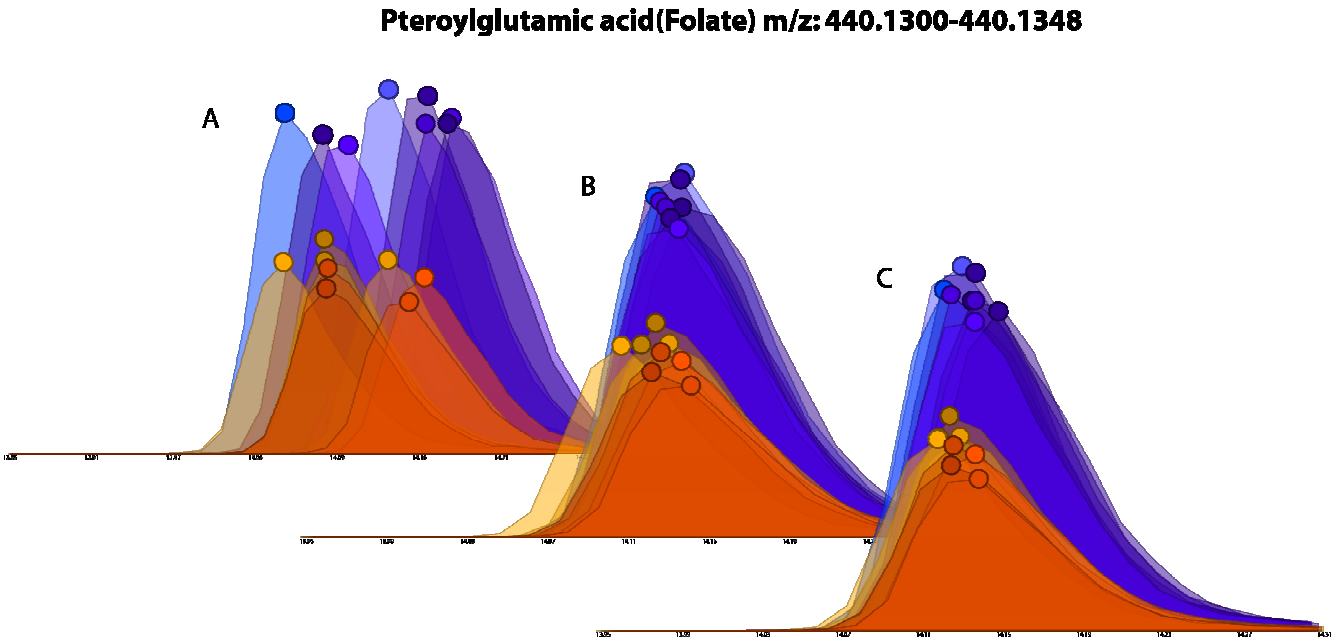


Supplementary Figure 1: Two iterations of alignment. Shown are sixteen EICs in the m/z and retention time range of folate from a viral infection time course. (A) Before alignment. (B) First iteration of alignment. The alignment was based on 2000 high intensity peaks (>5000 ion counts) found in all samples. (C) Second iteration of alignment. Complete list of alignment parameters used is listed below.

Peak Selection Criteria (peaks that are used to create the alignment):

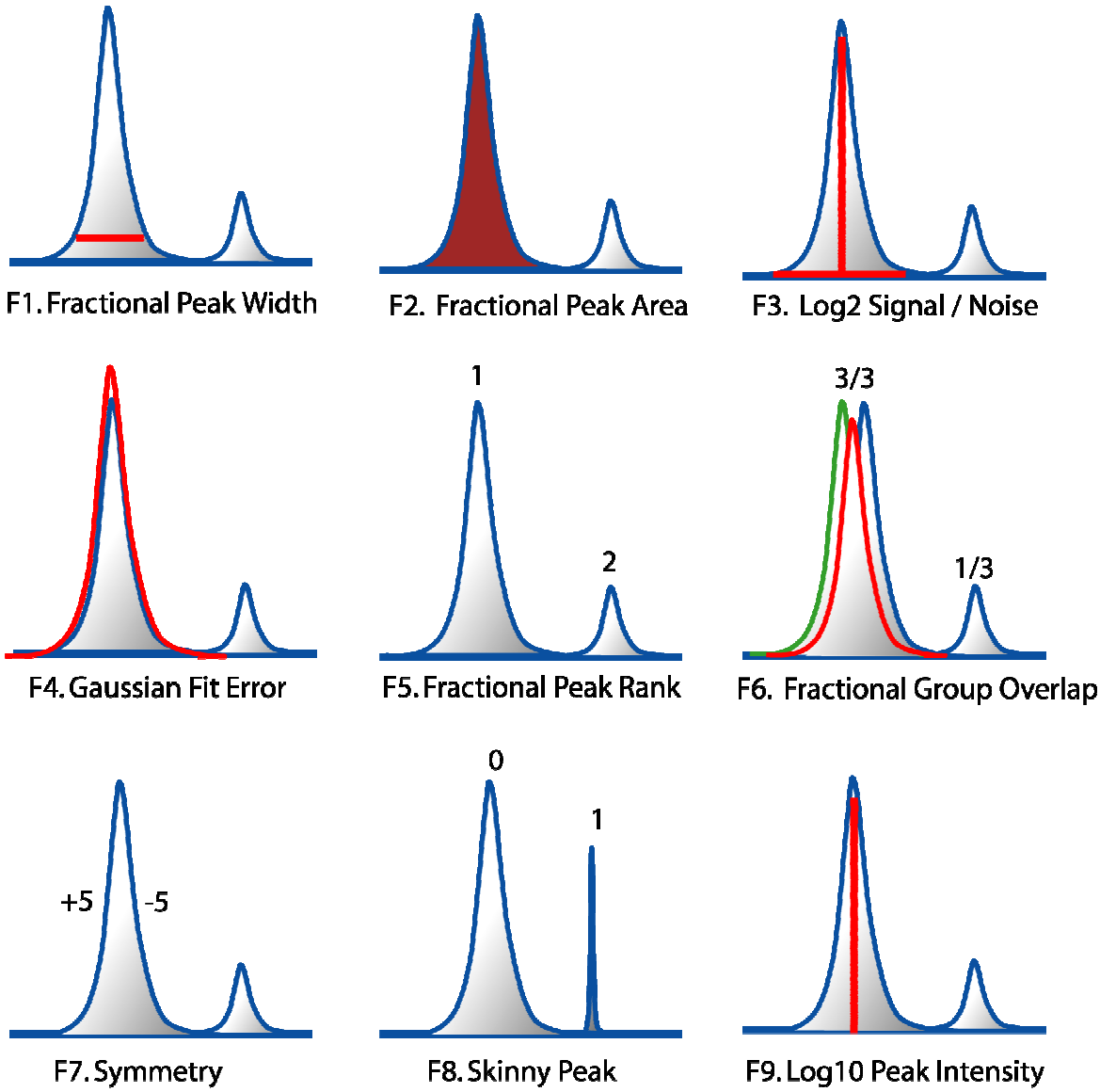
1. Minimum Peak Intensity is 5000 ions
2. Minimum Peak S/N Ratio is 5
3. Minimum Peak Width is 5 scans

Peak Grouping (peak groups that are used to create the alignment):

1. Peak grouping retention time window is 20 scans (peaks that are within ± 20 scans of the median peak center are grouped together)
2. Group must contain at least 2 good peaks.
3. Maximum number of groups used in the alignment is 2000 (groups are ranked by intensity)

Alignment Algorithm:

Maximum number of alignment iterations is 10
Fitting using polynomial of degree 3



Supplementary Figure 2: Peak features used for quality scoring. F1: Fractional Peak Width = peak width at baseline normalized by total number of scans in EIC with nonzero intensity; F2: Fractional Peak Area = peak area normalized by total area of EIC; F3: Log2 Signal to Noise (S/N) = Standard S/N ratio, normalized by maximum S/N ratio found for any compound and log2 transformed; F4: Gaussian Fit Error = Root mean square difference between observed shape and best fitting Gaussian curve; F5: Fractional Peak Rank = peak rank upon sorting peaks within EIC by area, normalized by number of peaks in the EIC; F6: Fractional Group Overlap = number of overlapping peaks from other samples normalized by the total number of samples; F7: Symmetry = count of scans increasing in intensity plus of scans decreasing in intensity scaled by peak width as per Formula 1 below; F8: Skinny Peak = True (1) if peak width is less than 3 scans, else false (0); F9: Log10 Peak Intensity = log10 of peak height.

Peak Symmetry score = (nSteps-abs(nPos-nNeg) / nSteps * log2(nSteps) where:

nPos : count of scans increasing in intensity

nNeg: count of scans decreasing in intensity

nSteps: nPos + nNeg;

Example: Symmetric peak, with +5 and -5: score = 3.3

Asymmetric peak with +1 and -5 : score = 0.8

Mass slice detection, EIC extraction, Peak detection, Peak scoring, and Peak grouping Benchmark
Computer: (Intel 6600 2.4ghz, 2 cores with 8 gb ram)

Peak Detection Settings

Mass Slice Detection		
Mass Domain Resolution	20 ppm	
Time Domain Resolution	10 scans	
EIC Processing		
Smoothing Window	10 scans	
Peak Grouping Window	0.5 min	
		12.5
Peak Scoring Parameters		11.875
Minimum Number of "good" peaks in group	2 peaks	11.875
Minimum Signal/Baseline Ratio	2	
Minimum Peak Width	3 scans	
Minimum Signal/Blank Ratio	2	
Minimum Peak Intensity	5000 ions	

Results	#Files	Memory Usage	Run Time	#Mass Slices	#EICs	#Peaks	#Groups
Using One Core							
Dataset: 16 centroided mzXML files, ~12 Mb each	**16**	**300 MB**	**21.09 sec**	**5628**	**90,000**	**137,295**	**5680**
Dataset: 32 centroided mzXML files, ~12 Mb each	**32**	**480 MB**	**46.00 sec**	**7132**	**228,000**	**346,296**	**6561**
Dataset: 48 centroided mzXML files, ~12 Mb each	**48**	**670 MB**	**64.0 sec**	**7086**	**340,000**	**523,878**	**6603**
Using Two Core							
Dataset: 16 centroided mzXML files, ~12 Mb each	**16**	**300 MB**	**11.06 sec**	**5628**	**90,000**	**137,295**	**5680**
Dataset: 32 centroided mzXML files, ~12 Mb each	**32**	**480 MB**	**28.08 sec**	**7132**	**228,000**	**346,296**	**6561**
Dataset: 48 centroided mzXML files, ~12 Mb each	**48**	**670 MB**	**38.05 sec**	**7086**	**340,000**	**523,878**	**6603**

Supplementary Table 1: Benchmark of Maven memory and CPU usage. The memory and speed of the program was benchmarked on three sets of files (16 samples, 32 samples, and 48 samples) from viral infection dataset. All files ware loaded into memory and peak detection algorithms was executed using settings show in the table above. Baseline memory consumption of the program (physical memory used without any files loaded) was ~ 120 MB, with additional 12Mb of usage for each loaded file. The performance was evaluated using the same computer operating on a single CPU and operating on two CPU cores. We find that overall performance scales roughly linearly with number of samples and number of CPUs used.