

Supplementary table 2: The complete list of peptides sequence along with energy values from MD simulations and VQE in kcal/mol,

Sequence	MD simulation	VQE
SPKHQED	2.915233	-7.9411
PSKDEHQ	-0.67593	-4.8295
DEHSQPK	4.48123	-9.5645
HKESDQP	2.05636	-8.0953
HSQPKDE	-3.61588	-1.2545
EKSPQHD	1.550641	-5.5649
HKDEPSQ	-0.67148	-4.7118
PSQHEKD	2.93161	-3.7896
DPKEHSQ	1.004534	-8.8733
DKPHQES	-3.13837	-8.353
HPDSQEK	-5.90379	-7.7257
SPHDQEK	3.556734	-4.4087
PKSEHQ	4.961891	-7.2669
DKESHQP	0.433324	-3.1401
SDPHQEK	0.293955	-2.3136
DPSHQKE	-1.11082	-2.9701
QSEHPDK	2.424853	-6.5226
SDQEHPK	-0.30439	-4.8151
KSQHPED	-0.98913	-6.0559
DSPQEKH	2.130704	-9.4248
QESDKPH	-3.39623	-8.1321
EHPQDSK	6.425594	-5.1767
PDQSEHK	0.442289	-6.9541
HSPKDQE	2.684608	-6.2522
KDQHSPE	0.442289	0.1422
PSDQKHE	-3.32972	-6.9541
DQEPHKS	4.947848	-5.2716
SPQEHDK	6.763119	-6.8982
PQKESHD	1.129353	-5.1026
PSDQKEH	6.929236	-6.223
KPSDEHQ	6.847186	-6.1646
EHKDQPS	6.597468	-4.512
QPEKHSD	5.776667	-7.9411
KDEQHSP	-2.4917	-9.7869
DSQHEPK	2.613003	-9.6108
EPKSQDH	5.289009	-9.9342
PQDESKH	6.249033	-2.8924
QPEKSDH	6.034505	-5.1026
QPEDHKS	6.395389	-2.2908
EDPKHSQ	5.44417	-4.552

KPHESDQ	-2.4727	-7.0993
PDHEQKS	6.621226	-3.8521
ESPKDHQ	6.487823	-7.7691
SDQPKHE	7.262528	-2.3767
QHDKESP	1.215829	-2.5936
EPQHDKS	6.349942	-4.8748
DPKEQSH	6.584153	-2.2355
HSQDEPK	-3.70421	-8.0409
DHQSKEP	6.457652	-7.7223
HEQSKPD	-3.82131	-7.1515