nanomaterials

MDPI

Supplementary Material

The effect of oligomerization on a solid-binding peptide binding to silica-based materials

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$$\Delta\varepsilon_{\text{de-randomised}} = \frac{\Delta\varepsilon_{\text{exp}} - \frac{\#_{RC}}{\#_{\text{exp}}}\Delta\varepsilon_{RC}}{1 - \frac{\#_{RC}}{\#_{\text{exp}}}} \quad (1)$$

$$\Delta\varepsilon_{\text{exp}} = \frac{\#_{\text{de-randomised}}\,\Delta\varepsilon_{\text{de-randomised}} + \#_{RC}\,\Delta\varepsilon_{RC}}{\#_{\text{de-randomised}} + \#_{RC}} = \frac{\#_{\text{de-randomised}}\,\Delta\varepsilon_{\text{derandomised}} + \#_{RC}\,\Delta\varepsilon_{RC}}{\#_{\text{exp}}}$$

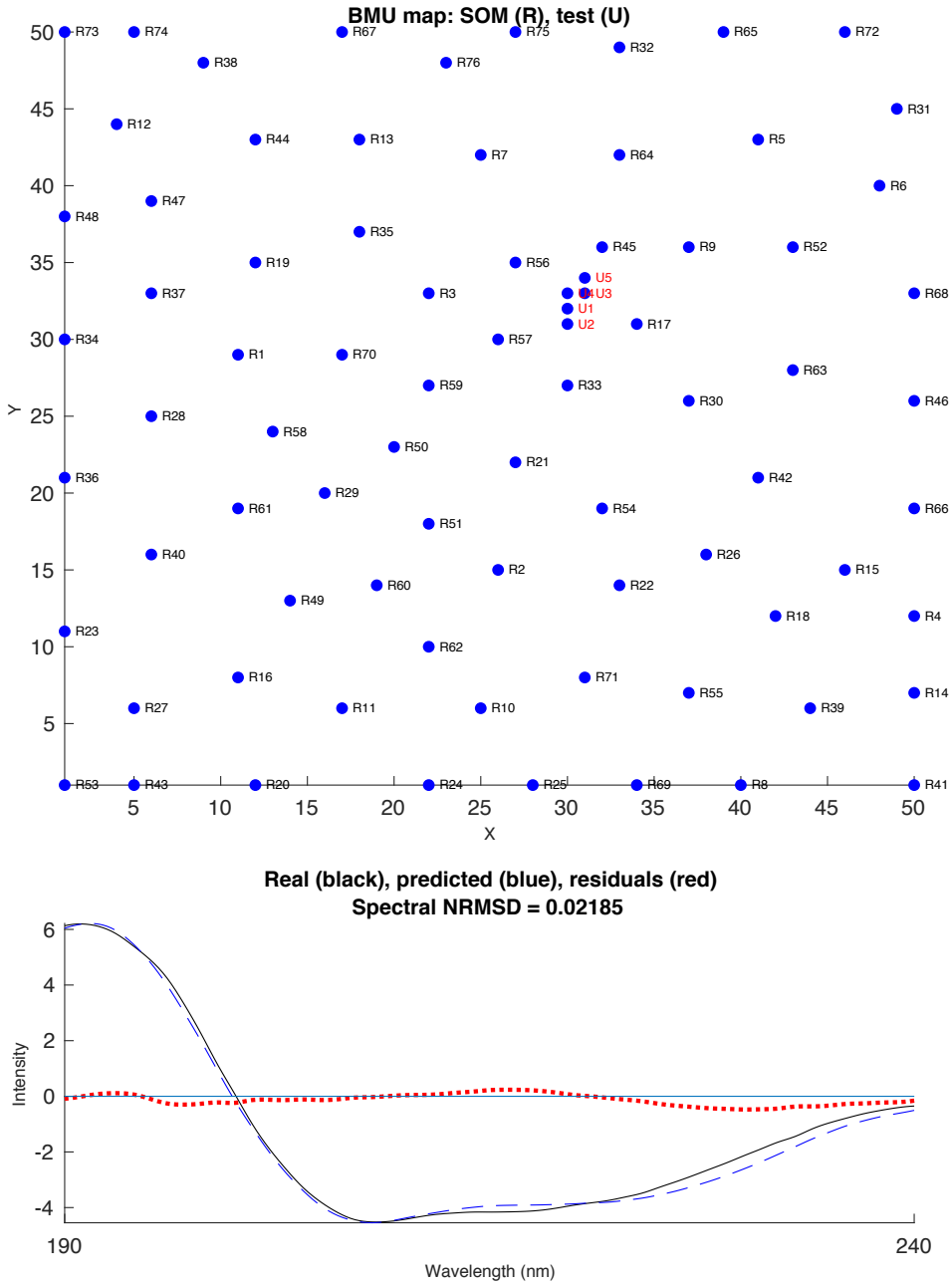
$$\Delta\varepsilon_{\text{exp}}(\#_{\text{de-randomised}} + \#_{RC}) = \#_{\text{de-randomised}}\,\Delta\varepsilon_{\text{de-randomised}} + \#_{RC}\,\Delta\varepsilon_{RC}$$

$$\Delta\varepsilon_{\text{de-randomised}} = \frac{\Delta\varepsilon_{\text{exp}}(\#_{\text{de-randomised}} + \#_{RC}) - \#_{RC}\,\Delta\varepsilon_{RC}}{\#_{\text{de-randomised}}}$$

$$= \frac{\#_{\text{exp}}(\Delta\varepsilon_{\text{exp}} - \frac{\#_{RC}}{\#_{\text{exp}}}\Delta\varepsilon_{RC})}{\#_{\text{exp}} - \#_{RC}}$$

$$= \frac{\Delta\varepsilon_{\text{exp}} - \frac{\#_{RC}}{\#_{\text{exp}}}\Delta\varepsilon_{RC}}{1 - \frac{\#_{RC}}{\#_{\text{exp}}}}$$

Equation S1. Derivation of Equation (1) of main text where *RC* denotes random coil, # denotes number of residues, exp denotes the full protein on which data were collected, and de-randomized denotes the core of the protein when the linkers and any extra unfolded residues are removed.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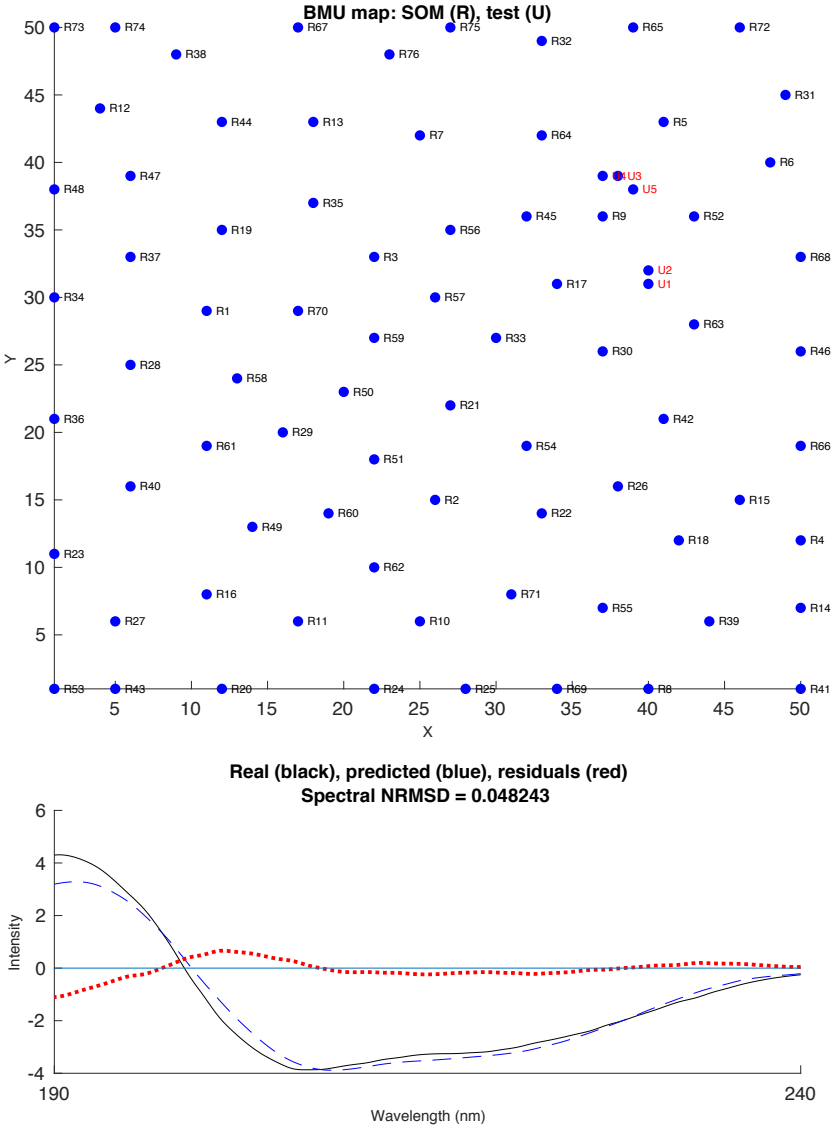
R32
R38 R76
R31
R12
R44 R13 R5
R7 R64
R6
R47
R48
R35
R45 R9 R52
R19 R56
U5
R37 R3 U4 U3 R68
U1
U2 R17
R34 R57
R1 R70
R63
R59 R33
R30 R46
R28
R58
R50
R21
R36 R42
R29
R61 R54 R66
R51
R40 R26
R2 R15
R60 R22
R49
R18 R4
R23
R62
R16 R71
R55 R14
R27 R11 R10 R39
R53 R43 R20 R24 R25 R69 R8 R41
X
Y
Real (black), predicted (blue), residuals (red)
Spectral NRMSD = 0.02185
Intensity
Wavelength (nm)

(a)


BMU map: SOM (R), test (U)
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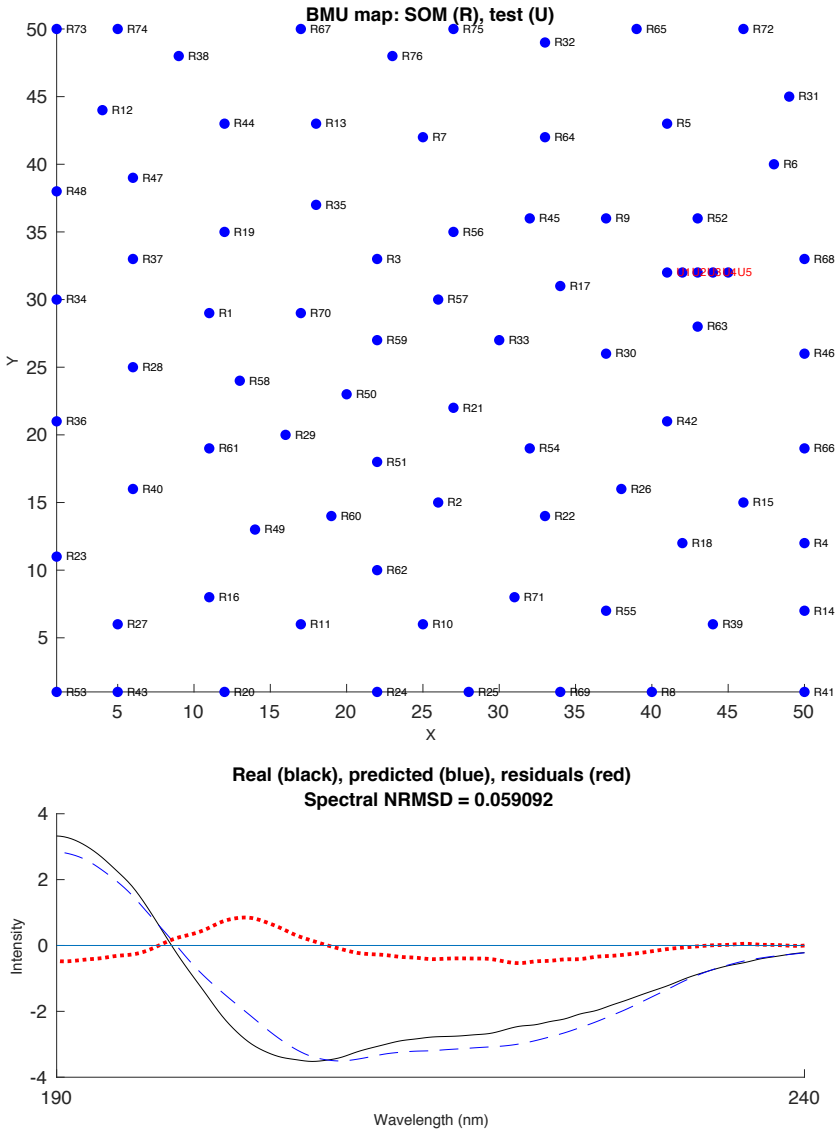
Y
Real (black), predicted (blue), residuals (red)
Spectral NRMSD = 0.048243
Intensity
Wavelength (nm)

(b)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R31
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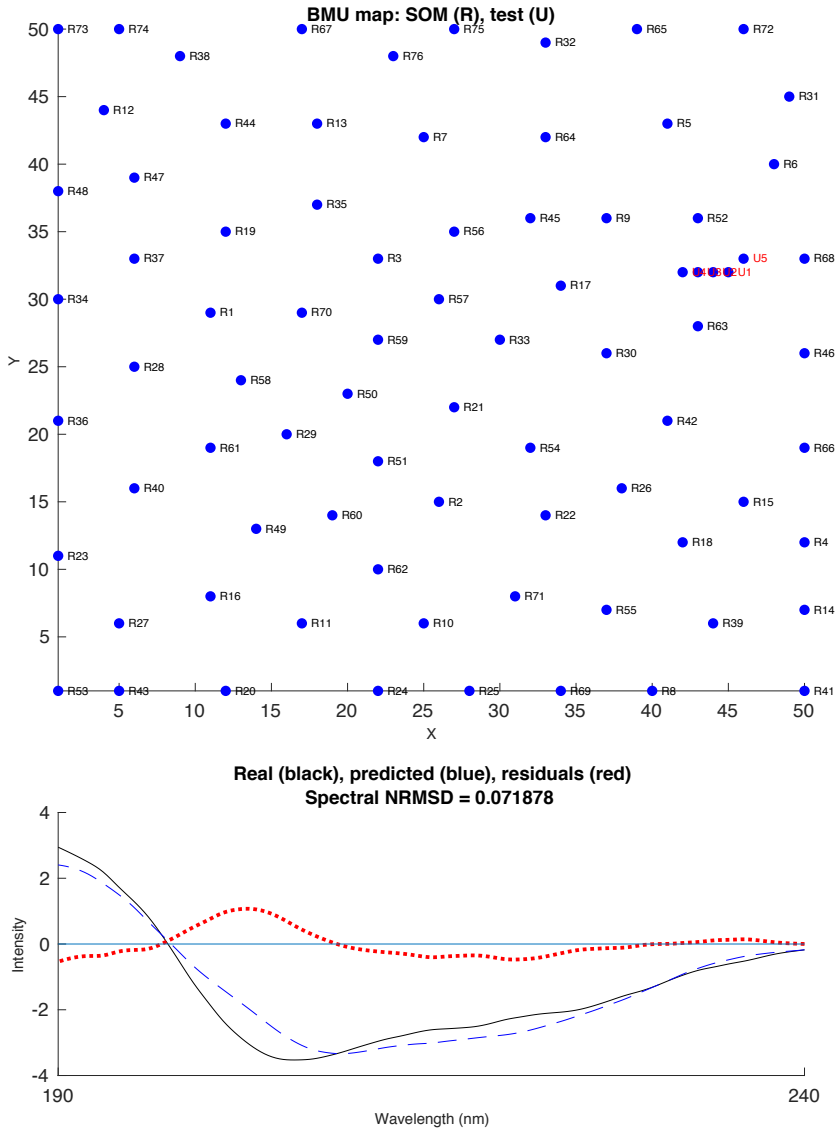
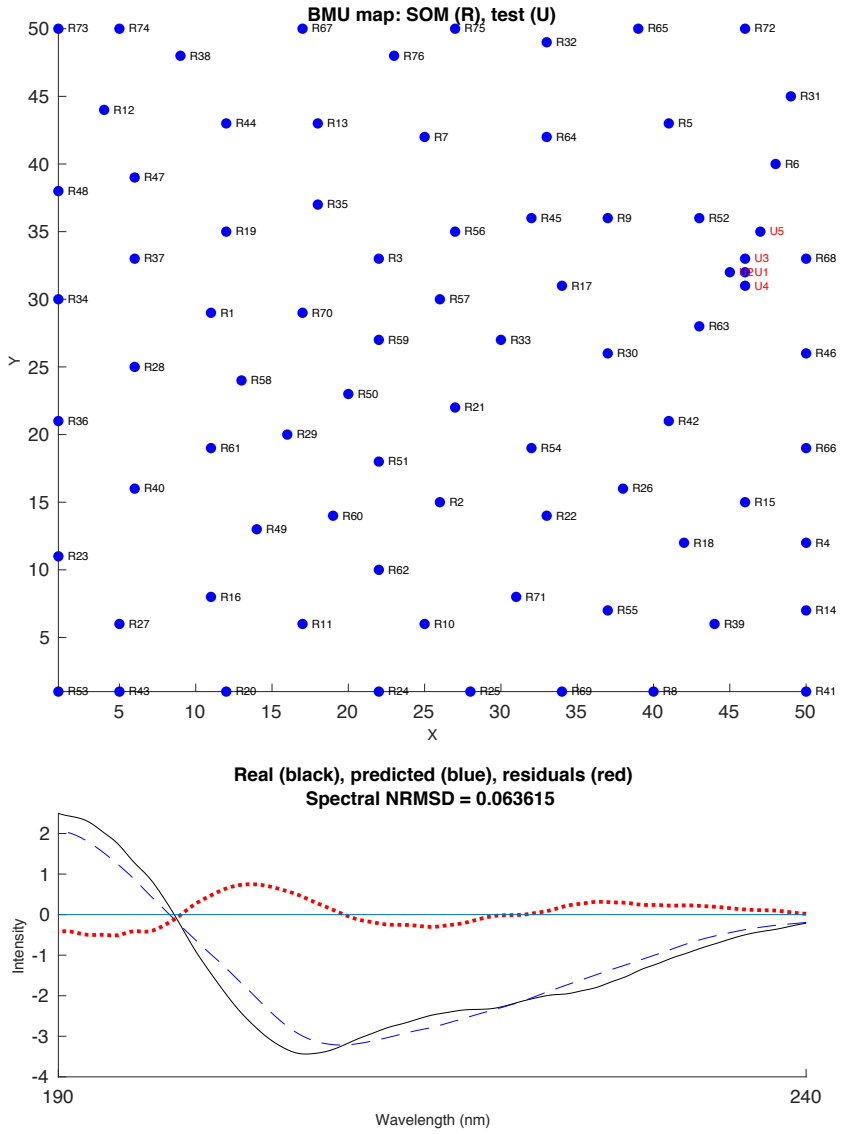
R6
R47
R48
R35
R45 R9 R52
R19 R56
R37 R3 R68
R17
R34 R57
R1 R70 R63
R59 R33 R30 R46
R28
R58
R50
R21
R36 R42
R29
R61 R54 R66
R51
R40 R26
R2 R15
R60 R22
R49
R18 R4
R23
R62
R16 R71
R55 R14
R27 R11 R10 R39
R53 R43 R20 R24 R25 R69 R8 R41
Y
X
Real (black), predicted (blue), residuals (red)
Spectral NRMSD = 0.059092
Intensity
Wavelength (nm)

(c)


BMU map: SOM (R), test (U)
X
Y
Real (black), predicted (blue), residuals (red)
Spectral NRMSD = 0.071878
Intensity
Wavelength (nm)

(d)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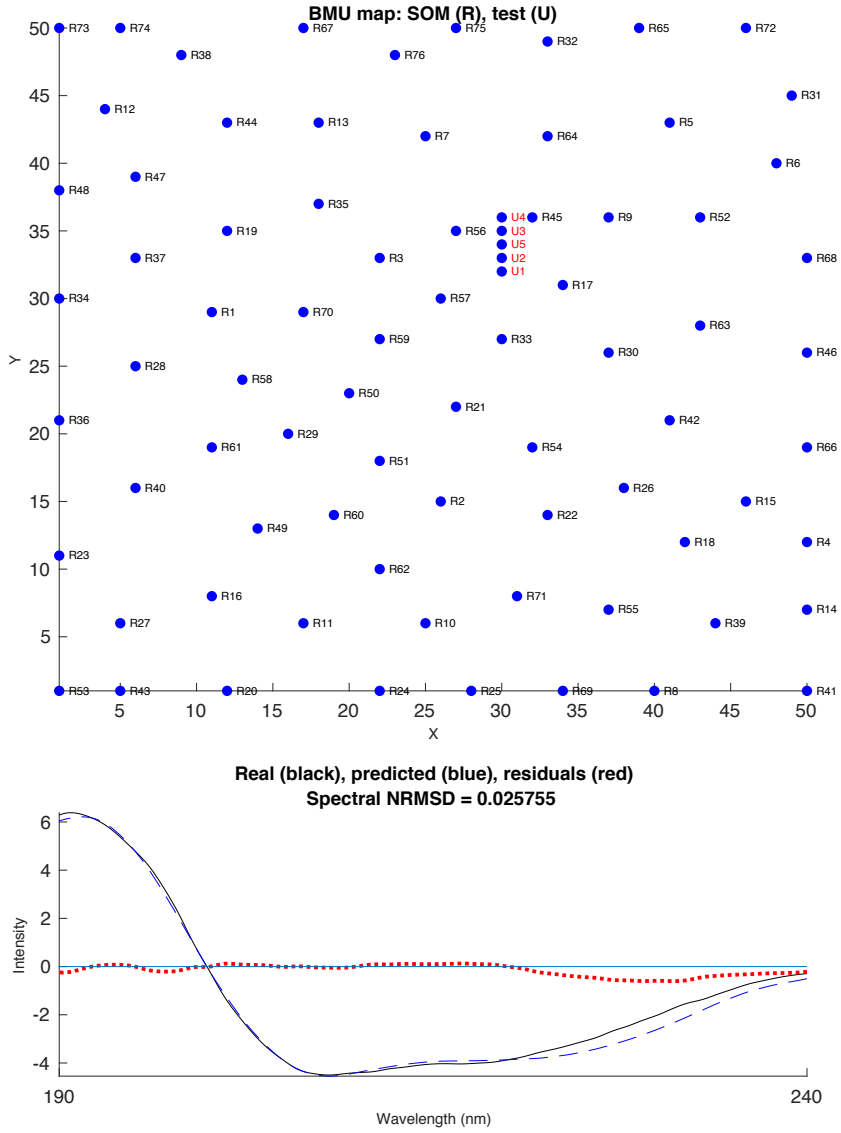
R32
R38 R76
R31
R12
R44 R13 R5
R7 R64
R6
R47
R48
R35
R45 R9 R52
R19 R56 U5
R37 R3 U3 R68
U2 U1
R17 U4
R34 R57
R1 R70
R63
R59 R33
R30 R46
R28
R58
R50
R21
R42
R36
R29
R61 R54 R66
R51
R40 R26
R2 R15
R60 R22
R49
R18 R4
R23
R62
R16 R71
R55 R14
R27 R11 R10 R39
R53 R43 R20 R24 R25 R69 R8 R41
Y
X
Real (black), predicted (blue), residuals (red)
Spectral NRMSD = 0.063615
Intensity
Wavelength (nm)

(e)


BMU map: SOM (R), test (U)
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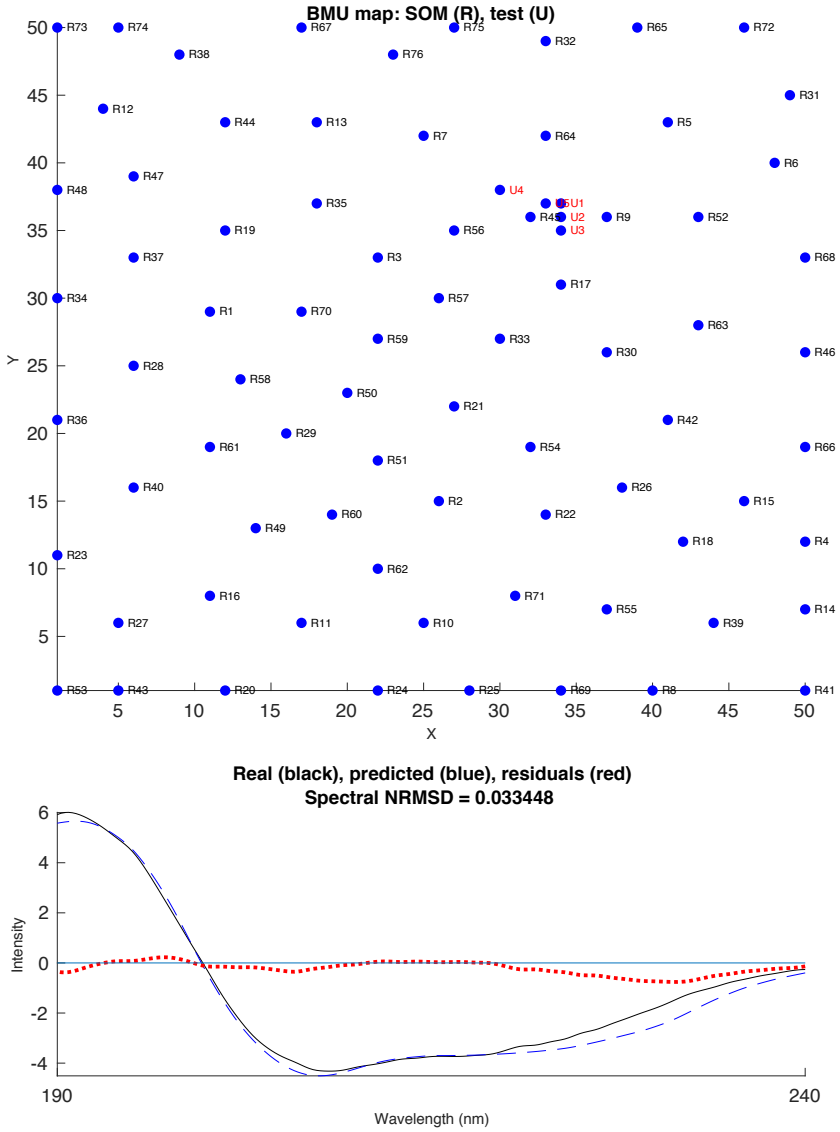
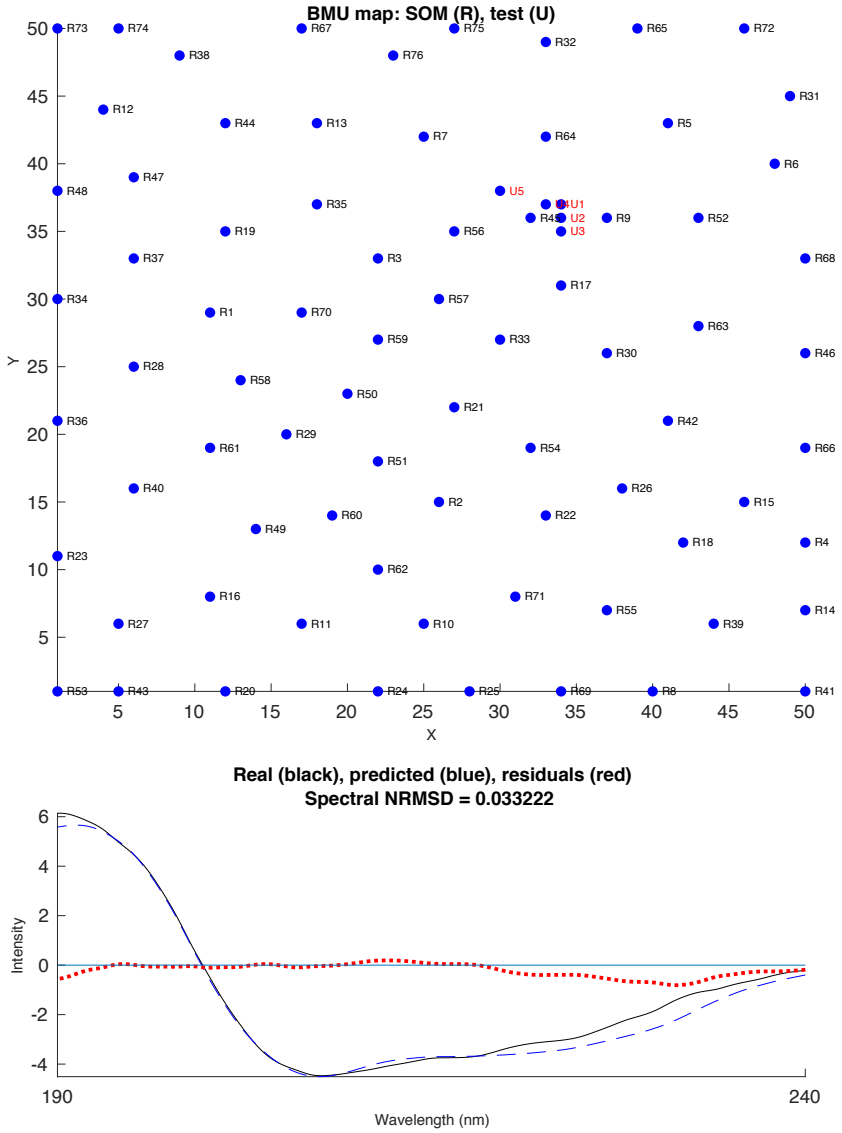
R38 R76
R31
R12 R44 R13 R5
R7 R64
R6
R47
R48
R35
U4 R45 R9 R52
R19 R56 U3
U5
R37 R3 U2 R68
U1
R17
R34 R1 R70 R57
R63
R59 R33
R30 R46
R28
R58
R50
R21
R36 R42
R29
R61 R54 R66
R51
R40 R26
R2 R15
R60 R22
R49
R18 R4
R23
R62
R16 R71
R55 R14
R27 R11 R10 R39
R53 R43 R20 R24 R25 R69 R8 R41
Y
X
Real (black), predicted (blue), residuals (red)
Spectral NRMSD = 0.025755
Intensity
Wavelength (nm)

(f)


BMU map: SOM (R), test (U)
X
Y
Real (black), predicted (blue), residuals (red)
Spectral NRMSD = 0.033448
Intensity
Wavelength (nm)

(g)


BMU map: SOM (R), test (U)
R73 R74 R67 R75 R32 R65 R72
R38 R76
R31
R12 R44 R13 R7 R64 R5
R6
R47
R48 U5
R35 U4 U1
R45 U2 R9 R52
R19 R56 U3
R37 R3 R68
R17
R34 R57
R1 R70
R63
R59 R33
R30 R46
R28
R58
R50
R21
R36 R42
R29
R61 R54 R66
R51
R40 R26
R2 R15
R60 R22
R49
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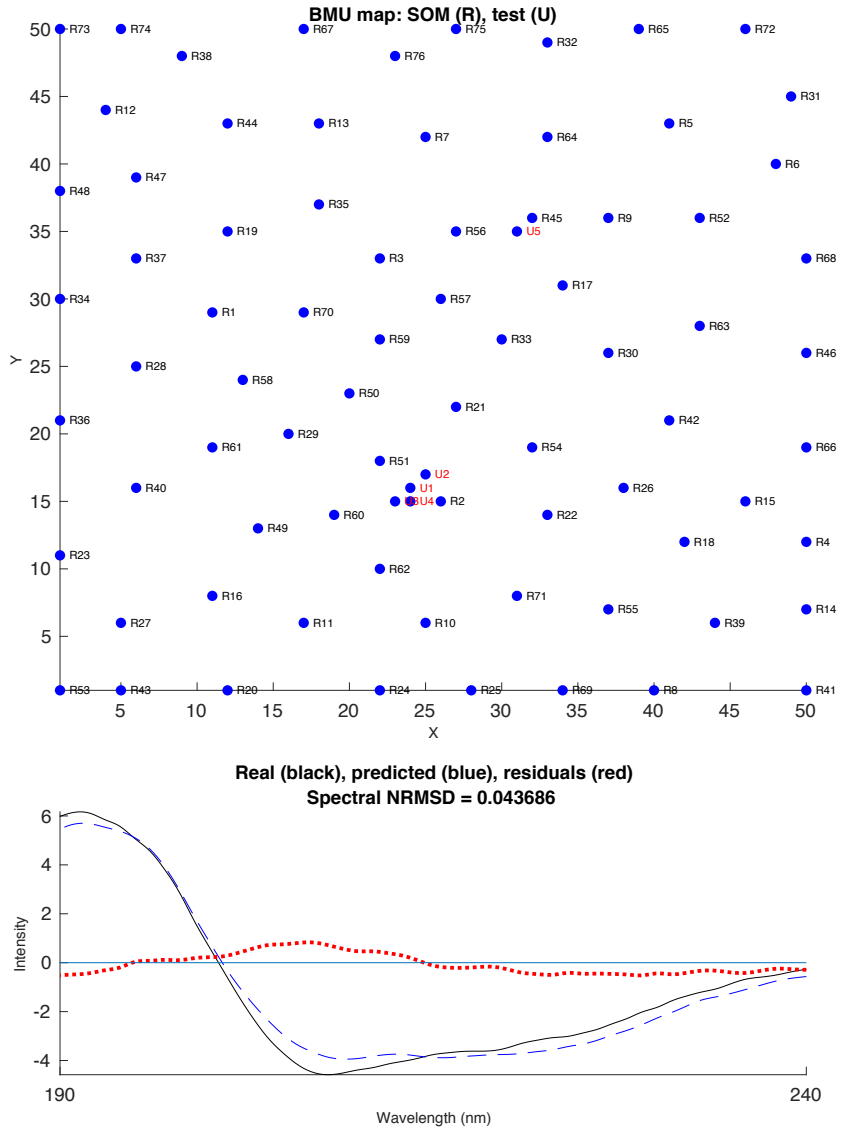
R23
R62
R16 R71
R55 R14
R27 R11 R10 R39
R53 R43 R20 R24 R25 R69 R8 R41
Y
X
Real (black), predicted (blue), residuals (red)
Spectral NRMSD = 0.033222
Intensity
Wavelength (nm)

(h)



(i)

Figure S1. SOMSpec output for (a) PG, (b) 1×LPG, (c) 2×LPG, (d) 3×LPG, (e) 4×LPG, (f) 1×LPG–0.22 random coil, (g) 2×LPG–0.31 random coil, (h) 3×LPG–0.36 random coil, (i) 4×LPG-0.40 random coil

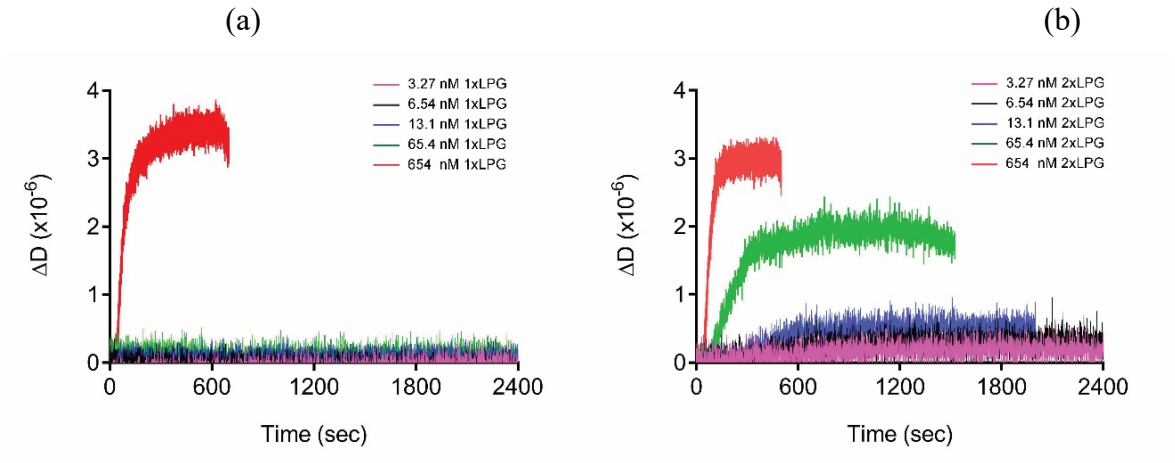


Figure S2. ΔD vs time for the 3rd overtone of the absorbed **(a)** 1xLPG and **(b)** 2xLPG on silica coated QCM-D crystals at various concentrations (3.27–654 nM). The measurement was performed in three steps at a flow rate of 150 μL/mL: baseline formation (1 × PBS buffer), adsorption of protein samples until saturation, and washing (1 × PBS buffer) to remove of unbound protein. Three independent measurements were performed for each concentration.

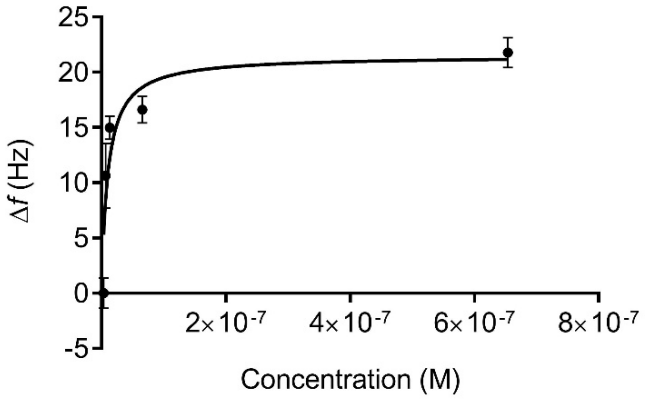


Figure S3. Langmuir adsorption isotherm for the adsorption of 3×LPG to silica surface. The data were fitted as per a single-site specific binding model, giving a binding affinity/equilibrium dissociation constant (K_D)= 53.23±4.5 nM.

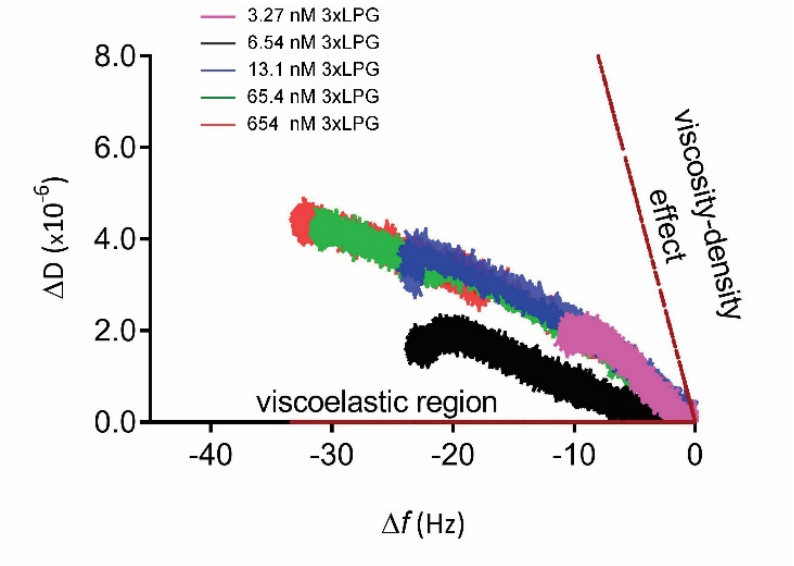


Figure S4. D*f* plot for the binding of 3×LPG to silica . The dotted lines indicate the pure elastic mass and viscosity-density responses indicating the data lie within the viscoelastic region.

Supplementary Table S1. Truncated derivatives of 4×LPG with different linker repeats and their physicochemical properties.

	Mw (kDa)[a]	**pI**[b]	**Charge**[c]	**GRAVY**[d]
Protein				
PG	21.363	4.58	–14.0	–0.56
1×LPG	23.443	4.69	–13.8	–0.69
2×LPG	25.797	4.94	–10.5	–0.78
3×LPG	28.151	5.25	–7.3	–0.85
4×LPG	30.504	5.80	-4.1	–0.91
Linker region without PG				
1×L	3.232	10.94	3.2	–1.27
2×L	5.586	11.38	6.4	–1.43
3×L	7.939	11.50	9.6	–1.50
4×L	10.293	11.57	12.9	–1.54

[a] Theoretical molecular weight (Mw)*

[b] Theoretical isoelectric point (pI)*

[c] Theoretical charge at pH 7.0*

[d] Theoretical grand average hydropathicity (GRAVY)†

* Values calculated using Protein calculator v3.4 (http://protcalc.sourceforge.net/)

† Values calculated using Protein GRAVY (https://www.bioinformatics.org/sms2/protein_gravy.html)