

SUPPLEMENTARY MATERIAL

**XPS and ToF-SIMS Investigation of α -Helical and β -Strand Peptide
Adsorption onto SAMs**

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Table S1: PCA Scores for LK β 15 adsorbed onto methyl and carboxyl SAMs. Percent variance for each PC is also shown. The letter in each sample name denotes the type of SAM (M for methyl and C for carboxyl). The number denotes the peptide adsorption concentration in mg/mL. Samples labeled M and C are the bare SAMs without adsorbed peptide.

Samples	PC 1 Scores	PC 2 Scores
C – 0.05	-0.010	0.136
C – 0.05	0.004	0.127
C – 0.05	0.047	0.083
C – 0.05	-0.002	0.138
C – 0.05	0.011	0.116
C – 0.05	-0.009	0.144
C – 0.05	-0.016	0.152
C – 0.05	-0.006	0.140
C – 0.05	-0.013	0.145
C – 0.001	0.019	0.110
C – 0.001	0.030	0.092
C – 0.001	0.059	0.070
C – 0.001	0.012	0.108
C – 0.001	0.020	0.107
C – 0.001	0.051	0.077
C – 0.001	0.057	0.071
C – 0.001	0.067	0.062
C – 0.001	0.050	0.077
C – 0.001	0.057	0.070
C	-0.272	-0.029
C	-0.271	-0.031
C	-0.255	-0.025
C	-0.268	-0.010
C	-0.267	-0.011
C	-0.268	-0.009
M – 0.3	0.053	-0.074
M – 0.3	0.051	-0.074
M – 0.3	0.053	-0.075
M – 0.3	0.054	-0.071
M – 0.3	0.186	-0.054
M – 0.3	0.193	-0.063
M – 0.3	0.196	-0.076
M – 0.3	0.158	-0.022
M – 0.3	0.168	-0.030
M – 0.05	0.056	-0.070
M – 0.05	0.060	-0.075
M – 0.05	0.059	-0.072
M – 0.05	0.061	-0.068
M – 0.05	0.192	-0.089
M – 0.05	0.203	-0.097

M - 0.05	0.196	-0.096
M - 0.05	0.209	-0.105
M - 0.05	0.206	-0.105
M	-0.308	-0.102
M	-0.301	-0.100
M	-0.294	-0.093
M	-0.107	-0.095
M	-0.096	-0.105
M	-0.073	-0.100
Percent Variance	69	24

Table S2: PCA Loadings for LK β 15 adsorbed onto methyl and carboxyl SAMs. The peak subset indicates whether the peak is from the lysine peak list (K), leucine peak list (L) or from both (B).

Peak label	Peak subset	Peak mass	PC 1 Loadings	PC 2 Loadings
NH ₃	K	17.0266	-0.02	0.01
NH ₄	K	18.0344	-0.61	-0.34
CH ₂ N	K	28.0187	-0.04	0.16
CH ₄ N	K	30.0344	0.07	0.67
CH ₅ N	K	31.0422	-0.01	0.05
C ₂ H ₆ N	B	44.0500	-0.25	-0.16
C ₂ H ₇ N	K	45.0579	-0.07	-0.04
C ₃ H ₆ N	K	56.0500	-0.11	0.04
C ₅ H ₁₀ N	K	84.0813	0.61	-0.58
C ₅ H ₁₂ N	L	86.0970	0.42	0.19