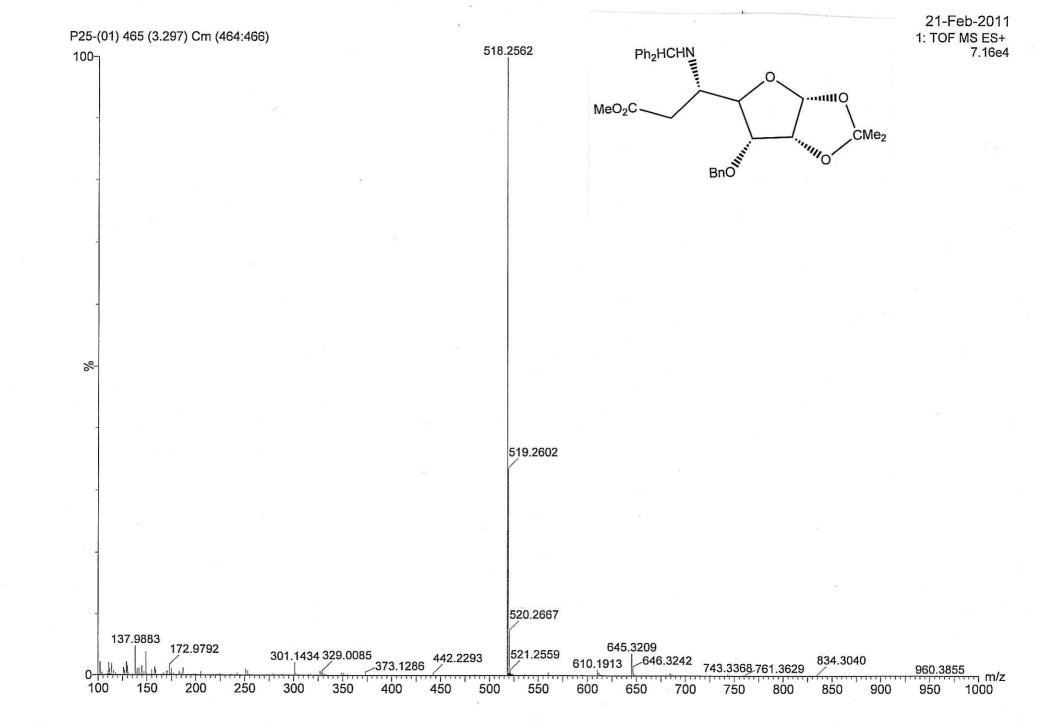
Supplementary Material (ESI) for Green Chemistry This journal is (c) The Royal Society of Chemistry 2011



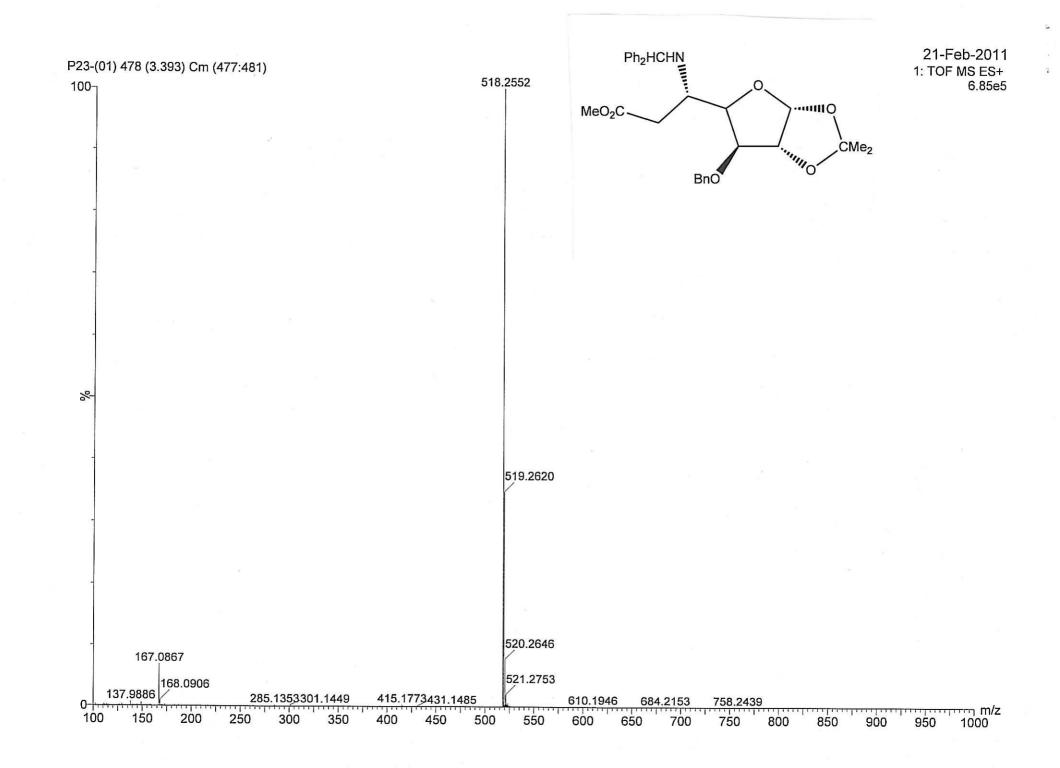
Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron lons 1279 formula(e) evaluated with 13 results within limits (up to 20 best isotopic matches for each mass) Elements Used: C: 0-70 H: 0-150 N: 0-15 O: 0-15 21-Feb-2011 1: TOF MS ES+ P25-(01) 465 (3.297) Cm (464:466)

100-				518.2562							1.100	
- - - %—				519,2602	,							
-				313.2002								
137.9883	172.9792 301.	1434_329.0085	442.2293	520.2667	645.3209	684.2048	743.3368	307.33	39			n/z
100	200 3	00 40	00	500	600	700	800		900		1000	
Minimum: Maximum:		5.0	10.0	-1.5 50.0								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	For	nula			
	518.2543 518.2556 518.2529 518.2596 518.2596 518.2601 518.2588 518.2575 518.2561 518.2548 518.2548 518.2534 518.2534 518.2606	1.9 4.6 0.6 3.3 -3.9 -3.4 -3.9 -2.6 -1.3 0.1 1.4 2.8 -4.4	3.7 8.9 1.2 6.4 -7.5 -6.6 -7.5 -5.0 -2.5 0.2 2.7 5.4 -8.5	14.5 15.5 19.5 20.5 5.5 23.5 16.5 11.5 6.5 1.5 7.5 2.5 -1.5	177.0 179.4 180.1 182.0 182.6 183.2 183.5 184.1 184.8 186.0 186.4 188.1	0.2 2.6 3.2 5.2 5.8 6.4 6.7 7.3 8.0 9.2 9.6 11.3		C31 C27 C32 C28 C24 C37 C22 C21 C20 C19 C16 C15 C9	H36 H32 H28 H40 H32 H28 H32 H36 H36 H36 H36	N7 N5 N11	011 0 05 09 013	

Page 1

7.16e+004



1 4 A

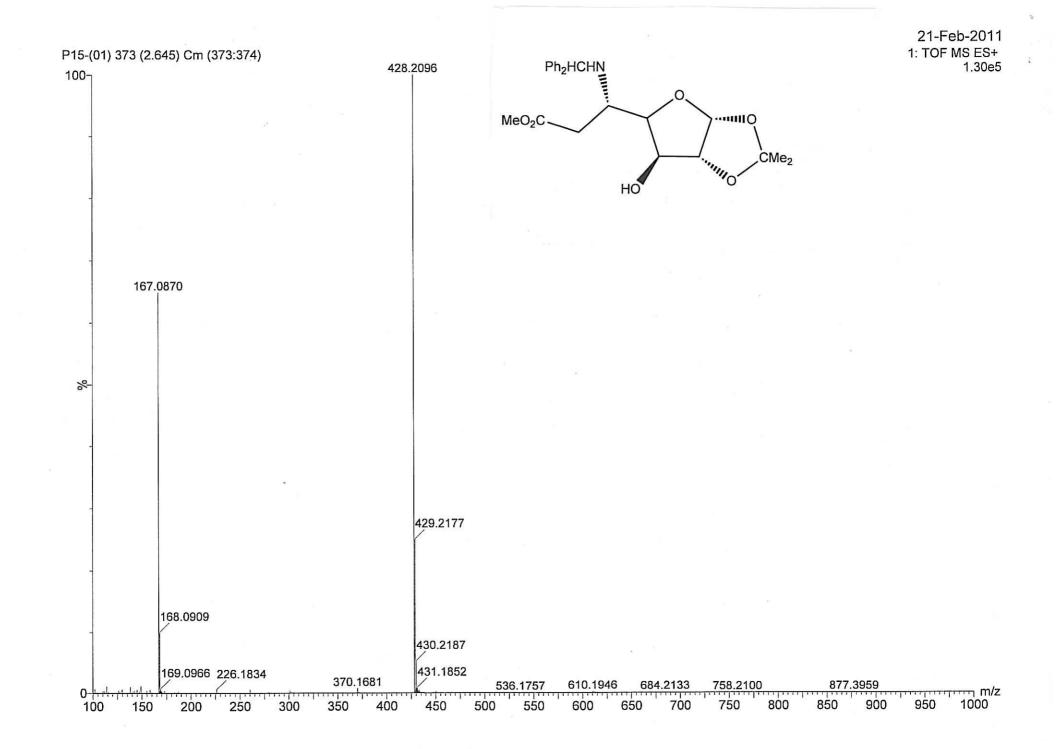
1

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 1279 formula(e) evaluated with 14 results within limits (up to 20 best isotopic matches for each mass) Elements Used: C: 0-70 H: 0-150 N: 0-15 O: 0-15 21-Feb-2011 1: TOF MS ES+ P23-(01) 478 (3.393) Cm (477:481)

	57									6.85e+005
100-7				518.2552						
-										
%-				519.262	D					
-										
0	7.0867	.1353 350.1617 4	15.1773,438.	520.264 2554		1	758.2439	1		
100	200	300 4	100	500	600	700	800	er (†)	900	m/z بريم m/z 1000
Minimum:				-1.5						
Maximum:		5.0	10.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT	(Norm)	Form	ula	
518.2552	518.2543	0.9	1.7	14.5	343.0	0.0		C31	Н36	N OG
	518.2556	-0.4	-0.8	19.5	346.6	3.7		C32	H32	N5 O2
	518.2516	3.6	6.9	15.5	348.2	5.2		C27	H32	N7 04
	518.2529	2.3	4.4	20.5	348.2	5.3		C28	H28	N11
	518.2502	5.0	9.6	10.5	349.2	6.2		C26	H36	N3 O8
	518.2596	-4.4	-8.5	23.5	349.7	6.7		C37	H32	N3
	518.2601	-4.9	-9.5	5.5	350.1	7.2		C24	H40	N 011
	518.2601	-4.9	-9.5	16.5	351.5	8.6		C22	H28	N15 O
	518.2588	-3.6	-6.9	11.5	351.8	8.8		C21	H32	N11 05
	518.2575	-2.3	-4.4	6.5	352.1	9.2		C20	H36	N7 09
	518.2561	-0.9	-1.7	1.5	352.6	9.6		C19	H40	N3 013
	518.2548	0.4	0.8	7.5	354.0	11.1		C16	H32	N13 07
	518.2534	1.8	3.5	2.5	354.3	11.4		C15	H36	N9 011
	518.2507	4,5	8.7	3.5	356.0	13.0		C11	H32	N15 O9

Page 1



1

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

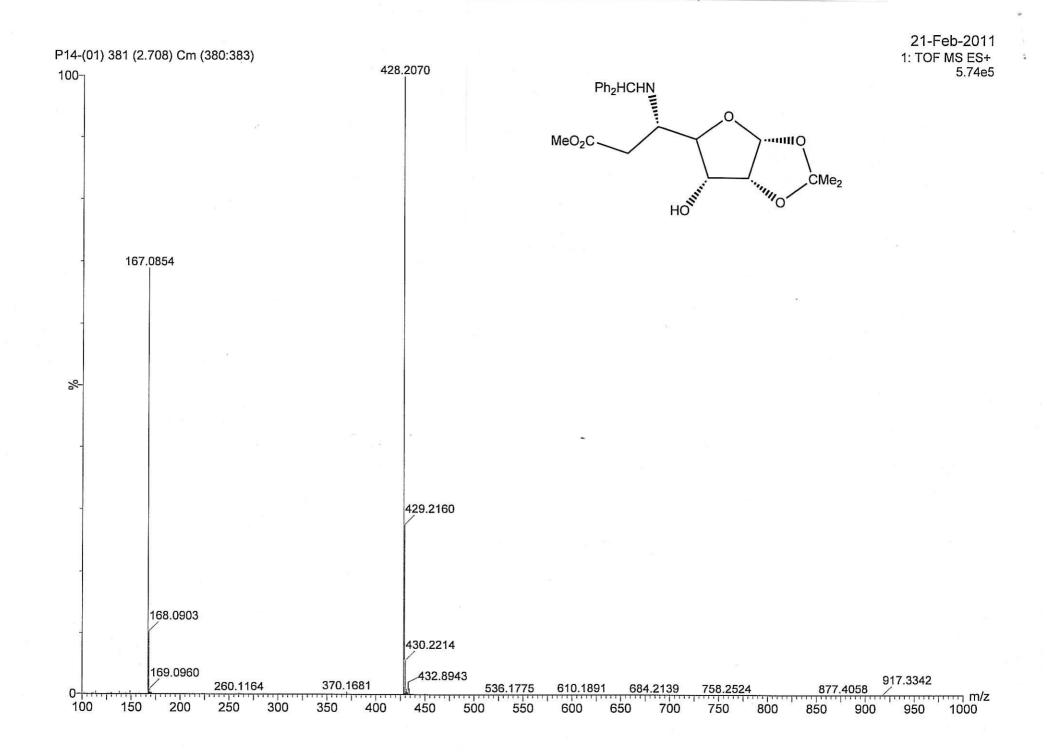
Monoisotopic Mass, Even Electron Ions 993 formula(e) evaluated with 10 results within limits (up to 20 best isotopic matches for each mass) Elements Used: C: 0-70 H: 0-150 N: 0-15 O: 0-15 21-Feb-2011 1: TOF MS ES+

P15-(01) 373 (2.645) Cm	(373:374)
-------------------------	-----------

1.30e+005

100			428.2096					1.30e+005
16	7.0870							
%-								
-			429.21	77				
-	168.0909	1102	430.21	87				
0	226.1834 260	.1163 370.168		536.1757		84.2133 758.2100	877.3959	m/z
100		300 4	100	500	600	700 800	900	1000
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm	Formula	
428.2096	428.2073	2.3	5.4	10.5	210.3	0.2	C24 H30 N C	06
	428.2087	0.9	2.1	15.5	212.8	2.7	C25 H26 N5	02
	428.2132	-3.6	-8.4	1.5	212.8	2.7	C17 H34 N C	011
	428.2060	3.6	8.4	16.5	213.1	3.1	C21 H22 N11	
	428.2127	-3.1	-7.2	19.5	214.7	4.6	C30 H26 N3	
	428.2132	-3.6	-8.4	12.5	214.7	4.6	C15 H22 N15	0
	428.2118	-2.2	-5.1	7.5	214.8	4.8	C14 H26 N11	05
	428.2105	-0.9	-2.1	2.5	215.3	5.2	C13 H30 N7	09
	428.2078	1.8	4.2	3.5	217.4	7.3		07
	428.2065	3.1	7.2	-1.5	217.8	7.7	C8 H30 N9 C	011

Page 1



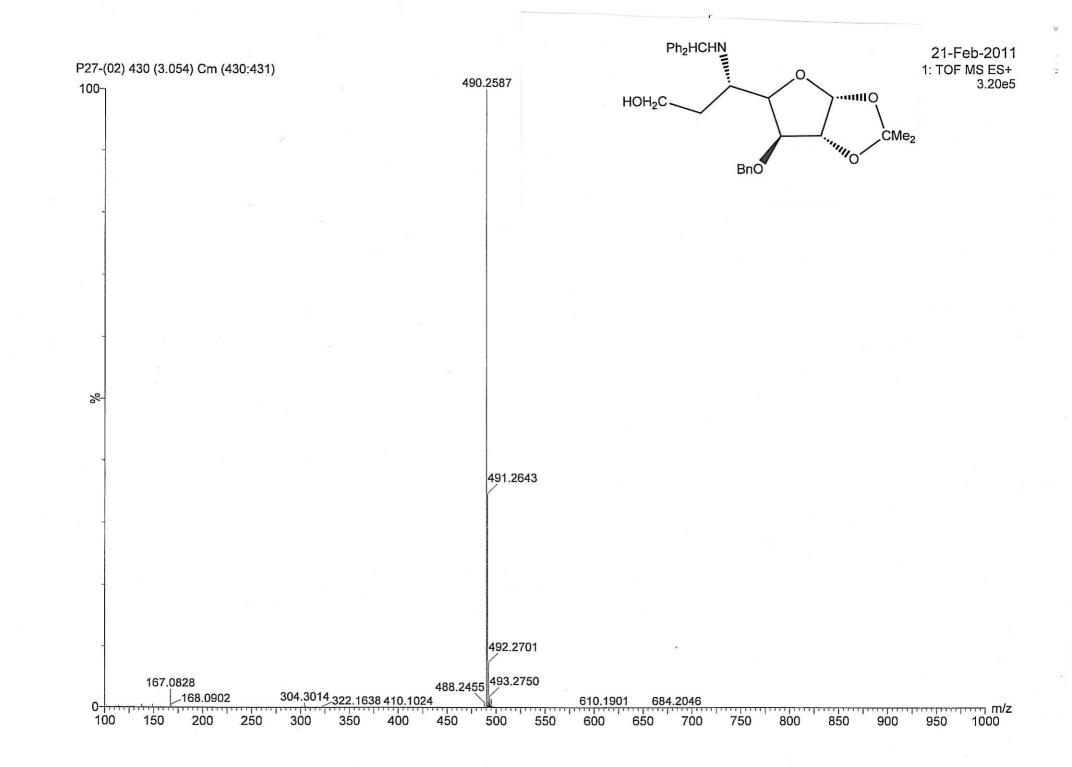
5

Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 993 formula(e) evaluated with 9 results within limits (up to 20 best isotopic matches for each mass) Elements Used: C: 0-70 H: 0-150 N: 0-15 O: 0-15 21-Feb-2011 1: TOF MS ES+ P14-(01) 381 (2.708) Cm (380:383)

								5.74e+005
100 -				428.207	70			
-								
-								
%-								
-				42	29.2160			
-								
417.	5073 419.3439 ^{420.377}		426.1953 42	\	430.2214	402.0040	2435.6075.43	7.0683
0-111-0	418.0 420.0 4	22.0 424.		428.0	430.0	432.0 434.0		38.0 440.0
	10.0 420.0 4	22.0 424.	-20.0	420.0	400.0	452.0 454.0	430.0 4	30.0 440.0
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
212		22.77			120	*		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula	
428.2070	428.2073	-0.3	-0.7	10.5	406.0	0.1	C24 H30	N OG
	428.2087	-1.7	-4.0	15.5	408.6	2.7	C25 H26	N5 02
	428,2046	2.4	5.6	11.5	410.3	4.4	C20 H26	N7 04
	428.2060	1.0	2.3	16.5	410.5	4.5	C21 H22	
	428.2033	3.7	8.6	6.5	411.1	5.2	C19 H30	N3 08
	428.2105	-3.5	-8.2	2.5	414.1	8.1	C13 H30	N7 09
	428.2078	-0.8	-1.9	3.5	415.5	9.6	C9 H26	N13 07
	428.2065	0.5	1.2	-1.5	415.9	10.0	C8 H30	N9 011
	428.2038	3.2	7.5	-0.5	417.1	11.2	C4 H26	N15 O9

Page 1



-03

1.3

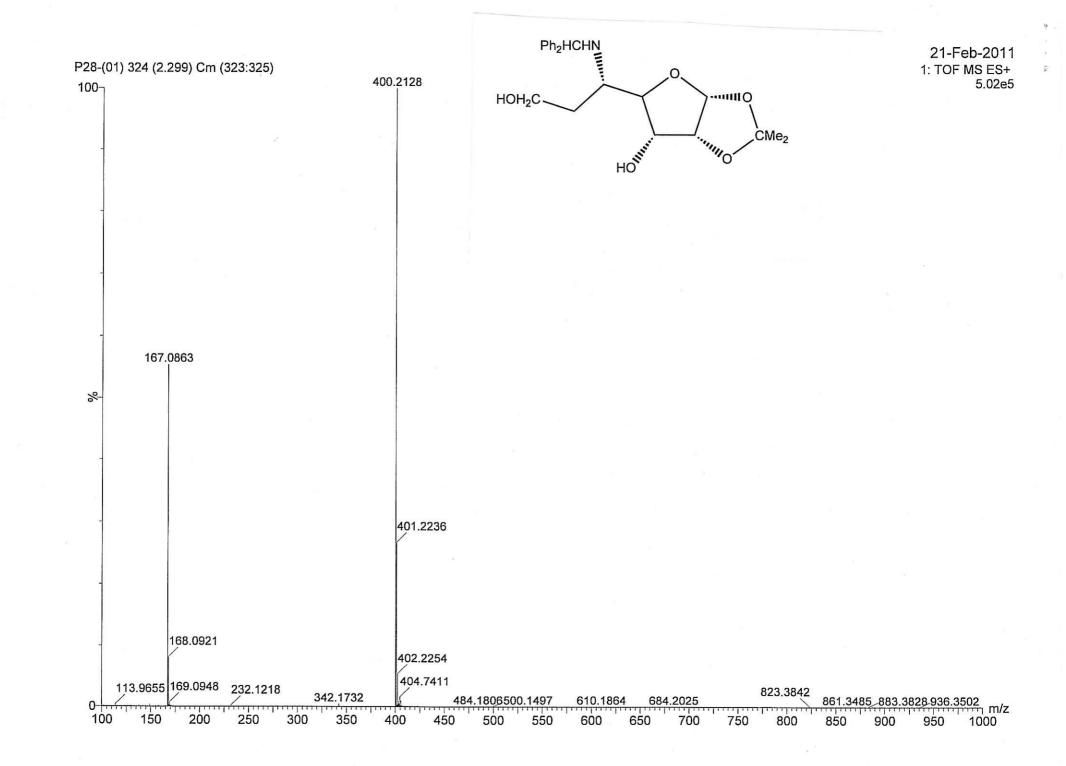
Single Mass Analysis Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 1191 formula(e) evaluated with 21 results within limits (up to 20 best isotopic matches for each mass) Elements Used: C: 0-70 H: 0-150 N: 0-15 O: 0-15 21-Feb-2011 P27-(02) 430 (3.054) Cm (430:431) 1: TOF MS ES+

100-			49	0.2587					5.200+005
-									
-									
%-				491.2643					
]				Y					
-				492.2701					
	.0828	304.3014 355.07	38 488.245	55	610.1901 6	84.2046			
0 -\ 100	200	tifiiii fairi	00	-)*	600		800	900	<u>הירידן m/z</u> 1000
100	200	500 40	00	500	000	700	000	500	1000
Minimum:				-1.5					
Maximum:		5.0	20.0	50.0					
Maga	Colo Mode	- De	PPM	DBE	i-FIT	; DTM (No	rm) Form		
Mass	Calc. Mass	mDa	PPM	DBE	T-FTI	i-FIT (No	rm) Form	ula	
490.2587	490.2593	-0.6	-1.2	13.5	212.9	0.1	C30	H36	N 05
	490.2607	-2.0	-4.1	18.5	215.4	2.7	C31	H32	N5 O
	490.2495	9.2	18.8	18.5	215.5	2.8	C32	H32	N3 02
	490.2567	2.0	4.1	14.5	218.1	5.4	C26	H32	N7 O3
	490.2535	5.2	10.6	22.5	218.9	6.2	C37	H32	N
	490.2553	3.4	6.9	9.5	219.0	6.3	C25	H36	N3 07
	490.2679	-9.2	-18.8	14.5	219.0	6.3	C25	H32	N9 O2
	490.2666	-7.9	-16.1	9.5	219.7	7.0	C24	H36	N5 06
	490.2652	-6.5	-13.3	4.5	220.4	7.7	C23	H40	N 010
	490.2540	4.7	9.6	15.5	221.0	8.3	C22	H28	N13 O
	490.2526	6.1	12.4	10.5	221.4	8.7	C21	H32	N9 05
	490.2652	-6.5	-13.3	15.5	221.5	8.8	C21	H28	N15
	490.2639	-5.2	-10.6	10.5	221.8	9.1	C20	H32	N11 04
	490.2513	7.4	15.1	5.5	222.0	9.3	C20	H36	N5 09
	490.2625	-3.8	-7.8	5.5	222.2	9.5	C19	H36	N7 08
	490.2500	8.7	17.7	0.5	222.6	9.9	C19	H40	N 013
	490.2612	-2.5	-5.1	0.5	222.7	10.0	C18	H40	N3 012
	490.2500	8.7	17.7	11.5	223.3	10.6	C17	H28	N15 O3
	490.2599	-1.2	-2.4	6.5	223.8	11.1	C15	H32	N13 06
	490.2585	0.2	0.4	1.5	224.0	11.3	C14	H36	N9 010

Page 1

3.20e+005



ciementa	I Composition F	Report									Page 1
Tolerance Element pr	ass Analysis = 20.0 PPM / DB ediction: Off isotope peaks use			50.0							
Monoisotopi 894 formula Elements U C: 0-70 H 21-Feb-2011		on lons results v O: 0-18		to 20 best i	sotopic ma	atches	for each		28-(01) 32	4 (2 299)	Cm (323:325)
1: TOF MS E	S+								20 (01) 02	. (2.200)	0111 (020.020)
100-7			400.2128	3							5.02e+005
- - - %			401	.2236							
-											
0 342.173	32 355.0736 363.1153	388.30	92399.8854	2.2254 422.	2095 438	8.1906	444.2422	47	70.1866 4	84.1806	500.1497,
0 ^{-342.173} 340	32 355.0736 363.1153 350 360 370	388.309 	92 399.8854 40 390 400		արողուղ	8.1906 440	444.2422 444.2422 450	47 460	nduuduu	84.1806 30 49	500.1497 m/z 0 500
340 Minimum:		380	32399.8854 / 390 400	422 410 420 -1.5	արողուղ	mum	funding	munun	nduuduu	ليسليسا	
0 -1		mini	32399.8854	422. 410 420	արողուղ	mum	funding	munun	nduuduu	ليسليسا	
340 Minimum:		380	32399.8854 / 390 400	422 410 420 -1.5	արողուղ	mum	funding	460	nduuduu	30 49	
0-4	2350.0736 350 360 370 Calc. Mass 400.2124	380 5.0 mDa 0.4	22399.8854 390 400 20.0 PPM 1.0	422 410 420 -1.5 50.0 DBE 9.5	i-FIT 339.4	mum	450 i-FIT 0.2	460	470 4 Formul C23 H	a 30 N	0 500 05
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137	380 5.0 mDa 0.4 -0.9	20.0 20.0 PPM 1.0 -2.2	422. 410 420 -1.5 50.0 DBE 9.5 14.5	i-FIT 339.4 341.3	mum	450 i-FIT 0.2 2.1	460	Formul C23 H C24 H	a 30 49 30 19 20 N 26 N	0 500 05 5 0
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097	380 5.0 mDa 0.4 -0.9 3.1	20.0 20.0 PPM 1.0 -2.2 7.7	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5	i-FIT 339.4 341.3 343.0	mum	450 i-FIT 0.2 2.1 3.8	460	Formul C23 H C24 H C19 H	a 30 49 30 49 20 N 26 N 26 N 26 N 26 N 7	0 500 05 5 0 7 03
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2084	380 5.0 mDa 0.4 -0.9 3.1 4.4	20.0 20.0 PPM 1.0 -2.2 7.7 11.0	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5	i-FIT 339.4 341.3 343.0 343.5	mum	450 i-FIT 0.2 2.1 3.8 4.3	460	Formul C23 H C24 H C19 H C18 H	a 30 49 30 49 230 N 26 N 26 N 30 N 30 N	0 500 05 5 0 7 03
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2084 400.2065	380 5.0 mDa 0.4 -0.9 3.1 4.4 6.3	20.0 20.0 PPM 1.0 -2.2 7.7 11.0 15.7	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5 18.5	i-FIT 339.4 341.3 343.0 343.5 343.5	mum	450 i-FIT 0.2 2.1 3.8 4.3 4.3	460	Formul C23 H C24 H C19 H C30 H	a 30 49 30 49 30 N 26 N 30 N 30 N 30 N 30 N	05 5 0 7 03 8 07
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2084 400.2065 400.2196	380 5.0 mDa 0.4 -0.9 3.1 4.4 6.3 -6.8	20.0 20.0 PPM 1.0 -2.2 7.7 11.0 15.7 -17.0	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5 18.5 5.5	i-FIT 339.4 341.3 343.0 343.5 343.5 344.0	mum	450 i-FIT 0.2 2.1 3.8 4.3 4.3 4.3 4.8	460	Formul C23 H C24 H C19 H C18 H C30 H C17 H	a 30 49 30 49 26 N5 26 N7 30 N3 26 N 30 N5	05 5 0 7 03 8 07 5 06
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2084 400.2065 400.2196 400.2183	380 5.0 mDa 0.4 -0.9 3.1 4.4 6.3 -6.8 -5.5	20.0 20.0 PPM 1.0 -2.2 7.7 11.0 15.7 -17.0 -13.7	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5 18.5 5.5 0.5	i-FIT 339.4 341.3 343.0 343.5 343.5 344.0 344.7	mum	450 i-FIT 0.2 2.1 3.8 4.3 4.3 4.3 5.5	460	Formul C23 H C24 H C19 H C18 H C30 H C17 H C16 H	a 30 49 30 49 30 N 26 N 30 N 30 N 30 N 30 N 5 34 N	05 5 0 7 03 8 07 5 06 010
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2084 400.2065 400.2196 400.2183 400.2070	380 5.0 mDa 0.4 -0.9 3.1 4.4 6.3 -6.8 -5.5 5.8	20.0 20.0 PPM 1.0 -2.2 7.7 11.0 15.7 -17.0 -13.7 14.5	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5 18.5 5.5 0.5 11.5	i-FIT 339.4 341.3 343.0 343.5 343.5 344.0 344.7 345.3	mum	450 i-FIT 0.2 2.1 3.8 4.3 4.3 4.3 4.3 5.5 6.1	460	Formul C23 H C24 H C19 H C18 H C30 H C17 H C16 H C15 H	a 30 49 30 49 30 N 26 N 30 N 30 N 30 N 30 N 34 N 22 N1	05 5 0 7 03 5 07 5 06 010 .3 0
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2084 400.2065 400.2196 400.2183 400.2070 400.2057	380 5.0 mDa 0.4 -0.9 3.1 4.4 6.3 -6.8 -5.5 5.8 7.1	20.0 20.0 PPM 1.0 -2.2 7.7 11.0 15.7 -17.0 -13.7 14.5 17.7	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5 18.5 5.5 18.5 5.5 11.5 6.5	i-FIT 339.4 341.3 343.0 343.5 343.5 344.0 344.7 345.3 345.7	mum	450 i-FIT 0.2 2.1 3.8 4.3 4.3 4.3 4.8 5.5 6.1 6.4	460	Formul C23 H C24 H C19 H C18 H C10 H C17 H C16 H C15 H C14 H	a 30 49 30 49 30 N 26 N 30 N 30 N 30 N 30 N 34 N 22 N1 26 N 9	05 5 0 7 03 5 07 5 06 010 .3 0 05
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2084 400.2065 400.2183 400.2070 400.2057 400.2057 400.2183	380 5.0 mDa 0.4 -0.9 3.1 4.4 6.3 -6.8 -5.5 5.8 7.1 -5.5	20.0 20.0 PPM 1.0 -2.2 7.7 11.0 15.7 -17.0 -13.7 14.5 17.7 -13.7	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5 18.5 5.5 18.5 5.5 11.5 6.5 11.5	i-FIT 339.4 341.3 343.0 343.5 343.5 344.0 344.7 345.3 345.7 345.8	mum	450 i-FIT 0.2 2.1 3.8 4.3 4.3 4.3 4.3 5.5 6.1 6.4 6.6	460	Formul C23 H C24 H C19 H C18 H C17 H C16 H C15 H C15 H C14 H	a 30 49 30 49 26 N5 26 N7 30 N3 26 N 30 N5 34 N 22 N1 26 N9 22 N1	05 5 0 7 03 6 07 5 06 010 .3 0 05 .5
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2065 400.2183 400.2070 400.2070 400.2057 400.2057 400.2183 400.2183 400.2169	380 5.0 mDa 0.4 -0.9 3.1 4.4 6.3 -6.8 -5.5 5.8 7.1 -5.5 -4.1	20.0 20.0 PPM 1.0 -2.2 7.7 11.0 15.7 -17.0 -13.7 14.5 17.7 -13.7 -10.2	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5 18.5 5.5 18.5 5.5 11.5 6.5 11.5 6.5	i-FIT 339.4 341.3 343.0 343.5 343.5 344.0 344.7 345.3 345.7 345.8 346.0	mum	450 i-FIT 0.2 2.1 3.8 4.3 4.3 4.3 4.3 5.5 6.1 6.4 6.4 6.6 6.8	460	Formul C23 H C24 H C19 H C18 H C17 H C16 H C15 H C15 H C14 H C14 H C13 H	a 30 49 30 49 26 N5 26 N7 30 N3 26 N 30 N5 34 N 22 N1 26 N9 22 N1 26 N1	05 5 0 7 03 5 07 5 06 010 .3 0 0 05 .5 .1 04
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2065 400.2183 400.2070 400.2070 400.2057 400.2057 400.2183 400.2169 400.2156	380 5.0 mDa 0.4 -0.9 3.1 4.4 6.3 -6.8 -5.5 5.8 7.1 -5.5 -4.1 -2.8	20.0 20.0 PPM 1.0 -2.2 7.7 11.0 15.7 -17.0 -13.7 14.5 17.7 -13.7 -13.7 -10.2 -7.0	422. 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5 18.5 5.5 18.5 5.5 11.5 6.5 11.5 6.5 1.5 1.5	i-FIT 339.4 341.3 343.0 343.5 343.5 344.0 344.7 345.3 345.7 345.8 346.0 346.4	mum	450 i-FIT 0.2 2.1 3.8 4.3 4.3 4.3 4.3 4.5 5.5 6.1 6.4 6.4 6.6 8 7.2	460	Formul C23 H C24 H C19 H C18 H C17 H C16 H C15 H C15 H C15 H C14 H C14 H C14 H C14 H C13 H C12 H	a 30 49 30 49 30 N 26 N 30 N 326 N 30 N 30 N 30 N 22 N 1 26 N 22 N 1 26 N 30 N 30 N 30 N 30 N	05 5 0 7 03 5 07 5 06 010 .3 0 0 05 .5 .1 04
0-innpung 340 Minimum: Maximum: Mass	Calc. Mass 400.2124 400.2137 400.2097 400.2065 400.2183 400.2070 400.2070 400.2057 400.2057 400.2183 400.2183 400.2169	380 5.0 mDa 0.4 -0.9 3.1 4.4 6.3 -6.8 -5.5 5.8 7.1 -5.5 -4.1	20.0 20.0 PPM 1.0 -2.2 7.7 11.0 15.7 -17.0 -13.7 14.5 17.7 -13.7 -10.2	422 410 420 -1.5 50.0 DBE 9.5 14.5 10.5 5.5 18.5 5.5 18.5 5.5 11.5 6.5 11.5 6.5	i-FIT 339.4 341.3 343.0 343.5 343.5 344.0 344.7 345.3 345.7 345.8 346.0	mum	450 i-FIT 0.2 2.1 3.8 4.3 4.3 4.3 4.3 5.5 6.1 6.4 6.4 6.6 6.8	460	Formul C23 H C24 H C19 H C18 H C17 H C16 H C15 H C15 H C14 H C14 H C13 H	a 30 49 30 49 30 N 26 N 30 N 30 N 30 N 30 N 22 N 22 N 22 N 22 N 30 N 30 N 30 N 5 N 30 N 5 N 30 N 5 N 5 N 5 N 5 N 5 N 5 N 5 N 5	05 50 703 507 506 010 30 55 104 08 06