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Article

Understanding the Free Energy Landscape of Phase Separation in Lipid Bilayer using Weighted Ensemble Molecular Dynamics

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ABSTRACT

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SIGNIFICANCE

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INTRODUCTION

This is a place holder article template for our future paper. For time being, I will be using this space to publish all the plots that are being generated as a part of the analysis.

METHODS

Will be updating this section soon!

Standard Molecular Dynamics

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Weighted Ensemble Molecular Dynamics

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RESULTS

All Figures

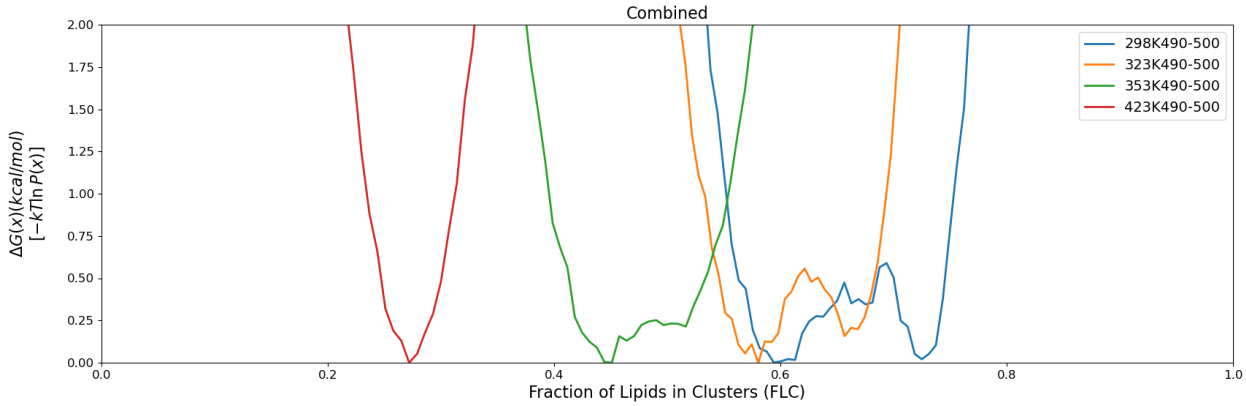

Figure 1: Free Energy Landscape of **DIPC** system. Data from all four replica has been combined using w_multi_west tool. All the FES are calculated by averaging over the iteration window 490 - 500. Note that 353K is an interesting outlier

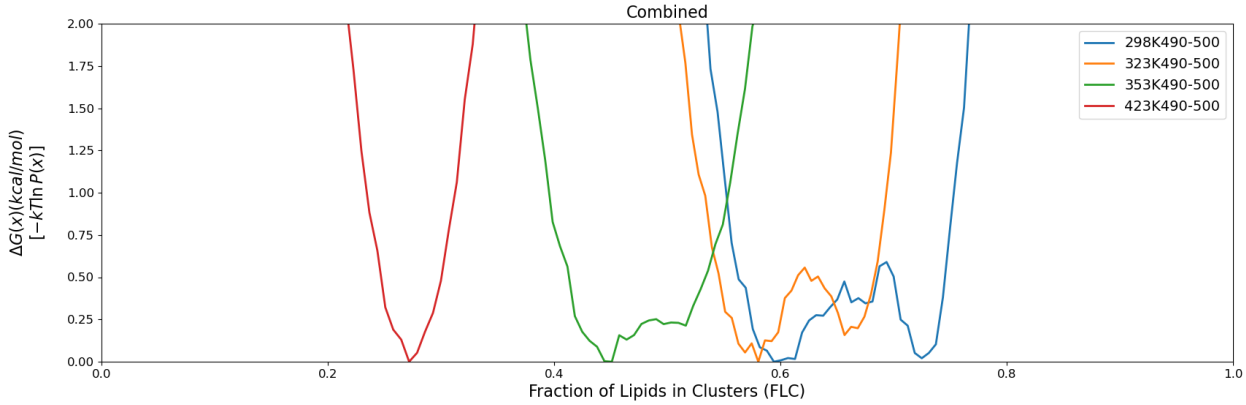

Figure 2: Free Energy Landscape of **DIPC** system. Data from all four replica has been combined using w_multi_west tool. All the FES are calculated by averaging over the iteration window 490 - 500.

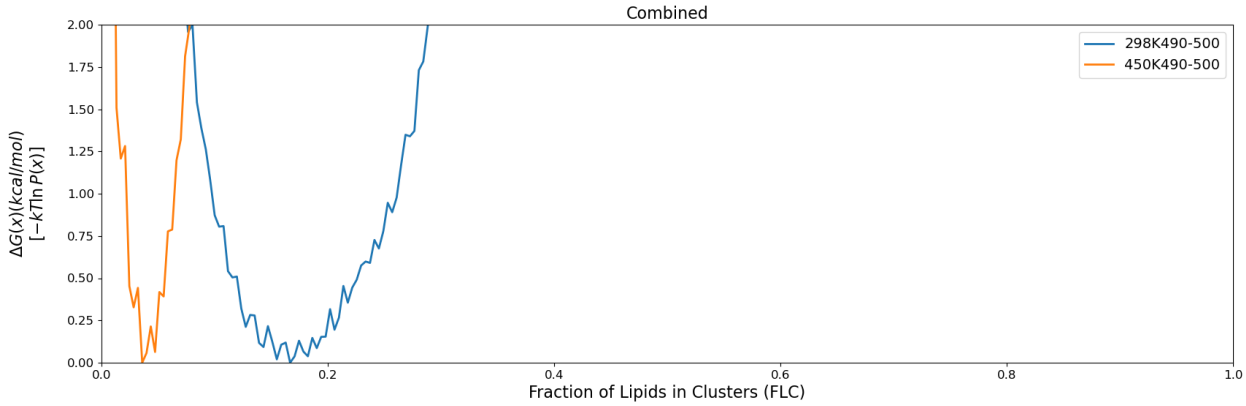

Figure 3: Free Energy Landscape of **POPC** system. Data from all four replica has been combined using w_multi_west tool. All the FES are calculated by averaging over the iteration window 490 - 500.

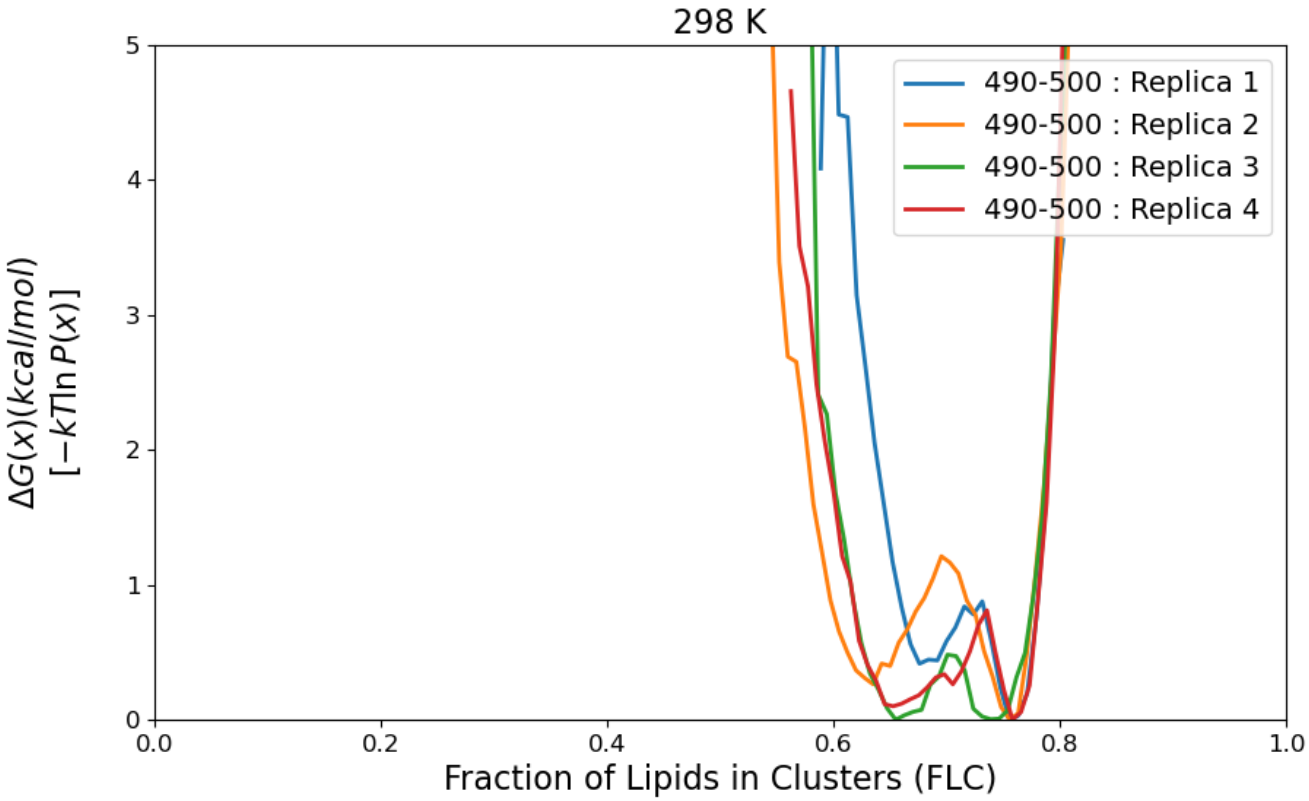

Figure 4: Free Energy Landscape of **DAPC** system for different replica at 298K. All the FES are calculated by averaging over the iteration window 490 - 500.

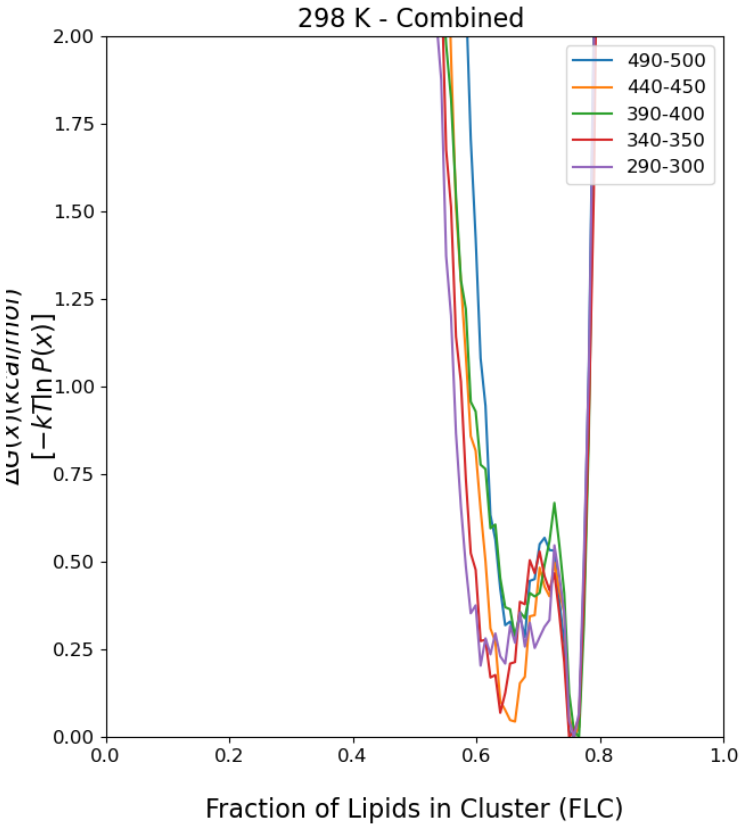

Figure 5: Convergence of Free Energy Landscape of **DAPC** system for combined replica at 298K. All the FES are calculated by averaging over the iteration window 490 - 500.

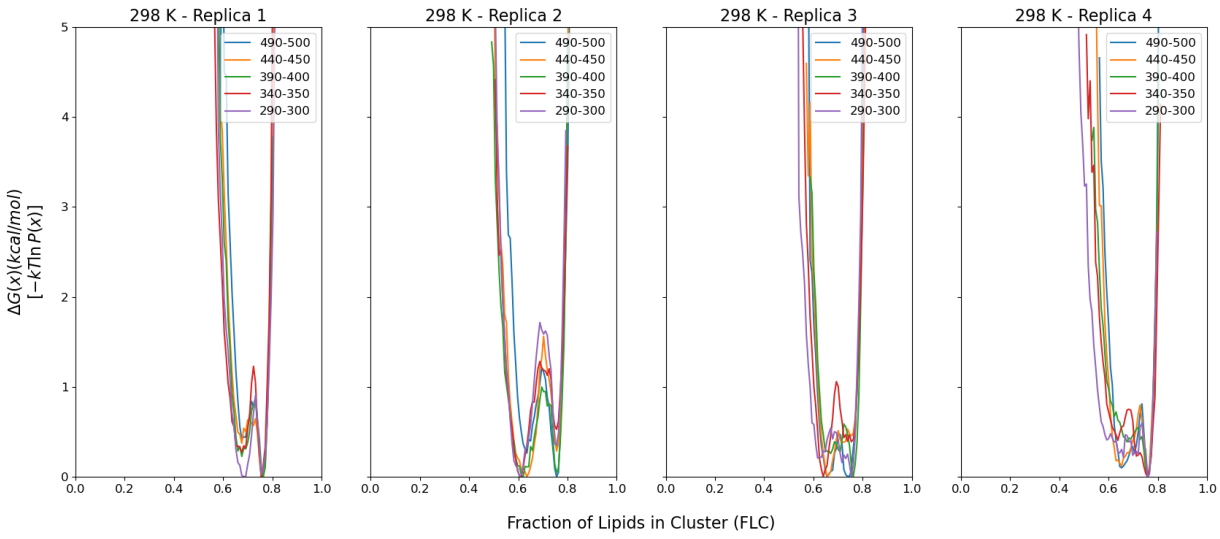

Figure 6: Convergence of Free Energy Landscape of **DAPC** system for different replica at 298K. All the FES are calculated by averaging over the iteration window 490 - 500.

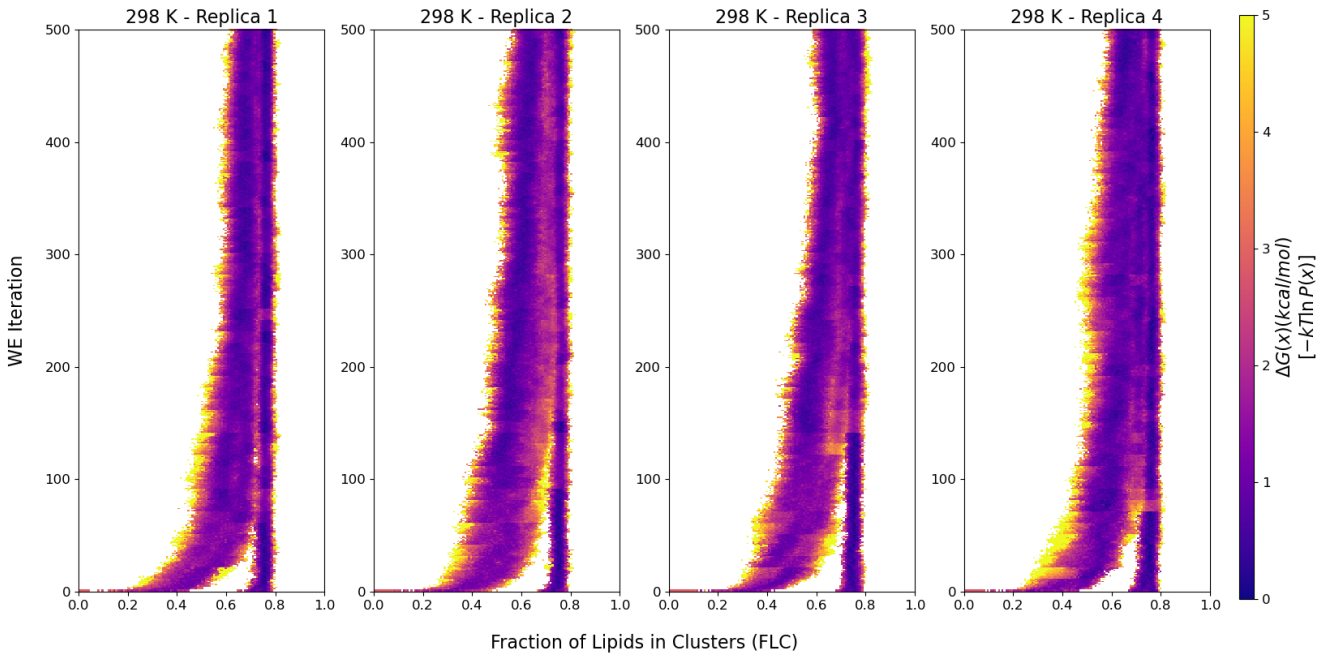

Figure 7: Evolution of Free Energy Landscape of **DAPC** system for different replica at 298K.

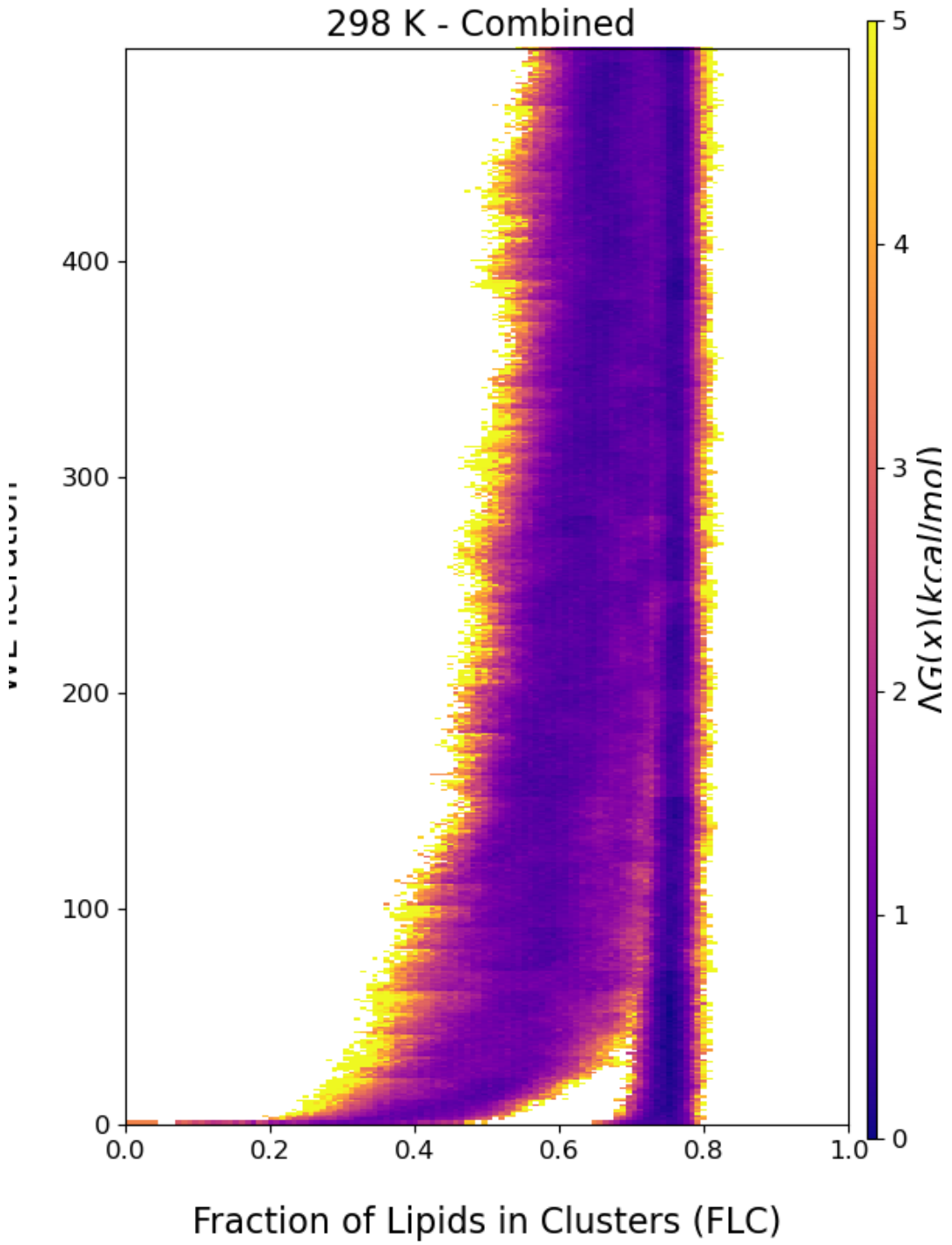

Figure 8: Evolution of Free Energy Landscape of **DAPC** system for combined replica at 298K using w_multi_tool.

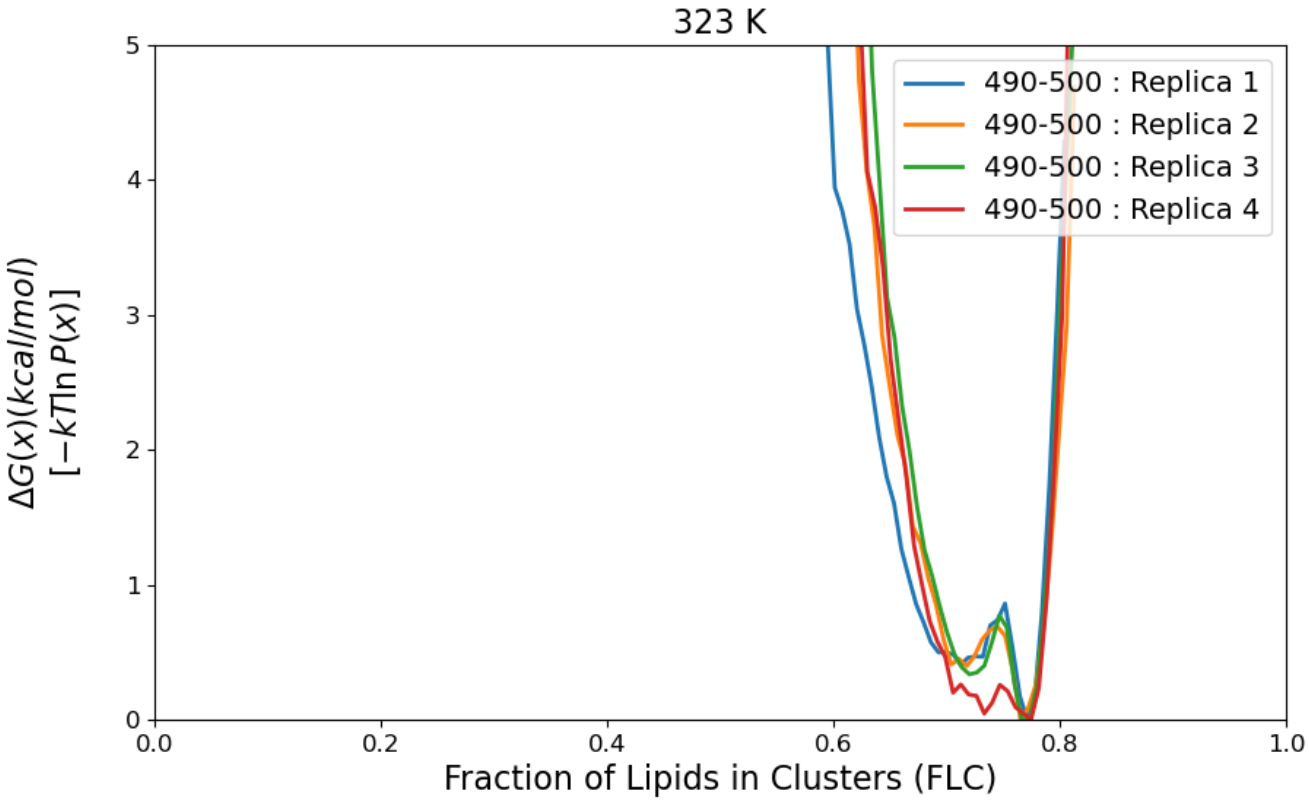

Figure 9: Free Energy Landscape of **DAPC** system for different replica at 323K. All the FES are calculated by averaging over the iteration window 490 - 500.

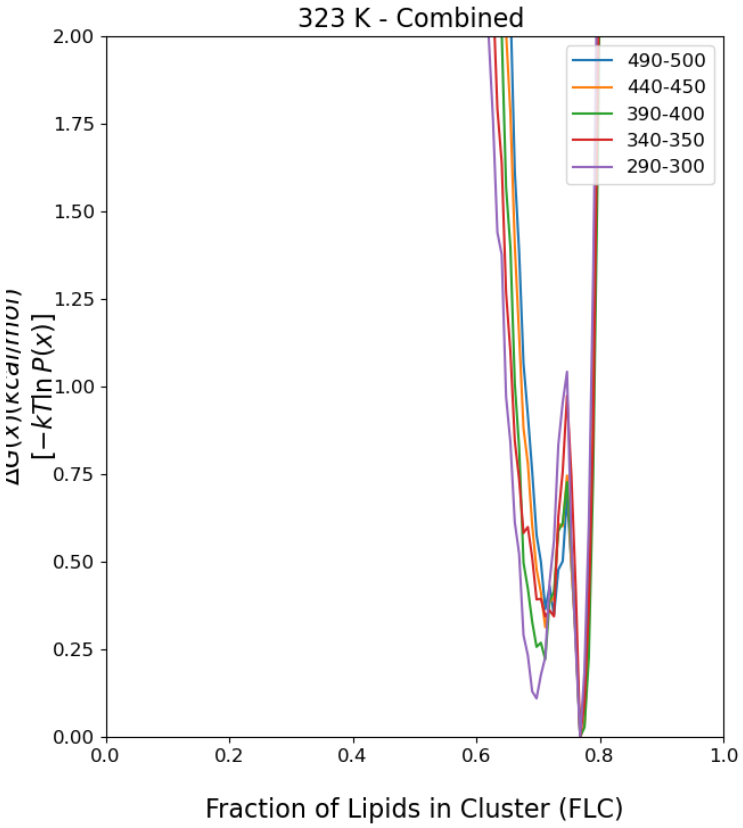

Figure 10: Convergence of Free Energy Landscape of **DAPC** system for combined replica at 323K. All the FES are calculated by averaging over the iteration window 490 - 500.

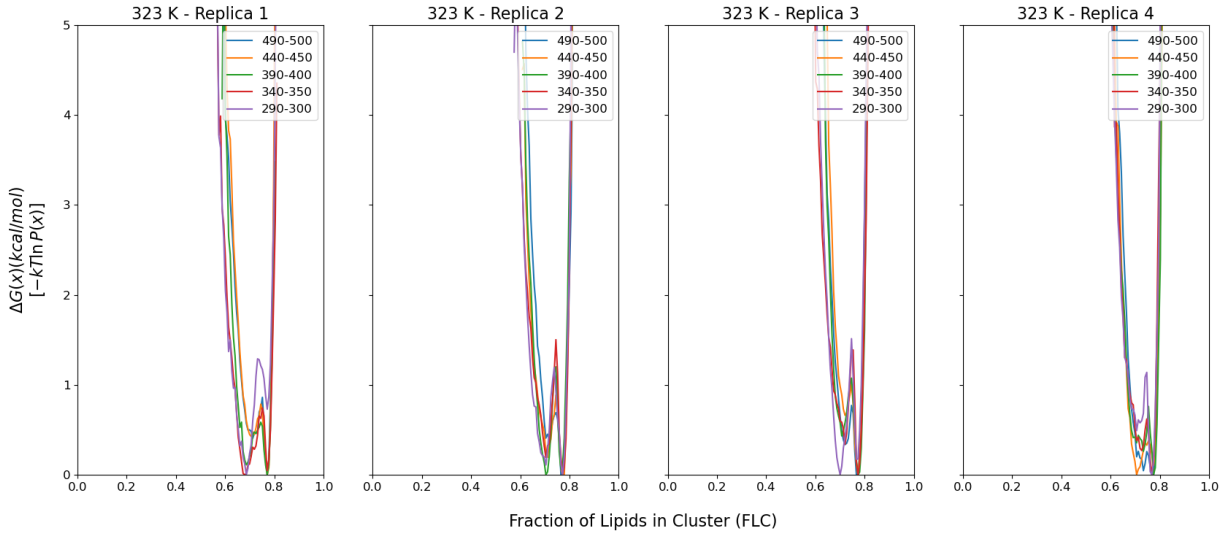

Figure 11: Convergence of Free Energy Landscape of **DAPC** system for different replica at 323K. All the FES are calculated by averaging over the iteration window 490 - 500.

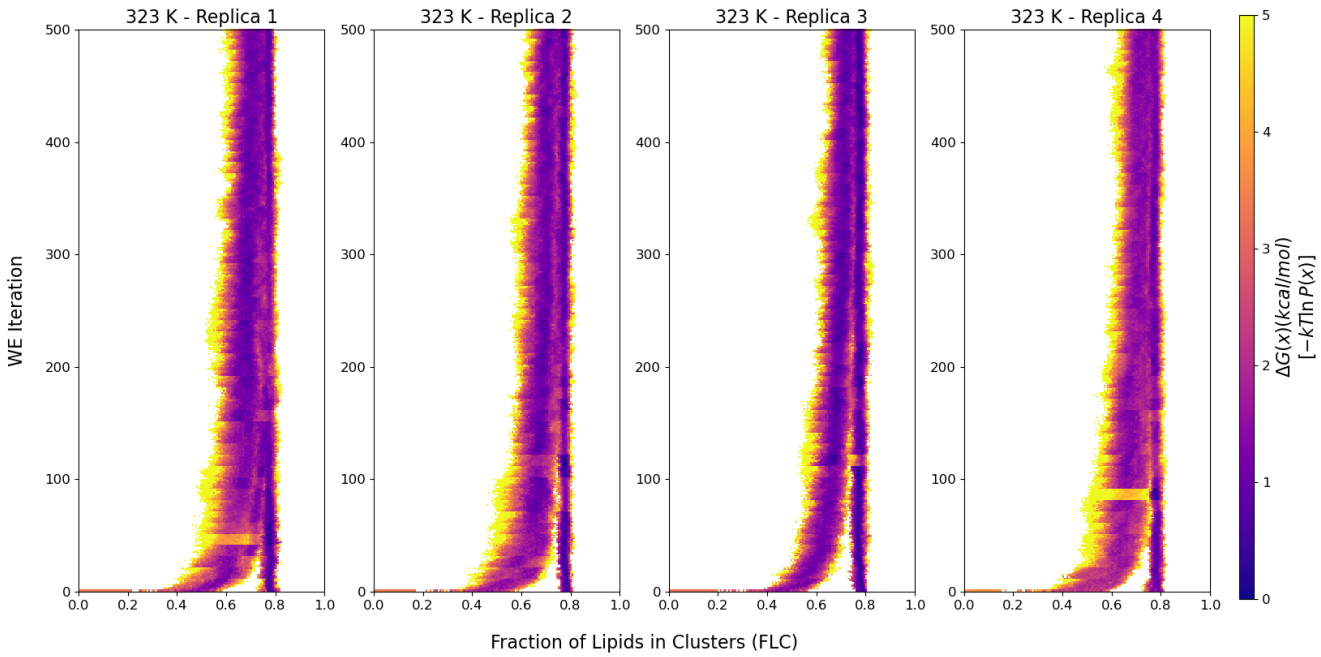

Figure 12: Evolution of Free Energy Landscape of **DAPC** system for different replica at 323K.

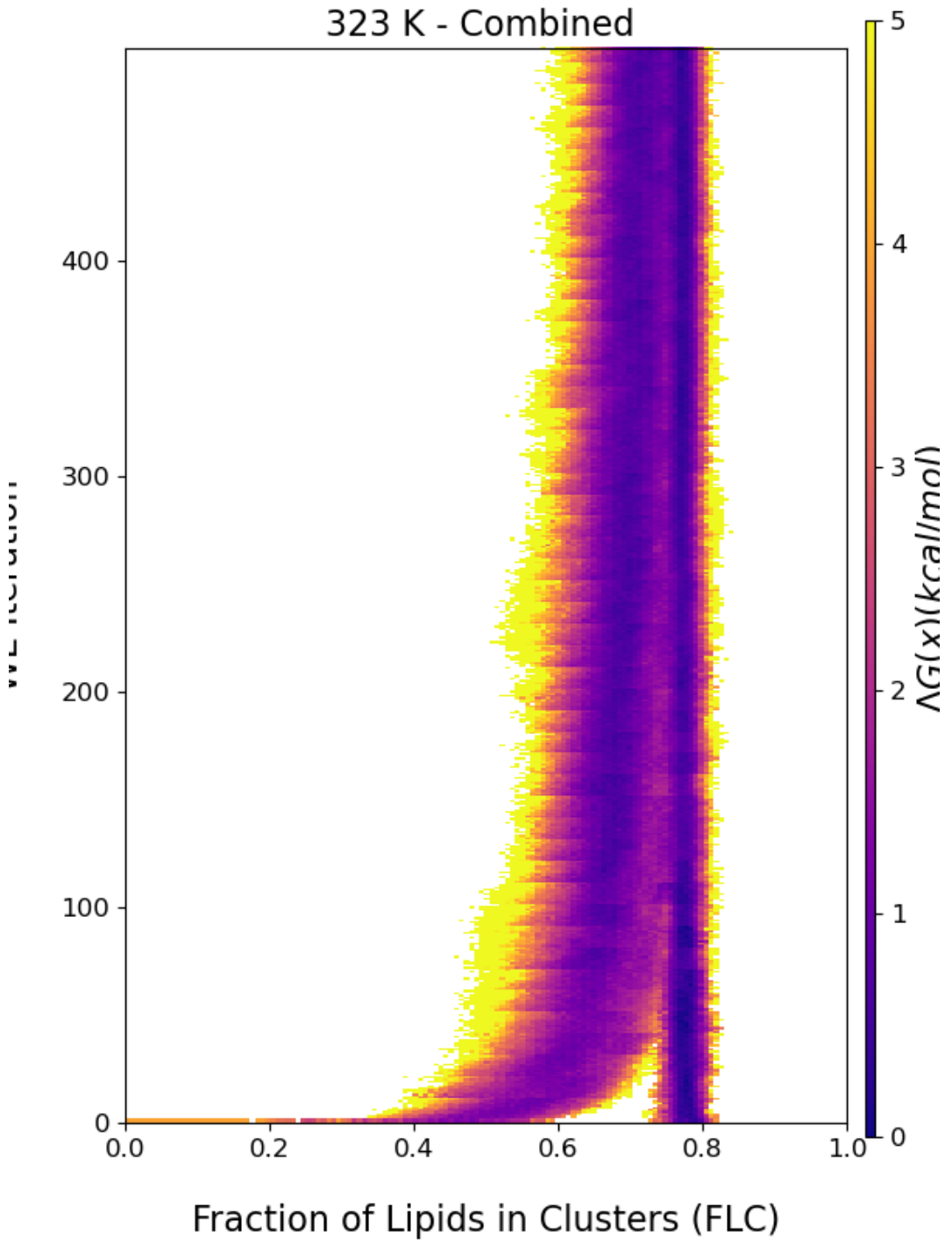

Figure 13: Evolution of Free Energy Landscape of **DAPC** system for combined replica at 323K using w_multi_tool.

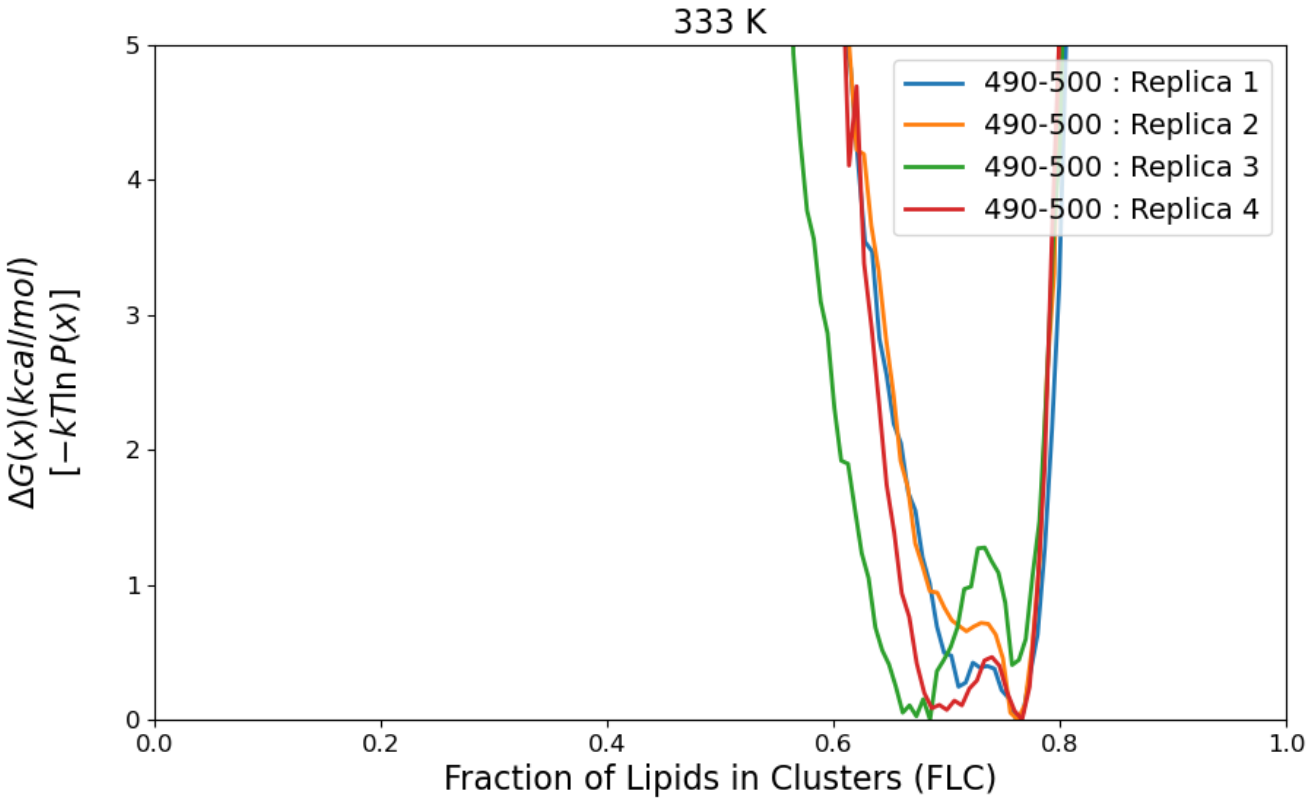

Figure 14: Free Energy Landscape of **DAPC** system for different replica at 333K. All the FES are calculated by averaging over the iteration window 490 - 500.

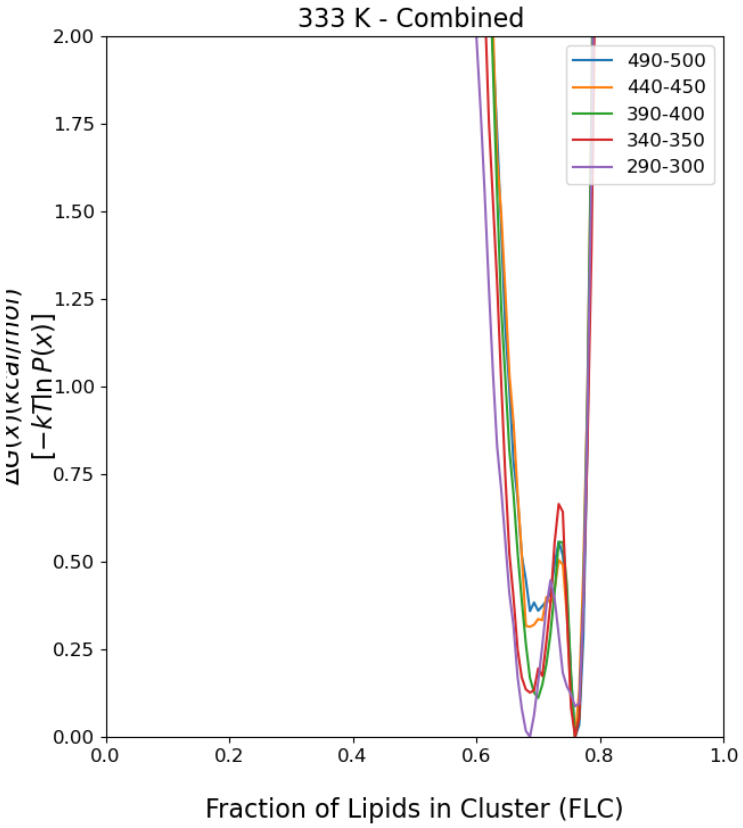

Figure 15: Convergence of Free Energy Landscape of **DAPC** system for combined replica at 333K. All the FES are calculated by averaging over the iteration window 490 - 500.

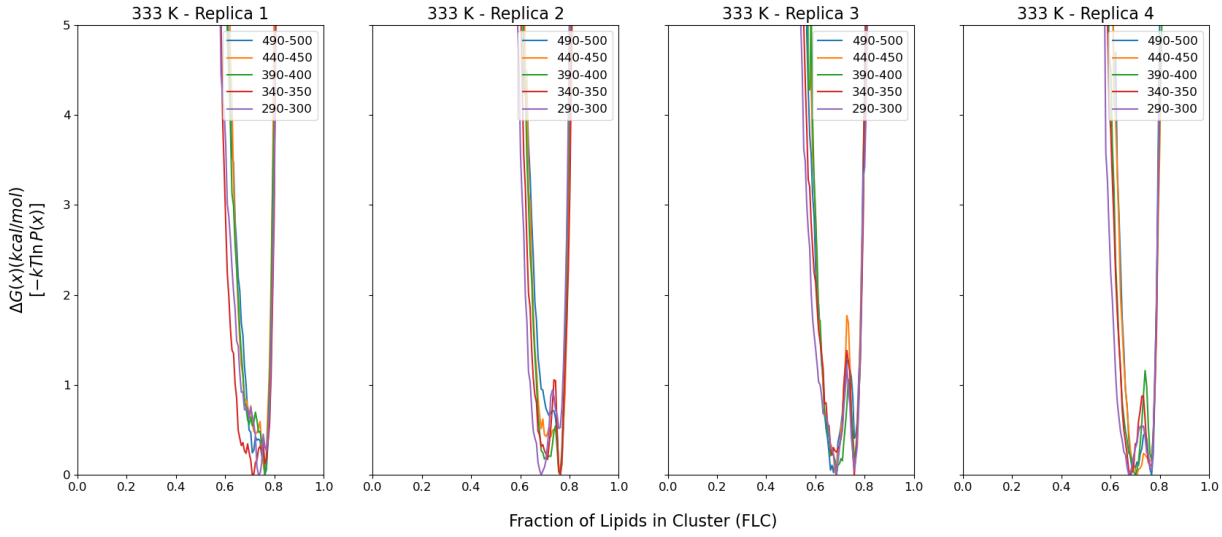

Figure 16: Convergence of Free Energy Landscape of **DAPC** system for different replica at 333K. All the FES are calculated by averaging over the iteration window 490 - 500.

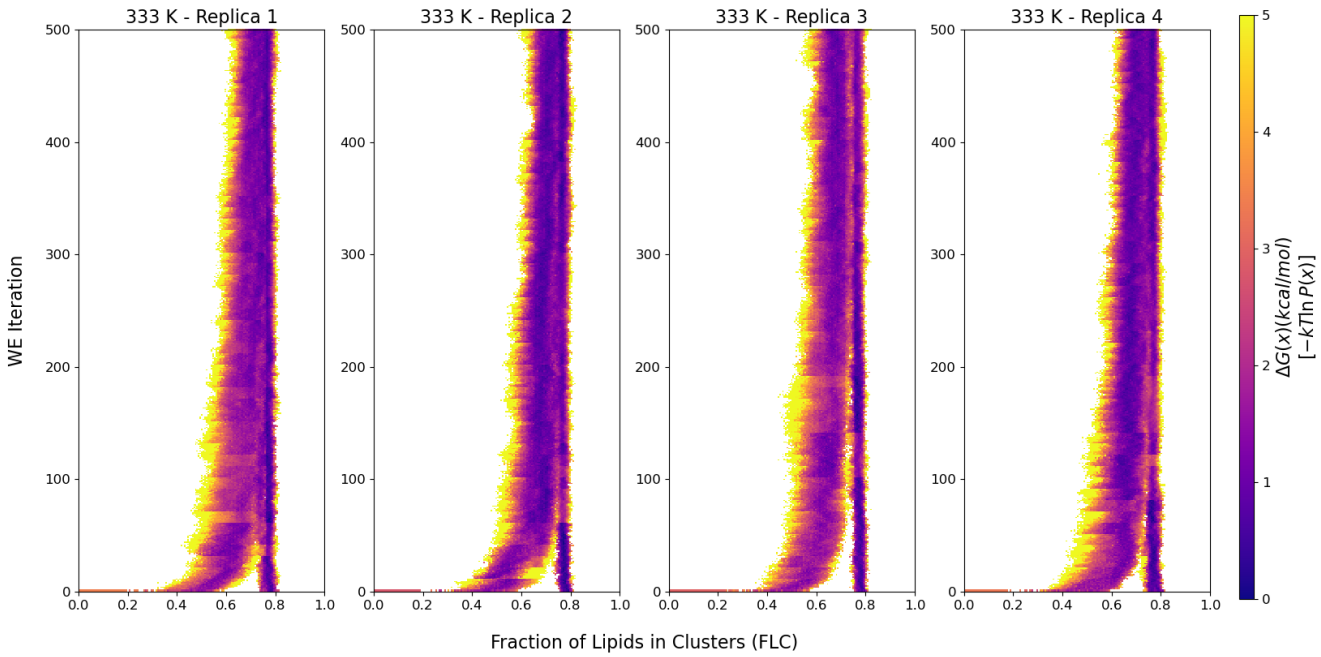

Figure 17: Evolution of Free Energy Landscape of **DAPC** system for different replica at 333K.

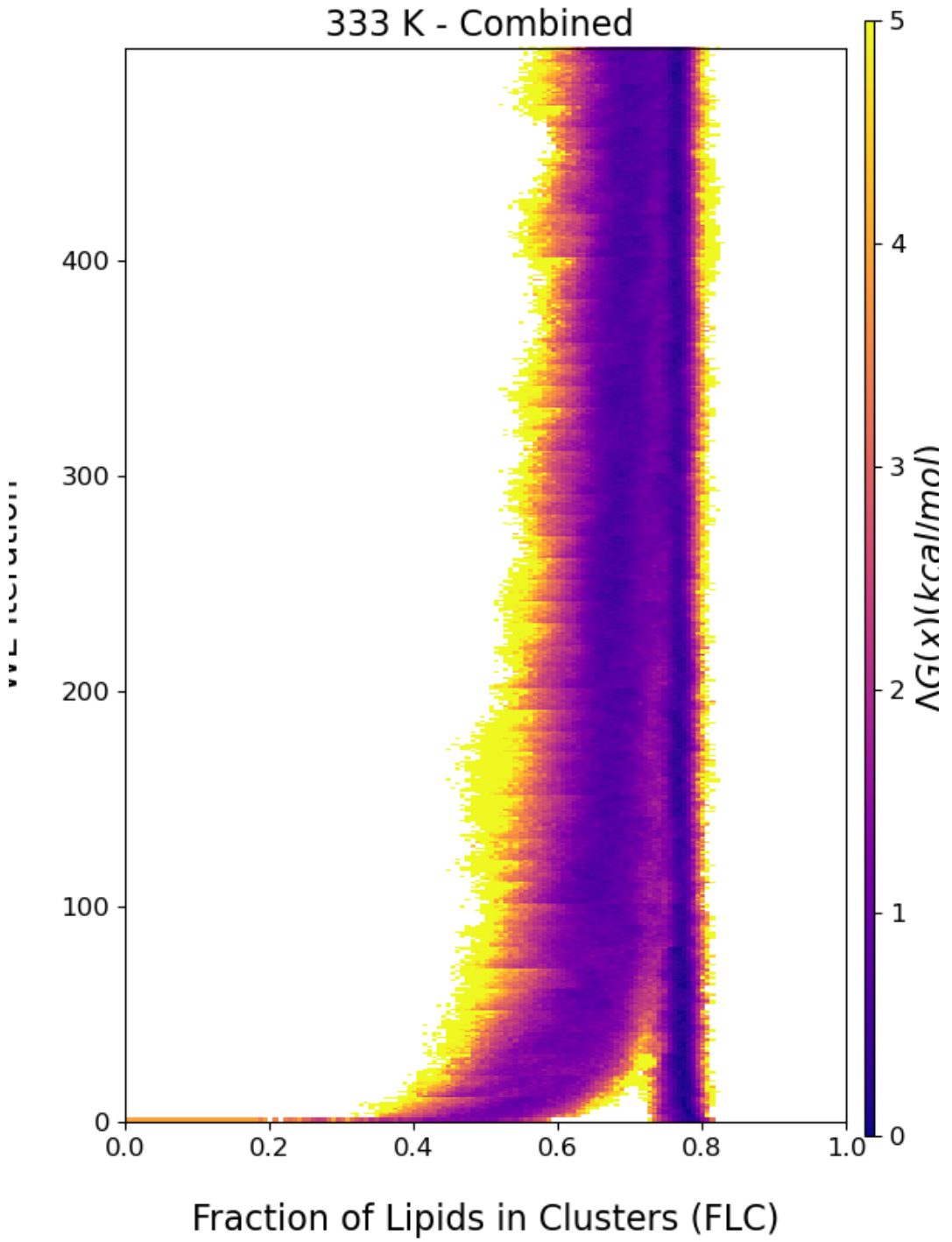

Figure 18: Evolution of Free Energy Landscape of **DAPC** system for combined replica at 333K using w_multi_tool.

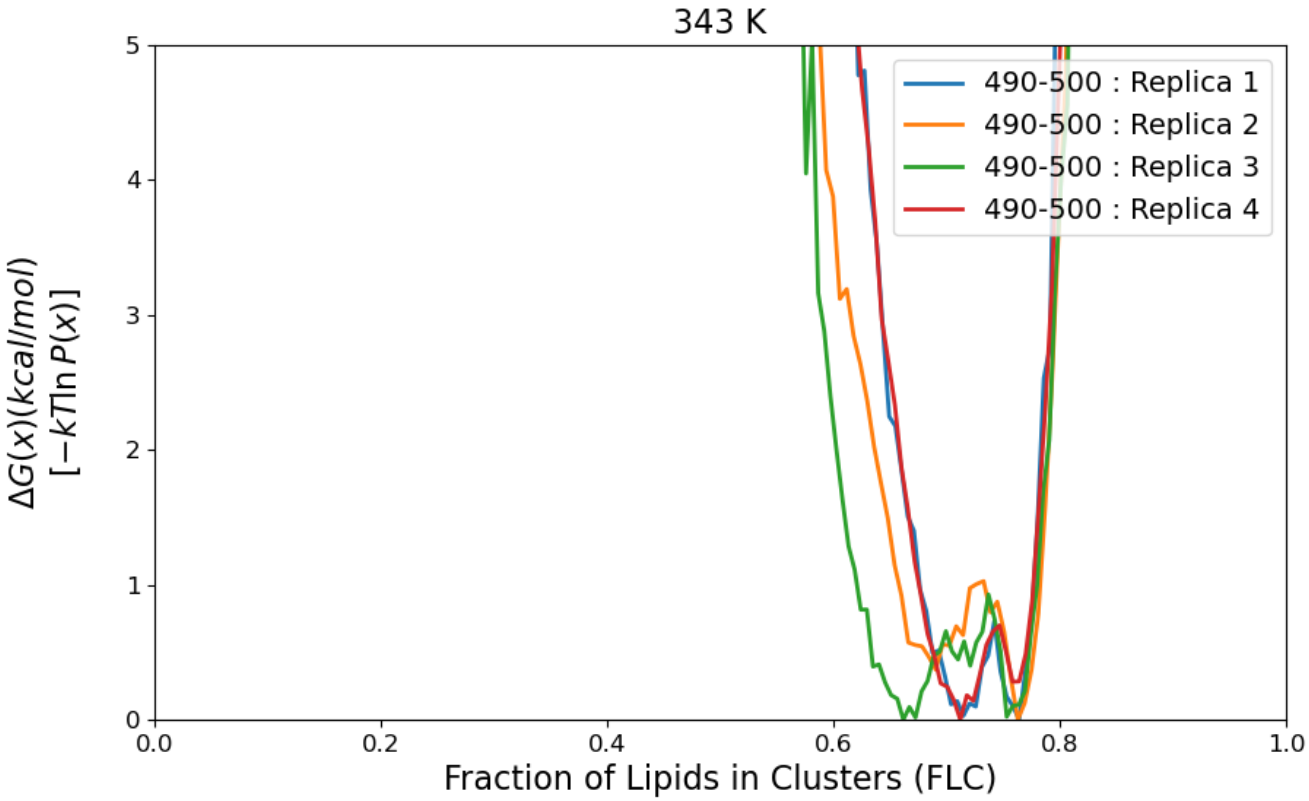

Figure 19: Free Energy Landscape of **DAPC** system for different replica at 343K. All the FES are calculated by averaging over the iteration window 490 - 500.

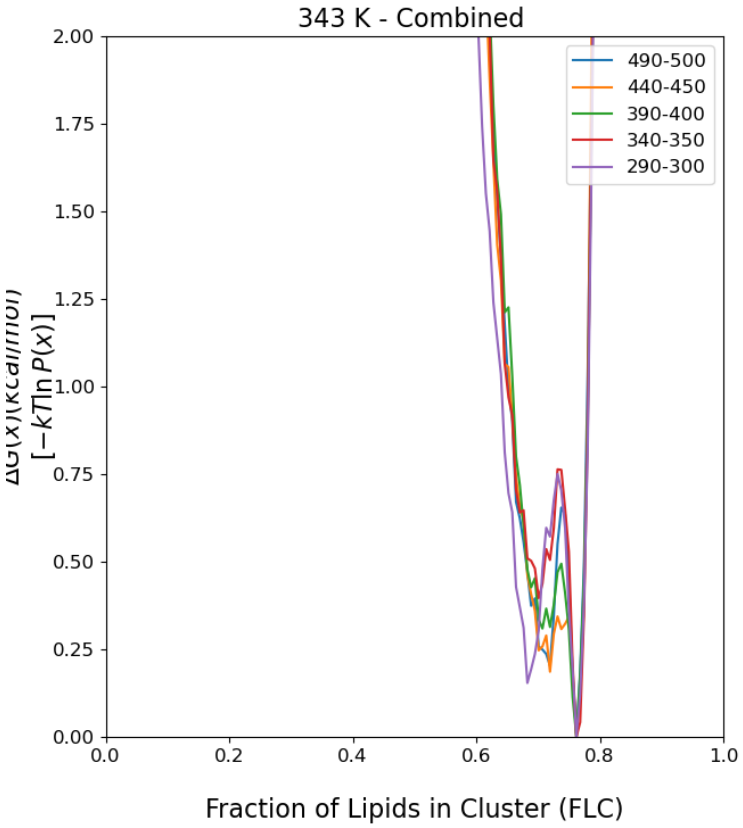

Figure 20: Convergence of Free Energy Landscape of **DAPC** system for combined replica at 343K. All the FES are calculated by averaging over the iteration window 490 - 500.

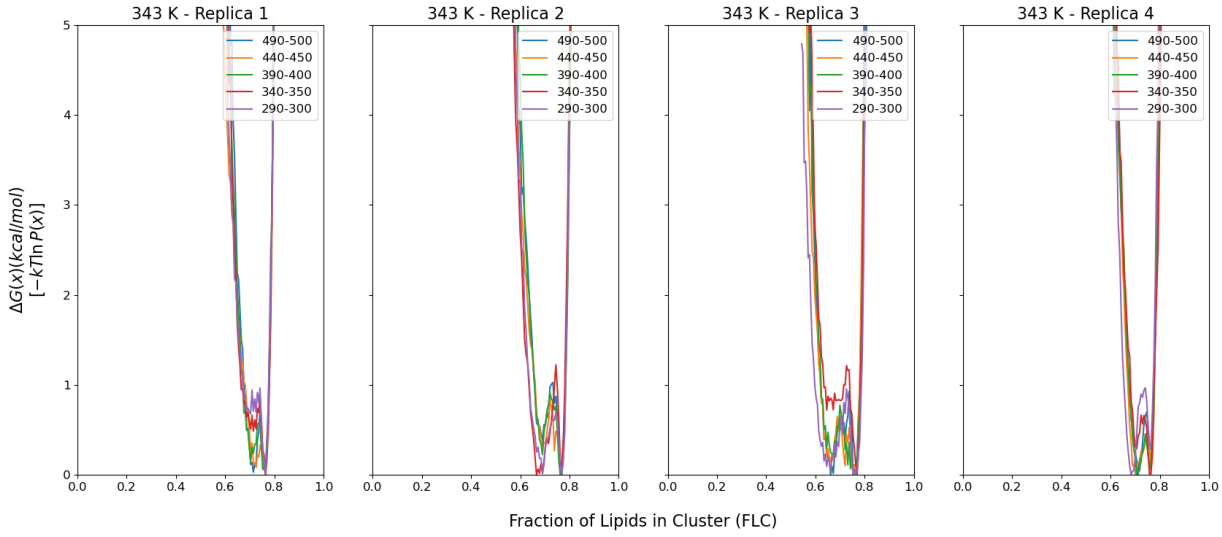

Figure 21: Convergence of Free Energy Landscape of **DAPC** system for different replica at 343K. All the FES are calculated by averaging over the iteration window 490 - 500.

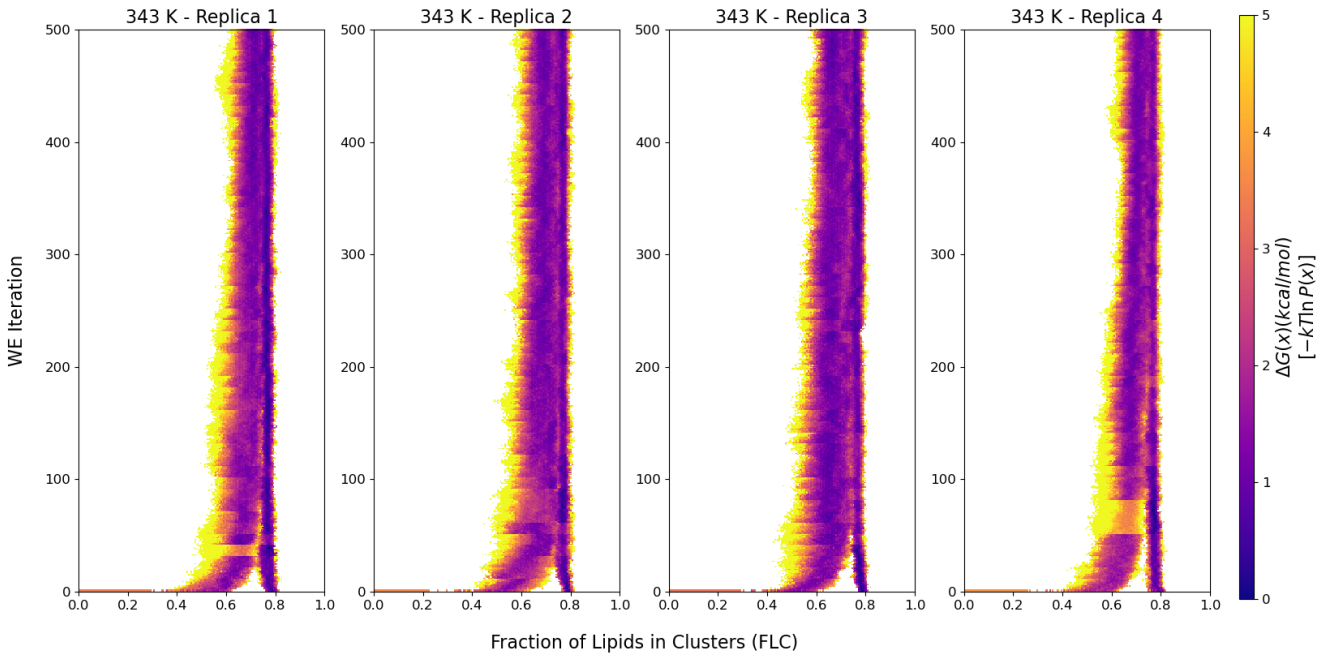

Figure 22: Evolution of Free Energy Landscape of **DAPC** system for different replica at 343K.

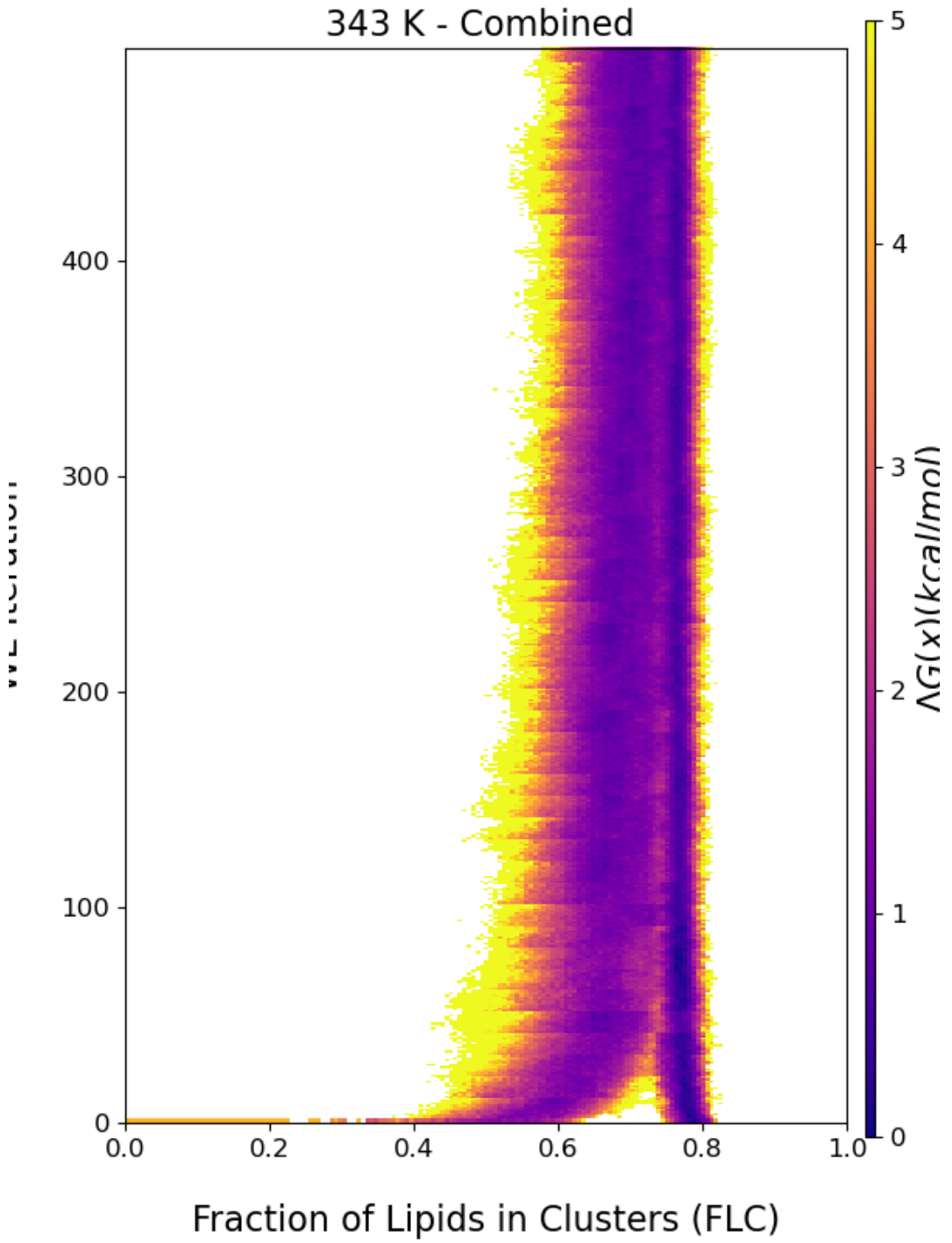

Figure 23: Evolution of Free Energy Landscape of **DAPC** system for combined replica at 343K using w_multi_tool.

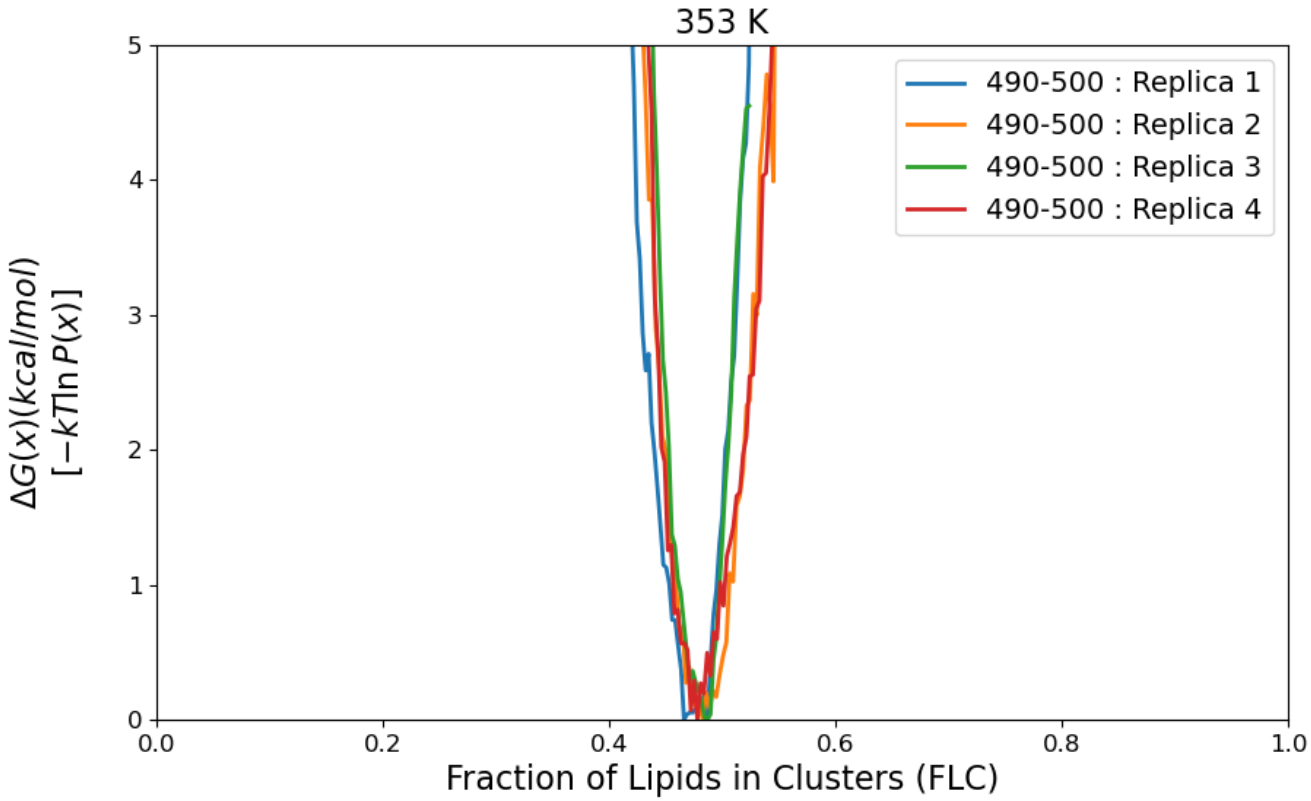

Figure 24: Free Energy Landscape of **DAPC** system for different replica at 353K. All the FES are calculated by averaging over the iteration window 490 - 500.

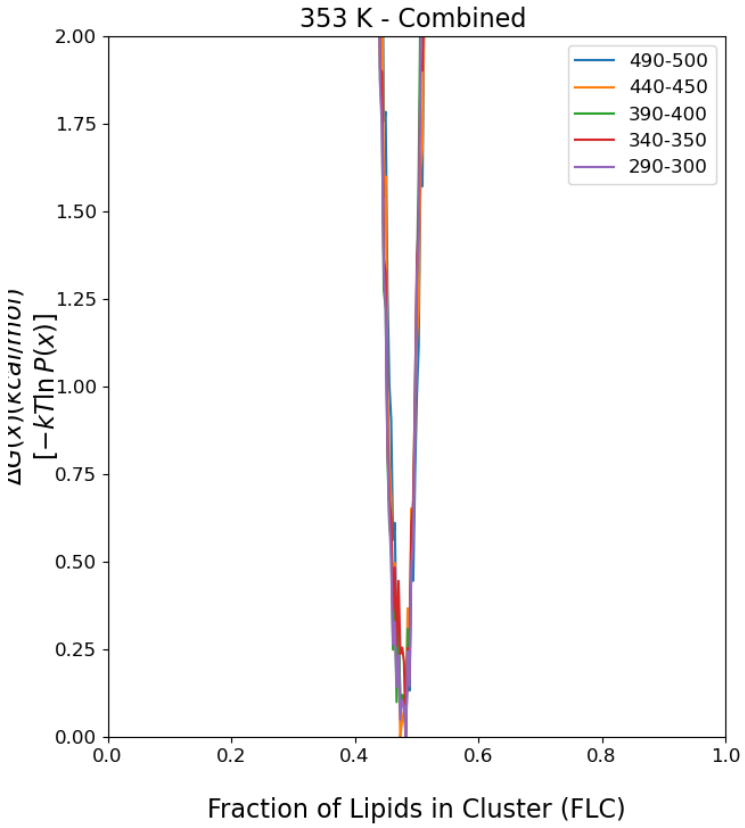

Figure 25: Convergence of Free Energy Landscape of **DAPC** system for combined replica at 353K. All the FES are calculated by averaging over the iteration window 490 - 500.

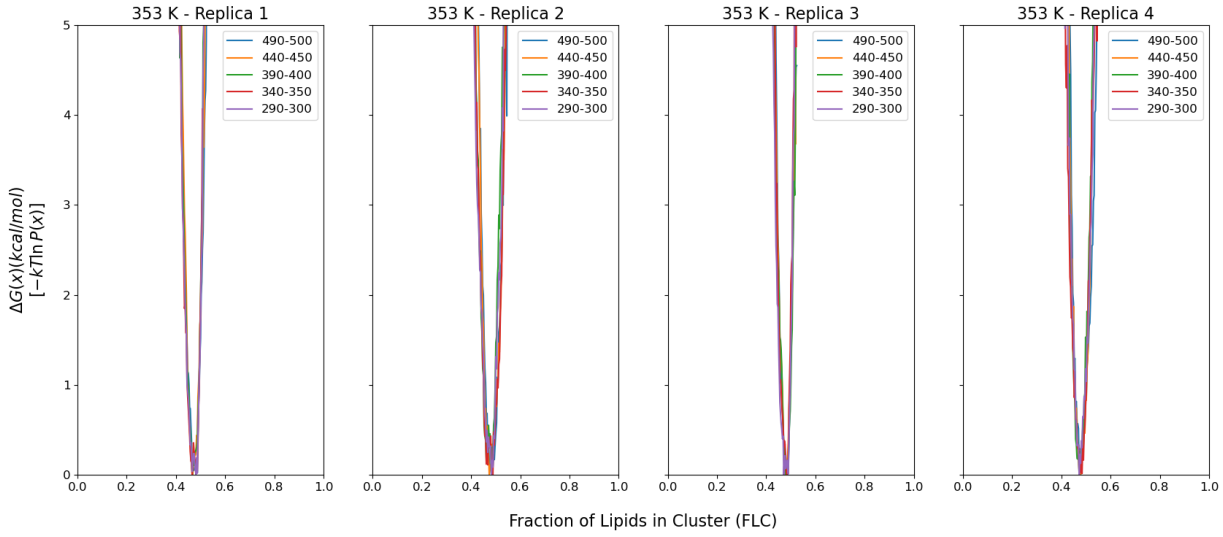

Figure 26: Convergence of Free Energy Landscape of **DAPC** system for different replica at 353K. All the FES are calculated by averaging over the iteration window 490 - 500.

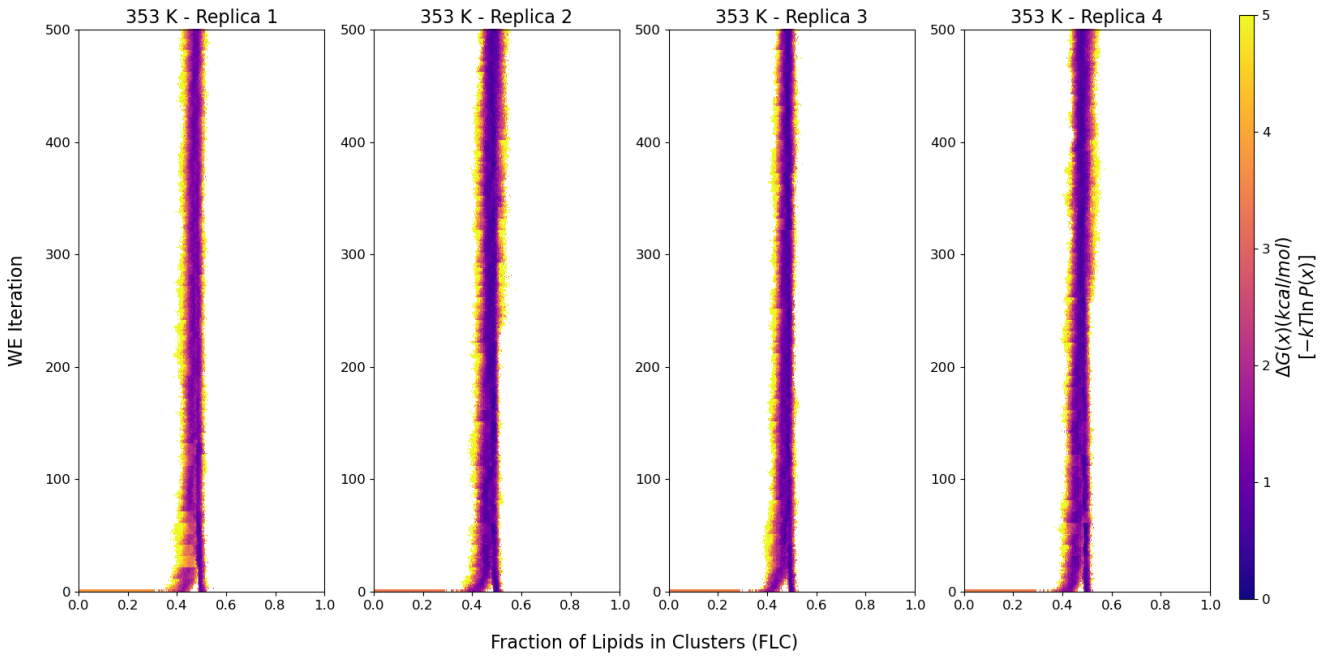

Figure 27: Evolution of Free Energy Landscape of **DAPC** system for different replica at 353K.

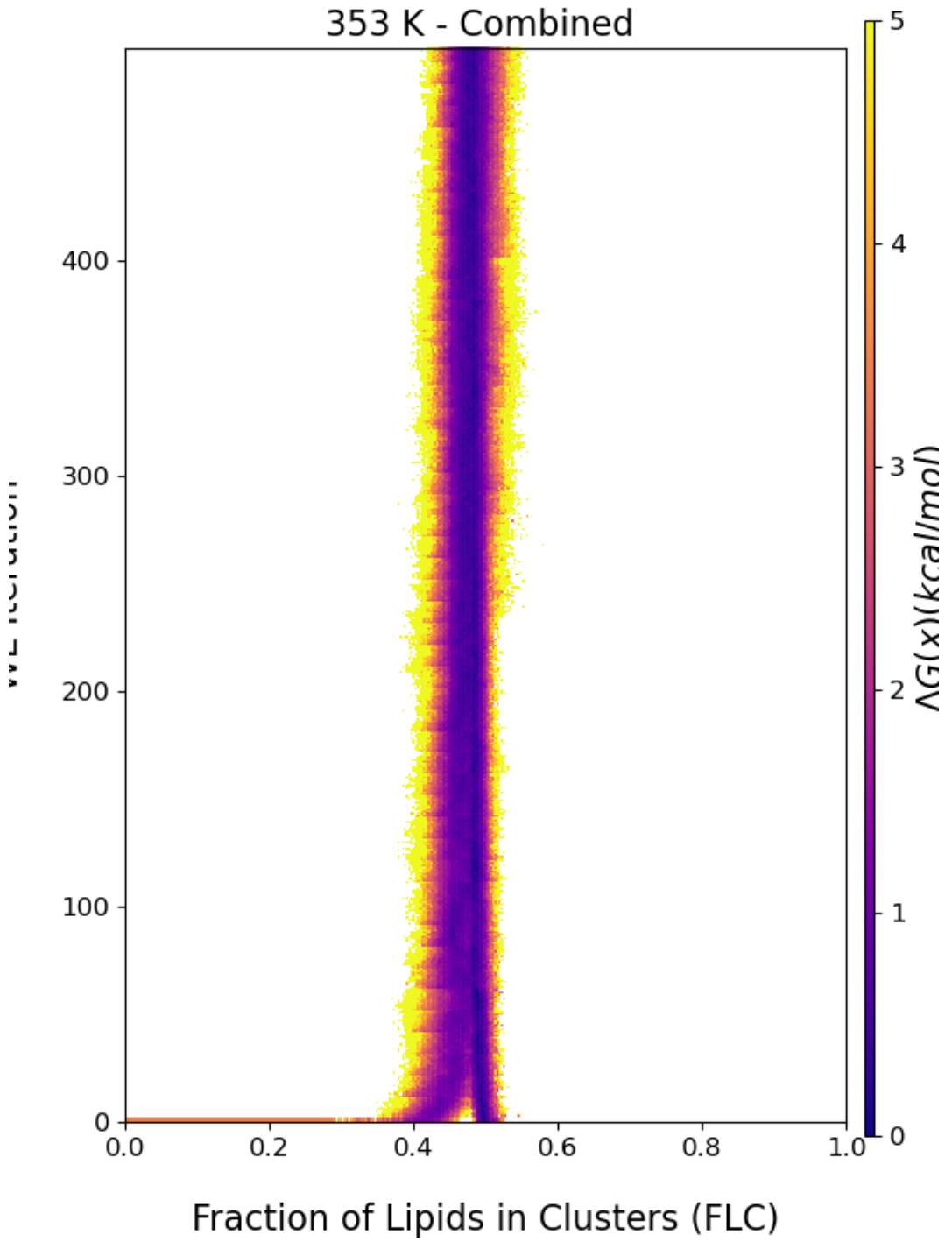

Figure 28: Evolution of Free Energy Landscape of **DAPC** system for combined replica at 353K using w_multi_tool.

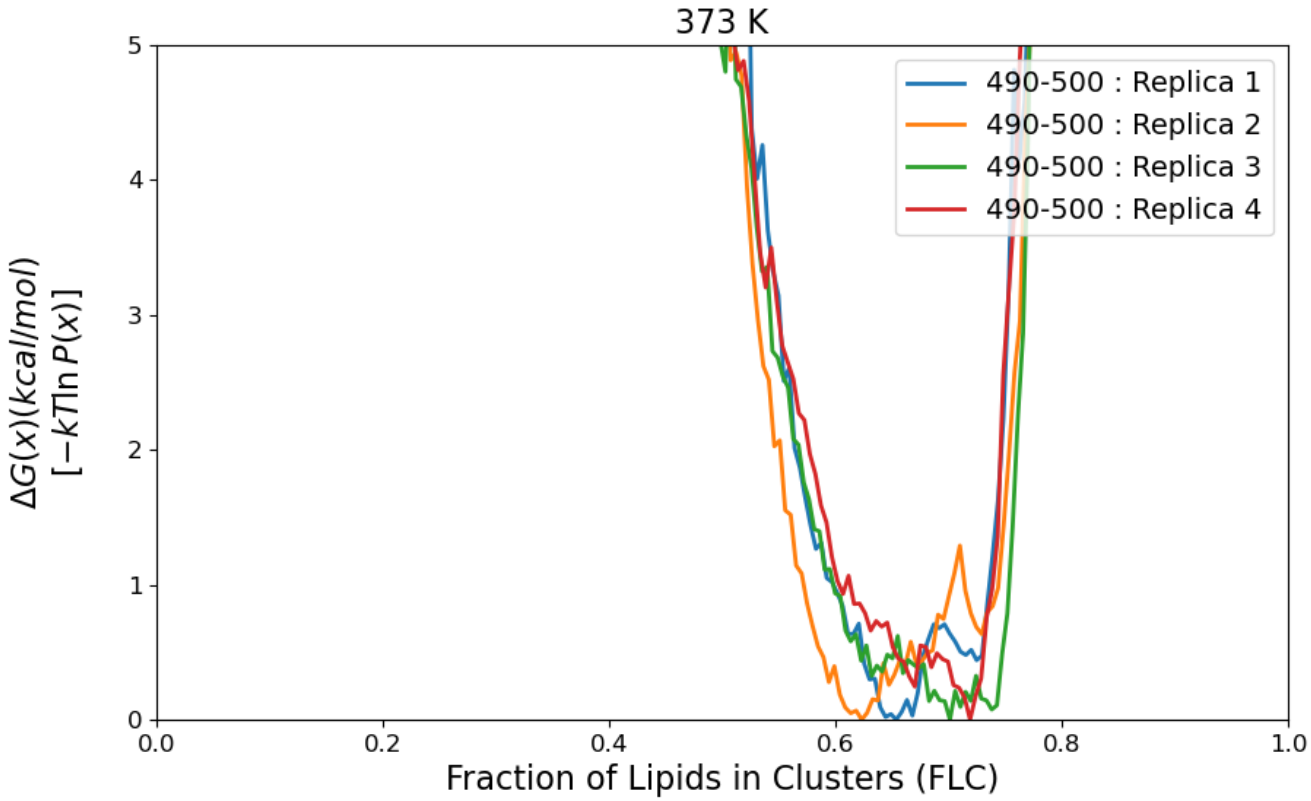

Figure 29: Free Energy Landscape of **DAPC** system for different replica at 373K. All the FES are calculated by averaging over the iteration window 490 - 500.

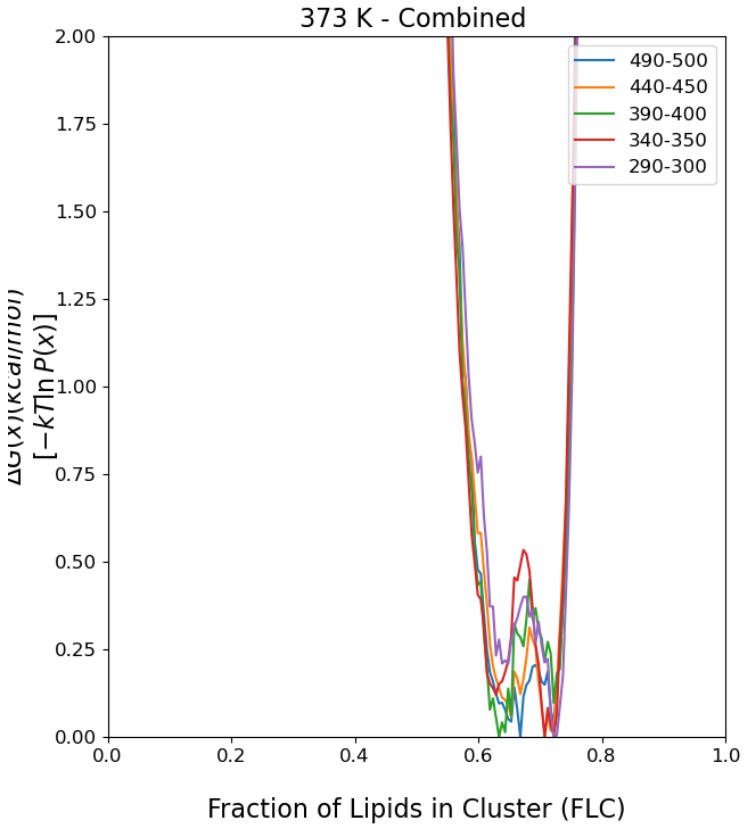

Figure 30: Convergence of Free Energy Landscape of **DAPC** system for combined replica at 373K. All the FES are calculated by averaging over the iteration window 490 - 500.

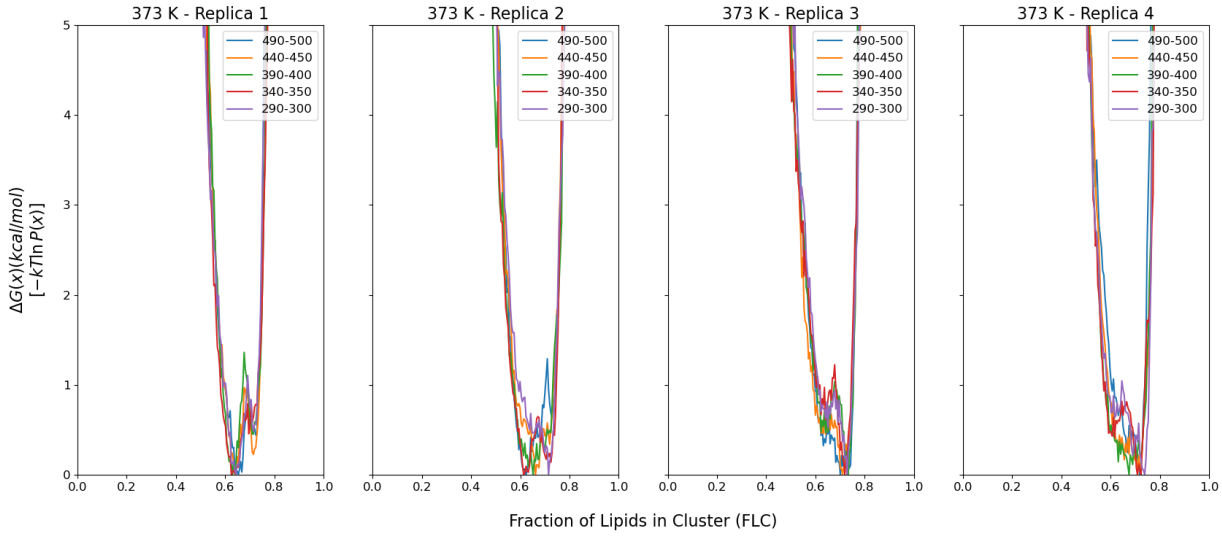

Figure 31: Convergence of Free Energy Landscape of **DAPC** system for different replica at 373K. All the FES are calculated by averaging over the iteration window 490 - 500.

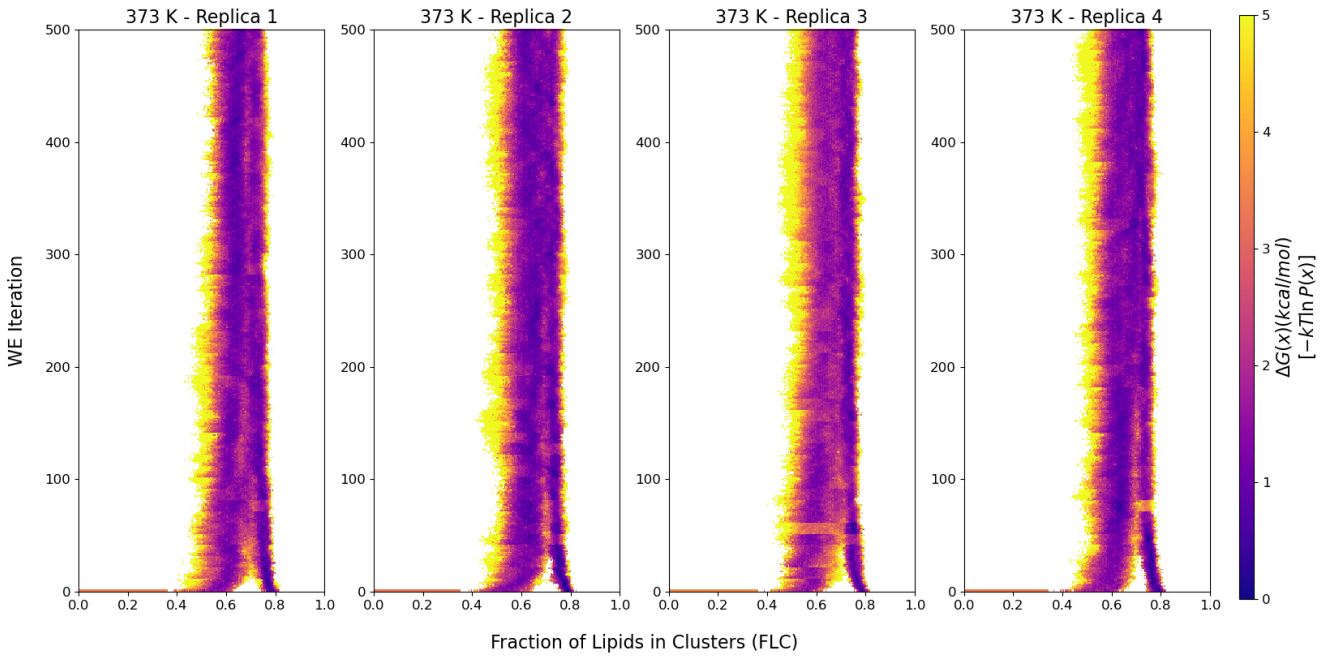

Figure 32: Evolution of Free Energy Landscape of **DAPC** system for different replica at 373K.

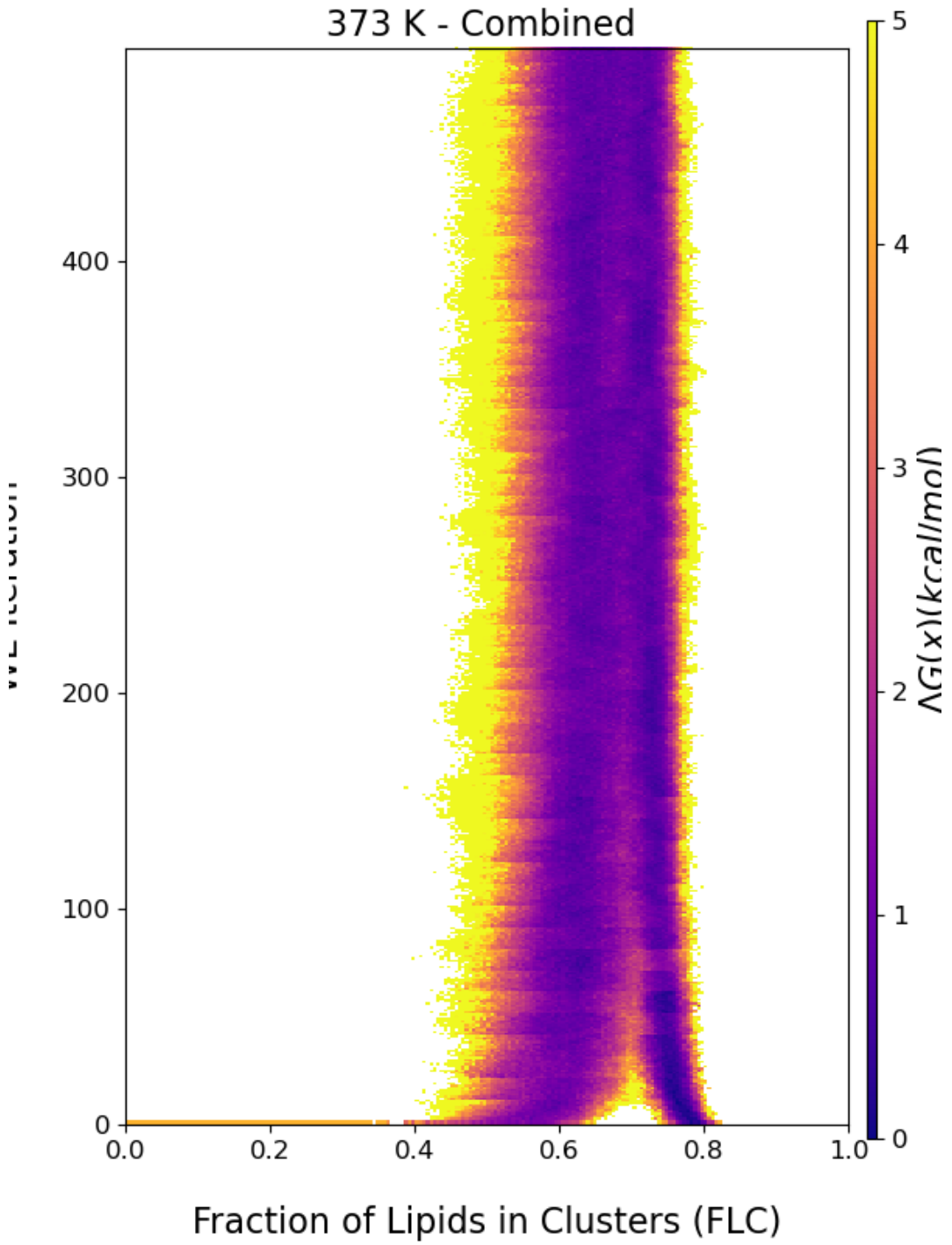

Figure 33: Evolution of Free Energy Landscape of **DAPC** system for combined replica at 373K using w_multi_tool.

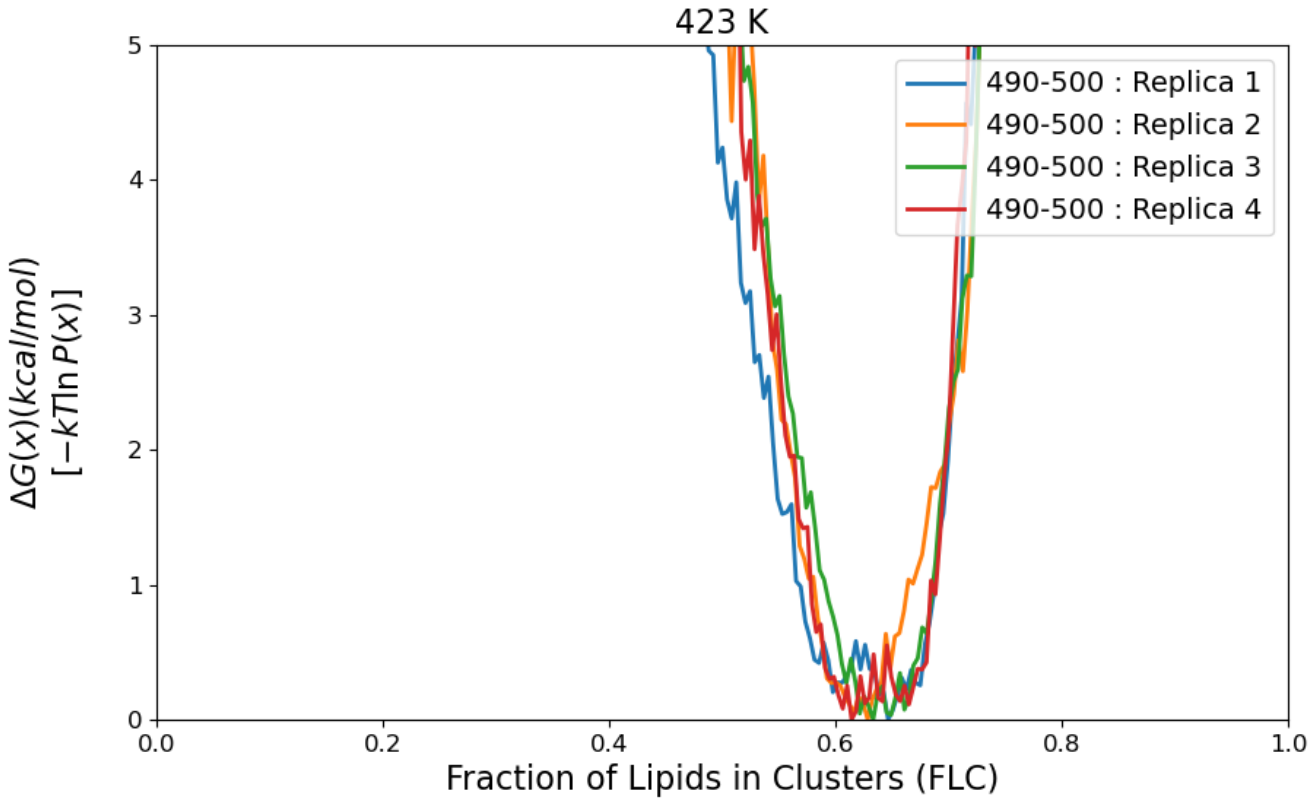

Figure 34: Free Energy Landscape of **DAPC** system for different replica at 423K. All the FES are calculated by averaging over the iteration window 490 - 500.

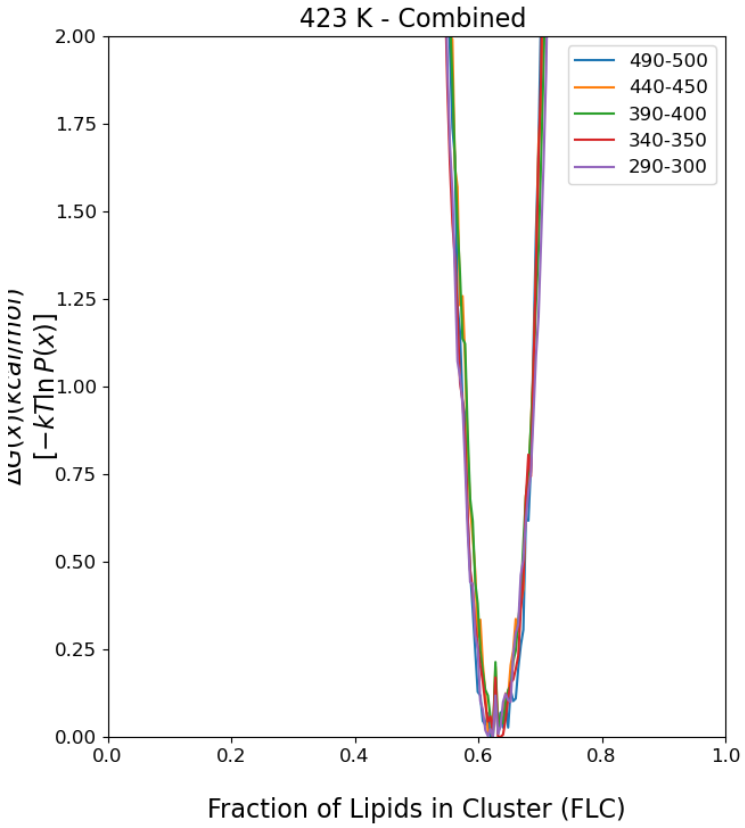

Figure 35: Convergence of Free Energy Landscape of **DAPC** system for combined replica at 423K. All the FES are calculated by averaging over the iteration window 490 - 500.

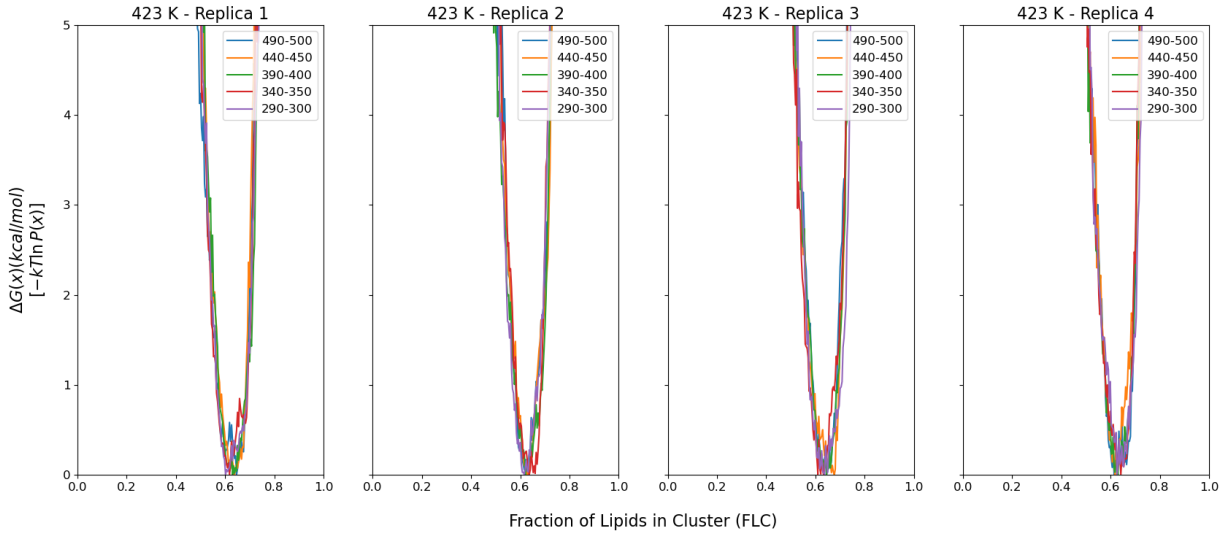

Figure 36: Convergence of Free Energy Landscape of **DAPC** system for different replica at 423K. All the FES are calculated by averaging over the iteration window 490 - 500.

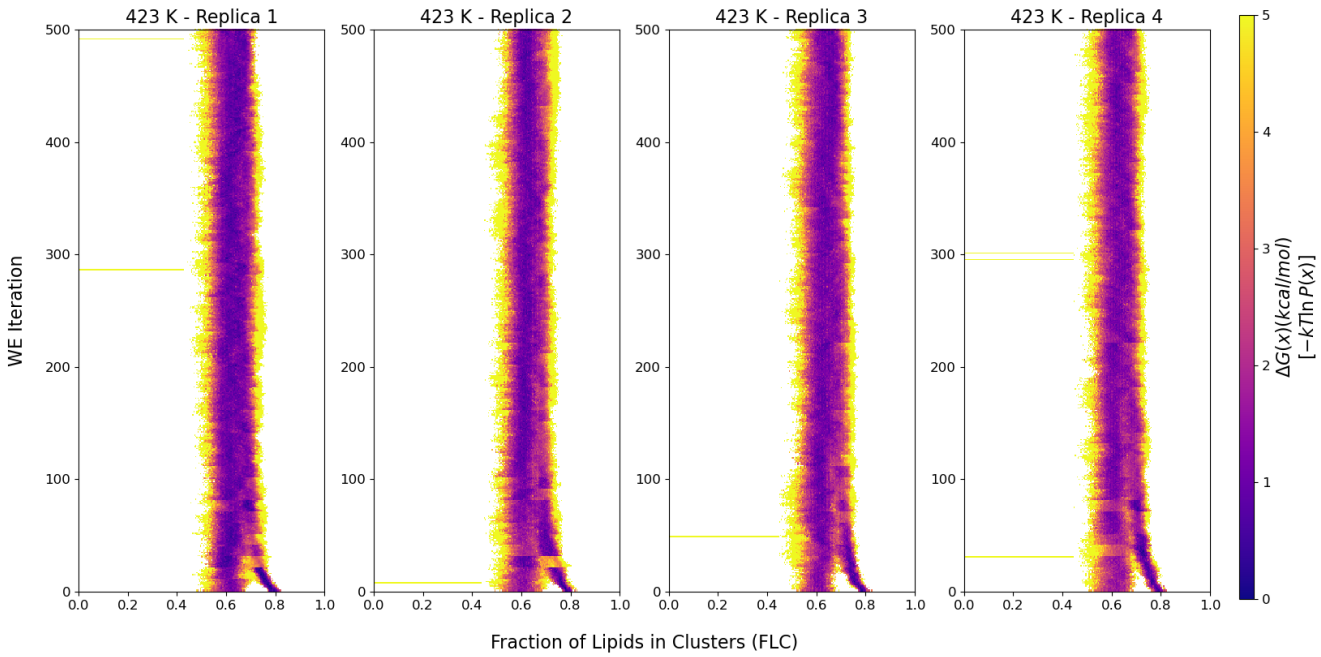

Figure 37: Evolution of Free Energy Landscape of **DAPC** system for different replica at 423K.

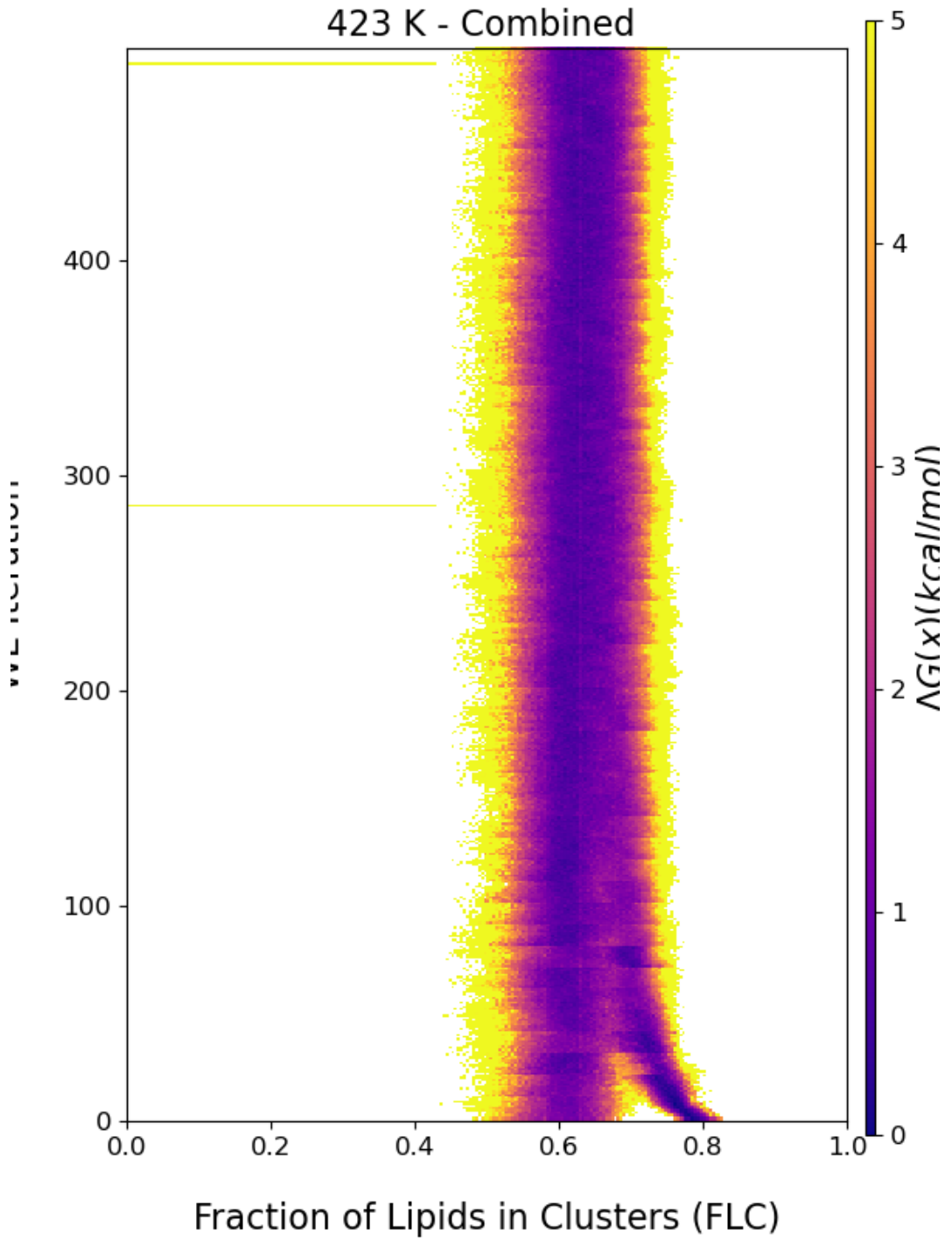

Figure 38: Evolution of Free Energy Landscape of **DAPC** system for combined replica at 423K using w_multi_tool.

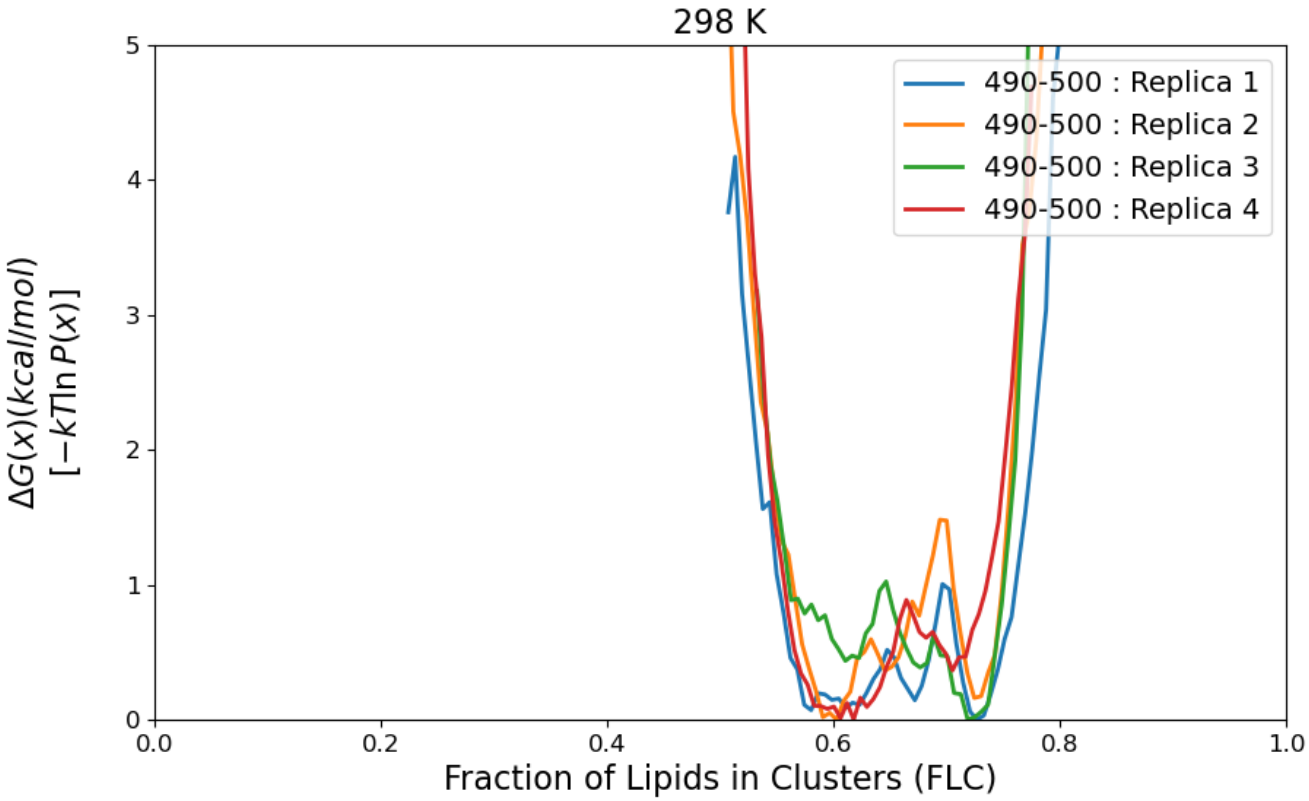

Figure 39: Free Energy Landscape of **DIPC** system for different replica at 298K. All the FES are calculated by averaging over the iteration window 490 - 500.

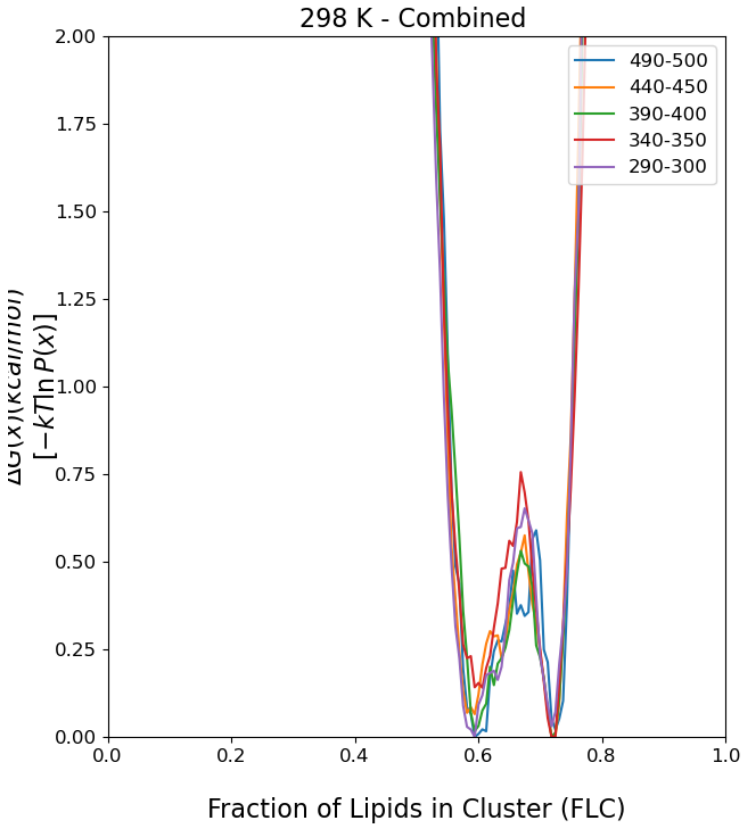

Figure 40: Convergence of Free Energy Landscape of **DIPC** system for combined replica at 298K. All the FES are calculated by averaging over the iteration window 490 - 500.

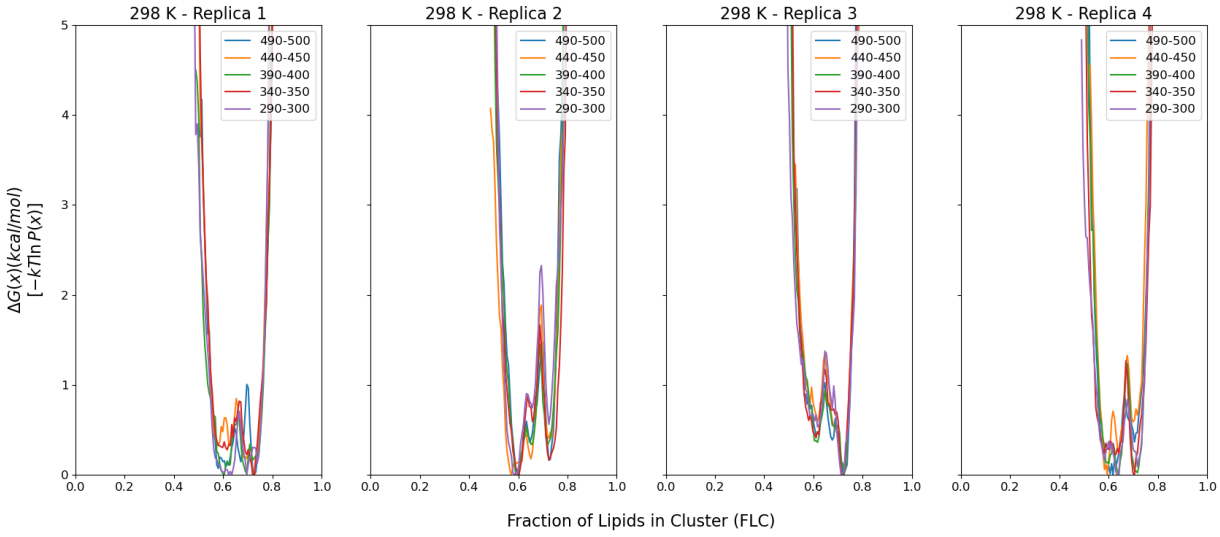

Figure 41: Convergence of Free Energy Landscape of **DIPC** system for different replica at 298K. All the FES are calculated by averaging over the iteration window 490 - 500.

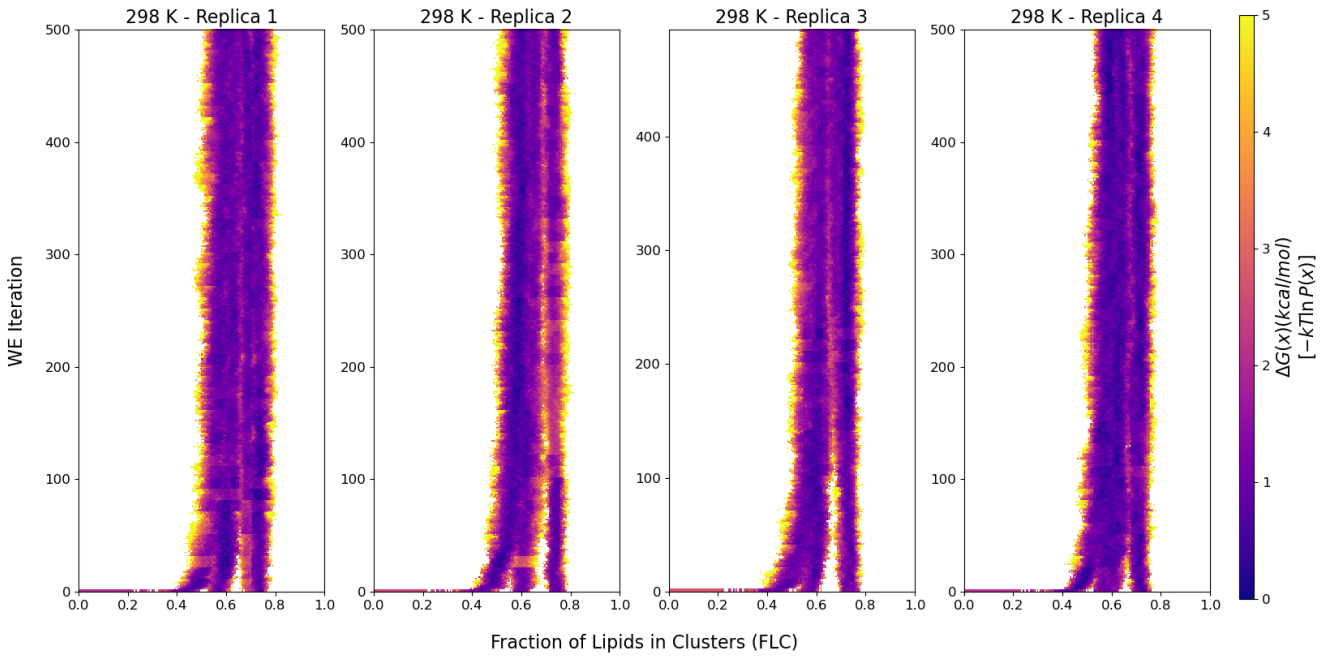

Figure 42: Evolution of Free Energy Landscape of **DIPC** system for different replica at 298K.

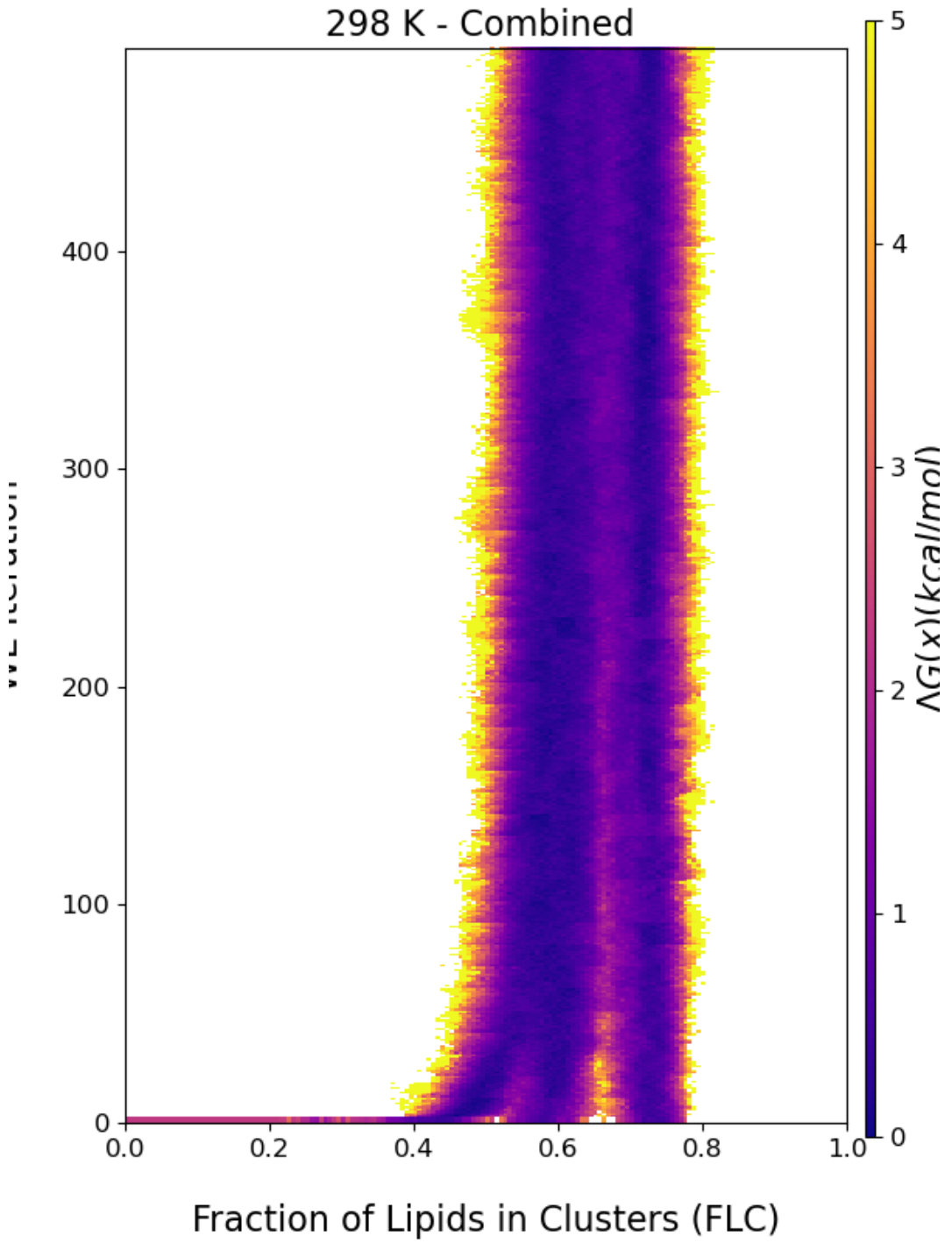

Figure 43: Evolution of Free Energy Landscape of **DIPC** system for combined replica at 298K using w_multi_tool.

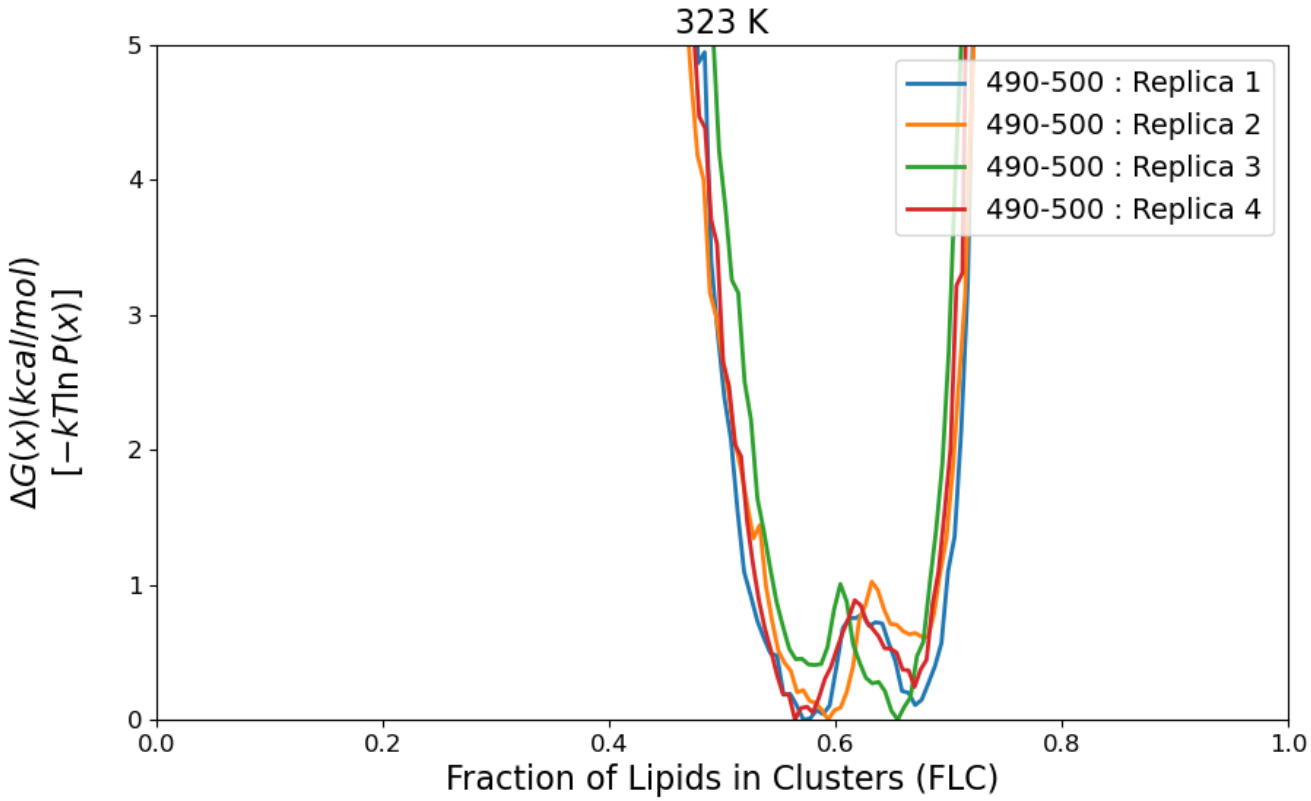

Figure 44: Free Energy Landscape of **DIPC** system for different replica at 323K. All the FES are calculated by averaging over the iteration window 490 - 500.

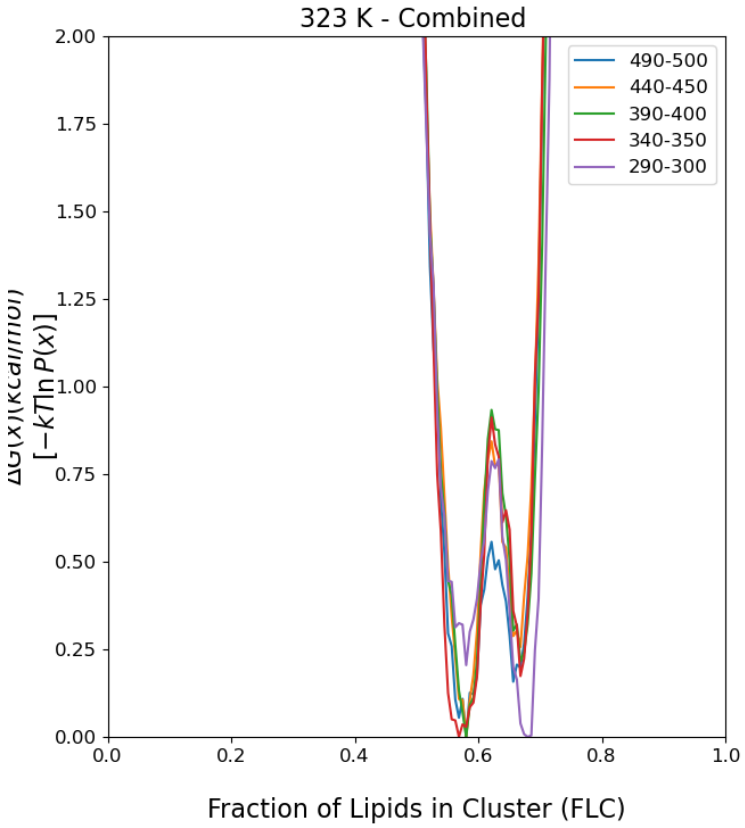

Figure 45: Convergence of Free Energy Landscape of **DIPC** system for combined replica at 323K. All the FES are calculated by averaging over the iteration window 490 - 500.

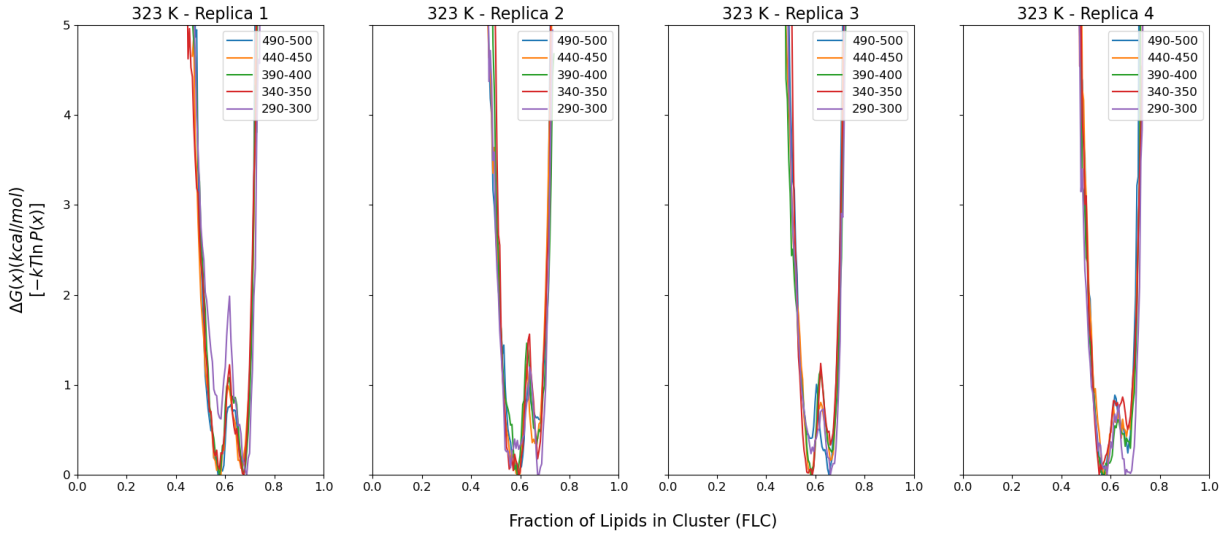

Figure 46: Convergence of Free Energy Landscape of **DIPC** system for different replica at 323K. All the FES are calculated by averaging over the iteration window 490 - 500.

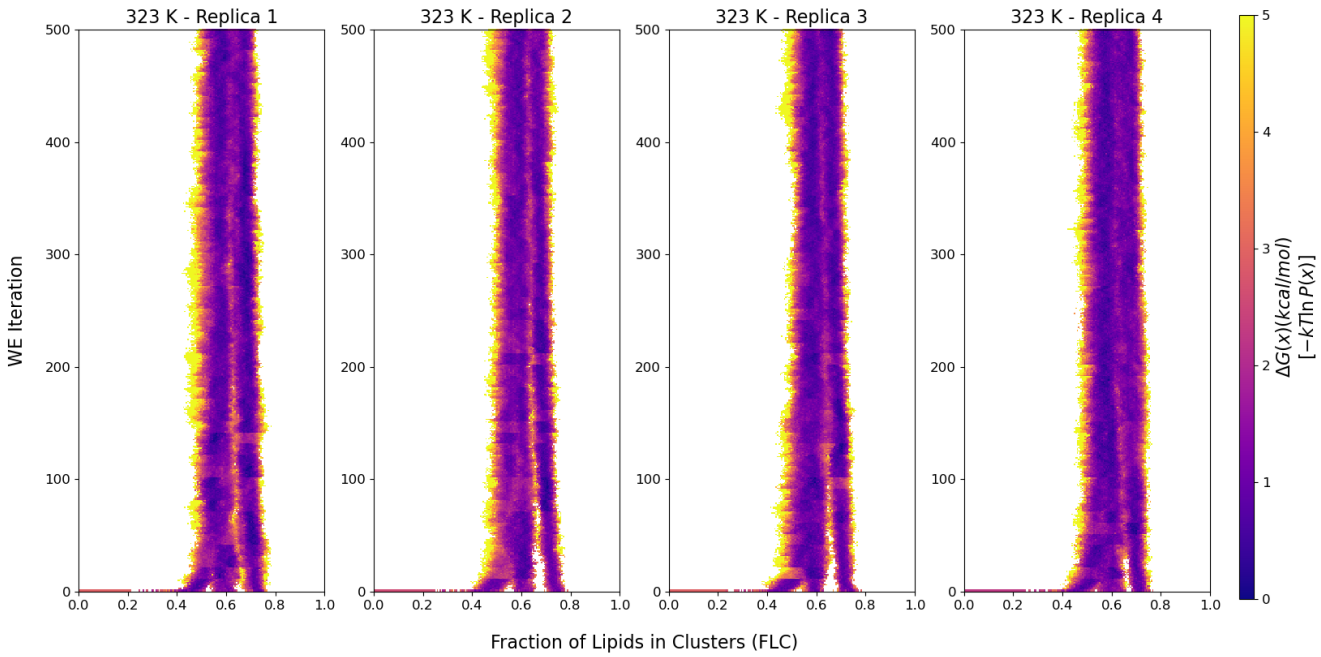

Figure 47: Evolution of Free Energy Landscape of **DIPC** system for different replica at 323K.

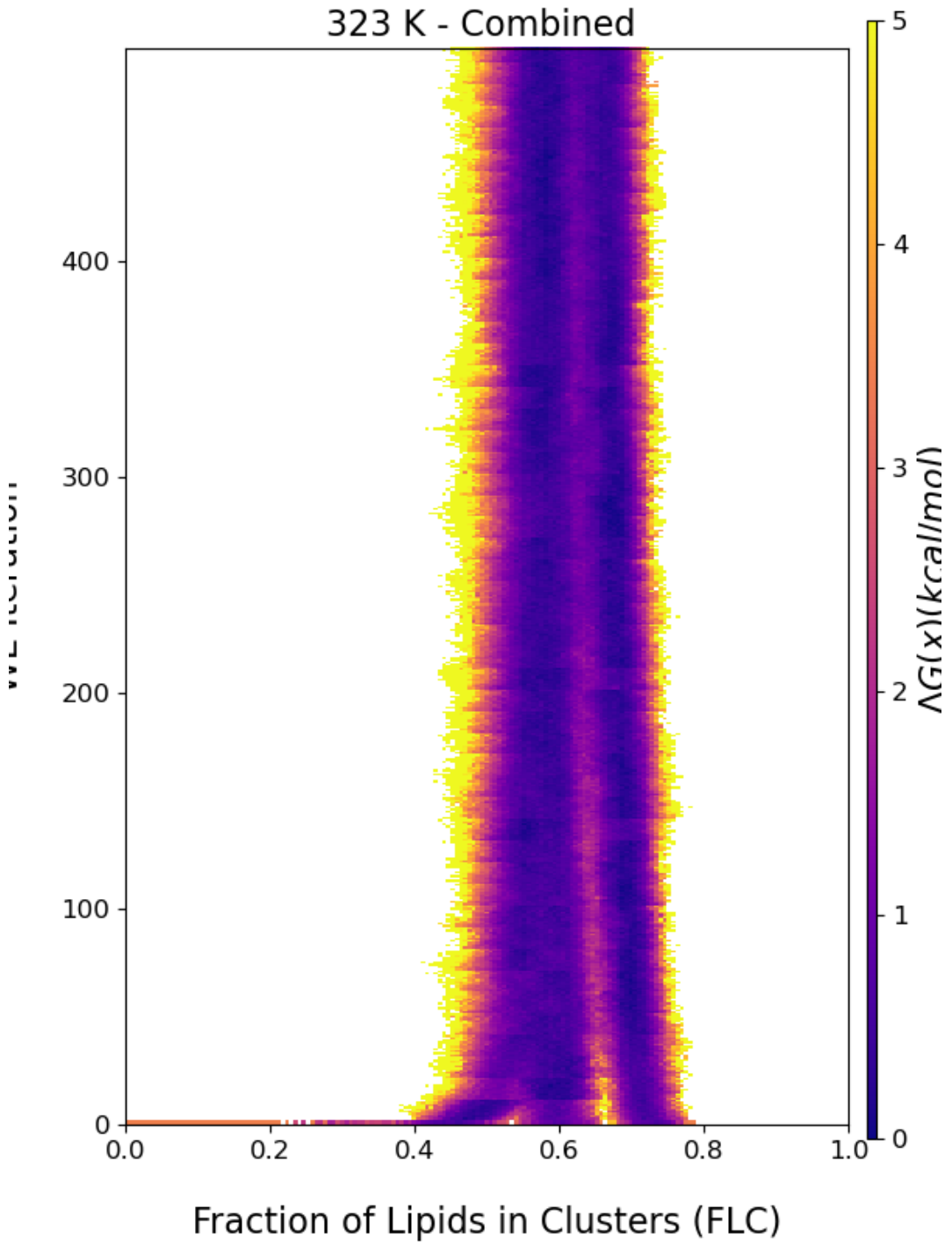

Figure 48: Evolution of Free Energy Landscape of **DIPC** system for combined replica at 323K using w_multi_tool.

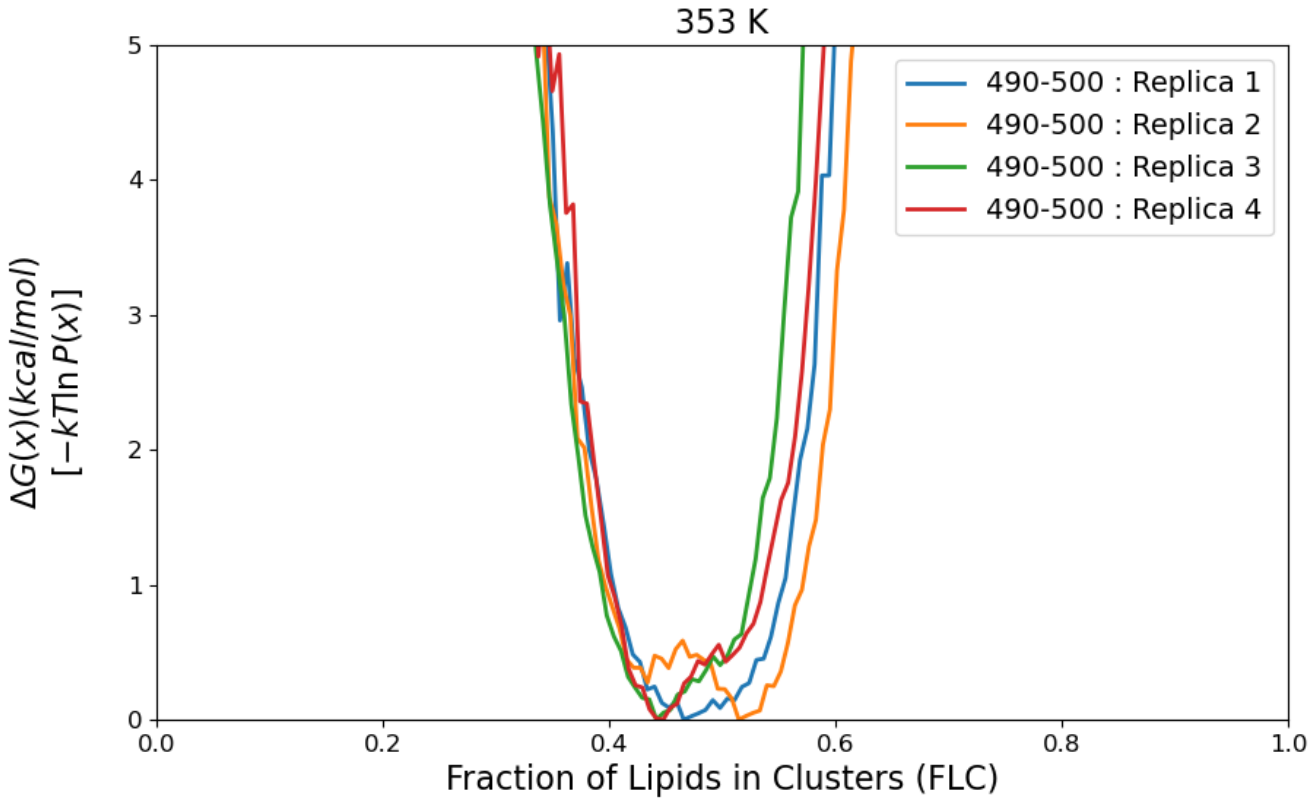

Figure 49: Free Energy Landscape of **DIPC** system for different replica at 353K. All the FES are calculated by averaging over the iteration window 490 - 500.

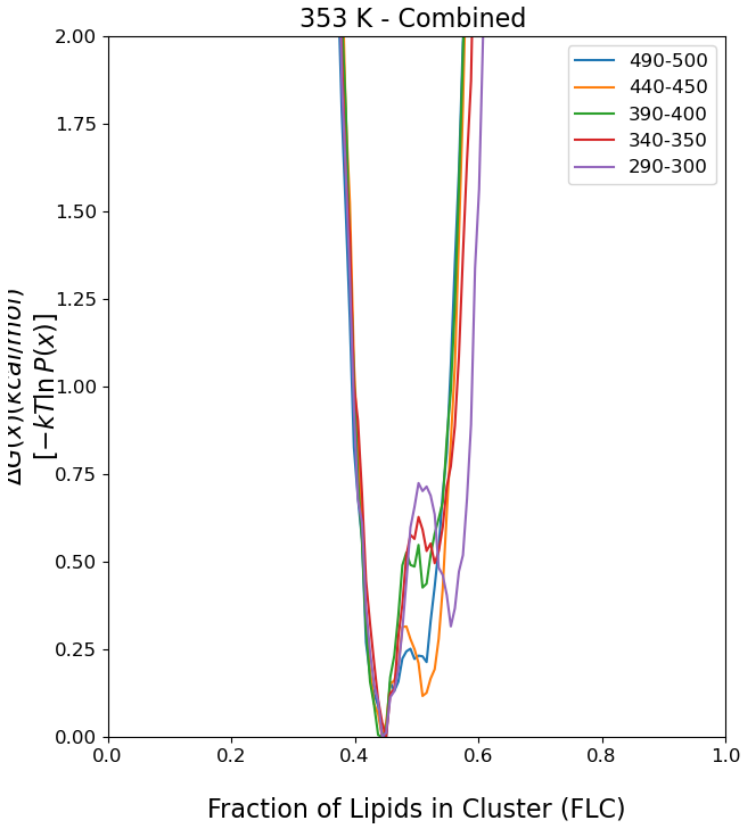

Figure 50: Convergence of Free Energy Landscape of **DIPC** system for combined replica at 353K. All the FES are calculated by averaging over the iteration window 490 - 500.

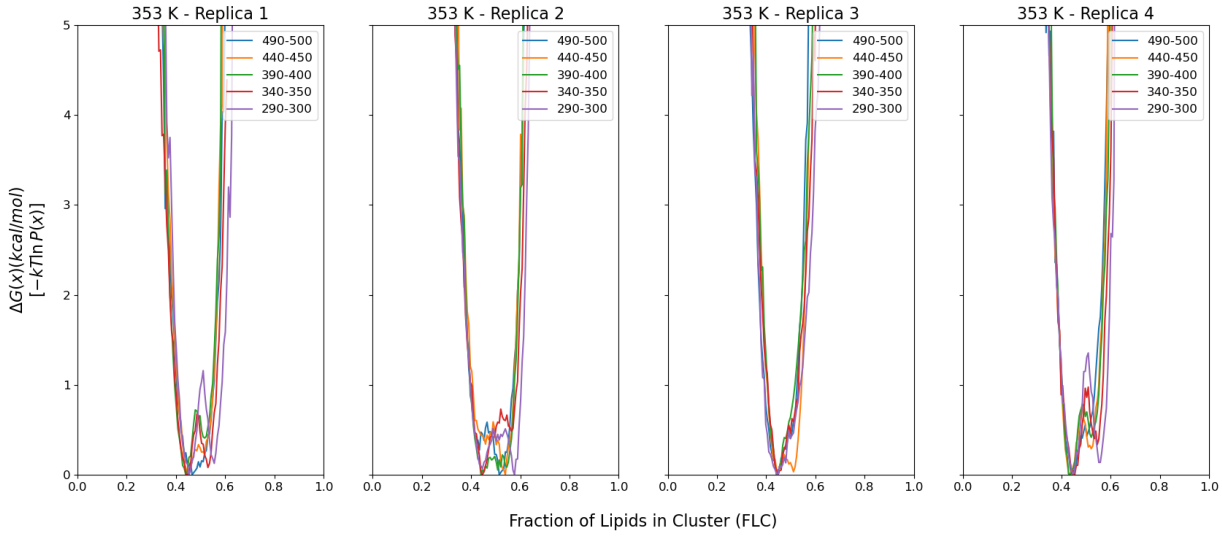

Figure 51: Convergence of Free Energy Landscape of **DIPC** system for different replica at 353K. All the FES are calculated by averaging over the iteration window 490 - 500.

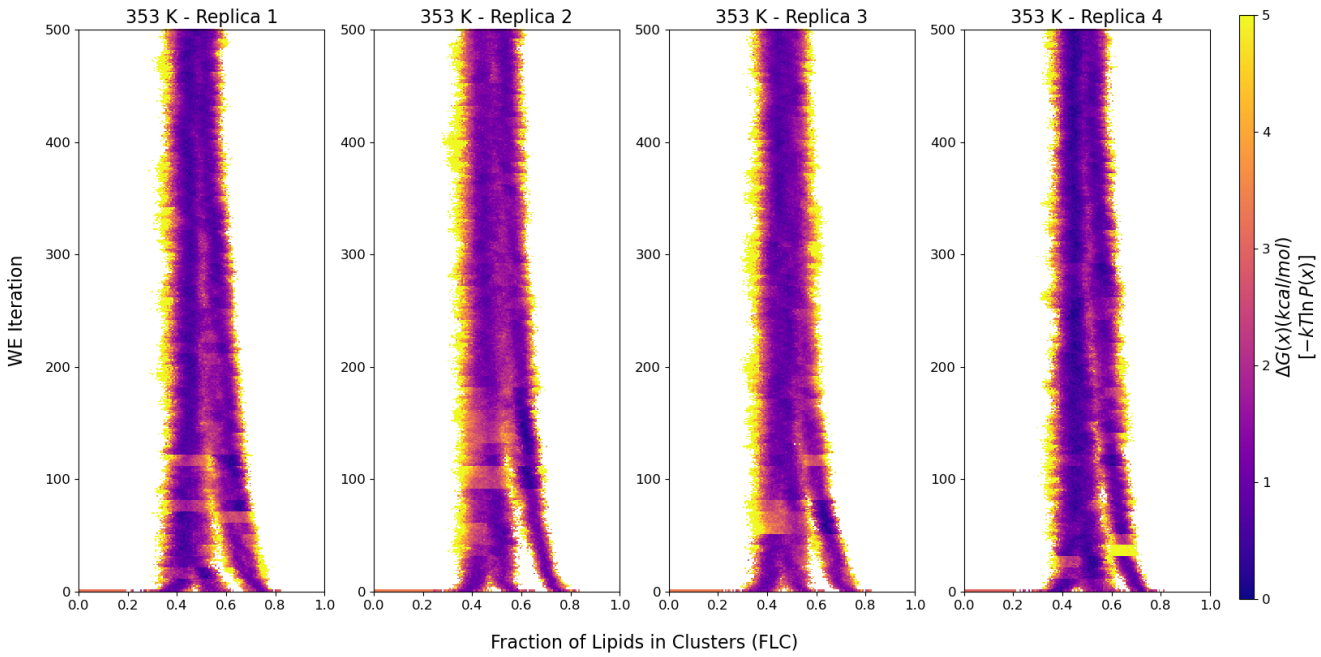

Figure 52: Evolution of Free Energy Landscape of **DIPC** system for different replica at 353K.

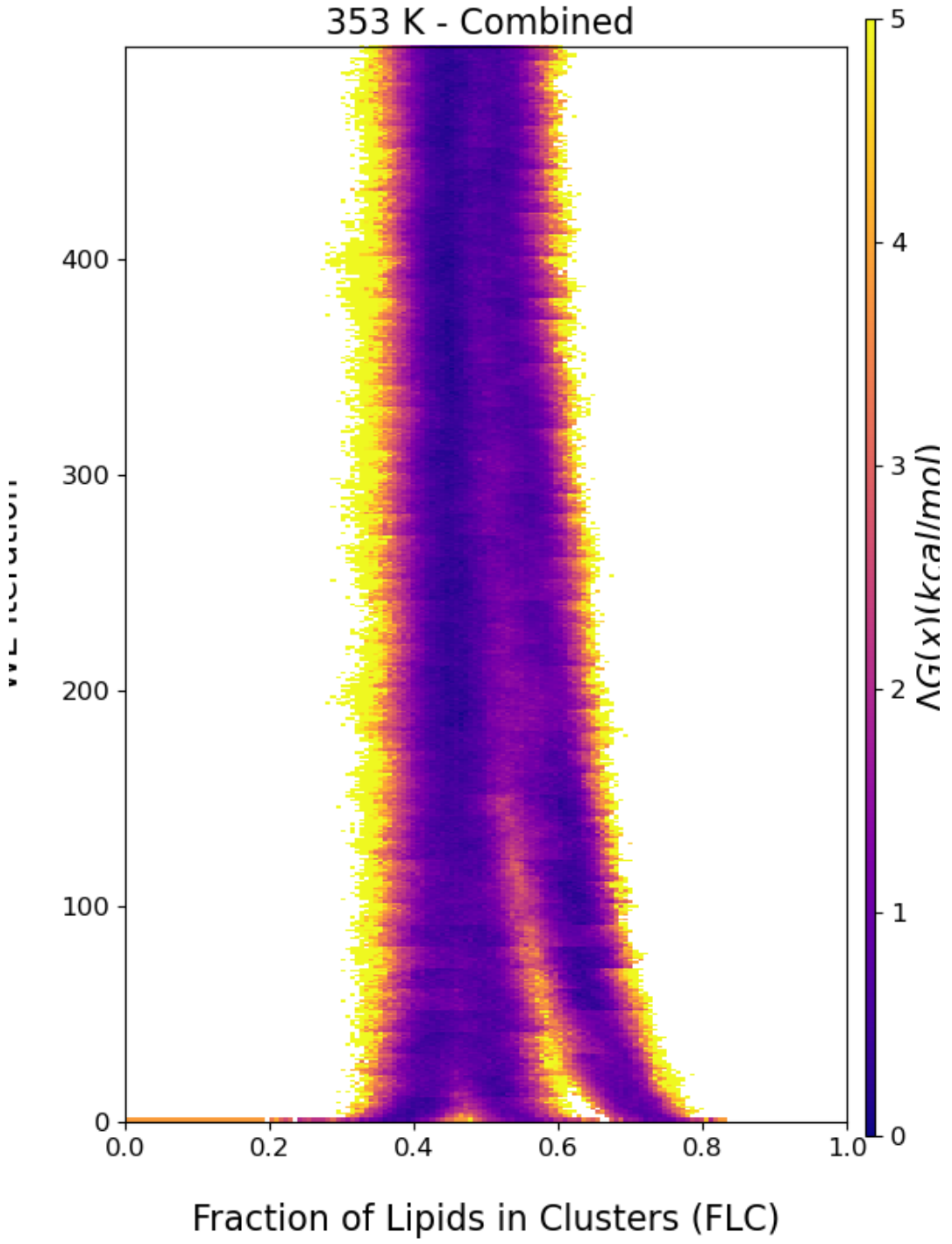

Figure 53: Evolution of Free Energy Landscape of **DIPC** system for combined replica at 353K using w_multi_tool.

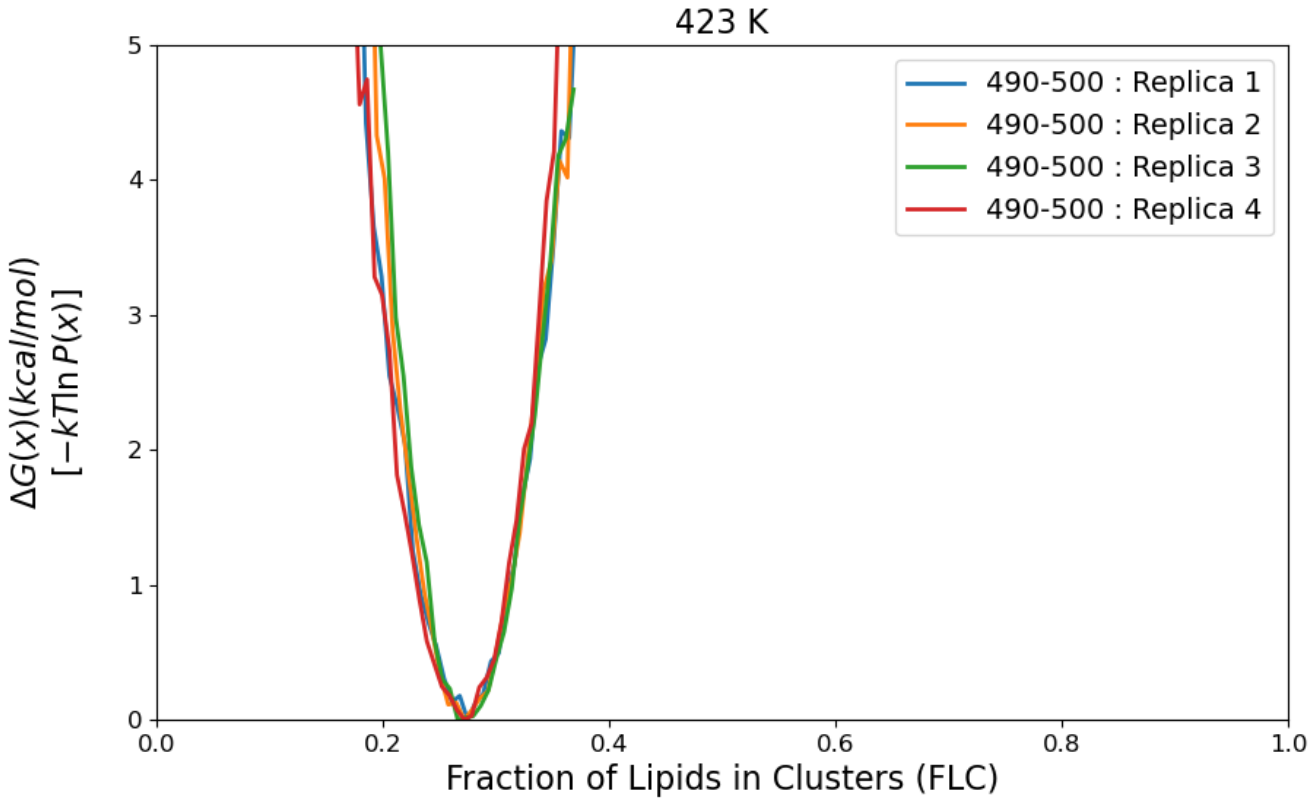

Figure 54: Free Energy Landscape of **DIPC** system for different replica at 423K. All the FES are calculated by averaging over the iteration window 490 - 500.

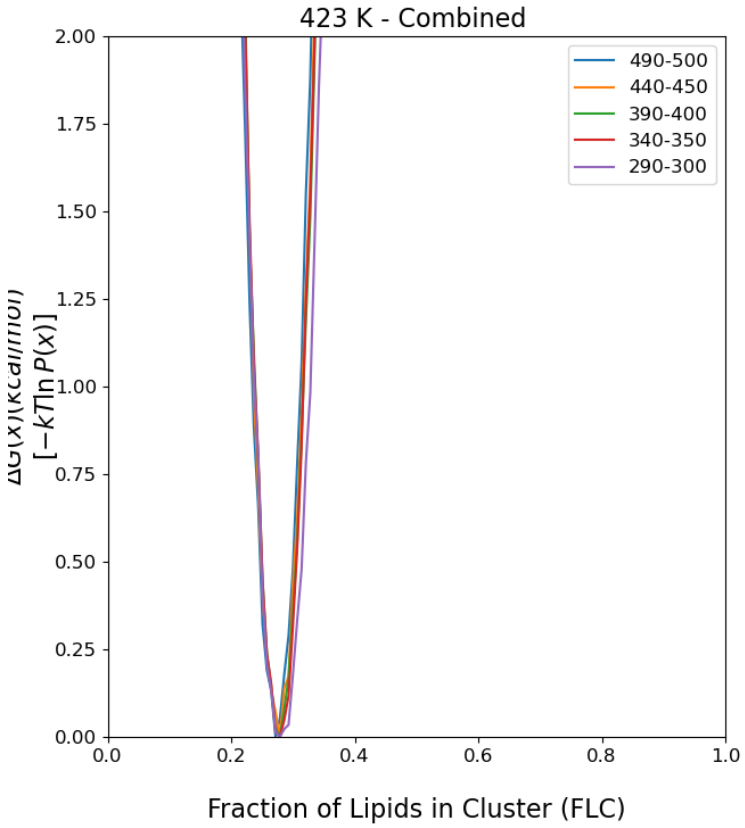

Figure 55: Convergence of Free Energy Landscape of **DIPC** system for combined replica at 423K. All the FES are calculated by averaging over the iteration window 490 - 500.

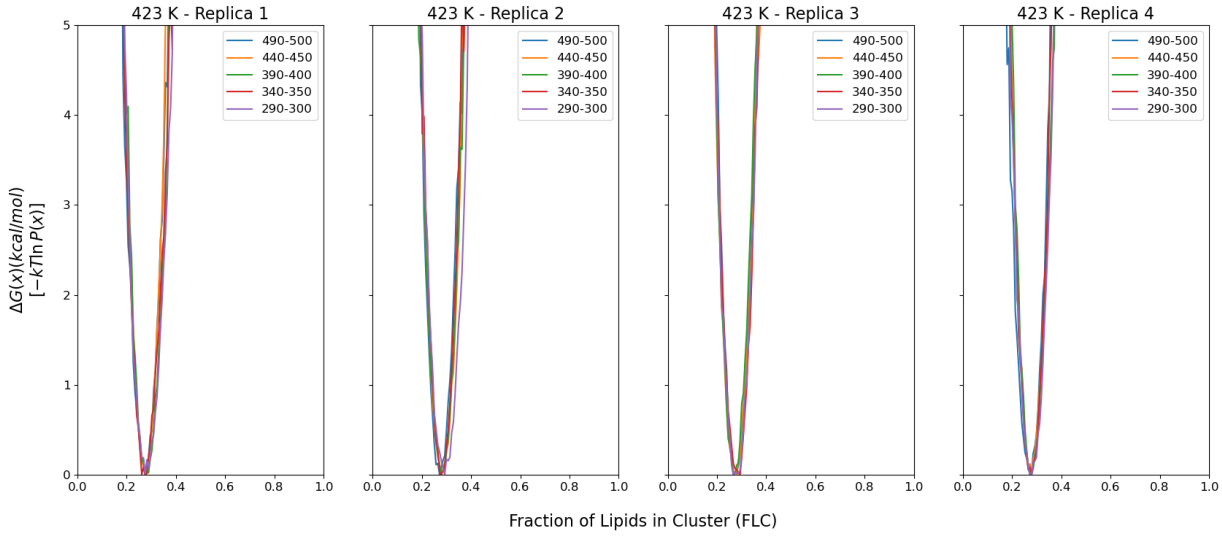

Figure 56: Convergence of Free Energy Landscape of **DIPC** system for different replica at 423K. All the FES are calculated by averaging over the iteration window 490 - 500.

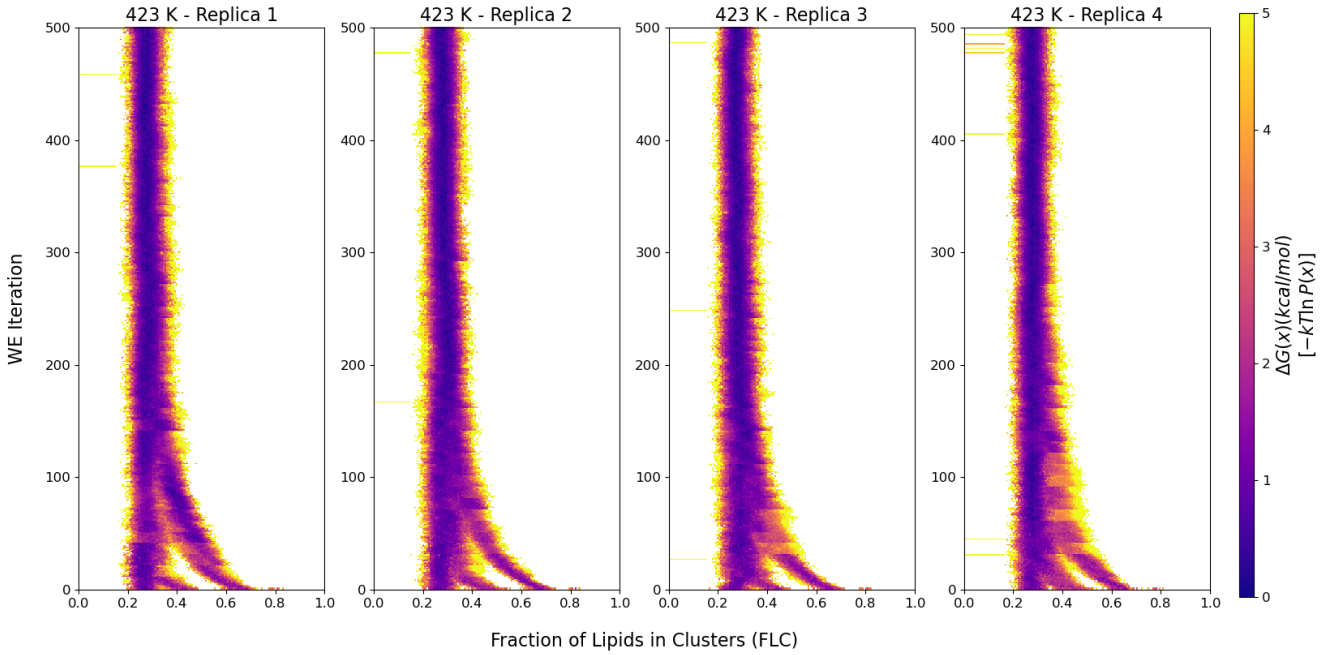

Figure 57: Evolution of Free Energy Landscape of **DIPC** system for different replica at 423K.

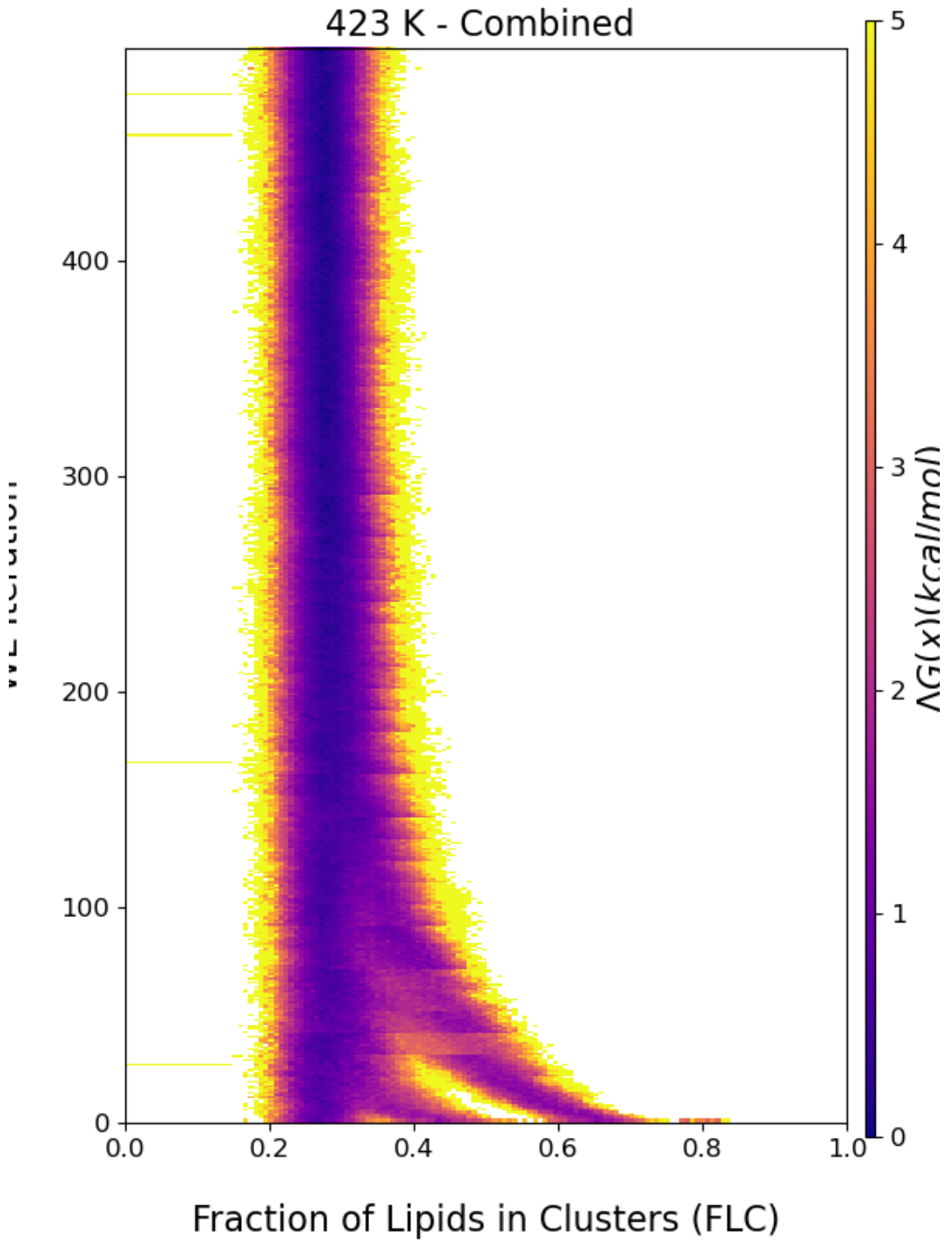

Figure 58: Evolution of Free Energy Landscape of **DIPC** system for combined replica at 423K using w_multi_tool.

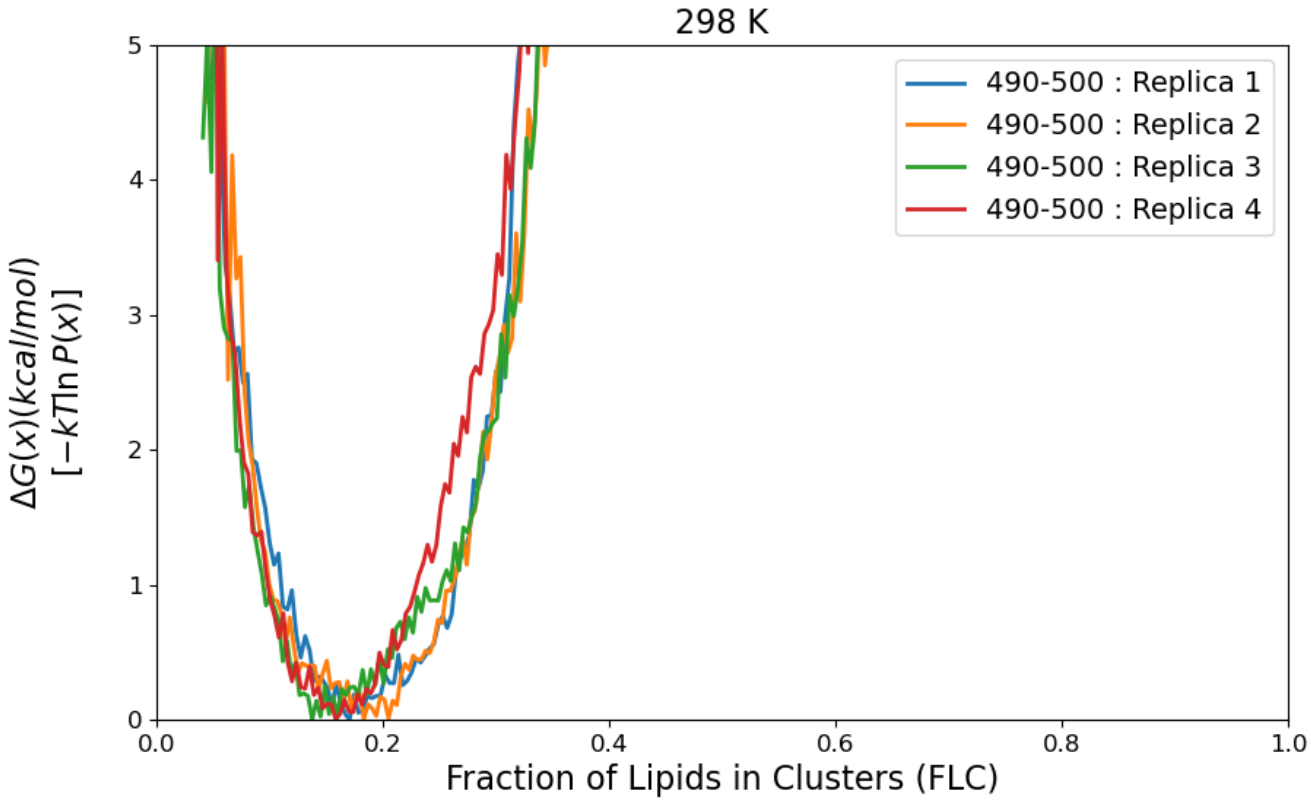

Figure 59: Free Energy Landscape of **POPC** system for different replica at 298K. All the FES are calculated by averaging over the iteration window 490 - 500.

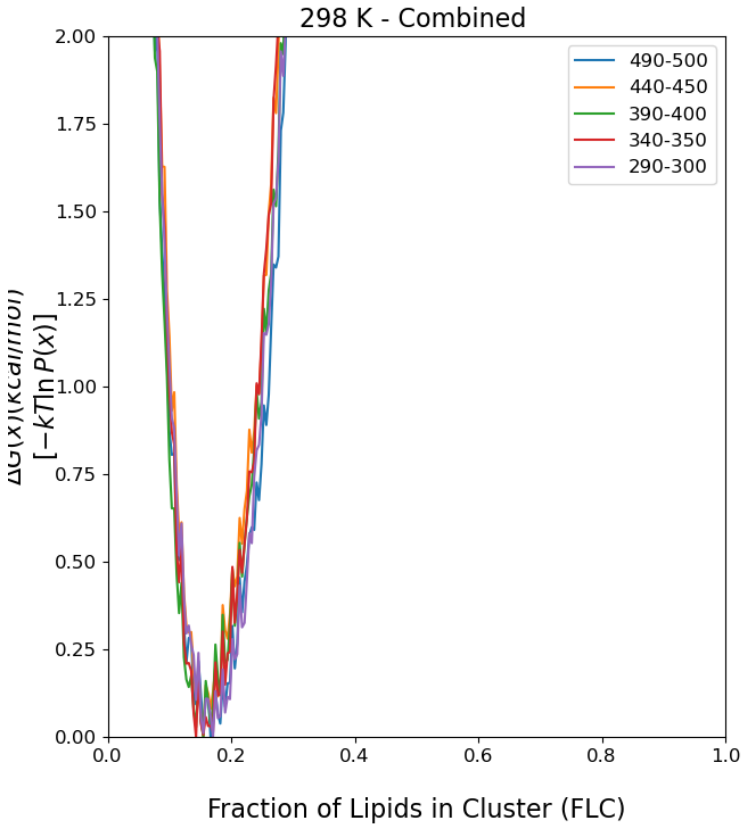

Figure 60: Convergence of Free Energy Landscape of **POPC** system for combined replica at 298K. All the FES are calculated by averaging over the iteration window 490 - 500.

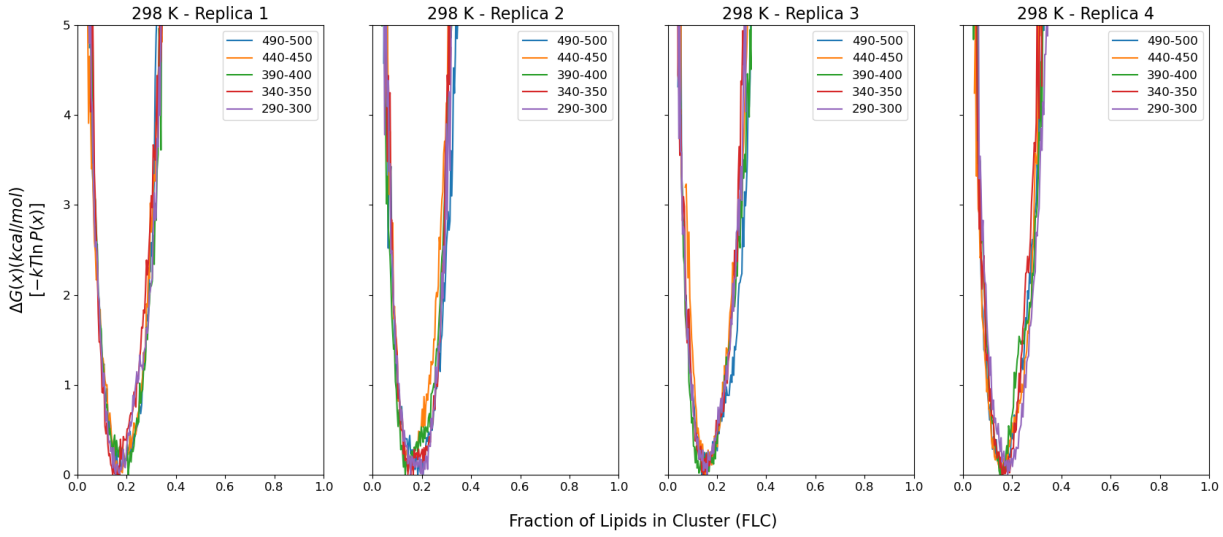

Figure 61: Convergence of Free Energy Landscape of **POPC** system for different replica at 298K. All the FES are calculated by averaging over the iteration window 490 - 500.

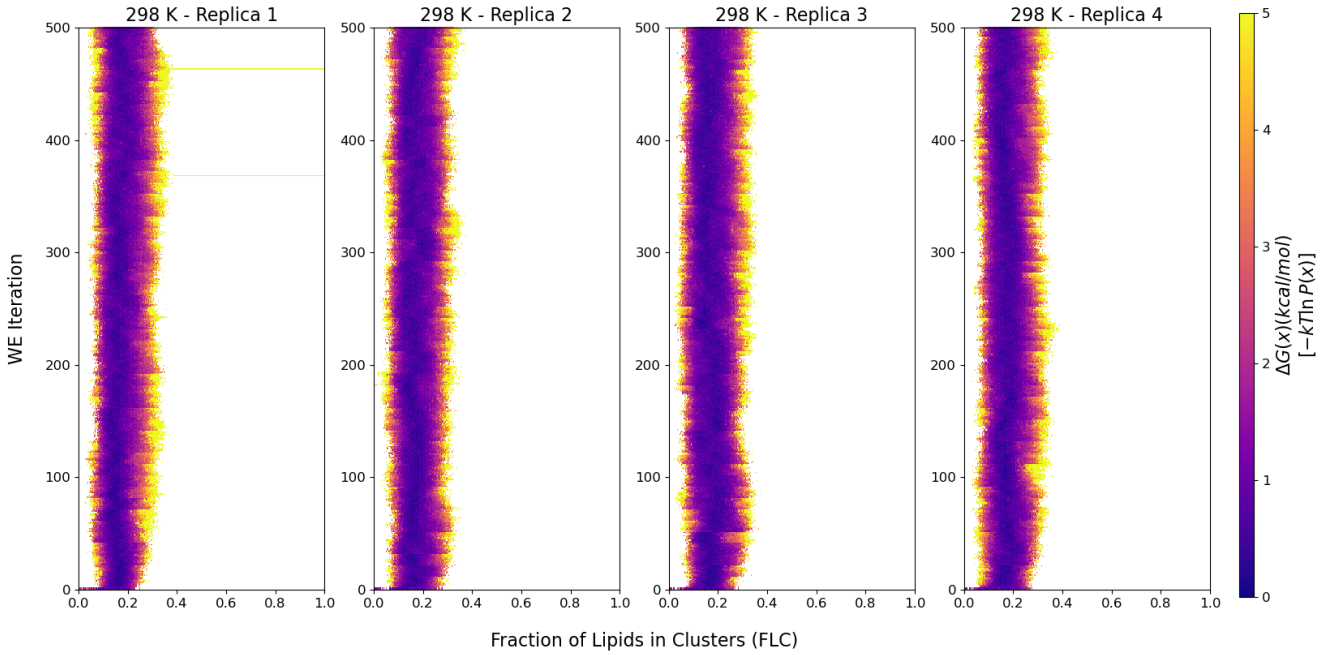

Figure 62: Evolution of Free Energy Landscape of **POPC** system for different replica at 298K.

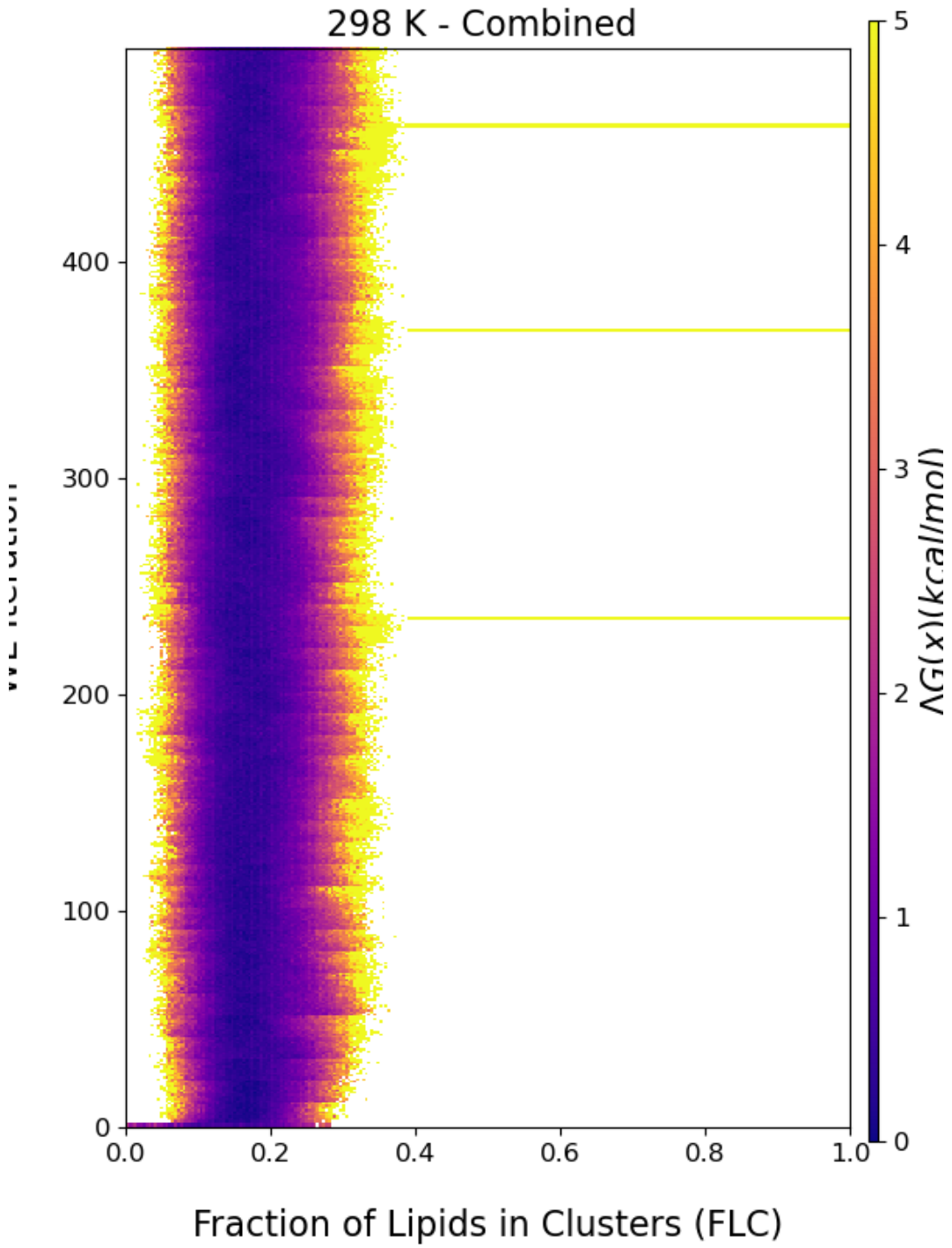

Figure 63: Evolution of Free Energy Landscape of **POPC** system for combined replica at 298K using w_multi_tool.

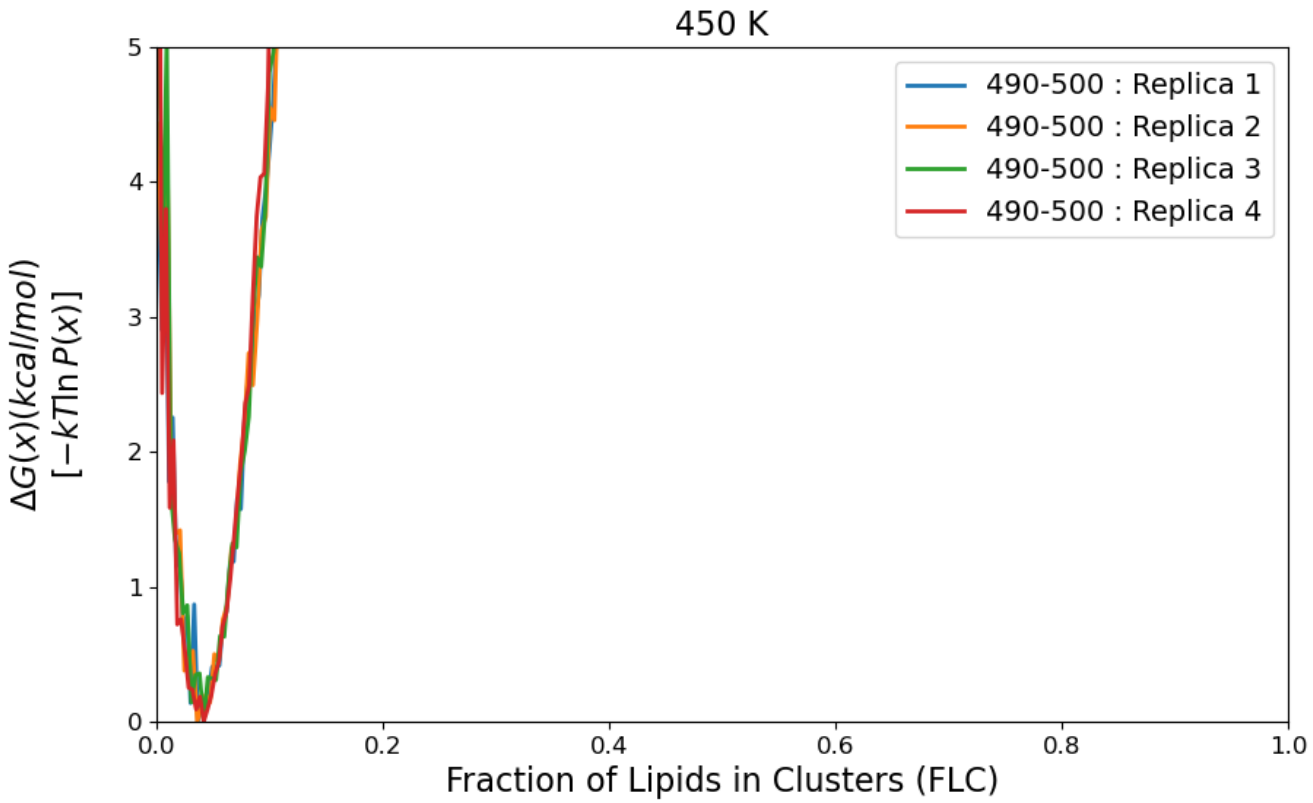

Figure 64: Free Energy Landscape of **POPC** system for different replica at 450K. All the FES are calculated by averaging over the iteration window 490 - 500.

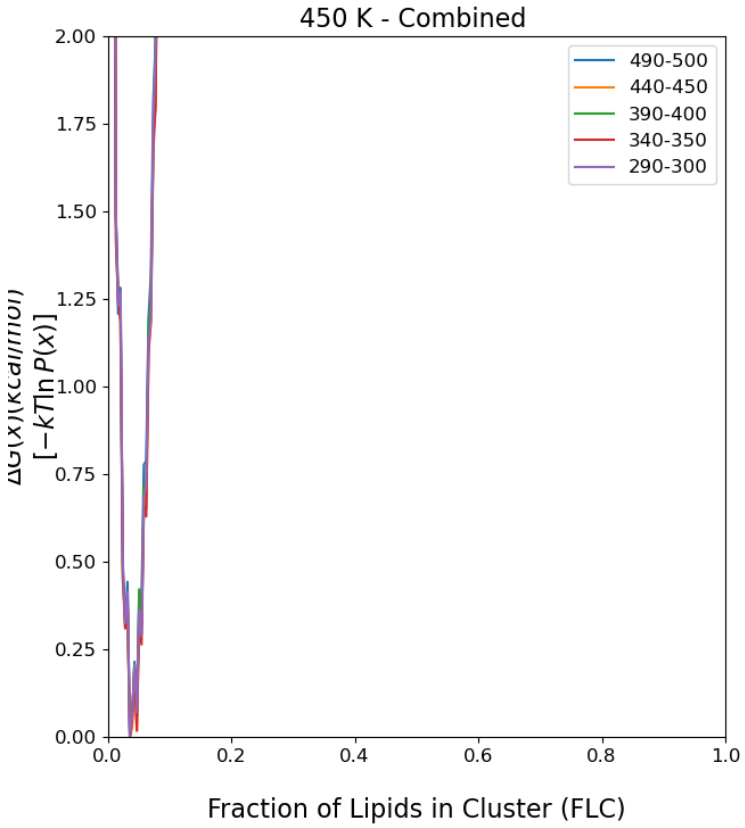

Figure 65: Convergence of Free Energy Landscape of **POPC** system for combined replica at 450K. All the FES are calculated by averaging over the iteration window 490 - 500.

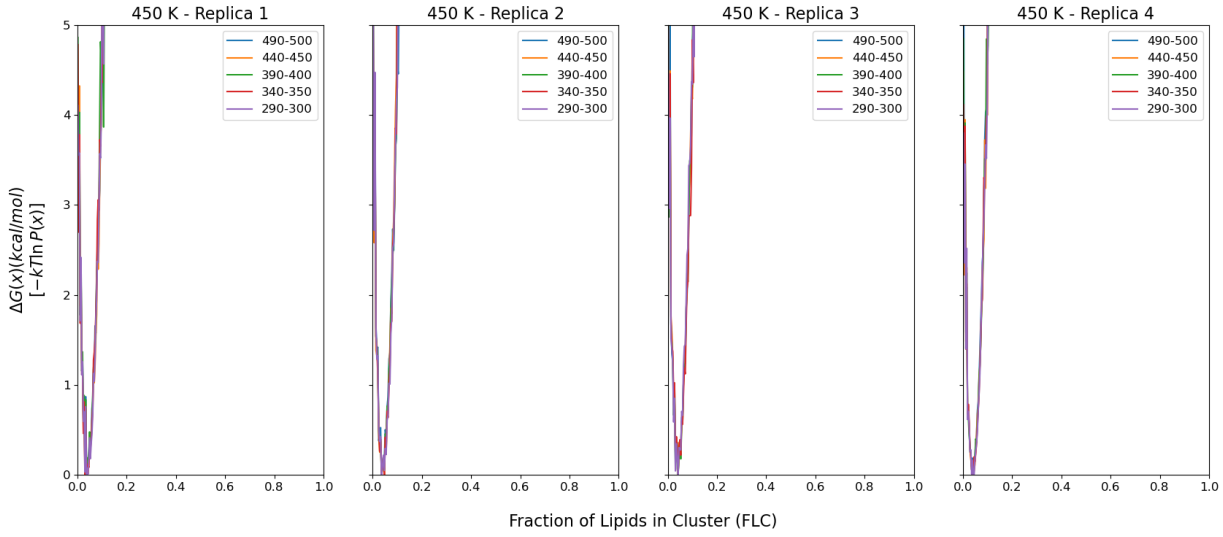

Figure 66: Convergence of Free Energy Landscape of **POPC** system for different replica at 450K. All the FES are calculated by averaging over the iteration window 490 - 500.

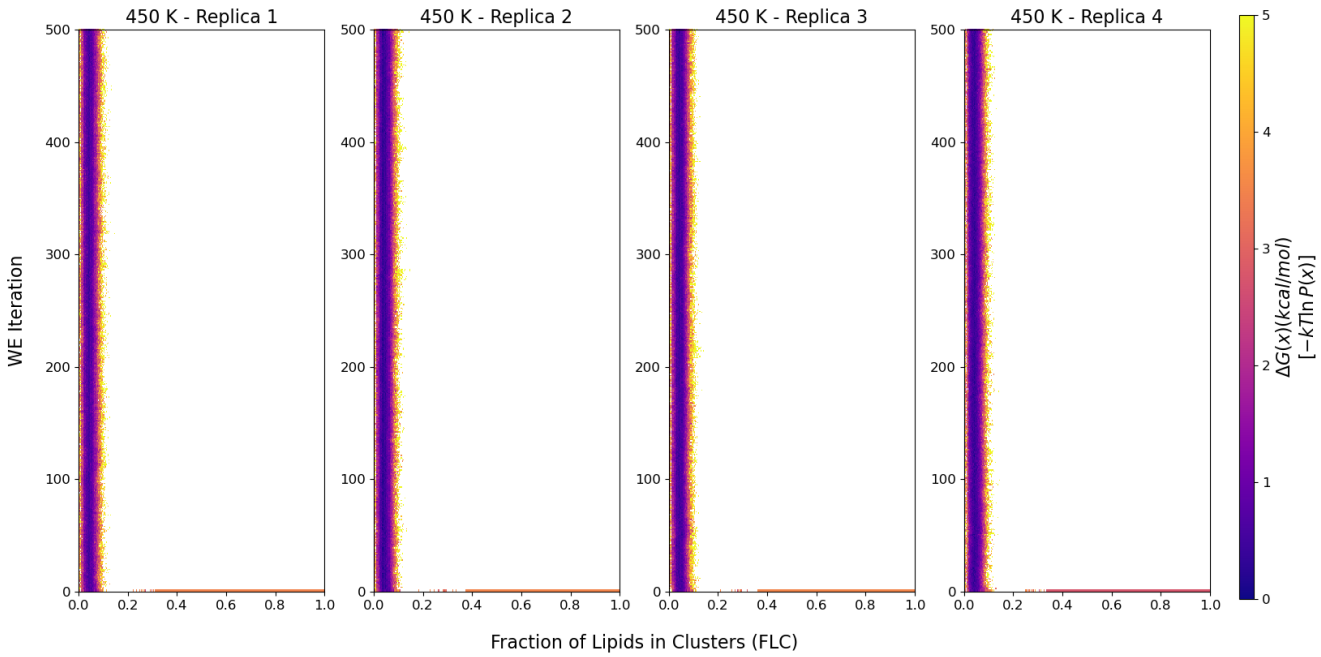

Figure 67: Evolution of Free Energy Landscape of **POPC** system for different replica at 450K.

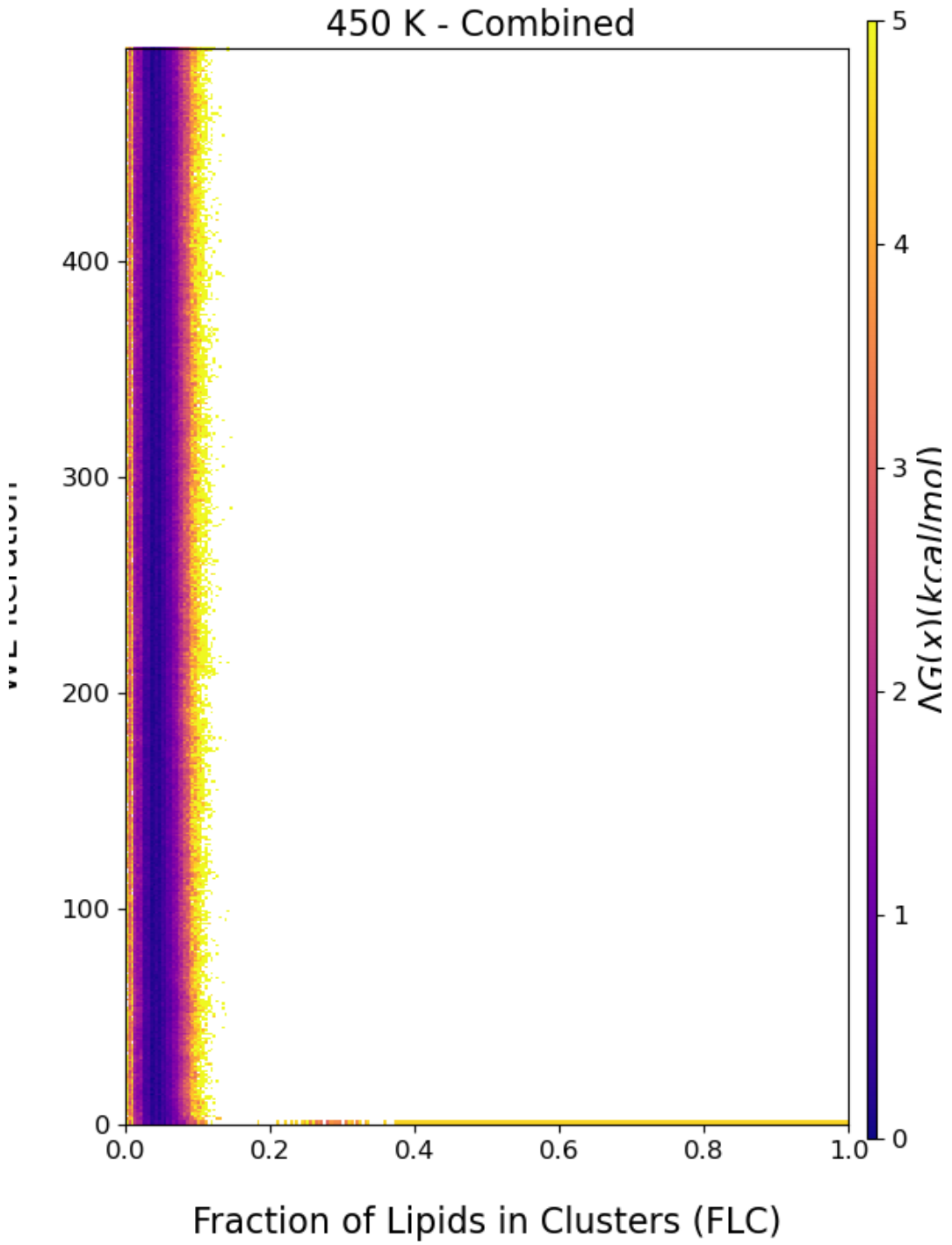

Figure 68: Evolution of Free Energy Landscape of **POPC** system for combined replica at 450K using w_multi_tool.