Chemical Composition of Teeth

DENTAL CHEMISTRY

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Sample preparation

Mechanical methods

A diamond saw or cutting disc is usually used to obtain layers of enamel or dentine or thin sections of longitudinal or horizontal planes for use as slides in light microscopy or electron probe analysis.

Large amounts of dentine or enamel material are usually prepared by using a diamond griding wheel with great care to avoid contaminating thr desired material.

Flotation technique of Manly and Hodge

Once the tooth has been pulverized , the more dense enamel particles can be separated from the dentine by using a flotation or centerfuge-flotation technique. The particles are interoduced into a solution of acetone –bromo – from having a specific gravity of 2.70. enamel having a density of 2.92±0.1 settles during centrifugation or flotation, while the lighter dentine with a density of about 2.40

floats on the surface permitting either fraction to be readily collected(see figure). A single separation gives enamel and dentine of 99% purity as determined by a refractive index method. Cementum, density 2/03, can also be separated by this technique.

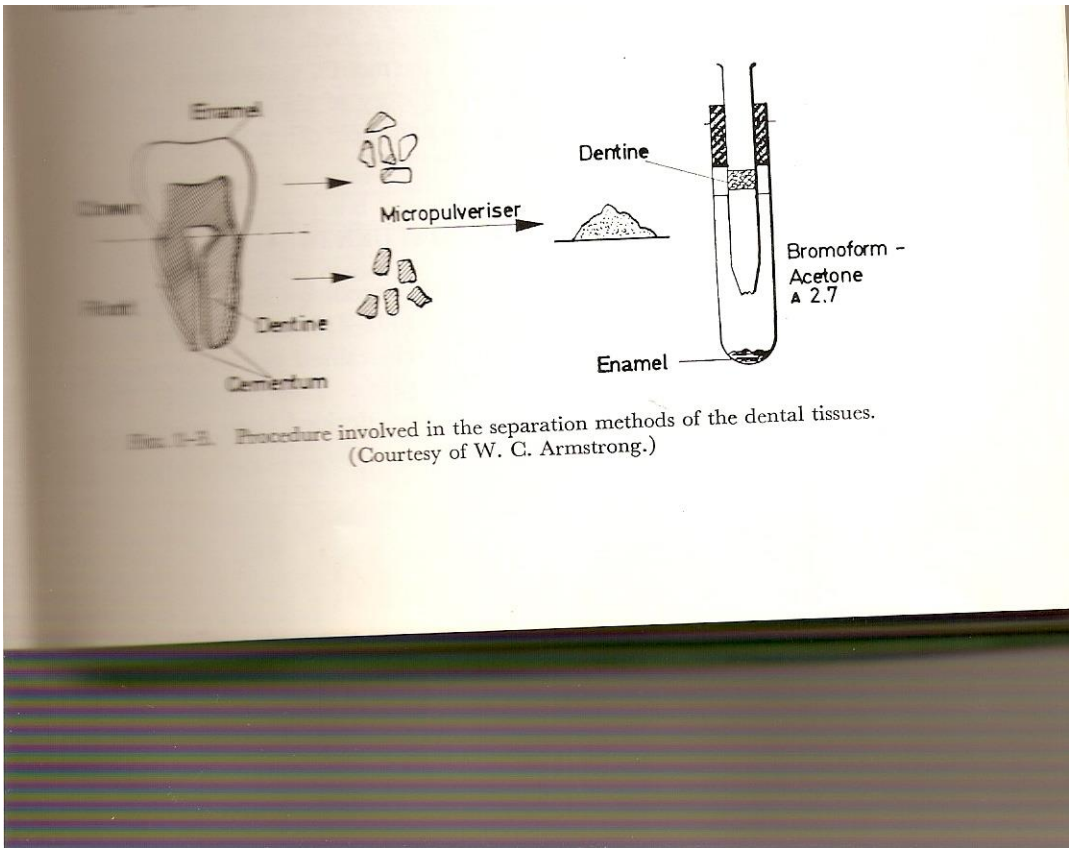

Fig. 11-3. Procedure involved in the separation methods of the dental tissues. (Courtesy of W. C. Armstrong.)

Chemical methods

Acids have been used to etch away successive layers of enamel and dentine to give either solutions of the desired soluble material or pure residues of wanted material. By adjusting the strength of the acid and the etching time, any thickness from as low as 10 microns may be achieved.

Chemical composition

A tooth unlike a shaker full of recrystalized salts, has no single, constant, chemical stoichiometry. It has been constituted and shaped by unique genetic and biochemical individual and therefore can be varied as nature will permit.

One reporting the composition of a tooth one must constantly keep in mind the effects of diet, position in the mouth , geographical locality, age, condition of the tooth and medical history of

the contributing individual. In the instances where these facts and their effects are known, they will be noted.

Inorganic constituents

Tooth analysis

In 1973 Lefever and Hodge reported the values intable for the chemical analysis of teeth. Their data permitted the following conclusions:

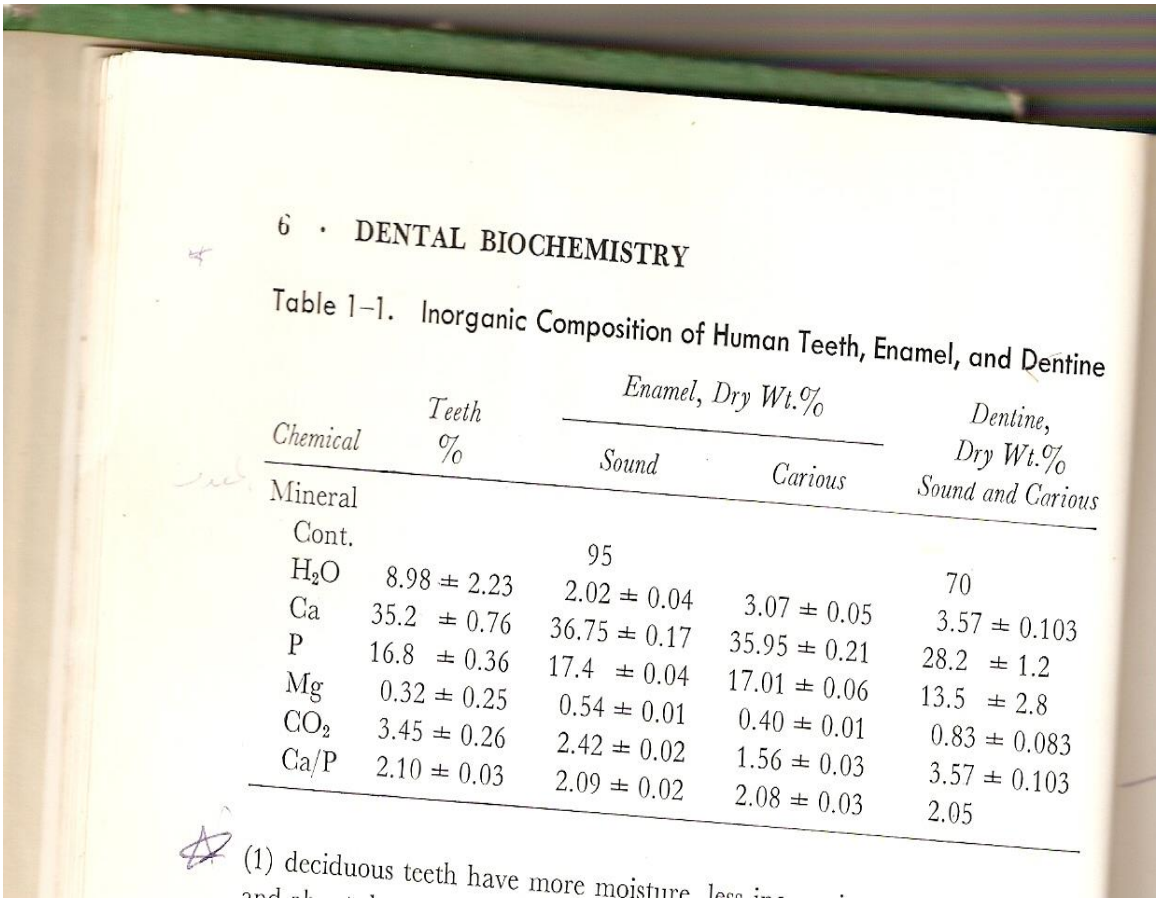

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Table 1–1. Inorganic Composition of Human Teeth, Enamel, and Dentine

Chemical	Teeth %	Enamel, Dry Wt.%		Dentine, Dry Wt.%
		Sound	Carious	Sound and Carious
Mineral		95		70
Cont.				
H_2O	8.98 ± 2.23	2.02 ± 0.04	3.07 ± 0.05	3.57 ± 0.103
Ca	35.2 ± 0.76	36.75 ± 0.17	35.95 ± 0.21	28.2 ± 1.2
P	16.8 ± 0.36	17.4 ± 0.04	17.01 ± 0.06	13.5 ± 2.8
Mg	0.32 ± 0.25	0.54 ± 0.01	0.40 ± 0.01	0.83 ± 0.083
CO_2	3.45 ± 0.26	2.42 ± 0.02	1.56 ± 0.03	3.57 ± 0.103
Ca/P	2.10 ± 0.03	2.09 ± 0.02	2.08 ± 0.03	2.05

(1) deciduous teeth have more moisture, less in-

1- Deciduous teeth have more moister, less inorganic residue , Ca and P, and about the same carbonate content as permanent.
2- There is little differences, except in moister content, between sound and carious teeth.
3- Age causes no change in the chemical constitution of teeth.
4- There is little chemical difference between teeth from male and female patients
5- Increasing severity of pyorrhea may cause a decrease in the carbonate content of teeth.
6- The composition of teeth substance is remarkably constant.

Calcium and phosphorus

Ca/P retio are slightly lower in carious than in sound enamel(table). Sound enamel from age groups beyond 30 years has a lower Ca/P ratio(1.97) than sound enamel from the younger age group(2.07).

As can be ssen from the table thr Ca/P ratio of enamel and dentines lies between that of octacalcium phosphate , $Ca_8H_2(PO_4)+5H_2O$, 1.72 and hydroxyapatite, $Ca_{10}(PO_4)_6(OH)_2$,2.15. possible intermidate compounds include hydrated tricalcium phosphate . two theories have been formulated to explain the continuous series of apatitic calcium phosphate.

1- The absorption theory, in which acid phosphate groups absorb to microcrystalline hydroxyapatite.
2- The defect theory, which proposes that hydrogen ions in hydroxapatite are substituted for Ca ions.

Water:

Enamel humidified to 100% relative humidity loses 1.7% and 2.1% by weigh of water at 61 and 100C, respectively. The use of nuclear magnetic resonance (NMR) revealed that heating to 200C was insufficient to dehydrate dental enamel.

Carbohydrate

Carbon dioxide (carbonate), unlike zinc, lead or fluoride , has a reverse distribution pattern. An ealier study gave the content of the outer enamel surface to be about 1.5% by weight increasing in smooth (concave) curve to about 2.9% by weight that the dentino-enamel junction (DEJ).

Magnesium

Brudevold and his co-workers showed that that the surface enamel has a lower Mg content than the body on intact enamel , 30-60 versus 60-74mM per gm.

Fluoride

Most investigators agree that the caries –inhibiting effect of fluoride is due to its relatively high concentration in the surface layer of the enamel .

The continuous drinking of water containing 0.1-0.5 ppm of fluoride by person under 20 years of age caused the level of surface enamel fluoride to rise from 419 to 3,370ppm. A degree of caries protections occurs when one hydroxyl group of hydroxyapatite ions is replaced by a fluoride per surface unit cell.

The inhibition of caries found in fluoride areas is due to the presence of fluoride alone and not to change in other enamel components.

Fluoride concentration in deciduous teeth follows a pattern similar to that in permanent teeth, although the level in the enamel surface to approximately 30 microns in depth are lower than in the permanent teeth.

Chloride

Chloride is capable of exchanging with the hydroxyl group of hydroxyapatite but is not fixed in calcified tissues.

Strontium

The uptake of strontium occurs prior to eruption , probably during tooth formation , since their is no change in concentration with age. The level of strontium concentration is about constant in the surface and subsurface enamel.

Vanadium

Vanadium was not considered as one of the essential trace elements but, after showing that is necessary for the growing rat. In 1972 it was added to the list of elements essential for life.

Lead

Deciduous teeth have been found to give an excellent indication of the lead accumulation in individual children.

Studies on whole teeth indicate that

1. The amount of lead increase at a fairly uniform rate through age 50(11 to27ppm), when a rapid increase occurs that levels off (50-55ppm) until age 79.
2. There is little different in assimilation by males and females.
3. Urban residents had lower levels than those of sub-urban or rural residents.
4. Ancient teeth (A.D. 200-600) had low metal level and no age correlation (5.3 to 2.9ppm).
5. Cadmium (3.1 to 5.8 ppm0 and zinc (1.6 to 3.6 ppm) levels showed no correlation with age.

Trace elements

Trace elements can be divided into three categories:

Table 1–2. Trace Elemental Composition of Sound Human Enamel and Dentine in Micrograms/Gram (PPM) (Numbers Indicate Mean ± Standard Error)

		Enamel		*Dentine*
Elements	*Symbol*	*1*	*2*	*3*
Aluminum	Al	12.5 ± 2.94	86.13 ± 4.54	68.6 ± 22.5
Antimony	Sb	0.13 ± 0.01	0.96 ± 0.69	0.69 ± 0.41
Barium	Ba	4.2 ± 0.60	125.11 ± 23.68	129.05 ± 54.69
Boron	B	5.0 ± 1.51		94.33 ± 11.47
Bromine	Br	1.12 ± 0.12	33.79 ± 5.71	114.37 ± 2.80
Cadmium	Cd	0.51 ± 0.12		
Chloride	Cl	6022 ± 723	3200 ± 100	350 ± 30
Chromium	Cr	3.2 ± 0.80	1.02 ± 0.51	1.99 ± 0.84
Cobalt	Co		0.13 ± 0.13	1.11 ± 0.27
Copper	Cu	4.20 ± 3.01		
Fluorine	F	293 ± 34		
Gold	Au		0.11 ± 0.07	0.07 ± 0.04
Iron	Fe	4.4 ± 0.95	118.27 ± 71.65	93.38 ± 35.05
Lead	Pb	3.6 ± 0.24		
Lithium	Li	1.13 ± 0.13		
Magnesium	Mg	1670 ± 120	2800 ± 100	8700 ± 300
Manganese	Mn	0.28 ± 0.03	0.59 ± 0.05	0.63 ± 0.05
Molybdenum	Mo	7.2 ± 1.35		
Niobium	Nb	0.28 ± 0.03		
Potassium	K	401 ± 31		
Rubidium	Rb	0.39 ± 0.03		
Selenium	Se	0.27 ± 0.02		
Silver	Ag	0.35 ± 0.07	0.56 ± 0.29	2.19 ± 0.84
Sodium	Na		7000 ± 100	5500 ± 300
Sulfur	S	281 ± 20		
Strontium	Sr	81 ± 11	111.19 ± 9.86	94.33 ± 11.47
Tin	Sn	0.21 ± 0.04		
Vanadium	V	0.036 ± 0.037[3]		
Zinc	Zn	293 ± 34		

1. Losee, F. L., Cutress, T. W., and Brown, R., Caries Res., *8*, 123–134, 1974.
2. Retief, D. H., and Cleaton-Jones, P. E., Arch. Oral Biol., *16*, 1257, 1971.
3. Curzon, M. E. J., Losee, F. L., Brown, R., and Taylor, H. E., Arch. Oral Biol., *19*, 1161–1165, 1974.

1. Those which apper to have no biological role and which are present in tissue only as adventitious contamination from the environment.

2. Those elements which appear to be essential to the enzymatic processes of living cell(eg. Fe,Zn,Cu,I,Mo,I,Co,Mn,Se).
3. Elements which are probably essential nutrients but whose metabolic action in not clear (e,g. F,Br,Ba,Sr).

Trace elements may assist in reducing caries by altering tooth solubility , by changing tooth morphology , or by altering the size and or shape of the crystallites and ultimately, the enamel structure.

Organic constituents

Citrate

Citrate occurs in greater concentration in the surface and junction enamel than in the body of the enamel going from value 3.5mM/gm to 1.1 and back to about 4.4mM/gm. Whether the distribution varies with age has not yet been determined.

Citrate , which has been found in all mineralized tissues, may be

1- An accidental co precipitation component of calcium phosphates.
2- In a citrate- containing arginine-rich peptide .
3- In the form of phosphate or pyrophosphoric-citrate.

Lactate

Lactate follows almost the same distribution and content as citrate and it is possible that both are located primarily in the water in the enamel since a comparison shows similar curves.

Table 1–3. Organic Constituents of Human Sound and Carious Enamel, Dentine and Bone

	Enamel Dry %		*Dentine Dry %*	*Bone Dry %*
	Sound	*Carious*	*Sound and Carious*	
Lactic	0.01 –0.03		0.15	
Citrate	0.10 ± 0.02		0.8 – 0.9	0.82–1.25
Total Organic	1.53 –3.80	3.65–6.98	19–21	24–27
N	0.073–0.077		3.4 – 3.5	4.15–4.97
Protein	0.194–0.275	0.64–1.89	18.2	15–27
Collagen	0.09		17–18	23
Insoluble Protein			0.2	1–2
Carbohydrate	0.015 ± 0.005	0.18	0.2 – 0.6*	0.04
Mucopoly-saccharide	0.1		0.2	0.24–0.4
Lipid	0.6	0.04–0.18	0.2	0.1

* In carious dentine this value is 4%

Nitrogen

The amount of nitrogen can be used as a measure of the concentration of organic material in areas of the tooth. The scientists found that there is no change with the age in the N concentration in enamel except that occurring in the last decade of life when measured on a weight basies. There is no theoretical basis to except that the organic material in a tooth should change with age. Possible alter ations may occur from external source through cracks and voids which would be more numerous in the order tooth due to wear and tear. Teeth over 50 years old differ from younger teeth by having:

1- Greater N concentration in the surface enamel , 0.15% versus 0.1%.
2- Greater N concentration at the dentino enamel junction 0.2% versus ca. 0.12%
3- Lower N concentration in the body of the enamel for a greater depth, ca.0.04%versus ca.0.07%N.

Protein in teeth

In discussing the enamel proteins, attention must ber given to the age of the tooth because of major differences observed between the developing (immature) and the mature tooth. These differences include

1-total protein content.

2-solubility

3-aminiacid composition

The total protein content of human enamel diminishes from approximately 15 to 20% in the developing tooth to about 0.05 to 0.2% at maturity. A similar large decrease in the enamel protein content of the maturing bovine tooth has been observed. An absolute loss of 90% in the weight of enamel protein during maturation has been demonstrated. The process responsible for the loss is unknown.

PROTEIN MATRIX OF DENTINE AND CEMENTUM

The decalcified matrix of human and bovine dentine is composed esse
tially of collagen. Dentinal protein possesses the distinctive wide-angle x-ra

Table 2–2. Amino Acid Composition of Some Collagens

	Dentine		*Cementum*	*Tendon*
Amino Acid	*Human*[1]	*Bovine*[2]	*Bovine*[3]	*Bovine*[4]
	Residues of Amino Acids/1000 Residues			
3-Hydroxyproline	—		1	2
4-Hydroxyproline	99	99	105	90
Aspartic acid	46	50	50	47
Theonine	17	17	19	17
Serine	33	38	39	34
Proline	116	118	124	120
Glutamic acid	74	71	80	74
Glycine	329	326	307	331
Alanine	112	125	115	112
Valine	25	21	21	23
Half-cystine	0	0	<0.5	0
Methionine	5	4	3	5
Isoleucine	9	11	12	12
Leucine	24	25	27	27
Tyrosine	6	4	3	5
Phenylalanine	16	12	14	14
Hydroxylysine	10	9	11	9
Lysine	22	19	25	22
Histidine	5	5		3
Arginine	52	47	51	51

[1] From Piez, K. A.: Amino Acid Composition of Some Calcified Proteins, Scien
841, 1961.

[2] From Veis, A. and Schleuter, R. J.: The Macromolecular Organization of
Matrix Collagen, Biochemistry, *3*, 1650, 1964.

[3] From Glimcher, M. J., Friberg, U. A., and Levine, P. T.: The Identificati
Characterization of a Calcified Layer of Coronal Cementum in Erupted Bovine
J. Ultrastruct. Res., *10*, 76, 1964.

[4] From Lidsky, M. D., Sharp, J. T., and Rudee, M. L.: Isolation, Chemical C
tion, and Demonstration of Collagen with an Unusual Hydroxylysine : Hydroxy
Ratio, Arch. Biochem., *121*, 496, 1967.

COLLAGEN

Collogen is the major protein of the extracellular connective tissues and functions as a structural protein serving principally as the prime mechanical support of tissues. The amount of collagen varies from one species to another and from tissue to tissue within the same species. Collagen content of normal human dentine has been estimated to be 18% by dry weight.

Physicochemical properties

From the standpoint of protein structure, collagen is an unique molecules.

Structure

In the native state, most collagen is insoluble. However , native soluble collagen can be obtained in vitro under certain conditions.

A collogen monomer consists of three polypeptide chains, each chain being twisted into a left-handed helix. The three helices in turn from a right-hunderd helix. The three helixes in turn from a right –handed super or major helix.

Biosynthesis of collagen

Collagen is formed by several steps:

Hydroxylation of proline and lysine

Helix formation

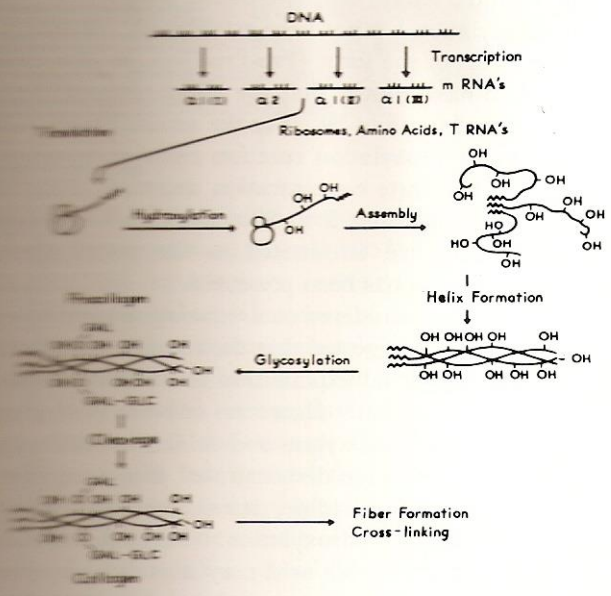
Glycosylation

Transport and secretion

’procollagen-collagen conversion

Fiber formation

cross-linking



...illustrating the steps involved in biosynthesis of functional ... and Matukas, V. J.: Biosynthesis of Collagen, Fed. Proc.,

CARBIHYDRATE OF TEETH

Various attempts have been made to extract and characterize the carbohydrate- containing components of teeth.

It was found that the dentine-cementum and enamel fractions of human teeth contain respectively 0.08 and 0.03% total aminosugar. Of these amounts glucose amine represents 42 and 47% of the total, respectively in dentine –cementum also contained a third compound (accounting for 15% of total hexamine).

In some tissues, the synthesis of glycosamine requires not glutamine but ammonia, as indicated by fallowing reaction;

NH_3 +fructose-6- phosphate ↔ glycosamine-6- phosphate +H_2O

The glycoamineglycons are high molecular weight hetropolysaccaride they may be conveniently represented by a ; (repeating unit) which is repeating many times to produce chains of different length eight different GAG((glycosaminoglycans) have been isolated and characterized on the **basis of**

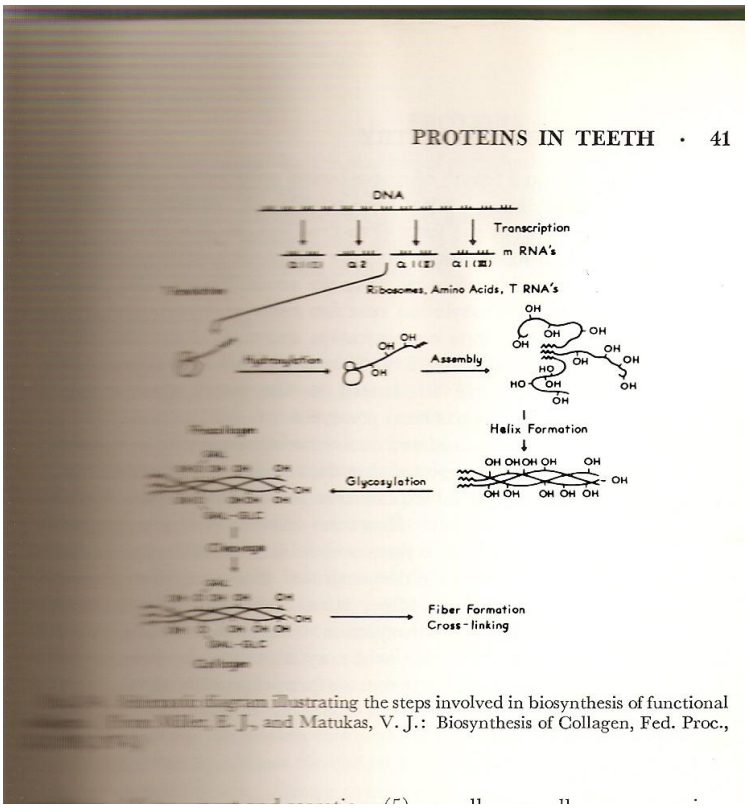
1- **The structure of repeating unit.**
2- **Optical rotation**
3- Solubility in alcoholic solutions
4- Enzymatic degradation

The acidic character of these compounds is due to the presence of three different functional group

Carboxylin (-COOH)

Ester sulfhate(-O-SO_4H)

Sulfonamide(-N-SO_3H)



and Matukas, V. J.: Biosynthesis of Collagen, Fed. Proc.,

LIPIDS IN TEETH AND MEMBERANCE

The presence of phosphatidyl serine was confirmed in carious dentin. Since this lipid was not wextracted from non carious material, a possible binding of inorganic salt by lipid was suggested, which prompted lipid analysis of deter mineralized dentin matrix. Lipid extracts of sound and EDTA- dermineralized dentin were separated and quantitated, the results of which are shown in table:

lipid was identified as
ment. No phosphatidyl serine, phosphatidyl inositol, or phosphatidic a
was extracted from the tissue until after demineralization. Quite compara
results were obtained with enamel. This again suggests a high degree
association between phospholipids and mineral. Similar observations w
made by Odutuga and Prout with human teeth. Enamel and dentin c
tain 0.51% and 0.33% total lipid, respectively.

Total fatty acids have been extracted from fossil teeth as old as 230,000,
years. Over 60% of the fatty acids were present as palmitic, stearic, a

Table 4–1. Comparison of the Lipid Content of Sound Dentin Prepared by Two Extraction Procedures

	I†	*II*‡
Total lipid weight	40.90*	176.60
Cholesterol esters	2.89	4.14
Free cholesterol	3.42	6.53
Triglycerides	1.59	1.61
Diglycerides	0.75	1.15
Monoglycerides	0.45	0.80
Phospholipids	0.45	4.95

* All values based on mg per 100 gm of dried dentin.
† Chloroform-methanol extraction.
‡ EDTA decalcification.

Fat soluble vitamins

Vitamins A,D,E, and K are found associated with the lipid fraction of foods and their absorption into the body depend upon the presence of bile for emulsification. The structure of the fat soluble vitamins are shown in figure.

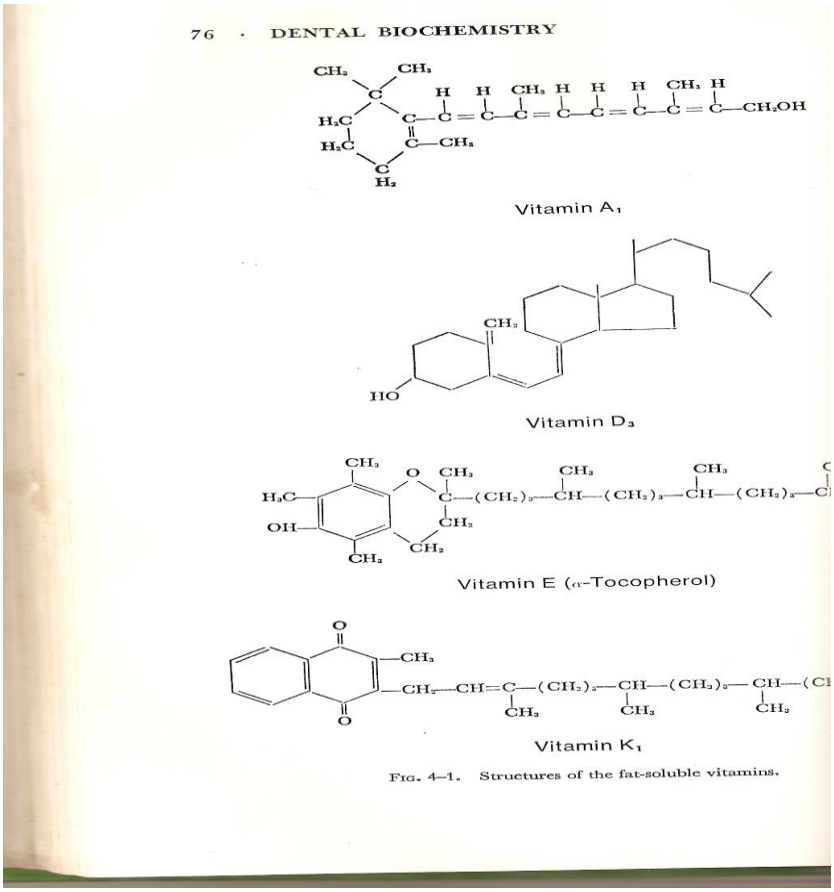
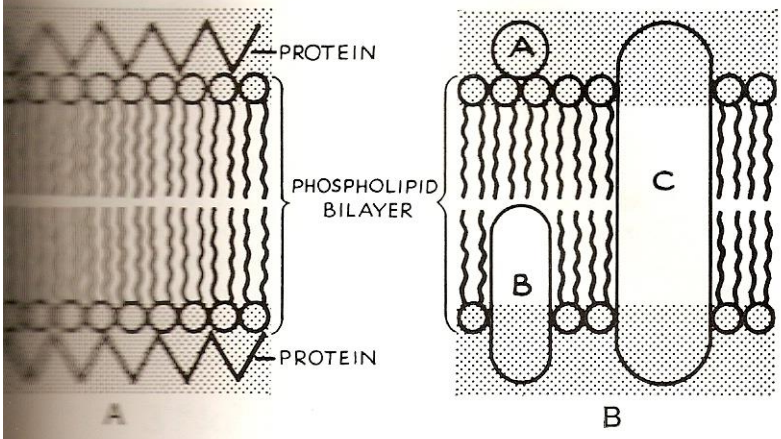


FIG. 4–1. Structures of the fat-soluble vitamins.

Lipids in membranes

Structure

Basically the phospholipids are the molecules that define membrane structure. These compounds are amphipathic in nature, which means that they contain both polar and polar regions.



Diagrams of membrane models. A, Unit membrane of Robertson. B, Lipid- mosaic model in which A represents hydrophilic proteins, B represents , and C represents predominantly hydrophobic proteins which are part continuum.