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Analysis and prediction of defects in UV photo-initiated polymer microarrays – Electronic supplementary information

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Table ESI1 List of top 20 molecular descriptors and the corresponding regression coefficient (RC) associated with promoting (positive RC) or preventing (negative RC) a particular defect for PLS models describing the total number of defects. Descriptors prefixed with 'Δ' relate to the difference in the molecular descriptor of the monomer components, whereas non-prefixed descriptors relate to the average value of the molecular descriptors of the monomer components.

Positive regression coefficient		Negative regression coefficient	
Regression coefficient	Molecular descriptor	Regression coefficient	Molecular descriptor
0.56	Δkhs.ssCH$_2$	-1.11	ΔC$_3$sp2
0.52	BCUTw.1l	-0.97	ΔtopoShape
0.50	Δkhs.sCH$_3$	-0.38	khs.aaCH
0.45	C$_3$sp2	-0.38	ΔBCUTw.1h
0.45	HybRatio	-0.33	LipinskiFailures
0.44	ΔBCUTw.1l	-0.30	ΔVC.4
0.33	ΔECCEN	-0.30	Δkhs.ssO
0.32	khs.sCH$_3$	-0.26	ΔSC.4
0.31	VC.4	-0.24	ΔVC.3
0.30	ΔVP.1	-0.24	C$_2$sp3
0.28	Δbpol	-0.24	SCH.5
0.26	ΔBCUTp.1h	-0.24	khs.sssCH
0.25	ΔnAtom	-0.24	VCH.5
0.25	ΔWPATH	-0.23	BCUTc.1h
0.24	ΔVP.4	-0.22	ΔATSc4
0.24	ΔVP.3	-0.22	ΔnHBDon
0.23	Δapol	-0.21	Δkhs.dssC
0.23	ΔKier3	-0.21	ΔSCH.3
0.23	BCUTc.1l	-0.21	SCH.6
0.21	VC.3	-0.21	ΔLipinskiFailures

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Table ESI2 List of top 20 molecular descriptors and the corresponding regression coefficient (RC) associated with promoting (positive RC) or preventing (negative RC) a particular defect for PLS models describing each defect. Descriptors prefixed with 'Δ' relate to the difference in the molecular descriptor of the monomer components, whereas non-prefixed descriptors relate to the average value of the molecular descriptors of the monomer components.

Non-Circular		Spreading		Rough		Chemical heterogeneity		Diameter	
Regression coefficient	Molecular descriptor	Regression coefficient	Molecular descriptor	Regression coefficient	Molecular descriptor	Regression coefficient	Molecular descriptor	Regression coefficient	Molecular descriptor
0.20	C_3sp2	0.26	Δkhs.ssCH_2	0.38	ΔFMF	0.16	HybRatio	176	ΔBCUTw.1l
0.12	Δkhs.ssCH_2	0.23	HybRatio	0.18	BCUTw.1l	0.15	ΔC_1sp3	145	C_3sp2
0.10	ΔBCUTw.1l	0.23	khs.sCH_3	0.16	ALogp2	0.14	ΔBCUTp.1h	121	khs.sCH_3
0.08	ΔECCEN	0.21	Δkhs.sCH_3	0.15	C_3sp2	0.11	Δkhs.dO	113	HybRatio
0.08	ΔVP.4	0.20	VC.4	0.12	ALogP	0.08	BCUTc.1l	111	ΔBCUTp.1h
0.08	ΔVP.1	0.17	C_3sp2	0.11	WPATH	0.08	ΔBCUTw.1l	101	BCUTw.1l
0.07	ΔVP.3	0.16	ΔBCUTw.1l	0.11	ΔECCEN	0.08	Δbpol	94	Δkhs.sCH_3
0.06	Δbpol	0.14	BCUTw.1l	0.11	Δkhs.ssCH_2	0.07	ΔAMR	75	Δkhs.ssCH_2
0.06	khs.dssC	0.13	VC.3	0.10	Δkhs.sCH_3	0.06	ΔnAtom	65	Δbpol
0.06	ΔVP.7	0.12	ΔKier3	0.09	SC.4	0.06	Δapol	65	VC.4
0.06	BCUTw.1l	0.12	C_4sp3	0.09	BCUTc.1l	0.06	BCUTw.1l	59	ΔVP.4
0.06	Δkhs.sCH_3	0.11	BCUTc.1l	0.09	khs.ssssC	0.06	ΔTopoPSA	59	C_4sp3
0.06	Δkhs.aaCH	0.11	Δbpol	0.08	SC.3	0.05	ΔnAtomLAC	56	ΔVP.1
0.05	khs.sCH_3	0.10	ΔBCUTp.1h	0.08	SC.6	0.05	SC.5	56	ΔVP.5
0.05	ΔnAtom	0.10	ΔnAtom	0.08	VC.3	0.05	SC.6	55	ΔnAtom
0.05	khs.ssO	0.10	ΔVP.1	0.08	ΔVP.4	0.05	khs.sssN	54	ΔVP.3
0.05	Δapol	0.09	Δapol	0.08	SC.5	0.05	khs.sCH_3	53	Δapol
0.05	ΔC_3sp3	0.08	ΔMLogP	0.08	VC.4	0.04	ΔWTPT.4	51	ΔATSc3
0.05	HybRatio	0.08	C_1sp3	0.08	ΔBCUTc.1l	0.04	XLogP	51	C_1sp3
0.05	ΔVP.5	0.08	ΔVP.3	0.08	ΔBCUTc.1h	0.04	Δkhs.sCH_3	51	ΔLipinskiFailures
-0.26	ΔC_3sp2	-0.43	ΔC_3sp2	-0.27	ΔtopoShape	-0.21	ΔFMF	-143	ΔtopoShape
-0.24	ΔtopoShape	-0.24	LipinskiFailures	-0.25	ΔC_3sp2	-0.12	ΔC_3sp2	-140	ΔC_3sp2
-0.12	Δkhs.dssC	-0.21	ΔtopoShape	-0.18	Δkhs.dssC	-0.11	ΔVC.3	-86	ΔnHBΔon
-0.12	khs.sssN	-0.16	ΔSCH.3	-0.14	ΔATSc3	-0.11	ΔBCUTw.1h	-86	ΔnHBΔon
-0.11	ΔBCUTw.1h	-0.14	Δkhs.ssO	-0.14	ΔBCUTw.1h	-0.10	Δkhs.sssCH	-79	ΔVC.3
-0.09	ΔnHBΔon	-0.12	VCH.5	-0.13	ΔLipinskiFailures	-0.10	ΔtopoShape	-76	ΔSC.4
-0.09	ΔnHBΔon	-0.11	SCH.5	-0.12	C_2sp3	-0.09	ΔVC.4	-72	ΔALogp2
-0.07	ΔVC.4	-0.11	BCUTc.1h	-0.12	ΔC_1sp3	-0.08	BCUTc.1h	-68	ΔATSc5
-0.07	ΔATSc5	-0.11	ΔBCUTc.1l	-0.11	ΔSC.5	-0.08	ΔSC.4	-65	ΔALogP
-0.07	ΔnAtomLAC	-0.11	ΔBCUTc.1h	-0.09	ΔVPC.4	-0.08	ΔC_3sp3	-64	ΔATSc4
-0.07	C_3sp3	-0.11	fragC	-0.09	BCUTc.1h	-0.08	ΔnAtomLC	-62	ΔSC.3
-0.07	SCH.5	-0.11	khs.aaCH	-0.09	ΔSPC.4	-0.07	ΔSC.3	-61	Δkhs.dCH_2
-0.07	VCH.5	-0.10	SCH.6	-0.08	WTPT.2	-0.07	ΔSP.2	-60	khs.dsCH
-0.06	Δkhs.dCH_2	-0.10	ΔC_3sp3	-0.08	ΔnAtomLAC	-0.07	FMF	-57	C_3sp3
-0.06	khs.sssCH	-0.10	ΔVAdjMat	-0.08	khs.aaCH	-0.07	ΔZagreb	-53	FMF
-0.06	khs.aaCH	-0.10	ΔATSm2	-0.08	Δkhs.sF	-0.06	ΔVAdjMat	-51	ΔSP.2
-0.06	VP.7	-0.09	ΔnAtomLC	-0.07	ΔVC.4	-0.06	WTPT.4	-51	Δkhs.ssO
-0.06	fragC	-0.09	ΔWTPT.4	-0.07	BCUTw.1h	-0.06	khs.aaCH	-51	Δkhs.dssC
-0.06	ΔATSc3	-0.09	ΔSP.2	-0.07	ATSc4	-0.06	Δkhs.sF	-49	SCH.5
-0.05	ΔATSc4	-0.09	ΔATSc1	-0.07	SCH.6	-0.06	khs.ssO	-48	VCH.5

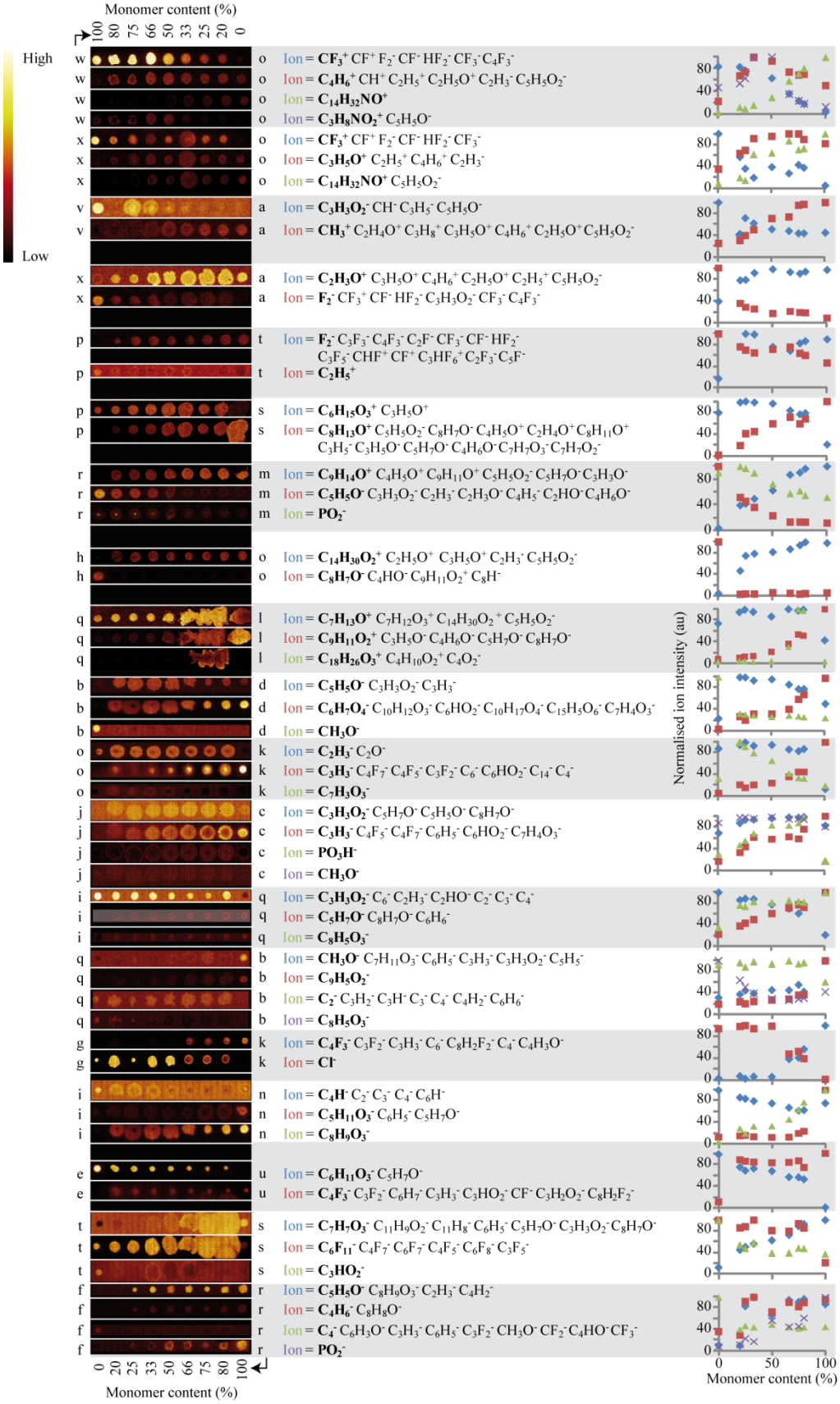

Fig. ESI1 ToF-SIMS images of each copolymer pair within the odd spot array with various ions mapped. The intensity scale is shown on the left. For each image the intensity was scaled to maximise the contrast for each ion, thus, the scale is arbitrary for each image. All ions that gave a similar image are shown to the right of each image. The intensity of the ion in bold is shown in the chemical maps/graphs.

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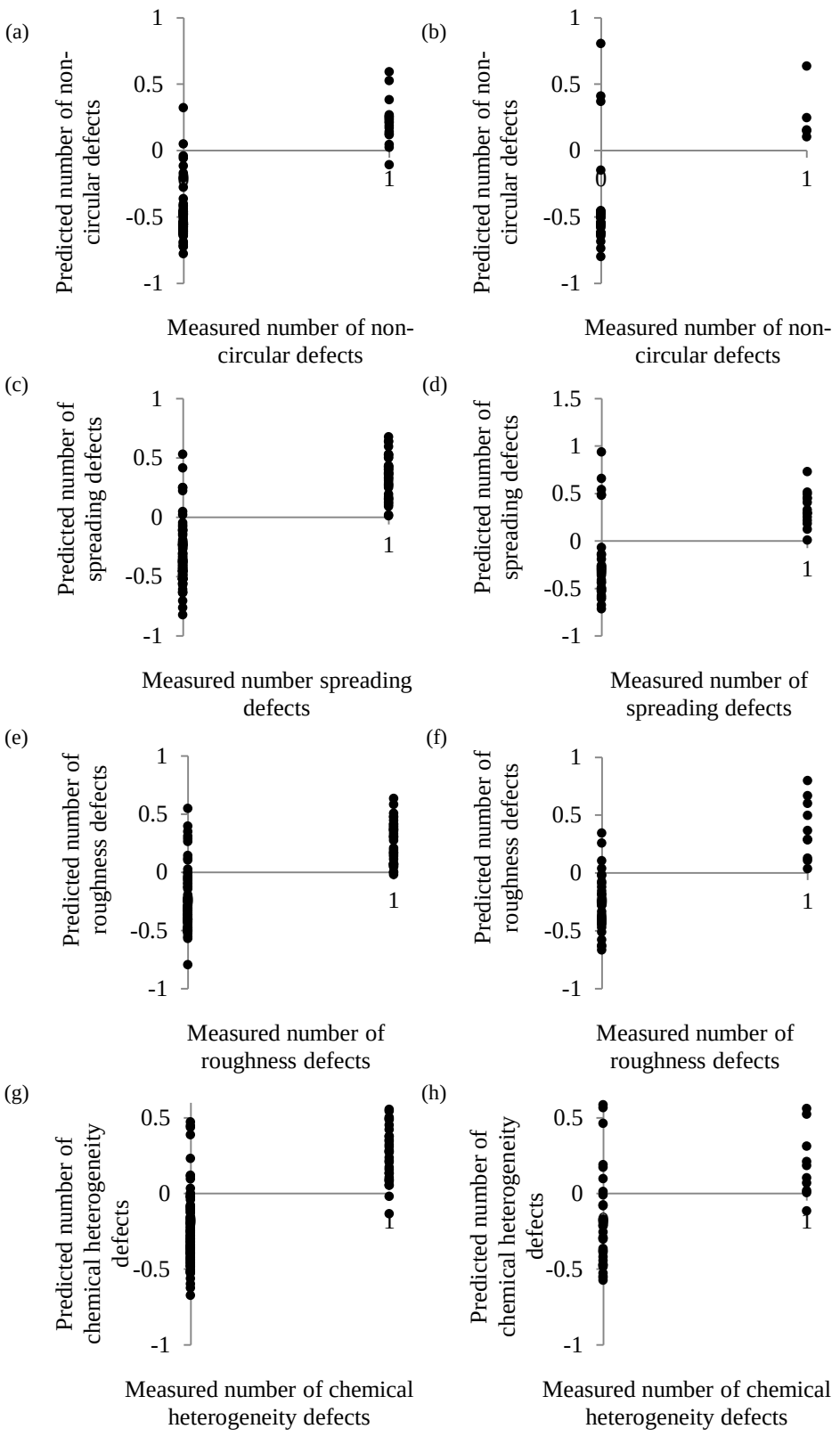

Fig. ESI2 PLS regression model prediction of the occurrence of defects (a-b) non-circular, (c-d) spreading, (e-f) roughness, and (g-h) chemical heterogeneity. Model calculated for the (a, c, e, g) training set and (b, d, f, h) test set. The number of correct predictions (positive = defect present, negative = defect absent) is (a) 97.7%, (b) 92.9%, (c) 94.6%, (d) 88.1%, (e) 90.7%, (f) 90.5%, (g) 90.7, (h) 81.0%.

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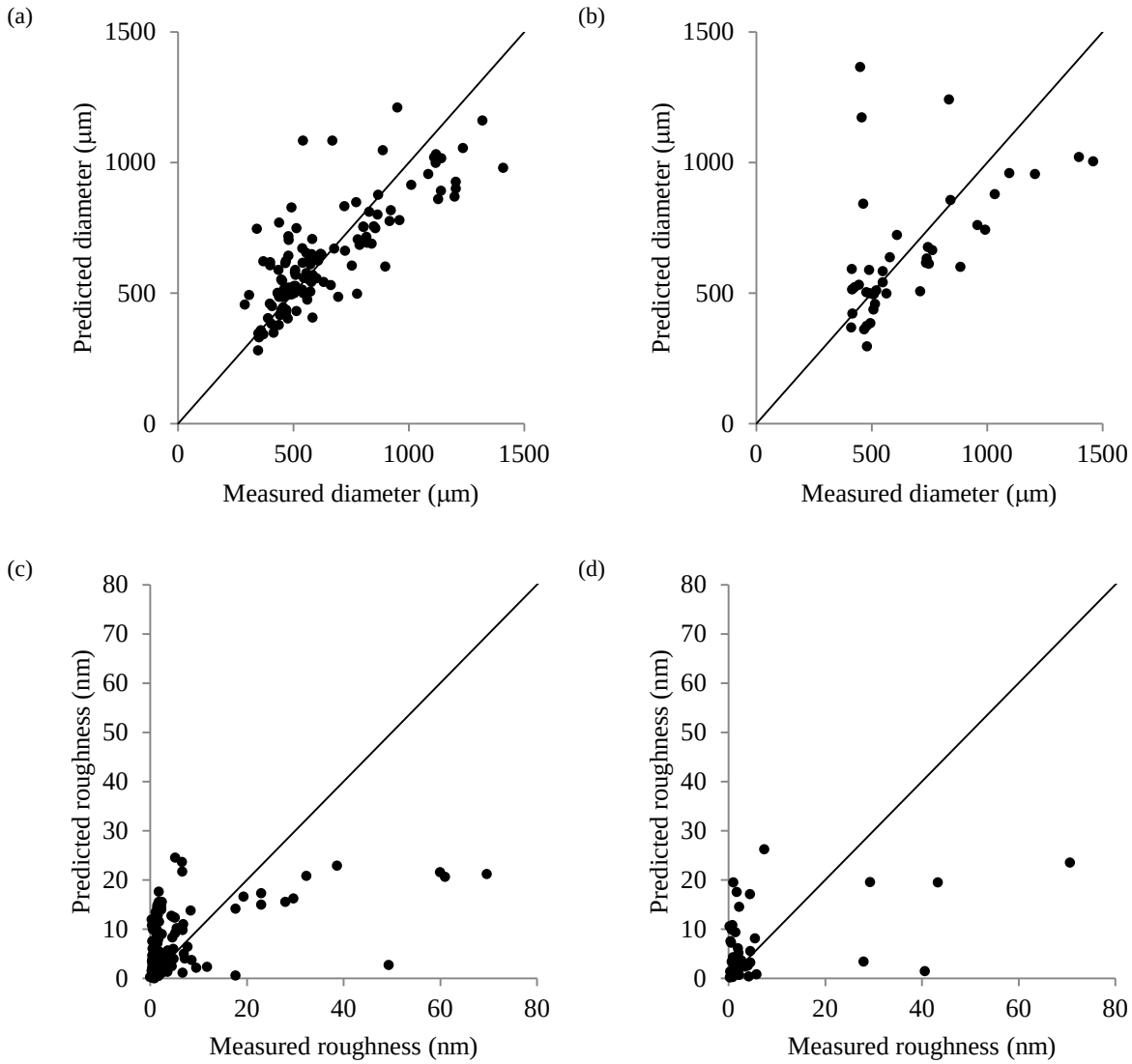

Fig. ESI3 PLS regression model prediction of the (a-b) diameter and (c-d) roughness of polymer spots, calculated for the (a, c) training set and (b, d) test set. R^2 value = (a) 0.42, (b) -0.01, (c) -1.50 and (d) -2.29.

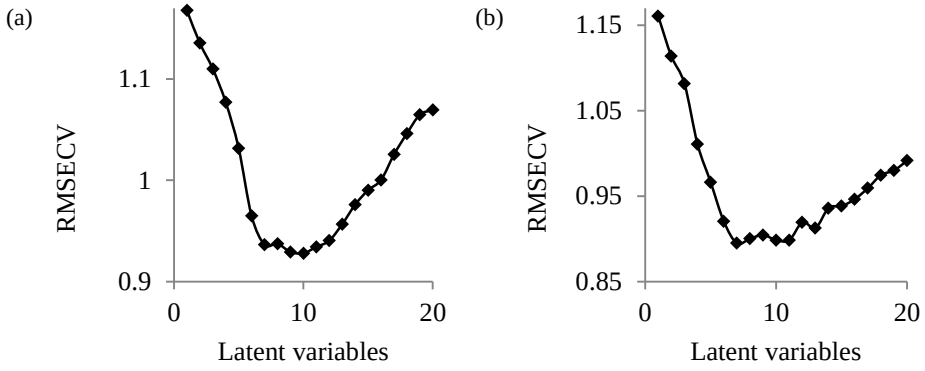

Fig. ESI4 Root mean square error of cross validation (RMSECV) curves for PLS models. (a) First model produced with 244 x-variables. (b) Second model produced with 166 x-variables. A minimum of the RMSECV curve at the lowest number of latent variables (7) was used to determine the number of latent variables to be used for the formation of a model.