

Supplementary Materials: Ergochromes: Heretofore Neglected Side of Ergot Toxicity

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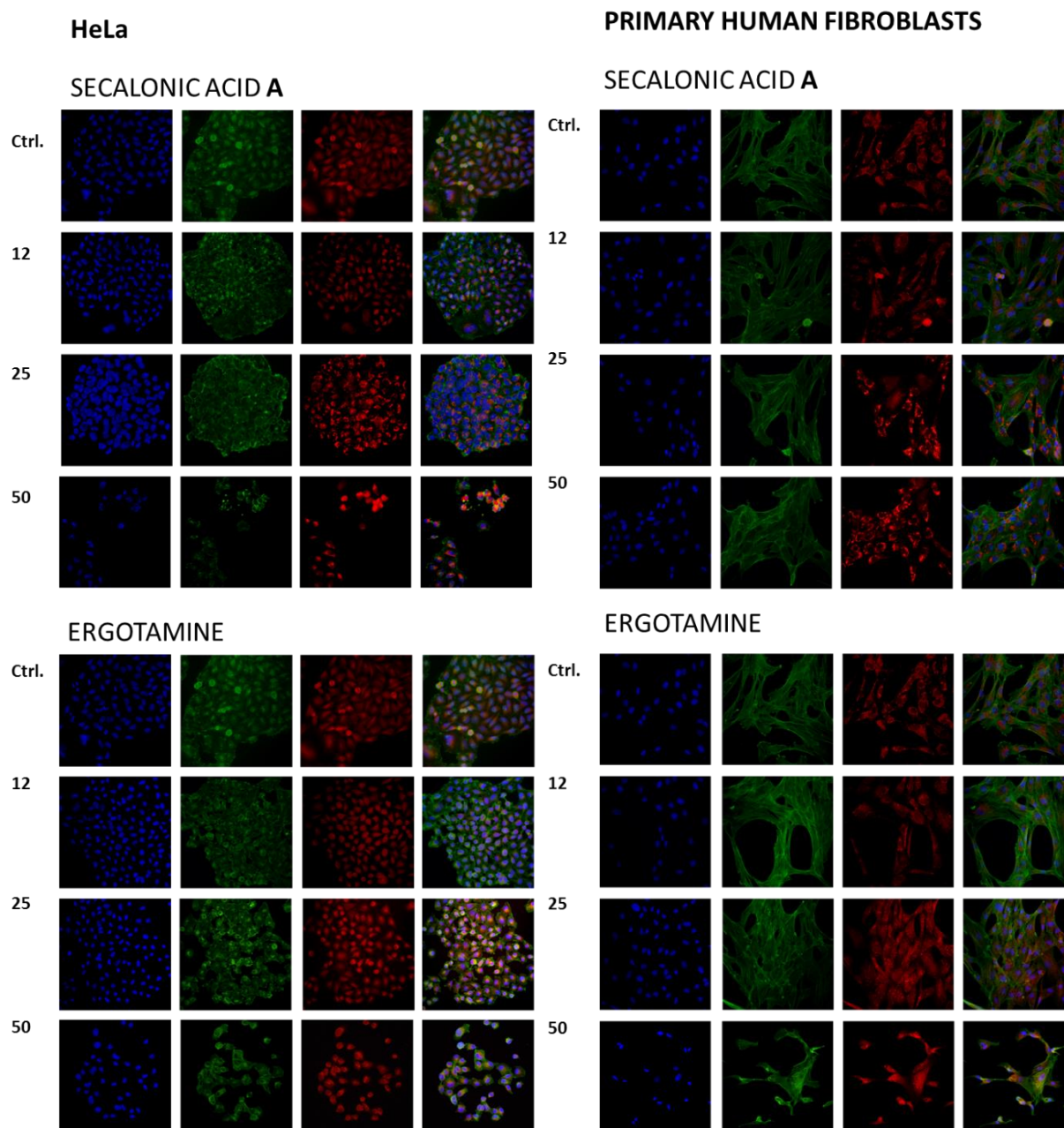
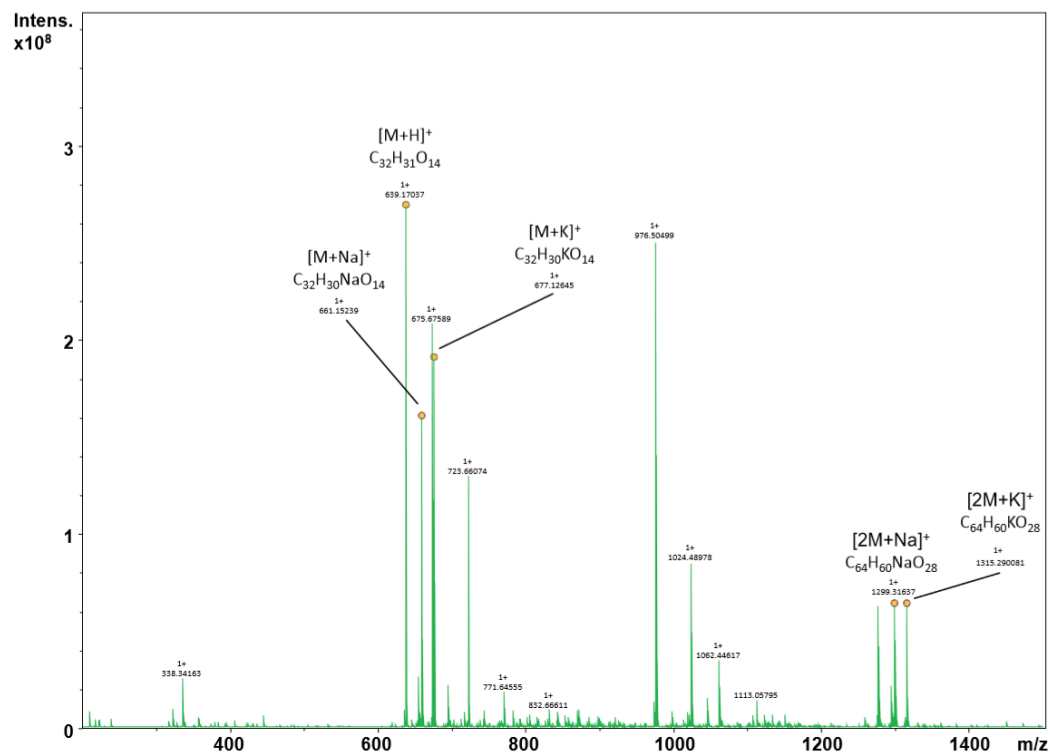
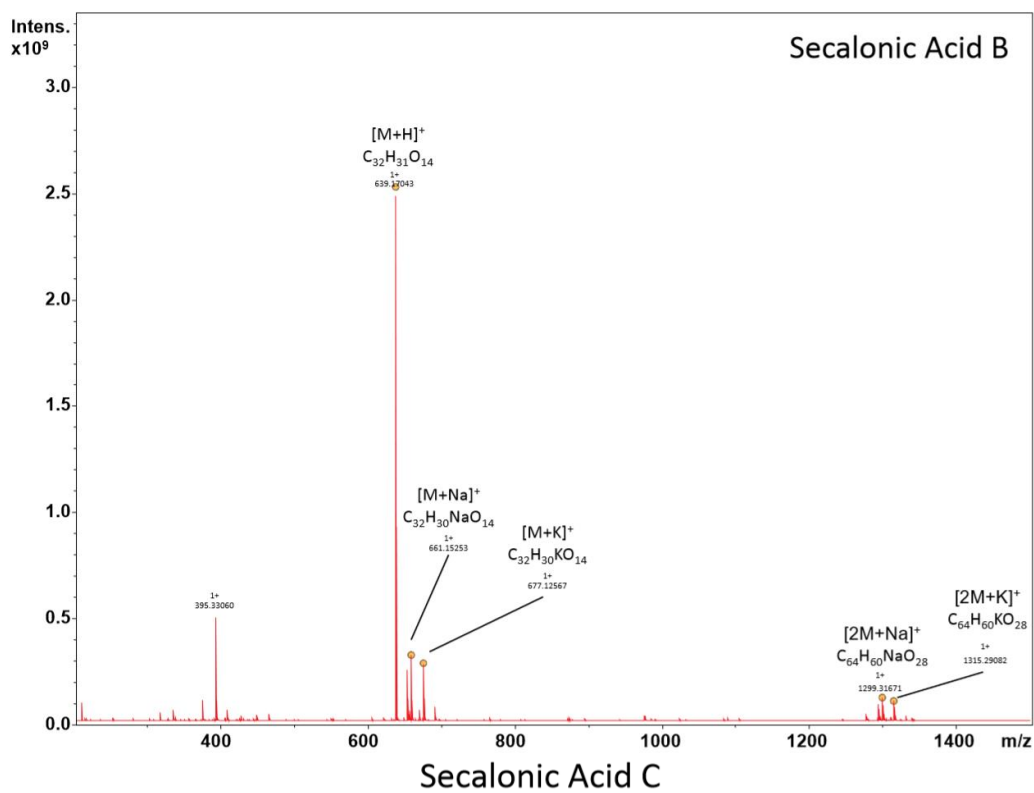


Figure S1. Cell cultures grown on glass coverslips were treated for 24 h with secalonic acid A or ergotamine and in vivo incubated with MitoTracker® Red CMXRos, fixed, permeabilized and labelled with Phalloidin-Alexa Fluor®488. Magnification 20x.



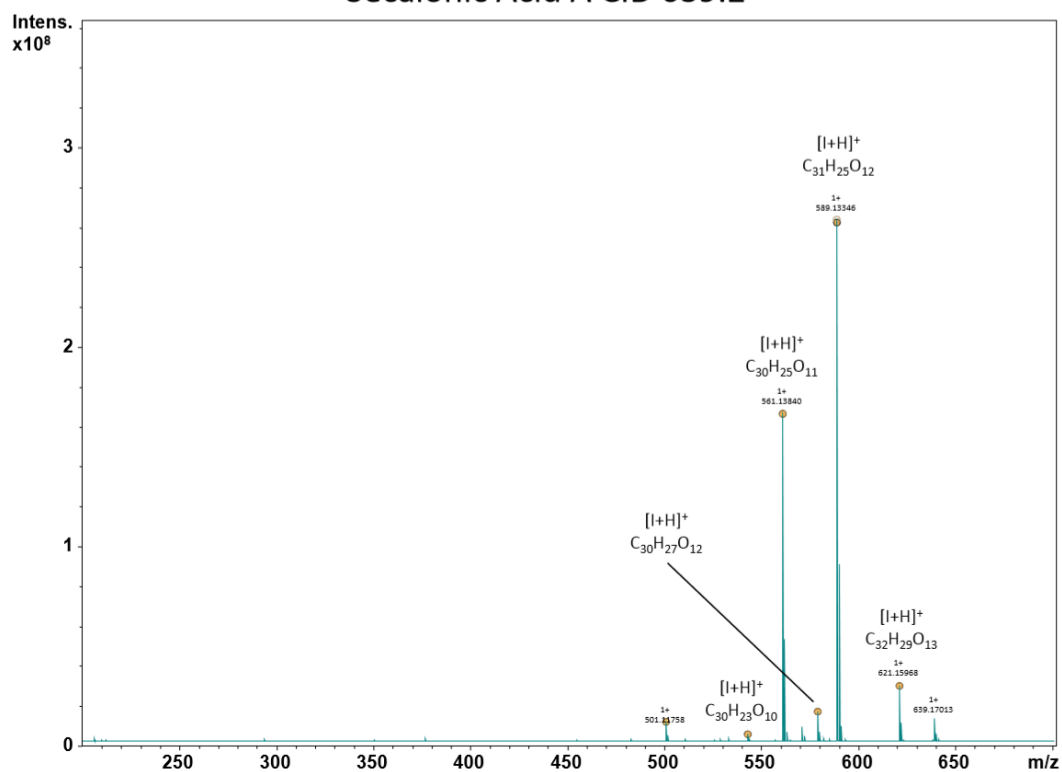
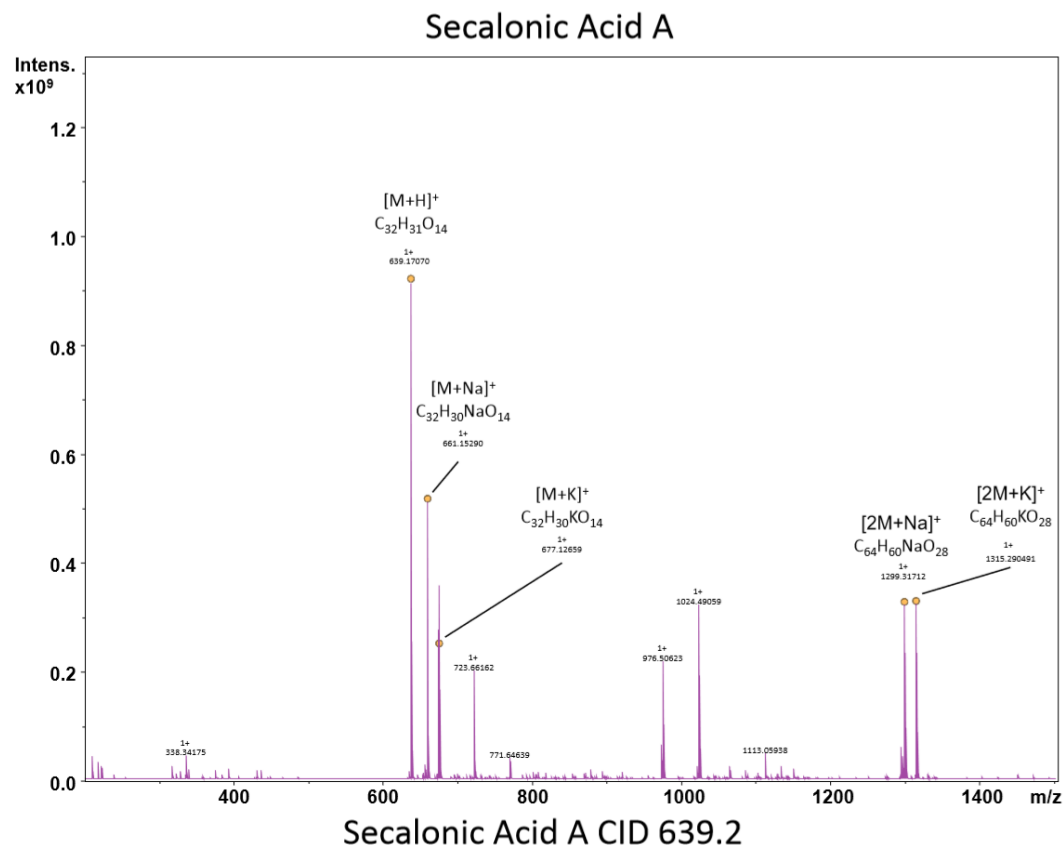


Figure 2. FTMS data for Secalonic Acid A–C.

Table S2. NMR data for Secalonic acid A–C.

Atom	SA A		SA B		SA C	
Number	δ_c	m	δ_c	m	δ_c	m _c
1	158.44	s	160.32	s	160.89	s
2	117.21	s	119.32	s	119.96	s
3	140.13	d	141.05	d	141.66	d
4	107.39	d	108.55	d	109.14	d
4a	158.81	s	158.75	s	159.31	s
5	75.13	d	71.81	d	72.44	d
6	29.80	d	29.50	d	30.11	d
7	35.72	t	33.46	t	34.07	t
8	178.11	s	181.54	s	182.10	s
8a	101.61	s	101.48	s	102.07	s
9	186.47	s	189.00	s	189.59	s
9a	106.21	s	107.59	s	108.23	s
10a	85.07	s	86.02	s	86.63	s
6-Me	17.65	q	17.76	q	18.33	q
10a-CO	169.92	s	172.25	s	172.83	s
10a-OMe	52.72	q	54.12	q	54.66	q
1'					160.87	s
2'					119.28	s
3'					141.88	d
4'					109.16	d
4'a					160.82	s
5'					77.82	d
6'					31.36	d
7'					37.45	t
8'					180.07	s
8a'					103.52	s
9'					189.15	s
9'a					108.40	s
10'a					86.74	s
6'-Me					18.80	q
10'a-CO					171.71	s
10'a-OMe					54.10	q

m – multiplicity

Table S3. ¹H NMR data for Secalonic acid A–C.

Atom	SA A			SA B			SA C		
Number	δ _H	m _H	J [Hz]	δ _H	m _H	J [Hz]	δ _H	m	J [Hz]
3	7.456	d	8.5	7.431	dd	0.4, 8.4	7.416	d	8.5
4	6.626	d	8.5	6.553	d	8.4	6.538	d	8.5
5	3.812	dd	5.8, 11.1	4.068	dd	1.7, 3.2	4.071	d	1.5
6	2.309	dddq	6.2, 6.5, 10.9, 11.1	2.085	m	-	2.083	m	-
7	2.660	dd	6.2, 19.3	2.414	m	-	2.410	m	-
	2.471	dd	10.9, 19.3	-	-	-	-		
1-OH	11.602	s	-	11.728	d	0.4	11.720	s	-
5-OH	6.001	d	5.8	3.690	dd	1.4, 3.2	n.d.		
6-Me	1.038	d	6.5	1.090	d	6.8	1.090	d	6.6
8-OH	13.601 [†]	br s	-	13.908	s	-	13.906 [†]	br s	-
10a-OMe	3.607	s	-	3.666	s	-	3.661	s	-
3'							7.440	d	8.4
4'							6.595	d	8.4
5'							3.854	d	10.9
6'							2.410	m	-
7'							2.687	dd	5.6, 18.6
							2.359	m	10.8, 18.6
1'-OH							11.582	s	-
5'-OH							n.d.		
6'-Me							1.090	d	6.6
8'-OH							13.680 [†]	br s	-
10'a-OMe							3.634	s	-

[†]—tentative assignment, n.d. - not detected, m - multiplicity