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Correlation of Skin Feel of Emollients to Their Chemical Structure

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Synopsis—It has been found possible to quantitate the SKIN FEEL of cosmetics by use of a Skin Feel Index (SFI) proposed by the authors. This index is the ratio of Initial Slip of a product (scale 1–5) to its Total End Feel (scale 4–20) after complete dry-out on the skin. SFI values were determined for 85 cosmetic EMOLLIENTS comprising 14 chemical groups, each incorporated in a standard base at 37% of the total "residue" left on the skin by this base after evaporation of its water content. Effects of molecular weight, "oiliness," polarity, unsaturation, and chain branching were studied. Due to the unavailability of some "key" compounds, a detailed statistical or graphical analysis was not possible, but definite trends could nevertheless be observed as various factors (such as chain length or polarity) were systematically varied in this initial study.

Introduction

Attempting to correlate the chemical structure of raw materials with various properties of cosmetic interest (such as skin feel, sheen on the hair, or effect on viscosity of lotions) has always fascinated the cosmetic chemist. However, measuring the influence of various changes in chemical structure implies the ability to measure numerical changes in other properties of these raw materials. Properties such as skin feel or odor, however, have generally been considered to be subjective in nature, and not amenable to numerical description. This has been a major stumbling block.

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Where it is possible to measure properties instrumentally (e.g., viscosity changes or hair sheen), numerical values are obtained which can be arranged into orderly tables or depicted graphically. Grouping of data allows the investigator to seek meaningful relationships, or to compare them with some external factor which may also be changing—i.e., molecular structure.

In the case of skin feel, no one heretofore has attempted to assign numerical values; the situation was analagous to trying to describe odor changes verbally. Some words, such as "oily" or "dry-velvety" or "waxy," are over-used; others, such as "scroopy" (the textile chemist's description of the somewhat rough, soft-draggy feel of raw silk), may be unfamiliar to most persons. In an attempt to become more precise, word modifiers are introduced to describe varying degrees of oiliness or velvetiness, etc. This often results in very complicated circumlocutions and language which mean different things to different investigators. Worst of all, such verbal descriptions cannot be ranked or summed up as can a series of numerical values.

Various groups of compounds can be ranked in order of their increasing dryness, oiliness, dragginess, or tackiness on the skin. One cannot give absolute values to such properties, but it certainly can be decided whether one compound is oilier or more tacky *than another.* By systematic evaluation of many small homologous series of compounds (ranking for changes in skin feel within each such small series), it should be possible to discern trends of changes in skin feel which relate to chemical structure. For example, when a series of isopropyl esters are used as emollients in a particular lotion, what is the effect on skin feel of the molecular weight of the fatty alcohol portion of the ester molecule, of branching the fatty alcohol portion of the molecule, or of successively increasing the degree of unsaturated bonding in a particular series of C_{18} esters? This investigation was an attempt to answer questions of this type.

Experimental

At first, the ranking of various series of lotions, each containing the test emollient at a fixed percentage, was tried. Later, a numerical (1 to 5) rating system for each of various qualities was adopted.

Each test series was limited to 4–6 samples, the number that could comfortably be applied to the inside of the tester's arm at one time. Emollients were not tested "pure," but incorporated at 7% in a basic lotion whose oil phase totalled 14%, which deposited an 18.9% total residue

Table I
Base Formula

Oil phase	
7.0%	Emollient
4.0	Glyceryl monostearate (pure)
3.0	Stearic acid XXX
Water phase	
4.0	Propylene glycol USP
0.5	Triethanolamine
0.4	Sodium lauryl sulfate
81.1	Water
100.0%	

Oil phase = 14%
Residue on skin = 18.9%
Emollient = 37% of residue

on the skin (Table I). Thus, once the water had evaporated, the residual film left on the skin contained 37% of the emollient under study. Each lotion (or cream) was aged at least 48 hours before being evaluated, to allow any crystal structure which was going to develop to do so. Members of a series being compared were about the same age when evaluated.

Approximately equal amounts of the creams or lotions were applied one by one to the inner arm. Each was evaluated individually as it went through the complete cycle (from wet Initial Feel to dry End Feel) before applying another to the skin. Successive changes in skin feel were noted as they occurred. To facilitate this process a work sheet was used (as shown in Fig. 1, filled out for PEG 200 monooleate).

This evaluation form uses language reminiscent of that used in perfumery. In place of "top note" Initial Feel is described, which includes such factors as the slip and texture of the cream. Middle Feel describes the cream's behavior during rub-out, factors such as absorption time, or whether it has a watery "break." Finally, End Feel (equivalent to "base notes" in perfumery) occurs only after complete dry-out and is described by words such as "oily," "tacky," "waxy," "draggy," "smooth," and "rich."

Samples were always tested "blind." Each evaluator was requested to make note of his various sensations from the initial "wet" feel to the final "dry" stage, and then to rank that particular series in respect to anything he considered significant—such as variation in Initial Slip, in final End Feel, in oiliness or tackiness, etc. After the evaluation and

EMOLLIENT PEG 200 MONO OLEATE

Source Van Dyk (EMULSYNT 2180) MW Sap Value 111 = mw 505.4

Structure 30 Day Viscosity (25°C) 7810 cps

$$HO\,(C_2H_4O)_3\,C_2H_4O-\overset{O}{\overset{\|}{C}}-(CH_2)_7CH=CH(CH_2)_7CH_3$$

PEG 200 Carbons ≅ 8
Oleate Carbons = 18
Total C = 26±

EVALUATION IN EMULSION BASE # #37-8-1

Product Appearance, type, etc somewhat shiny, almost translucent
Flowing cream. Gelatinous consistency

RATE ALL QUALITIES ON 1-5 SCALE (remarks in parenthesis = 1/3/5 ratings)

	date	11/18	11/24	12/2
	evaluator	CPR	RJG	Reg
A) INITIAL FEEL (Cream on skin)				
SLIP (slight/medium/much)		3	4	4+
TEXTURE of Cream (light/medium/heavy)		2	2	3
DESCRIBE IN WORDS (thin, pasty, lardy, etc.)		thin, gelatinous		
B) MIDDLE FEEL (Cream's behavior)				
"BREAK" QUALITY (watery/no change/oily)		3	3	3
"ABSORPTION" TIME (short/medium/prolonged)		3	3	3
CHANGE IN TEXTURE (becomes lighter/no change/heavier)		5	5	4
LUBRICANT QUALITIES (tacky/drags/"rolls")		5	4	4
DESCRIBE IN WORDS (waxy, lardy, etc.)		whitens very much		
C) END FEEL (Skin-Feel after complete Dry-Out)				
SMOOTHNESS (poor/good/velvety rich)		4	4	4
FRICTION (tacky/skids/drag/sl.drag/slip)		5	4	3+
OILINESS (dry/waxy/oily)		4	4	3
MOISTNESS (dry/neutral/dewy)		4	3	4+
DESCRIBE IN WORDS (raspy, lardy, rich, etc.)				

CPR – 3/17
RJG – 4/15
Reg – 4/15

SFI = 3.7/15.7

Figure 1. Typical work sheet

ranking were complete, the identity of emollients being tested in that particular series was revealed to the evaluator.

All emollients were tested in a base chosen with several specific purposes in mind: First, we wanted a typical cosmetic formula familiar to most cosmetic chemists. In an earlier test series, it was found that persons asked to evaluate emollients did so with considerably better discern-

ment if these were incorporated in a typical cream or lotion, rather than trying to feel them "pure."

The second requirement of the base formula was that it be stable, with emollient content as high (37%) as practicable, so that the primary feel would be that of the emollient under test. Deliberate use was made of a TEA-stearate soap emulsifier system containing excess stearic acid to provide a "background" raspiness and drag which each emollient had to "overcome" before it could score well. Additional emulsion stability was provided by a generous amount of glyceryl monostearate, to insure that we would not obtain mixed (O/W + W/O or O/W/O) emulsions, which have a peculiar skin feel all of their own.

Table II shows the evaluation of a Control Lotion, where water was substituted for the 7% emollient used in all other tests. This table also shows details of the numerical rating system used to determine the Skin

Table II

Control Lotion (No Emollient)

Viscosity (25°C) = 912 cps

Oil phase	
4.0%	Glyceryl monostearate (pure)
3.0	Stearic acid XXX
Water phase	
4.0	Propylene glycol
0.5	Triethanolamine
0.4	Sodium lauryl sulfate
88.1	Water
100.0%	

Initial Slip = 4.0

(Scale 1–5 = *slight* to *much* slip)

End Feel = 10.5

(Skin Feel after complete dry-out, the summation of four factors, each judged on a 1–5 scale. Total End Feel scale is therefore 4–20).

		End Feel Ratings				
		1	2	3	4	5
Smoothness	2.5	Poor	Fair	Good	Smooth	Velvety rich
Friction	3.0	Tacky	Skids	Drag	Sl. drag	Slips
Oiliness	3.0	Dry	Dry/waxy	Waxy	Oily/waxy	Oily
Moistness	2.0	Very dry	Sl. dry	Neutral	Sl. moist	Dewy
	= 10.5					

Skin Feel Index (SFI) = 4.0/10.5

Feel Index (SFI) of various emollients. The SFI is the ratio of Initial Slip/Total End Feel.

Initial Slip was considered very important, and was rated *per se,* on a 1–5 scale (slight to much slip).

Middle Feel could not be ranked reproducibly, since qualities such as "absorption time" are highly variable, depending on skin type. Creams would "rub in" quicker on a dry skin than on an oily skin, and absorption time varied greatly with the location to which cream is applied. Palms, for example, absorb very little.

End Feel was divided into four subcategories, as shown in Table II. With very little practice it is possible to describe quite reproducibly the sensations of smoothness, friction, oiliness, and moistness. The same investigator was able to repeat his own results at any given time, or his own results a week or a month later, or the results of other investigators. Overall SFI scores were reproducible within approximately 10 to 15%. This reproducibility is the primary justification for presenting the data which follow.

The SFI evaluation procedure relieves us of the necessity to ask dozens or hundreds of persons to evaluate each product. The SFI scores of over 85 different cosmetic emollients are reported below.

Results

The Control Lotion (no emollient, Table II) showed an Initial Slip = 4.0. Its End Feel score of 10.5 is the sum of the following four component scores:

Smoothness	2.5	(fair to good smoothness)
Friction	3.0	(drags)
Oiliness	3.0	(waxy)
Moistness	2.0	(slightly dry)
	10.5	(out of a possible score of 20.0)

This control lotion was almost perfect for our purposes, since it gave quite average results (SFI = 4.0/10.5). Its Middle Feel was also quite mediocre, showing values of 3.0 for "break" quality, medium "absorption time," and a 3.5 value for "change in texture." This lotion becomes extremely draggy during the transition period to complete dry out.

Materials which show SFI scores *below* the 4.0/10.5 Control Lotion score are likely to worsen the skin feel of emulsion cosmetics. Materials showing substantially *higher* scores can presumably improve them.

A relatively emollient material, PEG 200 monooleate (whose "work sheet" is shown in Fig. 1), is used to illustrate the complete evaluation procedure.

The POLYOL MONOESTERS OF OLEIC ACID, in general, are a uniformly poor group in terms of skin feel (Table III). Only the PEG 200 monooleate (SFI = 4.0/15.7) gave a decent result. All except PPG 2000 oleate are either water-soluble or water-dispersible (a property which seems to be unfavorable to final skin feel). In this particular series, PEG 200 monooleate gave a considerably better End Feel (15.7) than PPG 2000 monooleate (11.3), even though the latter is not water-soluble. In the case of PPG 2000 monooleate, however, oleic acid represents only 12% of the molecular weight, compared to 54% in PEG 200 monooleate. Apparently, greater "oiliness" is favorable to high End Feel scores. If this is true, it may be possible to correlate End Feel with HLB values of emollients.

The approximate molecular weight of each emollient was determined from saponification values where available, and from the theoretical structure otherwise. The number of carbons in the homolog portion of each series is also shown in the tables. Viscosities of the finished products (7% emollient in "Base Formula") were recorded after each cream or lotion had aged approximately 30 days.

HLB, hydroxyl values, per cent branching (% side chains/total mol wt) and iodine values (degree of unsaturation) were among the other factors considered in attempting to correlate Skin Feel with chemical structure in this initial study.

POLYOL POLYESTERS OF OLEIC ACID (Table III) apparently present the same problems as the polyol monoesters of oleic acid. None of them are very good, in spite of their greater molecular weight resulting from esterification of polymerized glycerol. All of these esters formed heavy, pasty, or gelatinous lotions. Polyol esters of fatty acids are *not* usually used as emollients for this reason; they were included in this study only to help find correlations to chemical structure.

The greater the water solubility of emollients, the more Initial Slip they give to emulsions containing them and, usually, the poorer the End Feel. In contrast, the oilier they are, the better their End Feel. This will be seen dramatically in the next group of emollients to be considered.

FATTY ALCOHOL ESTERS OF OLEIC ACID (Table III) show an immediate improvement in final skin feel over the two series of *polyol* esters of oleic acid. Even the least efficacious fatty alcohol oleic ester, hexadecyl oleate (End Feel = 13.0), was substantially better than 90% of

Table III

Esters of Oleic Acid

$CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH$

C_{18} Acid; Mol Wt 276

Polyol Monoesters:	Approx Mol wt	Polyol Carbons	Viscosity (Lotion)(cps)	
Glyceryl monooleate	350	3	4580	
PEG 200 monooleate	506	8±	7810	
Triglyceryl monooleate	498	9	8290	
PEG 600 monooleate	863	26±	182	
PEG 1540 monooleate	1753	69±	30	
PPG 2000 monooleate	2244	102±	2560	
Polyol Polyesters:				
Diglyceryl dioleate	682	6	2092	
PEG 400 dioleate	916	17±	2688	
Decaglyceryl tetraoleate	1791	30	7940	
Decaglyceryl octaoleate	2822	30	2300	
Decaglyceryl decaoleate	3339	30	2180	
Fatty Alcohol Esters:				(% Branching)
n-Decyl oleate	410	10	5320	...
Isodecyl oleate	410	10	6180	3.6
Hexadecyl oleate	500	16	5300	17.0
Oleyl oleate	526	18	6860	...
Isostearyl oleate	528	18	5780	2.8

	Initial Slip (Scale 1–5)		Total End Feel (Scale 4–20)	
Polyol Monoester Skin Feels:	PEG 1540	1.3	PEG 1540	7.3
	PEG 600	2.2	Triglyceryl	7.7
	Glyceryl	3.5	Glyceryl	8.3
	Triglyceryl	3.7	PEG 600	8.7
	PEG 200	4.0	PPG 2000	11.3
	PPG 2000	4.0	PEG 200	15.7
Polyol Polyester Skin Feels:	PEG 400 di-	3.5	Decaglyceryl tetra-	8.5
	Decaglyceryl octa-	4.0	Decaglyceryl octa-	9.3
	Decaglyceryl deca-	4.0	Diglyceryl di-	11.3
	Decaglyceryl tetra-	4.3	Decaglyceryl deca-	11.5
	Diglyceryl di-	4.8	PEG 400 di-	14.5
Fatty Alcohol Ester Skin Feels:	Isostearyl	3.0	Hexadecyl	13.0
	Isodecyl	3.5	Isostearyl	15.0
	Oleyl	4.0	*n*-Decyl	17.0
	Hexadecyl	4.0	Isodecyl	17.0
	n-Decyl	4.5	Oleyl	18.5

all the polyol esters of oleic acid tested. Within this subgroup, there seems to be no correlation between End Feel and molecular weight, nor with per cent branching. The best End Feel was obtained from oleyl oleate, but we do not think that this richer skin feel is due to the additional unsaturation. As a group, all these fatty alcohol esters of oleic acid gave rich Initial Feel and slip, as well as rich End Feel.

For the ESTERS OF STEARIC ACID (Table IV), it should be noted that the End Feel score for PEG 1000 monostearate is less than half that of the fatty alcohol monostearates. The best End Feel score was obtained from butyl stearate, where stearic acid represents almost 83% of the molecule. Branching, in this series, did not seem to improve End Feel substantially. The poor performance of PEG 1000 monostearate may be due in some measure to the almost watery viscosity lotion which it produced.

Table IV

Esters of Stearic Acid XXX

55% C_{16} acid—$CH_3(CH_2)_{14}COOH$ } Commercial
45% C_{18} acid—$CH_3(CH_2)_{16}COOH$ } Stearic (Mol Wt 270)

	Approx Mol Wt	Carbons on Alcohol	Viscosity (Lotion)(cps)	% Branching
Butyl stearate	326	4	2144	...
Isodecyl stearate	410	10	5230	3.7
Hexadecyl stearate	494	16	2322	17.2
PEG 1000 monostearate	1247	44±	39	...

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
PEG 1000	3.0	PEG 1000	6.5
Butyl	3.5	Isodecyl	16.3
Hexadecyl	4.0	Hexadecyl	17.0
Isodecyl	4.5	Butyl	17.0

Unfortunately, we were not able to obtain the same ESTERS OF ISOSTEARIC ACID (Table V) as were available to us for stearic acid. Therefore, it is difficult to compare the two series. The only ester common to both acids, that of isodecyl alcohol, shows the isostearic ester to be somewhat better, as would be expected. Note again that the two polyol esters gave substantially worse End Feels than the fatty alcohol esters in this series.

ESTERS OF LINOLEIC ACID are shown in Table VI. Linoleic is another C_{18} acid, structurally identical to oleic acid except for an additional double bond. Table VI shows that such extra unsaturation appears

Table V

Esters of Isostearic Acid

CH_3
$CH_3CH\text{-}(CH_2)_{14}COOH$ = 73%
isoC_{16} = 7%
n-C_{16}/C_{18} = 20%
} Commercial Isostearic Acid (Mol Wt 280)

	Approx Mol Wt	Carbons on Alcohol	Viscosity (Lotion)(cps)	% Branching
Isopropyl isostearate	327	3	5800	9.4
Glyceryl monoisostearate	336	3	2348	4.5
Isodecyl isostearate	420	10	2544	7.1
n-Decyl isostearate	420	10	2360	3.5
PEG 600 monoisostearate	862	26±	118	1.8

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
PEG 600	3.5	Glyceryl	11.1
n-Decyl	3.5	PEG 600	13.5
Glyceryl	4.3	*n*-Decyl	16.5
Isopropyl	4.5	Isopropyl	16.8
Isodecyl	5.0	Isodecyl	17.8

Table VI

Esters of Linoleic Acid

$CH_3(CH_2)_4CH{=}CHCH_2CH{=}CH(CH_2)_7COOH$

C_{18} Acid (Mol Wt 261)

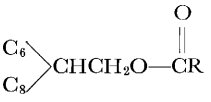
	Approx Mol Wt	Carbons on Alcohol	Viscosity (Lotion)(cps)	% Branching
Isopropyl linoleate	303	3	1144	4.9
Propylene glycol linoleate	319	3	5450	. . .
Decyl linoleate	401	10	7900	. . .
Hexadecyl linoleate	485	16	9900	17.6
PEG 400 linoleate	643	17±	277	. . .
PEG 4000 linoleate	4243	180±	207	. . .

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Isopropyl	3.0	PEG 4000	8.0
Decyl	3.0	Propylene glycol	11.0
Propylene glycol	3.5	PEG 400	12.0
PEG 4000	3.5	Hexadecyl	12.5
Hexadecyl	3.5	Isopropyl	13.0
PEG 400	4.5	Decyl	14.5

to reduce End Feel scores, and therefore usefulness as cosmetic emollients. On the other hand, since oleic acid esters performed better than stearic esters, a little unsaturation is apparently good.

Table VII

Hexadecyl Alcohol and Esters



	Approx Mol Wt	Carbons on Fatty Acid	Viscosity (Lotion)(cps)	% Branching
Hexadecyl alcohol	242	0	790	35.1
Hexadecyl laurate	424	12	7100	20.1
Hexadecyl myristate	437	14	7150	19.5
Hexadecyl linoleate	485	18	5130	17.6
Hexadecyl oleate	500	18	5300	17.0
Hexadecyl stearate	508	18	2322	16.7

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Laurate	3.0	Laurate	10.0
Alcohol	3.3	Linoleate	12.5
Linoleate	3.5	Oleate	13.0
Oleate	4.0	Alcohol	17.0
Stearate	4.0	Stearate	17.0
Myristate	4.3	Myristate	17.3

HEXADECYL ALCOHOL itself gives excellent End Feel, even though it produced a relatively low viscosity lotion (Table VII). Esterifying with oleic or linoleic acids substantially decreases performance. Esterifying with stearic or myristic acids does not affect End Feel at all, but does increase Initial Slip slightly. Esterifying with lauric acid decreases performance. Unsaturation tended to decrease performance in this series.

Three liquid (isoalcohol) ESTERS OF MYRISTIC ACID were available for test, as well as one waxy one, myristyl myristate (Table VIII). On the whole, they all performed well. As expected, the three liquid isoesters gave somewhat better results than the solid normal ester.

LAURIC ACID ESTERS seem to be poor emollients (Table IX).

ESTERS OF ADIPIC ACID show extraordinarily good skin feel (Table X). All of these are diesters, since adipic acid is a dicarboxy acid; the percentage of fatty alcohol or polyol in the molecule is therefore substantially higher than in monoesters. Results were so uniform in this series that it was difficult to draw any conclusions on the effect of systematically varying the structure of adipates.

ESTERS OF LACTIC ACID also show uniformly excellent results, except for stearyl lactate, which performed poorly (Table XI). Isostearyl lactate shows an End Feel score of 17.5, 50% higher than that of the

Table VIII

Esters of Myristic Acid
$CH_3(CH_2)_{12}COOH$
C_{14} Acid (Mol Wt 228)

	Approx Mol Wt	Carbons on Fatty Alcohol	Viscosity (Lotion)(cps)	% Branching
Isopropyl	271	3	2276	5.6
Myristyl	448	14	24,700	...
Hexadecyl	437	16	7150	19.5
Isostearyl	479	18	7350	3.2

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Myristyl	3.5	Myristyl	16.3
Isostearyl	4.0	Isopropyl	17.0
Isopropyl	4.3	Hexadecyl	17.3
Hexadecyl	4.3	Isostearyl	18.3

Table IX

Esters of Lauric Acid
$CH_3(CH_2)_{10}COOH$
C_{12} Acid (Mol Wt 200)

	Approx Mol Wt	Carbons on Alcohol	Viscosity (Lotion)(cps)	% Branching
Decyl laurate	340	10	6060	...
Hexadecyl laurate	424	16	7100	20.1
PEG 200 dilaurate	565	8±	2208	...
PEG 400 monolaurate	582	17±	217	...

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
PEG 400 monolaurate	2.0	Hexadecyl laurate	10.0
PEG 200 dilaurate	3.0	PEG 400 laurate	10.5
Hexadecyl laurate	3.0	PEG 200 dilaurate	14.0
Decyl laurate	4.3	Decyl laurate	15.0

stearyl lactate (11.8). Although their molecular weights are theoretically identical, the two esters we tested differed slightly (as determined from actual saponification values), presumably due to different sources of raw materials. Oleyl lactate, also a C_{18} ester, gave an even higher End Feel score than isostearyl lactate. The two solid lactate esters gave only fair results, while all of the liquid lactates were excellent.

A group of SATURATED FATTY ALCOHOLS was examined (Table XII). Here again, the pattern was similar: liquid alcohols gave better results than the solid ones. Furthermore, of the three liquid fatty alcohols evaluated, the two iso liquid fatty alcohols gave substantially

Table X

Esters of Adipic Acid

$HOOC(CH_2)_4COOH$

C_6 Acid (Mol Wt 146)

	Approx Mol Wt	Carbons on Alcohol	Viscosity (Lotion)(cps)	% Branching
Dimethyl adipate	174	2	884	...
Dipropyl adipate	228	6	1382	...
Diisopropyl adipate	228	6	800	13
Dibutyl adipate	258	8	1080	...
Diethylhexyl adipate	370	16	1000	16
Di-PEG 350 adipate	810	30±	750	...

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Dimethyl	4.2	Di-PEG 350	15.3
Dipropyl	4.4	Dimethyl	16.3
Diisopropyl	4.5	Diethylhexyl	17.8
Di-PEG 350	5.0	Dipropyl	18.5
Diethylhexyl	5.0	Dibutyl	18.8
Dibutyl	5.0	Diisopropyl	18.8

Table XI

Esters of Lactic Acid

$CH_3CH(OH)COOH$

C_3 Acid (Mol Wt 90)

	Approx Mol Wt	Carbons on Fatty Alcohol	Viscosity (Lotion)(cps)	% Branching
Lauryl lactate	258	12	7800	...
Myristyl lactate	324	14	28,300	...
Cetyl lactate	310	16	25,000	...
Stearyl lactate	373	18	32,500	...
Isostearyl lactate	353	18	5180	4.3
Oleyl lactate	356	18	4600	...
Linear alcohol lactate	276	(12–15)	7000	...

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Stearyl	3.0	Stearyl	11.8
Myristyl	3.7	Cetyl	16.0
Cetyl	4.0	Lauryl	17.3
Isostearyl	4.0	Myristyl	17.4
C_{12}–C_{15}	4.0	Isostearyl	17.5
Oleyl	4.8	C_{12}–C_{15}	18.0
Lauryl	5.0	Oleyl	18.3

Table XII
Saturated Fatty Alcohols

	Approx Mol Wt	Carbons	Viscosity (Lotion)(cps)	% Branching
Linear (primary)	207	(12–15)	75,000	...
Myristyl (natural)	214	14	>100,000	...
Hexadecyl	242	16	790	35.1
Cetyl (natural)	242	16	71,800	...
Isostearyl	271	18	9200	5.6
Stearyl (natural)	271	18	58,700	...

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Stearyl	1.8	Cetyl	7.5
Myristyl	1.8	Myristyl	12.0
Cetyl	2.0	Stearyl	12.4
C_{12}–C_{15}	2.9	C_{12}–C_{15}	14.0
Hexadecyl	3.3	Hexadecyl	17.0
Isostearyl	3.5	Isostearyl	17.3

Table XIII
Unsaturated Fatty Alcohols

	Approx Mol Wt	Carbons	Viscosity (Lotion)(cps)
Oleyl	269	18	6520
Ricinoleyl	285	18	2304
Erucyl	325	22	66,400
Lanolin "alcohols"	385	27±	39,500

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Ricinoleyl	3.0	Lanolin alcohols	11.5
Erucyl	3.0	Ricinoleyl	12.5
Lanolin alcohols	3.5	Oleyl	14.5
Oleyl	4.5	Erucyl	16.5

better SFI values than the normal liquid fatty alcohol. It is interesting to note the enormous range of viscosities generated in this group—from less than 1,000 cps (using hexadecyl alcohol) to over 100,000 cps using myristyl alcohol.

The UNSATURATED FATTY ALCOHOLS were surprisingly mediocre in their performance as emollients (Table XIII). Erucyl alcohol, a C_{22} soft waxy material, gave the best results of this group. Oleyl alcohol, as would be expected, gave better results than stearyl. Isostearyl alcohol performs even better than oleyl, while ricinoleyl alcohol—even though a liquid—performs no better than stearyl, a hard wax. Once again, we see

Table XIV
Hydrocarbons

	Approx Mol Wt	Carbons	Viscosity (Lotion)(cps)
Mineral oil (65/75)	335	23±	9000
Squalene	411	30	8680
Squalane	423	30	6140
White petrolatum	500	35	6810
Paraffin wax (130°F)	400		6430

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Paraffin	4.0	Paraffin	7.0
Mineral oil	4.3	Petrolatum	10.0
Petrolatum	5.0	Squalane	14.3
Squalane	5.0	Mineral oil	16.5
Squalene	5.0	Squalene	17.3

the influence of unsaturated bonds and additional groups such as the hydroxy. Polar groups often reduced the value of cosmetic emollients. The poor performance shown by the lanolin alcohols in this lotion (perhaps due to their high melting point) may surprise some formulators; however, their usual cosmetic use is for other properties than skin feel.

The emollient value of HYDROCARBONS apparently depends greatly on their melting points (Table XIV). Solid paraffin (mp 55°C) gives very poor results, semisolid petrolatum gives fair results, and medium viscosity mineral oil was quite good. The saturated squalane gives an End Feel slightly poorer than medium viscosity mineral oil, whereas the unsaturated squalene gives excellent End Feel. The ideal emollient (structurally) would appear to be one with a fairly long hydrocarbon chain having some unsaturation and branching, as illustrated perhaps by squalene. The SFI of squalene was 5.0/17.3.

ANIMAL AND VEGETABLE OILS were also evaluated (Table XV). Lanolin oil (also known as "liquid lanolin") gave one of the lowest End Feel scores of any material tested in this study. Castor and mink oils (both highly unsaturated) also gave poor scores; on the other hand, squalene and Jojoba oils (also highly unsaturated) produced extraordinarily high scores. Triglyceride oils generally performed more poorly than the hydrocarbons or high molecular weight esters, both of which are "oilier" in their molecular structure. The poor influence of polar (hydroxy) groups is seen once again in this series; the triglyceride oils did not perform as well as the fatty ester oils.

Table XV
Animal and Vegetable Oils

	Composition	Approx Mol Wt	Viscosity (Lotion) (cps)
Animal			
Egg oil	62% glycerides, 33% phosphates, 5% sterols	...	6760
Lanolin oil	Cholesterol, triterpenes, fatty acids	...	4680
Mink oil	C_{14}–C_{20} unsaturated triglycerides	852	9800
Squalene	C_{30} unsaturated aliphatic hydrocarbon	411	8680
Squalane	C_{30} saturated aliphatic hydrocarbon	423	6140
Vegetable			
Jojoba	Liquid wax (C_{20}–C_{22} esters)(half unsat.)	609	6880
Peanut	Triglycerides	864	10,010
Castor	90% ricinoleic triglyceride	935	6560
Safflower	Highly unsaturated triglycerides	942	11,300

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Castor	3.5	Lanolin oil	6.5
Jojoba	3.5	Castor	11.4
Mink	3.5	Mink	13.0
Egg	3.8	Egg	14.3
Peanut	4.0	Squalane	14.3
Safflower	4.0	Peanut	15.5
Lanolin oil	4.5	Safflower	15.5
Squalane	5.0	Squalene	17.3
Squalene	5.0	Jojoba	18.0

LANOLIN DERIVATIVES performed erratically (Table XVI). As previously noted, liquid lanolin gives very poor End Feel (6.5). Pure "lanolin alcohols" and lanolin alcohols ricinoleate are next (about 12.0), while lanolin itself gives a score of 15.8, substantially better than the control lotion containing no emollient, but still not very good in comparison to the better emollients. Other lanolin derivatives (the acetate, a hydrocarbon extract, and isopropyl lanolate) gave fairly good results (16–17). The best of this series was isopropyl lanolate, which produced an End Feel almost 50% better than lanolin alcohols themselves.

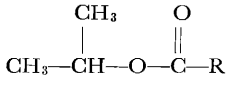
Table XVII is a regrouping of previous data to show all the ISOPROPYL ESTERS together. These were often the best of each series originally tested. Note that isopropyl ricinoleate, with its hydroxy group as well as double unsaturation, and the linoleate, also with two unsaturated bonds, performed quite poorly. Isopropyl azelate, an odd-carbon (C_9) fatty acid ester, gave a slightly better result than the sebacate, an even-carbon (C_{10}) fatty acid ester of approximately the same molecular

Table XVI
Lanolin and Derivatives

	Viscosity (Lotion)(cps)
Lanolin (anhyd. USP)	7860
Liquid lanolin (oil)	4680
Lanolin alcohols	39,500
Lanolin alcohols hydrocarbon extract	10,720
Lanolin alcohols acetate	13,560
Lanolin alcohols ricinoleate	8100
Isopropyl lanolate	6400

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Hydrocarbon extract	3.0	Liquid lanolin	6.5
Alcohols	3.5	Alcohols	11.5
Acetate	3.8	Ricinoleate	12.5
Ricinoleate	4.5	Lanolin	15.8
Lanolin	4.5	Acetate	16.3
Liquid lanolin	4.5	Hydrocarbon extract	16.5
Isopropyl lanolate	5.0	Isopropyl lanolate	16.8

Table XVII
Isopropyl Esters



	Approx Mol Wt	Carbons on Fatty Acid	Viscosity (Lotion)(cps)	% Branching
Isopropyl myristate	271	14	2276	5.6
Isopropyl palmitate	299	16	5540	5.1
Isopropyl linoleate	320	18	1144	4.7
Isopropyl isostearate	321	18	5800	9.4
Isopropyl ricinoleate	337	18	4530	4.4
Isopropyl lanolate		(10–32)	6400	?
Diisopropyl adipate	228	6	800	13.1
Diisopropyl azelate	272	9	2040	11.0
Diisopropyl sebacate	286	10	6580	10.5

Initial Slip (Scale 1–5)		End Feel (Scale 4–20)	
Linoleate	3.0	Ricinoleate	12.4
Sebacate	4.0	Linoleate	13.0
Palmitate	4.0	Sebacate	15.3
Myristate	4.3	Azelate	16.3
Isostearate	4.5	Isostearate	16.8
Adipate	4.5	Lanolate	16.8
Lanolate	4.8	Myristate	17.0
Azelate	4.8	Palmitate	18.3
Ricinoleate	5.0	Adipate	18.8

weight. On the other hand, the fact that both of these are diesters did not help them as much, apparently, as increasing the length of the fatty chain (isostearate, myristate, and palmitate isopropyl esters). Finally, note that the "best of the best" was diisopropyl adipate, with an End Feel score of 18.8. It is striking that the isopropyl ester giving the *poorest* End Feel (isopropyl ricinoleate) was the best in terms of Initial Slip, a pattern which was observed repeatedly throughout this study.

Summary and Conclusions

It is possible to quantitate skin feel of cosmetics, and to do so reasonably reproducibly—whether the same investigator repeats his own work at various time intervals or the work of another investigator.

From the work to date, we can draw a few "intuitive" conclusions, not yet backed by rigorous graphic or statistical analysis. Such analyses must await evaluation of further samples, not available at the time of this initial study. The intuitive conclusions include our belief that molecular weight *per se* is not relevant to final skin feel, but that "oiliness" (HLB?) is. This is evidenced by the fact that the presence of polar groups generally gives very negative effects. Some degree of unsaturation and/or chain branching was usually helpful, perhaps due to the "liquefying effect" such structural changes produced, lowering the melting point of the residual oil phase left on the skin.

Viscosity of the final test product had to be at certain minimum levels, otherwise results were poor. Physical factors of this type may "mask" the more purely chemical effects, obtained by systematically varying the structure of cosmetic emollients.

Finally (and we are really not quite sure why), isopropyl alcohol esters of most fatty acids were outstanding as a group. They were invariably at or near the top of each series in which they were tested.

Many of the trends demonstrated in this study have been known through practical experience in the past, or known "intuitively" by experienced cosmetic formulators. Now, however, being able to assign numerical values to skin feel makes it possible to study the subject systematically, and to estimate the additive skin feel effect of a series of ingredients proposed for a cosmetic formula. Also, we can now begin to choose emulsifiers and other cosmetic components on a known skin feel basis, considering their SFI index as well as HLB, solubility, etc. With this approach, it may be possible to custom-design molecules for certain

desired skin feel properties, just as drug and dye manufacturers now add desired antiseptic or chromophoric groups to molecules which have other functions as well.

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APPENDIX I

Source of Emollients Tested

Chemical Name	Trade Name	Source
Butyl stearate		Stoney Mueller Inc.
Castor oil, USP	Crystal	Baker Castor Oil Co.
Cetyl alcohol (natural)		M. Michel & Co.
Cetyl lactate	Ceraphyl 28	Van Dyk & Co.
Decaglyceryl decaoleate		Drew Chemical Co.
Decaglyceryl octaoleate		Drew Chemical Co.
Decaglyceryl tetraoleate		Drew Chemical Co.
Decyl isostearate		Experimental
Decyl laurate		Experimental
Decyl linoleate		Experimental
Decyl oleate	Ceraphyl 140	Van Dyk & Co.
Dibutyl adipate		Experimental
Diethyl hexyl adipate		Experimental
Diglyceryl dioleate		Experimental
Diisopropyl adipate	Ceraphyl 230	Van Dyk & Co.
Diisopropyl azelate		Experimental
Diisopropyl sebacate		Experimental
Dimethyl adipate		Experimental
Di-PEG 350 adipate		Experimental
Dipropyl adipate		Experimental
Egg oil		Viobin Corporation
Erucyl alcohol	Adol 22	Archer Daniels & Co.
Glyceryl monoisostearate	Emery 3771D	Emery Industries Inc.
Hexadecyl alcohol (Cosmetic Grade)		Enjay Chemical Co.
Hexadecyl laurate		Experimental
Hexadecyl linoleate		Experimental
Hexadecyl myristate		Experimental
Hexadecyl oleate		Experimental
Hexadecyl stearate		Experimental
Isodecyl isostearate		Experimental
Isodecyl oleate	Ceraphyl 140-A	Van Dyk & Co.
Isodecyl stearate		Experimental
Isopropyl isostearate	Emery 3770D	Emery Industries Inc.
Isopropyl lanolate	Amerlate P	Amerchol Div., CPC
Isopropyl linoleate	Ceraphyl IPL	Van Dyk & Co.
Isopropyl myristate		Ruger Chemical Co.
Isopropyl palmitate	Propal	Robinson Wagner & Co.
Isopropyl ricinoleate		Experimental
Isostearyl alcohol	Adol 66	Ashland Chemical Co.

APPENDIX I (continued)

Chemical Name	Trade Name	Source
Isostearyl lactate		Experimental
Isostearyl myristate		Experimental
Isostearyl oleate		Experimental
Jojoba oil		Experimental
Lanolin (anhydrous, USP)		Robinson Wagner & Co.
Lanolin alcohols	Ceralan	Robinson Wagner & Co.
Lanolin alcohols acetate	Acetulan	Amerchol Div., CPC
Lanolin alcohols hydrocarbon extract	Amerchol L-101	Amerchol Div., CPC
Lanolin alcohols ricinoleate	Ricilan B	Amerchol Div., CPC
Lauryl lactate	Ceraphyl 31	Van Dyk & Co.
Linear alcohol lactate	Ceraphyl 41	Van Dyk & Co.
Liquid lanolin	Lantrol	Malmstrom Chemical Co.
Mineral oil 65/75	Carnation	Sonneborn Div., Witco
Mink oil	Emulan	Emlin Inc.
Myristyl alcohol (natural)		Proctor & Gamble Inc.
Myristyl lactate	Ceraphyl 50	Van Dyk & Co.
Myristyl myristate	Ceraphyl 424	Van Dyk & Co.
Oleyl alcohol	Novol	Croda, Inc.
Oleyl lactate		Experimental
Oleyl oleate		Experimental
Paraffin wax (130°F)		Int'l Wax Ref'g Co.
Peanut oil		Drew Foods Ref'g Co.
Petrolatum (white)		Sonneborn Div., Witco
PEG 200 dilaurate		Experimental
PEG 200 monooleate	Emulsynt 2180	Van Dyk & Co.
PEG 400 dioleate	Emulsynt 600	Van Dyk & Co.
PEG 400 linoleate		Experimental
PEG 400 monolaurate	Emulsynt 1060	Van Dyk & Co.
PEG 600 monoisostearate	Emery 3969D	Emery Industries Inc.
PEG 600 monooleate	Emulsynt 710	Van Dyk & Co.
PEG 1000 monostearate	Cerasynt 840	Van Dyk & Co.
PEG 1540 monooleate	Emulsynt 910	Van Dyk & Co.
PEG 4000 linoleate		Experimental
Polypropylene glycol 2000 monooleate	Emcol F26-46	Witco Chemical Co.
Propylene glycol linoleate		Experimental
Ricinoleyl alcohol		Baker Co.
Safflower oil		Pacific Vegetable Oil Corp.
Stearyl alcohol (natural)		M. Michel & Co.
Stearyl lactate		Experimental
Squalane	Robane	Robeco Chemical Co.
Squalene		Robeco Chemical Co.
Triglyceryl monooleate		Drew Chemical Co.