SI Appendix A.   Comparative execution-time benchmark

Both InsPecT and spectral networks analysis were benchmarked on the same desktop machine running the Linux operating system on an Intel® Pentium® 4 CPU at a clock speed of 2.8GHz with 1 Gb of RAM. As thoroughly described in the main text, the IKKβ dataset has 11,760 MS/MS spectra and the Lens dataset has 27,154 MS/MS spectra. The dbHuman database referenced in Table A-1 is a subset of Swiss-Prot containing 13,749 *homo sapiens* protein sequences (April 20, 2006). When searching for modified peptides, InsPecT was run in *blind* search mode, i.e. assuming that the list of possible modifications is not known in advance.

database	max. # modifications	IKKβ dataset		Lens dataset	
		dbIKKβ	dbHuman	dbLens	dbHuman
# proteins		35	13,749	107	13,749
InsPecT	0	4	55	8	106
InsPecT	1	10	2585	55	5514
InsPecT	2	1754	n/a	n/a	n/a
Spectral networks	0-3+	9		31	

Table A-1: Running times for MS/MS spectra identification using spectral network analysis vs. InsPecT. Two smaller databases were defined containing only the sequences for the proteins present in the corresponding sample: dbIKKβ contains IKKβ, proteases and common contaminants; dbLens contains multiple human lens proteins, proteases and common contaminants (note that, in general, these conveniently small subsets are not known in advance). Running times are shown in minutes (rounded to the closest integer), 'n/a' means that the running time exceeds 2880 minutes (2 days).