ADVANCED MATERIALS

Supporting Information

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Discovery of Novel Materials with Broad Resistance to Bacterial Attachment Using Combinatorial Polymer Microarrays

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Table SI1. A complete list of *F* for *P. aeruginosa* (PA), *S. aureus* (SA) and UPEC on 116 homopolymers.

Monomer name	CAS number	F_{PA}	F_{SA}	F_{UPEC}
Poly(propylene glycol) diacrylate	52496-08-9	754429.5	618577.25	824092
Hydroxypropyl methacrylate	27813-02-1	433914.5	711057.75	0
Glycidyl methacrylate	106-91-2	1741128.75	1782278	2714390.25
Tetrahydrofurfuryl methacrylate	2455-24-5	0	103008	0
Di(ethylene glycol) ethyl ether acrylate	7328-17-8	21966911.25	1654367.25	1433283.25
Ethyl acrylate	140-88-5	1012726.75	766487.5	0
Butylamino carbonyl oxy ethyl acrylate	63225-53-6	6237787.75	715478.25	0
Ethylene glycol diacrylate	2274-11-5	109084.25	0	498060.75
Butoxyethyl methacrylate	13532-94-0	1714099.5	314256.5	66308.5
Methyl 3-hydroxy-2-methylenebutyrate	18020-65-0	1766908.5	2938696.75	5149233.25
Lauryl methacrylate	142-90-5	909323.25	363109	0
Ethylene glycol dicyclopentenenyl ether acrylate	65983-31-5	0	0	0
Hexafluoroisopropyl acrylate	2160-89-6	0	0	0
Bisphenol A glycerolate diacrylate	4687-94-9	0	0	0
Hexadecafluoro-9-(trifluoromethyl)decyl acrylate	15577-26-1	0	0	555656.5
Butyl methacrylate	97-88-1	916898.75	0	0
Pentafluoropropyl methacrylate	45115-53-5	775170.25	0	2064009.25
Ethylhexyl methacrylate	688-84-6	904171.5	98102	138594.75
Tert-butylcyclohexylacrylate	84100-23-2	0	0	0
Trimethylolpropane ethoxylate triacrylate	28961-43-5	0	0	7047425.75
Tribromophenyl methacrylate	37721-71-4	107533.5	0	68788.75
Ethylhexyl acrylate	103-11-7	0	0	521716
Dodecafluoroheptyl acrylate	2993-85-3	440423.5	0	0
Glycidyl acrylate		0	16379370.5	19791401.25
Ethylene glycol phenyl ether methacrylate	10595-06-9	0	0	0
Ethylene glycol methyl ether methacrylate	6976-93-8	2244432	168695.5	134959
Isobutyl acrylate	106-63-8	1718564	0	0
Butanediol diacrylate	1070-70-8	190340.25	0	304926.75
Bisphenol A propoxylate diacrylate	67952-50-5	5607400.25	0	0
Hexanediol ethoxylate diacrylate		0	350850.75	894851.5
Hydroxybutyl methacrylate	29008-35-3	369537.75	99599.5	0
Methyl methacrylate	35233-69-3	907155.25	0	928746
Octafluoropentyl methacrylate	355-93-1	614640.5	141157.5	0
Ethoxyethyl acrylate	106-74-1	11317679.25	419539	553358
Butyl acrylate	141-32-2	800073.5	0	0
Tricyclodecane-dimethanol diacrylate	42594-17-2	38699380	0	8907386.5
Dimethylamino-propyl acrylate	18526-07-3	25452568.75	0	0
Hydroxyethyl methacrylate	868-77-9	1751339.5	1224119	0
Heptadecafluorodecyl methacrylate	1996-88-9	1306635.75	0	242799.25
Cyclohexyl methacrylate	101-43-9	0	0	0
Diethylamino ethyl acrylate	2426-54-2	1992917.25	2416031.5	0
Neopentyl glycol diacrylate	2223-82-7	0	0	0
Trimethylolpropane benzoate diacrylate	79720-88-0	51865256.25	0	25900022
Octafluoropentyl acrylate	376-84-1	1165353.25	0	0
Dimethylamino-ethyl methacrylate	2867-47-2	8060612.5	3456221.25	1512849
Isodecyl methacrylate	29964-84-9	0	0	0
Norbornyl methacrylate	29753-02-4	0	0	0
Isobornyl acrylate	5888-33-5	68441.5	0	21997.25
Neopentyl glycol propoxylate diacrylate	84170-74-1	96317	125316	0
Heptadecafluorodecyl acrylate	27905-45-9	435058.75	63671.25	0
Chloro-2-hydroxy-propyl methacrylate	13159-52-9	0	0	0
Hydroxybutyl acrylate	2478-10-6	10417065.75	3802876.5	0
Benzyl 2-n-propyl acrylate	118785-93-6	1477152.25	359933.5	0
Ethylene glycol dicyclopentenenyl ether methacrylate	68586-19-6	0	0	304428.25
Trimethylcyclohexyl methacrylate	7779-31-9	0	0	0
Hexyl acrylate	2499-95-8	739271.5	0	0
Methyl-1,2-ethanediyl bis[oxy(methyl-2,1-ethanediyl)]diacrylate	42978-66-5	183188.5	0	235104.25

Table SI1 continued

Monomer name	CAS number	F_{PA}	F_{SA}	F_{UPEC}
Dipentaerythritol penta/hexa-acrylate	60506-81-2	43415355.75	0	58059977
Hexafluorobutyl acrylate	54052-90-3	0	0	1701424
Di(ethylene glycol) methyl ether methacrylate	45103-58-0	9216204.75	530792.75	0
Decyl methacrylate	3179-47-3	351097.5	183753	0
Hexafluoroisopropyl methacrylate	3063-94-3	1637504.75	0	0
Di(ethylene glycol) 2-ethylhexyl ether acrylate	117646-83-0	4093941.5	370736.5	223306.75
Trimethylhexyl acrylate	2664-55-3	0	0	0
Hexadecafluoro-2-hydroxy-10-(trifluoromethyl)undecyl methacrylate	88752-37-8	0	0	538505.75
Tridecafluorooctyl acrylate	17527-29-6	0	0	0
Isobutyl methacrylate	97-86-9	1185691.25	0	0
Dodecafluoro-7-(trifluoromethyl)-octyl acrylate	50836-65-2	0	0	0
Isobornyl methacrylate	7534-94-3	0	0	0
Isooctyl acrylate	29590-42-9	2693980.5	392728.5	20692547.25
Ethylene glycol methyl ether acrylate	3121-61-7	3953855	0	0
Trimethylolpropane triacrylate	15625-89-5	222450.5	0	0
Tridecafluoro-2-hydroxynonyl acrylate	127377-12-2	0	0	0
Allyl methacrylate	96-05-9	0	0	0
Hexyl methacrylate	142-09-6	966920.75	267395.25	0
Furfuryl methacrylate	3454-28-2	1753791.5	0	0
Tert-butyl acrylate	1663-39-4	0	0	0
Di(ethylene glycol) diacrylate	4074-88-8	211690.75	0	1644977.5
Trimethylolpropane propoxylate triacrylate	53879-54-2	127742.75	34733.25	377753.25
Trimethylolpropane ethoxylate methyl ether diacrylate	302911-84-8	0	1320333.75	2121488.25
Dimethylamino-ethyl acrylate	2439-35-2	2334129.5	0	155051.5
Ethyl 2-ethylacrylate	3070-65-3	2479766.5	1614326	1384790.75
Trimethylsilyloxy)ethyl methacrylate	17407-09-9	4294533.5	3093099	1861807.5
Tris(trimethylsilyloxy)-silyl propyl methacrylate	17096-07-0	4753286.75	2541511.75	1432574.5
Propargyl acrylate	10477-47-1	299912	0	1541442.75
Phosphoric acid 2-hydroxyethyl methacrylate ester	52628-03-2	31395036	4025800.75	4008903.25
Pentaerythritol triacrylate	3524-68-3	54435981.75	0	45707543.25
Hexafluoropent-1,5-diyl diacrylate		0	0	179989
Ethoxyethyl methacrylate	2370-63-0	2200640	258512.25	0
Vinyl methacrylate	4245-37-8	1688333.75	0	266091.5
Heptafluorobutyl methacrylate	13695-31-3	1493673.75	770116	0
Ethylene glycol phenyl ether acrylate	48145-04-6	219987	317283.75	576887.75
Tetrahydrofurfuryl acrylate	2399-48-6	15725596.5	2671600	1833627.5
Bisphenol A propoxylate glycerolate diacrylate	105650-05-3	0	0	1095889
Methyl acrylate	96-33-3	1463499.25	0	0
Ter-butyl methacrylate	585-07-9	1254612.25	0	91615.75
Tridecafluorooctyl methacrylate	2144-53-8	0	0	0
Methylthioethyl methacrylate	14216-23-0	586413.25	0	0
Isodecyl acrylate	1330-61-6	0	0	0
Tetra(ethylene glycol) diacrylate	17831-71-9	45421976.25	0	0
Glycerol 1,3-diglycerolate diacrylate	60453-84-1	6956927.25	1113226.25	0
Pentafluoropropyl acrylate	356-86-5	0	1596591.5	0
Ethyl methacrylate	97-63-2	0	0	0
Diethylaminoethyl methacrylate	105-16-8	3831227.75	639972.5	0
Phenyl methacrylate	2177-70-0	782439.5	509511.75	0
Lauryl acrylate	2156-97-0	1664645	0	0
Hexamethylene diacrylate	13048-33-4	137956.5	0	0
Epoxidized acrylate	91722-14-4	0	287844	648727.5
Poly(propylene glycol) methyl ether acrylate	83844-54-6	72901982	1036268.5	1154413.75
Perfluorodecyl acrylate	27905-45-9	0	0	0
Ethyl 2-propylacrylate	3550-06-9	881380.25	0	637083.25
Benzyl methacrylate	2495-37-6	0	0	0
Zirconium carboxyethyl acrylate	123633-53-4	11429964.25	3030234.5	17686331.25
Heptafluorobutyl acrylate	424-64-6	5257760.75	0	0
Bisphenol F ethoxylate diacrylate	120750-67-6	0	0	956104.75
Poly(propylene glycol) acrylate	50858-51-0	15668694	991637.25	1410742.75

Table SI2. List of bacterial strains isolated from clinical infections.

Strain number	Strain	Source	Hit material	% reduction in bacterial coverage
TS-3	*S. aureus*	Perineal wound	10 (100%)	98.0
TS-4	*S. aureus*	Recurrent boils	10 (100%)	98.0
TS-10	*S. aureus*	Abdominal wound	NA	NA
TS-11	*S. aureus*	Fistula infection	11:4 (4:1)	99.7
40-1	*P. aeruginosa*	Wound	NA	NA
81-2	*P. aeruginosa*	Wound	10 (100%)	79.1
82-2	*P. aeruginosa*	Wound	7:6 (4:1)	95.2
92-2	*P. aeruginosa*	Wound	11:4 (4:1)	98.0
94-2	*P. aeruginosa*	Wound	NA	NA

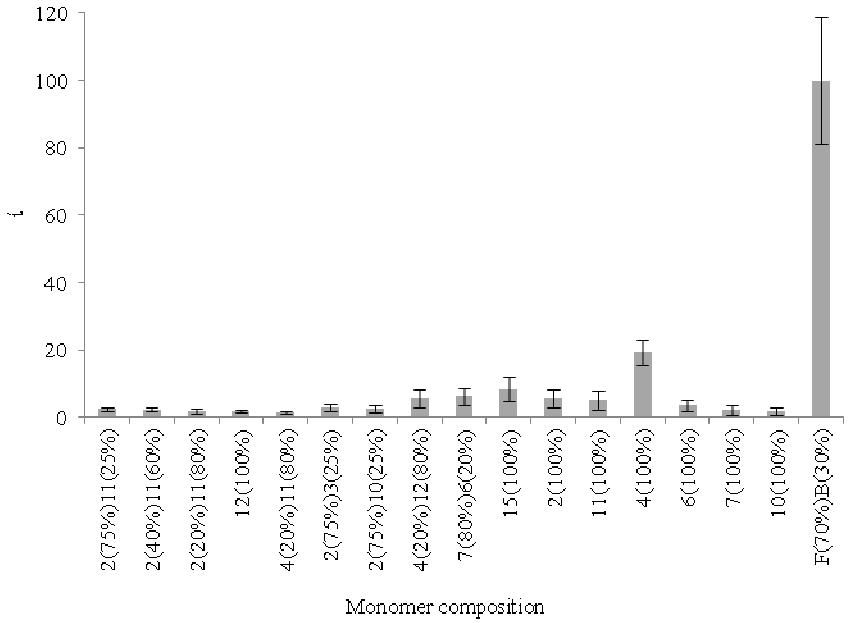

Figure SI1. Material scale out: i for each of the hit formulations. The monomer numbers given refers to the monomers in Figure 1b(i). The error bars equal ± one standard deviation unit, n = 60.

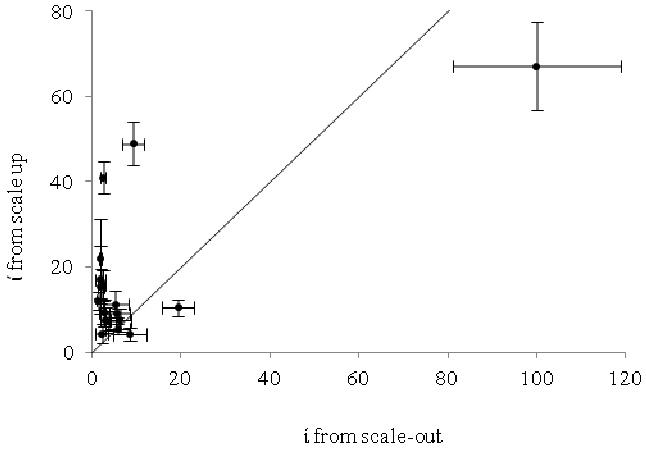

Figure SI2. Comparison of the biological performance of scaled up and scaled out samples. Error bars equal ± one standard deviation units, n = 3 for scale-up and whilst n = 60 for scale out. The y=x line is drawn as a guide.[1]

[1] A significantly different biological performance was observed for 4 of the 18 materials studied after scale up, specifically copolymers neopentyl glycol diacrylate (2) (75%) and *tert*-butylcyclohexyl acrylate (11) (25%), 2(40%)11(60%), 2(20%)11(80%), 4(20%)11(80%) and the homopolymers 12 (Figure SI2). It should be noted that some of the variance between the two assays is caused by the different staining procedures used. On the microarray all bacteria are labeled with GFP, thus the fluorescence signal will be representative of the total number of bacteria. On the polymer coupons the SYTO17 dye will stain both intracellular and extracellular DNA. Furthermore, the quantification is of coverage rather than total fluorescence, thus 3D structures will increase the value of the former measurement in comparison with the latter measurement. Despite this limitation, we have previously shown the two assays are comparable.[11] All the copolymers with varied performance contain monomer 11, however, the homopolymer of monomer 11 showed a relatively small change in performance between the two assays, with an i of 5.3% ± 2.8% on the microarray and 11.2% ± 3.1% as a polymer coupon. We have previously observed changes in the surface chemistry of polymeric materials after scale up due to the surface enrichment of a specific pendant group due to the altered surface area to volume ratio that occurs upon scale up. This effect is more pronounced in copolymers where the two components may phase separate or surface segregate.[11]

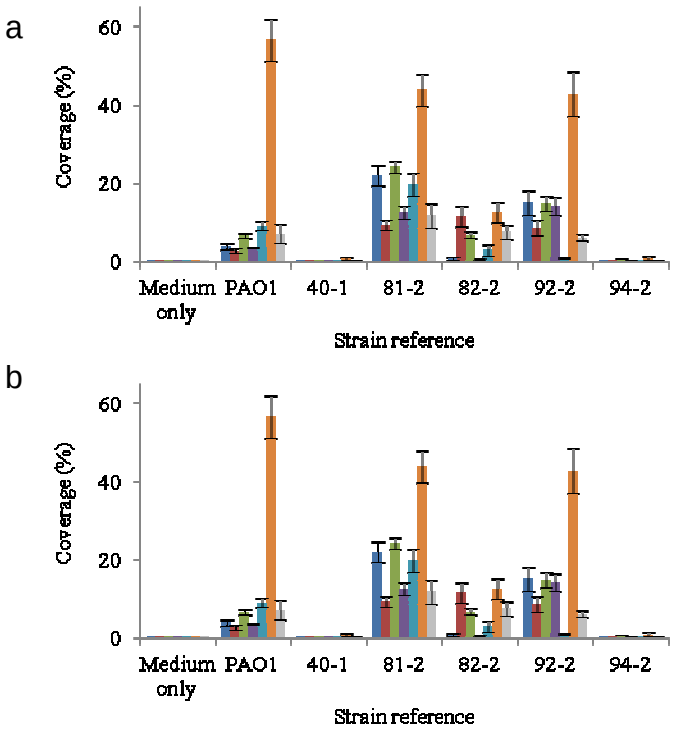

Figure SI3. Bacterial coverage of clinical isolates on scaled up hits. The composition of materials studied was monomers 2 (100%, ■), 15 (100%, ■), 7 (100%, ■), 7:6 (4:1, ■), 11:4 (4:1, ■), glass (■), silver hydrogel (■). The materials were cultured with (a) *P. aeruginosa* or (b) *S. aureus* strains. Error bars equal ± one standard deviation unit, n = 5.