

Supramolecular Adenosine-Based Skin Delivery System for Hair

Regulation and Restoration

Yixuan Tang^{1#}, Weihao Gao^{1#}, Hongwei Fu², Tianqi Liu^{1*}, Zhenyuan Wang³,

Lujie Yu³, Xiangli Liu¹, Mi Wang^{1*}, Jichuan Zhang^{1*}, Jiaheng Zhang^{1,3*}

*¹College of Frontier Sciences, School of Materials Science and Engineering,
Harbin Institute of Technology, Shenzhen 518055, China*

*²School of Chemistry and Chemical Engineering, Nanjing University of
Science and Technology, Nanjing 210094, China*

³Shenzhen Shinehigh Innovation Technology Co., Ltd., Shenzhen;

These authors contributed equally to this work.

** To whom correspondence should be addressed.*

zhangjiaheng@hit.edu.cn;

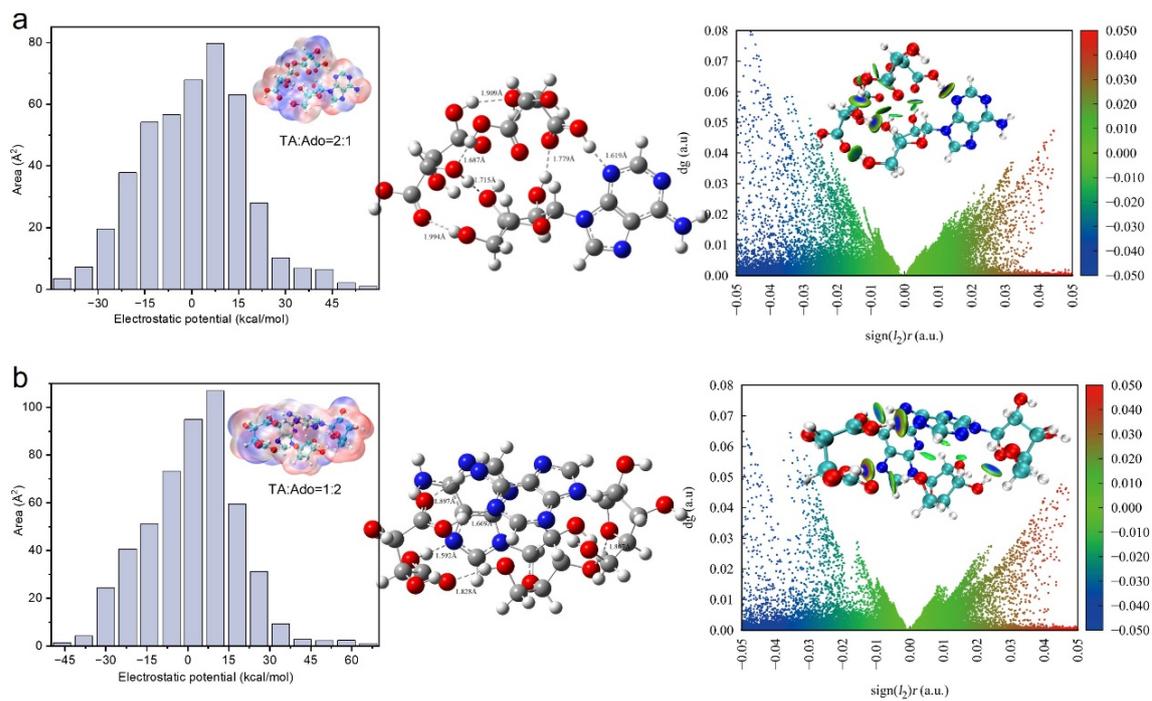


Figure S1. ESP simulation calculation. a. TA:Ado = 2:1. b. A:Ado = 1:2.

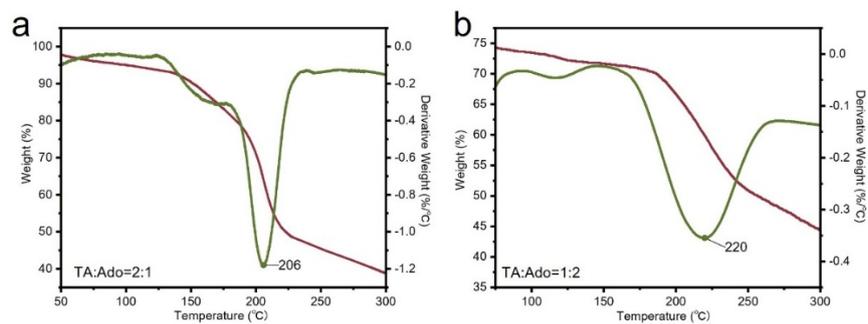


Figure S2. TGA and DTG images. a. TA:Ado = 2:1. b. TA:Ado = 1:2.

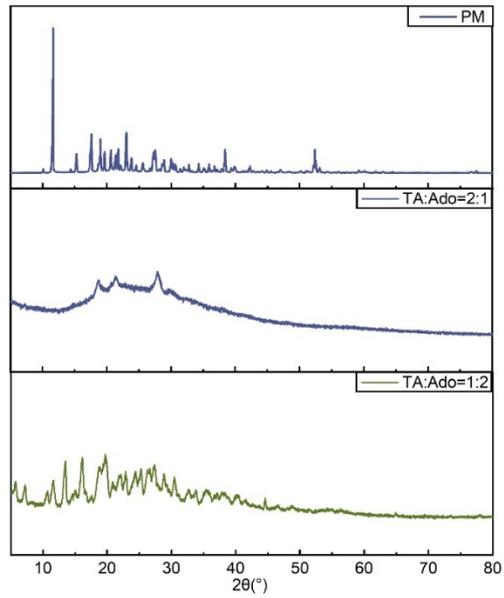


Figure S3. XRD images of TA:Ado=2:1, TA:Ado=1:2.

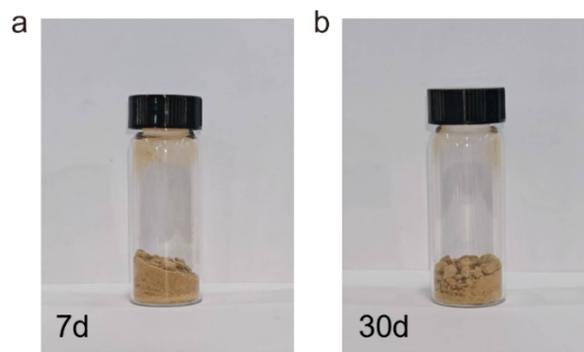


Figure S4. Observation on the Stability of TA-Ado Cocrystal.

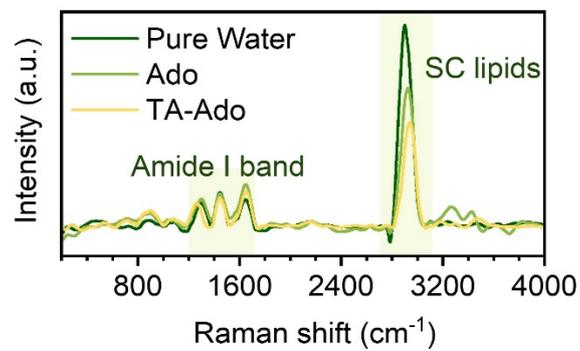


Figure S5. Raman spectra of porcine skin samples after treatment with pure water, Ado, and TA-Ado.

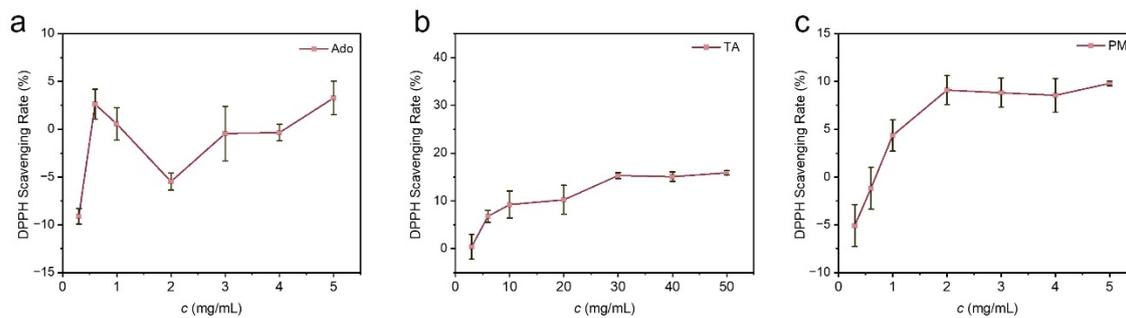


Figure S6. Curve of DPPH free radical scavenging rate varying with sample. a. Ado. b. TA. c. PM.

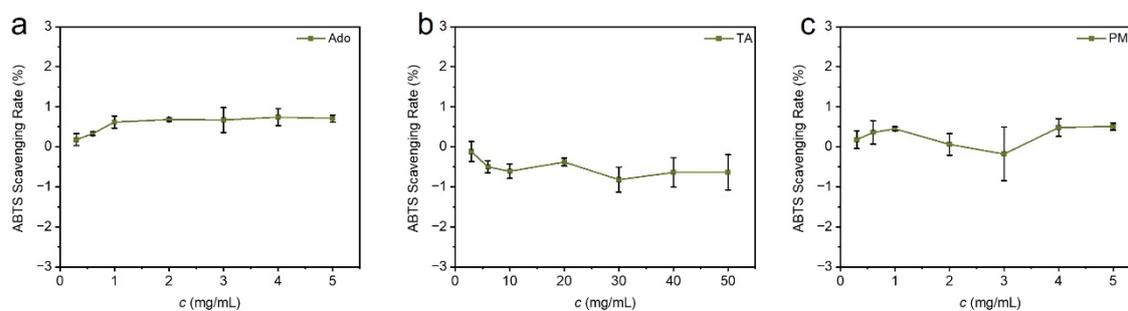


Figure S7. Curve of ABTS free radical scavenging rate varying with sample. a. Ado. b. TA. c. PM.

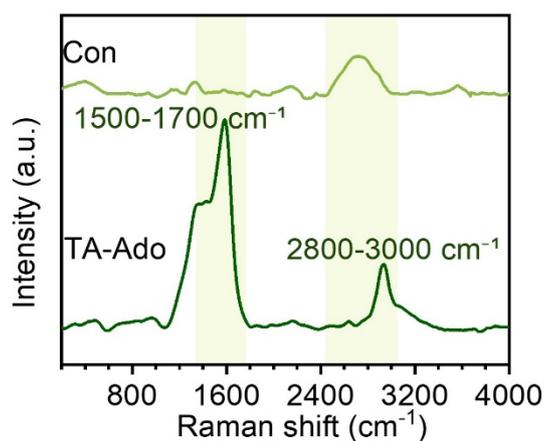


Figure S8. Raman spectra of damaged hair strands treated with TA-Ado shampoo and untreated damaged hair strands.

Table S1. Stability test results

	0D	180D
Ado content (wt%)	54.67	54.59
pH	3.5	3.5
Melting point (°C)	100-140	100-140

Table S2. Human Patch Test: rating Scales of Skin Reactions.

Rating Levels	Skin Reaction Types
0	Negative Reaction
1	Suspected Reaction: Only faint erythema
2	Weakly Positive Reaction (Erythema Reaction): Erythema, infiltration, edema, and possible papules
3	Strongly Positive Reaction (Herpetic Reaction): Erythema, infiltration, edema, papules, herpes; The reaction may extend beyond the test area
4	Extremely Strongly Positive Reaction (Confluent Herpetic Reaction): Obvious erythema, severe infiltration, edema, confluent herpes; The reaction extends beyond the test area

Table S3. Human Patch Test: number of People by Different Skin Reaction Grades in Patch Test.

Group	Observation Time	Number of People by Different Skin Reaction Grades in Patch Test				
		0	1	2	3	4
TA-Ado	0.5h	31	0	0	0	0
	24h	31	0	0	0	0
	48h	31	0	0	0	0
Blank Control	0.5h	31	0	0	0	0
	24h	31	0	0	0	0
	48h	31	0	0	0	0

Table S4. Evaluation Indicators of the Questionnaire on Repair and Soothing Effects After Using TA - Ado Shampoo. 0.5h

	Evaluation Indicator
A	The intensity and frequency of skin stinging, itching, and tightness are significantly reduced.
B	Helps soothe redness after use.
C	Helps soothe tightness after use.
D	Helps soothe desquamation after use.
E	Helps soothe stinging after use.
F	Helps soothe itching after use.
G	Helps soothe burning sensation after use.
H	Helps improve skin discomfort such as itching and pain caused by dryness.
I	After use, it helps reduce skin redness and relieve the feeling of tightness.

Table S5. Regulatory Effects and Functions of 5 α -Reductase, NF- κ B Pathway and TGF- β 2.

	Core biological function	Regulatory Effects of TA-Ado	Corresponding Efficacy
5α-reductase	Converts testosterone to DHT.	Dose-dependent inhibition	Reduced sebum secretion (Figure 5c) and decreased hair loss (Figure 5e)
NF-κB pathway	Activates the transcription of pro-inflammatory cytokines and mediates inflammatory responses.	Inhibition via activation of adenosine A ₁ /A ₂ A receptors	Alleviated scalp inflammation (81.82% of subjects reported reduced stinging/itching, Figure 5b)
TGF-β2	A key pro-inflammatory and profibrotic cytokine.	Significant downregulation (Figure 3I)	Relieved skin sensitivity symptoms and improved scalp barrier function

Table S6. Evaluation Indicators of the Questionnaire on User Experience After Using TA-Ado Shampoo.

	Evaluation Indicator
A	Satisfied with the smell of the product.
B	Richness of foam when using the product.
C	Smoothness of wet hair when using the product.
D	Smoothness of hair after blow - drying with the product.
E	The product is gentle and non – irritating.
F	After using the product, it feels that it soothes the scalp and improves redness.
G	After using the product, it feels that it soothes the scalp and improves dry itching.
H	The product has an oil - controlling effect when used.
I	After using the product, it has a refreshing and non - greasy effect.
J	After using the product, it improves hair loss and shedding.
K	I am satisfied with the product as a whole.
L	Will recommend this product to friends around me.