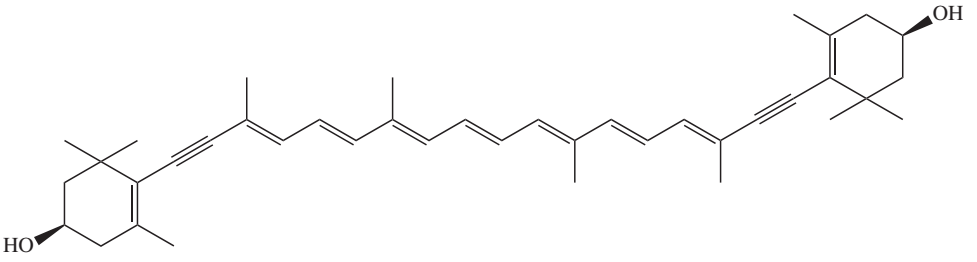
3 Xanthophylls

Alloxanthin

Recommended abbreviation: Allo (Al)

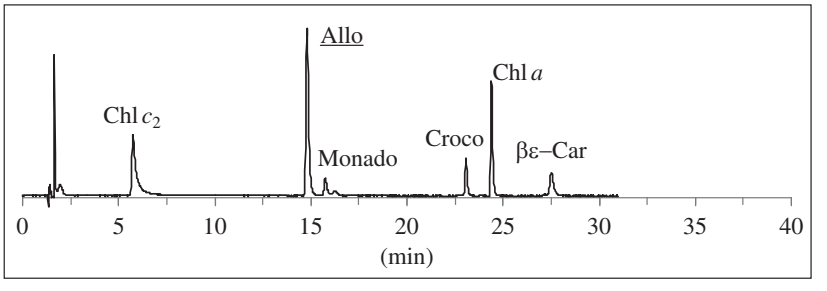
IUPAC: (3*R*,3′*R*)-7,8,7′,8′-Tetradehydro-β,β-carotene-3,3′-diol

Molecular formula: $C_{40}H_{52}O_2$ **Molecular weight:** 564.84

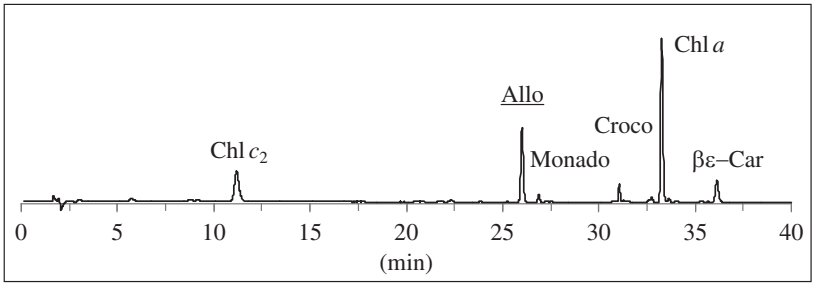


Biological occurrence	Major in cryptophytes, found in two chlorophytes (see Chapter 1, this volume)
Source culture	*Chroomonas salina* (cryptophyte)
Alteration products	Easily isomerizes to the more stable 9,9′-di*cis* isomer [43]
Biosynthetically related to	Diadino
Occurs together with	Chl c_2, βε-Car, Croco, Monado

HPLC chromatogram of *Chroomonas salina* (system 1)



HPLC chromatogram of *Rhodomonas baltica* (system 2)

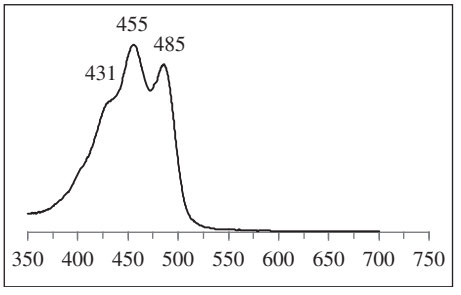


UV-Vis spectra (see also reference spectra below)

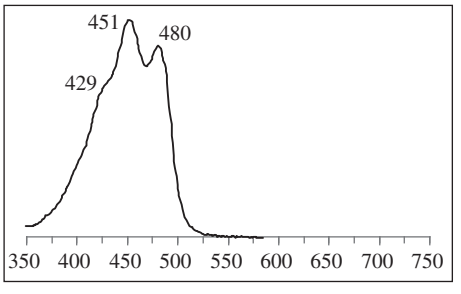
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(428), *454*, 484	50	[145]
Diethyl ether	(430), *451*, 481	44	[133]
Ethanol	(427), *450*, 478	29	[87]
Hexane	(427), *451*, 480	n.d.	[37]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		216 (at 464 nm, in benzene) [43] 250 (at 454 nm, in acetone) [109]	

Reference spectra

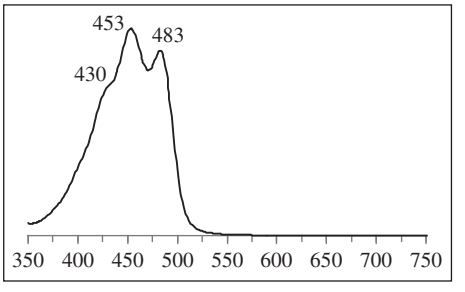
In acetone



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	564.398 $[M]^+$ (50), 549 $[M\text{-}15]^+$ (1), 546 $[M\text{-}18]^+$ (1), 119 (14), 105 (18), 91 (25), 41 (100)	[43]

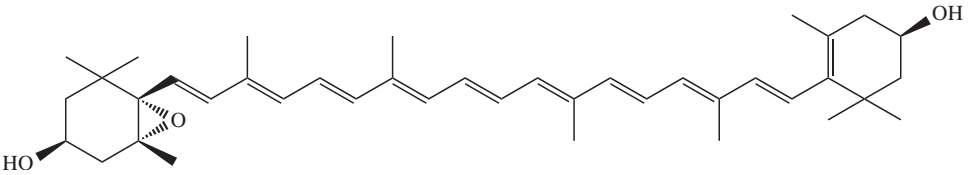
Remarks

Antheraxanthin

Recommended abbreviation: Anth (An)

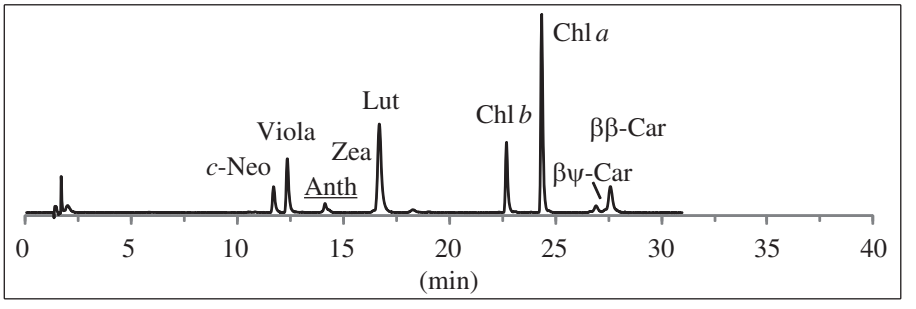
IUPAC: (3*S*,5*R*,6*S*,3′*R*)-5,6-Epoxy-5,6-dihydro-β,β-carotene-3,3′-diol

Molecular formula: $C_{40}H_{56}O_3$ **Molecular weight:** 584.87

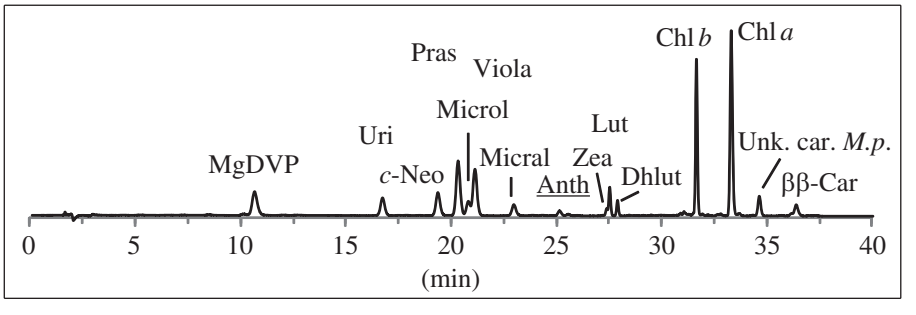


Biological occurrence	Minor pigment in chlorophytes, prasinophytes, trebouxiophytes, mesostigmatophytes, chlorarachniophytes, and some chrysophytes and eustigmatophytes. Also found in seaweeds and plants. Major in anthers of some flowers [78]
Source culture	*Dunaliella tertiolecta* (chlorophyte)
Alteration products	Undergoes rearrangement to Mutato in weakly acidic solutions. *Cis*-isomers
Biosynthetically related to	Biosynthetic intermediate between Zea and Viola
Occurs together with	Zea, Viola

HPLC chromatogram of *Dunaliella tertiolecta* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)

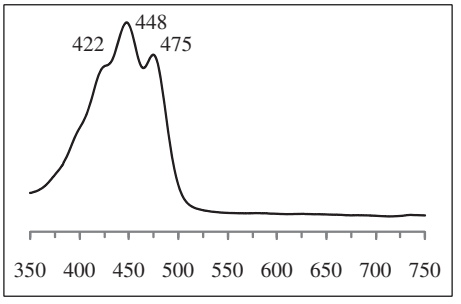


UV-Vis spectra (see also reference spectra below)

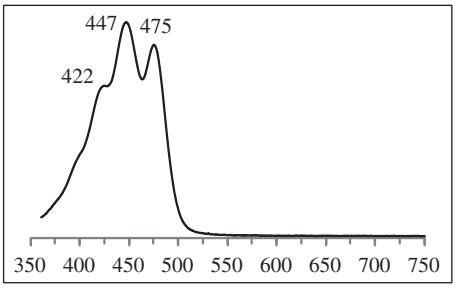
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(422), *448*, 475	29	[72]
Ethanol	422, *444*, 472	54	[152]
Hexane	420, *444*, 472	n.d.	[85]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		235 (at 446 nm, ethanol)	[84]

Reference spectra

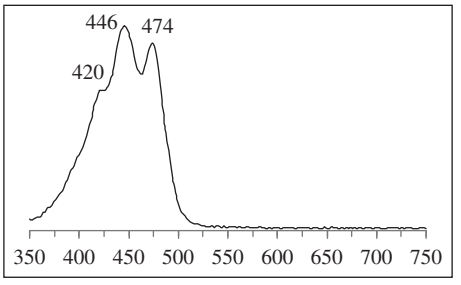
In acetone



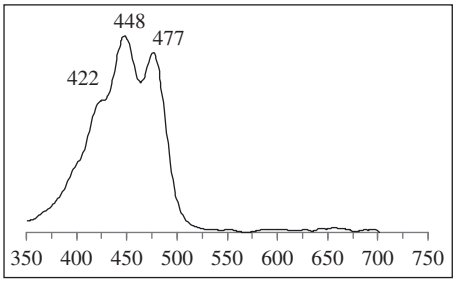
In ethanol



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	584 $[M]^+$ (60), 504 $[M-80]^+$ (30), 492 $[M-92]^+$ (6), 221 (30), 181 (10), 43 (100)	[127]

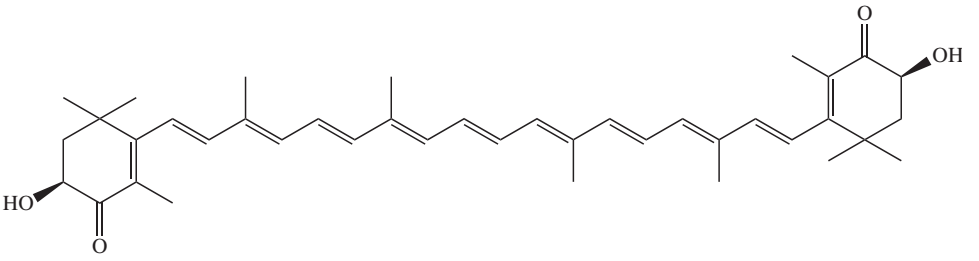
Remarks Part of a 'xanthophyll cycle' (see Chapter 11, this volume). May be present in diatoms under prolonged high light stress [123]

Astaxanthin

Recommended abbreviation: Asta (As)

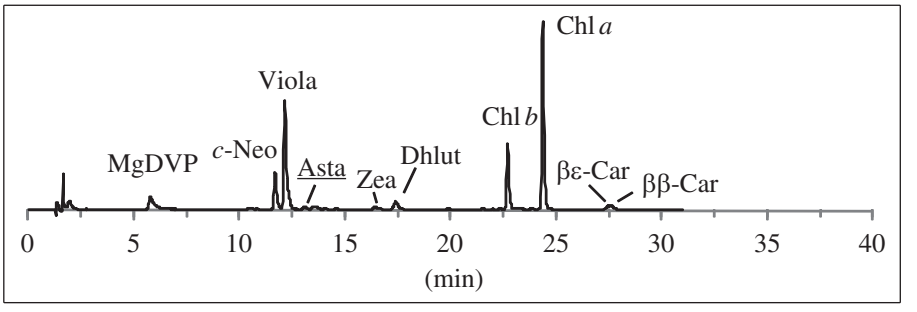
IUPAC: (3*S*,3′*S*)-3,3′-Dihydroxy-β,β-carotene-4,4′-dione

Molecular formula: $C_{40}H_{52}O_4$ **Molecular weight:** 596.84

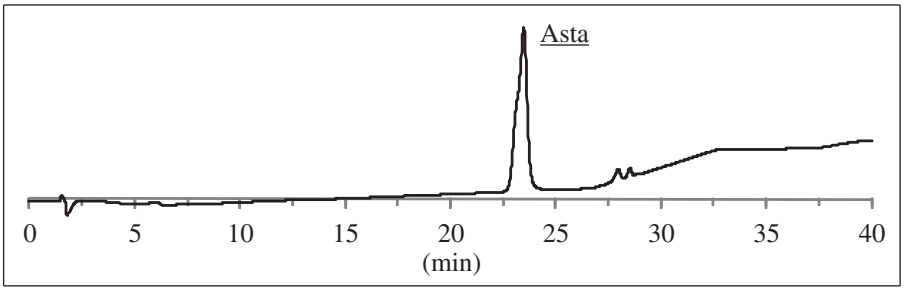


Biological occurrence	Present in some chlorophytes, but major (mainly as mono- and diesters of fatty acids) in some of these upon nitrogen starvation. Major in salmonids and crustaceans [78, 79]
Source culture	Synthetic (see Appendix E, this volume)
Alteration products	*Cis*-isomers; astacene (oxidation product)
Biosynthetically related to	Zea, Cantha
Occurs together with	

HPLC chromatogram of *Pycnococcus provasolii* (system 1)



HPLC chromatogram of synthetic astaxanthin (system 2)

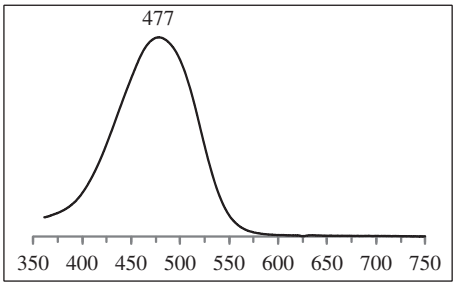


UV-Vis spectra (see also reference spectra below)

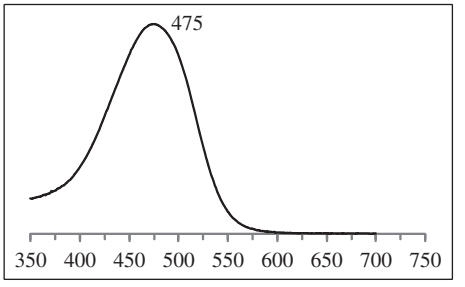
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	475	-	[82]
Ethanol	476	-	[33]
Hexane	466–467	-	[41]
Methanol	470–472	-	[41]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		206 (at 473 nm, methanol)	[79]

Reference spectra

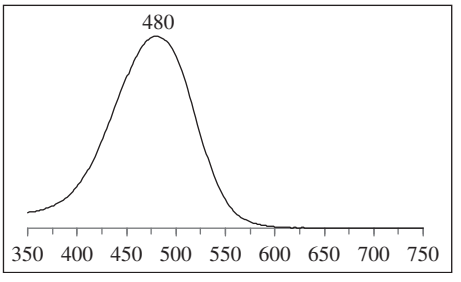
In acetone



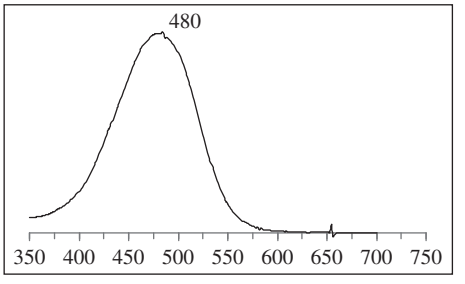
In methanol



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

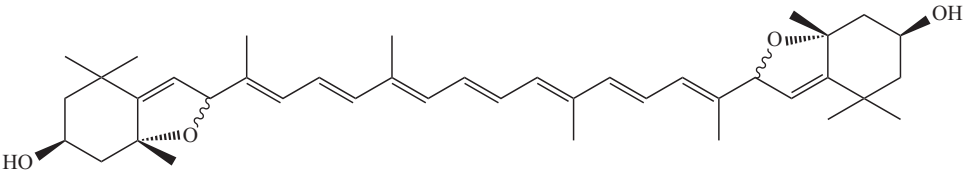
Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	596 $[M]^+$ (7), 580 $[M\text{-}16]^+$ (9), 564 $[M\text{-}16\text{–}16]^+$ (6), 133 (56), 109 (24), 91 (100)	[55]
Remarks	Mixtures of (3*S*,3′*S*), (3*R*,3′*R*) and (3*R*,3′*S*)-Asta are common in aquatic animals [15]. Esterification will change polarity and hence retention time		

Auroxanthin

Recommended abbreviation: Auro (Au)

IUPAC: (3*S*,5*R*,8*RS*,3′*S*,5′*R*,8′*RS*)-5,8:5′,8′-Diepoxy-5,8,5′,8′-tetrahydro-β,β-carotene-3,3′-diol

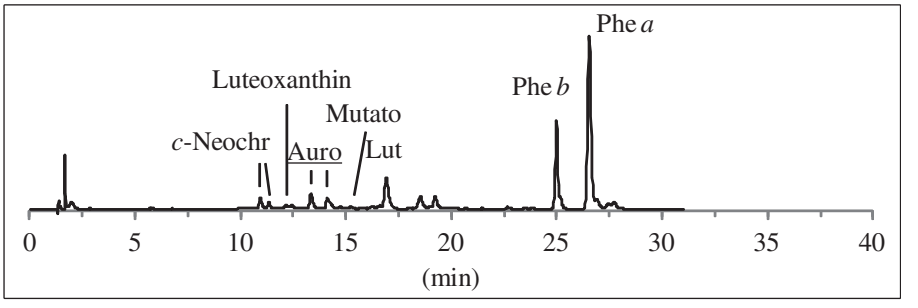
Molecular formula: $C_{40}H_{56}O_4$ **Molecular weight:** 600.87



(Always occurs as a mixture of the three (3*S*,5*R*,8*R*,3′*S*,5′*R*,8′*R*), (3*S*,5*R*,8*R*,3′*S*,5′*R*,8′*S*) and (3*S*,5*R*,8*S*,3′*S*,5′*R*,8′*S*) optical isomers)

Alteration product of	Viola. The acid-catalysed rearrangement occurs in slightly acidic extracts, especially in prasinophyte extracts [91]
Source culture	*Dunaliella tertiolecta* (chlorophyte)
Alteration products	*Cis*-isomers
Synthetically related to	Viola
Occurs together with	Luteoxanthin, Neochr

HPLC chromatogram of acidified *Dunaliella tertiolecta* (system 1)



HPLC chromatogram (system 2)

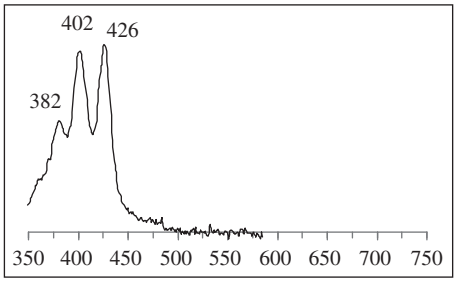
NO DATA AVAILABLE

UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	380, 401, *425*	125	[51]
Ethanol	379, *400*, 425	92	[136]
Hexane	380, 400, 425	n.d.	[167]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		181 (at 403 nm, ethanol) [114]	

Reference Spectra

In HPLC solvent system 1



In HPLC solvent system 2

NO DATA AVAILABLE

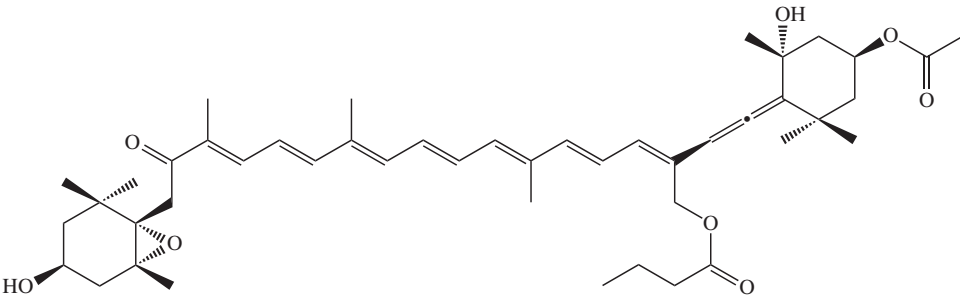
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	600 $[M]^+$ (44), 584 $[M\text{-}16]^+$ (22), 582 $[M\text{-}18]^+$ (11), 568 $[M\text{-}16\text{–}16]^+$ (12), 221 (100), 181 (68)	[51]
Remarks	Turns green on silica TLC (partly ionised to a blue oxonium ion)		

19′-Butanoyloxyfucoxanthin **Recommended abbreviation: But-fuco (BF)**

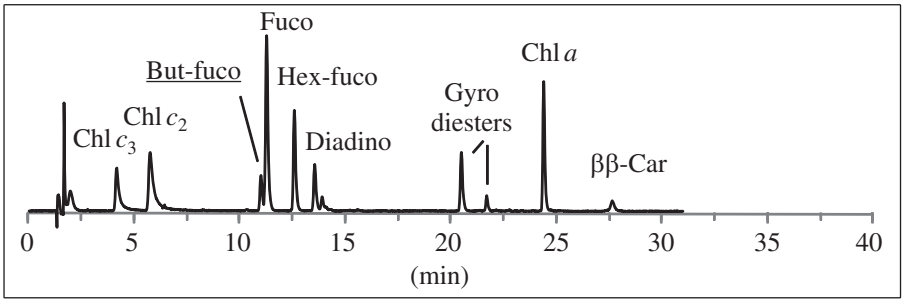
IUPAC: (3*S*,5*R*,6*S*,3′*S*,5′*R*,6′*R*)-19′-Butanoyloxy-5,6-epoxy-3′-ethanoyloxy-3,5′-dihydroxy-6′,7′-didehydro-5,6,7,8,5′,6′-hexahydro-β,β-caroten-8-one

Molecular formula: $C_{46}H_{64}O_8$ **Molecular weight:** 745.00

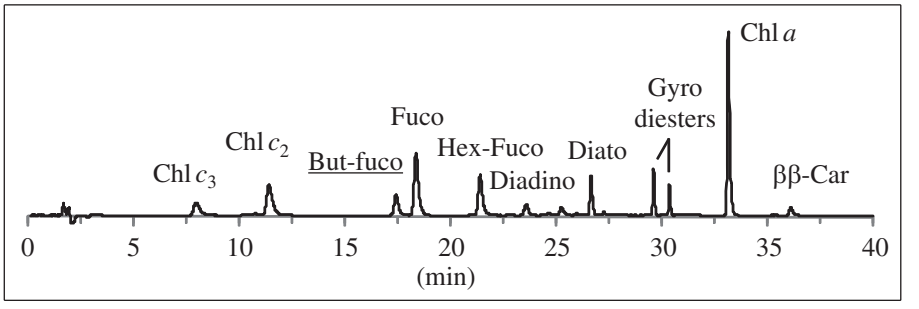


Biological occurrence	Dominant pigment in pelagophytes and dictyochophytes. Also present in some haptophytes; trace amounts in dinoflagellates Pigment Type 2 (see Chapter 1)
Source culture	*Pelagococcus subviridis* (pelagophyte)
Alteration products	*Cis*-isomers
Biosynthetically related to	Fuco, Hex-fuco, and other alkanoyloxy-derivatives of Fuco
Occurs together with	Chl c_2, Fuco, Diato, Diadino

HPLC chromatogram of *Karlodinium micrum* (system 1)



HPLC chromatogram of *Karlodinium micrum* (system 2)



UV-Vis spectra (see also reference spectra below)

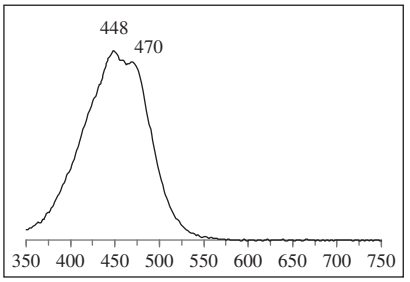
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(423), *446*, 472	37	[23]
Ethanol	*446*, 470	18	[173]
Hexane	(426), *446*, 473	57	[23]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks	

Reference spectra

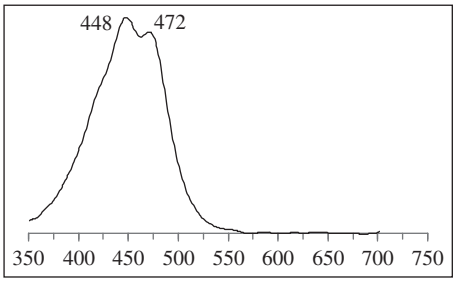
In acetone

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
APCI	Ion trap	767 $[M+Na]^+ \rightarrow$ 679 $[M+Na-88]^+ \rightarrow$ 661 $[M+Na-88-18]^+$, 619 $[M+Na-88-60]^+$, 525	[5]

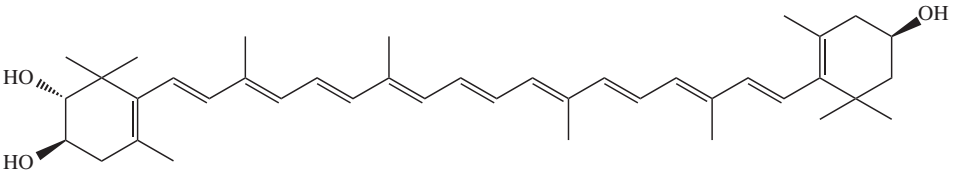
Remarks $d = 147$ L g^{-1} cm^{-1} (at 445 nm in acetone; calc. from Fuco) is recommended, as no value has been determined for But-fuco [109]. Several other, minor alkanoyloxyfucoxanthins have been reported [5]

Caloxanthin

Recommended abbreviation: Calo (Cal)

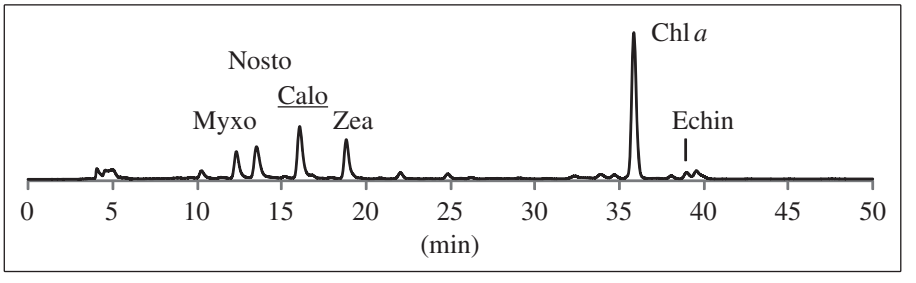
IUPAC: (2*R*,3*R*,3′*R*)-β,β -Carotene-2,3,3′-triol

Molecular formula: $C_{40}H_{56}O_3$ **Molecular weight:** 584.87



Biological occurrence	Major characteristic carotenoid from some cyanobacteria (Cyano-1, Chapter 1), e.g. *Anacystis nidulans* and *Chlorogloeopsis fritschii*
Source culture	*Chlorogloeopsis fritschii* (cyanobacteria)
Alteration products	*Cis*-isomers
Biosynthetically related to	ββ-Car, Zea, Nosto
Occurs together with	Nosto, Zea

HPLC chromatogram of a *Chlorogloeopsis fritschii* (system 3)



HPLC chromatogram (system 2)

NO DATA AVAILABLE

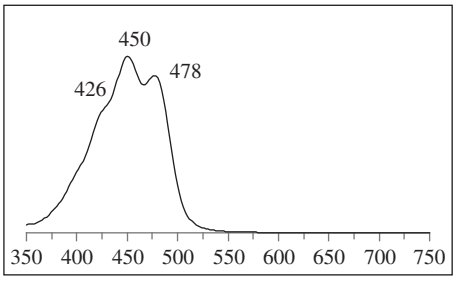
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(430), *454*, 481	n.d.	[33]
Ethanol	(425), *450*, 478	n.d.	[146]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

Reference spectra
In acetone

NO DATA AVAILABLE

In HPLC solvent system 3



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	584 $[M]^+$ (100), 566 $[M-18]^+$ (10), 492 $[M-92]^+$ (13), 478 $(M-106)^+$ (3), 133 (24), 91 (43), 83 (22), 62 (42)	[33]

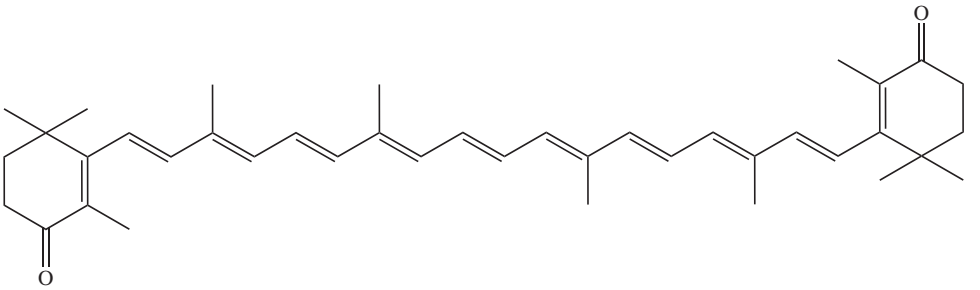
Remarks $d = 238\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in ethanol; calc. from Zea) is recommended, as no value has been determined for Calo

Canthaxanthin

Recommended abbreviation: Cantha (Ct)

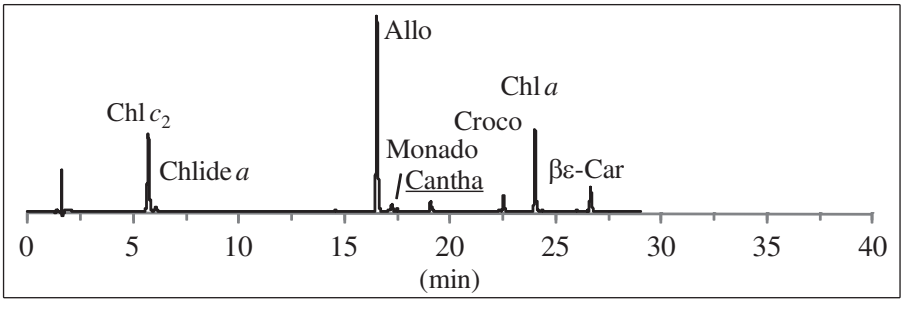
IUPAC: β,β-Carotene-4,4′-dione

Molecular formula: $C_{40}H_{52}O_2$ **Molecular weight:** 564.84

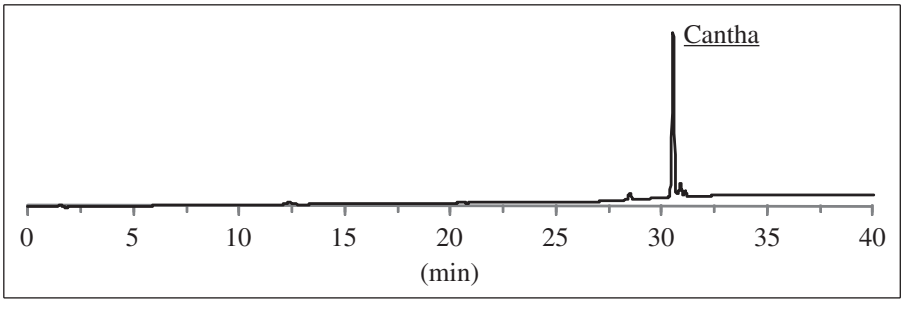


Biological occurrence	Minor or trace pigment in eustigmatophytes, cyanobacteria (Cyano-1) and some dinoflagellates. Detected in some cultures of chlorophytes, diatoms and prymnesiophytes. Major in some chlorophytes upon nitrogen starvation [78]
Source culture	Synthetic (see Appendix E, this volume)
Alteration products	*Cis*-isomers
Biosynthetically related to	ββ-Car, Echin, Asta
Occurs together with	

HPLC chromatogram of *Guillardia theta* – canthaxanthin: internal standard (system 1)



HPLC chromatogram of synthetic canthaxanthin (system 2)



UV-Vis spectra (see also reference spectra below)

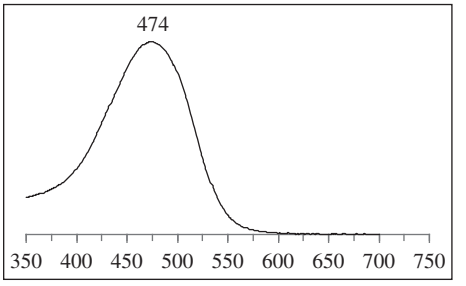
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	468	-	[82]
Ethanol	478	-	[135]
Hexane	468	-	[54]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		220 (at 469 nm, cyclohexane)	[155]

Reference spectra

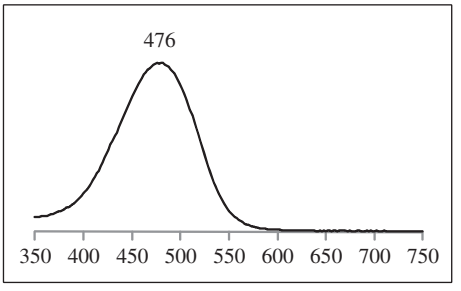
In acetone

For spectrum in acetone, see [109]

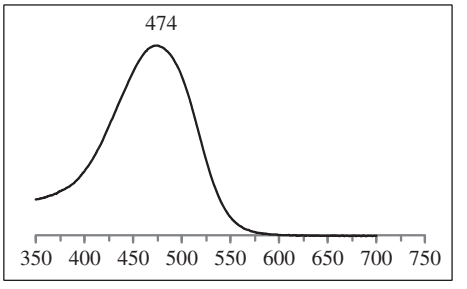
In methanol



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	564 $[M]^+$ (41), 562 $[M-2]^+$ (2), 472 $[M-92]^+$ (7), 458 $[M-106]^+$ (2), 91 (19), 83 (100)	[55]

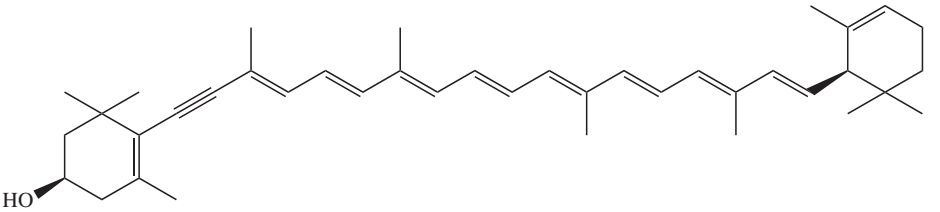
Remarks

Crocoxanthin

Recommended abbreviation: Croco (Co)

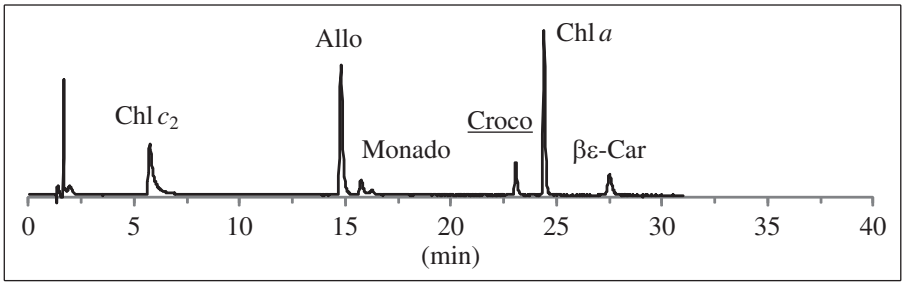
IUPAC: (3*R*,6′*R*)-7,8-Didehydro-β,ε-caroten-3-ol

Molecular formula: $C_{40}H_{54}O$ **Molecular weight:** 550.86

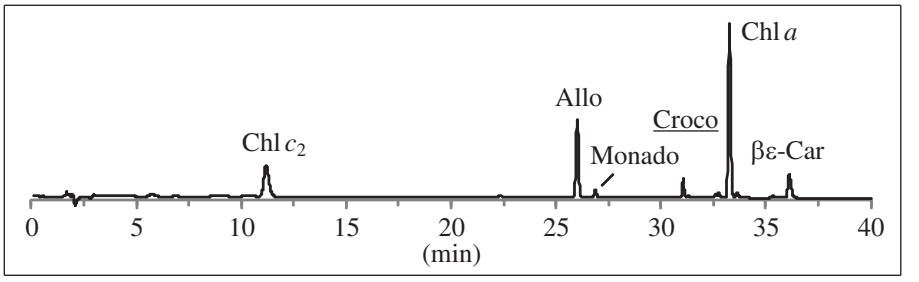


Biological occurrence	Cryptophytes only (minor carotenoid)
Source culture	*Chroomonas salina* (cryptophyte)
Alteration products	Easily isomerises to the more stable 9-*cis* isomer [43]
Biosynthetically related to	Monado
Occurs together with	Allo, Monado

HPLC chromatogram of *Chroomonas salina* (system 1)



HPLC chromatogram of *Rhodomonas baltica* (system 2)

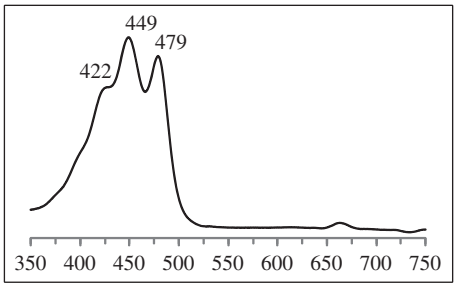


UV-Vis spectra (see also reference spectra below)

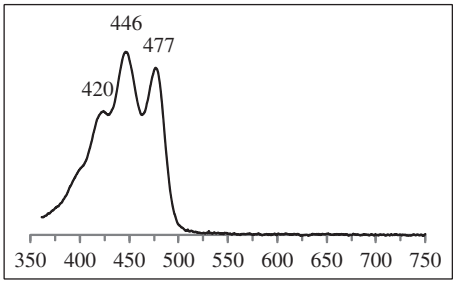
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Diethyl ether	428, *445*, 475	58	[133]
Ethanol	(421), *443*, 472	62	[87]
Hexane	422, *445*, 475	69	[35]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks	

Reference spectra

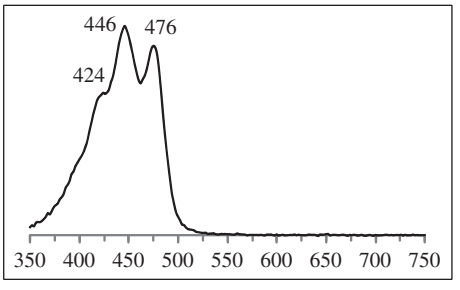
In acetone



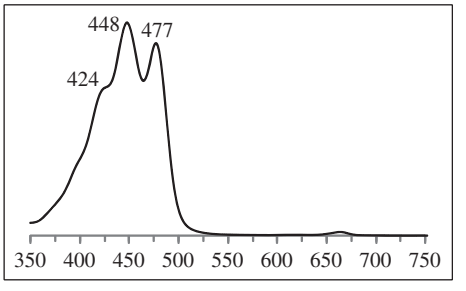
In hexane



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	550.421 $[M]^+$ (100), 535 $[M-15]^+$ (2), 532 $[M-18]^+$ (1), 494 $[M-56]^+$ (<1), 458 [M-92, 2], 444 [m*, 550 → 494], 119 (17), 105 (21), 92 (26)	[43]

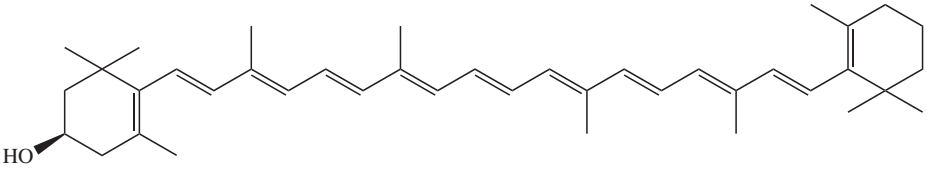
Remarks $d = 237\,L\,g^{-1}\,cm^{-1}$ (at 445 nm in hexane; calc. from Diadino) is recommended, as no value has been determined for Croco. In ethanol, use the value for β,β–carotene: $d = 250\,L\,g^{-1}\,cm^{-1}$ (at 443 nm) [45, 109]

Cryptoxanthin

Recommended abbreviation: Cryp (Cy)

IUPAC: (3*R*)-β,β-Caroten-3-ol

Molecular formula: $C_{40}H_{56}O$ **Molecular weight:** 552.87

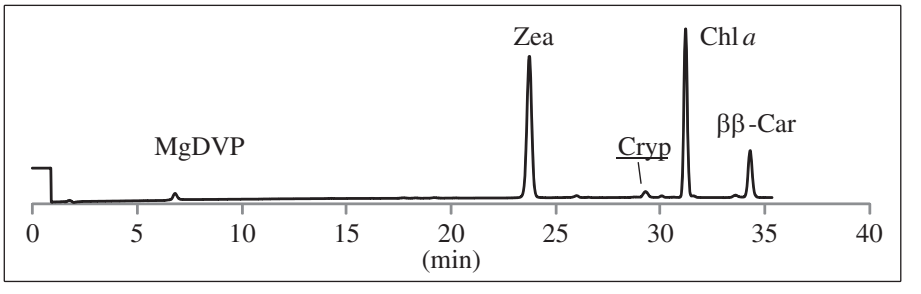


Biological occurrence	Dominant pigment in glaucocystophytes, minor pigment in some cyanobacteria (Cyano-1) and prochlorophytes (*Prochloron* spp., Cyano-3) (see Chapter 1, this volume)
Source culture	*Prochloron* spp.
Alteration products	*Cis*-isomers
Biosynthetically related to	The biosynthetic intermediate between ββ-Car and Zea
Occurs together with	ββ-Car, Zea

HPLC chromatogram (system 1)

NO DATA AVAILABLE

HPLC chromatogram of *Synechococcus* sp. (system 2)

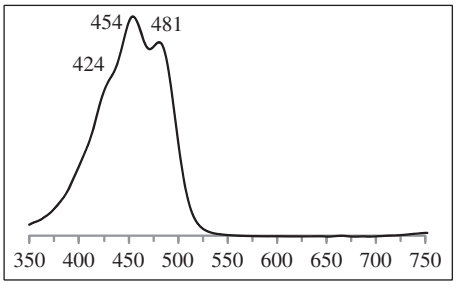


UV-Vis spectra (see also reference spectra below)

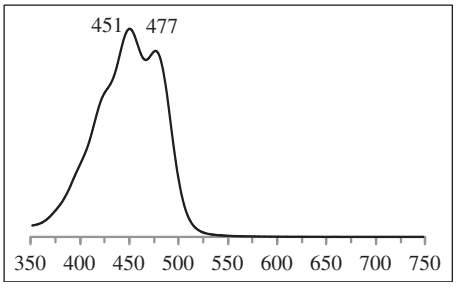
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(427), *450*, 475	n.d.	[64]
Ethanol	(428), *449*, 473	30	[86]
Hexane	(427), *452*, 478	43	[180]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		246 (at 452 nm, hexane) [180] 250 (at 452 nm, ethanol) [45]	

Reference spectra

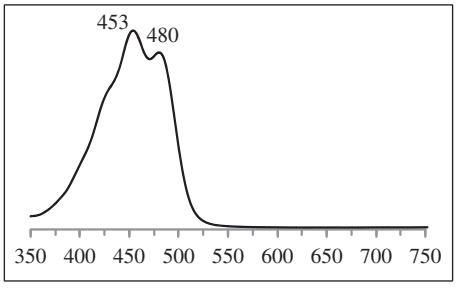
In acetone



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	552 $[M]^+$ (85), 550 $[M-2]^+$ (11), 534 $[M-18]^+$ (100), 460 $[M-92]^+$ (2), 442 $[M-18–92]^+$ (3), 267 $[M-18]^+$ (8), 105 (55)	[20]

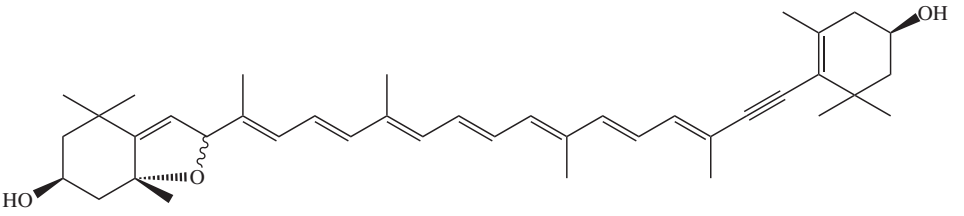
Remarks

Diadinochrome

Recommended abbreviation: Diadchr (Ddc)

IUPAC: (3*S*,5*R*,8*RS*,3′*R*)-5,8-Epoxy-7′,8′-didehydro-5,8-dihydro-β,β-carotene-3,3′-diol

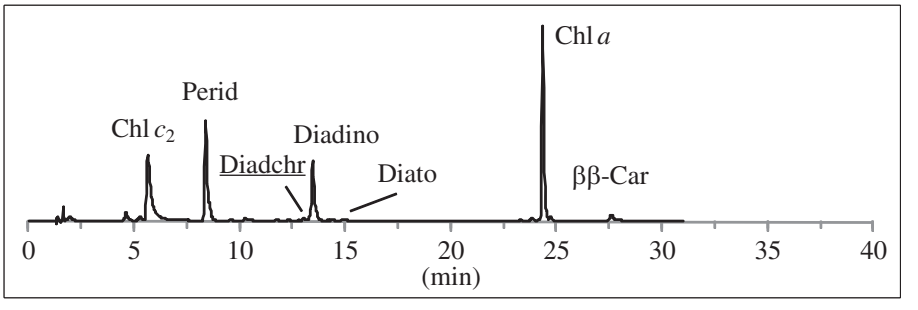
Molecular formula: $C_{40}H_{54}O_3$ **Molecular weight:** 582.85



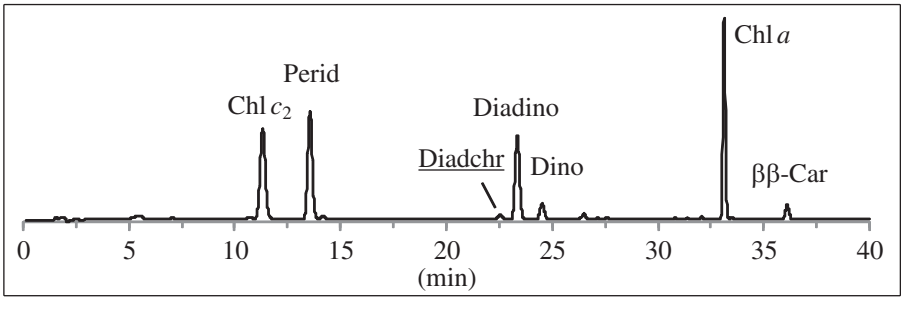
(Always occurs as a mixture of the two (3*S*,5*R*,8*R*,3′*R*) and (3*S*,5*R*,8*S*,3′*R*) optical isomers)

Alteration product of	Diadino. The acid-catalysed reaction occurs in slightly acidic extracts [91]
Source culture	*Amphidinium carterae* (dinoflagellate)
Alteration products	*Cis*-isomers
Synthetically related to	Diadino
Occurs together with	Diadino

HPLC chromatogram of *Amphidinium carterae* (system 1)



HPLC chromatogram of *Scrippsiella trochoidea* (system 2)



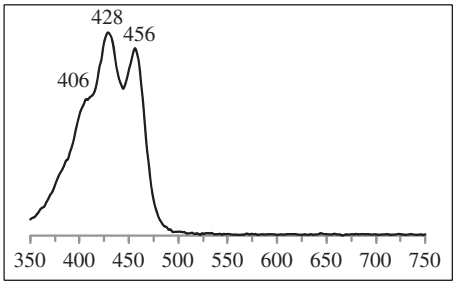
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	405, *427*, 454	48	[91]
Diethyl ether	(402), *425*, 452	n.d.	[60]
Ethanol	409, *430*, 457	n.d.	[53]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks	

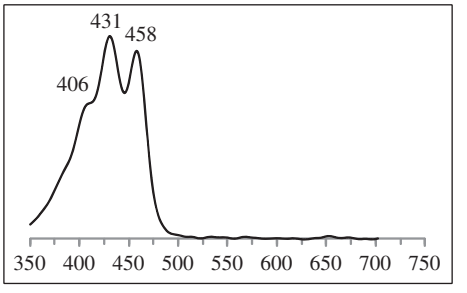
Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	582 $[M]^+$ (68), 580 $[M-2]^+$ (27), 566 $[M-16]^+$ (4), 564 $[M-18]^+$ (7), 502 $[M-80]^+$ (18), 243 (46), 221 (100), 181 (50), 165 (62)	[91]

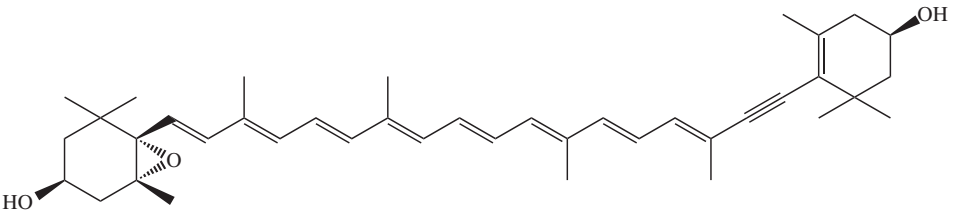
Remarks $d = 210\,L\,g^{-1}cm^{-1}$ (at 427 nm in acetone) is recommended, as no value has been determined for Diadchr

Diadinoxanthin

Recommended abbreviation: Diadino (Dd)

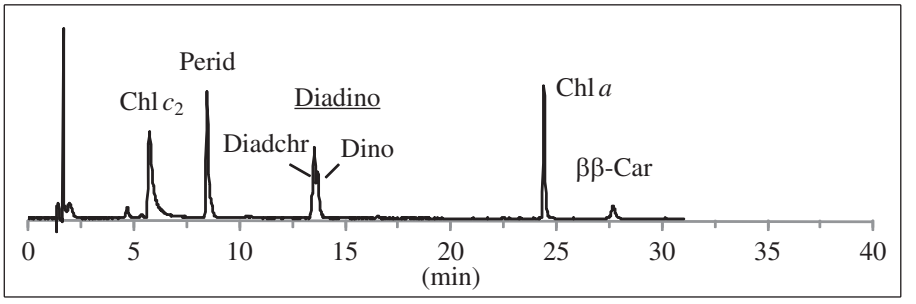
IUPAC: (3*S*,5*R*,6*S*,3′*R*)-5,6-Epoxy-7′,8′-didehydro-5,6-dihydro-β,β-carotene-3,3′-diol

Molecular formula: $C_{40}H_{54}O_3$ **Molecular weight:** 582.85

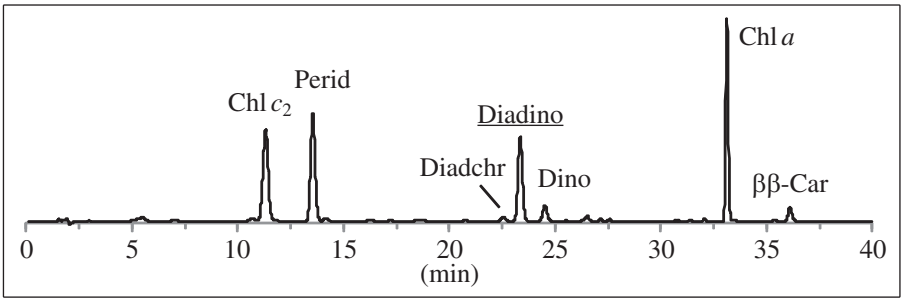


Biological occurrence	Dominant pigment in bolidophytes, diatoms, euglenophytes, haptophytes, pelagophytes, phaeothamniophytes, dictyochophytes (silicoflagellates) and some dinoflagellates. Minor in xanthophytes (see Chapter 1, this volume)
Source culture	*Amphidinium carterae* (dinoflagellate), *Phaeodactylum tricornutum* (diatom)
Alteration products	Undergoes rearrangement to Diadchr in weakly acidic solutions. *Cis*-isomers
Biosynthetically related to	Diato
Occurs together with	Diato, Fuco and derivatives, Peri

HPLC chromatogram of *Gymnodinium catenatum* (system 1)



HPLC chromatogram of *Scrippsiella trochoidea* (system 2)



UV-Vis spectra (see also reference spectra below)

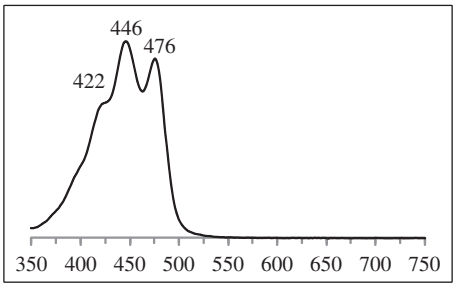
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(428), *449*, 479	75	[25]
Diethyl ether	424, *446*, 477	n.d.	[61]
Ethanol	(424), *445*, 476	64	[122]
Hexane	(421), *445*, 475	63	[122]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		224 (at 448 nm, acetone) [112]	

Reference spectra

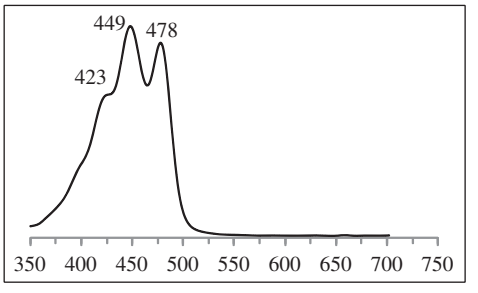
In acetone

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	582 $[M]^+$ (100), 567 $[M-15]^+$ (6), 564 $[M-18]^+$ (3), 502 $[M-80]^+$ (20), 490 $[M-92]^+$ (14), 487 $[M-15–80]^+$ (10), 475 $[M-15–92]^+$ (4), 221 (50), 181 (26)	[25]

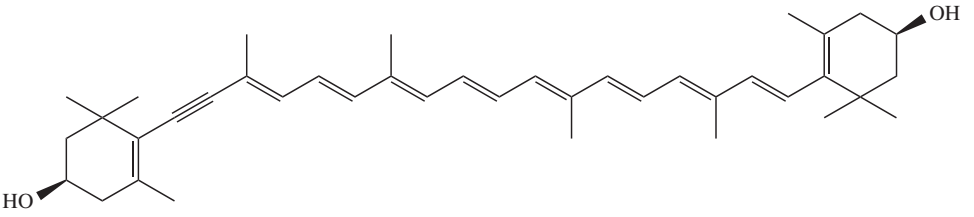
Remarks The recommended *d* value is the average of the two values given in [112]. Part of a 'xanthophyll cycle' (see Chapter 11 this volume)

Diatoxanthin

Recommended abbreviation: Diato (Dt)

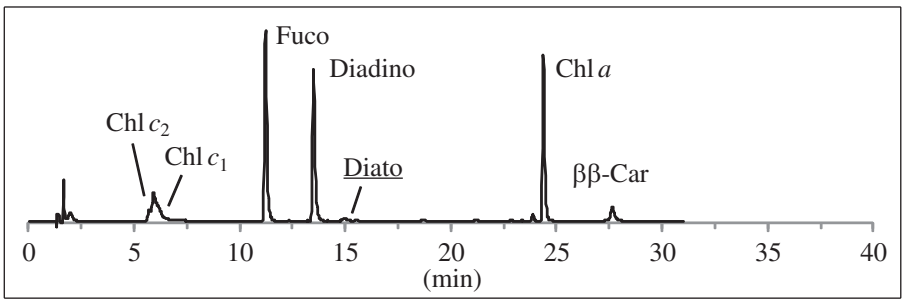
IUPAC: (3*R*,3′*R*)-7,8-Didehydro-β,β-carotene-3,3′-diol

Molecular formula: $C_{40}H_{54}O_2$ **Molecular weight:** 566.86

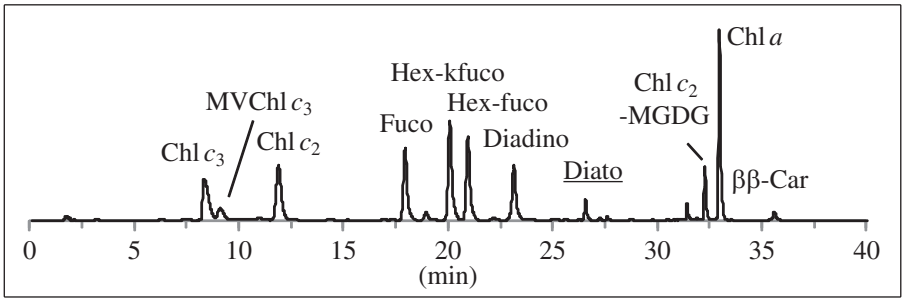


Biological occurrence	Minor pigment in euglenophytes, diatoms, bolidophytes, haptophytes, dictyochophytes, pelagophytes and some dinoflagellates
Source culture	*Amphidinium carterae* (dinoflagellate)
Alteration products	Easily isomerises to the more stable 9-*cis* isomer [43]
Biosynthetically related to	Diadino
Occurs together with	Diadino, Fuco and derivatives, Peri

HPLC chromatogram of *Pavlova gyrans* (system 1)



HPLC chromatogram of *Emiliania huxleyi* (system 2)



UV-Vis spectra (see also reference spectra below)

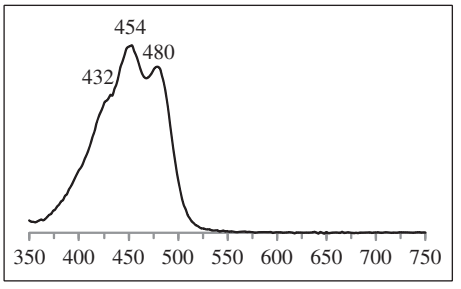
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	430, *453*, 480	42	[92]
Ethanol	(428), *452*, 478	n.d.	[130]
Hexane	(426), *451*, 480	31	[145]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		272 (at 453 nm, acetone) [92]	

Reference spectra

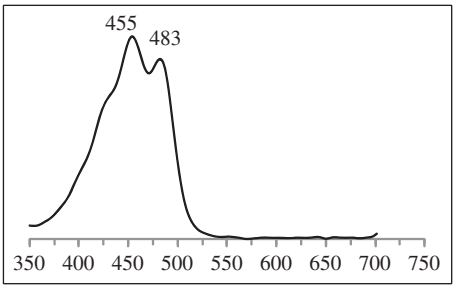
For spectrum in acetone, see [109]

For spectrum in hexane, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	566 $[M]^+$ (100), 548 $[M-18]^+$ (11), 474 $[M-92]^+$ (6), 408 $[M-158]^+$ (5), 283 (15), 119 (31), 43 (34)	[92]

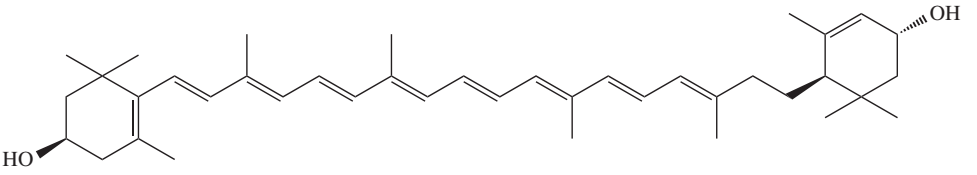
Remarks Part of a 'xanthophyll cycle' (see Chapter 11 this volume)

Dihydrolutein

Recommended abbreviation: Dhlut (Dl)

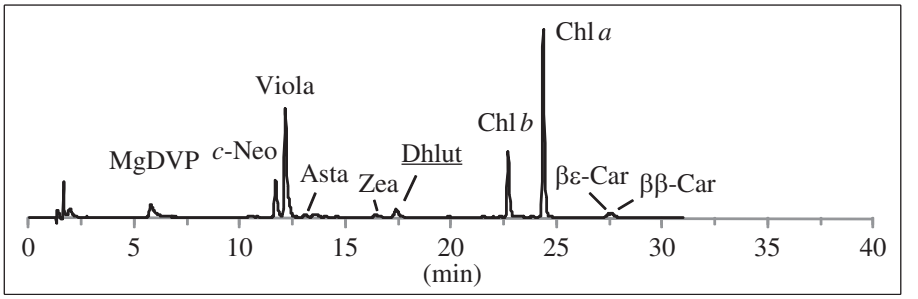
IUPAC: (3*R*,3′*R*,6′*R*)-7′,8′-Dihydro-β,ε-carotene-3,3′-diol

Molecular formula: $C_{40}H_{58}O_2$ **Molecular weight:** 570.89

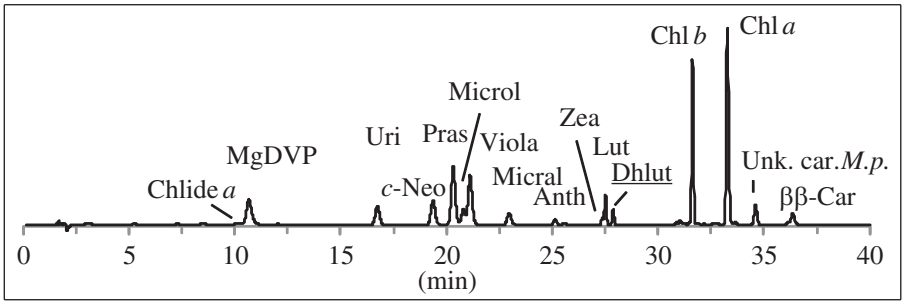


Biological occurrence	Only encountered in prasinophytes Pigment Type 3 [50]
Source culture	*Pseudoscourfieldia marina* (prasinophyte)
Alteration products	*Cis*-isomers
Biosynthetically related to	Lut (?), Microl, Micral, Uri
Occurs together with	Pras, Microl, Micral, Uri, Chl *b*, MgDVP

HPLC chromatogram of *Pycnococcus provasolii* (system 1)



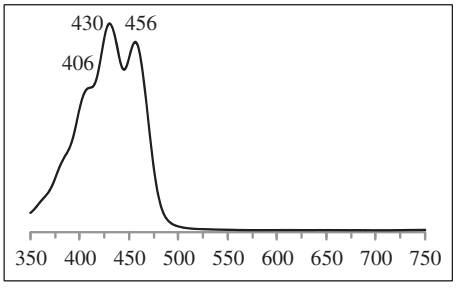
HPLC chromatogram of *Micromonas pusilla* (system 2)



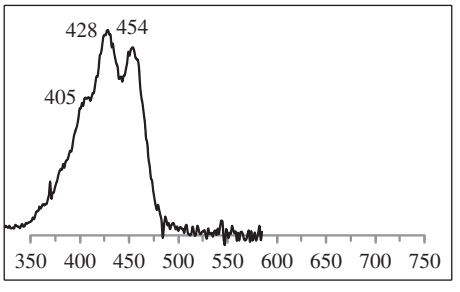
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III/II)	Ref.
Acetone	(402), *426*, 452	47	[50]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks	

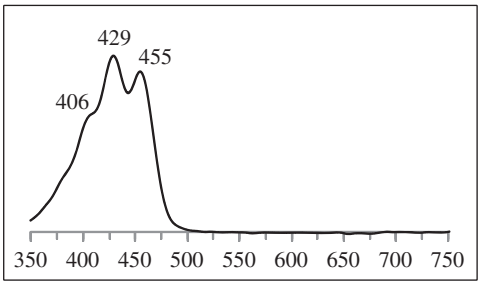
Reference spectra
In acetone



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	570 $[M]^+$ (100), 552 $[M-18]^+$ (35), 478 $[M-92]^+$ (4)	[52]

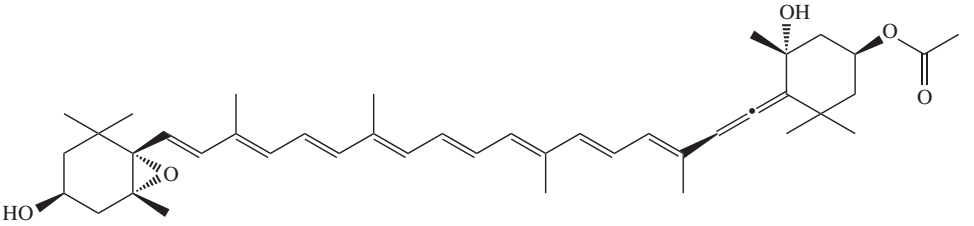
Remarks Structure not proven by NMR
$d = 229\,L\,g^{-1}cm^{-1}$ (at λ_{max} in ethanol, calc. from Mut) is recommended, as no *d* has been determined for Dhlut

Dinoxanthin

Recommended abbreviation: Dino (Dn)

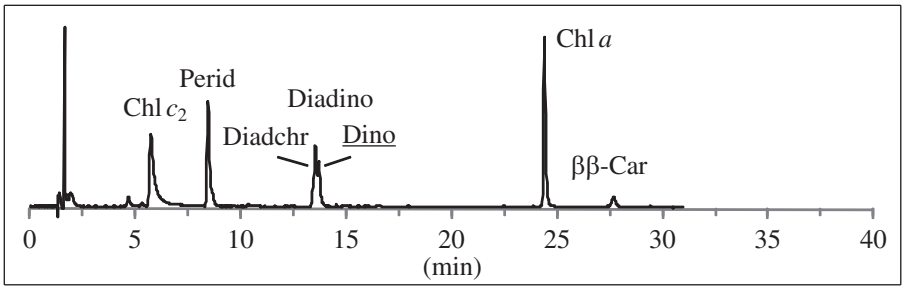
IUPAC: (3*S*,5*R*,6*S*,3′*S*,5′*R*,6′*R*)-5,6-Epoxy-3′-ethanoyloxy-6′,7′-didehydro-5,6,5′,6′-tetrahydro-β,β-carotene-3,5′-diol

Molecular formula: $C_{42}H_{58}O_5$ **Molecular weight:** 642.91

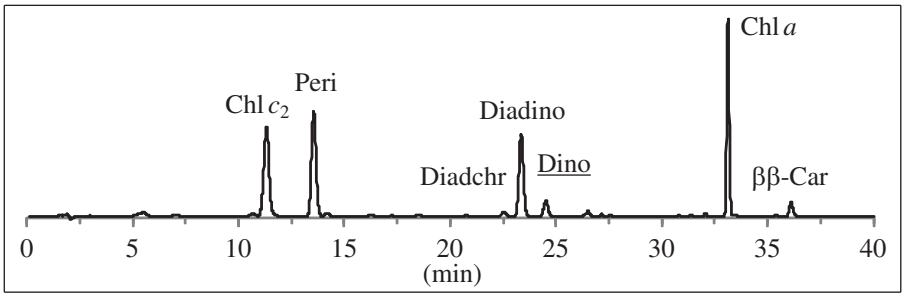


Biological occurrence	Minor pigment in Peri-containing dinoflagellates. Occasionally found in trace in various chromophyte cultures
Source culture	*Amphidinium carterae* (dinoflagellate)
Alteration products	Undergoes rearrangement to Dinochr in weakly acidic solutions. *Cis*-isomers
Biosynthetically related to	Neo, Viola
Occurs together with	Peri (if dinoflagellates)

HPLC chromatogram of *Gymnodinium catenatum* (system 1)



HPLC chromatogram of *Scrippsiella trochoidea* (system 2)



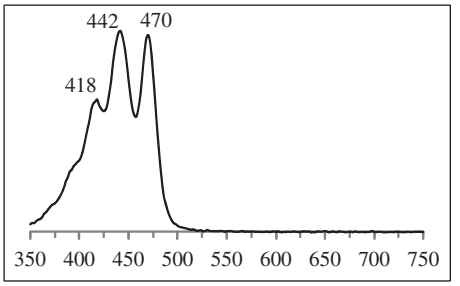
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	418, *442*, 471	86	[145]
Ethanol	417, *441*, 470	85	[145]
Hexane	416, *439*, 469	83	[122]
Methanol	416, *438*, 467	76	[122]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks	

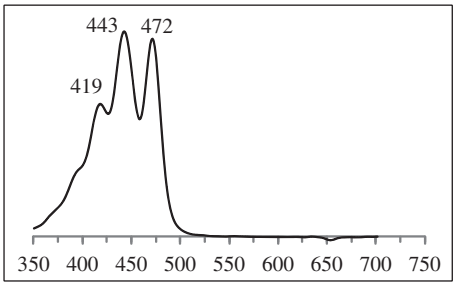
Reference spectra

For spectrum in acetone, see [109] For spectrum in ethanol, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	642 $[M]^+$ (3), 624 $[M\text{-}18]^+$ (11), 606 $[M\text{-}18\text{–}18]^+$ (7), 221 (100), 181 (64)	[18]

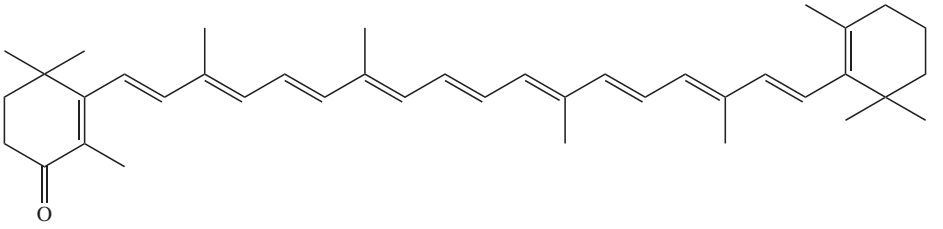
Remarks As *d* has not been determined for Dino, a value based on *t*-Neo was calculated: $d = 222\,L\,g^{-1}cm^{-1}$ (at 441 nm, ethanol). Note spectral similarity with Viola (but Dino is slightly red-shifted). Dinochrome is formed from Dino in slightly acidic extracts: [18, 22, 25]

Echinenone

Recommended abbreviation: Echin (Ec)

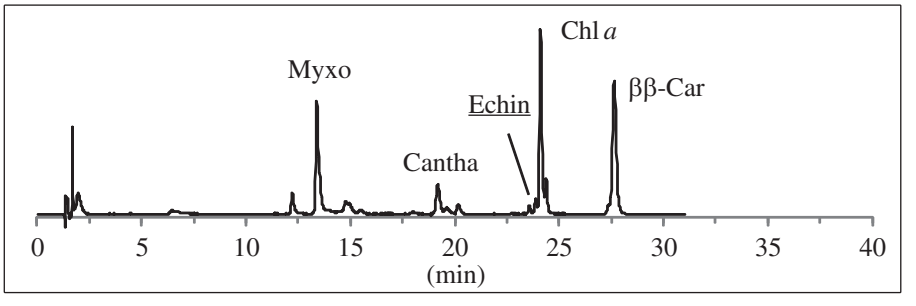
IUPAC: β,β-Caroten-4-one

Molecular formula: $C_{40}H_{54}O$ **Molecular weight:** 550.86

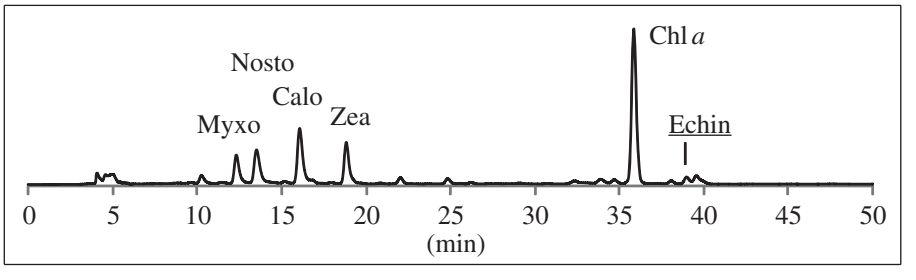


Biological occurrence	Minor pigment in some prochlorophytes (Cyano-3) and cyanobacteria (Cyano-1, Chapter 1). Occasional traces in algal cultures from several other classes
Source culture	*Oscillatoria agardhii (rubescens)* (cyanobacteria)
Alteration products	*Cis*-isomers
Biosynthetically related to	ββ-Car, Cantha, Asta
Occurs together with	

HPLC chromatogram *Nodularia spumigena* (system 1)



HPLC chromatogram *Chlorogloeopsis fritschii* (system 3)

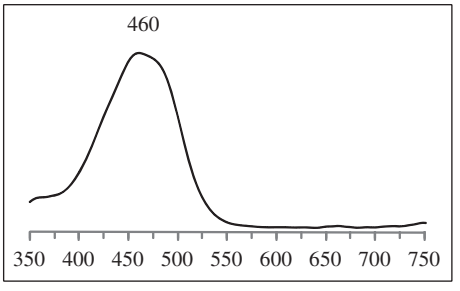


UV-Vis spectra (see also reference spectra below)

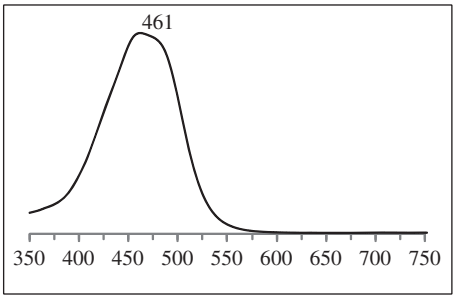
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	*459*, (475)	-	[88]
Diethyl ether	(430), *452*, (472)	-	[59]
Ethanol	461	-	[86]
Hexane	458	-	[135]
Methanol	460	-	[159]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		216 (at 458 nm, hexane) [68]	

Reference spectra

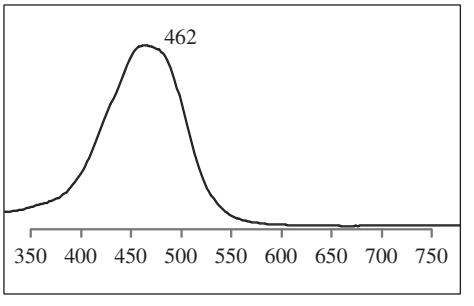
In acetone



In HPLC solvent system 2



In HPLC solvent system 3



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	550 $[M]^+$ (100), 534 $[M-16]^+$ (10), 458 $[M-92]^+$ (6), 444 $[M-106]^+$ (2), 189 (16)	[59]

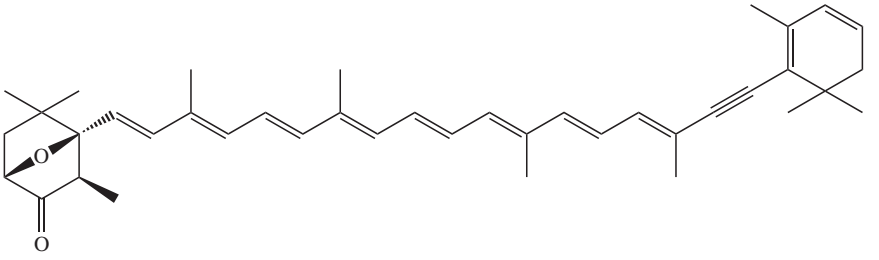
Remarks

Eutreptiellanone

Recommended abbreviation: Eutr (Eu)

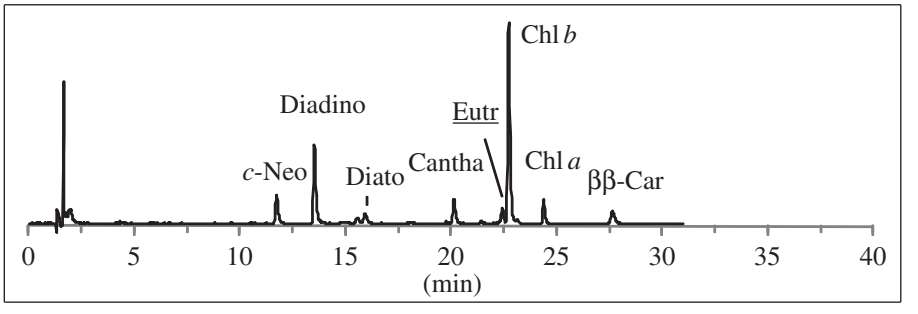
IUPAC: (3*S*,5*R*,6*S*)-3,6-Epoxy-3′,4′,7′,8′-tetradehydro-5,6-dihydro-β,β-caroten-4-one

Molecular formula: $C_{40}H_{50}O_2$ **Molecular weight:** 562.82

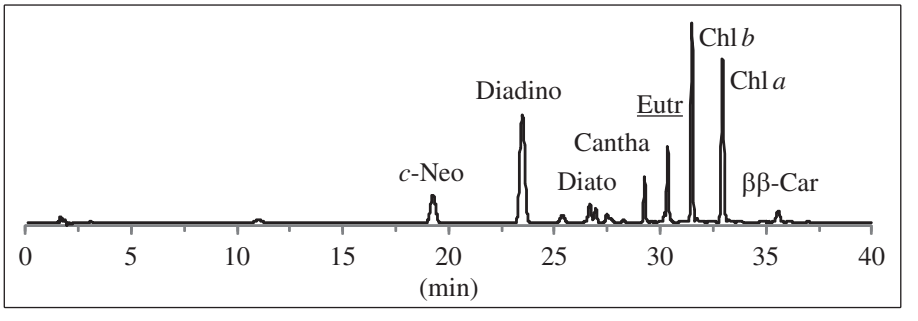


Biological occurrence	Only as major carotenoid in *Eutreptiella gymnastica*
Source culture	*Eutreptiella gymnastica* (euglenophyte)
Alteration products	*Cis*-isomers
Biosynthetically related to	Other carotenoids from *Eutreptiella gymnastica*
Occurs together with	Chl *b*, Diato, Diadino

HPLC chromatogram of *Eutreptiella* cf. *gymnastica* (system 1)



HPLC chromatogram of *Eutreptiella gymnastica* (system 2)



UV-Vis spectra (see also reference spectra below)

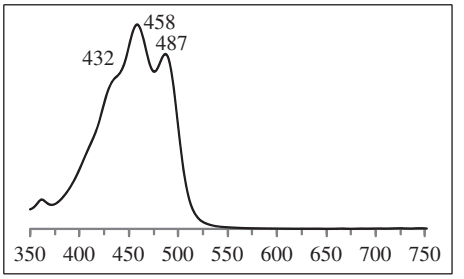
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(441), *461*, 491	47	[17]
Diethyl ether	(434), *457*, 483	48	[58]
Petroleum ether	(438), *458*, 487	50	[17]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d.	

Reference spectra

In HPLC solvent system 1

NO DATA AVAILABLE

In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	562.3808 $[M]^+$ (100), 547 $[M\text{-}15]^+$ (6), 506.3188 $[M\text{-}56]^+$ (2), 491.2956 $[M\text{-}56\text{–}18]^+$ (2), 470 $[M\text{-}92]^+$ (2), 455 $[M\text{-}92\text{–}15]^+$ (2), 261 (12)	[58]

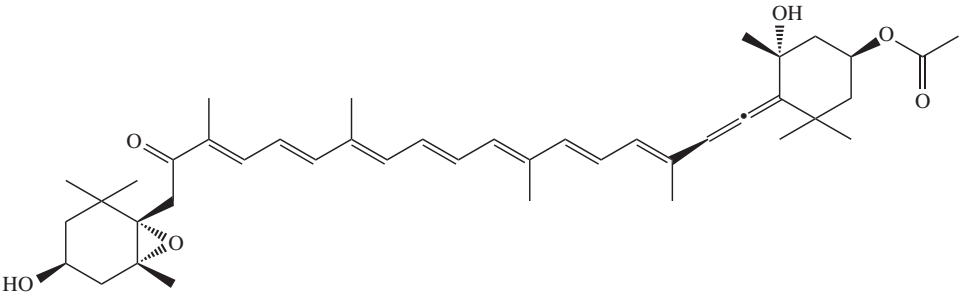
Remarks 'Unknown 1′ in ref. [17]
$d = 220\,L\,g^{-1}\,cm^{-1}$ (at 461 nm in acetone) is recommended, as no value has been determined for Eutr

Fucoxanthin

Recommended abbreviation: Fuco (F)

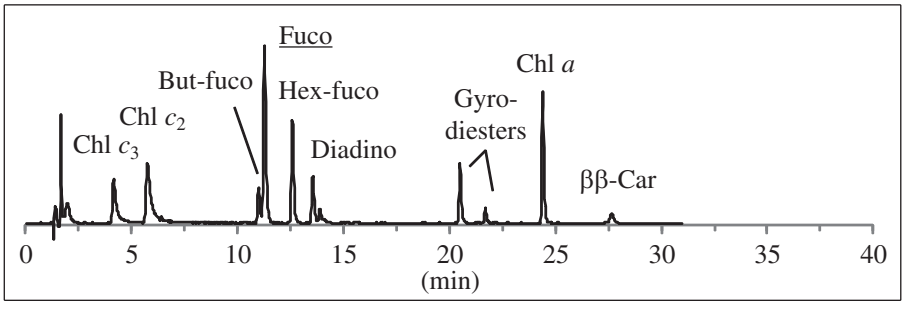
IUPAC: (3*S*,5*R*,6*S*,3′*S*,5′*R*,6′*R*)-5,6-Epoxy-3′-ethanoyloxy-3,5′-dihydroxy-6′,7′-didehydro-5,6,7,8,5′,6′-hexahydro-β,β-caroten-8-one

Molecular formula: $C_{42}H_{58}O_6$ **Molecular weight:** 658.91

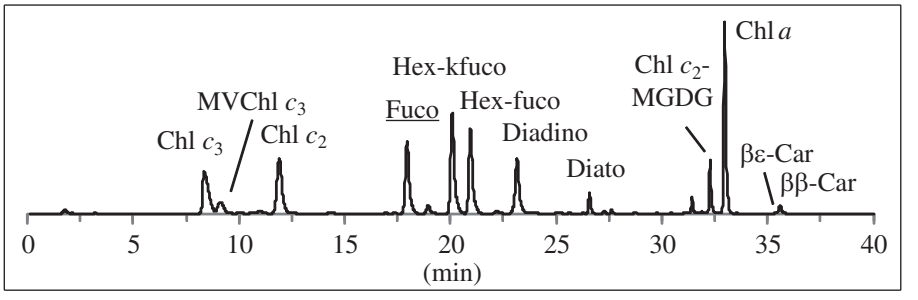


Biological occurrence	Dominant carotenoid in most algal classes of the Red Algal lineage (see Chapter 1, this volume) and brown seaweeds
Source culture	*Phaeodactylum tricornutum* (diatom)
Alteration products	*Cis*-isomers
Biosynthetically related to	Neo, Hex-fuco, But-fuco, Hex-kfuco, Kfuco
Occurs together with	Hex-fuco, But-fuco, Diato, Diadino, Viola, Zea, Chl *c*s

HPLC chromatogram of *Karlodinium micrum* (system 1)



HPLC chromatogram of *Emiliania huxleyi* (system 2)

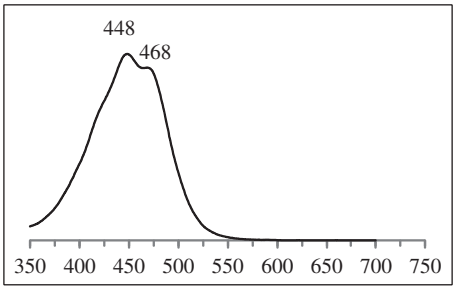


UV-Vis spectra (see also reference spectra below)

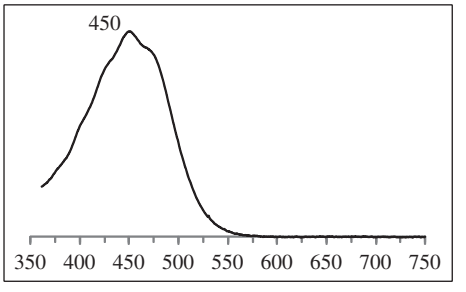
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(420), *444*, 467	5	[89]
Diethyl ether	*446*, 470	3	[173]
Ethanol	*449*, (467)		[174]
Hexane	(428), *446*, 475	40	[89]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		166 (at 443 nm, acetone) [90]	

Reference spectra

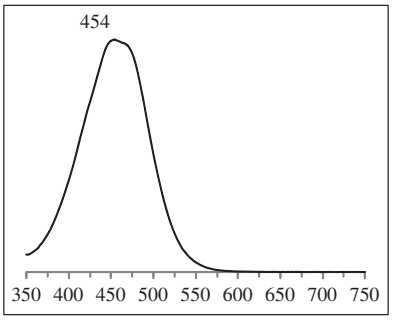
In acetone



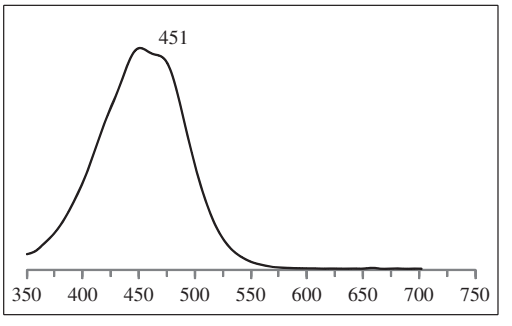
In ethanol



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
APCI	Ion trap	681 $[M+Na]^+ \rightarrow$ 527 $[M+Na\text{-}154]^+ \rightarrow$ 467 $[M+Na\text{-}154\text{–}60]^+$	[5]

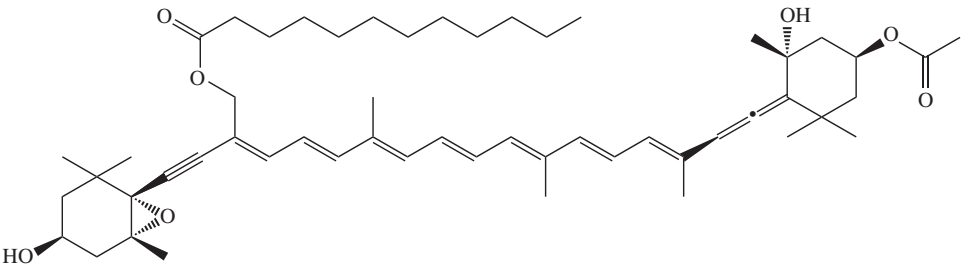
Remarks 4-ketofucoxanthin has also been encountered as a minor pigment in a few haptophytes [49]

Gyroxanthin dodecanoate ethanoate (one of several gyroxanthin diesters)

Recommended abbreviation: Gyro-de (Gd)

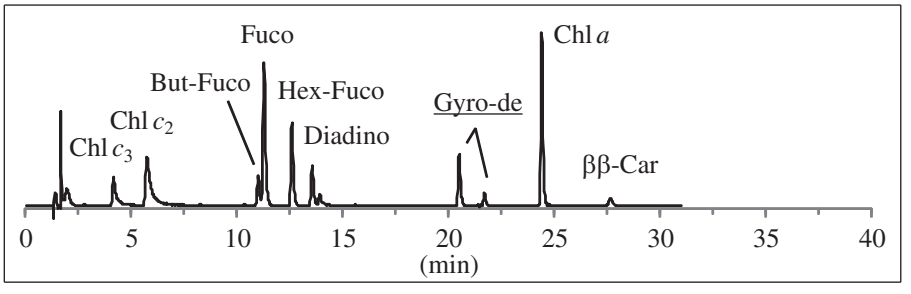
IUPAC: (3*S*,5*R*,6*S*,3′*S*,5′*R*,6′*R*)-19-Dodecanoyloxy-5,6-epoxy-3′-ethanoyloxy-7,8,6′,7′-tetradehydro-5,6,5′,6′-tetrahydro-β,β-carotene-3,5′-diol

Molecular formula: $C_{54}H_{78}O_7$ **Molecular weight:** 839.19

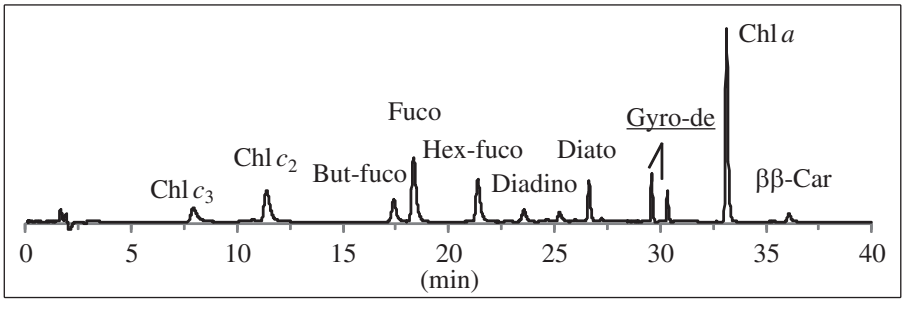


Biological occurrence	A major carotenoid in dinoflagellates Pigment Type 2, minor in pelagophytes and coccolithophytes (see Chapter 1)
Source culture	*Karenia brevis* (dinoflagellate)
Alteration products	Easily isomerises to the more stable 9-*cis* isomer [21]
Biosynthetically related to	Dino?
Occurs together with	Fuco, Diato, Diadino, various Fuco derivatives, Chl *c*s

HPLC chromatogram of *Karlodinium micrum* (system 1)



HPLC chromatogram of *Karlodinium micrum* (system 2)

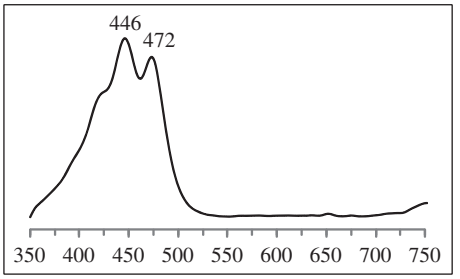


UV-Vis spectra (see also reference spectra below)

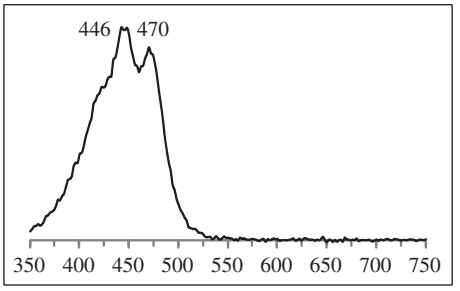
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(423), *444*, 472	55	[21]
Hexane	418, *442*, 470	76	[21]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks	

Reference spectra

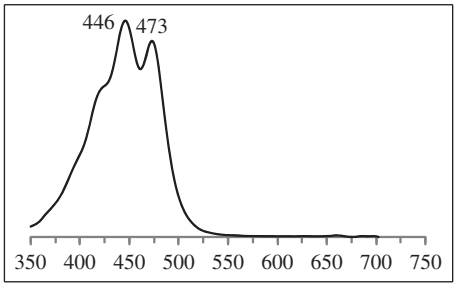
In acetone



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

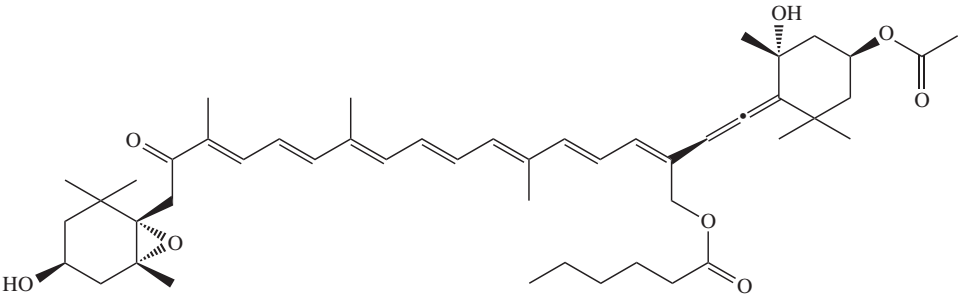
Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
ESI$^+$	Ion trap	861 $[M+Na]^+ \rightarrow$ 661 $[M+Na\text{-}200]^+ \rightarrow$ 555 $[M+Na\text{-}200\text{–}106]^+$, 643 $[M+Na\text{-}200\text{–}18]^+$, 601 $[M+Na\text{-}200\text{–}60]^+$, 569 $[M+Na\text{-}200\text{–}92]^+$	[178]

Remarks $d = 183\,L\,g^{-1}\,cm^{-1}$ (at 444 nm in acetone; calc. from an average carotenoid value of 250) is recommended, as no value has been determined for Gyro-de [21] Other gyroxanthin diesters also found (see the chromatograms shown) [21, 24]

19′-Hexanoyloxyfucoxanthin **Recommended abbreviation: Hex-fuco (HF)**

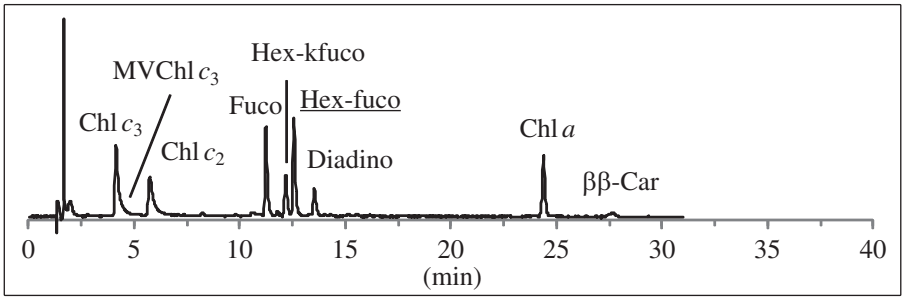
IUPAC:(3*S*,5*R*,6′*S*,3′*S*,5′*R*,6′*R*)-5,6-Epoxy-3′-ethanoyloxy-19′-hexanoyloxy-3, 5′-dihydroxy -6′,7′-didehydro-5,6,7,8,5′,6′-hexahydro-β,β-caroten-8-one

Molecular formula: $C_{48}H_{68}O_8$ **Molecular weight:** 773.05

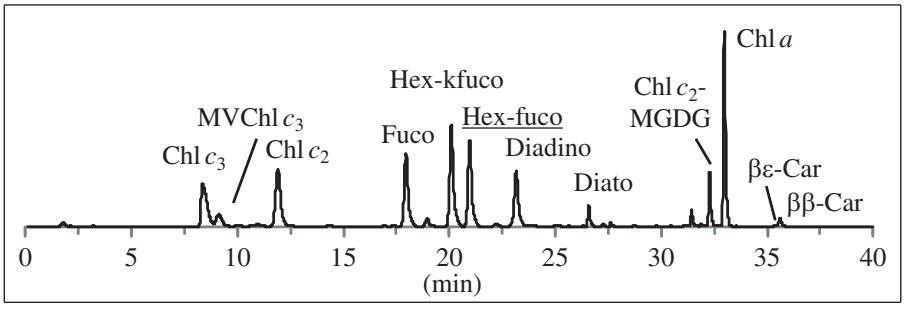


Biological occurrence	Major in many haptophytes and dinoflagellates Pigment Type 2 (see Chapter 1, this volume)
Source culture	*Emiliania huxleyi* (coccolithophyte), strain CS-57
Alteration products	*Cis*-isomers
Biosynthetically related to	Fuco, But-fuco, Hex-kfuco
Occurs together with	Fuco, other Fuco-derivatives, Diato, Diadino, Chl *c*s

HPLC chromatogram of *Emiliania huxleyi* (system 1)



HPLC chromatogram of *Emiliania huxleyi* (system 2)



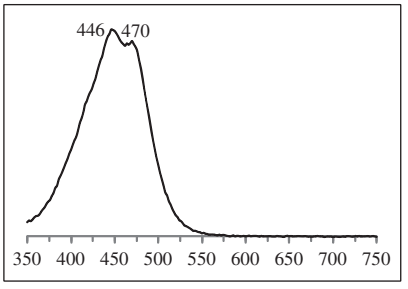
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	420, *443*, 463	40	[16]
Hexane	(423), *445*, 474	64	[22]
Methanol	443		[7]
Recommended specific absorption coefficient *d* (L $g^{-1}cm^{-1}$)		n.d., see Remarks	

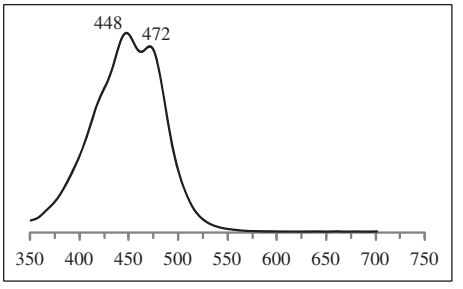
Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

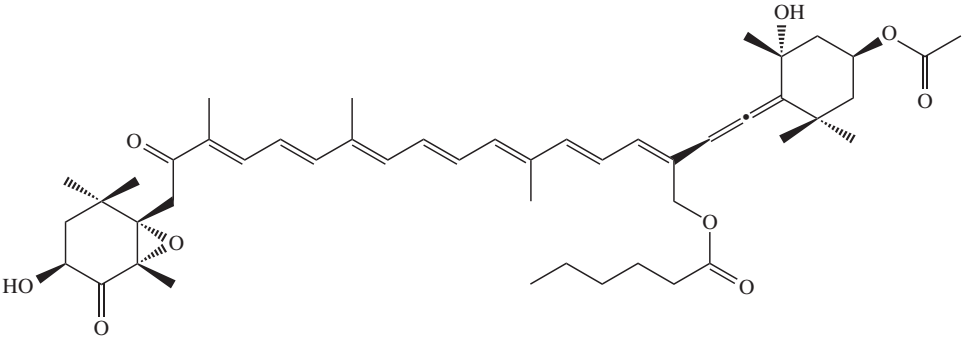
Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
APCI	Ion trap	795 $[M+Na]^+ \rightarrow$ 679 $[M+Na\text{-}116]^+ \rightarrow$ 661 $[M+Na\text{-}116\text{–}18]^+$, 619 $[M+Na\text{-}116\text{–}60]^+$, 525	[5]

Remarks $d = 142\ L\ g^{-1}cm^{-1}$ (at 445 nm in acetone; calc. from Fuco) is recommended, as no value has been determined for Hex-fuco [109]. Several other, minor alkanoyloxyfucoxanthins have been reported [5]

19′-Hexanoyloxy-4-ketofucoxanthin **Recom. abbrev.: Hex-kfuco (HKf)**

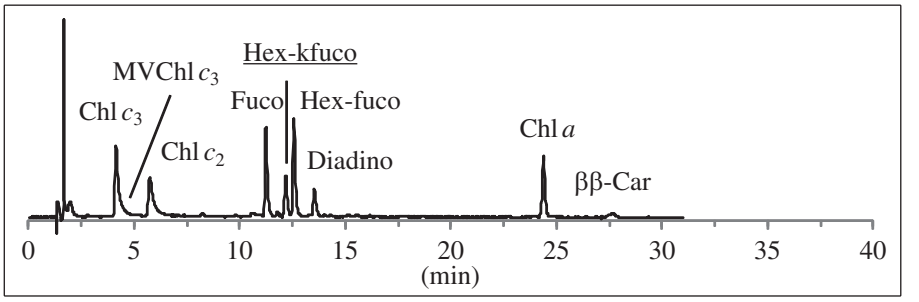
IUPAC: (3*S*,5*S*,6*S*,3′*S*,5′*R*,6′*R*)-5,6-Epoxy-3′-ethanoyloxy-19′-hexanoyloxy-3,5′-dihydroxy-6′,7′-didehydro-5,6,7,8,5′,6′-hexahydro-β,β-carotene-4,8-dione

Molecular formula: $C_{48}H_{66}O_9$ **Molecular weight:** 787.03

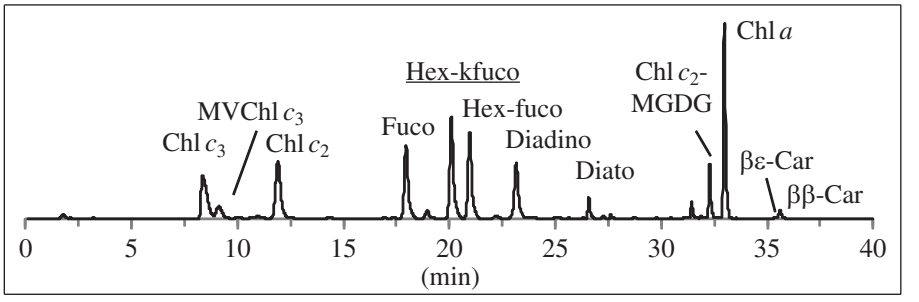


Biological occurrence	Major in some haptophytes (see Chapter 1, this volume)
Source culture	*Ochrosphaera neopolitana* (coccolithophyte) [180], strain CS-285 [8]
Alteration products	*Cis*-isomers. Degrades upon storage in acetone [49]
Biosynthetically related to	Fuco, Kfuco
Occurs together with	Fuco, Diato, Diadino, Chl *c*s

HPLC chromatogram of *Emiliania huxleyi* (system 1)



HPLC chromatogram of *Emiliania huxleyi* (system 2)

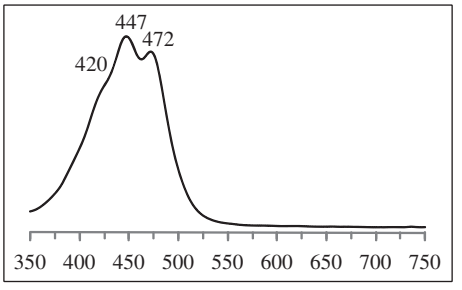


UV-Vis spectra (see also reference spectra below)

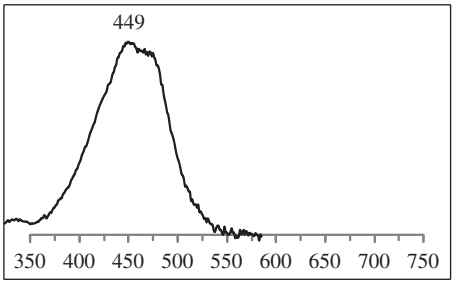
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(420), *443*, 467	38	[49]
Methanol	*443*, 465	28	[49]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks	

Reference spectra

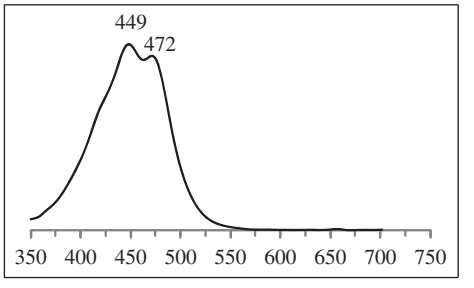
In acetone



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
APCI	Ion trap	809 $[M+Na]^+ \rightarrow$ 693 $[M+Na\text{-}116]^+$, 675 $[M+Na\text{-}116\text{–}18]^+$, 633, 525	[5]

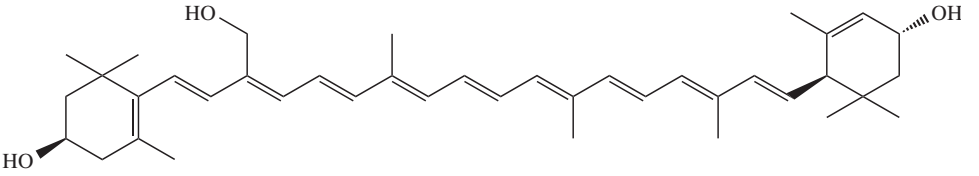
Remarks Former name = 4-keto-19′-hexanoyloxyfucoxanthin [49]
$d = 139\,L\,g^{-1}\,cm^{-1}$ (at 443 nm in acetone; calc. from Fuco) is recommended, as no value has been determined for Hex-kfuco.
Earlier misidentified as 19′-hexanoyloxyparacentrone 3-acetate

Loroxanthin

Recommended abbreviation: Loro (Lo)

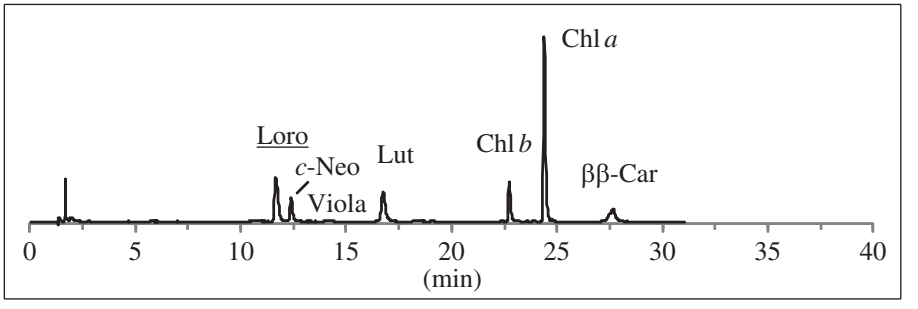
IUPAC: (3*R*,3′*R*,6′*R*)-β,ε-Carotene-3,19,3′-triol

Molecular formula: $C_{40}H_{56}O_3$ **Molecular weight:** 584.87

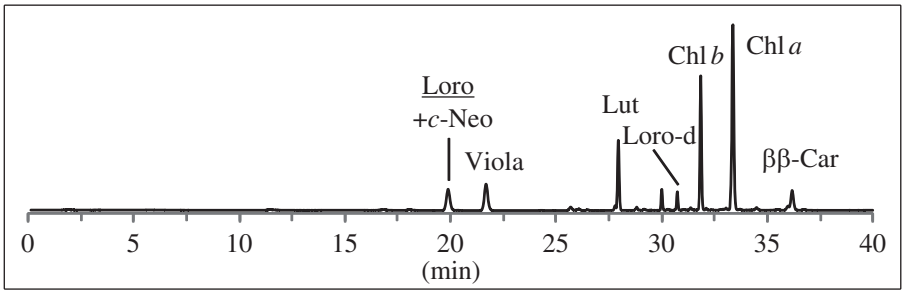


Biological occurrence	Minor pigment in some chlorophytes and prasinophytes
Source culture	*Pyramimonas parkeae* (prasinopyte) [71], CCMP 724 [164]
Alteration products	*Cis*-isomers
Biosynthetically related to	βε-Car, Lut, Loro-d, Siph
Occurs together with	βε-Car, Lut, Loro-d, Neo, Chl *b*

HPLC chromatogram of an *unidentified chlorophyte* (system 1)



HPLC chromatogram of *Tetraselmis suecica* (system 2)

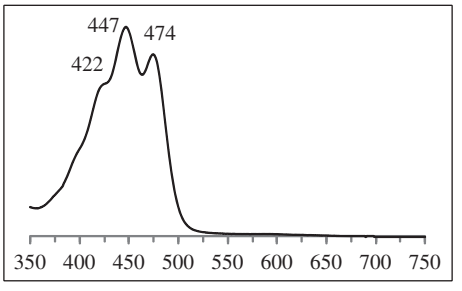


UV-Vis spectra (see also reference spectra below)

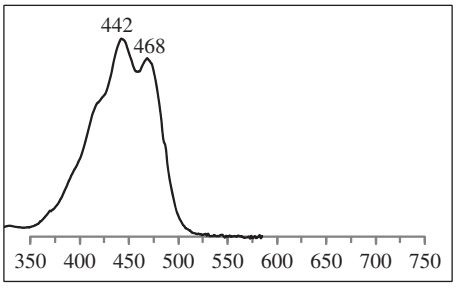
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(424), *447*, 472	44	[132]
Diethyl ether	(422), *444*, 472	48	[71]
Ethanol	(425), *446*, 473	n.d.	[116]
Hexane	423, *445*, 473	58	[71]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks	

Reference spectra

In acetone



In HPLC solvent system 1



In HPLC solvent system 2

NO DATA AVAILABLE

Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
ESI^+	Ion trap	584 $[M]^+ \rightarrow$ 566 $[M\text{-}18]^+$, 492 $[M\text{-}92]^+$, 474 $[M\text{-}92\text{–}18]^+$, 446 $[M\text{-}138]^+$, 428 $[M\text{-}138\text{–}18]^+$	[71]

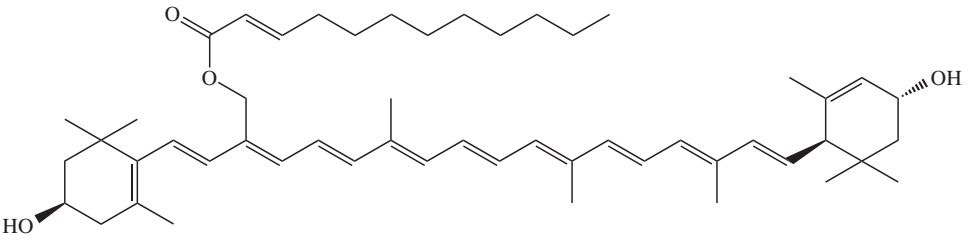
Remarks $d = 245\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in dioxane; calc. from Lut) is recommended, as no value has been determined for Loro. In ethanol, use the value for lutein corrected for the difference in molecular weight: $d = 248$ $Lg^{-1}cm^{-1}$ (at 445 nm)

Loroxanthin dodecenoate

Recommended abbreviation: Loro-d (Lod)

IUPAC: (3*R*,3′*R*,6′*R*)-19-(Dodec-2-enoyloxy)-β,ε-carotene-3,3′-diol

Molecular formula: $C_{52}H_{76}O_4$ **Molecular weight:** 765.16

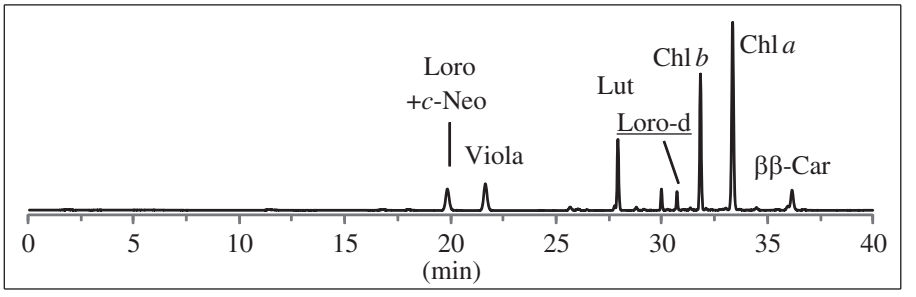


Biological occurrence	Minor in some prasinophytes, also encountered in an euglenophyte and a chlorarachniophyte
Source culture	*Pyramimonas parkeae* (prasinophyte) [139], CCMP 724 [164]
Alteration products	*Cis*-isomers
Biosynthetically related to	βε-Car, Loro, Lut, Siph esters
Occurs together with	βε-Car, Lut, Loro, Neo, Chl *b*

HPLC chromatogram (system 1)

NO DATA AVAILABLE

HPLC chromatogram of *Tetraselmis suecica* (system 2)

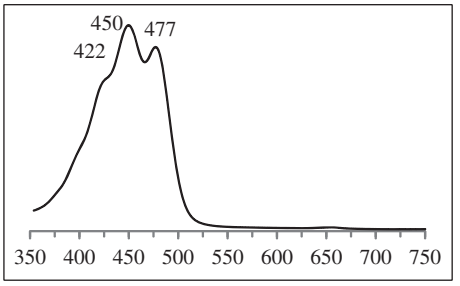


UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(423), *449*, 477	42	[71]
Hexane	422, *446*, 474	64	[71]
Methanol	*445*, 471	42	[139]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks	

Reference spectra

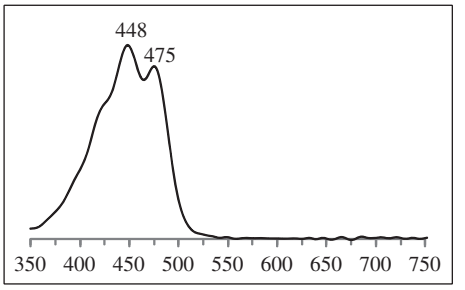
In acetone



In HPLC solvent system 1

NO DATA AVAILABLE

In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
ESI^+	Ion trap	764 $[M]^+$, 747 $[M+H\text{-}18]^+ \rightarrow$ 729 $[M+H\text{-}18\text{–}18]^+$, 549 $[M+H\text{-}18\text{–}198]^+$, 531 $[M+H\text{-}18\text{–}18\text{–}198]^+$	[71]

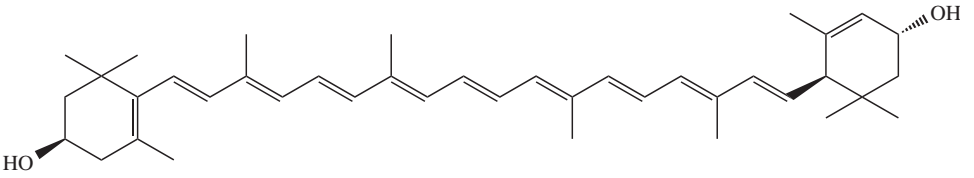
Remarks Other alkenoylloroxanthins have also been encountered [65]
$d = 187\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in dioxane; calc. from Lut) is recommended, as no value has been determined for Loro-d. In ethanol, use the value for lutein, corrected for the difference in molecular weight: $d = 190\ L\ g^{-1}\ cm^{-1}$ (at λ_{max})

Lutein

Recommended abbreviation: Lut (L)

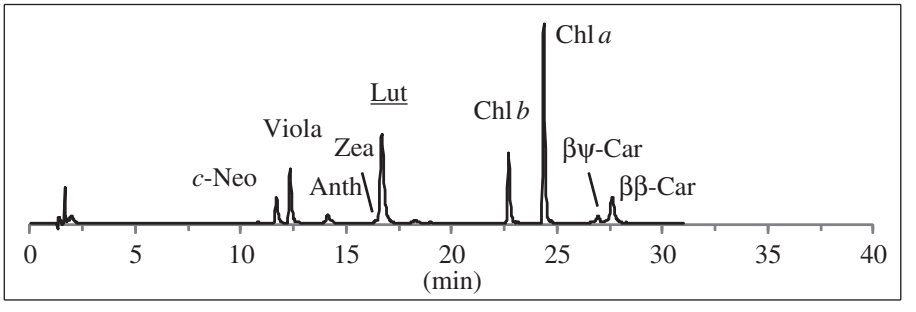
IUPAC: (3*R*,3′*R*,6′*R*)-β,ε-Carotene-3,3′-diol

Molecular formula: $C_{40}H_{56}O_2$ **Molecular weight:** 568.87

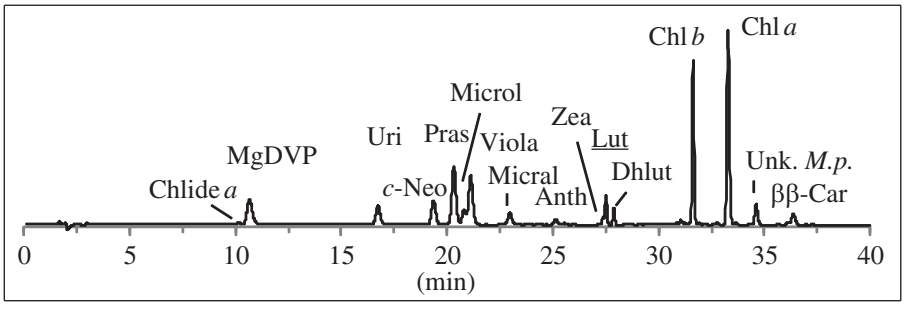


Biological occurrence	Dominant pigment in chlorophytes, chlorarachniophytes and prasinophytes. Minor in mesostigmatophytes. Also in red seaweeds, green leaves and some flowers
Source culture	*Dunaliella tertiolecta* (chlorophyte); *Tetraselmis suecica* (prasinophyte)
Alteration products	*Cis*-isomers
Biosynthetically related to	βε-Car, Loro, Siph, Loro and Siph esters, Dhlut?
Occurs together with	βε-Car, Zea, Viola, Neo, Chl *b*

HPLC chromatogram of *Dunaliella tertiolecta* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)



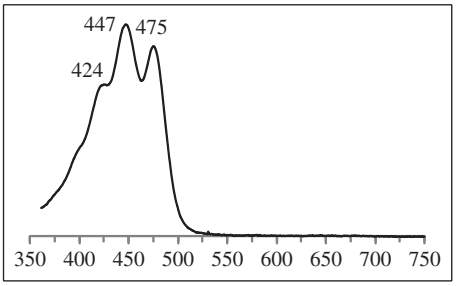
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	425, *448*, 476	67	[109]
Ethanol	422, *445*, 474	62	[86]
Hexane	421, *445*, 474	76	[109]
Methanol	(422), *443*, 470	62	[160]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		252 (at 453 nm, dioxane) [128] 255 (at 445 nm, ethanol) [148]	

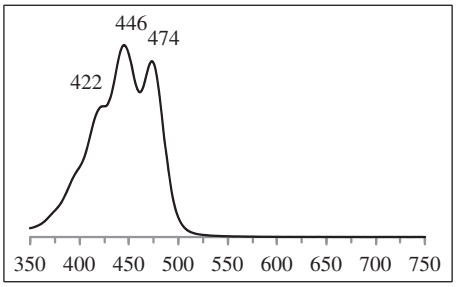
Reference spectra

For spectrum in acetone, see [109]

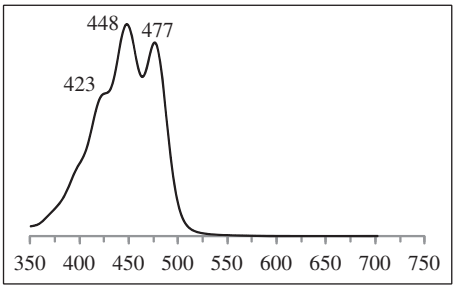
In ethanol



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	568 $[M]^+$ (23), 550 $[M\text{-}18]^+$ (31), 512 $[M\text{-}56]^+$ (1), 476 $[M\text{-}92]^+$ (8), 462 $[M\text{-}106]^+$ (5), 458 $[M\text{-}92\text{–}18]^+$ (12), 415 $[M\text{-}153]^+$ (2), 392 (29), 324 (41), 91 (100)	[55]

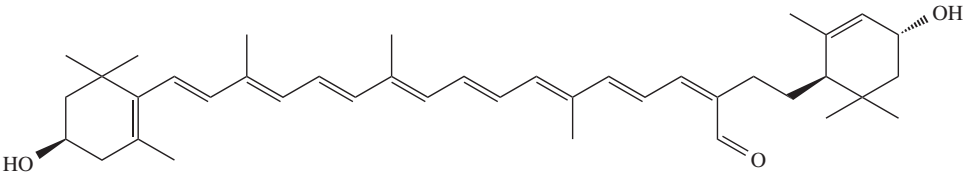
Remarks The name 'Xanthophyll' is found in older literature. Lutein and lutein epoxide are part of a 'xanthophyll cycle': see Chapter 11 this volume

Micromonal

Recommended abbreviation: Micral (Mia)

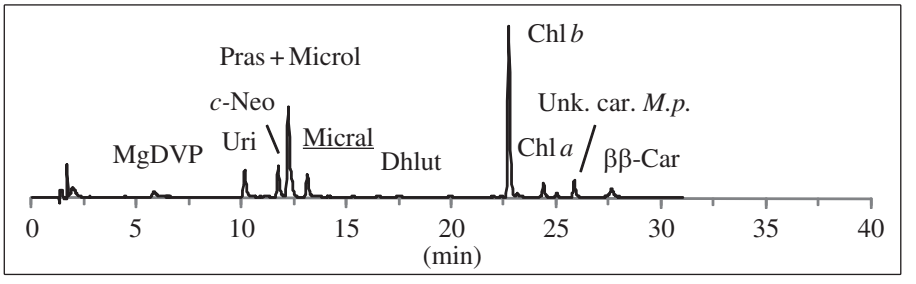
IUPAC: (3*R*,3′*R*,6′*R*)-3,3′-Dihydroxy-7′,8′-dihydro-β,ε-caroten-19′-al

Molecular formula: $C_{40}H_{56}O_3$ **Molecular weight:** 584.87

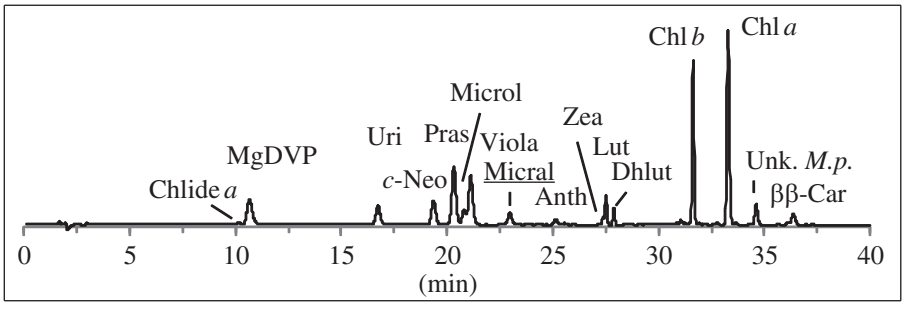


Biological occurrence	Dominant pigment in prasinophytes Pigment Type 3B (Chapter 1, this volume)
Source culture	*Micromonas pusilla* (prasinophyte)
Alteration products	*Cis*-isomers
Biosynthetically related to	Lut (?), Dhlut, Microl, Uri
Occurs together with	Pras, Microl, Dhlut, Uri, Chl *b*, MgDVP

HPLC chromatogram of *Micromonas pusilla* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)

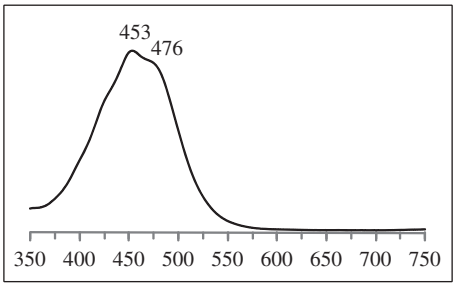


UV-Vis spectra (see also reference spectra below)

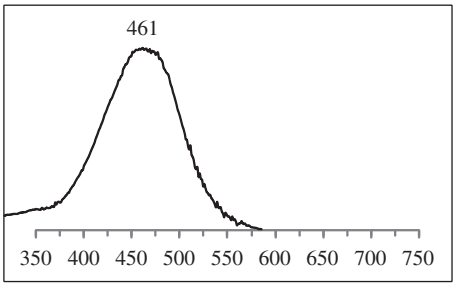
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(423), *449*, (472)	-	[52]
Diethyl ether	(422), *447*, (470)	-	[52]
Hexane	(425), *449*, (474)	-	[52]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

Reference spectra

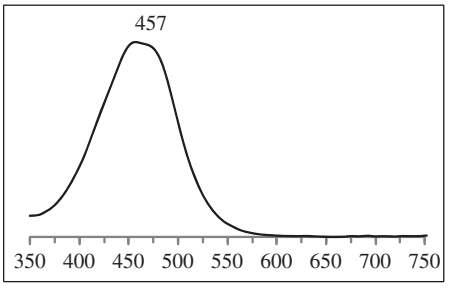
In acetone



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	584 $[M]^+$ (74), 566 $[M\text{-}18]^+$ (100), 548 $[M\text{-}18\text{–}18]^+$ (12), 538 $[M\text{-}46]^+$ (10), 492 $[M\text{-}92]^+$ (6), 478 $[M\text{-}106]^+$ (6), 444 $[M\text{-}138]^+$ (6), 431 $[M\text{-}153]^+$ (8)	[52]

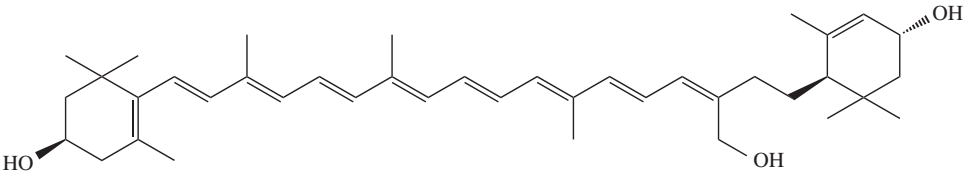
Remarks $d = 195\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in ethanol) is recommended, as no value has been determined for Micral

Micromonol

Recommended abbreviation: Microl (Mio)

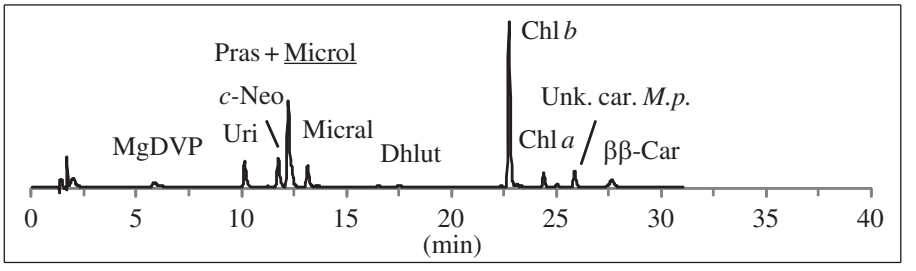
IUPAC: (3*R*,3′*R*,6′*R*)-7′,8′-Dihydro-β,ε-carotene-3,3′,19′-triol

Molecular formula: $C_{40}H_{58}O_3$ **Molecular weight:** 586.89

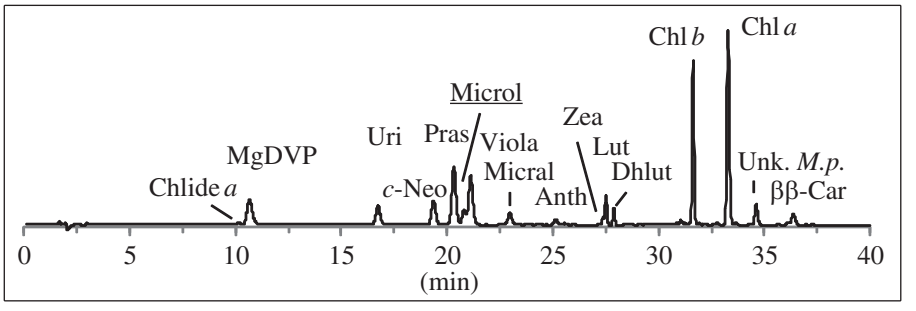


Biological occurrence	Minor pigment in prasinophytes Pigment Type 3B (Chapter 1, this volume)
Source culture	*Micromonas pusilla* (prasinophyte)
Alteration products	*Cis*-isomers
Biosynthetically related to	Lut (?), Dhlut, Micral, Uri
Occurs together with	Pras, Micral, Dhlut, Uri, Chl *b*, MgDVP

HPLC chromatogram of *Micromonas pusilla* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)



UV-Vis spectra (see also reference spectra below)

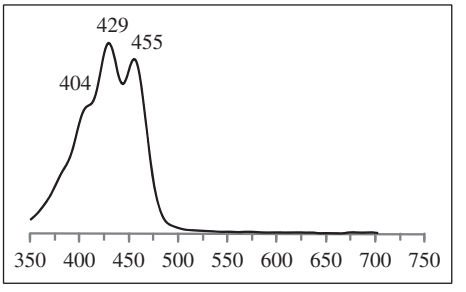
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(406), *427*, 452	54	[52]
Ethanol	(403), *424*, 450	49	[52]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

Reference spectra

In HPLC solvent system 1

NO DATA AVAILABLE

In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	586 $[M]^+$ (100), 568 $[M\text{-}18]^+$ (26), 550 $[M\text{-}18\text{–}18]^+$ (14), 532 $[M\text{-}18\text{–}18\text{–}18]^+$ (5), 494 $[M\text{-}92]^+$ (5), 480 $[M\text{-}106]^+$ (4), 446 $[M\text{-}140]^+$ (19)	[52]

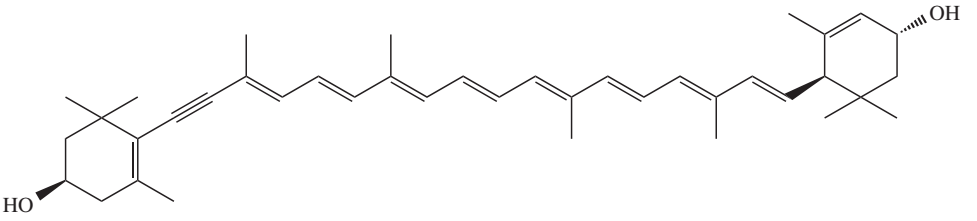
Remarks $d = 223\ L\ g^{-1}\ cm^{-1}$ (at 424 nm in ethanol; calc. from Mutato) is recommended, as no value has been determined for Microl

Monadoxanthin

Recommended abbreviation: Monado (Mo)

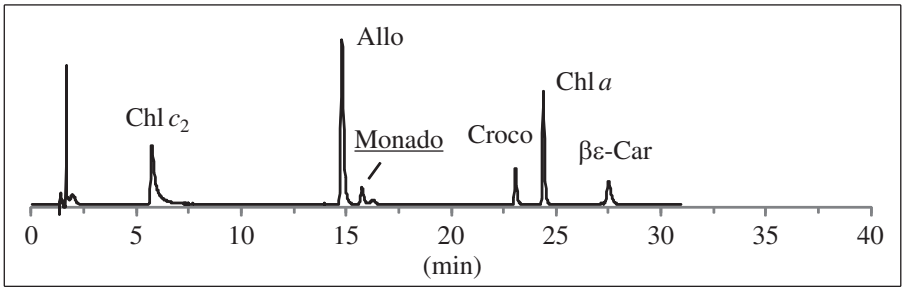
IUPAC: (3*R*,3′*R*,6′*R*)-7,8-Didehydro-β,ε-carotene-3,3′-diol

Molecular formula: $C_{40}H_{54}O_2$ **Molecular weight:** 566.86

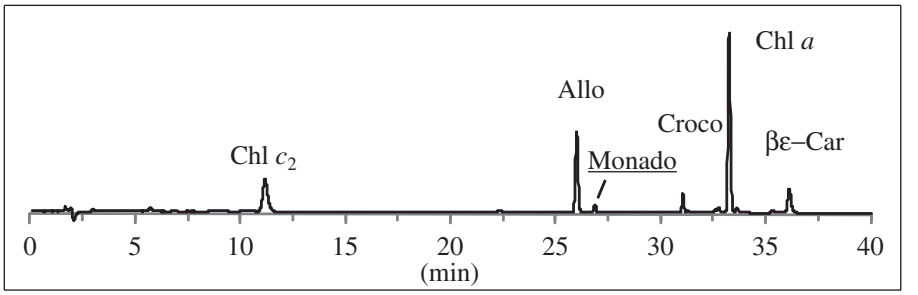


Biological occurrence	Minor pigment in cryptophytes; also present in two chlorophytes (see Chapter 1, this volume)
Source culture	*Chroomonas salina* (cryptophyte)
Alteration products	Easily isomerizes to the more stable 9-*cis* isomer [43]
Biosynthetically related to	Croco
Occurs together with	Allo, Croco

HPLC chromatogram of *Chroomonas salina* (system 1)



HPLC chromatogram of *Rhodomonas baltica* (system 2)

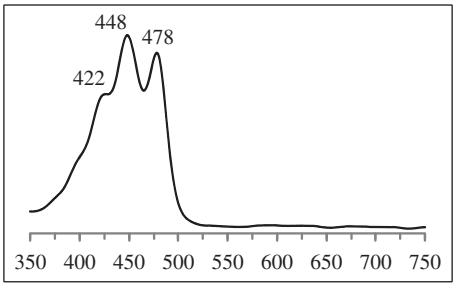


UV-Vis spectra (see also reference spectra below)

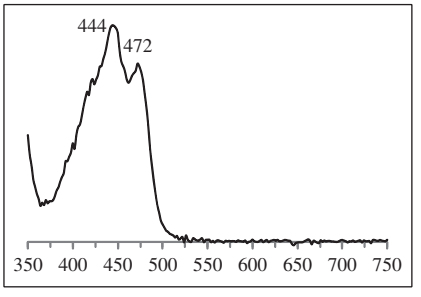
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Diethyl ether	428, *446*, 475	60	[133]
Ethanol	424, *447*, 477	n.d.	[37]
Hexane	422, *445*, 475	72	[35]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

Reference spectra

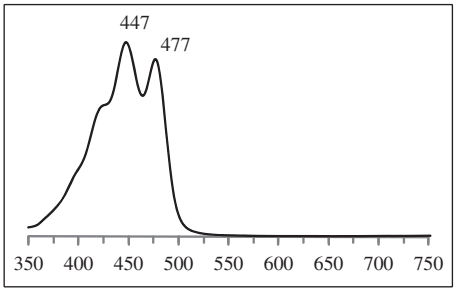
In acetone



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	566.411 $[M]^+$ (100), 548 $[M\text{-}18]^+$ (17), 533 $[M\text{-}18\text{–}15]^+$ (2), 530 $[M\text{-}18\text{–}18]^+$ (<1), 474 $[M\text{-}92]^+$ (4), 460 $[M\text{-}106]^+$ (2), 119 (34), 105 (42), 91 (56)	[43]

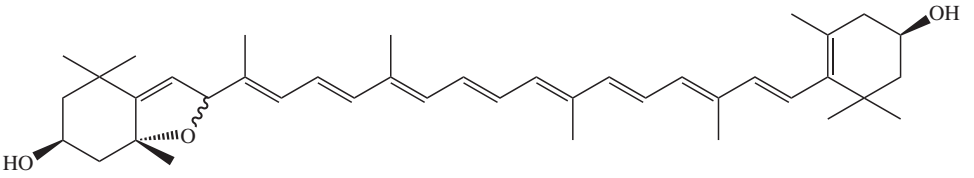
Remarks $d = 230\ L\ g^{-1}\ cm^{-1}$ (at 445 nm in hexane; calc. from Diadino) is recommended, as no value has been determined for Monado

Mutatoxanthin

Recommended abbreviation: Mutato (Mu)

IUPAC: (3*S*,5*R*,8*RS*,3′*R*)-5,8-Epoxy-5,8-dihydro-β,β-carotene-3,3′-diol

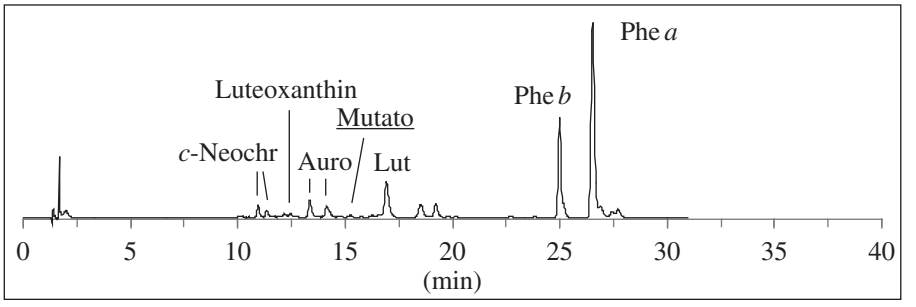
Molecular formula: $C_{40}H_{56}O_3$ **Molecular weight:** 584.87



Always occurs as a mixture of the two (3*S*,5*R*,8*R*,3′*R*) and (3*S*,5*R*,8*S*,3′*R*) optical isomers)

Alteration product of	Anth. The acid-catalysed rearrangement occurs in slightly acidic extracts, especially in prasinophyte extracts [91]
Source culture	*Dunaliella tertiolecta* (chlorophyte)
Alteration products	*Cis*-isomers
Synthetically related to	Anth
Occurs together with	Zea, Auro, Neochr

HPLC chromatogram of acidified *Dunaliella tertiolecta* (system 1)



HPLC chromatogram (system 2)

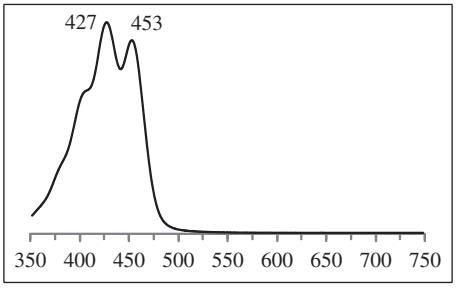
NO DATA AVAILABLE

UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Ethanol	404, *427*, 453	n.d.	[81]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		224 (at 430 nm, ethanol)	[119]

Reference spectra

In HPLC solvent system 1



In HPLC solvent system 2

NO DATA AVAILABLE

Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	584 $[M]^+$ (6), 566 $[M-18]^+$ (4), 550 $[M-34]^+$ (2), 504 $[M-80]^+$ (7), 492 $[M-92]^+$ (2), 221 (40), 181 (26), 43 (100)	[20]

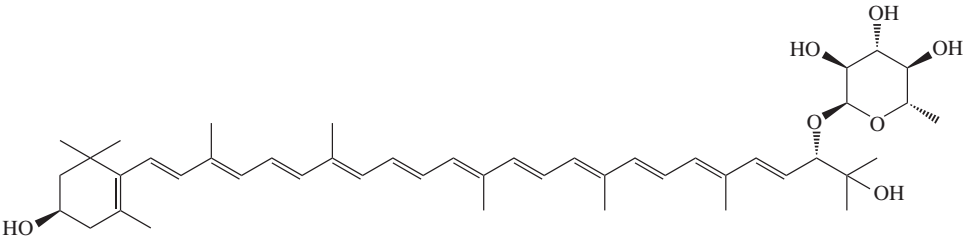
Remarks

Myxol quinovoside

Recommended abbreviation: Myxo (My)

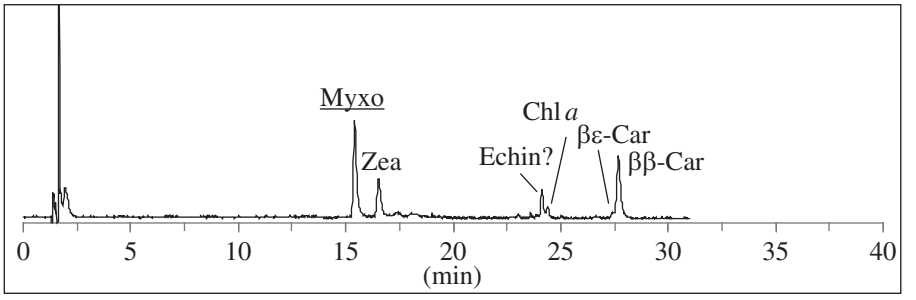
IUPAC: (3*R*,2′*S*)-2′-(6-Deoxy-α-L-glucopyranosyloxy)-3′,4′-didehydro-1′,2′-dihydro-β,ψ-carotene-3,1′-diol (trivial name: Myxoxanthophyll – see Remarks)

Molecular formula: $C_{46}H_{66}O_7$ **Molecular weight:** 731.01

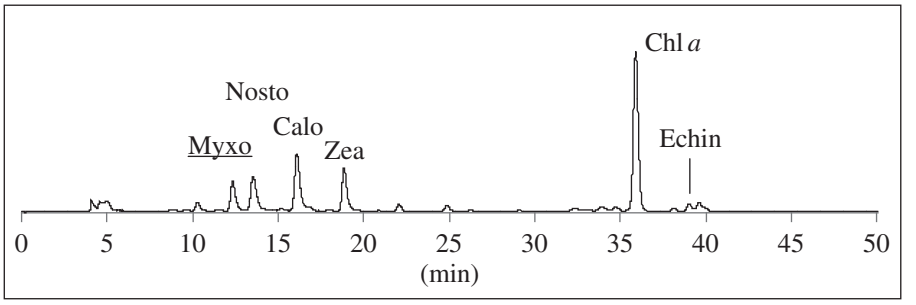


Biological occurrence	A dominant carotenoid in certain cyanobacteria (Cyano-1, Chapter 1)
Source culture	*Oscillatoria agardhii (rubescens)* (cyanobacteria)
Alteration products	*Cis*-isomers
Biosynthetically related to	βψ-Car, Kmyxo
Occurs together with	ββ-Car, Echin, Kmyxo, Oscil

HPLC chromatogram of *Synechococcus* sp. (system 1)



HPLC chromatogram of *Chlorogloeopsis fritschii* (system 3)

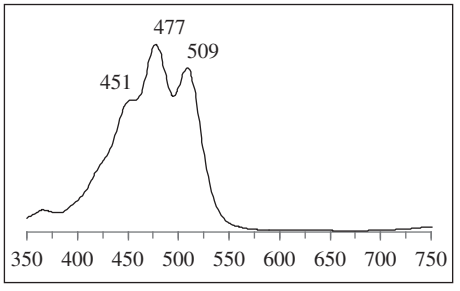


UV-Vis spectra (see also reference spectra below)

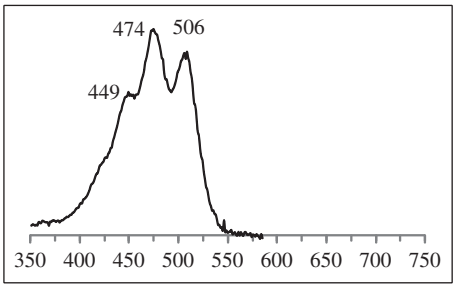
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(450), *478*, 510	57	[94]
Methanol	446, *472*, 502	55	[1]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		216 (at 478 nm, acetone) [94]	

Reference spectra

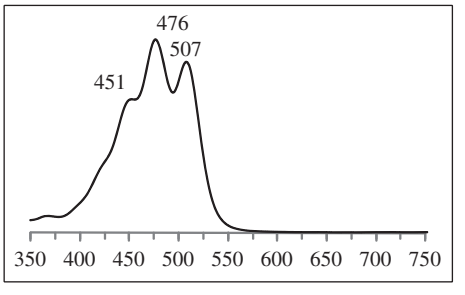
In acetone



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	730.4852 $[M]^+$ (2), 584 $[M\text{-}146]^+$ (2), 566 (7), 550 (8), 474 $[M\text{-}256]^+$ (3), 462 $[M\text{-}268]^+$ (8), 444 $[M\text{-}286]^+$ (15), 419 $[M\text{-}311]^+$ (7), 327 $[M\text{-}403]^+$ (15)	[94]

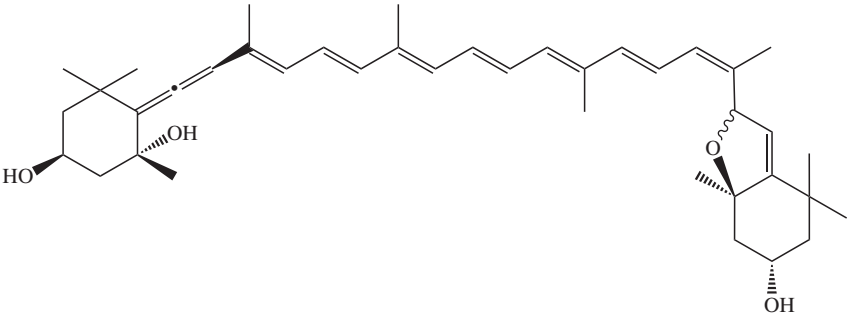
Remarks The name 'myxoxanthophyll' is recommended when the sugar moiety is unknown. Other myxol glycosides and 4-keto forms have been reported [1, 65, 142, 159]. Cyanobacterial myxoxanthophylls are unusual because they are glycosylated on the 2′-OH position of the ψ end of the molecule [80]

9′-*cis*-Neochrome

Recommended abbreviation: *c*-Neochr (*c*Nc)

IUPAC: 9′-*cis*-(3*S*,5*R*,6*R*,3′*S*,5′*R*,8′*RS*)-5′,8′-Epoxy-6,7-didehydro-5,6,5′,8′-tetrahydro-β,β-carotene-3,5,3′-triol

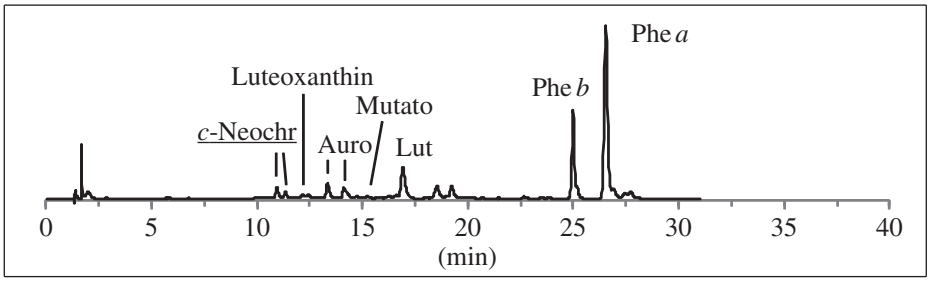
Molecular formula: $C_{40}H_{56}O_4$ **Molecular weight:** 600.87



(Always occurs as a mixture of the two (3*S*,5*R*,6*R*,3′*S*,5′*R*,8′*R*) and (3*S*,5*R*,6*R*,3′*S*,5′*R*,8′*S*) optical isomers)

Alteration product of	*c*-Neo. The acid-catalysed rearrangement occurs in slightly acidic extracts, especially in prasinophyte extracts [91]
Source culture	*Dunaliella tertiolecta* (chlorophyte)
Alteration products	*Trans*-isomer, other *cis*-isomers
Synthetically related to	*c*-Neo
Occurs together with	Auro, Mutato

HPLC chromatogram of acidified *Dunaliella tertiolecta* (system 1)



HPLC chromatogram (system 2)

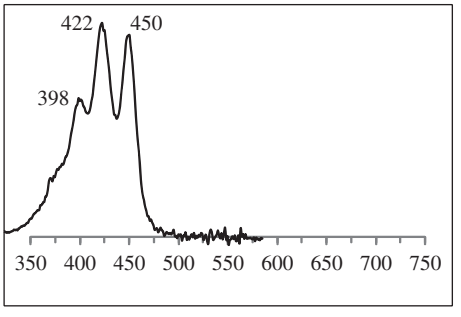
NO DATA AVAILABLE

UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	398, *422*, 450	88	[91]
Diethyl ether	399, 422, *449*	n.d.	[32]
Ethanol	401, *424*, 451	n.d.	[39]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		227 (at 424 nm, ethanol) [39]	

Reference spectra

In HPLC solvent system 1



In HPLC solvent system 2

NO DATA AVAILABLE

Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
	see Remarks		

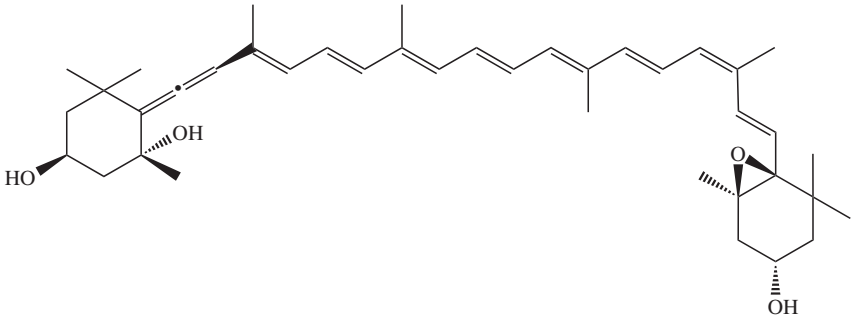
Remarks For MS, see *c*-Neo

9′-*cis*-Neoxanthin

Recommended abbreviation: *c*-Neo (*c*N)

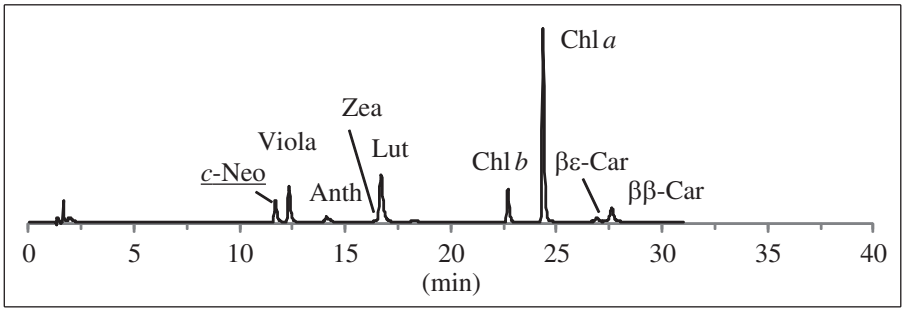
IUPAC: 9′-*cis*-(3*S*,5*R*,6*R*,3′*S*,5′*R*,6′*S*)-5′,6′-Epoxy-6,7-didehydro-5,6,5′,6′-tetrahydro-β,β-carotene-3,5,3′-triol

Molecular formula: $C_{40}H_{56}O_4$ **Molecular weight:** 600.87

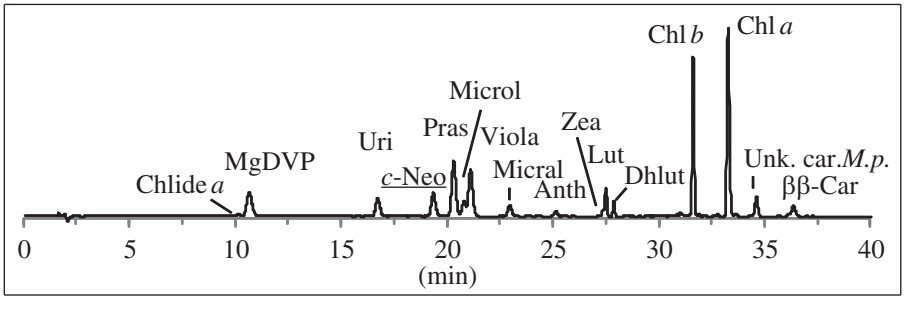


Biological occurrence	Dominant pigment in chlorophytes, prasinophytes and in dinoflagellates Pigment Type 5. Minor in euglenophytes, chlorarachniophytes and trebouxiophytes. Also in green leaves
Source culture	*Dunaliella tertiolecta* (chlorophyte)
Alteration products	Undergoes rearrangement to *c*-Neochr in weakly acidic solutions. *Trans*-isomer, *cis*-isomers
Biosynthetically related to	Zea, Anth, Viola, *t*-Neo
Occurs together with	Chl *b*, Lut, Viola, Zea

HPLC chromatogram of *Dunaliella tertiolecta* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)



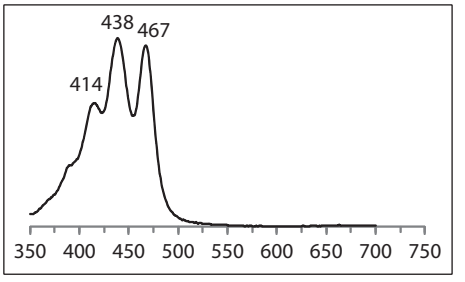
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	413, *438*, 466	87	[17]
Diethyl ether	414, *437*, 465	82	[91]
Ethanol	413, *437*, 466	87	[10]
Hexane	411, *435*, 463	97	[109]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		233 (at 437 nm, ethanol) [10]	

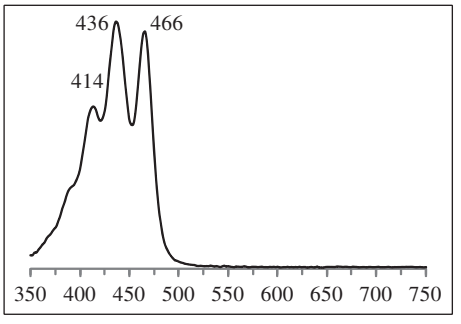
Reference spectra

For spectrum in acetone, see [109]

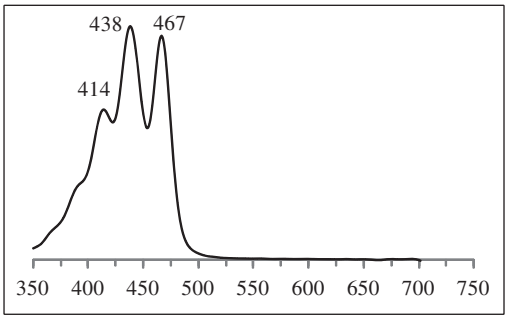
In ethanol



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	Magnetic sector	600 $[M]^+$ (100), 449 $[M\text{-}151]^+$ (6), 393 $[M\text{-}207]^+$ (20), 391 $[M\text{-}209]^+$ (12), 339 (10), 313 (9), 171 (12)	[28]

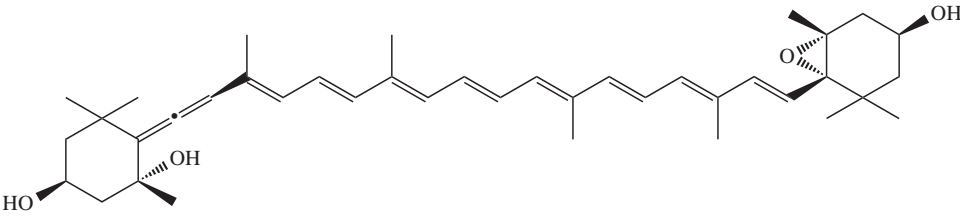
Remarks Do not confuse with all-*trans*-Neoxanthin (see its data sheet)

all-*trans*-Neoxanthin

Recommended abbreviation: ***t*-Neo (*t*N)**

IUPAC: (3*S*,5*R*,6*R*,3′*S*,5′*R*,6′*S*)-5′,6′-Epoxy-6,7-didehydro-5,6,5′,6′-tetrahydro-β,β-carotene-3,5,3′-triol

Molecular formula: $C_{40}H_{56}O_4$ **Molecular weight:** 600.87

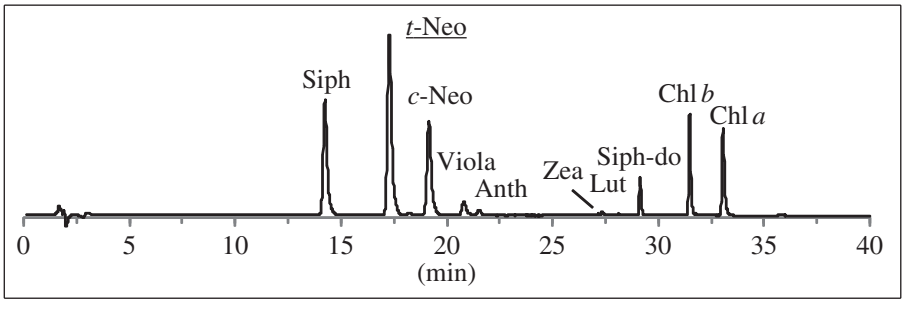


Biological occurrence	Dominant pigment in mesostigmatophytes. Also in various petals and fruits [158]
Source culture	*Mesostigma viride* (mesostigmatophyte) [177], NIES-296 [162]
Alteration products	Undergoes rearrangement to *trans*-Neochr in weakly acidic solutions. *Cis*-isomers
Biosynthetically related to	Zea, Anth, Viola, *c*-Neo
Occurs together with	Chl *b*, Siph esters, Viola

HPLC chromatogram (system 1)

NO DATA AVAILABLE

HPLC chromatogram of *Codium tomentosum* (system 2)



UV-Vis spectra (see also reference spectra below)

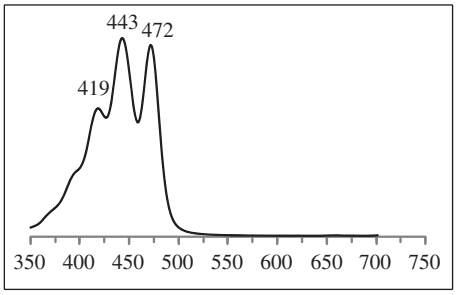
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	416, *440*, 469	84	[151]
Ethanol	418, *442*, 471	91	[9]
Hexane	416, *440*, 469	94	[109]
Recommended specific absorption coefficient *d* ($L\ g^{-1}cm^{-1}$)		238 (at 442 nm, ethanol) [9]	

Reference spectra

In HPLC solvent system 1

NO DATA AVAILABLE

In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
	see Remarks		

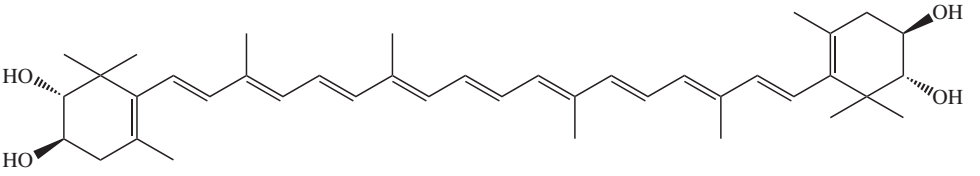
Remarks For MS, see *c*-Neo.
Occurs together with *c*-Neo in some prasinophytes [47]

Nostoxanthin

Recommended abbreviation: Nosto (Nos)

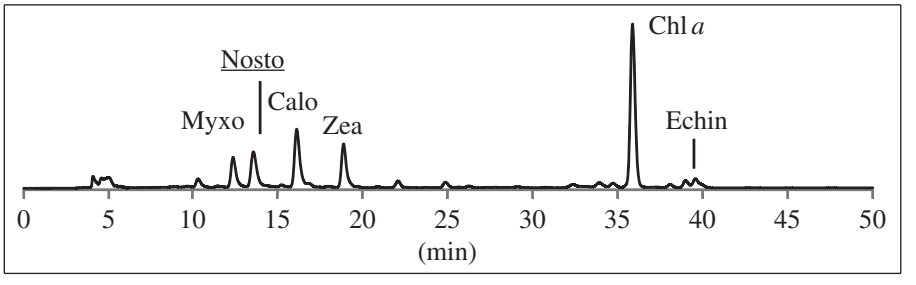
IUPAC: (2*R*,3*R*,2′*R*,3′*R*)-β,β-Carotene-2,3,2′,3′-tetrol

Molecular formula: $C_{40}H_{56}O_4$ **Molecular weight:** 600.87



Biological occurrence	Characteristic carotenoid from some cyanobacteria (Cyano-1, Chapter 1), e.g. *Anacystis nidulans* and *Chlorogloeopsis fritschii*
Source culture	*Chlorogloeopsis fritschii* (cyanobacteria)
Alteration products	*Cis*-isomers
Biosynthetically related to	ββ-Car, Zea, Calo
Occurs together with	Calo, Zea

HPLC chromatogram of *Chlorogloeopsis fritschii* (system 3)



HPLC chromatogram (system 2)

NO DATA AVAILABLE

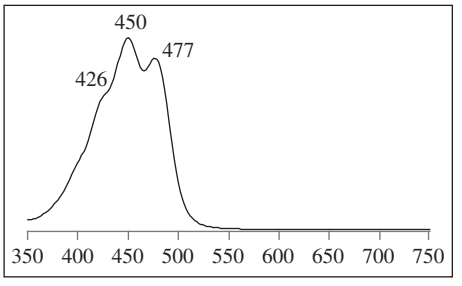
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(431), *453*, 480	n.d.	[33]
Ethanol	429, *449*, 477	n.d.	[117]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

Reference spectra
In acetone

NO DATA AVAILABLE

In HPLC solvent system 3



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	600 $[M]^+$ (100), 584 $[M\text{-}16]^+$ (31), 568 $[M\text{-}16\text{–}16]^+$ (2), 508 $[M\text{-}92]^+$ (11), 494 $[M\text{-}106]^+$ (2), 492 $[M\text{-}16\text{–}92]^+$ (2), 133 (22), 91 (33), 69 (25)	[33]

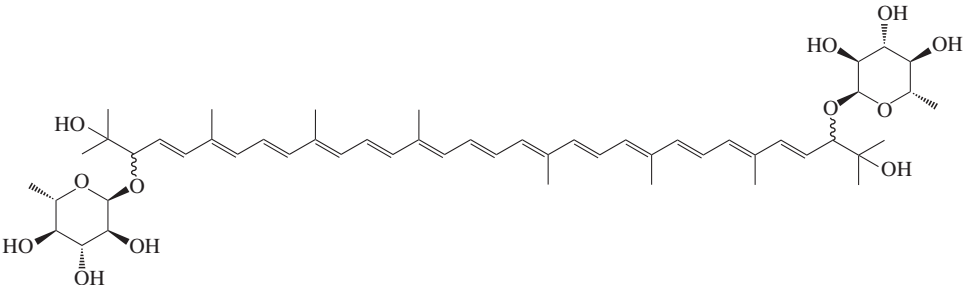
Remarks: $d = 232\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in ethanol; calc. from Zea) is recommended, as no value has been determined for Nosto

Oscillol diquinovoside

Recommended abbreviation: Oscil (O)

IUPAC: 2,2′-Di-(6-deoxy-α-L-glucopyranosyloxy)-3,4,3′,4′-tetradehydro-1,2,1′,2′-tetrahydro-ψ,ψ-carotene-1,1′-diol (trivial name: Oscillaxanthin – see Remarks)

Molecular formula: $C_{52}H_{76}O_{12}$ **Molecular weight:** 893.15

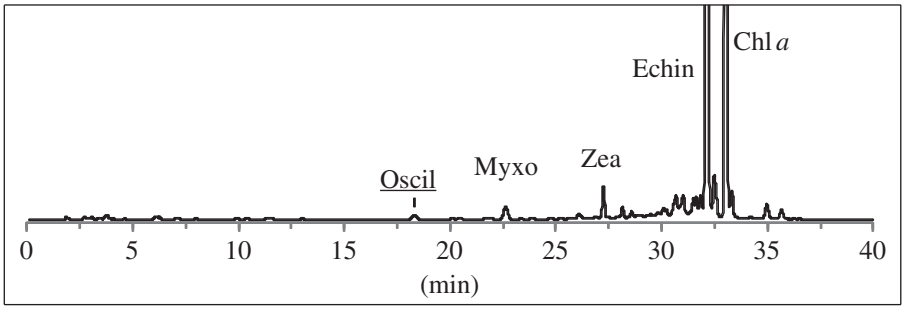


Biological occurrence	Characteristic carotenoid in some cyanobacteria (Cyano-1, Chapter 1)
Source culture	*Oscillatoria agardhii (rubescens)* (cyanobacteria)
Alteration products	*Cis*-isomers
Biosynthetically related to	Lyco
Occurs together with	ββ-Car, Echin, Myxo

HPLC chromatogram (system 1)

NO DATA AVAILABLE

HPLC chromatogram of *Oscillatoria agardhii* var. Kolbotnvatn (system 2)



UV-Vis spectra (see also reference spectra below)

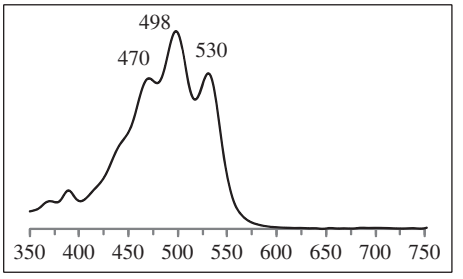
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	470, *499*, 534	n.d.	[67]
Ethanol	468, *492*, 526	59	[153]
Methanol	464, *491*, 525	42	[1]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		75 (at 490 nm, in 90% methanol: 10% pyridine) [95]	

Reference spectra

In HPLC solvent system 1

NO DATA AVAILABLE

In HPLC solvent system 2



Mass spectra

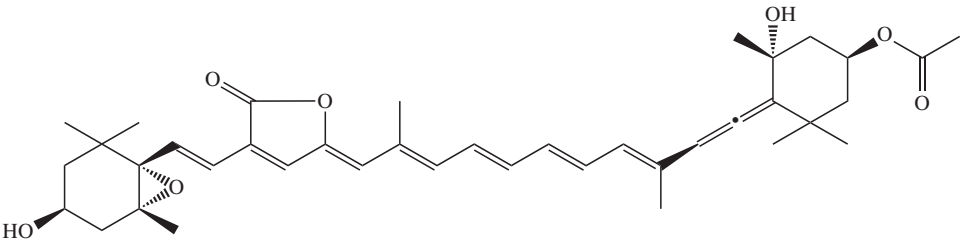
Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FD	Double focusing	892 $[M]^+$	[166]
Remarks	The name 'oscillaxanthin' is recommended when the sugar moiety is unknown. Other oscillol diglycosides have been reported [e.g. 1, 166]. Chirality at C-2,2′ is disputed [135, 165, 166]		

Peridinin

Recommended abbreviation: Peri (P)

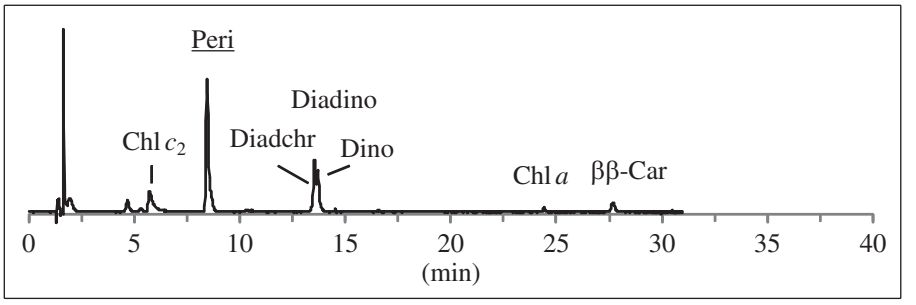
IUPAC: (3*S*,5*R*,6*S*,3′*S*,5′*R*,6′*R*)-5,6-Epoxy-3′-ethanoyloxy-3,5′-dihydroxy-6′,7′-didehydro-5,6,5′,6′-tetrahydro-12′,13′,20′-trinor-β,β-caroten-19,11-olide

Molecular formula: $C_{39}H_{50}O_7$ **Molecular weight:** 630.81

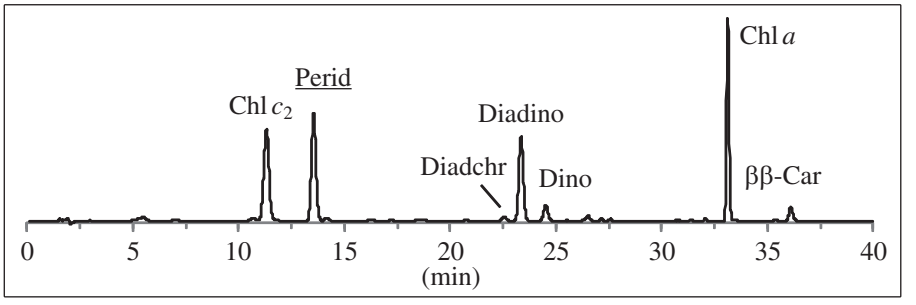


Biological occurrence	Major carotenoid in dinoflagellates Pigment Type 1 (Chapter 1)
Source culture	*Amphidinium carterae* (dinoflagellate)
Alteration products	Undergoes rearrangement to the corresponding furanoxide in acidic solutions, but Peri is more stable than other epoxides [115]. *Cis*-isomers
Biosynthetically related to	*trans*-Neo, Dino
Occurs together with	Chl c_2, Diadino, Diato, Dino, P457

HPLC chromatogram of *Gymnodinium catenatum* (system 1)



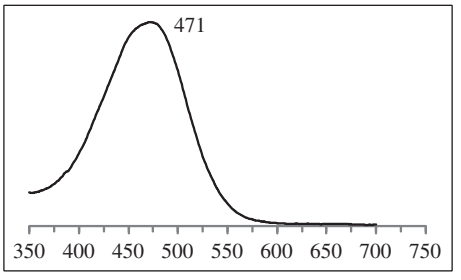
HPLC chromatogram of *Scrippsiella trochoidea* (system 2)



UV-Vis spectra (see also reference spectra below)

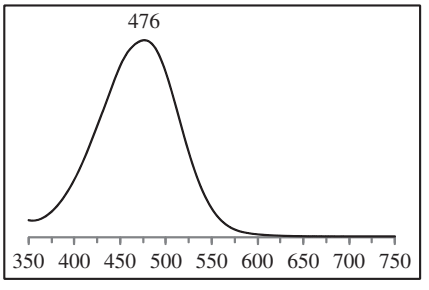
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	465	-	[118]
Ethanol	475	-	[150]
Hexane	(430), *454*, 483	74	[118]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		135 (at 475 nm, ethanol) [150] 134 (at 466 nm, acetone) [106]	

Reference spectra
In acetone

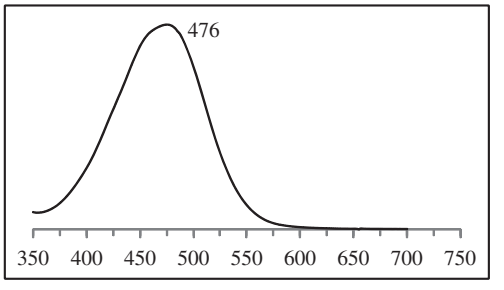


For spectrum in hexane and ethanol, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	630 $[M]^+$ (36), 612 $[M\text{-}18]^+$ (30), 594 $[M\text{-}18\text{–}18]^+$ (2), 570 $[M\text{-}60]^+$ (9), 552 $[M\text{-}18\text{–}60]^+$ (8), 538 $[M\text{-}92]^+$ (6), 234 (20), 221 (10), 181 (33), 169 (100)	[118]

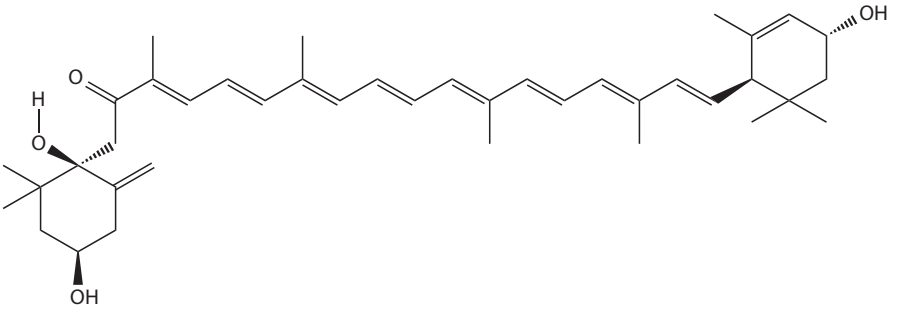
Remarks Peri furanoxide elutes right after Peri in HPLC solvent system 1

Prasinoxanthin

Recommended abbreviation: Pras (Pr)

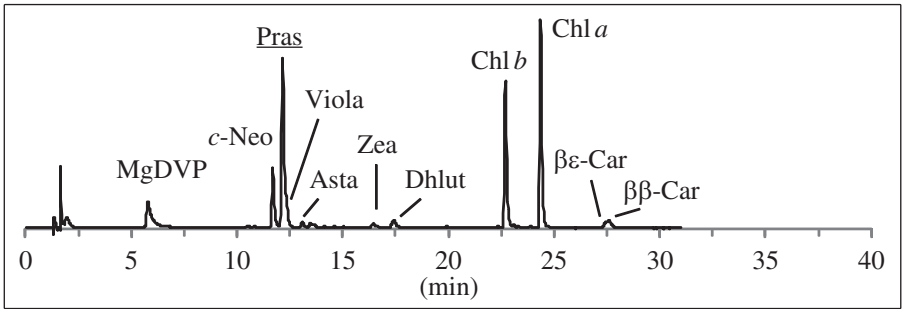
IUPAC: (3*S*,6*R*,3′*R*,6′*R*)-3,6,3′-Trihydroxy-7,8-dihydro-γ,ε-caroten-8-one

Molecular formula: $C_{40}H_{56}O_4$ **Molecular weight:** 600.87

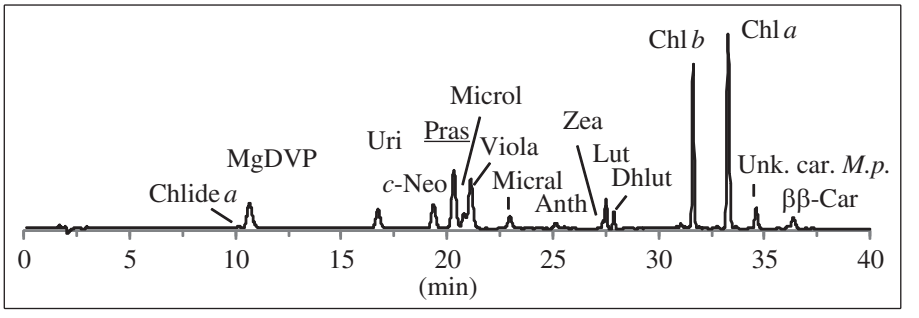


Biological occurrence	Dominant pigment in prasinophytes Pigment Types 3A and 3B. Occasionally found in dinoflagellates Pigment Type 5 (see Chapter 1, this volume)
Source culture	*Pycnococcus provasolii* (prasinophyte)
Alteration products	*Cis*-isomers
Biosynthetically related to	Lut?
Occurs together with	Chl *b*, ββ-Car, βε-Car, Dhlut, Micral, *cis*-Neo, *trans*-Neo, Uri

HPLC chromatogram of *Pycnococcus provasolii* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)



UV-Vis spectra (see also reference spectra below)

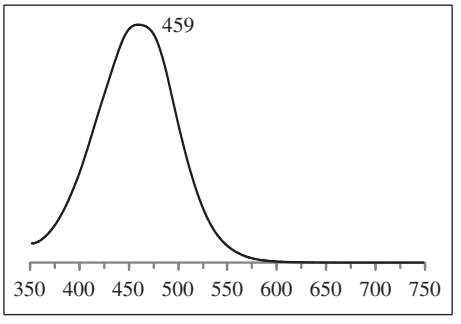
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(427), *448*, (468)	-	[51]
Diethyl ether	*446*, (466)	-	[62]
Ethanol	*451*, 470	1	[48]
Hexane	(429), *452*, (480)	-	[52]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

Reference spectra

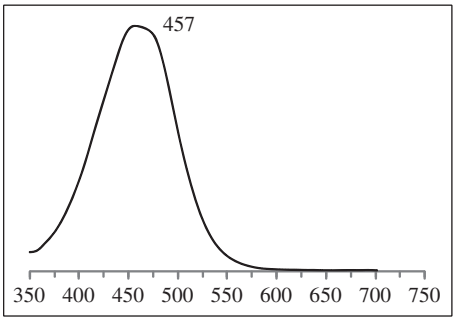
For spectrum in acetone, see [109]

For spectrum in hexane, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	600 $[M]^+$ (2), 582 $[M\text{-}18]^+$ (2), 446.3186 $[M\text{-}154]^+$ (100), 428 $[M\text{-}154\text{–}18]^+$ (21), 308 $[M\text{-}154\text{–}138]^+$ (6)	[51]

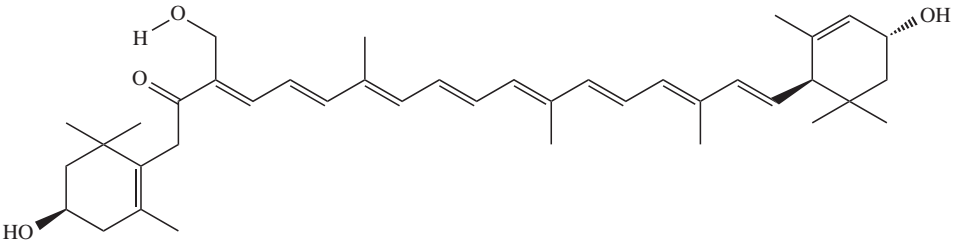
Remarks $d = 182\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in acetone, calc. from Fuco) is recommended, as no value has been determined for Pras

Siphonaxanthin

Recommended abbreviation: Siph (S)

IUPAC: (3*R*,3′*R*,6′*R*)-3,19,3′-Trihydroxy-7,8-dihydro-β,ε-caroten-8-one

Molecular formula: $C_{40}H_{56}O_4$ **Molecular weight:** 600.87

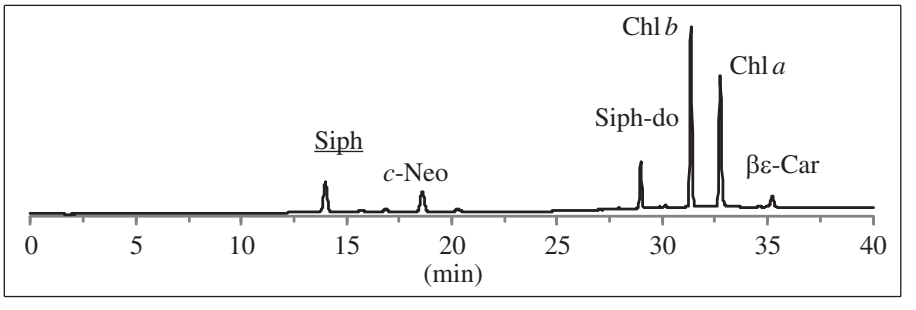


Biological occurrence	Dominant pigment in prasinophytes Pigment Type 2B and mesostigmatophytes. Minor in chlorophytes Pigment Type 2 (see Chapter 1, this volume). Also in siphonous green seaweeds
Source culture	*Mesostigma viride* (mesostigmatophyte) [177], NIES-296 [162]
Alteration products	*Cis*-isomers
Biosynthetically related to	Lut, Loro, Siph esters
Occurs together with	Chl *b*, Neo, Siph esters

HPLC chromatogram (system 1)

NO DATA AVAILABLE

HPLC chromatogram of *Codium fragile* (system 2)



UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	*441*, (461)	–	[50]
Diethyl ether	*441*, (464)	–	[58]
Ethanol	~448	–	[169]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

Reference spectra

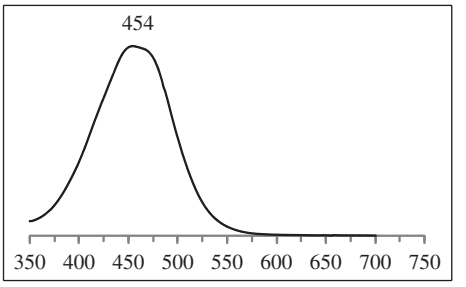
For spectrum in acetone, see [109]

For spectrum in hexane, see [109]

In HPLC solvent system 1

NO DATA AVAILABLE

In HPLC solvent system 2



Mass spectra

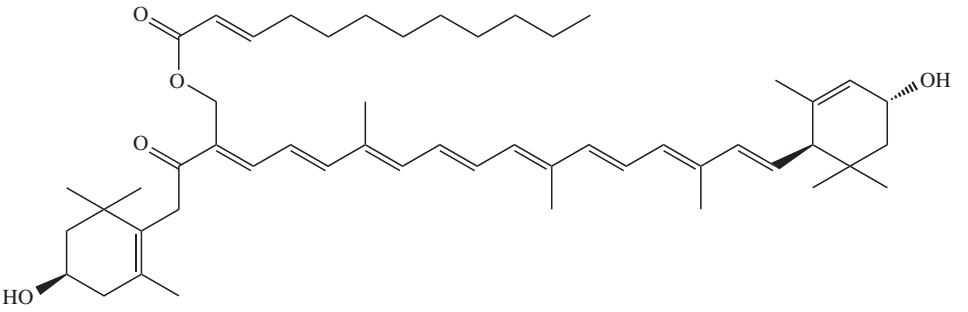
Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	600 $[M]^+$ (100), 584 $[M-16]^+$ (9), 582 $[M-18]^+$ (19), 572 $[M-28]^+$ (8), 564 $[M-18-18]^+$ (4), 494 $[M-106]^+$ (1)	[58]

Remarks $d = 182\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in acetone, calc. from Fuco) is recommended, as no value has been determined for Siph

Siphonaxanthin dodecenoate **Recommended abbreviation: Siph-do (Sdo)**

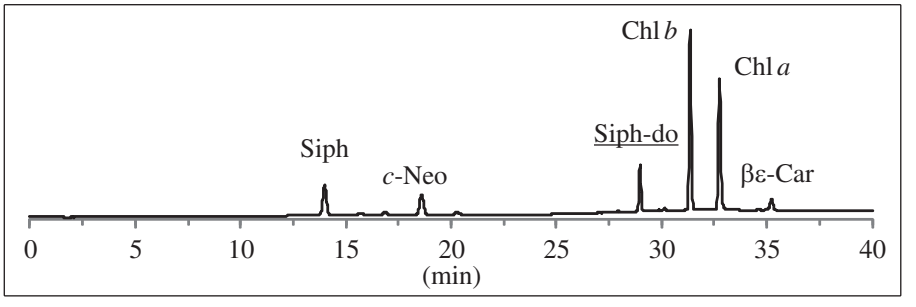
IUPAC: (3*R*,3′*R*,6′*R*)-19-(*trans*-Dodec-2-enoyloxy)-3,3′-dihydroxy-7,8-dihydro-β,ε-caroten-8-one

Molecular formula: $C_{52}H_{76}O_5$ **Molecular weight:** 781.16

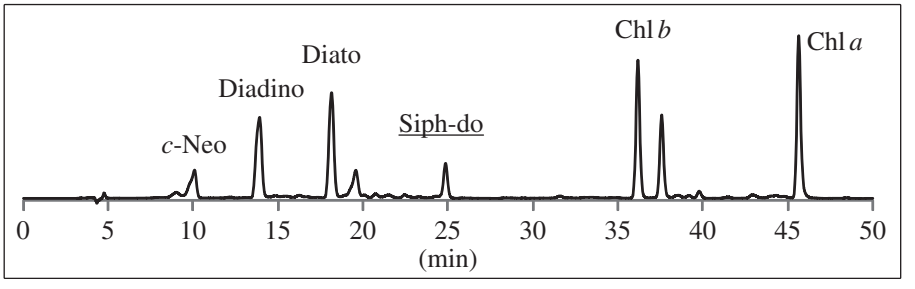


Biological occurrence	Dominant pigment (esters) in mesostigmatophytes, occasional in prasinophytes Pigment Type 2B and minor in chlorophytes Pigment Type 2. Also in siphonous green seaweeds
Source culture	*Pyramimonas amylifera* (prasinophyte) [50], PLY 246 [163]
Alteration products	*Cis*-isomers
Biosynthetically related to	Lut, Loro, Loro-d, Siph
Occurs together with	Chl *b*, Hsiph esters, Neo, Siph, Viola

HPLC chromatogram *Codium fragile* (system 2)



HPLC chromatogram of *Eutreptiella gymnastica* (system 3)

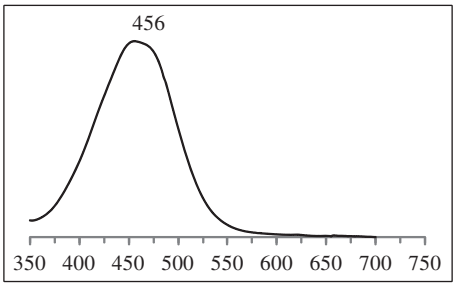


UV-Vis spectra (see also reference spectra below)

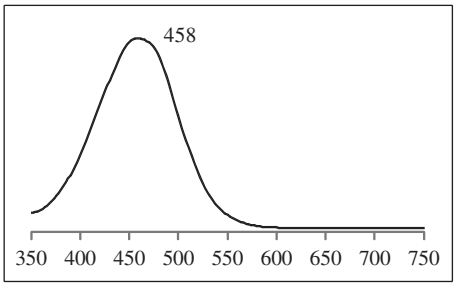
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	*448*, (463)	-	[50]
Diethyl ether	448	-	[58]
Ethanol	456	-	[169]
Recommended specific absorption coefficient *d* ($L\ g^{-1}cm^{-1}$)		n.d., see Remarks	

Reference spectra

In HPLC solvent system 2



In HPLC solvent system 3



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	780 $[M]^+$ (59), 762 $[M\text{-}18]^+$ (29), 688 $[M\text{-}92]^+$ (5), 582 $[M\text{-}180\text{–}18]^+$ (42), 568 $[M\text{-}180\text{–}18\text{–}18]^+$ (56), 180 (100)	[50]

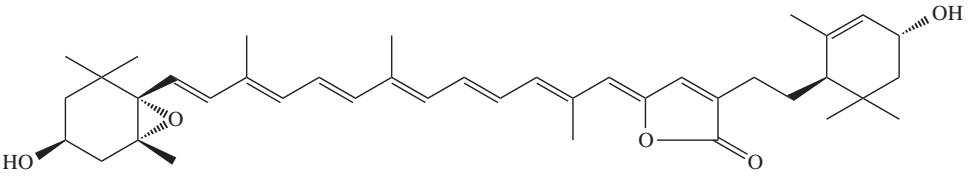
Remarks The name 'Siphonein' was erroneously given to this compound in earlier studies [31]. Other esters of siphonaxanthin and 6′-hydroxysiphonaxanthin have also been encountered [50, 175, 176], including siphonein (= Siph 19-dodecanoate). $d = 140\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in acetone, calc. from Fuco) is recommended, as no value has been determined for Siph-do

Uriolide

Recommended abbreviation: Uri (U)

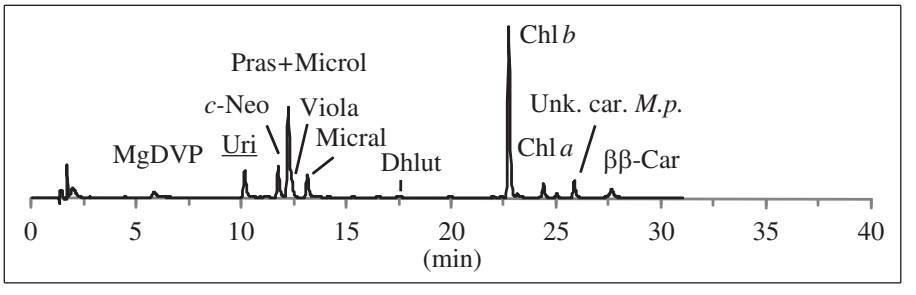
IUPAC: (3*S*,5*R*,6*S*,3′*R*,6′*R*)-5,6-Epoxy-3,3′-dihydroxy-5,6,7′,8′-tetrahydro-β,ε-caroten-19′,11′-olide

Molecular formula: $C_{40}H_{54}O_5$ **Molecular weight:** 614.85

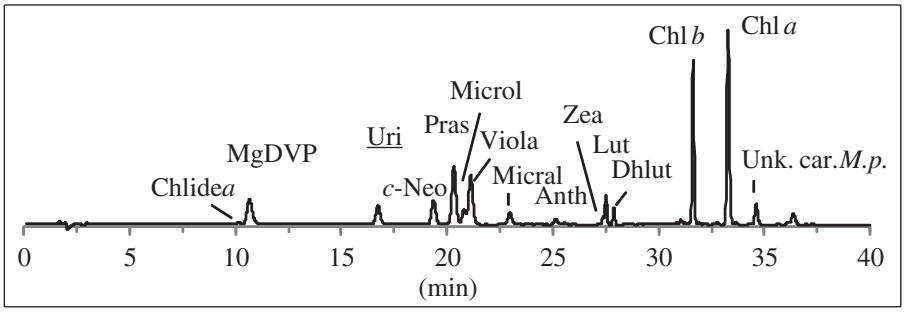


Biological occurrence	Dominant pigment in prasinophytes Pigment Type 3B (see Chapter 1, this volume)
Source culture	*Mantoniella squamata* (prasinophyte) [48], CCAP1965/1 [42]
Alteration products	Undergoes rearrangement to Uri-fur in weakly acidic solutions. *Cis*-isomers
Biosynthetically related to	Dhlut, Microl, Micral
Occurs together with	Chl *b*, MgDVP, Dhlut, Micral, Microl, Neo, Pras

HPLC chromatogram of *Micromonas pusilla* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)

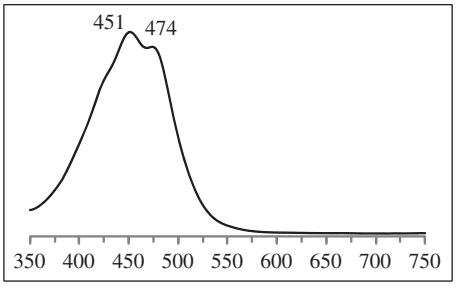


UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	*448*, 472	11	[63]
Hexane	(427), *448*, 478	38	[63]
Methanol	*448*, 470	2	[63]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

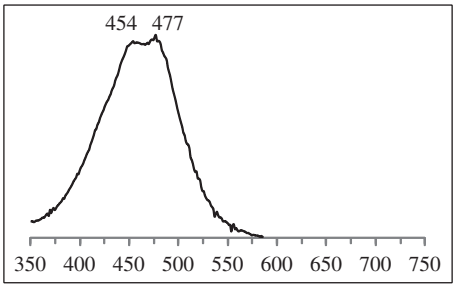
Reference spectra

In acetone

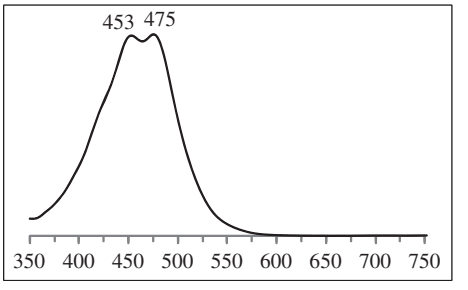


NO DATA AVAILABLE

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	614 $[M]^+$ (30), 596 $[M\text{-}18]^+$ (50), 534 $[M\text{-}80]^+$ (25), 522 $[M\text{-}92]^+$ (35), 516 $[M\text{-}80\text{–}18]^+$ (25), 504 $[M\text{-}92\text{–}18]^+$ (15), 221 (100)	[63]

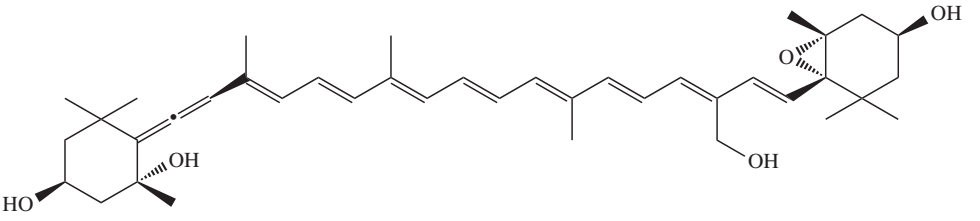
Remarks $d = 140\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in ethanol) is recommended, as no value has been determined for Uri. Uriolide furanoxide forms in slightly acidic conditions, which usually occur with prasinophyte extracts [63]

Vaucheriaxanthin

Recommended abbreviation: Vauch (Va)

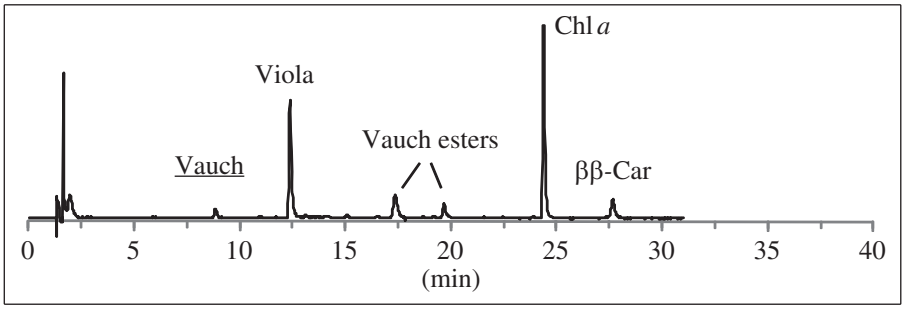
IUPAC: (3*S*,5*R*,6*R*,3′*S*,5′*R*,6′*S*)-5′,6′-Epoxy-6,7-didehydro-5,6,5′,6′-tetrahydro-β,β-carotene-3,5,3′,19′-tetrol

Molecular formula: $C_{40}H_{56}O_5$ **Molecular weight:** 616.87

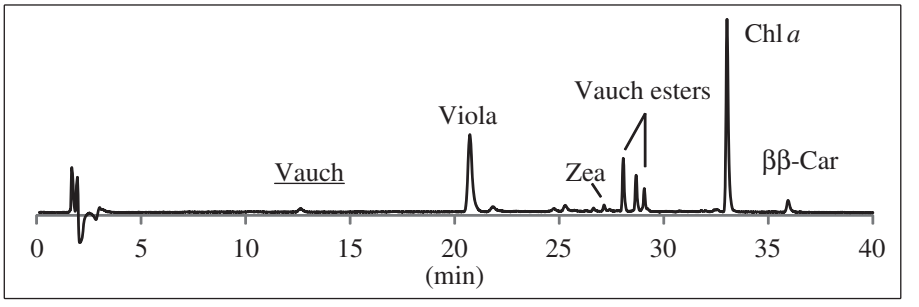


Biological occurrence	Dominant pigment in eustigmatophytes (see Chapter 1)
Source culture	*Nannochloropsis oculata* (eustigmatophyte)
Alteration products	Undergoes rearrangement to Vauchfur in weakly acidic solutions [91]. *Cis*-isomers
Biosynthetically related to	Zea, Anth, Viola, Neo, Vauch-eo, Vauch esters
Occurs together with	Vauch esters

HPLC chromatogram of *Nannochloropsis oculata* (system 1)



HPLC chromatogram of *Nannochloropsis gaditana* (system 2)



UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	416, *438*, 466	54	[47]
Ethanol	419, *442*, 471	78	[152]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks.	

Reference spectra

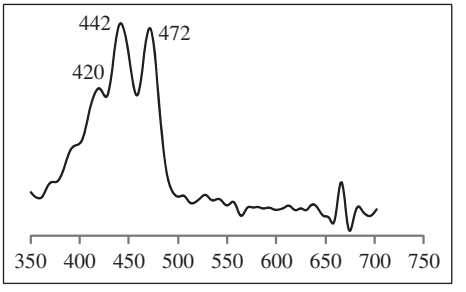
For spectrum in acetone, see [109]

For spectrum in hexane, see [109]

In HPLC solvent system 1

NO DATA AVAILABLE

In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	616 $[M]^+$ (11), 598 $[M\text{-}18]^+$ (11), 580 $[M\text{-}18\text{–}18]^+$ (19), 562 $[M\text{-}18\text{–}18\text{–}18]^+$ (30), 544 $[M\text{-}18\text{–}18\text{–}18\text{–}18]^+$ (21), 197 (73), 181 (100)	[47]

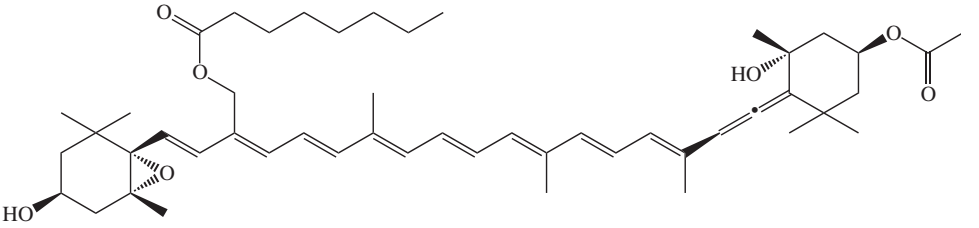
Remarks $d = 232\ L\ g^{-1}\ cm^{-1}$ (at 442 nm, ethanol) is recommended (calc. from *trans*-Neo), as no value has been determined for Vauch. Vaucheriaxanthin furanoxide is formed in slightly acidic extracts [91]

Vaucheriaxanthin ethanoate octanoate

Recom. abbreviation: Vauch-eo

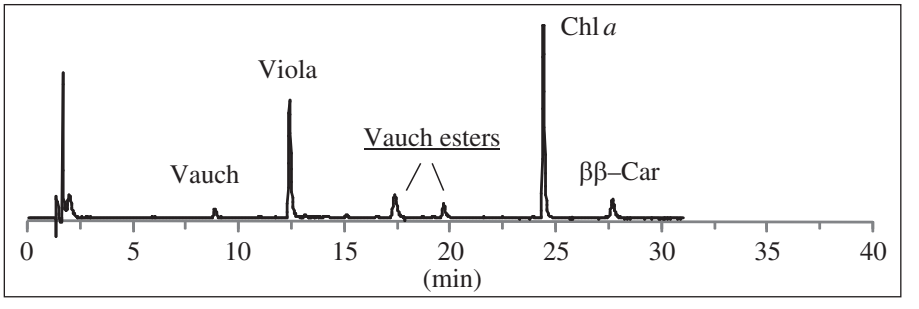
IUPAC: (3*S*,5*R*,6*S*,3′*S*,5′*R*,6′*R*)-5,6-Epoxy-3′-ethanoyloxy-19-octanoyloxy-6′,7′-didehydro-5,6,5′,6′-tetrahydro-β,β-carotene-3,5′-diol

Molecular formula: $C_{50}H_{72}O_7$ **Molecular weight:** 785.10

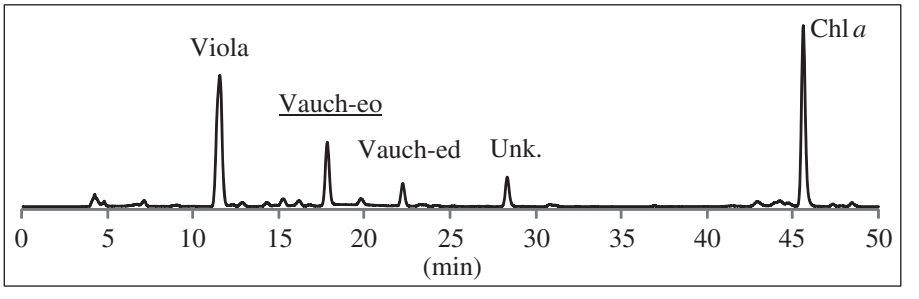


Biological occurrence	Dominant pigment in eustigmatophytes, minor in xanthophytes (see Chapter 1, this volume)
Source culture	*Nannochloropsis oculata* (eustigmatophyte)
Alteration products	Undergoes rearrangement to Vauch-eo-fur in weakly acidic solutions [91]. *Cis*-isomers
Biosynthetically related to	Zea, Anth, Viola, Neo, Vauch
Occurs together with	Vauch

HPLC chromatogram of *Nannochloropsis oculata* (system 1)



HPLC chromatogram of *Nannochloropsis oculata* (system 3)



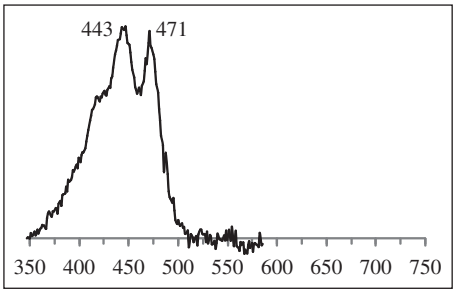
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	422, *445*, 471	33	[47]
Ethanol	419, *442*, 471	80	[152]
Hexane	419, *442*, 471	64	[109]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d., see Remarks.	

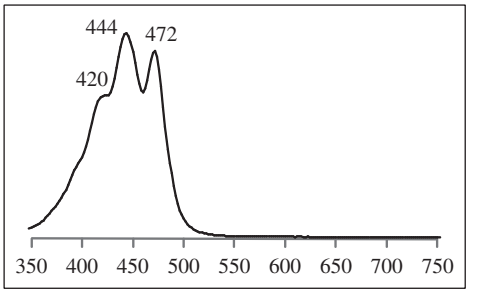
Reference spectra

For spectrum in acetone, see [109] For spectrum in hexane, see [109]

In HPLC solvent system 1



In HPLC solvent system 3



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	784 $[M]^+$ (6), 766 $[M\text{-}18]^+$ (3), 706 $[M\text{-}18\text{–}60]^+$ (2), 640 $[M\text{-}18\text{–}126]^+$ (15), 197 (58), 181 (100)	[47]

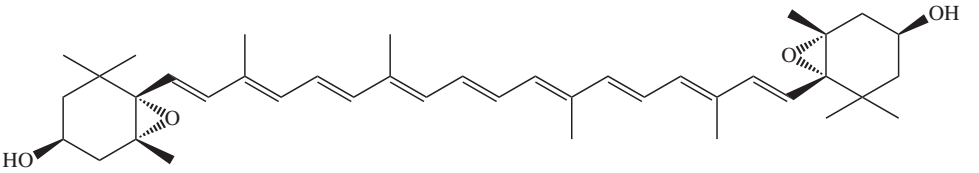
Remarks Former name: vaucheriaxanthin 3-acetate 19′-octanoate. Found also in mixture with vaucheriaxanthin ethanoate decanoate (Vauch-ed) [47]. Other esters and their acid-catalysed forms exist: [91]. $d = 182$ L g^{-1} cm^{-1} (at 442 nm, ethanol) is recommended (calc. from *trans*-Neo), as no value has been determined for Vauch-eo

Violaxanthin

Recommended abbreviation: Viola (V)

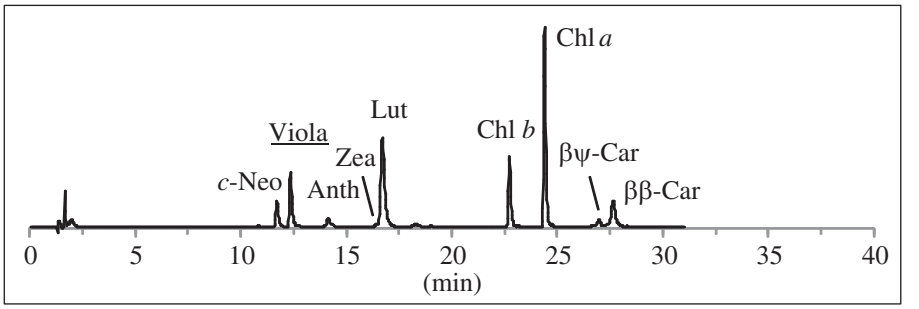
IUPAC: (3*S*,5*R*,6*S*,3′*S*,5′*R*,6′*S*)-5,6:5′,6′-Diepoxy-5,6,5′,6′-tetrahydro-β,β-carotene-3,3′-diol

Molecular formula: $C_{40}H_{56}O_4$ **Molecular weight:** 600.87

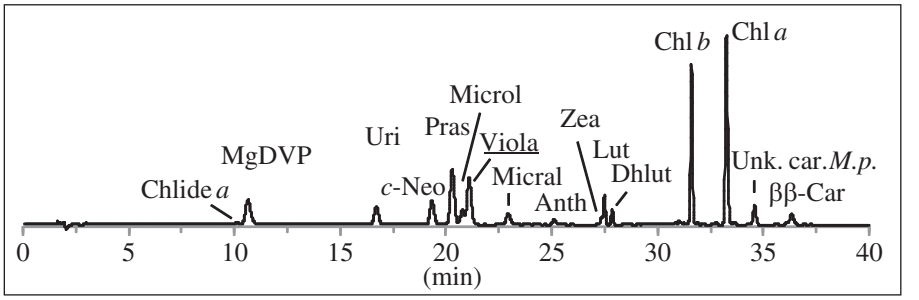


Biological occurrence	Dominant pigment in chrysophytes, eustigmatophytes, synurophytes, mesostigmatophytes, chlorophytes, prasinophytes, and dinoflagellates Pigment Type 5. Minor in chlorarachniophytes, pinguiophytes and raphidophytes (see Chapter 1, this volume). Also present in higher plants and brown seaweeds
Source culture	*Dunaliella tertiolecta* (chlorophyte)
Alteration products	Undergoes rearrangement to Luteoxanthin and Auro in weakly acidic solutions. *Cis*-isomers
Biosynthetically related to	ββ-Car, Cryp, Zea, Anth, Neo
Occurs together with	Anth, Neo

HPLC chromatogram of *Dunaliella tertiolecta* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)

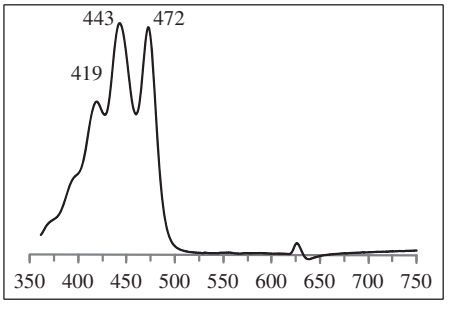


UV-Vis spectra (see also reference spectra below)

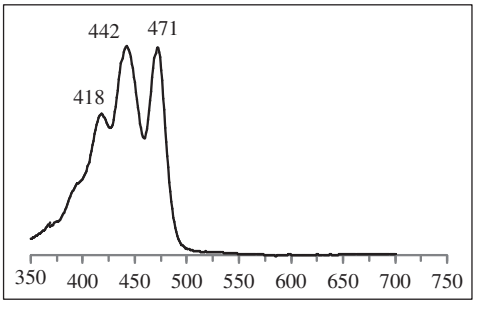
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	415, *438*, 467	79	[91]
Ethanol	417, *440*, 469	93	[152]
Hexane	417, *440*, *470*	100	[145]
Methanol	415, *436*, 466	90	[160]
Recommended specific absorption coef. *d* (L $g^{-1}cm^{-1}$)	254 (at 437 nm in diethyl ether:methylbutane:ethanol 5:5:2) [4] 255 (at 443 nm in ethanol) [44]		

Reference spectra

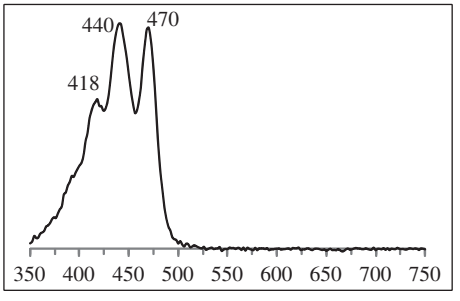
In acetone



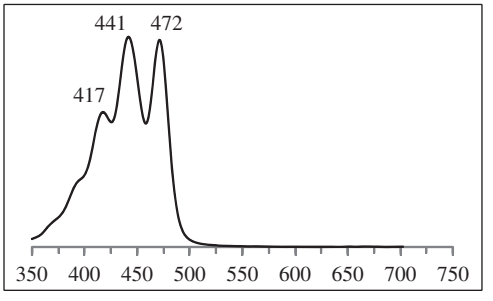
In ethanol



In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
CI	Magnetic sector	601 $[M+1]^+$ (47), 583 $[M+1–18]^+$ (36), 565 $[M+1–18–18]^+$ (22), 510 (35), 509 $[M+1–92]^+$, 221 (27), 181 (100)	[4]

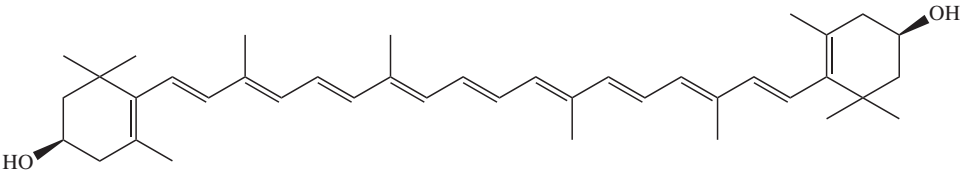
Remarks Part of a 'xanthophyll cycle': see Chapter 11. May be present in diatoms under prolonged high light stress [123]. Transforms into luteoxanthin and auroxanthin in slightly acidic extracts, particularly in prasinophytes [91]

Zeaxanthin

Recommended abbreviation: Zea (Z)

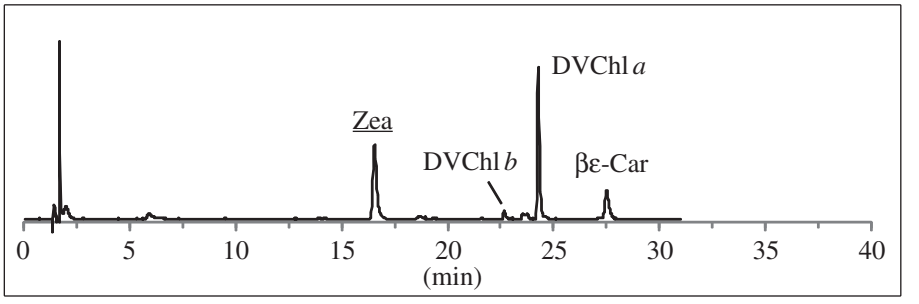
IUPAC: (3*R*,3′*R*)-β,β-Carotene-3,3′-diol

Molecular formula: $C_{40}H_{56}O_2$ **Molecular weight:** 568.87

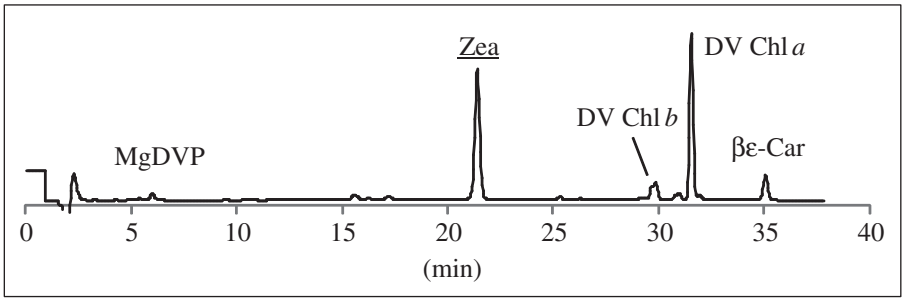


Biological occurrence	Dominant pigment in cyanobacteria, chrysophytes, eustigmatophytes, pelagophytes, rhodophytes and dinoflagellates Pigment Type 5. Minor in pinguiophytes, raphidophytes, chlorarachniophytes, chlorophytes, prasinophytes and trebouxiophytes. Occasional in dictyochophytes and dinoflagellates Pigment Type 3 (see Chapter 1, this volume)
Source culture	*Synechococcus* sp. (DC-2) (cyanobacteria)
Alteration products	*Cis*-isomers
Biosynthetically related to	ββ-Car, Cryp, Anth, Viola, Neo
Occurs together with	

HPLC chromatogram of *Prochlorococcus* sp. (system 1)



HPLC chromatogram of *Prochlorococcus* sp. (system 2)



UV-Vis spectra (see also reference spectra below)

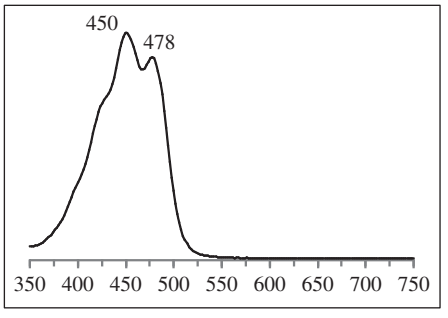
Solvent	λ_{max} (nm)	Band ratio (% III:II)	Ref.
Acetone	(428), *454*, 481	33	[145]
Ethanol	(428), *450*, 478	26	[152]
Hexane	(424), *450*, 478	46	[145]
Methanol	(429), *449*, 475	25	[160]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		245 (at 453 nm, ethanol) [148]	

Reference spectra

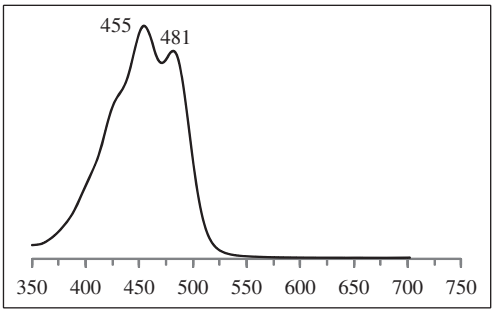
For spectrum in acetone, see [109]

For spectrum in hexane, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
EI	Magnetic sector	568 $[M]^+$ (100), 550 $[M\text{-}18]^+$ (84), 532 $[M\text{-}18\text{–}18]^+$ (5), 489 $[M\text{-}79]^+$ (1), 476 $[M\text{-}92]^+$ (13), 462 $[M\text{-}106]^+$ (1), 458 $[M\text{-}18\text{–}92]^+$ (11), 410 $[M\text{-}158]^+$ (5)	[19]
Remarks	Part of a 'xanthophyll cycle' – see Chapter 11, this volume. May be present in diatoms under prolonged high light stress [123]		

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