Electronic Supplementary Material (ESI) for Biomaterials Science.

Electronic Supplementary Information

Microencapsulation of Alcohol-Solvents and High-Content Actives for Efficient Transdermal Delivery

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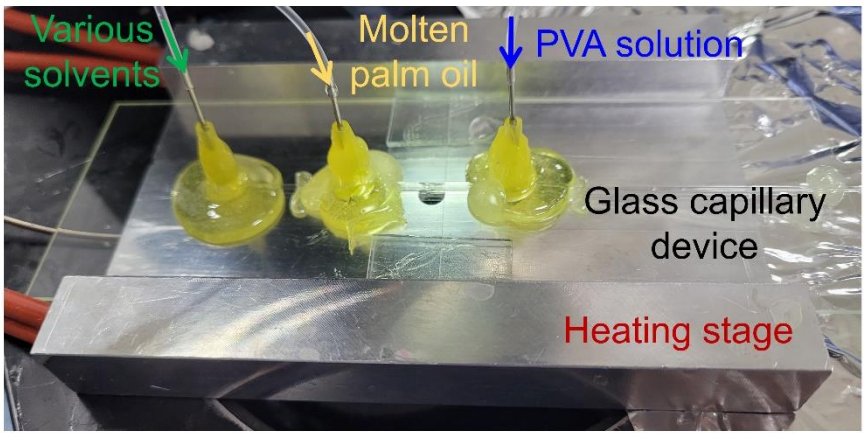

Fig. S1 Photograph of the device and the detailed setup used for the production of palm oil-based microcapsules.

Table S1. Hansen solubility parameters (HSP) of palm oil, PEGDA, water, EtOH, and DPG.

		[a]δ_d ($MPa^{1/2}$)	[a]δ_p ($MPa^{1/2}$)[b]	[a]δ_h ($MPa^{1/2}$)[c]
Solute	Palm oil	17.7	3.5	3.7
	PEGDA	17.0	10.7	8.9
Solvent	Water	15.5	16.0	42.3
	Ethanol	15.8	8.8	19.4
	DPG	16.5	10.6	17.7

[a]Values reported elsewhere.[15-18] δ_d, δ_p, and δ_h each indicates dispersion solubility parameter, polar solubility parameter, and hydrogen bonding solubility parameter, respectively.

Table S2. Relative energy difference (RED) results of palm oil and PEGDA acquired by calculating the ratio of HSP distance (R_a) between the solute and various solvents to the interaction radius (R_0) of the solute.

	Interaction radius (R_0)[a]	HSP distance between solute-solvents (R_a)			Relative energy difference (RED)/(Score)[b]		
		Water	Ethanol	DPG	Water	Ethanol	DPG
Palm oil	4.7	40.8	17.0	15.9	8.7 (0)	3.6 (0)	3.4 (0)
PEGDA	22	34.0	10.9	8.9	1.54 (0)	0.5 (1)	0.4 (1)

[a]Values reported elsewhere.[15-18] [b]Score 1: good solvent, and score 0: poor solvent.

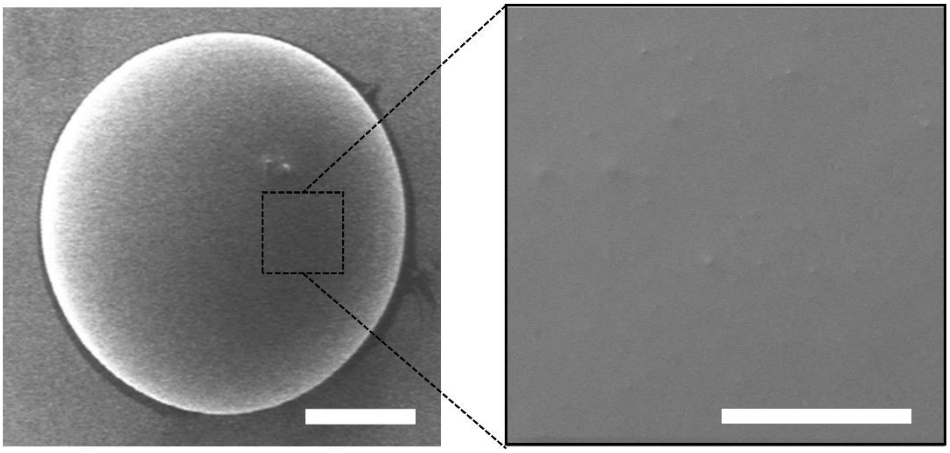

Fig. S2 Low and high magnification scanning electron micrographs (SEM) of the palm oil-based microcapsule and its surface topology. Scale bars each represent 100 and 10 µm for the left and right SEM, respectively.

Table S3. Composition of NC, WC, WC+D, and DC formulations containing niacinamide and adenosine. The niacinamide and adenosine amount in the microcapsule was determined using high-performance liquid chromatography (HPLC, Ultimate 3000, Dionex). All formulations contain equal amount of niacinamide and adenosine and the total amount of DPG in WC+D and DC formulations are identical. Additives are ethylenediaminetetraacetic acid (EDTA) and preservatives.

Component		NC	WC	WC+D	DC
Microcapsule (core)	Niacinamide	-	0.2	0.2	0.2
	Adenosine	-	0.04	0.04	0.04
	Dipropylene glycol (DPG)	-	-	-	0.38
	Water	-	0.76	0.76	0.38
Niacinamide		2	1.8	1.8	1.8
Adenosine		0.04	-	-	-
DPG		-	-	5	4.62
Butylene glycol (1,3-BG)		5	5	5	5
Cetearyl Alcohol		2	2	2	2
Cetyl Alcohol		1	1	1	1
Cetyl Palmitate/Sorbitan Olivate/Sorbitan Palmitate		1	1	1	1
Caprylic/Capric Triglyceride		5	5	5	5
Ceramide NP		0.5	0.5	0.5	0.5
Stearic acid		0.5	0.5	0.5	0.5
Oleic acid		0.3	0.3	0.3	0.3
Water		To 100	To 100	To 100	To 100
Additive		q.s	q.s	q.s	q.s

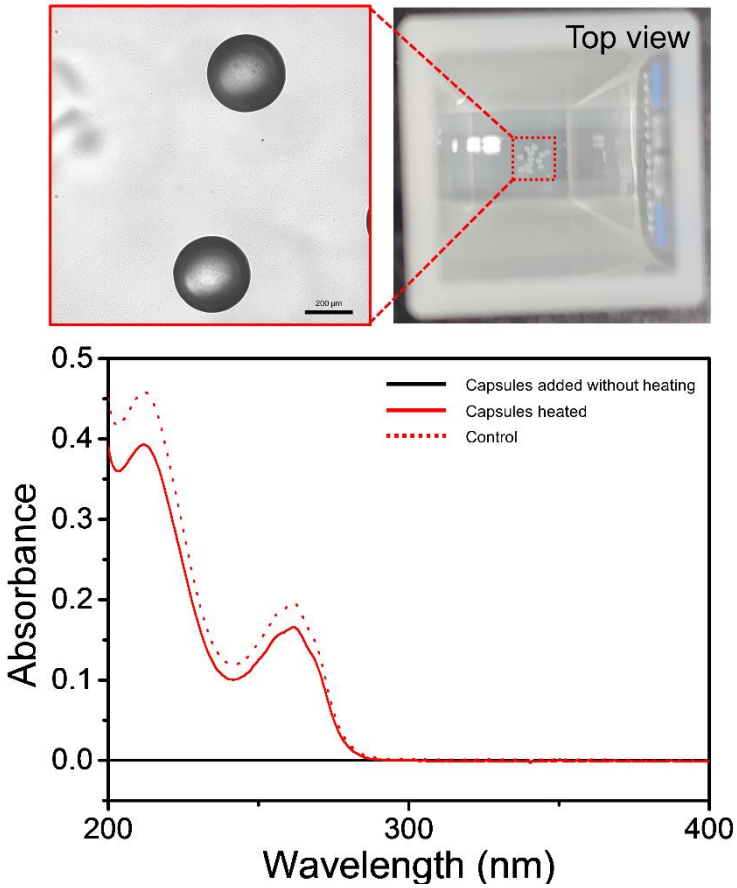

Fig. S3 Top-view photograph of the microcapsule suspension in a quartz cuvette, micrograph and UV-Vis spectra of the microcapsule suspension containing niacinamide and adenosine before and after heating. Black spectrum shows negligible absorbance even after 1 months of storage which indicates minimal leakage of actives from the microcapsule without additional heating. The red solid spectrum shows two characteristics peaks at wavelength of 212 and 262 nm which increases after heating. This indicates the thermally triggered release of encapsulated niacinamide and adenosine from the microcapsules. The red dotted spectrum represents the control where all niacinamide and adenosine encapsulated in the water capsule is released into the aqueous continuous phase.

Table S4. Human primary skin irritation test using ICDRG guidelines. The degree of skin irritation is scored as follows: (-) = no reaction, 1 = slight erythema, either spotty or diffuse, 2 = moderate uniform erythema, 3 = intense erythema with edema; 4= intense erythema with edema and vesicles.

Formulation type	Number of participants	Degree of skin irritation		Overall evaluation
		After 30 min	After 24 hr	
NC	32	-	-	No irritation
WC	32	-	-	No irritation
WC+D	31	-	-	No irritation
DC	31	-	-	No irritation