

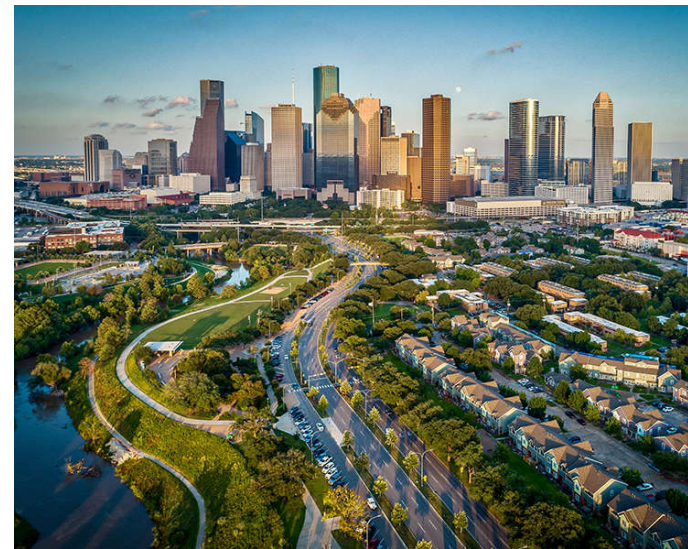
Connecting the Prots: Analyzing Crosslinked Data in a Core Lab Using Mascot

Susan T. Weintraub, Ph.D.

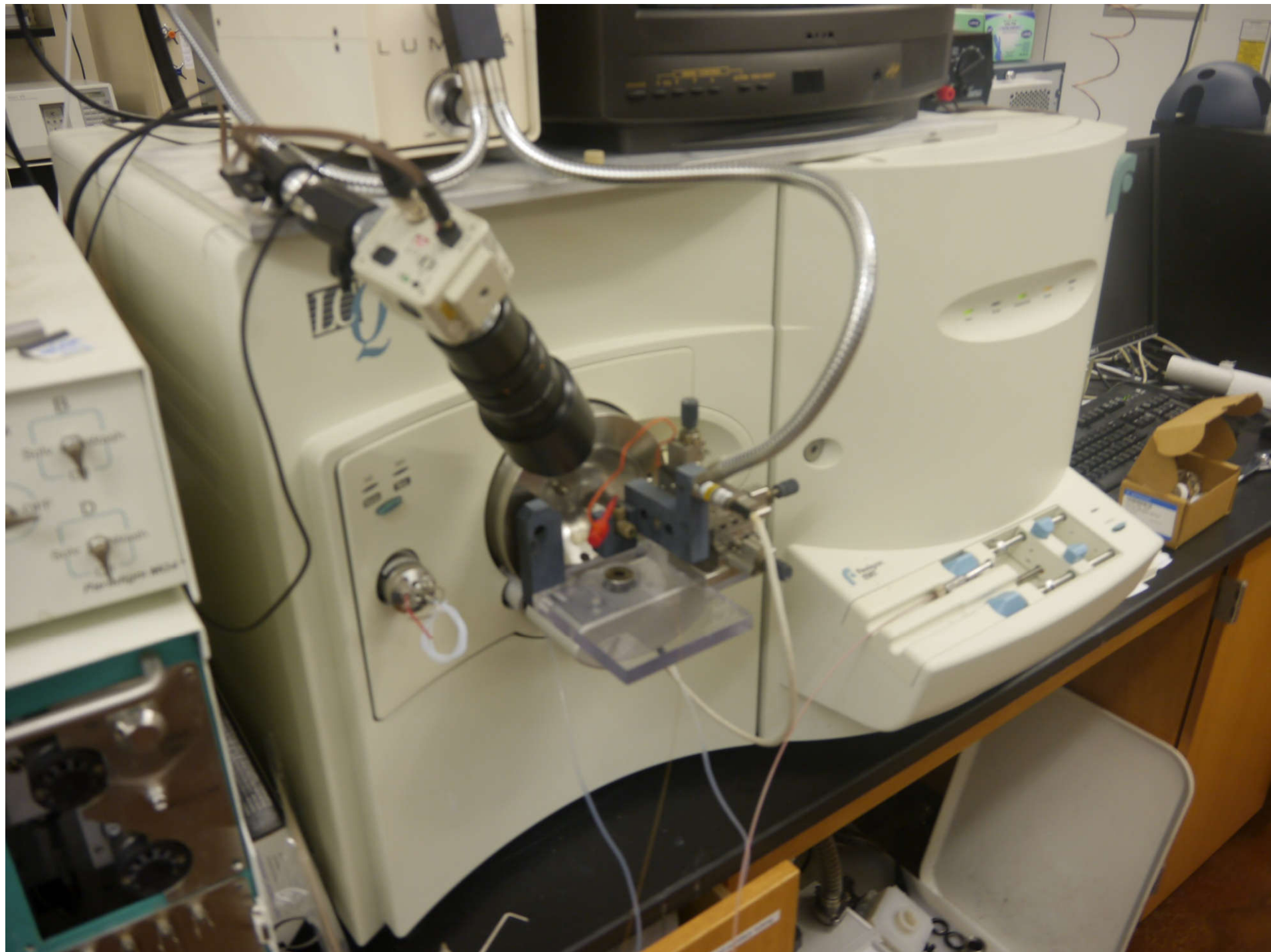
University of Texas Health Science Center
at San Antonio



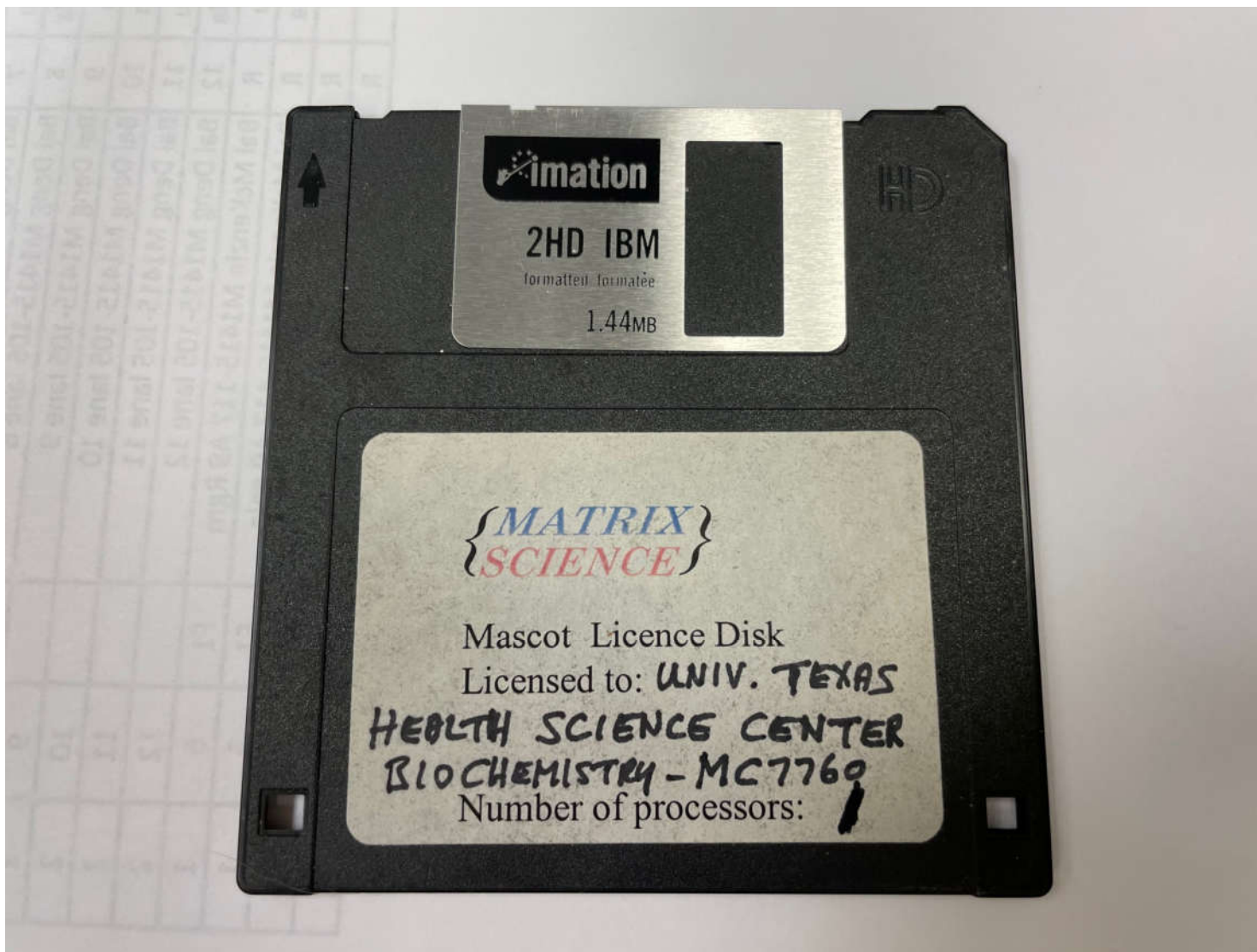
San Antonio - ASMS 2016



Houston - ASMS 2023



Mascot - the early days



Keys to success for cross-linking MS

Work with someone who knows how to prepare cross-linked proteins.

Have purified proteins (enriched or recombinant) of known sequence.

Use an appropriate cross-linking agent.

DSSO is a great choice for many experiments.

Off-line fractionation of *proteins* may be needed.

Separate proteins on a 1-D gel for in-gel digestion and MS analysis.

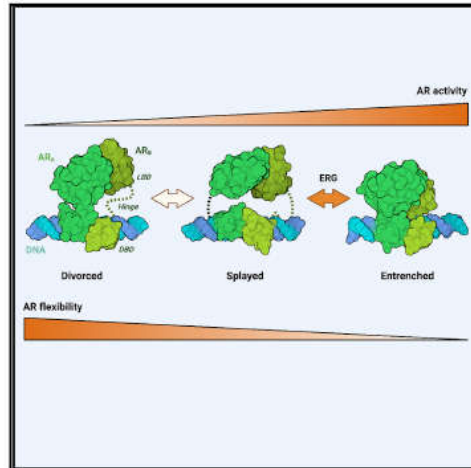
Analyze peptides on a high-performance mass spectrometer.

Use Mascot for database searching and cross-link determination.

Molecular Cell

Allosteric interactions prime androgen receptor dimerization and activation

Graphical abstract



Authors

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Arnaud Vanden Broeck,
Justin R. LaClair, ...,
Susan T. Weintraub, Sebastian Klinge,
Charles L. Sawyers

Correspondence

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sawyers@mskcc.org (C.L.S.)

In brief

Molecular features regulating DNA binding and the transactivation activities of the androgen receptor (AR) and the greater steroid receptor family have remained elusive. Using cryo-EM and mass spectrometry, Wasmuth et al. reveal a tunable mode of dimerization and define allosteric surfaces important for AR activities and development.

Highlights

- DNA-bound AR dimers exhibit conformational plasticity
- Allostericity between AR domains promotes DNA binding and transactivation
- Allosteric surfaces are mutated in partial androgen insensitivity syndrome
- The ERG oncoprotein and AR's hinge enhance binding to non-canonical DNA sequences



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Article

Molecular Cell

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Article

Allosteric interactions prime androgen receptor dimerization and activation

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<https://doi.org/10.1016/j.molcel.2022.03.035>

SUMMARY

The androgen receptor (AR) is a nuclear receptor that governs gene expression programs required for prostate development and male phenotype maintenance. Advanced prostate cancers display AR hyperactivation and transcriptome expansion, in part, through AR amplification and interaction with oncoprotein cofactors. Despite its biological importance, how AR domains and cofactors cooperate to bind DNA has remained elusive. Using single-particle cryo-electron microscopy, we isolated three conformations of AR bound to DNA, showing that AR forms a non-obligate dimer, with the buried dimer interface utilized by ancestral steroid receptors repurposed to facilitate cooperative DNA binding. We identify novel allosteric surfaces which are compromised in androgen insensitivity syndrome and reinforced by AR's oncoprotein cofactor, ERG, and by DNA-binding motifs. Finally, we present evidence that this plastic dimer interface may have been adopted for transactivation at the expense of DNA binding. Our work highlights how fine-tuning AR's cooperative interactions translate to consequences in development and disease.

INTRODUCTION

Androgen receptor (AR) signaling is a tightly controlled and multifaceted process, regulated through an orchestra of intramolecular and external cues. A better understanding of the rules governing AR activation is of great importance, as multiple pathologies are associated with aberrant AR transcriptional output, including prostate cancer and androgen insensitivity syndrome (AIS). That these disorders present with a spectrum of physical and molecular phenotypes (Cancer Genome Atlas Research Network, 2015; Jeske et al., 2007; La Spada et al., 1991; Lee et al., 2019; McPhaul et al., 1992; Robinson et al., 2015) suggests AR can exist in fully and partly primed states.

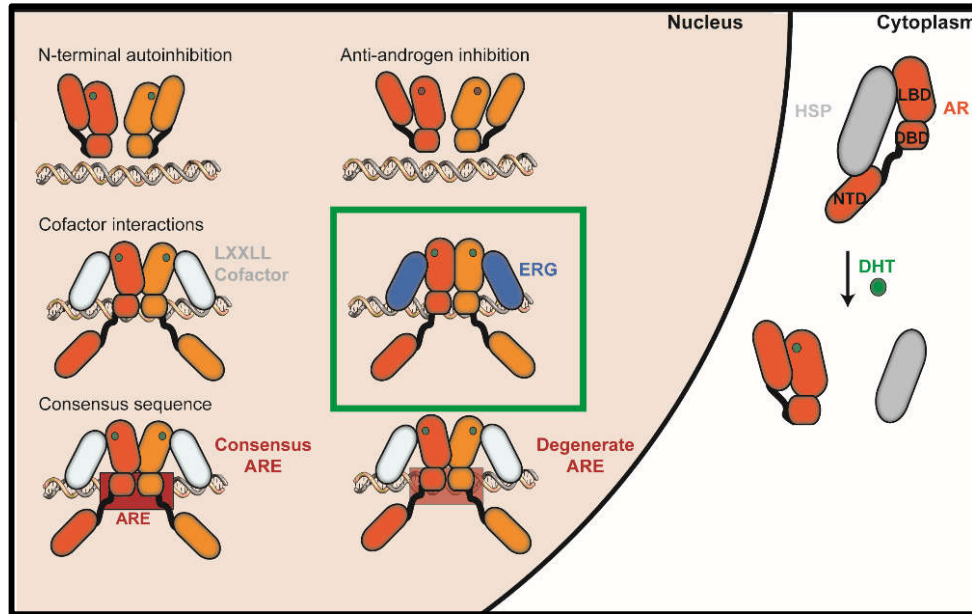
A type I nuclear receptor (NR) and member of the 3-ketosteroid receptor (3K-SR) subfamily, AR encodes an approximately 100-kilodalton (kDa) protein with an intrinsically disordered N-terminal domain (NTD), a DNA-binding domain (DBD), a flexible hinge, and a ligand binding domain (LBD) (Figure S1A) (Wakum et al., 2019). Androgens, including dihydrotestosterone (DHT)

and testosterone, bind to AR's LBD in the cytosol and facilitate AR's nuclear translocation.

The nuclear AR binds both palindromic and direct repeats of DNA hexamers known as androgen response elements (AREs) to activate its gene expression program, and is further regulated through association with numerous protein cofactors that bind the NTD or LBD through LXXLL and related motifs (Brooke et al., 2008; Wakum et al., 2018). AR can tolerate higher levels of sequence degeneracy within its ARE, an important feature required for normal development and a unique feature among steroid receptors (Adler et al., 1993; Sahu et al., 2014), with 70% of its cisrome comprised half-sites and up to 99% exhibiting some level of degeneracy (Massie et al., 2007; Wilson et al., 2016; Yu et al., 2010). Although many of these sites are not normally associated with active transcription, the overexpression of AR cofactors in prostate cancer is thought to activate expression of pro-proliferative genes at those lower affinity degenerate sites (Chen et al., 2013; Jin et al., 2014; Liu et al., 2017; Mao et al., 2019; Wasmuth et al., 2020).

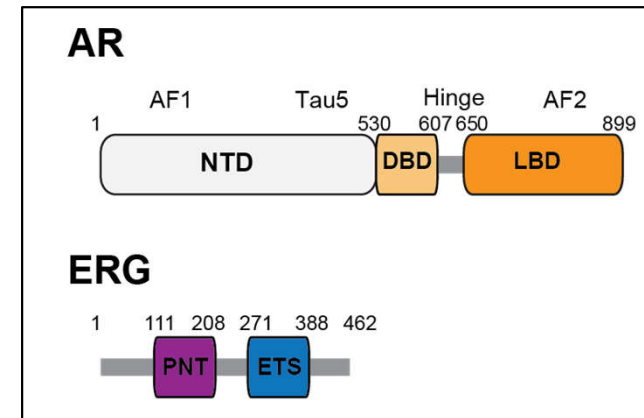


Androgen receptor



AR regulation in the cytoplasm and nucleus

AR, androgen receptor
 ERG, transcriptional regulator ERG



NTD, N-terminal domain
 DBD, DNA binding domain
 LBD, ligand binding domain

Domain structure of AR and ERG

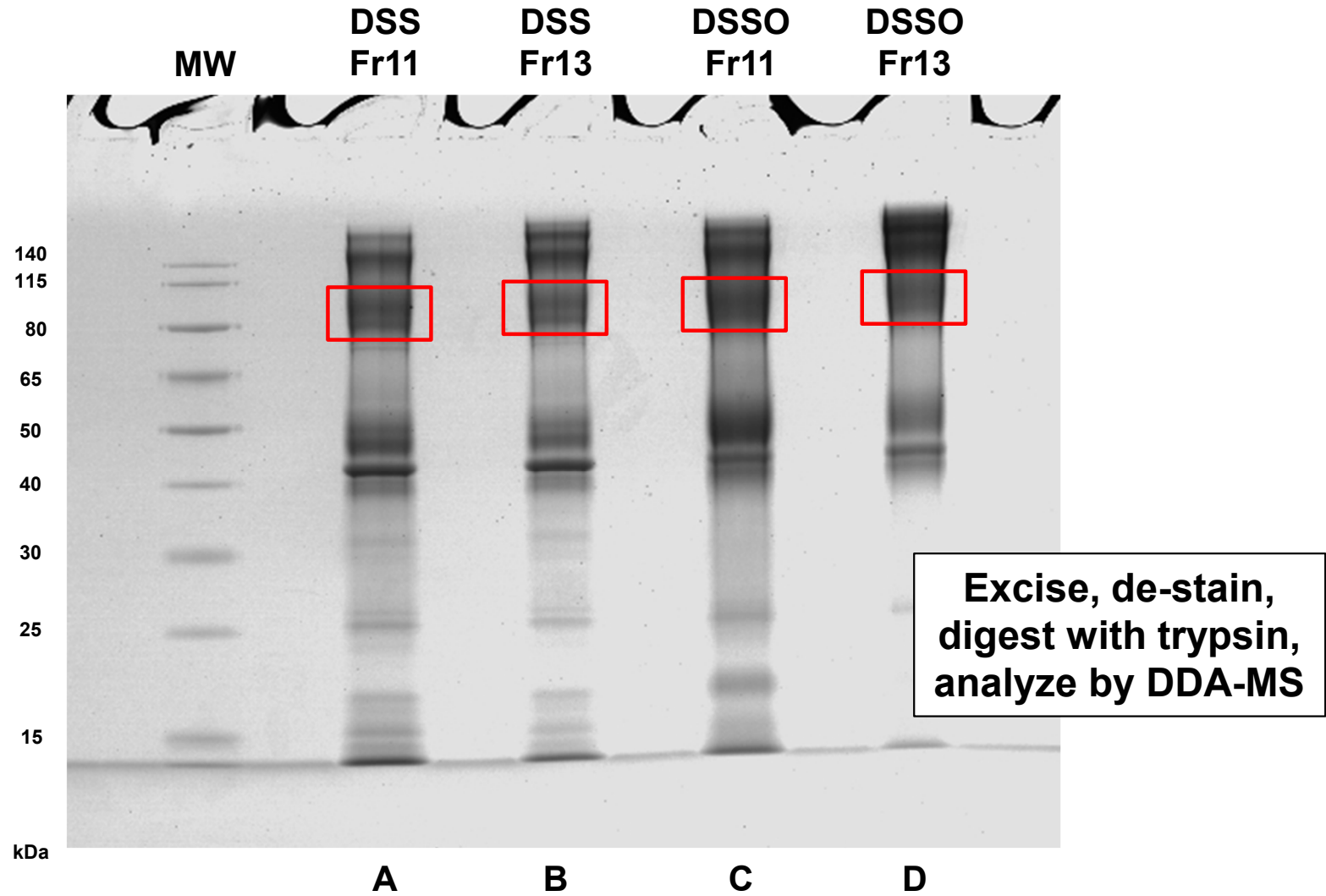
Be sure you have the correct sequences

>EWas01 Androgen receptor (530-899) (AR), mouse, NP_038504.1, **GS** N-terminus
GSDYYFPPQKTCLICGDEASGCHYGALTCGSCKVFFKRAAEGKQKYL CASRNDCTIDKFRRKNCPSCLRKCYEAGMTL
GARKLKKLGNLKLQEEGENSNAGSP TEDPSQKMTVSHIEGYECQPIFLNVLEAIEPGVVCAGHDNNQPDSFAALLSSLN
ELGERQLVHVVKWAKALPGFRNLHVDDQMAVIQYSWMGLMVFAMGWSFTNVNSRMLYFAPDLVFNEYRMHKSARMYSQC
VRMRHLSQEFGWLQITPQEF LCMKALLLFSIIPVDGLKNQKFFDEL RMNYIKELDRIIACKRKNPTSCSRRFYQLTKLL
DSVQPIARELHQFTFDLLIKSHMVSVD FPEMMAEIIISVQVPKILSGKVKPIYFHTQ

>EWas02 ERG isoform 2, human, NP_004440.1, **GS** N-terminus
GSMIQTVDPAAHIKEALSVVSEDQSLFECAYGTPHLAKTEMTASSSSDYGQTSKMSPRVPQQDWLSQPPARVTIKMEC
NPSQVNGSRNSPDECSVAKGGKMGVSPDTVGMNYGSYMEEKHMPPPNMTTNERRVIVPADPTLWSTDHVRQWLEWAVKE
YGLPDVNILLFQONIDGKELCKMTKDDFQRLTPSYNADILLSHLHYLRETPLPHLTSDDVDKALQNSPRLMHARN**TD**LPY
EPPRRSAWTGHGHPTPQSKAAQPS PSTVPKTEDQRPQLDPYQILGPTSSRLANPGSGQIQWLWQFLLELLSDSSNSSCIT
WEGTNGEFKMTDPDEVARRWGERKSKPNMNYDKLSRALRYYYDKNIMTKVHGKRYAYKFDFHGIAQALQPHPPESSLYK
YPSDLPYMGSYHAHPQKMN FVAPHPALPVTSSSFFAAPNPYWNSPTGGIYPNTRLPTSHMPSHLGTY Y

>MSL02 sp|P11308-3|ERG_HUMAN Isoform 2 of Transcriptional regulator ERG OS=Homo
sapiens OX=9606 GN=ERG
MIQTVDPAAHIKEALSVVSEDQSLFECAYGTPHLAKTEMTASSSSDYGQTSKMSPRVPQQDWLSQPPARVTIKMECNP
SQVNGSRNSPDECSVAKGGKMGVSPDTVGMNYGSYMEEKHMPPPNMTTNERRVIVPADPTLWSTDHVRQWLEWAVKEYG
LPDYNILLFQONIDGKELCKMTKDDFQRLTPSYNADILLSHLHYLRETPLPHLTSDDVDKALQNSPRLMHARN**TGGA****AFI**
FPNTSVYPEATQRITTRPLPYEPPRRSAWTGHGHPTPQSKAAQPS PSTVPKTEDQRPQLDPYQILGPTSSRLANPGSG
QIQWLWQFLLELLSDSSNSSCITWEGTNGEFKMTDPDEVARRWGERKSKPNMNYDKLSRALRYYYDKNIMTKVHGKRYAY
KFDFHGIAQALQPHPPESSLYKYPSDLPYMGSYHAHPQKMN FVAPHPALPVTSSSFFAAPNPYWNSPTGGIYPNTRLPT
TSHMPSHLGTY Y

Cross-linked AR and ERG



BioRad Criterion XT MOPS 12% SDS-PAGE reducing gel, colloidal Coomassie blue

Search against a non-specific database

MATRIX SCIENCE MASCOT Search Results **SwissProt**

User : Sam Pardo
E-mail : pardo@uthscsa.edu
Search title : Olsen Wasmuth M2021-005 201003Sols03_C3.raw (SwissProt) trypsin-1 Ox(M) Carb(C) D(NQ) Ac(Protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003Sols03_C3.raw
Database : SwissProt 2019_10 (561,356 sequences; 201,858,328 residues)
Timestamp : 4 Oct 2020 at 21:14:10 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

- Search parameters
- Score distribution
- Modification statistics for all protein families
- Legend

Protein Family Summary

Format Significance threshold p< 0.05 Max. number of families AUTO [\[help\]](#)
Target FDR (overrides sig. threshold) (not set) FDR type PSM
Display non-sig. matches Min. number of sig. unique sequences 1
Show Percolator scores Dendrograms cut at 0
Preferred taxonomy All entries

Sensitivity and FDR (reversed protein sequences)

Proteins (293) [Report Builder](#) [Unassigned \(47484\)](#) [\[permalink\]](#)

Protein families 1-10 (out of 285)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [29](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains Find Clear

▶ 1		1 ERG_HUMAN	36607	Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=ERG PE=1 SV=2
		2 FLII_BOVIN	1597	Friend leukemia integration 1 transcription factor OS=Bos taurus OX=9913 GN=FLI1 PE=2 SV=1
▶ 2		1 ANDR_MOUSE	21698	Androgen receptor OS=Mus musculus OX=10090 GN=Ar PE=1 SV=1
		2 PRGR_RANDY	85	Progesterone receptor OS=Rana dybowskii OX=71582 GN=pgr PE=1 SV=1

Search against a non-specific database

MATRIX SCIENCE MASCOT Search Results **SwissProt**

User : Sam Pardo
E-mail : pardo@uthscsa.edu
Search title : Olsen Wasmuth M2021-005 201003Sols03_C3.raw (SwissProt) trypsin-1 Ox(M) Carb(C) D(NQ) Ac(Protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003Sols03_C3.raw
Database : SwissProt 2019_10 (561,356 sequences; 201,858,328 residues)
Timestamp : 4 Oct 2020 at 21:14:10 GMT

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 Target FDR (overrides sig. threshold) (not set) FDR type PSM
 Display non-sig. matches Min. number of sig. unique sequences 1
 Show Percolator scores Dendrograms cut at 0

1 ERG_HUMAN 36607 Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=ERG PE=1 SV=2
2 FLI1_BOVIN 1597 Friend leukemia integration 1 transcription factor OS=Bos taurus OX=9913 GN=FLI1 PE=2 SV=1

1 ANDR_MOUSE 21698 Androgen receptor OS=Mus musculus OX=10090 GN=Ar PE=1 SV=1
2 PRGR_RANDY 85 Progesterone receptor OS=Rana dybowskii OX=71582 GN=pgr PE=1 SV=1

▶2 **1 ANDR_MOUSE** 21698 Androgen receptor OS=Mus musculus OX=10090 GN=Ar PE=1 SV=1
2 PRGR_RANDY 85 Progesterone receptor OS=Rana dybowskii OX=71582 GN=pgr PE=1 SV=1

Add a database with the recombinant sequences

MATRIX SCIENCE MASCOT Search Results **SwissProt and "MSLdb"**

User : Sam Pardo
E-mail : pardo@uthscsa.edu
Search title : Olsen Wasmuth M2021-005 201003Sols03_C3.raw (MSLdb; SwissProt) trypsin-1 Ox(M) Carb(C) D(NQ) Ac(protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac. 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003Sols03_C3.raw
Databases : 1: SwissProt 2019_10 (561,356 sequences; 201,858,328 residues)
2: MSLdb 200921 (578 sequences; 213,622 residues)
Timestamp : 5 Oct 2020 at 12:09:43 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

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- Score distribution
- Modification statistics for all protein families
- Legend

Protein Family Summary

Format Significance threshold p< 0.05 Max. number of families AUTO [\[help\]](#)
Target FDR (overrides sig. threshold) (not set) FDR type PSM
Display non-sig. matches Min. number of sig. unique sequences 1
Show Percolator scores Dendrograms cut at 0
Preferred taxonomy All entries

Sensitivity and FDR (reversed protein sequences)

Proteins (295) [Report Builder](#) [Unassigned \(47408\)](#) [s_permalink](#)

Protein families 1-10 (out of 285)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [29](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains Find Clear

1

1	2::EWas02	36828	ERG isoform 2, Full-length, GS N-terminus, human
2	1::ERG_HUMAN	36605	Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=ERG PE=1 SV=2
3	1::FLI1_BOVIN	1597	Friend leukemia integration 1 transcription factor OS=Bos taurus OX=9913 GN=FLI1 PE=2 SV=1

Add a database with the recombinant sequences

MATRIX SCIENCE MASCOT Search Results **SwissProt and "MSLdb"**

User : Sam Pardo
E-mail : pardo@uthscsa.edu
Search title : Olsen Wasmuth M2021-005 201003Sols03_C3.raw (MSLdb; SwissProt) trypsin-1 Ox(M) Carb(C) D(NQ) Ac(protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac. 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003Sols03_C3.raw
Databases : 1: SwissProt 2019_10 (561,356 sequences; 201,858,328 residues)
2: MSLdb 200921 (578 sequences; 213,622 residues)
Timestamp : 5 Oct 2020 at 12:09:43 GMT

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Protein Family Summary

Format	Significance threshold p<	0.05	Max. number of families	AUTO	[help]
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	Display non-sig. matches	<input type="checkbox"/>	Min. number of sig. unique sequences	1	
	Show Percolator scores	<input type="checkbox"/>	Dendrograms cut at	0	
	Preferred taxonomy	All entries			

► Sensitivity and FDR (reversed protein sequences)

Proteins (295) [Report Builder](#) [Unassigned \(47408\)](#) [s_permalink](#)

Protein families 1-10 (out of 285)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [29](#) [Next](#) [Expand all](#) [Collapse all](#)

- 1 2::EWAs02** 6828 ERG isoform 2, Full-length, GS N-terminus, human
- 2 1::ERG_HUMAN** 6605 Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=ERG PE=1 SV=2
- 3 1::FLI1_BOVIN** 1597 Friend leukemia integration 1 transcription factor OS=Bos taurus OX=9913 GN=FLI1 PE=2 SV=1

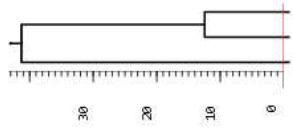
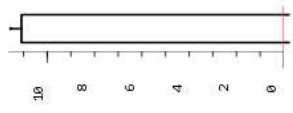
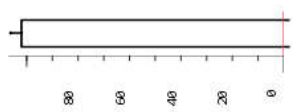
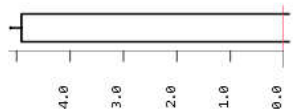
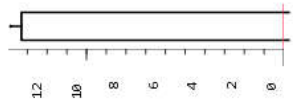
Proteins from the expression system are likely to be present

Proteins (295) [Report Builder](#) [Unassigned \(47408\)](#) [s_permalink](#)

Protein families 1–10 (out of 285)

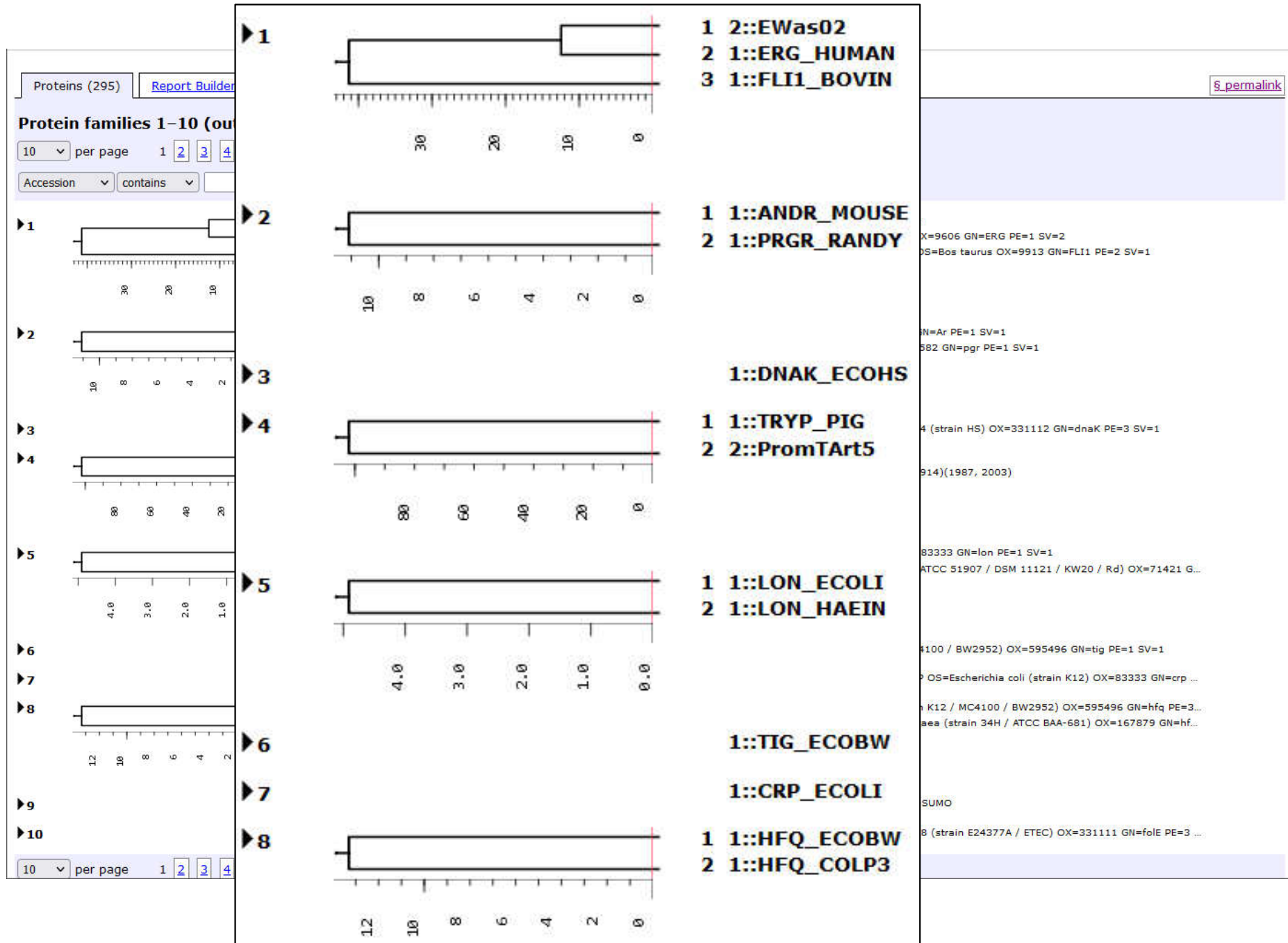
10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [29](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains Find Clear

▶ 1		<p>1 2::EWAS02 2 1::ERG_HUMAN 3 1::FLI1_BOVIN</p>	<p>36828 ERG isoform 2, Full-length, GS N-terminus, human 36605 Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=ERG PE=1 SV=2 1597 Friend leukemia integration 1 transcription factor OS=Bos taurus OX=9913 GN=FLI1 PE=2 SV=1</p>
▶ 2		<p>1 1::ANDR_MOUSE 2 1::PRGR_RANDY</p>	<p>21696 Androgen receptor OS=Mus musculus OX=10090 GN=Ar PE=1 SV=1 85 Progesterone receptor OS=Rana dybowskii OX=71582 GN=pgr PE=1 SV=1</p>
▶ 3		1::DNAK_ECOHS	<p>3730 Chaperone protein DnaK OS=Escherichia coli O9:H4 (strain HS) OX=331112 GN=dnaK PE=3 SV=1</p>
▶ 4		<p>1 1::TRYP_PIG 2 2::PromTart5</p>	<p>3280 Trypsin OS=Sus scrofa OX=9823 PE=1 SV=1 1592 Promega trypsin artifact 5 K to R mods (2239.1, 2914)(1987, 2003)</p>
▶ 5		<p>1 1::LON_ECOLI 2 2::LON_HAEIN</p>	<p>3151 Lon protease OS=Escherichia coli (strain K12) OX=83333 GN=lon PE=1 SV=1 260 Lon protease OS=Haemophilus influenzae (strain ATCC 51907 / DSM 11121 / KW20 / Rd) OX=71421 G...</p>
▶ 6		1::TIG_ECOBW	<p>1128 Trigger factor OS=Escherichia coli (strain K12 / MC4100 / BW2952) OX=595496 GN=tig PE=1 SV=1</p>
▶ 7		1::CRP_ECOLI	<p>1059 cAMP-activated global transcriptional regulator CRP OS=Escherichia coli (strain K12) OX=83333 GN=crp ...</p>
▶ 8		<p>1 1::HFQ_ECOBW 2 2::HFQ_COLP3</p>	<p>836 RNA-binding protein Hfq OS=Escherichia coli (strain K12 / MC4100 / BW2952) OX=595496 GN=hfq PE=3... 285 RNA-binding protein Hfq OS=Colwellia psychrerythraea (strain 34H / ATCC BAA-681) OX=167879 GN=hf...</p>
▶ 9		2::YGup04	<p>823 Tagged-SMARCA4-ATPase domain 731-1394-His6-SUMO</p>
▶ 10		1::GCH1_ECO24	<p>524 GTP cyclohydrolase 1 OS=Escherichia coli O139:H28 (strain E24377A / ETEC) OX=331111 GN=folE PE=3 ...</p>

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [29](#) [Next](#) [Expand all](#) [Collapse all](#)

Proteins from the expression system are likely to be present



Use specific databases and add cross-linker (DSSO) variable mods to verify reaction

MATRIX SCIENCE MASCOT Search Results

User : S.T. Weintraub
E-mail : weintraub@uthscsa.edu
Search title : Olsen Wasmuth M2021-005 Distiller update201003S0ls03_C3.raw (MSLdb UniProt_E_coli Con Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003S0ls03_C3.raw
Databases : 1: MSLdb 230513 (685 sequences; 267,424 residues) **MLdb UniProt_Ecoli_ref**
2: Contaminants_minus_Bos_taurus 20120713_20210211 (124 sequences; 62,564 residues) **Contaminants_minus bos taurus**
3: UniProt_E_coli 20180227 (6,130 sequences; 1,398,442 residues)
Timestamp : 25 May 2023 at 23:52:19 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

- Search parameters
- Score distribution
- Modification statistics for all protein families
- Legend

Protein Family Summary

Format Significance threshold p< 0.05 Max. number of families AUTO [\[help\]](#)
Target FDR (overrides sig. threshold) (not set) FDR type PSM
Display non-sig. matches Min. number of sig. unique sequences 1
Show Percolator scores Dendrograms cut at 0
Preferred taxonomy All entries

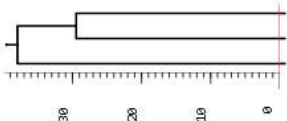
Sensitivity and FDR (reversed protein sequences)

Proteins (212) [Report Builder](#) [Unassigned \(45376\)](#) [§ permalink](#)

Protein families 1-10 (out of 207)

10 per page 1 2 3 4 5 6 ... 21 [Next](#) [Expand all](#) [Collapse all](#)

Accession contains Find Clear

1 

1 1::EWas02	73770	ERG isoform 2, human, NP_004440.1, GS N-terminus
2 1::MSL02	73156	sp P11308-3 ERG_HUMAN Isoform 2 of Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=ER...
3 1::DLib03	3054	EWS-FLI1_human-BirA_E_coli-3xHA

Use specific databases and add cross-linker (DSSO) variable mods to verify reaction

[Search parameters](#)
[Score distribution](#)
[Modification statistics for all protein families](#)
[Legend](#)

Protein Family Summary

Format Significance threshold p< Max. number of families [\[help\]](#)
 Target FDR (overrides sig. threshold) FDR type
 Display non-sig. matches Min. number of sig. unique sequences
 Show Percolator scores Dendrograms cut at
 Preferred taxonomy

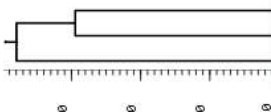
[Sensitivity and FDR \(reversed protein sequences\)](#)

Proteins (212) [Report Builder](#) [Unassigned \(45376\)](#) [§ permalink](#)

Protein families 1-10 (out of 207)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [21](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains [Find](#) [Clear](#)

1 

1	1::EWas02	73770	ERG isoform 2, human, NP_004440.1, GS N-terminus
	1::MSL02	73156	sp P11308-3 ERG_HUMAN Isoform 2 of Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=E...
	1::DLib03	3054	EWS-FLI1_human-BirA_E_coli-3xHA

2 **1::EWas04** 41962 Androgen receptor, mouse, NP_038504.1, GS N-terminus

	Score	Mass	Matches	Sequences	emPAI	
2.1	1::EWas04	41962	99758	2035 (2035)	50 (50)	281.04 Androgen receptor, mouse, NP_038504.1, GS N-terminus
	1 same set of 1::EWas04					
	1::EWas01	41962	43527	2035 (2035)	50 (50)	Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

1943 peptide matches (238 non-duplicate, 1705 duplicate)
 Auto-fit to window

Query	Dupes	Observed	Mr (expt)	Mr (calc)	ppm	M	Score	Expect	Rank	U	Peptide
966	3	411.1831	820.3517	820.3497	2.41	0	49	2e-05	1	U	K.NPTSCSR.R
980	6	411.7644	821.5143	821.5123	2.43	0	39	0.00013	1	U	R.QLVHVVK.W
993	1	412.2580	822.5015	822.4963	6.33	0	31	0.00072	1	U	R.QLVHVVK.W + Deamidated (NQ)
1664	4	433.1906	864.3667	864.3647	2.31	0	43	0.0001	1	U	R.NDCTIDK.F

Use specific databases and add cross-linker (DSSO) variable mods to verify reaction

MATRIX SCIENCE MASCOT Search Results

Protein View: EWas01

Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

Database: MSLdb
Score: 41962
Monoisotopic mass (M_r): 43527
Calculated pI: 8.90

Sequence similarity is available as [an NCBI BLAST search of EWas01 against nr](#).

Search parameters

MS data file: M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003S01s03_C3.raw
Enzyme: Trypsin: cuts C-term side of KR unless next residue is P.
Fixed modifications: [Carbamidomethyl \(C\)](#)
Variable modifications: [Acetyl \(Protein N-term\)](#), [Deamidated \(NQ\)](#), [Oxidation \(M\)](#), [Xlink:DSSO\[175\] \(K\)](#), [Xlink:DSSO\[176\] \(K\)](#)

Protein sequence coverage: 94%

Matched peptides shown in **bold red**.


1 GSDYYFPPQK **TCLICGDEAS GCHYGALTCG SCRVEFKRAA EGRQRYLCAS**
51 **RNDCTIDKFR RKNCPSCRLR KCYEAGMTLG ARKLLKLGNL KLQEEGENSN**
101 **AGSPTEDEPSQ KMTVSHIEGY ECQPIFLNVL EAIEPGVVCA GHDNNQPDFS**
151 **AALLSSLNEL GERQLVHVVK WAKALPGFRN LHVDDQMAVI QYSWMGLMVF**
201 **AMGWRSTNV NSRMLYFAPD LVFNEYRMHK SRMYSQCVRM RHLSQEFGLW**
251 **QITPQEFPCM KALLLSIIP VDGLRNQKFF DELRMNYIKE LDRIACKRK**
301 **NPTSCSRRFY QLTKLLDSVQ PIARELHQFT PDLLIKSHMV SVDFFEMMAE**
351 **IISVQVPEIL SGKVRPIYFH TQ**

Unformatted sequence string: [372 residues](#) (for pasting into other applications).

Sort by residue number increasing mass decreasing mass
Show matched peptides only predicted peptides also

Query	Start - End	Observed	Mr (expt)	Mr (calc)	ppm	M	Score	Expect	Rank	U	Peptide
36445	11 - 33	859.6807	2576.0202	2576.0223	-0.80	0	47	6.3e-05	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36446	11 - 33	859.6819	2576.0239	2576.0223	0.62	0	34	0.0013	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36449	11 - 33	1289.0206	2576.0266	2576.0223	1.70	0	70	3.7e-07	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36452	11 - 33	859.6830	2576.0273	2576.0223	1.95	0	72	2.2e-07	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36454	11 - 33	859.6832	2576.0277	2576.0223	2.09	0	29	0.0042	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36456	11 - 33	859.6832	2576.0277	2576.0223	2.13	0	27	0.0064	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36457	11 - 33	859.6834	2576.0283	2576.0223	2.34	0	47	7.8e-05	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36460	11 - 33	859.6835	2576.0286	2576.0223	2.44	0	19	0.046	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36462	11 - 33	859.6836	2576.0291	2576.0223	2.64	0	60	4e-06	1	U	K.TCLICGDEASGCHYGALTCGSCK.V

Use specific databases and add cross-linker (DSSO) variable mods to verify reaction

 **MASCOT Search Results**

Protein View: EWas01

Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

Database: MSLdb
Score: 41962
Monoisotopic mass (M_r): 43527
Calculated pI: 8.90

Sequence similarity is available as an NCBI BLAST search of EWas01 against nr

MS data file: M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003S01s03_C3.raw
Enzyme: Trypsin: cuts C-term side of KR unless next residue is P.
Fixed modifications: [Carbamidomethyl \(C\)](#)
Variable modifications: [Acetyl \(Protein N-term\)](#), [Deamidated \(NQ\)](#), [Oxidation \(M\)](#), [Xlink:DSSO\[175\] \(K\)](#), [Xlink:DSSO\[176\] \(K\)](#)

Protein sequence coverage: 94%

Matched peptides shown in **bold red**.

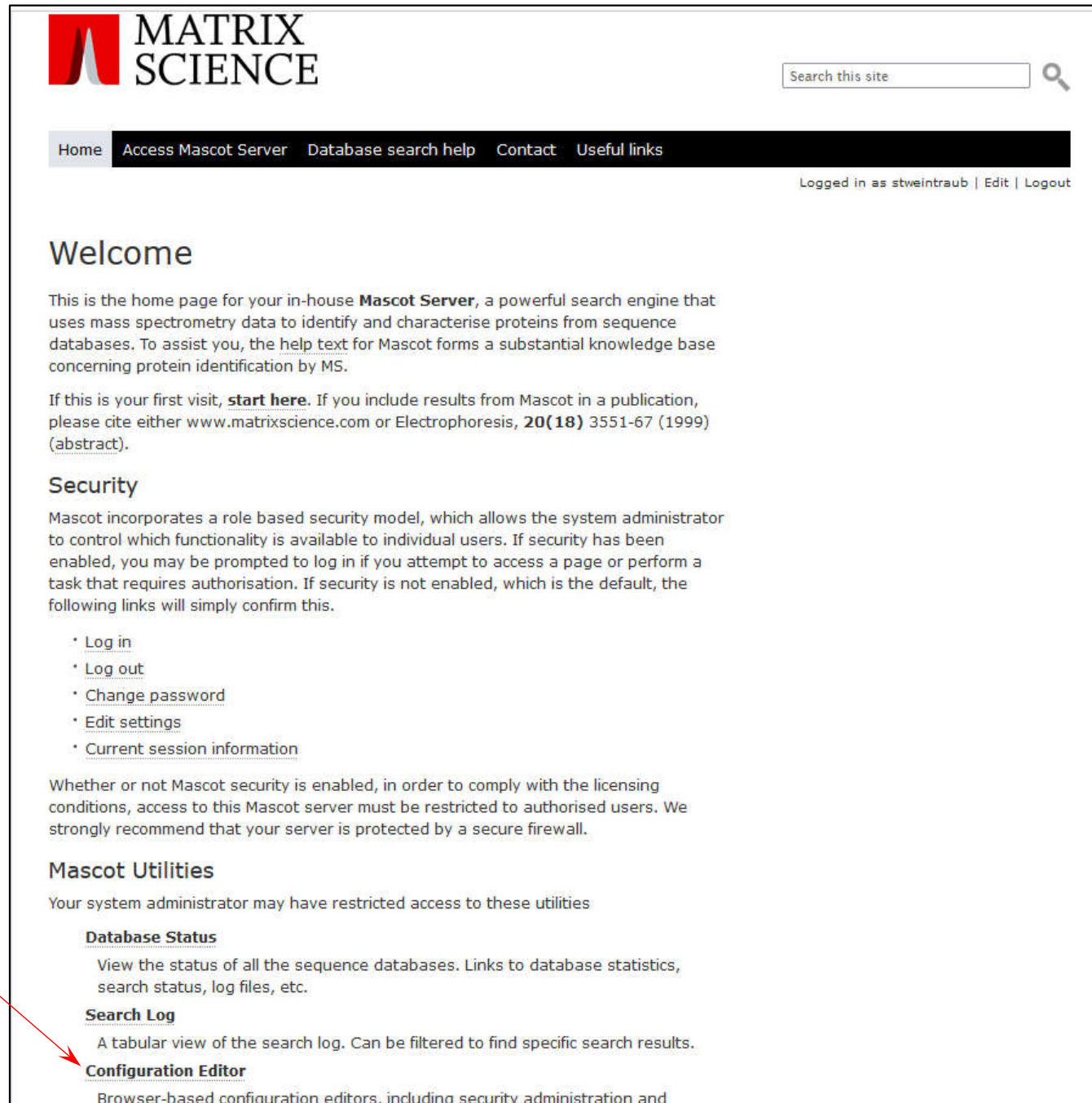
1 GSDYYFPPQK **TCLICGDEAS GCHYGALTCG SCKVFFKRAA EGKQKYL CAS**
51 **RNDCTIDKFR RKNCPSCRLR KCYEAGMTLG ARKLKRLGNL KLQEEGENSN**
101 **AGSPTEDPSQ KMTVSHIEGY ECQPIFLNVL EAIEPGVVCA GHDNNQPDSF**
151 **AALLSSLNEL GERQLVHVVK WAKALPGFRN LHVDDQMAVI QYSWMGLMVF**
201 **AMGWSFTNV NSRMLYFAPD LVFN EYRMHK SRMYSQCVRM RHLSQEF GWL**
251 **QITPQEF LCM KALLLFSIIP VDGLKNQKFF DELRMNYIKE LDRIIACKRK**
301 **NPTSCSRRFY QLTKLLDSVQ PIARELHQFT FDLLIKSHMV SVDFPEMMAE**
351 **IISVQVPKIL SGKVKPIYFH TQ**

36452	11 - 33	859.6830	2576.0273	2576.0223	1.95 0	72	2.2e-07	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36454	11 - 33	859.6832	2576.0277	2576.0223	2.09 0	29	0.0042	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36456	11 - 33	859.6832	2576.0277	2576.0223	2.13 0	27	0.0064	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36457	11 - 33	859.6834	2576.0283	2576.0223	2.34 0	47	7.8e-05	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36460	11 - 33	859.6835	2576.0286	2576.0223	2.44 0	19	0.046	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
36462	11 - 33	859.6836	2576.0291	2576.0223	2.64 0	60	4e-06	1	U	K.TCLICGDEASGCHYGALTCGSCK.V


Use specific databases and add cross-linker (DSSO) variable mods to verify reaction

28764	308 - 324	742.0673	2223.1800	2223.1722	3.54	2	33	0.0048	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28765	308 - 324	742.0673	2223.1800	2223.1722	3.55	2	29	0.012	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28770	308 - 324	742.0674	2223.1804	2223.1722	3.70	2	22	0.041	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28771	308 - 324	556.8024	2223.1804	2223.1722	3.72	2	32	0.0057	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
28772	308 - 324	742.0674	2223.1804	2223.1722	3.73	2	28	0.016	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28773	308 - 324	742.0675	2223.1807	2223.1722	3.83	2	33	0.0047	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
28775	308 - 324	556.8025	2223.1807	2223.1722	3.86	2	40	0.00085	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28779	308 - 324	742.0677	2223.1814	2223.1722	4.14	2	45	0.00028	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28780	308 - 324	742.0677	2223.1814	2223.1722	4.16	2	22	0.03	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
28781	308 - 324	556.8026	2223.1814	2223.1722	4.17	2	32	0.0045	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
28785	308 - 324	742.0679	2223.1818	2223.1722	4.35	2	24	0.011	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28786	308 - 324	742.0679	2223.1819	2223.1722	4.37	2	25	0.011	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
28787	308 - 324	742.0679	2223.1820	2223.1722	4.41	2	20	0.049	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28791	308 - 324	742.0680	2223.1822	2223.1722	4.52	2	22	0.045	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
28792	308 - 324	742.0680	2223.1822	2223.1722	4.52	2	18	0.048	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28793	308 - 324	742.0681	2223.1824	2223.1722	4.62	2	34	0.0042	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
28796	308 - 324	742.0682	2223.1827	2223.1722	4.76	2	21	0.032	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
28797	308 - 324	742.0682	2223.1829	2223.1722	4.82	2	24	0.036	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28800	308 - 324	742.0685	2223.1838	2223.1722	5.24	2	45	0.00027	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28801	308 - 324	742.0685	2223.1838	2223.1722	5.24	2	30	0.008	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28802	308 - 324	742.0688	2223.1845	2223.1722	5.53	2	36	0.0024	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
28804	308 - 324	742.0694	2223.1865	2223.1722	6.44	2	36	0.0024	1	U	R.RFYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
28819	308 - 324	742.3952	2224.1639	2224.1562	3.46	2	18	0.02	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[176] (K)
28820	308 - 324	742.3956	2224.1649	2224.1562	3.91	2	39	0.00047	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[176] (K)
28821	308 - 324	742.3956	2224.1651	2224.1562	4.02	2	35	0.0039	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[176] (K)
28822	308 - 324	742.3957	2224.1653	2224.1562	4.10	2	38	0.0007	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[176] (K)
28825	308 - 324	742.3968	2224.1685	2224.1562	5.55	2	42	0.00058	1	U	R.RFYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[176] (K)
20798	309 - 324	631.3516	1891.0330	1891.0567	-12.5	1	34	0.00062	1	U	R.FYQLTKLLDSVQPIAR.E
20799	309 - 324	946.5378	1891.0611	1891.0567	2.33	1	45	0.0001	1	U	R.FYQLTKLLDSVQPIAR.E
20800	309 - 324	631.3614	1891.0624	1891.0567	3.02	1	70	2.5e-07	1	U	R.FYQLTKLLDSVQPIAR.E
20801	309 - 324	631.3615	1891.0628	1891.0567	3.20	1	44	0.00011	1	U	R.FYQLTKLLDSVQPIAR.E
20802	309 - 324	946.5389	1891.0632	1891.0567	3.44	1	61	2.3e-06	1	U	R.FYQLTKLLDSVQPIAR.E
20803	309 - 324	631.3632	1891.0678	1891.0567	5.86	1	68	3.8e-07	1	U	R.FYQLTKLLDSVQPIAR.E
20804	309 - 324	946.5417	1891.0688	1891.0567	6.38	1	41	0.00017	1	U	R.FYQLTKLLDSVQPIAR.E
24791	309 - 324	689.7047	2066.0924	2066.0870	2.59	1	48	3.7e-05	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[175] (K)
24792	309 - 324	689.7054	2066.0943	2066.0870	3.51	1	38	0.00035	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[175] (K)
24793	309 - 324	1034.0553	2066.0960	2066.0870	4.36	1	36	0.0004	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[175] (K)
24808	309 - 324	690.0324	2067.0755	2067.0710	2.15	1	34	0.002	1	U	R.FYQLTKLLDSVQPIAR.E + Deamidated (NQ); Xlink:DSSO[175] (K)
24809	309 - 324	1034.5452	2067.0758	2067.0710	2.32	1	46	0.00031	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
24810	309 - 324	690.0326	2067.0761	2067.0710	2.43	1	35	0.0033	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
24811	309 - 324	517.7764	2067.0763	2067.0710	2.56	1	34	0.0047	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
24812	309 - 324	1034.5455	2067.0764	2067.0710	2.61	1	34	0.0045	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
24814	309 - 324	690.0330	2067.0771	2067.0710	2.91	1	50	0.00011	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
24815	309 - 324	690.0330	2067.0772	2067.0710	2.96	1	44	0.00048	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
24817	309 - 324	690.0330	2067.0772	2067.0710	2.99	1	36	0.0031	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
24818	309 - 324	690.0331	2067.0774	2067.0710	3.08	1	24	0.029	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
24819	309 - 324	690.0331	2067.0774	2067.0710	3.08	1	38	0.002	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)
24820	309 - 324	690.0331	2067.0774	2067.0710	3.08	1	38	0.002	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[176] (K)

Set up cross-linking method



MATRIX SCIENCE

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Welcome

This is the home page for your in-house **Mascot Server**, a powerful search engine that uses mass spectrometry data to identify and characterise proteins from sequence databases. To assist you, the [help text](#) for Mascot forms a substantial knowledge base concerning protein identification by MS.

If this is your first visit, [start here](#). If you include results from Mascot in a publication, please cite either www.matrixscience.com or *Electrophoresis*, **20(18)** 3551-67 (1999) ([abstract](#)).

Security

Mascot incorporates a role based security model, which allows the system administrator to control which functionality is available to individual users. If security has been enabled, you may be prompted to log in if you attempt to access a page or perform a task that requires authorisation. If security is not enabled, which is the default, the following links will simply confirm this.

- [Log in](#)
- [Log out](#)
- [Change password](#)
- [Edit settings](#)
- [Current session information](#)

Whether or not Mascot security is enabled, in order to comply with the licensing conditions, access to this Mascot server must be restricted to authorised users. We strongly recommend that your server is protected by a secure firewall.

Mascot Utilities

Your system administrator may have restricted access to these utilities

- **[Database Status](#)**
View the status of all the sequence databases. Links to database statistics, search status, log files, etc.
- **[Search Log](#)**
A tabular view of the search log. Can be filtered to find specific search results.
- **[Configuration Editor](#)**
Browser-based configuration editors, including security administration and

Mascot Configuration

S.T. Weintraub [Logout](#)

Amino Acids	Amino Acid Data
Modifications	Modification definitions
Symbols	Symbols used in chemical formulae
Linkers	Linker definitions
Enzymes	Enzyme definitions
Instruments	Fragmentation Rules
Quantitation	Quantitation Methods
Crosslinking	Crosslinking Methods
Configuration Options	Global Options in mascot.dat
Database Manager	Sequence databases, Parse Rules and automated downloads
Security	Security Administration Pages

Mascot Configuration: Crosslinking Methods

S.T. Weintraub [Logout](#)

Crosslinking Methods

Name	Strategy			
None	None			
Disulfide bridge in Lysozyme	Brute-force	Copy	Delete	Print
EDC MND1_ARATH+HOP2_ARATH	Brute-force	Copy	Delete	Print
HSA Xlink:DSS	Brute-force	Copy	Delete	Print
Xlink:Glutaraldehyde	Brute-force	Copy	Delete	Print
Wasmuth Xlink:DSS	Brute-force	Copy	Delete	Print
Wasmuth EWas01AR_EWas02ERG Xlink:DSSO	Brute-force	Copy	Delete	Print
Wasmuth EWas01AR_EWas03FOXA1 Xlink:DSSO	Brute-force	Copy	Delete	Print
Wasmuth EWas01AR_EWas02ERG_EWas03FOXA1 Xlink:DSSO	Brute-force	Copy	Delete	Print
Wasmuth EWas01AR_DNAK Xlink:DSSO	Brute-force	Copy	Delete	Print
Wasmuth EWas02ERG_EWas03FOXA1 Xlink:DSSO	Brute-force	Copy	Delete	Print
Wasmuth EWas04FL_AR_EWas04FL_AR Xlink:DSSO	Brute-force	Copy	Delete	Print
Wasmuth EWas04FL_AR_EWas03FOXA1 Xlink:DSSO	Brute-force	Copy	Delete	Print
Gupta_Yogesh_YGup12_Nsp16wt_YGup14_Nsp10wt_Xlink:BS3	Brute-force	Copy	Delete	Print
Sung PSun20BLM_PSun21CTC1_PSun22STN1 Xlink:DSSO	Brute-force	Copy	Delete	Print
Sung PSun20BLM_PSun21CTC1_PSun22STN1 Xlink:DSS	Brute-force	Copy	Delete	Print
Gupta_Yogesh YGup15Primase Xlink:DSSO	Brute-force	Copy	Delete	Print
Wasmuth EWas01AR_EWas02ERG Xlink:DSS	Brute-force	Copy	Delete	Print
Wasmuth EWas01AR_W1FT18_DNAK Xlink:DSSO	Brute-force	Copy	Delete	Print
Wasmuth EWas03FOXA1_W1FT18_DNAK Xlink:DSSO	Brute-force	Copy	Delete	Print

[New crosslinking method](#)

[Main menu](#)

Set up cross-linking method

S.T. Weintraub

Edit Crosslinking Method:Wasmuth EWas01AR_EWas02ERG Xlink:DSSO

Name

Name Description

Method

Property	Value	Action
Strategy	Brute-force ▾	
InterLink	<input checked="" type="checkbox"/>	
IntraLink	<input checked="" type="checkbox"/>	
LoopLink	<input checked="" type="checkbox"/>	
Linkers	Linker : <input type="text" value="Xlink:DSSO (K)"/>	
	Monolink : <input type="text" value="W"/> <input type="text" value="M"/> <input type="text" value="I"/> <input type="text" value="S"/>	DoesNotPairWith : <input type="text" value="Xlink:DSSO (K)"/> <input type="text" value="Xlink:DSSO (Protein N-term)"/> <input type="button" value="Delete"/>
	Linker : <input type="text" value="Xlink:DSSO (Protein N-term)"/>	
	Monolink : <input type="text" value="W"/> <input type="text" value="M"/> <input type="text" value="I"/> <input type="text" value="S"/>	DoesNotPairWith : <input type="text" value="Xlink:DSSO (K)"/> <input type="text" value="Xlink:DSSO (Protein N-term)"/> <input type="button" value="Delete"/>
Accessions	Database name : <input type="text"/>	Accession : <input type="text" value="EWas01"/> <input type="button" value="Delete"/>
	Database name : <input type="text"/>	Accession : <input type="text" value="EWas02"/> <input type="button" value="Delete"/> <input type="button" value="Add parameter"/>
Filters	Name : <input type="text" value="MinLen"/>	Value : <input type="text" value="3"/> <input type="button" value="Delete"/> <input type="button" value="Add parameter"/>
Settings	<input type="button" value="Add parameter"/>	

Set up cross-linking method

Edit Crosslinking Method: Wasmuth
EWas01AR_EWas02ERG Xlink:DSSO

S.T. Weintraub Logout

Name
Name: Description:

Method

Property	Value
Strategy	Brute-force
InterLink	<input checked="" type="checkbox"/>
IntraLink	<input checked="" type="checkbox"/>
LoopLink	<input checked="" type="checkbox"/>

Linkers

Linker	Value	Action
Linker :	Xlink:DSSO (K)	
Monolink :	W M I S	DoesNotF
Linker :	Xlink:DSSO (Protein N-term)	
Monolink :	W M I S	DoesNotF

Accessions

Database name	Accession	Action
<input type="text"/>	<input type="text"/>	delete
<input type="text"/>	<input type="text"/>	delete

Filters

Name	Value	Action
MinLen	3	Delete

Settings Add parameter

Xlink Method Selection

- Xlink:DSSO (K)
- Xlink:DMP (K)
- Xlink:DMP (Protein N-term)
- Xlink:DST (K)
- Xlink:DST (Protein N-term)
- Xlink:DSS (K)
- Xlink:DSS (Protein N-term)
- Xlink:DSSO (K)
- Xlink:DSSO (Protein N-term)
- Xlink:EGS (K)
- Xlink:EGS (Protein N-term)
- Xlink:BuUrBu (K)
- Xlink:BuUrBu (Protein N-term)
- Xlink:DTBP (K)
- Xlink:DTBP (Protein N-term)
- Xlink:DTSSP (K)
- Xlink:DTSSP (Protein N-term)
- Xlink:SMCC (C)
- Xlink:SMCC (K)
- Xlink:SMCC (Protein N-term)

Action

delete

delete

delete

delete

Add parameter

Add parameter

Re-search using a cross-linking method

MATRIX SCIENCE MASCOT Search Results

User : S.T. Weintraub
E-mail : weintraub@uthscsa.edu
Search title : Olsen Wasmuth M2021-005 Distiller update201003Sols03_C3.raw (MSLdb UniProt_E_coli Contam_minus_Bt) trypsin-2 DSSO175(K) DSSO176(K) Ox(M) Carb(C) D(NQ) Ac(Protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003Sols03_C3.raw
Databases : **1:** MSLdb 230513 (685 sequences; 267,424 residues)
2: Contaminants_minus_Bos_taurus 20120713_20210211 (124 sequences; 62,564 residues)
3: UniProt_E_coli 20180227 (6,130 sequences; 1,398,442 residues)
Timestamp : 25 May 2023 at 23:52:19 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

Not what you expected? Try [the select summary](#).

- Search parameters
- Score distribution
- Modification statistics for all protein families
- Legend

Protein Family Summary

Format	Significance threshold p<	0.05	Max. number of families	AUTO	[help]
	Target FDR (overrides sig. threshold)	(not set)	FDR type	PSM	
	Display non-sig. matches	<input type="checkbox"/>	Min. number of sig. unique sequences	1	
	Show Percolator scores	<input type="checkbox"/>	Dendrograms cut at	0	
	Preferred taxonomy	All entries			

Sensitivity and FDR (reversed protein sequences)

Proteins (212) [Report Builder](#) [Unassigned \(45376\)](#) [\[permalink\]](#)

Protein families 1-10 (out of 207)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [21](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains Find Clear

1

1	1::EWas02	73770	ERG isoform 2, human, NP_004440.1, GS N-terminus
2	1::MSL02	73156	sp P11308-3 ERG_HUMAN Isoform 2 of Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=E...
3	1::DLib03	3054	EWS-FLI1_human-BirA_E_coli-3xHA

Re-search using a cross-linking method



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MASCOT MS/MS Ions Search

Your name	weintraub	Email	weintraub@uthscsa.edu
Search title	Olsen Wasmuth M2021-005 Distiller update201003S0ls03_C3.raw (MSLdb Unif		
Database(s)	Contaminants_minus_Bos_taurus (^ MSLdb (AA) UniProt_E_coli (AA)	> <	Amino acid (AA) ^ Ab_plus Bacillus_thuringiensis contaminants cRFP GAG_mouse_UniProt Mycobacterium_tuberculosis NCBIprot Papio_anubis Phage_0105phi7-2
Taxonomy	All entries		
Enzyme	Trypsin	Allow up to	2 missed cleavages
Quantitation	None		
Crosslinking	None		
Fixed modifications	Carbamidomethyl (C)	> <	(SCS)Ni cofactor, oxidized (K) (SCS)Ni cofactor, reduced (K) Acetyl (K) Acetyl (N-term) Amidated (C-term) Amidated (Protein C-term) Ammonia-loss (N-term C) Carbamidomethyl (N-term) Carbamidomethyl:2H(2)13C(2) Carbamyl (K) Carbamyl (N-term)
	Display all modifications <input type="checkbox"/>		
Variable modifications	Acetyl (Protein N-term) Deamidated (NQ) Oxidation (M) Xlink:DSSO[175] (K)	> <	

Re-research using a cross-linking method - revise title

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MASCOT MS/MS Ions Search

Your name: Email:

Search title

MSLdb (AA) UniProt_E_coli (AA)

Ab_plus
Bacillus_thuringiensis
contaminants
cRFP
GAG_mouse_UniProt
Mycobacterium_tuberculosis
NCBIprot
Papio_anubis
Phage_0105phi7-2

Taxonomy

Enzyme **Allow up to** missed cleavages

Quantitation

Crosslinking

Fixed modifications Carbamidomethyl (C)

Display all modifications

Variable modifications Acetyl (Protein N-term) Deamidated (NQ) Oxidation (M) Xlink:DSSO[175] (K)

(SCS)Ni cofactor, oxidized (K)
(SCS)Ni cofactor, reduced (K)
Acetyl (K)
Acetyl (N-term)
Amidated (C-term)
Amidated (Protein C-term)
Ammonia-loss (N-term C)
Carbamidomethyl (N-term)
Carbamidomethyl:2H(2)13C(2)
Carbamyl (K)
Carbamyl (N-term)

Remove variable mods

MASCOT MS/MS Ions Search

Your name	<input type="text" value="weintraub"/>	Email	<input type="text" value="weintraub@uthscsa.edu"/>
Search title	<input type="text" value="rs 55591 XLink DSSO EWas01_EWas02 tryp-2 -mods Olsen Wasmuth M2021-0"/>		
Database(s)	<input type="text" value="Contaminants_minus_Bos_taurus (AA)"/> <input type="text" value="MSLdb (AA)"/> <input type="text" value="UniProt_E_coli (AA)"/>	<input type="button" value=">"/> <input type="button" value="<"/>	<input type="text" value="Amino acid (AA)"/> <input type="text" value="Ab_plus"/> <input type="text" value="Bacillus_thuringiensis"/> <input type="text" value="contaminants"/> <input type="text" value="cRFP"/> <input type="text" value="GAG_mouse_UniProt"/> <input type="text" value="Mycobacterium_tuberculosis"/> <input type="text" value="NCBIprot"/> <input type="text" value="Papio_anubis"/> <input type="text" value="Phage_0105phi7-2"/>
Taxonomy	<input type="text" value="All entries"/>		
Enzyme	<input type="text" value="Trypsin"/>	Allow up to	<input type="text" value="2"/> missed cleavages
Quantitation	<input type="text" value="None"/>		
Crosslinking	<input type="text" value="None"/>		
Fixed modifications	<input type="text" value="Carbamidomethyl (C)"/>	<input type="button" value=">"/> <input type="button" value="<"/>	<input type="text" value="(SCS)Ni cofactor, oxidized (K)"/> <input type="text" value="(SCS)Ni cofactor, reduced (K)"/> <input type="text" value="Acetyl (K)"/> <input type="text" value="Acetyl (N-term)"/> <input type="text" value="Acetyl (Protein N-term)"/> <input type="text" value="Amidated (C-term)"/> <input type="text" value="Amidated (Protein C-term)"/> <input type="text" value="Ammonia-loss (N-term C)"/> <input type="text" value="Carbamidomethyl (N-term)"/> <input type="text" value="Carbamidomethyl:2H(2)13C(2)"/> <input type="text" value="Carbamyl (K)"/>
	Display all modifications <input type="checkbox"/>		
Variable modifications	<input type="text" value="Oxidation (M)"/>	<input type="button" value=">"/> <input type="button" value="<"/>	

Select cross-linking method

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MASCOT

Your name

Search title

Database(s)

Taxonomy

Enzyme

Quantitation

Crosslinking

Fixed modifications

Display all modifications

Variable modifications

Modification list:

- (SCS)Ni cofactor, oxidized (K)
- (SCS)Ni cofactor, reduced (K)
- Acetyl (K)
- Acetyl (N-term)
- Acetyl (Protein N-term)
- Amidated (C-term)
- Amidated (Protein C-term)
- Ammonia-loss (N-term C)
- Carbamidomethyl (N-term)
- Carbamidomethyl:2H(2)13C(2)
- Carbamyl (K)

Search results list:

- Disulfide bridge in Lysozyme
- EDC MND1_ARATH+HOP2_ARATH
- HSA Xlink:DSS
- Xlink:Glutaraldehyde
- Wasmuth Xlink:DSS
- Wasmuth EWas01AR_EWas02ERG Xlink:DSSO
- Wasmuth EWas01AR_EWas03FOXA1 Xlink:DSSO
- Wasmuth EWas01AR_EWas02ERG_EWas03FOXA1 Xlink:DSSO
- Wasmuth EWas01AR_DNAK Xlink:DSSO
- Wasmuth EWas02ERG_EWas03FOXA1 Xlink:DSSO
- Wasmuth EWas04FL_AR_EWas04FL_AR Xlink:DSSO
- Wasmuth EWas04FL_AR_EWas03FOXA1 Xlink:DSSO
- Gupta_Yogesh_YGup12_Nsp16wt_YGup14_Nsp10wt_Xlink:BS3
- Sung PSun20BLM_PSun21CTC1_PSun22STN1 Xlink:DSSO
- Sung PSun20BLM_PSun21CTC1_PSun22STN1 Xlink:DSS
- Gupta_Yogesh YGup15Primase Xlink:DSSO
- Wasmuth EWas01AR_EWas02ERG Xlink:DSS
- Wasmuth EWas01AR_W1FT18_DNAK Xlink:DSSO
- Wasmuth EWas03FOXA1_W1FT18_DNAK Xlink:DSSO

Oops - no decoy search when using a cross-linking method

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MASCOT MS/MS Ions Search

Your name weintraub **Email** weintraub@uthscsa.edu

Search title rs 55591 XLink DSSO EWas01_EWas02 tryp-2 -mods Olsen Wasmuth M2021-0

Database(s) Contaminants_minus_Bos_taurus (, ^
MSLdb (AA) >
UniProt_E_coli (AA) <

Amino acid (AA) Ab_plus
Bacillus_thuringiensis
contaminants

🌐 g1200mas-ap01wp.win.uthscsa.edu

Error: Cannot combine Decoy with Crosslinking

[OK](#)

Taxonomy All entries

Enzyme Trypsin **Allow up to** 2 missed cleavages

Quantitation None

Crosslinking Wasmuth EWas01AR_EWas02ERG Xlink:DSS

Fixed modifications Carbamidomethyl (C) >
<

Variable modifications Oxidation (M) >
<

Display all modifications

(SCS)Ni cofactor, oxidized (K)
(SCS)Ni cofactor, reduced (K)
Acetyl (K)
Acetyl (N-term)
Acetyl (Protein N-term)
Amidated (C-term)
Amidated (Protein C-term)
Ammonia-loss (N-term C)
Carbamidomethyl (N-term)
Carbamidomethyl:2H(2)13C(2)
Carbamyl (K)

Ready to search

Your name **Email**

Search title

Database(s)

Contaminants_minus_Bos_taurus (^	>	Amino acid (AA)
MSLdb (AA)	<	Ab_plus
UniProt_E_coli (AA)		Bacillus_thuringiensis
		contaminants
		cRFP
		GAG_mouse_UniProt
		Mycobacterium_tuberculosis
		NCBIprot
		Papio_anubis
		Phage_0105phi7-2

Taxonomy

Enzyme **Allow up to** missed cleavages

Quantitation

Crosslinking

Fixed modifications

Carbamidomethyl (C)	>	(SCS)Ni cofactor, oxidized (K)
	<	(SCS)Ni cofactor, reduced (K)
		Acetyl (K)
		Acetyl (N-term)
		Acetyl (Protein N-term)
		Amidated (C-term)
		Amidated (Protein C-term)
		Ammonia-loss (N-term C)
		Carbamidomethyl (N-term)
		Carbamidomethyl:2H(2)13C(2)
		Carbamyl (K)

Display all modifications

Variable modifications

Oxidation (M)	>	
	<	

Peptide tol. **# ¹³C**

MS/MS tol.


Peptide charge 1+, 2+ and 3+ **Monoisotopic** **Average**

Data file

Data format Mascot generic

Instrument **Error tolerant**

Decoy **Target PSM FDR**



Search results - Xlink EWas01AR-EWas02ERG

MATRIX SCIENCE MASCOT Search Results

User :
E-mail :
Search title : rs 55591 XLink DSSO EWas01_EWas02 tryp-2 -mods Olsen Wasmuth M2021-005 Distiller update201003Sols03_C3.raw (MSLdb UniProt_E_coli Contam_minus_Bt) trypsin-2 DSSO175(K) DSSO176(K) Ox(M) Carb(C) D(NQ) Ac(Protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003Sols03_C3.raw
Databases : **1**: Contaminants_minus_Bos_taurus 20120713_20210211 (124 sequences; 62,564 residues)
2: MSLdb 230513 (685 sequences; 267,424 residues)
3: UniProt_E_coli 20180227 (6,130 sequences; 1,398,442 residues)
Timestamp : 26 May 2023 at 00:36:17 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

▶ **Search parameters**
▶ **Score distribution**
▶ **Modification statistics for all protein families**
▶ **Legend**

Protein Family Summary

Format Significance threshold p< 0.05 Max. number of families AUTO [\[help\]](#)
Display non-sig. matches Min. number of sig. unique sequences 1
Dendrograms cut at 0
Preferred taxonomy All entries

▶ **Sensitivity**

Proteins (185) [Report Builder](#) [Unassigned \(45933\)](#) [s_permalink](#)

Protein families 1-10 (out of 179)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [18](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains [Find](#) [Clear](#)

▶ **1**

1 2::EWas02 69353 ERG isoform 2, human, NP_004440.1, GS N-terminus
3 2::DLib03 2939 EWS-FLI1_human-BirA_E_coli-3xHA
2 2::MSL02 67101 sp|P11308-3|ERG_HUMAN Isoform 2 of Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=E...

▶ **2**

2::EWas01 43554 Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

Search results - Xlink EWas01AR-EWas02ERG

MATRIX SCIENCE MASCOT Search Results

Protein View: EWas01

Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

Database: MSLdb
 Score: 43554
 Monoisotopic mass (M_r): 43527
 Calculated pI: 8.90

Sequence similarity is available as [an NCBI BLAST search of EWas01 against nr](#).

Search parameters

MS data file: M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003S01s03_C3.raw
 Enzyme: Trypsin: cuts C-term side of KR unless next residue is P.
 Fixed modifications: [Carbamidomethyl \(C\)](#)
 Variable modifications: [Oxidation \(M\)](#)
 Linkers: [Xlink:DSSO \(K\)](#), [Xlink:DSSO \(Protein N-term\)](#)

Protein sequence coverage: 100%

Matched peptides shown in **bold red**.

1 GSDYYFPPQK TCLICGDEAS GCHYGALTCG SCKVFFKRAA EGKQKYL CAS
 51 RNDCTIDKFR RRNCPSCRLR KCYEAGMTLG ARKLRKLGNL KLQEEGENSN
 101 AGSPTEDPSQ KMTVSHIEGY ECQPIFLNVL EAIEPGVVCA GHDNNQPDSF
 151 AALLSSLNEL GERQLVHVVK WAKALPGFRN LHVDDQMAVI QYSWMGLMVF
 201 AMGWSFTNV NSRMLYFAPD LVPNEYRMHK SRMYSQCVRM RHLSQEFQWL
 251 QITPQEFPCM KALLLSIIP VDGLKNQKFF DELRMNYIKE LDRIACKRKR
 301 NPTSCSRRFY QLTKLLDSVQ PIARELHQFT PDLLIKSHMV SVDFPEMMAE
 351 IISVQVFKIL SGKVKPIYFH TQ

Unformatted sequence string: [372 residues](#) (for pasting into other applications).

Sort by residue number increasing mass decreasing mass
 Show matched peptides only predicted peptides also

Query	Start-End	Observed	Mr (expt)	Mr (calc)	ppm	M	M	Score	Expect	Rank	U	Peptide
33394	1 - 10	824.3640	2470.0702	2470.0457	9.92	0	0	17	0.025	1		-.GSDYYFPPQK.T Protein N-term<-Xlink:DSSO->K2 SKPNMNYDK[2::EWas02] + Oxidation (M)
33396	1 - 10	824.3643	2470.0711	2470.0457	10.3	0	0	15	0.043	1		-.GSDYYFPPQK.T Protein N-term<-Xlink:DSSO->K2 SKPNMNYDK[2::EWas02] + Oxidation (M)
33398	1 - 10	824.3648	2470.0724	2470.0457	10.8	0	0	16	0.034	1		-.GSDYYFPPQK.T Protein N-term<-Xlink:DSSO->K2 SKPNMNYDK[2::EWas02] + Oxidation (M)
36445	11 - 33	859.6807	2576.0202	2576.0223	-0.80	0	-	47	5.5e-05	1	U	K.TCLICGDEASGCHYGALTCGSK.V
36446	11 - 33	859.6819	2576.0239	2576.0223	0.62	0	-	34	0.0012	1	U	K.TCLICGDEASGCHYGALTCGSK.V
36449	11 - 33	1289.0206	2576.0266	2576.0223	1.70	0	-	70	3.4e-07	1	U	K.TCLICGDEASGCHYGALTCGSK.V

Search results - Xlink EWas01AR-EWas02ERG



Protein View: EWas01

Androgen receptor (530-899)(AR)

Database: MSLdb
 Score: 43554
 Monoisotopic mass (M_r): 43527
 Calculated pI: 8.90

Sequence similarity is available as [an NCBI](#)

Search parameters

MS data file: M:\Olsen_Shaun
 Enzyme: Trypsin: cuts C-
 Fixed modifications: [Carbamidomethyl](#)
 Variable modifications: [Oxidation \(M\)](#)
 Linkers: [Xlink:DSSO \(K\)](#)

Protein sequence coverage: 100%

Matched peptides shown in **bold red**.

1 **GSDYYFPPQK** **TCLICGDEAS** **GCHYGALTCG**
 51 **RNDCTIDKFR** **RRNCPSCLLR** **KCYEAGMTLG**
 101 **AGSPTEDPSQ** **KMTVSHIEGY** **ECQPIFLNVL**
 151 **AALLSSLNEL** **GERQLVHVVK** **WAKALPGFRN**
 201 **AMGWSFTNV** **NSRMLYFAPD** **LVFNEYRMHK**
 251 **QITPQEFPCM** **KALLFSIIP** **VDGLKNQKFF**
 301 **NPTSCSRRFY** **QLTKLLDSVQ** **PIARELHQFT**
 351 **IISVQVPKIL** **SGKVKPIYFH** **TQ**

Search parameters

MS data file: M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003S01s03_C3.raw
 Enzyme: Trypsin: cuts C-term side of KR unless next residue is P.
 Fixed modifications: [Carbamidomethyl \(C\)](#)
 Variable modifications: [Oxidation \(M\)](#)
 Linkers: [Xlink:DSSO \(K\)](#), [Xlink:DSSO \(Protein N-term\)](#)

Protein sequence coverage: 100%

Matched peptides shown in **bold red**.

1 **GSDYYFPPQK** **TCLICGDEAS** **GCHYGALTCG** **SKVFFKRAA** **EGKQKYL CAS**
 51 **RNDCTIDKFR** **RRNCPSCLLR** **KCYEAGMTLG** **ARKLKLGNL** **KLQEEGENSN**
 101 **AGSPTEDPSQ** **KMTVSHIEGY** **ECQPIFLNVL** **EAIEPGVVCA** **GHDNNQPSDF**
 151 **AALLSSLNEL** **GERQLVHVVK** **WAKALPGFRN** **LHVDDQMAVI** **QYSWMGLMVF**
 201 **AMGWSFTNV** **NSRMLYFAPD** **LVFNEYRMHK** **SRMYSQCVRM** **RHLSQEFQWL**
 251 **QITPQEFPCM** **KALLFSIIP** **VDGLKNQKFF** **DELRMNYIKE** **LDRIIACKRK**
 301 **NPTSCSRRFY** **QLTKLLDSVQ** **PIARELHQFT** **FDLLIKSHMV** **SVDFPEMMAE**
 351 **IISVQVPKIL** **SGKVKPIYFH** **TQ**

ppm	M	M	Score	Expect	Rank	U	Peptide
9.92	0	0	17	0.025	1		-.GSDYYFPPQK.T Protein N-term<-Xlink:DSSO->K2 SKPNMNYDK[2::EWas02] + Oxidation (M)
10.3	0	0	15	0.043	1		-.GSDYYFPPQK.T Protein N-term<-Xlink:DSSO->K2 SKPNMNYDK[2::EWas02] + Oxidation (M)
10.8	0	0	16	0.034	1		-.GSDYYFPPQK.T Protein N-term<-Xlink:DSSO->K2 SKPNMNYDK[2::EWas02] + Oxidation (M)
-0.80	0	-	47	5.5e-05	1	U	K.TCLICGDEASGCHYGALTCGSCK.V
0.62	0	-	34	0.0012	1	U	K.TCLICGDEASGCHYGALTCGSCK.V

Search results - Xlink EWas01AR-EWas02ERG

4860	309 - 324	690.0338	2067.0797	2067.0710	4.20	1 -	30	0.0016	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4861	309 - 324	690.0339	2067.0798	2067.0710	4.21	1 -	22	0.0083	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4862	309 - 324	690.0339	2067.0798	2067.0710	4.21	1 -	28	0.0073	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4863	309 - 324	690.0339	2067.0798	2067.0710	4.24	1 -	25	0.005	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4864	309 - 324	1034.5472	2067.0798	2067.0710	4.26	1 -	52	2.1e-05	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4865	309 - 324	690.0339	2067.0799	2067.0710	4.27	1 -	38	0.00028	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4866	309 - 324	690.0339	2067.0799	2067.0710	4.28	1 -	24	0.02	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4867	309 - 324	690.0339	2067.0799	2067.0710	4.30	1 -	31	0.0064	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4868	309 - 324	690.0340	2067.0801	2067.0710	4.37	1 -	30	0.0014	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4869	309 - 324	690.0340	2067.0801	2067.0710	4.39	1 -	19	0.017	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4870	309 - 324	690.0340	2067.0801	2067.0710	4.39	1 -	19	0.016	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4871	309 - 324	690.0340	2067.0802	2067.0710	4.42	1 -	49	2.5e-05	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4872	309 - 324	690.0340	2067.0802	2067.0710	4.43	1 -	27	0.0033	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4873	309 - 324	1034.5474	2067.0802	2067.0710	4.45	1 -	23	0.014	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4874	309 - 324	690.0340	2067.0803	2067.0710	4.49	1 -	23	0.0068	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4875	309 - 324	690.0341	2067.0804	2067.0710	4.50	1 -	39	0.00024	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4876	309 - 324	690.0341	2067.0805	2067.0710	4.58	1 -	21	0.0096	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4877	309 - 324	690.0341	2067.0805	2067.0710	4.58	1 -	28	0.0023	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4878	309 - 324	690.0341	2067.0805	2067.0710	4.59	1 -	30	0.0016	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4879	309 - 324	690.0341	2067.0806	2067.0710	4.62	1 -	31	0.0013	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4880	309 - 324	690.0342	2067.0807	2067.0710	4.65	1 -	41	0.00024	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4881	309 - 324	690.0342	2067.0807	2067.0710	4.68	1 -	20	0.013	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4882	309 - 324	690.0342	2067.0808	2067.0710	4.72	1 -	20	0.014	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4883	309 - 324	690.0342	2067.0808	2067.0710	4.73	1 -	27	0.0033	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4884	309 - 324	1034.5477	2067.0808	2067.0710	4.74	1 -	34	0.00058	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4885	309 - 324	690.0342	2067.0809	2067.0710	4.78	1 -	18	0.031	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4886	309 - 324	690.0343	2067.0810	2067.0710	4.79	1 -	45	6e-05	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4887	309 - 324	690.0343	2067.0810	2067.0710	4.84	1 -	25	0.021	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4888	309 - 324	1034.5478	2067.0810	2067.0710	4.84	1 -	45	6e-05	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4889	309 - 324	690.0344	2067.0815	2067.0710	5.04	1 -	38	0.00026	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4890	309 - 324	1034.5482	2067.0818	2067.0710	5.23	1 -	34	0.00077	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4891	309 - 324	690.0346	2067.0819	2067.0710	5.23	1 -	25	0.0058	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
4892	309 - 324	1034.5546	2067.0946	2067.0710	11.4	1 -	14	0.048	1	U	R.FYQLTKLLDSVQPIAR.E + Xlink:DSSO[W]
39633	309 - 324	681.8586	2723.4054	2723.4105	-1.85	1 1	15	0.036	1	R	FYQLTKLLDSVQPIAR.E K314<-Xlink:DSSO->K5 WGERK[2::Ewas02]
43921	309 - 324	796.1778	3180.6820	3180.6681	4.35	1 0	33	0.00074	1	U	R.FYQLTKLLDSVQPIAR.E K314<-Xlink:DSSO->K365 K.VKPIYFHTQ.-
47377	309 - 324	951.7306	3802.8930	3802.8732	5.23	1 2	27	0.031	1	R	FYQLTKLLDSVQPIAR.E K314<-Xlink:DSSO->K1 KSKPNMNYDKLSR[2::Ewas02] + K3<-Xlink:DSSO[I]->K10; Oxidation (M)
49033	309 - 324	1058.7566	4230.9972	4230.9759	5.05	1 1	44	8.1e-05	1	U	R.FYQLTKLLDSVQPIAR.E + 2 Oxidation (M)
49401	309 - 324	1096.3159	4381.2345	4381.2264	1.85	1 1	49	2.5e-05	1	U	[2::Ewas02]ETPLPHLTSDDVDKALQNSPR K14<-Xlink:DSSO->K314 R.FYQLTKLLDSVQPIAR.E
50325	309 - 324	921.4772	4602.3497	4602.3329	3.66	1 1	42	0.00011	1	U	[2::Ewas02]SAWTGHGHTPQS KAAQSPSTVPK K14<-Xlink:DSSO->K314 R.FYQLTKLLDSVQPIAR.E
50326	309 - 324	921.4779	4602.3530	4602.3329	4.36	1 1	20	0.013	1	U	[2::Ewas02]SAWTGHGHTPQS KAAQSPSTVPK K14<-Xlink:DSSO->K314 R.FYQLTKLLDSVQPIAR.E
4842	315 - 324	556.3279	1110.6413	1110.6397	1.42	0 -	35	0.00037	1	U	K.LLDSVQPIAR.E
4843	315 - 324	556.3281	1110.6417	1110.6397	1.78	0 -	20	0.011	1	U	K.LLDSVQPIAR.E
4844	315 - 324	556.3281	1110.6417	1110.6397	1.81	0 -	32	0.00072	1	U	K.LLDSVQPIAR.E
4845	315 - 324	556.3282	1110.6419	1110.6397	2.03	0 -	22	0.0066	1	U	K.LLDSVQPIAR.E

Search results - Xlink EWas01AR-EWas02ERG

Peptide View

MS/MS Fragmentation of **ETPLPHLTSDDVDKALQNSP** K14<-Xlink:DSSO->K6 **FYQLTKLLDSVQPIAR**

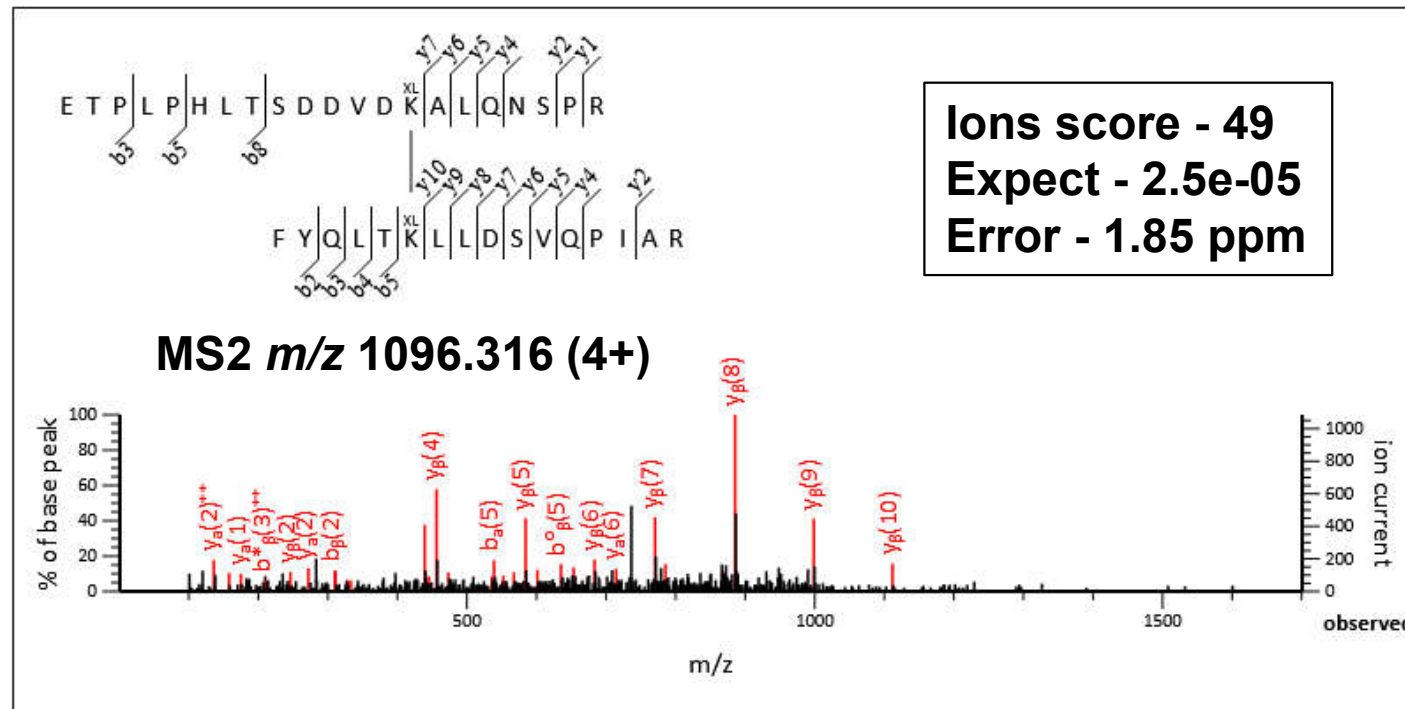
Found in **EWas02** in **MSLdb**, ERG isoform 2, human, NP_004440.1, GS N-terminus

Found in **EWas01** in **MSLdb**, Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

Match to Query 49401: 4381.234496 from(1096.315900,4+) intensity(29940.8160) scans(52769) rawscans(sn52769) rtinseconds(6033.2714) index(43834)

Title: 43835: Scan 52769 (rt=100.555) [M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003SOIs03_C3.raw]

Data file M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003SOIs03_C3.raw



Label all possible matches Label matches used for scoring

Monoisotopic mass of neutral linked peptide Mr(calc) : 4381.2264

Monoisotopic mass of neutral free alpha peptide Mr(calc): 2332.1659

Monoisotopic mass of neutral free beta peptide Mr(calc) : 1891.0567

Fixed modifications: Carbamidomethyl (C) (apply to specified residues or termini only)

Intact link : Alpha K14<-Xlink:DSSO->K6 Beta

Ions Score: 49 Expect: 2.5e-05

Matches : 37/366 fragment ions using 77 most intense peaks ([help](#))

Search results - Xlink EWas01AR-EWas02ERG

Peptide View

MS/MS Fragmentation of **ETPLPHLTSDDVDK**KL**ALQNSP**RL **Xlink:DSSO->K1** **KNCPCSR**

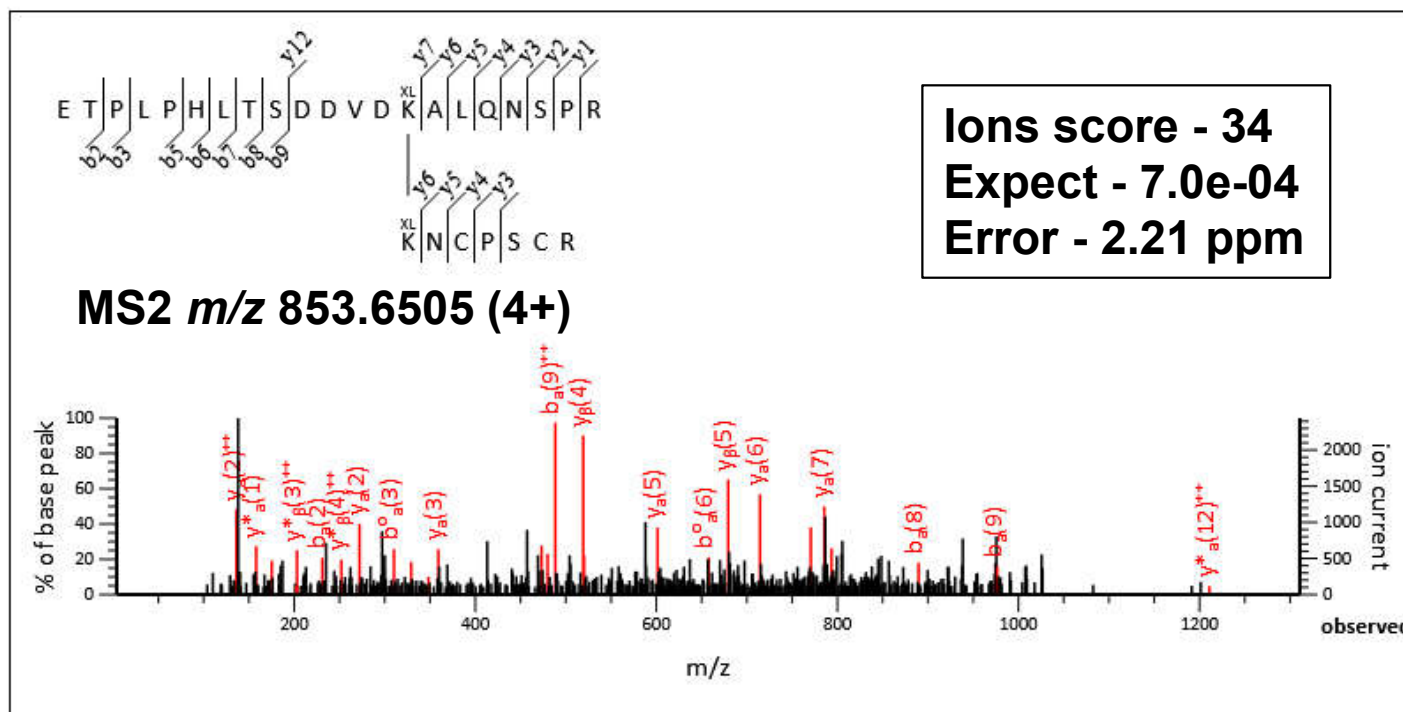
Found in **EWas02** in **MSLdb**, ERG isoform 2, human, NP_004440.1, GS N-terminus

Found in **EWas01** in **MSLdb**, Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

Match to Query 45029: 3410.572856 from(853.650490,4+) intensity(131677.4200) scans(30748) rawscans(sn30748) rtinseconds(4011.8647) index(24223)

Title: 24224: Scan 30748 (rt=66.8644) [M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003SOIs03_C3.raw]

Data file M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003SOIs03_C3.raw



3.98

to

1310.81



Label all possible matches Label matches used for scoring

Monoisotopic mass of neutral linked peptide Mr(calc) : 3410.5653

Monoisotopic mass of neutral free alpha peptide Mr(calc): 2332.1659

Monoisotopic mass of neutral free beta peptide Mr(calc) : 920.3956

Fixed modifications: Carbamidomethyl (C) (apply to specified residues or termini only)

Intact link : Alpha K14<-Xlink:DSSO->K1 Beta

Ions Score: 34 Expect: 0.00071

Matches : 29/270 fragment ions using 63 most intense peaks [\(help\)](#)

Search results - Xlink EWas01AR-EWas02ERG

Peptide View

MS/MS Fragmentation of **ETPLPHLTSDDVDKALQNSPK**←Xlink:DSSO→**KI** KNCPSCR

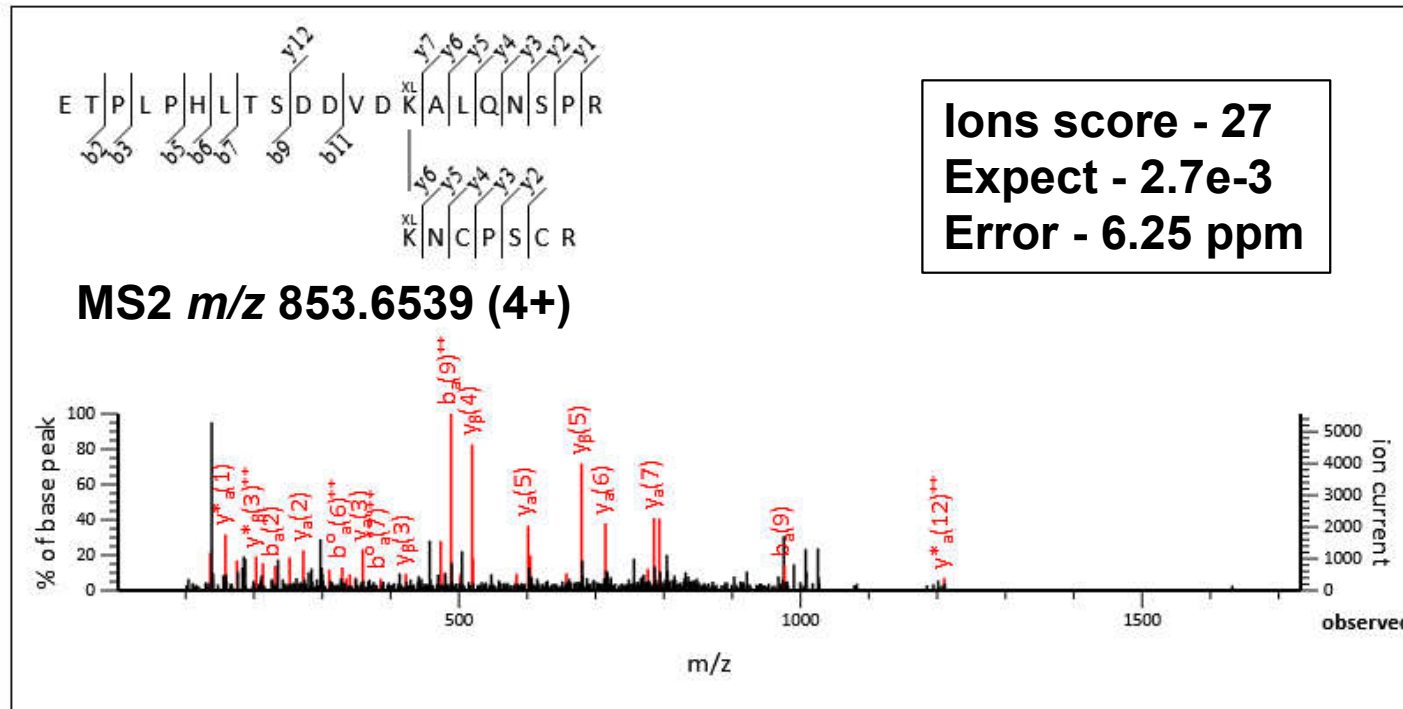
Found in **EWas02** in **MSLdb**, ERG isoform 2, human, NP_004440.1, GS N-terminus

Found in **EWas01** in **MSLdb**, Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

Match to Query 45032: 3410.586656 from(853.653940,4+) intensity(172497.6000) scans(30980) rawscans(sn30980) rtinseconds(4030.1333) index(24440)

Title: 24441: Scan 30980 (rt=67.1689) [M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003S0Is03_C3.raw]

Data file M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003S0Is03_C3.raw



1.14

to

1731.96



Label all possible matches Label matches used for scoring

Monoisotopic mass of neutral linked peptide Mr(calc) : 3410.5653

Monoisotopic mass of neutral free alpha peptide Mr(calc): 2332.1659

Monoisotopic mass of neutral free beta peptide Mr(calc) : 920.3956

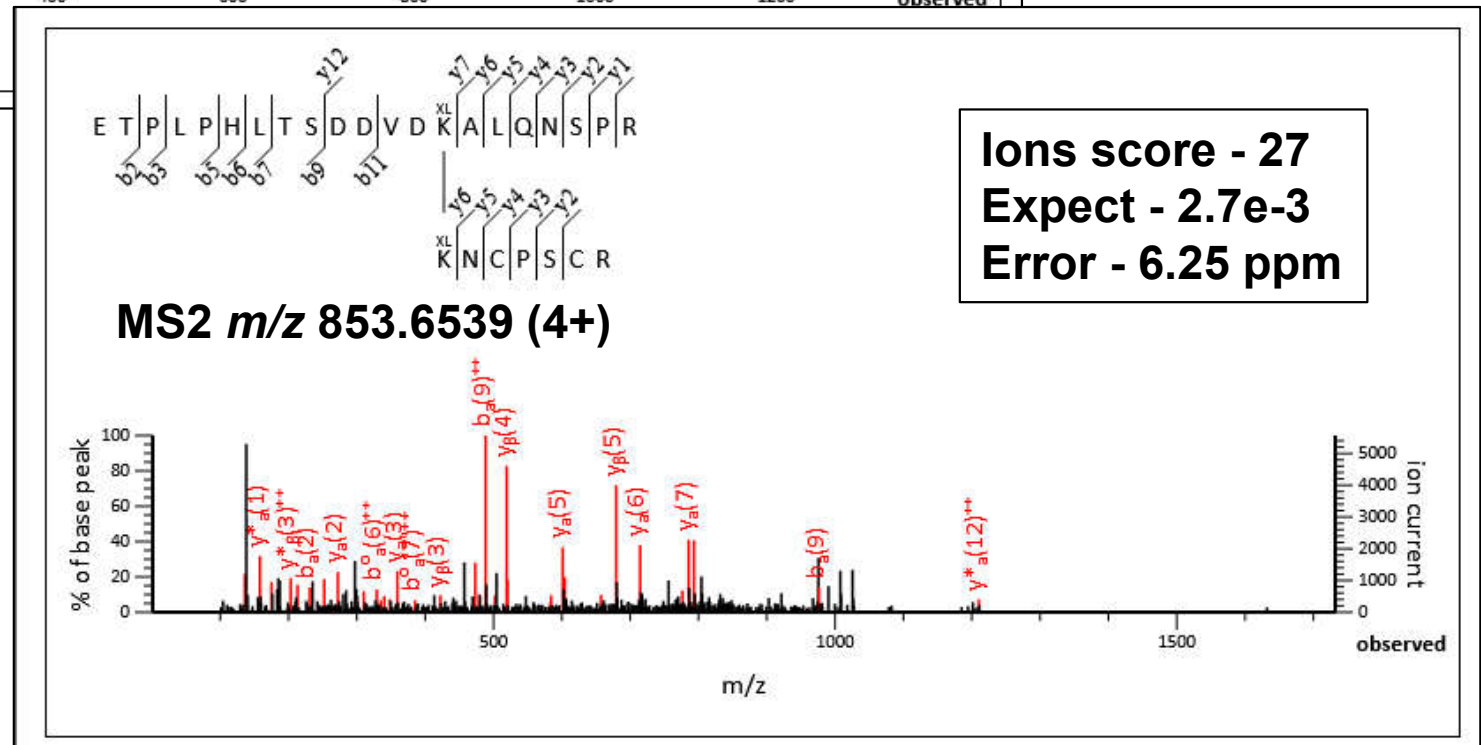
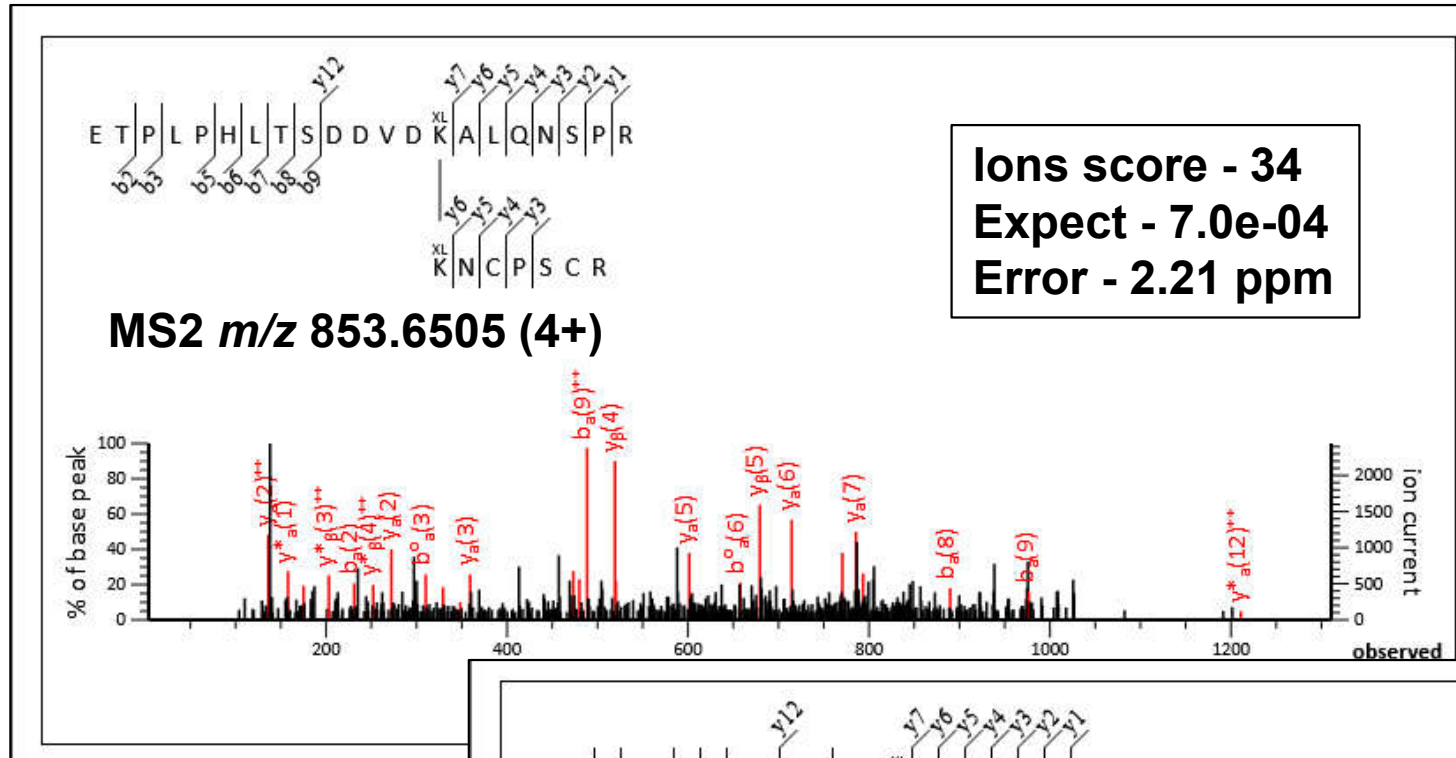
Fixed modifications: Carbamidomethyl (C) (apply to specified residues or termini only)

Intact link : Alpha K14<-Xlink:DSSO->K1 Beta

Ions Score: 27 Expect: 0.0027

Matches : 38/270 fragment ions using 88 most intense peaks [\(help\)](#)


Search results - Xlink EWas01AR-EWas02ERG



Export search results for xiVIEW

MATRIX SCIENCE MASCOT Search Results

User :
E-mail :
Search title : rs 55591 XLink DSSO EWas01_EWas02 tryp-2 -mods Olsen Wasmuth M2021-005 Distiller update201003Sols03_C3.raw (MSLdb UniProt_E_coli Contam_minus_Bt) trypsin-2 DSSO175(K) DSSO176(K) Ox(M) Carb(C) D(NQ) Ac(Protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003Sols03_C3.raw
Databases : **1:** Contaminants_minus_Bos_taurus 20120713_20210211 (124 sequences; 62,564 residues)
2: MSLdb 230513 (685 sequences; 267,424 residues)
3: UniProt_E_coli 20180227 (6,130 sequences; 1,398,442 residues)
Timestamp : 26 May 2023 at 00:36:17 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML 

▸ Search parameters
▸ Score distribution
▸ Modification statistics for all protein families
▸ Legend

Protein Family Summary

Format Significance threshold p< 0.05 Max. number of families AUTO [\[help\]](#)
Display non-sig. matches Min. number of sig. unique sequences 1
Dendrograms cut at 0
Preferred taxonomy All entries

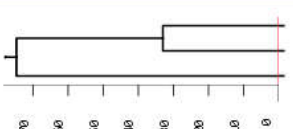
▸ Sensitivity

Proteins (185) [Report Builder](#) [Unassigned \(45933\)](#) [\[permalink\]](#)

Protein families 1-10 (out of 179)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [18](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains Find Clear

▸ 1  **1 2::EWas02** 69353 ERG isoform 2, human, NP_004440.1, GS N-terminus
3 2::DLib03 2939 EWS-FLI1_human-BirA_E_coli-3xHA
2 2::MSL02 67101 sp|P11308-3|ERG_HUMAN Isoform 2 of Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=E...

▸ 2 **2::EWas01** 43554 Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

Export search results for xiVIEW

MATRIX SCIENCE MASCOT Search Results

User :
E-mail :
Search title : rs 55591 XLink DSSO EWas01_EWas02 trypan-2 -mods Olsen Wasmuth M2021-005 Distiller update201003Sols03_C3.raw (MSLdb UniProt_E_coli Contam_minus_Bt) trypsin-2 DSSO175(K) DSSO176(K) Ox(M) Carb(C) D(NQ) Ac(Protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, Sul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003Sols03_C3.raw
Databases : 1: Contaminants_minus_Bos_taurus 20120713_20210211 (124 sequences; 62,564 residues)
2: MSLdb 230513 (685 sequences; 267,424 residues)
3: UniProt_E_coli 20180227 (6,130 sequences; 1,398,442 residues)
Timestamp : 26 May 2023 at 00:36:17 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As **XML**

- XML
- CSV
- mzIdentML
- FASTA
- xiVIEW-CSV
- Mascot DAT File
- MGF Peak List

Search parameters
Score distribution
Modification statistics for all protein families
Legend

Protein Family Summary

Format Significance threshold p< 0.05 Max. number of families
Display non-sig. matches Min. number of sig. unique sequences 1 [\[help\]](#)
Dendrograms cut at 0
Preferred taxonomy All entries

Sensitivity

Proteins (185) [Report Builder](#) [Unassigned \(45933\)](#) [\[permalink\]](#)

Protein families 1-10 (out of 179)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [18](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains [Find](#) [Clear](#)

1

Family	Score
1	~65
2	~35
3	~25

1 2::EWas02 69353 ERG isoform 2, human, NP_004440.1, GS N-terminus
3 2::DLib03 2939 EWS-FLI1_human-BirA_E_coli-3xHA
2 2::MSL02 67101 sp|P11308-3|ERG_HUMAN Isoform 2 of Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=E...

2 **2::EWas01** 43554 Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

Export search results for xiVIEW

MATRIX SCIENCE MASCOT Search Results

User :
E-mail :
Search title : rs 55591 XLink DSSO EWas01_EWas02 tryp-2 -mods Olsen Wasmuth M2021-005 Distiller update201003Sols03_C3.raw (MSLdb UniProt_E_coli Contam_minus_Bt) trypsin-2 DSSO175(K) DSSO176(K) Ox(M) Carb(C) D(NQ) Ac(Protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, Sul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003Sols03_C3.raw
Databases : 1: Contaminants_minus_Bos_taurus 20120713_20210211 (124 sequences; 62,564 residues)
2: MSLdb 230513 (685 sequences; 267,424 residues)
3: UniProt_E_coli 20180227 (6,130 sequences; 1,398,442 residues)
Timestamp : 26 May 2023 at 00:36:17 GMT

Re-search All Non-significant Unassigned [\[help\]](#) **Export** As xiVIEW-CSV

Search parameters
Score distribution
Modification statistics for all protein families
Legend

Protein Family Summary

Format Significance threshold p < 0.05 Max. number of families AUTO [\[help\]](#)
Display non-sig. matches Min. number of sig. unique sequences 1
Dendrograms cut at 0
Preferred taxonomy All entries

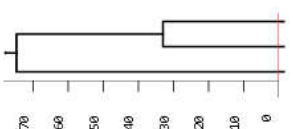
Sensitivity

Proteins (185) [Report Builder](#) [Unassigned \(45933\)](#) [s_permalink](#)

Protein families 1-10 (out of 179)

10 per page 1 [2](#) [3](#) [4](#) [5](#) [6](#) ... [18](#) [Next](#) [Expand all](#) [Collapse all](#)

Accession contains [Find](#) [Clear](#)

1  1 2::EWas02 69353 ERG isoform 2, human, NP_004440.1, GS N-terminus
3 2::DLib03 2939 EWS-FLI1_human-BirA_E_coli-3xHA
2 2::MSL02 67101 sp|P11308-3|ERG_HUMAN Isoform 2 of Transcriptional regulator ERG OS=Homo sapiens OX=9606 GN=E...

2 2::EWas01 43554 Androgen receptor (530-899)(AR), mouse, NP_038504.1, GS N-terminus

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Export format

Significance threshold $p <$ at identity homology

Display non-significant matches

Max. number of hits

Min. number of sig. unique sequences

Protein scoring Standard MudPIT

Group protein families

Require bold red

* Occasionally requires information to be retrieved from external utilities, which can be slow



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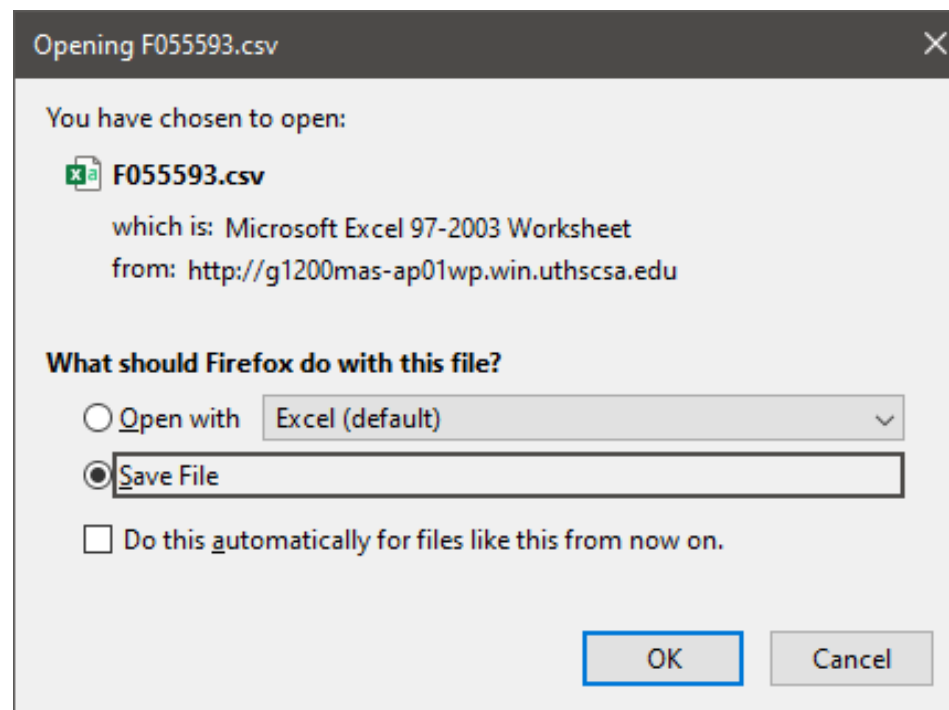
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Opening F055593.csv

You have chosen to open:

 **F055593.csv**
which is: Microsoft Excel 97-2003 Worksheet
from: <http://g1200mas-ap01wp.win.uthscsa.edu>

What should Firefox do with this file?

Open with Excel (default)

Save File

Do this automatically for files like this from now on.

OK Cancel

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[Help](#)

Export format	xiVIEW-CSV
Significance threshold p <	XML
Display non-significant matches	CSV
Max. number of hits	mzIdentML
Min. number of sig. unique sequences	FASTA
Protein scoring	xiVIEW-CSV
Group protein families	Mascot DAT File
Require bold red	MGF Peak List

entity homology

DPIT

* Occasionally requires information to be retrieved from external utilities, which can be slow

Show command line arguments

Export search results

Export search results for xiVIEW



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Export format

Significance threshold $p <$ at identity homology

Display non-significant matches

Max. number of hits

Min. number of sig. unique sequences

Protein scoring Standard MudPIT

Include same-set protein hits
(additional proteins that span
the same set of peptides)

Include sub-set protein hits
(additional proteins that span
a sub-set of peptides)

Group protein families

Require bold red

* Occasionally requires information to be retrieved from external utilities, which can be slow.

[Show command line arguments](#)

[Export search results](#)

Export search results for xiVIEW



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Mascot database search > Access Mascot Server > Export search results

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Export search results

[Help](#)

Export format: **FASTA** ▼

Significance threshold $p <$

Display non-significant matches

Max. number of hits

Min. number of sig. unique sequences

Protein scoring: identity **homology**

Include same-set protein hits (additional proteins that span the same set of peptides)

Include sub-set protein hits (additional proteins that span a sub-set of peptides)

Group protein families

Require bold red

Export format dropdown menu options:
XML
CSV
mzIdentML
FASTA
xiVIEW-CSV
Mascot DAT File
MGF Peak List

* Occasionally requires information to be retrieved from external utilities, which can be slow

Show command line arguments

Export search results

Export search results for xiVIEW

MATRIX SCIENCE

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Export format: MGF Peak List

Output spectra in:

- original order (for use with mzIdentML or mzTab)
- Mascot query order

Show command line arguments Export search results

Export search results for xiVIEW



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Mascot database search > Access Mascot Server > Export search results Logged in as weintraub | [Edit](#) | [Logout](#)

Export search results [Help](#)

Export format:

Output spectra in:
 original order (for use with mzIdentML or mzTab)
 Mascot query order

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MY DATA

SIGN OUT

DEMO

MZIDENTML

CSV FORMATS

PRIVACY

RAPPSILBER
LABORATORY

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Home

xiVIEW is a web-based visualisation tool for the analysis of cross-linking / mass spectrometry results, it is independent of the search software used. It provides multiple, linked views of the data, including:

- 2D network ([xiNET](#) or circular)
- the supporting annotated spectra using [xiSPEC](#).
- 3D structure view using [NGL](#).

The [video tutorials](#) give an overview of xiVIEW's many features.

xiVIEW is an open source project on [GitHub](#). Report issues and request features [here](#).

When using xiVIEW please cite: [Graham, M., Combe, C. W., Kolbowski, L. & Rappsilber, J. xiView: A common platform for the downstream analysis of Crosslinking Mass Spectrometry data. doi: 10.1101/561829.](#)

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SIGN OUT

DEMO

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4 CHOOSE FILE(S)

SUBMIT DATA

Identification file: Select a mzIdentML or csv file to upload

Peak list file(s): No peak list file(s) selected - spectra will be unavailable

Sequence file: No FASTA file selected, protein identifiers must be UniprotKB accession numbers

xiView accepts three types of input data:

i. Peptide Identifications (required)

Supported file formats: [mzIdentML](#) (file extension must be '.mzid') and [Comma Separated Values](#) (file extension '.csv').

ii. Peak Lists (optional)

Supported file formats: [mzML](#), [mgf](#), and [ms2](#) (& zip/gz archives of these). File extension must be '.mzML', '.mgf', '.ms2' or '.zip'.

If peak list data is uploaded then it must be complete, i.e. all spectra identified must be present, or the upload process will result in an error.

mzML tip: Filter out MS1 spectra to reduce file size and upload/parsing time. (e.g. 'MS level 2-' in [MSconvert](#))

iii. Protein Sequences (optional)

Supported file formats: [FASTA](#) (file extension must be '.fasta'), sequences can also be contained in mzIdentML files.

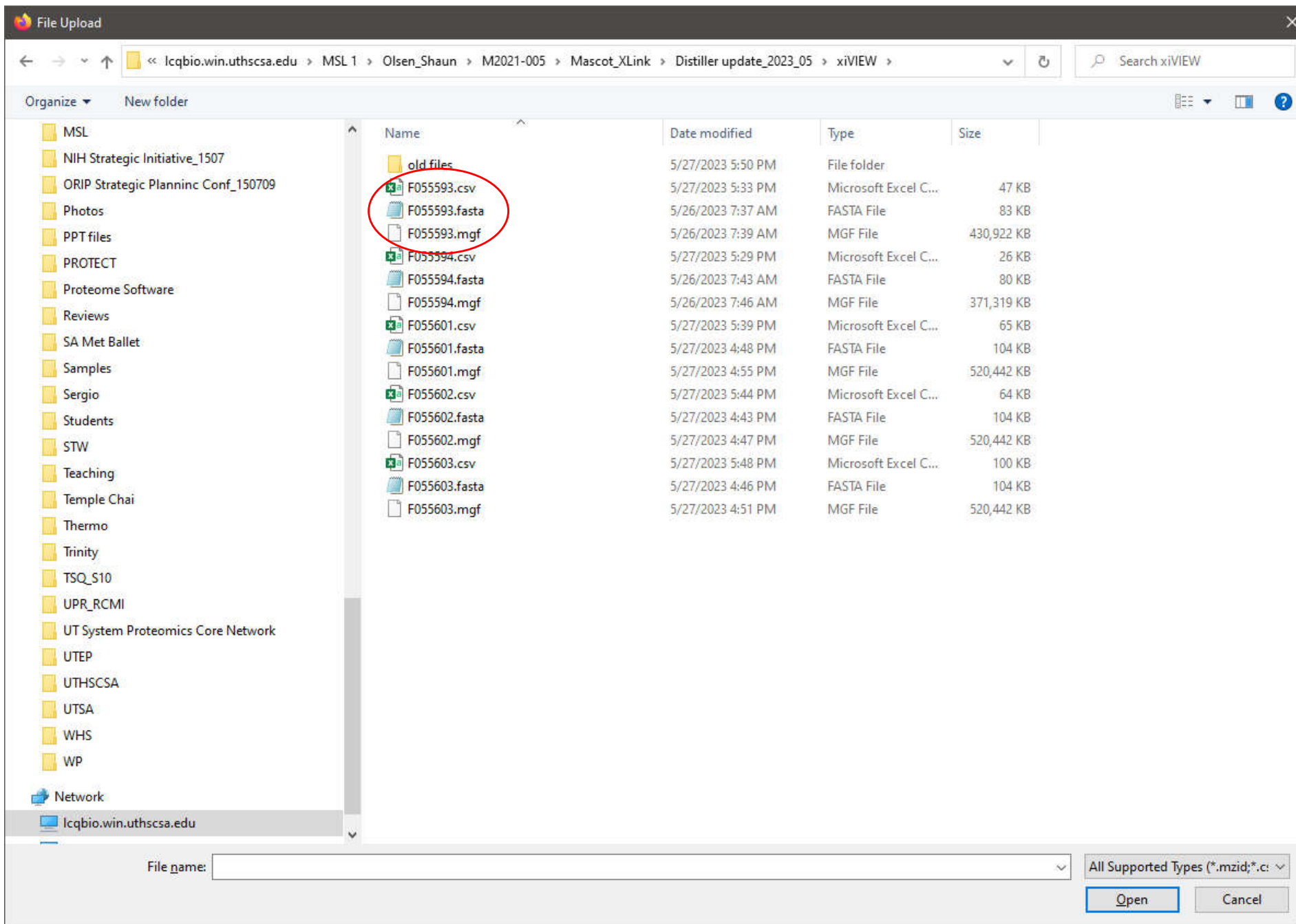
If you do not provide a FASTA file, then your protein IDs must be valid UniProtKB accession numbers.

If you do provide a FASTA file, then your protein IDs must all match identifiers in the FASTA file.

- **Only the peptide identifications file is required**, but without uploading peak lists you won't be able to inspect the supporting spectra using [xiSPEC](#).
- There is a 10GB size limit on uploaded files.

EXAMPLE DATA SETS

Upload files into xiVIEW



Submit files for xiVIEW

xiVIEW

HOME
UPLOAD
MY DATA
SIGN OUT

DEMO
MZIDENTML
CSV FORMATS
PRIVACY

RAPPSILBER
LABORATORY

Supported by
wellcome trust

Upload

[Data upload video tutorial](#)

CHOOSE FILE(S) 100% **SUBMIT DATA**

Identification file:	F055593.csv ✓
Peak list file(s):	F055593.mgf ✓
Sequence file:	F055593.fasta ✓

xiView accepts three types of input data:

i. Peptide Identifications (required)

Supported file formats: [mzIdentML](#) (file extension must be '.mzid') and [Comma Separated Values](#) (file extension '.csv').

ii. Peak Lists (optional)

Supported file formats: [mzML](#), [mgf](#), and [ms2](#) (& zip/gz archives of these). File extension must be '.mzML', '.mgf', '.ms2' or '.zip'.

If peak list data is uploaded then it must be complete, i.e. all spectra identified must be present, or the upload process will result in an error.

mzML tip: Filter out MS1 spectra to reduce file size and upload/parsing time. (e.g. 'MS level 2-' in [MSconvert](#))

iii. Protein Sequences (optional)

Supported file formats: [FASTA](#) (file extension must be '.fasta'), sequences can also be contained in mzIdentML files.

If you do not provide a FASTA file, then your protein IDs must be valid UniProtKB accession numbers.

If you do provide a FASTA file, then your protein IDs must all match identifiers in the FASTA file.

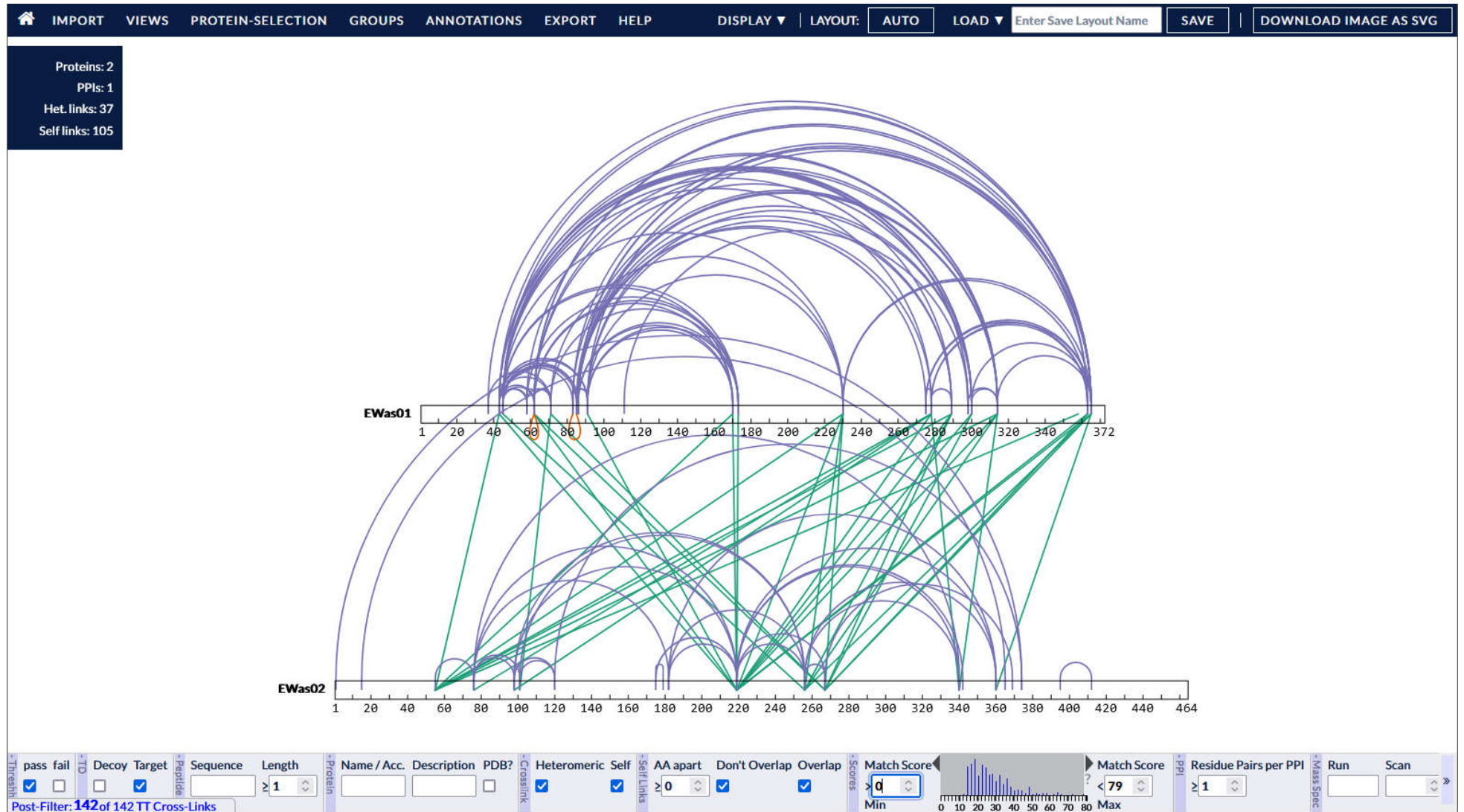
- **Only the peptide identifications file is required**, but without uploading peak lists you won't be able to inspect the supporting spectra using [xiSPEC](#).
- There is a 10GB size limit on uploaded files.

EXAMPLE DATA SETS

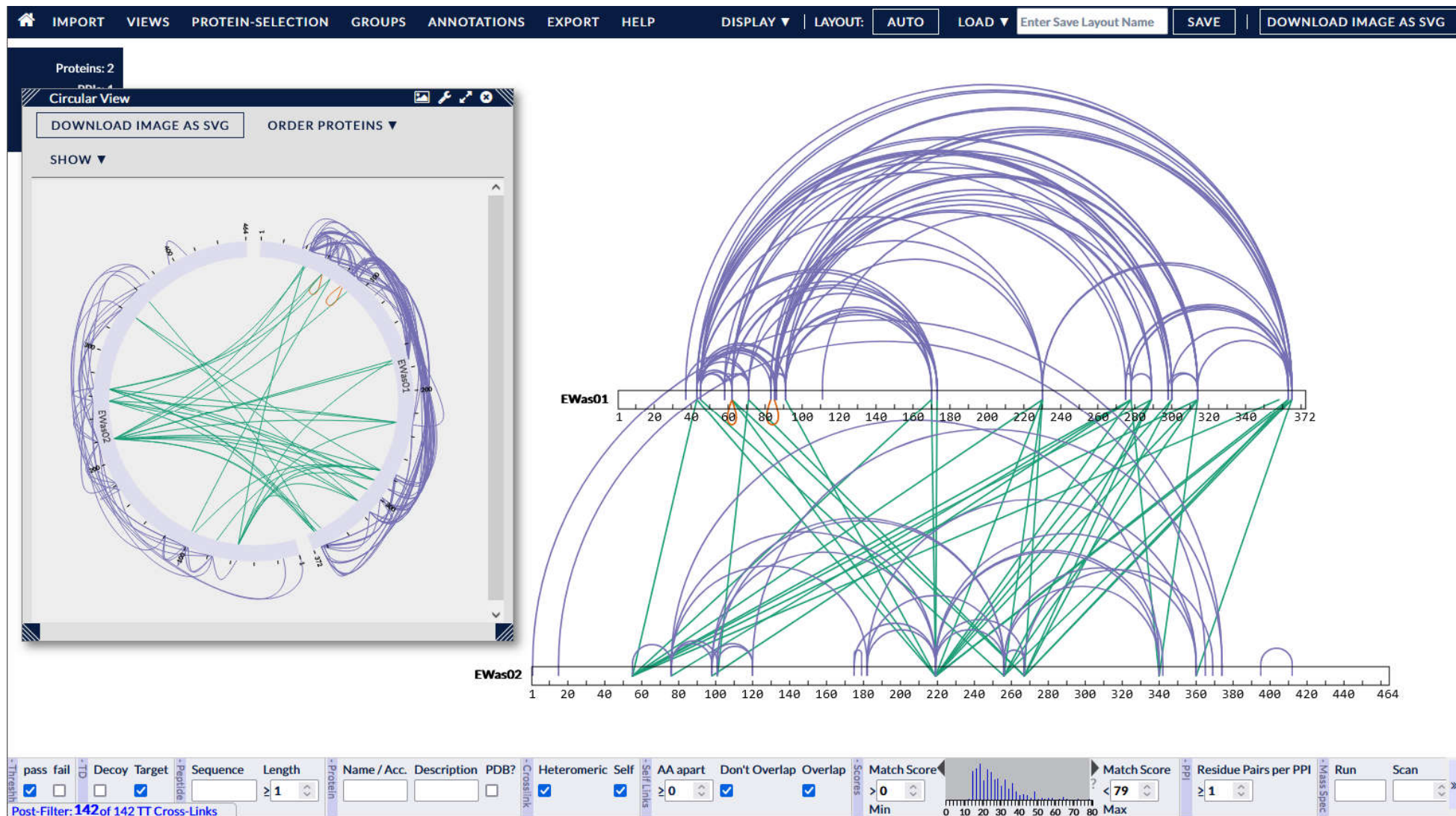
Open results file in xiVIEW

<< HOME STWEINTRAUB 'S DATA UPLOAD DATA HELP SIGN OUT AGGREGATE						
Page Number <input type="text" value="1"/> of 3						
Visualise Network	Spectra Only	Upload Time	Upload Error	Warnings	Agg Group	Delete
<input type="text"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	CLEAR ↓	
F055603.csv	View Spectra	2023-05-27 23:07			<input type="text"/>	DELETE
F055602.csv	View Spectra	2023-05-27 23:03			<input type="text"/>	DELETE
F055601.csv	View Spectra	2023-05-27 23:00			<input type="text"/>	DELETE
F055594.csv	View Spectra	2023-05-27 22:57			<input type="text"/>	DELETE
F055593.csv	View Spectra	2023-05-27 22:54			<input type="text"/>	DELETE
F055600.csv	View Spectra	2023-05-27 22:44			<input type="text"/>	DELETE
F055599.csv	View Spectra	2023-05-27 22:34			<input type="text"/>	DELETE
F055266.csv	View Spectra	2023-03-29 22:23			<input type="text"/>	DELETE
F055012.csv	View Spectra	2023-01-13 20:37			<input type="text"/>	DELETE
F055012.mzid	View Spectra	2023-01-13 20:28			<input type="text"/>	DELETE
F051211.csv	View Spectra	2022-05-31 17:38			<input type="text"/>	DELETE
F054048.csv	View Spectra	2022-05-17 19:39			<input type="text"/>	DELETE
F054047.csv	View Spectra	2022-05-17 19:30			<input type="text"/>	DELETE
F054046.csv	View Spectra	2022-05-17 19:26			<input type="text"/>	DELETE
F054045.csv	View Spectra	2022-05-17 19:23			<input type="text"/>	DELETE
F054044.csv	View Spectra	2022-05-17 19:22			<input type="text"/>	DELETE
F054042.csv	View Spectra	2022-05-17 19:18			<input type="text"/>	DELETE
F054041.csv	View Spectra	2022-05-17 19:16			<input type="text"/>	DELETE
F053907.csv	View Spectra	2022-04-20 19:03			<input type="text"/>	DELETE


xiVIEW - linear view



xiVIEW - circular view and linear view



Mascot search results - score distribution

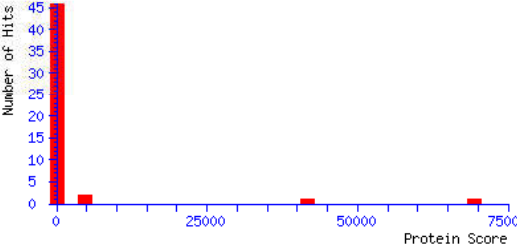
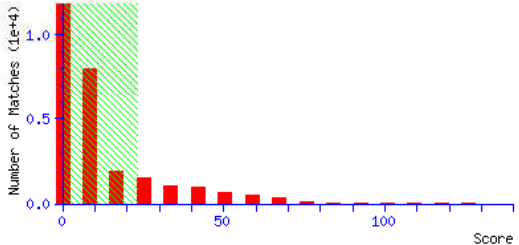


MASCOT Search Results

User :
E-mail :
Search title : rs 55591 XLink DSSO EWas01_EWas02 tryp-2 -mods Olsen Wasmuth M2021-005 Distiller update201003SOls03_C3.raw (MSLdb UniProt_E_coli Contam_minus_Bt) trypsin-2 DSSO175(K) DSSO176(K) Ox(M) Carb(C) D(NQ) Ac(Protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003SOls03_C3.raw
Databases : 1: Contaminants_minus_Bos_taurus 20120713_20210211 (124 sequences; 62,564 residues)
2: MSLdb 230513 (685 sequences; 267,424 residues)
3: UniProt_E_coli 20180227 (6,130 sequences; 1,398,442 residues)
Timestamp : 26 May 2023 at 00:36:17 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

► **Search parameters**
▼ **Score distribution**



Peptide score distribution. Ions score is $-10 \log(P)$, where P is the probability that the observed match is a random event. There are **5,096** peptide matches above identity threshold and **6,266** matches above homology threshold for **52,199** queries. On average, individual ions scores > 23 (beyond green shading) indicate **identity or extensive homology** ($p < 0.05$).

[Deprecated] Protein score distribution. Score distribution for family members in the first 50 proteins. Protein scores are derived from ions scores as a non-probabilistic basis for ranking protein families.

► **Modification statistics for all protein families**
► **Legend**

Protein Family Summary

Format Significance threshold $p <$ Max. number of families [\[help\]](#)
Display non-sig. matches Min. number of sig. unique sequences
Dendrograms cut at
Preferred taxonomy:

Mascot search results - score distribution

MATRIX SCIENCE MASCOT Search Results

User :
E-mail :
Search title : rs 55591 XLink DSSO EWas01_EWas02 tryp-2 -mods Olsen Wasmuth M2021-005 Distiller update201003SOIs03_C3.raw (MSLdb UniProt_E_coli Contam_minus_Bt) trypsin-2 DSSO175(K) DSSO176(K) Ox(M) Carb(C) D(NQ) Ac(Protein N-term) (Olsen Wasmuth M2021-005 DSSO Frac 11, Band C3, cOT_TS_cIT_ddHCD, 30min, 5ul, GB3)
MS data file : M:\Olsen_Shaun\M2021-005\Xcalibur\201003\201003SOIs03_C3.raw
Databases : **1:** Contaminants_minus_Bos_taurus 20120713_20210211 (124 sequences; 62,564 residues)
2: MSLdb 230513 (685 sequences; 267,424 residues)
3: UniProt_E_coli 20180227 (6,130 sequences; 1,398,442 residues)
Timestamp : 26 May 2023 at 00:36:17 GMT

Re-search All Non-significant Unassigned [\[help\]](#) Export As XML

▶ **Search parameters**
▼ **Score distribution**

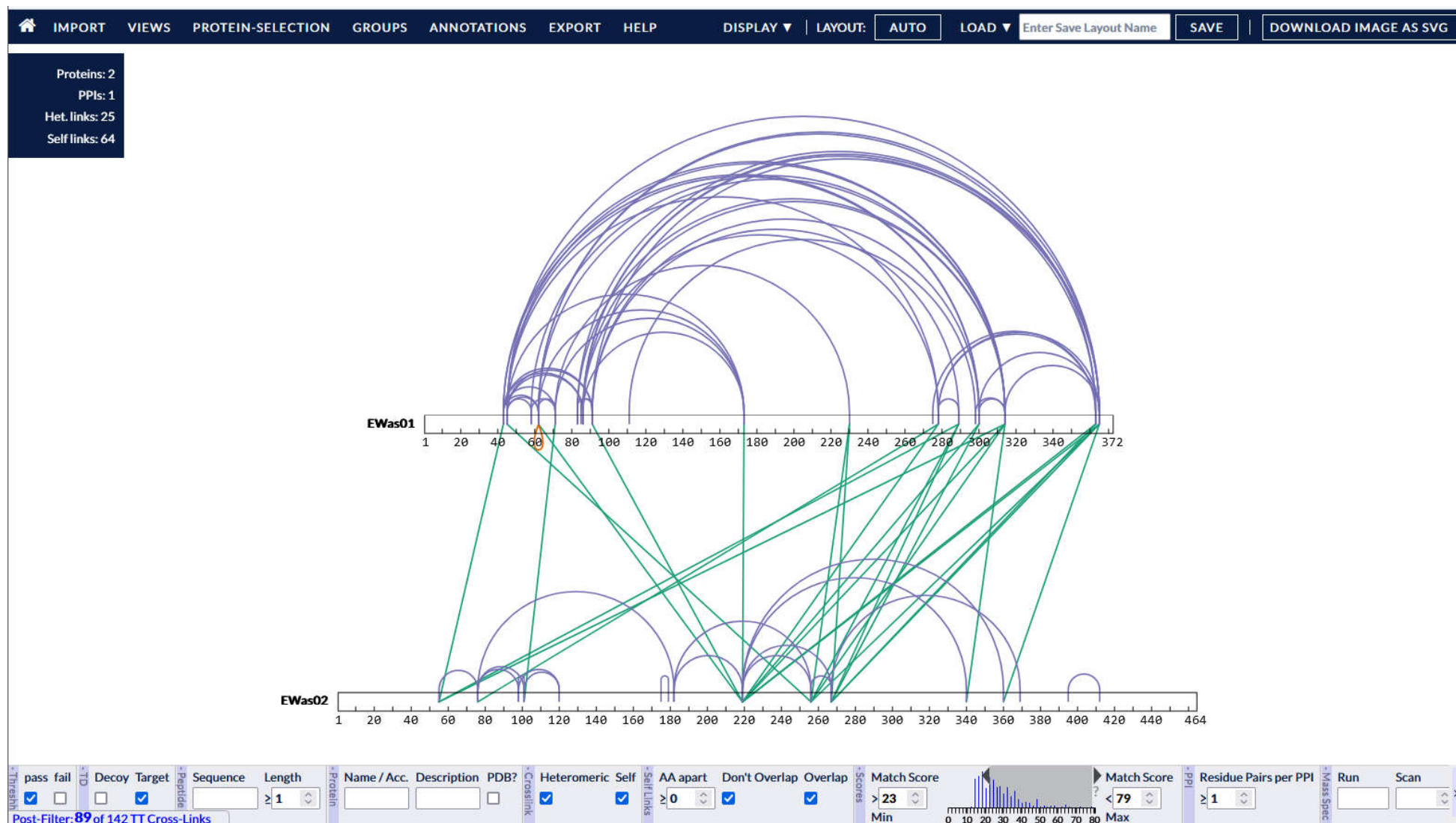
Peptide score distribution. Ions score is $-10 \log(P)$, where P is the probability that the observed match is a random event. There are **5,096** peptide matches above identity threshold and **6,266** matches above homology threshold for **52,199** queries. On average, individual ions scores > 23 (beyond green shading) indicate **identity or extensive homology** ($p < 0.05$).

core distribution for protein scores are derived from protein scores for ranking protein

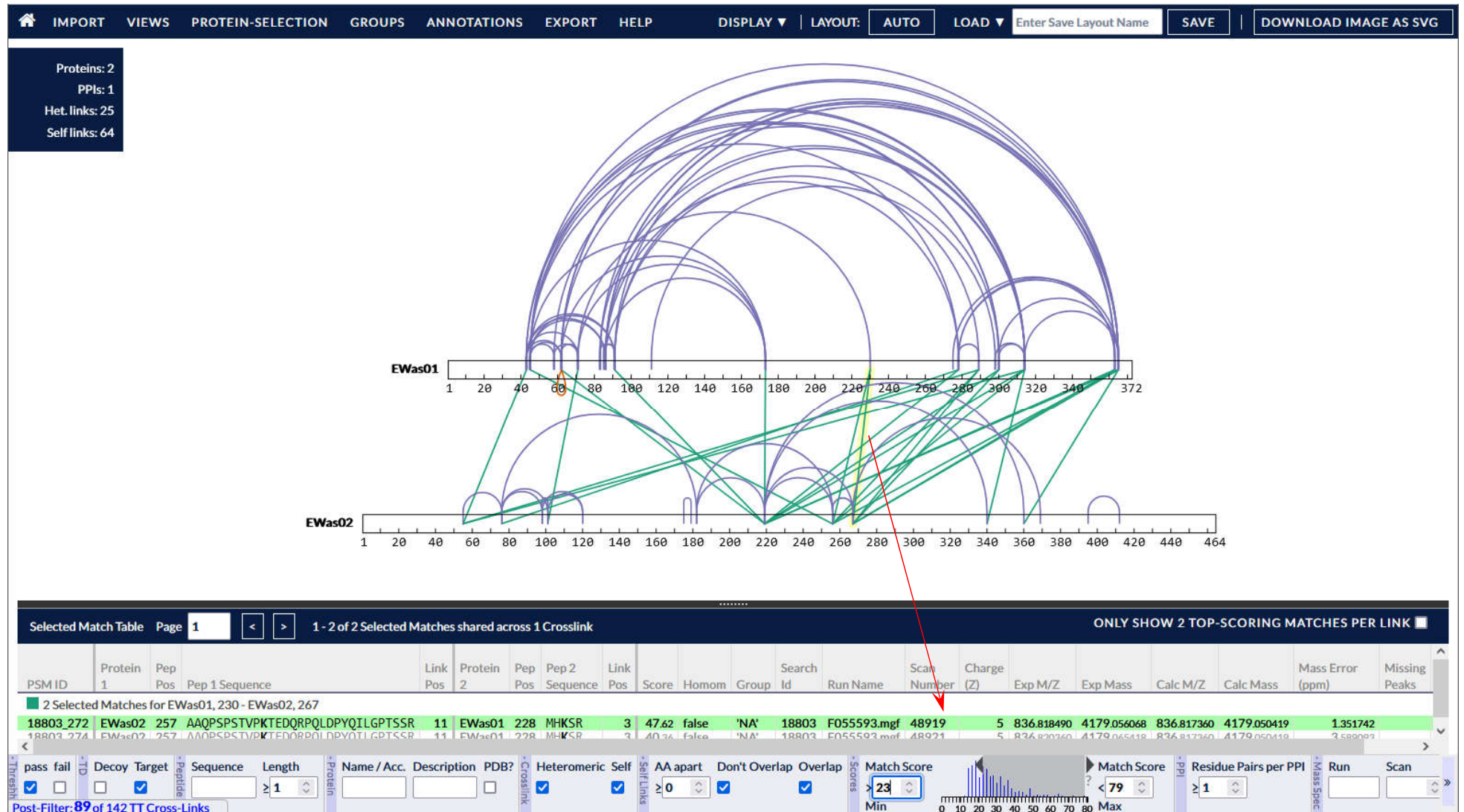
Protein Family Summary

Format Significance threshold $p <$ Max. number of families [\[help\]](#)
Display non-sig. matches Min. number of sig. unique sequences
Dendrograms cut at
Preferred taxonomy:

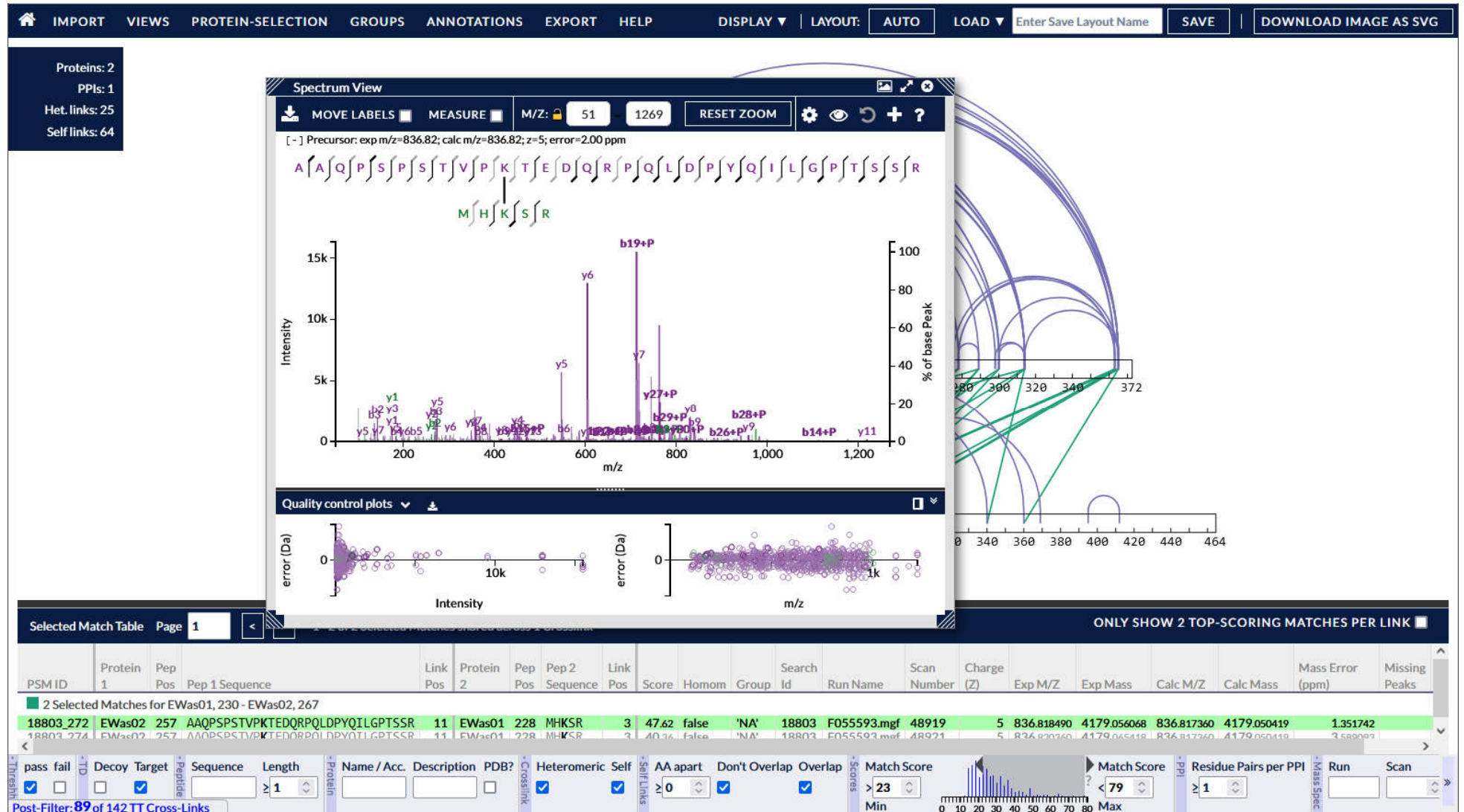
xiVIEW - linear view with minimum match score set to 23



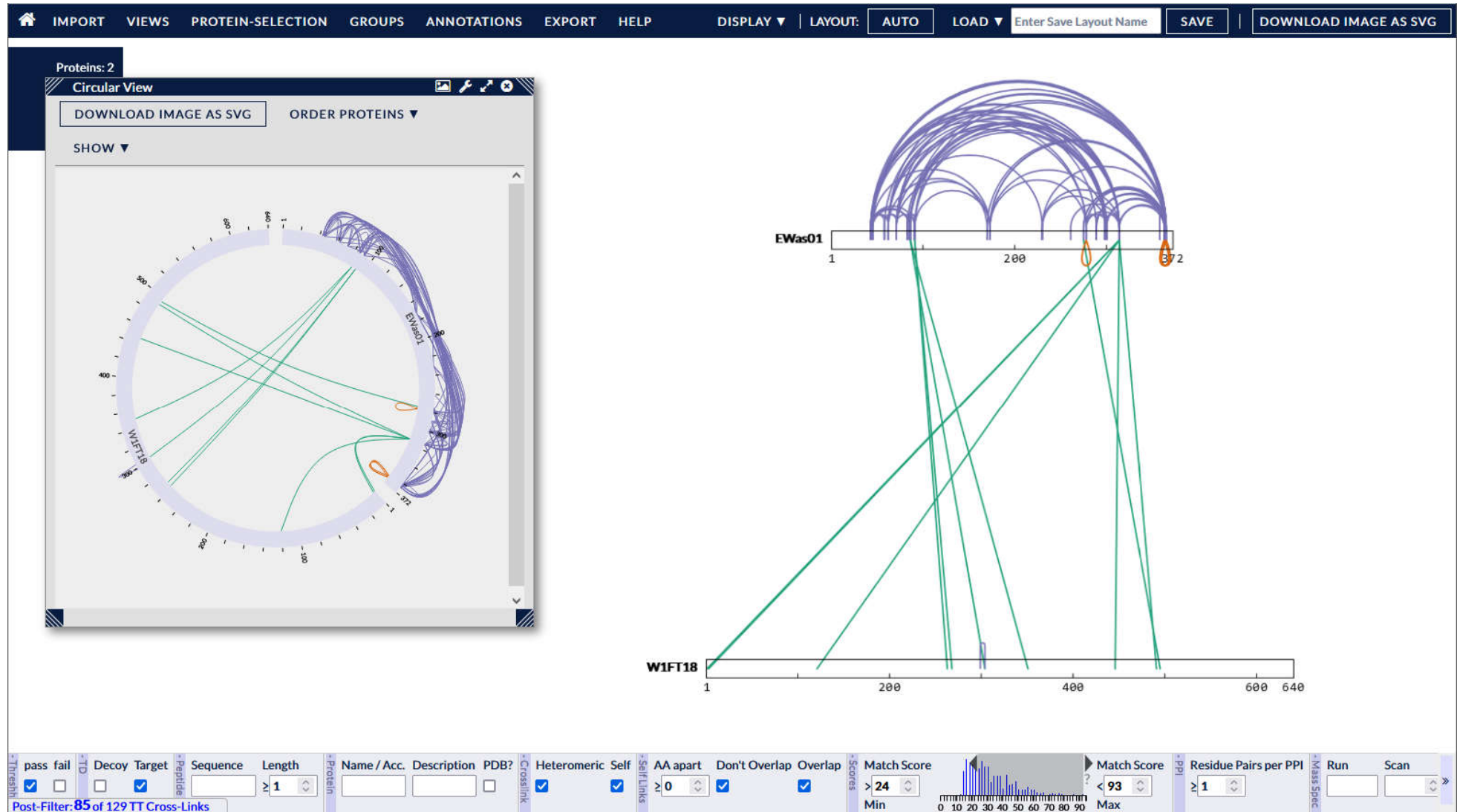
xiVIEW - linear view with minimum match score set to 23



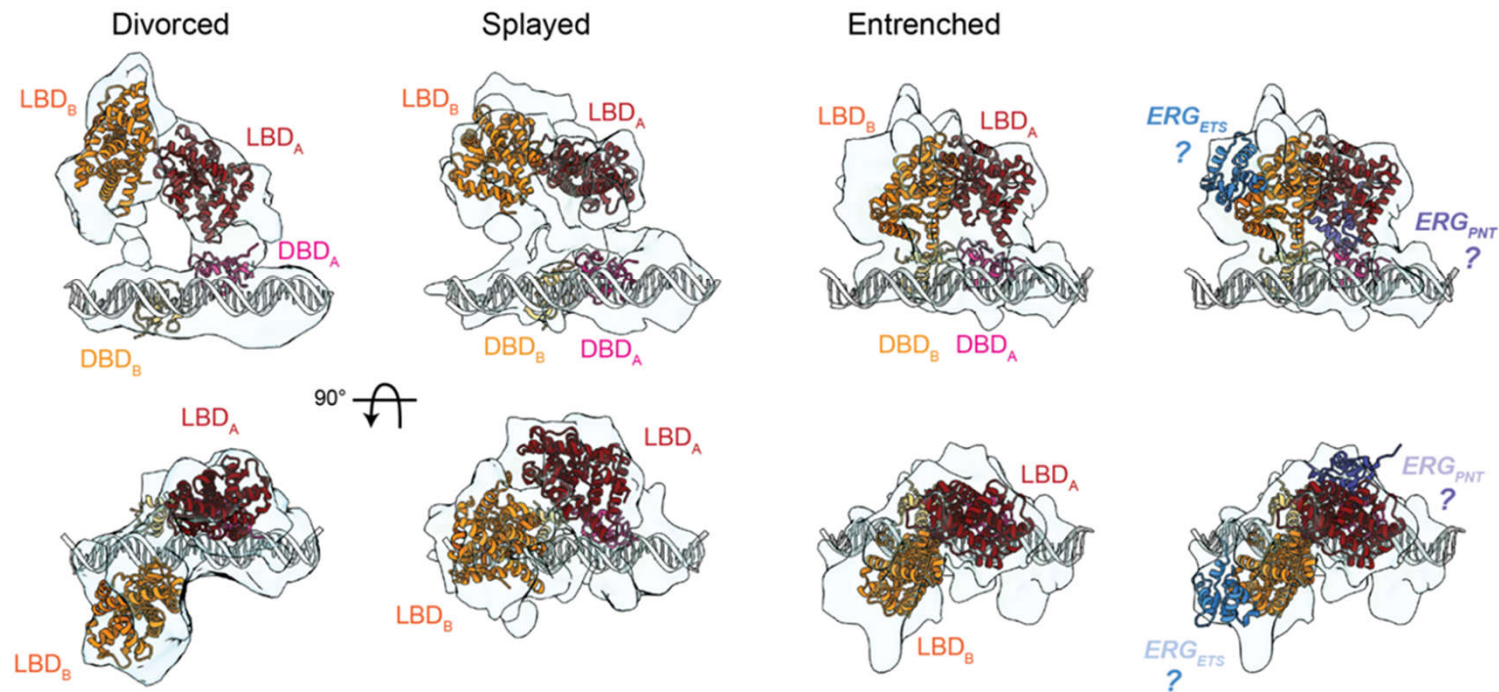
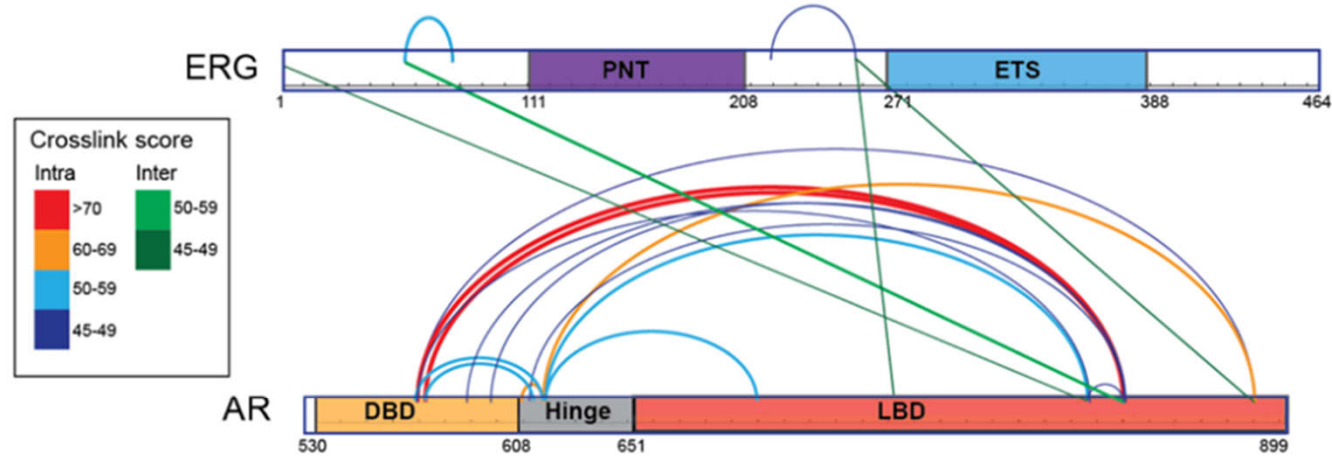
xiVIEW - annotated cross-linked peptide spectrum



AR cross-linked with E. coli chaperone DNAK



ERG modulates AR activity through association with the AR LBD



ABRF iPRG 2020 cross-linking study

This tutorial focuses on these three pipeline steps.

Step #3: Click Update Page to finish.

Select which peptide sequence to overlay on the spectrum from these tabs.



- Study divided into two parts.
- Part 1: Participants given self-guided, graphical tutorials (Mascot or Kojak) that instruct them on how to complete data analysis on half the study data.
- Part 2: Participants apply what they learned in Part 1 to the remaining data. They can use the same analysis pipelines, or explore new tools.
- No prior knowledge of crosslinking analysis is required to participate.

Acknowledgements



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Dana Molleur

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