Supporting Information

Prediction of Broad-spectrum Pathogen Attachment to Coating Materials for Biomedical Devices

Paulius Mikulskis†, Andrew Hook†, Adam A. Dundas†¶, Derek Irvine¶, Olutoba Sanni†, Daniel Anderson#, Robert Langer#, Morgan R. Alexander†, Paul Williams§ and David A. Winkler&†**

† School of Pharmacy, University of Nottingham, Nottingham NG7 2RD, UK.

§ Centre for Biomolecular Sciences, School of Life Sciences, University of Nottingham, Nottingham NG7 2RD, UK.

¶ Faculty of Engineering, University of Nottingham, Nottingham NG7 2RD, UK

 # Koch Institute for Integrative Cancer Research, MIT, Cambridge MA, 02139-4307, USA

& Department of Chemistry and Physics, La Trobe Institute for Molecular Science, La Trobe University, Kingsbury Drive, Melbourne, Victoria 3086, Australia; Monash Institute for Pharmaceutical Sciences, Parkville 3052, Australia; School of Chemical and Physical Sciences, Flinders University 5046, Australia

Corresponding authors email addresses: d.winkler@latrobe.edu.au; david.winkler@monash.edu; morgan.alexander@nottingham.ac.uk

Table S1. Computed molecular descriptors used in the models

Descriptor	PA	SA	UPEC	Multi (linear)	Multi (BRANN)
ATSC2s	✓			✓	✓
ATSC4s		✓			
ATSC6s	✓			✓	✓
ATSC7s		✓			
ATSC8s	✓	✓		✓	✓
CENT		✓			
CSI	✓				
GMTIV		✓	✓		
IDMT	✓	✓	✓		
J_X	✓	✓	✓		
IDET	✓				
P_VSA_LogP_3		✓		✓	✓
P_VSA_LogP_4	✓	✓		✓	✓
P_VSA_MR_1	✓			✓	✓
P_VSA_MR_2	✓	✓		✓	✓

Descriptor	PA	SA	UPEC	Multi (linear)	Multi (BRANN)
P_VSA_MR_5			✓		
P_VSA_i_3		✓		✓	✓
P_VSA_s_6	✓		✓	✓	✓
P_VSA_ppp_con	✓	✓			
P_VSA_ppp_L	✓				
P_VSA_ppp_cyc					
P_VSA_ppp_ter	✓			✓	✓
T(O..O)			✓		
SMTIV		✓			
TIE	✓		✓		
TIC1		✓		✓	✓
TIC2				✓	✓
TIC5	✓			✓	✓
Wi_Dt	✓	✓		✓	
Wap		✓			
Wi_Dz(v)			✓	✓	✓

Descriptor	**PA**	**SA**	**UPEC**	**Multi (linear)**	**Multi (BRANN)**
ZM1Kup	✓			✓	✓
ZM2Per		✓		✓	✓
ZM2Kup				✓	✓
QW_L	✓				
Wi_D/Dt				✓	✓
I_{SA}				✓	✓
I_{PA}				✓	✓
I_{UPEC}				✓	✓

Table S2. Explanation of molecular descriptors

Molecular descriptor	Description
ATSC2s	Centred Broto-Moreau autocorrelation of lag 2 weighted by I-state
ATSC4s	Centred Broto-Moreau autocorrelation of lag 4 weighted by I-state
ATSC6s	Centred Broto-Moreau autocorrelation of lag 6 weighted by I-state
ATSC7s	Centred Broto-Moreau autocorrelation of lag 7 weighted by I-state
ATSC8s	Centred Broto-Moreau autocorrelation of lag 8 weighted by I-state
CENT	Centralization
CSI	Eccentric connectivity index
GMTI	Gutman Molecular Topological Index
GMTIV	Gutman Molecular Topological Index by valence vertex degrees
IDET	Total information content on the distance equality
IDMT	Total information content on the distance magnitude
J_X	Balaban-like index from chi matrix
P_VSA_LogP_3[1]	P_VSA-like on LogP, bin 3
P_VSA_LogP_4	P_VSA-like on LogP, bin 4
P_VSA_MR_1	P_VSA-like on Molar Refractivity, bin 1

Molecular descriptor	Description
P_VSA_MR_2	P_VSA-like on Molar Refractivity, bin 2
P_VSA_MR_5	P_VSA-like on Molar Refractivity, bin 5
P_VSA_i_3	P_VSA-like on ionization potential, bin 3
P_VSA_ppp_L	P_VSA-like on potential pharmacophore points, L - lipophilic
P_VSA_ppp_con	P_VSA-like on potential pharmacophore points, conjugated atoms
P_VSA_ppp_cyc	P_VSA-like on potential pharmacophore points, atoms in rings
P_VSA_ppp_ter	P_VSA-like on potential pharmacophore points, terminal atoms
P_VSA_s_6	P_VSA-like on I-state, bin 6
QW_L	Quasi-Wiener index (Kirchhoff number) from Laplace matrix
SMTIV	Schultz Molecular Topological Index by valence vertex degrees
T(O..O)	Sum of topological distances between O..O
TIC1[2]	Total Information Content index (neighbourhood symmetry of 1-order)
TIC2	Total Information Content index (neighbourhood symmetry of 2-order)
TIC5	Total Information Content index (neighbourhood symmetry of 5-order)
TIE	E-state topological parameter
Wap	All-path Wiener index

Molecular descriptor	Description
Wi_D/Dt	Wiener-like index from distance/detour matrix
Wi_Dt	Wiener-like index from detour matrix (detour index)
Wi_Dz(v)	Wiener-like index from Barysz matrix weighted by VdW volume
ZM1Kup	First Zagreb index by Kupchik vertex degrees
ZM2Kup	Second Zagreb index by Kupchik vertex degrees
ZM2Per	Second Zagreb index by perturbation vertex degrees

Table S3. Experimental ToF-SIMS ion peak features used in modelling.

Descriptor	**PA**	**SA**	**UPEC**	**Multi-pathogen (linear)**	**Multi**-pathogen **(BRANN)**	**Ion present in monomers** (Figure S1 for monomer names)
C^-	X					All
$C_{13}H_9^+$		X				All but 5
$C_2H_3^+$	X			X	X	All
$C_2H_3O^-$		X				All
$C_2H_3O^+$		X				All but 5
$C_2H_4^+$		X				All
$C_2H_4N^+$			X			E; 8,12,13,15 from contamination
$C_2H_5^+$	X		X			5
$C_2H_5O^+$	X					All but 5, A, B, C, D, E, F
$C_2H_5O_4^+$	X	X				6
C_2HO	X					All
C_3H^-	X			X	X	5, 6, 7, A, B, E, F
$C_3H_3^+$	X	X		X	X	All
$C_3H_3O^+$	X	X		X	X	All
$C_3H_3O_2^-$	X	X				All
$C_3H_5O^+$	X					3, 6
$C_3H_6^+$			X			All

Descriptor	**PA**	**SA**	**UPEC**	**Multi-pathogen (linear)**	**Multi-**pathogen **(BRANN)**	**Ion present in monomers** (Figure S1 for monomer names)
$C_3H_7^+$	X	X		X	X	All
$C_3H_7O_2^+$		X				3,6,16, A,E
C_3HO^+		X		X	X	All but 3, 4, 5, 6, 9, B
C_4H^+	X			X	X	7, 9, 14, D, F
$C_4H_{12}NO^+$	X					E
$C_4H_3^+$			X			1,2,4,5,6,16
$C_4H_6^+$	X		X			All
$C_4H_6O^+$	X	X				12
$C_4H_6O_2^+$		X				All but 5,14,B,C,D,F
$C_4H_7^+$		X		X	X	All
$C_4H_7O_2^+$	X					3
$C_5H_3^+$	X					7, 14
$C_5H_6O^+$		X				All
$C_5H_7^+$			X			All
$C_5H_7O_2^+$	X					All
$C_5H_8O_2^+$	X					All
$C_5H_9^+$			X			All
$C_6H_{11}^+$	X			X	X	1, 4, 5, 6, 11, 13, A

Descriptor	**PA**	**SA**	**UPEC**	**Multi-pathogen (linear)**	**Multi**-pathogen **(BRANN)**	**Ion present in monomers** (Figure S1 for monomer names)
$C_6H_{13}^+$	X					All
$C_6H_2^+$		X				1,4,7,8,9,10,13,14,15,B,D,F
$C_6H_5^+$	X					7, 14
$C_6H_5O^-$			X			7
$C_6H_6O^+$	X			X	X	7
$C_7H_{13}^+$	X					All
$C_7H_5O^+$	X					14
$C_8H_{12}^+$	X					All
$C_8H_9O^+$	X			X	X	7, 9
$C_9H_{13}^+$	X					All
CH_3^+			X			All
CH_5O+		X				14,16
CHO+	X	X		X	X	All but 5
WCA			X	X	X	N/A
I_{SA}				X	X	N/A
I_{PA}				X	X	N/A
I_{UPEC}				X	X	N/A

Table S4. Correlation of molecular descriptors with logF

PA		**SA**		**UPEC**	
ATSC2s	0.18	ATSC4s	-0.09	ATSC4s	-0.22
ATSC6s	0.07	ATSC7s	0.07	ATSC7s	-0.11
ATSC7s	0.19	ATSC8s	-0.05	ATSC8s	-0.18
ATSC8s	0.08	CENT	-0.01	CENT	-0.03
CENT	0.35	CSI	0.00	GMTI	-0.02
CSI	0.37	GMTIV	0.00	GMTIV	0.00
GMTI	0.34	IDMT	-0.01	IDMT	-0.03
GMTIV	0.37	J_X	0.00	J_X	0.02
IDET	0.38	P_VSA_LogP_3	0.41	P_VSA_LogP_4	-0.05
IDMT	0.34	P_VSA_LogP_4	-0.13	P_VSA_MR_2	-0.10
J_X	0.36	P_VSA_MR_2	-0.10	P_VSA_MR_5	0.01
P_VSA_LogP_4	0.28	P_VSA_i_3	-0.02	P_VSA_s_6	0.11
P_VSA_MR_1	0.37	P_VSA_ppp_con	0.04	T(O..O)	0.03
P_VSA_MR_2	0.21	SMTIV	0.00	TIE	0.03
P_VSA_MR_5	0.31	TIC1	-0.01	Wi_Dt	-0.03
P_VSA_MR_6	0.15	Wap	-0.04	Wi_Dz(v)	-0.02

PA		SA		UPEC	
P_VSA_ppp_L	0.13	Wi_Dt	-0.01	ZM1Kup	-0.02
P_VSA_ppp_con	0.12	ZM2Per	-0.01	ZM2Kup	-0.04
P_VSA_ppp_cyc	0.10				
P_VSA_ppp_ter	0.13				
P_VSA_s_6	0.36				
QW_L	0.34				
SMTIV	0.36				
TIC2	0.37				
TIC5	0.38				
TIE	0.36				
Wi_D/Dt	0.39				
Wi_Dt	0.34				
Wi_Dz(v)	0.34				
ZM1Kup	0.39				

Table S5. Correlation of experimental feature descriptors with logF (>0.5 in bold)

PA						**SA**		**UPEC**	
C^-	-0.05	$C_3H_3O_2^-$	0.09	$C_5H_7O_2^+$	-0.02	CHO^+	-0.17	CH_3^+	0.17
CH^+	-0.09	$C_3H_5^+$	-0.22	$C_5H_8O_2^+$	0.26	CH_5O^+	-0.17	**$C_2H_4N^+$**	**0.52**
CH^-	0.02	$C_3H_5O^+$	0.38	$C_6H_{10}^+$	-0.19	$C_{13}H_9^+$	0.02	$C_2H_5^+$	-0.32
CHO^+	0.01	$C_3H_5O_2^+$	0.16	$C_6H_{11}^+$	-0.07	$C_2H_3^-$	-0.34	$C_3H_6^+$	0.06
CH_2F^+	-0.01	$C_3H_7^+$	-0.21	$C_6H_{12}O_2^+$	0.03	$C_2H_3O^+$	-0.01	$C_4H_3^+$	-0.07
$C_{10}H_{11}^+$	0.03	C_4H^+	0.03	$C_6H_{13}^+$	0.01	$C_2H_3O^-$	0.08	**$C_4H_5^+$**	**-0.54**
$C_{10}H_{11}O^+$	0.10	C_4H^-	0.19	$C_6H_5^+$	0.04	$C_2H_4^+$	-0.33	$C_5H_7^+$	-0.48
$C_{10}H_{14}^+$	0.29	**$C_4H_6^+$**	**-0.50**	$C_6H_6O^+$	0.10	$C_2H_5O_4^+$	0.35	$C_5H_9^+$	-0.44
$C_{12}H_{15}^+$	-0.16	$C_4H_6O^+$	-0.31	$C_7H_{13}^+$	-0.06	C_3HO^+	0.11	$C_6H_5O^-$	0.20
C_2H^+	-0.10	$C_4H_7O_2^+$	0.39	$C_7H_5O^+$	0.00	$C_3H_3^+$	-0.17	**WCA**	**-0.51**
C_2HO^-	0.30	$C_4H_8^+$	-0.37	$C_7H_6O^+$	0.01	$C_3H_3O^+$	-0.11		
$C_2H_2O_2^-$	0.08	$C_4H_8O^+$	0.25	$C_8H_{12}^+$	-0.05	$C_3H_3O_2^-$	0.07		
$C_2H_3^-$	-0.43	$C_4H_9O^+$	0.01	$C_8H_9O^+$	0.05	$C_3H_7^+$	-0.12		
$C_2H_5^+$	-0.22	$C_5H_{10}^+$	-0.24	$C_9H_{11}O_2^+$	-0.08	$C_3H_7O_2^+$	0.29		
$C_2H_5O^+$	0.21	$C_5H_{12}N^+$	0.08	$C_9H_{13}^+$	-0.07	$C_4H_6O^+$	-0.15		
$C_2H_5O_4^+$	0.32	$C_5H_{12}NO^+$	0.19	$C_9H_{15}^+$	-0.04	$C_4H_6O_2^+$	-0.10		
C_3H^-	0.26	$C_5H_2^+$	0.03	F^-	0.01	$C_4H_7^+$	-0.32		

PA						SA		UPEC
$C_3H_3^+$	-0.43	$C_5H_3^+$	0.01	OF^-	0.31	$C_5H_6O^+$	0.08	
$C_3H_3O^+$	-0.30	$C_5H_5O^+$	-0.34	WCA	-0.39	$C_6H_2^+$	0.25	

Table S6 Composition and pathogen attachment (expressed as log mCherry fluorescence, logF) of the smaller polymer library used for model validation

Polymer number (Figure S6)	*Monomer 1*	*% monomer 1*	*% TBCHA (Figure S6)*	*Measured F mCherry*	*log measured F mCherry*
P1	DdMA	100	0	730	2.86
P2	LMA	100	0	259	2.41
P3	CyDMA	100	0	735	2.87
P4	GMA	100	0	854	2.93
P5	LMMA	100	0	848	2.93
P6	EGPhEA	100	0	1251	3.10
P7	CHMA	100	0	411	2.61
P8	PhMA	100	0	1675	3.22
P9	HPhOPA	100	0	2669	3.43
P10	DdMA	83.3	16.6	623	2.79
P11	LMA	83.3	16.6	273	2.44
P12	CyDMA	83.3	16.6	643	2.81
P13	GMA	83.3	16.6	901	2.95
P14	LMMA	83.3	16.6	673	2.83
P15	EGPhEA	83.3	16.6	448	2.65
P16	CHMA	83.3	16.6	694.0	2.84
P17	PhMA	83.3	16.6	1557	3.19
P18	HPhOPA	83.3	16.6	2788	3.45
P19	DdMA	66.6	33.3	682	2.83
P20	LMA	66.6	33.3	439	2.64
P21	CyDMA	66.6	33.3	816	2.91
P22	GMA	66.6	33.3	887	2.95
P23	LMMA	66.6	33.3	405	2.61
P24	EGPhEA	66.6	33.3	423	2.63
P25	CHMA	66.6	33.3	725	2.86

Polymer number (Figure S6)	*Monomer 1*	*% monomer 1*	*% TBCHA (Figure S6)*	*Measured F mCherry*	*log measured F mCherry*
P26	PhMA	66.6	33.3	1355	3.13
P27	HPhOPA	66.6	33.3	2118	3.33
P28	DdMA	50	50	570	2.76
P29	LMA	50	50	442	2.65
P30	CyDMA	50	50	668	2.83
P31	GMA	50	50	694	2.84
P32	LMMA	50	50	688	2.84
P33	EGPhEA	50	50	550	2.74
P34	CHMA	50	50	675	2.83
P35	PhMA	50	50	895	2.95
P36	HPhOPA	50	50	1280	3.11
P37	DdMA	33.3	66.6	1023	3.01
P38	LMA	33.3	66.6	na	
P39	CyDMA	33.3	66.6	na	
P40	GMA	33.3	66.6	354	2.55
P41	LMMA	33.3	66.6	450	2.65
P42	EGPhEA	33.3	66.6	656	2.82
P43	CHMA	33.3	66.6	591	2.77
P44	PhMA	33.3	66.6	732	2.86
P45	HPhOPA	33.3	66.6	1017	3.01
P46	DdMA	16.7	83.3	893	2.95
P47	LMA	16.7	83.3	642	2.81
P48	CyDMA	16.7	83.3	326	2.51
P49	GMA	16.7	83.3	720	2.86
P50	LMMA	16.7	83.3	190	2.28
P51	EGPhEA	16.7	83.3	530	2.72
P52	CHMA	16.7	83.3	298	2.47
P53	PhMA	16.7	83.3	614	2.79

Polymer number (Figure S6)	*Monomer 1*	*% monomer 1*	*% TBCHA (Figure S6)*	*Measured F mCherry*	*log measured F mCherry*
P54	HPhOPA	16.7	83.3	826	2.92
P55	tBCHA	100	0	693	2.84
P56	NpMAe	100	0	855	2.93
P57	BMA	100	0	1075	3.03
P58	NpMAe	50	50	742	2.87
P59	BnMA	50	50	967	2.99
P60	MEdMSPNH	100	0	457	2.66
P61	MEdMSPNH	50	50	445	2.65

Table S7 Composition and pathogen attachment (expressed as log mCherry fluorescence, logF) of the larger polymer library used for model validation

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
CHMA	67	Cddm	33	188	2.27
tBCHA	67	LMM	33	331	2.52
EGDPEA	67	4MpM	33	430	2.63
CiM	67	4MbM	33	395	2.60
4IpbM	67	EGDPEA	33	349	2.54
4NbM	67	Cddm	33	1196	3.08
CM	67	LMM	33	505	2.70
4MpM	67	4MpM	33	631	2.80
PM	67	4MbM	33	452	2.65
2EhM	67	EGDPEA	33	315	2.50
GM	67	Cddm	33	511	2.71
DdMA	67	LMM	33	551	2.74
Cddm	67	4MpM	33	427	2.63
4MbM	100			318	2.50
MEdMSPNH	100			493	2.69
4MpM	25	HPhOPA	75	2059	3.31
4MbM	25	PhMA	75	629	2.80
EGDPEA	25	DEGMA	75	717	2.86
Cddm	25	MEdMSPNH	75	799	2.90
LMM	50	HPhOPA	50	495	2.69
4MpM	50	PhMA	50	912	2.96
4MbM	50	DEGMA	50	588	2.77
CHMA	67	LMM	33	262	2.42
tBCHA	67	4MpM	33	491	2.69
EGDPEA	67	64MbM	33	447	2.65

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
CiM	67	EGDPEA	33	336	2.53
4MbM	67	Cddm	33	503	2.70
4NbM	67	LMM	33	1279	3.11
CM	67	4MpM	33	400	2.60
4MpM	67	4MbM	33	381	2.58
PM	67	EGDPEA	33	360	2.56
LMM	67	Cddm	33	390	2.59
GM	67	LMM	33	390	2.59
DdMA	67	4MpM	33	605	2.78
Cddm	67	4MbM	33	407	2.61
Cddm	100			378	2.58
BnMA	100			161	2.21
4MbM	25	HPhOPA	75	847	2.93
EGDPEA	25	PhMA	75	680	2.83
Cddm	25	BnMA	75	453	2.66
LMM	25	MEdMSPNH	75	459	2.66
4MpM	50	HPhOPA	50	1682	3.23
4MbM	50	PhMA	50	720	2.86
EGDPEA	50	DEGMA	50	698	2.84
CHMA	67	4MpM	33	185	2.27
tBCHA	67	4MbM	33	470	2.67
EGDPEA	67	EGDPEA	33	447	2.65
4IpbM	67	Cddm	33	343	2.53
4MbM	67	LMM	33	378	2.58
4NbM	67	4MpM	33	617	2.79
CM	67	4MbM	33	431	2.63
4MpM	67	EGDPEA	33	391	2.59
2EhM	67	6Cddm	33	321	2.51

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
LMM	67	LMM	33	299	2.47
GM	67	4MpM	33	579	2.76
DdMA	67	4MbM	33	417	2.62
Cddm	67	EGDPEA	33	357	2.55
LMM	100			333	2.52
EGDPEA	25	HPhOPA	75	889	2.95
Cddm	25	DEGMA	75	397	2.60
LMM	25	BnMA	75	562	2.75
4MpM	25	MEdMSPNH	75	699	2.84
4MbM	50	HPhOPA	50	568	2.75
EGDPEA	50	PhMA	50	463	2.67
Cddm	50	BnMA	50	594	2.77
CHMA	67	4MbM	33	338	2.53
tBCHA	67	EGDPEA	33	265	2.42
CiM	67	Cddm	33	336	2.53
4IpbM	67	LMM	33	339	2.53
4MbM	67	4MpM	33	346	2.54
4NbM	67	4MbM	33	360	2.56
CM	67	EGDPEA	33	431	2.63
PM	67	Cddm	33	355	2.55
2EhM	67	LMM	33	381	2.58
LMM	67	4MpM	33	359	2.55
GM	67	4MbM	33	453	2.66
DdMA	67	EGDPEA	33	392	2.59
4MpM	100			528	2.72
EGDPEA	75	MEdMSPNH	25	592	2.77
Cddm	25	PhMA	75	518	2.71
LMM	25	DEGMA	75	667	2.82

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
4MpM	25	BnMA	75	521	2.72
4MbM	25	MEdMSPNH	75	1143	3.06
EGDPEA	50	HPhOPA	50	426	2.63
Cddm	50	DEGMA	50	468	2.67
LMM	50	BnMA	50	762	2.88
CHMA	67	EGDPEA	33	255	2.41
EGDPEA	67	Cddm	33	320	2.51
CiM	67	LMM	33	305	2.48
4IpbM	67	4MpM	33	307	2.49
4MbM	67	4MbM	33	503	2.70
4NbM	67	EGDPEA	33	442	2.65
4MpM	67	Cddm	33	545	2.74
PM	67	LMM	33	379	2.58
2EhM	67	4MpM	33	430	2.63
LMM	67	4MbM	33	358	2.55
GM	67	EGDPEA	33	318	2.50
Cddm	67	Cddm	33	505	2.70
PhMA	100			626	2.80
Cddm	25	HPhOPA	75	379	2.58
LMM	25	PhMA	75	731	2.86
4MpM	25	DEGMA	75	618	2.79
4MbM	25	BnMA	75	460	2.66
EGDPEA	25	MEdMSPNH	75	927	2.97
Cddm	50	PhMA	50	610	2.78
LMM	50	DEGMA	50	545	2.74
4MpM	50	BnMA	50	586	2.77
tBCHA	67	Cddm	33	293	2.47
EGDPEA	67	LMM	33	332	2.52

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
CiM	67	4MpM	33	348	2.54
4IpbM	67	4MbM	33	330	2.52
4MbM	67	EGDPEA	33	336	2.53
CM	67	Cddm	33	461	2.66
4MpM	67	LMM	33	436	2.64
PM	67	4MpM	33	326	2.51
2EhM	67	4MbM	33	395	2.60
LMM	67	EGDPEA	33	341	2.53
DdMA	67	Cddm	33	548	2.74
Cddm	67	LMM	33	381	2.58
LMM	25	HPhOPA	75	677	2.83
4MpM	25	PhMA	75	665	2.82
4MbM	25	DEGMA	75	670	2.83
EGDPEA	25	BnMA	75	249	2.40
Cddm	50	HPhOPA	50	748	2.87
LMM	50	PhMA	50	739	2.87
4MpM	50	DEGMA	50	628	2.80
4MbM	50	BnMA	50	167	2.22
CHMA	67	DdMA	33	186	2.27
tBCHA	67	2EhM	33	401	2.60
EGDPEA	67	CM	33	412	2.61
CiM	67	4IpbM	33	357	2.55
4IpbM	67	tBCHA	33	372	2.57
CM	67	2EhM	33	582	2.76
4MpM	67	CM	33	692	2.84
PM	67	4IpbM	33	593	2.77
2EhM	67	6tBCHA	33	400	2.60
GM	67	DdMA	33	373	2.57

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
DdMA	67	2EhM	33	496	2.70
Cddm	67	CM	33	464	2.67
4IpbM	100			270	2.43
tBCHA	100			313	2.50
DEGMA	100			483	2.68
CM	25	HPhOPA	75	1688	3.23
4IpbM	25	PhMA	75	537	2.73
tBCHA	25	DEGMA	75	679	2.83
DdMA	25	MEdMSPNH	75	804	2.91
2EhM	50	HPhOPA	50	494	2.69
CM	50	PhMA	50	574	2.76
4IpbM	50	DEGMA	50	496	2.70
CHMA	67	2EhM	33	291	2.46
tBCHA	67	CM	33	708	2.85
EGDPEA	67	4IpbM	33	302	2.48
CiM	67	tBCHA	33	401	2.60
4MbM	67	DdMA	33	482	2.68
4NbM	67	2EhM	33	1697	3.23
CM	67	CM	33	874	2.94
4MpM	67	4IpbM	33	365	2.56
PM	67	tBCHA	33	615	2.79
LMM	67	DdMA	33	340	2.53
GM	67	2EhM	33	410	2.61
DdMA	67	CM	33	523	2.72
Cddm	67	4IpbM	33	398	2.60
DdMA	100			333	2.52
4IpbM	25	HPhOPA	75	634	2.80
tBCHA	25	PhMA	75	561	2.75

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
DdMA	25	BnMA	75	676	2.83
2EhM	25	MEdMSPNH	75	724	2.86
CM	50	HPhOPA	50	1022	3.01
4IpbM	50	PhMA	50	357	2.55
tBCHA	50	DEGMA	50	471	2.67
CHMA	67	33CM	33	341	2.53
tBCHA	67	4IpbM	33	374	2.57
EGDPEA	67	tBCHA	33	328	2.52
4IpbM	67	DdMA	33	437	2.64
4MbM	67	2EhM	33	379	2.58
4NbM	67	CM	33	2274	3.36
CM	67	4IpbM	33	346	2.54
4MpM	67	tBCHA	33	473	2.67
2EhM	67	DdMA	33	571	2.76
LMM	67	2EhM	33	372	2.57
GM	67	CM	33	424	2.63
DdMA	67	4IpbM	33	397	2.60
Cddm	67	tBCHA	33	389	2.59
2EhM	100			347	2.54
tBCHA	25	HPhOPA	75	773	2.89
DdMA	25	DEGMA	75	477	2.68
2EhM	25	BnMA	75	405	2.61
CM	25	MEdMSPNH	75	937	2.97
4IpbM	50	HPhOPA	50	535	2.73
tBCHA	50	PhMA	50	442	2.64
DdMA	50	5BnMA	50	528	2.72
CHMA	67	4IpbM	33	287	2.46
tBCHA	67	tBCHA	33	386	2.59

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
CiM	67	DdMA	33	491	2.69
4IpbM	67	2EhM	33	313	2.50
4MbM	67	CM	33	405	2.61
CM	67	tBCHA	33	421	2.62
PM	67	DdMA	33	556	2.75
2EhM	67	2EhM	33	444	2.65
LMM	67	CM	33	547	2.74
GM	67	4IpbM	33	380	2.58
DdMA	67	tBCHA	33	400	2.60
CM	100			426	2.63
tBCHA	75	MEdMSPNH	25	710	2.85
DdMA	25	PhMA	75	578	2.76
2EhM	25	DEGMA	75	579	2.76
CM	25	BnMA	75	473	2.67
4IpbM	25	MEdMSPNH	75	952	2.98
tBCHA	50	HPhOPA	50	546	2.74
DdMA	50	DEGMA	50	474	2.68
2EhM	50	BnMA	50	349	2.54
CHMA	67	tBCHA	33	209	2.32
EGDPEA	67	DdMA	33	401	2.60
CiM	67	2EhM	33	307	2.49
4IpbM	67	CM	33	450	2.65
4MbM	67	4IpbM	33	327	2.51
4NbM	67	tBCHA	33	1417	3.15
4MpM	67	DdMA	33	523	2.72
PM	67	2EhM	33	512	2.71
2EhM	67	33CM	33	489	2.69
LMM	67	4IpbM	33	477	2.68

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
GM	67	tBCHA	33	404	2.61
Cddm	67	DdMA	33	477	2.68
DdMA	25	HPhOPA	75	1066	3.03
2EhM	25	PhMA	75	538	2.73
CM	25	DEGMA	75	543	2.73
4IpbM	25	BnMA	75	564	2.75
tBCHA	25	MEdMSPNH	75	959	2.98
DdMA	50	PhMA	50	558	2.75
2EhM	50	DEGMA	50	457	2.66
CM	50	BnMA	50	510	2.71
tBCHA	67	DdMA	33	362	2.56
EGDPEA	67	2EhM	33	293	2.47
CiM	67	CM	33	477	2.68
4IpbM	67	4IpbM	33	362	2.56
4MbM	67	tBCHA	33	378	2.58
CM	67	DdMA	33	747	2.87
4MpM	67	2EhM	33	492	2.69
PM	67	CM	33	439	2.64
2EhM	67	4IpbM	33	400	2.60
LMM	67	tBCHA	33	413	2.62
DdMA	67	DdMA	33	557	2.75
Cddm	67	2EhM	33	502	2.70
2EhM	25	HPhOPA	75	991	3.00
CM	25	PhMA	75	628	2.80
4IpbM	25	DEGMA	75	575	2.76
tBCHA	25	BnMA	75	400	2.60
DdMA	50	HPhOPA	50	911	2.96
2EhM	50	PhMA	50	466	2.67

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
CM	50	DEGMA	50	545	2.74
4IpbM	50	BnMA	50	326	2.51
CHMA	67	GM	33	315	2.50
tBCHA	67	PM	33	592	2.77
EGDPEA	67	4NbM	33	1512	3.18
CiM	67	CiM	33	238	2.38
4IpbM	67	CHMA	33	341	2.53
CM	67	PM	33	702	2.85
PM	67	CiM	33	249	2.40
2EhM	67	CHMA	33	415	2.62
GM	67	GM	33	417	2.62
DdMA	67	PM	33	769	2.89
Cddm	67	4NbM	33	615	2.79
CiM	100			185	2.27
CHMA	100			244	2.39
4NbM	254	HPhOPA	75	1930	3.29
CiM	25	PhMA	75	373	2.57
CHMA	25	DEGMA	75	487	2.69
GM	25	MEdMSPNH	75	573	2.76
PM	50	HPhOPA	50	612	2.79
4NbM	50	PhMA	50	270	2.43
CiM	50	DEGMA	50	304	2.48
CHMA	67	PM	33	241	2.38
tBCHA	67	4NbM	33	1021	3.01
EGDPEA	67	CiM	33	251	2.40
CiM	67	CHMA	33	332	2.52
4MbM	67	GM	33	368	2.57
4NbM	67	PM	33	2990	3.48

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
CM	67	4NbM	33	1090	3.04
4MpM	67	CiM	33	258	2.41
PM	67	CHMA	33	611	2.79
LMM	67	GM	33	349	2.54
GM	67	PM	33	620	2.79
DdMA	67	4NbM	33	416	2.62
Cddm	67	CiM	33	322	2.51
GM	100			333	2.52
CiM	25	HPhOPA	75	496	2.70
CHMA	25	PhMA	75	483	2.68
GM	25	BnMA	75	409	2.61
PM	25	MEdMSPNH	75	3849	3.59
CiM	50	PhMA	50	429	2.63
CHMA	50	DEGMA	50	405	2.61
tBCHA	67	CiM	33	288	2.46
EGDPEA	67	CHMA	33	293	2.47
4IpbM	67	GM	33	345	2.54
4MbM	67	PM	33	697	2.84
4NbM	67	4NbM	33	2136	3.33
CM	67	CiM	33	264	2.42
4MpM	67	CHMA	33	492	2.69
2EhM	67	GM	33	403	2.60
LMM	67	PM	33	697	2.84
GM	67	4NbM	33	2543	3.41
DdMA	67	CiM	33	437	2.64
Cddm	67	CHMA	33	455	2.66
PM	100			590	2.77
CHMA	25	HPhOPA	75	1005	3.00

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
GM	25	DEGMA	75	439	2.64
PM	25	BnMA	75	585	2.77
4NbM	25	MEdMSPNH	75	653	2.81
CiM	50	HPhOPA	50	295	2.47
CHMA	50	PhMA	50	263	2.42
GM	50	BnMA	50	478	2.68
CHMA	67	CiM	33	214	2.33
tBCHA	67	CHMA	33	491	2.69
CiM	67	GM	33	298	2.47
4IpbM	67	PM	33	351	2.54
4NbM	67	CiM	33	1146	3.06
CM	67	CHMA	33	683	2.83
PM	67	GM	33	545	2.74
2EhM	67	PM	33	559	2.75
LMM	67	4NbM	33	618	2.79
GM	67	CiM	33	387	2.59
DdMA	67	CHMA	33	471	2.67
CHMA	75	MEdMSPNH	25	322	2.51
GM	25	PhMA	75	425	2.63
PM	25	DEGMA	75	1136	3.06
4NbM	25	BnMA	75	816	2.91
CiM	25	MEdMSPNH	75	277	2.44
CHMA	50	HPhOPA	50	812	2.91
GM	50	DEGMA	50	628	2.80
PM	50	BnMA	50	914	2.96
CHMA	67	CHMA	33	289	2.46
EGDPEA	67	GM	33	414	2.62
CiM	67	PM	33	222	2.35

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
4IpbM	67	4NbM	33	1118	3.05
4MbM	67	CiM	33	348	2.54
4MpM	67	GM	33	430	2.63
PM	67	PM	33	202	2.31
2EhM	67	4NbM	33	793	2.90
LMM	67	CiM	33	341	2.53
GM	67	CHMA	33	418	2.62
Cddm	67	GM	33	383	2.58
GM	25	HPhOPA	75	835	2.92
PM	25	PhMA	75	619	2.79
4NbM	25	DEGMA	75	746	2.87
CiM	25	BnMA	75	437	2.64
CHMA	25	MEdMSPNH	75	529	2.72
GM	50	PhMA	50	355	2.55
PM	50	DEGMA	50	279	2.45
tBCHA	67	GM	33	263	2.42
EGDPEA	67	PM	33	242	2.38
CiM	67	4NbM	33	275	2.44
4IpbM	67	CiM	33	418	2.62
4MbM	67	CHMA	33	338	2.53
CM	67	GM	33	589	2.77
4MpM	67	PM	33	624	2.79
PM	67	4NbM	33	1451	3.16
2EhM	67	CiM	33	339	2.53
LMM	67	CHMA	33	505	2.70
DdMA	67	GM	33	536	2.73
Cddm	67	PM	33	680	2.83
PM	25	HPhOPA	75	942	2.97

Monomer 1 (Figure S7)	*% monomer 1*	*Monomer 2 (Figure S7)*	*% monomer 2*	*Measured F mCherry*	*log measured F mCherry*
4NbM	25	PhMA	75	798	2.90
CiM	25	DEGMA	75	499	2.70
CHMA	25	BnMA	75	472	2.67
GM	50	HPhOPA	50	707	2.85
PM	50	PhMA	50	303	2.48
4NbM	50	DEGMA	50	578	2.76
CiM	50	BnMA	50	100	2.00

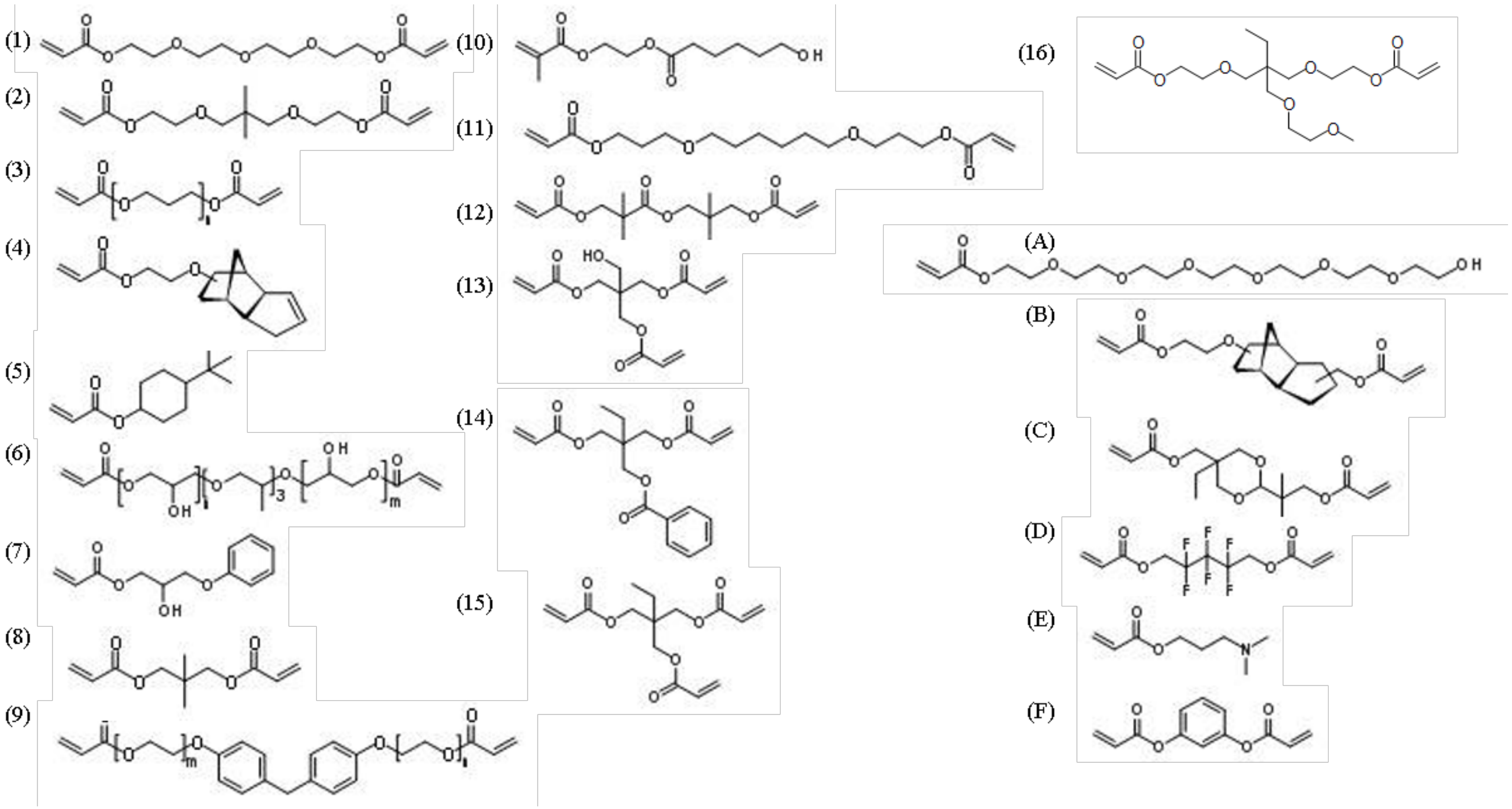


Figure S1. Monomer structures of commercially available compounds employed in the micro array fabrication. The co-polymers were formed by combining monomers 1-15 with monomers A-F in different volume ratios then exposing the mixture to UV.

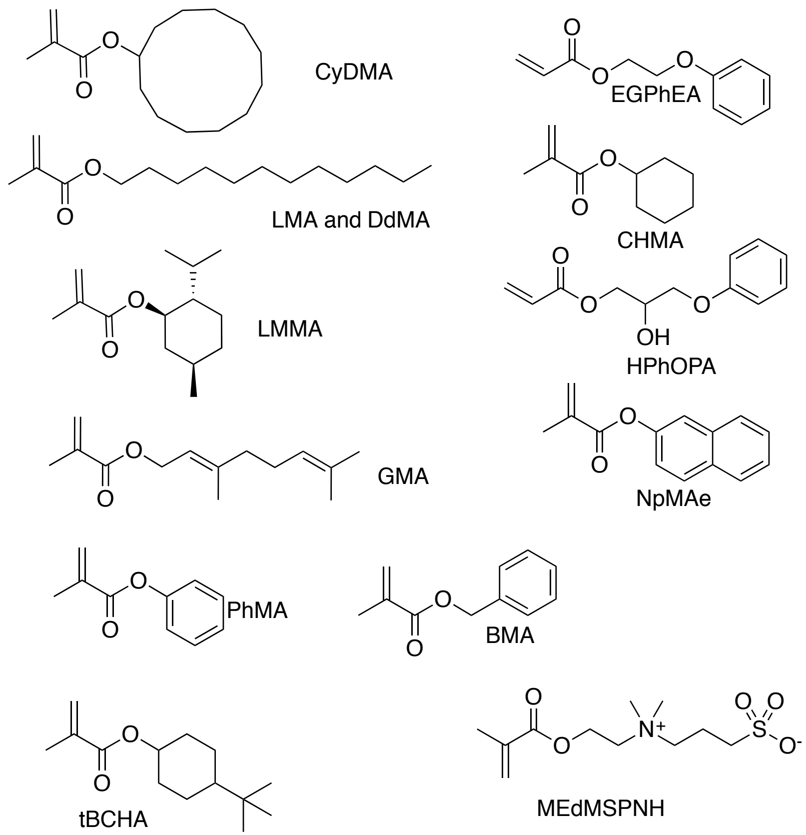
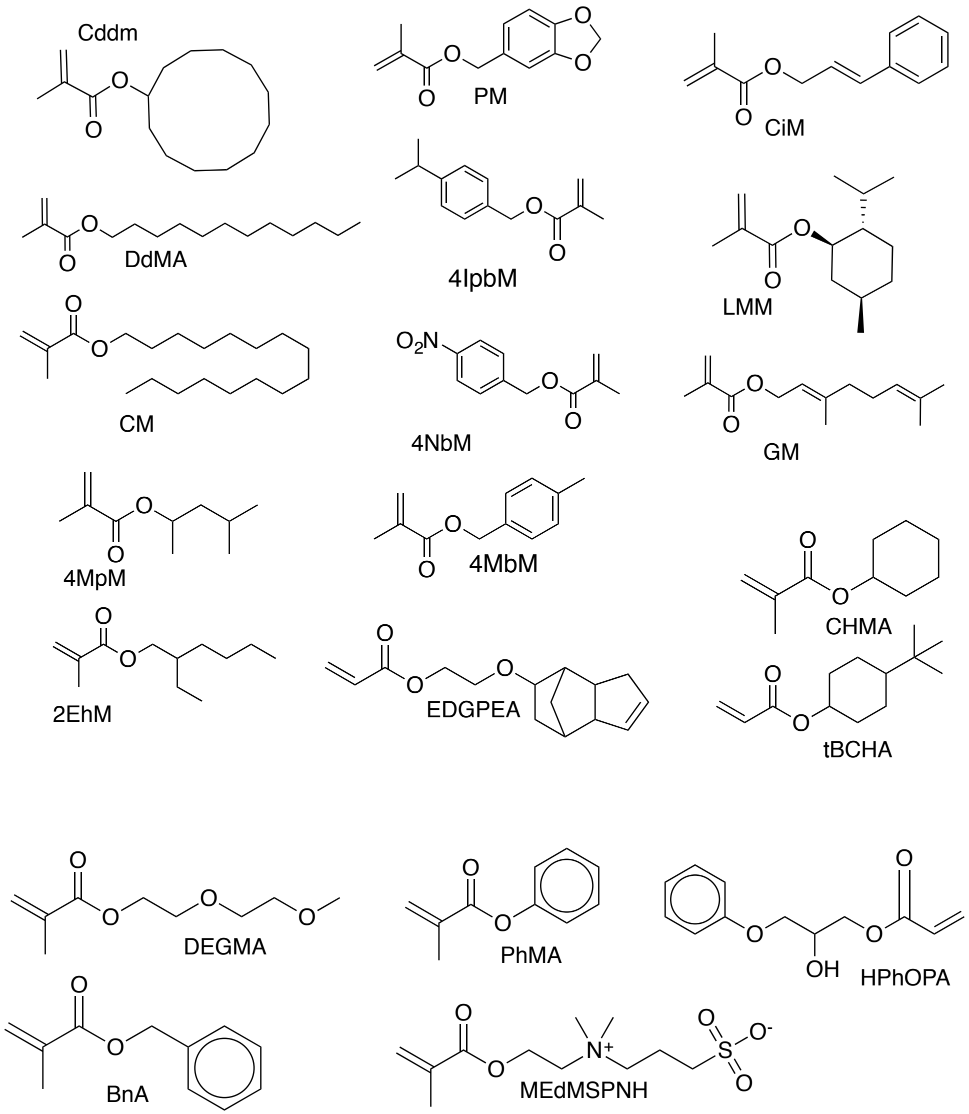


Figure S2. Structures of monomers used to generate smaller polymer library used to validate model predictions for mCherry-transformed pathogens


Cddm
PM
CiM
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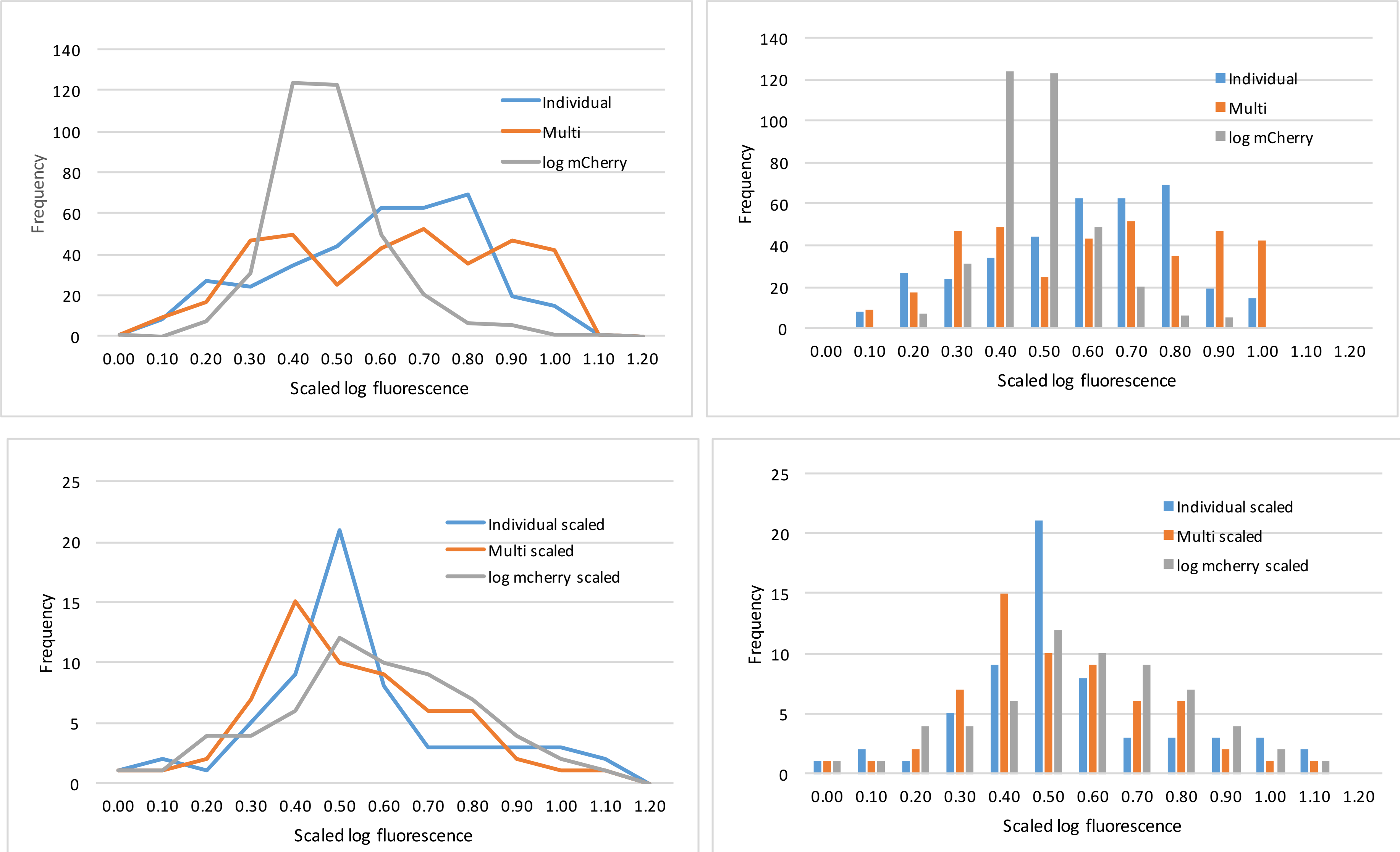
4IpbM
LMM
CM
O_2N
4NbM
GM
4MpM
4MbM
CHMA
2EhM
EDGPEA
tBCHA
DEGMA
PhMA
OH
HPhOPA
BnA
MEdMSPNH

Figure S3. Structures of monomers used to generate larger polymer library used to validate model predictions for mCherry-transformed pathogens



Individual
Multi
log mCherry
Frequency
Scaled log fluorescence
Individual scaled
Multi scaled
log mcherry scaled

Figure S4. Graph (left) and histograms (right) of distributions of normalized pathogen adhesion predicted by the individual, multi-pathogen and log mCherry fluorescence data for PA (top panels) and UPEC (bottom panels).

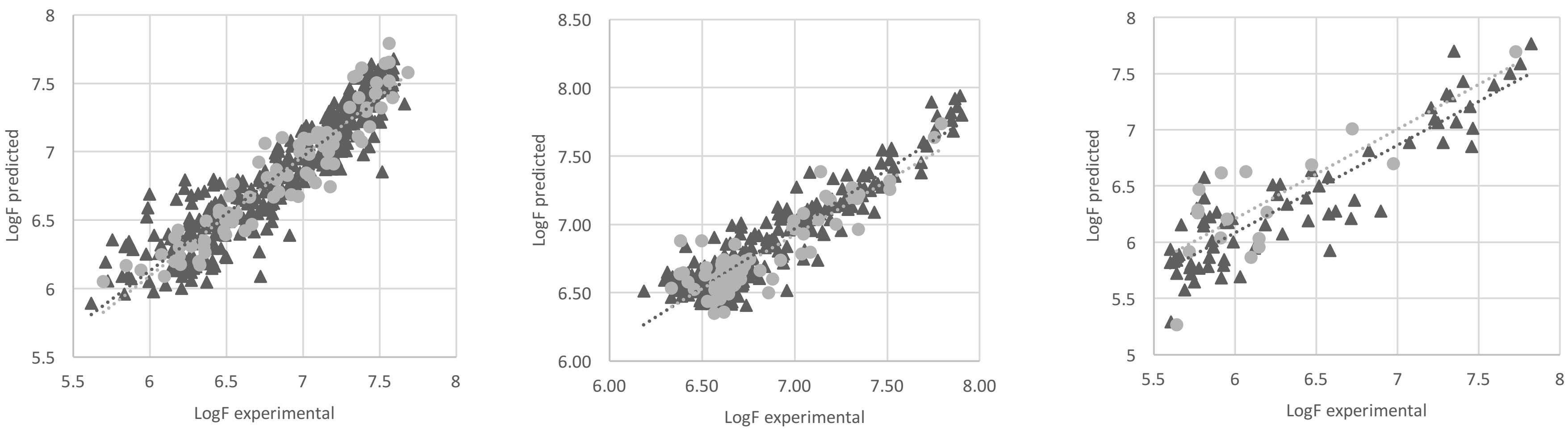


Figure S5. Measured and predicted attachment of PA, SA and UPEC for individual pathogens using molecular descriptors, training set (triangles), test set (circles).

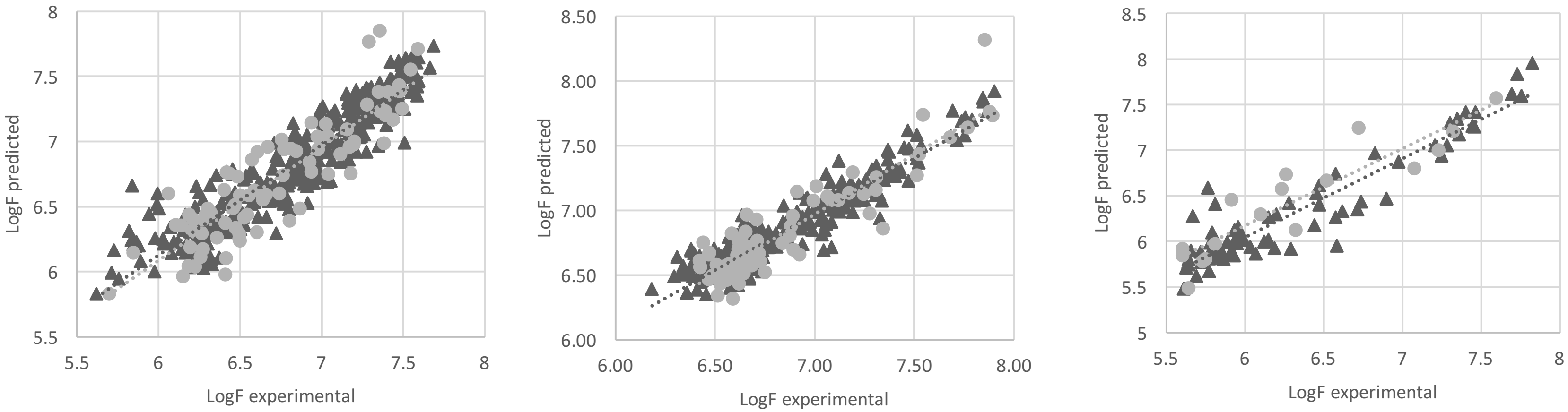
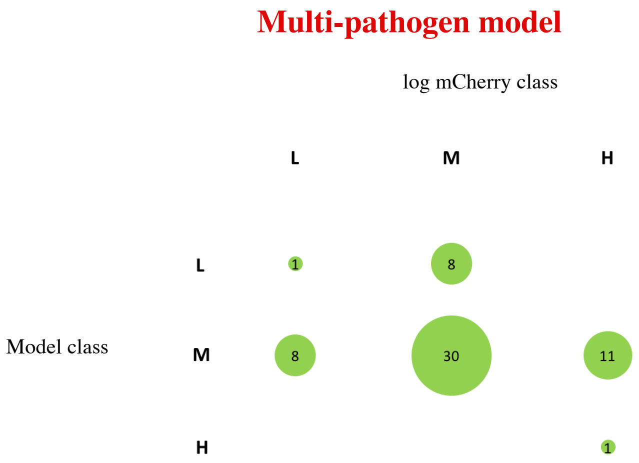
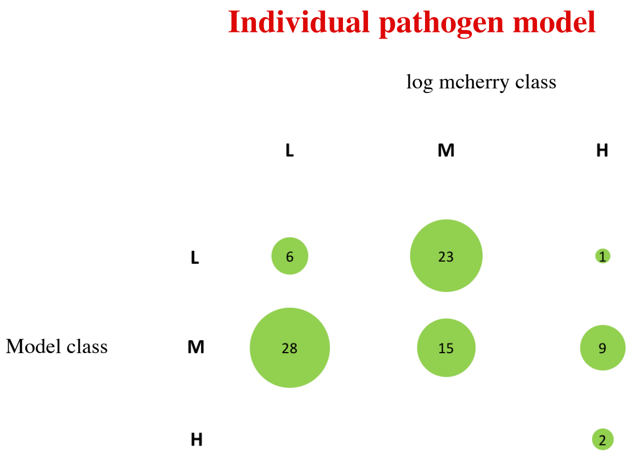


Figure S6. Measured and predicted attachment of PA, SA and UPEC for individual pathogens using experimental feature descriptors, training set (triangles), test set (circles).

PA attachment

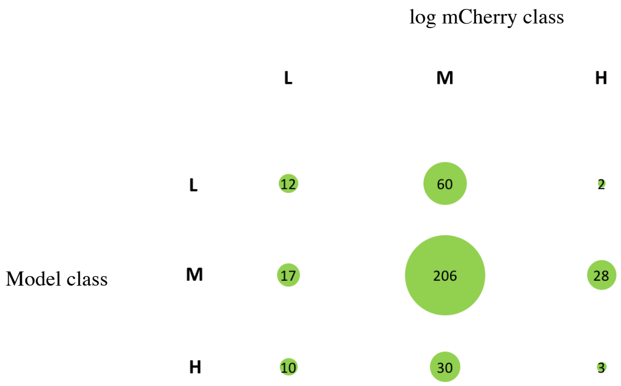
Polymer array 1



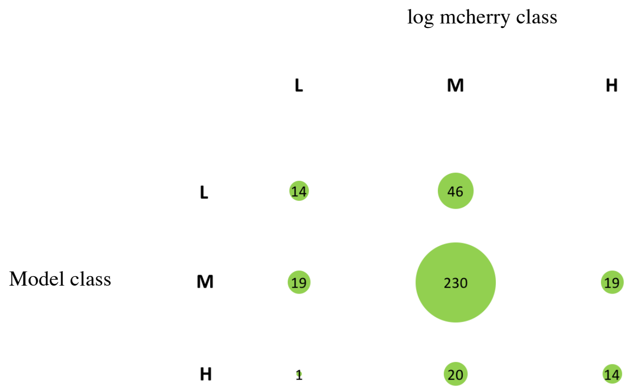


Polymer array 2

Multi-pathogen model



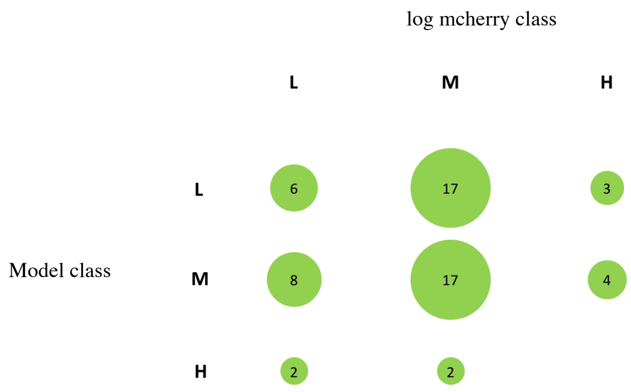
Individual pathogen model



UPEC

Polymer array 1

Multi-pathogen model



Individual pathogen model

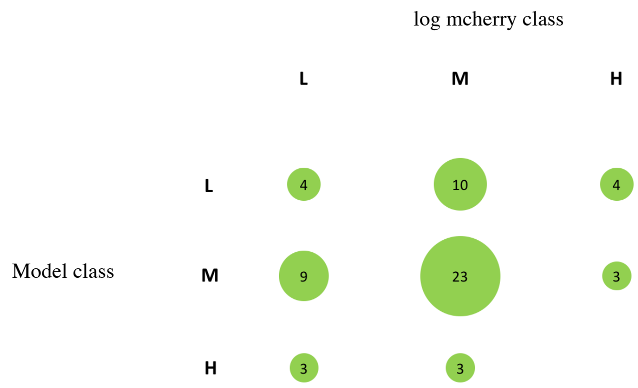


Figure S7. Truth tables for the three class predictions of pathogen attachment to a new polymer array where the pathogen adhesion was assessed by the brightness of the mCherry fluorescence.

References

1. Labute, P., A widely applicable set of descriptors. *J. Mol. Graph. Model.* **2000,** *18* (4-5), 464-477.

2. Raychaudhury, C.; Ray, S. K.; Ghosh, J. J.; Roy, A. B.; Basak, S. C., Discrimination of Isomeric Structures Using Information Theoretic Topological Indexes. *J. Comput. Chem.* **1984,** *5* (6), 581-588.