toxics

Supplementary Materials: Pharmacokinetics and the Dermal Absorption of Bromochlorophene, A Cosmetic Preservative Ingredient, in Rats

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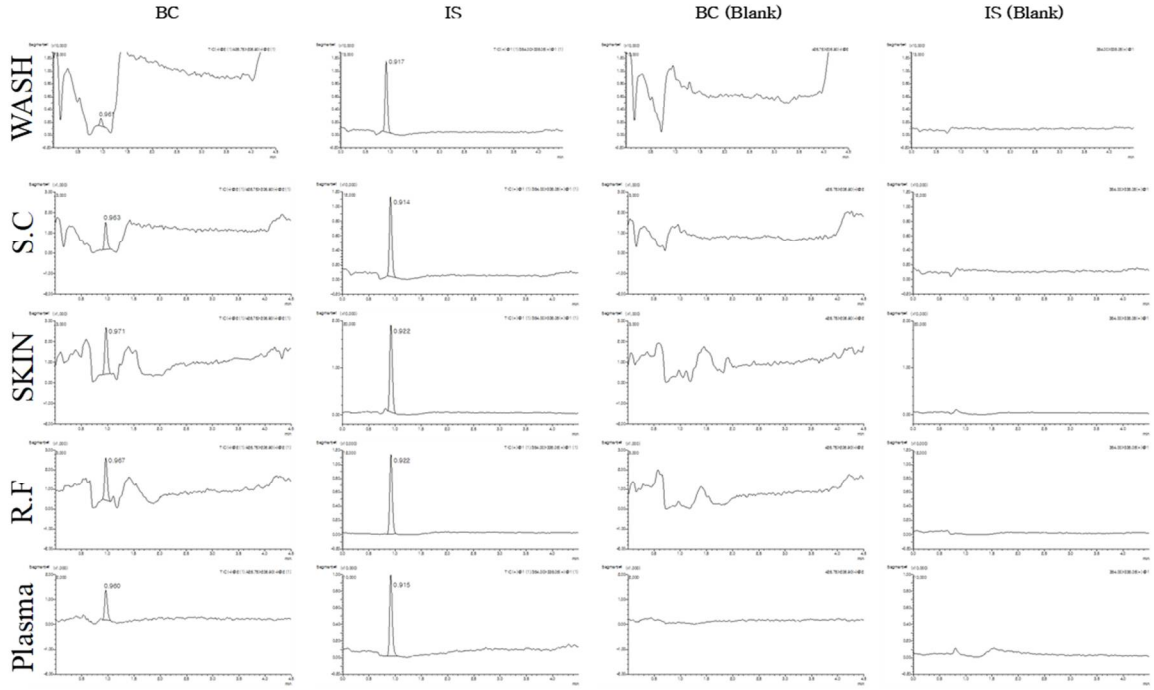


Figure S1. Representative MRM chromatograms of BCP and IS at LLOQ in WASH, SC, SKIN, RF, and plasma.

Table S1. Physicochemical properties of BCP.

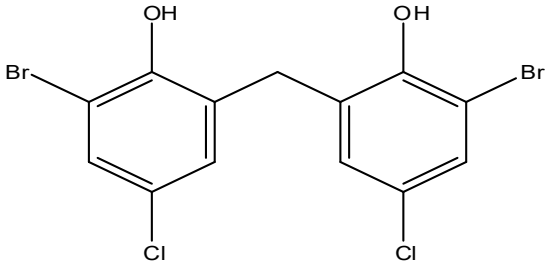
Structure of chemical		
INCI name	Bromochlorophene	
EINECS name	2,2'-Methylenbis (6-bromo-4-chlorophenol)	
CAS number	15435-29-7	
EC number	239-446-8	
Molecular formula	$C_{13}H_8Br_2Cl_2O_2$	
Molar mass	426.92	
Solubility in water	< 5 mg/L	
Log P_{ow}	6.12	
Effect of preservative	gram-positive bacteria	good
	gram-negative bacteria	moderate
	yeasts / moulds	inadequate
	head-space pretection	no

Table S2. Contents of gel and cream formulations containing 1 % BCP.

Content	Gel (%,w/w)	Cream (%,w/w)
Distilled water	75.4	54
Glycerin	23.6	4
Grape seed oil		28
Benzyl alcohol		5
Olive glutinate		3
Hydroxypropyl cyclodextrin		5
Bromochlorophene	1	1
Total	100	100

Table S3. Analytical conditions of BCP and IS of LC-MS/MS.

	Bromochlorophene	**Felodipine (IS)**
Instrument		
HPLC	LC-30AD-1 and -2, SIL-30AC, CTO-20AC (Shimadzu, Kyoto, Japan)	
MS/MS	LCMS-8050 (Shimadzu, Kyoto, Japan)	
Column	Zorbax SB-C8 (150 × 2.1 mm, i.d. 3.5 μm , Agilent, USA)	
Guard column	Security Guard Cartridges RP-1 (4 × 3.0 mm; Phenomenex, CA, USA)	
Chromatographic condition		
Mobile phase	95% ACN in 0.1% formic acid	
Column oventemperature (°C)	40	
Autosampler temperature (°C)	10	
Flow rate (mL/min)	0.5	
Running time (min)	4.5	
Injection volume (mL)	5	
MSMS condition		
Ionization mode	Electro spray ionization, multi reaction monitoring	
Polarity	Negative	Positive
Mass transition (m/z)	426.75 → 206.90	384.00 → 338.05
Dwell time (ms)	100	100
Q1 pre vias	19	-13
Q3 pre vias	21	-25
Collision energy (V)	26	-14
Gas flow (L/min)	10	
Neubulizing gas flow (L/min)	3	
Source temperature (°C)	300	