A critical evaluation of random copolymer mimesis of homogeneous antimicrobial peptides

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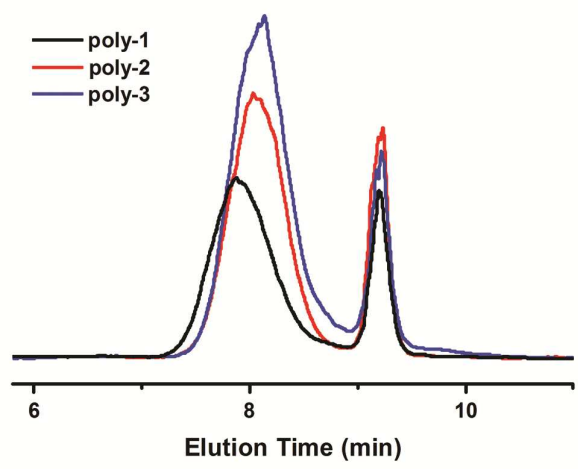
1. Figure S1. GPC elution characterization of the as-prepared MA-co-AEMA copolymers after de-protection. The GPC spectra (acetic acid/acetate buffer + 20% acetonitrile, calibrated with polystyrene standard) were obtained from a Waters 515 Pump and Waters 2410 Refractive Index Detector.



2. Table S1. Average molecular weights and polydispersities of the polymer SMAMPs according to GPC analysis.

copolymer	Mn (GPC)	Mw/Mn (PDI)
poly-1	2930	1.79
poly-2	2380	1.52
poly-3	2040	1.63

3. Figure S2. The Log P versus polymer side chain length, L, for the methacrylate monomers from published octanol-H_2O partition coefficient measurements.

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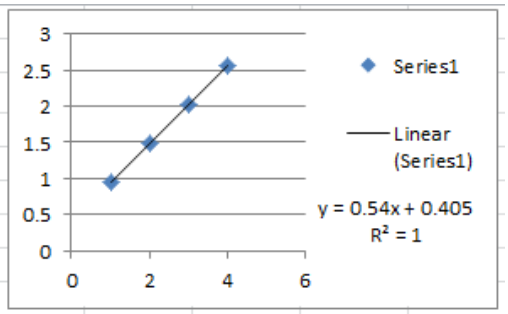
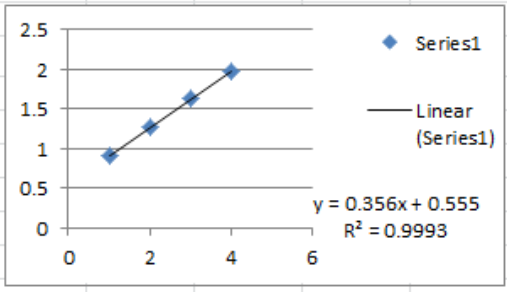
J Biomed. Mater. Res. (1983) 17, 945

	L_{alkyl}	Log P	ΔG = 2.3*RT*LogP
MMA	1	0.945	1.2878
EMA	2	1.485	2.0237
nPMA	3	2.025	2.7596
nBMA	4	2.565	3.4955
amine			-1.0981



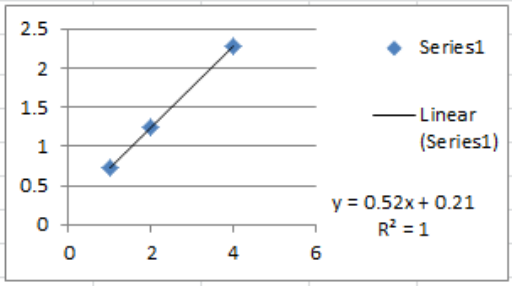
J. Biomed. Mater. Res. (1997) 37, 517

	L_{alkyl}	Log P	ΔG = 2.3*RT*LogP
MMA	1	0.9	1.2265
EMA	2	1.28	1.7443
nPMA	3	1.63	2.2213
nBMA	4	1.97	2.6846
amine			-0.8937



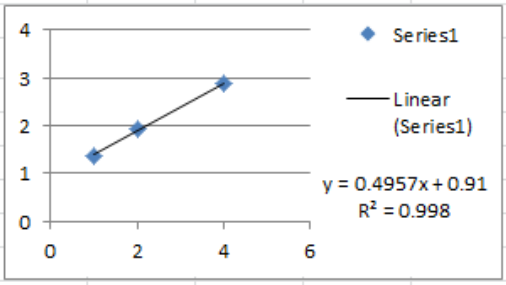
J. Biomed. Mater. Res. (1981) 15, 787

	L_{alkyl}	Log P	ΔG = 2.3*RT*LogP
MMA	1	0.73	0.9948
EMA	2	1.25	1.7034
nPMA	3		
nBMA	4	2.29	3.1207
amine			-1.3639

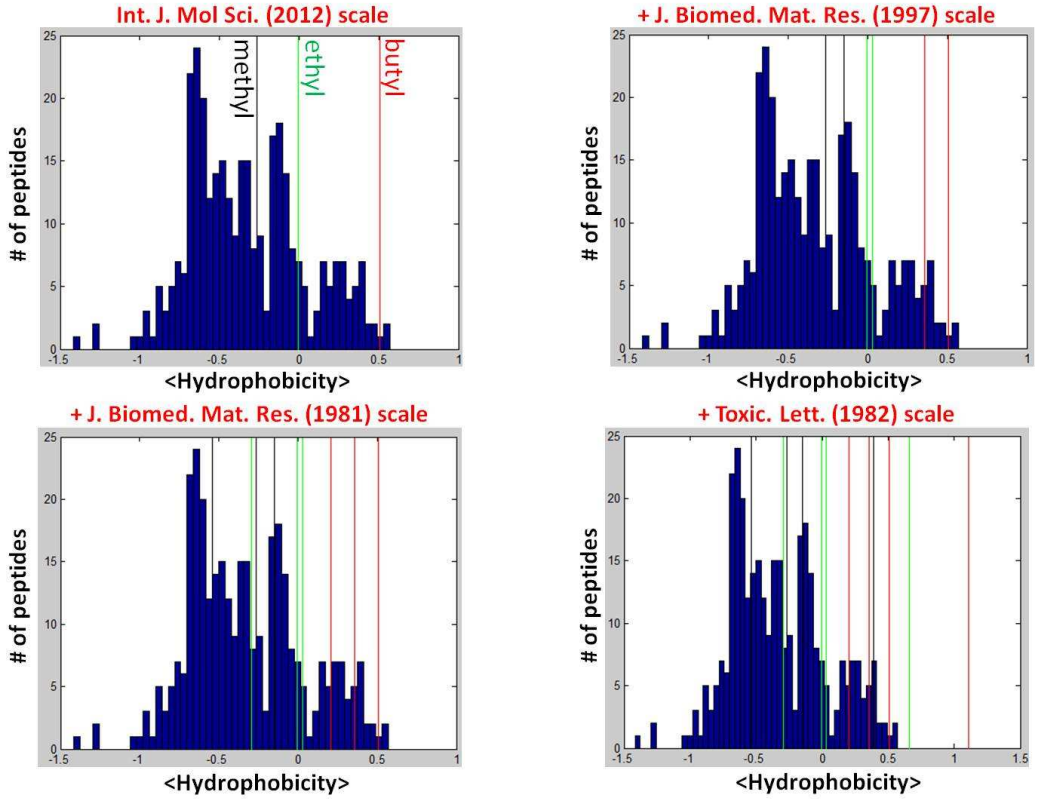


Toxicol. Lett. (1982) 11, 125

	L_{alkyl}	Log P	ΔG = 2.3*RT*LogP
MMA	1	1.38	1.8806
EMA	2	1.94	2.6437
nPMA	3		
nBMA	4	2.88	3.9247
amine			-0.4099



4. Figure S3. Comparison on <Hydrophobicity> of SMAMPs and AMPs using methacrylate hydrophobicity scales from different references [1-4]. The differences we observe between the random methacrylate copoplymer SMAMPs and natural AMPs are robust, and do not depend on details of the scale used.



References

1. Fujisawa, S.; Kadoma, Y. *International Journal of Molecular Sciences* **2012,** 13, (1), 758-773.
2. Yoshii, E. *Journal of Biomedical Materials Research* **1997,** 37, (4), 517-524.
3. Fujisawa, S.; Masuhara, E. *Journal of Biomedical Materials Research* **1981,** 15, (6), 787-793.
4. Hideji, T.; Kazuo, H. *Toxicology Letters* **1982,** 11, (1–2), 125-129.