

**Multiscale Design Principles for Noncovalent Heteroaryl Phosphonate
Inhibitors Targeting NDM-1**

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Supplementary Information

Figure S1. Bar plots depicting the average atomic distances corresponding to the data shown in Table 2.

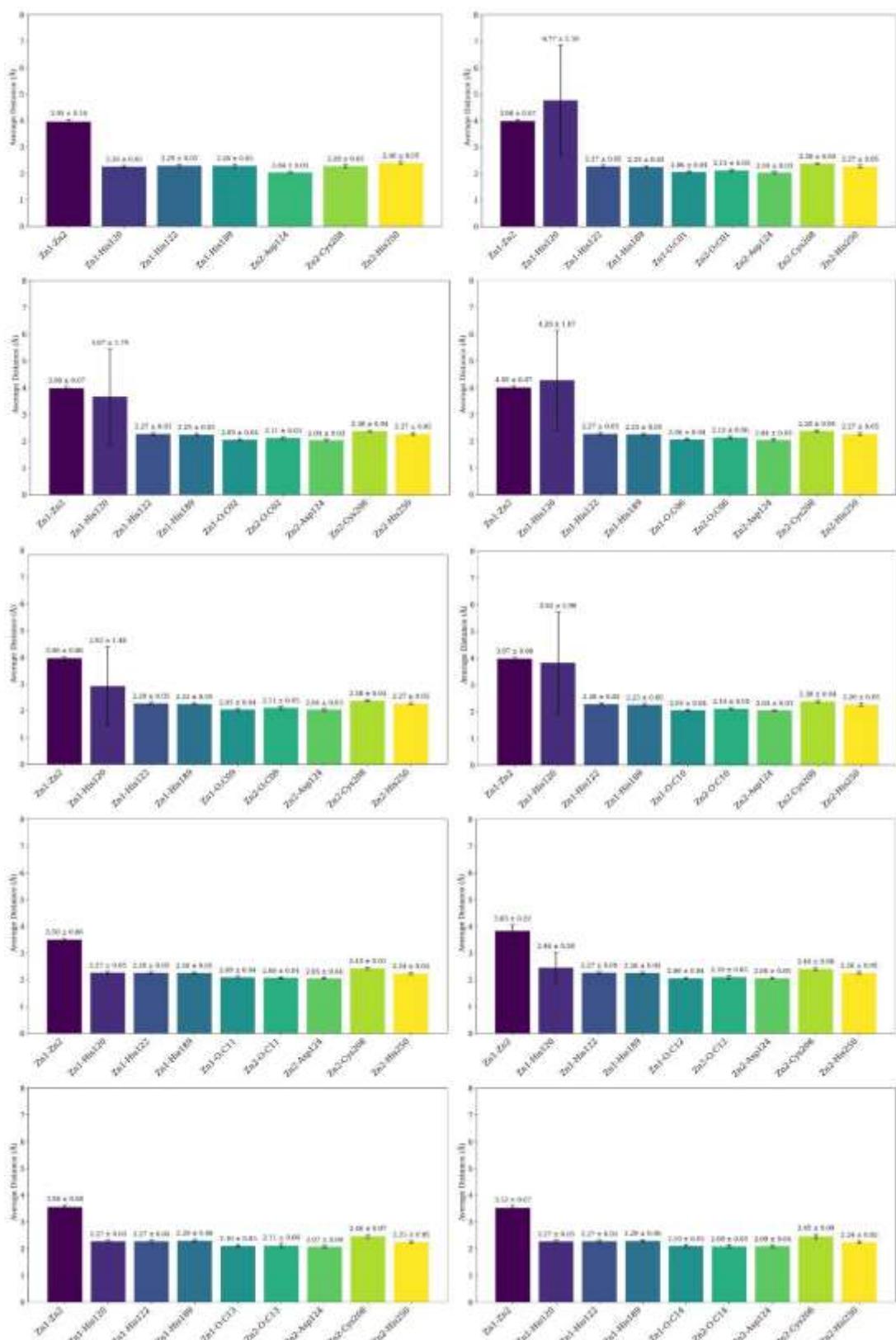


Figure S2. RMSD plots for all NDM-1 systems (in triplicate).

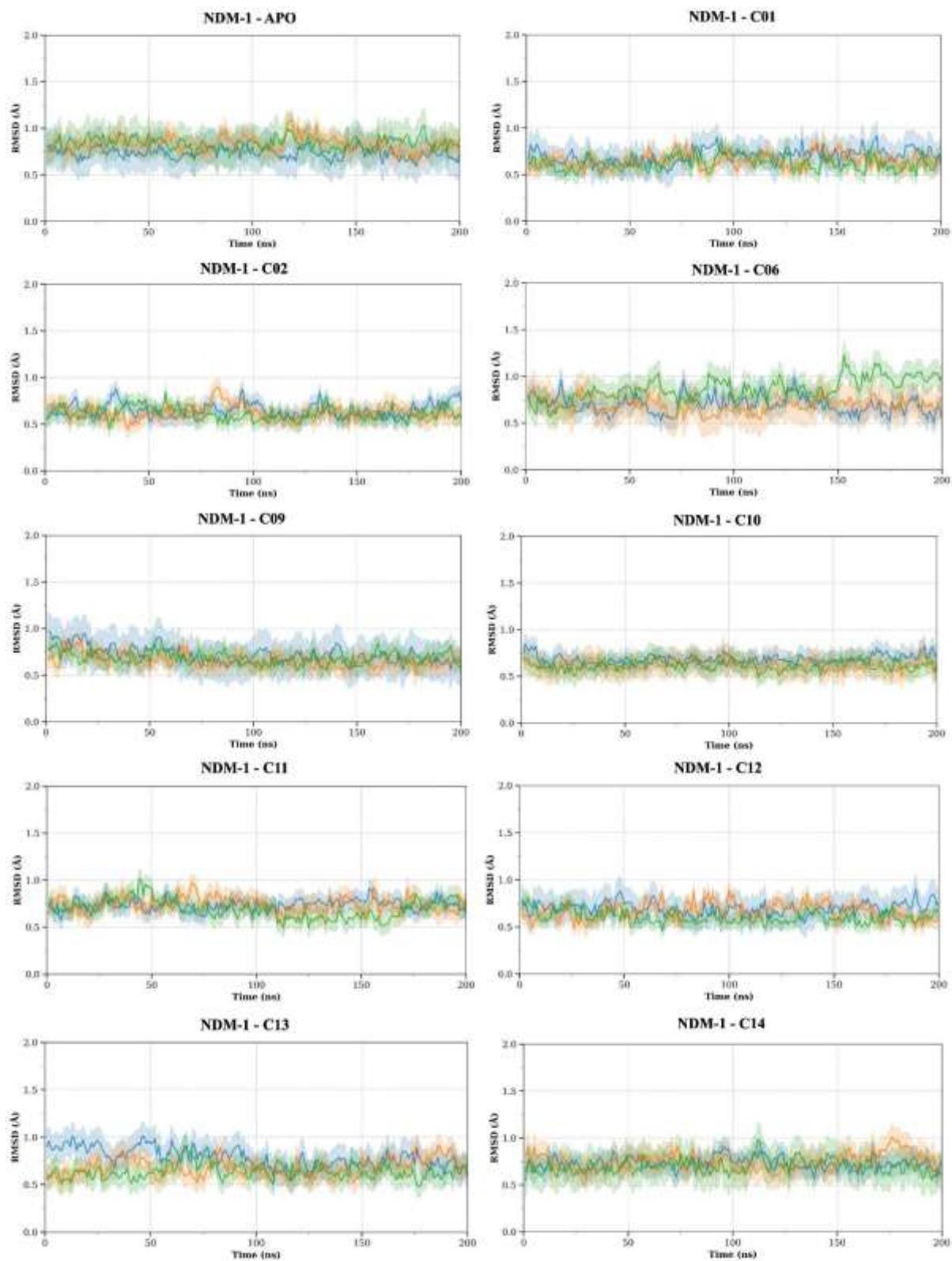


Figure S3. RMSF plots for all NDM-1 systems (in triplicate).

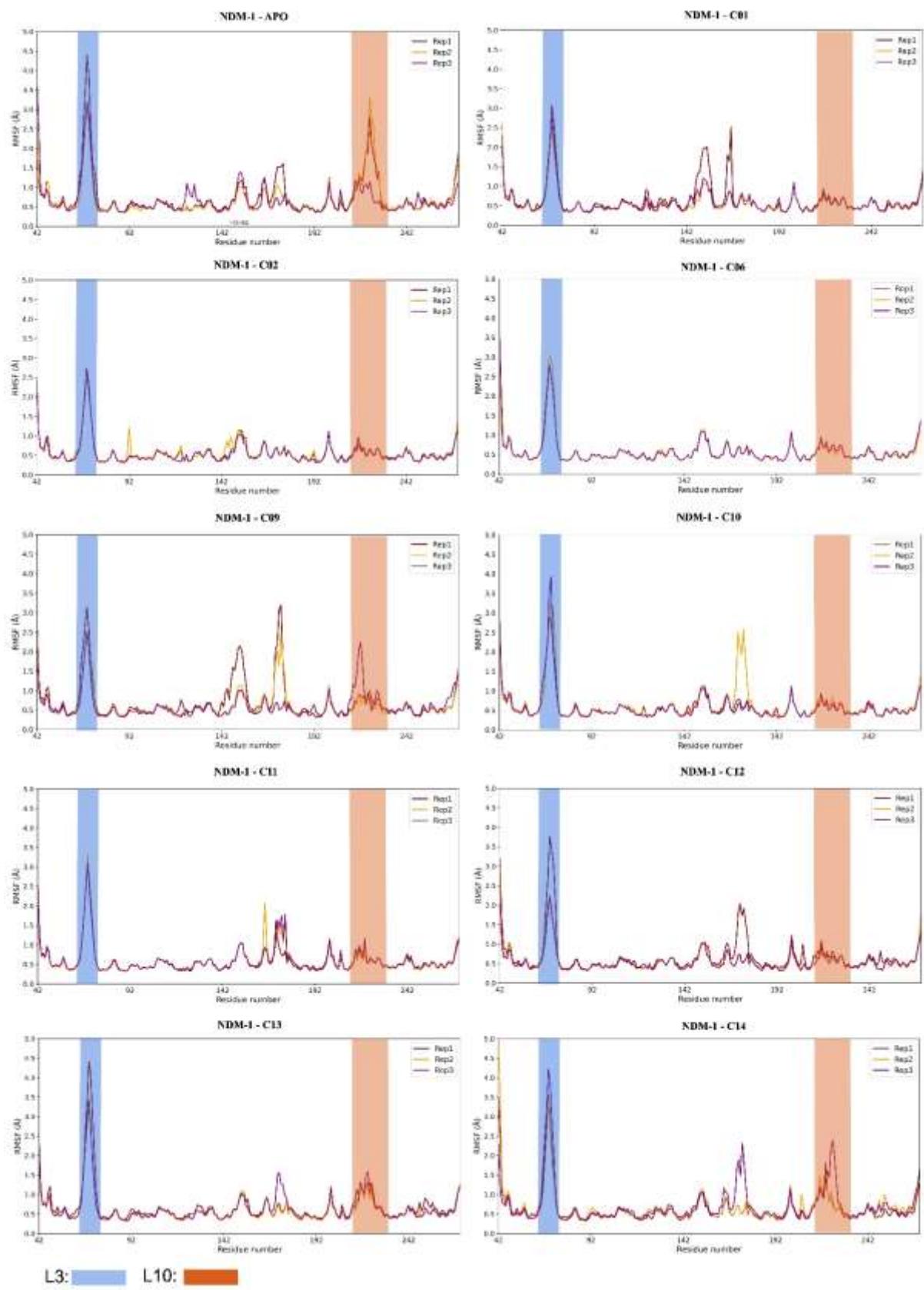


Figure S4. PCA plots for all NDM-1 systems (in triplicate).

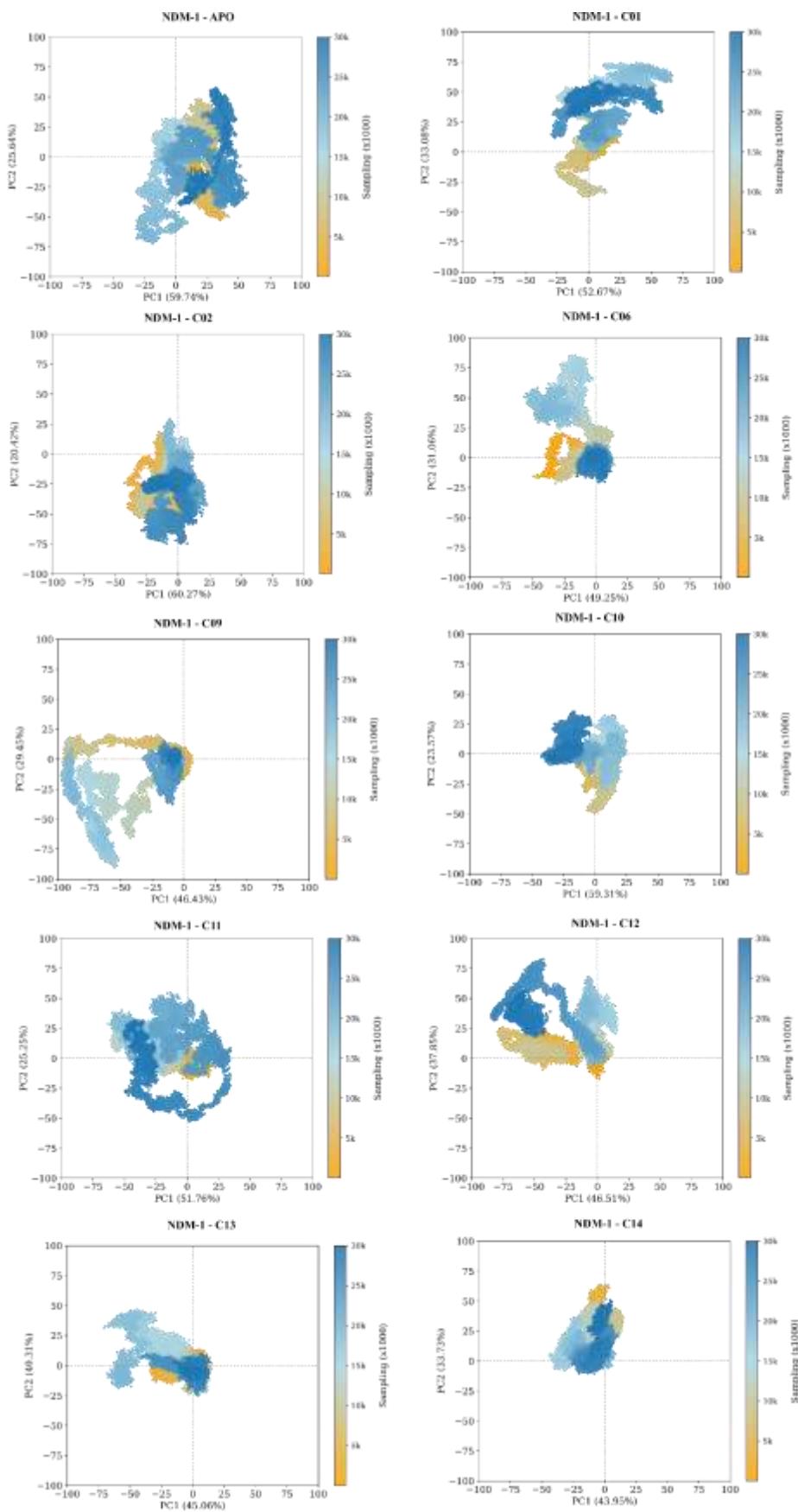


Figure S5. FEL plots for all NDM-1 systems (in triplicate).

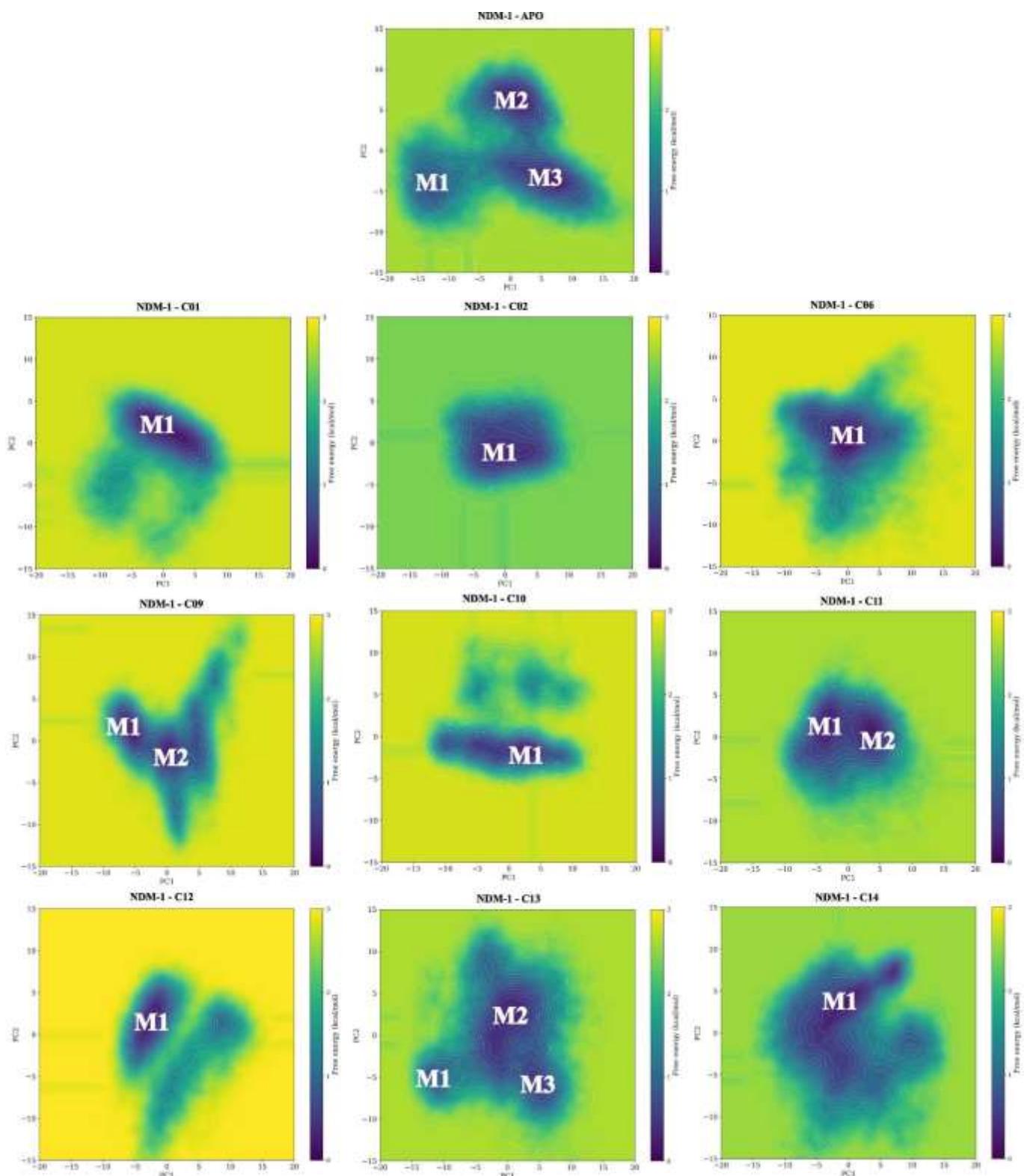


Figure S6. Linear regression plots for A) ΔG_{EXP} versus E_{vdW} and B) ΔG_{EXP} versus ΔE_{vdW} .

All values are reported in kcal/mol.

