SI Legends

Fig. S1. A. Inactivation of wild-type OhrR (□), sc OhrR WT-WT (△), or WT-C15S scOhrR (×) in the presence of 0.5 mM Cys. As a control, the comparatively slow inactivation of OhrR in the absence of Cys is also shown (◇). B. Inactivation of OhrR (□), scOhrR WT-WT (△) or WT-C15S scOhrR (×) in the presence of 0.5 mM BSH.

Fig. S2. *S*-bacillithiolated BrxB C54A does not transfer BSH to OhrR. Immunoblot analysis usig anti-BSH antibodies to follow protein *S*-bacillithiolation. Purified OhrR-SSB (lane 1) and BrxB C54A-SSB (lane 2) are shown as controls. BSH does not de-bacillithiolate OhrR-SSB (lane 3), but incubation with BrxB C54A leads to de-bacillithiolation and transfer of the BSH moiety to BrxB (lane 4). The reverse reaction, transfer of BSH from BrxB C54A-SSB to OhrR is not observed (lane 5).

Table S1: Detected MetE-SSB sites by Orbitrap LC-MS/MS analysis before and after reduction by BrxA and BrxB in an in vitro Brx-assay. His-tagged MetE was expressed and purified from *E. coli* cells, in vitro bacillithiolated using BSSB and purified as described in the Methods section. MetE-SSB was reduced by purified BrxA and BrxB for 1 hour. The MetE-SSB control reaction and MetE-SSB that was treated with BrxA and BrxB were separated by SDS-PAGE. The MetE-SSB bands and the BrxA and BrxB bands were tryptically in gel-digested. The resulting MetE-SSB peptides were analyzed using LTQ Orbitrap Velos LC-MS/MS analysis as described in the Methods section (Chi et al., 2011). The Scaffold search results are shown and the Table includes the Xcorr, deltaCn scores,m/z of the precursor ions, neutral molecular masses of the peptides, peptide mass deviations (delta ppm) of all detected bacillithiolated peptides in MetE. The CID MS/MS spectrum of the modified Cys peptides are shown,with the b and y ion series labeled in red and blue, respectively. Two replicates each for the Brx assay using MetE-SSB were performed and the averages and SEM are shown for the bacillithiolated Cys peptides of MetE before and after Brx reduction in the Table below that is used for the Figure 5.

Table S2: Detected BrxA-SSB sites by Orbitrap LC-MS/MS analysis before and after reduction of MetE-SSB by BrxA in the in vitro Brx-assay. His-tagged MetE was expressed and purified from *E. coli* cells, in vitro bacillithiolated using BSSB and purified as described in the Methods section. MetE-SSB was reduced by purified BrxA for 1 hour. The MetE-SSB control reaction and MetE-SSB that was treated with BrxA and BrxB were separated by SDS-PAGE. The MetE-SSB bands and the BrxA and BrxB bands were tryptically in gel-digested. The resulting BrxA-SSB peptides were analyzed using LTQ Orbitrap Velos LC-MS/MS analysis as described in the Methods section (Chi et al., 2011). The Scaffold search results are shown and the Table includes the Xcorr, deltaCn scores,m/z of the precursor ions, neutral molecular masses of the peptides, peptide mass deviations (delta ppm) of all detected bacillithiolated peptides in BrxA. The CID MS/MS spectrum of the modified Cys peptides are shown,with the b and y ion series labeled in red and blue, respectively. Two replicates each for the Brx assay using MetE-SSB were performed and the averages and SEM are shown for the bacillithiolated Cys peptides of BrxA before and after Brx reduction of MetE-SSB in the Table below that is used for the Figure 5.

Table S3: Detected BrxB-SSB sites by Orbitrap LC-MS/MS analysis before and after reduction of MetE-SSB by BrxB in the in vitro Brx-assay. His-tagged MetE was expressed and purified from *E. coli* cells, in vitro bacillithiolated using BSSB and purified as described in the Methods section. MetE-SSB was reduced by purified BrxB for 1 hour. The MetE-SSB control reaction and MetE-SSB that was treated with BrxA and BrxB were separated by SDS-PAGE. The MetE-SSB bands and the BrxA and BrxB bands were tryptically in gel-digested. The resulting BrxB-SSB peptides were analyzed using LTQ Orbitrap Velos LC-MS/MS analysis as described in the Methods section (Chi et al., 2011). The Scaffold search results are shown and the Table includes the Xcorr, deltaCn scores,m/z of the precursor ions, neutral molecular masses of the peptides, peptide mass deviations (delta ppm) of all detected bacillithiolated peptides in BrxB. The CID MS/MS spectrum of the modified Cys peptides are shown,with the b

and y ion series labeled in red and blue, respectively. Two replicates each for the Brx assay using MetE-SSB were performed and the averages and SEM are shown for the bacillithiolated Cys peptides of BrxB before and after Brx reduction of MetE-SSB in the Table below that is used for the Figure 5.

Table S4: BrxB C54A with the Cys52-SSB site (upper figure) and BrxA C55A with Cys53-SSB site (bottom figure) *in vivo*. FLAG-tagged BrxB C54A and BrxA C55A proteins were purified from *B. subtilis* cells after NaOCl-stress, separated by SDS-PAGE and the Brx bands tryptically digested.The resulting peptides were analyzed using LTQ Orbitrap Velos LC-MS/MS analysis as described in the Methods section (Chi et al., 2011). The Scaffold search results are shown and the Table includes the Xcorr, deltaCn scores, m/z of the precursor ions, neutral molecular masses of the peptides, peptide mass deviations (delta ppm) of the S-bacillithiolated Cys52 peptide in BrxB C54A and Cys53 in BrxA C55A. The CID MS/MS spectra are shown with the b and y ion series labeled in red and blue, respectively.
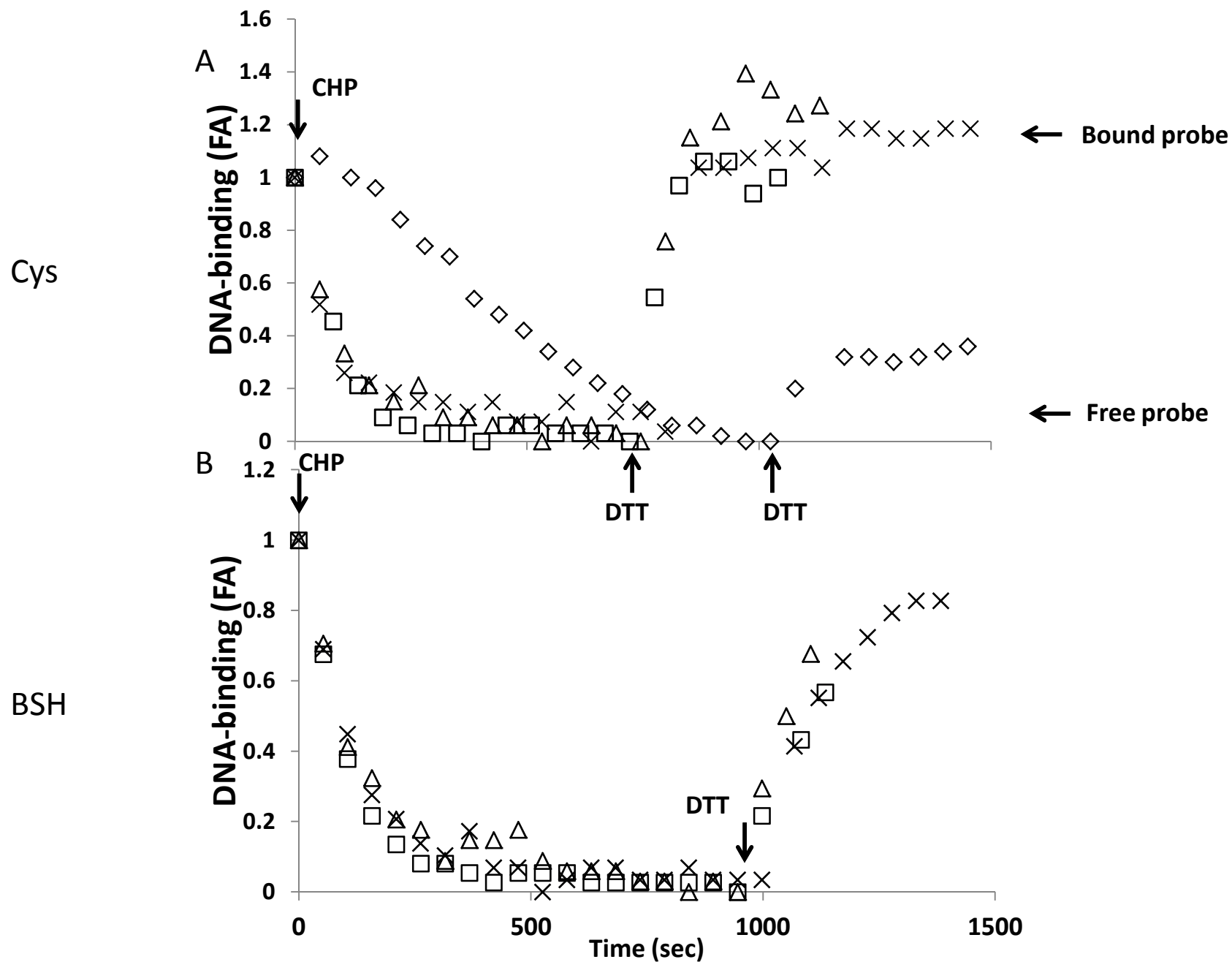
Fig. SI 1. . Inactivation of OhrR (□), scOhrR WT-WT (△) or WT-C15S scOhrR (✕) in the presence of 0.5 mM L-Cys (A) or BSH (B). As a control, the comparatively slow inactivation of OhrR in the absence of thiols is also shown (◇).

Fig. S2: *S*-bacillithiolated BrxB C54A does not transfer BSH to OhrR.

	M	OhrR-SSB	BrxB C54A-SSB	OhrR-SSB + BSH	OhrR-SSB + BrxB C54A	OhrR + BrxB C54A-SSB	BrxB+ BSH	

20 kDa →   ← BrxB-SSB
                          ← OhrR-SSB

     1   2   3   4 5 6

Table S1: MetE-SSB reduction by BrxA and BrxB in vitro (SI to MetE-SSB peptide informations to Fig. 5)

Sequence	Prob	SEQUEST XCorr	SEQUEST ΔCn	NTT	Modifications	Observed	Actual Mass	Charge	ΔAMU	ΔPPM	TIC	Start	Stop	Spectrum ID
MetE-SSB control Replicate-1														
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.1836	0.7028	2	~ (+396)	944.7602	2831.2588	3	0.003419	1.207	14,591.20	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.12392.12392.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.0592	0.7896	2	~ (+396)	944.7584	2831.2533	3	-0.002075	-0.7327	26,578.30	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.12343.12343.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.2177	0.6941	2	~ (+396)	944.7583	2831.2531	3	-0.002258	-0.7974	27,220.40	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.12306.12306.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9997	0.7969	2	~ (+396)	944.7592	2831.2556	3	0.0003057	0.1079	13,520.70	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.12267.12267.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.0461	0.6715	2	~ (+396)	944.7579	2831.2520	3	-0.003356	-1.185	6,669.91	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.11394.11394.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.5867	0.7053	2	~ (+396)	944.7578	2831.2514	3	-0.003906	-1.379	7,123.97	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.11338.11338.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	3.5058	0.5981	2	~ (+396)	944.7575	2831.2507	3	-0.004638	-1.638	8,693.21	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.11184.11184.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.3561	0.6894	2	~ (+396)	944.7612	2831.2619	3	0.006531	2.306	11,118.70	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.11068.11068.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.5656	0.6957	2	~ (+396)	944.7571	2831.2496	3	-0.005737	-2.026	8,588.09	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.11034.11034.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.0674	0.7613	2	~ (+396)	944.7601	2831.2584	3	0.003052	1.077	11,691.60	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10990.10990.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.5114	0.7231	2	~ (+396)	944.7550	2831.2432	3	-0.01215	-4.288	12,948.00	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10884.10884.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9779	0.6684	2	~ (+396)	944.7634	2831.2685	3	0.01312	4.633	13,677.00	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10845.10845.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.8058	0.7143	2	~ (+396)	944.7588	2831.2547	3	-0.0006103	-0.2155	12,763.80	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10802.10802.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.0123	0.7767	2	~ (+396)	944.7579	2831.2520	3	-0.003356	-1.185	11,207.90	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10742.10742.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.0021	0.7254	2	~ (+396)	944.7594	2831.2564	3	0.001038	0.3664	17,197.90	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10660.10660.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.1924	0.6948	2	~ (+396)	944.7564	2831.2474	3	-0.007934	-2.801	16,668.40	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10619.10619.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.1576	0.7643	2	~ (+396)	944.7605	2831.2597	3	0.004334	1.53	17,913.90	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10576.10576.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.2905	0.7977	2	~ (+396)	944.7609	2831.2608	3	0.005433	1.918	21,582.60	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10496.10496.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.7834	0.6853	2	~ (+396)	944.7557	2831.2452	3	-0.01013	-3.577	19,462.80	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10456.10456.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.5139	0.6994	2	~ (+396)	944.7586	2831.2540	3	-0.001342	-0.4739	16,986.40	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10384.10384.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9454	0.7078	2	~ (+396)	944.7587	2831.2544	3	-0.0009763	-0.3447	28,884.20	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10344.10344.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9607	0.6636	2	~ (+396)	944.7545	2831.2417	3	-0.01361	-4.805	27,961.80	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10242.10242.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9153	0.7267	2	~ (+396)	944.7619	2831.2639	3	0.008546	3.017	31,832.80	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10203.10203.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.3433	0.7273	2	~ (+396)	944.7619	2831.2639	3	0.008546	3.017	33,131.10	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10163.10163.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.0397	0.6821	2	~ (+396)	944.7561	2831.2465	3	-0.008849	-3.124	40,008.80	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10120.10120.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.1553	0.7324	2	~ (+396)	944.7601	2831.2584	3	0.003052	1.077	39,504.60	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.10048.10048.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9204	0.7729	2	~ (+396)	944.7604	2831.2595	3	0.004151	1.466	50,752.70	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.09983.09983.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.2939	0.6514	2	~ (+396)	944.7551	2831.2436	3	-0.01178	-4.159	55,685.70	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.09942.09942.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.2380	0.7827	2	~ (+396)	944.7574	2831.2503	3	-0.005004	-1.767	77,989.70	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.09871.09871.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.0692	0.7421	2	~ (+396)	944.7584	2831.2534	3	-0.001891	-0.6678	91,589.50	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.09826.09826.3.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	100%	4.0605	0.7869	2	Ox (+16), ~ (+396)	1424.6305	2847.2464	2	-0.003813	-1.339	14,667.10	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.08868.08868.2.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	5.3098	0.7701	2	Ox (+16), ~ (+396)	950.0927	2847.2561	3	0.005879	2.064	1.12E+07	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.08854.08854.3.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	5.9281	0.7620	2	Ox (+16), ~ (+396)	950.0905	2847.2497	3	-0.0005303	-0.1862	458115	702	723	130610_V3_P5_KB_MetE_SSB_co_2_2.08802.08802.3.dta
(R)cVRPPVIYGDVEFIEPMTVK(D)	96%	4.1406	0.6886	2	~ (+396)	896.7585	2687.2538	3	0.0002747	0.1022	106475	520	539	130610_V3_P5_KB_MetE_SSB_co_2_2.08379.08379.3.dta
(R)cVRPPVIYGDVEFIEPMTVK(D)	96%	5.0547	0.6595	2	~ (+396)	896.7588	2687.2547	3	0.00119	0.4426	382327	520	539	130610_V3_P5_KB_MetE_SSB_co_2_2.08312.08312.3.dta
(R)cVRPPVIYGDVEFIEPmTVK(D)	96%	3.8629	0.6606	2	~ (+396), Ox (+16)	902.0899	2703.2479	3	-0.0005613	-0.2076	366930	520	539	130610_V3_P5_KB_MetE_SSB_co_2_2.07605.07605.3.dta
(R)FWVNPDcGLK(T)	98%	2.4407	0.6298	2	~ (+396)	787.8284	1573.6422	2	-0.0008463	-0.5375	627771	724	733	130610_V3_P5_KB_MetE_SSB_co_2_2.06505.06505.2.dta
(R)FWVNPDcGLK(T)	99%	2.3836	0.7030	2	~ (+396)	787.8287	1573.6429	2	-0.0001133	-0.07196	1579570	724	733	130610_V3_P5_KB_MetE_SSB_co_2_2.06442.06442.2.dta
(R)FWVNPDcGLK(T)	98%	2.2077	0.6300	2	~ (+396)	787.8278	1573.6411	2	-0.001944	-1.235	51,795.60	724	733	130610_V3_P5_KB_MetE_SSB_co_2_2.06047.06047.2.dta
MetE-SSB control Replicate-2														
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.7813	0.7129	2	~ (+396)	944.7587	2831.2544	3	-0.0009763	-0.3447	14,522.70	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.12192.12192.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.4939	0.7352	2	~ (+396)	944.7592	2831.2558	3	0.0004887	0.1725	15,950.40	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.12138.12138.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.2838	0.7359	2	~ (+396)	944.7582	2831.2527	3	-0.002624	-0.9266	6,764.73	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.12101.12101.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	3.3597	0.6547	2	~ (+396)	944.7565	2831.2478	3	-0.007568	-2.672	7,946.10	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.10964.10964.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9609	0.7191	2	~ (+396)	944.7551	2831.2434	3	-0.01196	-4.224	10,002.50	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.10737.10737.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.6705	0.7493	2	~ (+396)	944.7599	2831.2580	3	0.002686	0.9482	12,010.30	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.10641.10641.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.6133	0.7155	2	~ (+396)	944.7617	2831.2633	3	0.007996	2.823	12,158.20	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.10531.10531.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9583	0.6872	2	~ (+396)	944.7581	2831.2525	3	-0.002807	-0.9912	15,069.60	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.10241.10241.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.4027	0.7612	2	~ (+396)	944.7607	2831.2604	3	0.005067	1.789	34,427.50	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.10037.10037.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.0872	0.7923	2	~ (+396)	944.7558	2831.2456	3	-0.009765	-3.448	39,167.30	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09888.09888.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.4802	0.7841	2	~ (+396)	944.7574	2831.2503	3	-0.005004	-1.767	50,801.60	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09819.09819.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.3476	0.7687	2	~ (+396)	944.7585	2831.2536	3	-0.001708	-0.6032	68,761.10	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09734.09734.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.3652	0.7367	2	~ (+396)	944.7605	2831.2597	3	0.004334	1.53	88,926.80	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09692.09692.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.4537	0.7465	2	~ (+396)	944.7596	2831.2571	3	0.001771	0.6252	141096	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09589.09589.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.1091	0.7170	2	~ (+396)	944.7593	2831.2560	3	0.0006717	0.2372	396402	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09520.09520.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.2440	0.7625	2	~ (+396)	944.7604	2831.2595	3	0.004151	1.466	3445940	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09457.09457.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	99%	4.6707	0.6470	2	~ (+396)	1416.6361	2831.2577	2	0.002333	0.8236	206331	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09436.09436.2.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9272	0.7971	2	~ (+396)	944.7603	2831.2589	3	0.003602	1.272	101589	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09403.09403.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.1418	0.7355	2	~ (+396)	944.7595	2831.2566	3	0.001221	0.431	132187	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09341.09341.3.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	3.7532	0.5885	2	Ox (+16), ~ (+396)	950.0922	2847.2548	3	0.004597	1.614	42,864.50	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09304.09304.3.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	4.1360	0.6756	2	Ox (+16), ~ (+396)	950.0927	2847.2563	3	0.006062	2.128	47,558.80	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09242.09242.3.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	5.0509	0.7564	2	Ox (+16), ~ (+396)	950.0887	2847.2444	3	-0.00584	-2.05	84,118.20	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09175.09175.3.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	4.8773	0.7392	2	Ox (+16), ~ (+396)	950.0904	2847.2494	3	-0.0008963	-0.3147	73,714.60	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.09066.09066.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.9155	0.7641	2	~ (+396)	944.7604	2831.2593	3	0.003968	1.401	65,018.50	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.08921.08921.3.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	5.0802	0.7408	2	Ox (+16), ~ (+396)	950.0914	2847.2525	3	0.002217	0.7783	1049810	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.08890.08890.3.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	5.0467	0.8003	2	Ox (+16), ~ (+396)	950.0914	2847.2525	3	0.002217	0.7783	2279640	702	723	130610_V3_P5_KB_MetE_SSB_co_1_1.08828.08828.3.dta
(R)cVRPPVIYGDVEFIEPMTVK(D)	96%	4.1941	0.7213	2	~ (+396)	896.7588	2687.2545	3	0.001007	0.3745	125845	520	539	130610_V3_P5_KB_MetE_SSB_co_1_1.08392.08392.3.dta
(R)cVRPPVIYGDVEFIEPMTVK(D)	96%	4.9455	0.6422	2	~ (+396)	896.7572	2687.2498	3	-0.003754	-1.397	155388	520	539	130610_V3_P5_KB_MetE_SSB_co_1_1.08338.08338.3.dta
(R)cVRPPVIYGDVEFIEPmTVK(D)	96%	3.5225	0.6580	2	~ (+396), Ox (+16)	902.0902	2703.2488	3	0.0003547	0.1312	224515	520	539	130610_V3_P5_KB_MetE_SSB_co_1_1.07664.07664.3.dta
(R)FWVNPDcGLK(T)	98%	2.1774	0.6548	2	~ (+396)	787.8275	1573.6405	2	-0.002555	-1.623	45,024.10	724	733	130610_V3_P5_KB_MetE_SSB_co_1_1.06135.06135.2.dta
(R)FWVNPDcGLK(T)	98%	2.1758	0.6774	2	~ (+396)	787.8284	1573.6422	2	-0.0008463	-0.5375	463282	724	733	130610_V3_P5_KB_MetE_SSB_co_1_1.06504.06504.2.dta
(R)FWVNPDcGLK(T)	98%	2.4610	0.6334	2	~ (+396)	787.8289	1573.6432	2	0.0001307	0.083	1461860	724	733	130610_V3_P5_KB_MetE_SSB_co_1_1.06566.06566.2.dta
MetE-SSB + BrxB-Replicate-1														
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	6.0773	0.7597	2	~ (+396)	944.7606	2831.2600	3	0.0047	1.659	336186	702	723	130610_V3_P5_KB_MetE_SSB_BrxB_2_10.10784.10784.3.dta
MetE-SSB + BrxB-Replicate-2														
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.3880	0.7508	2	~ (+396)	944.7593	2831.2560	3	0.0006717	0.2372	262115	702	723	130610_V3_P5_KB_MetE_SSB_BrxB_1_9.09550.09550.3.dta
(R)cVRPPVIYGDVEFIEPMTVK(D)	96%	4.0088	0.7085	2	~ (+396)	896.7578	2687.2514	3	-0.002106	-0.7835	120023	520	539	130610_V3_P5_KB_MetE_SSB_BrxB_1_9.08524.08524.3.dta
(R)FWVNPDcGLK(T)	97%	2.2891	0.5738	2	~ (+396)	787.8287	1573.6428	2	-0.0002353	-0.1494	129435	724	733	130610_V3_P5_KB_MetE_SSB_BrxB_1_9.06660.06660.2.dta
MetE-SSB + BrxA-Replicate-1														
(R)FWVNPDcGLK(T)	98%	2.1824	0.6655	2	~ (+396)	787.8289	1573.6432	2	0.0001307	0.083	201913	724	733	130610_V3_P5_KB_MetE_SSB_BrxA_2_8.06904.06904.2.dta
(R)cVRPPVIYGDVEFIEPMTVK(D)	96%	5.0063	0.6117	2	~ (+396)	896.7567	2687.2483	3	-0.005218	-1.941	94,112.40	520	539	130610_V3_P5_KB_MetE_SSB_BrxA_2_8.08691.08691.3.dta
(R)cVRPPVIYGDVEFIEPMTVKDTVYAQSLTSK(H)	99%	3.7219	0.6908	2	~ (+396)	971.2198	3880.8500	4	0.003614	0.9309	614560	520	550	130610_V3_P5_KB_MetE_SSB_BrxA_2_8.08920.08920.4.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	5.1725	0.8070	2	Ox (+16), ~ (+396)	950.0901	2847.2484	3	-0.001811	-0.6359	77,108.30	702	723	130610_V3_P5_KB_MetE_SSB_BrxA_2_8.09192.09192.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	4.4482	0.7399	2	~ (+396)	944.7596	2831.2571	3	0.001771	0.6252	188968	702	723	130610_V3_P5_KB_MetE_SSB_BrxA_2_8.09687.09687.3.dta
MetE-SSB + BrxA-Replicate-2														
(R)FWVNPDcGLK(T)	99%	2.5236	0.6809	2	~ (+396)	787.8281	1573.6416	2	-0.001456	-0.9248	123356	724	733	130610_V3_P5_KB_MetE_SSB_BrxA_1_7.07303.07303.2.dta
(R)FWVNPDcGLK(T)	98%	2.2705	0.6444	2	~ (+396)	787.8297	1573.6448	2	0.001718	1.091	122362	724	733	130610_V3_P5_KB_MetE_SSB_BrxA_1_7.07242.07242.2.dta
(R)cVRPPVIYGDVEFIEPMTVK(D)	96%	4.0816	0.5925	2	~ (+396)	896.7578	2687.2516	3	-0.001923	-0.7154	67,739.60	520	539	130610_V3_P5_KB_MetE_SSB_BrxA_1_7.09229.09229.3.dta
(R)cVRPPVIYGDVEFIEPMTVK(D)	96%	4.9484	0.6823	2	~ (+396)	896.7560	2687.2463	3	-0.007233	-2.691	92,183.30	520	539	130610_V3_P5_KB_MetE_SSB_BrxA_1_7.09173.09173.3.dta
(R)VPSTEEMYNIIVDALAVcPTDR(F)	96%	5.0634	0.7676	2	~ (+396)	944.7595	2831.2567	3	0.001404	0.4956	793243	702	723	130610_V3_P5_KB_MetE_SSB_BrxA_1_7.10280.10280.3.dta
(R)VPSTEEmYNIIVDALAVcPTDR(F)	96%	5.4257	0.7453	2	Ox (+16), ~ (+396)	950.0893	2847.2461	3	-0.004192	-1.472	180550	702	723	130610_V3_P5_KB_MetE_SSB_BrxA_1_7.09709.09709.3.dta

Peptide sequence	Spectral counts				Spectral counts				Spectral counts			
MetE-Cys-peptides-SSB	MetE-co1	MetE-co2	MetE-Av	SD	MetE+BrxA-1	MetE+BrxA-2	MetE+BrxA-Av	SD	MetE+BrxB-1	MetE+BrxB-2	MetE+BrxB-Av	SD
(R)FWVNPDc730(BSH)GLK(T)	3.0	3.0	3.0	0.0	1.0	2.0	1.5	0.7	0.0	1.0	0.5	0.7
(R)c520(BSH)VRPPVIYGDVEFIEPmTVK(D)	3.0	3.0	3.0	0.0	2.0	2.0	2.0	0.0	0.0	1.0	0.5	0.7
(R)VPSTEEMYNIIVDALAVc719(BSH)PTDR(F)	33.0	28.0	30.5	3.5	2.0	2.0	2.0	0.0	1.0	1.0	1.0	0.0

Legend to Table S1: Detected MetE-SSB sites by Orbitrap LC-MS/MS analysis before and after reduction by BrxA and BrxB in an in vitro Brx-assay. His-tagged MetE was expressed and purified from E. coli cells, in vitro bacillithiolated using BSSB and purified as described in the Methods section. MetE-SSB was reduced by purified BrxA and BrxB for 1 hour. The MetE-SSB control reaction and MetE-SSB that was treated with BrxA and BrxB were separated by SDS-PAGE. The MetE-SSB bands and the BrxA and BrxB bands were tryptically in gel-digested. The resulting MetE-SSB peptides were analyzed using LTQ Orbitrap Velos LC-MS/MS analysis as described in the Methods section (Chi et al., 2011). The Scaffold search results are shown and the Table includes the Xcorr, deltaCn scores, m/z of the precursor ions, neutral molecular masses of the peptides, peptide mass deviations (delta ppm) of all detected bacillithiolated peptides in MetE. The CID MS/MS spectrum of the modified Cys peptides are shown, with t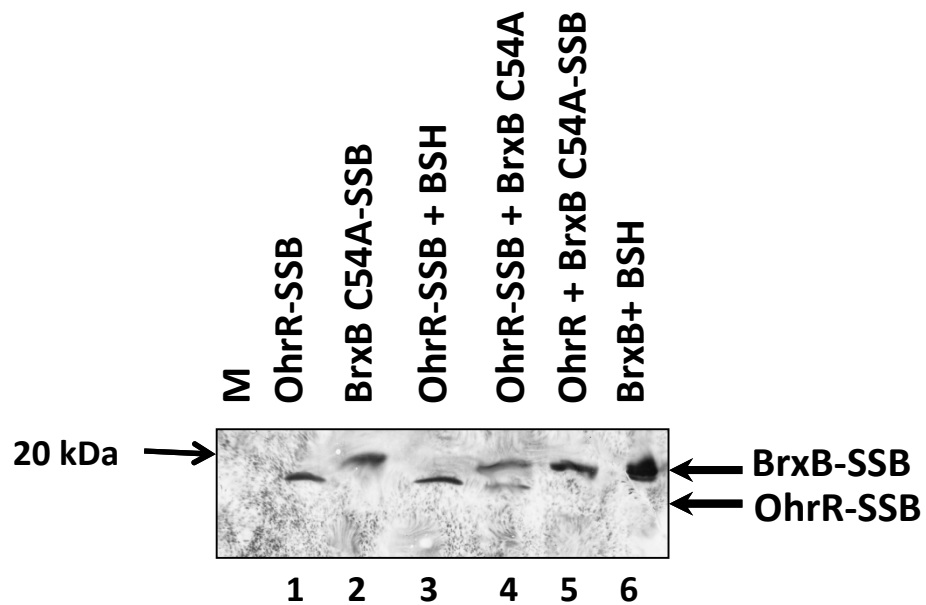he b and y ion series labeled in red and blue, respectively. Two replicates each for the Brx assay using MetE-SSB were performed and the averages and SEM are shown for the bacillithiolated Cys peptides of MetE before and after Brx reduction in the Table below that is used for the Figure 5.

Table S2: BrxA-SSB peptides after in vitro MetE-SSB reduction by BrxA (SI to BrxA-SSB peptide informations to Fig. 5)

Sequence	Prob	SEQUEST XCorr	SEQUEST ΔCn	NTT	Modifications	Observed	Actual Mass	Charge	ΔAMU	ΔPPM	TIC	Start	Stop	Spectrum ID
BrxA Cys53-SSBpeptide Replicate-1														
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.3439	0.6705	2	~ (+396), IAM (+57)	1,222.5602	2,443.1058	2	0.002811	1.15	241284	41	61	130610_V3_P5_KB_BrxA_1_3.07377.07377.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.0093	0.6601	2	~ (+396), IAM (+57)	611.7833	2,443.1042	4	0.001199	0.4907	1368120	41	61	130610_V3_P5_KB_BrxA_1_3.07419.07419.4.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.4746	0.6879	2	~ (+396), IAM (+57)	1,222.5591	2,443.1036	2	0.0006144	0.2514	94,579.60	41	61	130610_V3_P5_KB_BrxA_1_3.07442.07442.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.6582	0.6814	2	~ (+396), IAM (+57)	1,222.5610	2,443.1075	2	0.00452	1.85	64,280.30	41	61	130610_V3_P5_KB_BrxA_1_3.07509.07509.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.5244	0.6873	2	~ (+396), IAM (+57)	1,222.5593	2,443.1041	2	0.001102	0.451	23,773.80	41	61	130610_V3_P5_KB_BrxA_1_3.07601.07601.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.6067	0.5882	3	~ (+396), IAM (+57)	815.3757	2,443.1052	3	0.002188	0.8954	969805	41	61	130610_V3_P5_KB_BrxA_1_3.07670.07670.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.3809	0.5930	2	~ (+396), IAM (+57)	815.3754	2,443.1043	3	0.001273	0.521	861204	41	61	130610_V3_P5_KB_BrxA_1_3.07733.07733.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9883	0.6012	3	~ (+396), IAM (+57)	815.3742	2,443.1008	3	-0.002206	-0.9024	881644	41	61	130610_V3_P5_KB_BrxA_1_3.07862.07862.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9292	0.6176	2	~ (+396), IAM (+57)	815.3759	2,443.1059	3	0.002921	1.195	393074	41	61	130610_V3_P5_KB_BrxA_1_3.08238.08238.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	5.1324	0.6490	2	~ (+396), IAM (+57)	815.3751	2,443.1034	3	0.0003574	0.1462	325125	41	61	130610_V3_P5_KB_BrxA_1_3.08427.08427.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.6976	0.5816	2	~ (+396), IAM (+57)	815.3749	2,443.1028	3	-0.0001916	-0.0784	276282	41	61	130610_V3_P5_KB_BrxA_1_3.08492.08492.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.1542	0.6129	2	~ (+396), IAM (+57)	815.3755	2,443.1046	3	0.001639	0.6708	290393	41	61	130610_V3_P5_KB_BrxA_1_3.08595.08595.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.1945	0.6068	2	~ (+396), IAM (+57)	815.3754	2,443.1043	3	0.001273	0.521	315465	41	61	130610_V3_P5_KB_BrxA_1_3.08659.08659.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0174	0.5937	2	~ (+396), IAM (+57)	815.3751	2,443.1034	3	0.0003574	0.1462	366688	41	61	130610_V3_P5_KB_BrxA_1_3.08721.08721.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0835	0.5977	2	~ (+396), IAM (+57)	815.3754	2,443.1045	3	0.001456	0.5959	495890	41	61	130610_V3_P5_KB_BrxA_1_3.08973.08973.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.7850	0.6616	2	~ (+396), IAM (+57)	815.3751	2,443.1043	3	0.0005404	0.2211	502974	41	61	130610_V3_P5_KB_BrxA_1_3.09099.09099.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	95%	3.8743	0.4706	2	~ (+396), IAM (+57)	815.3770	2,443.1090	3	0.006033	2.469	548015	41	61	130610_V3_P5_KB_BrxA_1_3.09162.09162.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0708	0.6076	2	~ (+396), IAM (+57)	815.3760	2,443.1063	3	0.003287	1.345	381624	41	61	130610_V3_P5_KB_BrxA_1_3.09607.09607.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9460	0.6302	2	~ (+396), IAM (+57)	815.3755	2,443.1048	3	0.001822	0.7456	361430	41	61	130610_V3_P5_KB_BrxA_1_3.09669.09669.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.3289	0.6000	2	~ (+396), IAM (+57)	1,222.5636	2,443.1126	2	0.009647	3.947	11,465.60	41	61	130610_V3_P5_KB_BrxA_1_3.09716.09716.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.7169	0.6441	2	~ (+396), IAM (+57)	815.3760	2,443.1061	3	0.003104	1.27	400496	41	61	130610_V3_P5_KB_BrxA_1_3.09733.09733.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0753	0.6044	2	~ (+396), IAM (+57)	815.3756	2,443.1050	3	0.002005	0.8205	387159	41	61	130610_V3_P5_KB_BrxA_1_3.09793.09793.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0443	0.5498	2	~ (+396), IAM (+57)	815.3752	2,443.1037	3	0.0007234	0.296	360887	41	61	130610_V3_P5_KB_BrxA_1_3.09856.09856.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.9546	0.4937	2	~ (+396), IAM (+57)	815.3755	2,443.1046	3	0.001639	0.6708	385756	41	61	130610_V3_P5_KB_BrxA_1_3.10024.10024.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.6452	0.6249	2	~ (+396), IAM (+57)	815.3756	2,443.1050	3	0.002005	0.8205	362143	41	61	130610_V3_P5_KB_BrxA_1_3.10076.10076.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	95%	3.5188	0.4936	2	~ (+396), IAM (+57)	815.3750	2,443.1032	3	0.0001744	0.07135	301162	41	61	130610_V3_P5_KB_BrxA_1_3.10294.10294.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.5350	0.5500	2	~ (+396), IAM (+57)	815.3753	2,443.1041	3	0.00109	0.4461	213113	41	61	130610_V3_P5_KB_BrxA_1_3.10419.10419.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.5287	0.6572	2	~ (+396), IAM (+57)	1,222.5542	2,443.0938	2	-0.009152	-3.744	6,865.67	41	61	130610_V3_P5_KB_BrxA_1_3.10546.10546.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9731	0.5564	2	~ (+396), IAM (+57)	815.3749	2,443.1030	3	-8.606E-06	-0.003521	157244	41	61	130610_V3_P5_KB_BrxA_1_3.10636.10636.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.6843	0.6101	2	~ (+396), IAM (+57)	815.3755	2,443.1048	3	0.001822	0.7456	140262	41	61	130610_V3_P5_KB_BrxA_1_3.10720.10720.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.8956	0.5092	2	~ (+396), IAM (+57)	815.3748	2,443.1024	3	-0.0005576	-0.2281	107074	41	61	130610_V3_P5_KB_BrxA_1_3.10877.10877.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.5205	0.6364	2	~ (+396), IAM (+57)	815.3748	2,443.1024	3	-0.0005576	-0.2281	84,877.60	41	61	130610_V3_P5_KB_BrxA_1_3.10993.10993.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0513	0.6006	2	~ (+396), IAM (+57)	815.3751	2,443.1034	3	0.0003574	0.1462	83,911.10	41	61	130610_V3_P5_KB_BrxA_1_3.11029.11029.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0520	0.6034	2	~ (+396), IAM (+57)	815.3749	2,443.1028	3	-0.0001916	-0.0784	67,207.40	41	61	130610_V3_P5_KB_BrxA_1_3.11148.11148.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.8423	0.5685	2	~ (+396), IAM (+57)	815.3752	2,443.1039	3	0.0009064	0.3708	66,001.70	41	61	130610_V3_P5_KB_BrxA_1_3.11190.11190.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	4.0039	0.5066	2	~ (+396), IAM (+57)	815.3751	2,443.1034	3	0.0003574	0.1462	39,954.80	41	61	130610_V3_P5_KB_BrxA_1_3.11383.11383.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.8891	0.6026	2	~ (+396), IAM (+57)	815.3752	2,443.1037	3	0.0007234	0.296	46,409.80	41	61	130610_V3_P5_KB_BrxA_1_3.11467.11467.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.3444	0.5927	2	~ (+396), IAM (+57)	815.3750	2,443.1032	3	0.0001744	0.07135	39,217.70	41	61	130610_V3_P5_KB_BrxA_1_3.11575.11575.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.8041	0.6216	2	~ (+396), IAM (+57)	815.3748	2,443.1026	3	-0.0003746	-0.1533	34,236.80	41	61	130610_V3_P5_KB_BrxA_1_3.11619.11619.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.7241	0.6553	2	~ (+396), IAM (+57)	815.3753	2,443.1041	3	0.00109	0.4461	25,763.10	41	61	130610_V3_P5_KB_BrxA_1_3.11654.11654.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9120	0.6346	2	~ (+396), IAM (+57)	815.3747	2,443.1023	3	-0.0007416	-0.3034	24,972.80	41	61	130610_V3_P5_KB_BrxA_1_3.11759.11759.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.2106	0.6055	2	~ (+396), IAM (+57)	815.3754	2,443.1043	3	0.001273	0.521	21,838.30	41	61	130610_V3_P5_KB_BrxA_1_3.11829.11829.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.1453	0.6061	2	~ (+396), IAM (+57)	815.3754	2,443.1043	3	0.001273	0.521	18,615.70	41	61	130610_V3_P5_KB_BrxA_1_3.11891.11891.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.1762	0.6342	2	~ (+396), IAM (+57)	815.3755	2,443.1046	3	0.001639	0.6708	100723	41	61	130610_V3_P5_KB_BrxA_1_3.12570.12570.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.9277	0.5359	2	~ (+396), IAM (+57)	815.3749	2,443.1028	3	-0.0001916	-0.0784	131345	41	61	130610_V3_P5_KB_BrxA_1_3.12627.12627.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.3097	0.5720	2	~ (+396), IAM (+57)	815.3749	2,443.1028	3	-0.0001916	-0.0784	83,757.60	41	61	130610_V3_P5_KB_BrxA_1_3.12679.12679.3.dta
BrxA Cys53-SSBpeptide Replicate-2														
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.8498	0.5580	2	~ (+396), IAM (+57)	815.3748	2,443.1024	3	-0.0005576	-0.2281	859066	41	61	130610_V3_P5_KB_BrxA_2_4.07657.07657.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.2945	0.6787	2	~ (+396), IAM (+57)	1,222.5602	2,443.1058	2	0.002811	1.15	180191	41	61	130610_V3_P5_KB_BrxA_2_4.07681.07681.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.9780	0.5462	2	~ (+396), IAM (+57)	815.3777	2,443.1112	3	0.008231	3.368	3.08E+07	41	61	130610_V3_P5_KB_BrxA_2_4.07720.07720.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.6019	0.6776	2	~ (+396), IAM (+57)	1,222.5599	2,443.1053	2	0.002323	0.9506	334056	41	61	130610_V3_P5_KB_BrxA_2_4.07741.07741.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.8530	0.5517	2	~ (+396), IAM (+57)	815.3766	2,443.1079	3	0.004935	2.019	8700520	41	61	130610_V3_P5_KB_BrxA_2_4.07783.07783.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.2054	0.5820	2	~ (+396), IAM (+57)	611.7833	2,443.1040	4	0.0009554	0.3909	492841	41	61	130610_V3_P5_KB_BrxA_2_4.07786.07786.4.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.3958	0.7172	2	~ (+396), IAM (+57)	1,222.5598	2,443.1051	2	0.002079	0.8508	90,325.70	41	61	130610_V3_P5_KB_BrxA_2_4.07808.07808.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.7661	0.6333	2	~ (+396), IAM (+57)	815.3767	2,443.1083	3	0.005301	2.169	5454350	41	61	130610_V3_P5_KB_BrxA_2_4.07846.07846.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.1478	0.6044	2	~ (+396), IAM (+57)	1,222.5603	2,443.1061	2	0.003055	1.25	65,303.30	41	61	130610_V3_P5_KB_BrxA_2_4.07874.07874.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.7299	0.7332	2	~ (+396), IAM (+57)	1,222.5588	2,443.1031	2	0.0001264	0.05171	47,159.80	41	61	130610_V3_P5_KB_BrxA_2_4.07938.07938.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9094	0.6504	2	~ (+396), IAM (+57)	815.3763	2,443.1070	3	0.004019	1.645	2631210	41	61	130610_V3_P5_KB_BrxA_2_4.07973.07973.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.4741	0.6674	2	~ (+396), IAM (+57)	1,222.5612	2,443.1078	2	0.004764	1.949	39,725.00	41	61	130610_V3_P5_KB_BrxA_2_4.08004.08004.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	5.1103	0.7374	2	~ (+396), IAM (+57)	1,222.5594	2,443.1043	2	0.001346	0.5509	22,234.70	41	61	130610_V3_P5_KB_BrxA_2_4.08072.08072.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	95%	3.4385	0.4919	2	~ (+396), IAM (+57)	815.3757	2,443.1052	3	0.002188	0.8954	1937220	41	61	130610_V3_P5_KB_BrxA_2_4.08099.08099.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.6439	0.7077	2	~ (+396), IAM (+57)	1,222.5601	2,443.1056	2	0.002567	1.05	48,769.50	41	61	130610_V3_P5_KB_BrxA_2_4.08135.08135.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.4069	0.6498	2	~ (+396), IAM (+57)	1,222.5586	2,443.1026	2	-0.0003616	-0.148	34,527.20	41	61	130610_V3_P5_KB_BrxA_2_4.08261.08261.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.2165	0.7207	2	~ (+396), IAM (+57)	1,222.5602	2,443.1058	2	0.002811	1.15	19,333.20	41	61	130610_V3_P5_KB_BrxA_2_4.08325.08325.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.0795	0.5503	2	~ (+396), IAM (+57)	1,222.5588	2,443.1031	2	0.0001264	0.05171	21,067.60	41	61	130610_V3_P5_KB_BrxA_2_4.08385.08385.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.3213	0.6148	2	~ (+396), IAM (+57)	1,222.5553	2,443.0960	2	-0.006954	-2.845	19,281.50	41	61	130610_V3_P5_KB_BrxA_2_4.08452.08452.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.7171	0.6486	2	~ (+396), IAM (+57)	1,222.5532	2,443.0919	2	-0.0111	-4.543	17,273.40	41	61	130610_V3_P5_KB_BrxA_2_4.08536.08536.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.8117	0.6997	2	~ (+396), IAM (+57)	815.3752	2,443.1039	3	0.0009064	0.3708	1273030	41	61	130610_V3_P5_KB_BrxA_2_4.08540.08540.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.5784	0.5943	2	~ (+396), IAM (+57)	815.3762	2,443.1068	3	0.003836	1.57	1058740	41	61	130610_V3_P5_KB_BrxA_2_4.08603.08603.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.7328	0.6724	2	~ (+396), IAM (+57)	1,222.5608	2,443.1070	2	0.004032	1.65	18,903.80	41	61	130610_V3_P5_KB_BrxA_2_4.08621.08621.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	3.7702	0.6026	2	~ (+396), IAM (+57)	815.3754	2,443.1045	3	0.001456	0.5959	1286750	41	61	130610_V3_P5_KB_BrxA_2_4.08666.08666.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.4738	0.6671	2	~ (+396), IAM (+57)	1,222.5579	2,443.1012	2	-0.001827	-0.7474	21,503.90	41	61	130610_V3_P5_KB_BrxA_2_4.08703.08703.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.4346	0.6472	2	~ (+396), IAM (+57)	1,222.5598	2,443.1051	2	0.002079	0.8508	17,312.40	41	61	130610_V3_P5_KB_BrxA_2_4.08889.08889.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.1317	0.6132	2	~ (+396), IAM (+57)	815.3751	2,443.1035	3	0.0005404	0.2211	1040080	41	61	130610_V3_P5_KB_BrxA_2_4.08981.08981.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.6012	0.7035	2	~ (+396), IAM (+57)	1,222.5581	2,443.1017	2	-0.001339	-0.5477	20,096.10	41	61	130610_V3_P5_KB_BrxA_2_4.09057.09057.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.4770	0.6110	2	~ (+396), IAM (+57)	1,222.5575	2,443.1004	2	-0.00256	-1.047	17,313.90	41	61	130610_V3_P5_KB_BrxA_2_4.09137.09137.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.8072	0.6444	2	~ (+396), IAM (+57)	815.3754	2,443.1045	3	0.001456	0.5959	955352	41	61	130610_V3_P5_KB_BrxA_2_4.09149.09149.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.3862	0.6784	2	~ (+396), IAM (+57)	1,222.5632	2,443.1119	2	0.008915	3.648	20,461.70	41	61	130610_V3_P5_KB_BrxA_2_4.09207.09207.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.2250	0.6335	2	~ (+396), IAM (+57)	1,222.5585	2,443.1024	2	-0.0006066	-0.2482	21,310.80	41	61	130610_V3_P5_KB_BrxA_2_4.09262.09262.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.7327	0.6187	2	~ (+396), IAM (+57)	815.3751	2,443.1035	3	0.0005404	0.2211	1183100	41	61	130610_V3_P5_KB_BrxA_2_4.09276.09276.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9727	0.6068	2	~ (+396), IAM (+57)	815.3755	2,443.1046	3	0.001639	0.6708	1192320	41	61	130610_V3_P5_KB_BrxA_2_4.09401.09401.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.3419	0.6024	2	~ (+396), IAM (+57)	815.3752	2,443.1037	3	0.0007234	0.296	1177450	41	61	130610_V3_P5_KB_BrxA_2_4.09464.09464.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.1729	0.6521	2	~ (+396), IAM (+57)	815.3757	2,443.1054	3	0.002371	0.9702	1175490	41	61	130610_V3_P5_KB_BrxA_2_4.09526.09526.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.8730	0.5308	2	~ (+396), IAM (+57)	815.3779	2,443.1118	3	0.00878	3.592	1298480	41	61	130610_V3_P5_KB_BrxA_2_4.09592.09592.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	95%	4.5178	0.5667	2	~ (+396), IAM (+57)	815.3759	2,443.1057	3	0.002737	1.12	942410	41	61	130610_V3_P5_KB_BrxA_2_4.09779.09779.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.4129	0.6724	2	~ (+396), IAM (+57)	1,222.5632	2,443.1119	2	0.008915	3.648	24,132.50	41	61	130610_V3_P5_KB_BrxA_2_4.09881.09881.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.9040	0.5755	2	~ (+396), IAM (+57)	815.3757	2,443.1054	3	0.002371	0.9702	1052140	41	61	130610_V3_P5_KB_BrxA_2_4.09905.09905.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.9791	0.6442	2	~ (+396), IAM (+57)	611.7830	2,443.1030	4	-0.00002161	-0.00884	138546	41	61	130610_V3_P5_KB_BrxA_2_4.09931.09931.4.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.8523	0.6186	2	~ (+396), IAM (+57)	1,222.5602	2,443.1058	2	0.002811	1.15	21,358.30	41	61	130610_V3_P5_KB_BrxA_2_4.09958.09958.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.8988	0.6820	2	~ (+396), IAM (+57)	815.3759	2,443.1059	3	0.002921	1.195	1019020	41	61	130610_V3_P5_KB_BrxA_2_4.09969.09969.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.2036	0.7606	2	~ (+396), IAM (+57)	1,222.5553	2,443.0960	2	-0.006954	-2.845	18,340.20	41	61	130610_V3_P5_KB_BrxA_2_4.10133.10133.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.0258	0.6640	2	~ (+396), IAM (+57)	1,222.5642	2,443.1139	2	0.01087	4.447	23,963.10	41	61	130610_V3_P5_KB_BrxA_2_4.10188.10188.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.0448	0.5780	2	~ (+396), IAM (+57)	1,222.5565	2,443.0985	2	-0.004513	-1.846	19,755.50	41	61	130610_V3_P5_KB_BrxA_2_4.10300.10300.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	3.9801	0.6923	2	~ (+396), IAM (+57)	1,222.5619	2,443.1092	2	0.006229	2.549	12,180.50	41	61	130610_V3_P5_KB_BrxA_2_4.10373.10373.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.5208	0.6937	2	~ (+396), IAM (+57)	1,222.5546	2,443.0946	2	-0.008419	-3.444	13,653.80	41	61	130610_V3_P5_KB_BrxA_2_4.10427.10427.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.0078	0.6139	2	~ (+396), IAM (+57)	1,222.5618	2,443.1090	2	0.005985	2.449	22,465.40	41	61	130610_V3_P5_KB_BrxA_2_4.10516.10516.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.0893	0.6659	2	~ (+396), IAM (+57)	1,222.5701	2,443.1256	2	0.02259	9.241	22,187.40	41	61	130610_V3_P5_KB_BrxA_2_4.10564.10564.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.4008	0.5982	2	~ (+396), IAM (+57)	815.3756	2,443.1050	3	0.002005	0.8205	592521	41	61	130610_V3_P5_KB_BrxA_2_4.10642.10642.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.5736	0.6826	2	~ (+396), IAM (+57)	1,222.5553	2,443.0960	2	-0.006954	-2.845	12,596.50	41	61	130610_V3_P5_KB_BrxA_2_4.10670.10670.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.7696	0.6826	2	~ (+396), IAM (+57)	815.3762	2,443.1067	3	0.003653	1.495	553102	41	61	130610_V3_P5_KB_BrxA_2_4.10684.10684.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0368	0.6351	2	~ (+396), IAM (+57)	815.3746	2,443.1019	3	-0.001108	-0.4532	496621	41	61	130610_V3_P5_KB_BrxA_2_4.10725.10725.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.7836	0.5407	2	~ (+396), IAM (+57)	815.3755	2,443.1046	3	0.001639	0.6708	473452	41	61	130610_V3_P5_KB_BrxA_2_4.10808.10808.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9532	0.6496	2	~ (+396), IAM (+57)	815.3758	2,443.1056	3	0.002554	1.045	376538	41	61	130610_V3_P5_KB_BrxA_2_4.10892.10892.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.7736	0.6349	2	~ (+396), IAM (+57)	1,222.5610	2,443.1075	2	0.00452	1.85	13,261.50	41	61	130610_V3_P5_KB_BrxA_2_4.10915.10915.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.3561	0.6060	2	~ (+396), IAM (+57)	815.3757	2,443.1054	3	0.002371	0.9702	383272	41	61	130610_V3_P5_KB_BrxA_2_4.10976.10976.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.7922	0.6377	2	~ (+396), IAM (+57)	1,222.5562	2,443.0978	2	-0.005245	-2.146	10,279.90	41	61	130610_V3_P5_KB_BrxA_2_4.11001.11001.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.3396	0.6426	2	~ (+396), IAM (+57)	815.3754	2,443.1045	3	0.001456	0.5959	340285	41	61	130610_V3_P5_KB_BrxA_2_4.11018.11018.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.9074	0.6391	2	~ (+396), IAM (+57)	1,222.5656	2,443.1166	2	0.01355	5.546	11,318.80	41	61	130610_V3_P5_KB_BrxA_2_4.11075.11075.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.6898	0.6640	2	~ (+396), IAM (+57)	1,222.5621	2,443.1097	2	0.006718	2.749	7,398.84	41	61	130610_V3_P5_KB_BrxA_2_4.11219.11219.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.3724	0.5899	2	~ (+396), IAM (+57)	815.3757	2,443.1054	3	0.002371	0.9702	245012	41	61	130610_V3_P5_KB_BrxA_2_4.11270.11270.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	99%	4.2908	0.6805	2	~ (+396), IAM (+57)	1,222.5577	2,443.1009	2	-0.002071	-0.8472	7,357.08	41	61	130610_V3_P5_KB_BrxA_2_4.11324.11324.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	3.6816	0.6291	2	~ (+396), IAM (+57)	1,222.5645	2,443.1144	2	0.01136	4.646	5,978.21	41	61	130610_V3_P5_KB_BrxA_2_4.11424.11424.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	95%	3.5220	0.4553	2	~ (+396), IAM (+57)	815.3754	2,443.1045	3	0.001456	0.5959	190308	41	61	130610_V3_P5_KB_BrxA_2_4.11478.11478.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0162	0.5697	2	~ (+396), IAM (+57)	815.3754	2,443.1045	3	0.001456	0.5959	180412	41	61	130610_V3_P5_KB_BrxA_2_4.11520.11520.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9055	0.6038	2	~ (+396), IAM (+57)	815.3754	2,443.1043	3	0.001273	0.521	149149	41	61	130610_V3_P5_KB_BrxA_2_4.11729.11729.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.5372	0.5998	2	~ (+396), IAM (+57)	1,222.5581	2,443.1017	2	-0.001339	-0.5477	6,277.79	41	61	130610_V3_P5_KB_BrxA_2_4.11964.11964.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.4963	0.5024	2	~ (+396), IAM (+57)	815.3751	2,443.1035	3	0.0005404	0.2211	107216	41	61	130610_V3_P5_KB_BrxA_2_4.11972.11972.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	98%	4.1014	0.6342	2	~ (+396), IAM (+57)	815.3753	2,443.1041	3	0.00109	0.4461	92,617.60	41	61	130610_V3_P5_KB_BrxA_2_4.12049.12049.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.4723	0.5395	2	~ (+396), IAM (+57)	815.3748	2,443.1026	3	-0.0003746	-0.1533	97,424.80	41	61	130610_V3_P5_KB_BrxA_2_4.12085.12085.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.5388	0.5826	2	~ (+396), IAM (+57)	815.3758	2,443.1056	3	0.002554	1.045	68,841.80	41	61	130610_V3_P5_KB_BrxA_2_4.12125.12125.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.1306	0.6371	2	~ (+396), IAM (+57)	815.3755	2,443.1048	3	0.001822	0.7456	77,782.80	41	61	130610_V3_P5_KB_BrxA_2_4.12204.12204.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0407	0.6093	2	~ (+396), IAM (+57)	815.3749	2,443.1030	3	-8.606E-06	-0.003521	60,971.80	41	61	130610_V3_P5_KB_BrxA_2_4.12240.12240.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0617	0.6382	2	~ (+396), IAM (+57)	815.3751	2,443.1035	3	0.0005404	0.2211	61,097.30	41	61	130610_V3_P5_KB_BrxA_2_4.12277.12277.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9419	0.6525	2	~ (+396), IAM (+57)	815.3752	2,443.1037	3	0.0007234	0.296	56,583.80	41	61	130610_V3_P5_KB_BrxA_2_4.12355.12355.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.0746	0.5921	2	~ (+396), IAM (+57)	815.3752	2,443.1037	3	0.0007234	0.296	53,732.60	41	61	130610_V3_P5_KB_BrxA_2_4.12389.12389.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.7459	0.6227	2	~ (+396), IAM (+57)	815.3761	2,443.1063	3	0.00347	1.42	25,576.20	41	61	130610_V3_P5_KB_BrxA_2_4.12563.12563.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	96%	3.2792	0.5384	2	~ (+396), IAM (+57)	1,222.5566	2,443.0987	2	-0.004269	-1.746	8,743.72	41	61	130610_V3_P5_KB_BrxA_2_4.13243.13243.2.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.8317	0.6413	2	~ (+396), IAM (+57)	815.3752	2,443.1039	3	0.0009064	0.3708	164759	41	61	130610_V3_P5_KB_BrxA_2_4.13312.13312.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	4.1012	0.5957	2	~ (+396), IAM (+57)	815.3751	2,443.1035	3	0.0005404	0.2211	128145	41	61	130610_V3_P5_KB_BrxA_2_4.13353.13353.3.dta
(K)AEGTTLVVVNSVcGcAAGLAR(P)	97%	3.9375	0.6283	2	~ (+396), IAM (+57)	815.3760	2,443.1061	3	0.003104	1.27	63,249.40	41	61	130610_V3_P5_KB_BrxA_2_4.13391.13391.3.dta

Peptide sequence	Spectral counts			
	BrxA-SSB	BrxA-SSB-2	BrxA-SSB-Av	SD
(K)AEGTTLVVVNSVcGcAAGLAR(P)	45.0	82.0	63.5	26.2

Legend to Table S2: Detected BrxA-SSB sites by Orbitrap LC-MS/MS analysis before and after reduction of MetE-SSB by BrxA in the in vitro Brx-assay. His-tagged MetE was expressed and purified from E. coli cells, in vitro bacillithiolated using BSSB and purified as described in the Methods section. MetE-SSB was reduced by purified BrxA for 1 hour. The MetE-SSB control reaction and MetE-SSB that was treated with BrxA and BrxB were separated by SDS-PAGE. The MetE-SSB bands and the BrxA and BrxB bands were tryptically in gel-digested. The resulting BrxA-SSB peptides were analyzed using LTQ Orbitrap Velos LC-MS/MS analysis as described in the Methods section (Chi et al., 2011). The Scaffold search results are shown and the Table includes the Xcorr, deltaCn scores,m/z of the precursor ions, neutral molecular masses of the peptides, peptide mass deviations (delta ppm) of all detected bacillithiolated peptides in BrxA. The CID MS/MS spectrum of the modified Cys peptides are shown,with the b and y ion series labeled in red and blue, respectively. Two replicates each for the Brx assay using MetE-SSB were performed and the averages and SEM are shown for the bacillithiolated Cys peptides of BrxA before and after Brx reduction of MetE-SSB in the Table below that is used for the Figure 5.

Table S3: BrxB-SSB peptides after in vitro MetE-SSB reduction by BrxB (SI to BrxB-SSB peptide informations to Fig. 5)

Sequence	Prob	SEQUEST XCorr	SEQUEST ΔCn	NTT	Modifications	Observed	Actual Mass	Charge	ΔAMU	ΔPPM	TIC	Start	Stop	Spectrum ID
BrxB Cys52-SSB peptide 1														
(K)LQEAFEEYcEEV(-)	99%	3.5339	0.9781	2	~ (+396)	942.8559	1883.6972	2	0.0007077	0.3755	58,186.30	134	145	130610_V3_P5_KB_BrxB_1.5.06591.06591.2.dta
(K)LQEAFEEYcEEV(-)	99%	3.1124	0.9156	2	~ (+396)	942.8558	1883.6971	2	0.0005857	0.3108	92,802.40	134	145	130610_V3_P5_KB_BrxB_1.5.06631.06631.2.dta
(K)LQEAFEEYcEEV(-)	99%	3.0009	0.8836	2	~ (+396)	942.8558	1883.6970	2	0.0004637	0.246	45,494.70	134	145	130610_V3_P5_KB_BrxB_1.5.06677.06677.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.4764	0.8904	2	~ (+396)	942.8553	1883.6960	2	-0.0005133	-0.2724	21,657.90	134	145	130610_V3_P5_KB_BrxB_1.5.06856.06856.2.dta
(K)LQEAFEEYcEEV(-)	98%	2.5758	0.7802	2	~ (+396)	942.8548	1883.6950	2	-0.001489	-0.7902	25,277.80	134	145	130610_V3_P5_KB_BrxB_1.5.06948.06948.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.3117	0.891	2	~ (+396)	942.8550	1883.6955	2	-0.001001	-0.5313	12,915.20	134	145	130610_V3_P5_KB_BrxB_1.5.07008.07008.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.2767	0.9869	2	~ (+396)	942.8538	1883.6931	2	-0.003442	-1.826	11,019.00	134	145	130610_V3_P5_KB_BrxB_1.5.07095.07095.2.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	96%	3.6678	0.5241	2	~ (+396), IAM (+57)	797.3649	2389.0728	3	-0.002022	-0.8458	119590	41	60	130610_V3_P5_KB_BrxB_1.5.04815.04815.3.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	99%	4.5683	0.7697	2	~ (+396), IAM (+57)	1195.5454	2389.0763	2	0.00147	0.6152	38,826.60	41	60	130610_V3_P5_KB_BrxB_1.5.04841.04841.2.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	96%	3.5027	0.5008	2	~ (+396), IAM (+57)	797.3651	2389.0733	3	-0.001472	-0.6157	136079	41	60	130610_V3_P5_KB_BrxB_1.5.04901.04901.3.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	97%	3.7127	0.6231	2	~ (+396), IAM (+57)	797.3657	2389.0753	3	0.0005424	0.2269	61,904.50	41	60	130610_V3_P5_KB_BrxB_1.5.04943.04943.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	99%	4.3844	0.7465	2	~ (+396), IAM (+57)	1131.4972	2260.9798	2	0.00003539	0.01565	102764	42	60	130610_V3_P5_KB_BrxB_1.5.05626.05626.2.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	99%	4.2349	0.7763	2	~ (+396), IAM (+57)	1131.4971	2260.9796	2	-0.0002086	-0.09222	78,814.20	42	60	130610_V3_P5_KB_BrxB_1.5.05668.05668.2.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.5031	0.6333	2	~ (+396), IAM (+57)	754.6664	2260.9773	3	-0.00248	-1.096	395205	42	60	130610_V3_P5_KB_BrxB_1.5.05778.05778.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.791	0.7099	2	~ (+396), IAM (+57)	754.6670	2260.9791	3	-0.0006486	-0.2867	239572	42	60	130610_V3_P5_KB_BrxB_1.5.05862.05862.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.5648	0.6629	2	~ (+396), IAM (+57)	754.6666	2260.9780	3	-0.001748	-0.7726	160028	42	60	130610_V3_P5_KB_BrxB_1.5.05927.05927.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	4.0554	0.7564	2	~ (+396), IAM (+57)	754.6671	2260.9793	3	-0.0004656	-0.2058	88,924.90	42	60	130610_V3_P5_KB_BrxB_1.5.06031.06031.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.689	0.7073	2	~ (+396), IAM (+57)	754.6668	2260.9786	3	-0.001199	-0.5299	48,751.50	42	60	130610_V3_P5_KB_BrxB_1.5.06685.06685.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.6412	0.6866	2	~ (+396), IAM (+57)	754.6669	2260.9788	3	-0.00116	-0.449	40,367.40	42	60	130610_V3_P5_KB_BrxB_1.5.06728.06728.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.3639	0.6342	2	~ (+396), IAM (+57)	754.6679	2260.9819	3	0.002097	0.9272	41,799.80	42	60	130610_V3_P5_KB_BrxB_1.5.07075.07075.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.4168	0.7204	2	~ (+396), IAM (+57)	754.6673	2260.9801	3	0.0002664	0.1178	32,758.50	42	60	130610_V3_P5_KB_BrxB_1.5.07369.07369.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.3314	0.6307	2	~ (+396), IAM (+57)	754.6674	2260.9804	3	0.0006324	0.2796	43,543.50	42	60	130610_V3_P5_KB_BrxB_1.5.07833.07833.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.3249	0.7019	2	~ (+396), IAM (+57)	754.6675	2260.9806	3	0.0008154	0.3605	65,119.20	42	60	130610_V3_P5_KB_BrxB_1.5.08162.08162.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.5985	0.7397	2	~ (+396), IAM (+57)	754.6671	2260.9793	3	-0.0004656	-0.2058	65,215.30	42	60	130610_V3_P5_KB_BrxB_1.5.08346.08346.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.5049	0.6345	2	~ (+396), IAM (+57)	754.6677	2260.9813	3	0.001548	0.6845	56,668.40	42	60	130610_V3_P5_KB_BrxB_1.5.08389.08389.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.4963	0.6768	2	~ (+396), IAM (+57)	754.6671	2260.9795	3	-0.0002826	-0.1249	37,543.00	42	60	130610_V3_P5_KB_BrxB_1.5.08430.08430.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.3583	0.6423	2	~ (+396), IAM (+57)	754.6667	2260.9784	3	-0.001382	-0.6108	52,593.10	42	60	130610_V3_P5_KB_BrxB_1.5.08514.08514.3.dta
BrxB Cys52-SSB peptide 2														
(K)LQEAFEEYcEEV(-)	99%	3.4316	0.8598	2	~ (+396)	942.8557	1883.6969	2	0.0003417	0.1813	51,842.80	134	145	130610_V3_P5_KB_BrxB_2.6.06715.06715.2.dta
(K)LQEAFEEYcEEV(-)	99%	3.0351	0.962	2	~ (+396)	942.8558	1883.6971	2	0.0005857	0.3108	144311	134	145	130610_V3_P5_KB_BrxB_2.6.06752.06752.2.dta
(K)LQEAFEEYcEEV(-)	99%	3.2967	0.8768	2	~ (+396)	942.8557	1883.6969	2	0.0003417	0.1813	63,913.80	134	145	130610_V3_P5_KB_BrxB_2.6.06794.06794.2.dta
(K)LQEAFEEYcEEV(-)	98%	2.2245	0.7763	2	~ (+396)	942.8560	1883.6974	2	0.0008297	0.4402	120520	134	145	130610_V3_P5_KB_BrxB_2.6.06863.06863.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.8494	0.9073	2	~ (+396)	942.8559	1883.6972	2	0.0007077	0.3755	25,277.10	134	145	130610_V3_P5_KB_BrxB_2.6.06972.06972.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.8524	0.9192	2	~ (+396)	942.8552	1883.6959	2	-0.0006353	-0.3371	14,645.00	134	145	130610_V3_P5_KB_BrxB_2.6.07082.07082.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.9067	0.8804	2	~ (+396)	942.8560	1883.6975	2	0.0009517	0.505	12,190.50	134	145	130610_V3_P5_KB_BrxB_2.6.07141.07141.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.8557	0.9298	2	~ (+396)	942.8547	1883.6948	2	-0.001733	-0.9197	18,188.30	134	145	130610_V3_P5_KB_BrxB_2.6.07226.07226.2.dta
(K)LQEAFEEYcEEV(-)	99%	3.188	0.8686	2	~ (+396)	942.8575	1883.7004	2	0.003882	2.06	14,020.40	134	145	130610_V3_P5_KB_BrxB_2.6.07303.07303.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.9151	0.8249	2	~ (+396)	942.8548	1883.6950	2	-0.001489	-0.7902	7,671.48	134	145	130610_V3_P5_KB_BrxB_2.6.07350.07350.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.989	0.9129	2	~ (+396)	942.8562	1883.6978	2	0.001318	0.6992	10,647.40	134	145	130610_V3_P5_KB_BrxB_2.6.07402.07402.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.832	0.823	2	~ (+396)	942.8558	1883.6971	2	0.0005857	0.3108	7,076.55	134	145	130610_V3_P5_KB_BrxB_2.6.07454.07454.2.dta
(K)LQEAFEEYcEEV(-)	99%	2.6617	0.8108	2	~ (+396)	942.8552	1883.6959	2	-0.0006353	-0.3371	6,359.12	134	145	130610_V3_P5_KB_BrxB_2.6.07500.07500.2.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	98%	3.9843	0.6625	2	~ (+396), IAM (+57)	598.2766	2389.0773	4	0.002543	1.064	2224600	41	60	130610_V3_P5_KB_BrxB_2.6.04941.04941.4.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	99%	4.6822	0.8098	2	~ (+396), IAM (+57)	1195.5462	2389.0770	2	0.002203	0.9219	47,361.20	41	60	130610_V3_P5_KB_BrxB_2.6.04964.04964.2.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	96%	3.3174	0.5204	2	~ (+396), IAM (+57)	797.3648	2389.0726	3	-0.002205	-0.9224	76,825.80	41	60	130610_V3_P5_KB_BrxB_2.6.05078.05078.3.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	97%	3.5093	0.6215	2	~ (+396), IAM (+57)	797.3642	2389.0708	3	-0.004036	-1.688	43,178.70	41	60	130610_V3_P5_KB_BrxB_2.6.05120.05120.3.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	97%	3.7865	0.6226	2	~ (+396), IAM (+57)	797.3660	2389.0761	3	0.001274	0.5332	33,142.80	41	60	130610_V3_P5_KB_BrxB_2.6.05200.05200.3.dta
(K)KGTTLVMVNSVcGcAGGIAR(P)	97%	3.3969	0.6286	2	~ (+396), IAM (+57)	797.3649	2389.0730	3	-0.001838	-0.7688	16,898.90	41	60	130610_V3_P5_KB_BrxB_2.6.05460.05460.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	4.0277	0.7292	2	~ (+396), IAM (+57)	754.6681	2260.9824	3	0.002646	1.17	2797070	42	60	130610_V3_P5_KB_BrxB_2.6.05715.05715.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	99%	4.4324	0.7794	2	~ (+396), IAM (+57)	1131.4974	2260.9803	2	0.0005234	0.2314	83,898.10	42	60	130610_V3_P5_KB_BrxB_2.6.05718.05718.2.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	99%	3.7098	0.7638	2	~ (+396), IAM (+57)	1131.4971	2260.9796	2	-0.0002086	-0.09222	173347	42	60	130610_V3_P5_KB_BrxB_2.6.05760.05760.2.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	99%	4.0596	0.7845	2	~ (+396), IAM (+57)	1131.4886	2260.9627	2	-0.01705	-7.54	13,353.30	42	60	130610_V3_P5_KB_BrxB_2.6.05878.05878.2.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.6488	0.6807	2	~ (+396), IAM (+57)	754.6663	2260.9771	3	-0.002664	-1.178	407211	42	60	130610_V3_P5_KB_BrxB_2.6.05883.05883.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	99%	3.7252	0.8301	2	~ (+396), IAM (+57)	1131.4969	2260.9793	2	-0.0004536	-0.2005	6,833.28	42	60	130610_V3_P5_KB_BrxB_2.6.05975.05975.2.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.4147	0.7383	2	~ (+396), IAM (+57)	754.6671	2260.9795	3	-0.0002826	-0.1249	120646	42	60	130610_V3_P5_KB_BrxB_2.6.06090.06090.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.3109	0.6487	2	~ (+396), IAM (+57)	754.6672	2260.9797	3	-0.00009961	-0.04403	62,467.40	42	60	130610_V3_P5_KB_BrxB_2.6.06928.06928.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.7898	0.7048	2	~ (+396), IAM (+57)	754.6678	2260.9808	3	0.0009984	0.4414	41,627.80	42	60	130610_V3_P5_KB_BrxB_2.6.06973.06973.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.8421	0.6949	2	~ (+396), IAM (+57)	754.6673	2260.9801	3	0.0002664	0.1178	30,575.40	42	60	130610_V3_P5_KB_BrxB_2.6.07483.07483.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.3052	0.7186	2	~ (+396), IAM (+57)	754.6671	2260.9795	3	-0.0002826	-0.1249	62,485.90	42	60	130610_V3_P5_KB_BrxB_2.6.08590.08590.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.343	0.6749	2	~ (+396), IAM (+57)	754.6674	2260.9804	3	0.0006324	0.2796	36,372.70	42	60	130610_V3_P5_KB_BrxB_2.6.08922.08922.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	96%	3.516	0.5489	2	~ (+396), IAM (+57)	754.6680	2260.9821	3	0.00228	1.008	55,625.30	42	60	130610_V3_P5_KB_BrxB_2.6.09046.09046.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.471	0.7358	2	~ (+396), IAM (+57)	754.6677	2260.9813	3	0.001548	0.6845	45,343.30	42	60	130610_V3_P5_KB_BrxB_2.6.09169.09169.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.8978	0.6182	2	~ (+396), IAM (+57)	754.6681	2260.9824	3	0.002646	1.17	35,979.90	42	60	130610_V3_P5_KB_BrxB_2.6.09338.09338.3.dta
(K)GTTLVMVNSVcGcAGGIAR(P)	97%	3.4986	0.6428	2	~ (+396), IAM (+57)	754.6675	2260.9806	3	0.0008154	0.3605	20,987.10	42	60	130610_V3_P5_KB_BrxB_2.6.09506.09506.3.dta
(K)GTTLVmVNSVcGcAGGIAR(P)	97%	3.704	0.7032	2	Ox (+16), ~ (+396), IAM	759.9990	2276.9752	3	0.0005294	0.2324	750781	42	60	130610_V3_P5_KB_BrxB_2.6.05005.05005.3.dta
(K)GTTLVmVNSVcGcAGGIAR(P)	98%	4.1327	0.6396	2	Ox (+16), ~ (+396), IAM	1139.4955	2276.9764	2	0.001702	0.7473	42,769.20	42	60	130610_V3_P5_KB_BrxB_2.6.05029.05029.2.dta
(K)GTTLVmVNSVcGcAGGIAR(P)	97%	3.3622	0.6126	2	Ox (+16), ~ (+396), IAM	759.9931	2276.9575	3	-0.01723	-7.564	53,312.20	42	60	130610_V3_P5_KB_BrxB_2.6.05726.3.dta

Peptide sequence	Spectral counts			
	BrxB-SSB-1	BrxB-SSB-2	BrxB-SSB-Av	SD
(K)GTTLVMVNSVcGcAGGIAR(P)	20.0	25.0	22.5	3.5
(K)LQEAFEEYcEEV(-)	7	13	10.0	4.2

Legend to Table S3: Detected BrxB-SSB sites by Orbitrap LC-MS/MS analysis before and after reduction of MetE-SSB by BrxB in the in vitro Brx-assay. His-tagged MetE was expressed and purified from E. coli cells, in vitro bacillithiolated using BSSB and purified as described in the Methods section. MetE-SSB was reduced by purified BrxB for 1 hour. The MetE-SSB control reaction and MetE-SSB that was treated with BrxA and BrxB were separated by SDS-PAGE. The MetE-SSB bands and the BrxA and BrxB bands were tryptically in gel-digested. The resulting BrxB-SSB peptides were analyzed using LTQ Orbitrap Velos LC-MS/MS analysis as described in the Methods section (Chi et al., 2011). The Scaffold search results are shown and the Table includes the Xcorr, deltaCn scores,m/z of the precursor ions, neutral molecular masses of the peptides, peptide mass deviations (delta ppm) of all detected bacillithiolated peptides in BrxB. The CID MS/MS spectrum of the modified Cys peptides are shown,with the b and y ion series labeled in red and blue, respectively. Two replicates each for the Brx assay using MetE-SSB were performed and the averages and SEM are shown for the bacillithiolated Cys peptides of BrxB before and after Brx reduction of MetE-SSB in the Table below that is used for the Figure 5.

Table S4: Identification of Cys52-SSB in BrxB C54A and Cys53-SSB in BrxA C55A in vivo after immunoprecipitation

BrxB-Cys52-SSB

Sequence	Prob	SEQUEST XCorr	SEQUEST ΔCn	NTT	Modifications	Observed	Actual Mass	Charge	ΔAMU	ΔPPM	TIC	Start	Stop	Spectrum ID		
(K)GTTLVmVNSVcGAAGGIAR(P)	95%	3.0551	0.729	1	Ox (+16), ^ (+396)	730.3342	2187.9807	3	0.000076	0.03472	19,661.90	42	60	110328_OV3_P3_KG_HA_YqiWC54A_10.09955.09955.3.dta		
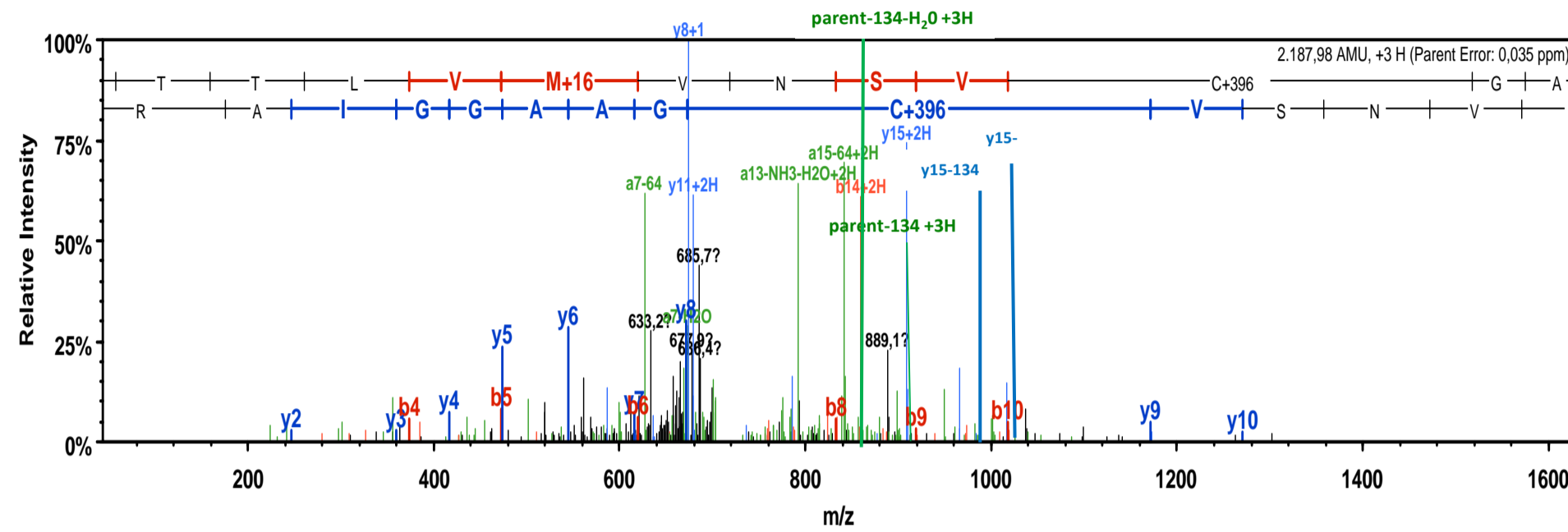
B	B Ions	B+2H	B-NH3	B-H2O	AA	Y Ions	Y+2H	Y-NH3	Y-H2O	Y
1	58.0				G	2.189,0	1.095,0	2.172,0	2.171,0	19
2	159,1			141.1	T	2.132,0	1.066,5	2.114,9	2.114,0	18
3	260.1			242.1	T	2.030,9	1.016,0	2.013,9	2.012,9	17
4	373.2			355.2	L	1.929,9	965,4	1.912,8	1.911,9	16
5	472.3			454.3	V	1.816,8	908,9	1.799,8	1.798,8	15
6	619.3	310.2		601.3	M+16	1.717,7	859,4	1.700,7	1.699,7	14
7	718.4	359,7		700.4	V	1.570,7	785,8	1.553,7	1.552,7	13
8	832.4	416,7	815.4	814.4	N	1.471,6	736,3	1.454,6	1.453,6	12
9	919.5	460,2	902,4	901.4	S	1.357,6	679,3	1.340,5	1.339,6	11
10	1.018,5	509,8	1.001,5	1.000,5	V	1.270,5	635,8	1.253,5		10
11	1.517,6	759,3	1.500,6	1.499,6	C+396	1.171,5	586,2	1.154,4		9
12	1.574,6	787,8	1.557,6	1.556,6	G	672,4	336,7	655,4		8
13	1.645,7	823,3	1.628,6	1.627,7	A	615,4	308,2	598,3		7
14	1.716,7	858,9	1.699,7	1.698,7	A	544,3	272,7	527,3		6
15	1.773,7	887,4	1.756,7	1.755,7	G	473,3		456,3		5
16	1.830,8	915,9	1.813,7	1.812,7	G	416,3		399,2		4
17	1.943,8	972,4	1.926,8	1.925,8	I	359,2		342,2		3
18	2.014,9	1.007,9	1.997,8	1.996,9	A	246,2		229,1		2
19	2.189,0	1.095,0	2.172,0	2.171,0	R	175,1		158,1		1

BrxA-Cys53-SSB

Sequence	Prob	SEQUEST XCorr	SEQUEST ΔCn	NTT	Modifications	Observed	Actual Mass	Charge	ΔAMU	ΔPPM	TIC	Start	Stop	Spectrum ID		
(K)AEGTTLVVVNSVC53(+BSH)GAAAGLAR(P)	95%	2.4157	0.5477	1	^ (+396)	785.7110	2354.1112	3	0.002285	0.9702	7,578.04	41	61	110327_OV3_P3_KG_HA_YphPC55A_10.11736.11736.3.dta		
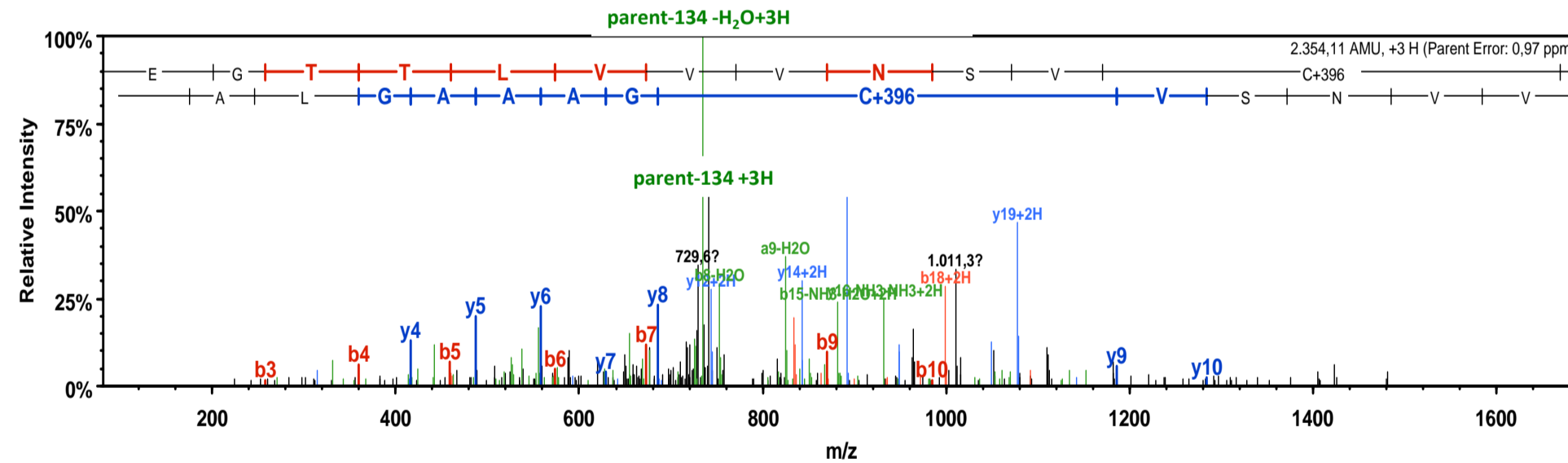
B	B Ions	B+2H	B-NH3	B-H2O	AA	Y Ions	Y+2H	Y-NH3	Y-H2O	Y
1	72.0				A	2.355,1	1.178,1	2.338,1	2.337,1	21
2	201.1			183.1	E	2.284,1	1.142,5	2.267,1	2.266,1	20
3	258.1			240.1	G	2.155,0	1.078,0	2.138,0	2.137,0	19
4	359.2			341.1	T	2.098,0	1.049,5	2.081,0	2.080,0	18
5	460.2			442.2	T	1.997,0	999,0	1.979,9	1.979,0	17
6	573.3	287.1		555.3	L	1.895,9	948,5	1.878,9	1.877,9	16
7	672.4	336,7		654.3	V	1.782,8	891,9	1.765,8	1.764,8	15
8	771.4	386,2		753.4	V	1.683,8	842,4	1.666,7	1.665,8	14
9	870.5	435,8		852.5	V	1.584,7	792,9	1.567,7	1.566,7	13
10	984.5	492,8	967,5	966.5	N	1.485,6	743,3	1.468,6	1.467,6	12
11	1.071,6	536,3	1.054,5	1.053,6	S	1.371,6	686,3	1.354,6	1.353,6	11
12	1.170,6	585,8	1.153,6	1.152,6	V	1.284,6	642,8	1.267,5		10
13	1.669,7	835,4	1.652,7	1.651,7	C+396	1.185,5	593,2	1.168,5		9
14	1.726,8	863,9	1.709,7	1.708,7	G	686,4	343,7	669,4		8
15	1.797,8	899,4	1.780,8	1.779,8	A	629,4	315,2	612,3		7
16	1.868,8	934,9	1.851,8	1.850,8	A	558,3	279,7	541,3		6
17	1.939,9	970,4	1.922,8	1.921,9	A	487,3		470,3		5
18	1.996,9	998,9	1.979,9	1.978,9	G	416,3		399,2		4
19	2.110,0	1.055,5	2.092,9	2.092,0	L	359,2		342,2		3
20	2.181,0	1.091,0	2.164,0	2.163,0	A	246,2		229,1		2
21	2.355,1	1.178,1	2.338,1	2.337,1	R	175,1		158,1		1

Legend to Table S4: BrxB C54A with the Cys52-SSB site (upper figure) and BrxA C55A with Cys53-SSB site (bottom figure) in vivo. FLAG-tagged BrxB C54A and BrxA C55A proteins were purified from B. subtilis cells after NaOCl-stress, separated by SDS-PAGE and the Brx bands tryptically digested.The resulting peptides were analyzed using LTQ Orbitrap Velos LC-MS/MS analysis as described in the Methods section (Chi et al., 2011). The Scaffold search results are shown and the Table includes the Xcorr, deltaCn scores, m/z of the precursor ions, neutral molecular masses of the peptides, peptide mass deviations (delta ppm) of the S-bacillithiolated Cys52 peptide in BrxB C54A and Cys53 in BrxA C55A. The CID MS/MS spectra are shown wth the b and y ion series labeled in red and blue, respectively.