DDM
ANN and Metaproteomics Update

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May 03, 2012

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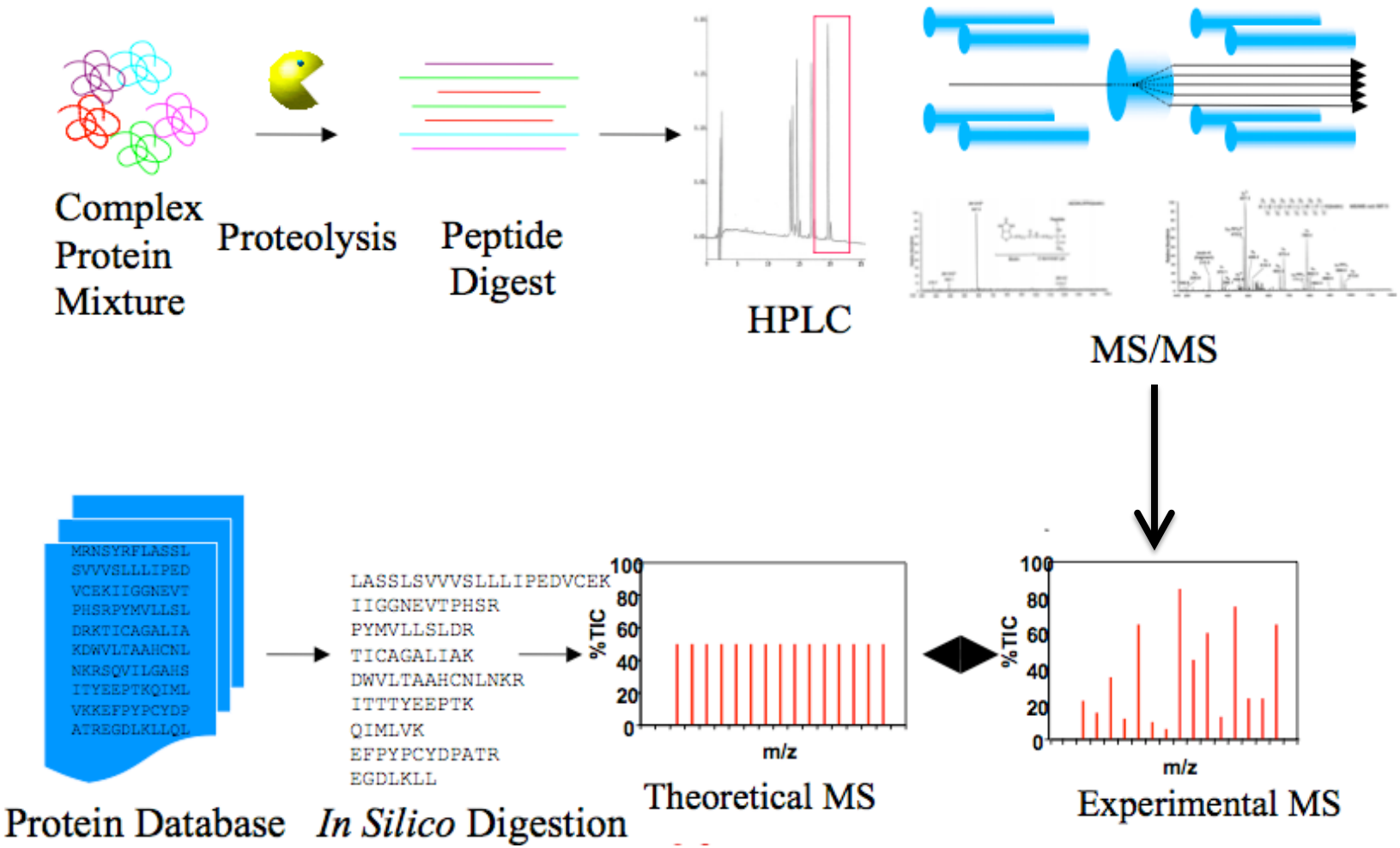
Summary From 4/19/12

- ANN paper
  - Submitted (returned for minor revisions)
  - iVIREONS webpages (Mike A.)
- Metaproteomics Paper
  - GAAS shows that small genomes are still prevalent
  - Found few proteins with strong MOWSE scores
  - MASCOT searches found no significant hits
  - Automate MP Analysis

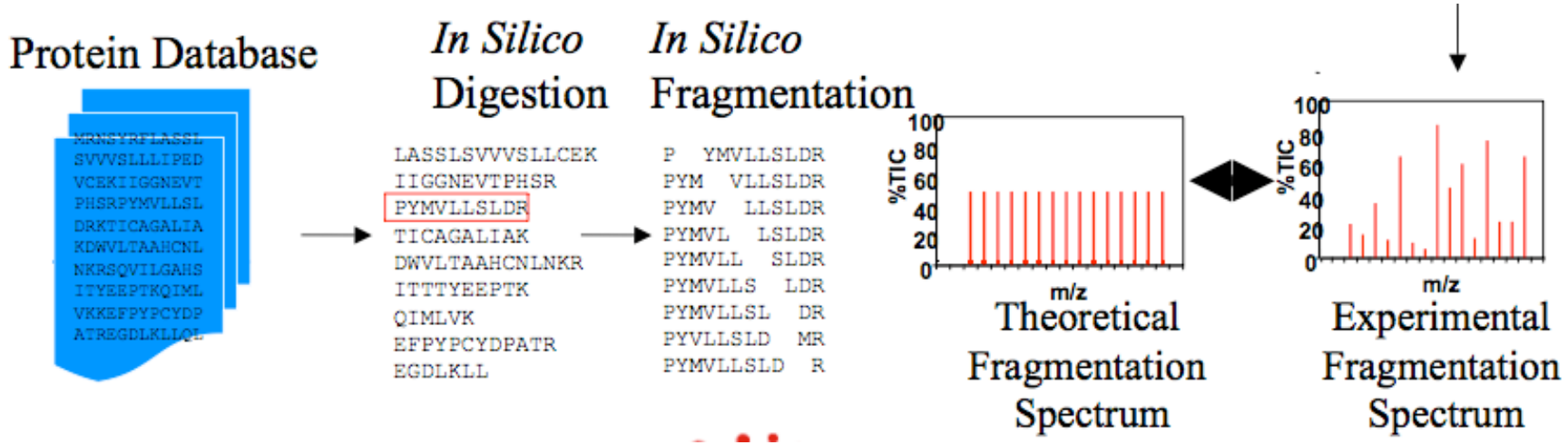
Work In Progress

- ANN paper
  - Reviewers' comments
- Metaproteomics Paper
  - Recalculate scores using fragment ion masses (SEQUEST)

Overview of MOWSE



ID Protein By Fragment Ion Spectra



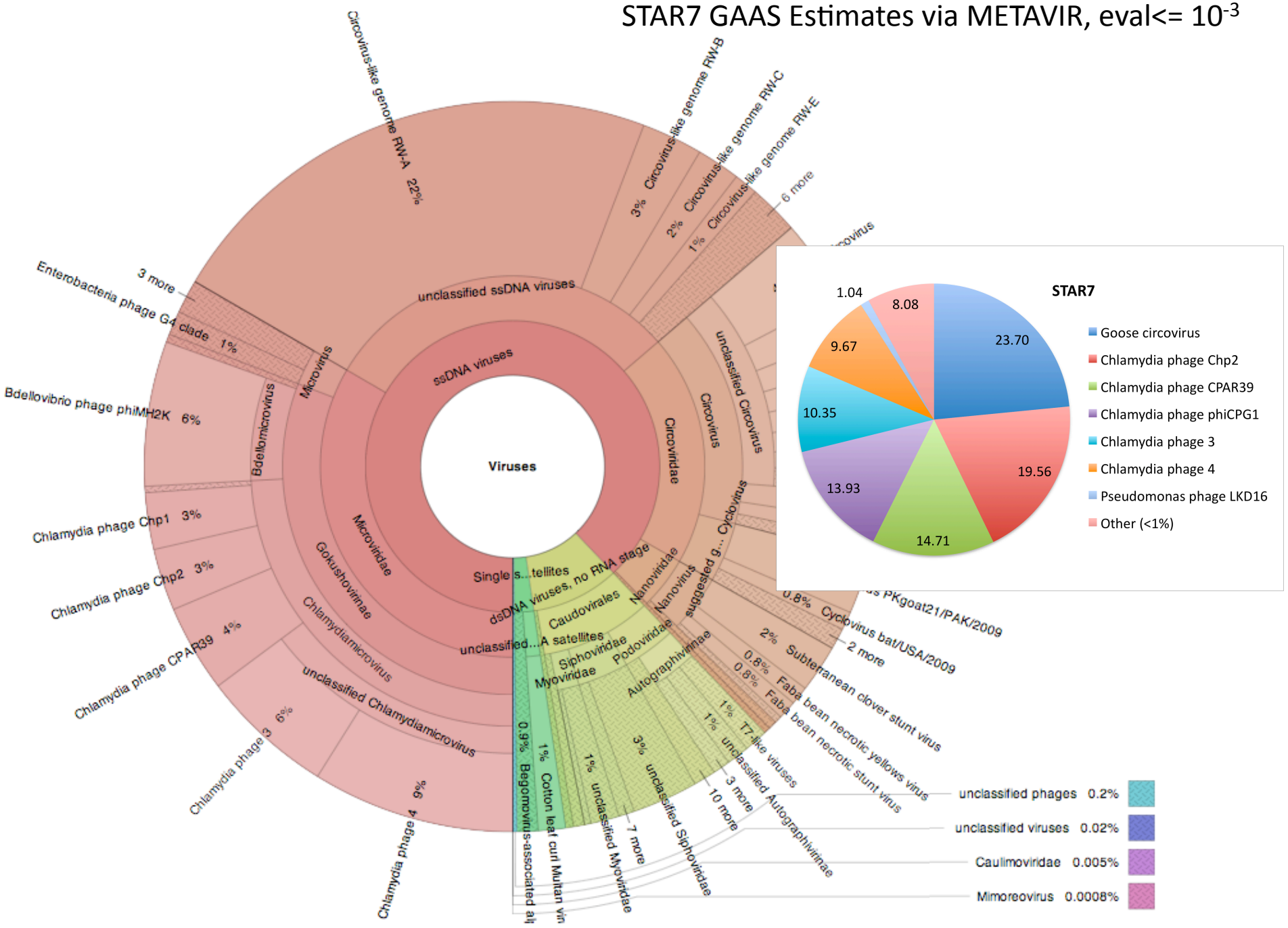
$\Longrightarrow$ SEQUEST

Jimmy K. Eng, Ashley L. McCormack, and John R. Yates, III (1994). "An Approach to Correlate Tandem Mass Spectral Data of Peptides with Amino Acid Sequences in a Protein Database". *J Am Soc Mass Spectrom* **5** (11): 976–989(Eng et al., 1994)

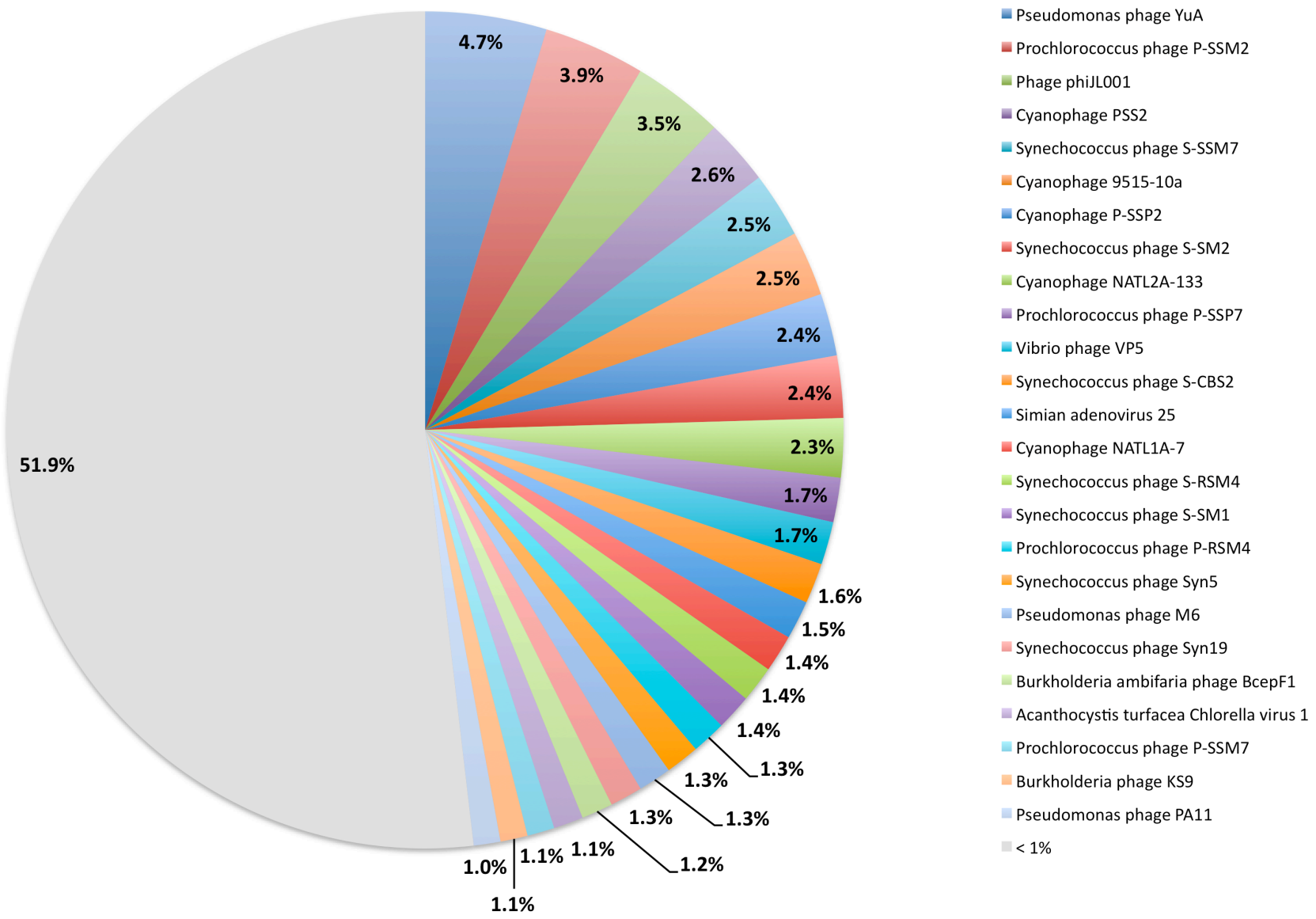
Summary of Work In Progress

- ANN paper
  - Address reviewers' comments
  - Fix Y-axes in supporting figure 14 (confidence inter.)
  - Finish iVIREONs (Mike A.)
- Metaproteomics Paper
  - Use SEQUEST algorithm for protein identification
  - Sequence statistics on 5965 and 5971
  - Incorporate new algorithms in automation scripts
  - Draft of paper to Emerald (Don & Alex)

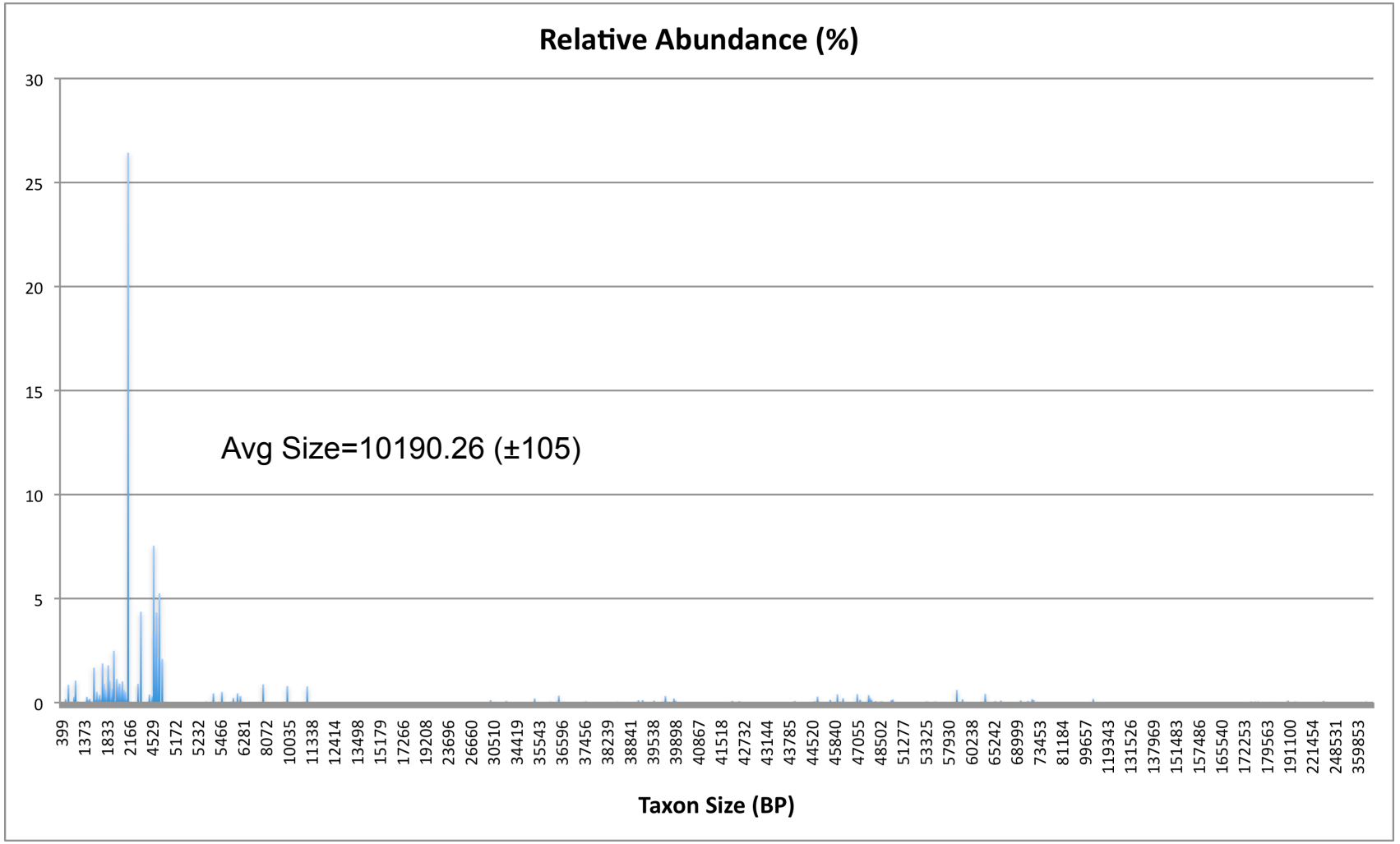
STAR7 GAAS Estimates via METAVIR, eval<= 10^{-3}



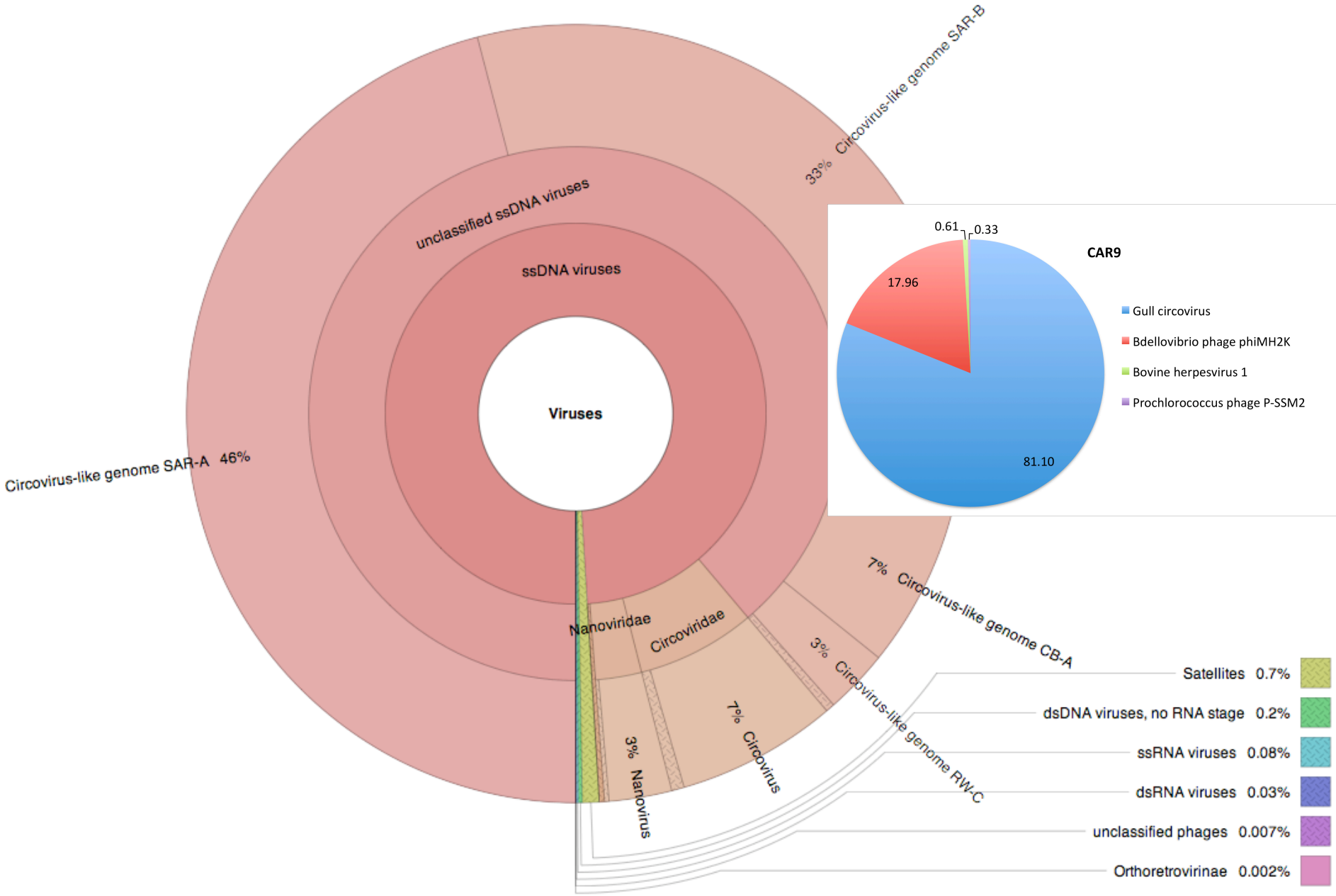
STAR7 GAAS Estimates
(minus Micro-, Nano-, and Circoviridae)



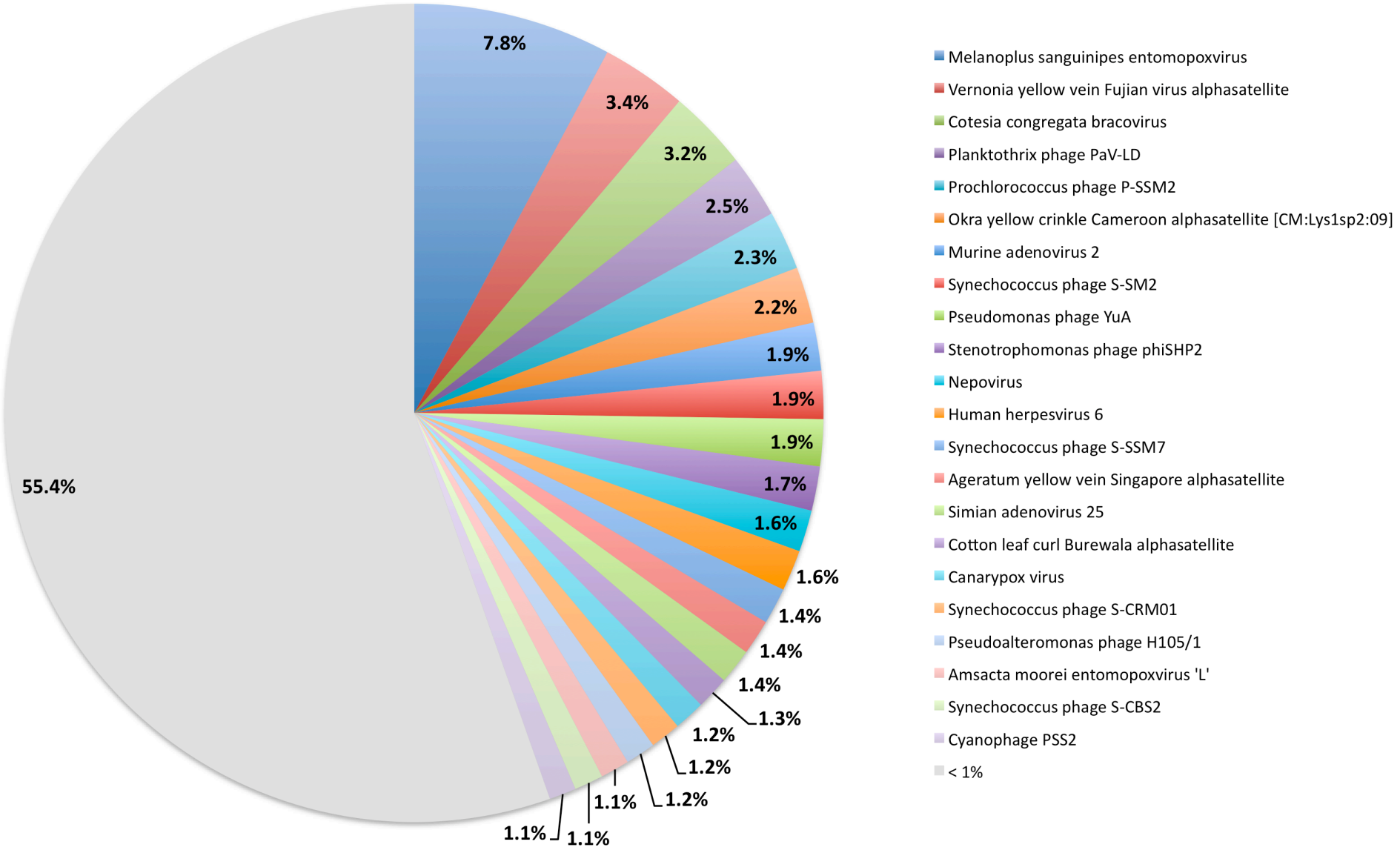
STAR7 Taxon Sizes



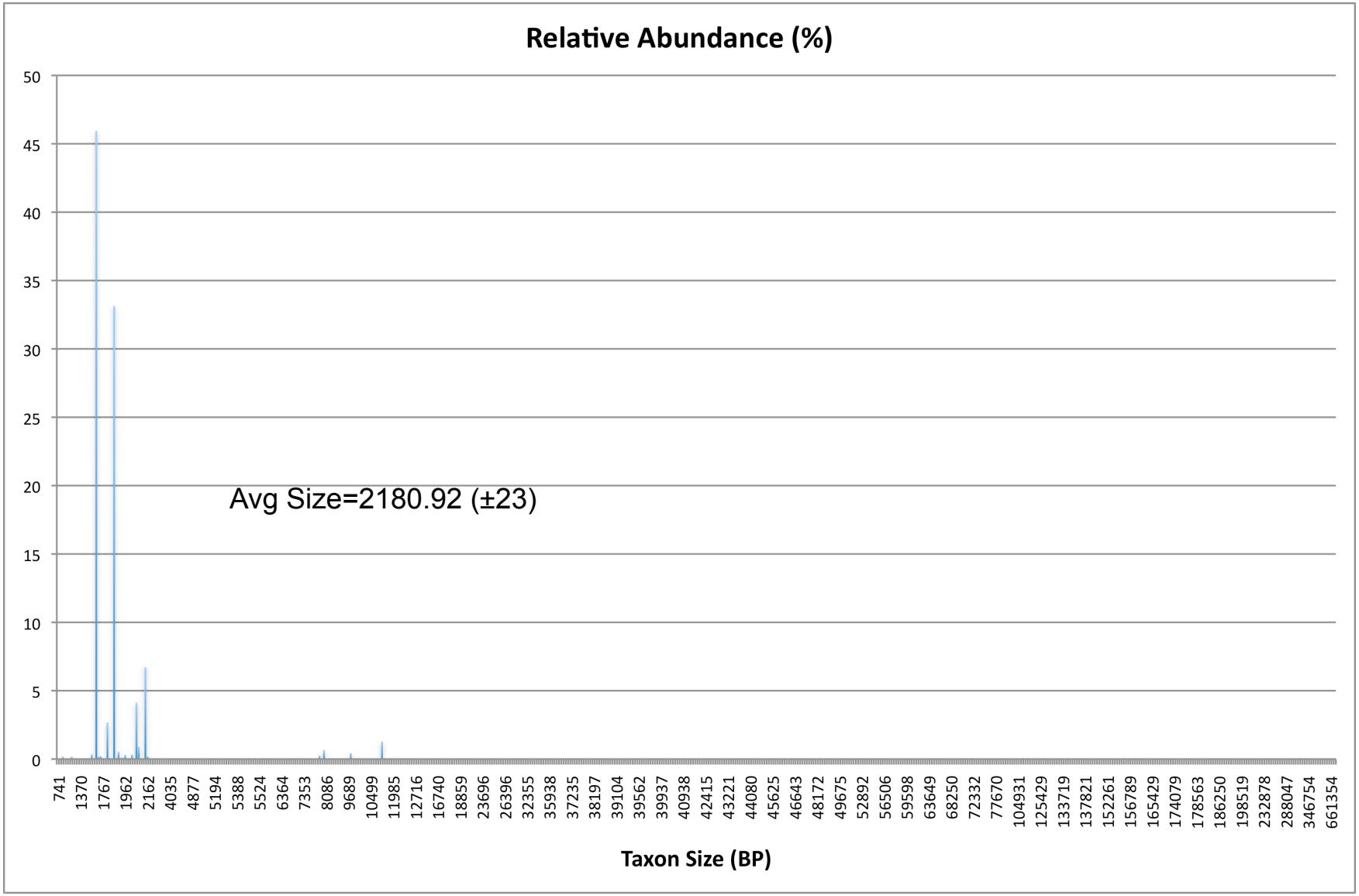
CAR9 GAAS Estimates via METAVIR – eval<= 10^{-3}



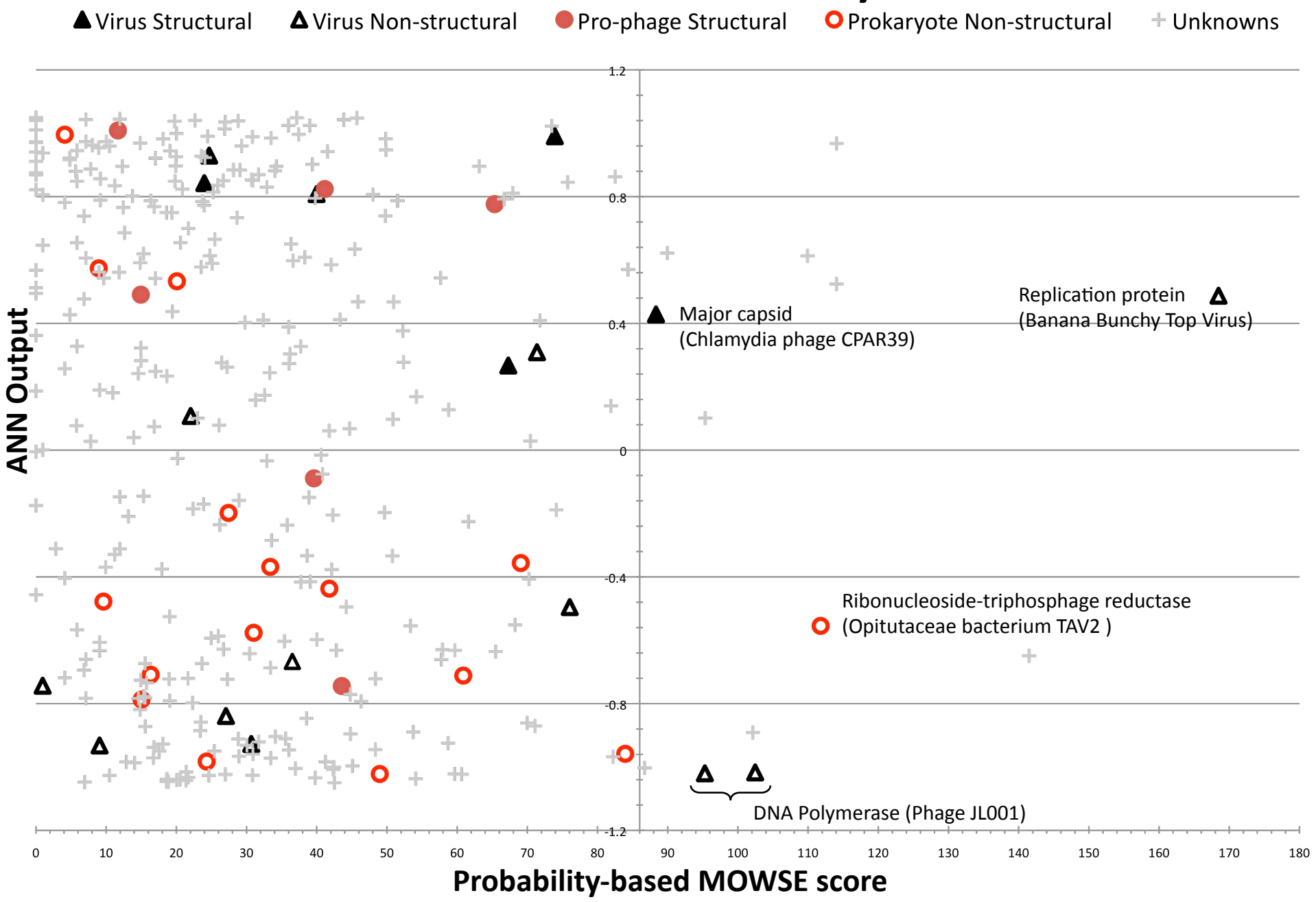
CAR9 GAAS Estimates
(minus Micro-, Nano-, and Circoviridae)



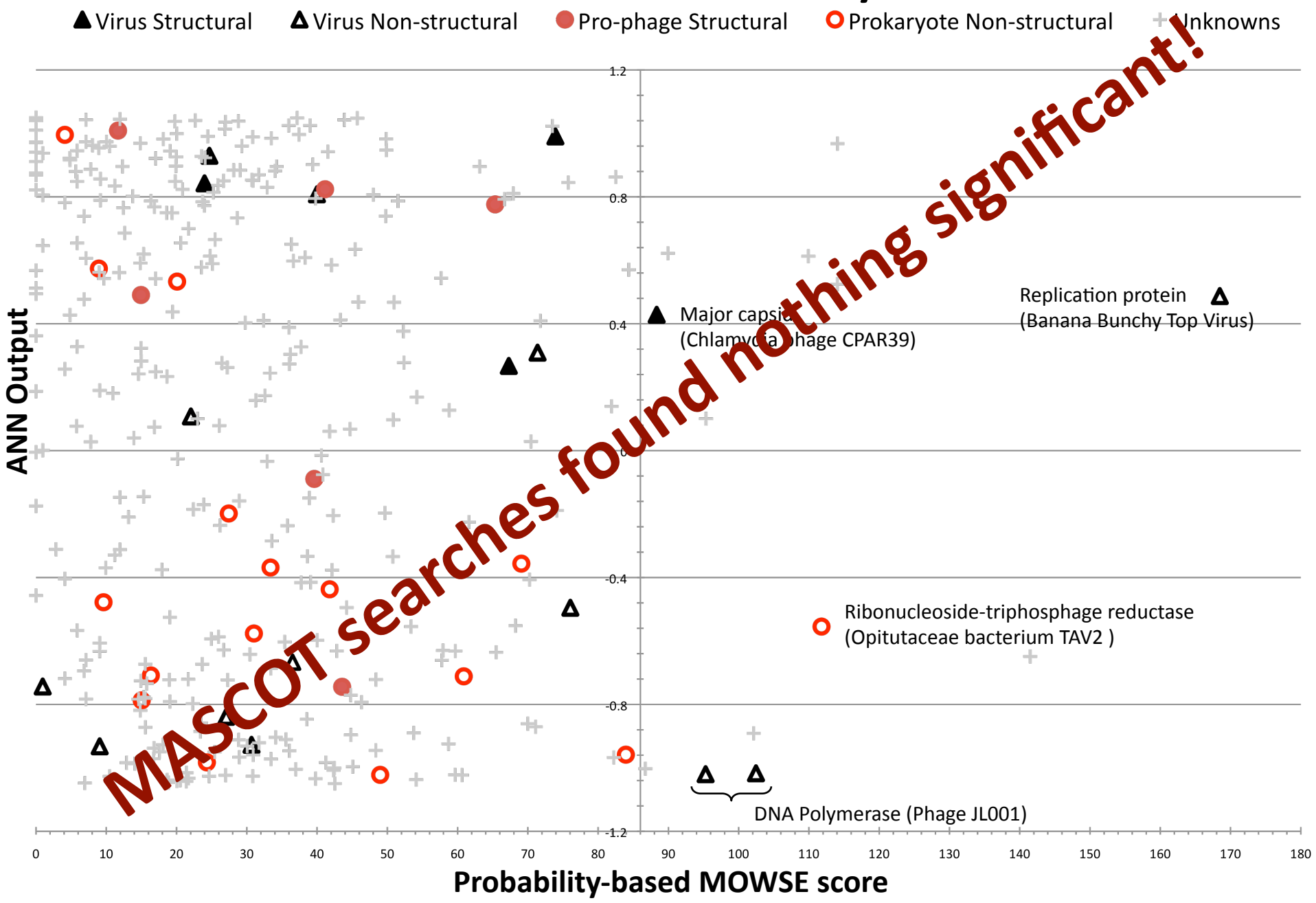
CAR9 Taxon Sizes



Protein Identification by MOWSE



Protein Identification by MOWSE



MASCOT Search Results - NR

MS data file : AnalysisStar7.mgf
Database : NCBInr 20120421 (17910093 sequences; 6147033692 residues)
Timestamp : 23 Apr 2012 at 11:25:01 GMT
Protein hits :

gi|11935049 keratin 1 [Homo sapiens]
gi|623409 keratin 10 [Homo sapiens]
gi|61740600 keratin, type I cytoskeletal 10 [Canis lupus familiaris]
gi|146741296 keratin 1 [Sus scrofa]
gi|351695070 Keratin, type II cytoskeletal 1, partial [Heterocephalus glaber]
gi|4159806 type II keratin subunit protein [Mus musculus]
gi|12859782 unnamed protein product [Mus musculus]
gi|136429 RecName: Full=Trypsin; Flags: Precursor
gi|348562686 PREDICTED: keratin, type I cytoskeletal 10-like [Cavia porcellus]
gi|348581121 PREDICTED: keratin, type II cytoskeletal 1-like [Cavia porcellus]
gi|435476 cytokeratin 9 [Homo sapiens]
gi|194037336 PREDICTED: keratin, type II cytoskeletal 1b [Sus scrofa]
gi|148727309 keratin, type II cytoskeletal 2 epidermal [Pan troglodytes]
gi|109099462 PREDICTED: keratin, type II cytoskeletal 6B-like [Macaca mulatta]
gi|149031970 rCG50690 [Rattus norvegicus]
gi|355698804 keratin 6A [Mustela putorius furo]
gi|73996461 PREDICTED: keratin, type II cytoskeletal 78 [Canis lupus familiaris]
gi|291334540 prophage LambdaCh01 coat protein [uncultured phage MedDCM-OCT-S04-C1220]
gi|52789 unnamed protein product [Mus musculus]
gi|293686

MS data file : AnalysisCar9.mgf
Database : NCBInr 20120421 (17910093 sequences; 6147033692 residues)
Timestamp : 23 Apr 2012 at 11:35:03 GMT
Protein hits :

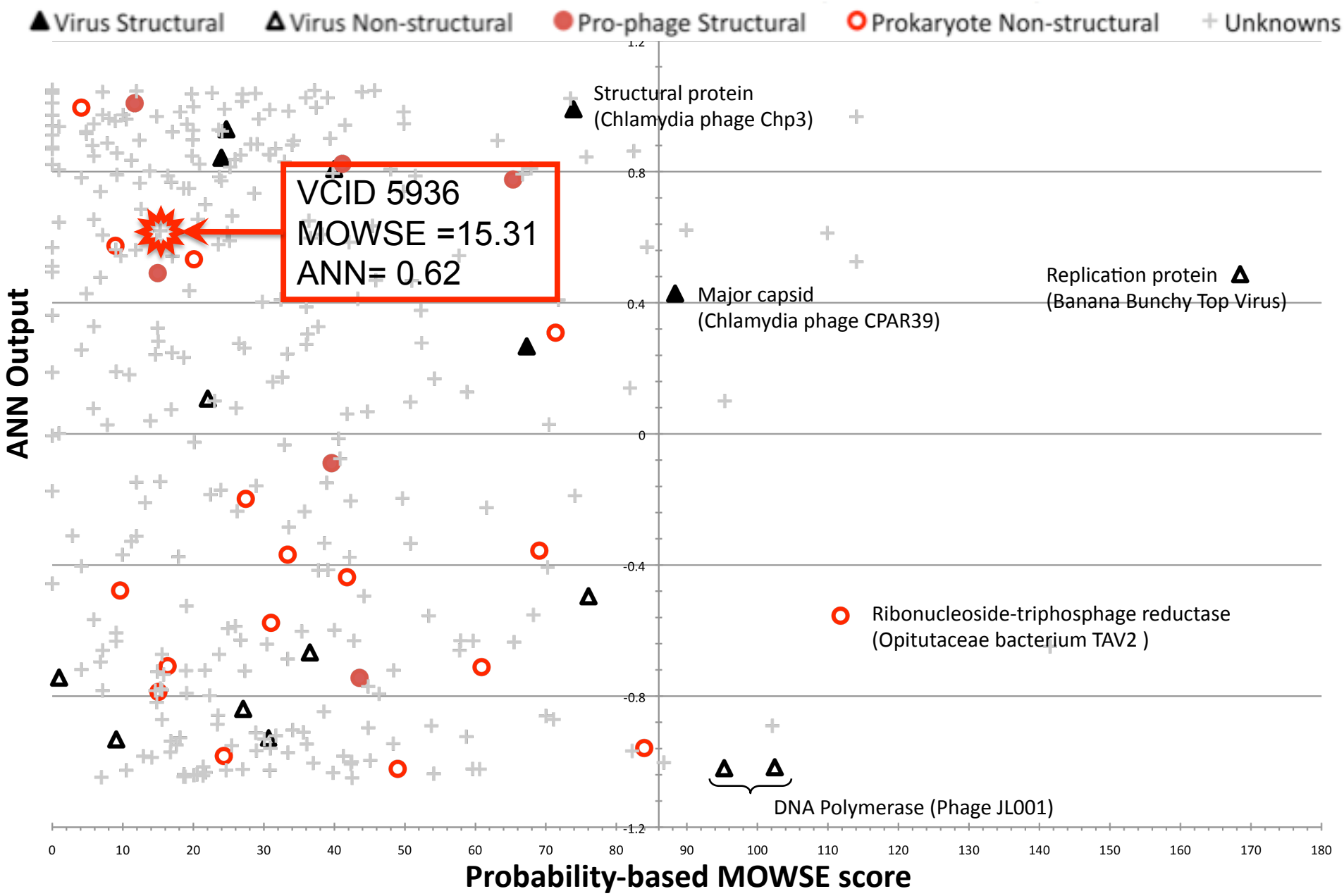
gi|160961491 keratin, type II cytoskeletal 1 [Pan troglodytes]
gi|291389217 PREDICTED: keratin 6A-like [Oryctolagus cuniculus]
gi|348581121 PREDICTED: keratin, type II cytoskeletal 1-like [Cavia porcellus]
gi|4159806 type II keratin subunit protein [Mus musculus]
gi|12859782 unnamed protein product [Mus musculus]
gi|291389225 PREDICTED: keratin 8-like [Oryctolagus cuniculus]
gi|136429 RecName: Full=Trypsin; Flags: Precursor
gi|47604942 keratin 75 [Gallus gallus]
gi|224099135 PREDICTED: similar to cytokeratin type II [Taeniopygia guttata]

No significant hits against STAR7 pORFs

MASCOT Hits to STAR7 Sequences

				MASCOT Hits			
				Peptide 1		Peptide2	
Seq ID	**BLASTP**	**ANN**	**MOWSE**	**E-val**	**Sequence**	**E-val**	**Sequence**
16031_6_2	hypothetical protein	-0.67	15.5518	2.1	ISEQAAVQMPMKTVASLIAMIAVGTWAYFGIHEK		
2146_6_2	hypothetical protein	0.97	7.10127	3.7	TEEYDGSTWTTKSNMGVSLYR		
26232_3_1	No hits found	0.59	25.1388	3.6	QIEKLFK	3	NQLRQYGLPAFANGGIVGMGPGQSR
4336_5_15	hypothetical protein	-0.33	11.2065	3.2	SSLVVGKR		
27756_6_69	hypothetical protein	0.27	36.0452	3.1	VQASIPVR		
28154_4_11	ribonucleoside-triphosphate reductase [Roseiflexus castenholzii DSM 13941]	0.31	71.3758	3	GKPEMGTFMR		
24501_1_5	hypothetical protein	0.28	52.3631	3	LEVKQLALPCR		
6482_3_19	structural protein [Chlamydia phage Chp2]	0.99	73.9156	2.6	LQDPEYLGGGSNR		
10190_1_1	hypothetical protein	-0.59	25.9649	2.3	EGNQQYALVDMKNE	1.9	GENPPEPQTEPLVTMFTK
4335_3_26	No hits found	0.10	50.8172	2.1	QRLPTMMQR		
24005_3_7	hypothetical protein	0.93	23.5737	2.1	SRAQFGDSMWTGAR		
2554_5_29	hypothetical protein	1.03	35.9551	1.8	DPDMGIMRPPPGMSRLPK		
4461_3_3	hypothetical protein	0.85	30.8636	1.7	KAAEER	5.1	KAAEER
13476_5_2	No hits found	-0.63	9.06241	1.7	LGMSVYR		
2565_3_14	hypothetical protein	0.30	36.2046	1.4	GLNVGFLAK		
21676_2_21	hypothetical protein	-0.66	57.755	1.1	VQELLKDEMIHRPR		
2890_4_64	hypothetical protein	1.05	37.1753	0.95	MALIPVTPPAGIVKNGTEYATK		
9341_2_6	hypothetical protein	-0.20	49.6547	0.61	EYVDTLNYNPPQTSSIEDNK		
11954_2_1	No hits found	1.04	26.9663	0.49	VSAKPGTNFTIWDTGERGELK		

ANN vs MOWSE (STAR7)



In Progress

- Metaproteomics Paper
  - Include METAVIR (GAAS, MDS, etc.) analysis with caveat, i.e. phi29 sequencing bias
  - Emphasize matches between the proteome and MG sequences (downplay MASCOT searches)
- Automate MP Analysis
- iVIREONS webpages (Mike A.)

Sequences cleaned by DECONSEQ

	STAR7	CAR9 (Broad + EnGenCore)
numAlignedReads	**824,055**	**513,540**
numAlignedBases	**84,240,446**	**27,494,474**
inferredReadError	2.17%	2.38%
numberAssembled	**125,866**	**1,261**
numberPartial	65,501	55,578
numberSingleton	150,062	118,170
numberRepeat	619,573	453,928
numberOutlier	13,115	2,773
numberTooShort	24,426	3,123
largeContigMetrics		
numberOfContigs	7,380	2,218
numberOfBases	7,524,259	2,028,489
avgContigSize	1,019	914
largestContigSize	15,940	6,912
allContigMetrics		
numberOfContigs	28,933	8,074
numberOfBases	13,543,709	3,738,919

CAR9 1st Attempt

Assembly Data	
#bases, %id	35,98
reads	41812
bases	15266925
overlaps found	28210
overlaps used	12143
aligned reads	13794
# of contigs	4615
avg contig size (largest)	521 (820)