activity in fraction I to be due to tritium water originating during glycine metabolism. Actually the radioactivities present in water distillates from liver and brain extracts were found to be almost the same as those in the respective fractions I (92% and 97%).

The shift of ^{3}H-activity from glycine to fraction I occurs also in kidney slices, though to a lesser extent (Table II). This can be explained by taking into consideration that tritium water originating in the slices exchanges with the excess of water of the incubation medium. The data concerning the distribution of radioactivity of the medium before and at the end of the incubation are in favour of this view.

From all these findings it is evident that the use of ^{3}H-labelled glycine seems not to be advisable in studies of glycine metabolism and in investigations concerning the role of glycine as a precursor substance[17].

Table II. ^{3}H- and ^{14}C-activity of medium (dpm/ml) before and after the incubation of kidney slices and percentage distribution of extract radioactivity (dpm/g wet weight) between glycine, serine and two other fractions

		^{3}H	^{14}C
Activity of medium prior to incubation		4,230,000	1,290,000
Activity of medium after incubation		4,000,000	880,000
Extract activity	dpm/g	9,270,000	4,046,000
Fraction I	%	36	13
Fraction II (serine)	%	9	14
Fraction III (glycine)	%	37	43
Fraction IV	%	19	29

Zusammenfassung. Die Radioaktivitätsverteilung von ^{3}H und ^{14}C nach Gabe von ^{3}H- und ^{14}C-Glycin weist sowohl in vivo als auch in vitro erhebliche Unterschiede auf. Unsere Resultate zeigen, dass die Aufnahme von Glycin und seine metabolischen Umsetzungen nicht mit 2-^{3}H-Glycin bestimmt werden können.

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Conformations of Amino Acids Calculated from Molecular Orbital Theory

The forces that govern the folding of a polypeptide chain in aqueous solution are poorly understood, although it has been suggested that the major influence may be conformation of individual amino acid residues with interaction between adjacent residues being of lesser importance[1]. We have used a quantum mechanical method developed by HOFFMANN[2] (extended Hückel molecular orbital) to calculate the energetically preferred conformation of amino acid residues and reported results for glycine, alanine, phenylalanine, and proline which agree with experimental data[3]. Previous calculations of minimum energy conformation of small molecules[4–6] using this method have in general correlated well with experimental data. A report of calculations of 2 amino acid residues using an extended Hückel approach has recently appeared[7], and here we report the results of calculations of 4 additional amino acid residues.

Methods. The N-acetyl amides of amino acids were the molecules considered as these simulate peptide bonds at each end of the amino acid residue. The bond lengths and angles of the backbone atoms were those of PAULING and COREY[8] and of the side chain were taken from X-ray crystallographic data compiled by SCHERAGA[9]. The molecular orbital parameters were those previously used[3]. The energy was calculated as a function of varying geometry of all freely rotating bonds until the energy minimum was obtained. Angles near the ϕ, minimum were refined to $\pm 15°$. The calculated minimum energy conformations (using the Ψ convention of EDSALL et al.[10]) of leucine, isoleucine, valine, and serine are shown in the Table along with secondary conformations having energies within 1 kcal/mole.

The ϕ, Ψ values of the calculated minimum energy conformations of amino acid residues can be compared

with ϕ, Ψ values of experimentally determined conformations. In some cases the data were obtained by X-ray crystallography but there is ample evidence that conformation in crystal and solution are similar[15]. Gramicidin S-A has been studied using nuclear magnetic resonance[16], and although the leucyl residue may be constrained by the cyclic nature of this decapeptide it is noteworthy that the observed conformation agrees with the calculated energy minimum at Ψ and is within 30° at ϕ.

The generally good agreement between calculated and experimental conformations suggests that the extended Hückel molecular orbital approach can be used to determine the preferred conformation of amino acid residues as an initial step towards understanding the forces involved in the folding of polypeptide chains.

Conformations of amino acid residues

Residue	Calculated[a]		Experimental conformations		Reference
	ϕ	Ψ	ϕ	Ψ	
L-Serine	60°	330°	61°	293°	11
	120°				
L-Isoleucine	60°	300°	38°	293°	12
	90°′		61°′	325°′	
L-Valine	60°	300°	38°	293°	13
	90°′		61°′	325°′	
			132°	123°	13
L-Leucine	60°	0°	132°	123°	14
			30°	0°	15

[a] 0° = 360°, angles listed are within 1 kcal/mole^{-1}.

Zusammenfassung. Die Konformation einiger natürlicher Aminosäuren wird auf Grund einer erweiterten Hückel-Molekular-Orbital-Theorie berechnet.

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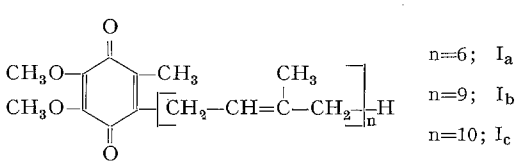
Coenzymes Q: Stimulants of the Phagocytic Activity in Rats and Immune Response in Mice

Coenzymes Q_9 (Ib) and Q_{10} (Ic) are present in shark livers[1], and we identified them in the hexane extracts of shark livers (Lemon shark *Negaprion brevirostris*), that had shown stimulation of the phagocytic activity in rats, increase in the antibody formation of mice vs sheep erythrocytes and modified other parameters of the reticuloendothelial system (RES)[2]. Since the activity of pure coenzymes Q has not been studied in these tests, we decided to investigate their action as stimulants of the RES.



n=6; I_a
n=9; I_b
n=10; I_c

Materials and methods. Pure, commercially available coenzymes Q_6 (Ia) and Q_{10} (Ic) were used for this study. Only pure material was used.

Phagocytic activity. Adult male CFN rats weighing 180 g were injected via the saphenous vein with the material to be tested as an emulsion in a 5% non-pyrogenic glucose solution containing Ninol (lauric diethanolamide) used as an emulsifier. In all cases the amount of Ninol used was 5% by weight of the substance under investigation. The Q_6 and Q_{10} emulsions contained 375 and 250 µg respectively of coenzyme per ml. They were prepared in a 500 ml Waring blender and initially homogenized for 45 sec. The smaller doses were injected first and the emulsion rehomogenized for 15 sec before proceeding to the next larger dose[3]. 10 animals were used for each dose and 10 animals were injected as controls

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[3] The method used to prepare the emulsion is of critical importance and it should always be the same in order to obtain reproducible results.