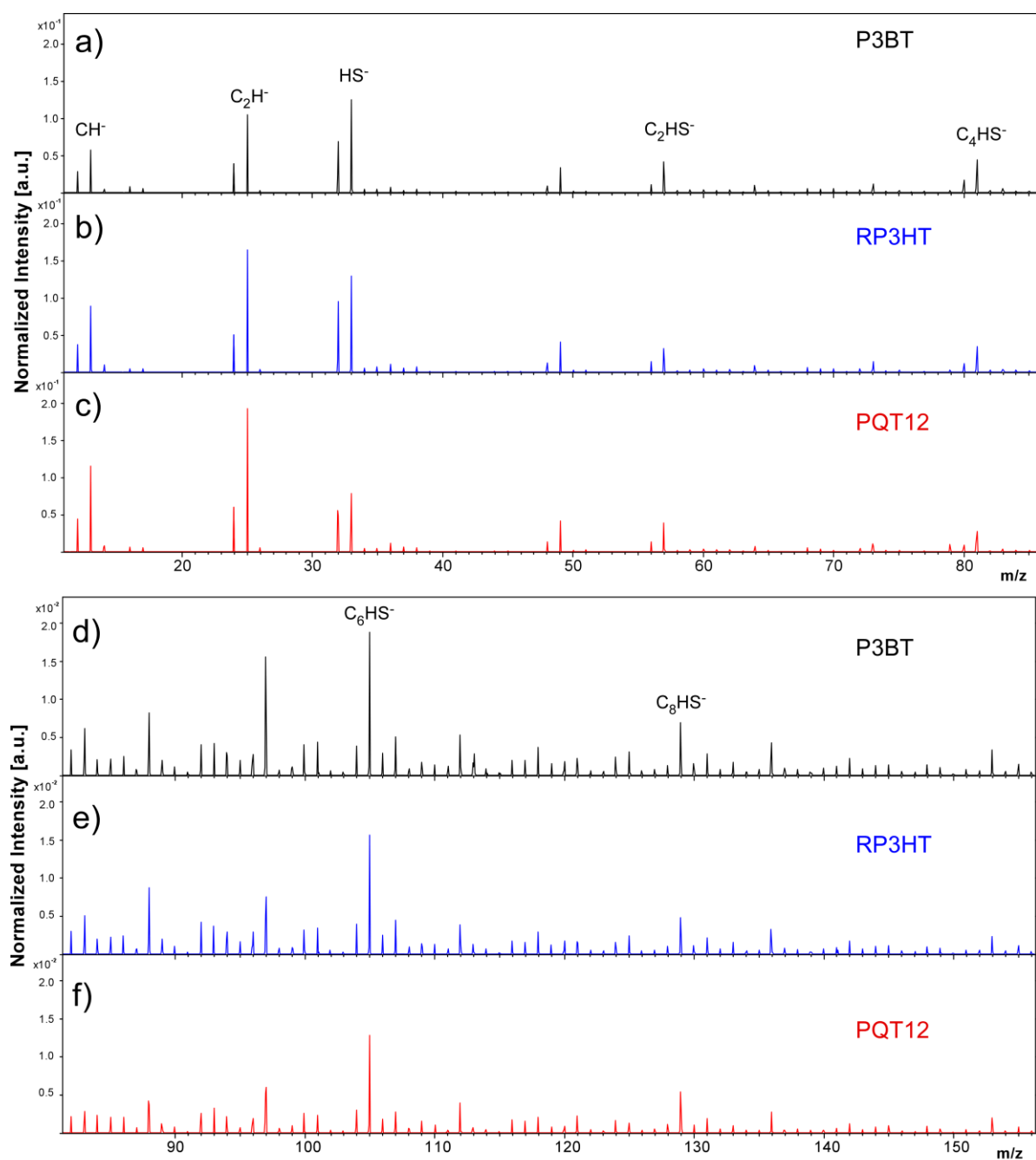# Orientation of biotin binding sites in streptavidin adsorbed onto the surface of polythiophene films

by K. Awsiuk*, P. Petrou, A. Thanassoulas, J. Raczkowska

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Figure S1. Representative negative ion ToF-SIMS spectra of P3BT (a, d), RP3HT (b, e) and PQT12 (c, f) surfaces. Signals distinguishing between different polythiophenes as determined from PCA (cf. Fig. 3b) are marked.

Table S1. ToF-SIMS signals selected for Principal Component Analysis from mass spectra of polythiophenes thin films prior to protein adsorption.

Secondary Ion	Mass
CH^-	13.01
C_2H^-	25.01
S^-	31.97
HS^-	32.98
C_3H^-	37.01
$C_3H_2^-$	38.02
CHS^-	44.98
C_4H^-	49.01
$C_4H_2^-$	50.01
$C_4H_3^-$	51.02
C_2S^-	55.97
C_2HS^-	56.98
C_5H^-	61.01
$C_5H_2^-$	62.02
C_6H^-	73.01
$C_6H_2^-$	74.01
$C_6H_3^-$	75.03
C_4HS^-	80.98
$C_4H_3S^-$	83.00
C_5S^-	91.97
C_5HS^-	92.98
C_8H^-	97.01
$C_8H_2^-$	98.01
C_6HS^-	104.98
$C_{10}H^-$	121.01
$C_{10}H_2^-$	122.01
C_8HS^-	128.98
$C_{10}SH^-$	152.98
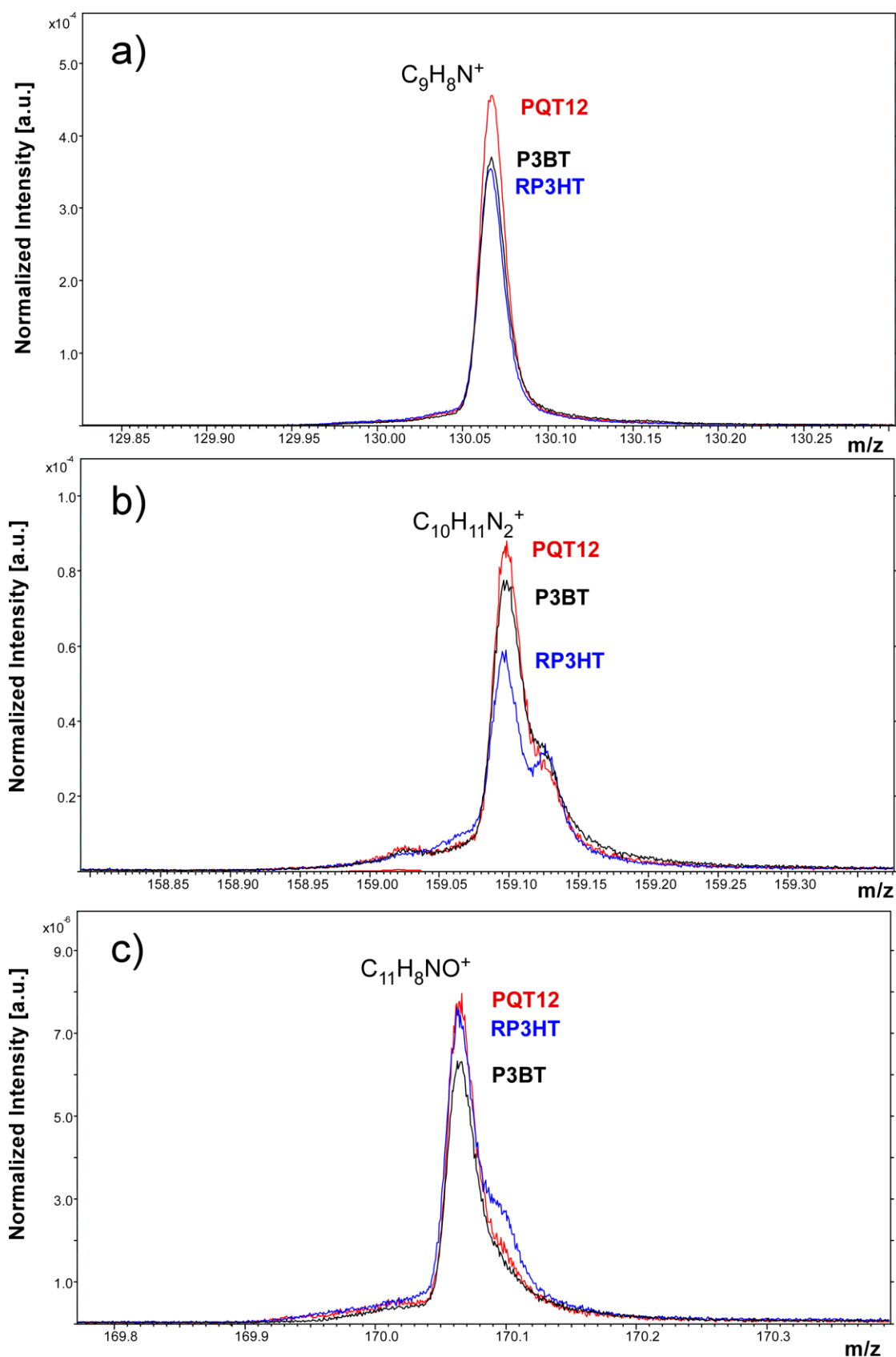
Figure S2. Representative normalized intensities of ToF-SIMS signal originating from tryptophan collected from streptavidin adsorbed into surface of different polythiophenes: a) $C_9H_8N^+$, b) $C_{10}H_{11}N_2^+$ and c) $C_{11}H_8NO^+$.

Table S2. ToF-SIMS signals selected for Principal Component Analysis from mass spectra of streptavidin adsorbed to polythiophenes thin films, their mass and amino acid origin.

| Secondary Ion	Mass	Amino acid origin
CH_4N^+	30.03	Gly
$CH_3N_2^+$	43.03	Arg
$C_2H_6N^+$	44.05	Ala
$C_3H_6N^+$	56.05	Lys
$C_4H_6N^+$	68.05	Pro
$C_4H_5O^+$	69.03	Thr
$C_3H_4NO^+$	70.03	Asn
$C_4H_8N^+$	70.07	Arg. Pro. Val
$C_3H_3O_2^+$	71.01	Ser
$C_4H_{10}N^+$	72.08	Val
$C_2H_7N_3^+$	73.07	Arg
$C_3H_8NO^+$	74.07	Thr
$C_4H_5N_2^+$	81.05	His
$C_4H_6N_2^+$	82.05	His
$C_5H_7O^+$	83.05	Val
$C_4H_6NO^+$	84.05	Gln. Glu
$C_5H_{10}N^+$	84.08	Lys
$C_5H_{12}N^+$	86.10	Ile. Leu
$C_3H_7N_2O^+$	87.06	Asn
$C_3H_6NO_2^+$	88.04	Asn. Asp
$C_4H_4NO_2^+$	98.02	Asn
$C_4H_{10}N_3^+$	100.09	Arg
$C_4H_{11}N_3^+$	101.09	Arg
$C_4H_8NO_2^+$	102.06	Glu
$C_7H_7O^+$	107.05	Tyr
$C_5H_8N_3^+$	110.07	His
$C_8H_{10}N^+$	120.08	Phe
$C_5H_{11}N_4^+$	127.10	Arg
$C_9H_8N^+$	130.07	Trp
$C_{10}H_{11}N_2^+$	159.09	Trp
$C_{11}H_8NO^+$	170.06	Trp
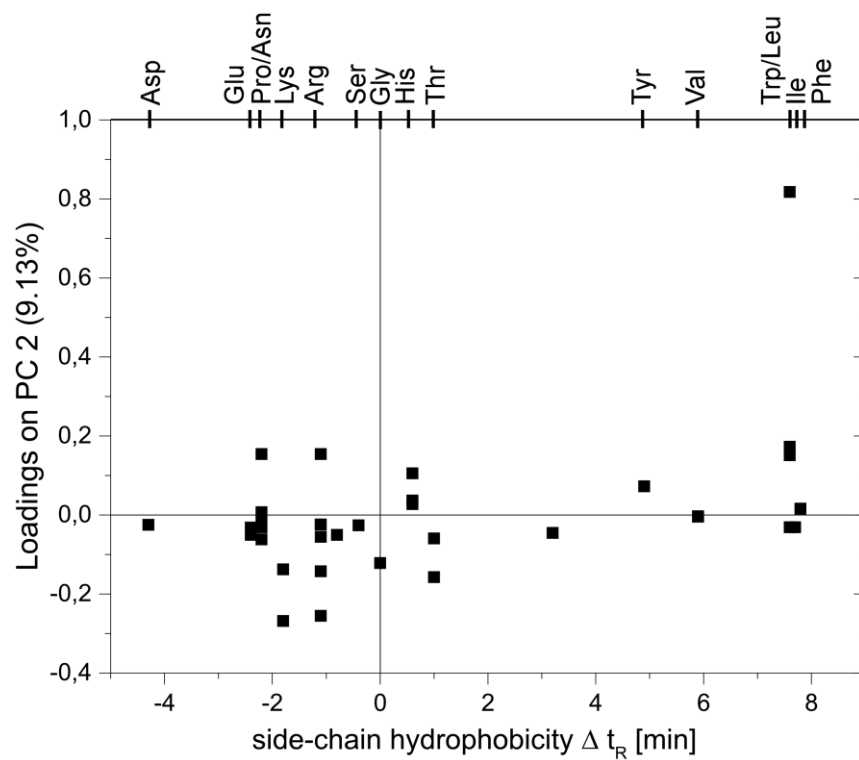
Figure S3. Hydrophobicity of amino acid side chains defined as the difference in retention time Δt_R relative to glycine peptide plotted against the loadings on PC 2.