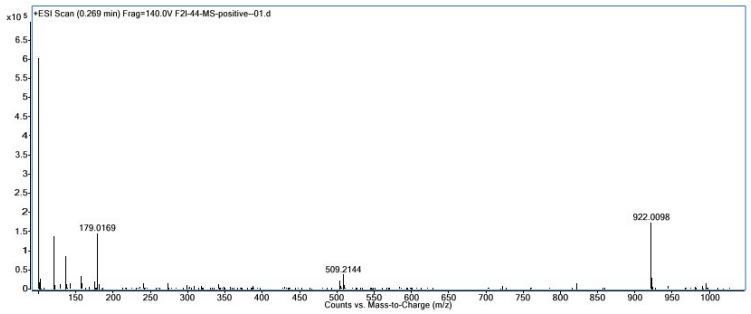


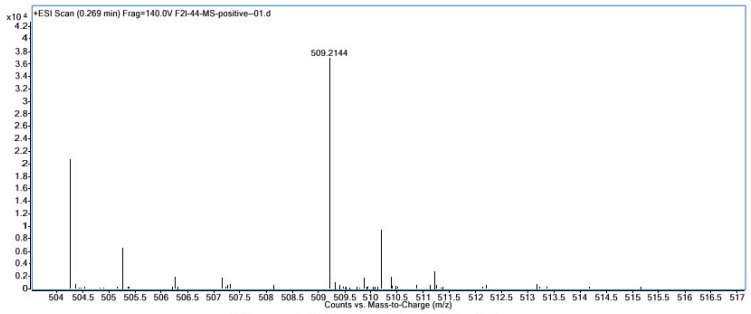
S32 ROSEY of Khasenegasin E (**5**)



Khasenegasin F (**6**)

S33 HR-ESI-MS of Khasenegasin F (**6**)

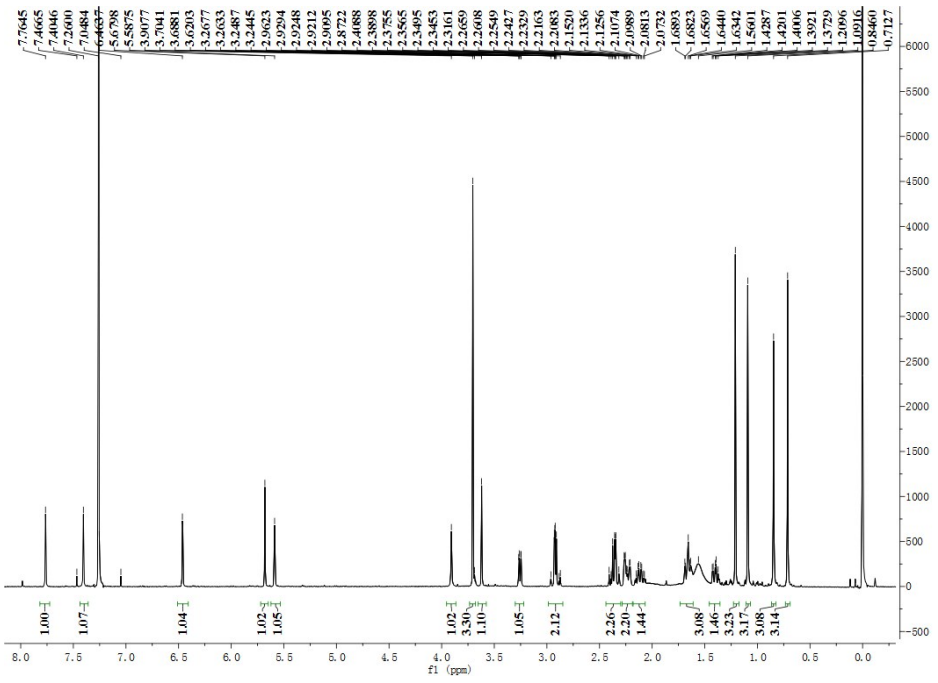




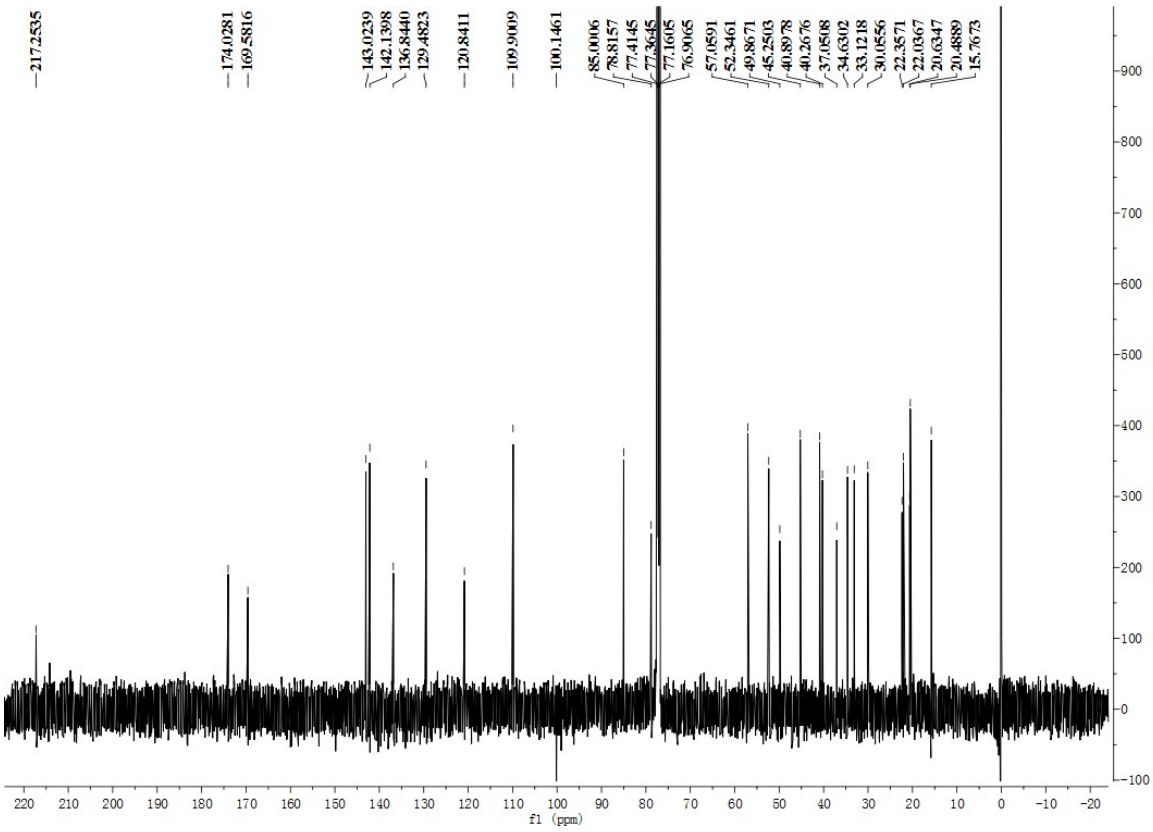
Elemental Composition Calculator

Target m/z:	509.2144	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C27H34NaO8		509.2146		0.42	

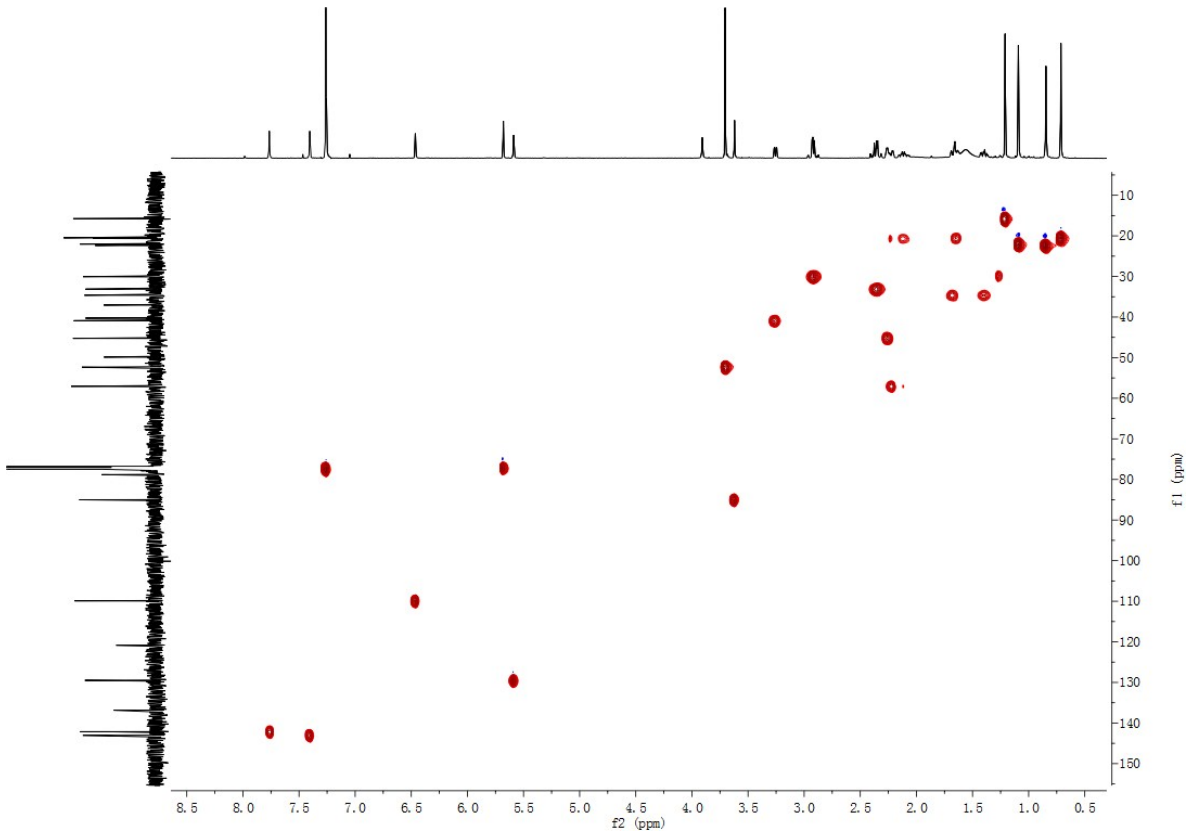
S34 ^{1}H NMR of Khasenegasin F (**6**)



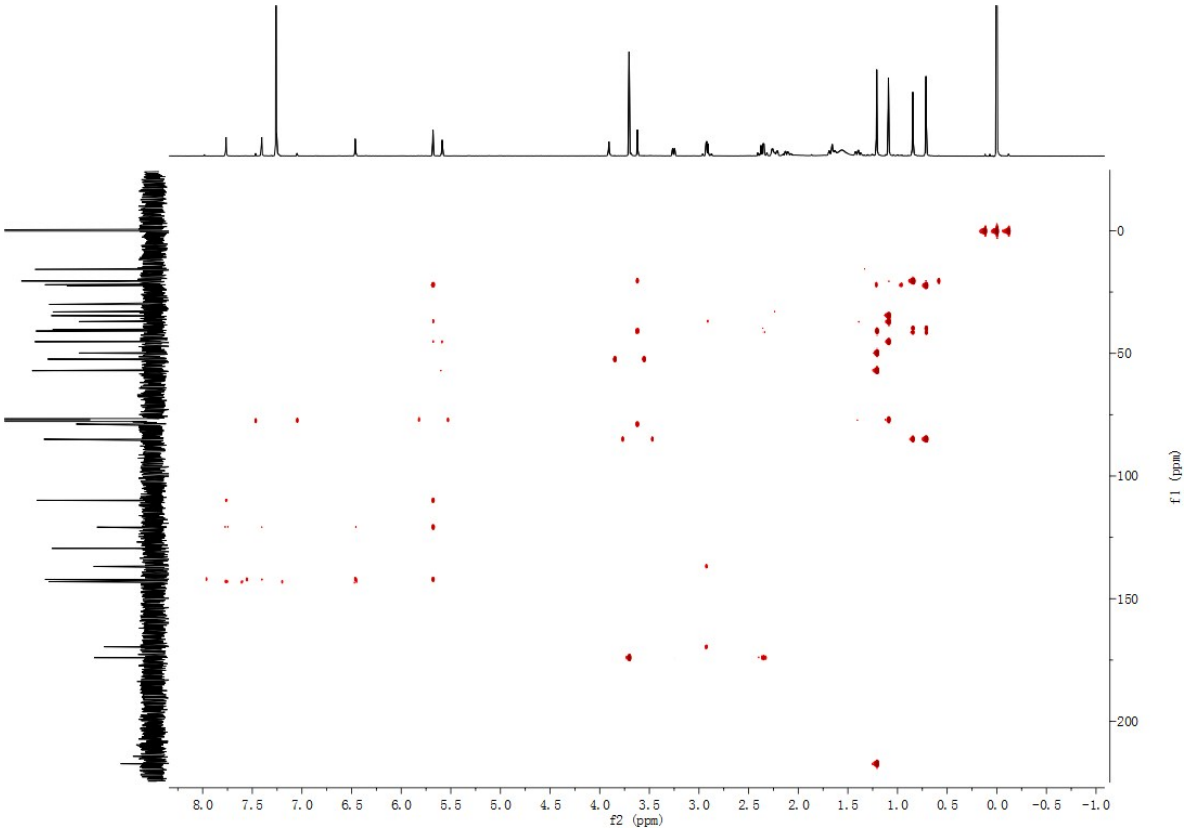
S35 ^{13}C NMR of Khasenegasin F (**6**)



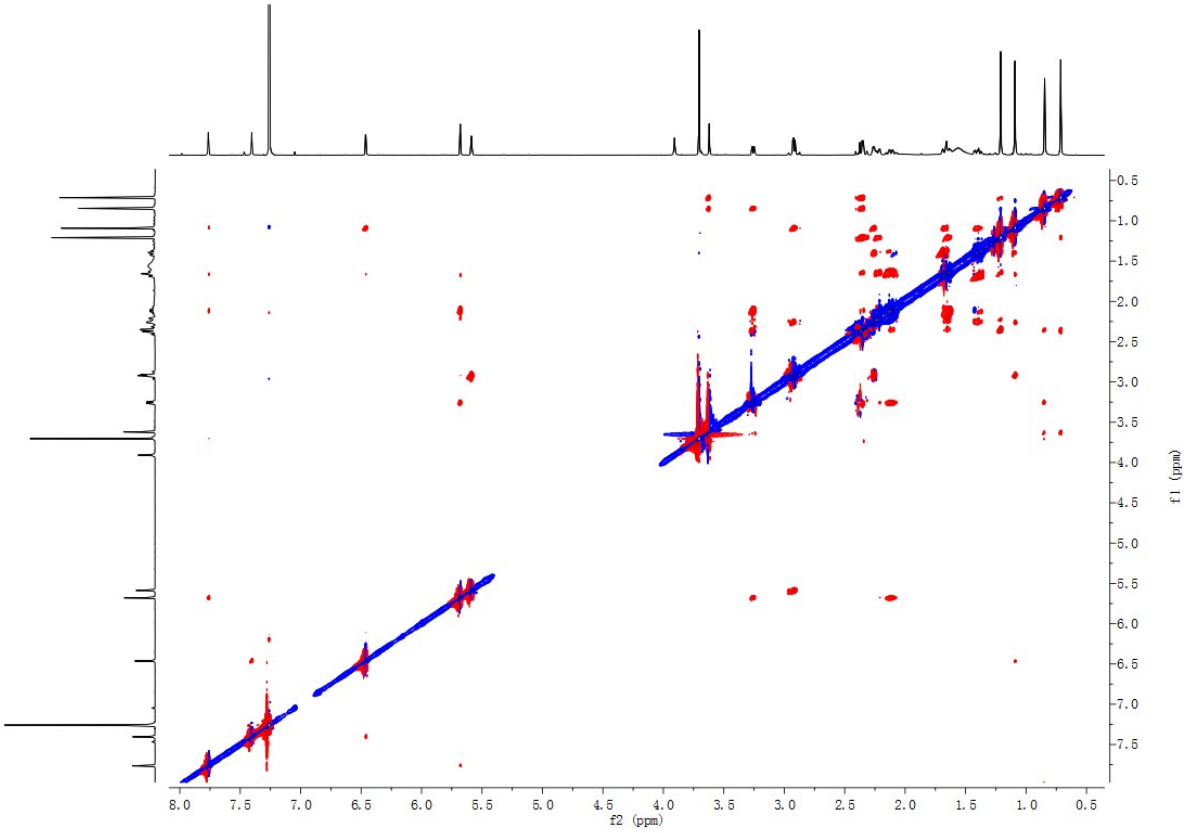
S36 HSQC of Khasenegasin F (**6**)



S37 HMBC of Khasenegasin F (**6**)

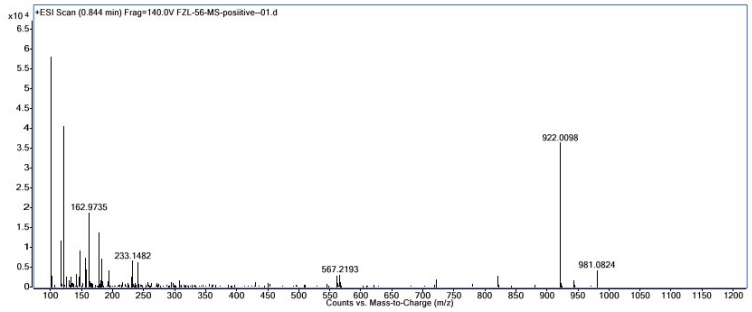


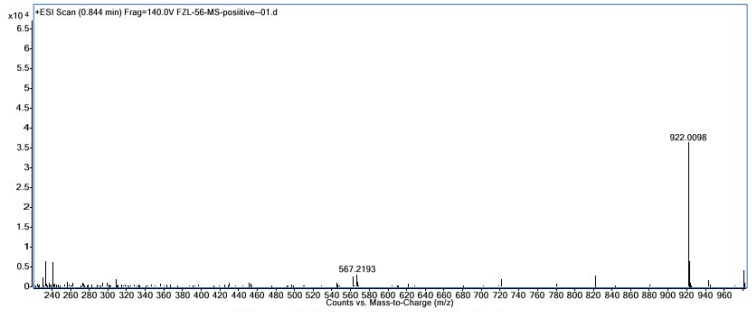
S38 ROSEY of Khasenegasin F (**6**)



Khasenegasin F (**7**)

S39 HR-ESI-MS of Khasenegasin F (**7**)

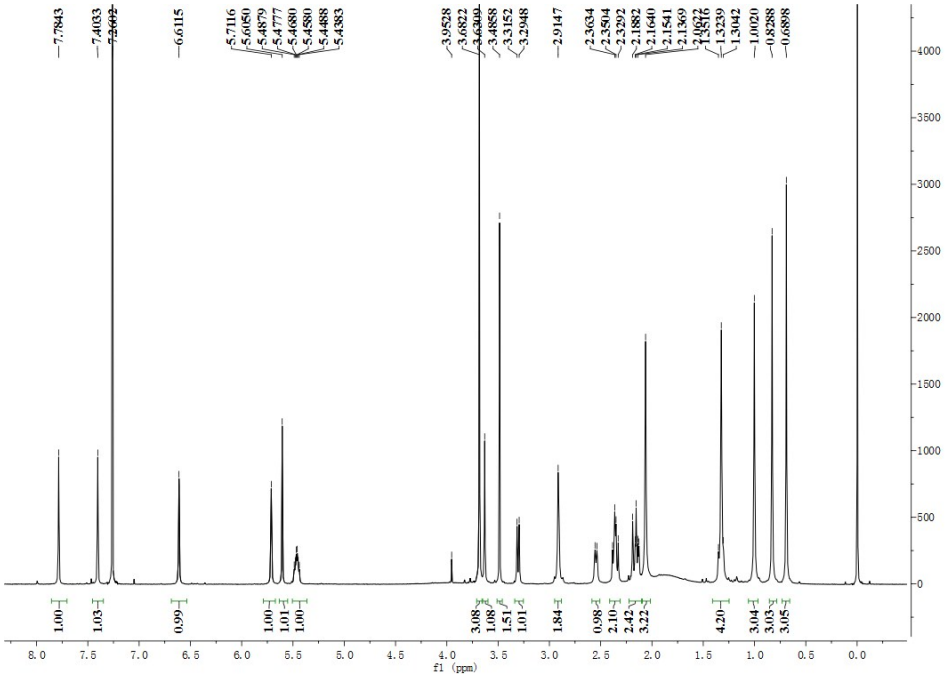




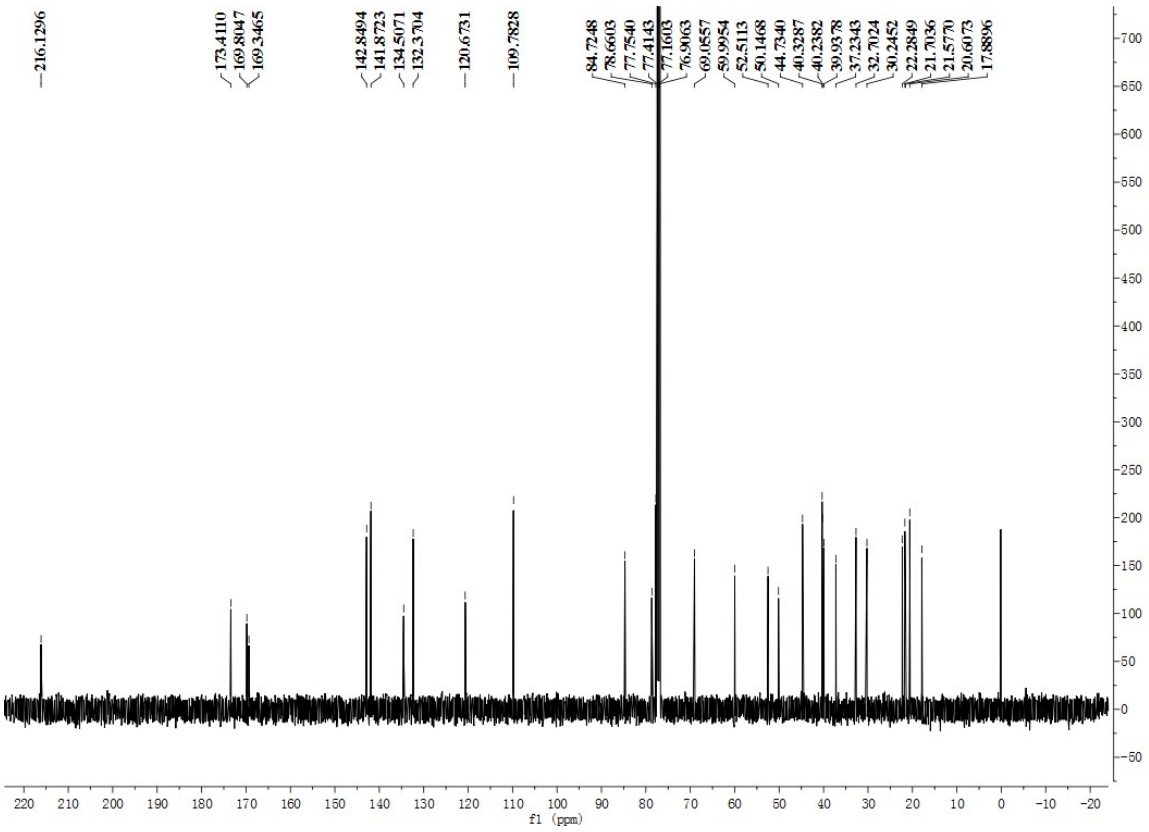
Elemental Composition Calculator

Target m/z:	567.2196	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C29H36NaO10		567.2201		0.81	

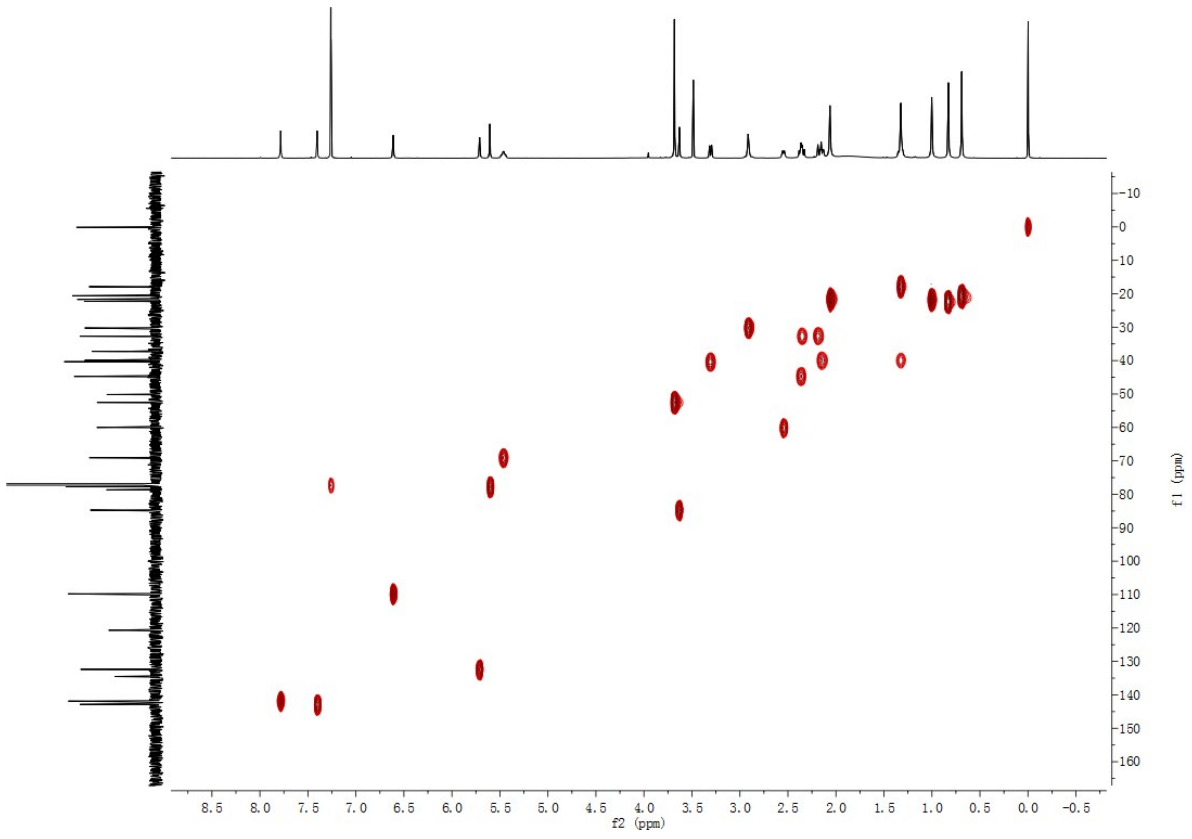
S40 ^{1}H NMR of Khasenegasin F (**7**)



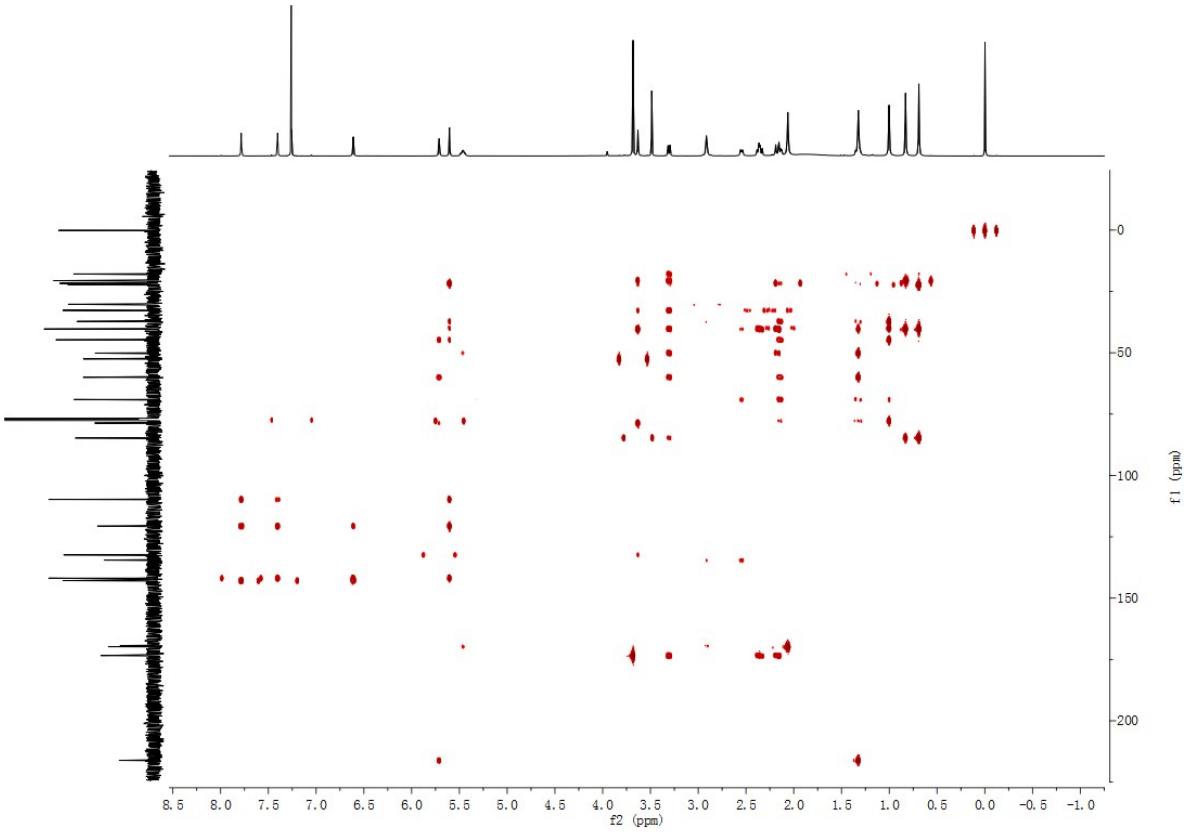
S41 ^{13}C NMR of Khasenegasin F (**7**)



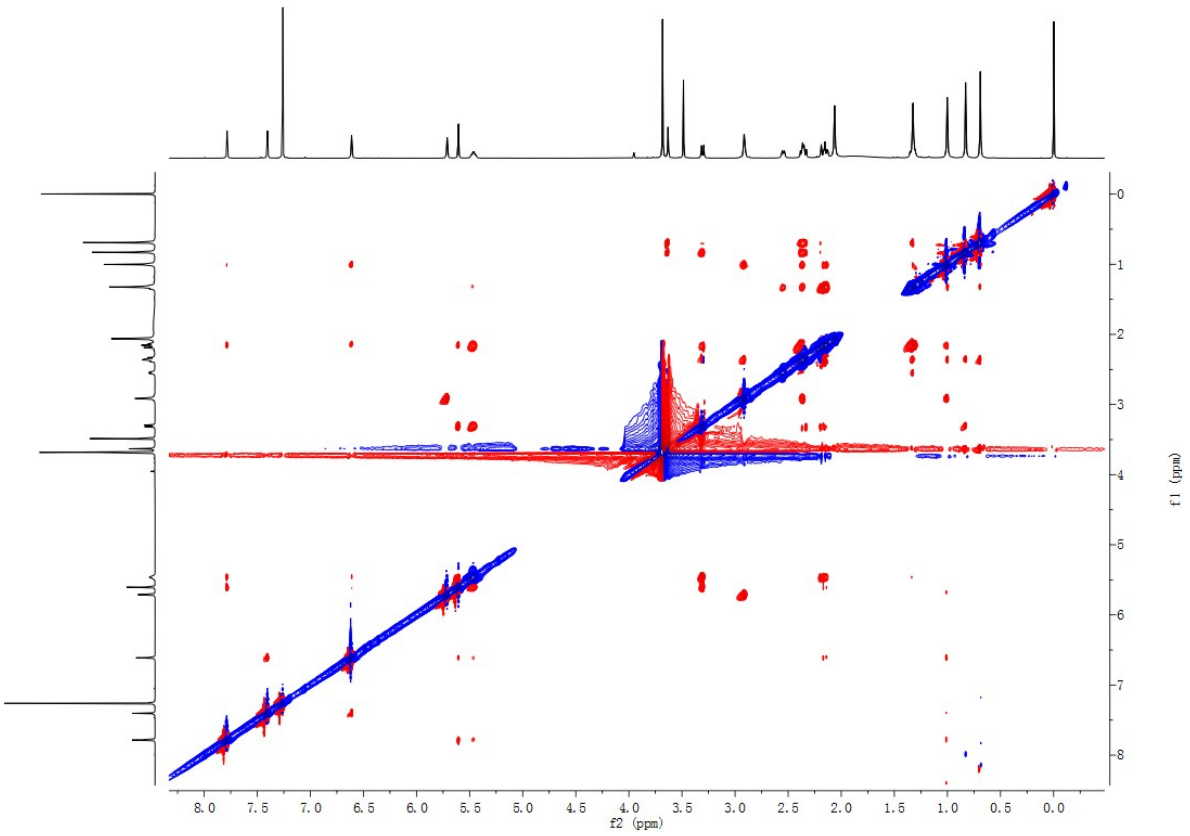
S42 HSQC of Khasenegasin F (**7**)



S43 HMBC of Khasenegasin F (**7**)

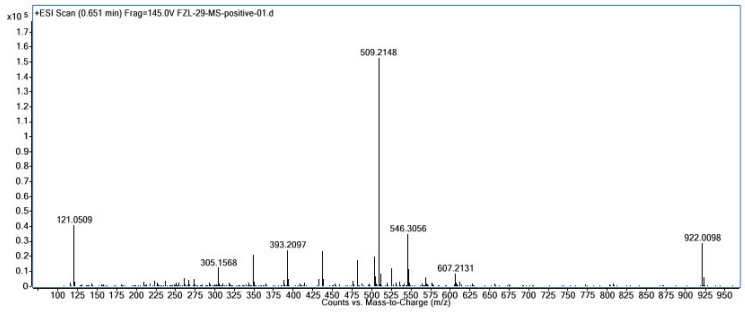


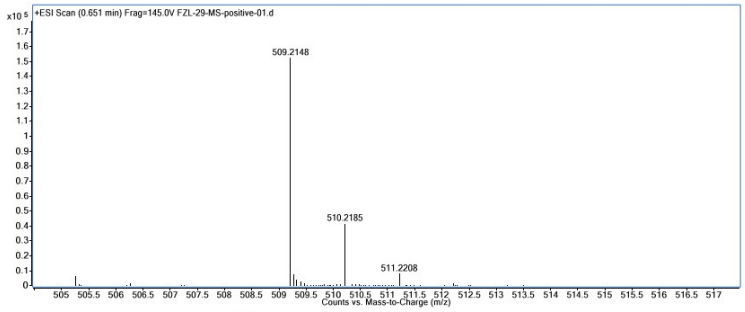
S44 ROSEY of Khasenegasin F (**7**)



Khasenegasin H (**8**)

S45 HR-ESI-MS of Khasenegasin H (**8**)

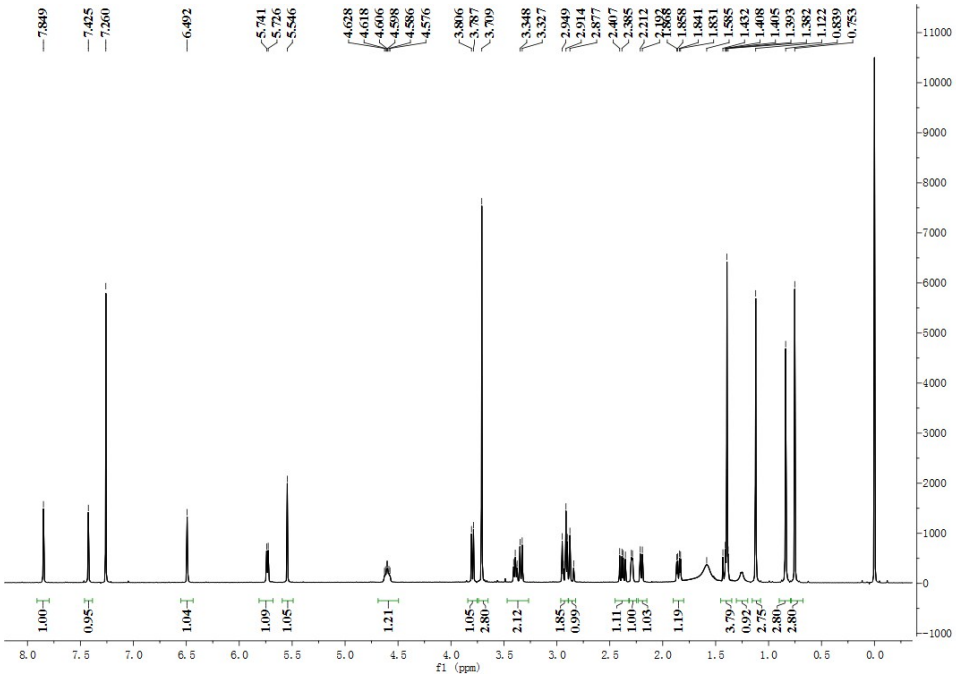




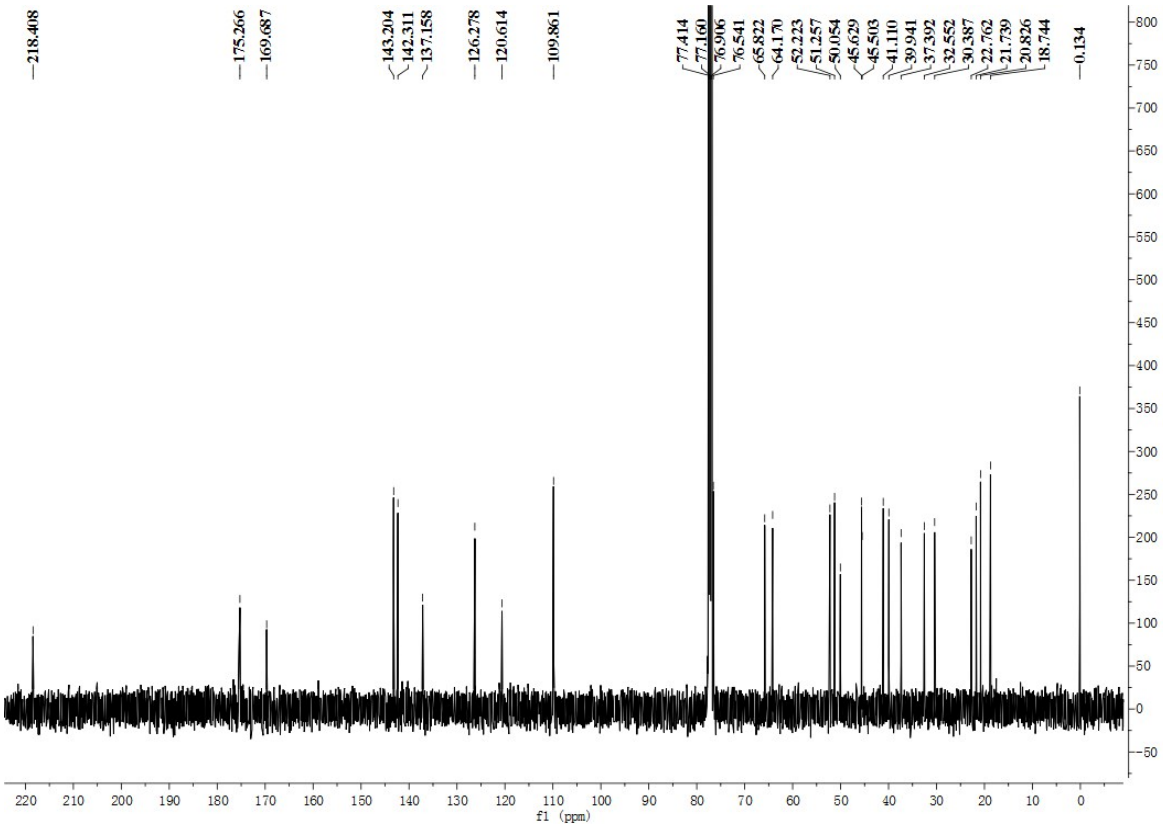
Elemental Composition Calculator

Target m/z:	509.2148	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C27H34NaO8		509.2146		-0.38	

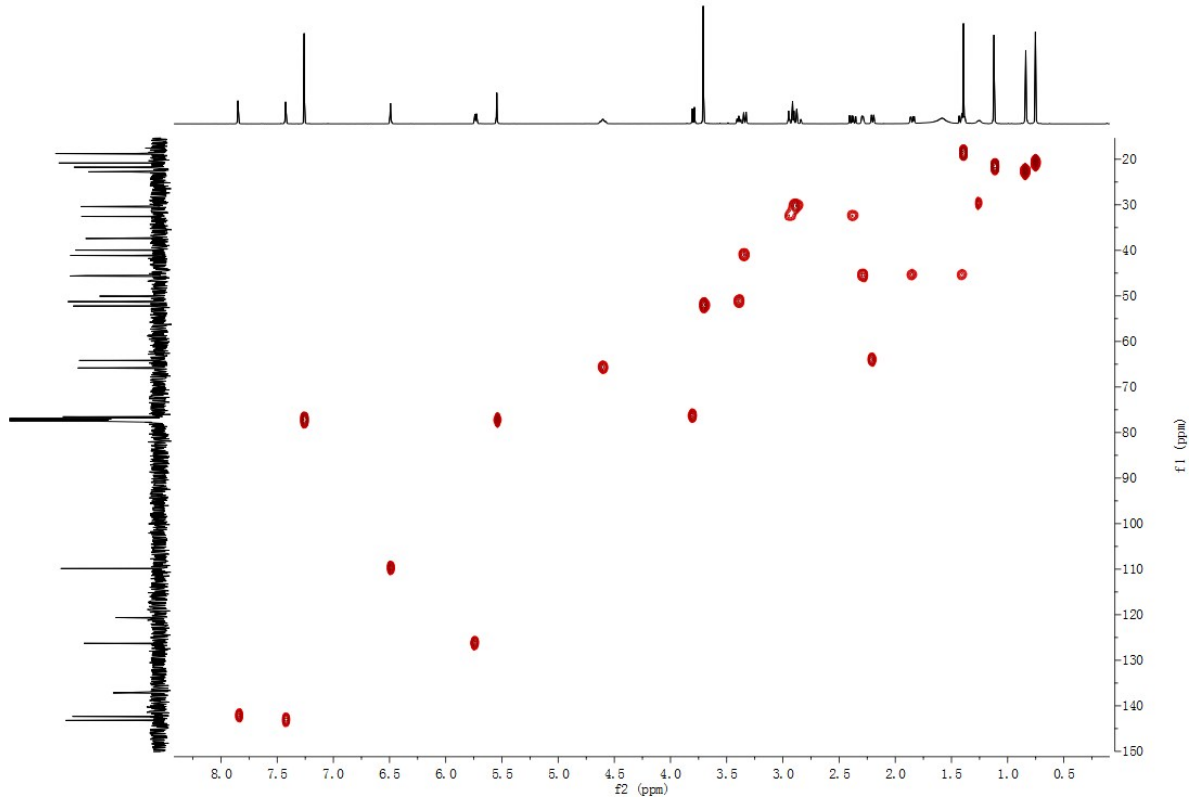
S46 ^{1}H NMR of Khasenegasin H (**8**)



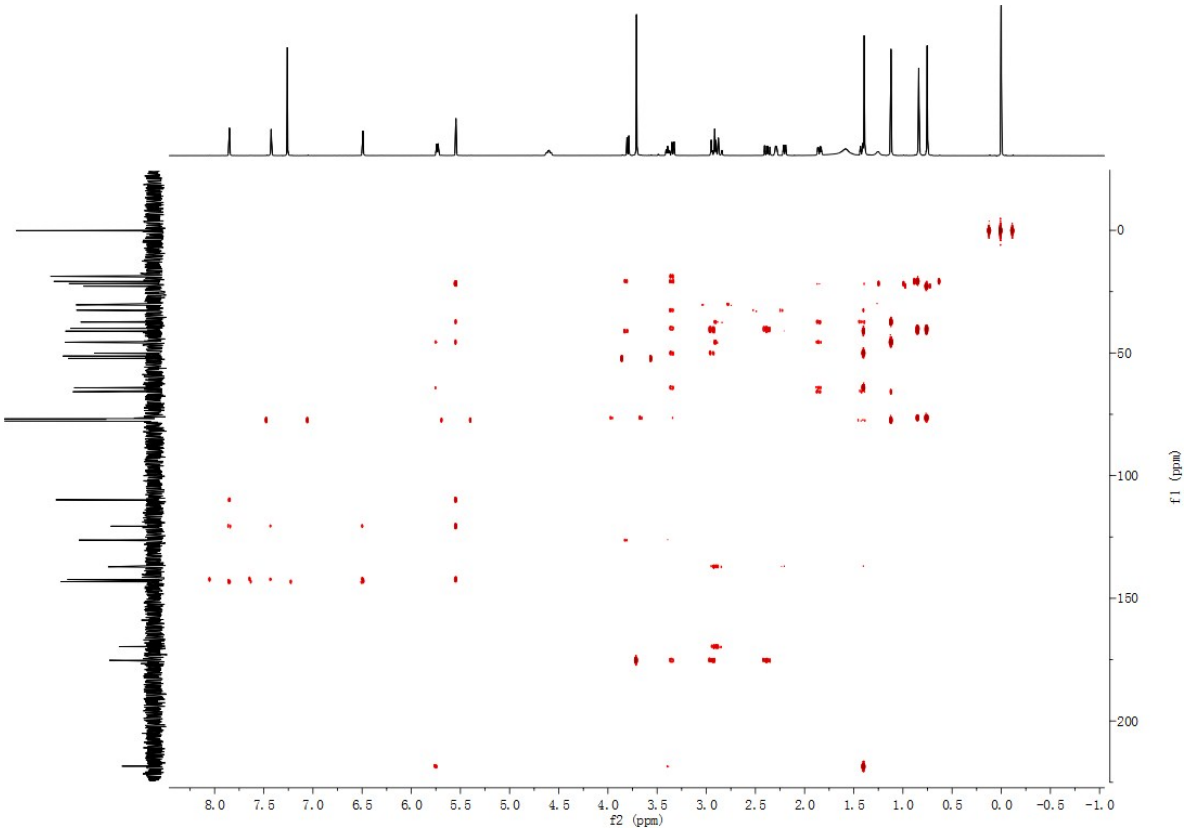
S47 ^{13}C NMR of Khasenegasin H (**8**)



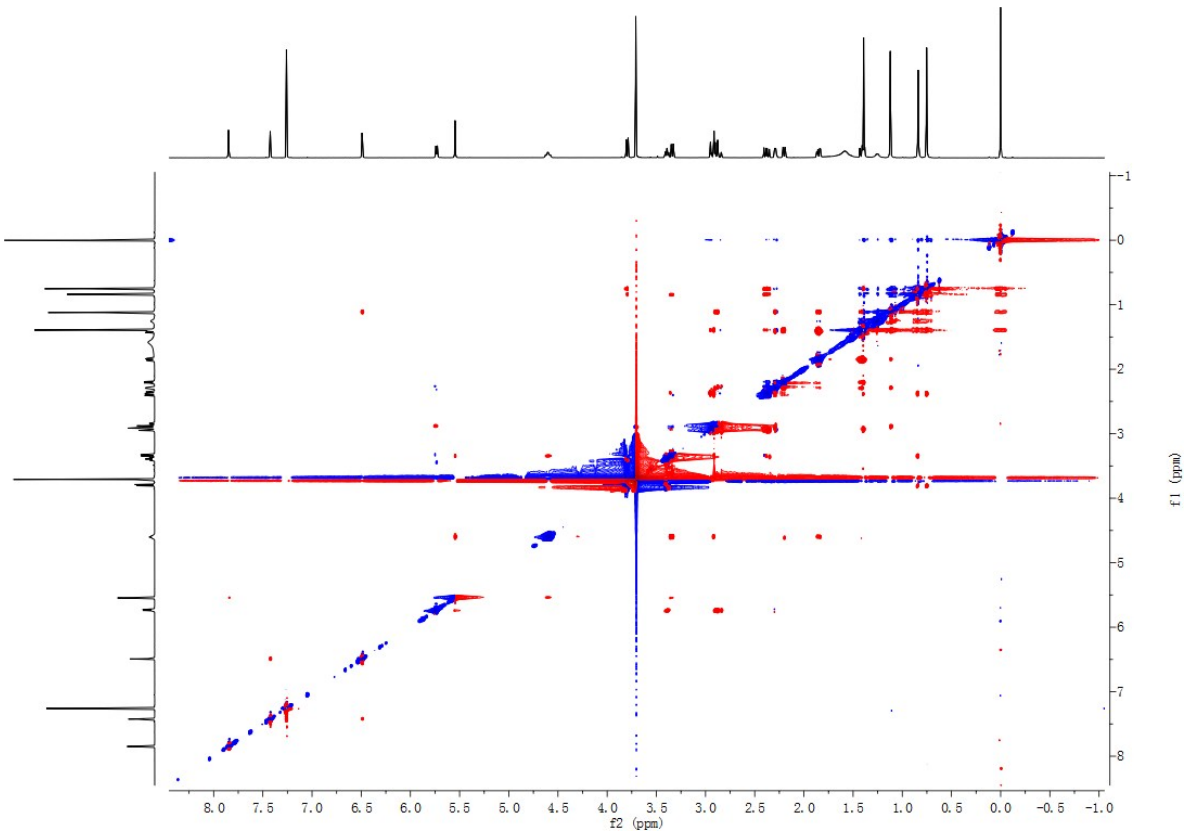
S48 HSQC of Khasenegasin H (**8**)



S49 HMBC of Khasenegasin H (**8**)

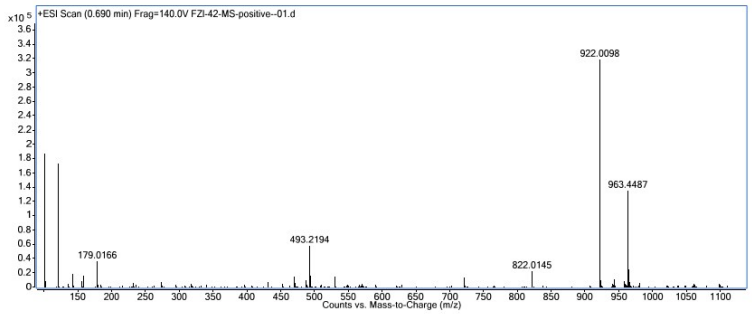


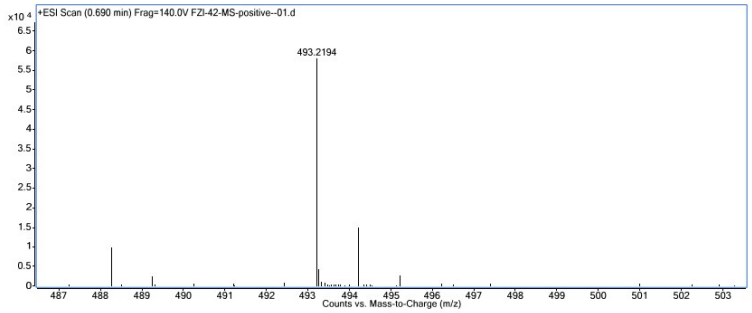
S50 ROSEY of Khasenegasin H (**8**)



Khasenegasin I (**9**)

S51 HR-ESI-MS of Khasenegasin I (**9**)

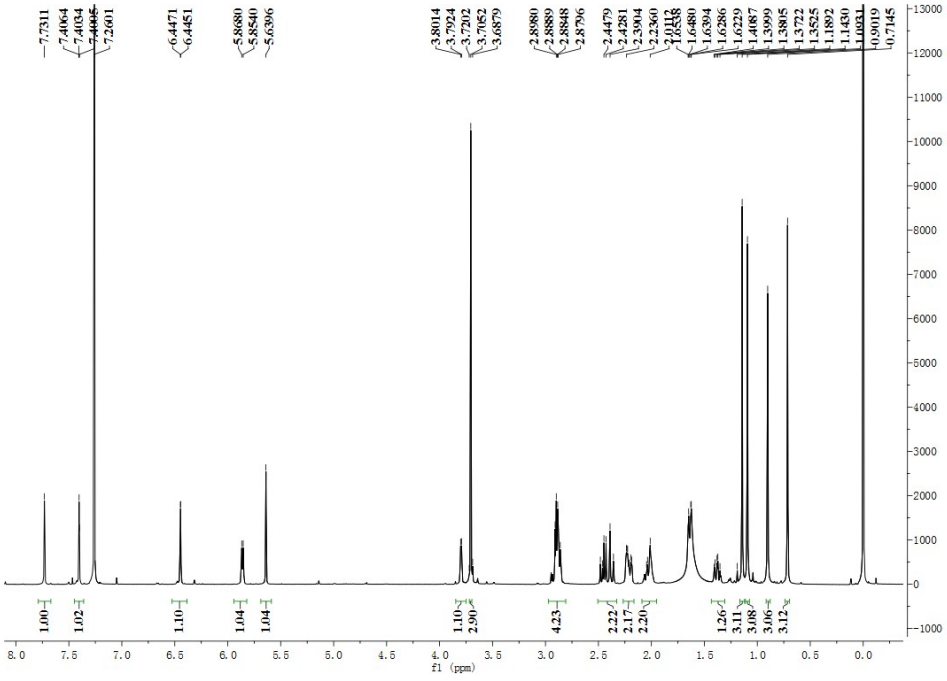




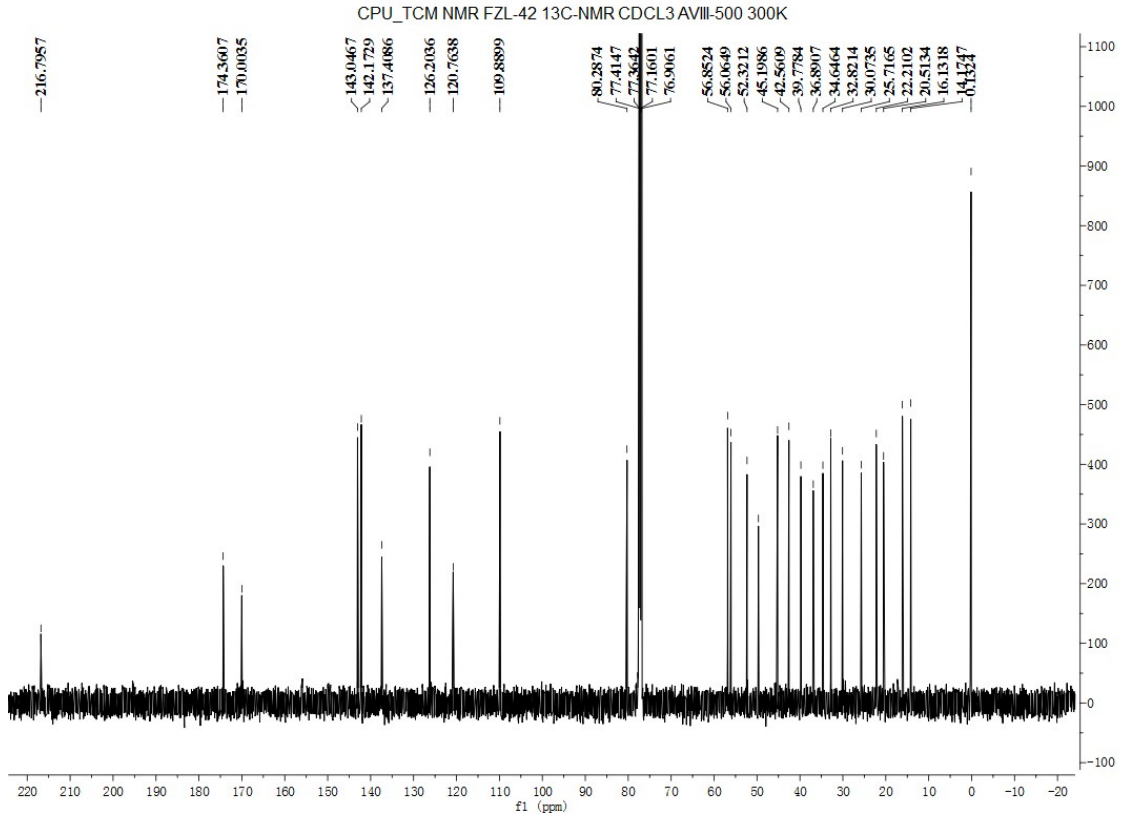
Elemental Composition Calculator

Target m/z:	493.2194	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); Cl (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C27H34NaO7		493.2197		0.51	

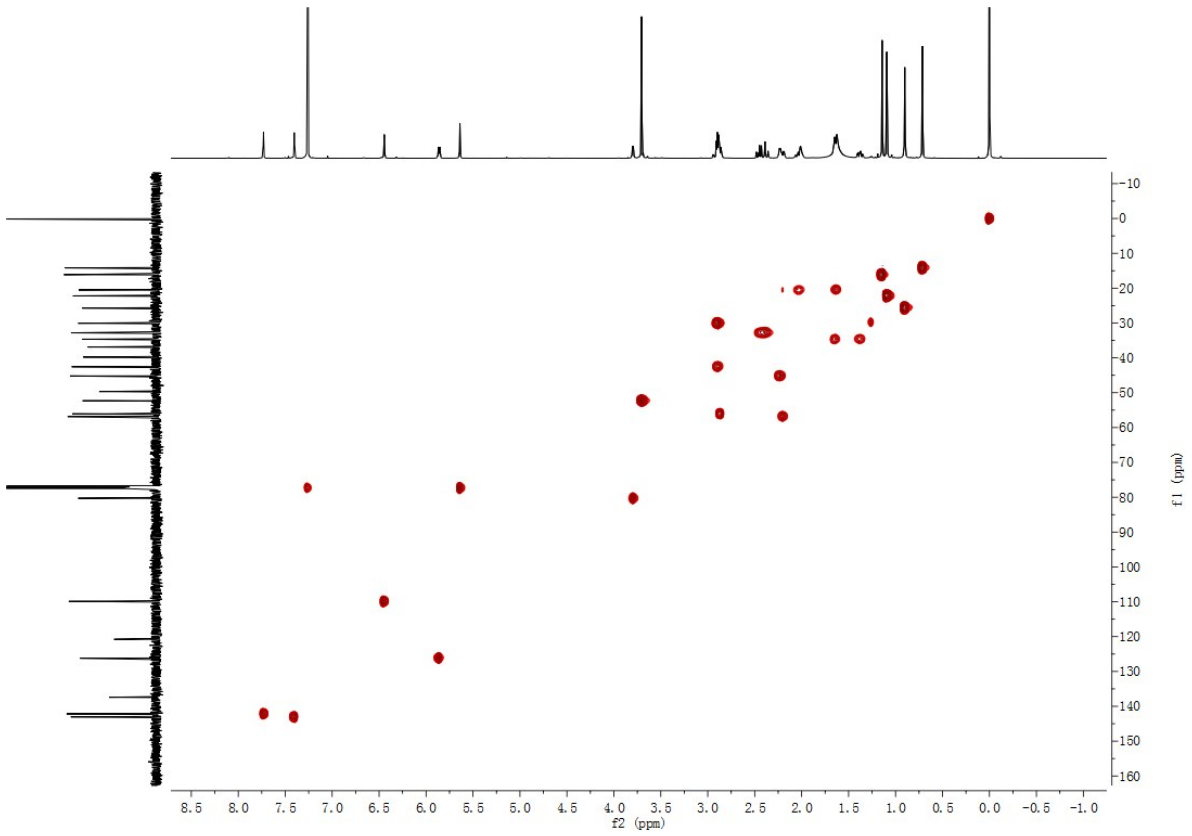
S52 ^{1}H NMR of Khasenegasin I (**9**)



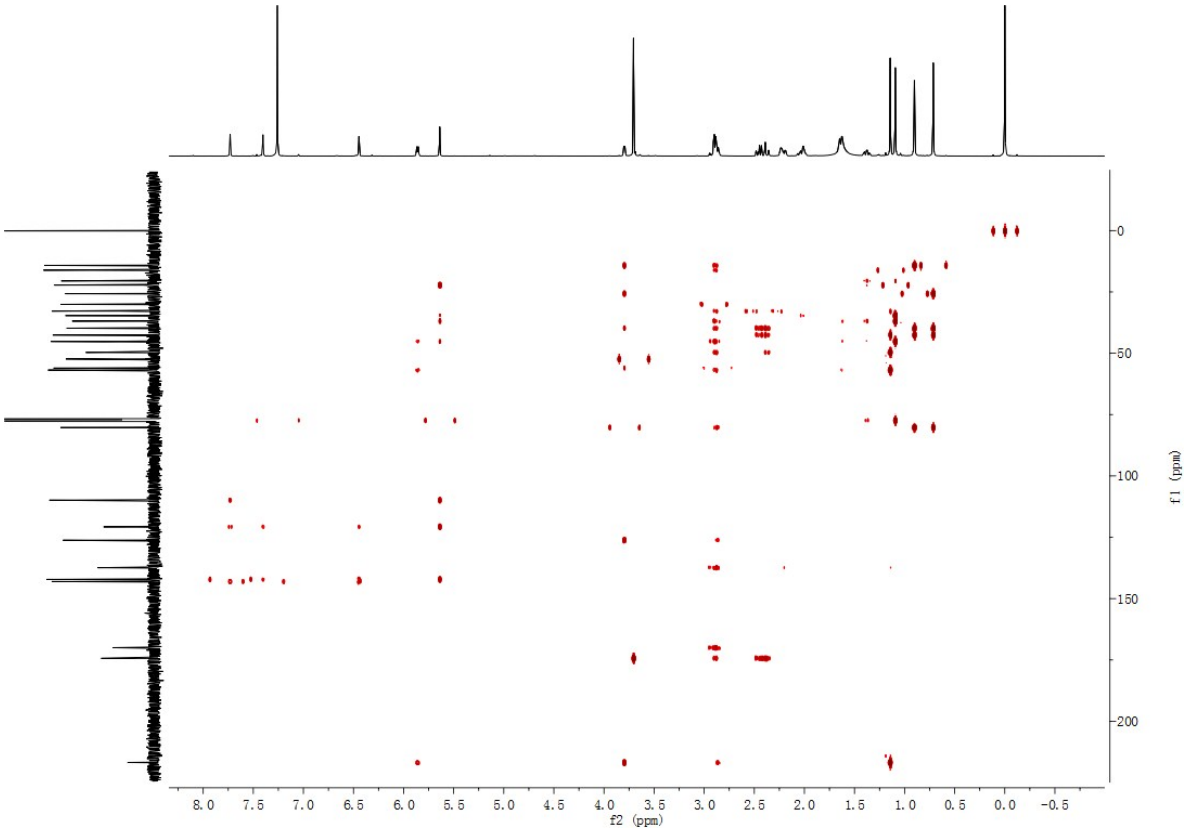
S53 ^{13}C NMR of Khasenegasin I (**9**)



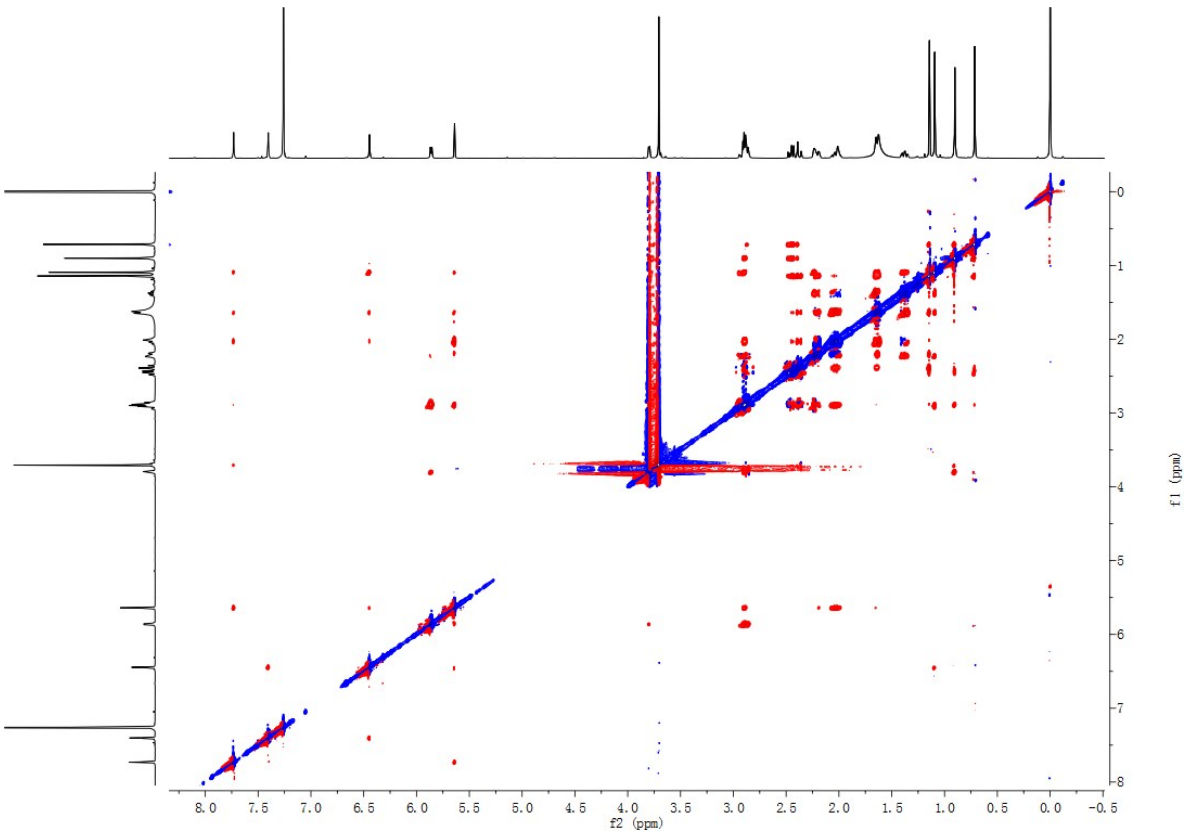
S54 HSQC of Khasenegasin I (**9**)



S55 HMBC of Khasenegasin I (**9**)

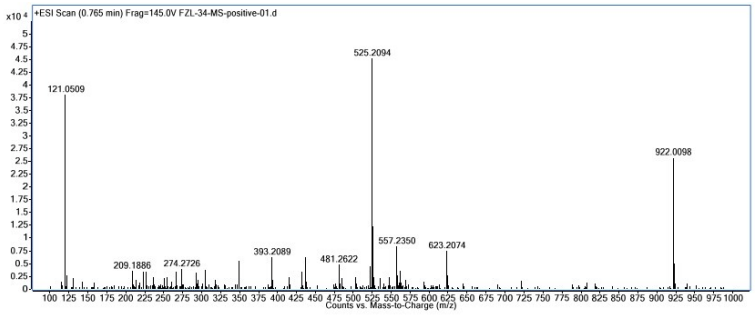


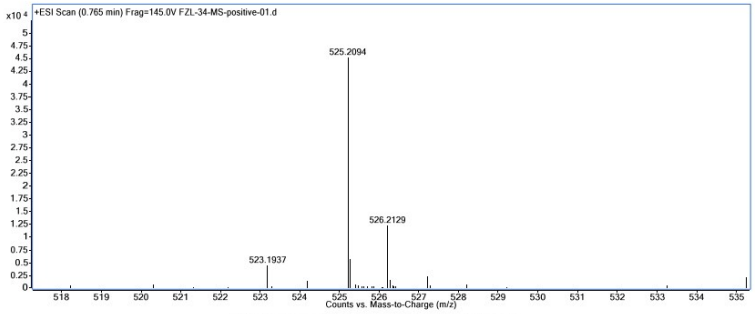
S56 ROSEY of Khasenegasin I (**9**)



Khasenegasin J (**10**)

S57 HR-ESI-MS of Khasenegasin J (**10**)

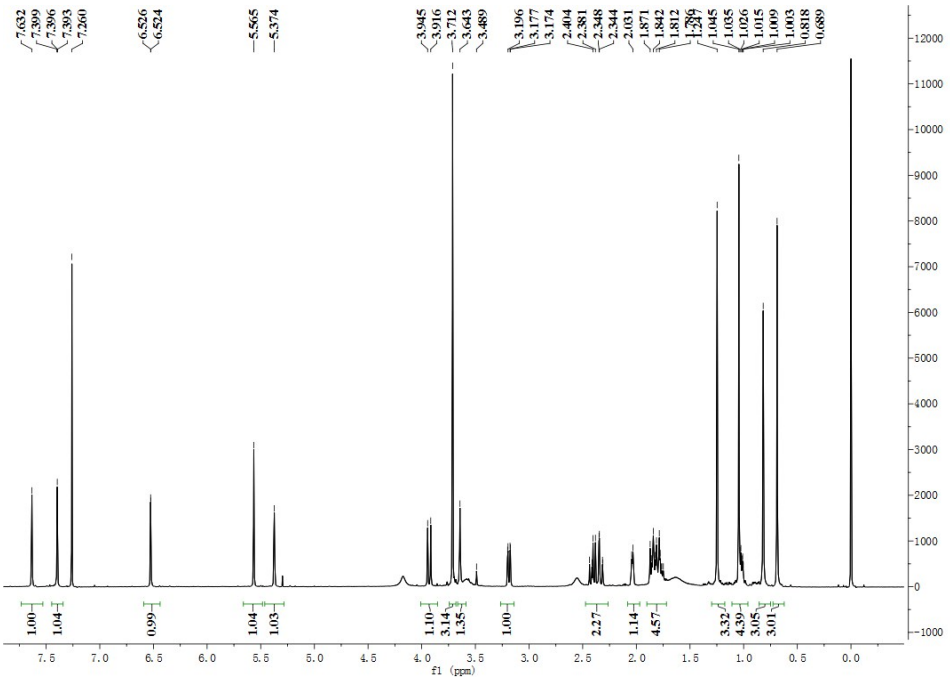




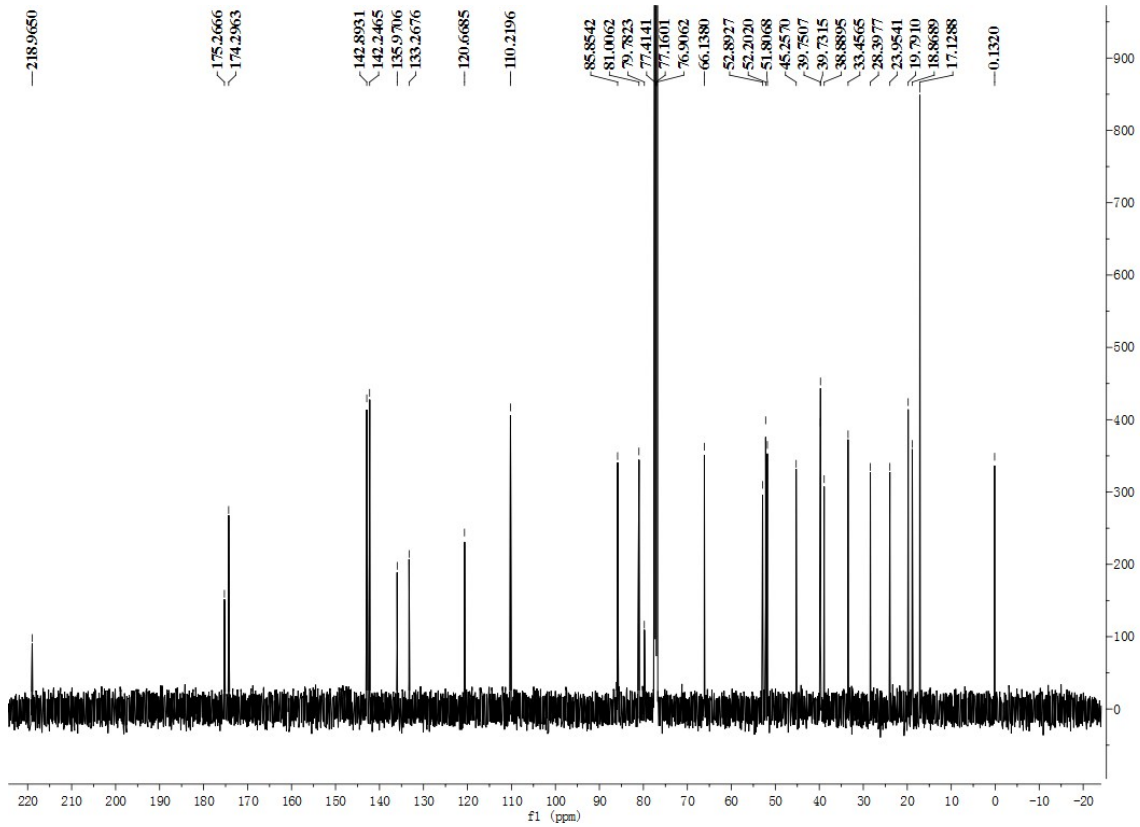
Elemental Composition Calculator

Target m/z:	525.2094	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C27H34NaO9		525.2095		0.19	

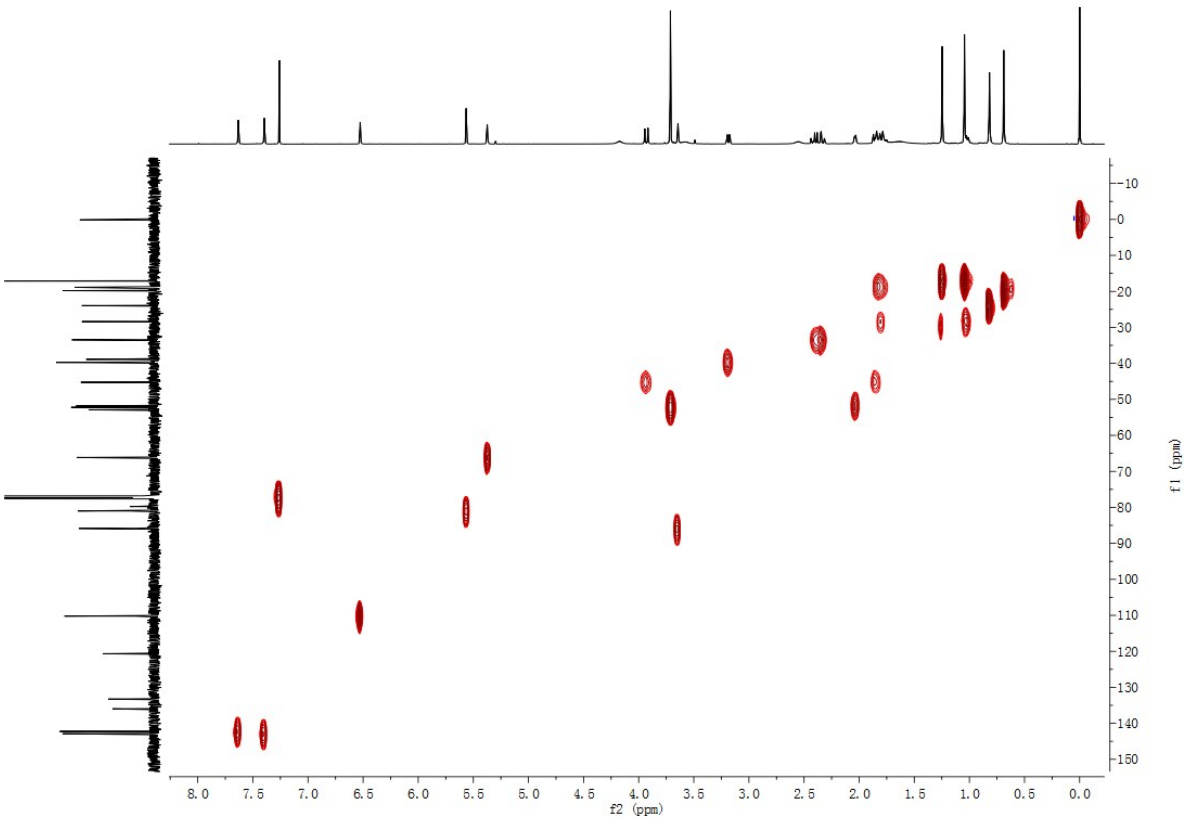
S58 ^{1}H NMR of Khasenegasin J (**10**)



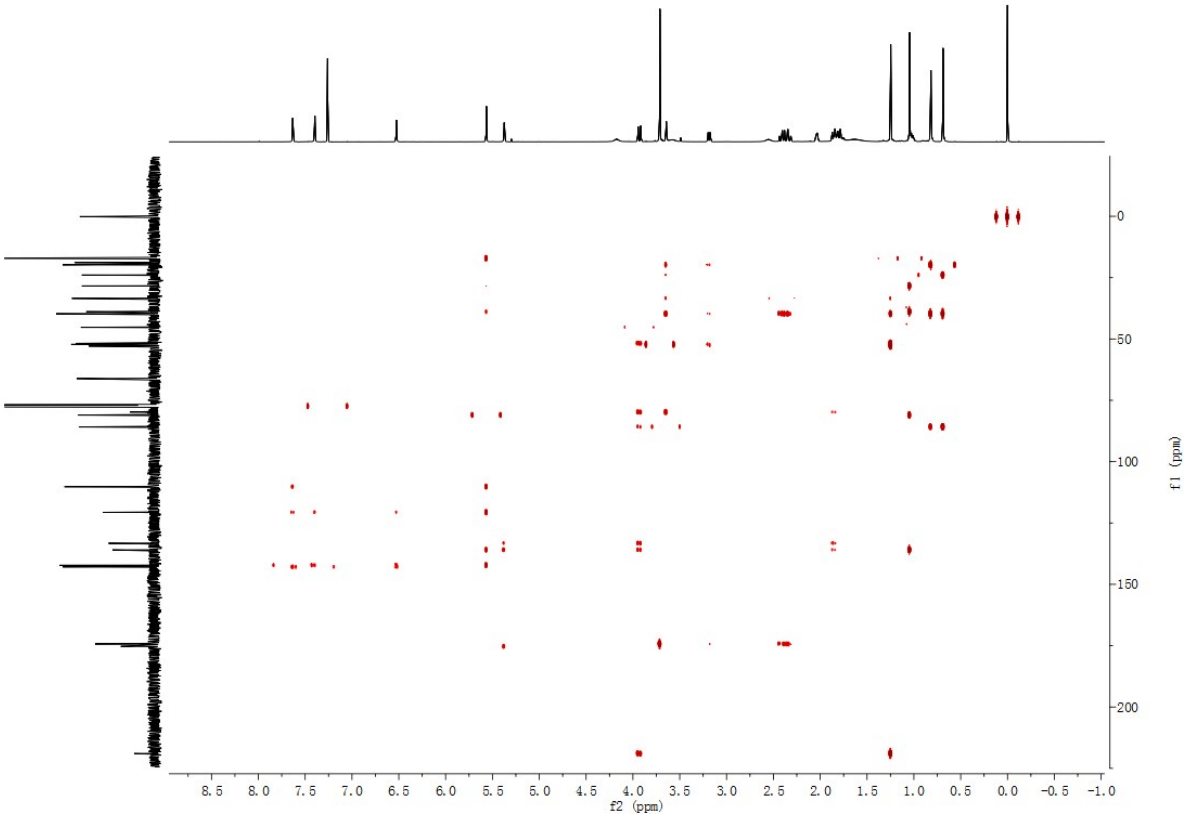
S59 ^{13}C NMR of Khasenegasin J (**10**)



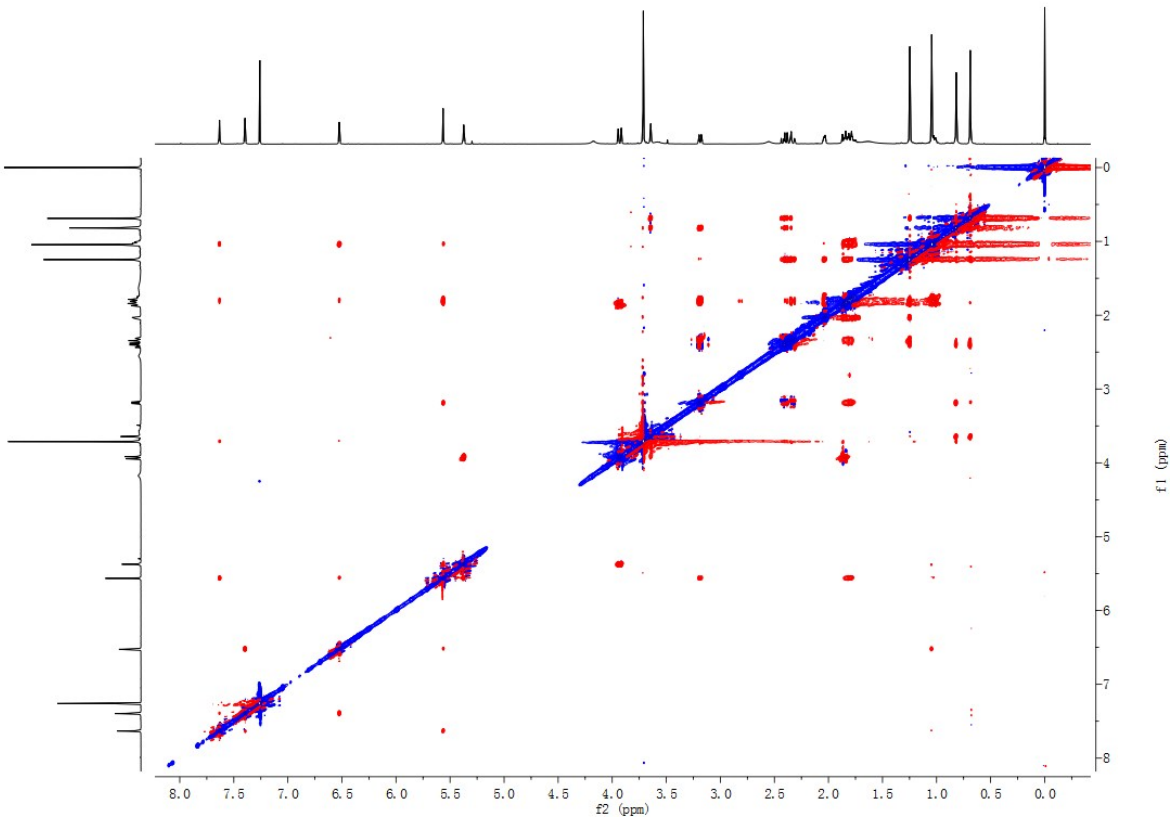
S60 HSQC of Khasenegasin J (**10**)



S61 HMBC of Khasenegasin J (**10**)

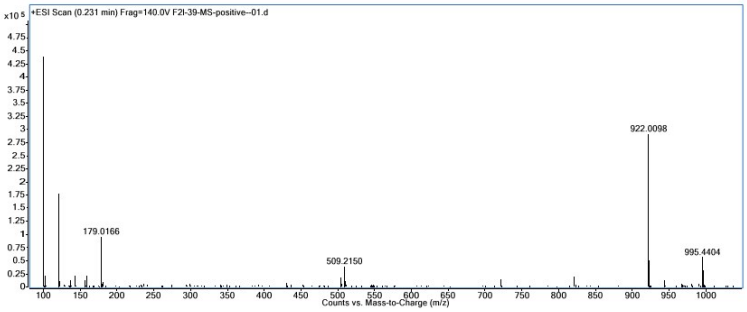


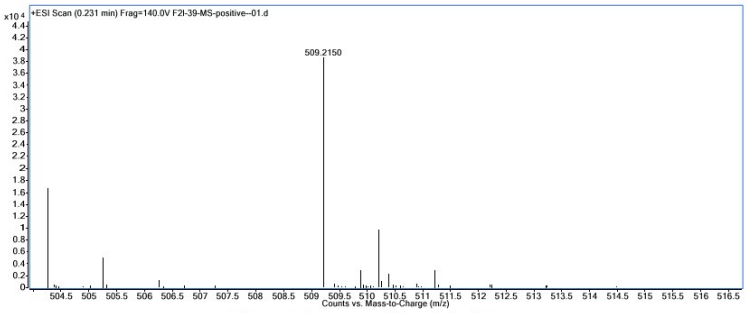
S62 ROSEY of Khasenegasin J (**10**)



Khasenegasin K (**11**)

S63 HR-ESI-MS of Khasenegasin K (**11**)

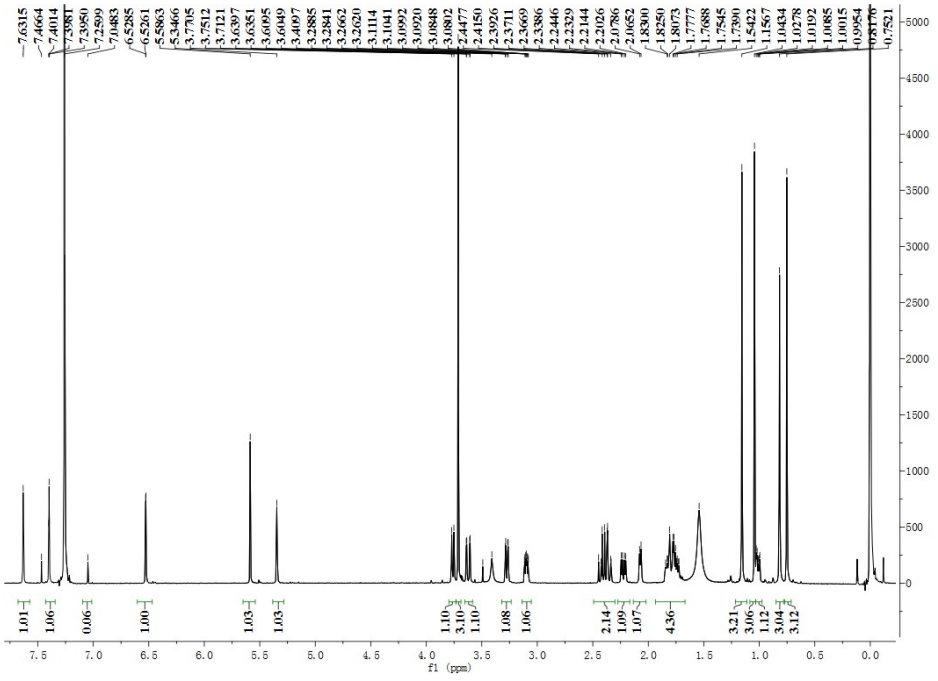




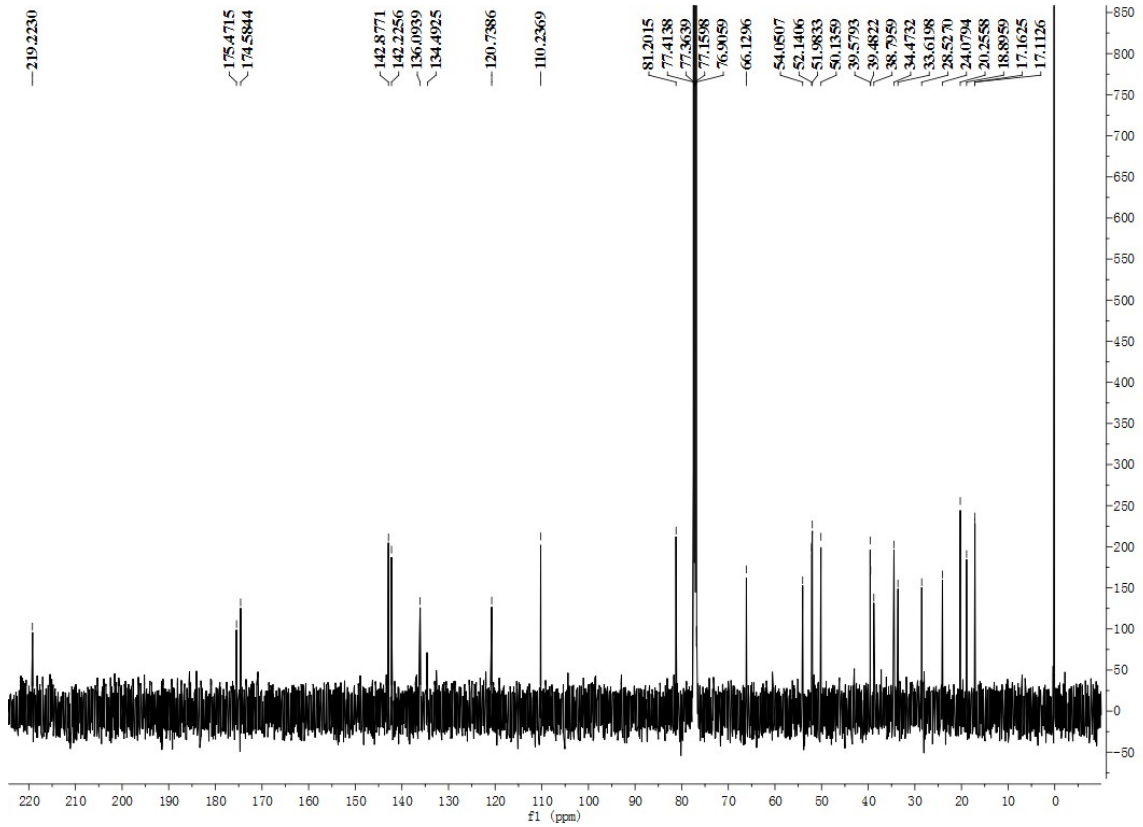
Elemental Composition Calculator

Target m/z:	509.2150	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C27H34NaO8		509.2146		-0.83	

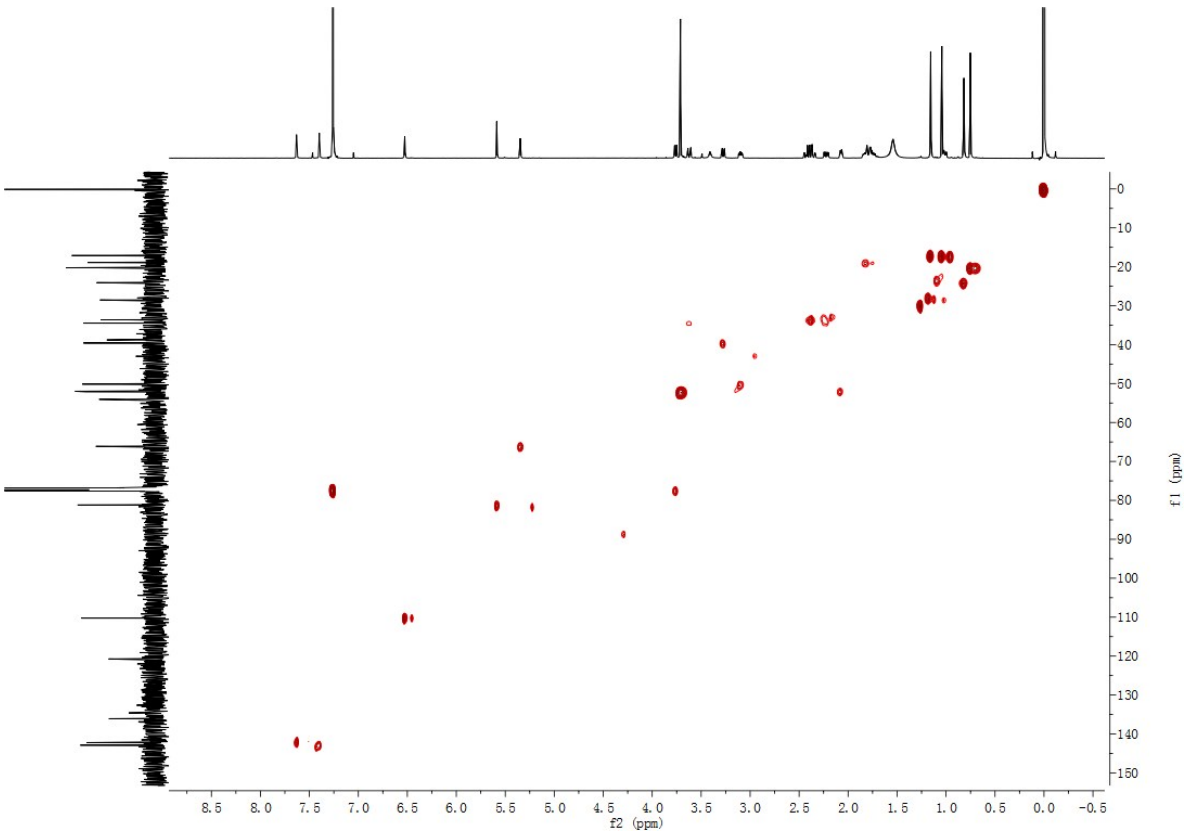
S64 ^{1}H NMR of Khasenegasin K (**11**)



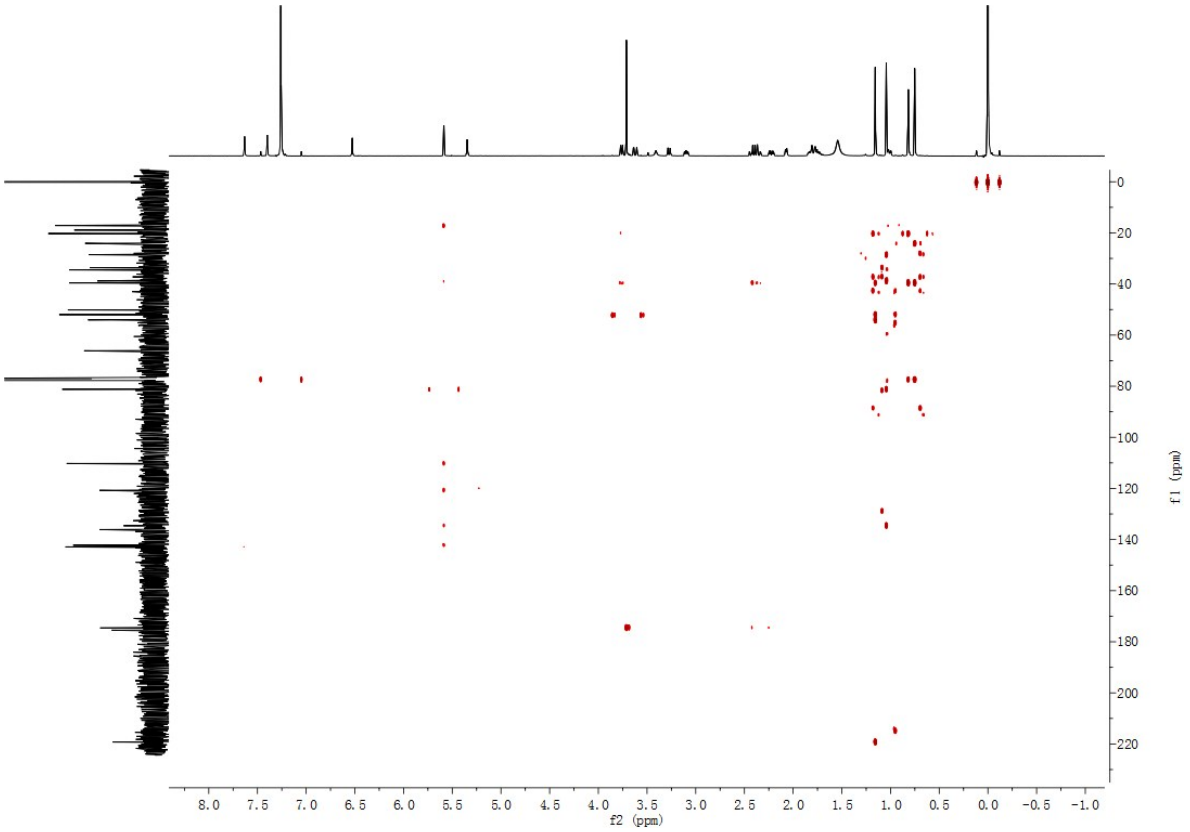
S65 ^{13}C NMR of Khasenegasin K (**11**)



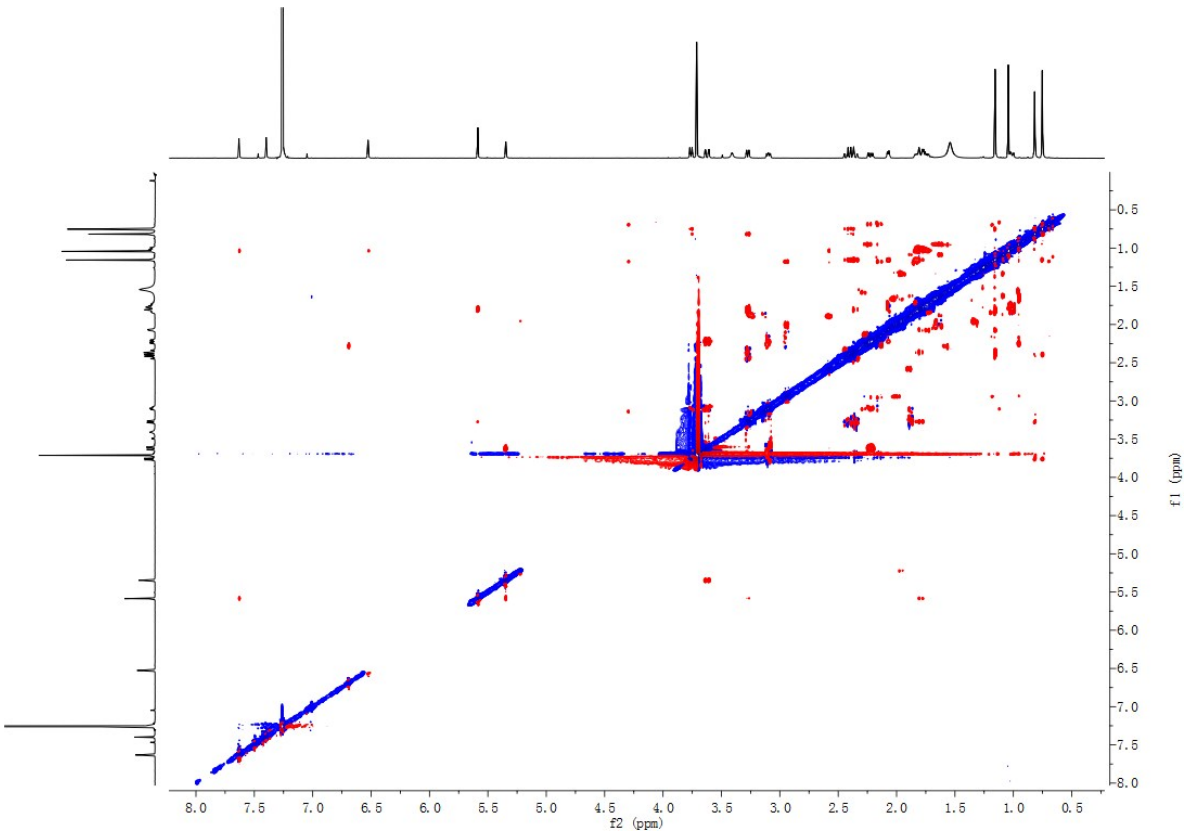
S66 HSQC of Khasenegasin K (**11**)



S67 HMBC of Khasenegasin K (**11**)

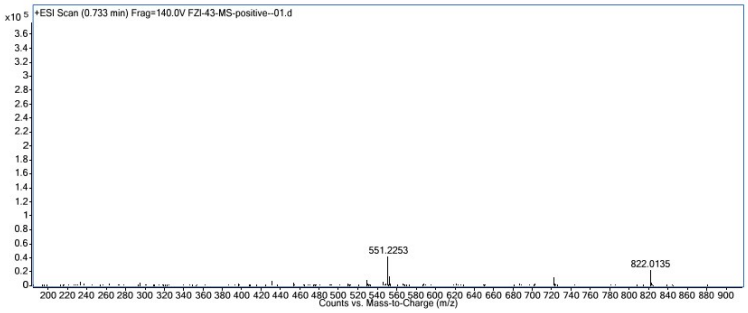


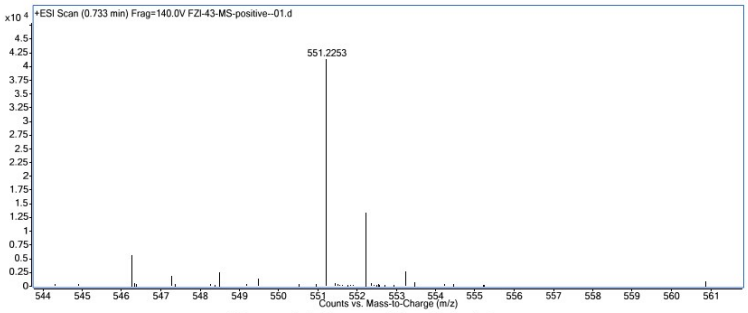
S68 ROSEY of Khasenegasin K (**11**)



Khasenegasin L (**12**)

S69 HR-ESI-MS of Khasenegasin L (**12**)

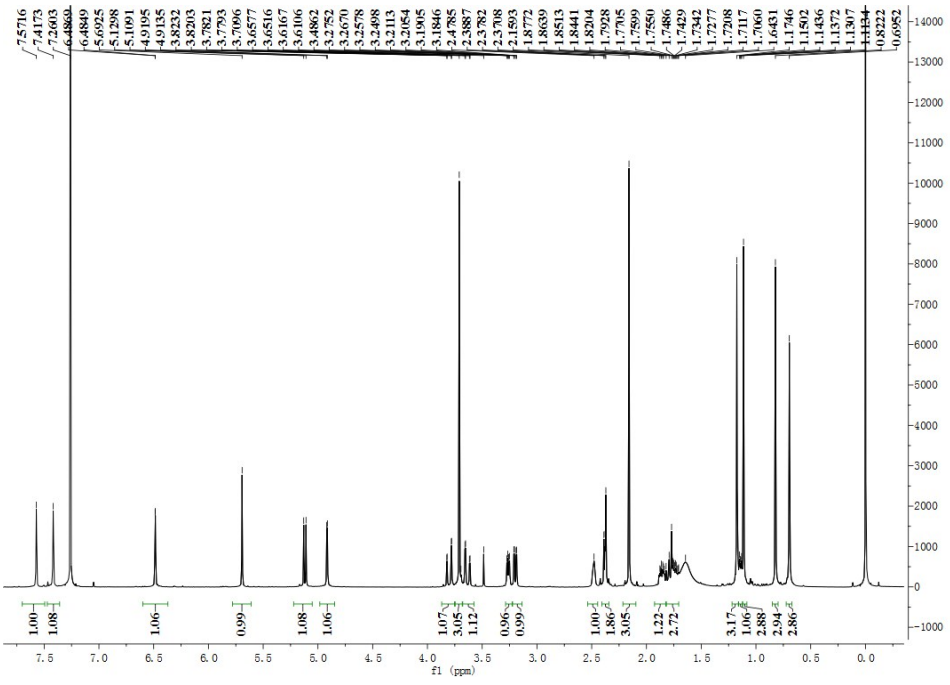




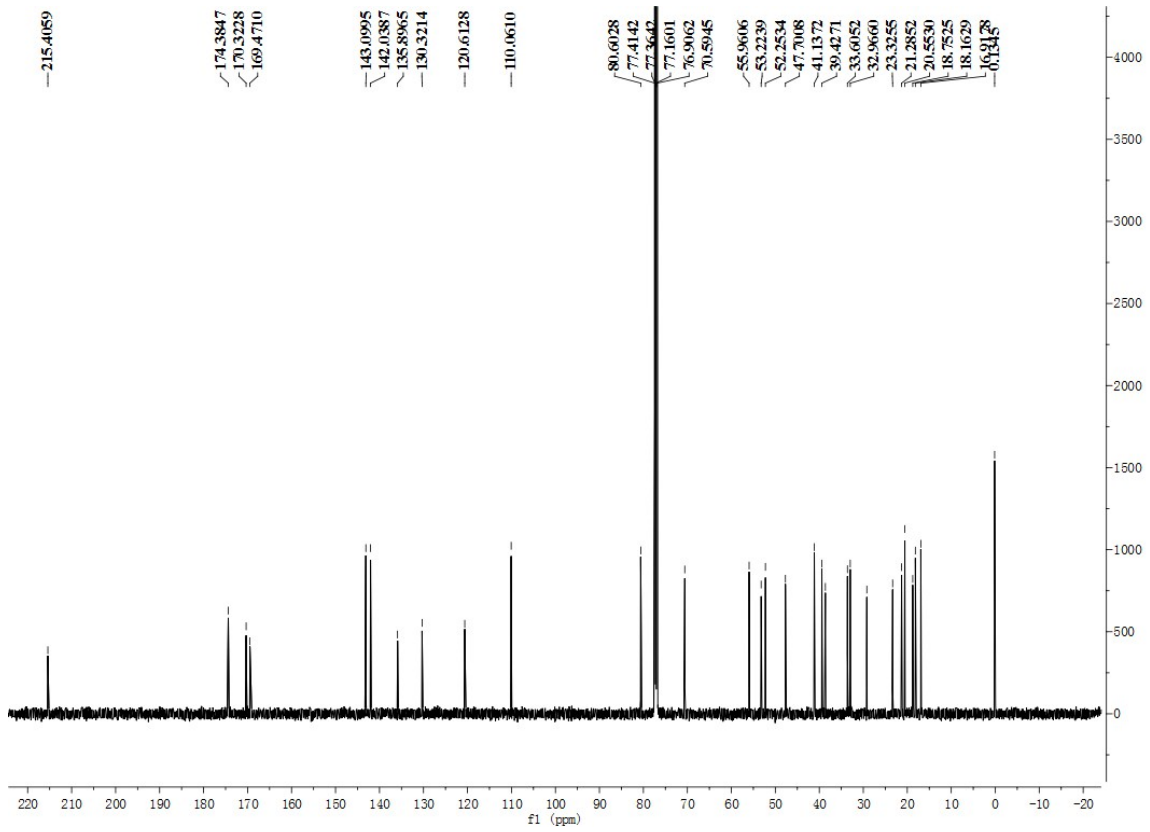
Elemental Composition Calculator

Target m/z:	551.2253	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); S (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C29H36NaO9		551.2252		-0.32	

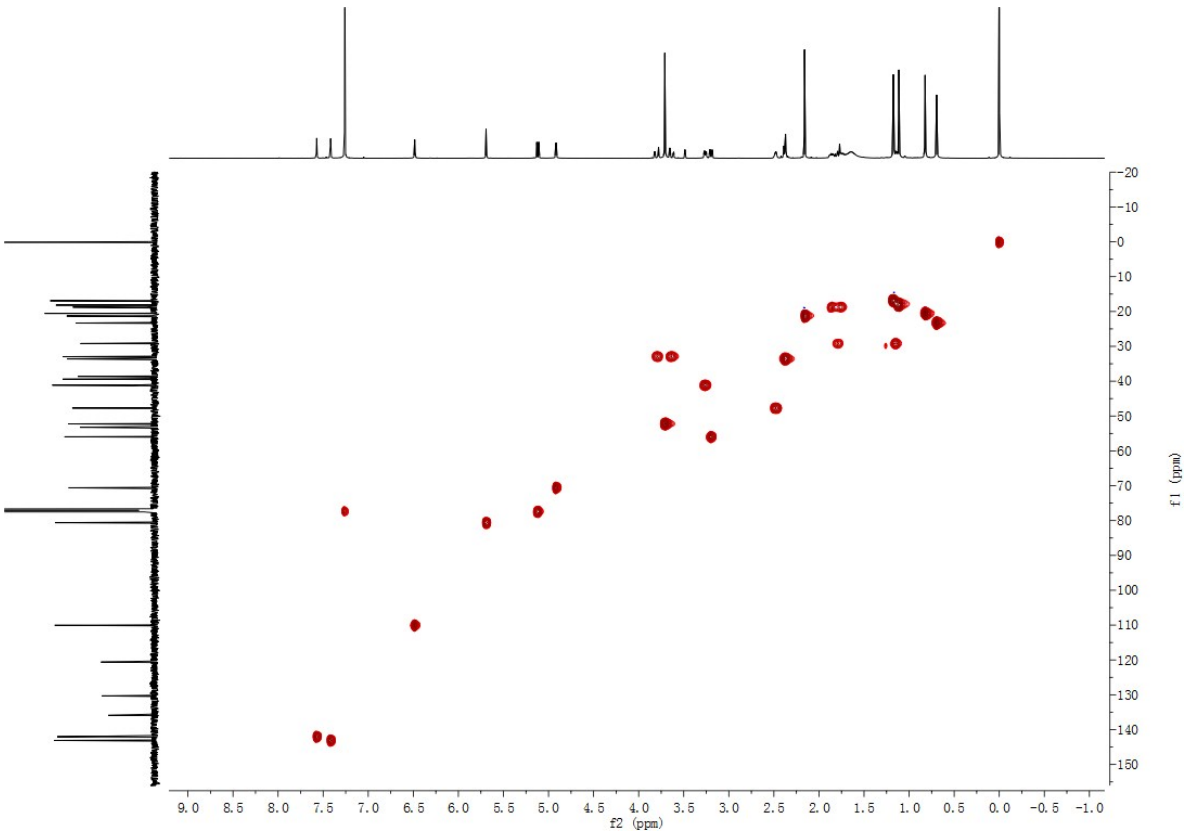
S70 ^{1}H NMR of Khasenegasin L (**12**)



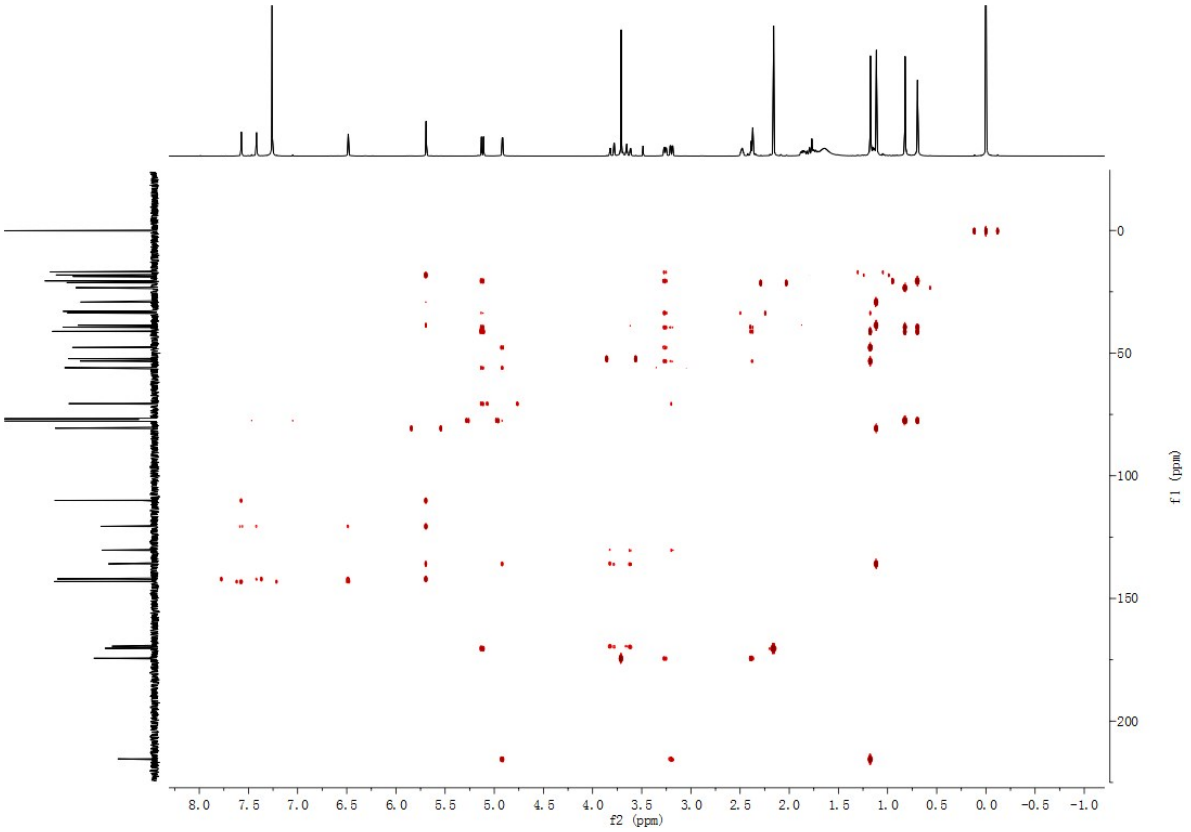
S71 ^{13}C NMR of Khasenegasin L (**12**)



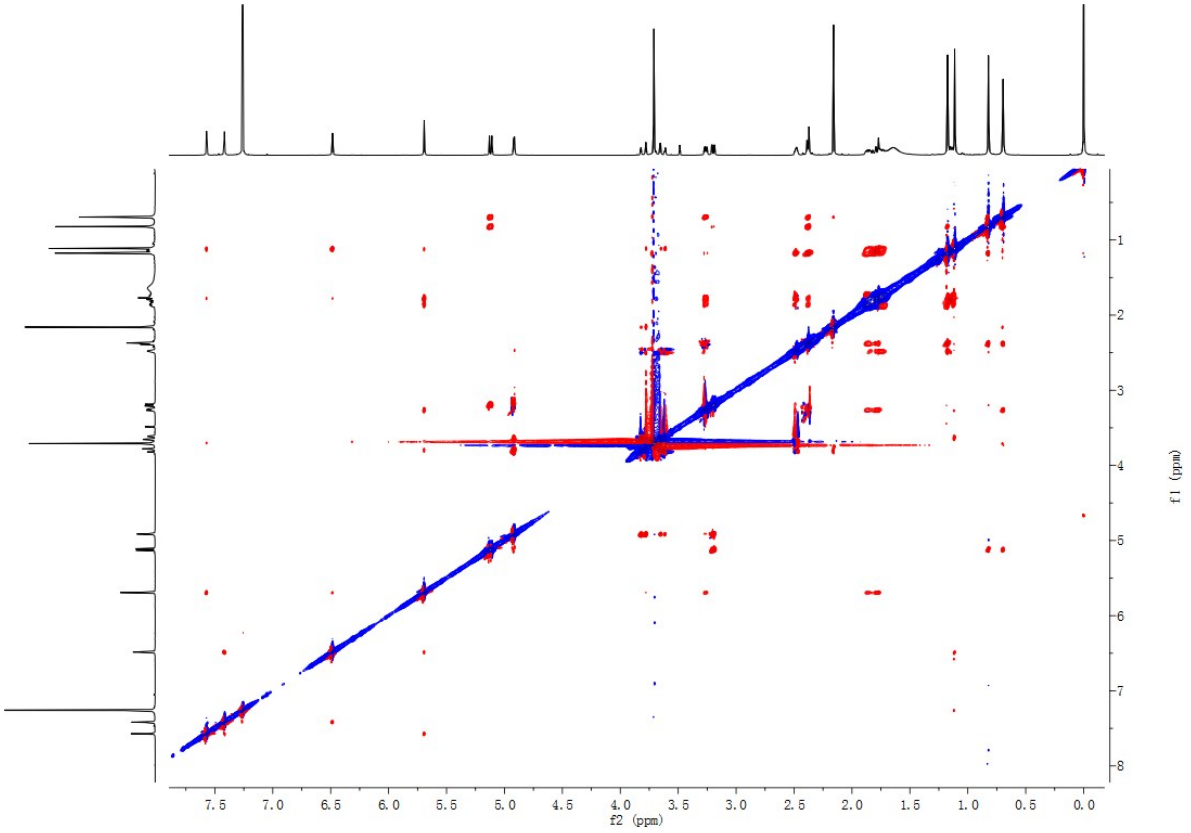
S72 HSQC of Khasenegasin L (**12**)



S73 HMBC of Khasenegasin L (**12**)

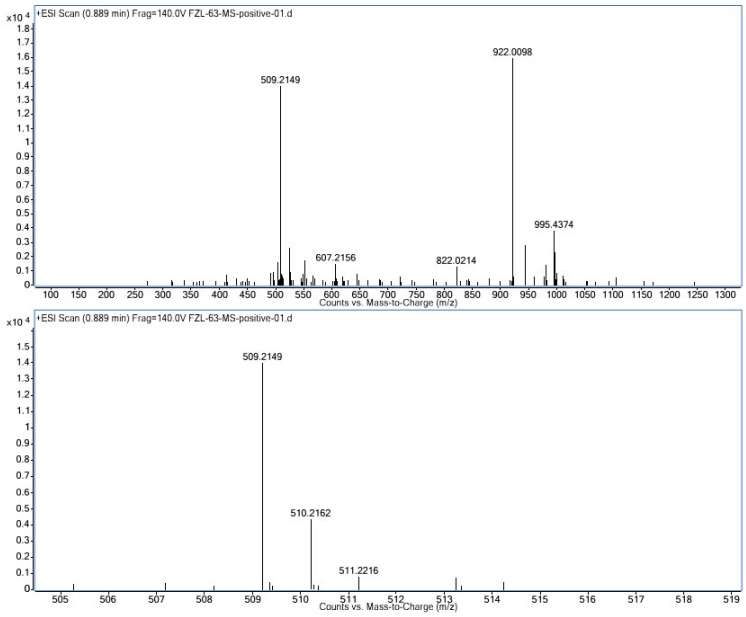


S74 ROSEY of Khasenegasin L (**12**)



Khasenegasin M (**13**)

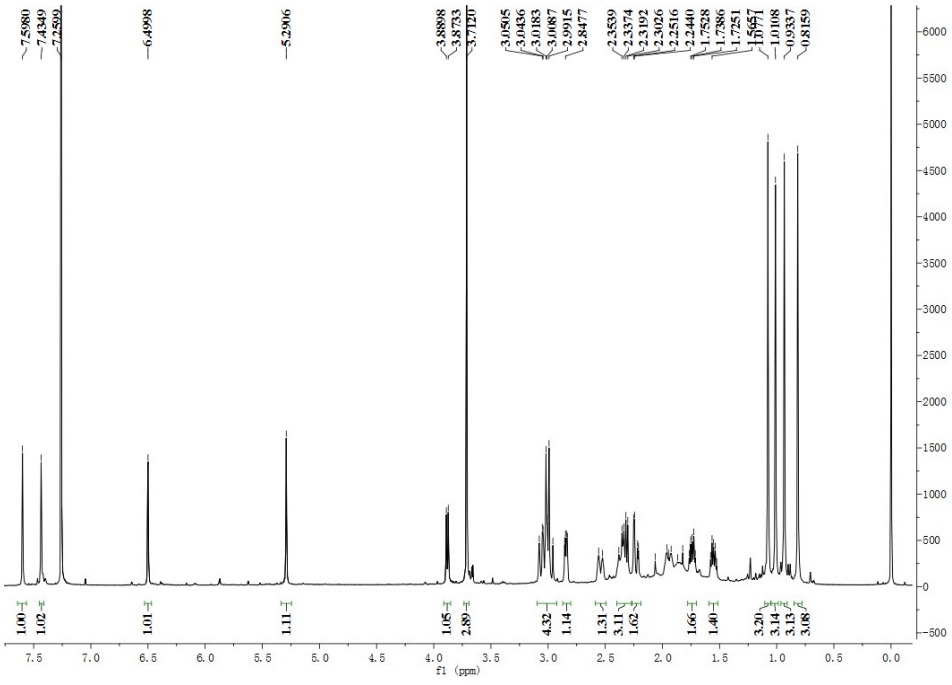
S75 HR-ESI-MS of Khasenegasin M (**13**)



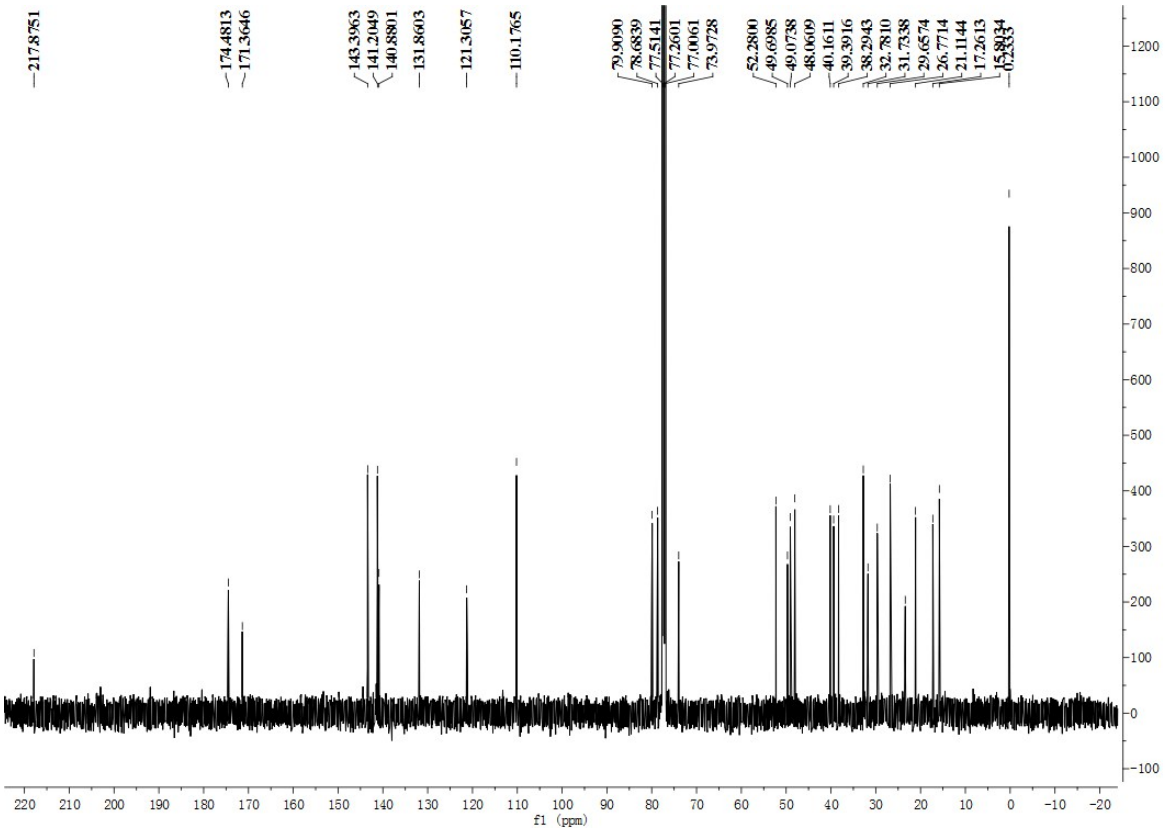
Elemental Composition Calculator

Target m/z:	509.2149	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5)			
Ion Formula		**Calcalated m/z**		**PPM Error**	
C27H34NaO8		509.2146		-0.67	

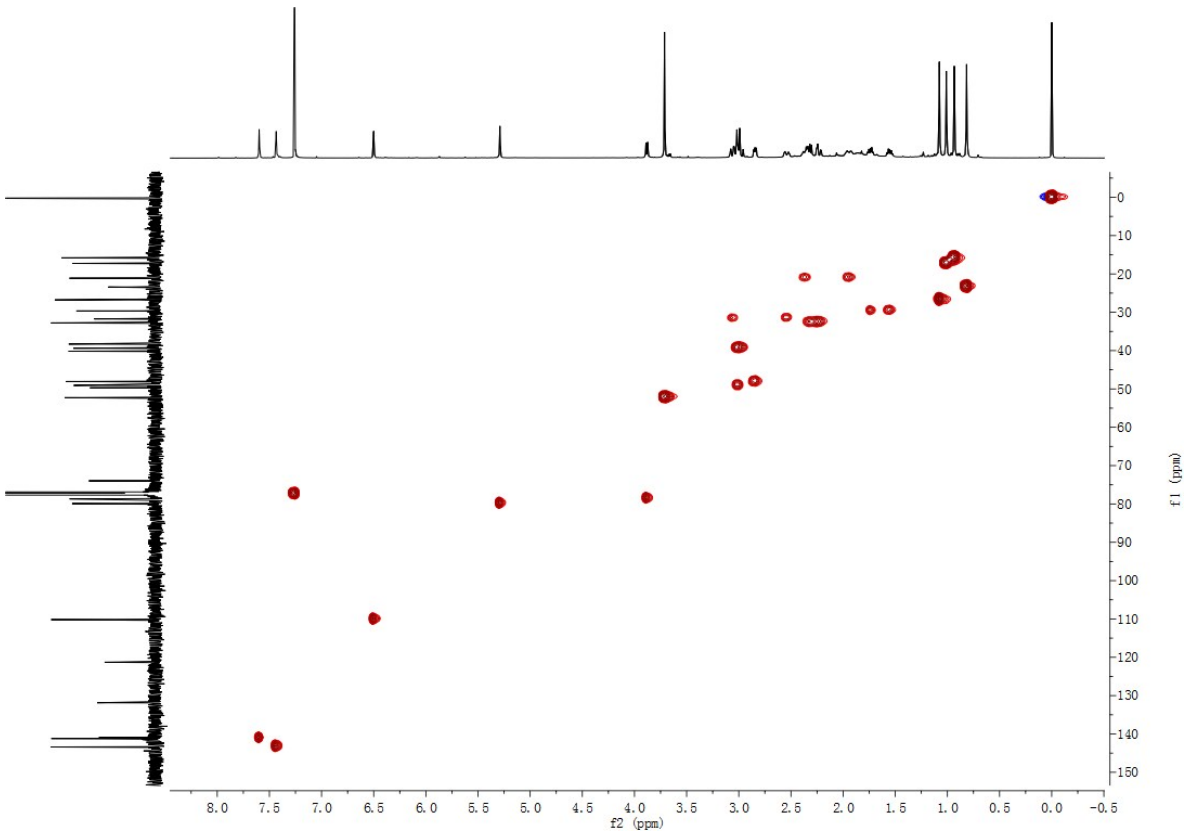
S76 ^{1}H NMR of Khasenegasin M (**13**)



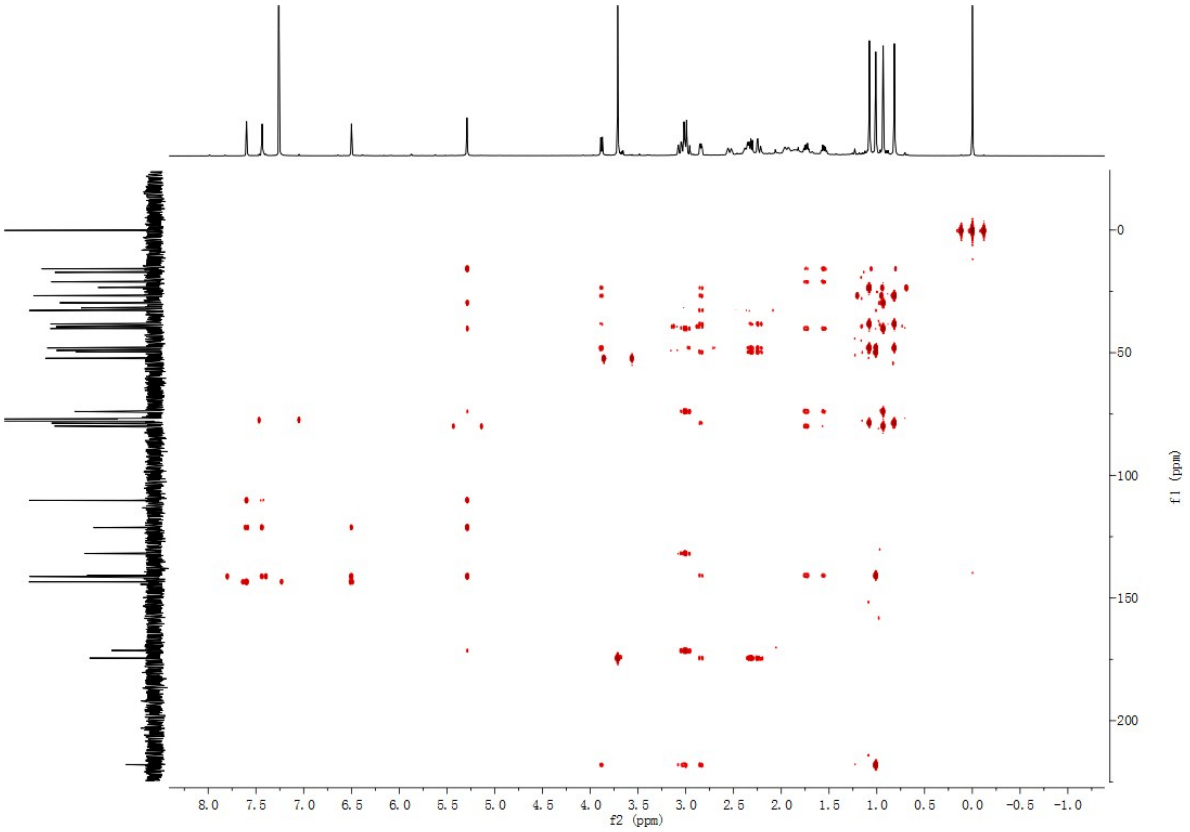
S77 ^{13}C NMR of Khasenegasin M (**13**)



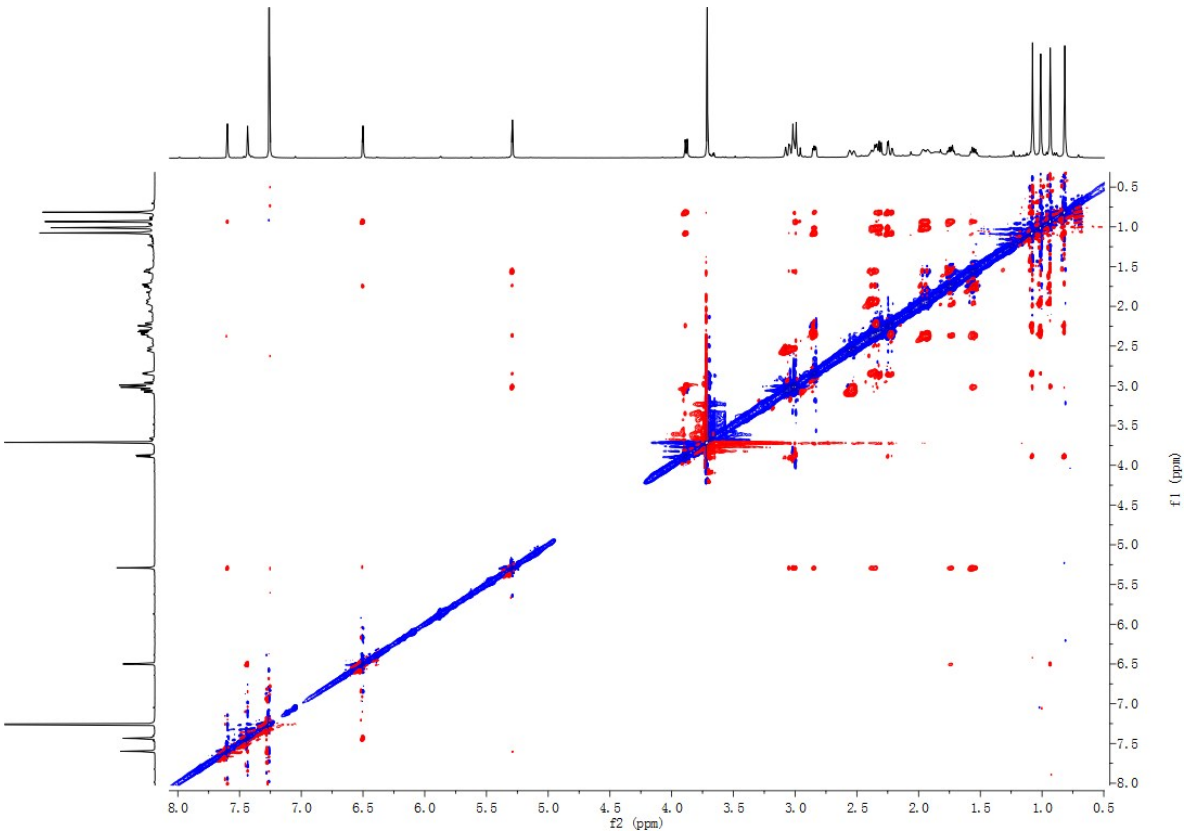
S78 HSQC of Khasenegasin M (**13**)



S79 HMBC of Khasenegasin M (**13**)

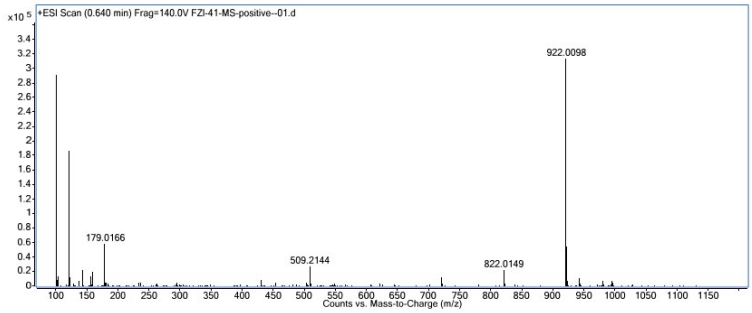


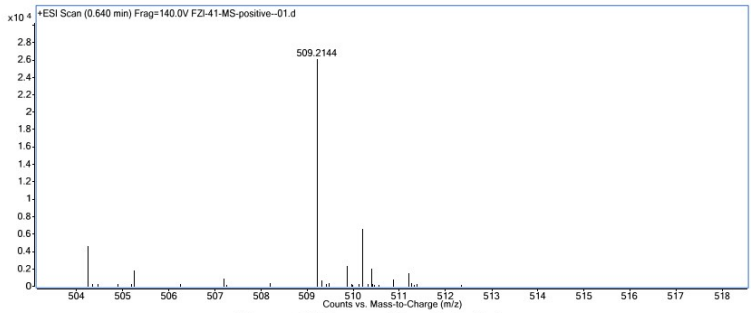
S80 ROSEY of Khasenegasin M (**13**)



Khasenegasin N (**14**)

S81 HR-ESI-MS of Khasenegasin N (**14**)

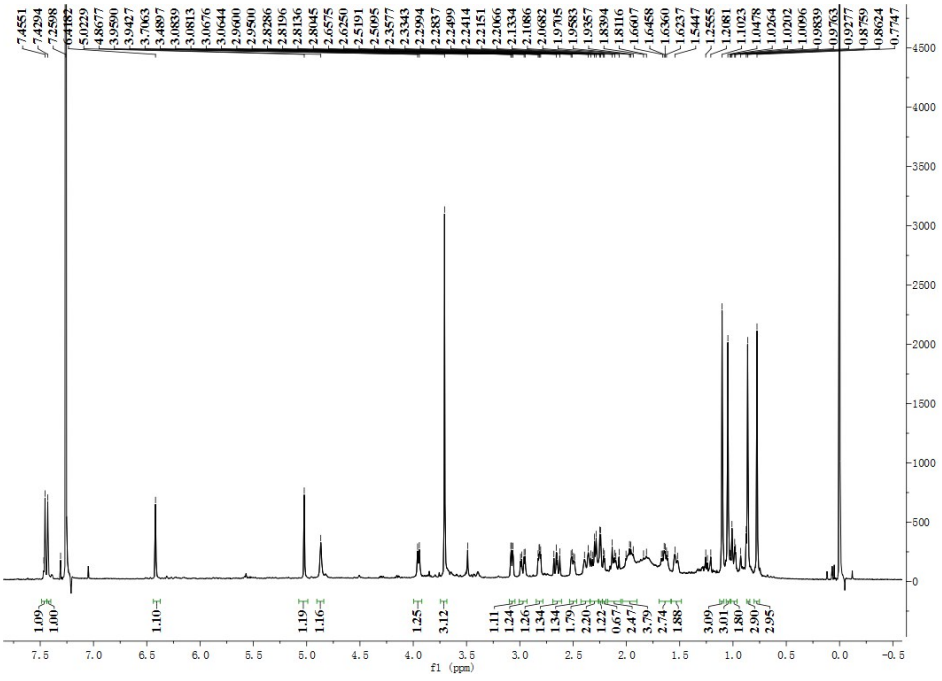




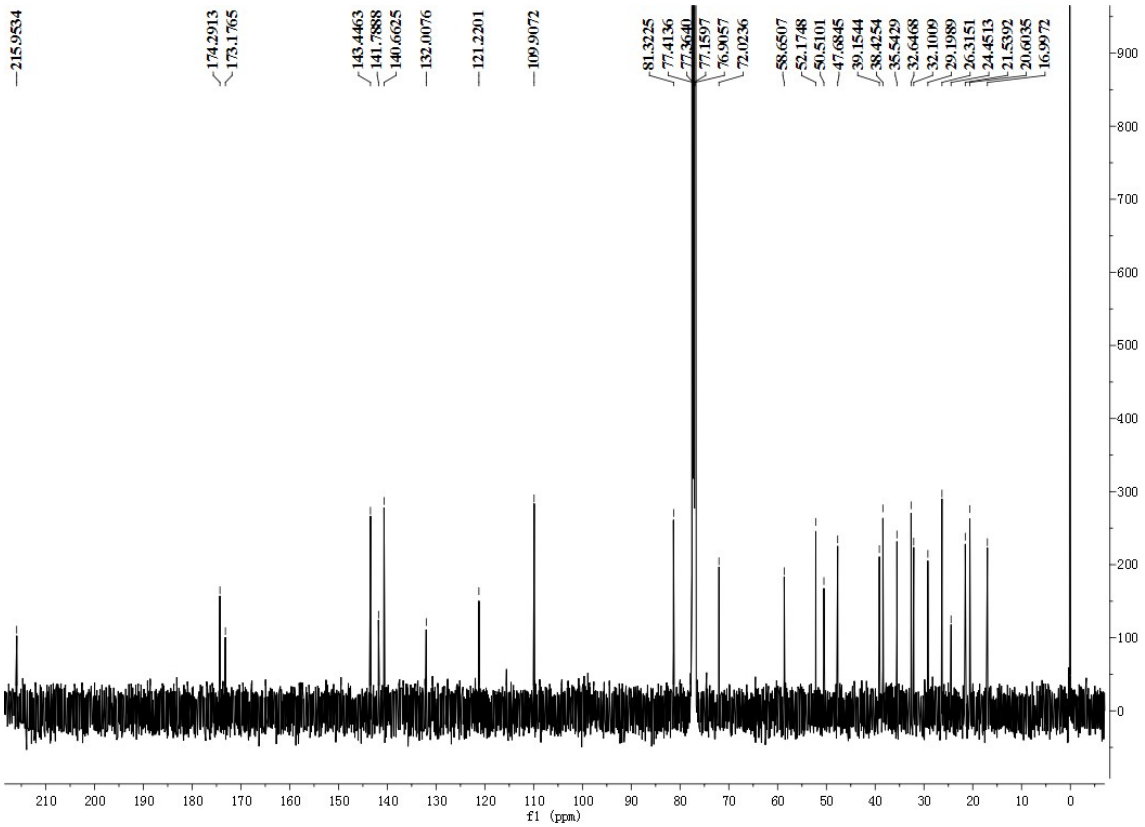
Elemental Composition Calculator

Target m/z:	509.2144	**Result type:**	Positive ions	**Species:**	$[M+Na]^+$
Elements:		C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5); Cl (0-5)			
Ion Formula		**Calculated m/z**		**PPM Error**	
C27H34NaO8		509.2146		0.39	

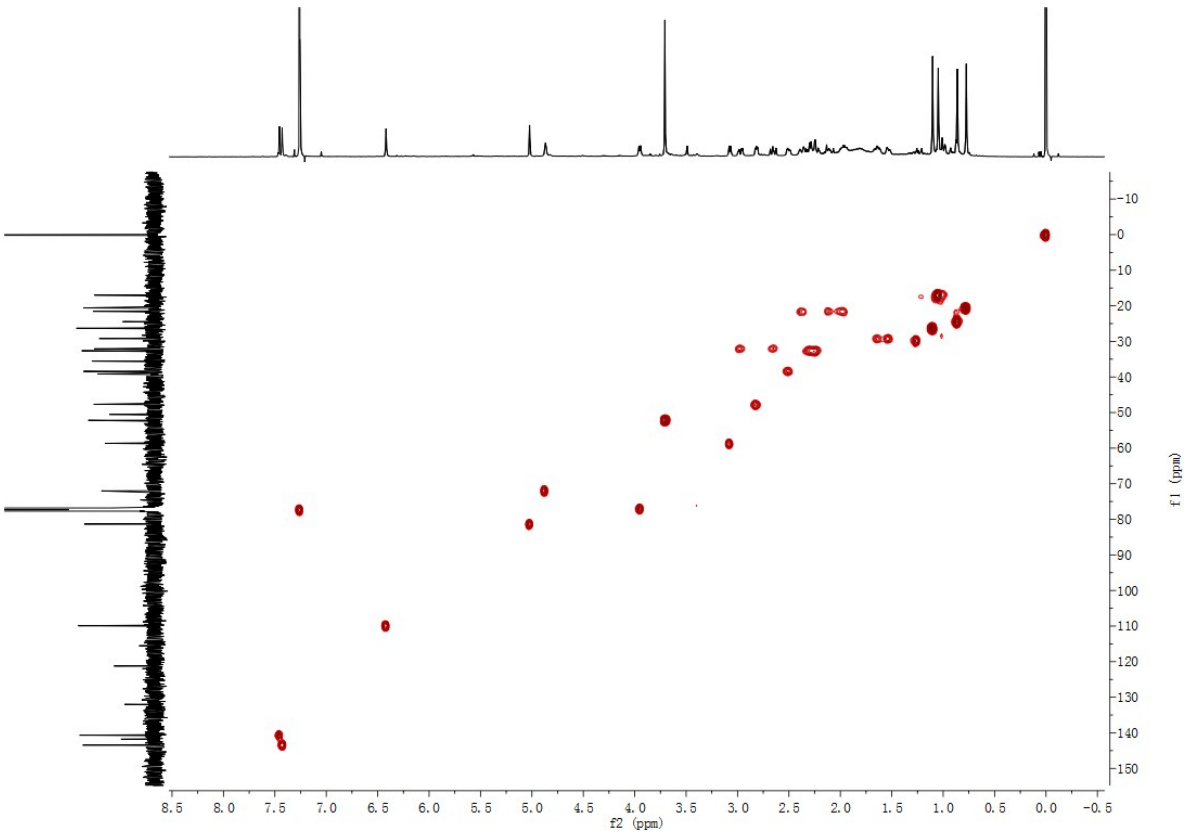
S82 ^{1}H NMR of Khasenegasin N (**14**)



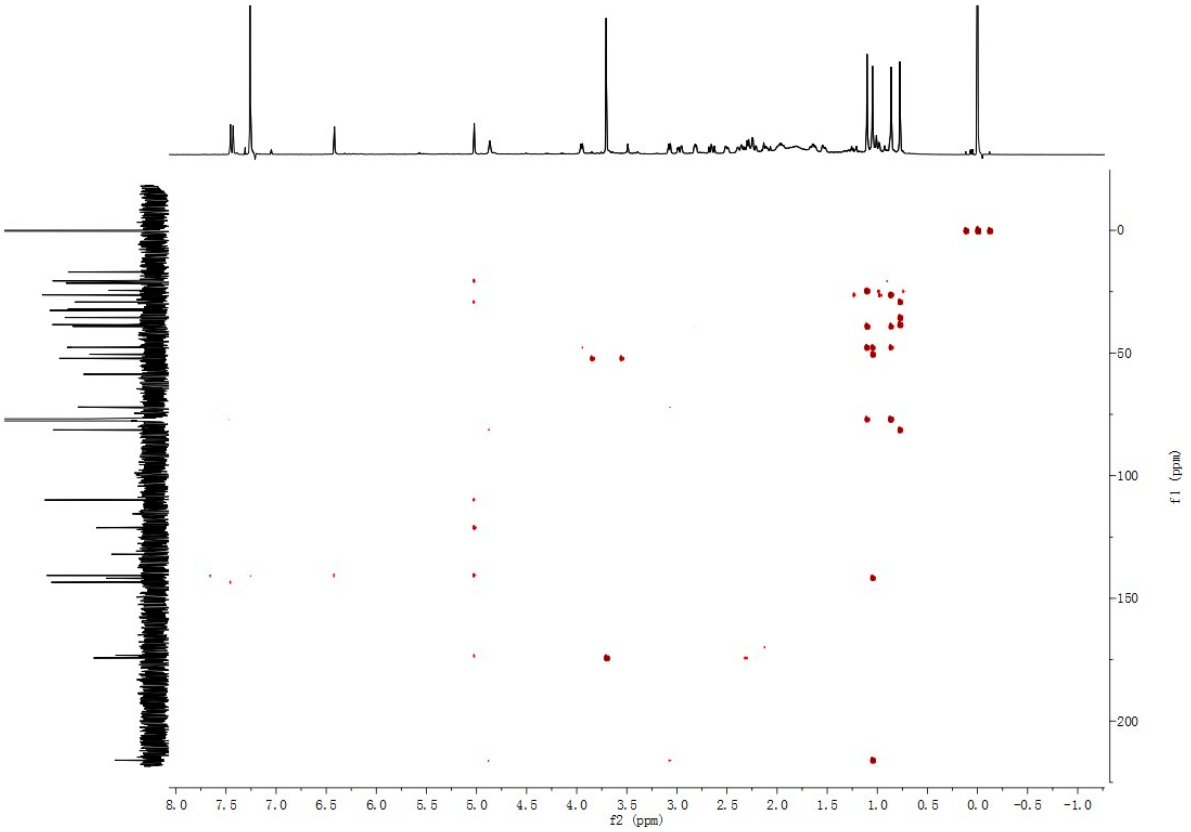
S83 ^{13}C NMR of Khasenegasin N (**14**)



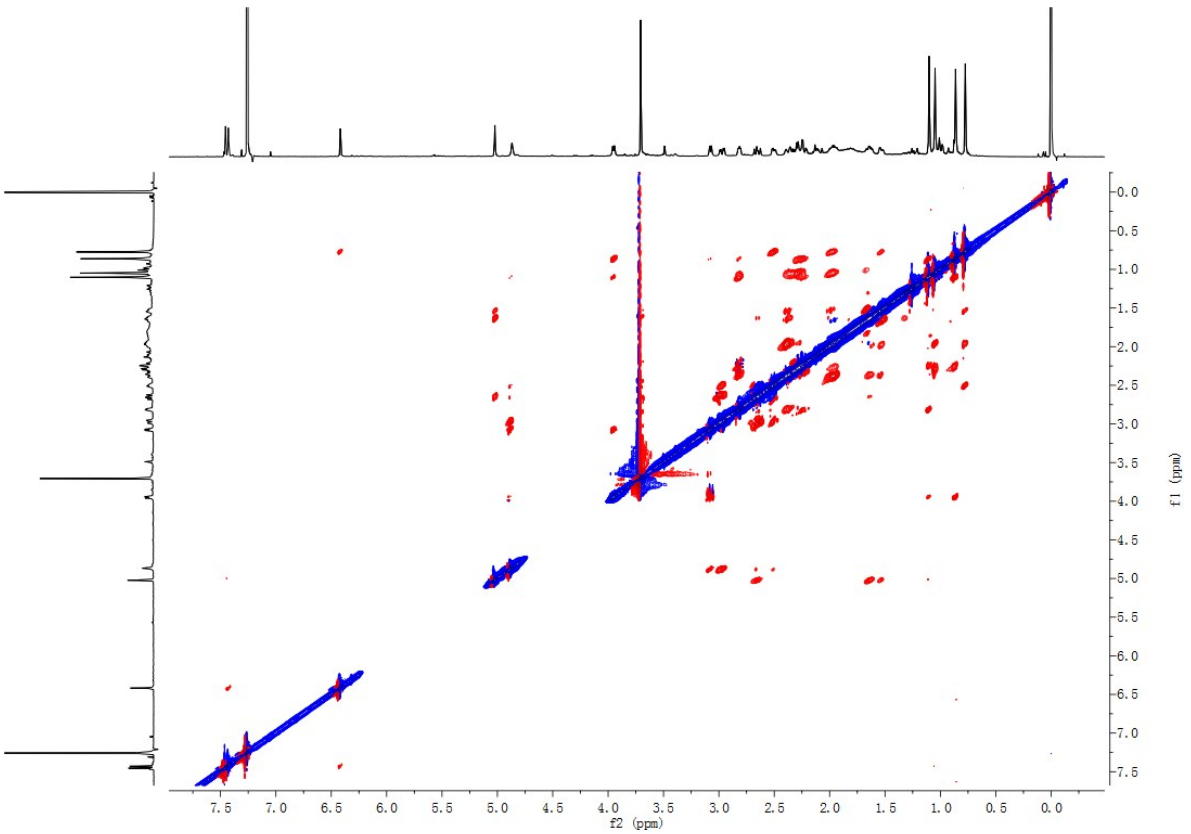
S84 HSQC of Khasenegasin N (**14**)



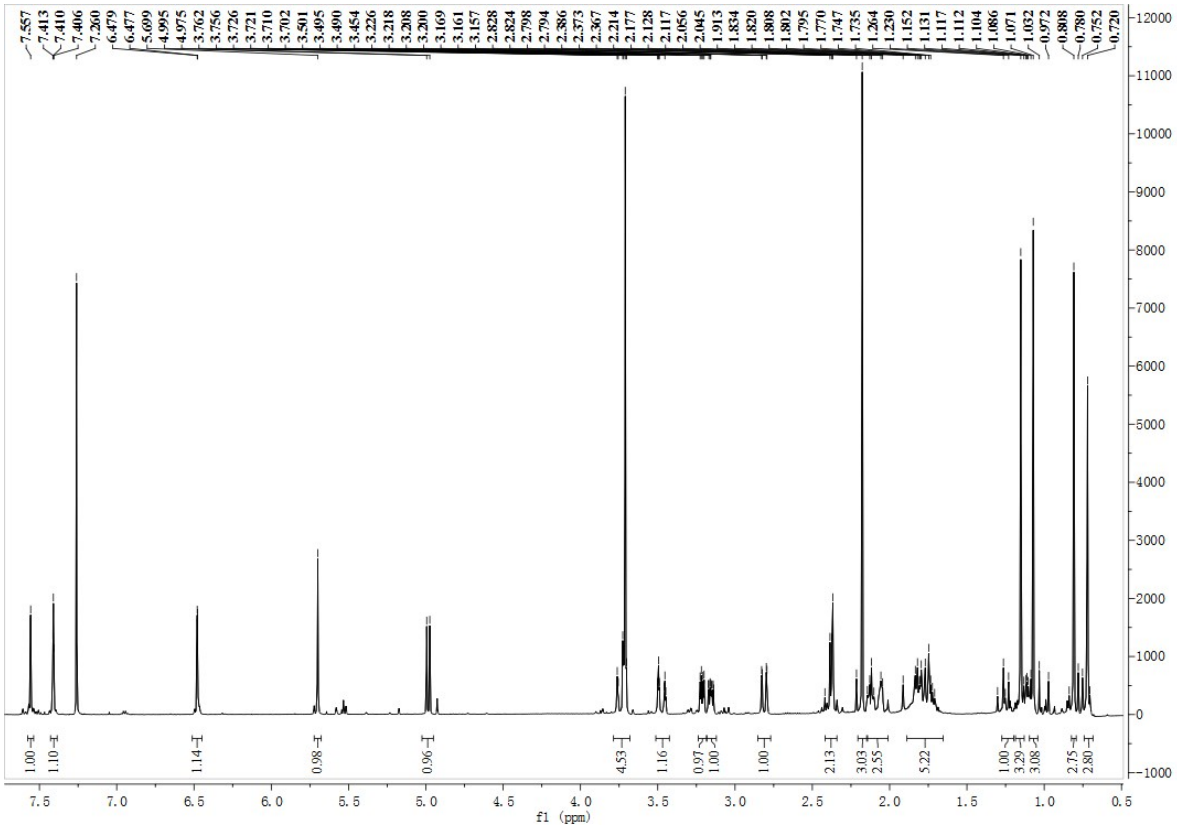
S85 HMBC of Khasenegasin N (**14**)



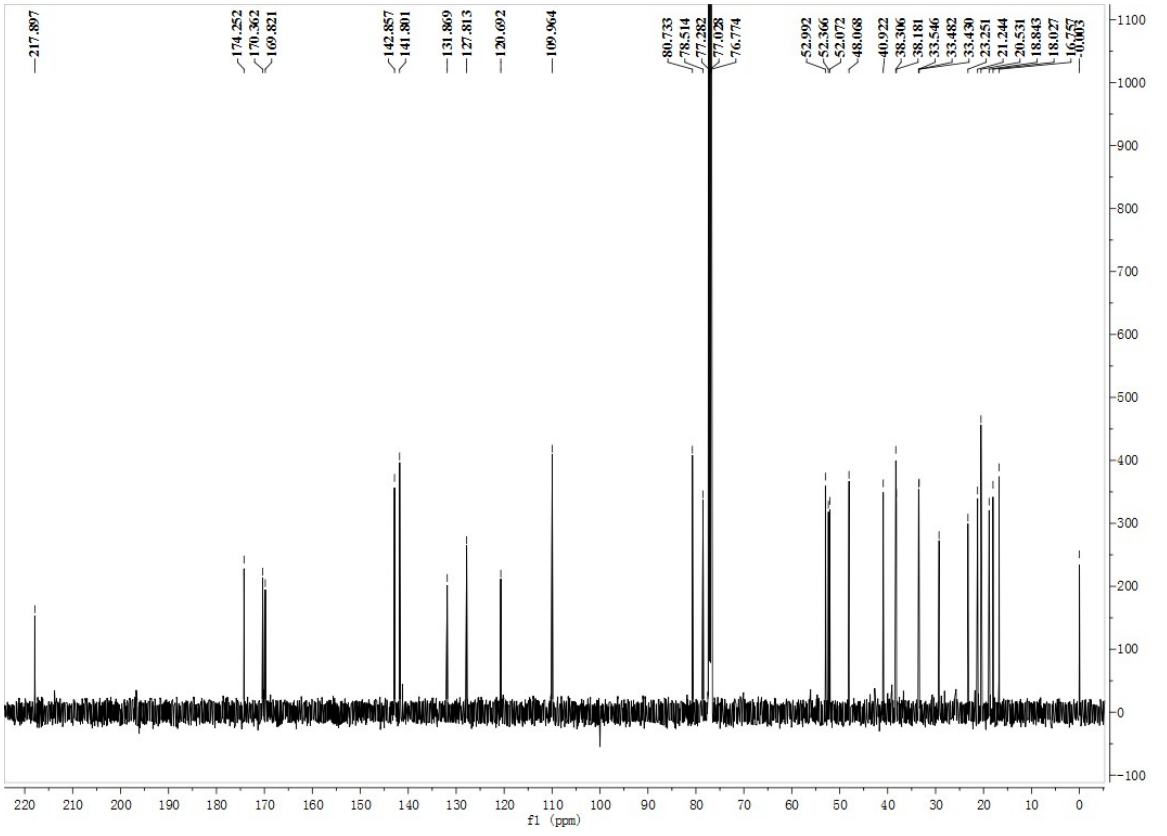
S86 ROSEY of Khasenegasin N (**14**)



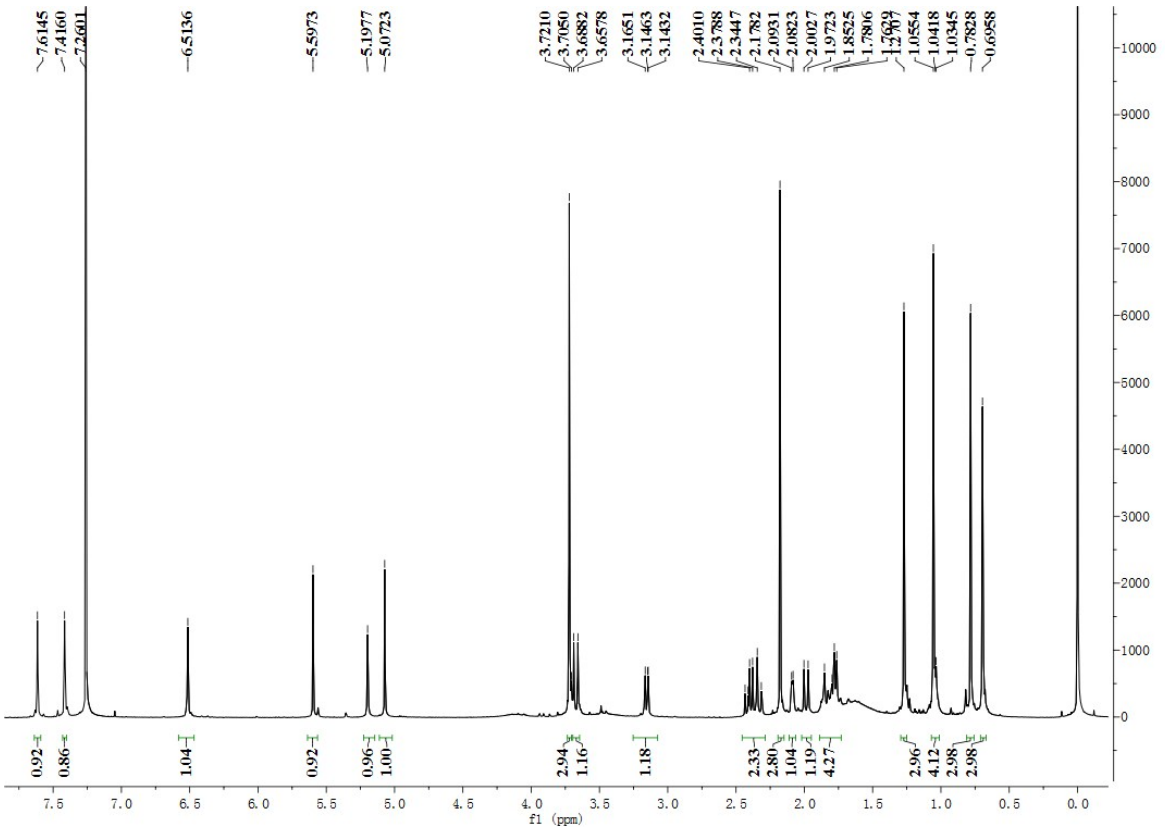
S87: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **15** (fissinolide)



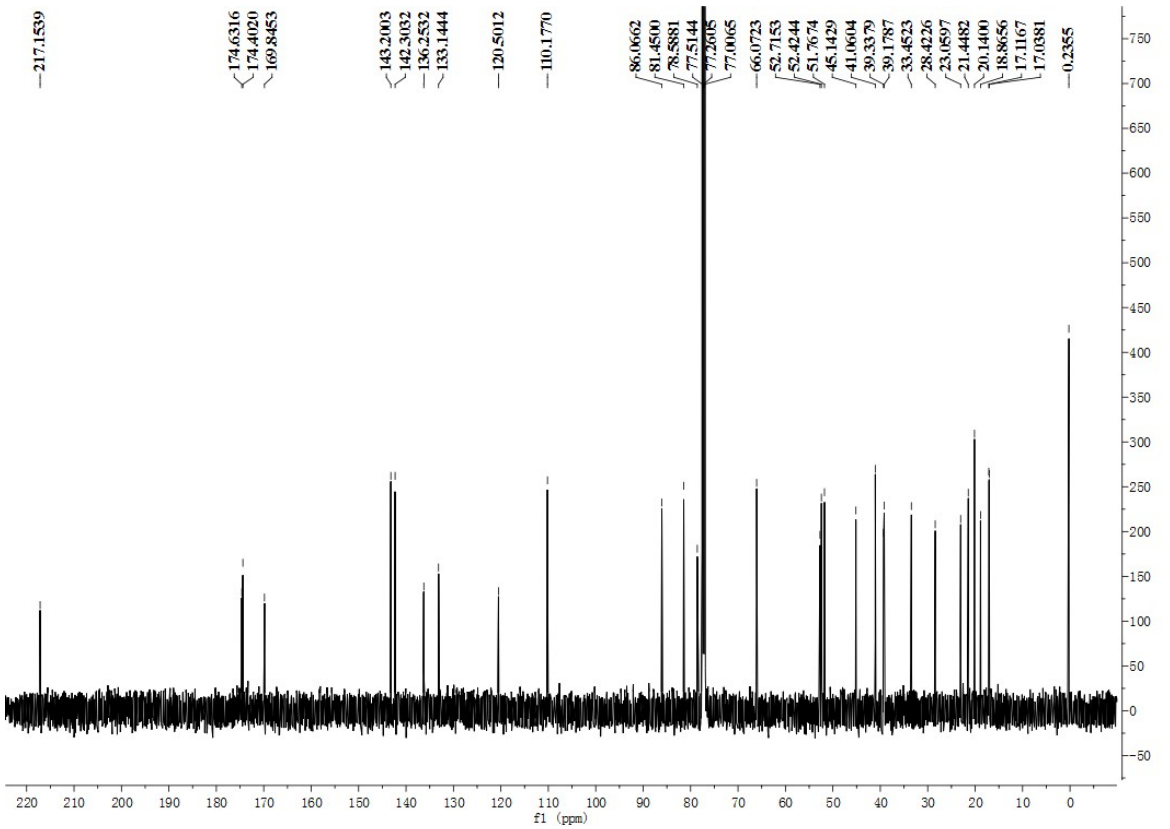
S88: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **15** (fissinolide)



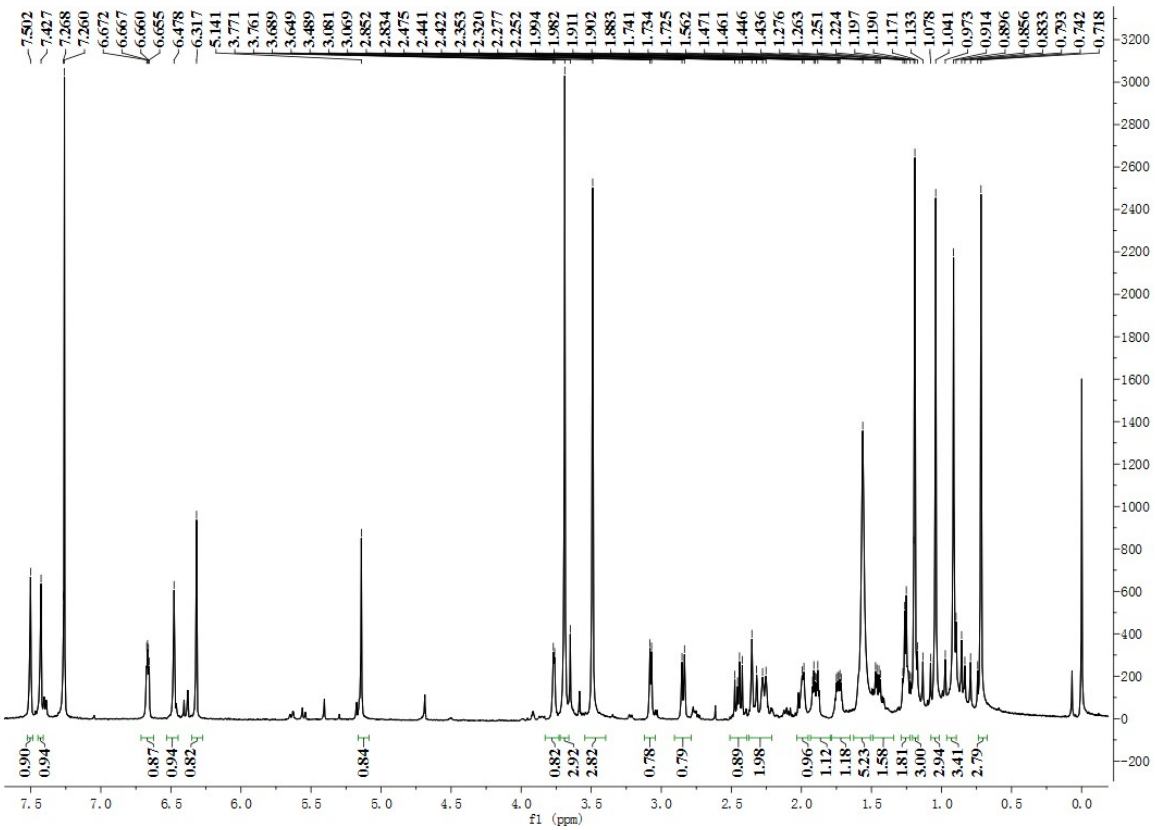
S89: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **16** (swietmanin F)



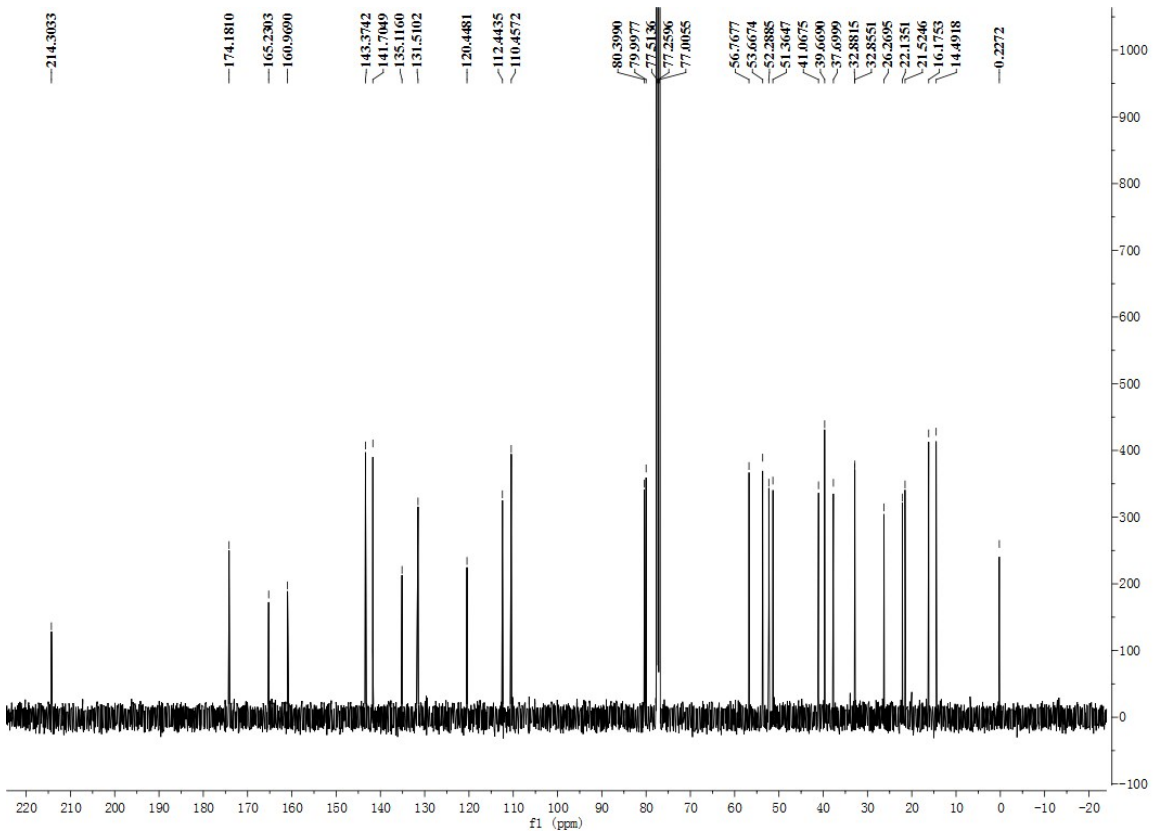
S90: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **16** (swietmanin F)



S91: ^{1}H-NMR (500 MHz, $CDCl_3$) Spectrum of Compound **17** (seneganolide A)



S92: ^{13}C-NMR (125 MHz, $CDCl_3$) Spectrum of Compound **17** (seneganolide A)



S93: NMR data comparing compound **15** with published NMR data (fissinolide)

	15		fissinolide published NMR data[a]	
Position	δ_H (multi, *J* in Hz)[b]	δ_C[c]	δ_H (multi, *J* in Hz)[d]	δ_C[e]
1		217.9		218.1
2	3.15, m	48.1	3.15, m	48.0
3	4.98, d (10.0)	78.5	4.95, d (10.5)	78.4
4		38.3		38.3
5	3.21, dd (9.0, 4.0)	40.9	3.22, m	40.8
6	2.40, dd (16.0, 9.0)	33.4	2.38, m	33.4
	2.35, br d (16.0)			
7		174.3		174.3
8		127.8		127.8
9	1.82, m	52.1	1.8*	52.2
10		52.4		53.0
11α	1.80, m	18.8	1.7*	18.8
11β	1.70, m		1.8*	
12α	1.80, m	29.3	1.0*	29.1
12β	1.00, m		1.8*	
13		38.2		38.1
14		131.9		131.8
15α	3.47, dt (21.0, 3.0)	33.5	3.48, dt (20, 2.5)	33.5
15β	3.75, m		3.80, dm (20)	
16		169.8		170.0
17	5.70, s	80.7	5.70, s	80.7
18	1.07, s, 3H	18.1	1.08, s, 3H	17.9
19	1.15, s, 3H	16.8	1.16, s, 3H	16.8
20		120.7		120.6
21	7.58, s	142.9	7.56, d (1.8)	142.9
22	6.48, d (1.5)	110.0	6.48, d (1.8)	109.9
23	7.41, t (1.5)	141.8	7.42, t (1.8)	141.8
28	0.81, s, 3H	20.5	0.81, s, 3H	20.5
29	0.70, s, 3H	23.3	0.72, s, 3H	23.2
30α	2.05, m	33.5	2.05, dm (15)	33.4
30β	2.81, dd (15.0, 2.0)		2.81 dd (15, 2.5)	
7-OCH_3	3.72, s, 3H	53.0	3.85, s, 3H	53.3
3-OAc	2.18. s, 3H	170.4	2.18, s, 3H	170.4
		21.2		21.3

[a] S. A. Khalid, G. M. Friedrichsen, A. Kharazmi, T. G. Theander, C. E. Olsen and S. B. Christensen, *Phytochemistry*, 1998, **49**, 1769-1772 ;. [b] measured in $CDCl_3$ at 500 MHz; [c] measured in $CDCl_3$ at 125 MHz; [d] measured in $CDCl_3$ at 300 MHz, * Severe overlapping of signals prevents a detailed interpretation of the coupling pattern. n.o. Not observed; [e]measured in $CDCl_3$ at 75 MHz.

S94: NMR data comparing compound **16** with published NMR data (swietmanin F)

	16		swietmanin F published NMR data[a]	
Position	δ_H (multi, *J* in Hz)[b]	δ_C[c]	δ_H (multi, *J* in Hz)[d]	δ_C[e]
1		216.9		216.9
2		78.6		78.3
3	5.07, s	86.1	5.07, s	85.7
4		39.3		39.0
5	3.16, dd (11.0, 1.5)	41.1	3.15, dd (11.1, 1.9)	40.7
6	2.40, dd (16.5, 11.0)	33.5	2.41, dd (16.5, 11.1)	33.1
	2.33, dd (16.5, 1.5)		2.33, dd (16.5, 1.9)	
7		174.4		174.1
8		133.1		132.8
9	2.09, br d (5.4)	51.8	2.08, br d (4.5)	51.4
10		52.7		52.4
11α	1.86, m	18.9	1.88, m	18.5
11β	1.80, m		1.80, m	
12α	1.12, m	28.4	1.12, m	28.0
12β	1.68, m		1.78, m	
13		39.2		38.9
14		136.3		135.9
15	5.20, s	66.1	5.02, s	65.7
16		174.6		174.4
17	5.60, s	81.5	5.60, s	81.1
18	1.06, s, 3H	17.1	1.06, s, 3H	16.9
19	1.27, s, 3H	17.0	1.27, s, 3H	16.7
20		120.5		120.1
21	7.61, s	142.3	7.62, br d (0.6)	142.0
22	6.51, br s	110.2	6.51, br t (0.9)	109.9
23	7.42, br s	143.2	7.42, br t (1.6)	142.9
28	0.78, s, 3H	23.1	0.78, s, 3H	22.7
29	0.70, s, 3H	20.1	0.69, s, 3H	19.8
30	3.66, d (15.2)	45.1	3.67, d (15.2)	44.8
	1.99, d (15.2)		1.99 d (15.2)	
7-OCH_3	3.72, s, 3H	52.4	3.72, s, 3H	52.2
3-OAc	2.18, s, 3H	169.8	2.18, s, 3H	169.6
		21.4		21.2

[a] B. D. Lin, T. Yuan, C. R. Zhang, L. Dong, B. Zhang, Y. Wu and J. M. Yue, *J. Nat. Prod.*, 2009, **72**, 2084–2090.[b] measured in $CDCl_3$ at 500 MHz; [c] measured in $CDCl_3$ at 125 MHz; [d] measured in $CDCl_3$ at 400 MHz; [e] measured in $CDCl_3$ at 125 MHz.

S95: NMR data comparing compound **17** with published NMR data (seneganolide A)

	17		seneganolide A published NMR data[a]	
Position	δ_H (multi, *J* in Hz)[b]	δ_C[c]	δ_H (multi, *J* in Hz)[d]	δ_C[e]
1		214.3		213.9
2	3.07, d (6.0)	56.8	3.07, d (5.9)	56.5
3	3.77, d (5.0)	80.4	3.77, d (5.2)	80.2
4		39.7		39.5
5	2.84, br d (9.0)	41.1	2.85, dd (9.7, 1.5)	40.9
6	2.44, dd (17.0, 9.0)	32.9	2.46, dd (16.8, 9.7)	32.7
	2.33, br d (17.0)		2.35, dd (17.2, 1.6)	
7		174.2		173.9
8		135.1		134.9
9	2.26, br d (12.5)	53.7	2.27, br dt (12.2, 2.8)	53.6
10		51.4		51.2
11α	1.73, ddd (12.5, 8.0, 4.5)	21.5	1.73, ddd (13.2,9.1,4.3)	21.3
11β	1.45 ddd (14.0,12.5, 5.0)		1.47, ddd (14.5,12.1,5.2)	
12α	1.26, m	32.9	1.26, ddd (14.1,11.0,5.3)	32.7
12β	1.90, dt (14.0, 4.5)		1.90, dt (14.1, 4.5)	
13		37.7		37.5
14		161.0		160.7
15	6.32, s	112.4	6.31, s	112.3
16		165.2		164.9
17	5.14, s	80.0	5.14, s	79.8
18	1.04, s, 3H	22.1	1.05, s, 3H	21.9
19	1.20, s, 3H	16.2	1.20, s, 3H	15.9
20		120.4		120.3
21	7.43, br s	141.7	7.50, d (1.5)	141.5
22	6.48, br s	110.5	6.48 br d (1.0)	110.2
23	7.50, br s	143.4	7.42, t (1.6)	143.2
28	0.91, s, 3H	26.3	0.92, s, 3H	26.1
29	0.72, s, 3H	14.5	0.72, s, 3H	14.2
30	6.66, dd (6.0, 2.5)	131.5	6.67, dd (6.0, 2.7)	131.2
7-OCH_3	3.69, s, 3H	52.3	3.69, s, 3H	52.0

[a] S. A. M. Abdelgaleil, T. Iwagawa, M. Doe and M. Nakatani, *Fitoterapia*, 2004, **75**, 566-572. [b] measured in $CDCl_3$ at 500 MHz; [c] measured in $CDCl_3$ at 125 MHz;[d] measured in $CDCl_3$ at 600 MHz; [e] measured in $CDCl_3$ at 150 MHz.