This investigation was supported by the
Swedish Research Council.

1. Ågren, G., de Verdier, C.H. and Glomset,
2. Ågren, G., de Verdier, C.H. and Glomset,
Scand. 10 (1956) 877.
4. Ågren, G. and de Verdier, C-H. To be
published.
7. Leloir, L. F. and Cardini, C. E. in Colowick
and Kaplan Methods of Enzymology
10 (1955) 1.
9. Di Stefano, V., Neuman, W. F. and Rouser,

**Mass Spectrometric Studies on**

**Amino Acid and Peptide**

**Derivatives**

**Carl-Ove Andersson**

Department of Medical Biochemistry,
Institute of Medical Chemistry, University of
Uppsala, Uppsala, Sweden, and Laboratory for
Mass Spectrometry, Kemiska Institutionen I,
Karolinska Institutet, Stockholm, Sweden

In the mass spectrum of a methyl ester of
the type RCH₂COOCH₃, the most prominent
peak is normally found at m/e 74 and is due
to a rearranged fragment C₅H₅NO₂⁺. A pro-
minent peak due to the alkyl fragment R⁺ is
only observed when carbon atom 3 is quater-
nary. The mass spectrum of the methyl ester of
an a-amino acid RCHNH₂COOCH₃ shows,
on the other hand, a very large peak due to
the ionized fragment RCHNH⁺. The mass
number of this fragment is different for all
amino-acids except the isomeric valines and
leucines.

The parent peaks are small but in the cases
so far examined allow a direct determination
of the molecular weight of the esters. A further
prominent peak occurs at m/e 88 corresponding
to the fragment -CHNH₄COOCH₃⁺.

Although several free amino-acids and simple
peptides can be brought into the gas phase
without decomposition, compounds with the
zwitterion structure have been found less suitable
for mass spectrometric analysis than com-
pounds in which either the amino group or
the carboxyl is protected. It has been found
possible to analyze peptides with protected
amino- and carboxyl groups. Thus N-triflu-
rroacetetyl-L-alanyl-L-phenylalnine methyl ester
² gives an excellent mass spectrum with a
parent peak at m/e 346 (calculated molecular
weight 346.3).

The high-mass, high-resolution mass spectro-
rometer thus seems to offer interesting possi-
bilities in the analysis of amino-acids and peptides.

It is intended to extend this work to other
amino-acid derivatives and to study the possi-
bility of analyzing mixtures. As carried out
at present one analysis requires about 100
micrograms of material.

1. Asselineau, J., Ryhage, R., and Stenhagen,
Soc. 77 (1955) 1678.
3. Weygand, F., Geiger, B. and Swedenh, W.
Angew. Chem. 68 (1956) 307.

**Infrared-spectroscopic Studies on**

**Bile Acids**

**I. Fischmeister**

Department of Medical Biochemistry,
Institute of Medical Chemistry, University of
Uppsala, Sweden

The poor solubility of the bile acids in the
nonpolar solvents required for infrared spec-
troscopy prevents their investigation in solu-
tion. We have therefore examined the spectra
of the solid substances pressed in potassium
bromide pellets. In the case of the bile acid
esters which can be examined both in solution
and in the solid state, the solid state spectra
are found to be more distinct, owing to the
fixed positions of the molecules in the crystal.

The spectra are sufficiently specific to allow
identification of each bile acid by infrared
spectroscopy. They are especially sensitive
to the number and position of the hydroxyl
groups in the skeleton. This is shown for the
series of cholic acid and its hydroxy deriv-
atives, for coprostanic acid and its 3,7- and
3,7,12-hydroxy derivatives as well as for pep-
tide conjugates of cholic acid and its hydroxy
derivatives with glycine and taurine. The
length of the side chain affects not only the
CH₂-vibrations but also those of the hydroxyl-
and carboxyl group, indicating differences in
the hydrogen bond pattern and/or different
degree of hydrogen bonding in the crystallized
compounds with different side chains.