

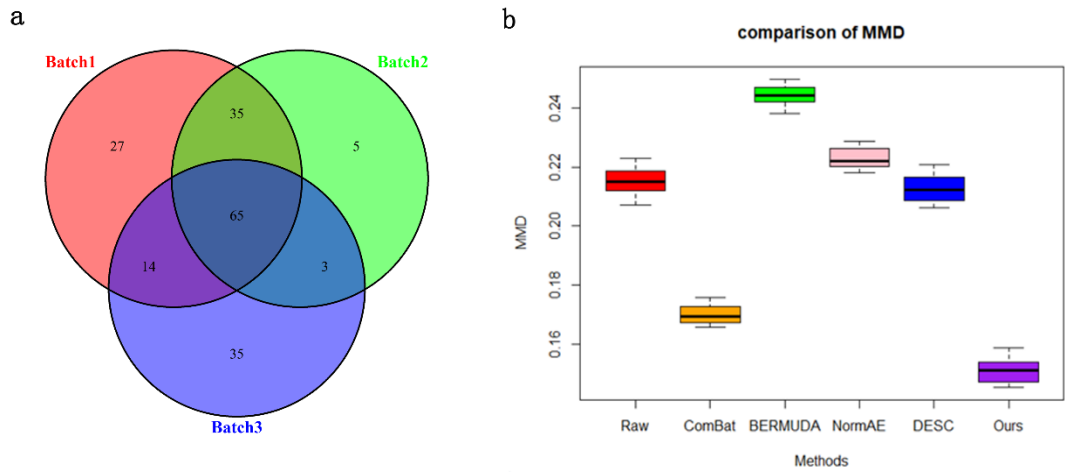


Fig. S1. **a** Venn diagram about the number of differential peak intersections within three batches on MI data. **b** Boxplot of the MMDs in six algorithms aiming at plate 3 and plate 4 on CHD data.

Table S1. Original classification results before averaging on the CHD data of MALDI MS.

a

Sample Level		Before Calibration				Joint Calibration			
		1	2	3	4	1	2	3	4
ACC	1, 2			0.609	0.550			0.739	0.744
	1, 3		0.762		0.688		0.794		0.732
	1, 4		0.721	0.789			0.829	0.779	
	2, 3	0.712			0.678	0.793			0.761
	2, 4	0.787		0.746		0.865		0.807	
	3, 4	0.696	0.786			0.817	0.822		
F-score	1, 2			0.721	0.683			0.758	0.744
	1, 3		0.818		0.749		0.805		0.759
	1, 4		0.794	0.809			0.858	0.821	
	2, 3	0.655			0.727	0.774			0.752
	2, 4	0.773		0.773		0.871		0.819	
	3, 4	0.609	0.814			0.815	0.851		
AUC	1, 2			0.579	0.551			0.739	0.744
	1, 3		0.737		0.689		0.798		0.732
	1, 4		0.691	0.787			0.816	0.764	
	2, 3	0.725			0.679	0.801			0.761
	2, 4	0.794		0.741		0.866		0.807	
	3, 4	0.713	0.778			0.821	0.811		
MCC	1, 2			0.221	0.189			0.477	0.488
	1, 3		0.544		0.431		0.593		0.476
	1, 4		0.469	0.576			0.658	0.568	
	2, 3	0.489			0.383	0.618			0.522
	2, 4	0.598		0.486		0.731		0.612	
	3, 4	0.493	0.564			0.642	0.642		

b

Pairwise		Target Source			
		1	2	3	4
ACC	1		0.799	0.701	0.643
	2	0.746		0.678	0.735
	3	0.793	0.701		0.816
	4	0.809	0.662	0.765	
F-score	1		0.837	0.709	0.699
	2	0.734		0.657	0.757
	3	0.776	0.669		0.812
	4	0.827	0.759	0.800	
AUC	1		0.784	0.704	0.644
	2	0.752		0.688	0.735
	3	0.802	0.719		0.816
	4	0.806	0.626	0.755	
MCC	1		0.601	0.407	0.311
	2	0.509		0.384	0.478
	3	0.617	0.457		0.632
	4	0.616	0.344	0.527	

1.0
0.1

a the cross-batch prediction of before and after multi-batch joint calibration. **b** the result of going through pairwise calibration.