Supporting Information for:

Biological Identification of Peptides that Specifically Bind to Poly(phenylene vinylene) Surfaces: Recognition of the Branched or Linear Structure of the Conjugated Polymer

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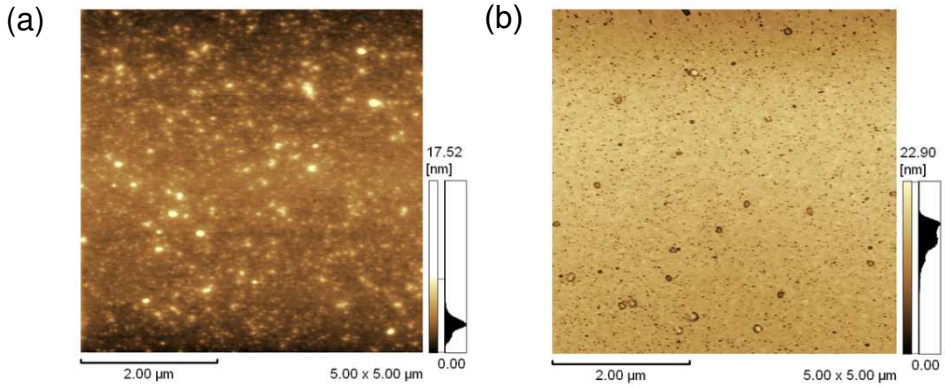
Peptide Synthesis. All amino acid derivatives, 1-hydroxybenzotriazole (HOBT), *O*-benzotriazole-*N,N,N',N'*-tetramethyl-uronium-hexafluoro-phosphate (HBTU), *N,N'*-diisopropylethylamine (DIEA), and the resins used for peptide synthesis were purchased from Novabiochem. All other chemicals and reagents were purchased from Nacalai Tesque. C-terminal amidated peptides (Hyp01, Hyp01-H1A, -T2A, -D3A, -W4A, -R5A, -L6A, -G7A, -T8A, -W9A, -H10A, -H11A, -S12A, Hyp04, Lin01) were synthesized by solid-phase synthesis using standard fluorenylmethoxycarbonyl (Fmoc) protocols starting with NovaSyn TGR resin. Briefly, the coupling reactions were performed with the resin (300 mg, amino group 0.2 mmol g^{-1}) and Fmoc amino acid derivatives (180 μmol) in the presence of HBTU (180 μmol), HOBt (180 μmol), and DIEA (360 μmol) in a *N*-methylpyrrolidone (NMP, 1.5 mL) and *N,N*-dimethylformamide (DMF, 0.5 mL) mixed solvent. The Fmoc groups were then removed by 20% piperidine-NMP. These steps were repeated sequentially until the desired sequences were obtained. After washing the resin with dichloromethane and methanol, the resins were dried in a vacuum for 4 hrs. The final peptides were cleaved from the resin, and all protecting groups were removed by the general trifluoroacetic acid (TFA) cleavage protocol. The peptide resin was mixed with a cleavage cocktail (triisopropylsilane 75 μL, distilled water 75 μL, and TFA 2.85 mL), and then stirred at room temperature for 2 hrs. The solution was filtered to remove the resin, and cooled diethyl ether was added to precipitate the peptide. The precipitate was washed five times with cooled diethyl ether, and the solvent was evaporated to give the crude product. The product was subsequently purified by reverse-phase high-performance liquid chromatography (ELITE LaChrom, Hitachi High-technologies) with a C18 column (Cosmosil 5C18-AR-300, 10 × 250 mm, Nacalai Tesque). The peptides were purified with a linear gradient of acetonitrile/water containing 0.05% TFA at a flow rate of 6 mL min^{-1}. After evaporation of the organic solvent and lyophilization, a white powder was obtained, and was confirmed by matrix-assisted laser desorption/ionization time-of-flight mass (MALDI-TOF MS, autoflex II TOF/TOF, Bruker Daltonics) spectrometry (Table S1)

Table S1. Synthesized peptide sequences and the results of MALDI-TOF MS.

Peptide	Sequence	m/z $[M+H]^+$ (found)	m/z $[M+H]^+$ (calcd.)
Hyp01	**HTDWRLGTWHHS**	1531.82	1531.72
Hyp01-H1A	**ATDWRLGTWHHS**	1465.71	1465.70
Hyp01-T2A	**HADWRLGTWHHS**	1501.83	1501.71
Hyp01-D3A	**HTAWRLGTWHHS**	1487.69	1487.73
Hyp01-W4A	**HTDARLGTWHHS**	1416.67	1416.68
Hyp01-R5A	**HTDWALGTWHHS**	1447.03	1446.66
Hyp01-L6A	**HTDWRAGTWHHS**	1489.68	1489.68
Hyp01-G7A	**HTDWRLATWHHS**	1546.54	1545.74
Hyp01-T8A	**HTDWRLGAWHHS**	1501.33	1501.71
Hyp01-W9A	**HTDWRLGTAHHS**	1416.61	1416.68
Hyp01-H10A	**HTDWRLGTWAHS**	1465.59	1465.70
Hyp01-H11A	**HTDWRLGTWHAS**	1465.41	1465.70
Hyp01-S12A	**HTDWRLGTWHHA**	1515.34	1515.73
Hyp04	**LLADTTHHRPWT**	1447.25	1446.75
Lin01	**ELWSIDTSAHRK**	1441.80	1441.75



Mean square roughness (R_a)
1.4 ± 0.3 nm
Surface area
25.06 ± 0.01 µm^2
Increase of surface area
0.25 ± 0.04 %

Mean square roughness (R_a)
1.5 ± 0.5 nm
Surface area
25.36 ± 0.16 µm^2
Increase of surface area
1.45 ± 0.64 %

Figure S1. AFM height images (5 × 5 µm) of the film surfaces of: (a) hypPPV and (b) linPPV on SPR substrates (SIA Kit Au, GE Healthcare). These two images were obtained by a SPM 9600 (Shimadzu) in air at room temperature. The mean square roughness (R_a) and surface area of each surface were determined by the attached software. The difference in the surface areas of hypPPV and linPPV was *ca.* 1%. Thus, the surface morphology has little effect on the amounts of bound peptides. The values of R_a and surface area are average values with standard deviations from five measurements in different regions (mean ± S.D.).

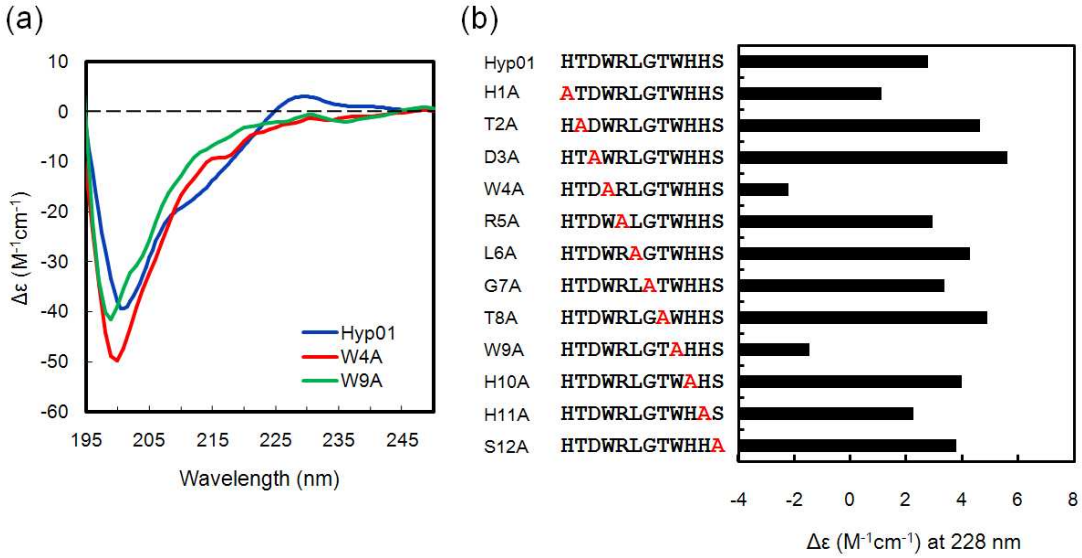


Figure S2. (a) CD spectra of the Hyp01, W4A, and W9A peptides. (b) Intensities at 228 nm of Ala-mutants of the Hyp01 peptide.

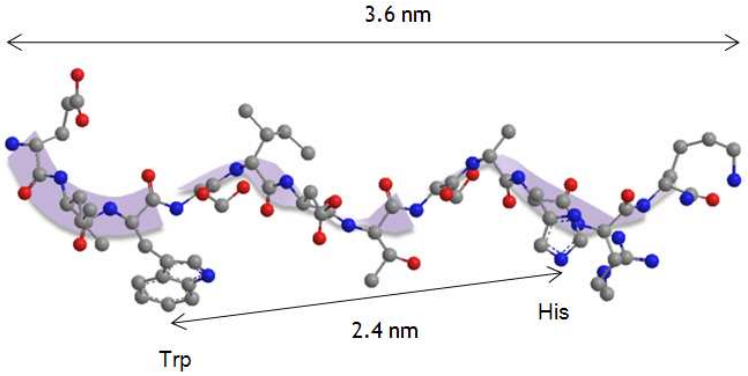


Figure S3. A possible conformation of the Lin01 peptide. The structure was modeled using Chem3D software (CambridgeSoft Corporation), and subjected to energy minimization by the molecular mechanics method (MM2). Hydrogen atoms were omitted for clarity. Blue: nitrogen; red: oxygen; gray: carbon. The distance between the Trp and His residues is 2.4 nm, which corresponds to that of benzene rings 4 repeating units in linPPV.