Supplementary Figure1. *Interface of* Citrullia*, showing each page from the program, where home page, analysis page, validation page, and quantification page can be picked from the left menu, while sub menus can be picked in the top of each page. From the analysis window, the following subpages can be accessed, general, parameters, modifications, and options. Furthermore, all the parameters from the X! Tandem search engine can be accessed by the analysis page. By selecting a peptide from the validation page, three windows can be opened, one for analysis of paired citrullinated peptides by the citrullinated peptide, one for analysis of the paired citrullinations by the arginine containing peptide, and one for single citrullinated peptides.*

Interface of *Citrullia*

CITRULLIA

Home

Analysis

Validation

Quantification

Validation

Citrullinations   Arginines   Lonely

Search Query:
Subject Spectra
Type: Modified
Name: Citrullination
Residue: [R]
Mass Change: + 0.9845
(From an identical unmodified peptide)

Complimentary Spectra
Type: Unmodified
Name: Arginine Containing
Residue: [R]
Mass difference: - 0.9845
(From the subject spectra parent mass)

Parent Mass Error:

0.05   Da

Find Spectra

Search Result:

Protein:	ScanID:	E-value:	Scans:	Sequence:
sp|B2RM93|CPG1_PO...	3986	0.00073	2	IKEGLTETTYR
sp|B2RM93|CPG1_PO...	3959	0.0062	2	IKEGLTETTYR
sp|B2RM93|CPG1_PO...	3971	0.0086	2	IKEGLTETTYR
sp|B2RM93|CPG1_PO...	4004	0.004	2	IKEGLTETTYR
tr|B2RHK9|B2RHK9_P...	4980	7.7E-07	2	LIDHLLSNYESDPR
sp|Q51817|KGP83_PO...	4948	4.8E-09	1	KLIAVPVGATPVVR
tr|B2RIM9|B2RIM9_P...	4680	2.7E-05	1	KINVQSLHVIPGR
tr|B2RMC1|B2RMC1_...	3282	1.4E-07	1	GSHEPVADNSTVAGR
tr|B2RHK9|B2RHK9_P...	2819	0.0048	6	AGNHTVQGATR

Spectra Validation - Citrullinations   - X

Spectrum ID: 3282

Citrullinated Peptide:
ID / Protein: 3282 / B2RMC1
Parent Mass: 1497.689
Charge-state: 2
Sequence: GSHEPVADNSTVAGR
E-value: 1.4E-07
Retention Time: 727 sec.
File Name: QEHF1_10226_DNL.mzXML.MGX

Arginine Peptide:
ID / Protein: 3173 / B2RMC1
Parent Mass: 1496.706
Charge-state: 3
Sequence: GSHEPVADNSTVAGR
E-value: 1.5E-06
Retention Time: 711 sec.
File Name: QEHF1_10236_DNL.mzXML.MGX

Next

Previous

Add

Remove

Export

B Ions   B-17 Ions   B-18 Ions   Y Ions   Y-17 Ions   Y-18 Ions   A Ions   Unidentified   Save   Reset Zoom

Intensity

m/z

a	b-18	b-17	b	Seq.	y	y-17	y-18
650.326	660.31	661.318	678.321	b7 "A" y9	891.417	874.414	873.406
765.353	775.337	776.345	793.348	b8 "D" y8	820.38	803.377	802.369
879.396	889.38	890.388	907.39	b9 "N" y7	705.353	688.35	687.342
966.428	976.412	977.42	994.422	b10 "S" y6	591.31	574.307	573.299
1067.475	1077.46	1078.467	1095.47	b11 "T" y5	504.278	487.275	486.267
1166.544	1176.528	1177.536	1194.539	b12 "V" y4	403.23	386.227	385.219

a	b-18	b-17	b	Seq.	y	y-17	y-18
30.034	40.018	41.026	58.029	b1 "G" y15	1496.709	1479.706	1478.698
117.066	127.05	128.058	145.061	b2 "S" y14	1439.687	1422.685	1421.677
254.125	264.109	265.117	282.12	b3 "H" y13	1352.655	1335.653	1334.645
383.167	393.152	394.16	411.162	b4 "E" y12	1215.596	1198.594	1197.586
480.22	490.204	491.212	508.215	b5 "P" y11	1086.554	1069.551	1068.543
579.289	589.273	590.281	607.283	b6 "V" y10	989.501	972.498	971.49

MS1 Scan of Modified Peptide
Retention Time: 726 sec.   Save   Reset Zoom

Intensity

m/z

MS1 Scan of Unmodified Peptide
Retention Time: 710 sec.   Save   Reset Zoom

Intensity

m/z
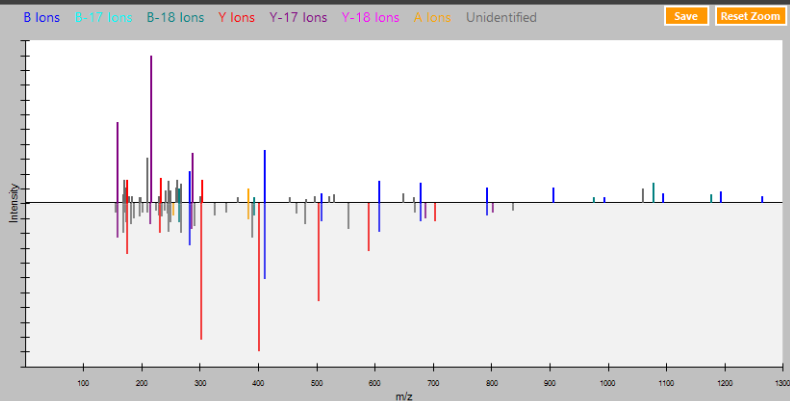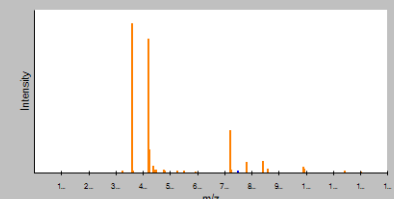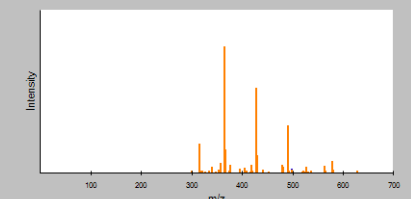
Citrullia

Citrullinations | Arginines | Lonely

Home
Analysis
Validation
Quantification

Validation

Search Query:
Subject Spectra
Type: Unmodified
Name: Arginine Containing
Residue: [R]
Mass Change: 0.0
(From an identical unmodified peptide)

Complimentary Spectra
Type: Modified
Name: Citrullination
Residue: [R]
Mass difference: + 0.9845
(From the subject spectra parent mass)

Parent Mass Error:
0.05   Da

Find Spectra

Search Result:

Protein:	ScanID:	E-value:	Scans:	Sequence:
tr|B2RH25|B2RH25_P...	2550	0.0013	2	RATTAPAPK
tr|B2RHH5|B2RHH5_P...	3903	0.00012	1	RQQELQDIQ
tr|B2RHH5|B2RHH5_P...	3933	5.6E-05	1	RQQELQDIQ
tr|B2RKY7|B2RKY7_PO...	3026	0.00098	1	RQQIIDK
tr|B2RKY7|B2RKY7_PO...	3023	0.0034	1	RQQIIDK
sp|B2RM93|CPG1_PO...	4247	4.4E-05	1	RTFGGVTMN
sp|B2RM93|CPG1_PO...	4251	0.00032	1	RTFGGVTMNG
tr|B2RMC1|B2RMC1_...	5097	0.00046	1	RVEVYILPNA
sp|B2RM93|CPG1_PO...	5091	2E-07	2	SDQVYGQIVGNDHYNEVFIGR
sp|B2RM93|CPG1_PO...	5063	5.4E-09	2	SDQVYGQIVGNDHYNEVFIGR
tr|B2RI00|B2RI00_PO...	2729	0.0028	1	SSVPGR
tr|B2RLB6|B2RLB6_P...	3962	0.0033	1	TEIKPGGSTLLR
sp|B2RM93|CPG1_PO...	3119	0.0059	2	TIHYER
tr|B2RK56|B2RK56_P...	4403	1.1E-05	2	TKVPGVFAAGDVADPHYR
tr|B2RK56|B2RK56_P...	4416	1.3E-10	2	TKVPGVFAAGDVADPHYR
tr|B2RLP4|B2RLP4_PO...	2928	0.00037	1	VQNNSVQQPR
tr|Q7MT61|Q7MT61_P...	2620	0.00013	1	YDSVHGR

Spectra Validation - Arginines

Spectrum ID: 5241

Next | Previous | **Add** | Remove

Arginine Peptide:
ID / Protein: 5241 / B2RM93
Parent Mass: 2410.136
Charge-state: 3
Sequence: SDQVYGQIVGNDHYNEVFIGR
E-value: 4.7E-10
Retention Time: 1177 sec.
File Name: QEHF1_10121_DNL.mzXML.MGX

Citrullinated Peptide:
ID / Protein: 5508 / B2RM93
Parent Mass: 2411.131
Charge-state: 3
Sequence: (SDQVYGQIVGNDHYNEVFIGR)
Retention Time: 1235 sec.
File Name: QEHF1_10127_DNL.mzXML.MGX
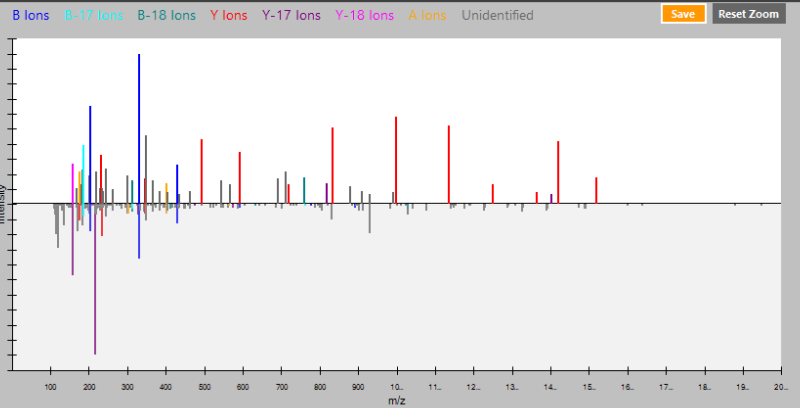(NB. The Sequence is in this case the potential sequence!)

Export

B Ions | B-17 Ions | B-18 Ions | Y Ions | Y-17 Ions | Y-18 Ions | A Ions | Unidentified | Save | Reset Zoom

a	b-18	b-17	b	Seq.	y	y-17	y-18
60.044	70.029	71.037	88.039	b1 "S" y21	2410.142	2393.139	2392.132
175.071	185.056	186.064	203.066	b2 "D" y20	2323.11	2306.107	2305.1
303.13	313.114	314.122	331.125	b3 "Q" y19	2208.083	2191.081	2190.073
402.198	412.183	413.19	430.193	b4 "V" y18	2080.025	2063.022	2062.014
565.262	575.246	576.254	593.257	b5 "Y" y17	1980.956	1963.954	1962.946
622.283	632.267	633.275	650.278	b6 "G" y16	1817.893	1800.89	1799.882

a	b-18	b-17	b	Seq.	y	y-17	y-18
1890.862	1900.846	1901.854	1918.857	b17 "V" y5	592.346	575.343	574.335
2037.93	2047.914	2048.922	2065.925	b18 "F" y4	493.277	476.275	475.267
2151.014	2160.999	2162.006	2179.009	b19 "I" y3	346.209	329.206	328.198
2208.036	2218.02	2219.028	2236.031	b20 "G" y2	233.125	216.122	215.114
2365.121	2375.106	2376.113	2393.116	b21 "R" y1	176.103	159.101	158.093

MS1 Scan of Unmodified Peptide
Retention Time: 1176 sec.   Save | Reset Zoom
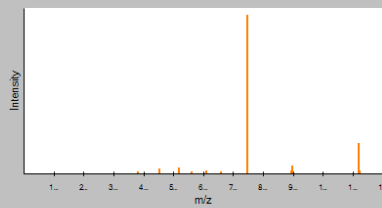
MS1 Scan of Modified Peptide
Retention Time: 1235 sec.   Save | Reset Zoom
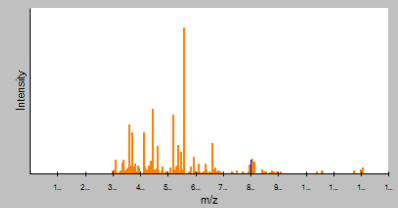
Citrullinations   Arginines   Lonely

Search Query:
Subject Spectra
Type: Modified
Name: Citrullination
Residue: [R]
Mass Change: + 0.9845
(From an identical unmodified peptide)

Find Spectra

Search Result:

Protein:	ScanID:	E-value:	Scans:	Sequence:
tr|B2RKG5|B2RKG5_P...	2847	0.00085	0	AGRIPK
tr|B2RIQ1|B2RIQ1_PO...	3948	5.3E-05	0	AHQTGAVNSHEHLIMPTIAMR
tr|B2RIQ1|B2RIQ1_PO...	4438	0.0038	0	AHQTGAVNSHEHLIMPTIAMR
tr|B2RHH7|B2RHH7_P...	6380	0.0087	0	AMNALVAEIESLR
tr|B2RHH7|B2RHH7_P...	6350	0.0017	0	AMNALVAEIESLR
sp|B2RM93|CPG1_PO...	6021	0.0079	0	DGKPTGTVAIIASTINQSWAS...
sp|B2RM93|CPG1_PO...	6180	0.00026	0	DGKPTGTVAIIASTINQSWAS...
sp|B2RM93|CPG1_PO...	6206	0.00021	0	DGKPTGTVAIIASTINQSWAS...
sp|B2RM93|CPG1_PO...	5991	0.00036	0	DGKPTGTVAIIASTINQSWAS...
tr|B2RJ70|B2RJ70_PO...	4149	0.0095	0	GKDTAGCYGEGLDLKR
sp|P59915|HAGA1_P...	4815	0.00011	0	HFGCTGIFR
tr|B2RI10|B2RI10_PO...	3082	0.0015	0	HLANPDGTR
sp|B2RIT0|DPP5_POR...	5391	4.7E-05	0	HSFELPDDLYR
sp|B2RIT0|DPP5_POR...	5334	2.2E-06	0	HSFELPDDLYR
sp|B2RIT0|DPP5_POR...	5360	3.3E-06	0	HSFELPDDLYR
tr|B2RKE1|B2RKE1_P...	4077	0.0043	0	HSSLVHFDGR
tr|B2RKE1|B2RKE1_P...	4049	0.0017	0	HSSLVHFDGR

Home

Analysis

Validation

Quantification

Validation

Spectra Validation – Lonely Citrullinations

- X

Spectrum ID: 2847

Citrullinated Peptide:
Parent Mass: 642.391
Charge-state: 2
Sequence: AGRIPK
E-value: 0.00085
Retention Time: 639 sec.
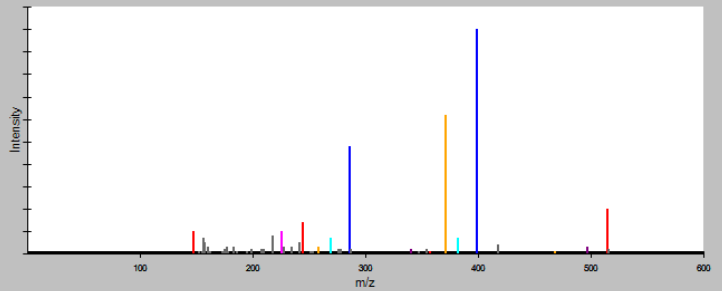File Name: QEHF1_10237_DNL.mzXML.MGX

Add   **Remove**

B Ions   B-17 Ions   B-18 Ions   Y Ions   Y-17 Ions   Y-18 Ions   A Ions   Unidentified   **Save**   **Reset Zoom**

Export

a	b-18	b-17	b	Seq.	y	y-17	y-18
44.049	54.034	55.042	72.044	b1 "A" y6	642.393	625.391	624.383
101.071	111.055	112.063	129.066	b2 "G" y5	571.356	554.353	553.346
258.156	268.14	269.148	286.151	b3 "R" y4	514.335	497.332	496.324
371.24	381.224	382.232	399.235	b4 "I" y3	357.25	340.247	339.239
468.293	478.277	479.285	496.288	b5 "P" y2	244.166	227.163	226.155
596.388	606.372	607.38	624.383	b6 "K" y1	147.113	130.11	129.102

MS1 Scan of Modified Peptide
Retention Time: 638 sec.

Save   **Reset Zoom**