Supplementary Data:

Figure 1: Quantum mechanical optimized monomeric polymers showcasing electropositive(blue) and electronegative potentials(red) A) Chitosan B) Pectin C) Cyclodextrin D) Alginate E) Dextrin
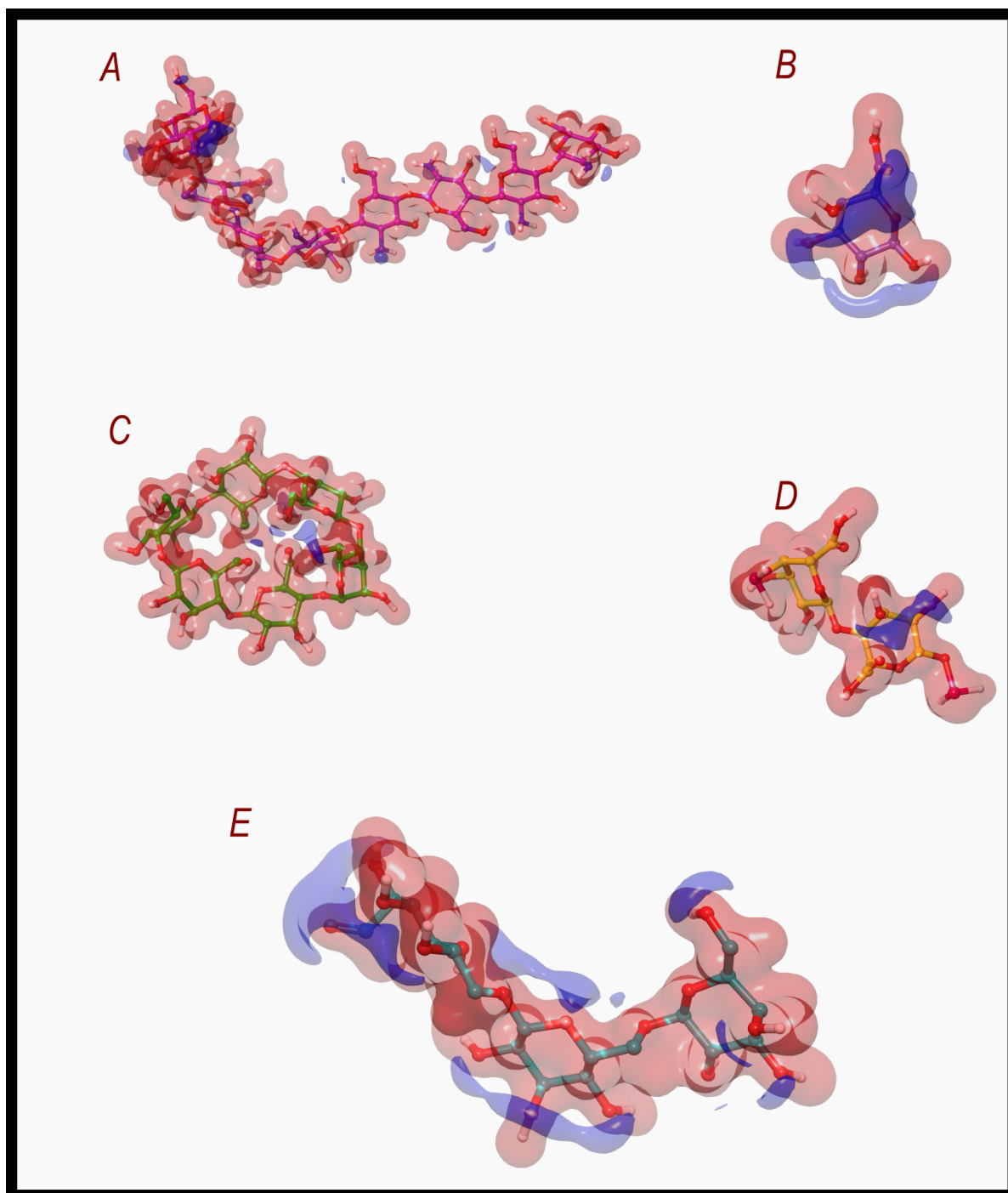
Figure 2: Root mean square deviations of Replica Runs of molecular dynamics calculations at 280 K :
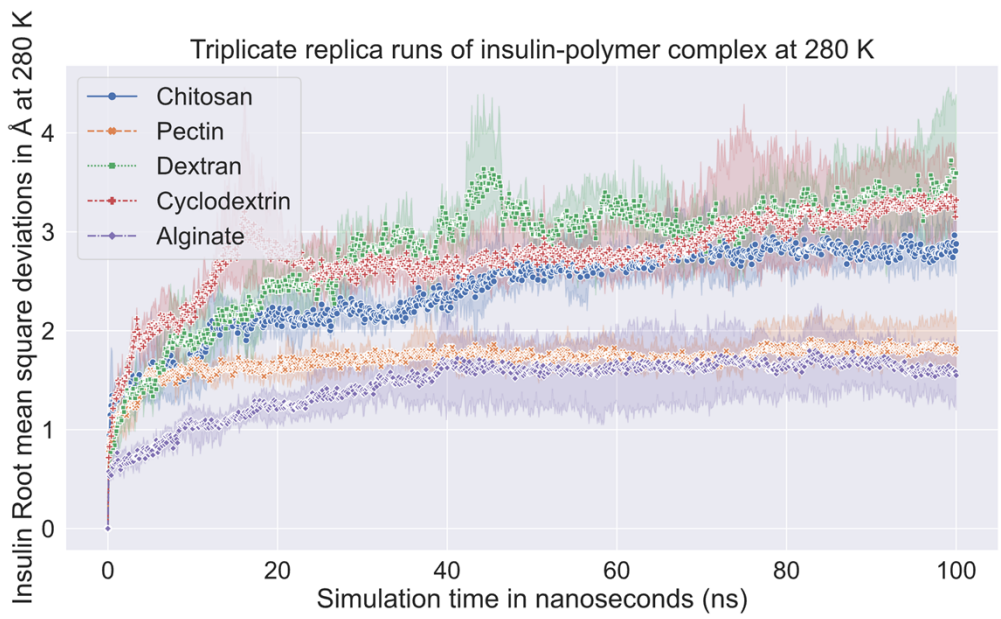

Triplicate replica runs of insulin-polymer complex at 280 K

Figure 3: Root mean square deviations of Replica Runs of molecular dynamics calculations at 280 K :

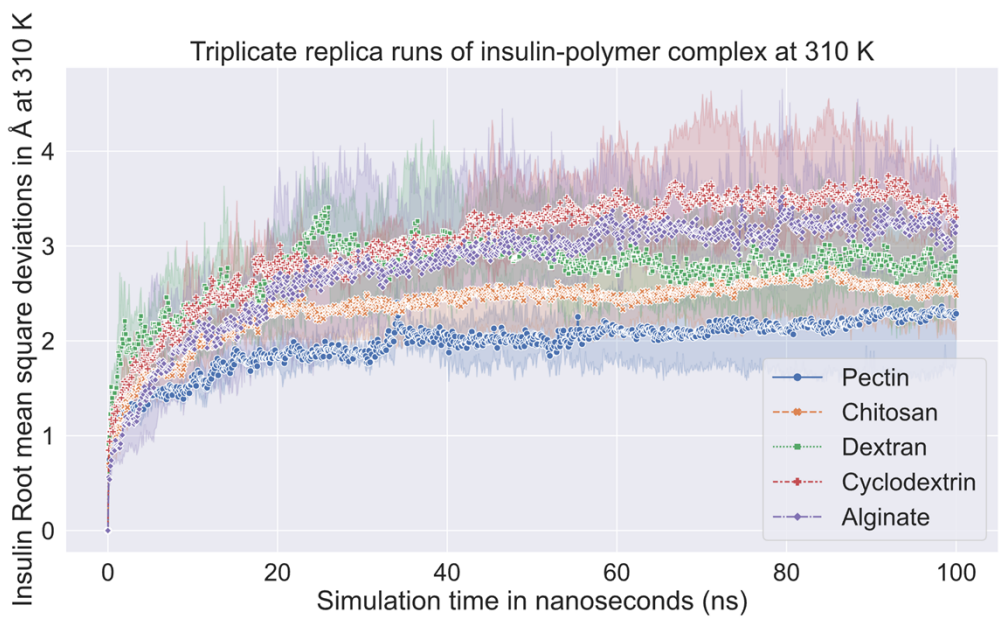Triplicate replica runs of insulin-polymer complex at 310 K

Figure 4 : Principal Component Analysis of computational formulation at 280K and 310 K:
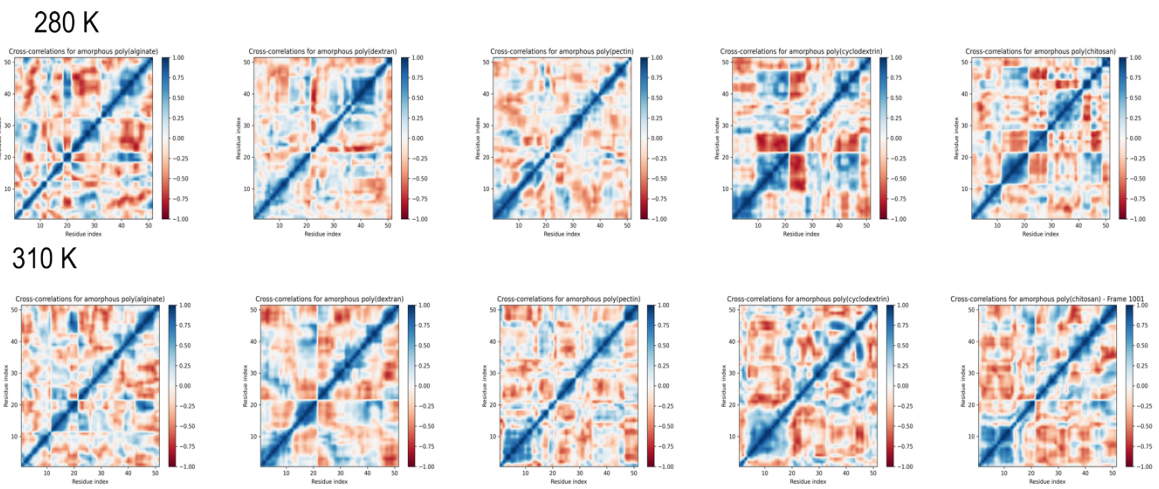
280 K

310 K

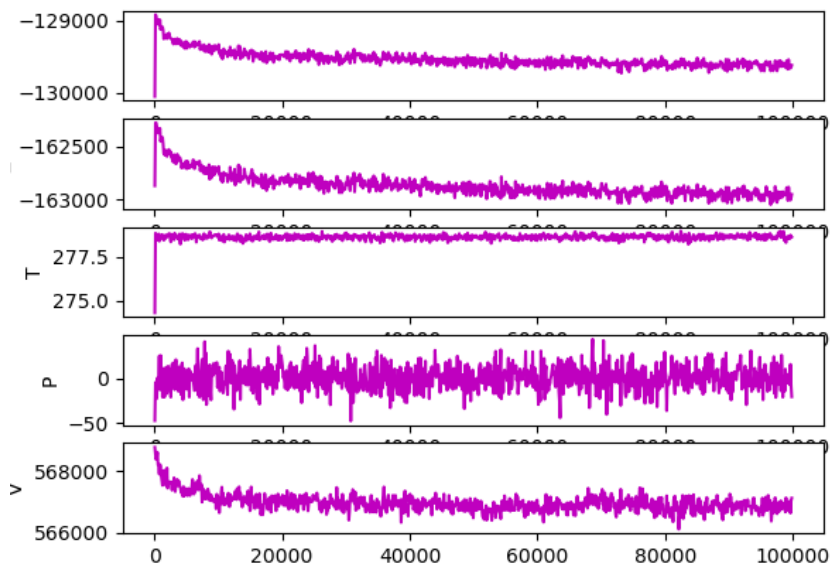**Figure 5: 280 K Cyclodextrin-insulin energetics analysis.**

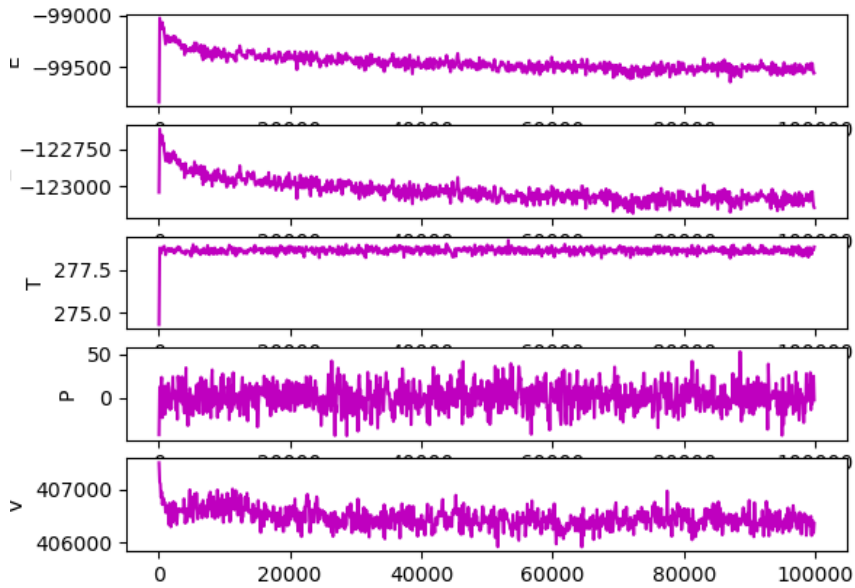**Figure 6 280 K Dextran – insulin formulation energetics analysis.**

Figure 7 : 280 K Pectin – insulin formulation energetics analysis.
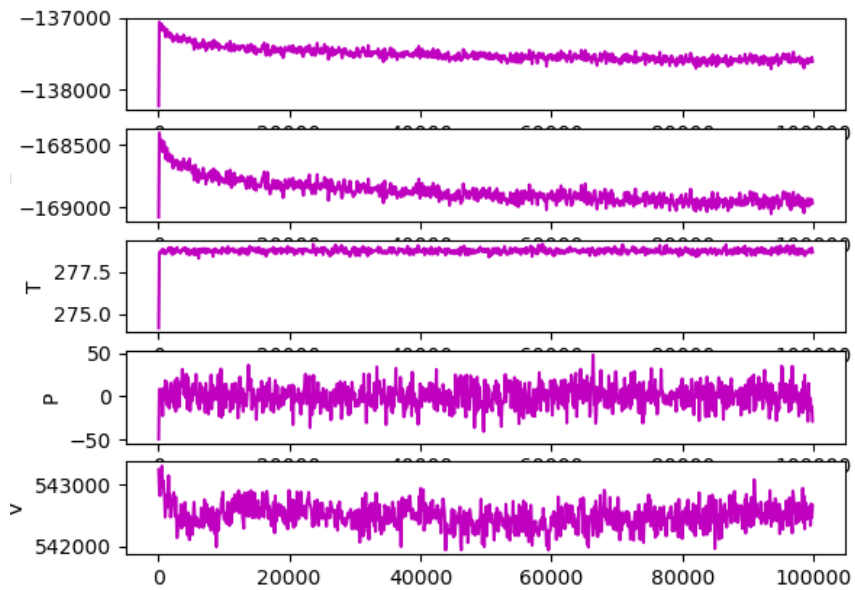
Figure 8 : 280 K Alginate- insulin formulation energetics analysis.
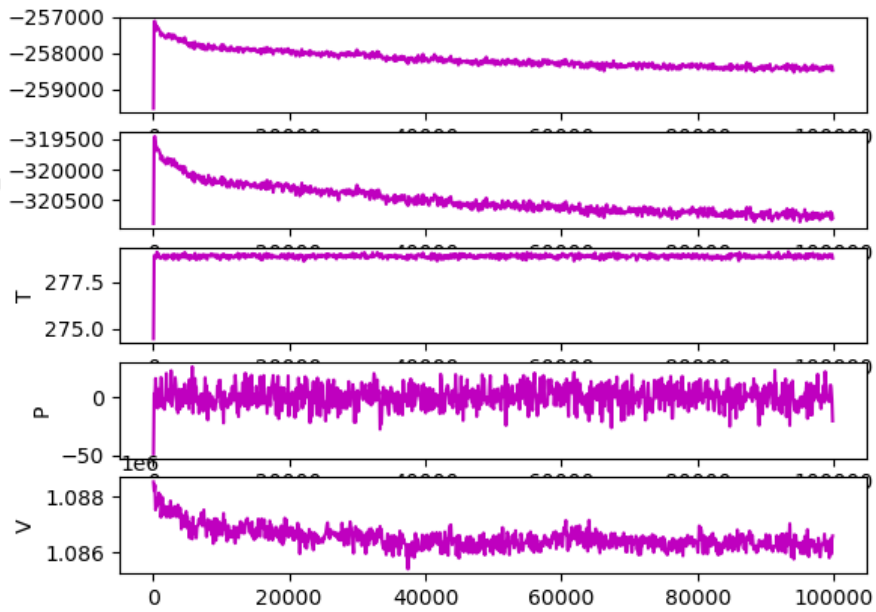

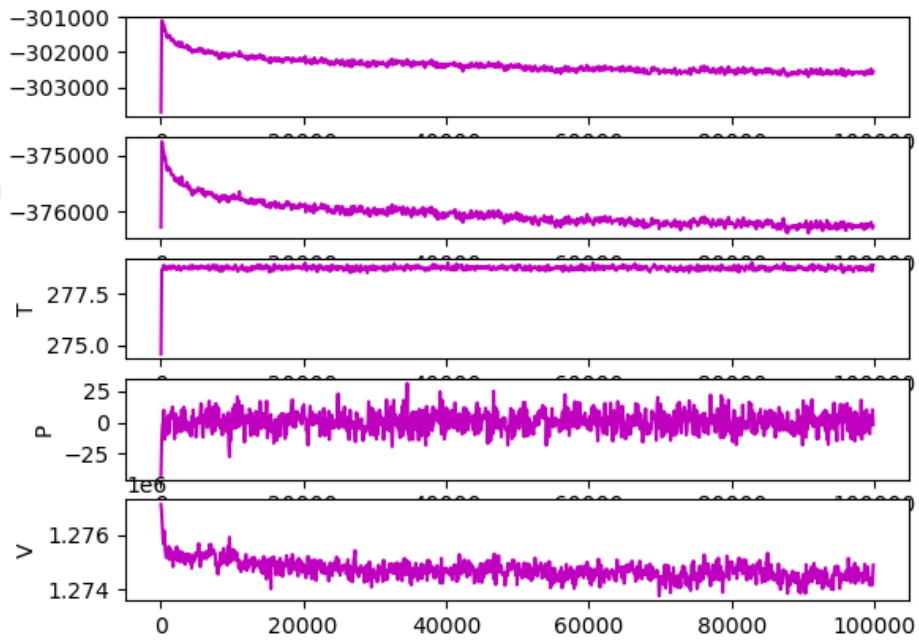**Figure 9: 280 K Chitosan – insulin formulation energetics analysis.**

Figure 10: 310 K Cyclodextrin-insulin energetics analysis.
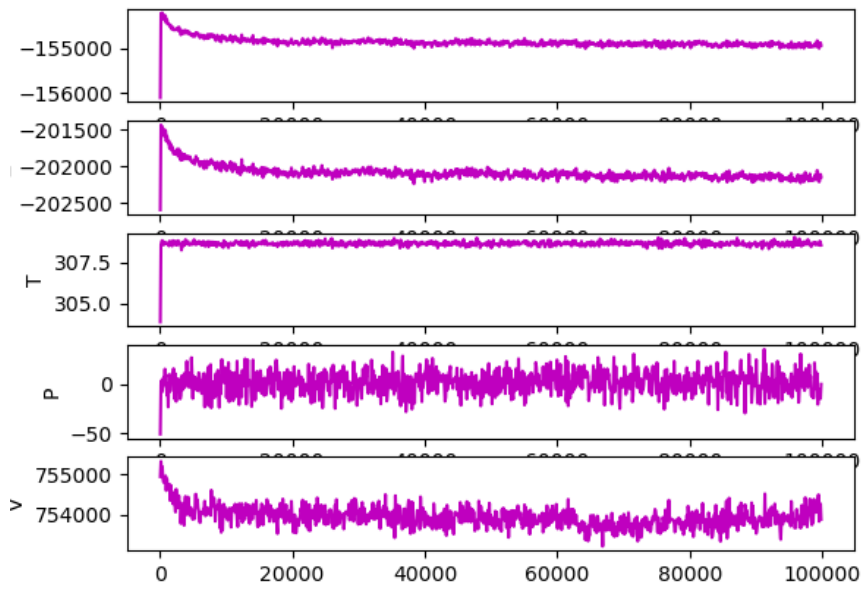

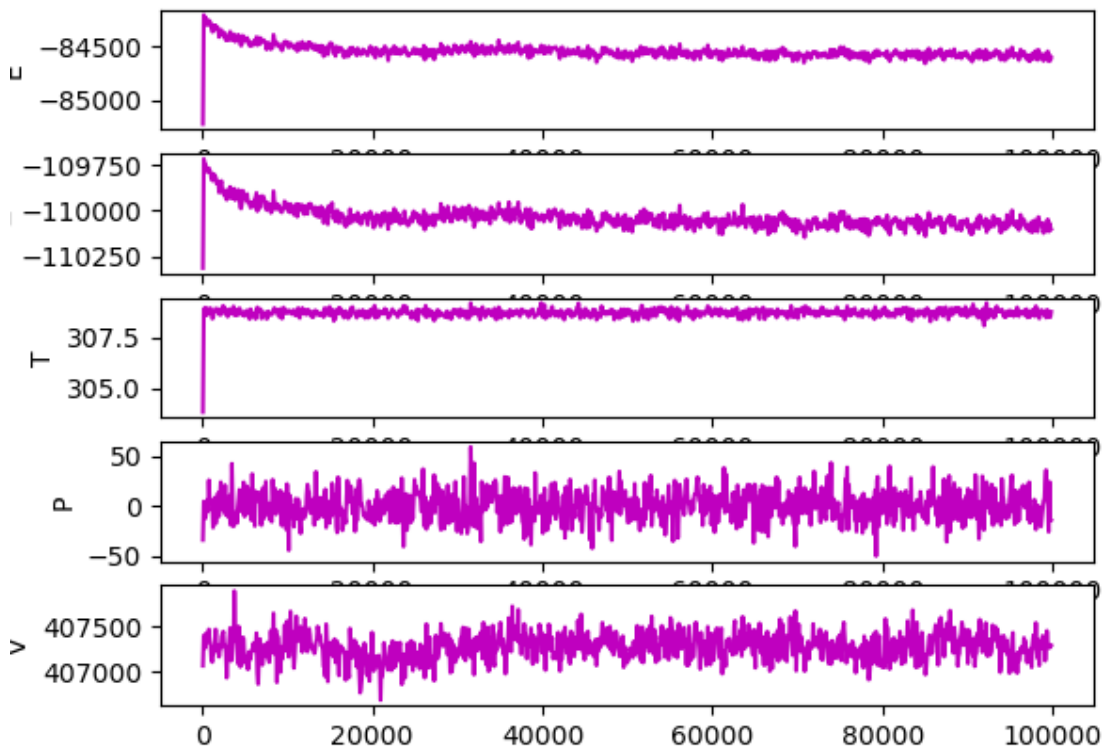**Figure 11 310 K Dextran – insulin formulation energetics analysis.**

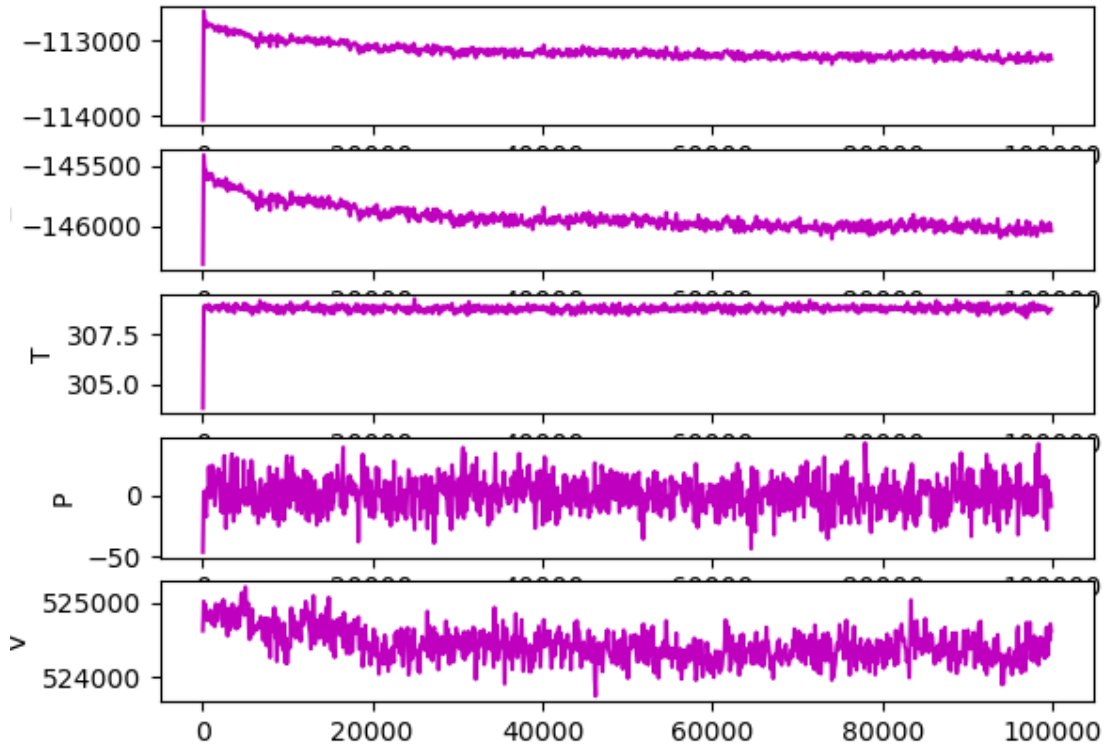**Figure 12 310 K Pectin – insulin formulation energetics analysis.**

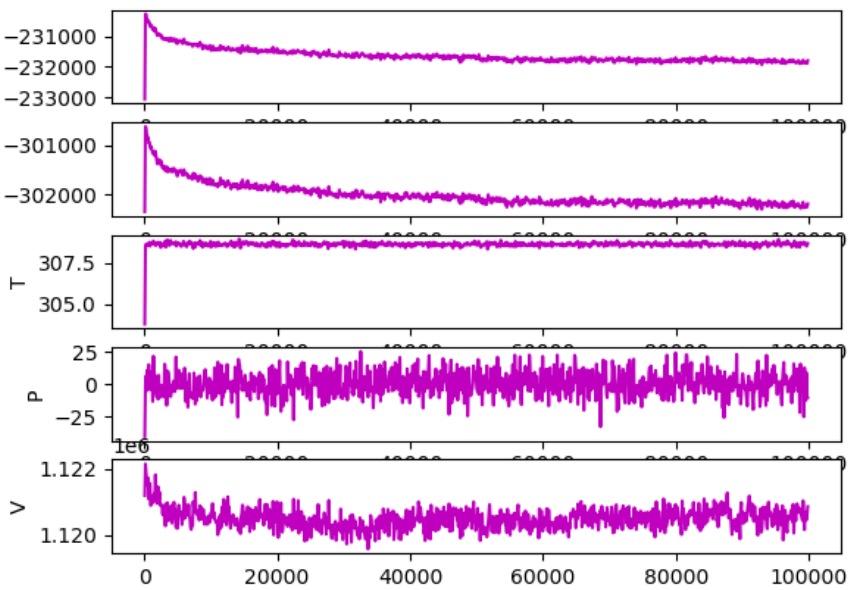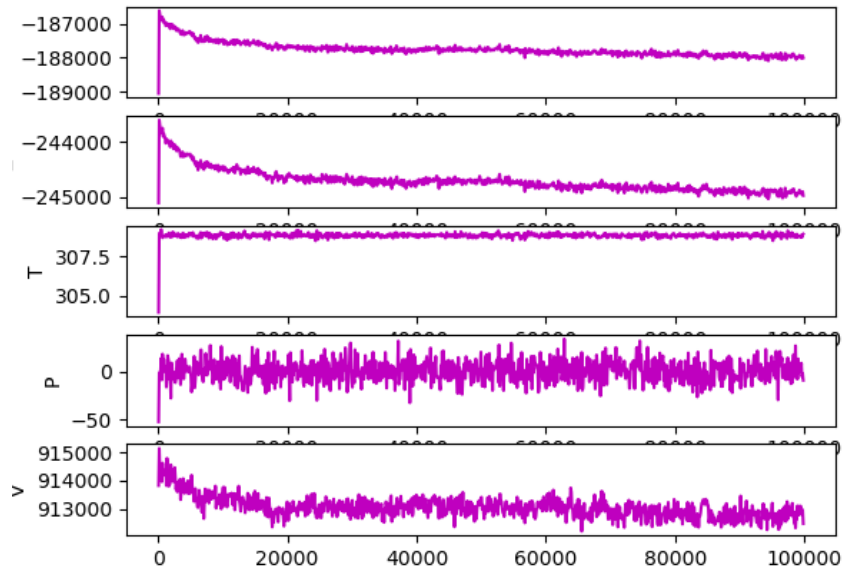**Figure 13: 310 Alginate- insulin formulation energetics analysis.**

Figure 14 310 K Chitosan – insulin formulation energetics analysis.

Tables:

Table 1: Quantum mechanical properties of monomer polymer units:

S.No	Polymer	QM Method	QM Basis	Number of canonical orbitals	Gas Phase Energy (Hartree)	HOMO	LUMO
1	alginate	DFT(b3lyp-d3)	6-31g**	498	-2054.658	-0.227401	-0.0345
2	chitosan	DFT(b3lyp-d3)	6-31g**	2075	-5622.280	-0.217256	-0.0108
3	cyclodextrin	DFT(b3lyp-d3)	6-31g**	1290	-3664.432	-0.200809	0.0308
4	dextran	DFT(b3lyp-d3)	6-31g**	670	-1908.615	-0.220565	-0.0232
5	pectin	DFT(b3lyp-d3)	6-31g**	245	-761.199	-0.237331	-0.0066