Supporting Information for "Param-Medic Breathes New Life into MS/MS Database Search by Optimizing Parameter Settings"

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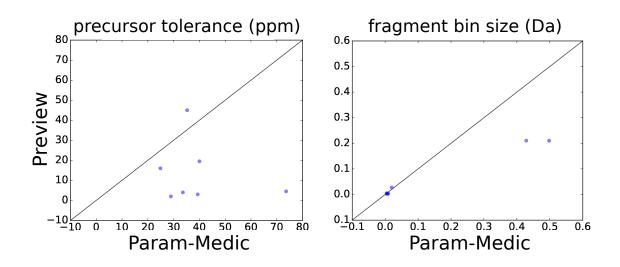


Figure 1: Comparing parameter estimates from Param-Medic and Preview. Scatter plots of parameter values estimated by Param-Medic (horizontal axis) and Preview (vertical axis) on all nine training and test experiments for which both tools returned values. Solid line represents 1:1 correspondence. Left: precursor error, r = -0.20. Right: fragment bin size, correlation coefficient r = 0.99. The fragment bin size estimates show high correlation (r = 0.99), though this value is largely driven by two outlier datasets. The precursor tolerance estimates are essentially uncorrelated (r = -0.20).