Supporting Information for the Article

Computational Design of Helical Artificial Metallopeptides: From Sequence to Activity in Pd-Peptide Systems

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Table of Contents

S1. Supplementary Figures

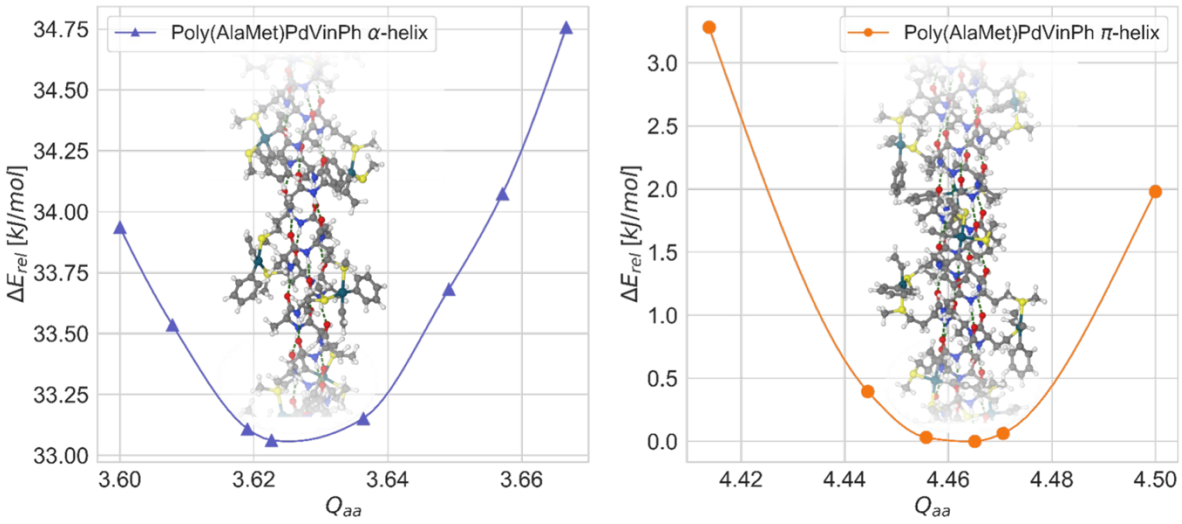

Figure S1. Potential energy surfaces near the minima of the π- and α-helical conformations of $[PhVinPd(Met\text{-}Ala)_2]_n$.

S2. Symmetry Reduction Procedure

If a monomer in the chain consists of a single amino acid, it is evident that Q corresponds to the number of amino acid residues per turn (Q_{aa}). However, when a monomer comprises multiple amino acids, an analogous mapping is not always straightforward. To address this, we will elaborate further on this specific case when the object's symmetry group is defined by a screw axis.

Suppose we have a structure described by a screw axis L_0 with defined parameters (Q_0, q_0, r_0, f_0) and monomer M_0. To replicate this structure using a new monomer M^N (repeated N times), we need to determine the generator of the new symmetry group and define the structure of the new monomer M^N, enabling subsequent modifications to its configuration.

The structure of the new monomer M^N is simply determined by applying the corresponding symmetry operations to the original monomer, namely:

$$\begin{aligned} \mathrm{M}^N &= \sum_{x=0}^{x=N-1} M_0\left(C_Q\middle|f\right)^x \\ &= \left[M_0\left(C_Q\middle|f\right)^0, M_0\left(C_Q\middle|f\right)^1, M_0\left(C_Q\middle|f\right)^2, \dots, M_0\left(C_Q\middle|f\right)^{N-1}\right] \\ &= \left[M_0, M_1, M_2, \dots, M_{N-1}\right] \end{aligned} \tag{s1}$$

Square brackets here denote a collection of atoms. Thus, the monomer $\boldsymbol{M^N}$ will contain $\boldsymbol{N}$ times more atoms than the original $\boldsymbol{M_0}$. Once the structure of the new monomer is obtained as a collection of fragments from the original, it becomes straightforward to modify each resulting fragment $\boldsymbol{M_x}$ to achieve the desired structure.

To determine the parameters $\boldsymbol{q_N}$, $\boldsymbol{r_N}$, $\boldsymbol{f_N}$ of the new group, we can refer to the following relationships:

$$\frac{1}{Q_N} = \left\{\frac{N}{Q_0}\right\} \; or \; 1 \tag{s2a}$$

$$f_N = Nf \tag{s2b}$$

Here, $\left\{\frac{N}{Q_0}\right\}$ denotes the fractional part of the number. If the result is an integer, 1 is used instead of 0. Using relationships 1b, 4 (main text), s2a, and s2b, we can derive the equations linking the original group parameters (q, r, f) to those of the group after scaling up the monomer:

$$q_N = \begin{cases} {}^{q}/_{N}, & \text{for q } mod \text{ N} = 0 \text{ and N} < q \\ 1, & \text{for } N \; mod \; q = 0 \; and \; N \geq q \\ {}^{q}/_{GCD(q,\ N)}, & otherwise \end{cases} \tag{s3a}$$

$$r_N = \begin{cases} 1, & \text{for } N \; mod \; q = 0 \; and \; N \geq q \\ q_N \left\{\frac{Nr}{q}\right\}, & otherwise \end{cases} \tag{s3b}$$

$$t_N = \begin{cases} t, & \text{for } q \; mod \; N = 0 \text{ and } N < q \\ {}^{Nt}/_{q}, & \text{for } N \; mod \; q = 0 \; and \; N \geq q \\ {}^{Nt}/_{\text{GCD}(q,\ N)}, & otherwise \end{cases} \tag{s3c}$$

These relationships are sufficient to determine the parameters of the new group. Thus, knowing the symmetry group and structural parameters allows us to construct a system with effectively the same structure but a modified monomer size. In this case, Q_0 serves as Q_{aa} (the number of amino acid residues per turn), while f_0 represents the average shift of amino acids within the new monomer, and h_0 corresponds to the average height of a turn composed not of the new monomer but of individual amino acids. These characteristics are explicitly used in subsequent sections of this work.