Bacterial Carotenoids

XXV. C_{50}-Carotenoids. 1. The Structure of *Dehydrogenans*-P439

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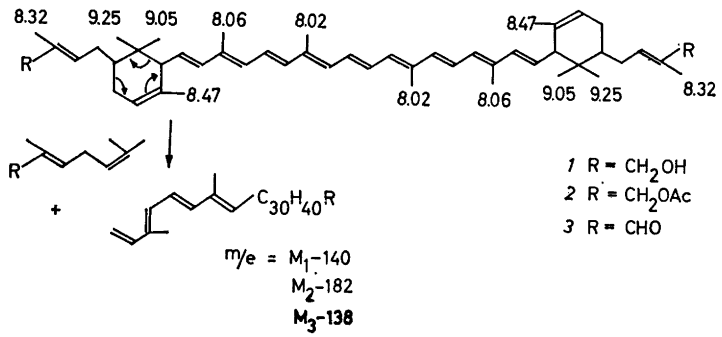
The first C_{50}-carotenoid encountered in nature was recently isolated from the non-photosynthetic bacterium *Flavobacterium dehydrogenans* Arnaudi.[1] The pigment was provisionally called *dehydrogenans*—P439.[2] Structure *1* is now suggested for this compound.

Further chemical studies along the lines previously reported [1] have confirmed the primary, allylic character of the two hydroxyl functions. Absence of isopropylidene groups was shown by quantitative ozonolysis.

Table 1. Proton magnetic resonance data for P439 (*1*).

Signal position in τ-value	Relative intensities[a]	Assignment
2.76		$CHCl_3$
3.38—3.93	*ca.* 12	in-chain olefinic H
4.38—4.68	*ca.* 6	olefinic H
5.98	4	$=C-CH_2OH$
7.52—7.83	*ca.* 8	allylic CH_2 and allylic CH
8.02	6	in-chain CH_3
8.06	6	in-chain/end-of-chain CH_3
8.32	*ca.* 6	CH_3 on double bond
8.47	*ca.* 6	CH_3 on double bond
8.75	(3)	Impurity?
9.05	6	*gem.* CH_3 in α-ring
9.25	6	*gem.* CH_3 in α-ring

[a] Average of two samples based on integrals and weight of cut-out areas.



Additional information was obtained by spectroscopic data (electronic, infrared-, mass-, and proton magnetic resonance spectra involving double resonance) of P439 (*1*), the diacetate (*2*), and the dialdehyde (*3*).

Proton magnetic resonance data of P439 are compiled in Table 1 and some assignments included on structure *1*. The spectrum had many features in common with that of ε-carotene.

Significant peaks in the mass spectrum of P439 ($M_1 = 704$) occurred at M_1-140, resulting from a rearrangement analogous to that observed for ε-carotene by Schwieter *et al.*[3] Corresponding peaks occurred at M_2-182 and M_3-138 for *2* and *3*, respectively.

Further details will be published.[4]

1. Liaaen Jensen, S. and Weeks, O. B. *Norweg. J. Chem. Mining Met.* **26** (1966) 130.
2. Weeks, O. B. and Garner, R. J. *Arch. Biochem. Biophys. In press.*
3. Schwieter, U., Bolliger, H. R., Chopard-dit Jean, L. H., Englert, G., Kofler, M., König, A., Planta, C. v., Rüegg, R., Vetter, W. and Isler, O. *Chimia* **19** (1965) 294.
4. Liaaen Jensen, S., Hertzberg, S., Weeks, O. B. W. and Schwieter, U. *Acta Chem. Scand. To be published.*

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