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(De	ca-B	DE)			•	•					THE SCIE	INCE OF WH
Elementa	al Compositio	n											_ 🗆 🗙
<u>File E</u> dit <u>V</u>	jew <u>P</u> rocess	Help											
	8 2 3	M 🗉		1									
Single N	lass Anal	ysis											
Toleranc	e = 5.0 PF	M/D	BE: mir	= -1.5, m	nax = 50.0)							
Isotope o	cluster para	ameters:	Separa	ation = 1.0) Abunda	ance = 1	.0%						
Monoisot	topic Mass,	Odd and	Even E	lectron lor	1S 		10	000 4		>			
522 TOPM	ulalej evalu	ated with	i z resul	ts within I	imits (all r	esuits lu	ρτοιυ	00) 101	reach i	nassj			
	-		DOM D	05 5		6	icore	C	но	79Br	81Br		
Mass	Calc. Mass	mDa		BE Pormu	la								
Mass 816.3335	Calc. Mass 816.3362 816.3372	-2.7 -3.7	-3.3 8 -4.5 9	85 (Formu 1.5 C12 F 1.5 C13 F	la IO2 79Br4 8 IO 79Br2 81	31Br4 1 1Br6 2		12 13	1 2 1 1	4	4		
Mass 816.3335	Calc. Mass 816.3362 816.3372	-2.7 -3.7	-3.3 8 -4.5 9	8.5 C12 H 8.5 C13 H	la IO2 79Br4 8 IO 79Br2 81	31Br4 1 1Br6 2		12 13	1 2 1 1	4 2	4 6		
Mass 816.3335	Calc. Mass 816.3362 816.3372	-2.7 -3.7	-3.3 8 -4.5 9	85 C12 F 1.5 C12 F 1.5 C13 F	la IO2 79Br4 8 IO 79Br2 81	31Br4 1 1Br6 2		12 13	1 2	4 2	4 6		
Mass 816.3335	Calc. Mass 816.3362 816.3372	-2.7 -3.7	-3.3 8 -4.5 9	85 C12 H	la O2 79Br4 8 O 79Br2 81	31Br4 1 1Br6 2		12 13	1 2 1 1	4	4 6		
Mass 816.3335	Calc. Mass 816.3362 816.3372	-2.7 -3.7	-3.3 8 -4.5 9	BE Formu N.5 C12 H N.5 C13 H	ia O2 79Br4 8 O 79Br2 8	31Br4 1 1Br6 2		12 13	1 2	4	4		
Mass 816.3335	Calc. Mass 816.3362 816.3372	-2.7 -3.7	-3.3 8 -4.5 9	8E Formu 8.5 C12 F 9.5 C13 F	la O2 79Br4 6 O 79Br2 8]	31Br4 1 1Br6 2		12	1 2	4 2	4 6		
Mass 816.3335	Calc. Mass 816.3362 816.3372	-2.7 -3.7	-3.3 6 -4.5 9	tryC18 2.1*	la I O2 79Br4 6 I O 79Br2 8 10 150	31Br4 1 1Br6 2		12 13	1 2	4	4	1: TO	- MO 50
Mass 816.3335 Deca BDE 1 SannSouKe	Calc. Mass 816.3362 816.3372 816.3372	100 CN/H	-3.3 8 -4.5 9 208ymme Cm ((576)	thyC18 2.1* 578+585:50	la I O2 798r4 8 I O 798r2 8 1 50 36)-(548:553 3335	31Br4 1 1Br6 2	»»	12 13	1 2	4	6	1: TO	F MS ES- 5.84e3
Mass 816.3335 Deca BDE 1 SannSouKe 100-	Calc. Mass 816.3362 816.3372	mDa -2.7 -3.7 100 CN/H i (13.440)	-3.3 & -4.5 S 20Symme Cm ((576) 81	tryC18 2.1* 578+585:56 4.3334	la I O2 79Br4 8 I O 79Br2 8 150 36)-(548:553 .3335 818.331	31Br4 1 1Br6 2 3+620:624 02	»»	12 13	1 2	4 2	4 6	1: TO	F MS ES- 5.84e3
Mass 816.3335 Deca BDE 1 SannSouKe	Calc. Mass 816.3362 816.3372	mDa -2.7 -3.7 100 CN/H i (13.440)	-3.3 E -4.5 S 20Symme Cm ((576: 81	tryC18 2.1* 578+585:51 816 4.3334	1002 798r4 8 1 00 798r2 81 1 00 798r2 81 150 36)-(548:553 3335 818:331 818:331	310r4 1 10r6 2 3+620:624	»	12 13	1 2	4 2	4 6	1: TO	F MS ES- 5.84e3
Deca BDE 1 SannSouke	Calc. Mass 816.3362 816.3372 91000 ppm 90/ enn10024 586	mDa -2.7 -3.7	-4.5 9 20Symme Cm ((576: 812.	be formula 5 c12 + 1 5 c13 + 1 thyC18 2.1* 578+585.51 816 4.3334 3361	la 1 02 798r4 8 1 0 798r2 8 150 150 150 150 150 150 150 150	31Br4 1 1Br6 2 3+620:624 02 1.3276	»»	12 13	1 2	4 2	6	1: TO	F MS ES- 5.84e3
Mass 816.3335 Deca BDE 1 SamSouKe 100 * 788	Cak. Mass 816.3362 816.3372 1000 ppm 90/ nn10024 586 1.5640 7,91.5657	mDa -2.7 -3.7	20Symme Cm ((576) 812.840 810.340 82.540 810.340 82.540 810.340	ttyC18 2.1* 578+58551 816 4.3334 3361	la 102 798r4 8 10798r2 8 150 150 (548:55: 3335 818.33 818.33	31Br4 1 1Br6 2 3+620:624 02 1.3276 822.3312	»»	12 13	<u>1 2</u> <u>1 1</u>	842.3	221 .	1: TO	F MS ES- 5.84e3
Mass 816.3335 Deca BDE SannSouKe	Cak. Mass 816.3362 816.3372 1000 ppm 90/ pm10024 586 1.5640 791.5657	100 CN/H	20Symme Cm ((576: 810.340	ttyC18 2.1* 578+58550 816 4.3334 3361	la 10 2798r4 8 1 0 798r2 81 150 150 (548:55: 3335 818.33 818.33 820	31Br4 1 1Br6 2 3+620:624 02 1.3276 822.3312 	»»	12 13	<u>1 2</u> 1 1 84.3245	842.3	4 6 221 ε	1: TOI	F MS ES- 5.84e3







ピーク (Deca	7の糸 〒BD	l成分 E)	析希	吉界	4	11.000	*	1			THE	SCIENCE	Aters of what's possible."
	💦 Elementa	l Composition										<u>- 🗆 ×</u>	
	File Edit Vi	ew Process <u>H</u> blend (ext	elp	[sat								
		ie si	<u> </u>	8									
	Toleranc Isotope o Monoisot 97 formul	e = 10.0 mD Iuster paran opic Mass, E a(e) evaluate	ia / neters ven El d with	DBE: Sep ectron 2 resi	min = aration lons ults wi	-1.5, max = 50.0 n = 1.0 Abundance : thin limits (all results)	= 1.0% (up to 10	100) fo	reac	:h ma	ss)		
	Mass	Calc. Mass	mDa	PPM	DBE	Formula	Score	С	н	0	79Br	81Br	
	656.5016	656.5025	-0.7	-1.1	9.5	C12 H 02 798r 818r5	1	12	1	1	1	5	
	Deca BDE 1 SannSouKe	000 ppm 90/10 nn10024 586 (*	0 CN/H 13,440)	20Sym Cm ((5	metryC 76:578	:18 2.1*150 +585:586)-(548:553+620:0	624))				1: TOF	MS ES-	
	100 %- 0- 620.0	626.5569 6: 630.0	37.4381	65 65 .640.55	54.5054 2.5062 539 650.0	656.5018 4 658.5026 660.4965 672.49 660.0 670.0 670.0	93 676.48 680.0	¹²¹ 68	5.486 1111 690.0	5 692.	4836 40.0	1.18e3	
	For Help, press	s F1											2007 Nihon Waters k.k.



ピーク 7の組成分析結果5	aters F WHAT'S POSSIBLE.
Remental Composition	
Elle Edit View Process Help	
Single Mass Analysis Tolerance = 10.0 mDa / DBE: min = -1.5 max = 50.0	
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%	
Monoisotopic Mass, Odd and Even Electron Ions 447 (annuloc) a valuated with 2 scoults within limits (all scoults (up to 1999) (as each moos)	
Mass Calc. Mass mDa PPM DBE Formula Score C H O 79Br 81Br 610.5634 610.5632 0.2 0.4 10.5 C12 04 3 12 4 1 4	
610.5622 1.2 2.0 9.5 C11 05 798/3 818/2 2 11 5 3 2 610.5612 2.2 3.7 8.5 C10 06 798/5 1 10 6 5	
Deca 8DE 1000 ppm 90/100 CN/H2OSymmetryC18 2.1*150 SamSouKenn10024 586 (13.440) Cm ((576:578+585:586)-(548:553+620:624)) 1: TOF MS ES- 610.5634 5.01e3	
608.5649 %-	
508.5233 540.5781 568.5773 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	
For Help, press F1	007 Nihon Waters k.k. 14





















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Isotope of Monoisot 234 form	cluster paran opic Mass, O ula(e) evaluat	neters: Sep add and Ever ted with 3 re:	aration = 1 Electron lo sults within	.0 Abundance = ins limits (all results)	1.0% (up to 1000) for e	ach mass)	
Mass	Calc. Mass	mDa PPM	DBE Form	ula	Score	С Н О 7	9Br 81Br
532.6550	532.6526 532.6517 532.6507	2.4 4.4 3.3 6.3 4.3 8.2	10.5 C12 9.5 C11 8.5 C10	H 04 818r4 H 05 798r2 818r2 H 06 798r4	1 2 2	12 1 4 11 1 5 10 1 6	4 2 2 4
Octa BDE 11 SannSouKe	000 ppm 90/10 nn10023 487 (0 CN/H2OSym 11.167) Cm (4)	metryC18 2.1* 30:487-(446:4	*150 :56+525:531)) 532.6550			1: TOF MS ES- 1.46e4
100			530.6	3572 534.6531			

