Electronic Supplementary Information
For

Searching low-energy conformers of neutral and protonated di-, tri-, and tetra-glycine with first-principle accuracy assisted by the use of neural network potentials

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Figure S1. Analyze ΔE1, ΔF1, ΔE2, and RMSD between min structures by NNP and M06-2X.

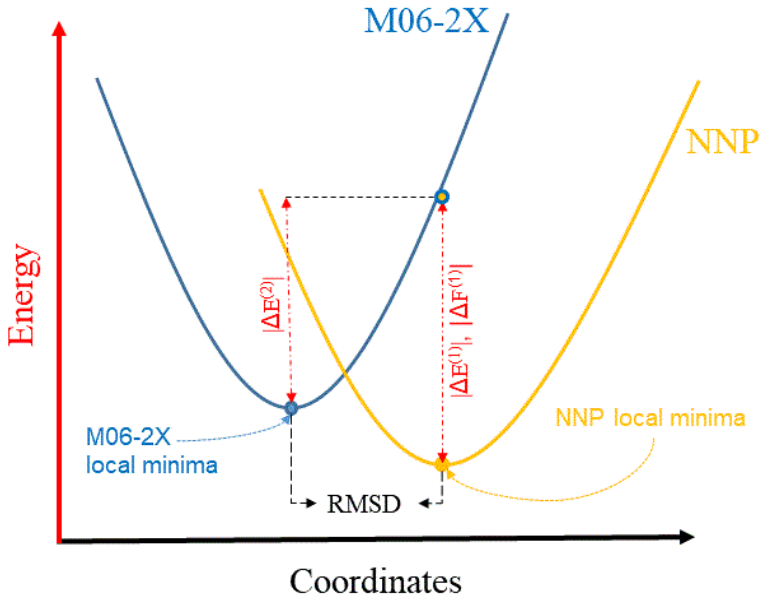


Figure S2. M06-2X minima of Gly_n_2-4 within 0-10 kJ/mol of ZPE-corrected energy.

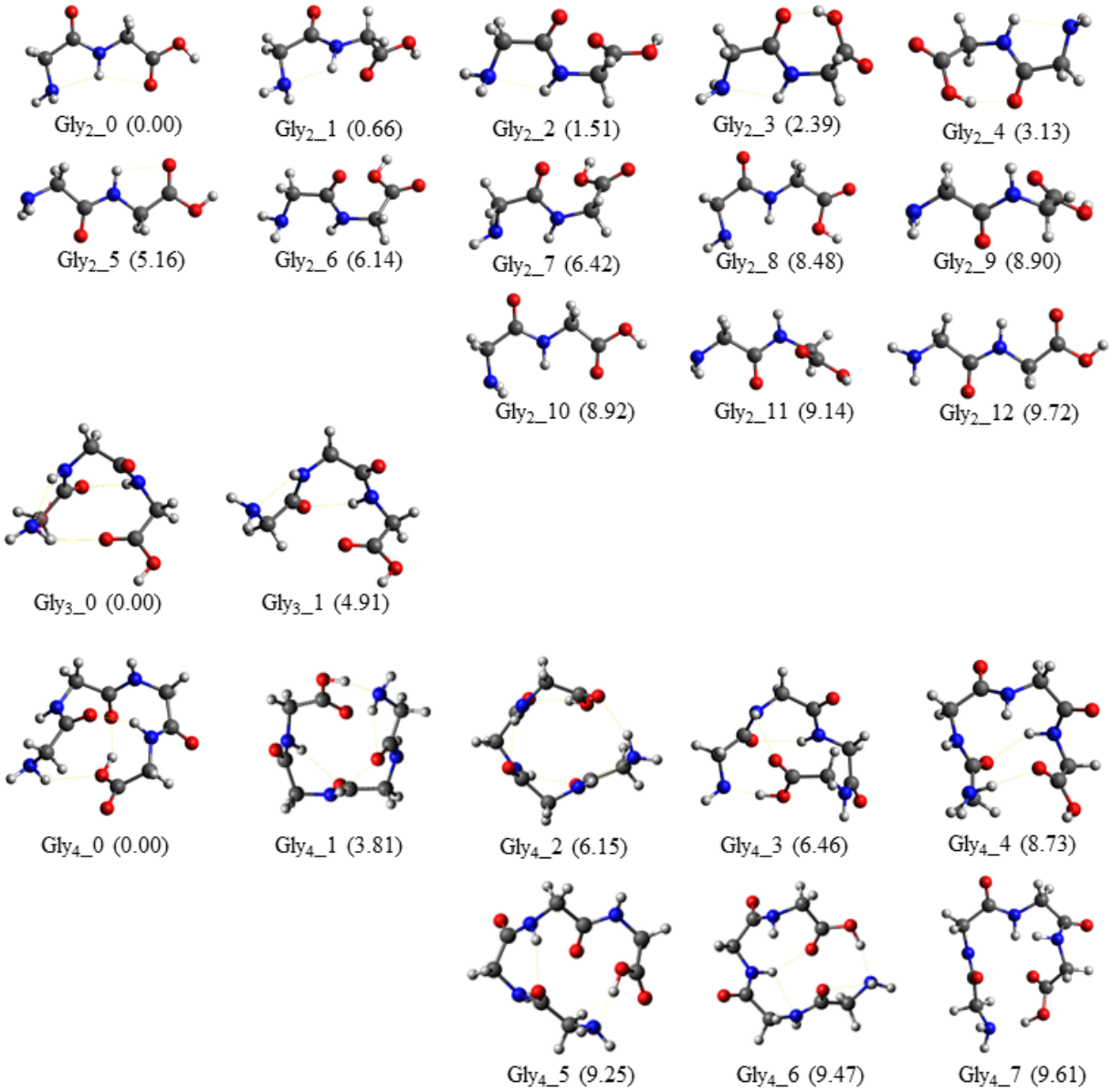


Figure S3. M06-2X minima of H^+Gly_n_2-4 within 0-10 kJ/mol of ZPE-corrected energy.

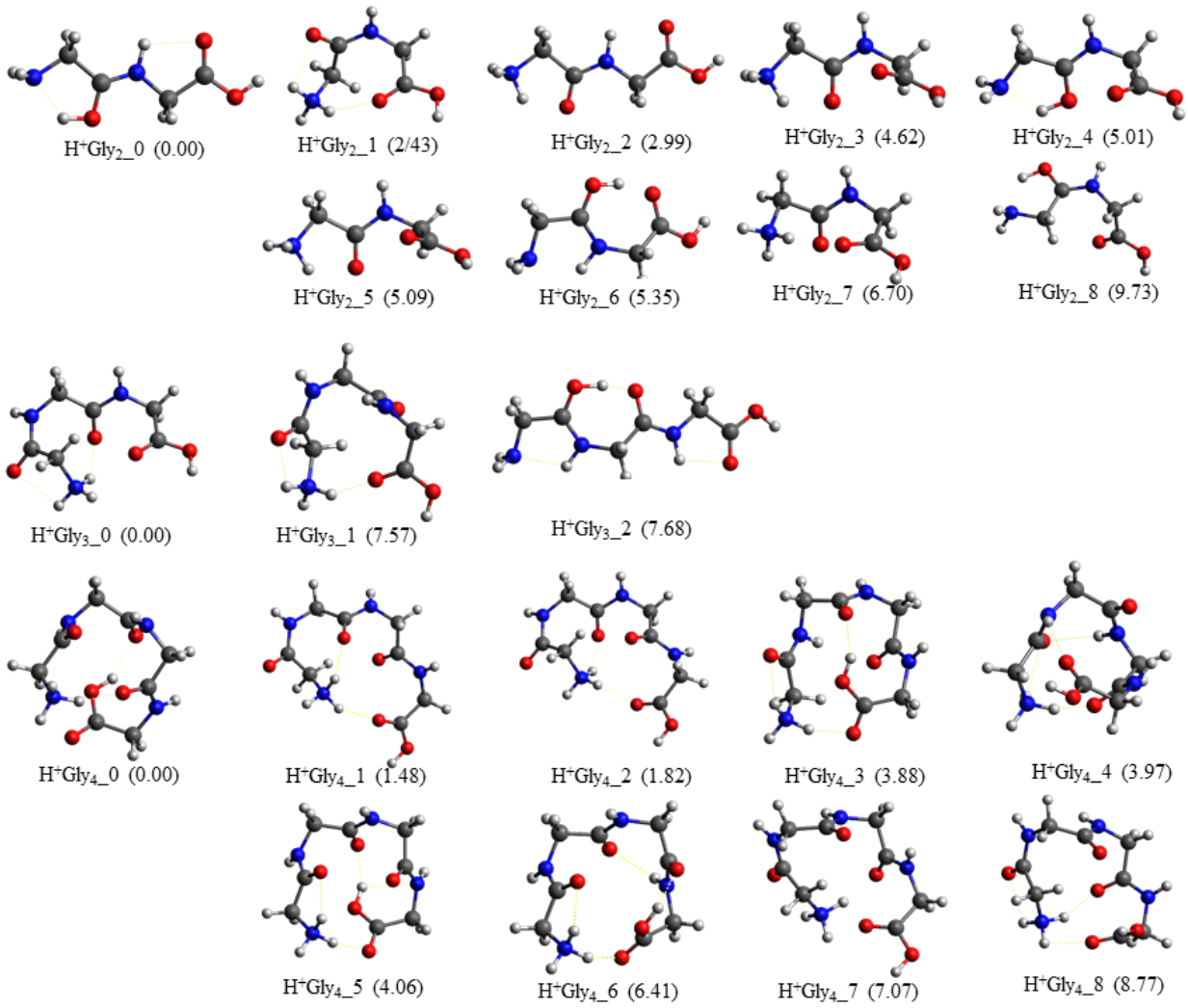


Figure S4. Root Mean Square Deviation (RMSD) between NNP-2 and M06-2X minima (Å).

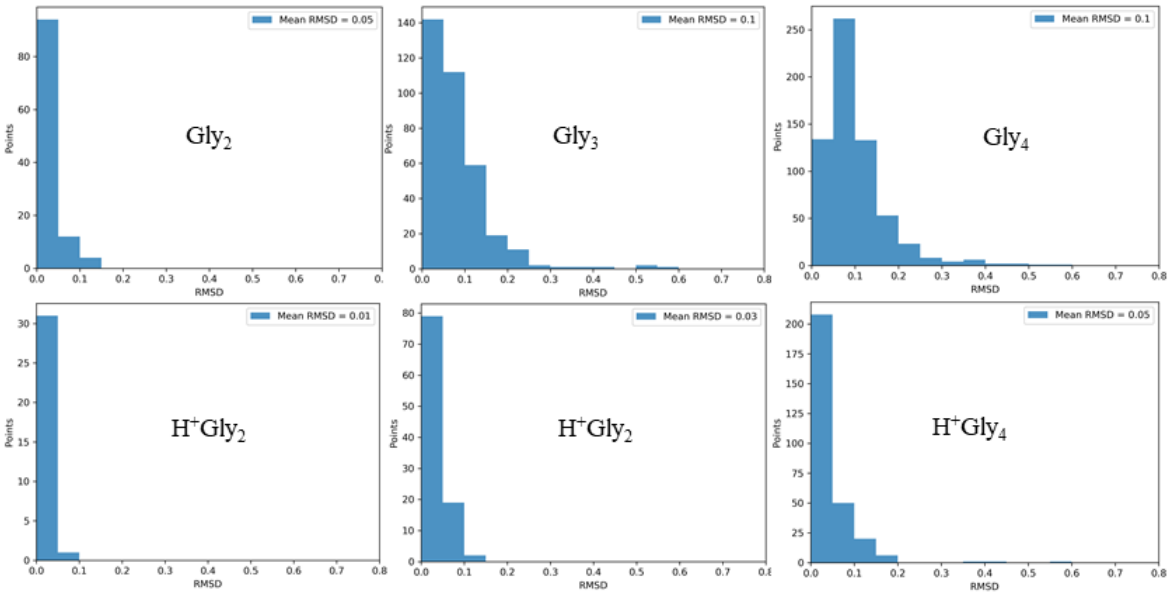


Figure S5. The correlation between NNP-2 energy (y-axis) and M06-2X energy (x-axis) of all NNP-2 stable configurations within 0-50 kJ/mol. The zero of the relative energies is calculated with respect to the lowest M06-2X energy (ΔE1 in Table 2).

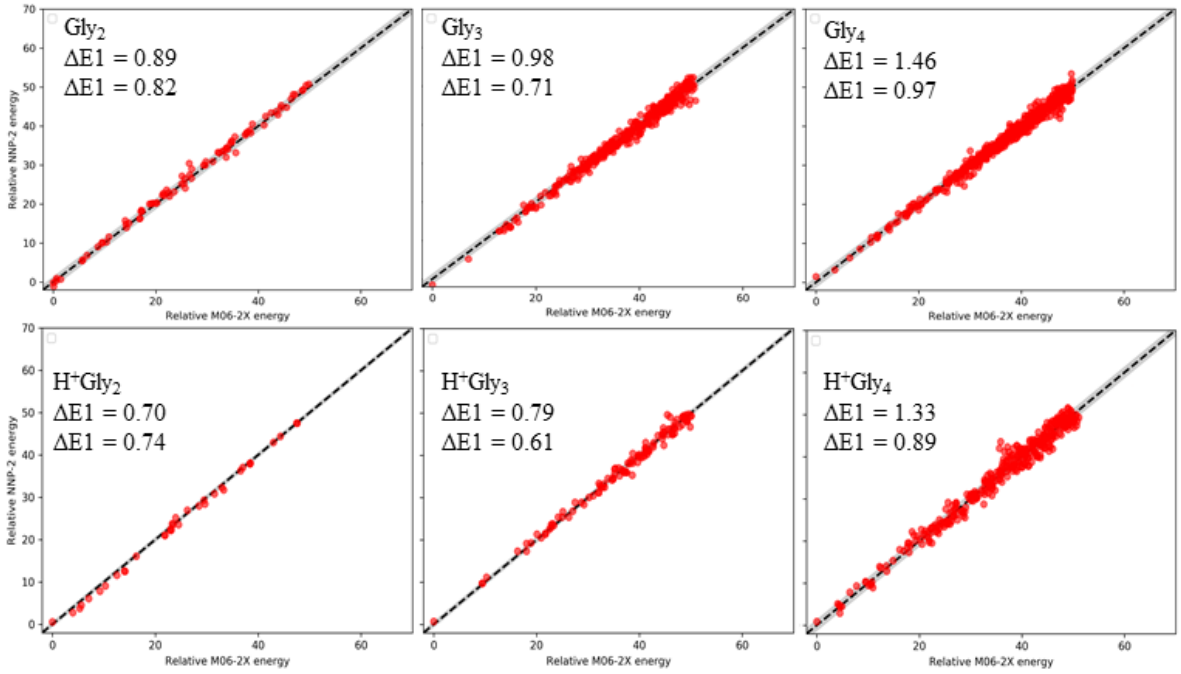


Figure S6. The energy histogram of Gly_n (left) and H+Gly_n (right) at M06-2X level.

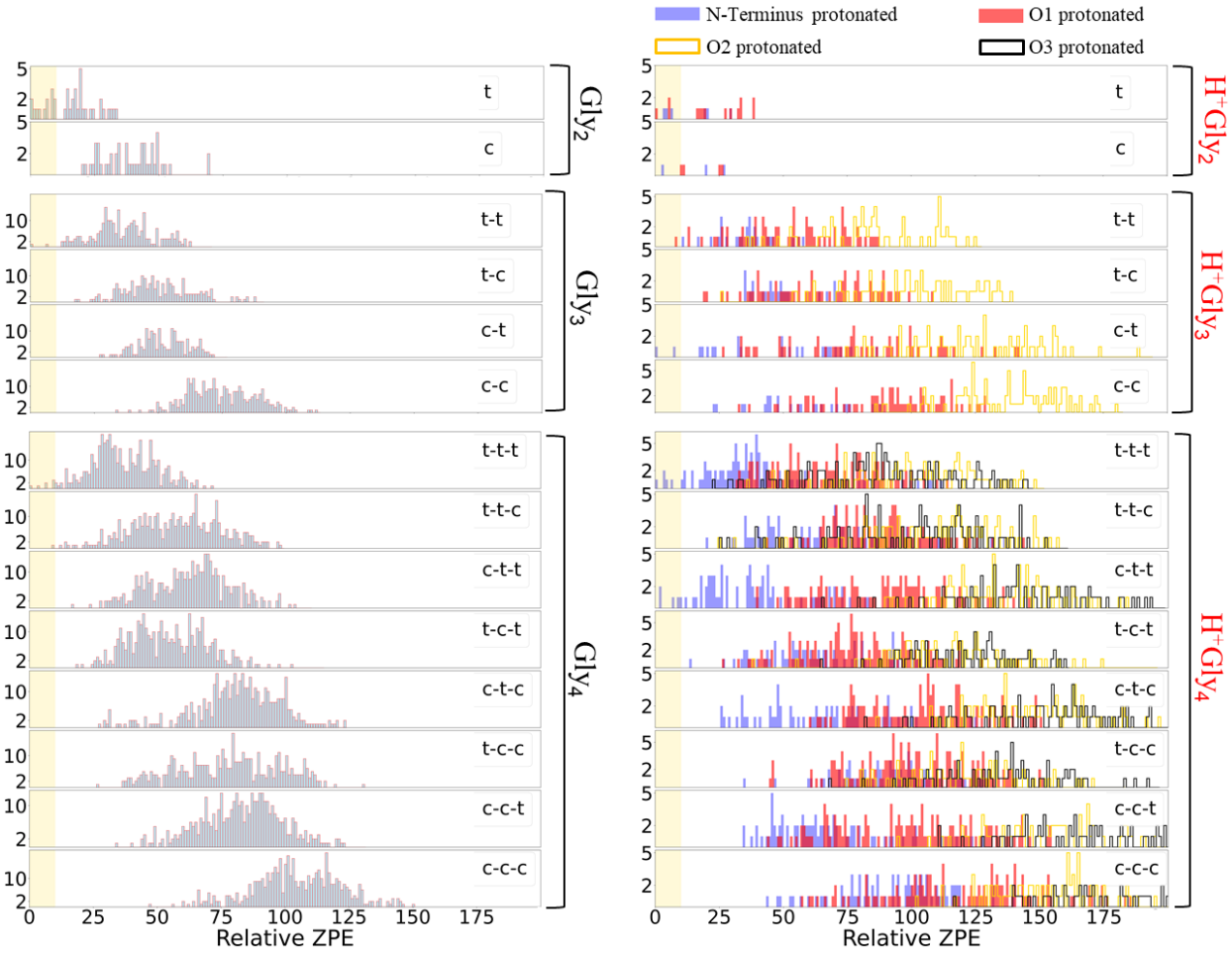
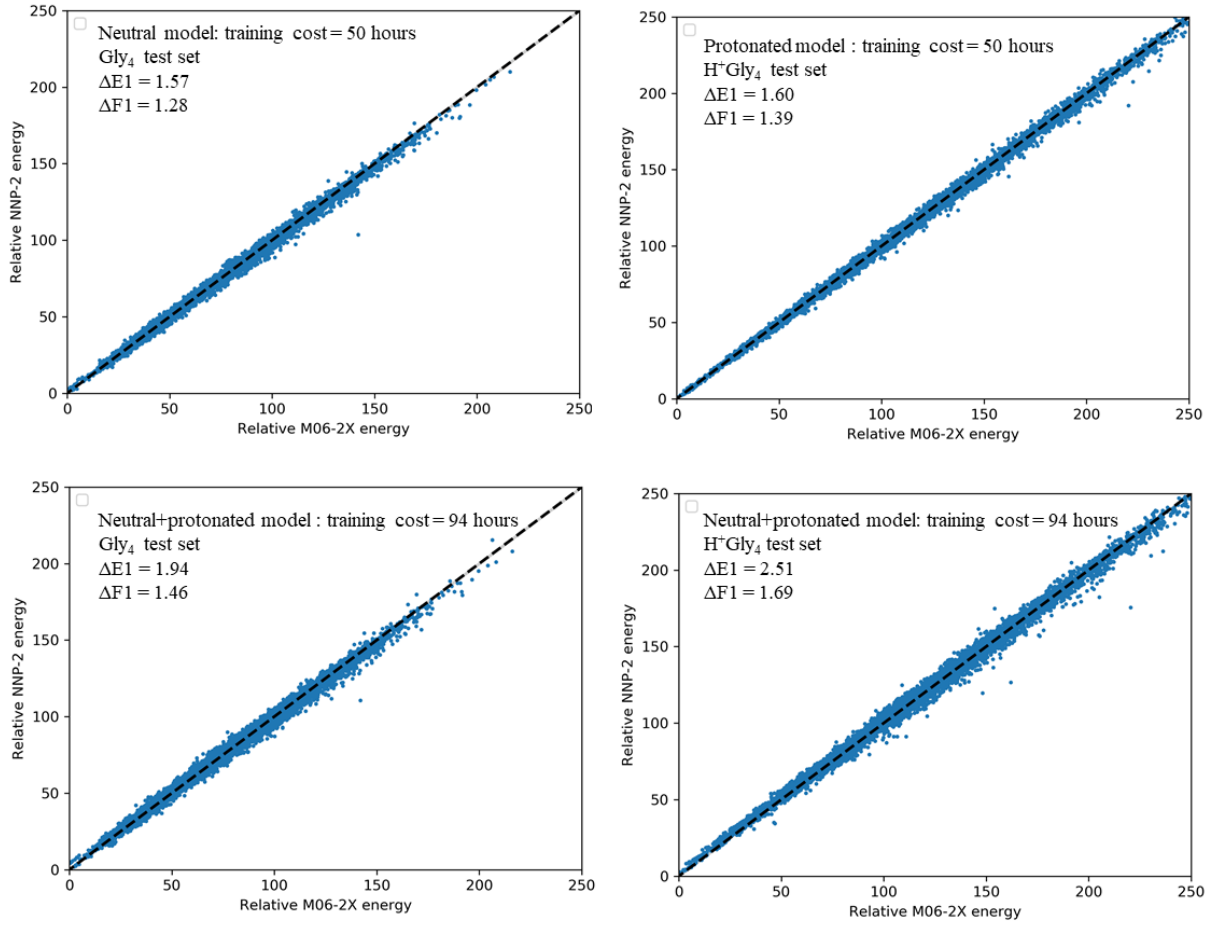


Figure S7. The prediction of the NNP-2 neutral model (top-left) and NNP-2 protonated model (top-right) model on the test set of Gly_4 and H^+Gly_4. The prediction of one neutral+protonated model (bottom) on the test set of Gly_4 and H^+Gly_4. The performance of the NNP-2 neutral or NNP-2 protonated model surpasses that of the neutral_protonated model trained on neutral+protonated data. The training duration for the NNP-2 neutral model or NNP-2 protonated model, which is 50 hours, is shorter than that of the neutral_protonated model, which takes 94 hours.



Amplitudes		0.1π	0.2π	0.3π	0.4π	0.5π
Gly_3	Trial structures	20k	20k	20k	20k	20k
	DFTB-3 min	3618	4117	4134	4082	3942
	DFTB-3 min (0-50)	3276	3682	3883	3484	3687

Table S1. Number of distinct DFTB-3 minima with varying amplitudes from 0.1π to 0.5π for Gly_3

Glycine	Gly_2	Gly_3	H^+Gly_2	H^+Gly_3
camB3LYP/def2TZVPP	55	119	48	107
M06-2X/6311+G(d,p)	87	146	55	110
MP2/6-311+G(d,p)	85	139	50	95

Table S2. Number of distinct minima at cam-B3LYP/def2TZVPP, M06-2X/6-311+G(d,p), and MP2/6-311+G(d,p) level (from 400 DFTB-3 minima)

	Name of peptide	NNP-0	NNP-1	NNP-2	Test set
The training set for Gly_n	Gly-2	1450	6543	6543	1613
	Gly-3	5622	15768	25263	5724
	Gly-4	8190	23433	27908	7607
The training set for H^+Gly_n	H^+Gly-2	1700	6752	6752	1629
	H^+Gly-3	4418	18593	25759	4262
	H^+Gly-4	6736	25863	27385	6915

Table S3. Number of training sets of the model's generations