Supporting Information for Publication:

Developing a Multiplexed Quantitative Cross-linking Mass Spectrometry Platform for Comparative Structural Analysis of Protein Complexes

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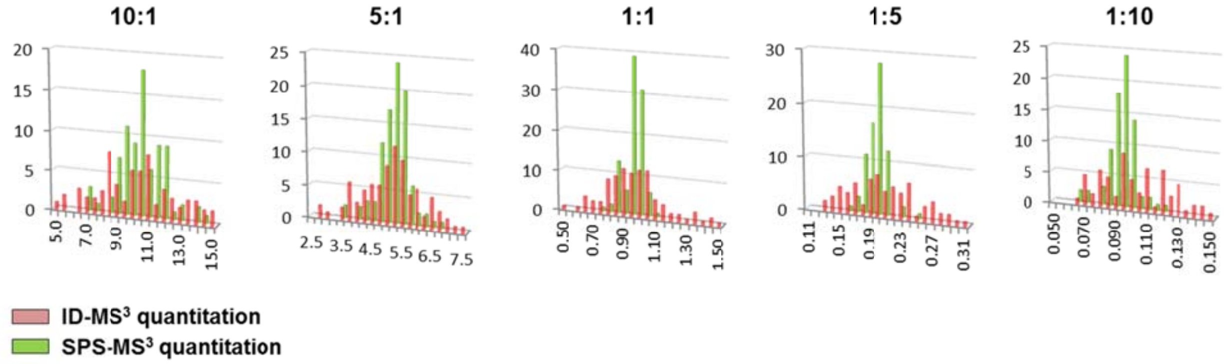

Figure S-1. Distribution of raw cross-link quantitative ratios across five input mixings using ID-SPS-MS3. Reporter ion ratios for TMT2-126:TMT2-127 as determined by ID-MS^3 (red) and SPS-MS^3 (green). For each mixing, quantitative ratios derived from SPS-MS^3 acquisitions clustered more tightly around average values than those derived from ID-MS^3 acquisitions. As a result, there was a corresponding decrease in standard deviation observed from MultiNotch acquisitions.

Table S-1. List of the Unique Cytochrome c K-K linkages Identified Using Different Acquisition Methods.

XL Residue 1	XL Residue 2	ID-MS^3	ID-MS^3 + SPS-MS^3
K6	K28	X	X
K6	K40	X	X
K6	K54	X	
K6	K87	X	X
K6	K88	X	X
K6	K89	X	X
K6	K100	X	X
K6	K101	X	X
K8	K14	X	
K8	K26	X	X
K8	K28	X	X
K8	K40	X	X
K8	K54	X	
K8	K73	X	
K8	K88	X	
K8	K89	X	
K8	K100	X	X
K8	K101	X	X
K9	K26		X
K9	K28	X	X
K9	K40	X	X
K9	K54	X	
K9	K73	X	
K9	K87	X	X
K9	K88	X	X
K9	K89	X	X
K9	K100	X	X
K9	K101		X
K14	K40	X	
K26	K26	X	X
K26	K28	X	X
K26	K40	X	X
K26	K54	X	X
K26	K73	X	X
K26	K80	X	
K26	K88	X	X
K26	K89	X	X

K26	K100	X	X
K28	K26	X	X
K28	K40	X	X
K28	K54	X	X
K28	K88		X
K28	K89	X	X
K28	K100	X	X
K40	K40	X	X
K40	K54	X	X
K40	K56	X	X
K40	K73	X	X
K40	K74	X	X
K40	K80	X	X
K40	K87	X	X
K40	K88	X	X
K40	K89	X	X
K40	K100	X	X
K40	K101	X	X
K54	K54	X	X
K54	K73	X	X
K54	K74	X	X
K54	K80	X	X
K54	K87	X	X
K54	K88	X	X
K54	K89	X	X
K54	K100	X	X
K56	K74	X	X
K56	K88	X	
K73	K74	X	X
K73	K80	X	X
K73	K87	X	X
K73	K88	X	X
K73	K89	X	X
K73	K100	X	
K74	K80		X
K74	K87	X	X
K74	K88	X	X
K74	K89	X	X
K74	K100	X	X
K80	K89	X	X
K80	K100	X	
K87	K89	X	X
K87	K100	X	X

K88	K100	X	X
K89	K100	X	X
K100	K100	X	X