T- and B-cell immunosuppressive activity of novel α-santonin analogs with humoral and cellular immune response in Balb/c mice

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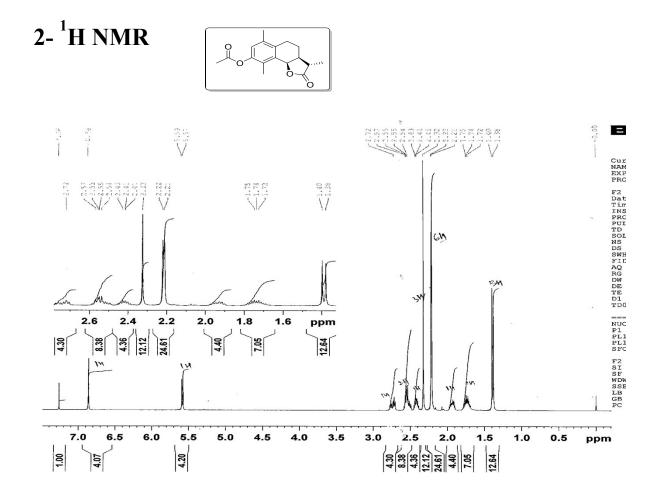
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Section A

General Methods

All the reagents and solvents for executing the present work were obtained from Sigma Aldrich. Dry DCM was prepared first by distilling it and then refluxing it over CaH₂ (5% w/v) for few hours and again distilled it and finally stored it over $4A^{\circ}$ molecular sieves for future use. Pyridine was dried over KOH for one week, then distilled and stored over $4A^{\circ}$ molecular sieves and used throughout the synthesis. All the chemical reactions were monitored by TLC on 0.25 mm silica gel 60 F254 plates (E. Merck) using 2% ceric ammonium sulphate solution as a spraying reagent for detection of the spots on the TLC. Purification of all the compounds was carried out by column chromatography using Silica gel 60-120 mesh stationary phase or by recrystillation. ¹H NMR and ¹³C NMR spectra were recorded on Bruker DPX 400 and DPX 500 instruments using CDCl₃ or CD₃OD as the solvents with TMS as internal standard. The chemical shifts were expressed in \overline{a} ppm and coupling constants in Hertz. High resolution mass spectra (HREIMS) were recorded on Agilent Technologies 6540 instrument.



Section B: ¹H NMR, ¹³C NMR, DEPT135 and HRMS spectra of compounds

2- HRMS

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IRM Calibration Status	1.11 (DA Method	daily_report.m
Comment				
Sample Group		Info.		

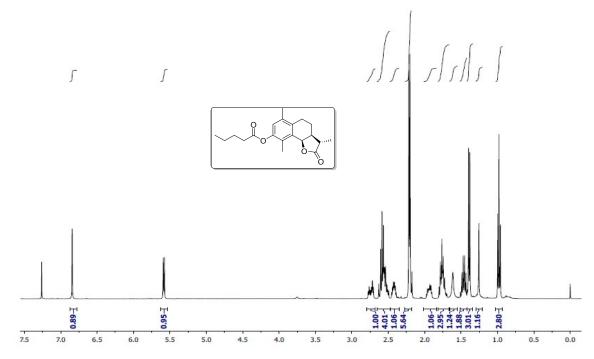
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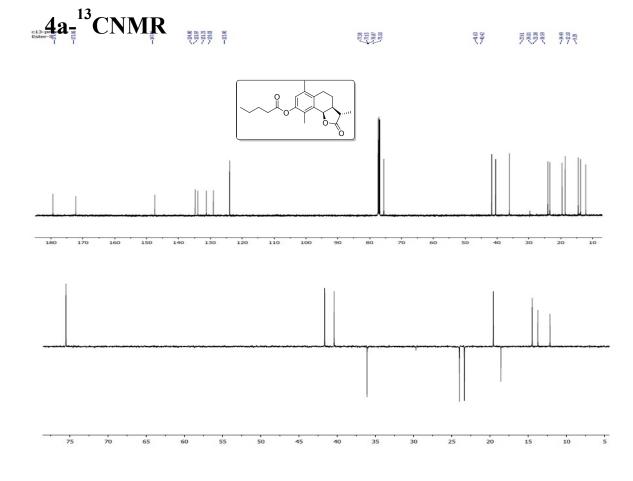
6200 series TOF/6500 series	
Q-TOF B.05.01 (B5125)	

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Compound La		m/z	RT	Algorithm	Mass			
Cpd 6: C17 H20	0 04	289.1451	0.26	Find by Molecula	r Feature 288.138	2		
					i			
IFE MS Spectrum								
							-	
x10 4 Cpd 6:	C17 H20 C	4: +ESI MFE	E Spectrum	(0.198-0.398 min)	Frag=135.0V SN-	AC.d		
1.2		5 SIST					1	
		17H210						
1.		2100						
0.8		5						
0.6								
0.4								
0.2								
0 4	200 250	300 350	400 450	500 550 600	650 700 750 8		-1	
	200 200		Counts	vs. Mass-to-Charg	je (m/z)	00 200 000 000		
160								
	Poak Liet							
1S Spectrum	Peak List	Formula		Ion				
1S Spectrum	Abund	Formula						
15 Spectrum	Abund 1262		01	(M+H)+	(a)			
AS Spectrum n/z z 289.1451 1	Abund 1262 24	3.54 C17 H21	01 04					
4S Spectrum 7/z z 289.1451 1 290.1499 1	Abund 1262 24 42	3.54 C17 H21 00.3 C17 H21 8.05 C17 H21	01 04	(M+H)+ (M+H)+				
4S Spectrum 7/z z 289,1451 1 290,1499 1 291,1572 1	Abund 1262 244 422 ope Matcl	3.54 C17 H21 00.3 C17 H21 8.05 C17 H21	01 04	(M+H)+ (M+H)+ (M+H)+	Calc Abund %	Abund Sum %	Calc Abund Sum %	
AS Spectrum n/z z 289,1451 1 290,1499 1 291,1572 1 Predicted Isot	Abund 1262 244 422 ope Matcl	3.54 C17 H21 00.3 C17 H21 8.05 C17 H21 h Table	04 04 04 Diff (ppm	(M+H)+ (M+H)+ (M+H)+	Calc Abund %	Abund Sum % 81.7	Calc Abund Sum %	82.46
AS Spectrum n/z z 289,1451 1 290,1499 1 291,1572 1 Predicted Isot	Abund 1262 244 422 0pe Matc	3.54 C17 H21 00.3 C17 H21 8.05 C17 H21 1 Table Calc m/z	04 04 04 Diff (ppm	(M+H)+ (M+H)+ (M+H)+			Calc Abund Sum %	82.46 15.49

--- End Of Report ---

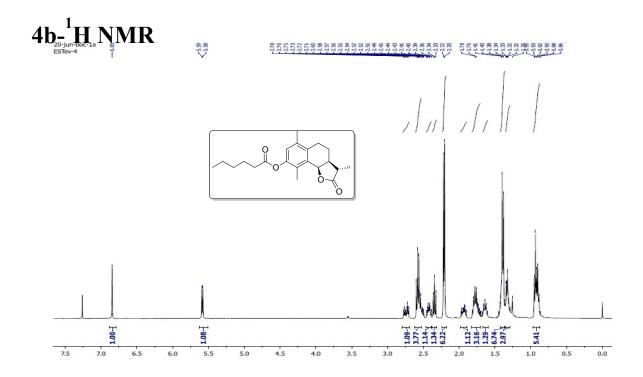
4a----H NMR



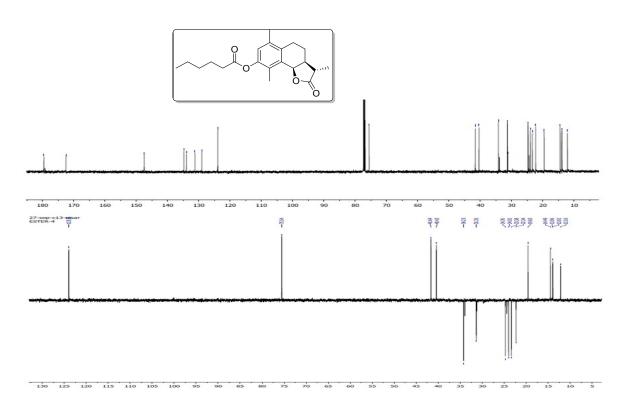


4a-HRMS

								FG Diff	DB Formula
	nd Label 30: C20 H26 O4	RT 0.343	Mass 330.1832	C20 H26		AFG Formula		(ppm) -0.22	C20 H26 04
	01 C20 H28 O4	0.343	330.1032	C20 H20		C20 H20 04		-0.22	C20 1120 04
Compound	Label	m/z	RT	Algorithm	Mass				
Cpd 30: C20		331.190			ar Feature 330.183	32			
MFE MS Spectr	(1000								
		04: +ESI	MFE Spectrum	n (0.228-0.762 n	nin) Frag=135.0V E	STER-10.d		1	
8-					,				
6		331.1904	20 47						
4			-		661.3722 C40 H53 08				
		1			5 5			1	
2					40 T				
0	-,,,,				k]	
0	150 200 25	0 300 3	350 400 450 Counts	500 550 600 vs. Mass-to-Cha	650 700 750 8 irge (m/z)	300 850 900 9	950		
0			350 400 450 Counts	500 550 600 vs. Mass-to-Cha	k	300 850 900 S	950		
0 MS Spectru	m Peak List	Form	nula	Ion	650 700 750 8 Irge (m/z)	300 850 900 S	950		
0 MS Spectru m/z 331.1904	m Peak List z Abund 1 8338	Form	nula H27 04	Ion (M+H)+	650 700 750 8 Irge (m/z)	800 850 900 9	950		
0 MS Spectru <i>m/z</i> 331.1904 332.194	m Peak List z Abund 1 8338 1 1667	Form 52.25 C20	nula H27 04 H27 04	Ion (M+H)+ (M+H)+	650 700 750 8 Irge (m/z)	300 850 900 9	950]	
0 MS Spectru <i>m/z</i> 331.1904 332.194 333.1971	m Peak List z Abund 1 83384 1 1667 1 234	Form 52.25 C20 59.95 C20 136.2 C20	nula H27 04 H27 04 H27 04 H27 04	Ion (M+H)+ (M+H)+ (M+H)+	4 650 700 750 8 Irige (m/z)	300 850 900 9	950]	
0 MS Spectru <i>m/z</i> 331.1904 332.194 333.1971 661.3722	z Abund 1 83384 1 1667 1 234 1 628	Form 52.25 C20 59.95 C20 136.2 C20 12.54 C40	nula H27 O4 H27 O4 H27 O4 H27 O4 H53 O8	Ion (M+H)+ (M+H)+	4 650 700 750 8 Irige (m/z)	300 850 900 s	950]	
0 MS Spectrum m/z 331.1904 333.1971 661.3722 662.3752	Z Abund 1 83384 1 16679 1 234 1 6283 1 2743	Form 52.25 C20 59.95 C20 136.2 C20 2.54 C40 24.81 C40	nula H27 O4 H27 O4 H27 O4 H27 O4 H53 O8	Ion (M+H)+ (M+H)+ (M+H)+	+	300 850 900 9	950		
0 MS Spectru <i>m/z</i> 331.1904 332.194 333.1971 661.3722	Z Abund 1 83384 1 16679 1 234 1 6283 1 2743	Form 52.25 C20 59.95 C20 136.2 C20 2.54 C40 24.81 C40	nula H27 O4 H27 O4 H27 O4 H53 O8 H53 O8	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+H) (2M+H)	+ +	300 850 900 9	950]	
MS Spectru m/z 331.1904 333.1971 661.3722 662.3752 Predicted Is	m Peak List 2 Abund 1 8338 1 1667 1 23 1 23 1 628 1 274 500pe Mate m/z	Form 52.25 C20 59.95 C20 136.2 C20 136.2 C20 12.54 C40 14.81 C40 h Table Calc m/z	nula H27 04 H27 04 H27 04 H53 08 H53 08 Diff (ppm	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+H) (2M+H) (2M+H)	+ + Calc Abund %	Abund Sum %		Calc Abund S	
MS Spectru m/z 331.1904 333.1971 661.3722 662.3752 Predicted Is	m Peak List z Abund 1 83384 1 16673 1 234 1 628 1 2743 5000pe Mate	52.25 C20 59.95 C20 136.2 C20 12.54 C40 14.81 C40 h Table	nula H27 04 H27 04 H27 04 H53 08 H53 08 Diff (ppm	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+H) (2M+H)	+ + Calc Abund %	Abund Sum %		Calc Abund S	79.61
MS Spectru m/z 331.1904 333.1971 661.3722 662.3752 Predicted Is	m Peak List 2 Abund 1 8338 1 1667 1 23 1 23 1 628 1 274 500pe Mate m/z	Form 52.25 C20 59.95 C20 136.2 C20 136.2 C20 12.54 C40 14.81 C40 h Table Calc m/z	nula H27 04 H27 04 H27 04 H53 08 H53 08 Diff (ppm 1904 -0	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+H) (2M+H) (2M+H)	L 700 750 8 n 650 700 750 8 rge (m/2) + + + Caic Abund % 0 100	Abund Sum %		Calc Abund S	79.61 17.59
0 MS Spectru <i>m/z</i> 331.1904 332.194 333.1971 661.3722 662.3752 Predicted Is	Peak List z Abund 1 8338 1 1667 1 233 1 628 1 274: sotope Mate m/z 331.1904 331.1904	Form 52.25 C20 59.95 C20 136.2 C20 136.2 C20 136.2 C40 14.81 C40 h Table Calc m/z 331.1	Inula H27 O4 H27 O4 H27 O4 H53 O8 H53 O8 Diff (ppm) 1904 -C 1938	Ion (M+H)+ (M+H)+ (M+H)+ (2M+H) (2M+H) (2M+H) (2M+H) (2M+H) (200) (201) (L 500 750 8 rige (m/2) 	Abund Sum %	80.98	Calc Abund S	79.61
0 MS Spectrui <i>m/z</i> 331.1904 332.194 333.1971 661.3722 662.3752 Predicted Is Isotope 1 2	m Peak List z Abund 1 8338 1 1667 1 234 1 628 1 274 sotope Mate m/z 331.1904 332.194	Form 52.25 C20 59.95 C20 136.2 C20 2.54 C40 44.81 C40 h Table Calc m/z 331.1 332.1	nula H27 04 H27 04 H53 08 H53 08 H53 08 Diff (ppm 1904 -C 1938 -C 1938 -C	Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)	+ + Calc Abund % 0 22.09 1 3.15	Abund Sum %	80.98 16.2	Calc Abund S	79.61 17.59
MS Spectru m/z 331.1904 332.194 333.1971 661.3722 662.3752 Predicted Is sotope 1 2 3 3	m Peak List z Abund 1 83384 1 1667 1 23 1 23 1 23 1 23 1 23 24 33 1.1904 333.1904 333.1971	Form 52.25 C20 59.95 C20 136.2 C20 2.54 C40 4.81 C40 h Table Calc m/z 331.1 332.1 333.1 333.1	Diff (ppm) 1936 1904 1904 1904 1905 1992	Ion (M+H)+ (M+H)+ (M+H)+ (2M+H) (2M+H	L 00 700 750 8 irge (m/2) + + Calc Abund % 0 100 0 22.09 1 3.15 6 0.34	Abund Sum %	80.98 16.2 2.28	Calc Abund S	79.61 17.59 2.5

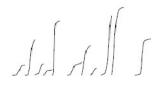


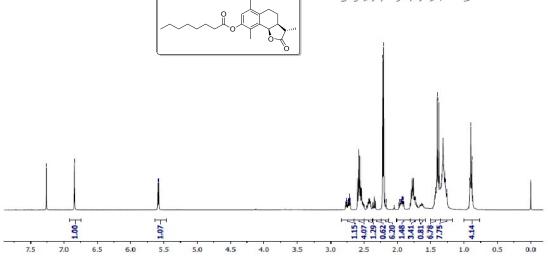


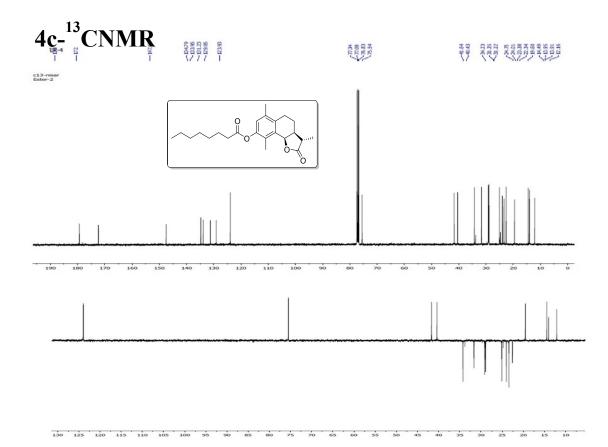


4b-HRMS

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Cod	nd Label 11: C21 H28 O4	0.344	344.2005	C21 H28 C		C21 H28 O4	-4.99	C21 H28 O4
Сра	11: CZI H28 04	0.344	377.2003	C21 1120 C		0211120 04	1.55	dir nico o i
					<u> </u>	· · · · · · · · · · · · · · · · · · ·		
Compound	Label	m/z	RT	Algorithm	Mass			
Cpd 41: C21	H28 O4	345.2077	0.344	Find by Molecula	r Feature 344.200	15		
	guarrae namaanton karanan karabu dikabukhan k		_	5 2 2 2		a munan una put		
IFE MS Spect							_	
x10 6 Cpd	41: C21 H28		E Spectru	m (0.202-0.920 m	n) Frag=135.0V E	STER-4.d	Į	
1-		104					1	
0.8		H29						
		345.2077 C21 H29 O4						
0.6 -		0						
0.4		1			57 C			
					88			
0.2					689.4056 C42 H57 O8			
	150 200 25	0 300 350	400 450 Counts	500 550 600 vs. Mass-to-Char	650 700 750 8 ge (m/z)	300 850 900 950		
0 J	m Peak List				1	300 850 900 950		
0 <u>MS Spectru</u> n/z	m Peak List	Formul	a	Ion	1	300 850 900 950 -	.	
0 J	m Peak List z Abund		a 04		1	300 850 900 950 -		
0 MS Spectru m/z 345.2077	m Peak List z Abund 1 97158 1 19131	Formul 5.25 C21 H29	a 04 04	Ion (M+H)+	1	300 850 900 950 -		
0 MS Spectru <i>n/z</i> 345.2077 346.2113	m Peak List z Abund 1 97156 1 19131 1 290 1 8776	Formul 5.25 C21 H29 0.58 C21 H29 88.8 C21 H29 8.53 C42 H57	a 04 04 04 04 08	Ion (M+H)+ (M+H)+	650 700 750 8 ge (m/z)	300 850 900 950 -		
0 MS Spectru m/z 345.2077 346.2113 347.2138 689.4056 690.409	z Abund 1 97156 1 19131 1 290 1 8776 1 4124	Formul 5.25 C21 H29 0.58 C21 H29 88.8 C21 H29 8.53 C42 H57 4.23 C42 H57	a 04 04 04 04 08	Ion (M+H)+ (M+H)+ (M+H)+	650 700 750 8	500 850 900 950 -		
0 MS Spectru n/z 345.2077 346.2113 347.2138 689.4056 690.409 Predicted I	z Abund 1 97155 1 19131 1 290 1 8776 1 4124 sotope Matc 94124	Formul 5.25 C21 H29 0.58 C21 H29 88.8 C21 H29 85.3 C42 H57 4.23 C42 H57 h Table	a 04 04 04 08 08	Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+	650 760 750 8	-		â 94
0 MS Spectru m/z 345.2077 346.2113 347.2138 689.4056 690.409	Peak List z Abund 1 97156 1 19131 1 290 1 8776 1 4124 sotope Matc m/z	Formul 5.25 C21 H29 0.58 C21 H29 88.8 C21 H29 85.3 C42 H57 4.23 C42 H57 h Table Calc m/z	a 04 04 04 08 08 Diff (ppn	Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+	650 700 750 8 ge (m/z)	Abund Sum %	Calc Abund	
0 MS Spectru m/z 345.2077 346.2113 347.2138 689.4056 690.409 Predicted I sotope 1	z Abund 1 97158 1 19133 1 290 1 8776 1 4124 sotope Matc m/z 345.2077 345.2077	Formul 5.25 C21 H29 0.58 C21 H29 88.8 C21 H29 88.53 C42 H57 4.23 C42 H57 h Table Calc m/z 345.20	a 04 04 08 08 08 Diff (ppn 5	Ion (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ 1) Abund % 4.89 100	650 760 750 8 go (m/2)	Abund Sum %	12	78.74
0 MS Spectru <i>n/z</i> 345.2077 346.2113 347.2138 689.4056 690.409 Predicted I sotope 1 2	z Abund 1 97156 1 19131 1 290 1 8776 1 4124 sotope Matc m/z 345.2077 346.2113	Formul. 5.25 C21 H29 0.58 C21 H29 88.58 C21 H29 88.53 C42 H57 h Table Caic m/z 346.209	a 04 04 08 08 Diff (ppn 5 4	Ion (M+H)+ (MH)+ (MH)+ (2M+H)+ (2M+H)+	650 760 750 8 ge (m/2) Calc Abund %	Abund Sum % 81. 15.	12 97	78.74 18.27
0 MS Spectru m/z 345.2077 346.2113 689.4056 690.409 Predicted I sotope 1 2 3 3 3 3 3 3 3 3 3 3 3 3 3	Peak List z Abund 1 97158 1 19131 1 290 1 19131 1 290 1 4124 sotope Matc m/z 345.2077 346.2113 347.2138 347.2138	Formul 5.25 C21 H29 0.58 C21 H29 88.8 C21 H29 88.8 C21 H29 4.23 C42 H57 h Table Calc m/z 345.20 346.209 347.212	a 04 04 04 08 08 Diff (ppn 5 - 4 - 2	Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (3.2 19.69 4.53	650 700 750 8 ge (m/z) Calc Abund % 100 23.2 3.39	Abund Sum % 81. 15. 2.	12 97 13	78.74
0 MS Spectru m/z 345.2077 346.2113 347.2138 689.4056 690.409 Predicted I sotope 1	z Abund 1 97158 1 19133 1 290 1 8776 1 4124 sotope Matc m/z 345.2077 345.2077	Formul 5.25 C21 H29 0.58 C21 H29 88.8 C21 H29 88.53 C42 H57 4.23 C42 H57 h Table Calc m/z 345.20	a 04 04 08 08 08 Diff (ppn 5	Ion (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ 1) Abund % 4.89 100	650 760 750 8 go (m/2)	Abund Sum %	12	78.74
0 MS Spectru <i>n/z</i> 345.2077 346.2113 347.2138 689.4056 690.409 Predicted I sotope 1 2	Peak List z Abund 1 97155 1 19131 1 290 1 19131 1 290 1 4124 sotope Matc m/z 345.2077 346.2113 347.2138 347.2138	Formul. 5.25 C21 H29 0.58 C21 H29 88.58 C21 H29 88.53 C42 H57 h Table Caic m/z 346.209	a 04 04 04 08 08 08 08 08 08 08 08 08 08	Ion (M+H)+ (MH)+ (MH)+ (2M+H)+ (2M+H)+	1 1 ge (m/2) 750 8	Abund Sum % 81. 15. 2. 0.	12 97 43 41	78.74 18.27 2.67

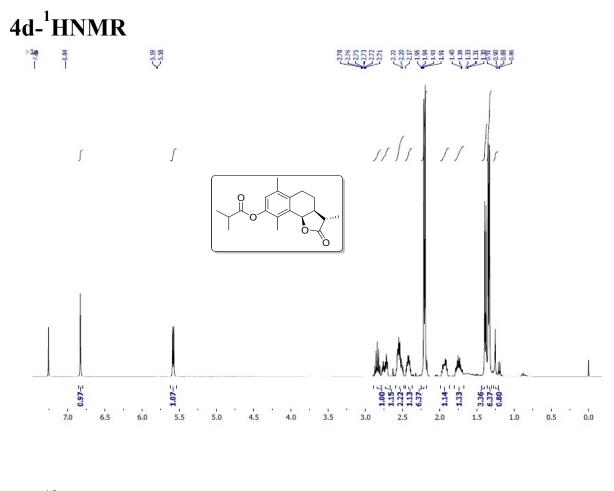


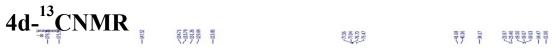


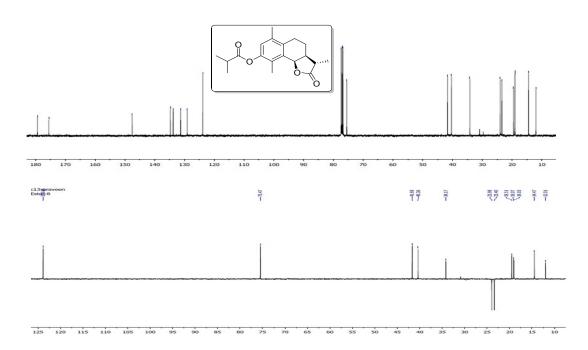


4c-HRMS

Compoun	able d Label	RT	Mass	Formula		IFG Formula	IFG Diff (ppm)	DB Formula
Cpd 26	: C23 H32 O4	0.344	372.2334	C23 H32 O	4	C23 H32 O4	-8.95	C23 H32 O4
Compound L		m/z		Algorithm	Mass			
Cpd 26: C23 H	32 04	373.2406	0.344	Find by Molecula	Feature 372.233	4		
				el Middel I Cludu i renovembro en usuron servicio				
IFE MS Spectru	n							
			E 0	- (0.027 1.001 ml	n) Frag=135.0V ES	TED 2 d	Г	
AIU - I	6: C23 H32			n (0.237-1.021 mi	n) Frag=135.0V Ed	51ER-2.0		
1-		8	ŏ					
0.8		3.24	2					
		373.2406	:23					
0.6			0		80			
0.4					745.4700 C46 H65 08			
					5.4 5.4			
0.2					2 A O			
0						<u>,,,,,</u>	Ļ	
11	0 200 25	0 300 350	400 450	500 550 600	650 700 750 8	800 850 900 950		
			Counts	va. 141833-10-Citat	36 (11/2)			
1S Spectrun								
m/z	z Abund	Formula		Ion				
	1 95206	5.63 C23 H33	04	(M+H)+				
373.2406		****						
373.2406 374.2443	1 21591	1.33 C23 H33		(M+H)+				
373.2406 374.2443 375.2469	1 21591 1 3438	1.33 C23 H33 4.83 C23 H33	04	(M+H)+				
373.2406 374.2443 375.2469 745.47	1 21591 1 3438 1 8025	1.33 C23 H33 4.83 C23 H33 7.11 C46 H65	04 08	(M+H)+ (2M+H)+				
373.2406 374.2443 375.2469 745.47 746.4734	1 21591 1 3438 1 8025 1 4463	1.33 C23 H33 4.83 C23 H33 7.11 C46 H65 7.95 C46 H65	04 08	(M+H)+				
373.2406 374.2443 375.2469 745.47 746.4734 Predicted Is	1 21591 1 3438 1 8025 1 4463 otope Mate	1.33 C23 H33 4.83 C23 H33 7.11 C46 H65 7.95 C46 H65 h Table	04 08 08	(M+H)+ (2M+H)+ (2M+H)+	Catc Abund %	Abund Sum %	Calc Abund Sum	%
373.2406 374.2443 375.2469 745.47 746.4734 Predicted Is	1 21591 1 3438 1 8025 1 4463 50000 Matc	1.33 C23 H33 4.83 C23 H33 7.11 C46 H65 7.95 C46 H65 h Table Calc m/z	04 08 08 Diff (ppm	(M+H)+ (2M+H)+ (2M+H)+	Calc Abund %	Abund Sum % 78.8		% 77.03
373.2406 374.2443 375.2469 745.47 746.4734 Predicted Is	1 21591 1 3438 1 8025 1 4463 0tope Mato <i>n/z</i> 373.2406	1.33 C23 H33 4.83 C23 H33 7.11 C46 H65 7.95 C46 H65 h Table Calc m/z 373.2373	04 08 08 Diff (ppm	(M+H)+ (2M+H)+ (2M+H)+ (2M+H)+				
373.2406 374.2443 375.2469 745.47 746.4734 Predicted Iso Isotope / 1	1 21591 1 3438 1 8025 1 4463 50000 Matc	1.33 C23 H33 4.83 C23 H33 7.11 C46 H65 7.95 C46 H65 h Table Calc m/z	04 08 08 Diff (ppm 3 -1	(M+H)+ (2M+H)+	100	78.8		77.03
373.2406 374.2443 375.2469 745.47 746.4734 Predicted Iso (sotope / 1 2	1 21591 1 3438 1 8025 1 4463 otope Mato <i>m/z</i> 373.2406 374.2443	1.33 C23 H33 4.83 C23 H33 7.11 C46 H65 7.95 C46 H65 h Table Calc m/z 373.2373 374.2407	04 08 08 Diff (ppm 3	(M+H)+ (2M+H)+	100 25.41	78.8 17.87		77.03 19.57



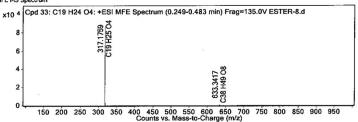




4d-HRMS

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 33: C19 H24 O4	0.344	316.1686	C19 H24 O4	C19 H24 O4	-3.7	C19 H24 O4
ompound Label	m/z	RT	Algorithm	Mass		

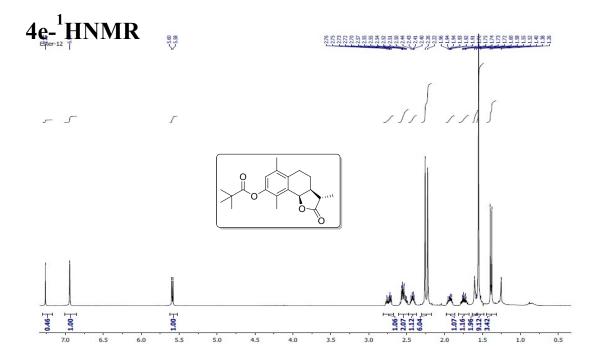
MET MC	Coortman	

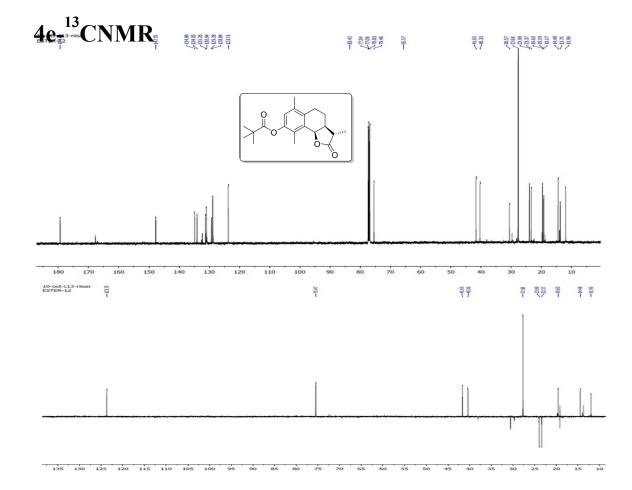


MS Spectrum Peak List

m/z	z	Abund	Formula		Ion	
317.1759	1	86736.3	C19 H25 O4		(M+H)+	L
318.1794	1	16992.7	C19 H25 O4		(M+H)+	L
319.1825	1	2939.97	C19 H25 O4		(M+H)+	l
633,3417	1	729.04	C38 H49 O8		(2M+H)+	l
634.344	1	351.9	C38 H49 O8		(2M+H)+	
Predicted I	sot	ope Matc	h Table			
Isotope	m/	z	Calc m/z	Diff (ppm)	Abund %	k
1		317,1759	317,1747	-3.58	100	Г

Predicted Is	sotope Matc	h Table					
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1	317.1759	317.1747	-3.58	100	100	81.31	80.71
2	318.1794	318.1781	-3.95	19.59	20.99	15.93	16.94
3	319.1825	319.1808	-5.24	3.39	2.91	2.76	2.35

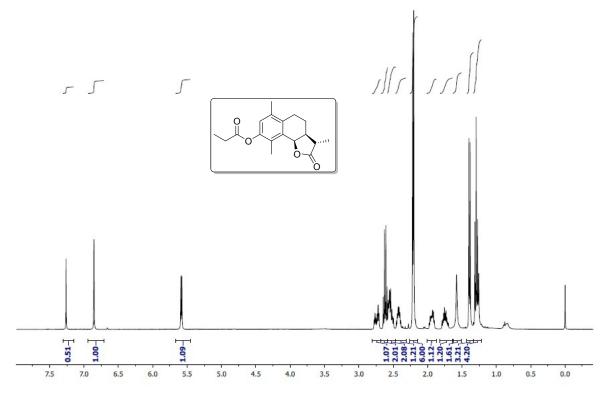




4e-HRMS

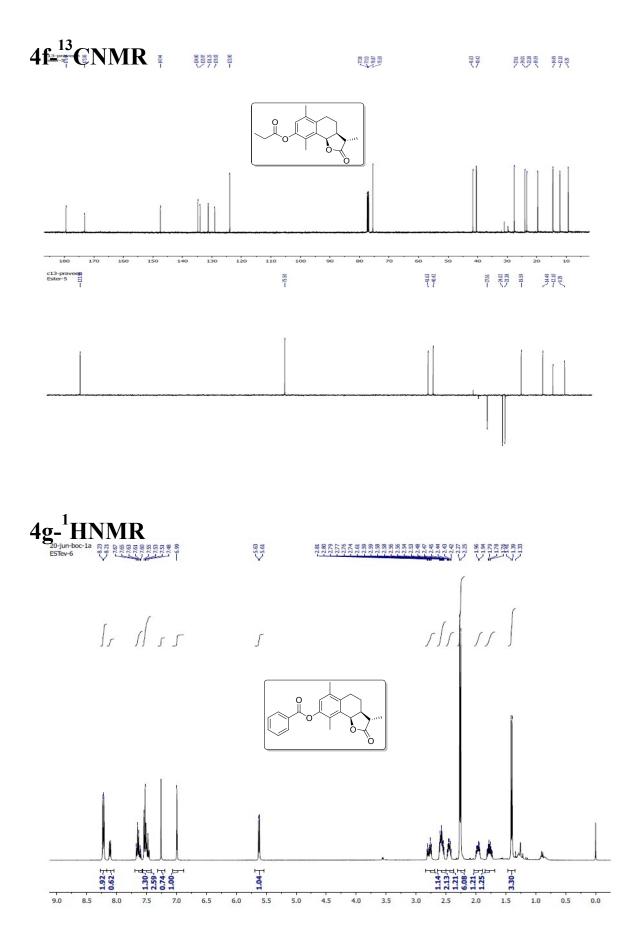
Compound Tal		RT	Mass	Form	la	MFG		IFG Diff (ppm)	DB Formul
	20 H26 O4		330.1815	C20 H2	5 04	C20	H26 O4	4.9	C20 H26 Q4
								<i>%</i>	
Compound Lat		m/z	RT	Algorithm		lass			
Cpd 33: C20 H20	5 04	331.188	7 0.341	Find by Molecu	lar Feature 3	30.1815			
e e anna mhanna an bhann à mhanh c'A tha na fair an an an an a n an tha an tha	1614 F T & T & T & T			3 		nennamours annandalhallti Ar Stedert B			
IFE MS Spectrum									
· · · · · · · · · · · · · · · · · · ·	C20 H26	04: +ESI	MEE Spectru	m (0.241-0.742	min) Frag=135	.0V E-12.d		7	
x10 5 Cpd 33: 3.5	0201120				,				
3		88							
2.5		331.1887	Ċ,		3				
2		č,							
1.5									
					661.3723 C40 H53 08			1	
1-					0H			1	
0.5		I			°.2			1	
0 4	200 25	0 300 3	50 400 450	500 550 60	0 650 700	750 800	850 900 950	-	
			Counts	s vs. Mass-to-Ch	arge (m/z)				
IS Spectrum	Peak List								
<i>n/z</i> z	Abund		nula	Ion					
331.1887 1	33444		H27 04	(M+H)					
332.1923 1		51.08 C20		(M+H)					
333.195 <u>1</u> 661.3723 <u>1</u>		2.89 C20		(M+H) (2M+H					
661.3723 1 662.3768 1		4.16 C40		(2M+F	·				
Predicted Isot			155 00						
sotope m/		Calc m/z	Diff (ppr	n) Abund %	Calc Abund	% Abu	ind Sum %	Calc Abund S	um %
	331.1887	331.	1904	4.96 1	00	100	80.16		79.63
1	332.1923	332.	1938	4.51 20.	98	22.09	16.82		17.59
1	332.1923			4.53 3.		2 4 5	2.47		2.51
1 2 3	333.195	333. 334.			08 69	3.15 0.34	0.56		0.27

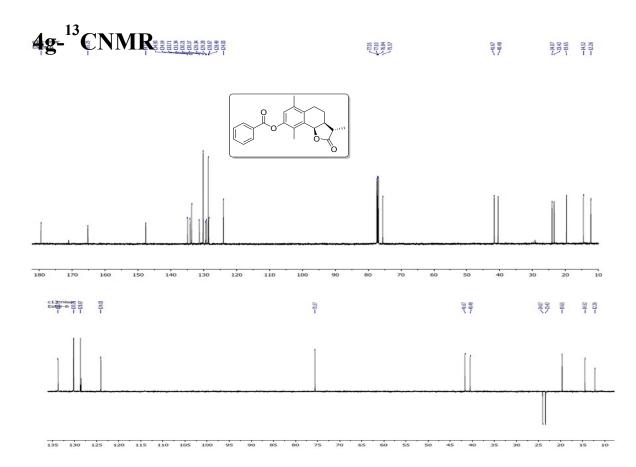
4f¹_{er-5}HNMR



4f-HRMS

Compound Compou			RT	Mass	<u> </u>	Formula	м		IFG Diff (ppm)	DB Formula
		H22 04	0.342	302.1523		C18 H22 O	4	C18 H22 O4	-1.62	C18 H22 O4
Compound	Label		m/z	RT	Algor	ithm	Mass			
Cpd 19: C18			303.1596	0.342	Find b	y Molecula	Feature 302.152	3		
	n ann ann ann ann a		A CARGONE SUCCESSION OF COMPANY			AND A DRIVEN MALE AND A DRIVEN				
IFE MS Spectr	um									
		18 H22	O4: +ESI MI	E Spectru	m (0.24	1-0.542 mi	n) Frag=135.0V ES	STER-5.d		
			6.0							
1.75			303.1596 C18 H23 O4							
1.5			303.							
1.25-			0							
0.75						605.3110 C36 H45 O8				
0.5						45				
0.25						36.05				
ہ لیے	160.0		2 200 250	400 450	600		660 700 750 8	00 850 900 950	-J	
	150 2	00 250	300 350	Counts	s vs. Ma	ass-to-Char	ge (m/z)	00 850 500 550		
1S Spectru	m Pea	ak List								
n/z		bund	Formul	а		Ion				
303.1596	1	18602	9.88 C18 H2	3 04		(M+H)+				
304.1627	1		9.66 C18 H2			(M+H)+				
305.1659	1		9.66 C18 H2			(M+H)+				
605.311	1		3.01 C36 H4			(2M+H)+				
606.3158			3.95 C36 H4	5 08		(2M+H)+				
				D:## (bund %	Calc Abund %	Abund Sum %	Calc Abund Sur	n %
Predicted I			Calc m/z	Diff (ppr	1.79	100	100			81.58
sotope	m/z		203 150							
Predicted Is sotope 1 2	3	03.1596 04.1627	303.159		-0.56	20.12	19,89	16.25		16.22



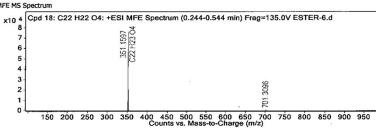


4g-HRMS

A	PT		F	NEC Formula	MFG Diff	DB Formula
Compound Label	RT	Mass	Formula	MFG Formula	(ppm)	
Cpd 18: C22 H22 O4	0.341	350.1525	C22 H22 O4	C22 H22 O4	-1.91	C22 H22 O4

Compound Label	m/z	RT	Algorithm	Mass
Cpd 18: C22 H22 O4	351.1597	0.341	Find by Molecular Feature	350.1525
		1		

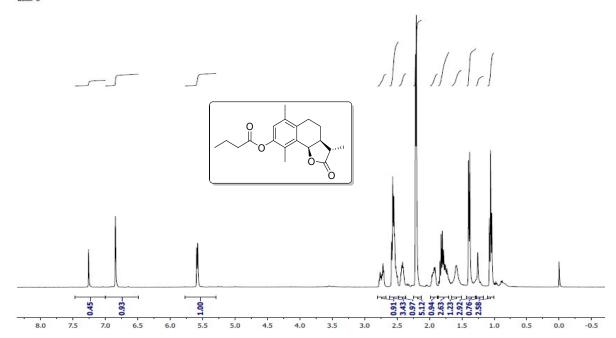
MFE MS Spectrum

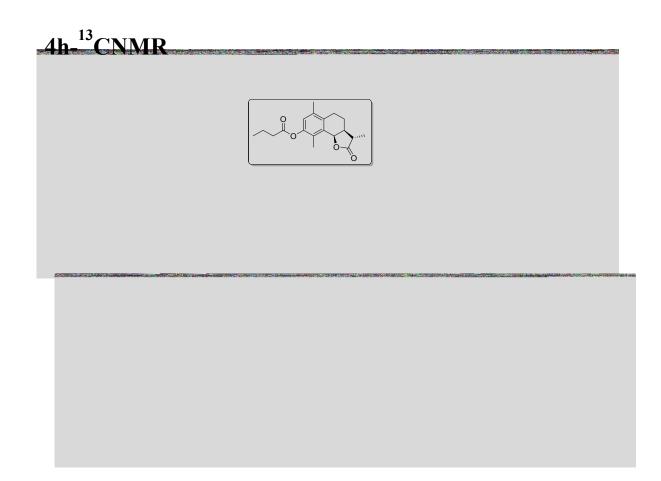


MS Spectru	m P	eak List						
m/z	z	Abund	Formula		Ion			
351.1597	1	7553	0.73 C22 H23	04	(M+H)+			
352.1631	1	2045	3.84 C22 H23	04	(M+H)+			
353.1665	1	365	6.73 C22 H23	04	(M+H)+			
701.3096	1	80	7.34		(2M+H)+			
702.3148	1	58	3.45		(2M+H)+			
Predicted Is	soto	pe Matc	h Table					
Isotope	m/2	r	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1		351.1597	351.1591	-1.88	100	100	75.44	77.98
2		352.1631	352.1625	-1.7	27.08	24.21	20.43	18.83
3		353.1665	353.1653	-3.33	4.84	3.62	3.65	2.83
4		354.1692	354.168	-3.3	0.63	0.41	0.48	0.32

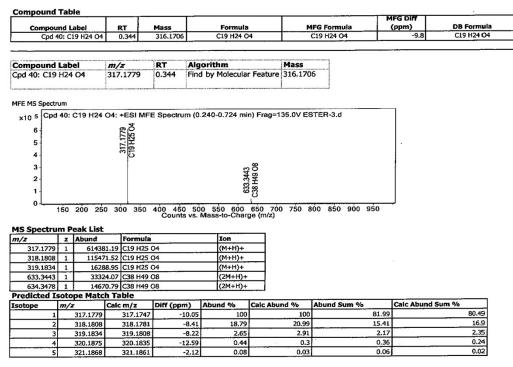
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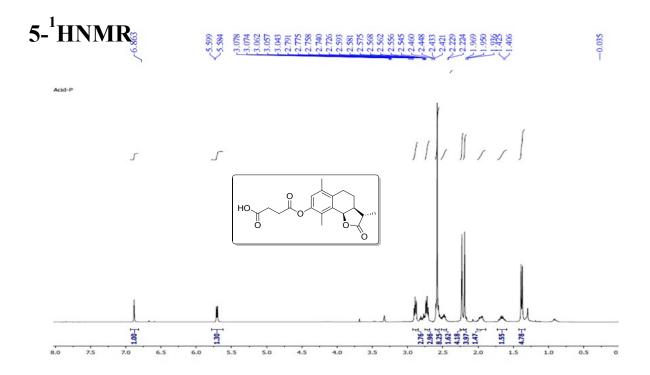


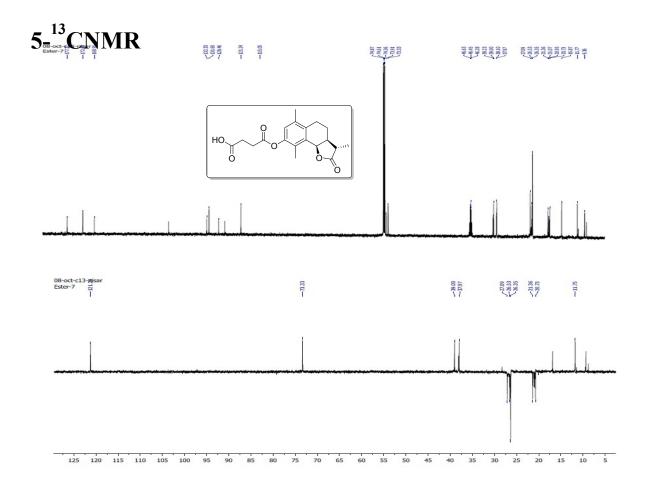




4h-HRMS







5-HRMS

Compound Table						
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 62: C19 H22 O6	0.359	346.143	C19 H22 O6	C19 H22 O6	-4.03	C19 H22 O6

Compound Label	m/z	RT	Algorithm	Mass
Cpd 62: C19 H22 O6	347.1524	0.359	Find by Molecular Feature	346.143

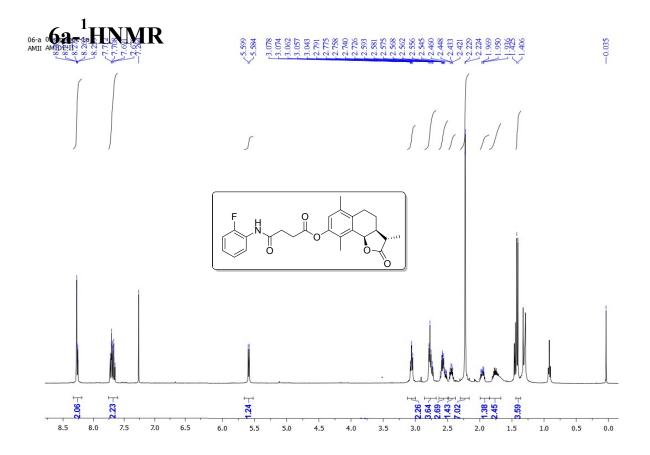
MFE MS Spectrum

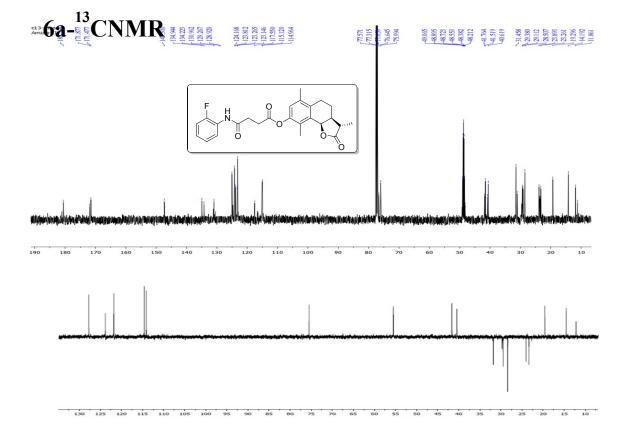
×10 ³	Cpd 62	: C19	H22 O	6: +E	SI MF	E Sp	ectrun	n (0.2	75-0.5	59 mi	n) Fra	ig=13	5.0V I	ESTE	R-7.d			
1.2					23 06													
1-					9 H													
0.8-					0													
0.6																		
0.4																		
0.2																		
0-	Ļ <u> </u>				<u> </u>													,
	150) 200	250	300	350	400 C	450 ounts	500 vs. Ma	550 ass-to	600 -Char	650 ge (m	700 /z)	750	800	850	900	950	

MS Spectrum Peak List

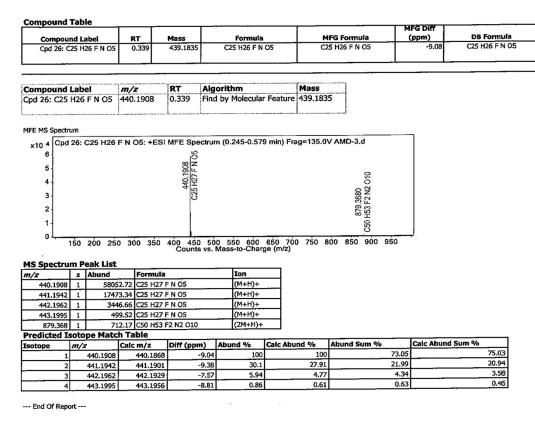
m/z	z	Abund	Formula		Ion
347.1524	1	1293.18	C19 H23 O6		(M+H)+
348.1537	1	387.41	C19 H23 O6		(M+H)+
349.1446	1	239.88	C19 H23 O6		(M+H)+
Predicted Is	soto	pe Matc	h Table		
Isotope	m/.	7	Calc m/z	Diff (ppm)	Abund %

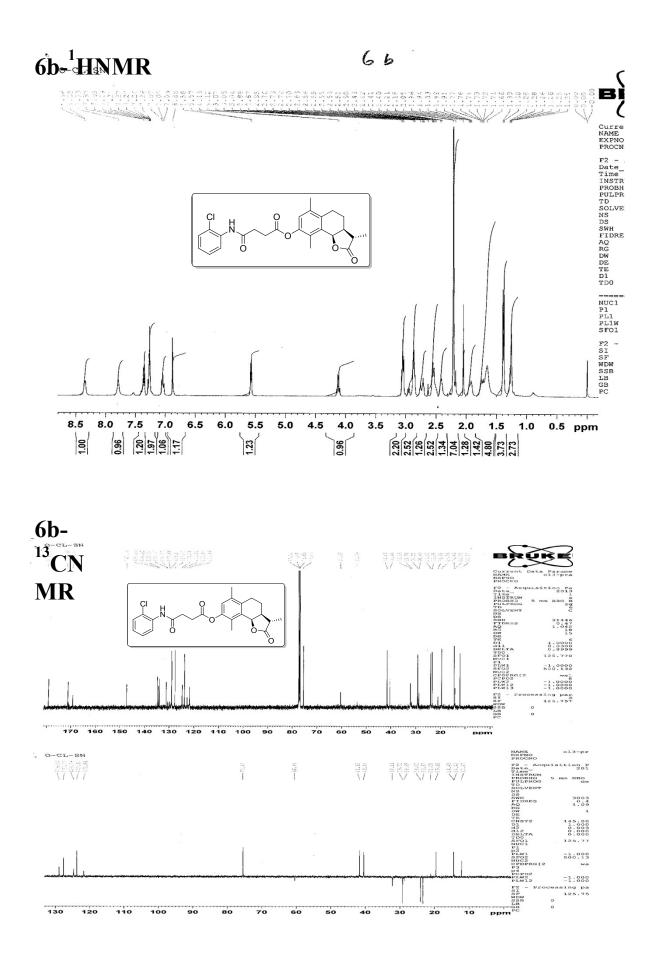
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
	1 347.1524	347.1489	-10.15	100	100	67.34	80.4
	2 348.1537	348.1523	-4.05	29.96	21.04	20.17	16.92
	349.1446	349.1548	29.01	18.55	3.34	12.49	2.68





6a-HRMS





6b-HRMS

					MFG Diff	
Compound Label	RT	Mass	Formula	MFG Formula	(ppm)	DB Formula
Cpd 22: C25 H26 Cl N O5	0.338	455.1517	C25 H26 CI N O5	C25 H26 CI N O5	-3.75	C25 H26 CI N O5

Compound Label	m/z	RT	Algorithm	Mass
Cpd 22: C25 H26 CI N O5	456.1589	0.338	Find by Molecular Feature	455.1517

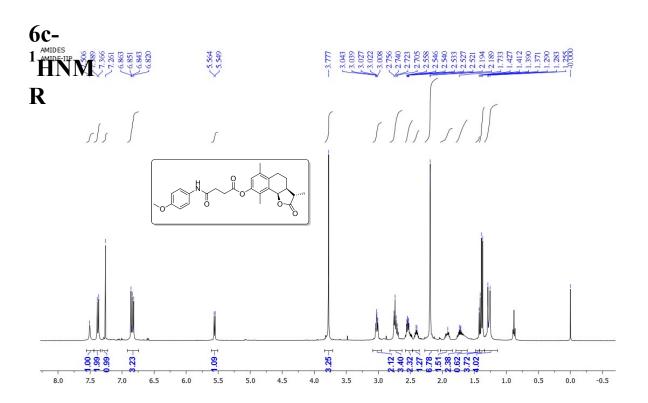
MFE MS Spectrum

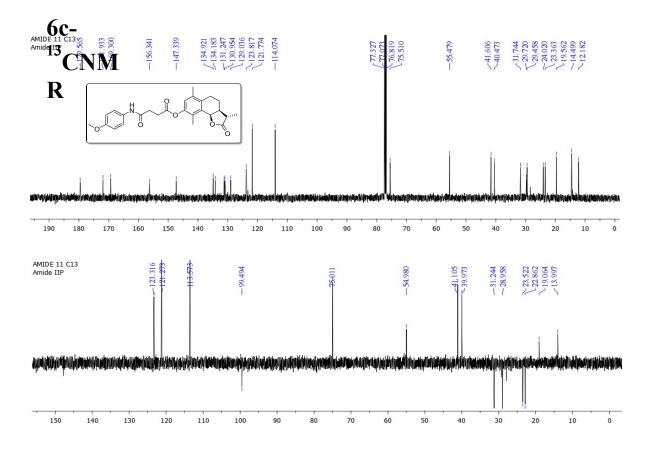
4 Cp	d 22:	C25 I	126 C	IN O	5: +E	SI MFI	E Spe	ctrum	(0.24	9-0.5	00 min) Fra	g=138	5.0V A	MD-4	.d	
i-							i c	8									
1							589 CI N /										
1							0.15	2									
							14 H	5									
ł							Č.	\$									
-																	
Ļ							_			·· (,
	150	200	250	300	350	400	450	500	550	600	650	700	750	800	850	900	950

Counts vs. Mass-to-Charge (m/z)

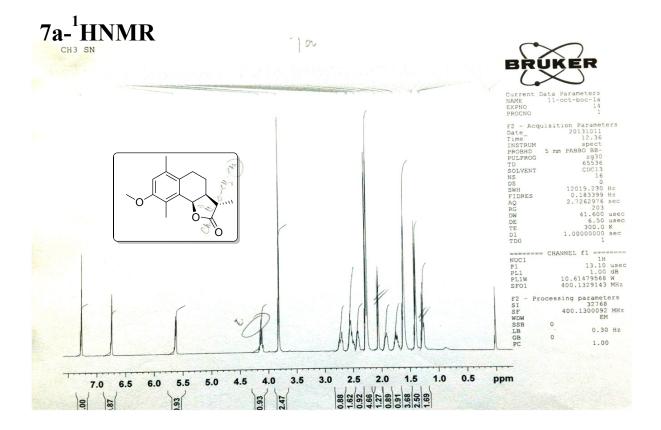
MS Spectrum Peak List

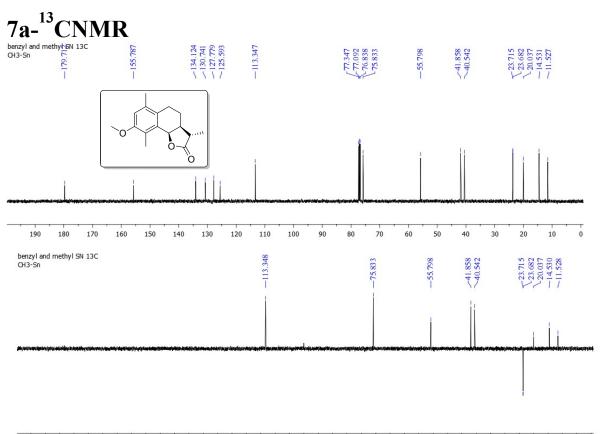
m/z	Z	Abund	Formula	(Ion]		
456.1589	1	1654	6.83 C25 H27	CI N O5	(M+H)+]		
457.1622	1	449	2.13 C25 H27	CI N O5	(M+H)+			
458.1571	1	665	1.85 C25 H27	CIN OS	(M+H)+			
459.1601	1	172	9.21 C25 H27	CI N 05	(M+H)+			
460.1649	1	42	6.22 C25 H27 (CI N O5	(M+H)+			
Predicted Is	soto	pe Matc	h Table					
Isotope	m/2	۵.	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %
1		456.1589	456.1572	-3.62	100	100	55.44	56.8
2	3	457.1622	457.1605	-3.7	27.15	27.91	15.05	15.82
3		458.1571	458,1555	-3.54	40.2	36.77	22.29	20.92
4		459.1601	459.1581	-4.36	10.45	9,54	5.79	5.42
5		460.1649	460.1607	-9.05	2.58	1.59	1.43	0,9





6c-HRM Smpound Table MFG Diff MFG Formula C26 H29 N O6 Compound Label Cpd 38: C26 H29 N O6 **DB** Formula RT Mass Formula C26 H29 N O6 (ppm) -5.57 0.341 451.202 C26 H29 N O6 **Compound Label** m/z RT Algorithm Mass Find by Molecular Feature 451.202 Cpd 38: C26 H29 N O6 452.2093 0.341 MFE MS Spectrum x10 4 Cpd 38: C26 H29 N O6: +ESI MFE Spectrum (0.240-0.557 min) Frag=135.0V AMD-2.d 452.2093 C26 H30 N O6 8 903.4136 2 H59 N2 O12 6 4 2 C52 0 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 Counts vs. Mass-to-Charge (m/z) MS Spectrum Peak List z z Abund 452.2093 1 8968 Formula Ion m/z 89683.57 C26 H30 N O6 27589.89 C26 H30 N O6 (M+H)+ 453.2126 1 (M+H)+(M+H)+ 5104.69 C26 H30 N O6 454.2153 1 3224.48 C52 H59 N2 O12 (2M+H)+ 903.4136 1 904.415 1 1707.49 C52 H59 N2 O12 (2M+H)+ Predicted Isotope Match Table Diff (ppm) Abund % Calc Abund % Abund Sum % Caic Abund Sum % Isotope m/z Calc m/z 100 100 72.47 74.03 452.2093 -5.51 452.2068 453.2126 453.2101 -5.45 30.76 29.06 22.3 21.51 2 3.93 454.2153 454.2128 -5.42 5.69 5.3 4.13 0.54 1.1 -11.65 1.52 0.72 4 455.2208 455.2155



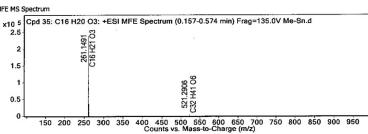


7a- HRMS

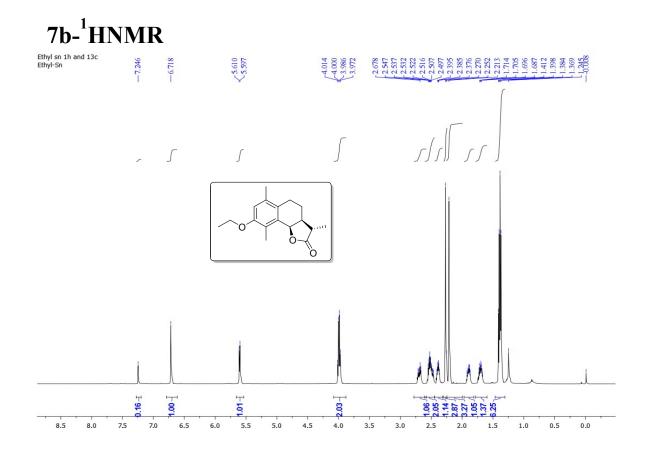
					MFG Diff	
Compound Label	RT	Mass	Formula	MFG Formula	(ppm)	DB Formula
Cpd 35: C16 H20 O3	0.342	260.1418	C16 H20 O3	C16 H20 O3	-2.16	C16 H20 O3

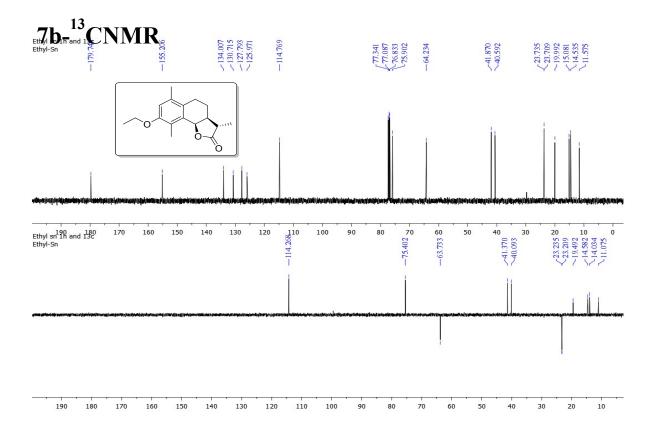
Compound Label	m/z	RT	Algorithm	Mass
Cpd 35: C16 H20 O3	261.1491	0.342	Find by Molecular Feature	260.1418
		L		

MFE MS Spectrum

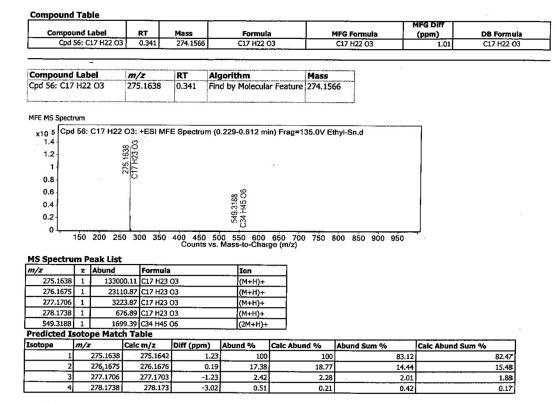


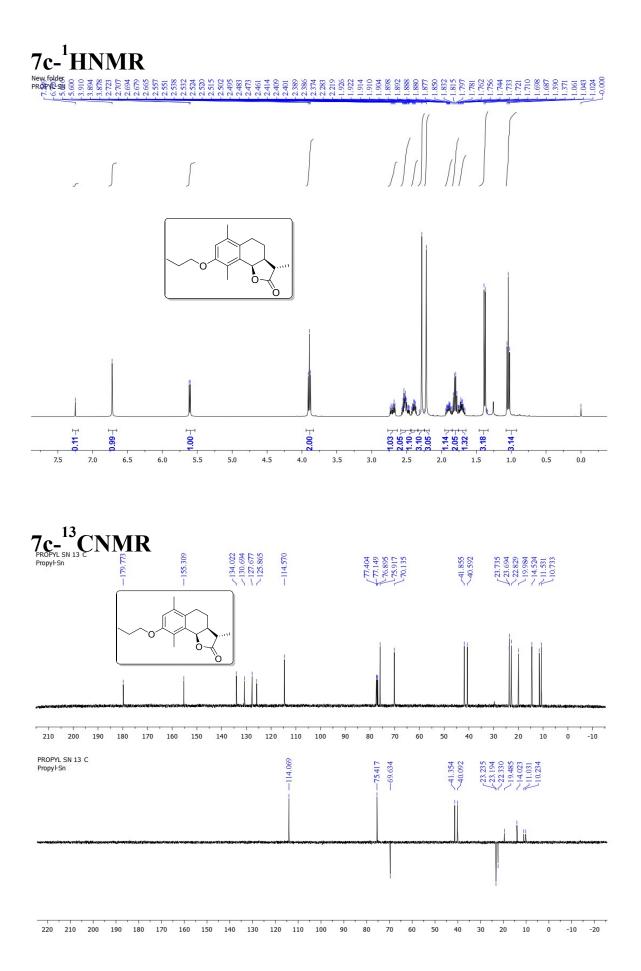
MS Spectru	m P	eak List											
m/z	z	Abund		Formula		1	lon	· .					
261.1491	1	23914	7.03	C16 H21 0	03		(M+H)+						
262.1524	1	3732	7.34	C16 H21 0	03	((M+H)+						
263.1557	1	462	5.03	C16 H21 0	03	(M+H)+						
521.2906	1	357	1.02	C32 H41 (26		2M+H)+	· .					
522.2935	1	109	6.33	C32 H41 (06	(2M+H)+						
Predicted Is	soto	pe Matci	n Ta	ble									
Isotope	m/2		Calc	m/z	Diff (ppm)	Abun	d %	Calc	Abund %	Abund Sum %		Calc Abund Sum %	
1		261.1491		261.1485	-2.13		100	2.6	100		84.84		83.38
2		262.1524		262.1519	-1.99		15.61		17.66		13.24		14.73
3		263.1557		263.1546	-4.28		1.93		2.08		1.64		1.74
4		264.1582		264.1572	-3.77		0.32		0.18		0.27		0.15





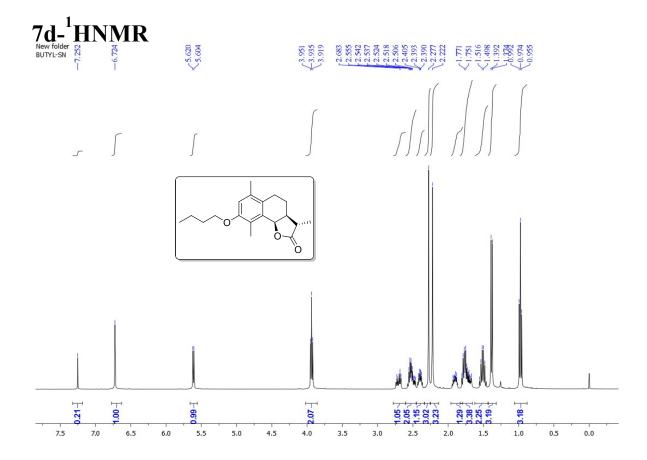
7b-HRMS

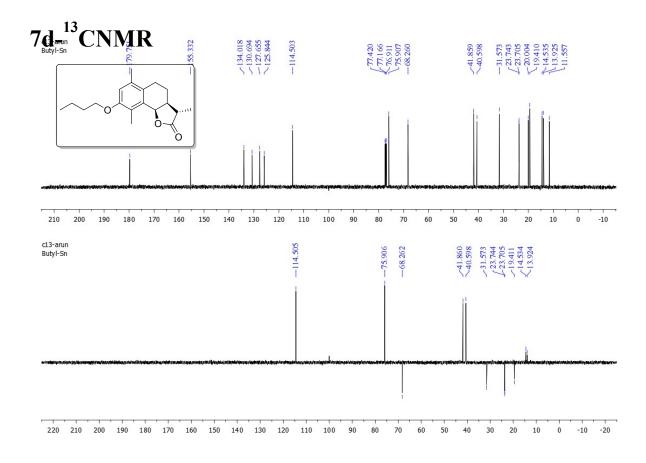




7c-HRMS

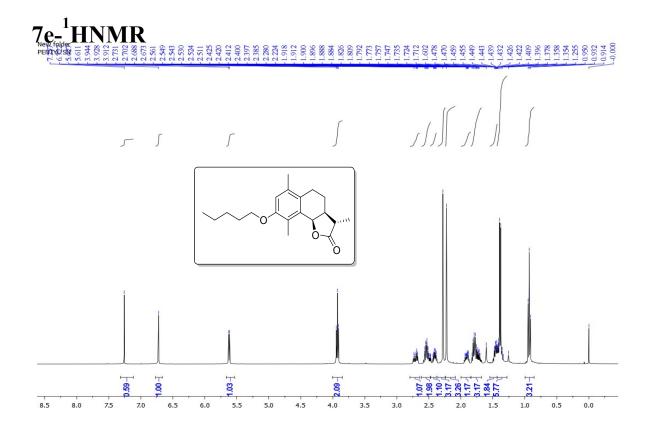
	mpou			RT	Mass	Form			G Formula		4FG Diff (ppm)	DB Formu
L	Cpd 4	8: C1	8 H24 O3	0.341	288.1739	C18 H24	03	C	18 H24 O3		-4.76	C18 H24 C
Compo	und	ahe	əf	m/z	RT	Algorithm		Mass				
Cpd 48:				289.1812		Find by Molecu						
Arked among water			Co. U. P. Mahamatan Indonesia	1			l	er av Mart, Nature & March 1				
MFE MS S	Spectru	m										
x10 5	Cpd	48: 0	C18 H24	O3: +ESI MI	E Spectrur	n (0.178-0.579 i	nin) Frag=13	5.0V Pro	p-Sn.d		7	
1				12							1	
0.8				289.1812 218 H25 03								
0.6				618							1	
						Q						
0.4				ſ		~ O					1	
						7.3517 H49 C					1	
0.2						577.3517 577.3517 C36 H49 O						
	, 1	50 :	200 250	0 300 350	400 450	00 550 500 500 550 600 500 550 600	650 700	750 80	0 850 900 s	950	ļ	
0.2				D 300 350	400 450 Counts	213617 200 520 600 vs. Mass-to-Cha) 650 700 arge (m/z)	750 80	0 850 900 s	950	ļ	
0.2 0		n Pe		0 300 350) 650 700 arge (m/z)	750 80	0 850 900 s	950	ļ	
0.2 0 MS Spec m/z 289.1	ctrun 1812	n Pe z /	ak List Abund 10184	Formula 9.02 C18 H25	a 03	500 550 600 vs. Mass-to-Cha Ion (M+H)+	· .	750 80	0 850 900 s	950	ļ	
0.2 0 MS Spee m/z 289.1 290.1	ctrun 1812 1848	n Pe z / 1	ak List Abund 10184 2240	Formula 9.02 C18 H25 1.21 C18 H25	a 03 03	500 550 600 vs. Mass-to-Cha Ion (M+H)-1 (M+H)-1	· · · · ·	750 80	0 850 900 s	950	ļ	
0.2 0 MS Spec m/z 289.1 290.1 291.1	ctrur 1812 1848 1877	n Pe z / 1 1	2240 326	Formula 9.02 C18 H25 1.21 C18 H25 8.99 C18 H25	a 03 03 03	500 550 600 vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+		750 80	0 850 900 s	950		
0.2 0 MS Spec m/z 289.1 290.1 291.1 292.1	ctrun 1812 1848 1877 1875	n Pe z / 1 1 1	2240 326 51	Formula 9.02 C18 H25 1.21 C18 H25 8.99 C18 H25 1.43 C18 H25	a 03 03 03 03 03	500 550 600 vs. Mass-to-Cha (M+H)-1 (M+H)-1 (M+H)-1 (M+H)-1 (M+H)-1		750 80	0 850 900 s	950	ļ	
0.2 0 MS Spec m/z 289.1 290.1 291.1 292.1 577.3	ctrur 1812 1848 1877 1875 3517	n Pe z / 1 1 1 1	2240 326 51 85	Formula 9.02 C18 H25 1.21 C18 H25 8.99 C18 H25 1.43 C18 H25 1.44 C36 H49	a 03 03 03 03 03	500 550 600 vs. Mass-to-Cha (M+H)+ (M+H)+ (M+H)+		750 80	0 850 900 s	950	ļ	
0.2 0 MS Spec m/z 289.1 290.1 291.1 292.1	ctrun 1812 1848 1877 1875 3517 ed Is	n Pe z / 1 1 1 1	Abund 10184 2240 326 51 85 De Matc	Formula 9.02 C18 H25 1.21 C18 H25 8.99 C18 H25 1.43 C18 H25 1.44 C36 H49 h Table	a 03 03 03 03 03 06	500 550 600 vs. Mass-to-Cha (M+H)-1 (M+H)-1 (M+H)-1 (M+H)-1 (M+H)-1 (M+H)-1	· · · · · · · · · · · · · · · · · · ·	х		950	Calc Abund 5	Sum %
0.2 0 MS Spee <i>m/z</i> 289.1 290.1 291.1 292.1 577.3 Predicte	ctrun 1812 1848 1877 1875 3517 ed Is	n Pe z / 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Abund 10184 2240 326 51 85 De Matc	Formula 9.02 C18 H25 1.21 C18 H25 8.99 C18 H25 1.43 C18 H25 1.44 C36 H49	a 03 03 03 03 06 Diff (ppm	500 550 600 vs. Mass-to-Cha (M+H)-1 (M+H)-1 (M+H)-1 (M+H)-1 (M+H)-1 (M+H)-1	+ Calc Abund	х	0 850 900 s		Calc Abund S	
0.2 0 MS Spee <i>m/z</i> 289.1 290.1 291.1 292.1 577.3 Predicte	ctrun 1812 1848 1877 1875 3517 ed Is	n Pe z 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2	ak List Abund 10184 2240 326 51 85 0e Matcl	Formula 9.02 C18 H25 1.21 C18 H25 1.43 C18 H25 1.43 C18 H25 1.44 C36 H49 h Table Calc m/z	a 03 03 03 03 03 06 Diff (ppm 3 -4	500 550 600 vs. Mass-to-Chi (M+H)- (M+H)- (M+H)- (M+H)- (M+H)- (ZM+H) (ZM+H)	+ Calc Abund	1 % A		79.55 17.5	Calc Abund 5	Sum %
0.2 0 MS Spee <i>m/z</i> 289.1 290.1 291.1 292.1 577.3 Predicte	ctrun 1812 1848 1877 1875 3517 ed Is	n Pe z / 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	ak List Abund 10184 2240 326 51 85 96 Matc 289.1812	Formula 9.02 C18 H25 1.21 C18 H25 8.99 C18 H25 1.43 C18 H25 1.44 C36 H49 h Table Calc m/z 289.1796	a 03 03 03 03 06 Diff (ppm 3 -4 2 -5	500 550 600 vs. Mass-to-Chi (M+H)- (M	Calc Abunc 0 9	1 % A		79.55	Calc Abund 5	81.57



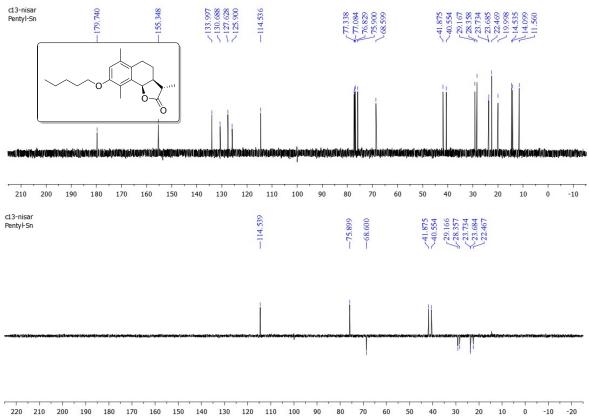


7d-HRMS

Compound		4	RT	Mass		Formula		м	FG Formula		(ppm)	D8 Formul
Cpd 3	7: C19 H	26 O3	0.339	302.1908		C19 H26 O	3		C19 H26 O3		-8.68	C19 H26 O3
									·······			
Compound	Label		n/z	RT	Algo	rithm		Mass				
Cpd 37: C19	H26 O3	3	03.1981	0.339	Find	by Molecula	r Feature	302.190	8			
						NUMBER OF A STREET OF STREET OF STREET	nyana ya manamoni manamar m	L				
IFE MS Spectro												
X10 - 1 -	37: C19	9 H26 O		E Spectru	n (0.2	40-0.574 mi	n) Frag=1	35.0V Bu	t-Sn.d			
1.2			303.1981 C19 H27 03									
1.			138									
0.8			9H 0 1 0 1 0									
			5									
0.6												
0.4						80						
0.2						605.3918						
						202						
0	50 20	0 250	300 350	400 450	500		650 700	750 8	00 850 90	950	-J	
	50 20	0 200	500 500	Counts	vs. M	ass-to-Char	ge (m/z)	, ,00 0	00 850 90			
IS Spectru	m Peak	List										
n/z	z Ab		Formula)		Ion				-		
303.1981	1	113229.	38 C19 H27	03		(M+H)+						
304.2013	1	23009.	55 C19 H27	03		(M+H)+						
305.2039	1	3184.	22 C19 H27	03		(M+H)+						
605.3918	1	1108.	51			(2M+H)+						
606.3932	1	406.	07			(2M+H)+						
redicted Is	otope	Match	Table									
sotope	m/z	C	alc m/z	Diff (ppr) A	bund %	Calc Abu	nd %	Abund Sum		Calc Abund S	
1	303	3.1981	303.1955		8.81	100		100		80.99		80.68
2	-	.2013	304.1989		7.98	20.32		20.97		16.46		16.92
3	305	.2039	305.2017		7.36	2.81		2.71		2.28		2.18
		.2081	306.2044		1.92	0.34		0.26		0.28		0.21







7e- HRMS

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 44: C20 H28 O3	0.342	316.2015	C20 H28 O3	C20 H28 O3	7.37	C20 H28 O3

Calc Abund Sum %

79.8

17.62

2.34

0.23

78.11

18.36

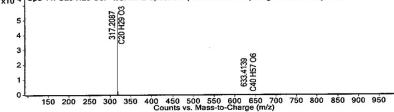
3.14

0.39

Compound Label	m/z	RT	Algorithm	Mass
Cpd 44: C20 H28 O3	317.2087	0.342	Find by Molecular Feature	316.2015
		-		1

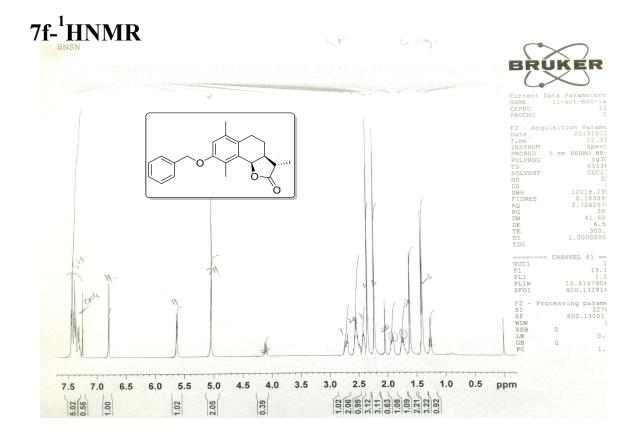
MFE MS Spectrum

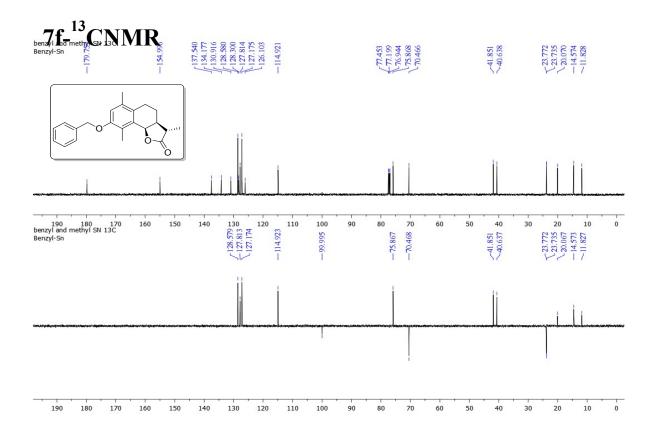
x10 4 Cpd 44: C20 H28 O3: +ESI MFE Spectrum (0.065-0.566 min) Frag=135.0V Pentyl-Sn.d



MS Spectrum Peak List

m/z	2	Abund	Fo	ormula			ton		
317.2087	1	5531	2.84 C	0 H29 (03		(M+H)+		
318,2124	1	1300	0.19 CZ	20 H29 (03		(M+H)+		
319.2166	1	221	9.97 C2	20 H29 (03		(M+H)+		
320.2222	1	27	78.22 C2	20 H29 (03		(M+H)+		
633.4139	1	46	6.63 C4	Ю H57 (06		(2M+H)+		
Predicted I	soto	pe Matc	h Tabl	e			100.0		
Isotope	m/2	7	Catc m	/z	Diff (ppm)	Abun	d %	Calc Abund %	Abund Sum %
1		317.2087	31	7.2111	7.73		100	100	
2		318.2124	31	8.2145	6.82	-	23.5	22.08	
		319.2166	31	9.2174	2.56		4.01	2.94	
4		320.2222	32	0.2201	-6.53		0.5	0.29	

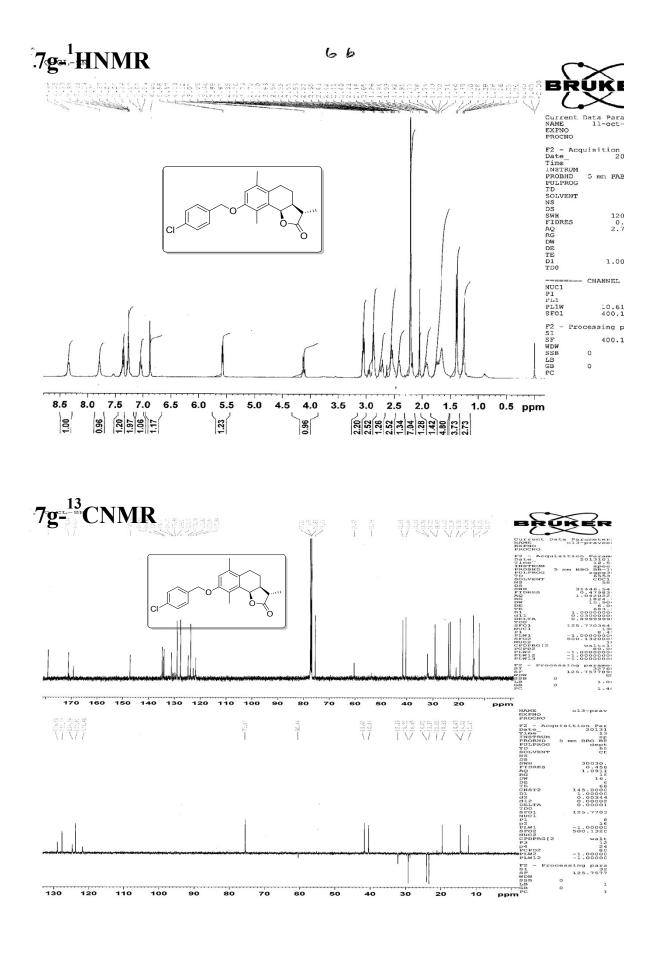




7f-HRMS

Compound T			Mage	Formula		MFG Formula	MFG (pp		DB Formula
Compound		RT 0.342	Mass	C22 H24 03		C22 H24 O3		-2.48	C22 H24 O3
Cpd 37	C22 H24 O3	0.342	530,1/34	C22 1124 0.	<u> </u>				
Compound L	abel	m/z	RT A	gorithm	Mass				
Cpd 37: C22 H		337.1807	0.342 Fir	nd by Molecular	Feature 336.17	34			
annana a ana anta 22.49 yang a mana sanisi ka 1	y / S.L. annymikensymmetri sender vik Al ktiv vy m	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	<u> </u>	gananana karaan kara m ayoo mananan ka dab	nya na faanaanaa ah kata talaatay masaana katata	we are no normalized			
MFE MS Spectrum	n						——————————————————————————————————————		
x10 5 Cpd 3	7: C22 H24	O3: +ESI MF	E Spectrum (0.235-0.569 mir) Frag=135.0V E	In-Sn.d			
3.5		337.1807 C22 H25 O3							
3-		12 12 12							
2.5		337							
2		P							
1.5					52				
1-					H40				
0.5					673.3525 C44 H49 O6				
		k		., ,,					
11	50 200 25	0 300 350	400 450 5 Counts vs	500 550 600 Mass-to-Char	650 700 750 te (m/z)	800 850 900	950		
40 Que e human	Deals Link								
MS Spectrun	z Abund	Formul	a	Ion					
337.1807	1 3604			(M+H)+					
338,1838		00.91 C22 H25		(M+H)+					
	1 121	49.19 C22 H25	03	(M+H)+					
673.3525		205.7 C44 H49		(2M+H)+					
674.3558		55.44 C44 H49	06	(2M+H)+					
Predicted Is	otope Mate					1		alc Abund Su	m 9/a
Isotope	m/z	Calc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	78.95	aic Abuna Su	78.15
1	337.1807				24		18.09	<u> </u>	18.91
2	338.1838				3.		2.66		2.67
3	339.1869						0.3		0.28
4	340,1899	340.188	-2.8	0.38	0.				

--- End Of Report ---



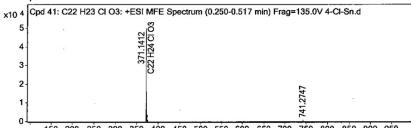
7g-HRMS

Compou	nd Table
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RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
0.341	370.134	C22 H23 CI O3	C22 H23 CI O3	-1.17	C22 H23 Cl O3
_					

Compound Label	m/z	RT	Algorithm	Mass
od 41: C22 H23 Cl O3	371.1412	0.341	Find by Molecular Feature	370.134

MFE MS Spectrum



150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 Counts vs. Mass-to-Charge (m/z)

MS Spectrum Peak List

z	Abund Formula		Ion	
1	49728.36	C22 H24 CI O3	(M+H)+	
1	14165.91	C22 H24 CI O3	(M+H)+	
1	15888.38	C22 H24 CI O3	(M+H)+	
1	3672.21	C22 H24 CI O3	(M+H)+	
1	902.98		(2M+H)+	
	1 1 1	1 49728.36 1 14165.91 1 15888.38 1 3672.21	1 49728.36 C22 H24 Cl O3 1 14165.91 C22 H24 Cl O3 1 15888.38 C22 H24 Cl O3 1 3672.21 C22 H24 Cl O3	

Isotope	٦	m/z	Catc m/z	Diff (ppm)	Abund %	Calc Abund %	Abund Sum %	Calc Abund Sum %	
8	1	371.1412	371.1408	-0.96	100	100	59.07	59.24	
	2	372.1446	372.1442	-0.93	28.49	24.18	16.83	14.33	
	3	373.1395	373.1388	-1.89	31.95	35.41	18.87	20.98	
	4	374.1419	374.1417	-0.52	7.38	8.09	4.36	4.79	
- (*	5	375.147	375.1444	-6.87	1.47	1.12	0.87	0.66	