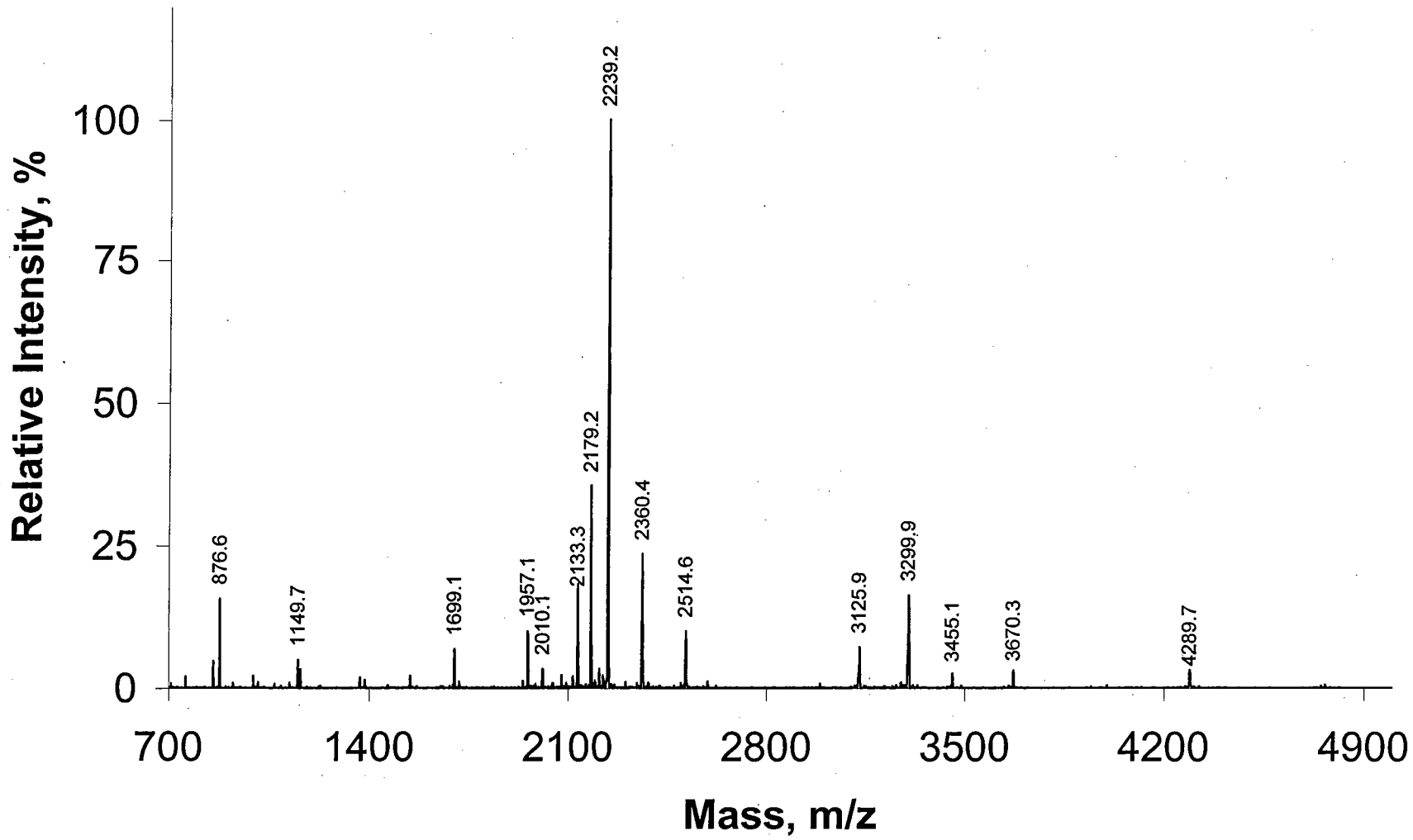
MALDI mass spectra of the trypsin digest of MRSL-36



C2

MRSL-36, Aldo-keto reductase family 1 member C2; # P52895

[1-323] m+H = 37112.117
Cleavage at KR trypsin digest

Small polar:	D(18)	E(23)	N(17)	Q(11)			
Large polar:	K(26)	R(15)	H(10)				
Small non-polar:	S(19)	T(7)	A(23)	G(15)			
Large non-polar:	L(36)	I(15)	V(27)	M(5)	F(13)	Y(14)	W(3)
Special:	C(7)	P(19)					

C[7] + 57.05 C[145] + 57.05 C[154] + 57.05 C[188] + 57.05
C[193] + 57.05 C[206] + 57.05 C[242] + 57.05

```
  1 M D S K y q c v k L N D G H F M P V L G F G T Y A P A E V P  30
 31 K s k A L E A V K l a i e a g f h h i d s a h v y n n e e q  60
 61 v g l a i r S K i a d g s v k R e d i f y t s k L W S N S H  90
 91 R P E L V R P A L E R s l k N L Q L D Y V D L Y L I H F P V 120
121 S V K P G E E V I P K d e n g k I L F D T V D L C A T W E A 150
151 M E K c k D A G L A K s i g v s n f n h r L L E M I L N K P 180
181 G L K y k p v c n q v e c h p y f n q r K I I d f c k S K d 210
211 i v l v a y s a l g s h r E E P W V D P N S P V L L E D P V 240
241 L C A L A K k H K r T P A L I A L R y q l q r G V V V L A K 270
271 s y n e q r l R q n v q v f e f q l t s e e m k A I D G L N 300
301 R n v r Y L T L D I F A G P P N Y P F S D E Y              323
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(1)	[1-4] = 480.212	(2)	[5-9] = 697.334	(3)	[10-31] = 2360.174
(4)	[32-33] = 234.145	(5)	[34-39] = 630.382	(6)	[40-66] = 3003.507
(7)	[67-68] = 234.145	(8)	[69-75] = 689.383	(9)	[76-76] = 175.119
(10)	[77-84] = 1002.478	(11)	[85-101] = 2060.115	(12)	[102-104] = 347.229
(13)	[105-131] = 3125.692	(14)	[132-136] = 562.247	(15)	[137-153] = 2041.961
(16)	[154-155] = 307.144	(17)	[156-161] = 574.320	(18)	[162-171] = 1130.570
(19)	[172-183] = 1368.828	(20)	[184-200] = 2239.017	(21)	[201-201] = 147.113
(22)	[202-207] = 795.407	(23)	[208-209] = 234.145	(24)	[210-223] = 1500.817
(25)	[224-246] = 2591.306	(26)	[247-247] = 147.113	(27)	[248-249] = 284.172
(28)	[250-250] = 175.119	(29)	[251-258] = 854.546	(30)	[259-263] = 707.384
(31)	[264-270] = 685.461	(32)	[271-276] = 796.358	(33)	[277-278] = 288.203
(34)	[279-294] = 1956.937	(35)	[295-301] = 758.416	(36)	[302-304] = 388.230
(37)	[305-323] = 2222.033				

MRSL-36 alternative

C1

human aldo-keto reductase family 1 member C1; Q04824

[1-323] m+H = 37222.197
Cleavage at KR trypsin digest

Small polar:	D(18)	E(23)	N(17)	Q(12)			
Large polar:	K(26)	R(17)	H(8)				
Small non-polar:	S(18)	T(8)	A(23)	G(15)			
Large non-polar:	L(36)	I(15)	V(26)	M(4)	F(13)	Y(14)	W(3)
Special:	C(8)	P(19)					

C[7] + 57.05	C[87] + 57.05	C[145] + 57.05	C[154] + 57.05
C[188] + 57.05	C[193] + 57.05	C[206] + 57.05	C[242] + 57.05

```
  1 M D S K y q c v k L N D G H F M P V L G F G T Y A P A E V P  30
 31 K s k A L E A T K I a i e a g f r H I D S A H L Y N N E E Q  60
 61 V G L A I R s k I A D G S V K r E D I F Y T S K I w c n s h  90
 91 r p e I v r p a I e r S L K n I q I d y v d I y I i h f p v 120
121 s v k p g e e v i p k D E N G K i I f d t v d I c a t w e a 150
151 v e k C K d a g I a k S I G V S N F N R r Q L E M I L N K P 180
181 G L K y k p v c n q v e c h p y f n q r K I I d f c k S K d 210
211 i v I v a y s a I g s h r E E P W V D P N S P V L L E D P V 240
241 L C A L A K k H K r T P A L I A L R y q I q r G V V V L A K 270
271 s y n e q r I R q n v q v f e f q I t s e e m k A I D G L N 300
301 R n v r Y L T L D I F A G P P N Y P F S D E Y              323
```

(1)	[1-4] = 480.212	(2)	[5-9] = 697.334	(3)	[10-31] = 2360.174
(4)	[32-33] = 234.145	(5)	[34-39] = 632.361	(6)	[40-47] = 876.494
(7)	[48-66] = 2179.089	(8)	[67-68] = 234.145	(9)	[69-75] = 689.383
(10)	[76-76] = 175.119	(11)	[77-84] = 1002.478	(12)	[85-101] = 2133.113
(13)	[102-104] = 347.229	(14)	[105-131] = 3125.692	(15)	[132-136] = 562.247
(16)	[137-153] = 2009.989	(17)	[154-155] = 307.144	(18)	[156-161] = 574.320
(19)	[162-170] = 993.511	(20)	[171-171] = 175.119	(21)	[172-183] = 1383.803
(22)	[184-200] = 2239.017	(23)	[201-201] = 147.113	(24)	[202-207] = 795.407
(25)	[208-209] = 234.145	(26)	[210-223] = 1500.817	(27)	[224-246] = 2591.306
(28)	[247-247] = 147.113	(29)	[248-249] = 284.172	(30)	[250-250] = 175.119
(31)	[251-258] = 854.546	(32)	[259-263] = 707.384	(33)	[264-270] = 685.461
(34)	[271-276] = 796.358	(35)	[277-278] = 288.203	(36)	[279-294] = 1956.937
(37)	[295-301] = 758.416	(38)	[302-304] = 388.230	(39)	[305-323] = 2222.033

matches to Aldo-keto reducatase family 1 member C2 (Swiss Prot accession number P52895)

Centroid Mass	Rel. Intensity	Potential Tryptic Peptide	Calc. Mass	Mass Error, ppm
876.556016	3.8			
1149.685008	1.4			
1699.11478	3.2	R[250-263]R	1699.012	60
1957.070689	6.5	Q[279-294]K	1956.937	68
2010.124666	2.0			
2076.257142	1.3			
2116.744381	1.1			
2133.256527	14.9			
2179.236178	31.2			
2209.511441	2.7	T[251-270]K	2209.354	71
2222.665889	1.1			
2239.16895	100.0	Y[184-200]R	2239.017	68
2360.355764	19.3	L[10-31]K	2360.174	77
2365.516735	1.1			
2514.582517	8.8			
3125.937087	7.9	N[105-131]K	3125.692	78
3299.918903	18.7			
3455.124272	2.2			
3670.262077	2.3			
4289.655005	1.4			

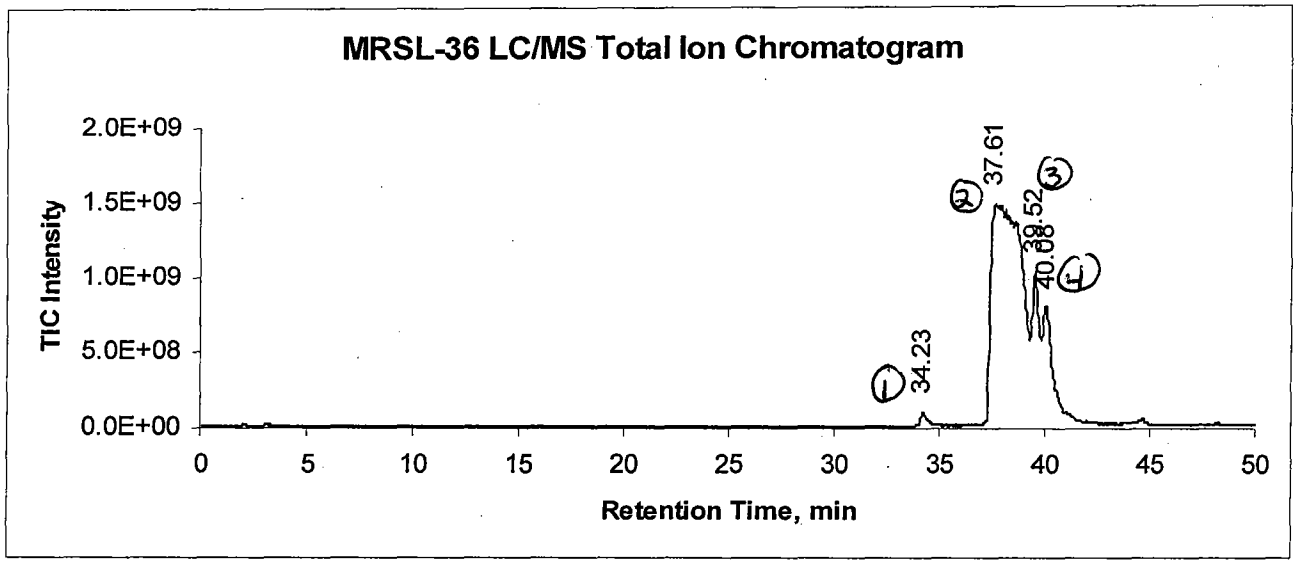
← many unassignable

matches to Aldo-keto reducatase family 1 member C1 (Swiss Prot accession number Q04828)

Centroid Mass	Rel. Intensity	Potential Tryptic Peptide	Calc. Mass	Mass Error, ppm
876.556016	3.8	I[40-47]R	876.494	71
1149.685008	1.4	S[162-171]R	1149.612	64
1699.11478	3.2	R[250-263]R	1699.012	60
1957.070689	6.5	Q[279-294]K	1956.937	68
2010.124666	2.0	I[137-153]K	2009.989	67
2076.257142	1.3			
2116.744381	1.1			
2133.256527	14.9	L[85-101]R	2133.113	67
2179.236178	31.2	H[48-66]R	2179.089	68
2209.511441	2.7	T[251-270]K	2209.354	71
2222.665889	1.1			
2239.16895	100.0	Y[184-200]R	2239.017	68
2360.355764	19.3	L[10-31]K	2360.174	77
2365.516735	1.1	R[250-270]K	2365.455	26
2514.582517	8.8	S[162-183]K	2514.397	74
3125.937087	7.9	N[105-131]K	3125.692	78
3299.918903	18.7			
3455.124272	2.2			
3670.262077	2.3	G[264-294]K	3669.905	97
4289.655005	1.4			

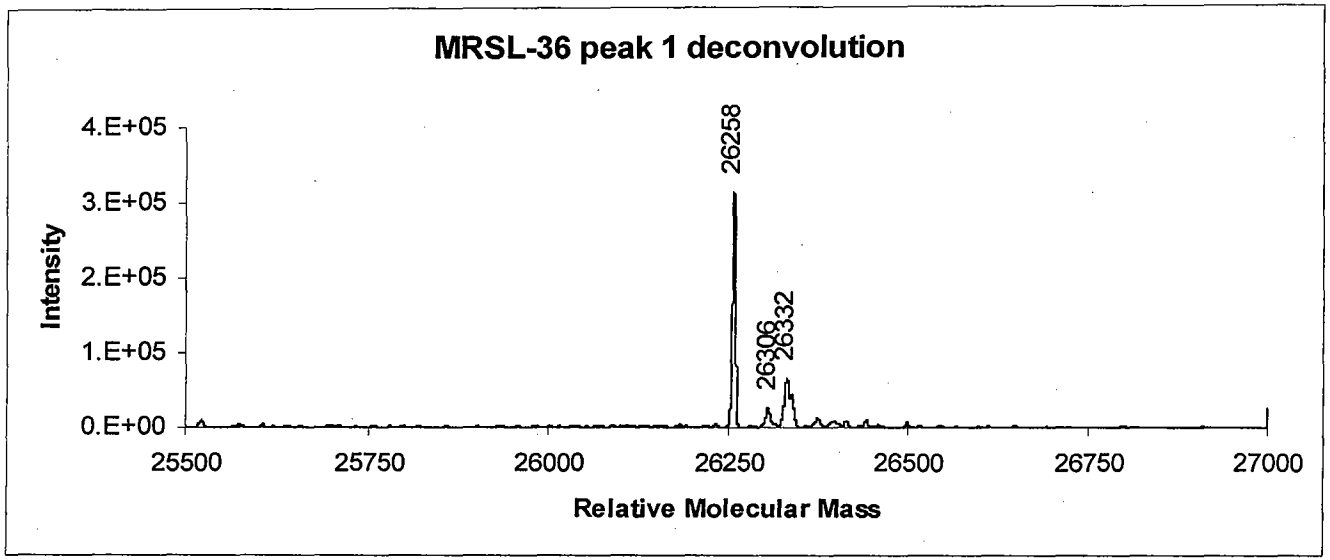
← good fit

but not protein we said it was

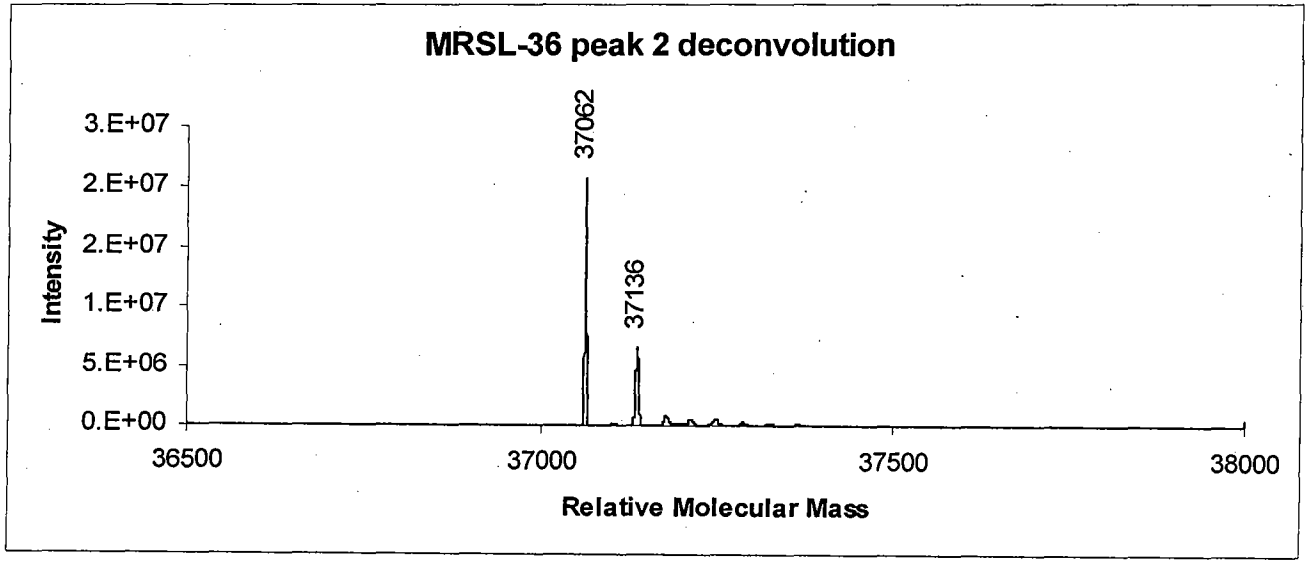


Column = Supelco Discovery BIO Wide Pore C5, 10 cm x 0.32 mm, 3 µm; #44493-01
Mobile Phase A = 0.05 % (v/v) trifluoroacetic acid in water
Mobile Phase B = 0.05 % (v/v) trifluoroacetic acid in acetonitrile
Method File = NCI Proteins-Polar
Column Temp = 50 °C
Injection Volume = 5 µL (full loop injection)

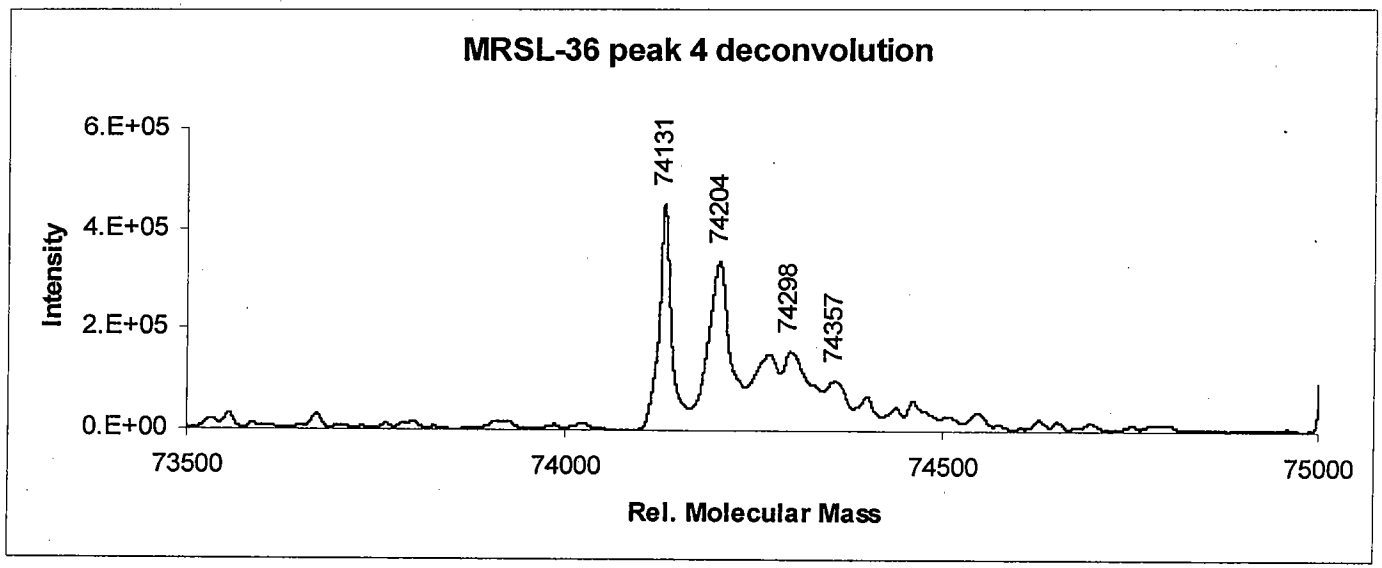
Time, min	% B	Flow, µL/min
0	15	6
5	15	6
45	60	6
50	95	6
55	95	6
56	15	6
80	15	6



Rel Molecular Mass	Intensity	Potential ID
26258	3.13E+05	
26306	2.62E+04	
26332	6.70E+04	



Rel. Molecular Mass	Intensity	Potential ID			
37062	2.07E+07	MRSL-36 Calculated Mr =		36735	(without disulfides)
37136	6.59E+06			36729	(with 3 disulfides)



Rel. Molecular Mass	Intensity	Potential ID
74131	4.51E+05	covalent dimer of Mr 37062 (MRSL-36 peak 2) species
74204	3.37E+05	
74298	1.56E+05	
74357	9.79E+04	