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Rapid, non-targeted discovery of biochemical transformation and biomarker candidates in oncovirus-infected cell lines using LAESI mass spectrometry

Bindesh Shrestha[a], Prabhakar Sripadi[a], Callee M. Walsh[b], Trust T. Razunguzwa[b], Matthew J. Powell,[b] Kylene Kehn-Hall,[c] Fatah Kashanchi[c] and Akos Vertes*[a]

[a]Department of Chemistry, W.M. Keck Institute of Proteomics Technology and Applications, The George Washington University, Washington D.C, USA. Fax: +1-202-994-5873 Tel: +1-202-994-2717; E-mail: vertes@gwu.edu

[b]Protea Biosciences, 955 Hartman Run Road, Morgantown, WV 26505

[c]Department of Molecular and Microbiology, National Center for Biodefense and Infectious Diseases, George Mason University, Manassas, VA 20110, USA.

Table S1. Putative assignments of ions corresponding to the numbered points found in the wings of the S-plotin Figure 2 and the histogram in Figure 3. Table S1 only shows the assignments selected on the basis of exhibiting the most variance in the mass spectra between the affected and control cell lines. Numerous other ions were also detected but did not show major changes between the two groups.

SN	Putative Assignments	Ion	Monoisotopic *m/z*	Measured Average *m/z*	Δm (mDa)	Factor of Change	
						Down regulated	Up regulated
1	unassigned			678.5152		7.2±2.1	
2	unassigned			707.5327		3.3±0.4	
3	PC(30:0)	$C_{38}H_{76}NO_8P+H^+$	706.5387	706.5423	3.6	3.1±0.3	
4	PE(34:2)	$C_{39}H_{74}NO_8P+H^+$	716.5230	716.5443	21.3	3.1±0.3	
5	thymosin β4	$C_{212}H_{350}N_{56}O_{78}S_1+7H^{+7}$	710.0806	710.0843	3.7	11.2±4.8	
6	PC(32:0)	$C_{40}H_{80}NO_8P+H^+$	734.5700	734.5634	-6.6	2.6±0.2	
7	PC(32:1)	$C_{40}H_{78}NO_8P+H^+$	732.5543	732.5581	3.8	1.8±0.1	
8	PC(32:2)	$C_{40}H_{76}NO_8P+H^+$	730.5387	730.5405	1.8	2.5±0.2	
9	unassigned			729.5273		3.1±0.4	
10	PC(32:3)	$C_{40}H_{74}NO_8P+H^+$	728.5230	728.5353	12.3	3.6±0.3	
11	unassigned			735.5429		2.3±0.2	
12	PC(34:3) PC(32:0)	$C_{42}H_{78}NO_8P+H^+$ $C_{40}H_{80}NO_8P+Na^+$	756.5543 756.5519	756.5322	-22.1 -19.7	1.9±0.1	
13	unassigned			755.5476		2.1±0.2	
14	PC(34:4)	$C_{42}H_{76}NO_8P+H^+$	754.5387	754.5399	1.2	1.9±0.1	
15	unassigned			781.5575		2.2±0.3	
16	PC(36:5)	$C_{44}H_{78}NO_8P+H^+$	780.5543	780.5441	-10.2	1.6±0.1	
17	thymosin β4	$C_{212}H_{350}N_{56}O_{78}S_1+6H^{+6}$	828.5954	828.5778	-17.6	2.5±0.4	
18	thymosin β4	$C_{212}H_{350}N_{56}O_{78}S_1+6H^{+6}$	828.2594	828.1824	-77.0	3.9±0.4	
19	unassigned			706.2482			8.0±0.1
20	PA (O-37:1)	$C_{40}H_{79}O_7P+H^+$	703.5641	703.5728	8.7		2.4±0.0
21	unassigned			747.5930			1.9±0.0
22	PC(35:1)	$C_{43}H_{84}NO_8P+H^+$	774.6012	774.6004	-0.8		2.2±0.0
23	PC(34:1)	$C_{42}H_{82}NO_8P+K^+$	798.5414	798.5606	19.2		1.9±0.0
24	unassigned			797.5982			2.0±0.0
25	PC(37:4)	$C_{45}H_{82}NO_8P+H^+$	796.5856	796.5830	-2.6		1.6±0.0
26	PC(39:4)	$C_{47}H_{86}NO_8P+H^+$	824.6170	824.5488	-68.2		1.8±0.1
27	thymosin β10	$C_{211}H_{353}N_{57}O_{76}S+6H^{+6}$	823.5976	823.5300	-67.6		2.3±0.0

[a] The monoisotopic masses were calculated using the NIST Isotope Calculator package (ISOFORM, Version 1.02) or MolE - Molecular Mass Calculator v2.02 (http://library.med.utah.edu/masspec/mole.htm). The measured *m/z* values were obtained by averaging *m/z* values in mass spectra from parallel samples.

[b] Glycerophosphocholines (PC), glycerophosphates (PA), and phosphatidylethanolamines (PE) species are identified by the total length of the acyl chain(s) and the number of double bonds in parentheses.

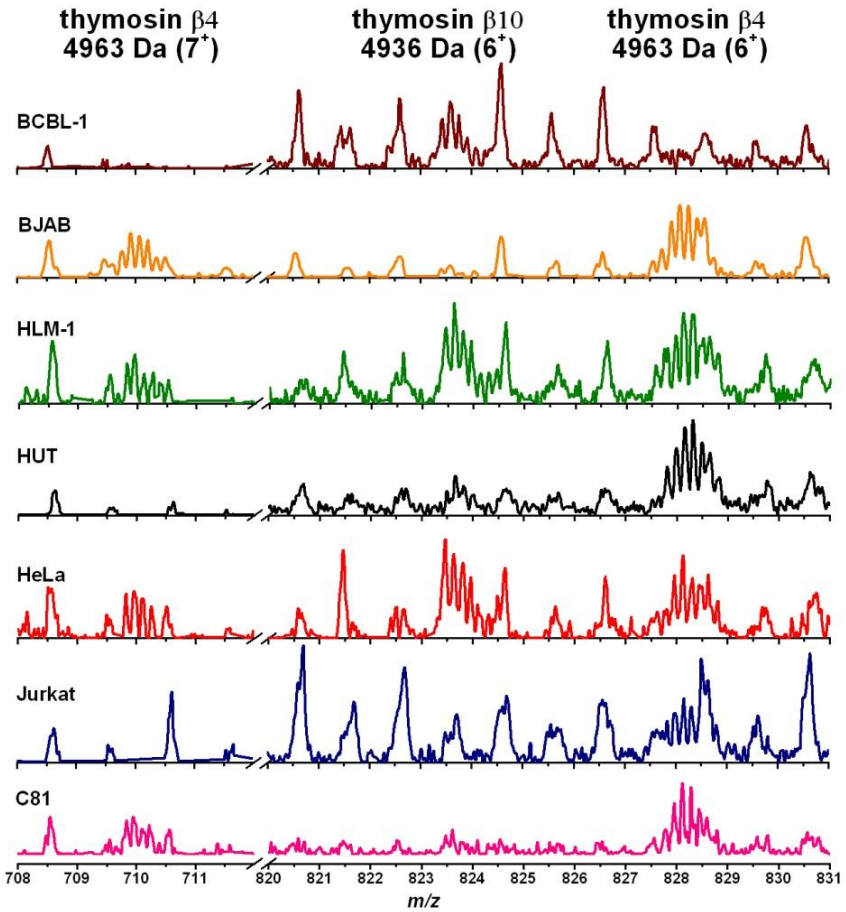

Fig. S1 LAESI-MS analysis of seven different cell lines indicates differences in expression of thymosin β4 and β10. Multiply-charged ion peaks with +6 charge state at ~ *m/z* 823 were assigned to thymosin β10. Ions with charge states of +7 and +6 at ~ *m/z* 710 and 828, respectively, were assigned to thymosin β4. Thymosin β4 expression is reduced in BCBL-1 cells, while thymosin β10 expression is reduced in BJAB cells.

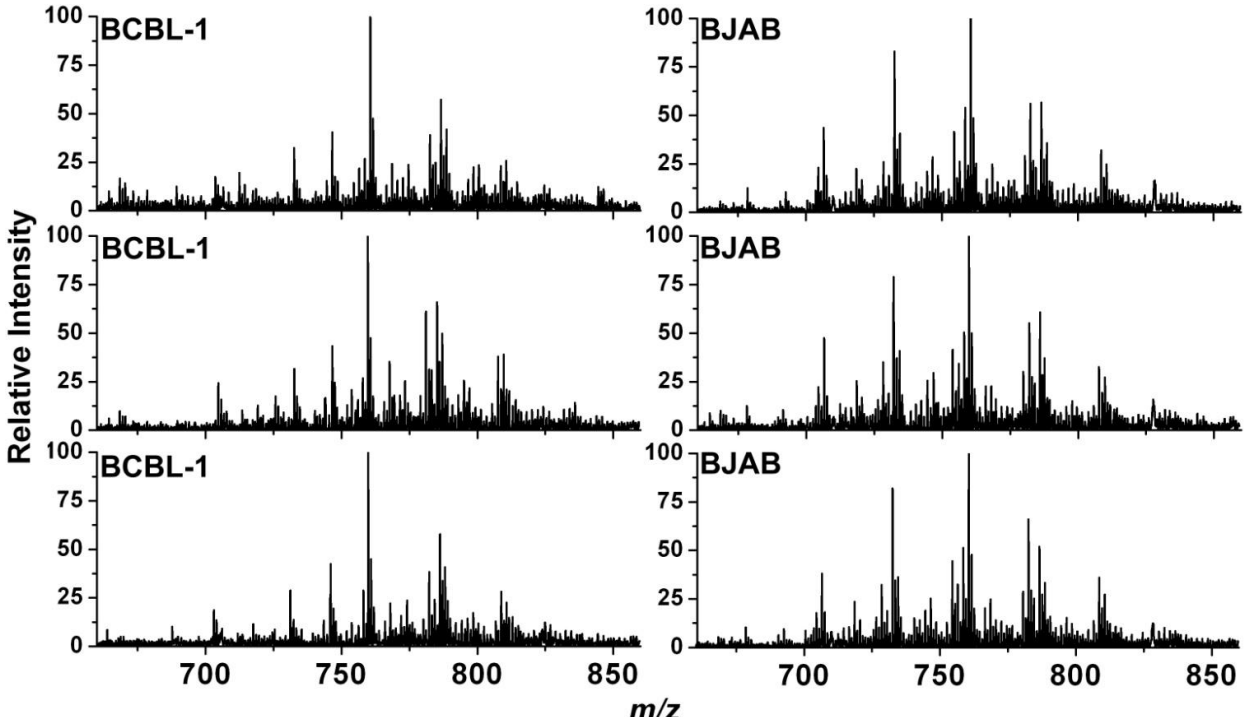

Fig. S2 Comparison of technical variance (spectra within columns) and biological variance (spectra between columns) for LAESI-MS analysis of BCBL-1 and BJAB cell pellets. Differences between the two cell-lines clearly exceed the variations for a given cell line.

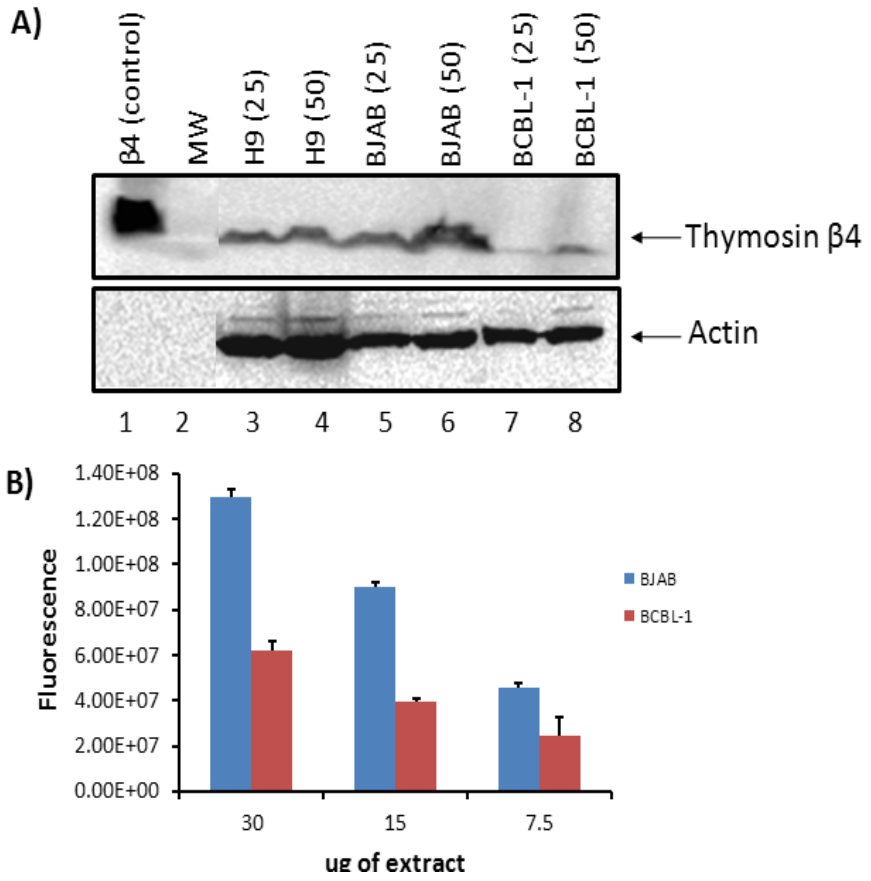

Fig. S3 A) Anti-Tβ4 western blot of lysates from H9 T-cells, BJAB, and BCBL-1 point to lower concentrations of Tβ4 in the infected B cells. B) Lysates from BJAB and BCBL-1 cells assayed for total PC indicate downregulation in the infected cells.