

IDENTIFICATION OF CORDYCEPIN, A METABOLITE OF CORDYCEPS MILITARIS,AS 3'-DEOXYADENOSINE

Edward A. Kaczka, Nelson R. Trenner, Byron Arison,  
Robert W. Walker and Karl Folkers

Merck Sharp & Dohme Research Laboratories  
Division of Merck & Co., Inc.  
Rahway, New Jersey

Received December 4, 1963

After the isolation of a crystalline compound from the fermentation broth of Aspergillus nidulans that showed inhibitory effects on KB cell cultures, the compound was identified as a deoxyadenosine. It was shown by comparative IR and NMR spectral data that the compound was not identical with 2'-deoxyadenosine and that the most likely structure was 3'-deoxyadenosine (Kaczka, et al., 196 ).

The proposed structure of cordycepin (Bentley, et al., 1951) is an adenine nucleoside containing a 3-deoxypentose with a branched chain; this structure is unacceptable for the structure of our product from Aspergillus nidulans according to the interpretation of the NMR spectrum.

Complete IR and NMR spectra of synthetic 3'-deoxyadenosine (Lee, et al., 1961) kindly furnished by Dr. L. Goodman of the Stanford Research Institute, and samples of cordycepin, kindly furnished by Professor R. A. Raphael of the University of Glasgow and Dr. Chester Stock of the Sloan-Kettering Institute, were compared.

The IR and NMR spectra of the active metabolite from Aspergillus nidulans, synthetic 3'-deoxyadenosine, and the two samples of cordycepin are identical.

It is possible, but doubtful, that a culture of Cordyceps militaris produced a product of the structure proposed by Bentley, et al., but it is noted that the structure proof for a branched-chain 3-deoxy-pentose derivative was inconclusive. The samples of the metabolic product of this microorganism which we have obtained is 3'-deoxyadenosine.

#### REFERENCES

- Bentley, H. R., Cunningham, K. G., and Spring, F. S., J. Chem. Soc., 2301 (1951).
- Kaczka, E. A., Dulaney, E. L., Gitterman, C. O., Woodruff, H. B., and Folkers, K., Biochem. Biophys. Res. Commun.
- Lee, W. W., Benítez, A., Anderson, C. D., Goodman, L., Baker, B. R., J. Am. Chem. Soc., 83, 1906 (1961).