

Supplementary Table 1 : Ground state energy values for each peptide at different time frames along with the least energy value and statistical data (Mean and Standard deviation). All the values in kcal/mol.

Sequence	native fold	10 ns	20 ns	30 ns	40 ns	50 ns	Ground state energy	Average	SD
SPKHQED	5.407077	3.966243	6.014085	2.915233	3.089983	4.442046	2.915233	4.305777833	1.131134987
PSKDEHQ	6.972349	9.663861	-0.675931	3.946321	2.684608	6.049854	-0.675931	4.773510333	3.29453184
DEHSQPK	7.012393	6.657722	4.48123	7.678857	5.636397	5.796853	4.48123	6.210575333	1.040046872
HKESDQP	7.466478	5.753732	6.01356	5.089129	10.85024	2.05636	2.05636	6.2049165	2.641535393
HSQPKDE	8.055986	5.753732	-3.615879	3.012663	5.594764	2.361442	-3.615879	3.527118	3.705614791
EKSPQHD	5.56788	11.116696	6.350452	1.550641	12.602904	5.138684	1.550641	7.054542833	3.740649692
HKDEPSQ	6.076479	6.302173	3.92134	7.40688	8.476853	-0.671484	-0.671484	5.252040167	2.99121303
PSQHEKD	9.517688	7.143742	2.93161	15.927405	8.683694	4.453413	2.93161	8.109592	4.174177289
DPKEHSQ	6.321006	8.738137	5.549719	1.004534	1.419166	2.54972	1.004534	4.263713667	2.815380479
DKPHQES	7.723148	8.564811	6.043709	6.981377	6.735242	-3.138369	-3.138369	5.484986333	3.936399372
HPDSQEK	9.093111	4.616299	4.988435	-1.123449	-5.903789	4.06354	-5.903789	2.622357833	4.834735839
SPHDQEK	12.916721	7.521786	3.556734	5.146238	10.872071	5.834956	3.556734	7.641417667	3.277553049
PDKSEHQ	11.644622	8.193781	6.457775	4.961891	13.386531	6.026088	4.961891	8.445114667	3.07277473
DKESHQP	11.523207	9.855357	1.005822	0.433324	3.47806	6.669131	0.433324	5.494150167	4.214496848
SDPHQEK	10.120324	11.315311	8.207976	8.339975	11.992648	0.293955	0.293955	8.378364833	3.875377526
DPSHQKE	10.657242	1.236293	4.23945	6.463002	2.622781	-1.110815	-1.110815	4.017992167	3.788048803
QSEHPDK	8.934646	6.862416	15.280032	2.424853	10.565863	7.928337	2.424853	8.6660245	3.876769428
SDQEHPK	11.391187	5.349911	-0.304389	8.393737	5.952933	6.805882	-0.304389	6.264876833	3.540092116
KSQHPED	6.326102	-0.989125	0.040175	5.784731	2.529962	1.06086	-0.989125	2.458784167	2.760286089
DSPQEKH	11.129083	3.669357	10.516065	6.579056	6.222502	2.130704	2.130704	6.7077945	3.278329313
QESDKPH	8.612147	-0.28275	-1.972835	-1.520819	-3.396226	1.352863	-3.396226	0.465396667	3.92680992
EHPQDSK	13.19072	13.089008	11.276032	10.075038	11.818986	6.425594	6.425594	10.97922967	2.298125932
PDQSEHK	10.620655	9.226217	10.561006	0.442289	1.278032	1.850898	0.442289	5.663182833	4.51444368

HSPKDQE	11.276032	10.075038	5.952933	6.597468	3.781458	2.684608	2.684608	6.727922833	3.09666903
KDQHSPE	10.620655	9.226217	10.561006	0.442289	1.278032	1.850898	0.442289	5.663182833	4.51444368
PSDQKHE	12.616123	3.670813	-3.329716	4.195982	2.529814	9.836114	-3.329716	4.919855	5.15192455
DQEPHKS	8.815527	8.799937	12.158175	9.489563	10.132634	4.947848	4.947848	9.057280667	2.159124279
SPQEHDK	11.640298	12.244345	9.959256	7.497296	10.712621	6.763119	6.763119	9.8028225	2.03079635
PQKESHD	8.674255	11.040177	8.099159	1.760201	4.524408	1.129353	1.129353	5.871258833	3.668299249
PSDQKEH	11.895736	11.848647	11.948491	10.103068	10.764607	6.929236	6.929236	10.58163083	1.770263622
KPSDEHQ	10.834974	10.209683	11.374826	10.090425	10.482144	6.847186	6.847186	9.973206333	1.461042054
EHKDQPS	9.775447	9.377655	10.437671	9.607306	9.886443	6.597468	6.597468	9.280331667	1.242717853
QPEKHS	8.342946	8.352432	9.29625	8.741272	8.962711	5.776667	5.776667	8.245379667	1.153279637
KDEQHSP	5.615922	15.427316	1.582222	-2.491703	-0.038854	5.156846	-2.491703	4.208624833	5.752855835
DSQHEPK	9.802065	9.227129	8.529255	7.015757	2.613003	11.94911	2.613003	8.1893865	2.898336649
EPKSQDH	9.162771	14.06668	7.73745	8.858127	5.289009	7.51708	5.289009	8.771852833	2.676132166
PQDESKH	13.119434	13.095499	11.097444	10.807969	10.92365	6.249033	6.249033	10.8821715	2.288511277
QPEKSDH	10.159377	10.144738	11.927128	9.842723	10.258785	6.034505	6.034505	9.727876	1.785717407
QPEDHKS	8.827511	9.911322	10.579173	9.366043	9.722636	6.395389	6.395389	9.133679	1.334604553
EDPKHSQ	8.014477	8.001585	8.8983	8.010057	8.194853	5.44417	5.44417	7.760573667	1.082708101
KPHESDQ	9.897802	8.661652	3.733366	8.813038	10.187323	-2.472702	-2.472702	6.470079833	4.533625611
PDHEQKS	11.886887	11.579765	11.531308	10.883191	11.30707	6.621226	6.621226	10.63490783	1.820568983
ESPKDHQ	11.705081	12.278388	11.735059	10.724276	10.840418	6.487823	6.487823	10.6285075	1.928078412
SDQPKHE	11.379248	9.530428	7.51126	9.486273	7.262528	8.850274	7.262528	9.003335167	1.380588233
QHDKESP	9.031651	10.158836	8.850503	5.128065	1.215829	10.146723	1.215829	7.4219345	3.24870949
EPQHDKS	9.388854	9.387776	10.410104	9.202874	9.487774	6.349942	6.349942	9.037887333	1.263806881
DPKEQSH	12.559475	12.544198	11.942953	10.818189	11.041549	6.584153	6.584153	10.91508617	2.049263861
HSQDEPK	9.104992	5.400356	-3.70421	3.552892	3.781458	10.732906	-3.70421	4.811399	4.636921955
DHQSKEP	9.704204	9.70365	10.399562	9.304164	9.588135	6.457652	6.457652	9.1928945	1.266787441
HEQSKPD	9.186759	6.925401	1.543514	-2.047041	6.039107	-3.82131	-3.82131	2.971071667	4.779123955