FT-IR Study of Some Carotenoids

by **Tamás Lóránd**, **József Deli**, **Péter Molnár**, and **Gyula Tóth***

Department of Medical Chemistry, University of Pécs, Medical School, P.O. Box 99, H-7601 Pécs

Some natural and semisynthetic carotenoids were examined by means of FT-IR spectroscopy. The IR bands of the characteristic functional groups (CH_3, CH_2, C=C, C=O, OH, *etc.*) were assigned when possible. Some special functional groups – without H-atoms – such as C=C=C, 'cross epoxides', *etc.*, which cannot be easily identified by ^{1}H-NMR methods, were also detected in the FT-IR spectra.

Introduction. – IR Spectroscopy played an important role in the structure verification of complex organic molecules during the period of 1950–1970. Later, structure elucidations were based mainly on NMR spectroscopy. This latter method has the advantage of giving a practically complete analysis, while the IR spectra provide information only about the characteristic functional groups. In addition, a complex organic molecule such as a carotenoid shows several IR bands according to the $(3n - 6)$ normal vibrations ($n =$ number of atoms of the molecule). The advent of FT-IR spectroscopy gave new impetus to the usage of IR spectroscopy. The fast and relatively cheap analysis, the requirement of only very small samples, the computerized data processing and data storage, and the usage of spectral data banks are some of the advantages of this analytical method. FT-IR Spectroscopy has not been widely applied to structure verification of carotenoids [1–4]. We wished to use it to further clarify the structures of some carotenoids. Additionally, we investigated some special carotenoids, *i.e.*, that contain functional groups without H-atoms.

Results and Discussion. – Examining the FT-IR spectra of 16 natural and semisynthetic carotenoids, the characteristic functional groups were assigned based on literature data (for the IR bands and assignments, see *Exper. Part*). The carotenoids were taken from our collection and were characterized earlier by their mass, CD, and NMR spectra. Some selected oxo-carotenoids (β-citraurin¹) (**1**), semi-β-carotenone 5,6-epoxide¹) (**2**), and capsorubin¹) (**3**)) were studied (see *Table*). The formyl group of **1** can be detected not only by the $\tilde{\nu}$(C=O) band at 1668 cm^{-1}, corresponding to the expected value of an $\alpha,\beta,\gamma,\delta$-unsaturated aldehyde, but also by the C(O)H) absorption at 2715 cm^{-1} [2]. The IR spectrum of **2** indicates the presence both of the conjugated (1672 cm^{-1}) and the nonconjugated keto group (1716 cm^{-1}) [5b]. Capsorubin (**3**) shows a CO band at 1665 cm^{-1}, in accordance with the literature value of conjugated carbonyl groups [5b].

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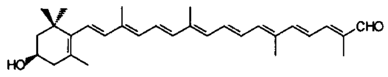
¹) For systematic names, see *Exper. Part.*



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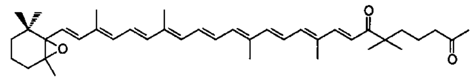

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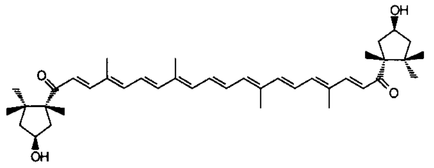

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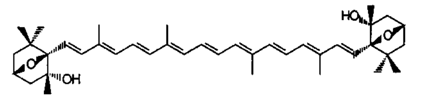

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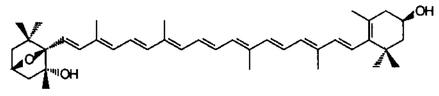

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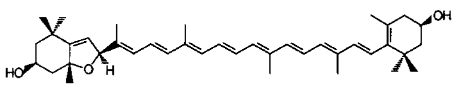

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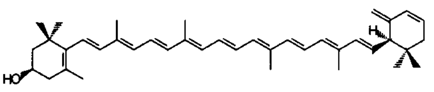

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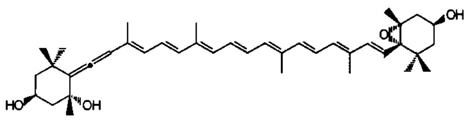

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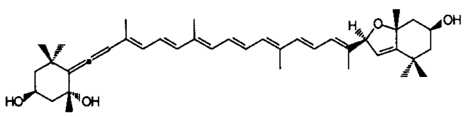

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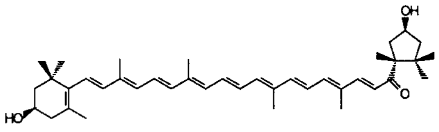

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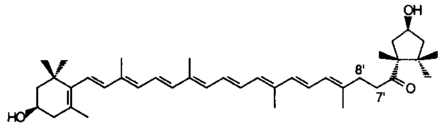

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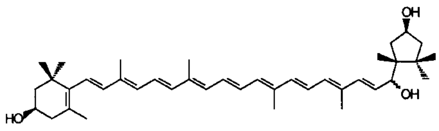

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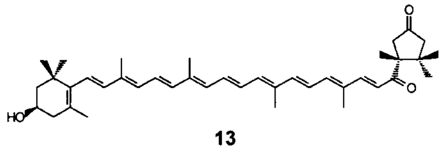

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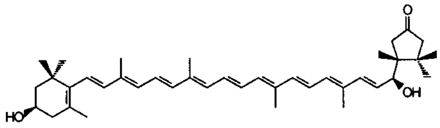

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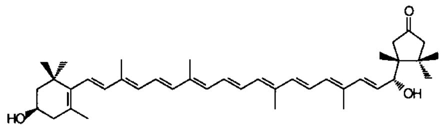

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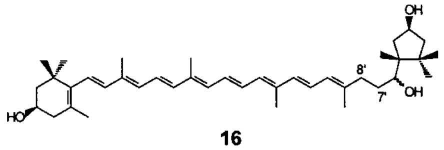

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Table. *Stretching Frequencies $\tilde{\nu}(CO)$ of the Carotenoids Examined*[1])

	Group	Position [cm^{-1}]
β-Citraurin (**1**)	$\tilde{\nu}$(CO), conj. aldehyde	1668
Semi-β-carotenone 5,6-epoxide (**2**)	$\tilde{\nu}$(CO), conj.	1672
	$\tilde{\nu}$(CO), aliph., nonconj.	1716
Capsorubin (**3**)	$\tilde{\nu}$(CO), conj.	1665
Capsanthin (**10**)	$\tilde{\nu}$(CO), conj.	1665
7′,8′-Dihydrocapsanthin (**11**)	$\tilde{\nu}$(CO), alkyl cycloalkyl ketone	1695
Capsanthone (**13**)	$\tilde{\nu}$(CO), conj.	1661
	$\tilde{\nu}$(CO), cyclopentanone	1743
(6′*S*)-Capsanthol-3′-one (**14**)	$\tilde{\nu}$(CO), cyclopentanone	1725
(6′*R*)-Capsanthol-3′-one (**15**)	$\tilde{\nu}$(CO), cyclopentanone	1729

Some special structural parts of carotenoids were identified by means of FT-IR methods. Two of our models contain a 'cross epoxide' group. These groups show a $\tilde{\nu}_{as}$(C−O−C) band at 1100 cm^{-1} (cycloviolaxanthin[1]) (**4**)) or at 1107 cm^{-1} (cucurbitaxanthin[1]) A (**5**)) [5c]. The presence of a furan moiety in mutatoxanthin[1]) (**6**) can be detected by the band at 3074 cm^{-1} assigned to the olefinic H-atom of the furan ring [6a]. In the spectrum of deoxylutein II[1]) (**7**), it is possible to detect the bands of the characteristic terminal methylene group (3083 cm^{-1} $\tilde{\nu}$(=CH$_2$) and 883 cm^{-1} γ(=CH)) [5d]. The allene group of neoxanthin[1]) ((9*Z*)-**8**) and neochrome[1]) ((9*Z*)-**9**) gives a weak, but well-detectable band at 1927 and at 1929 cm^{-1}, respectively ($\tilde{\nu}_{as}$(C=C=C)). In this spectral region, the maximum of the allene group does not overlap with any kind of other bands.

In the following, the carotenoid family of capsanthin (**10**), 7,8-dihydrocapsanthin (**11**), capsanthol (**12**), capsanthone (**13**), (6′*S*)- and (6′*R*)-capsanthol-3′-one (**14** and **15**) and 7′,8′-dihydrocapsanthol (**16**) is discussed[1]). Their spectra (see *Fig.*) corroborate their structures (see the assigned bands). In addition, by means of these spectra, it is possible to monitor simple reactions of carotenoids (see below).

Our starting material capsanthin (**10**) exhibits a $\tilde{\nu}$(C=O) band at 1665 cm^{-1} typical for a conjugated ketone (see **3**) [4a]. The reduction of the C(7′)=C(8′) bond of capsanthin (**10**) results in 7′,8′-dihydrocapsanthin (**11**) with a nonconjugated C=O group (1695 cm^{-1}) [5b], and there is a big change in the C=C region as compared to that of **10**. The position of the $\tilde{\nu}$(C=C) bands is changed and their intensity decreased in the less-conjugated compound **11**. On reduction of the C(6′)=O group of **10** yielding capsanthol (**12**), the $\tilde{\nu}$(C=O) band disappears, and changes in the ν(C=C) absorptions occur. The reduction of C(7′)=C(8′) bond of **12** yields the 7′,8′-dihydrocapsanthol (**16**) with similar changes in the C=C absorptions (1630–1570 cm^{-1}). The oxidation of OH−C(3′) of **10** provides capsanthone (**13**), with the new keto group at C(3′) giving rise to an absorption at 1743 cm^{-1}, corresponding to the literature values of cyclopentanones [5b]. The reduction of C(6′)=O of **13** yields the stereoisomeric (6′*S*)- and (6′*R*)-capsanthol-3′-ones (**14** and **15**). In the spectrum of **14**, the absorption of C(3′)=O is shifted to 1725 cm^{-1}, and there are changes in the C=C absorptions (decrease of intensities because of the less-conjugated character of **14** [6b]). The value of the $\tilde{\nu}$(C=O) band of **14** represents a decrease of 18 cm^{-1} compared to the parent capsanthone (**13**). This decrease and the frequency of the OH band (3421 cm^{-1}) refers

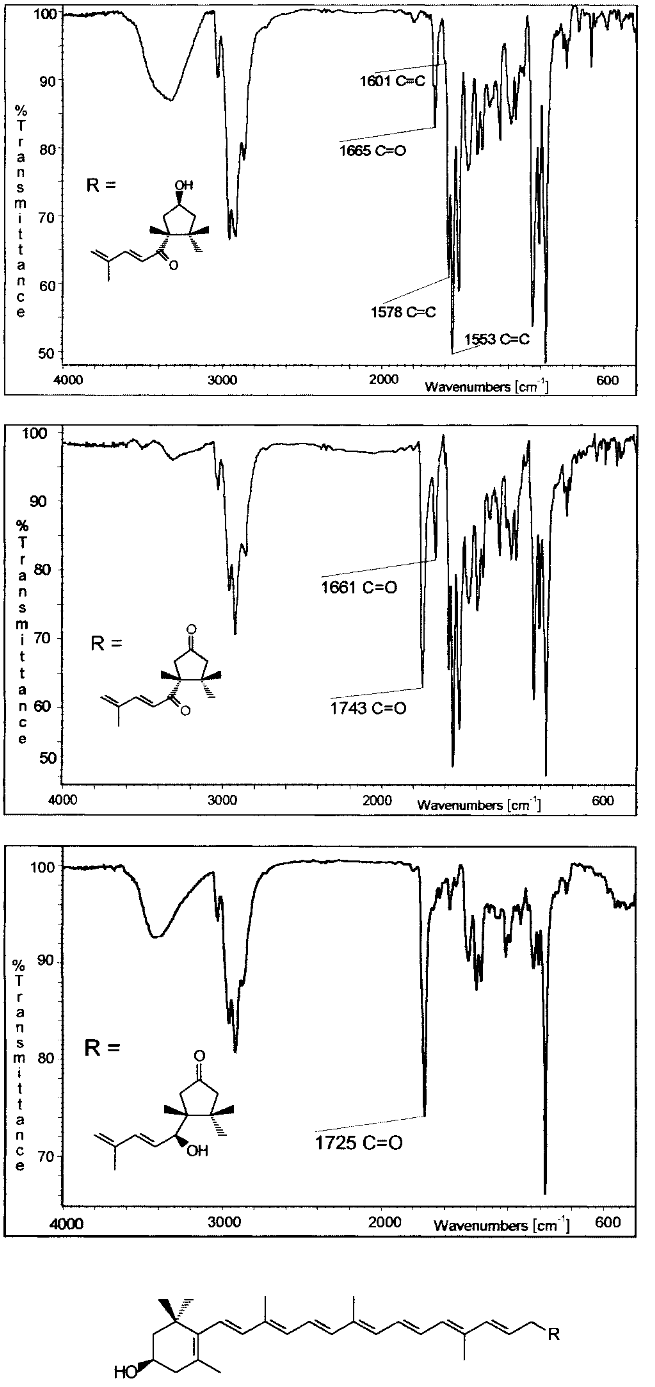

Figure. *FT-IR Spectra of capsanthin* (**10**), *capsanthone* (**13**), *and (6′*S*)-capsanthol-3′-one* (**14**)[1]) to a weak H-bond in compound **14** [5e]. For the other stereoisomer, (6′*R*)-capsanthol-3′-one (**15**), similar absorption maxima are observed ($\tilde{\nu}$(C=O) 1729 and $\tilde{\nu}$(OH) 3461 cm^{-1}), but the changes compared to the parent **13** are somewhat smaller, indicating the presence of a weaker H-bond in this case.

In conclusion, we were able to follow some simple chemical reactions by means of the FT-IR spectroscopic method. This method allows the identification of some special functional groups present in the end groups of carotenoids, *e.g.* 'cross epoxides', furan rings, *etc.* Some general remarks can be made in connection with the features of the spectra studied. A special characteristic of the oxo-carotenoids is that the carbonyl stretching bands appear to be much weaker than in most of the carbonyl compounds. On the other hand, the lack of the carbonyl group leads to the decrease of the conjugated C=C absorptions. However, FT-IR spectroscopy has some limitations; *e.g.*, we were not able to assign the bands of the epoxide group in compounds **2** and **8**.

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Experimental Part

1. *General.* FT-IR Spectra: KBr pellets; *Impact-400* spectrometer (*Nicolet*); *DTGS* detector in the region of 400–4000 cm^{-1}, resolution 4 cm^{-1}; 0.2-mg to 0.5-mg samples; $\tilde{\nu}$ indicates stretching, δ bending, and γ out-of-plane bending vibrations; intensities v*s*, *s*, *m*, and *w* correspond to 75–100%, 50–75%, 20–50%, and 0–20%, resp.

2. *β-Citraurin* (= *(3*R*)-3-Hydroxy-8′-apo-β-caroten-8′-al*; **1**). NMR, CD, and MS: [7]. IR: 967v*s* (γ(=CH), C=C *trans*), 1040*m* ($\tilde{\nu}$(C–O)), 1358*m* ($\delta_s(CH_3)$), 1380*m* ($\delta_s(CH_3)$), 1444*m* ($\delta_{as}(CH_3)$), 1567*m* ($\tilde{\nu}$(C=C)), 1610v*s* ($\tilde{\nu}$(C=C)), 1668 (v*s* $\tilde{\nu}$(C=O)), 2715*w* ($\tilde{\nu}$(C(O)H)), 2831*w* ($\tilde{\nu}_s(CH_2)$), 2864*m* ($\tilde{\nu}_s(CH_3)$), 2918*m* ($\tilde{\nu}_{as}(CH_2)$), 2956*m* ($\tilde{\nu}_{as}(CH_3)$), 3030*w* ($\tilde{\nu}$(=CH)), 3341*m* ($\tilde{\nu}$(OH)).

3. *Semi-β-carotenone 5,6-Epoxide* (= *5,6-Diepoxy-5,6-dihydro-5′,6′-seco-β,β-carotene-5′,6′-dione*; **2**). NMR, CD, and MS: [8][9]. IR: 967*s* (γ(=CH), C=C *trans*), 1363*m* ($\delta_s(CH_3)$), 1387*m* ($\delta_s(CH_3)$), 1438*m* ($\delta_{as}(CH_3)$), 1458*m* ($\delta_{as}(CH_3)$), 1559*s* ($\tilde{\nu}$(C=C)), 1583*m* ($\tilde{\nu}$(C=C)), 1655*m* ($\tilde{\nu}$(C=C)), 1672*m* ($\tilde{\nu}$(C=O), conj), 1716v*s* ($\tilde{\nu}$(C=O), nonconj.), 2852*s* ($\tilde{\nu}_s(CH_2)$), 2868*m* ($\tilde{\nu}_s(CH_3)$), 2923v*s* ($\tilde{\nu}_{as}(CH_2)$), 2953*s* ($\tilde{\nu}_{as}(CH_3)$), 3024*w* ($\tilde{\nu}$(=CH)).

4. *Capsorubin* (= *(*all-E*,3*S*,3′*S*,5*R*,5′*R*)-3,3′-Dihydroxy-κ,κ-carotene-6,6′-dione*; **3**). NMR, CD, and MS: [7]. IR: 961*m* (γ(=CH), C=C *trans*), 1051*s* ($\tilde{\nu}$(C–O)), 1375*m* ($\delta_s(CH_3)$), 1388*m* ($\delta_s(CH_3)$), 1454*m* ($\delta_{as}(CH_3)$), 1544v*s* ($\tilde{\nu}$(C=C)), 1583*m* (ν(C=C)), 1665*m* ($\tilde{\nu}$(C=O)), 2873*w* ($\tilde{\nu}_s(CH_3)$, $\tilde{\nu}_s(CH_2)$), 2936*m* ($\tilde{\nu}_{as}(CH_2)$), 2958*m* ($\tilde{\nu}_{as}(CH_3)$), 3036*w* ($\tilde{\nu}$(=CH), 3433*w* ($\tilde{\nu}$(OH)).

5. *Cycloviolaxanthin* (= *(*all-E*,3*S*,3′*S*,5*R*,5′*R*,6*R*,6′*R*)-3,6:3′,6′-Diepoxy-5,5′,6,6′-tetrahydro-β,β-carotene-5,5′-diol*; **4**). NMR, CD, and MS: [10]. IR: 965v*s* (γ(=CH), C=C *trans*), 1034*w* ($\tilde{\nu}$(C–O)), 1100*m* ($\tilde{\nu}_{as}$(C–O–C)), 1216*m* ($\tilde{\nu}(C(CH_3)_2)$), 1365*m* ($\delta_s(CH_3)$), 1386*w* ($\delta_s(CH_3)$), 1465*w* ($\delta_{as}(CH_3)$), 1479*w* ($\delta_{as}(CH_3)$), 1567*w* ($\tilde{\nu}$(C=C)), 1631*w* ($\tilde{\nu}$(C=C)), 2868*m* ($\tilde{\nu}_s(CH_3)$, $\tilde{\nu}_s(CH_2)$), 2920*m* ($\tilde{\nu}_{as}(CH_2)$), 2953*m* ($\tilde{\nu}_{as}(CH_3)$), 2980*m* ($\tilde{\nu}_{as}(CH_3)$), 3034*w* ($\tilde{\nu}$(=CH)), 3441*m* ($\tilde{\nu}$(OH)).

6. *Cucurbitaxanthin A* (= *(*all-E*,3*S*,3′*R*,5*R*,6*R*)-3,6-Epoxy-5,6-dihydro-β,β-carotene-3′,5-diol*; **5**). NMR, CD, and MS: [10]. IR: 964v*s* (γ(=CH), C=C *trans*), 1034*m* ($\tilde{\nu}$(C–O)), 1107*w* ($\tilde{\nu}_{as}$(C–O–C)), 1157*w* ($\tilde{\nu}(C(CH_3)_2$), 1217*w* ($\tilde{\nu}C(CH_3)_2$), 1366*m* ($\delta_s(CH_3)$), 1390*w* ($\delta_s(CH_3)$), 1445*m* ($\delta_{as}(CH_3)$), 1462*m* ($\delta_{as}(CH_3)$), 1565*w* ($\tilde{\nu}$(C=C)), 2866*s* ($\tilde{\nu}_s(CH_3)$, $\tilde{\nu}_s(CH_2)$), 2919*s* ($\tilde{\nu}_{as}(CH_2)$), 2954*m* ($\tilde{\nu}_{as}(CH_3)$), 3028*w* ($\tilde{\nu}$(=CH)), 3432*m* ($\tilde{\nu}$(OH).

7. *Mutatoxanthin* (= *(*all-E*,3*S*,3′*R*,5*R*,8*S*)-5,8-Epoxy-5,8-dihydro-β-β-carotene-3,3′-diol*; **6**). NMR, CD, and MS: [11]. IR: 965v*s* (γ(=CH), C=C *trans*), 1038*m* ($\tilde{\nu}$(C–O)), 1169*m* ($\tilde{\nu}(C(CH_3)_2$), 1206*m* ($\tilde{\nu}(C(CH_3)_2$), 1367*m* ($\delta_s(CH_3)$), 1387*m* ($\delta_s(CH_3)$), 1445*m* ($\delta_{as}(CH_3)$), 1570*w* ($\tilde{\nu}$(C=C)), 1650*w* ($\tilde{\nu}$(C=C)), 2850*s* ($\tilde{\nu}_s(CH_3)$, $\tilde{\nu}_s(CH_2)$), 2918v*s* ($\tilde{\nu}_{as}(CH_2)$), 2958*s* ($\tilde{\nu}_{as}(CH_3)$), 3026*w* ($\tilde{\nu}$(=CH)), 3074*w* (=CH of furan), 3336*m* ($\tilde{\nu}$(OH)), 3466*w* ($\tilde{\nu}$(OH)).

8. *Deoxylutein II* (= *(*all-E*,3*R*,6′*R*)-3′,4′-Didehydro-β,γ-caroten-3-ol*; **7**). NMR, CD, and MS: [12]. IR: 883*w* ($\gamma(=CH_2)$), 963v*s* (γ(=CH), C=C *trans*), 1364*m* ($\delta_s(CH_3)$), 1385*w* ($\delta_s(CH_3)$), 1447*m* ($\delta_{as}(CH_3)$), 1560*w*

($\tilde{\nu}(C{=}C)$), 1636*w* ($\tilde{\nu}(C{=}C)$), 2826*w* ($\tilde{\nu}_s(CH_2)$), 2865*m* ($\tilde{\nu}_s(CH_3)$), 2916*m* ($\tilde{\nu}_{as}(CH_2)$), 2959*m* ($\tilde{\nu}_{as}(CH_3)$), 3027*m* ($\tilde{\nu}(=CH)$, *trans*), 3083*w* ($\tilde{\nu}(=CH_2)$); 3311*w* ($\tilde{\nu}(OH)$).

9. *Neoxanthin* (=(3S,3′S,5R,5′R,6R,6′S,9Z)-*5′,6′-Epoxy-6,7-didehydro-5,5′,6,6′-tetrahydro-β,β-carotene-3,3′,5-triol*; (9*Z*)-**8**). NMR, CD, and MS: [7]. IR: 964v*s* ($\gamma(=CH)$, C=C *trans*), 1036*s* ($\tilde{\nu}(C{-}O)$), 1364*m* ($\delta_s(CH_3)$), 1377*m* ($\delta_s(CH_3)$), 1452*m* ($\delta_{as}(CH_3)$), 1539*w* ($\tilde{\nu}(C{=}C)$), 1561*w* ($\tilde{\nu}(C{=}C)$), 1570*w* ($\tilde{\nu}(C{=}C)$), 1927*w* ($\tilde{\nu}_{as}(C{=}C{=}C)$), 2868*m* ($\tilde{\nu}_s(CH_3)$, $\tilde{\nu}_s(CH_2)$), 2923*m* ($\tilde{\nu}_{as}(CH_2)$), 2959v*s* ($\tilde{\nu}_{as}(CH_3)$), 3029*w* ($\tilde{\nu}(=CH)$), 3367*m* ($\tilde{\nu}(OH)$).

10. *Neochrome* (=(3S,3′S,5R,5′R,6R,8′S,9Z)-*5′,8′-Epoxy-6,7-didehydro-5,5′,6,6′-tetrahydro-β,β-carotene-3,3′,5-triol*; (9*Z*)-**9**). NMR, CD, and MS: [7]. IR: 965*m* ($\gamma(=CH)$, C=C *trans*), 1046*m* ($\tilde{\nu}(C{-}O)$), 1365*w* ($\delta_s(CH_3)$), 1377*w* ($\delta_s(CH_3)$), 1450*w* ($\delta_{as}(CH_3)$), 1471*m* ($\delta_{as}(CH_3)$), 1651*w* ($\tilde{\nu}(C{=}C)$), 1929*w* ($\nu_{as}(C{=}C{=}C)$), 2850*s* ($\tilde{\nu}_s(CH_3)$, $\tilde{\nu}_s(CH_2)$), 2918v*s* ($\tilde{\nu}_{as}(CH_2)$), 2957*s* ($\tilde{\nu}_{as}(CH_3)$), 3028*w* ($\tilde{\nu}(=CH)$), 3410*m* ($\tilde{\nu}(OH)$).

11. *Capsanthin* (=(all-E,3R,3′S,5′R)-*3,3′-Dihydroxy-β,κ-caroten-6′-one*; **10**). NMR, CD, and MS: [7]. IR: 964v*s* ($\gamma(=CH)$, C=C *trans*), 1049v*s* ($\tilde{\nu}(C{-}O)$), 1184*m* ($\tilde{\nu}(C(CH_3)_2)$), 1254*m* ($\tilde{\nu}(C(CH_3)_2)$), 1365*m* ($\delta_s(CH_3)$), 1397*m* ($\delta_s(CH_3)$), 1455*m* ($\delta_{as}(CH_3)$), 1553v*s* ($\nu(C{=}C)$), 1578*s* ($\nu(C{=}C)$), 1601*w* ($\tilde{\nu}(C{=}C)$), 1665*m* ($\tilde{\nu}(C{=}O)$), 2867*m* ($\tilde{\nu}_s(CH_3)$, $\nu_s(CH_2)$), 2917*s* ($\tilde{\nu}_{as}(CH_2)$), 2956*s* ($\tilde{\nu}_{as}(CH_3)$), 3028*w* ($\tilde{\nu}(=CH)$), 3329*m* ($\tilde{\nu}(OH)$).

12. *7′,8′-Dihydrocapsanthin* (=(all-E,3R,3′S,5′R)-*7′,8′-Dihydro-3,3′-dihydroxy-β,κ-caroten-6′-one*; **11**). NMR, CD, and MS: [13]. IR: 970v*s* ($\tilde{\gamma}(=CH)$, C=C *trans*), 1045v*s* ($\tilde{\nu}(C{-}O)$), 1175*s* ($\tilde{\nu}(C(CH_3)_2$), 1207*s* ($\tilde{\nu}(C(CH_3)_2$), 1370*s* ($\delta_s(CH_3)$), 1458*s* ($\delta_{as}(CH_3)$), 1632*w* ($\tilde{\nu}(C{=}C$), 1695v*s* ($\nu(C{=}O)$), 2873*s* ($\tilde{\nu}_s(CH_3)$, $\nu_s(CH_2)$), 2933v*s* ($\tilde{\nu}_{as}(CH_2)$), 2961v*s* ($\tilde{\nu}_{as}(CH_3)$), 3031*w* ($\tilde{\nu}(=CH)$), 3340*m* ($\tilde{\nu}(OH)$), 3470*m* ($\tilde{\nu}(OH)$).

13. *Capsanthol* (=*β,κ-Carotene-3,3′,6′-triol*; **12**). NMR, CD, and MS: [14]. IR: 959v*s* ($\gamma(=CH)$, C=C *trans*), 1031*m* ($\tilde{\nu}(C{=}O)$), 1206*w* ($\tilde{\nu}(C(CH_3)_2)$), 1362*m* ($\delta_s(CH_3)$), 1394*m* ($\delta_s(CH_3)$), 1446*m* ($\delta_{as}(CH_3)$), 1465*m* ($\delta_{as}(CH_3)$), 1561*w* ($\tilde{\nu}(C{=}C)$), 2867*m* ($\tilde{\nu}_s(CH_3)$, $\nu_s(CH_2)$), 2918*s* ($\tilde{\nu}_{as}(CH_2)$), 2953*m* ($\tilde{\nu}_{as}(CH_3)$), 3026*w* ($\tilde{\nu}(=CH)$), 3330*m* ($\tilde{\nu}(OH)$).

14. *Capsanthone* (=(all-E,3R,5′R)-*3-Hydroxy-β,κ-carotene-3′,6′-dione*; **13**). NMR, CD, and MS: [15]. IR: 965v*s* ($\gamma(=CH)$, C=C *trans*), 1186*m* ($\tilde{\nu}(C(CH_3)_2)$), 1213*m* ($\tilde{\nu}(C(CH_3)_2)$), 1364*m* ($\delta_s(CH_3)$), 1397*m* ($\delta_s(CH_3)$), 1450*m* ($\delta_{as}(CH_3)$), 1552v*s* ($\tilde{\nu}(C{=}C)$), 1576*s* ($\tilde{\nu}(C{=}C)$), 1661 (*m*, $\tilde{\nu}(C{=}O)$, conj.), 1743*s* ($\tilde{\nu}(C{=}O)$, nonconj.), 2852*m* ($\tilde{\nu}_s(CH_2)$, $\nu_s(CH_3)$), 2917*s* ($\tilde{\nu}_{as}(CH_2)$), 2957*m* ($\tilde{\nu}_{as}(CH_3)$), 3025*w* ($\tilde{\nu}(=CH)$).

15. *(6′S)-Capsanthol-3′-one* (=(all-E,3R,5′R,6′S)-*3,6′-Dihydroxy-β,κ-caroten-3′-one*; **14**). NMR, CD, and MS: [14]. IR: 965v*s* ($\gamma(=CH)$, C=C *trans*), 1038*m* ($\tilde{\nu}(C{-}O)$), 1187*m* ($\tilde{\nu}(C(CH_3)_2)$), 1212*m* ($\tilde{\nu}(C(CH_3)_2)$), 1367*m* ($\delta_s(CH_3)$), 1446*m* ($\delta_{as}(CH_3)$), 1564*w* ($\tilde{\nu}(C{=}C)$), 1725*s* ($\tilde{\nu}(C{=}O)$), 2871*m* ($\tilde{\nu}_s(CH_3)$, $\nu_s(CH_2)$), 2918*s* ($\tilde{\nu}_{as}(CH_2)$), 2958*m* ($\tilde{\nu}_{as}(CH_3)$), 3027*w* ($\tilde{\nu}(=CH)$), 3421*w* ($\tilde{\nu}(OH)$).

16. *(6′R)-Capsanthol-3′-one* (=(all-E,3R,5′R,6′R)-*3,6′-Dihydroxy-β,κ-caroten-3′-one*; **15**). NMR, CD, and MS: [19]. IR: 965v*s* ($\gamma(=CH)$, C=C *trans*), 1046*m* ($\tilde{\nu}(C{-}O)$), 1184*w* ($\tilde{\nu}(C(CH_3)_2)$), 1220*m* ($\tilde{\nu}(C(CH_3)_2)$), 1362*m* ($\delta_s(CH_3)$), 1375*m* ($\delta_s(CH_3)$), 1461*w*, ($\delta_{as}(CH_3)$), 1561*w* ($\tilde{\nu}(C{=}C)$), 1729*s* ($\tilde{\nu}(C{=}O)$), 2850*m* ($\tilde{\nu}_s(CH_2)$), 2875*m* ($\tilde{\nu}_s(CH_3)$), 2918*m* ($\tilde{\nu}_{as}(CH_2)$), 2954*m* ($\tilde{\nu}_{as}(CH_3)$), 3025*w* ($\tilde{\nu}(=CH)$), 3461*w* ($\tilde{\nu}(OH)$).

17. *7′,8′-Dihydrocapsanthol* (=*7′,8′-Dihydro-β,κ-carotene-3,3′,6′-triol*; **16**). NMR, CD, and MS: [18]. IR: 964v*s* ($\gamma(=CH)$, C=C *trans*), 1040*s* ($\tilde{\nu}(C{-}O)$), 1171*w* ($\tilde{\nu}(C(CH_3)_2)$), 1206*w* ($\tilde{\nu}(C(CH_3)_2)$), 1364*m* ($\delta_s(CH_3)$), 1375*m* ($\delta_s(CH_3)$), 1445*m* ($\delta_{as}(CH_3)$), 1573*w* ($\tilde{\nu}(C{=}C)$), 1630*w* ($\tilde{\nu}(C{=}C)$), 2864*m* ($\tilde{\nu}_s(CH_3)$, $\tilde{\nu}(CH_2)$), 2920v*s* ($\tilde{\nu}_{as}(CH_2)$), 2950v*s*, ($\nu_{as}(CH_3)$), 3029*w* ($\tilde{\nu}(=CH)$), 3331*m* ($\tilde{\nu}(OH)$).

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