MOLECULAR CHAPERONES DNAK AND DNAJ SHARE PREDICTED BINDING SITES ON MOST PROTEINS IN THE *E. COLI* PROTEOME

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SUPPLEMENTAL FIGURES AND TABLES

Position	1	2	3	4	5	6	7	8	9	10	11	12	13
A	0.99	0.72	1.46	0.51	1.14	0.51	1.39	-0.15	1.46	0.06	0.41	1.50	0.91
C	0.99	0.96	0.94	0.96	0.99	-1.21	0.49	0.96	-4.21	0.99	0.51	0.52	0.53
D	-0.23	1.46	0.17	1.78	2.60	0.75	0.94	0.63	2.66	0.99	4.50	-0.36	-0.24
E	5.36	0.72	-0.06	1.60	0.61	1.07	1.02	2.17	0.39	-1.08	2.17	1.89	-1.74
F	-0.87	-0.89	2.08	-2.05	-1.40	-1.76	-3.30	-3.26	-2.30	-2.45	-3.26	-2.26	-0.02
G	-0.82	-0.32	-0.06	-0.85	-0.20	1.16	-1.23	1.05	2.04	-0.02	1.05	-0.85	0.90
H	0.54	-1.76	-0.06	0.51	-1.73	-0.04	0.49	1.16	1.95	0.54	-0.04	2.24	0.53
I	4.42	-0.20	-0.58	-0.62	-2.12	-0.46	-0.19	-3.21	-1.23	-0.87	-1.56	-0.84	-1.90
K	-1.47	-0.62	-1.17	-0.04	4.42	0.79	-0.34	2.47	0.23	0.82	0.39	0.80	-0.63
L	-0.73	0.40	-1.20	-0.75	-1.38	-0.16	2.73	0.40	-0.90	0.39	-1.47	-1.10	0.84
M	0.70	1.97	0.94	0.16	2.25	0.96	-0.78	1.97	2.86	0.18	-0.37	0.98	-0.74
N	-2.37	1.57	-0.06	-0.15	0.77	-1.28	-0.17	0.08	-1.45	1.90	0.75	1.24	1.80
P	0.39	0.16	1.57	-0.04	1.37	0.96	1.88	2.15	2.44	3.78	1.26	1.69	1.29
Q	0.77	-1.28	0.80	1.57	-0.14	0.82	-1.02	-1.43	0.80	-0.73	1.10	-0.03	0.53
R	-0.73	-1.15	-1.78	-1.21	-2.19	-1.76	-1.52	-2.21	-1.51	-0.12	-1.52	-1.19	-1.48
S	0.27	-0.87	0.86	0.25	-0.47	-0.13	2.12	2.68	1.41	0.36	0.41	-0.74	0.36
T	0.88	-0.26	1.55	0.20	-0.73	4.69	-0.90	-0.15	0.17	0.88	0.41	0.87	2.80
V	-0.31	1.60	1.49	1.35	3.49	0.34	-0.43	-0.04	0.32	-1.35	0.51	0.80	-0.82
W	-0.02	-0.04	-2.49	-2.47	-0.02	-4.48	-0.06	-0.04	-3.50	0.54	-2.47	-0.74	0.53
Y	-1.18	-1.31	-0.99	-0.26	-0.53	-0.97	2.86	0.34	-0.06	-1.18	-0.56	1.17	-0.24

Supplementary Table S1. $\Delta\Delta G_{binding}$ values for DnaJ's affinity to every amino acid at each possible position in a 13mer binding site.

Number of Proteins in Proteome	4,303
Number of Proteins with DnaK Sites	4,215
Total number of DnaK Sites	95,558
Average start point (% of protein length)	46.03 ± 28.53
Average $\Delta\Delta G_{binding}$	-7.43 ± 2.08
Average number of sites per protein	22.67 ± 18.66
% Binding site coverage	7.15 ± 4.16

Supplementary Table S2. Statistical analysis of DnaK Binding sites in *E. coli*

Number of Proteins in Proteome	4,303
Number of Proteins with DnaJ Sites	4,294
Total number of DnaJ Sites	224,530
Average start point (% of protein length)	47 ± 28
Average $\Delta\Delta G_{binding}$	-4.69 ± 2.27
Average number of sites per protein	52.29 ± 38.76
% Binding site coverage	16.29 ± 6.23

Supplementary Table S3. Statistical analysis of DnaJ Binding sites in *E. coli*

sp|P0A6A8|ACP_ECOLI Acyl carrier protein OS=Escherichia coli (strain K12) GN=acpP PE=1 SV=2
sp|C1P605|AZUC_ECOLI Uncharacterized protein AzuC OS=Escherichia coli (strain K12) GN=azuC PE=1 SV=1
sp|P0AE63|CHAB_ECOLI Cation transport regulator ChaB OS=Escherichia coli (strain K12) GN=chaB PE=1 SV=1
sp|P28307|CSGA_ECOLI Major curlin subunit OS=Escherichia coli (strain K12) GN=csgA PE=1 SV=3
sp|P0A9X9|CSPA_ECOLI Cold shock protein CspA OS=Escherichia coli (strain K12) GN=cspA PE=1 SV=2
sp|P36995|CSPB_ECOLI Cold shock-like protein CspB OS=Escherichia coli (strain K12) GN=cspB PE=2 SV=1
sp|P0A9Y6|CSPC_ECOLI Cold shock-like protein CspC OS=Escherichia coli (strain K12) GN=cspC PE=1 SV=2
sp|P0A972|CSPE_ECOLI Cold shock-like protein CspE OS=Escherichia coli (strain K12) GN=cspE PE=1 SV=2
sp|P0A978|CSPG_ECOLI Cold shock-like protein CspG OS=Escherichia coli (strain K12) GN=cspG PE=1 SV=1
sp|P0A986|CSPI_ECOLI Cold shock-like protein CspI OS=Escherichia coli (strain K12) GN=cspI PE=3 SV=1
sp|P27838|CYAY_ECOLI Protein CyaY OS=Escherichia coli (strain K12) GN=cyaY PE=1 SV=1
sp|P0ACF4|DBHB_ECOLI DNA-binding protein HU-beta OS=Escherichia coli (strain K12) GN=hupB PE=1 SV=1
sp|P0ABR1|DINI_ECOLI DNA-damage-inducible protein I OS=Escherichia coli (strain K12) GN=dinI PE=1 SV=1
sp|P0A9R4|FER_ECOLI 2Fe-2S ferredoxin OS=Escherichia coli (strain K12) GN=fdx PE=1 SV=2
sp|P0A8P3|FETP_ECOLI Probable Fe(2+)-trafficking protein OS=Escherichia coli (strain K12) GN=yggX PE=1 SV=2
sp|P0A6T9|GCSH_ECOLI Glycine cleavage system H protein OS=Escherichia coli (strain K12) GN=gcvH PE=1 SV=2
sp|P68688|GLRX1_ECOLI Glutaredoxin-1 OS=Escherichia coli (strain K12) GN=grxA PE=1 SV=1
sp|P0AC92|GNSA_ECOLI Protein gnsA OS=Escherichia coli (strain K12) GN=gnsA PE=3 SV=1
sp|P0A703|HYBF_ECOLI Probable hydrogenase nickel incorporation protein hybF OS=Escherichia coli (strain K12) GN=hybF PE=3 SV=1
sp|C1P619|ILVX_ECOLI Uncharacterized protein ilvX OS=Escherichia coli (strain K12) GN=ilvX PE=1 SV=1
sp|P0C0L9|ISCX_ECOLI Protein iscX OS=Escherichia coli (strain K12) GN=iscX PE=1 SV=1
sp|Q6BF86|LDRA_ECOLI Small toxic polypeptide ldrA/ldrC OS=Escherichia coli (strain K12) GN=ldrA PE=2 SV=1
sp|Q6BF87|LDRB_ECOLI Small toxic polypeptide ldrB OS=Escherichia coli (strain K12) GN=ldrB PE=2 SV=1
sp|Q6BF25|LDRD_ECOLI Small toxic polypeptide ldrD OS=Escherichia coli (strain K12) GN=ldrD PE=2 SV=1
sp|P0AD74|LPF2_ECOLI Phenylalanyl--tRNA ligase operon leader peptide OS=Escherichia coli (strain K12) GN=pheM PE=4 SV=1
sp|P0ADF0|LPFS_ECOLI Putative fruR/shl operon leader peptide OS=Escherichia coli (strain K12) GN=fruL PE=5 SV=1
sp|A8DYP9|LPFUR_ECOLI Fur leader peptide OS=Escherichia coli (strain K12) GN=uof PE=1 SV=1
sp|P0AD72|LPF_ECOLI Phe operon leader peptide OS=Escherichia coli (strain K12) GN=pheL PE=4 SV=1
sp|P60995|LPHI_ECOLI His operon leader peptide OS=Escherichia coli (strain K12) GN=hisL PE=3 SV=1
sp|P0ADF3|LPRH_ECOLI Putative rho operon leader peptide OS=Escherichia coli (strain K12) GN=rhoL PE=5 SV=1
sp|P0AD89|LPTN_ECOLI Tryptophanase leader peptide OS=Escherichia coli (strain K12) GN=tnaL PE=4 SV=1
sp|P0AD92|LPW_ECOLI Trp operon leader peptide OS=Escherichia coli (strain K12) GN=trpL PE=1 SV=1
sp|P0A917|OMPX_ECOLI Outer membrane protein X OS=Escherichia coli (strain K12) GN=ompX PE=1 SV=1
sp|P02338|PRTL_ECOLI Protamine-like protein OS=Escherichia coli (strain K12) GN=tpr PE=4 SV=2
sp|P69808|PTFB1_ECOLI Fructose-like phosphotransferase enzyme IIB component 1 OS=Escherichia coli (strain K12) GN=fryB PE=1 SV=1
sp|P37188|PTKB_ECOLI Galactitol-specific phosphotransferase enzyme IIB component OS=Escherichia coli (strain K12) GN=gatB PE=1 SV=2
sp|P0A7M9|RL31_ECOLI 50S ribosomal protein L31 OS=Escherichia coli (strain K12) GN=rpmE PE=1 SV=1
sp|P0A7N4|RL32_ECOLI 50S ribosomal protein L32 OS=Escherichia coli (strain K12) GN=rpmF PE=1 SV=2
sp|P0AFW2|RMF_ECOLI Ribosome modulation factor OS=Escherichia coli (strain K12) GN=rmf PE=1 SV=1
sp|P0AF90|RRAB_ECOLI Regulator of ribonuclease activity B OS=Escherichia coli (strain K12) GN=rraB PE=1 SV=1
sp|P07464|THGA_ECOLI Galactoside O-acetyltransferase OS=Escherichia coli (strain K12) GN=lacA PE=1 SV=1
sp|P0A8H8|YACG_ECOLI UPF0243 zinc-binding protein yacG OS=Escherichia coli (strain K12) GN=yacG PE=1 SV=1
sp|P0A8K5|YAEP_ECOLI UPF0253 protein yaeP OS=Escherichia coli (strain K12) GN=yaeP PE=1 SV=1
sp|P0AAS7|YBCJ_ECOLI Uncharacterized protein ybcJ OS=Escherichia coli (strain K12) GN=ybcJ PE=1 SV=1
sp|P0AAS9|YBDD_ECOLI Uncharacterized protein ybdD OS=Escherichia coli (strain K12) GN=ybdD PE=4 SV=1
sp|P0A8J4|YBED_ECOLI UPF0250 protein ybeD OS=Escherichia coli (strain K12) GN=ybeD PE=1 SV=1
sp|P41039|YBII_ECOLI Uncharacterized protein YbiI OS=Escherichia coli (strain K12) GN=ybiI PE=1 SV=1
sp|P0AAX3|YBIJ_ECOLI Uncharacterized protein YbiJ OS=Escherichia coli (strain K12) GN=ybiJ PE=3 SV=1

sp|P0AB14|YCCJ_ECOLI Uncharacterized protein yccJ OS=Escherichia coli (strain K12) GN=yccJ PE=4 SV=1
sp|P21361|YCIG_ECOLI Uncharacterized protein yciG OS=Escherichia coli (strain K12) GN=yciG PE=1 SV=1
sp|P58094|YCIX_ECOLI Uncharacterized protein yciX OS=Escherichia coli (strain K12) GN=yciX PE=4 SV=2
sp|A5A614|YCIZ_ECOLI UPF0509 protein yciZ OS=Escherichia coli (strain K12) GN=yciZ PE=3 SV=1
sp|P38394|YDAE_ECOLI Uncharacterized protein ydaE OS=Escherichia coli (strain K12) GN=ydaE PE=4 SV=1
sp|P0ACW0|YDAF_ECOLI Uncharacterized protein ydaF OS=Escherichia coli (strain K12) GN=ydaF PE=4 SV=1
sp|P0ACW8|YDFA_ECOLI Uncharacterized protein ydfA OS=Escherichia coli (strain K12) GN=ydfA PE=4 SV=1
sp|P29009|YDFB_ECOLI Uncharacterized protein ydfB OS=Escherichia coli (strain K12) GN=ydfB PE=1 SV=1
sp|P76231|YEAC_ECOLI Uncharacterized protein yeaC OS=Escherichia coli (strain K12) GN=yeaC PE=4 SV=2
sp|P76275|YEBW_ECOLI Uncharacterized protein yebW OS=Escherichia coli (strain K12) GN=yebW PE=4 SV=2
sp|P0AA31|YEDF_ECOLI UPF0033 protein yedF OS=Escherichia coli (strain K12) GN=yedF PE=1 SV=1
sp|P76322|YEDM_ECOLI Uncharacterized protein yedM OS=Escherichia coli (strain K12) GN=yedM PE=1 SV=1
sp|P33014|YEED_ECOLI UPF0033 protein yeeD OS=Escherichia coli (strain K12) GN=yeeD PE=3 SV=1
sp|P0AFT8|YEIW_ECOLI UPF0153 protein yeiW OS=Escherichia coli (strain K12) GN=yeiW PE=3 SV=1
sp|P77656|YFDK_ECOLI Uncharacterized protein yfdK OS=Escherichia coli (strain K12) GN=yfdK PE=4 SV=1
sp|P76516|YFDT_ECOLI Uncharacterized protein yfdT OS=Escherichia coli (strain K12) GN=yfdT PE=4 SV=1
sp|P52102|YFHL_ECOLI Uncharacterized ferredoxin-like protein yfhL OS=Escherichia coli (strain K12) GN=yfhL PE=1 SV=1
sp|Q46905|YGCO_ECOLI Ferredoxin-like protein ygcO OS=Escherichia coli (strain K12) GN=ygcO PE=3 SV=2
sp|P65292|YGDI_ECOLI Uncharacterized lipoprotein ygdI OS=Escherichia coli (strain K12) GN=ygdI PE=4 SV=1
sp|Q46789|YGEI_ECOLI Uncharacterized protein ygeI OS=Escherichia coli (strain K12) GN=ygeI PE=4 SV=1
sp|P0ADU2|YGIN_ECOLI Probable quinol monooxygenase ygiN OS=Escherichia coli (strain K12) GN=ygiN PE=1 SV=1
sp|P67624|YHEU_ECOLI UPF0270 protein yheU OS=Escherichia coli (strain K12) GN=yheU PE=3 SV=1
sp|P0ADW8|YHEV_ECOLI Uncharacterized protein yheV OS=Escherichia coli (strain K12) GN=yheV PE=4 SV=1
sp|C1P621|YJEV_ECOLI Uncharacterized protein yjeV OS=Escherichia coli (strain K12) GN=yjeV PE=1 SV=1
sp|P77087|YLCE_ECOLI Putative uncharacterized protein ylcE OS=Escherichia coli (strain K12) GN=ylcE PE=5 SV=1
sp|Q47268|YLCH_ECOLI Uncharacterized protein ylcH in lambdoid DLP12 prophage region OS=Escherichia coli (strain K12) GN=ylcH PE=4 SV=1
sp|P56614|YMDF_ECOLI Uncharacterized protein ymdF OS=Escherichia coli (strain K12) GN=ymdF PE=1 SV=1
sp|P0CD93|YMJD_ECOLI Putative uncharacterized protein ymjD OS=Escherichia coli (strain K12) GN=ymjD PE=5 SV=1
sp|P64448|YNBE_ECOLI Uncharacterized protein ynbE OS=Escherichia coli (strain K12) GN=ynbE PE=4 SV=1
sp|C1P600|YNBG_ECOLI Uncharacterized protein ynbG OS=Escherichia coli (strain K12) GN=ynbG PE=1 SV=1
sp|P76138|YNEL_ECOLI Putative HTH-type transcriptional regulator yneL OS=Escherichia coli (strain K12) GN=yneL PE=5 SV=1
sp|P0AEB7|YOAB_ECOLI RutC family protein yoaB OS=Escherichia coli (strain K12) GN=yoaB PE=3 SV=1
sp|P67338|YOAH_ECOLI UPF0181 protein yoaH OS=Escherichia coli (strain K12) GN=yoaH PE=3 SV=1
sp|Q2EET0|YPDJ_ECOLI Putative uncharacterized protein ypdJ OS=Escherichia coli (strain K12) GN=ypdJ PE=5 SV=1
sp|C1P610|YPDK_ECOLI Uncharacterized membrane protein ypdK OS=Escherichia coli (strain K12) GN=ypdK PE=1 SV=1
sp|A5A621|YPFM_ECOLI Uncharacterized protein ypfM OS=Escherichia coli (strain K12) GN=ypfM PE=1 SV=1
sp|C1P613|YQEL_ECOLI Uncharacterized protein yqeL OS=Escherichia coli (strain K12) GN=yqeL PE=1 SV=1
sp|P0A9W6|YRBA_ECOLI Uncharacterized protein YrbA OS=Escherichia coli (strain K12) GN=yrbA PE=1 SV=1
sp|C1P618|YRBN_ECOLI Uncharacterized protein yrbN OS=Escherichia coli (strain K12) GN=yrbN PE=1 SV=1
sp|P0AC51|ZUR_ECOLI Zinc uptake regulation protein OS=Escherichia coli (strain K12) GN=zur PE=1 SV=1

Supplementary Table S4. Proteins without a DnaK binding site.

sp|P36560|ASR_ECOLI Acid shock protein OS=Escherichia coli (strain K12) GN=asr PE=1 SV=3
sp|P60995|LPHI_ECOLI His operon leader peptide OS=Escherichia coli (strain K12) GN=hisL PE=3 SV=1
sp|P03061|LPIV_ECOLI IlvBN operon leader peptide OS=Escherichia coli (strain K12) GN=ivbL PE=4 SV=1
sp|P0AD86|LPT_ECOLI Thr operon leader peptide OS=Escherichia coli (strain K12) GN=thrL PE=3 SV=1
sp|P76096|MOKB_ECOLI Regulatory protein mokB OS=Escherichia coli (strain K12) GN=mokB PE=4 SV=1
sp|P64496|YOAG_ECOLI Protein yoaG OS=Escherichia coli (strain K12) GN=yoaG PE=1 SV=1
sp|C1P606|YOEI_ECOLI Uncharacterized protein yoeI OS=Escherichia coli (strain K12) GN=yoeI PE=1 SV=1
sp|C1P620|YSHB_ECOLI Uncharacterized protein yshB OS=Escherichia coli (strain K12) GN=yshB PE=1 SV=1
sp|P0AC51|ZUR_ECOLI Zinc uptake regulation protein OS=Escherichia coli (strain K12) GN=zur PE=1 SV=1

Supplementary Table S5. Proteins without a DnaJ binding site.

	DnaK	DnaJ
Number of Proteins with Unique Sites	1,701	4,112
Total number of Unique Binding Sites	4,526 (4.7%)	69,595 (31.0%)
Average start point (% of protein length)	47.76 ± 29.55	49.22 ± 27.80
Average $\Delta\Delta G_{\mathrm{binding}}$	-7.07 ± 1.84	-4.47 ± 2.12
Average number of sites per protein	2.66 ± 2.14	16.93 ± 14.26
% Binding site coverage	0.84 ± 1.01	5.32 ± 3.17

Supplementary Table S6. Statistical data regarding unique DnaJ and unique DnaK binding sites.

	K site with Overlapping J site	J site with Overlapping K site	Identical
Number of Proteins with Overlapping Sites	4,192	4,198	3,739
Total number Overlapping Sites	91,032 (95.3%)	154,935 (69.0%)	24,653 (J: 11%; K: 25.8%)
Average start point (% of protein length)	45.83 ± 28.41	46.07 ± 28.02	44.40 ± 28.82
Average $\Delta\Delta G_{\mathrm{binding}}$	-7.45 ± 2.09	-4.79 ± 2.32	J: -4.97 ± 2.41 K: -7.56 ± 2.16
Average number of sites per protein	21.72 ± 18.23	36.90 ± 30.78	6.59 ± 6.17
% Binding site coverage	6.81 ± 4.15	11.42 ± 6.60	2.12 ± 1.82

Supplementary Table S7. Statistical data regarding overlapping and identical DnaK/J binding sites.