Supporting Information

Residue-Dependent Adsorption of Model Oligopeptides on Gold

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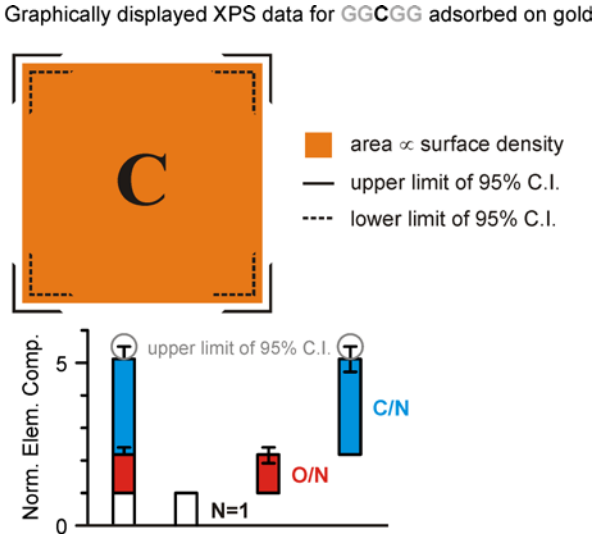

Figure S1. Explanatory diagram for graphical representation of the results of XPS analyses.

(Top) Square graphics used to represent the peptide surface densities in Figure 8. The area of the main colored square represents (is proportional to) the mean measured value. The upper and lower limits of the 95% C.I. are indicated by the outlines of larger (solid) and smaller (dashed) squares, respectively. To avoid overlapping lines, these larger and smaller squares are only indicated in this illustration by the outlines of their corners, rather than their entire perimeters. In Figure 8, the representation is further simplified by showing only the main colored square and the corner outlines of the larger (outer) square to indicate the positive (upper) limit of the 95% C.I.

(Bottom) Stacked columns used to represent elemental ratios in Figures 4 and 5. Each stacked column, as shown in the example on the left, represents 3 separate values. The bottom of the column (white) represents the nitrogen contents of the sample, set to unity in this representation. The middle of the column (red) represents the O/N ratio. The top of the column (blue) represents the C/N ratio. As the N contents is set to unity in this representation, the numerical values corresponding to the heights of the red and blue columns are equal to the measured O/N and C/N ratios. The red and blue columns have 95% C.I. error bars associated with them (as shown in the “unstacked” version of the plot on the right). In the stacked version, as used in Figures 4 and 5, on the positive (upper) limit is shown (highlighted at the top of the blue columns in this illustration).

Table S1. C/N and O/N XPS intensity ratios after gold substrates were incubated in 1.0 mM (GG–X–GG, X_5) or 0.5 mM (X_{10}) peptide solutions for 24 h. (mean ± 95% C.I.; $n \geq 3$)

	X	GG–X–GG				X_5				X_{10}			
		C/N*	C/N**	O/N*	O/N**	C/N*	C/N**	O/N*	O/N**	C/N*	C/N**	O/N*	O/N**
Polar	C	2.2	2.9 ± 0.4	1.0	1.2 ± 0.2								
	N	2.0	12.7 ± 4	1.0	5.6 ± 0.9								
	P	2.5	13.2 ± 3	1.0	4.4 ± 1	4.5	9.7 ± 2	1.0	2.8 ± 0.1				
	Q	2.1	10.1 ± 2	1.0	3.5 ± 0.4								
	S	2.2	12.7 ± 2	1.2	3.9 ± 0.7	2.8	8.2 ± 0.8	1.8	1.6 ± 0.4	2.9	6.9 ± 0.7	1.9	2.9 ± 0.1
	T	2.3	5.9 ± 0.7	1.2	2.3 ± 0.1								
	W	3.0	6.3 ± 0.7	0.9	1.9 ± 0.3								
	Y	3.2	11.0 ± 3	1.2	3.0 ±2								
Nonpolar	A	2.2	7.7 ± 0.6	1.0	2.2 ± 0.1	2.8	7.1 ± 0.2	1.0	2.3 ± 0.1				
	G	2.0	10.5 ± 1	1.0	2.9 ± 0.2	2.0	10.5 ± 1	1.0	2.9 ± 0.2	2.0	11.7 ± 0.5	1.0	3.9 ± 0.1
	I	2.7	15.1 ± 5	1.0	5.4 ± 3								
	L	2.7	5.0 ± 0.1	1.0	1.8 ± 0.1								
	M	2.5	7.7 ± 2	1.0	4.4 ± 0.3								
	V	2.5	7.5 ± 1	1.0	2.6 ± 0.3								
Charged	D	2.3	11.3 ± 0.4	1.3	4.2 ± 0.4	3.7	8.8 ± 0.5	2.7	4.6 ± 0.1	3.8	7.4 ± 0.7	2.8	3.0 ± 0.1
	E	2.5	7.9 ± 1	1.3	3.0 ± 0.2	4.5	9.3 ± 0.6	2.7	3.4 ± 0.1	4.7	7.0 ± 0.8	2.8	2.8 ± 0.1
	H	2.0	6.2 ± 0.6	0.8	2.2 ± 0.3								
	K	2.3	9.1 ± 0.5	0.9	3.6 ± 0.7	2.9	7.7 ± 0.9	0.5	1.7 ± 0.3	3.0	6.2 ± 0.2	0.5	3.0 ± 0.1
	R	1.8	6.3 ± 1	0.7	4.1 ± 0.8	1.5	4.4 ± 0.4	0.3	2.4 ± 0.1	1.5	4.5 ± 0.2	0.3	2.1 ± 0.1

*Theoretical ratios based on the chemical formulas, including terminal amidation and acetylation
**Measured atomic ratios

Table S2. Normalized N/Au XPS intensity ratios after gold substrates were incubated in 1mM peptide solutions for 24 h. (mean ± 95% C.I.; $n \geq 3$)

	Residue	GG–X–GG	X_5	X_{10}
Polar	C	0.172 ± 0.024	--	--
	N	0.030 ± 0.004	--	--
	P	0.043 ± 0.008	0.058 ± 0.009	--
	Q	0.053 ± 0.007	--	--
	S	0.036 ± 0.008	0.053 ± 0.004	0.105 ± 0.008
	T	0.108 ± 0.009	--	--
	W	0.068 ± 0.005	--	--
	Y	0.053 ± 0.017	--	--
Nonpolar	A	0.075 ± 0.006	0.095 ± 0.005	--
	G	0.045 ± 0.003	0.045 ± 0.003	0.057 ± 0.005
	I	0.047 ± 0.010	--	--
	L	0.110 ± 0.021	--	--
	M	0.062 ± 0.008	--	--
	V	0.077 ± 0.014	--	--
Charged	D	0.050 ± 0.004	0.051 ± 0.004	0.084 ± 0.010
	E	0.069 ± 0.003	0.043 ± 0.010	0.088 ± 0.005
	H	0.070 ± 0.010	--	--
	K	0.051 ± 0.005	0.041 ± 0.004	0.067 ± 0.003
	R	0.078 ± 0.013	0.035 ± 0.004	0.044 ± 0.004

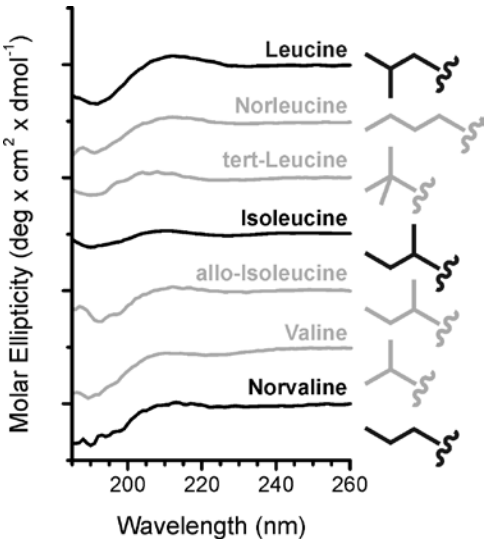

Figure S2. CD spectra of GG–X–GG peptides, where "X" is one of the structural isomers of leucine or valine. Solution CD spectra were measured at 0.5 mM peptide concentration in 10 mM sodium phosphate buffer (pH=7.0) in a 1-mm path quartz cuvette at 20°C. All spectra are normalized to show mean molar ellipticity per residue. Vertical offset is added to clarify the visual presentation: the molar ellipticity of each spectrum at 260 nm is approximately zero with the ticks representing 5,000 molar ellipticity units.

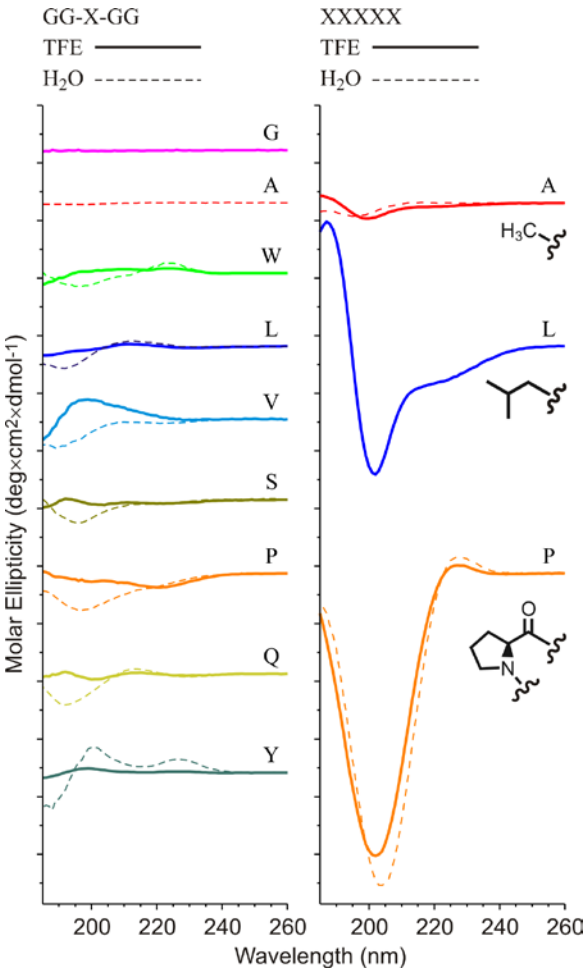

Figure S3. CD spectra of model oligopeptides in aqueous and organic solvents. Model GG–X–GG (left panel) and X_5 (right panel) peptides were measured at 0.5 mM concentration in 2,2,2-trifluoroethanol (TFE) or in aqueous 10 mM sodium phosphate (pH=7.0) in a 1-mm path quartz cuvette at 20°C. Spectra measured in TFE and PBS are indicated by solid and dashed lines, respectively; all the spectra are color-coded and labeled based on the "X" residues in GG–X–GG or X_5 sequences. All spectra are normalized to show mean molar ellipticity per residue. Vertical offset is added to clarify the visual presentation: the molar ellipticity of each spectrum at 260 nm is approximately zero with the ticks representing 5,000 molar ellipticity units.