Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Insights on peptides topology in the computational design of protein ligands: the example of lysozyme binding peptides

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time (ns)	binding site rank 1	2	3	4	5	6
0	P	P	P	P	P	P
5	P	P	P	P	P	B
10	P	P	P	B	P	P
15	P	B	R	P	P	B
20	P	B	P	P	R	B
25	P	P	P	B	B	B
30	P	B	P	P	B	B
35	P	B	B	P	P	P
40	P	B	P	R	P	P
45	P	P	P	B	R	B
50	P	B	B	P	P	P

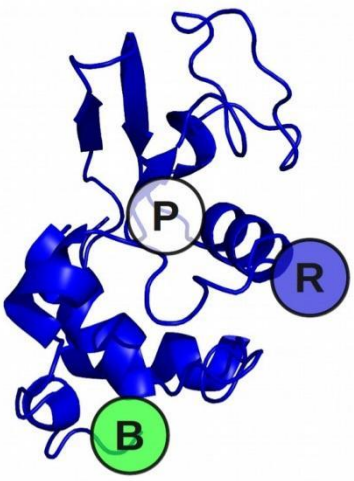

Figure S1. Identification and ranking of binding sites HuL for conformation sampled along 50ns molecular dynamics trajectory. Binding site are labelled as: pocket (P), right site (R, blue), and a bottom site (B, green).

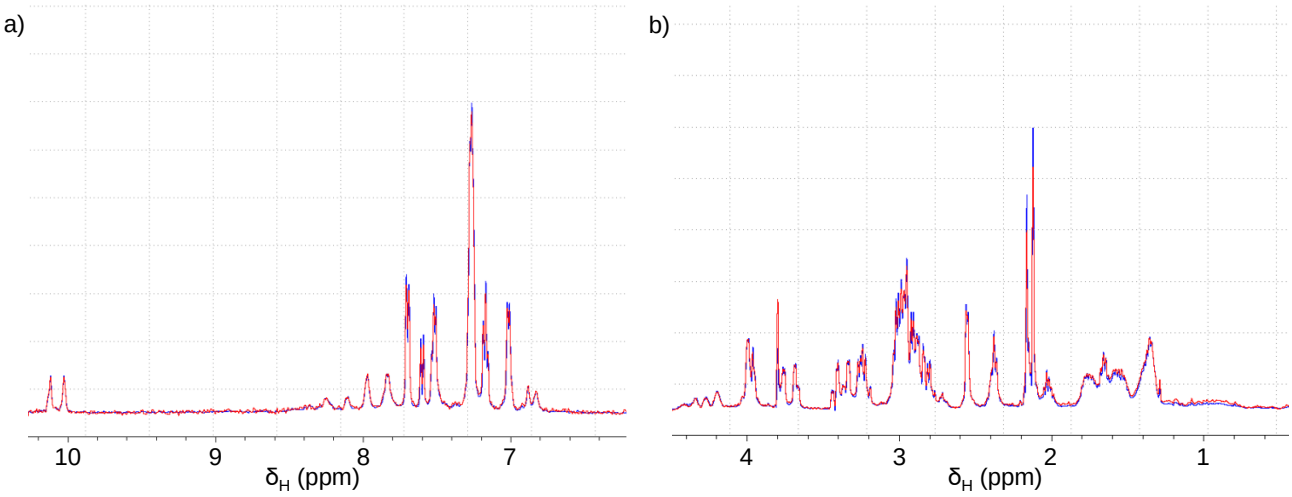

Figure S2. Overlay of a) aromatic and b) aliphatic 1H NMR spectra of peptide 140 at 0.2 mM (blue) and 0.6 mM (red). The spectra were scaled at the same intensity to better appreciate the unaltered peak linewidths.

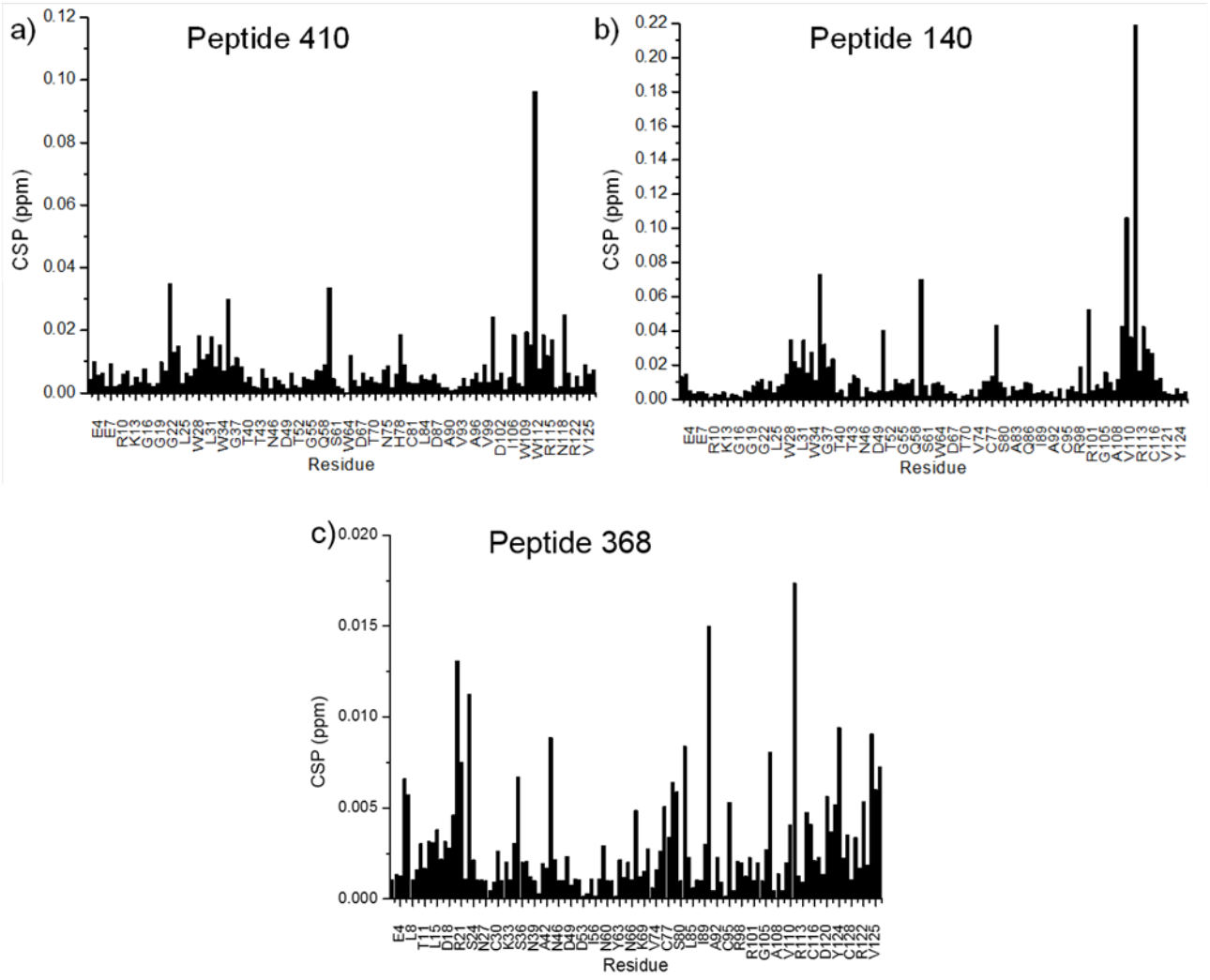

Figure S3. CSP bar plots recorded at protein/peptide ratio of 1/3 with a) peptide 410, b) peptide 140 and c) peptide 368. For the calculation of CSP see Experimental Section.

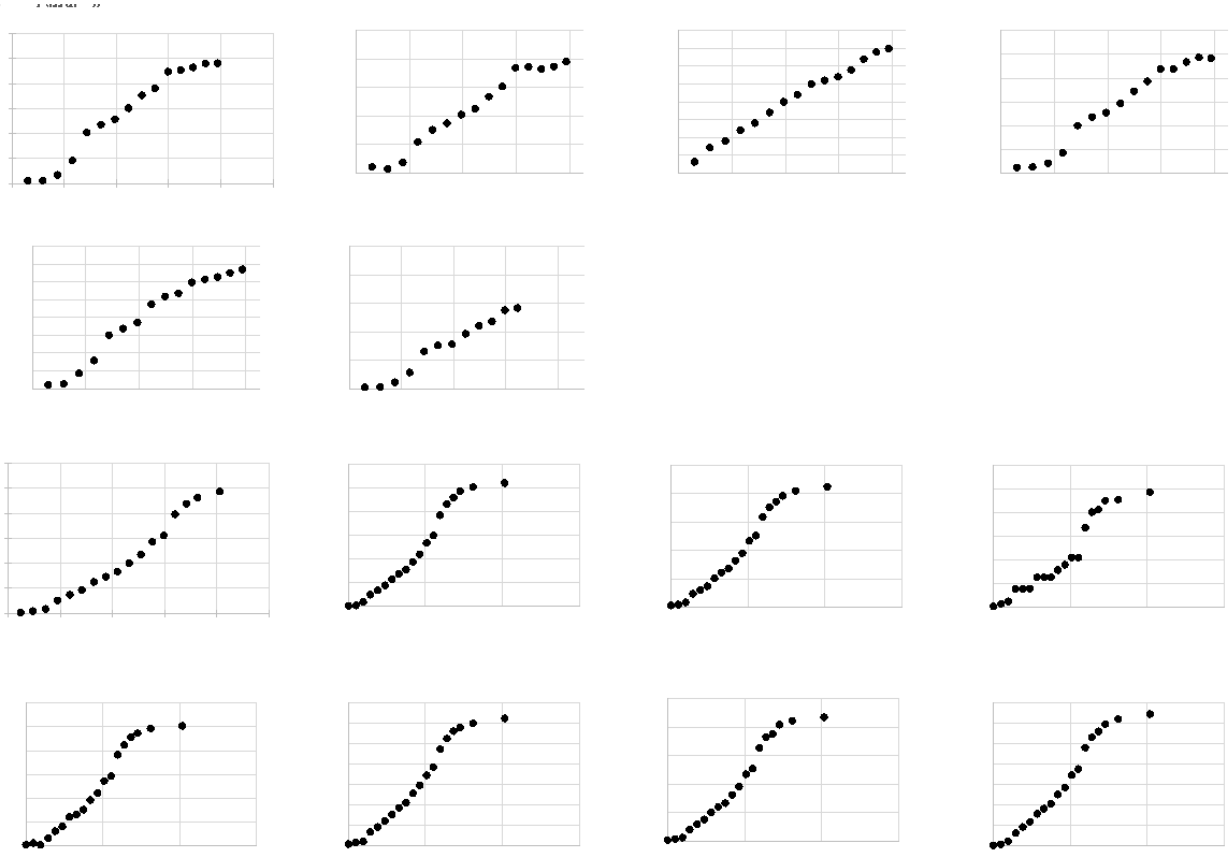

Figure S4. Representative CSP of selected residues with peptide 410 (a) and 140 (b) concentration. The HuL concentration was 299 μM with peptide 410 and 239 μM with peptide 140.

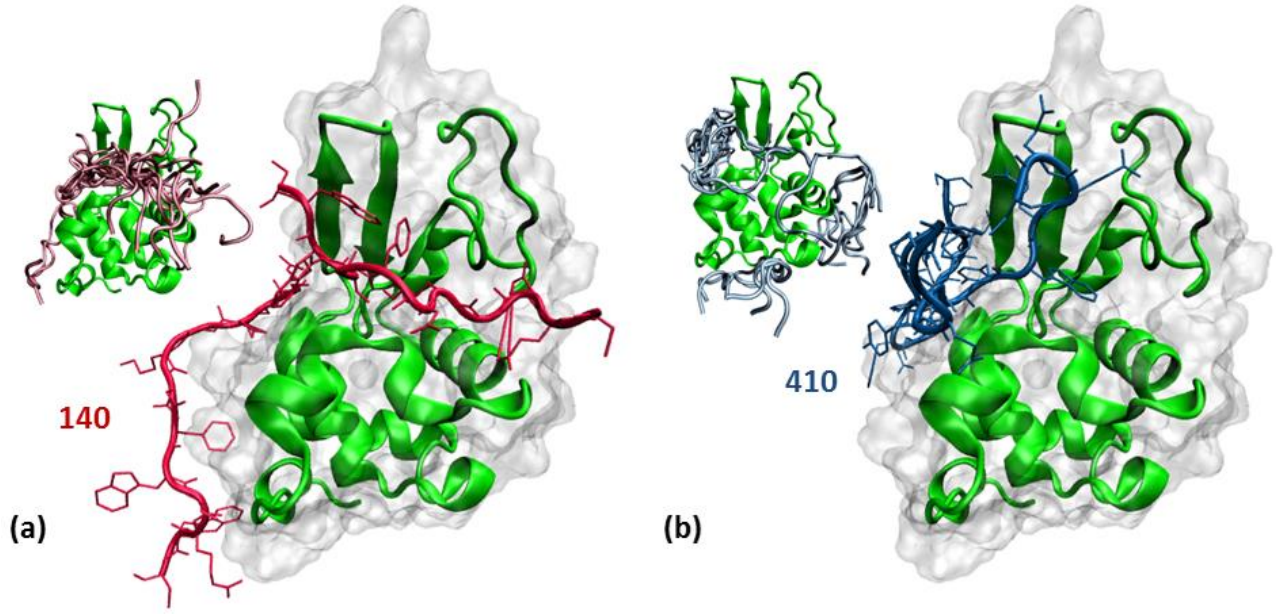

Figure S5. Blind docking results. Peptides140 (a) and 410 (b) representative docked conformations corresponding to the two most populated clusters as calculated from 80 AutoDock CrankPep (ADCP) runs with 2500000 steps each [1-2]. In the insets: the 20 lowest energy clusters.

References:

[1] Zhang, Yuqi, and Michel F. Sanner. "Docking flexible cyclic peptides with AutoDock CrankPep." *J. Chem. Theory. Comput.*, **2019**, 15(10), 5161-5168.

[2] Zhang, Yuqi, and Michel F. Sanner. "AutoDock CrankPep: combining folding and docking to predict protein–peptide complexes." *Bioinformatics*, **2019**, 35(24), 5121-5127.