# Supporting Information

## Multi-Scale In-silico Analysis of Phase Separation Behavior of FUS Mutants

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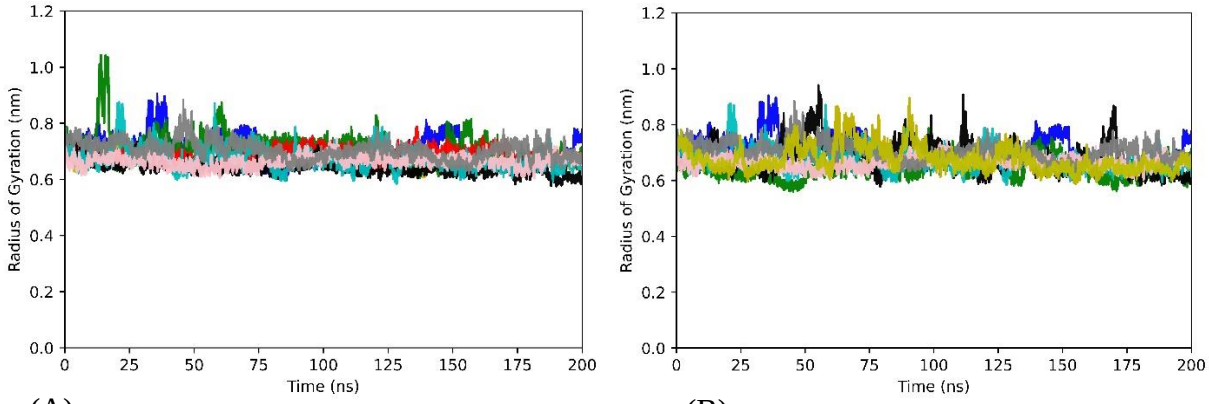
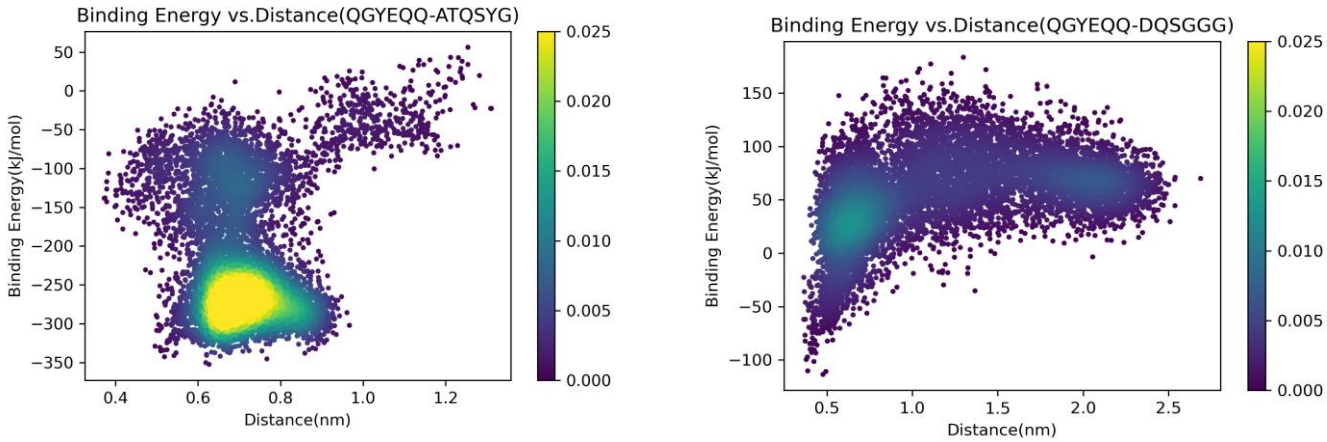
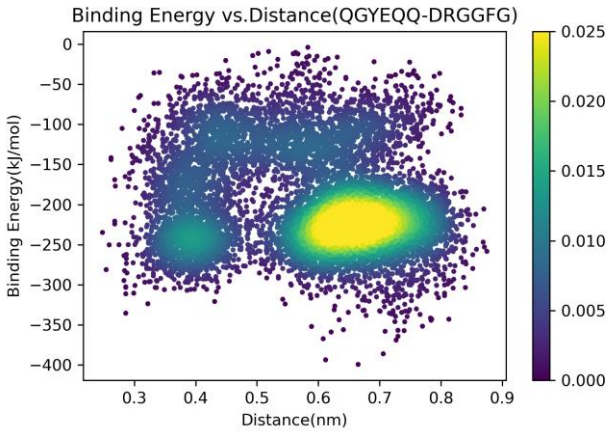


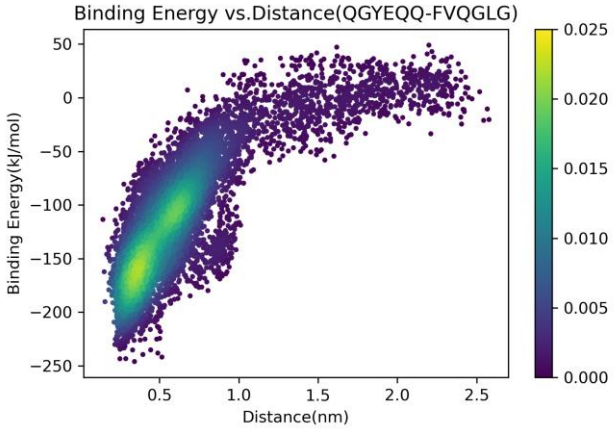

(A) (B)

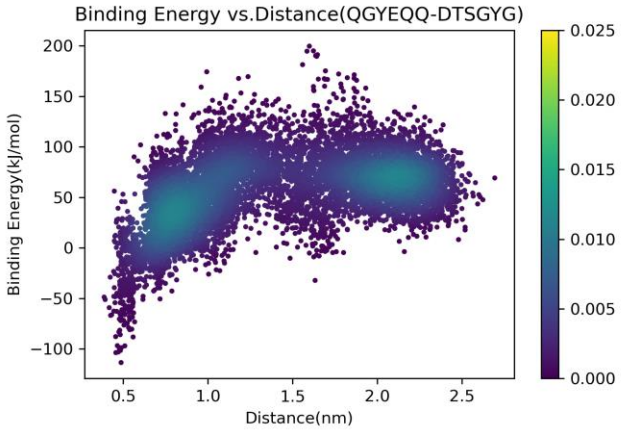
**Figure S1**: Convergence analysis of FUS mutant sticker complexes using the satbilty the radius of gyration of each sticker with relevant mutant sticker. (A) for G156E mutant complex with QGYEQQ (green: ATQSYG, red:SYSGYS, blue: DTSGYG, black: QNTGYG, yellow: STGGYG, purple: SSSGGG, light blue: DQSGGG,gray: GSGGYG, orange:GRGGSG, light yellow:RGGGRG, light green:GRGGMG, dark green:FVQGYG, dark red: GRGGRG, teal:RRGGRG, violet:GYRGRG, pink:DRGGFG)and (B) for R244C mutant complex with CGGGRG(green: ATQSYG, red:SYSGYS, blue: DTSGYG, black: QNTGYG, yellow: STGGYG, purple: SSSGGG, light blue: DQSGGG,gray: GSGGYG, orange:GRGGSG, light, light green:GRGGMG, dark green:FVQGYG,dark red:GRGGRG, teal:RRGGRG, violet:GYRGRG, pink:DRGGFG)

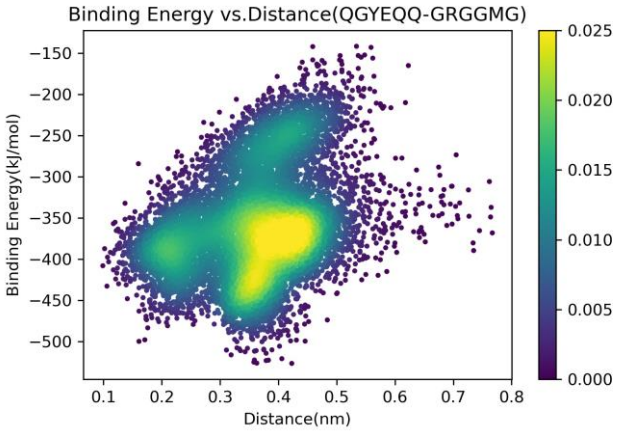
G156E mutation stickers




Binding Energy vs.Distance(QGYEQQ-DRGGFG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(QGYEQQ-FVQGLG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(QGYEQQ-DTSGYG)
Binding Energy(kJ/mol)
Distance(nm)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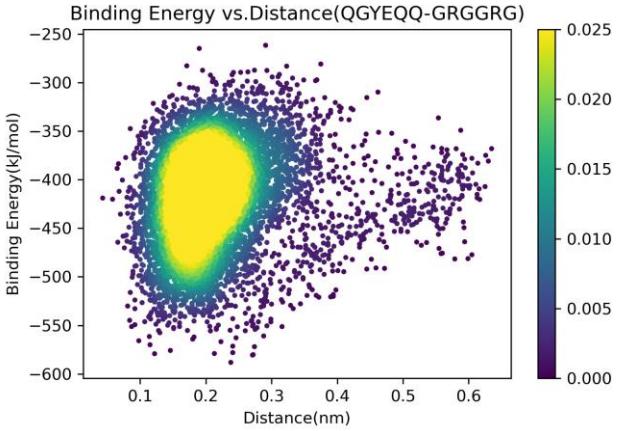
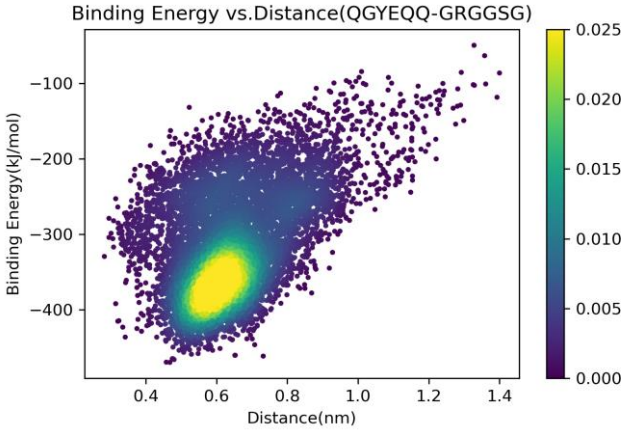
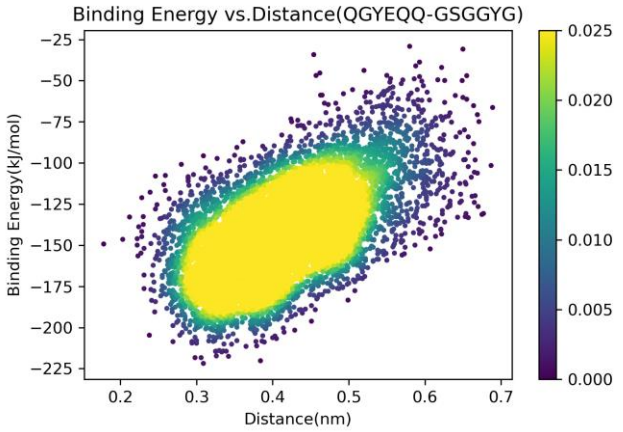
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(QGYEQQ-GRGGRG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(QGYEQQ-GRGGSG)
Binding Energy(kJ/mol)
Distance(nm)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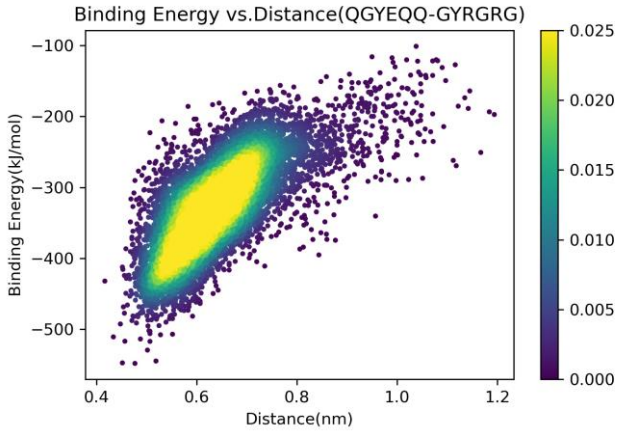
Binding Energy(kJ/mol)
Distance(nm)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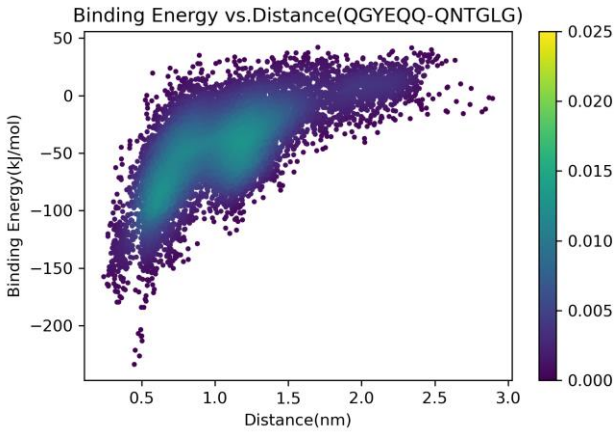
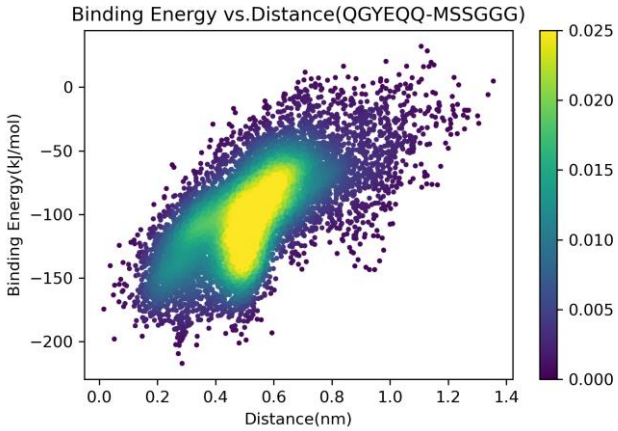
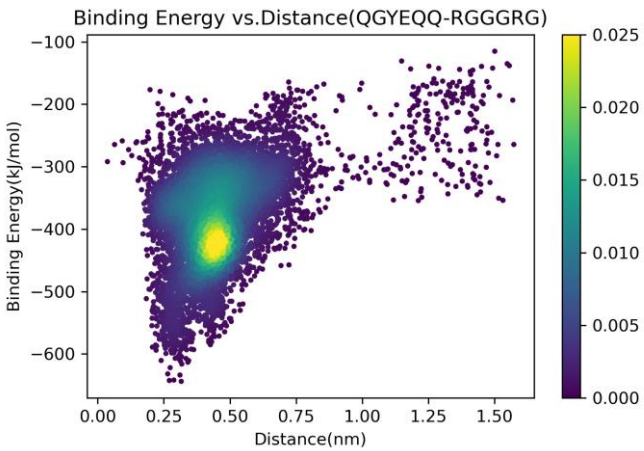
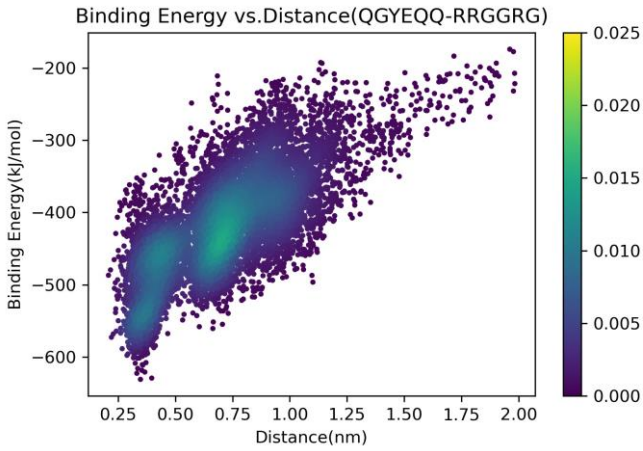
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(QGYEQQ-QNTGLG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(QGYEQQ-MSSGGG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(QGYEQQ-RGGGRG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(QGYEQQ-RRGGRG)
Binding Energy(kJ/mol)
Distance(nm)

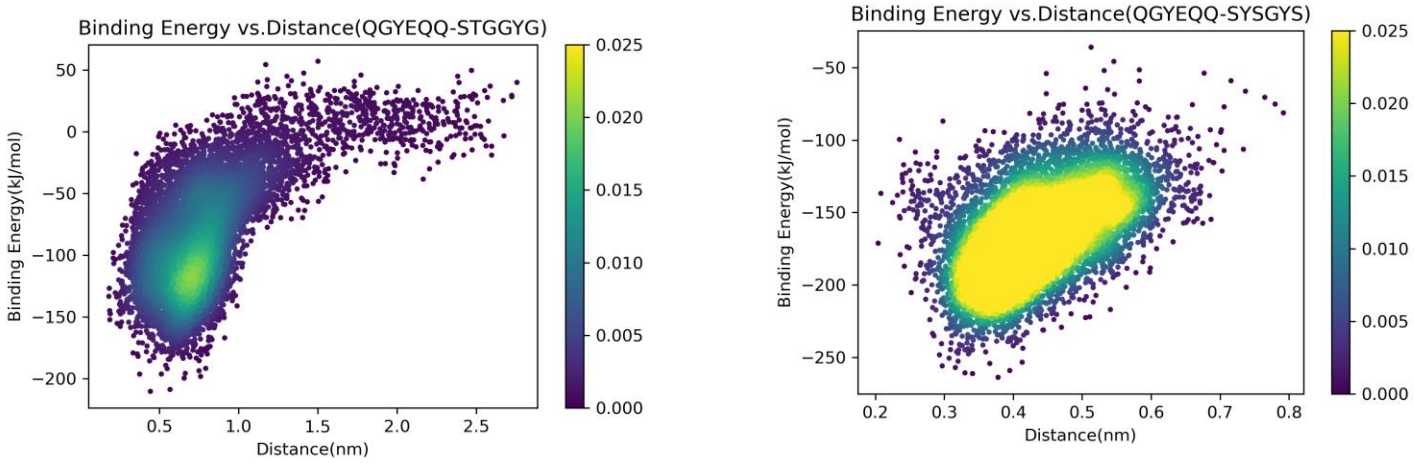
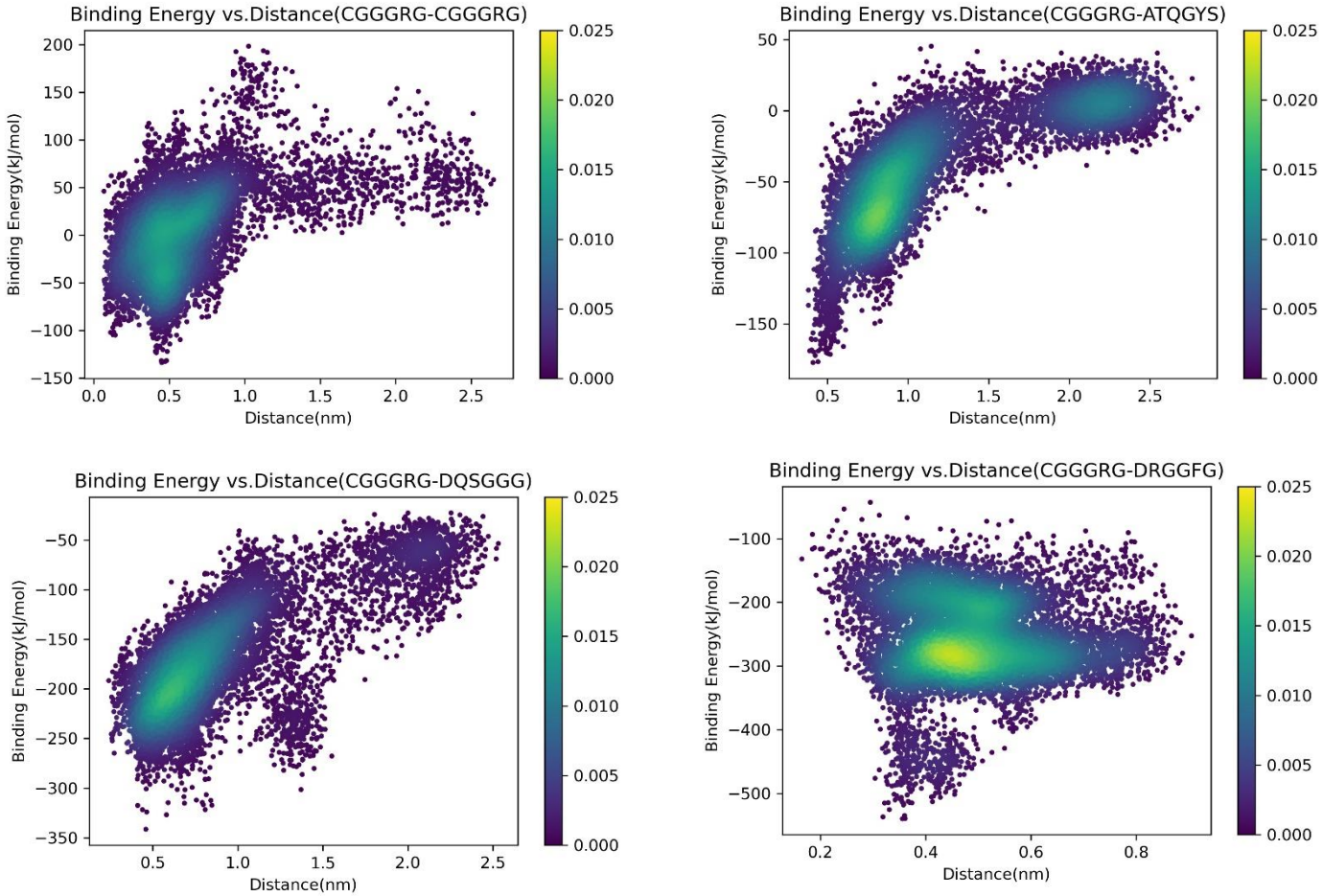
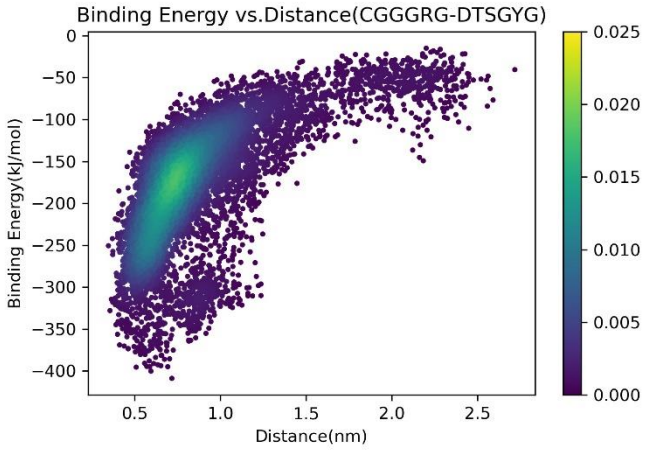
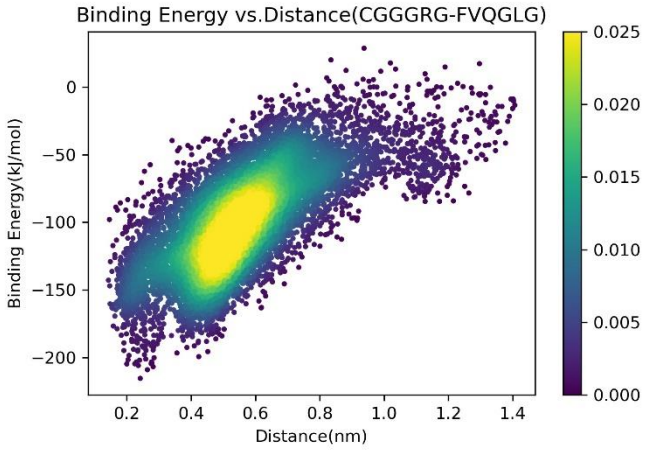
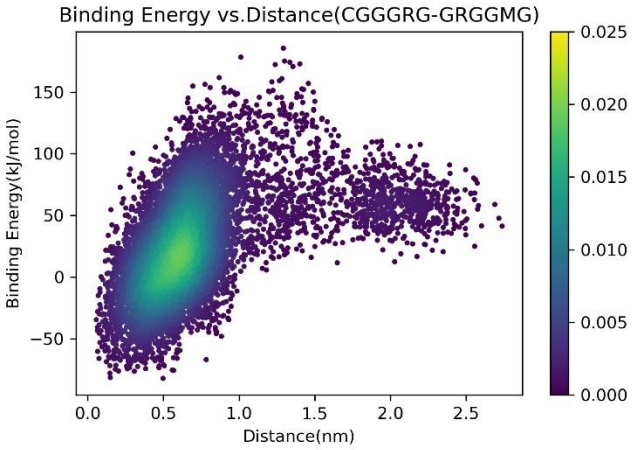


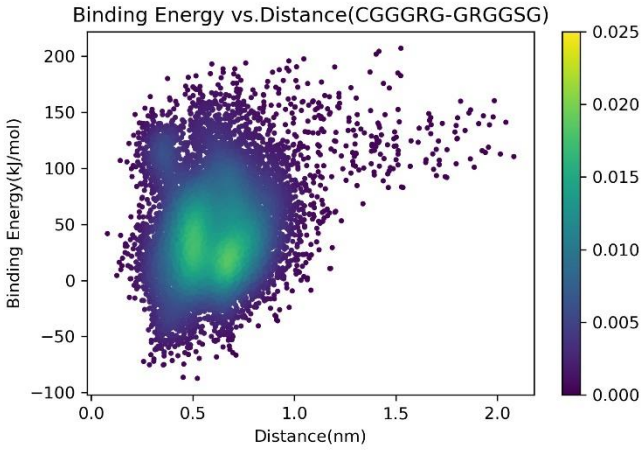

**Figure S2:** Homotypic binding energy distribution calculated by MMPBSA method using AA-MD simulation trajectories of 200 ns at 300K temperature of stickers (LARKS) extracted from LARKSdb as a function of centroid distance between a pair of hexapeptides for G156E mutation.

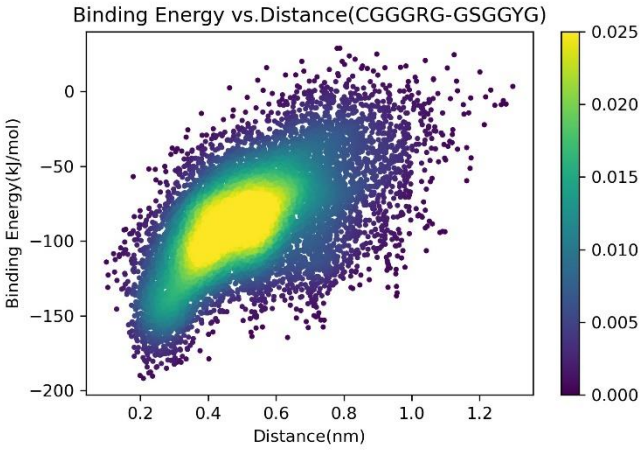


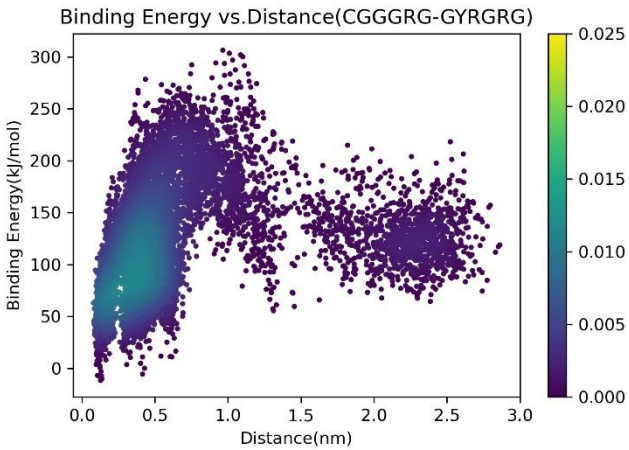

Binding Energy vs.Distance(CGGGRG-DTSGYG)
Binding Energy(kJ/mol)
Distance(nm)

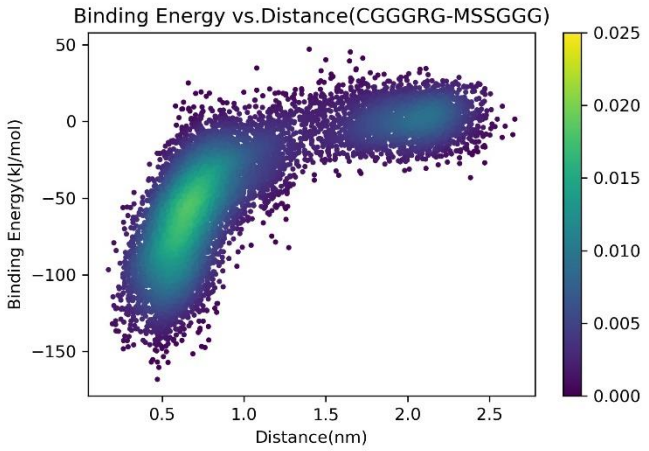

Binding Energy vs.Distance(CGGGRG-FVQGLG)
Binding Energy(kJ/mol)
Distance(nm)

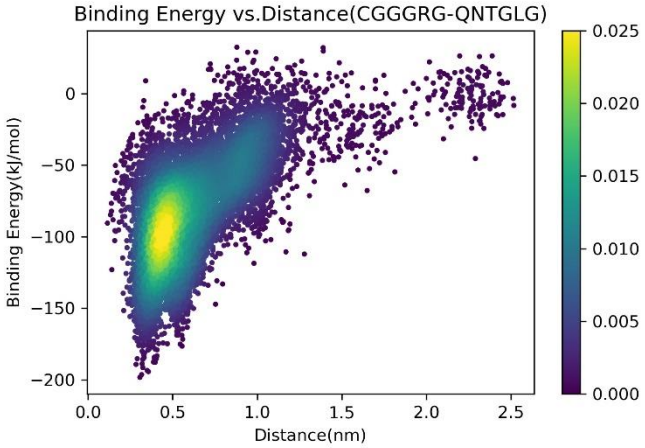

Binding Energy vs.Distance(CGGGRG-GRGGMG)
Binding Energy(kJ/mol)
Distance(nm)

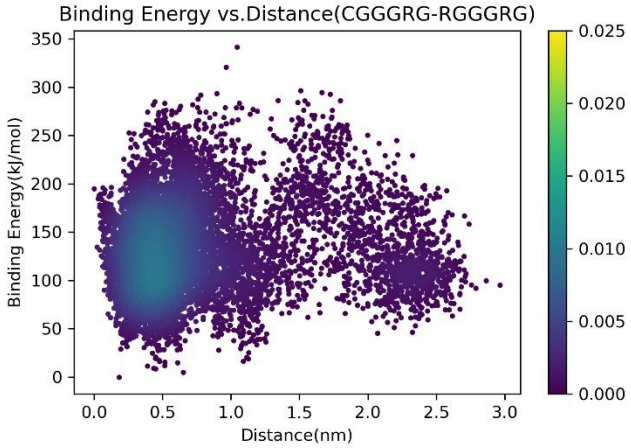

Binding Energy vs.Distance(CGGGRG-GRGGSG)
Binding Energy(kJ/mol)
Distance(nm)

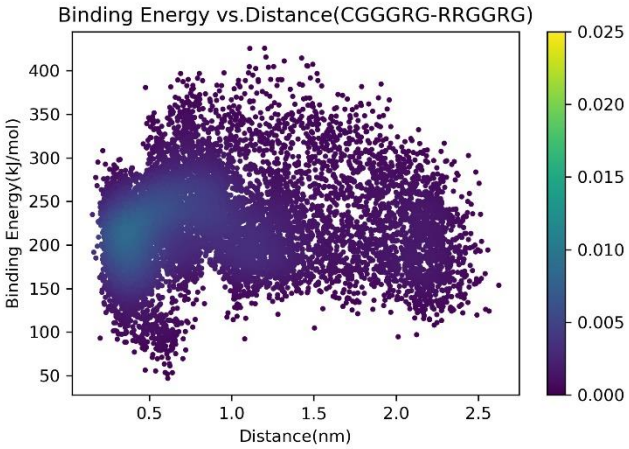

Binding Energy vs.Distance(CGGGRG-GSGGYG)
Binding Energy(kJ/mol)
Distance(nm)

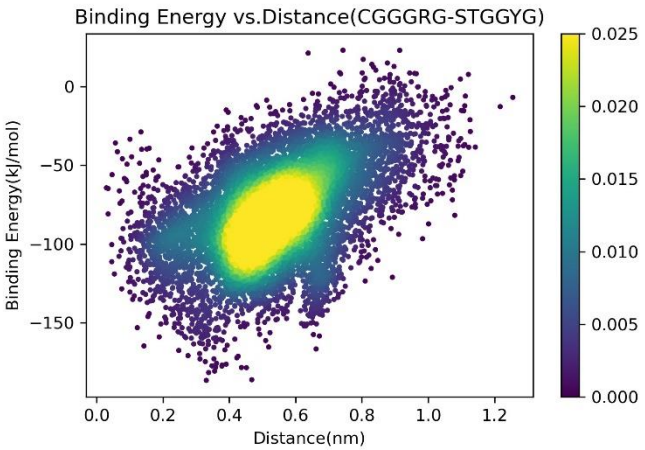

Binding Energy vs.Distance(CGGGRG-GYRGRG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(CGGGRG-MSSGGG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(CGGGRG-QNTGLG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(CGGGRG-RGGGRG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(CGGGRG-RRGGRG)
Binding Energy(kJ/mol)
Distance(nm)


Binding Energy vs.Distance(CGGGRG-STGGYG)
Binding Energy(kJ/mol)
Distance(nm)

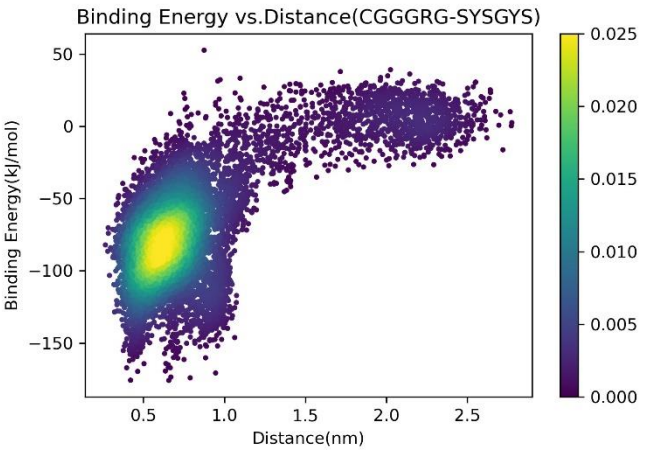
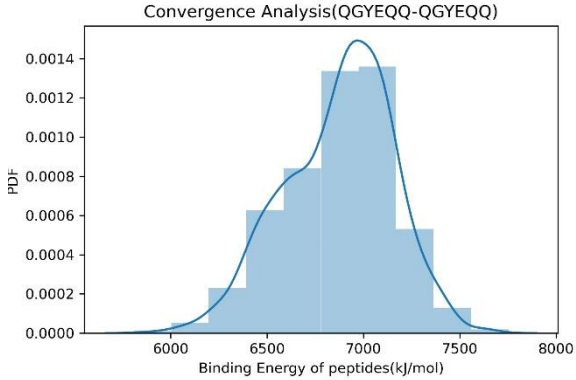
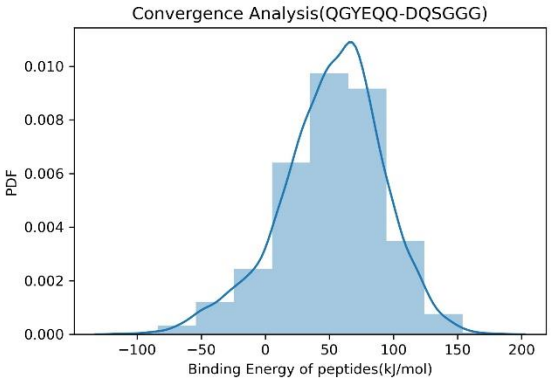
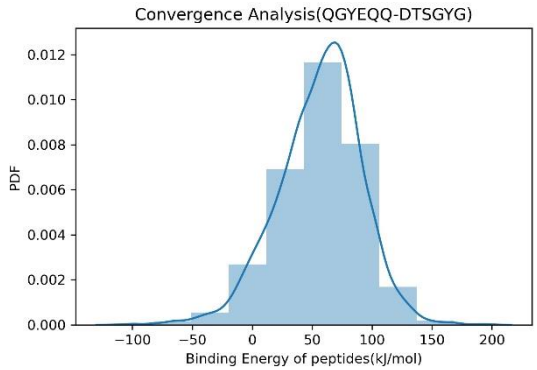
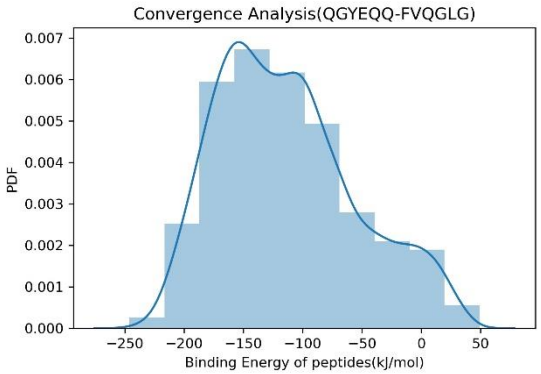

Binding Energy vs.Distance(CGGGRG-SYSGYS)
Binding Energy(kJ/mol)
Distance(nm)

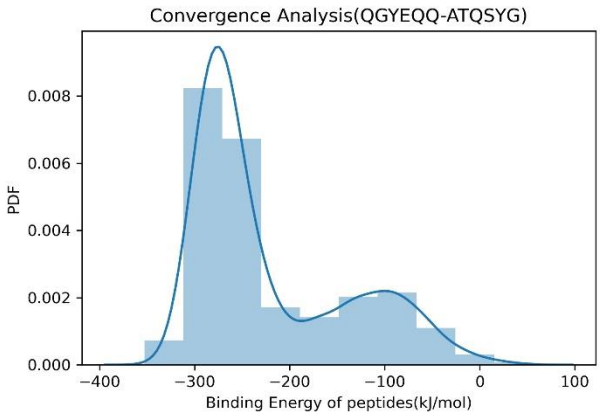
**Figure S3:** Homotypic binding energy distribution calculated by MMPBSA method using AA-MD simulation trajectories of 200 ns at 300K temperature of stickers (LARKS) extracted from LARKSdb as a function of centroid distance between a pair of hexapeptides for R244C mutation.

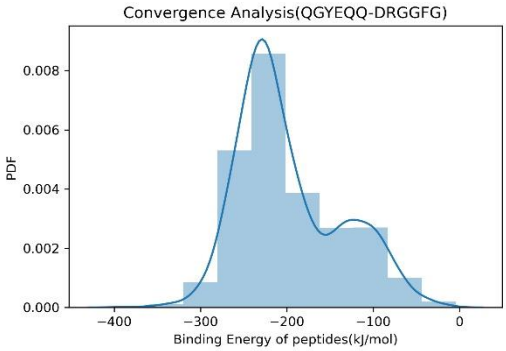


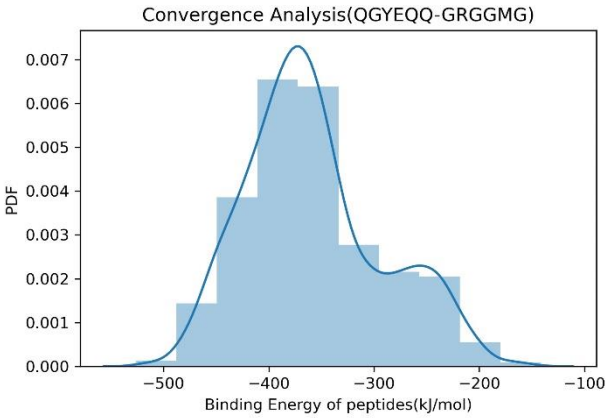



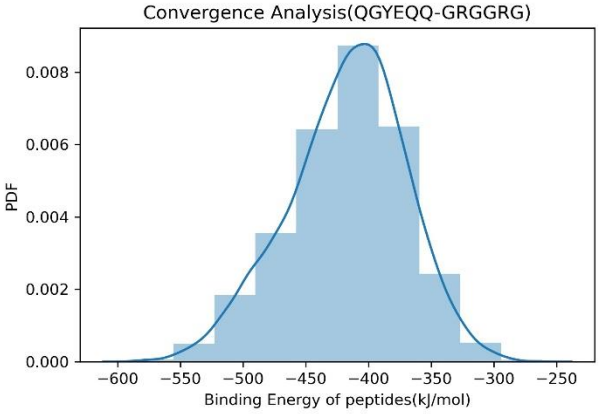



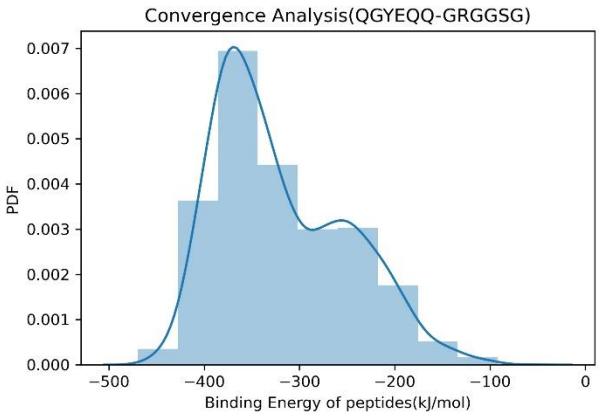

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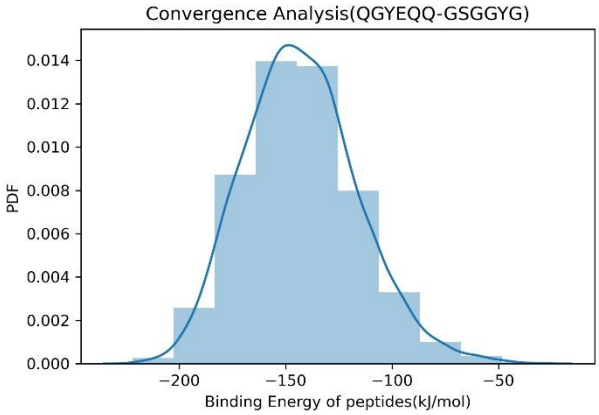
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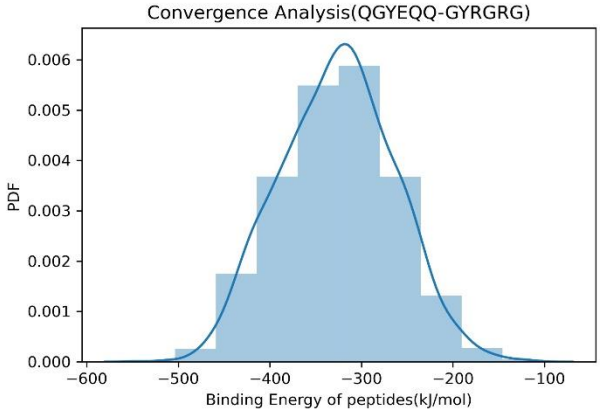
Binding Energy of peptides(kJ/mol)


Convergence Analysis(QGYEQQ-GYRGRG)
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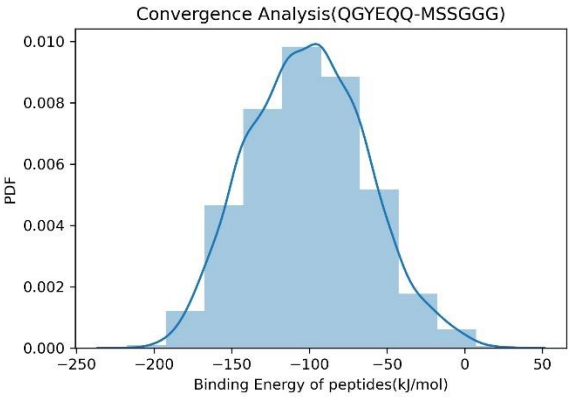
Binding Energy of peptides(kJ/mol)


Convergence Analysis(QGYEQQ-MSSGGG)
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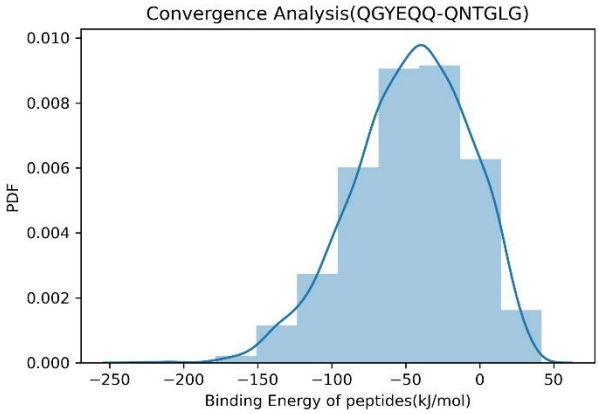
Binding Energy of peptides(kJ/mol)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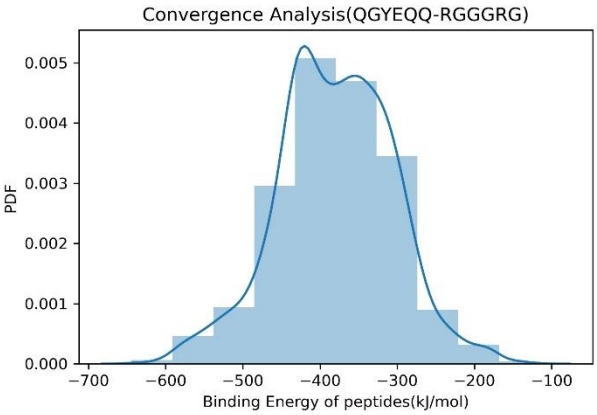
Binding Energy of peptides(kJ/mol)


Convergence Analysis(QGYEQQ-RGGGRG)
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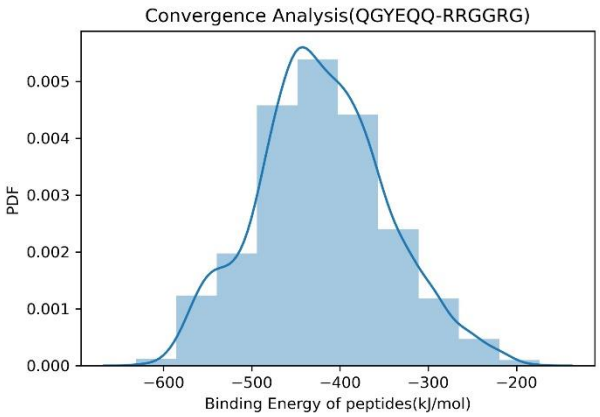
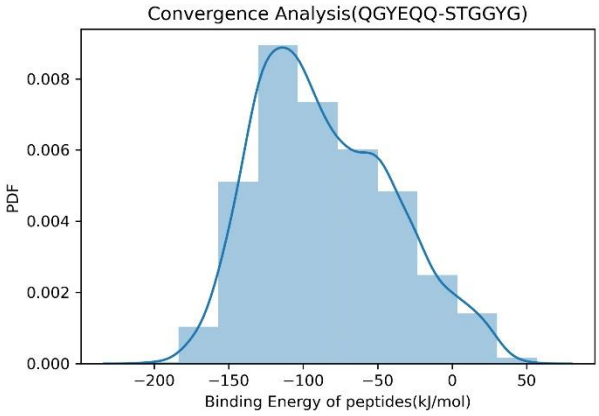
Binding Energy of peptides(kJ/mol)



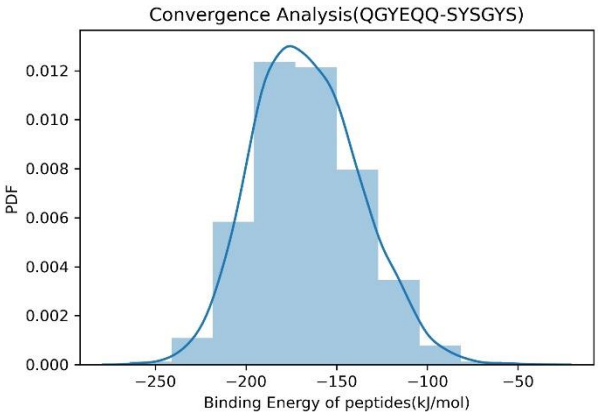
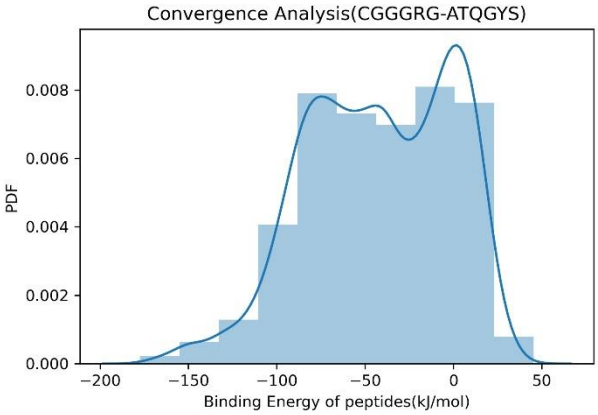
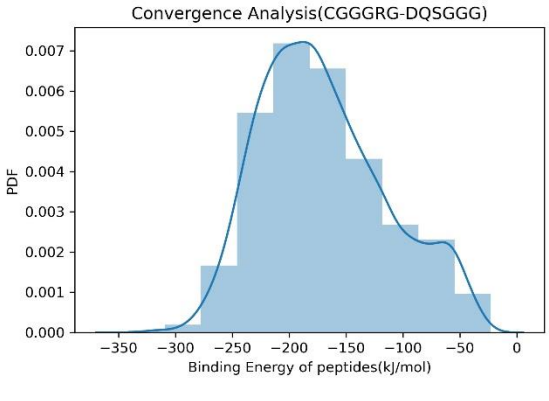
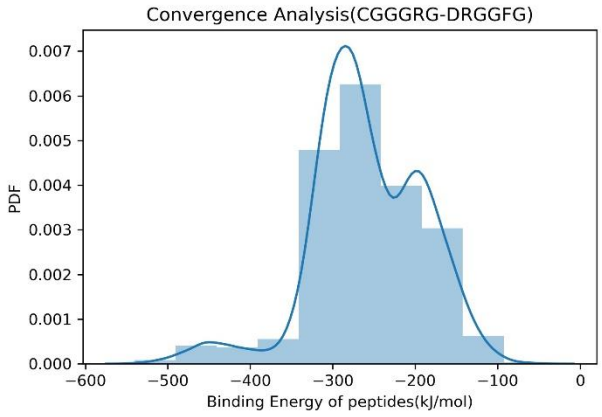
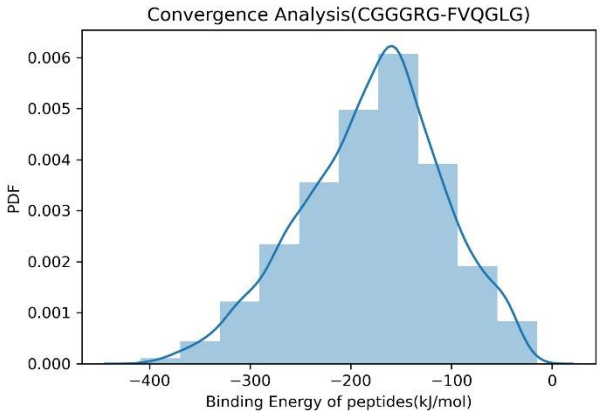



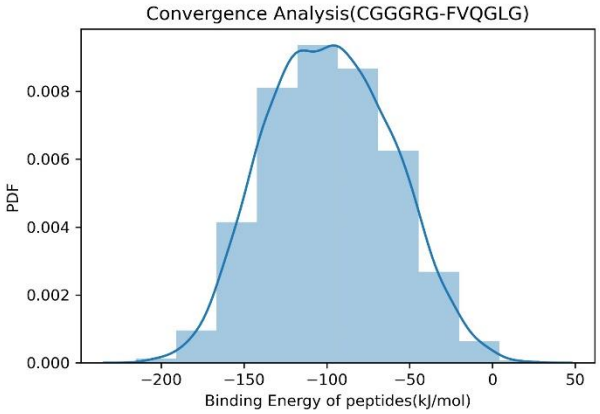

**Figure S4:** Histogram analysis of binding energy distribution of stickers estimated for G156E mutation

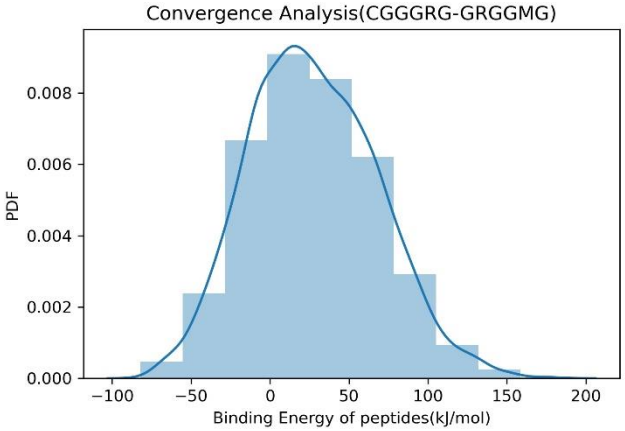


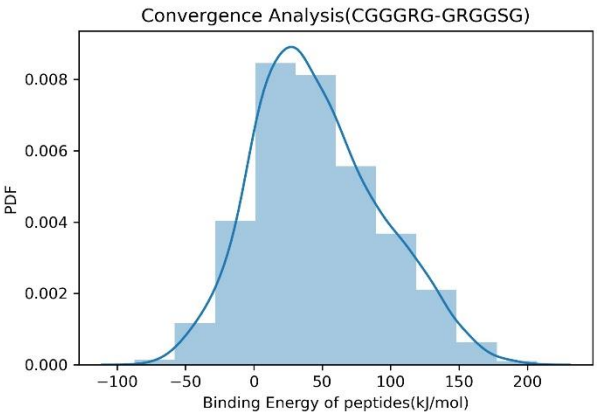



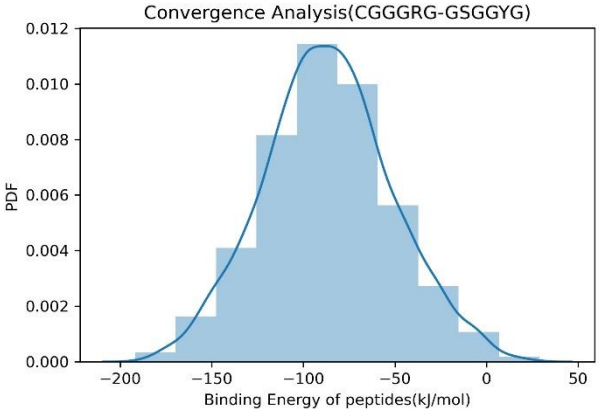

Convergence Analysis(CGGGRG-DRGGFG)
PDF
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
−600
−500
−400
−300
−200
−100
0
Binding Energy of peptides(kJ/mol)

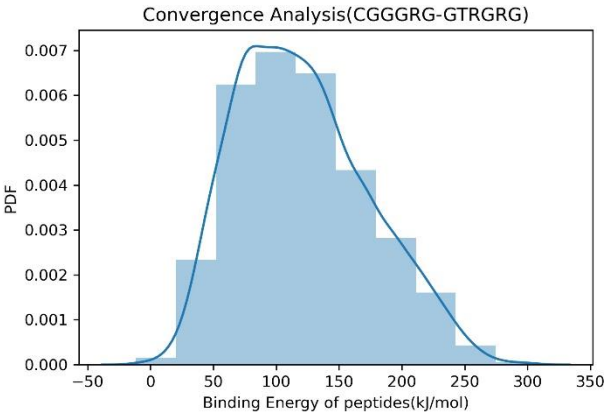

Convergence Analysis(CGGGRG-FVQGLG)
PDF
0.006
0.005
0.004
0.003
0.002
0.001
0.000
−400
−300
−200
−100
0
Binding Energy of peptides(kJ/mol)

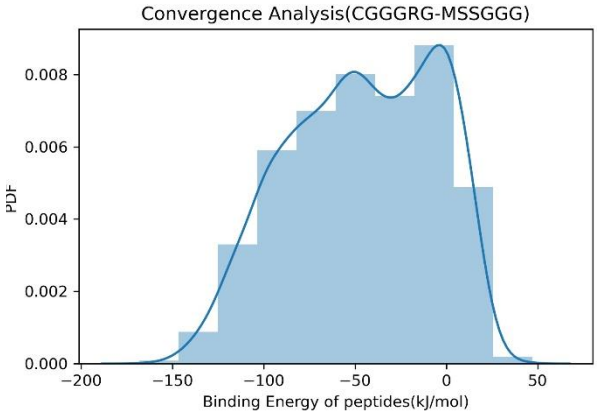

Convergence Analysis(CGGGRG-FVQGLG)
PDF
0.008
0.006
0.004
0.002
0.000
−200
−150
−100
−50
0
50
Binding Energy of peptides(kJ/mol)

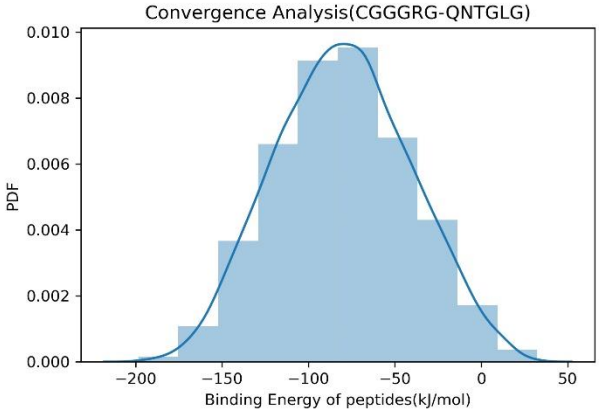

Convergence Analysis(CGGGRG-GRGGMG)
PDF
0.008
0.006
0.004
0.002
0.000
−100
−50
0
50
100
150
200
Binding Energy of peptides(kJ/mol)

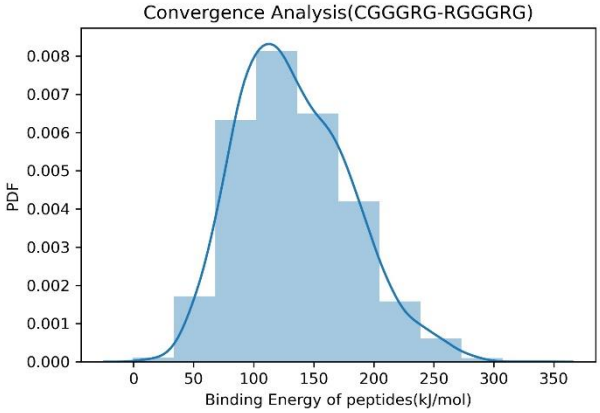

Convergence Analysis(CGGGRG-GRGGSG)
PDF
0.008
0.006
0.004
0.002
0.000
−100
−50
0
50
100
150
200
Binding Energy of peptides(kJ/mol)

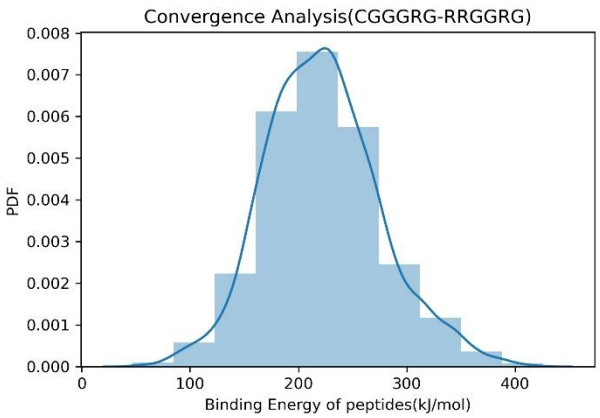

Convergence Analysis(CGGGRG-GSGGYG)
PDF
0.012
0.010
0.008
0.006
0.004
0.002
0.000
−200
−150
−100
−50
0
50
Binding Energy of peptides(kJ/mol)

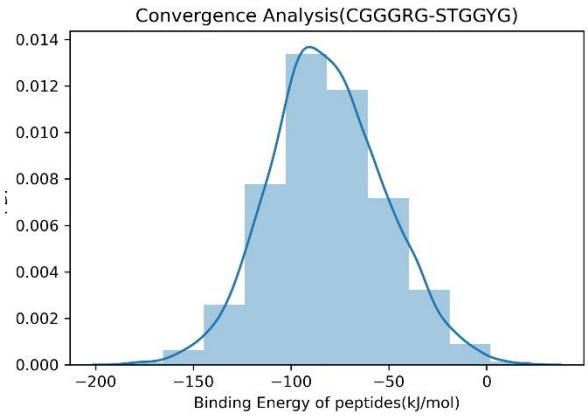

Convergence Analysis(CGGGRG-GTRGRG)
PDF
Binding Energy of peptides(kJ/mol)


Convergence Analysis(CGGGRG-MSSGGG)
PDF
Binding Energy of peptides(kJ/mol)


Convergence Analysis(CGGGRG-QNTGLG)
PDF
Binding Energy of peptides(kJ/mol)


Convergence Analysis(CGGGRG-RGGGRG)
PDF
Binding Energy of peptides(kJ/mol)


Convergence Analysis(CGGGRG-RRGGRG)
PDF
Binding Energy of peptides(kJ/mol)


Convergence Analysis(CGGGRG-STGGYG)
Binding Energy of peptides(kJ/mol)

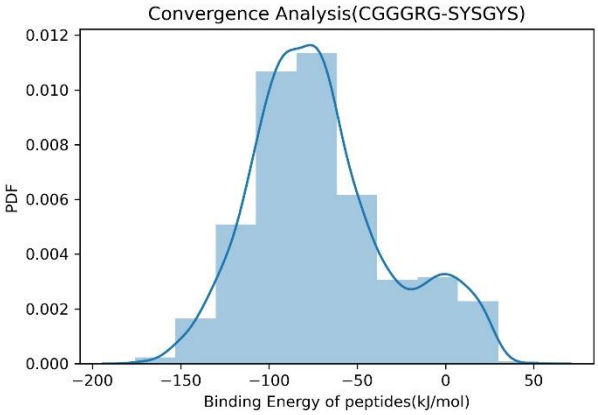



**Figure S5:** Histogram analysis of binding energy distribution of stickers estimated for R244C mutation