

Supplementary Information:  
Bayesian diversity control for batch-based phase diagram determination  
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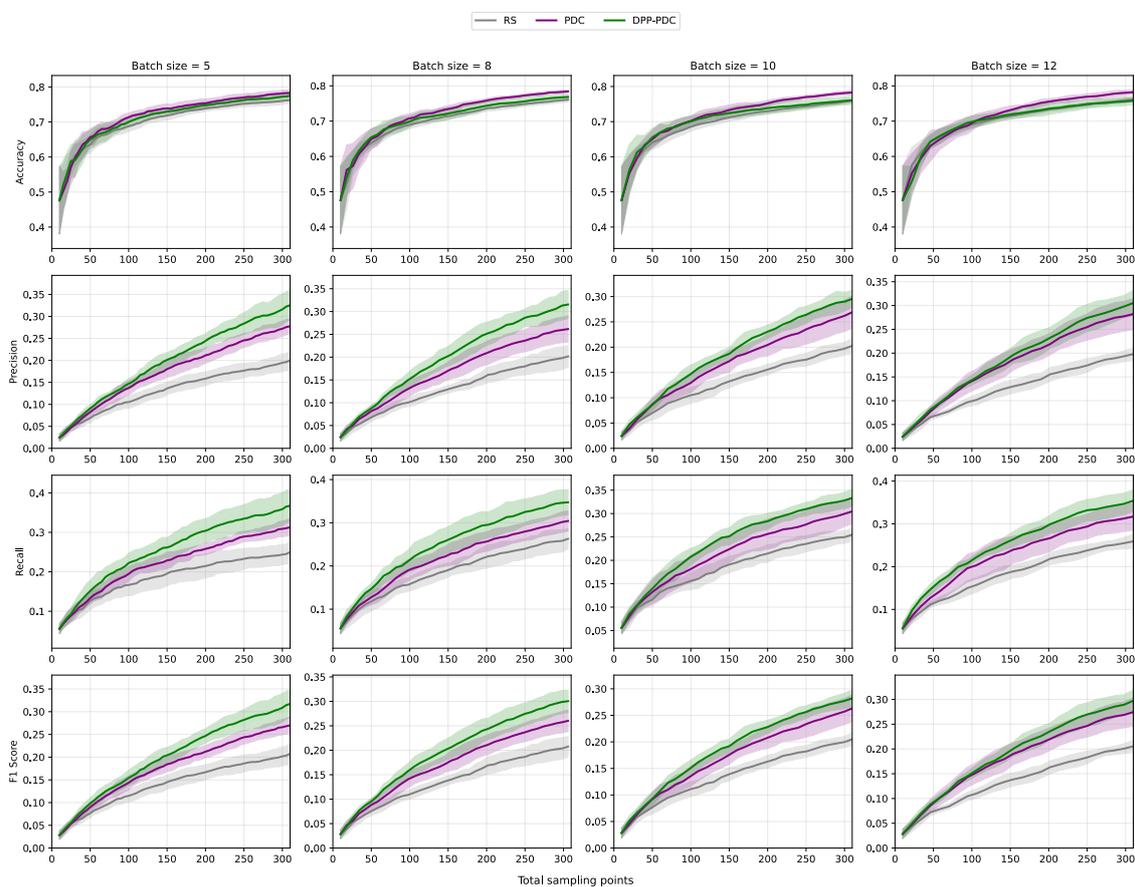
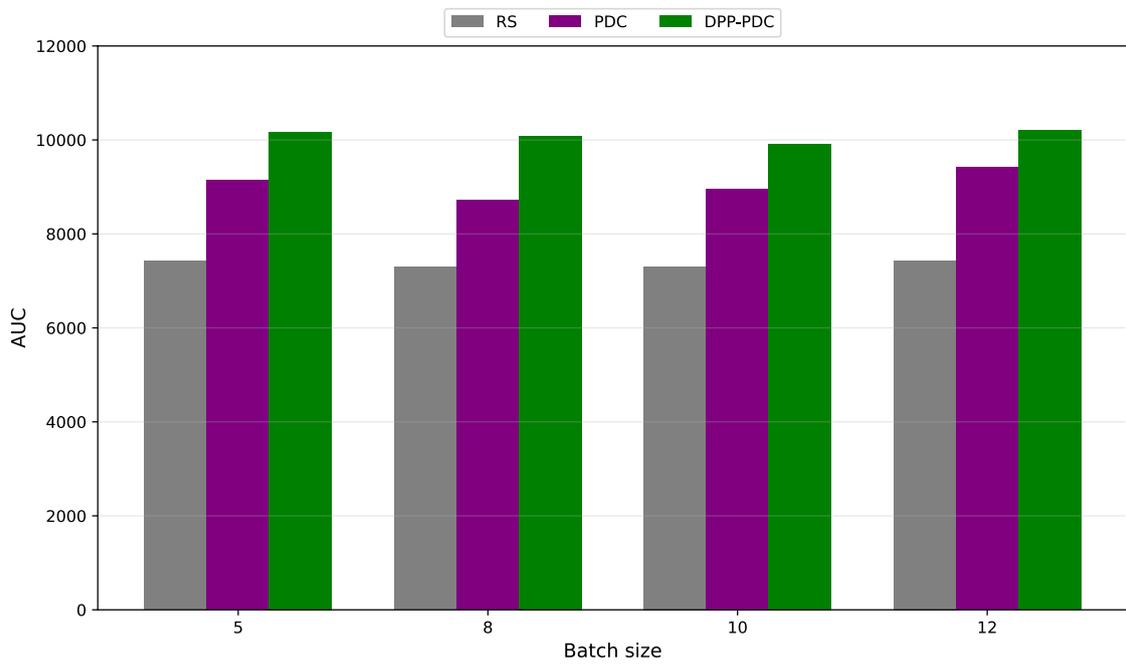
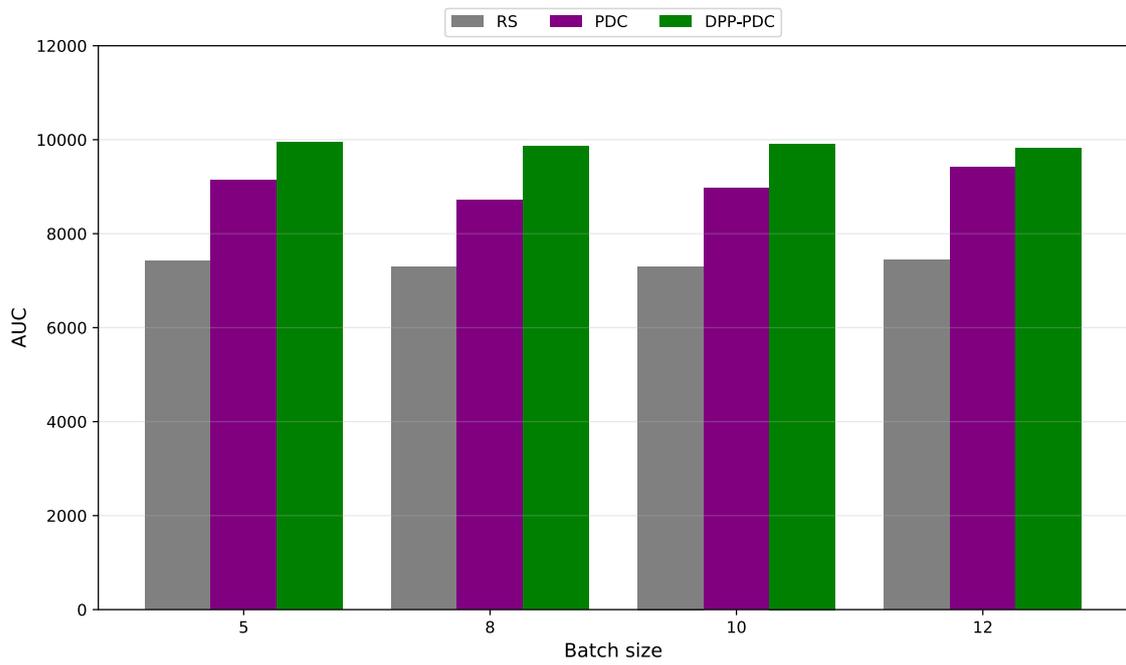


Figure S1: Evaluation of DPP-PDC in terms of accuracy, precision, recall and F1-score. The x-axis corresponds to the number of samples, and the y-axis shows the performance measure. RS stands for random sampling



(a)  $\mu = -5$ ,  $\omega = 3$



(b)  $\mu = -6$ ,  $\omega = 2$

Figure S2: Area under the phase discovery curve at different hyperparameter settings.

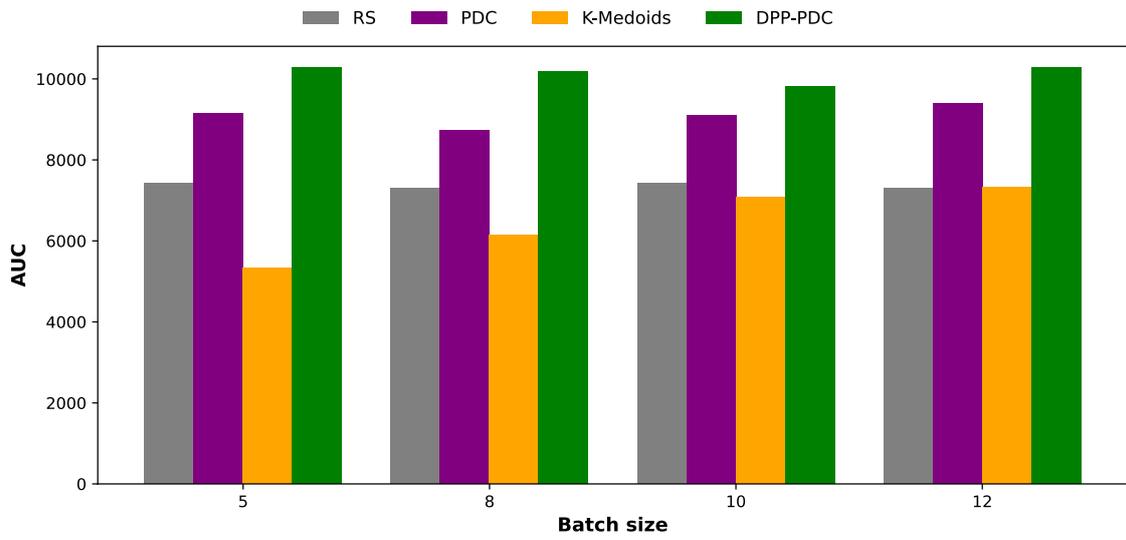


Figure S3: Comparison to K-medoids (Mancias et al., 2025). The batch size is 10. The cut-off parameter of K-medoids was set to 2.5% as instructed in the paper.