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Supplementary Information for

Article

Synthesis of Peptide-Immobilized Magnetic Beads, and Peptide Reactivity Assay for Assessing Skin Sensitization Utilizing Chromophore

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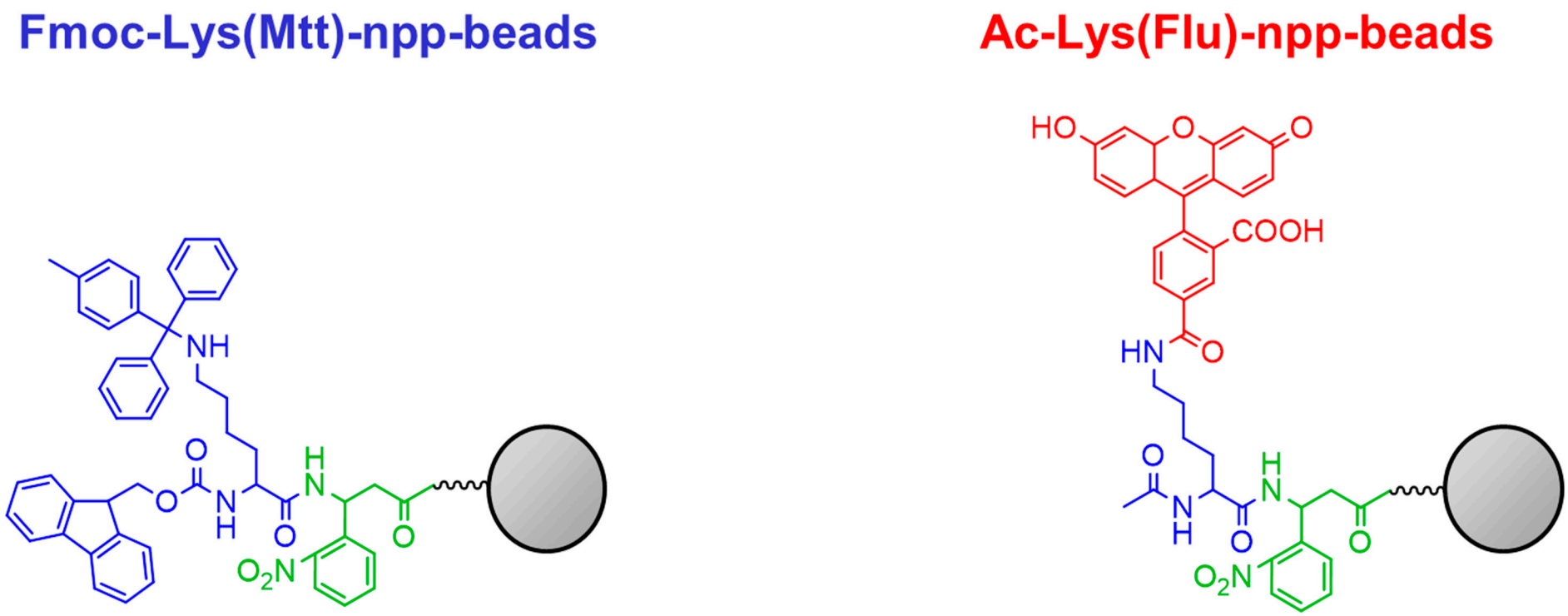

Figure S1. Structures of Fmoc-Lys(Mtt)-npp-beads and fluorescein tagged Ac-Lys(Flu)-npp-beads

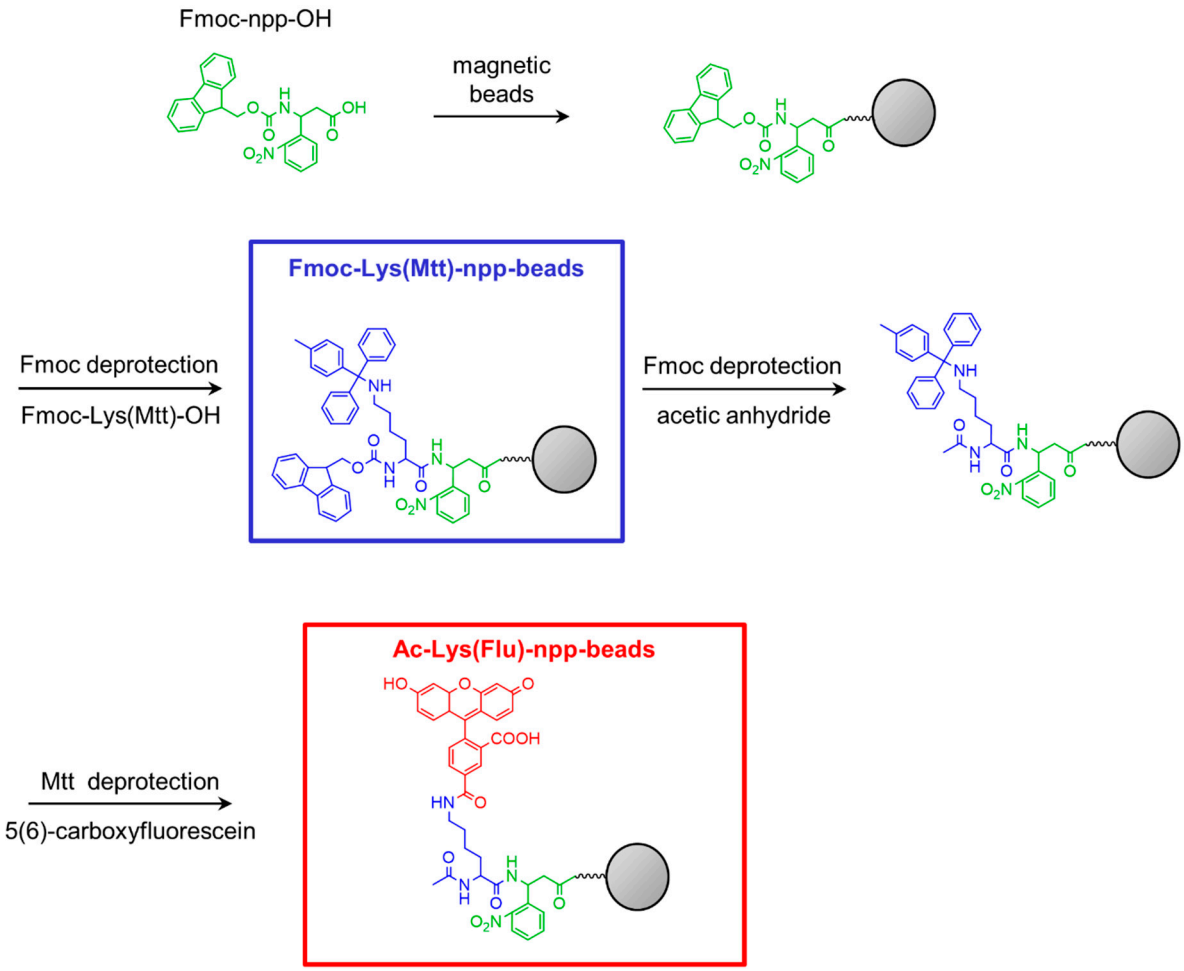

Figure S2. Synthesis of Fmoc-Lys(Mtt)-npp-beads and Ac-Lys(Flu)-npp-beads.

Table **S**1.Reactivity of test chemicals to Ac-Lys-beads determined by percent depletion

Test Chemicals	log Kow	LLNA Potency category	Mechanism	DPRA[a,b] Mean depletion ratio (%)	DPRA[a,b] Results[c]	ADRA[d] Depletion ratio (%)	ADRA[d] Results[e]	C-SPRA-MB Depletion ratio (%)	C-SPRA-MB Results[f]
p-Benzoquinone (BQ)	0.25	Extreme	Michael acceptor	95.0[a]	P	98.2[d]	P	92.5	P
Fluorescein-5-isothiocyanate (FITC)	4.69	Strong	Acyl-transfer	80.6[a]	P	100.0[d]	P	84.6	P
Benzylidene acetone (BA)	2.04	Moderate	Michael acceptor	48.1[a]	P	55.1[d]	P	75.0	P
5-Methyl-2-phenyl-2-hexenal (MPH)	3.77	Moderate	Michael acceptor /Schiff base	-	-	-	-	46.2	P
Undec-10-enal (UE)	4.12	Moderate	Schiff base	0.00[b]	N[g]	-	N[g]	67.5	P
-Amyl cinnamic aldehyde (ACA)	4.33	Weak	Michael acceptor /Schiff base	2.25[a]	N[g]	4.1[d]	N[g]	40.0	P
Dibutyl phthalate (DP)	4.61	Non-sensitizer	Non-binding	0.00[b]	N	-	N	9.7	N

[a]Data from Ref. 1. [b]Data from Ref. 2. [c]Threshold of 6.38% average peptide depletion was used to discriminate between 'P' (positive) and 'N' (negative). [d]Data from Ref. 3. [e]Threshold of 4.9 % mean peptide depletion was used to discriminate between 'P' (positive) and 'N' (negative). [f] Threshold of 20 % mean peptide depletion was used to discriminate between 'P' (positive) and 'N' (negative). [g]Although they are sensitizers, they showed "false negatives" in DPRA and ADRA.

References

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3. Fujita, M., Yamamoto, Y., Tahara, H., Kasahara, T., Jimbo, Y. and Hioki, T.: Development of a prediction method for skin sensitisation using novel cysteine and lysinederivatives, J. Pharmacol. Toxicol. Methods, **2014**, 70, 94–105.