Description of Additional Supplementary Files

Supplementary Data 1: Training performance (MAE_{tr} and R²_{tr}) of ten parallel ML experiments, trained based on three different number of datasets and four algorithms with 80-bit one-hot representation.

Supplementary Data 2: The top 8,000 AP_{HC} of tetrapeptides.

Supplementary Data 3: The top 8,000 C_g of tetrapeptides.

Supplementary Data 4: Mass spectrometry of 165 synthetic tetrapeptides.

Supplementary Data 5: Nuclear magnetic resonance spectroscopy and peak location and associated information of 165 synthetic tetrapeptides.

Supplementary Data 6: Transmission electron microscope morphologies of 165 synthetic tetrapeptide hydrogels/solutions.

Supplementary Data 7: Statistical results of gelation experiments of 165 synthetic tetrapeptides