

| File   | Parameter                   | Value  | Description  |
|--|-----------------------------|--|--|
| <b>iqpir.params</b><br>--No header line--<br>(like 2-channel but with some different parameters including sample_ratios) | sample_map                  | /full_path_to/sample_map.txt   | Required   |
|  | sample_channels             | /full_path_to/sample_channels.txt  | Optional to specify non-standard 6-plex channels   |
|  | sample_ratios               | /full_path_to/sample_ratios.txt  | --Required, presence triggers multiplex quant--  |
|  | email                       | me@u.washington.edu  | Required for receiving analysis messages   |
|  | xlinkprophetfile            | /full_path_to/iprophet-xl.pep.xml  | Required   |
|  | deadendprophetfile          | /full_path_to/Deadend_search/iprophet.pep.xml  | Optional   |
|  | fdr                         | 0.01   | Required   |
|  | filter_crit                 | composite probability  | Required   |
|  | iqpir_output_dir            | /full_path_to/multiplex/   | Required   |
|  | existing_xl_iqpirfiles      | /full_path_to_outputdir1(,full_path_to_outputdir2,...)                               | Optional to reuse iqpir.xls files in specified directories   |
|  | existing_deadend_iqpirfiles | /full_path_to_outputdir1(,full_path_to_outputdir2,...)                               | Optional to reuse iqpir.xls files in specified directories   |
| <b>sample_map</b><br>--No header line--<br>(like 2-channel, but without fwd/rev column)                                  | column 1                    | raw file name (without extension or full path)                                       | No header line   |
|  | column 2                    | sample number  | Multiplexed sample number so can separately quantify related 6-plex samples analyzed together with XLinkProphet                |
|  | column 3                    | biorep number  | Bioreps are independently normalized, unlike technical reps  |
| <b>sample_channels</b><br>--No header line--<br>(optional: specifies channel stump and reporter masses)                  | column 1                    | sample number  | No header line   |
|  | column 2                    | stump modification masses for each channel in increasing mass order, comma delimited | default value:<br>325.127386,327.134095,329.14080505,330.13784005,332.14454905,334.15125905 (2-channel: 325.127386,327.134095) |
|  | column 3                    | reporter masses for each channel, in decreasing mass order, comma delimited          | default value:<br>825.490275,821.47686,817.463,815.469,811.455947,807.442528 (2-channel: 811.455947,807.442528)                |
| <b>sample_ratios</b><br>--Requires header line--<br>(replaces 2-channel sample_def)                                      | column 1                    | sample   | Requires header line with sample, experiment condition, etc.   |
|  | column 2                    | experiment_condition   | How ratio is referred to on XLinkDB  |
|  | column 3                    | experiment_channel   | Specify numerator channel, e.g. 826 or 822 or..., etc  |
|  | column 4                    | reference_condition  |  |
|  | column 5                    | reference_channel  | Specify denominator channel, e.g. 826 or 822 or..., etc  |
|  | column 6                    | description  | Optional text to describe ratio  |
|  | column 7                    | normalize  | yes or no: Whether to center log2ratio distribution at 0   |