

Figure S1a. Bean plots (generated with BoxPlotR) showing the distribution of XiQ quantified fold-change ($\log_2(\text{H/L ratio})$) for cross-links in control and experimental samples for (A) SpyL32P +/- Im7 datasets, (B) SpyL32P +/- 8M Urea datasets, and (C) SpyL32P+Im7 +/- 8M Urea datasets. The fold-change of the reverse-labeled experimental sample is shown as $\log_2(\text{H/L ratio}) * (-1)$.

Fold-change in Cross-links (L+-U-)

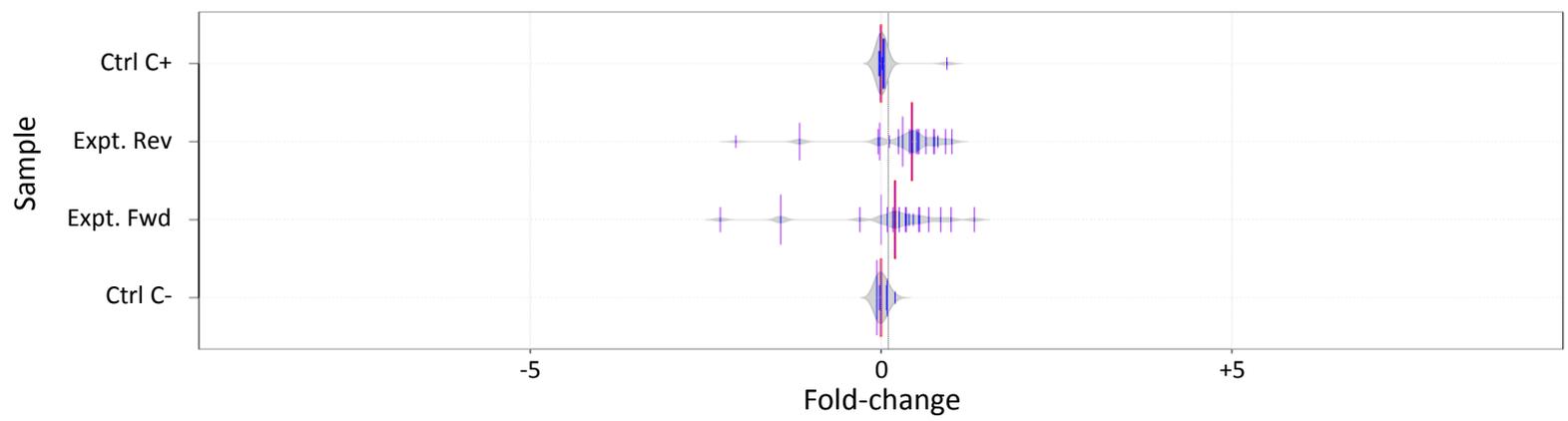


Figure S1b. Bean plots (generated with BoxPlotR) showing the distribution of XiQ quantified fold-change ($\log_2(\text{H/L ratio})$) for cross-links in control and experimental samples for FKBP25 F145A I223P +/- rapamycin datasets. The fold-change of the reverse-labeled experimental sample is shown as $\log_2(\text{H/L ratio}) * (-1)$.

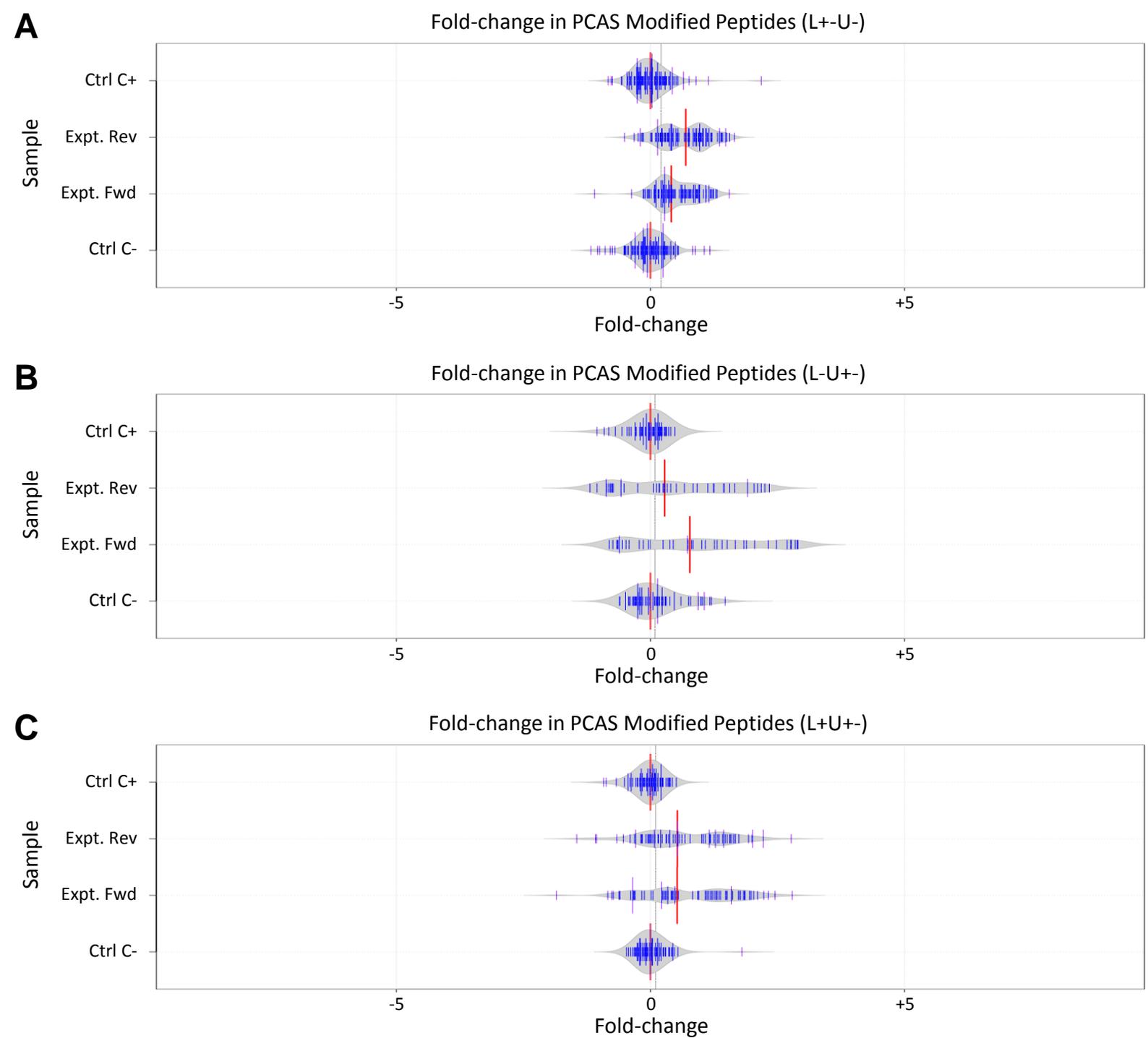


Figure S2a. Bean plots (generated with BoxPlotR) showing the distribution of XiQ quantified fold-change ($\log_2(\text{H/L ratio})$) for PCAS-modified peptides in control and experimental samples for (A) SpyL32P +/- Im7 datasets, (B) SpyL32P +/- 8M Urea datasets, and (C) SpyL32P+Im7 +/- 8M Urea datasets. The fold-change of the reverse-labeled experimental sample is shown as $\log_2(\text{H/L ratio}) * (-1)$.

Fold-change in PCAS Modified Peptides (L+-U-)

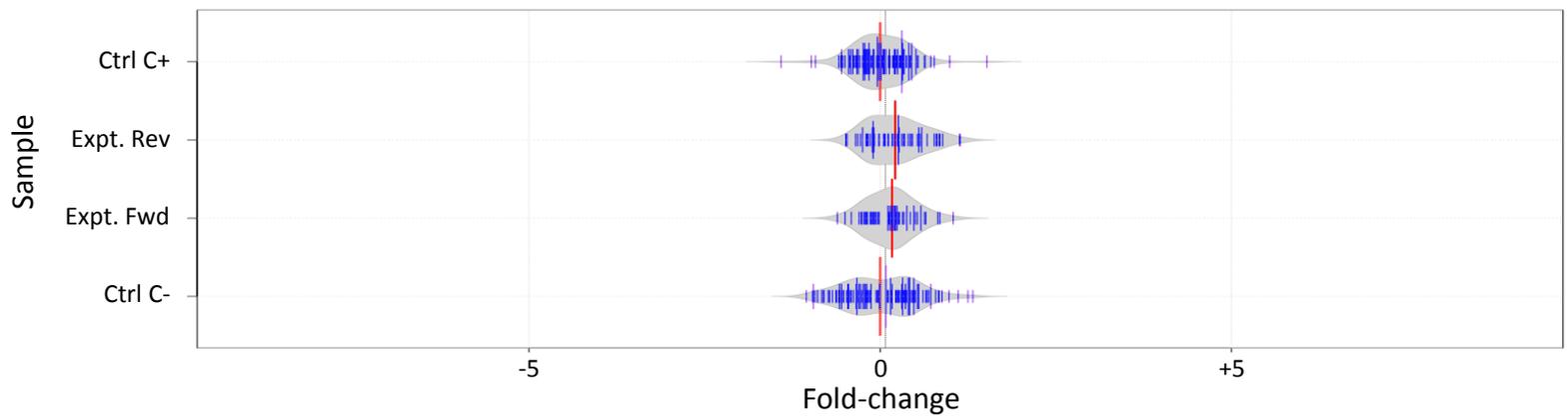


Figure S2b. Bean plots (generated with BoxPlotR) showing the distribution of XiQ quantified fold-change ($\log_2(\text{H/L ratio})$) for PCAS-modified peptides in control and experimental samples for FKBP25 F145A I223P +/- rapamycin datasets. The fold-change of the reverse-labeled experimental sample is shown as $\log_2(\text{H/L ratio}) * (-1)$.

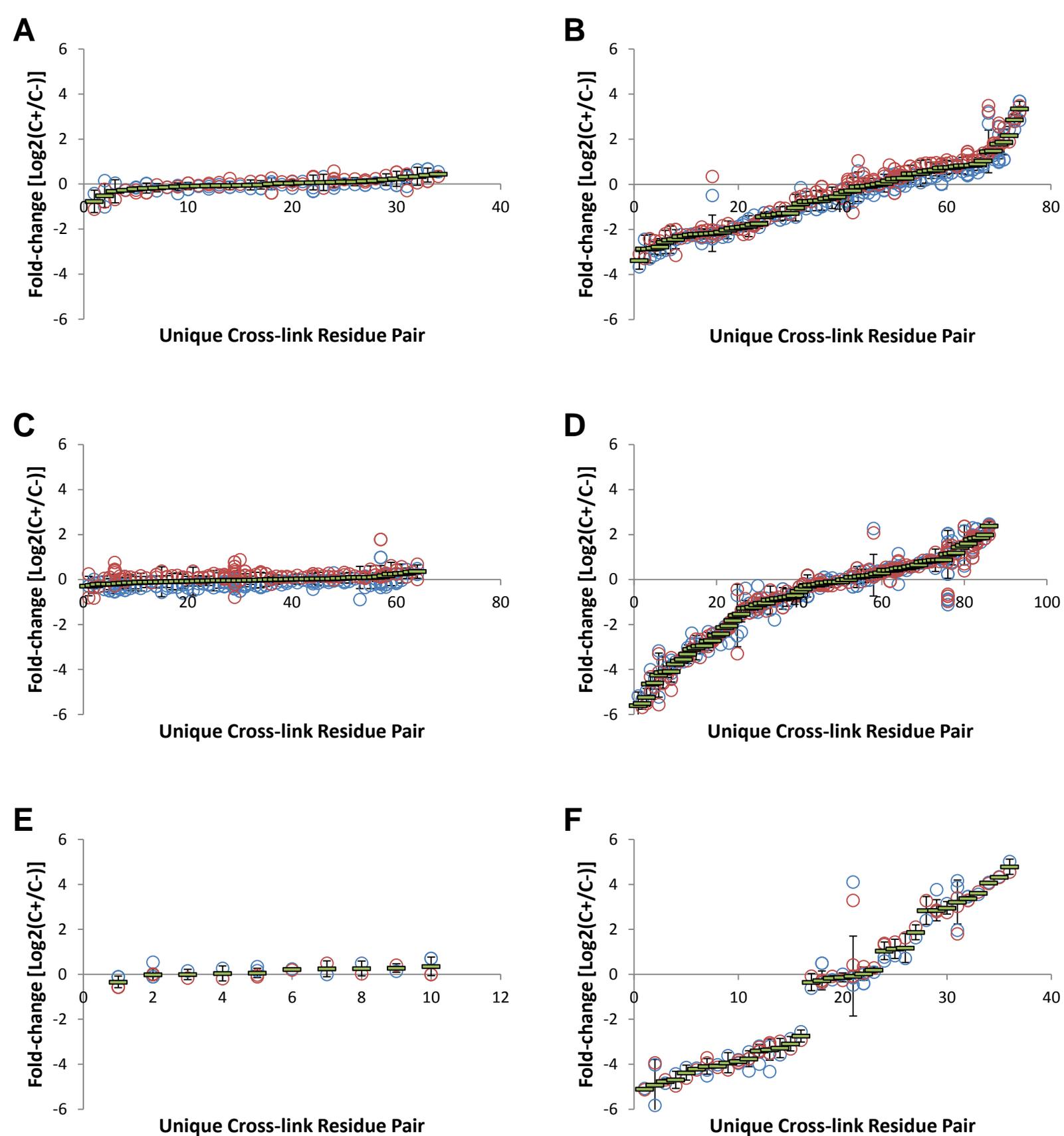


Figure S3a. Range of observed $\log_2(H/L)$ ratio for all quantified cross-links. Blue circles represent data for control condition(-) or experimental forward-labeled cross-links and red circles represent data for control condition(+) or experimental reverse-labeled cross-links. Green bars indicate median fold-change. The fold-change of the reverse-labeled experimental sample is shown as $\log_2(H/L) * (-1)$. (A) SpyL32P condition(+/- Im7) control samples. (B) SpyL32P condition(+/- Im7) experimental samples. (C) SpyL32P condition(+/- 8M Urea) control samples. (D) SpyL32P condition(+/- 8M Urea) experimental samples. (E) SpyL32P+Im7 condition(+/- 8M Urea) control samples. (F) SpyL32P+Im7 condition(+/- 8M Urea) experimental samples.

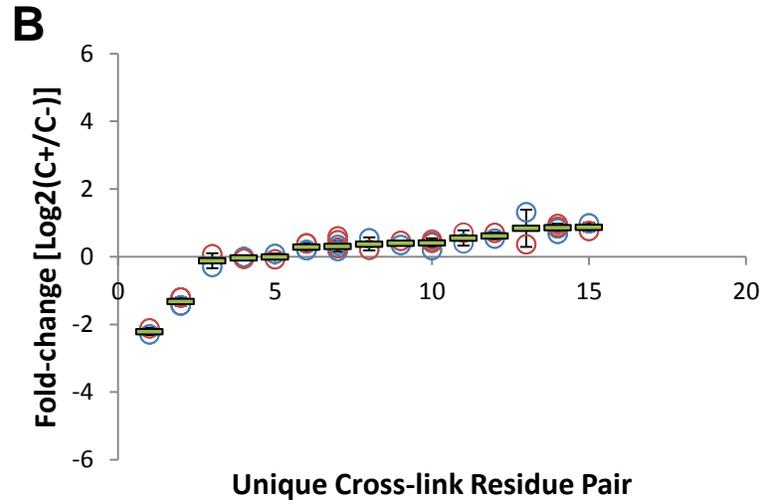
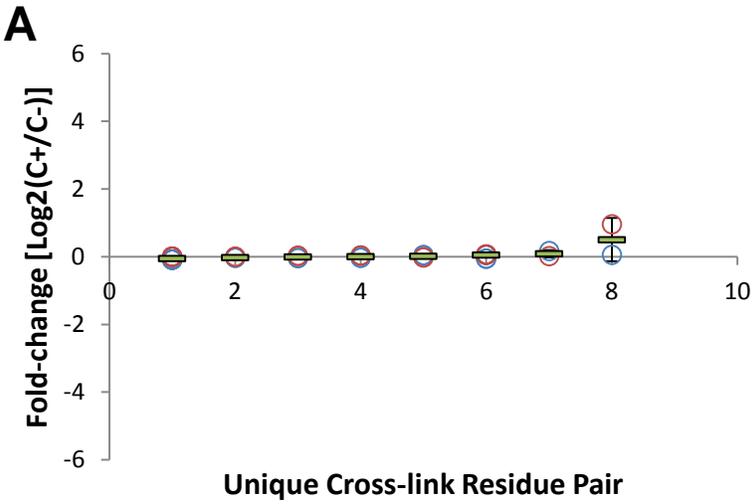


Figure S3b. Range of observed $\log_2(H/L)$ ratio for all quantified cross-links. Blue circles represent data for control condition(-) or experimental forward-labeled cross-links and red circles represent data for control condition(+) or experimental reverse-labeled cross-links. Green bars indicate median fold-change. The fold-change of the reverse-labeled experimental sample is shown as $\log_2(H/L) * (-1)$. **(A)** FKBP25 F145A I223P condition(+/- rapamycin) control samples. **(B)** FKBP25 F145A I223P condition(+/- rapamycin) experimental samples.

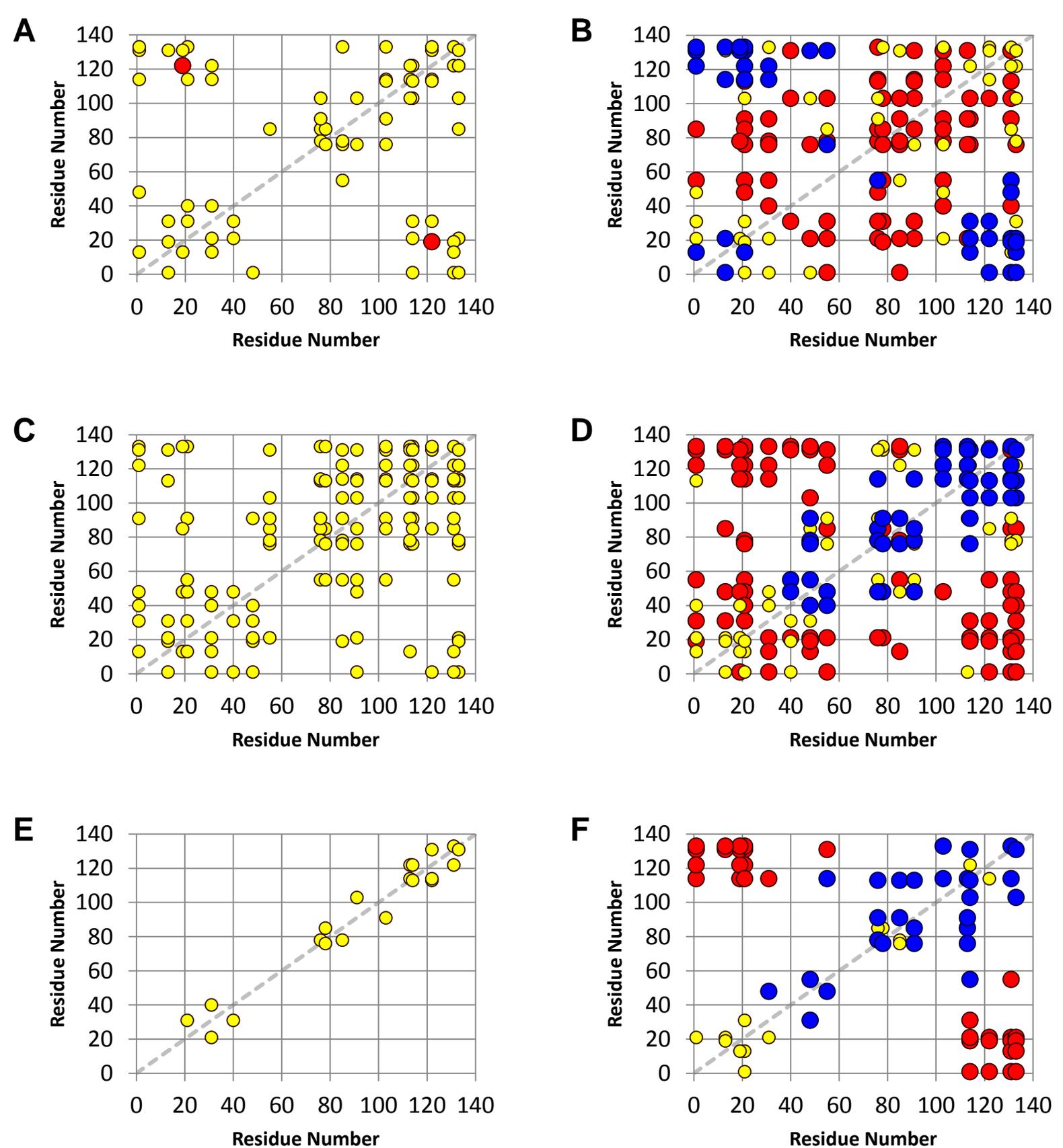


Figure S4a. Cross-link contact maps. **(A)** SpyL32P condition(+/- Im7) control samples. **(B)** SpyL32P condition(+/- Im7) experimental samples. **(C)** SpyL32P condition(+/- 8M Urea) control samples. **(D)** SpyL32P condition(+/- 8M Urea) experimental samples. **(E)** SpyL32P+Im7 condition(+/- 8M Urea) control samples. **(F)** SpyL32P+Im7 condition(+/- 8M Urea) experimental samples. Red circles indicate cross-links are enriched in condition(-). Blue circles indicate cross-links are enriched in condition(+). Yellow circles indicate no significant change between in cross-link abundance between condition(-) and condition(+). Thresholds for significance are reported in supplementary table 1.

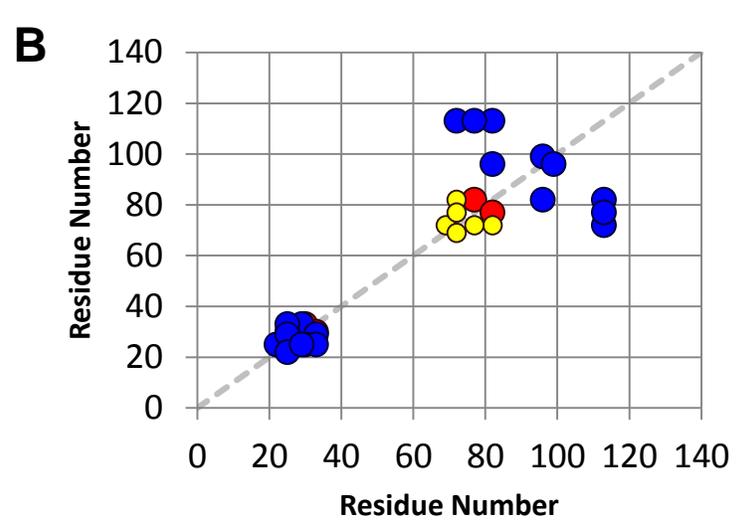
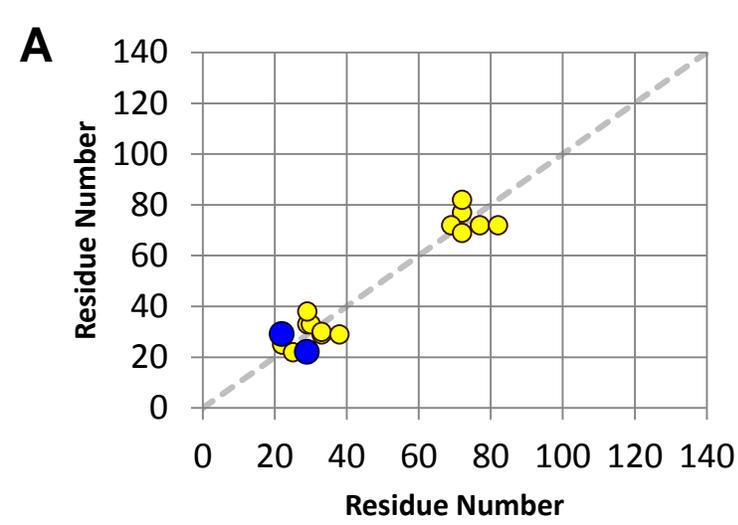


Figure S4b. Cross-link contact maps. **(A)** FKBP25 F145A I223P condition(+/- rapamycin) control samples. **(B)** FKBP25 F145A I223P condition(+/- rapamycin) experimental samples. Thresholds for significance are reported in supplementary table 1.

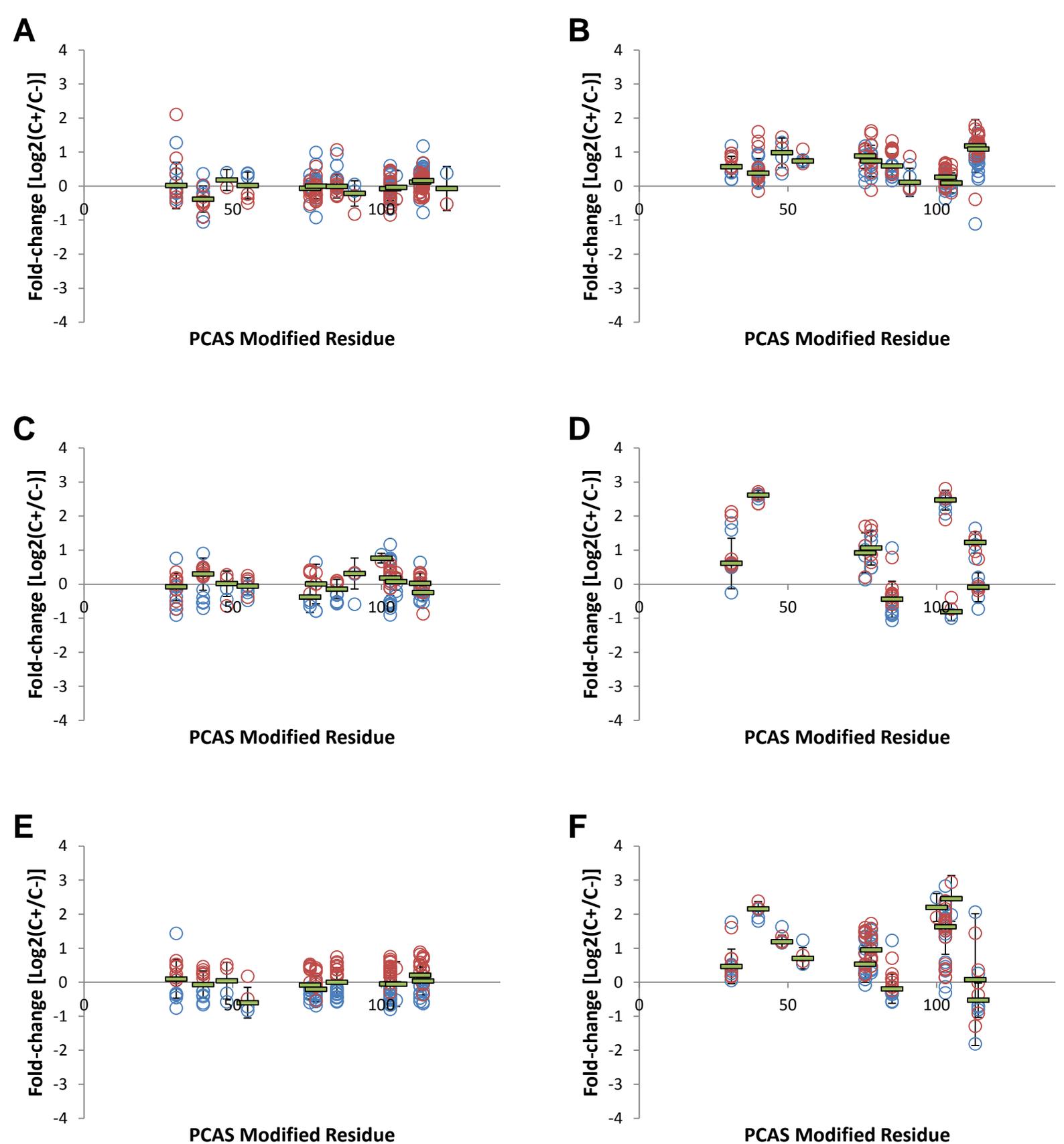


Figure S5a. Range of observed $\log_2(H/L)$ ratio for all quantified PCAS-modified peptides. Blue circles represent data for control condition(-) or experimental forward-labeled cross-links and red circles represent data for control condition(+) or experimental reverse-labeled cross-links. Green bars indicate median fold-change. The fold-change of the reverse-labeled experimental sample is shown as $\log_2(H/L \text{ ratio}) * (-1)$. **(A)** SpyL32P condition(+/- Im7) control samples. **(B)** SpyL32P condition(+/- Im7) experimental samples. **(C)** SpyL32P condition(+/- 8M Urea) control samples. **(D)** SpyL32P condition(+/- 8M Urea) experimental samples. **(E)** SpyL32P+Im7 condition(+/- 8M Urea) control samples. **(F)** SpyL32P+Im7 condition(+/- 8M Urea) experimental samples.

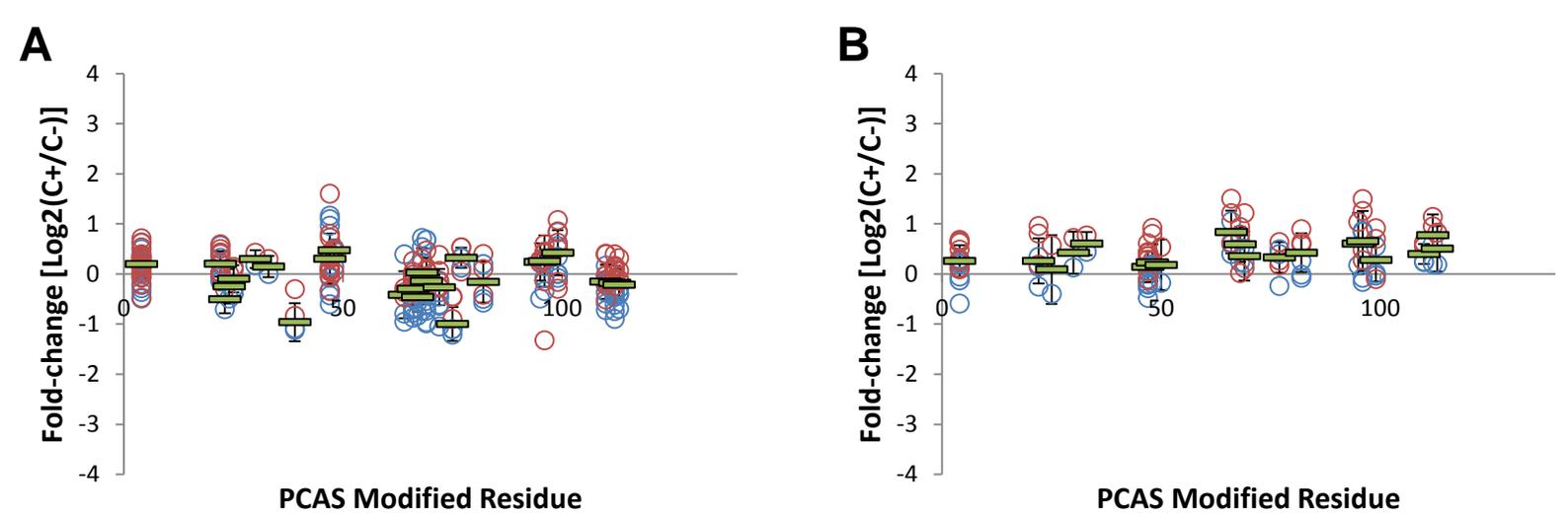


Figure S5b. Range of observed \log_2 (H/L ratio) for all quantified PCAS-modified peptides. Blue circles represent data for control condition(-) or experimental forward-labeled cross-links and red circles represent data for control condition(+) or experimental reverse-labeled cross-links. Green bars indicate median fold-change. The fold-change of the reverse-labeled experimental sample is shown as \log_2 (H/L ratio)*(-1). **(A)** FKBP25 F145A I223P condition(+/- rapamycin) control samples. **(B)** FKBP25 F145A I223P condition(+/- rapamycin) experimental samples.

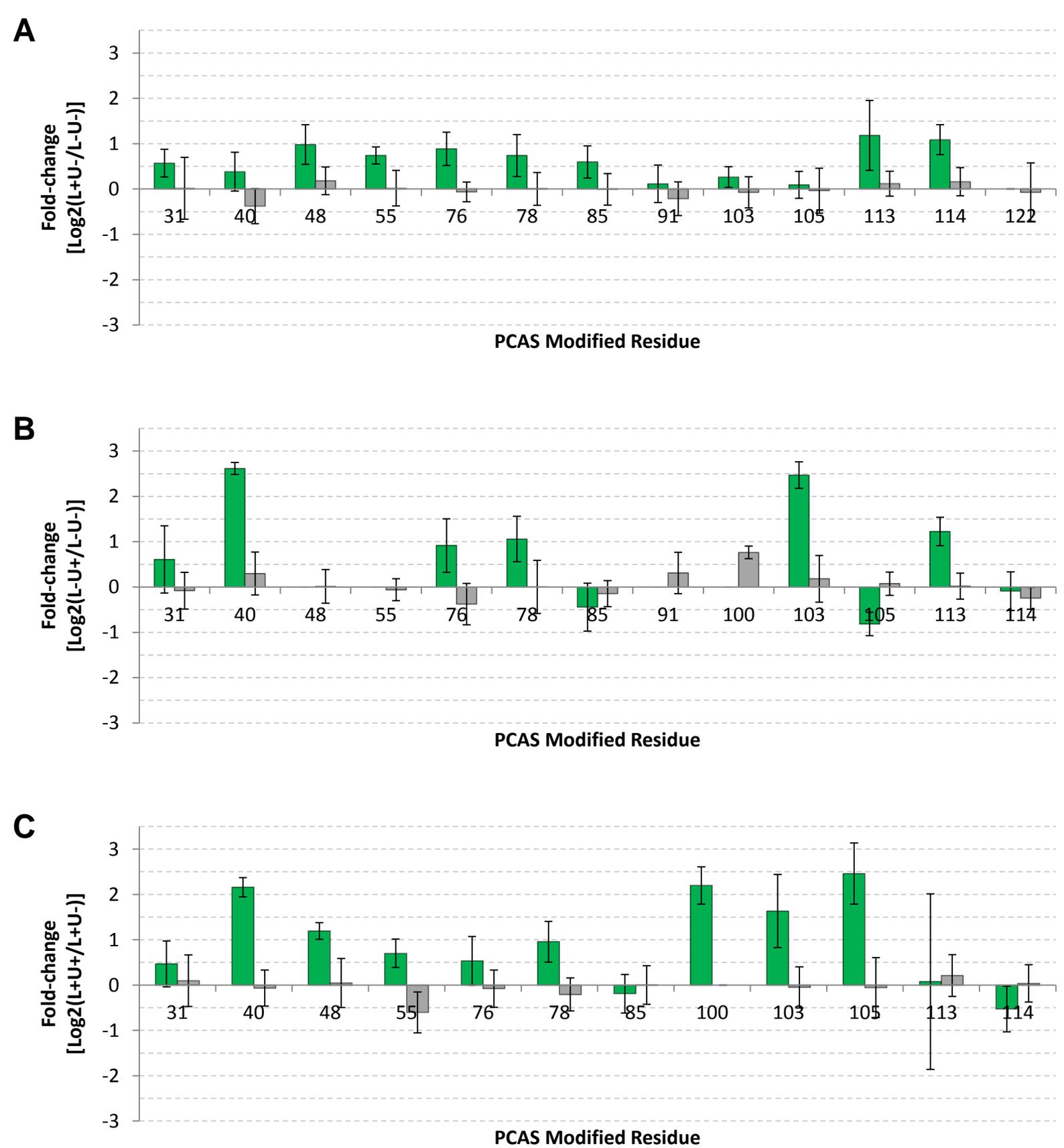


Figure S6a. Unique PCAS-modified residue fold-change column charts. **(A)** SpyL32P condition(+/- Im7) samples. **(B)** SpyL32P condition(+/- 8M Urea) samples. **(C)** SpyL32P+Im7 condition(+/- 8M Urea) samples. Experimental and control sample data are represented by green and grey bars, respectively. Error bars indicate standard error for all identified PCAS-modified peptides with modification on respective residue.

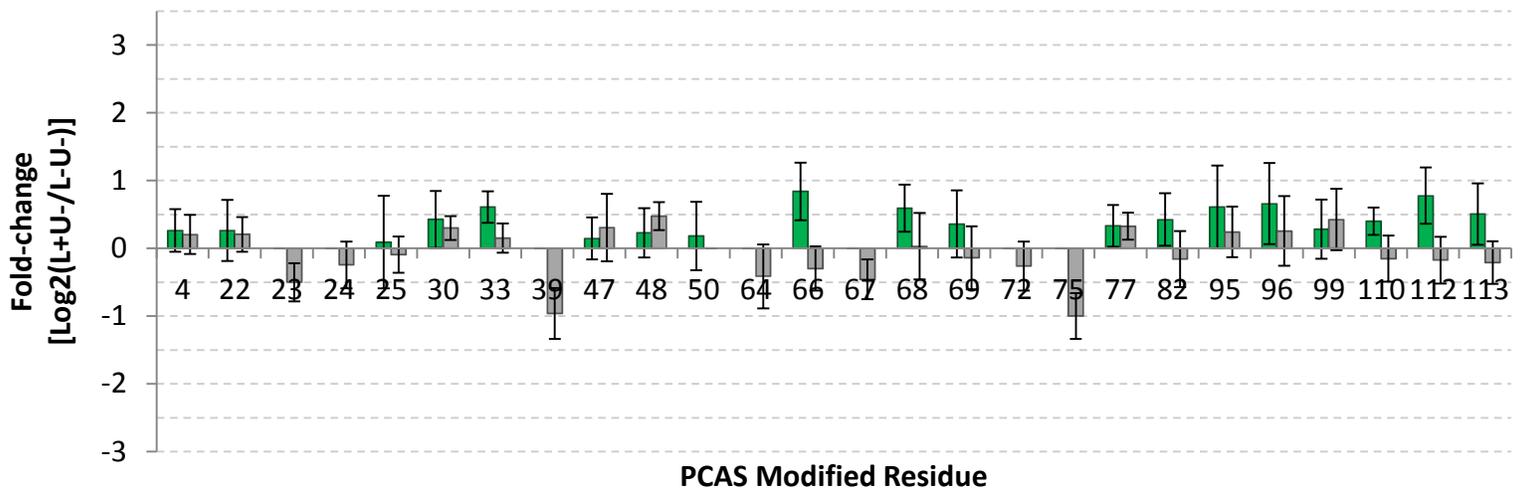


Figure S6b. Unique PCAS-modified residue fold-change column charts for FKBP25 F145A I223P condition(+/- rapamycin) control samples. Experimental and control sample data are represented by green and grey bars, respectively. Error bars indicate standard error for all identified PCAS-modified peptides with modification on respective residue.

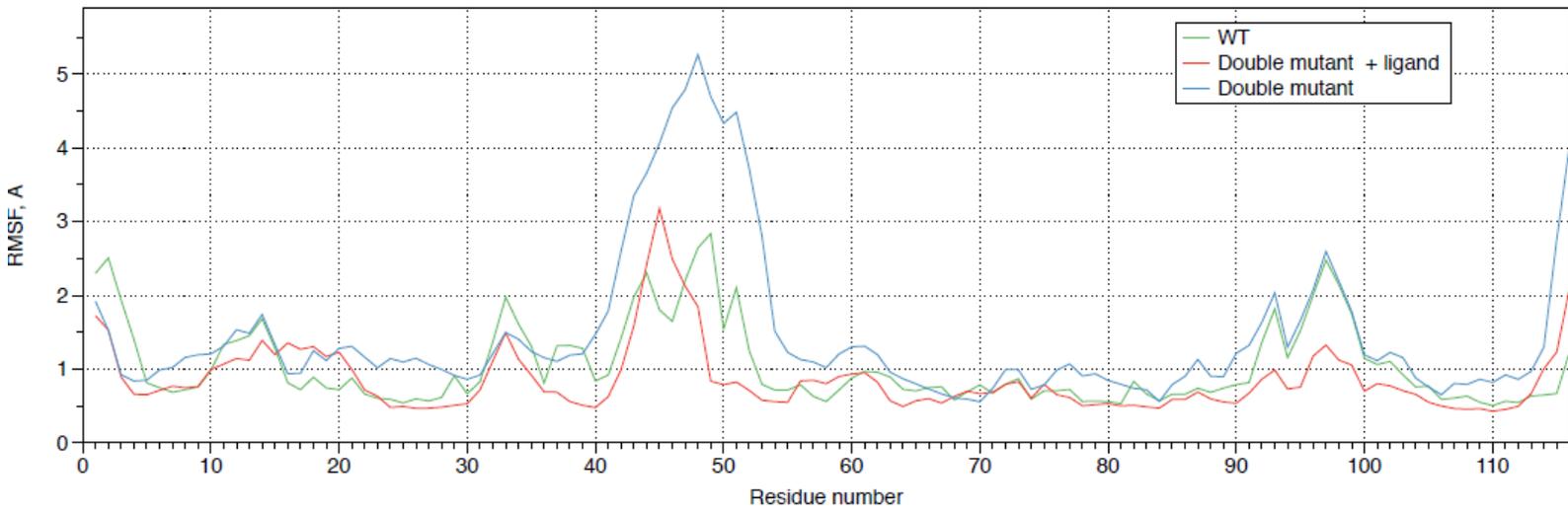


Figure S7. Main chain fluctuations along MD trajectory.

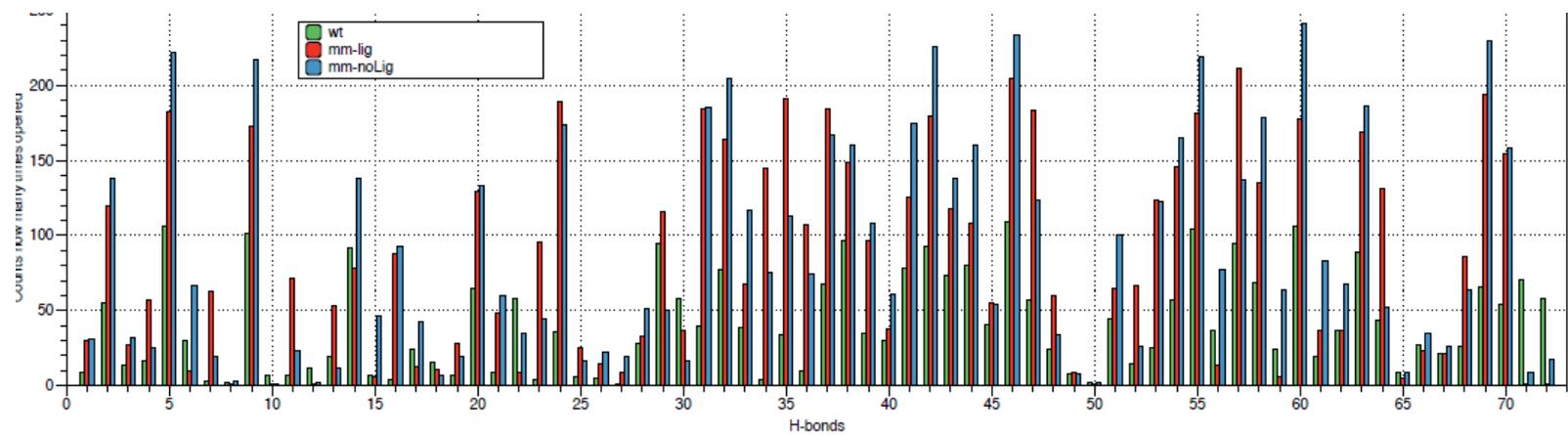


Figure S8. Frequencies of opening along MD trajectory of the backbone amide donor-acceptor pairs.

Table S1. Standard deviation of fold-change [$\text{Log}_2(\text{C+}/\text{C-})$] Significance thresholds used classification of corresponding $\text{log}_2(\text{H}/\text{L}$ ratio) medians as enriched in condition(-), condition(+), or unchanged are calculated as 2x the sample standard deviation.

Experiment	Control Condition(-) and Condition(+) Fold-change [$\text{Log}_2(\text{C+}/\text{C-})$] Sample Standard Deviation (s)	Experiment Forward and Reverse Significance Fold-change [$\text{Log}_2(\text{C+}/\text{C-})$] Threshold (+/-2s)
Spy qCL L+-U-	0.298	0.597
Spy qCL L-U+-	0.234	0.469
Spy qCL L+U+-	0.311	0.622
Spy SM L+-U-	0.373	0.746
Spy SM L-U+-	0.382	0.764
Spy SM L+U+-	0.280	0.561
FKBP qCL L+-U-	0.134	0.268
FKBP SM L+-U-	0.446	0.893
FKBP SM L-U+-	0.721	1.442
FKBP SM L+U+-	0.687	1.374

Table S2. Sample naming convention and conditions.

Sample #	Ligand	Urea	Isotopic Label
01	-	-	Light
02	-	-	Heavy
04	-	+	Light
05	-	+	Heavy
07	+	-	Light
08	+	-	Heavy
10	+	+	Light
11	+	+	Heavy

Table S3. Sample combination reference table.

Sample	L+U-	L-U+	L+U+
Ctrl Condition (-)	01-02	01-02	07-08
Experimental Forward Label	01-08	01-05	07-11
Experimental Reverse Label	02-07	02-04	08-10
Ctrl Condition (+)	07-08	04-05	10-11

S. Material. Summary Microsoft Excel workbooks of all quantitative cross-linking and surface modification results to be uploaded.

Name	Date modified	Type	Size
FKBP25_F145A_I223P_qCL_L+-U-.xlsb	11/7/2016 11:12 AM	Microsoft Excel Binary Worksheet	493 KB
FKBP25_F145A_I223P_SM_L+-U-.xlsb	11/6/2016 12:22 PM	Microsoft Excel Binary Worksheet	666 KB
FKBP25_F145A_I223P_SM_L+U+-U-.xlsb	11/7/2016 11:13 AM	Microsoft Excel Binary Worksheet	378 KB
FKBP25_F145A_I223P_SM_L-U+-U-.xlsb	11/7/2016 11:13 AM	Microsoft Excel Binary Worksheet	321 KB
SpyL32P_qCL_L+-U-.xlsb	11/7/2016 11:00 AM	Microsoft Excel Binary Worksheet	3,042 KB
SpyL32P_qCL_L+U+-U-.xlsb	11/7/2016 11:02 AM	Microsoft Excel Binary Worksheet	1,731 KB
SpyL32P_qCL_L-U+-U-.xlsb	11/7/2016 11:03 AM	Microsoft Excel Binary Worksheet	3,619 KB
SpyL32P_SM_L+-U-.xlsb	11/7/2016 11:08 AM	Microsoft Excel Binary Worksheet	773 KB
SpyL32P_SM_L+U+-U-.xlsb	11/7/2016 11:08 AM	Microsoft Excel Binary Worksheet	645 KB
SpyL32P_SM_L-U+-U-.xlsb	11/7/2016 11:09 AM	Microsoft Excel Binary Worksheet	624 KB

e.g.

1	quantified in	raw_name	scan_number	precursor_mz	precursor_charge	label	label_count	label_state	expected_shift	time_window	id	Scan Number	Ret Time	Obs Mass	Charge	PSM Mass	PPM Error	Score	dScore	Pep. Diff.	Peptide #1	Link #1	
2	CAXIGMR	20160720	5284	892.470327	2	6.020123	1	0	0	3	15242/5284	5284	55.682	1782.926	2	1782.916	-5.686	0.05	0.05	0	[128.07]SDYEA-FYLLK	-1	Int_T
3	CAXIGMR	20160720	2916	511.255343	3	6.020123	1	0	0	3	13337/2916	2916	37.458	1530.753	3	1530.758	3.1549	0.02	0.02	0	A-AGAAK[128.07]MFCOR	-1	SPyL
4	CAXIGMR	20160720	1863	900.473777	2	6.020123	1	0	0	3	12020/1863	1863	26.142	1798.933	2	1798.937	2.0705	1.33	1.33	0	LT-EPAAK[128.05]KMPATAE	-1	SPyL
5	CAXIGMR	20160720	###	910.452127	2	6.020123	1	0	0	3	14705/444	1863	49.373	1818.893	2	1818.894	2.4228	5.33	5.33	0	AMHDIASDTFQK[128.05]VK	-1	SPyL
6	CAXIGMR	20160720	4526	910.456727	2	6.020123	1	0	0	3	14745/4526	4526	49.434	1818.893	2	1818.894	-2.611	4.65	4.65	0	AMHDIASDTFQK[128.05]VK	-1	SPyL
7	CAXIGMR	20160720	###	607.304977	3	6.020123	1	0	0	3	15026/43	###	52.709	1818.893	3	1818.894	0.551	0.94	0.94	0	AMHDIASDTFQK[128.05]VK	-1	SPyL
8	CAXIGMR	20160720	3911	659.337277	3	6.020123	1	0	0	3	14306/3911	3911	44.773	1974.397	3	1974.399	2.6539	6.25	6.25	0	FAMHIIASDTFQK[128.05]VK	-1	SPyL
9	CAXIGMR	20160720	###	388.505927	2	6.020123	1	0	0	3	14313/393	###	44.848	1974.397	2	1974.395	-1.03	4.93	4.93	0	FAMHIIASDTFQK[128.05]VK	-1	SPyL
10	CAXIGMR	20160720	5486	388.505927	2	6.020123	1	0	0	3	15372/5486	5486	57.414	1974.397	2	1974.395	1.6274	0.25	0.25	0	FAMHIIASDTFQK[128.05]VK	-1	SPyL
11	CAXIGMR	20160720	1917	1055.43148	2	6.020123	1	0	0	3	12077/1917	1917	26.794	2108.368	2	2108.374	2.6036	3.43	3.43	0	[129.05]A-DTTPAARAKPFMMHKK	-1	SPyL
12	CAXIGMR	20160720	2210	703.39591	3	6.020123	1	0	0	3	12344/2210	2210	30.229	2108.368	3	2108.374	3.7735	5.03	5.03	0	SA-TTFAAPA-AK[128.05]PFMMHKK	-1	SPyL
13	CAXIGMR	20160720	2218	1055.43158	2	6.020123	1	0	0	3	12355/221	2218	30.323	2108.368	2	2108.374	2.4938	4.49	4.49	0	SA-TTFAAPA-AK[128.05]PFMMHKK	-1	SPyL
14	CAXIGMR	20160720	1553	574.282402	4	6.020123	1	0	0	3	11708/1553	1553	22.366	2293.101	4	2293.106	2.4965	3.76	3.76	0	SA-TTFAAPA-AKPFMMHKK[128.07]GK	-1	SPyL
15	CAXIGMR	20160720	1393	574.528452	4	6.020123	1	0	0	3	1531/1393	1393	20.21	2294.085	4	2294.091	2.4471	0.21	0.21	0	SA-TTFAAPA-AKPFMMHKK[128.05]GK	-1	SPyL
16	CAXIGMR	20160720	1723	765.701717	3	6.020123	1	0	0	3	11884/1723	1723	24.446	2294.084	3	2294.091	2.9468	5.74	5.74	0	SA-TTFAAPA-AKPFMMHKK[128.05]GK	-1	SPyL
17	CAXIGMR	20160720	1724	574.528802	4	6.020123	1	0	0	3	11886/1724	1724	24.457	2294.086	4	2294.091	1.8086	4.34	4.34	0	SA-TTFAAPA-AKPFMMHKK[128.05]GK	-1	SPyL
18	CAXIGMR	20160720	1725	1148.05128	2	6.020123	1	0	0	3	11889/1725	1725	24.462	2294.088	2	2294.091	0.9989	4.01	4.01	0	SA-TTFAAPA-AKPFMMHKK[128.05]GK	-1	SPyL
19	CAXIGMR	20160720	###	783.36681	3	6.020123	1	0	0	3	14570/43	###	47.643	2347.083	3	2347.085	0.8446	6.84	6.36	0	FQPHQMMF[K128.07]PNLTKA	-1	SPyL
20	CAXIGMR	20160720	###	1174.54738	2	6.020123	1	0	0	3	14572/43	###	47.668	2347.088	2	2347.085	1.6271	5.66	5.1	0	FQPHQMMF[K128.07]PNLTKA	-1	SPyL
21	CAXIGMR	20160720	4539	783.635677	3	6.020123	1	0	0	3	14754/4539	4539	43.533	2348.065	3	2348.069	1.3949	6.26	5.73	0	FQPHQMMF[K128.05]PNLTKA	-1	SPyL
22	CAXIGMR	20160720	###	818.762743	3	6.020123	1	0	0	3	14842/46	###	50.535	2453.266	3	2453.271	1.8575	3.36	1.45	0	IYNLTPGK[128.05]PNAFNEK	-1	SPyL
23	CAXIGMR	20160720	5063	844.108777	3	6.020123	1	0	0	3	1513/5063	5063	55.816	2523.305	3	2523.302	-1.119	8	8	0	AMHDIASDTFQK[128.07]IA-AIAIA	-1	SPyL
24	CAXIGMR	20160720	5268	844.435677	3	6.020123	1	0	0	3	1523/5268	5268	55.568	2530.285	3	2530.286	0.1885	7.17	7.37	0	AMHDIASDTFQK[128.05]IA-AIAIA	-1	SPyL
25	CAXIGMR	20160720	5269	633.578727	4	6.020123	1	0	0	3	15233/526	5269	55.577	2530.286	4	2530.286	-0.072	3.23	3.23	0	AMHDIASDTFQK[128.05]IA-AIAIA	-1	SPyL
26	CAXIGMR	20160720	5313	1266.15028	2	6.020123	1	0	0	3	15264/531	5313	55.325	2530.286	2	2530.286	-0.43	5.63	5.69	0	AMHDIASDTFQK[128.05]IA-AIAIA	-1	SPyL
27	CAXIGMR	20160720	###	634.054802	4	6.020123	1	0	0	3	14113/368	###	43.075	2532.19	4	2532.201	4.2439	6.39	5.26	0	K[128.07]GPHQMMF[K128.05]PNLTKA	-1	SPyL
28	CAXIGMR	20160720	3681	845.40081	3	6.020123	1	0	0	3	14293/368	3681	44.628	2533.181	3	2533.185	1.6874	8.08	6.28	0	GKFGPHQMMF[K128.05]PNLTKA	-1	SPyL
29	CAXIGMR	20160720	###	634.302977	4	6.020123	1	0	0	3	14293/368	###	44.636	2533.183	4	2533.185	0.8253	6.47	5.27	0	GKFGPHQMMF[K128.05]PNLTKA	-1	SPyL
30	CAXIGMR	20160720	5713	905.793643	3	6.020123	1	0	0	3	15496/571	5713	59.573	2714.359	3	2714.364	1.7743	3.14	3.14	0	AMMLAHMTGNK[128.07]YMLTPGK	-1	SPyL
31	CAXIGMR	20160720	5928	1958.68043	2	6.020123	1	0	0	3	15619/592	5928	61.777	2715.346	2	2715.348	0.6046	5.7	5.7	0	AMMLAHMTGNK[128.05]YMLTPGK	-1	SPyL
32	CAXIGMR	20160720	5110	948.491943	3	6.020123	1	0	0	3	15112/5110	5110	56.197	2842.454	3	2842.459	1.7111	6.09	4.35	0	KA-MLLA-MTGNK[128.07]YMLTPGK	-1	SPyL
33	CAXIGMR	20160720	5345	711.622977	4	6.020123	1	0	0	3	15230/534	5345	56.198	2842.463	4	2842.459	-1.398	8.77	6.87	0	AMMLAHMTGNK[128.07]YMLTPGK	-1	SPyL
34	CAXIGMR	20160720	###	711.865652	4	6.020123	1	0	0	3	15039/34	###	52.806	2843.434	4	2843.443	3.2861	7.18	5.41	0	K[128.05]AMMLAHMTGNK[128.05]YMLTPGK	-1	SPyL
35	CAXIGMR	20160720	5316	711.866477	4	6.020123	1	0	0	3	15308/531	5316	56.439	2843.445	4	2843.443	-0.664	6.24	4.54	0	KA-MLLA-MTGNK[128.05]YMLTPGK	-1	SPyL
36	CAXIGMR	20160720	5412	948.822577	3	6.020123	1	0	0	3	15329/541	5412	56.814	2843.446	3	2843.443	-1.055	6.47	4.83	0	KA-MLLA-MTGNK[128.05]YMLTPGK	-1	SPyL
37	CAXIGMR	20160720	5601	948.821243	3	6.020123	1	0	0	3	15430/560	5601	58.581	2843.446	3	2843.443	0.3621	5.3	4.84	0	AMMLAHMTGNK[128.05]YMLTPGK	-1	SPyL
38	CAXIGMR	20160720	4154	719.349127	4	6.020123	1	0	0	3	14467/415	4154	46.572	2873.37	4	2873.371	0.9358	6.66	6.66	0	FQPHQMMF[K128.05]PNLTKA	-1	SPyL
39	CAXIGMR	20160720	4170	958.796677	3	6.020123	1	0	0	3	14468/4170	4170	46.669	2873.368	3	2873.371	0.8835	7.94	7.94	0	FQPHQMMF[K128.05]PNLTKA	-1	SPyL
40	CAXIGMR	20160720	4301	719.348627	4	6.020123	1	0	0	3	14574/430	4301	47.677	2873.365	4	2873.371	1.6552	8.47	8.47	0	FQPHQMMF[K128.05]PNLTKA	-1	SPyL
41	CAXIGMR	20160720	5962	546.338977	2	6.020123	1	0	0	3	15564/596	5962	61.013	1090.663	2	1090.656	-5.944	0.12	0.02	0	YH134.05IA-AIAIA	-1	SPyL
42	CAXIGMR	20160720	4467	913.464127	2	6.020123	1	0	0	3	14704/446	4467	48.968	1624.914	2	1624.914	0.9343	5.19	5.19	0	AMHIIASDTFQK[128.05]VK	-1	SPyL
43	CAXIGMR	20160720	3927	661.344543	3	6.020123	1	0	0	3	14318/392	3927	44.893	1981.012	3	1981.015	1.8076	6.74	6.74	0	FAMHIIASDTFQK[128.05]VK	-1	SPyL
44	CAXIGMR	20160720	1746	1055.09918	2	6.020123	1	0	0	3	11939/1746	1746	24.674										

S. Material. Raw data to be uploaded.

e.g.

Name	Date modified	Type	Size
 20160426_FKBP25_F145A_I223P_1213.raw	4/28/2016 8:01 PM	Xcalibur Raw File	433,157 KB
 20160426_FKBP25_F145A_I223P_1312.raw	4/28/2016 10:09 PM	Xcalibur Raw File	365,506 KB
 20160426_FKBP25_F145A_I223P_ctrl.raw	4/28/2016 4:29 PM	Xcalibur Raw File	556,540 KB
 20160426_FKBP25_F145A_I223P_rap_ctrl.raw	4/28/2016 5:53 PM	Xcalibur Raw File	342,673 KB
 20160620_FKBP25_F145A_I223P_PCASurea_ctrl.raw	6/30/2016 2:10 PM	Xcalibur Raw File	442,843 KB
 20160620_FKBP25_F145A_I223P_PCASurea_DH.raw	6/30/2016 12:17 PM	Xcalibur Raw File	439,103 KB
 20160620_FKBP25_F145A_I223P_PCASurea_HD.raw	6/30/2016 10:24 AM	Xcalibur Raw File	422,603 KB
 20160620_FKBP25_F145A_I223P_PCASurea_urea_ctrl.raw	6/30/2016 3:34 PM	Xcalibur Raw File	438,311 KB
 20160620_FKBP25_F145A_I223P_rap_PCASurea_ctrl.raw	6/30/2016 9:12 PM	Xcalibur Raw File	429,375 KB
 20160620_FKBP25_F145A_I223P_rap_PCASurea_DH.raw	6/30/2016 7:19 PM	Xcalibur Raw File	408,323 KB
 20160620_FKBP25_F145A_I223P_rap_PCASurea_HD.raw	6/30/2016 5:26 PM	Xcalibur Raw File	388,318 KB
 20160620_FKBP25_F145A_I223P_rap_PCASurea_urea_ctrl.raw	6/30/2016 10:36 PM	Xcalibur Raw File	412,905 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_01-02_TDSol_OT_OT_TN.raw	7/21/2016 1:17 AM	Xcalibur Raw File	577,115 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_01-05_TDSol_OT_OT_TN.raw	7/21/2016 4:01 AM	Xcalibur Raw File	530,167 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_01-08_TDSol_OT_OT_TN.raw	7/21/2016 6:45 AM	Xcalibur Raw File	448,081 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_02-04_TDSol_OT_OT_TN.raw	7/21/2016 9:28 AM	Xcalibur Raw File	625,172 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_02-07_TDSol_OT_OT_TN.raw	7/21/2016 12:13 PM	Xcalibur Raw File	519,773 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_04-05_TDSol_OT_OT_TN.raw	7/21/2016 2:57 PM	Xcalibur Raw File	750,112 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_07-08_TDSol_OT_OT_TN.raw	7/21/2016 5:41 PM	Xcalibur Raw File	414,269 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_07-11_TDSol_OT_OT_TN.raw	7/21/2016 8:25 PM	Xcalibur Raw File	380,938 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_08-10_TDSol_OT_OT_TN.raw	7/21/2016 11:09 PM	Xcalibur Raw File	435,076 KB
 20160720_SpyL32P_qCL_DSA-12C6-13C6_100uM_10-11_TDSol_OT_OT_TN.raw	7/22/2016 1:53 AM	Xcalibur Raw File	832,665 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_01-02_PepSol_OT_OT_TN.raw	7/22/2016 5:04 PM	Xcalibur Raw File	513,535 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_01-05_PepSol_OT_OT_TN.raw	7/22/2016 7:48 PM	Xcalibur Raw File	721,328 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_01-08_PepSol_OT_OT_TN.raw	7/22/2016 10:32 PM	Xcalibur Raw File	697,070 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_02-04_PepSol_OT_OT_TN.raw	7/23/2016 1:16 AM	Xcalibur Raw File	706,956 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_02-07_PepSol_OT_OT_TN.raw	7/23/2016 3:59 AM	Xcalibur Raw File	649,897 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_04-05_PepSol_OT_OT_TN.raw	7/23/2016 6:43 AM	Xcalibur Raw File	684,078 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_07-08_PepSol_OT_OT_TN.raw	7/23/2016 9:27 AM	Xcalibur Raw File	673,614 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_07-11_PepSol_OT_OT_TN.raw	7/23/2016 12:11 PM	Xcalibur Raw File	688,429 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_08-10_PepSol_OT_OT_TN.raw	7/23/2016 2:55 PM	Xcalibur Raw File	632,741 KB
 20160720_SpyL32P_SM_PCAS-H4-D4_10mM_10-11_PepSol_OT_OT_TN.raw	7/23/2016 5:40 PM	Xcalibur Raw File	622,478 KB
 20160911_FKBP25_F145A_I223P_PCAS_sm_1213.raw	9/12/2016 12:18 AM	Xcalibur Raw File	737,683 KB
 20160911_FKBP25_F145A_I223P_PCAS_sm_1312.raw	9/12/2016 3:01 AM	Xcalibur Raw File	749,172 KB
 20160911_FKBP25_F145A_I223P_PCAS_sm_ctrl.raw	9/12/2016 5:44 AM	Xcalibur Raw File	696,162 KB
 20160911_FKBP25_F145A_I223P_PCAS_sm_rapctrl.raw	9/12/2016 8:27 AM	Xcalibur Raw File	734,700 KB

S. Material. PyMOL session files to be uploaded.

e.g.

Name	Date modified	Type	Size
 FKBP25_F145A_I223P_1pbk_with_I-TASSER_fused_Nterm__qCL__L+-U-_01.pse	11/8/2016 12:15 PM	PyMOL Session File	485 KB
 FKBP25_F145A_I223P_1pbk_with_I-TASSER_fused_Nterm__qCL+SM__L+-U-_01.pse	11/8/2016 12:17 PM	PyMOL Session File	486 KB
 FKBP25_F145A_I223P_1pbk_with_I-TASSER_fused_Nterm__SM__L+-U-_01.pse	11/8/2016 11:43 AM	PyMOL Session File	480 KB
 FKBP25_F145A_I223P_1pbk_with_I-TASSER_fused_Nterm__SM__L+U+-_01.pse	11/8/2016 11:44 AM	PyMOL Session File	479 KB
 FKBP25_F145A_I223P_1pbk_with_I-TASSER_fused_Nterm__SM__L-U+-_01.pse	11/8/2016 11:43 AM	PyMOL Session File	480 KB
 Spy Im7 for 20161014_02_qCL__L+-U-_01.pse	11/8/2016 11:55 AM	PyMOL Session File	1,501 KB
 Spy Im7 for 20161014_02_qCL__L+U+-_01.pse	11/8/2016 11:55 AM	PyMOL Session File	1,417 KB
 Spy Im7 for 20161014_02_qCL__L-U+-_01.pse	11/8/2016 11:55 AM	PyMOL Session File	1,522 KB
 Spy Im7 for 20161014_02_qCL+SM__L+-U-_01.pse	11/8/2016 11:53 AM	PyMOL Session File	1,501 KB
 Spy Im7 for 20161014_02_qCL+SM__L+U+-_01.pse	11/8/2016 11:55 AM	PyMOL Session File	1,416 KB
 Spy Im7 for 20161014_02_qCL+SM__L-U+-_01.pse	11/8/2016 11:54 AM	PyMOL Session File	1,522 KB
 Spy_Im7_for_20161014_02_SM__L+-U-_01.pse	11/8/2016 2:31 PM	PyMOL Session File	1,337 KB
 Spy_Im7_for_20161014_02_SM__L+U+-_01.pse	11/8/2016 2:33 PM	PyMOL Session File	1,337 KB
 Spy_Im7_for_20161014_02_SM__L-U+-_01.pse	11/8/2016 2:32 PM	PyMOL Session File	1,337 KB

S. Material. Kojak configuration.

Name	Date modified	Type	Size
 Kojak_qCL_Parameters.conf	11/9/2016 5:33 PM	CONF File	3 KB

e.g.

```
Kojak_qCL_Parameters.conf X
1 # Kojak version 1.5.1 parameter file
2
3 threads = 8
4
5 database = #Concatenated TARGET-DECOY(seq. reversal) of FKBP25_F145A_I223P or SpyL32P and Im7(7-45)
6
7 # FKBP25_F145A_I223P searches:
8 # >FKBP25_F145A_I223P
9 # MRGSHHHHHGLVPRGSMGPPKYTKSVLKKGDKTNFPKKGQVHVCHWYTGTLQDGTVDNINQTSAKKKKNAKPLSFKVGVGKVIKRGWDEALLTMSKGEKARLEIEPEWAYGKKKQPDAKIPPNAKLTFFVELVDPD
10 # >decoy_FKBP25_F145A_I223P
11 # DPDVLEVEFTLKNPPIKADPQGGKYAWPEIELRRAKEGKSMSTLLAEDWGRIVKGVGVKFSLPKANKKKKASTQINTDAVTDGQTLGTWYVCHVVDGKKPFNFKDGKLVSKTYKPPGMSGRPVLGHHHHHSGRM
12 # >SpyL32P
13 # SADITTAAPADAKPMHHHKGKFGPHQDMMFQDNLTDQAQKQIREIMKGQRDQMKRPPLEERRAMHDIASDTFDKVKAEAQIAKMEEQRKANMLAHMETQNKIYNILTPEQKKQFNANFEKRLTERPAAKGKMPATAE
14 # >Im7_7-45
15 # SISDYTEAEFVQLLKEIEKENVAATDDVLDVLLLEHFVKIT
16 # >decoy_SpyL32P
17 # EATAPMKGKAAPRETLRKEFNANFQKKQEPILINIKNQTEMHALMNAKRQEEMKAIQAEAKVKDFDSAIIDHMARREELPPRKMQRQGMIERIQKQADTLNPKDFMMDQHPGFKGHHMMPKADAPAAITTDAS
18 # >decoy_Im7_7-45
19 # TIKVFHELLVLDVDDTAAVNEKEIEKLLQVFEAETYDSIS
20
21 export_percolator = 1
22 export_pepXML = 1
23 percolator_version = 3.0
24
25 enrichment = 0
26 instrument = 0
27 MS1_centroid = 0
28 MS2_centroid = 0
29 MS1_resolution = 60000
30 MS2_resolution = 30000
31
32 cross_link = nK nK 110.0362342 DSA_Light
33 mono_link = nK 128.0706042
34 mono_link = nK 129.0546242
35 cross_link = nK nK 116.0563632 DSA_Heavy
36 mono_link = nK 134.0907332
37 mono_link = nK 135.0747532
38
39 diff_mods_on_xl = 1
40 max_mods_per_peptide = #1 for FKBP25_F145A_I223P 3 for SpyL32P
41 mono_links_on_xl = #0 for FKBP25_F145A_I223P 1 for SpyL32P
42 modification = M 15.9949
43
44 enzyme = [KR]|{P}
45
46 fragment_bin_offset = 0.0
47 fragment_bin_size = 0.03
48 ion_series_A = 0
49 ion_series_B = 1
50 ion_series_C = 0
51 ion_series_X = 0
52 ion_series_Y = 1
53 ion_series_Z = 0
54
55 decoy_filter = decoy
56 isotope_error = 1
57 max_misceavages = #5 for FKBP25_F145A_I223P 2 for SpyL32P
58 max_peptide_mass = #6000.0 for FKBP25_F145A_I223P 8000.0 for SpyL32P
59 min_peptide_mass = 400.0
60 max_spectrum_peaks = 0
61 ppm_tolerance_pre = #6.0 for FKBP25_F145A_I223P 10.0 for SpyL32P
62 prefer_precursor_pred = 2
63 spectrum_processing = 0
64 top_count = 300
65
66 truncate_prot_names = 0
67 turbo_button = 1
```