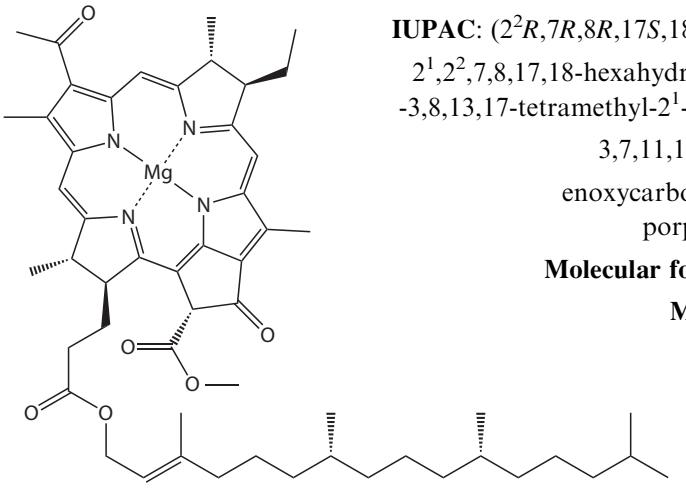
1 Chlorophylls

Bacteriochlorophyll *a*

Recommended abbreviation: BChl *a* (BCa)



IUPAC: (2^2R,7*R*,8*R*,17*S*,18*S*)-12-Ethanoyl-7-ethyl-2^1,2^2,7,8,17,18-hexahydro-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxo-18-{2-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-enoxycarbonyl]ethyl}cyclopenta[*at*]porphyrinatomagnesium(II)

Molecular formula: $C_{55}H_{74}N_4O_6Mg$

Molecular weight: 911.50

Biological occurrence	Chloroflexaceae, Chlorobiaceae and purple bacteria [141]
Source culture	*Rhodobacter sulfidophilus* (photosynthetic bacteria)
Alteration products	Various derivatives as for Chl *a* and Chl *b*
Biosynthetically related to	Chlide *a*, MgDVP
Occurs together with	See Table 3 in [120] for an overview

UV-Vis spectra

Solvent	**λ_{max} (nm)**	**Band ratio (blue:red ratio)**	**Ref.**
Acetone	358, 577, *770*	0.94	[140]
Diethyl ether	357, 392, 573, *770*	0.76	[140]
Ethanol	366, 607, *773*	0.94	[140]
Methanol	364, 530, 609, 695, *771*	0.79	[170]
Recommended specific absorption coefficient *d* ($L\,g^{-1}\,cm^{-1}$)		75.9 (at 770 nm, acetone) [140]	

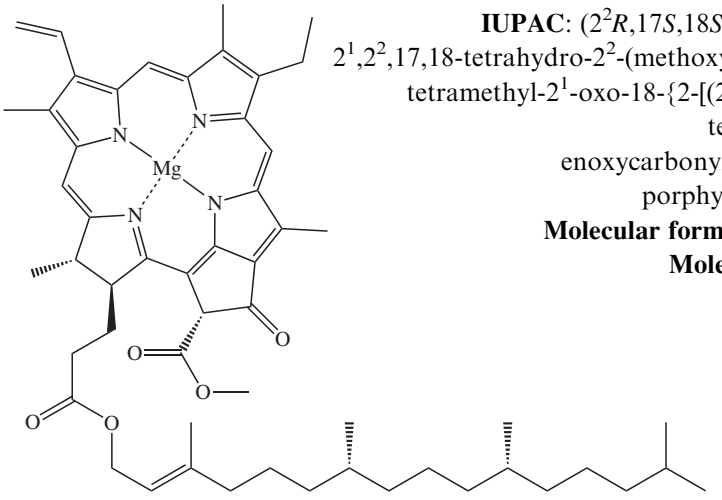
Mass spectra

Ionization technique	**Mass analyser type**	**Diagnostic ions (m/z, rel. intensity)**	**Ref.**
MALDI	TOF	910 $[M]^+ \rightarrow$ 632 $[M\text{-phytyl}]^+$	[156]

Remarks	Fluorescence: excitation 360 nm, emission 795 nm (ethanol) [40] Several other bacteriochlorophylls present in bacteria: see [141]

Chlorophyll *a*

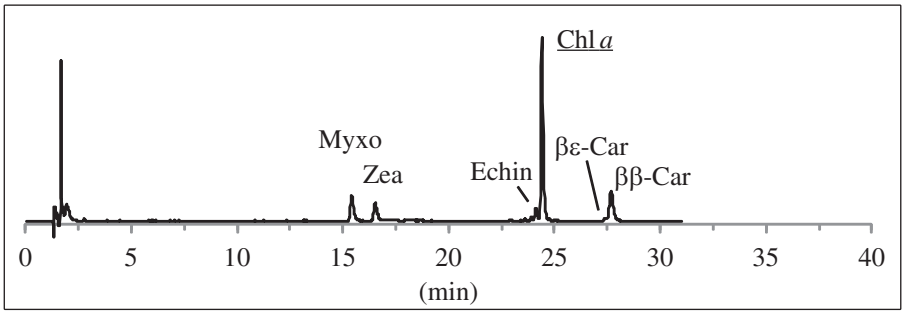
Recommended abbreviation: Chl *a* (C*a*)



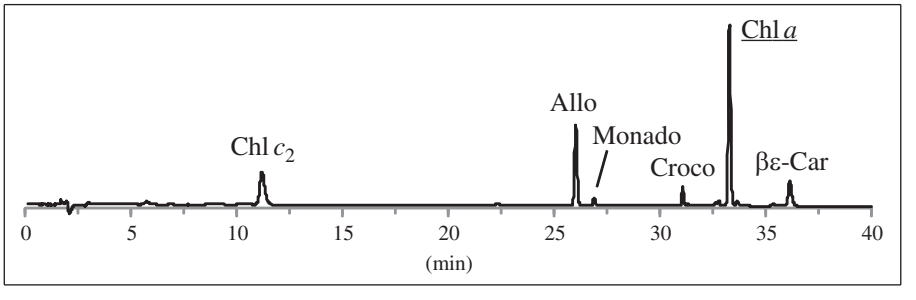
IUPAC: (2^2*R*,17*S*,18*S*)-12-Ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxo-18-{2-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-enoxycarbonyl]ethyl}cyclopenta[*at*]porphyrinatomagnesium(II)
Molecular formula: $C_{55}H_{72}N_4O_5Mg$
Molecular weight: 893.49

Biological occurrence	Characteristic pigment in all photosynthetic algae and plants
Source culture	*Chroomonas salina* (cryptophyte)
Alteration products	Chlide *a*, Pheide *a*, Phe *a*, Chl *a*′, Chl *a* allo, Pyro derivatives
Biosynthetically related to	Chl *b*, MgDVP
Occurs together with	

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



HPLC chromatogram of *Rhodomonas baltica* (system 2)

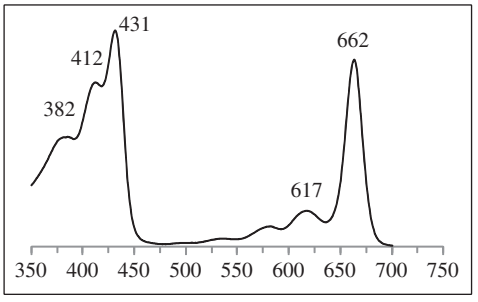


UV-Vis spectra (see also reference spectra below)

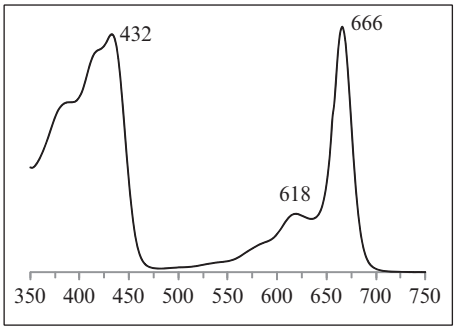
Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	383, 411, *430*, 534, 580, 617, 662	1.2	[145]
Diethyl ether	409, *428*, 495, 530, 575, 614, 660	1.3	[98]
95% Ethanol	414, 432, 618, 649, *664*	0.99	[121]
Methanol	432, 618, 652, *665*	0.97	[121]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		129 (at 428 nm, diethyl ether) [98] 87.7 (at 664 nm, 90% acetone) [107]	

Reference spectra

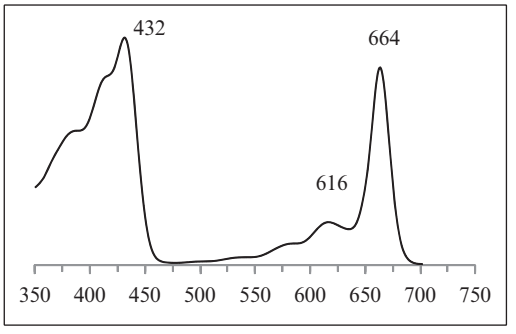
In acetone



In HPLC solvent system 1



In HPLC solvent system 2

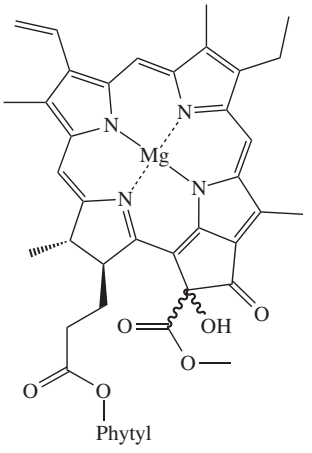


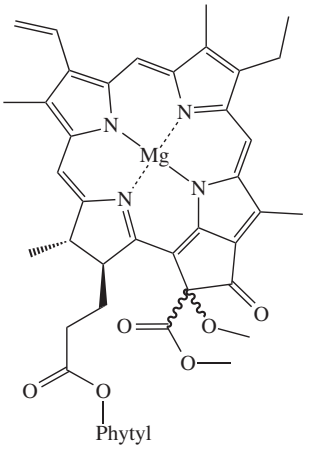
Mass spectra

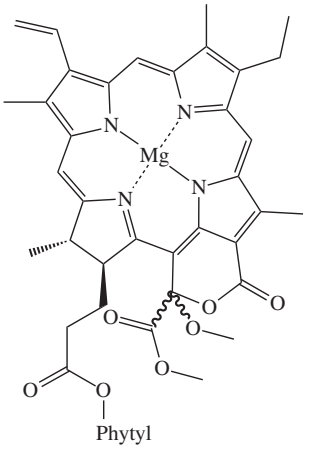
Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	Magnetic sector	892 $[M]^+$ (25), 614 [M-phytyl]$^+$ (100), 555 [M-337]$^+$ (39), 481 [M-60–351]$^+$ (29)	[27]
Remarks	Fluorescence: excitation 428 nm, emission 666 nm (diethyl ether) [26]		

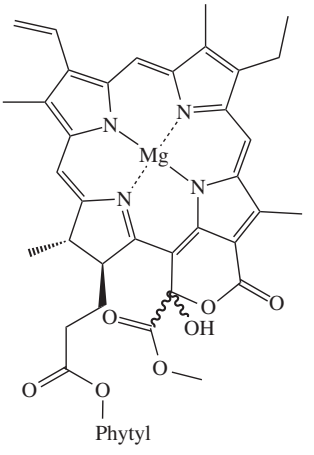
Chlorophyll *a* allomers

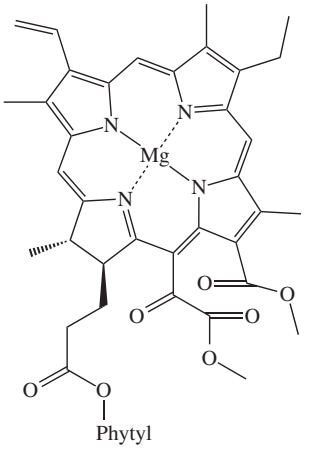
Recommended abbreviation: Chl *a* allo (C*a*al)





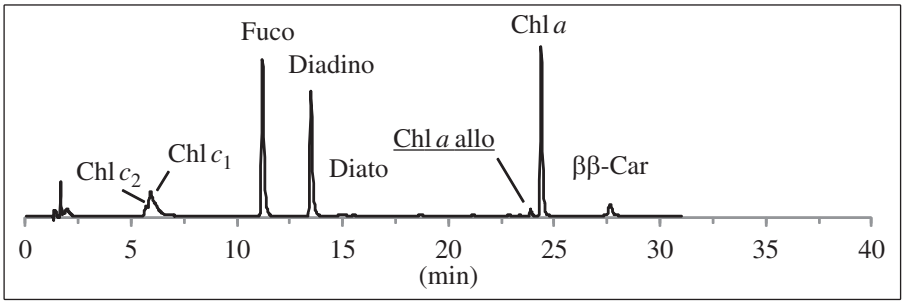




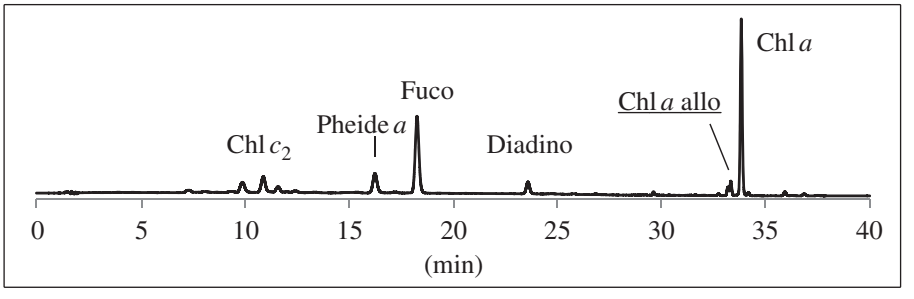


Alteration products of	Various oxidation products of Chl *a* [100, 172]
Source culture	*Chroomonas salina* (cryptomonad)
Alteration products	
Synthetically related to	Chl *a*
Occurs together with	

HPLC chromatogram of *Pavlova gyrans* (system 1)



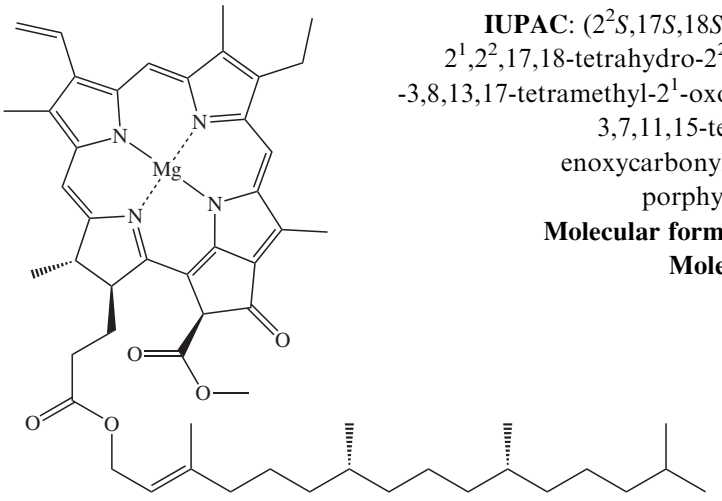
HPLC chromatogram of a coastal marine sample (system 2)



Remarks	Similar allomerization products also from other chlorophylls [100, 102, 172] *d*: assume identical to Chl *a*

Chlorophyll *a* epimer

Recommended abbreviation: Chl *a*′ (Ca′)



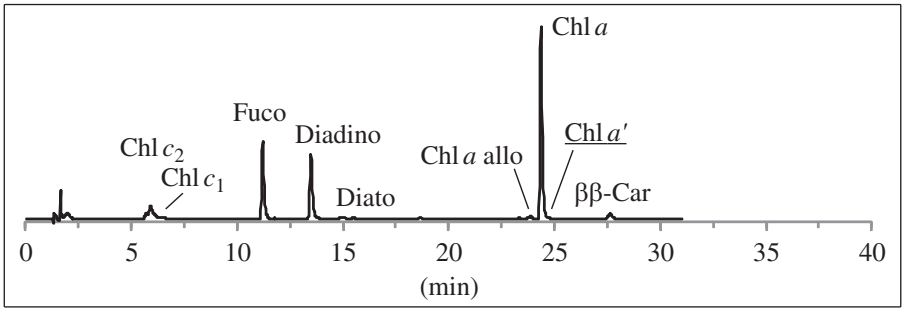
IUPAC: (2²*S*,17*S*,18*S*)-12-Ethenyl-7-ethyl-2¹,2²,17,18-tetrahydro-2²-(methoxycarbonyl)-3,8,13,17-tetramethyl-2¹-oxo-18-{2-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-enoxycarbonyl]ethyl}cyclopenta[*at*]porphyrinatomagnesium(II)

Molecular formula: $C_{55}H_{72}N_4O_5Mg$

Molecular weight: 893.49

Alteration product of	Chlorophyll *a*; occurs in slightly acidic or basic extracts using polar solvents
Source culture	*Chroomonas salina* (cryptomonad)
Alteration products	Chl *a*, Phe *a*′, Chl *a*′ allo, Pphe *a*
(Bio)synthetically related to	Chl *a*
Occurs together with	

HPLC chromatogram of *Pavlova lutheri* (system 1)



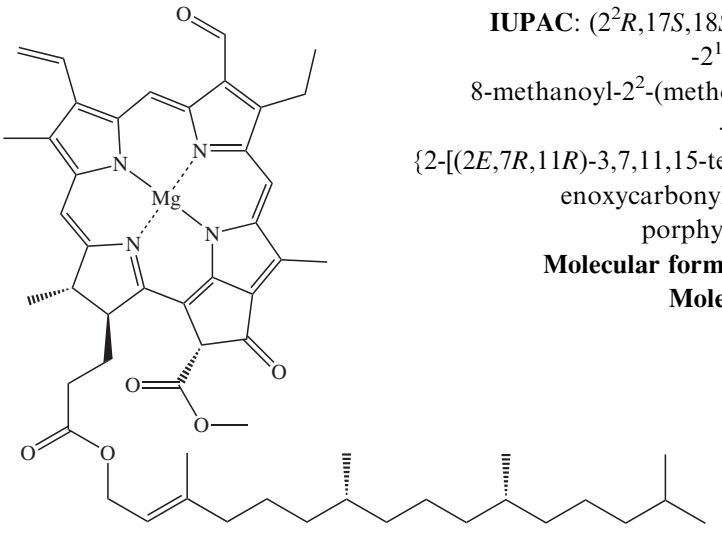
UV-Vis spectra and fluorescence spectra

For all practical purposes, identical with the parent chlorophyll

Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})	Assume identical to Chl *a*

Chlorophyll *b*

Recommended abbreviation: Chl *b* (C*b*)



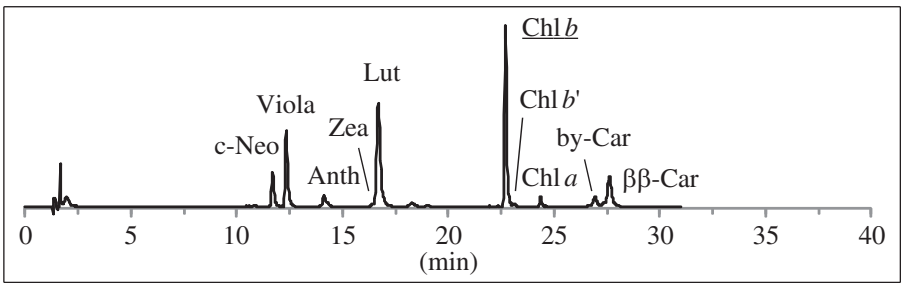
IUPAC: (2^2R,17*S*,18*S*)-12-Ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-8-methanoyl-2^2-(methoxycarbonyl)-3,13,17-trimethyl-2^1-oxo-18-{2-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-enoxycarbonyl]ethyl}cyclopenta[*at*]porphyrinatomagnesium(II)

Molecular formula: $C_{55}H_{70}N_4O_6Mg$

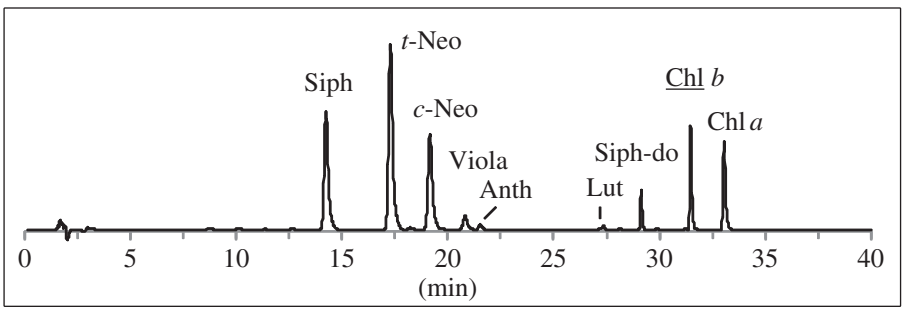
Molecular weight: 907.47

Biological occurrence	Dominant pigment in all classes of green algae, in higher plants and some prochlorophytes (Cyano-3, Chapter 1)
Source culture	*Dunaliella tertiolecta* (chlorophyte), *Pycnococcus provasolii* (prasinophyte)
Alteration products	Chlide *b*, Pheide *b*, Phe *b*, Chl *b*′, Chl *b* allo and pyro deriv.
Biosynthetically related to	Chl *a*, MgDVP
Occurs together with	Lut, Zea, Viola, *c*-Neo

HPLC chromatogram of *Dunaliella tertiolecta* (system 1)



HPLC chromatogram of *Codium tomentosum* (system 2)



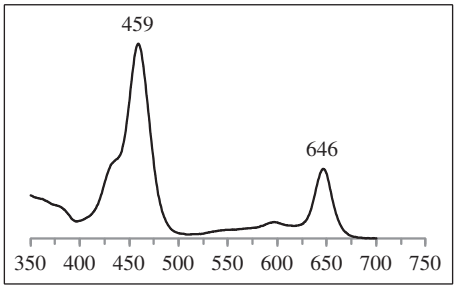
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*457*, 597, 646	2.8	[145]
Diethyl ether	428, *453*, 593, 642	2.8	[98]
95% Ethanol	*464*, 601, 649	2.6	[121]
Methanol	*469*, 603, 652	2.7	[121]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		176 (at 453 nm, diethyl ether) [98] 51.4 (at 647 nm. 90% acetone) [107]	

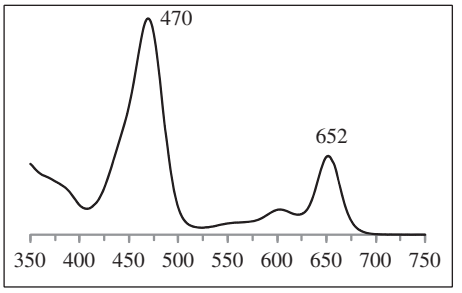
Reference spectra

For spectrum in acetone, see [109]

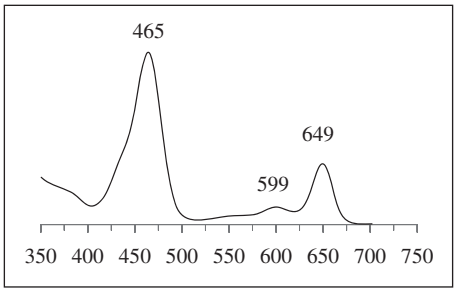
In 90% acetone



In HPLC solvent system 1



In HPLC solvent system 2

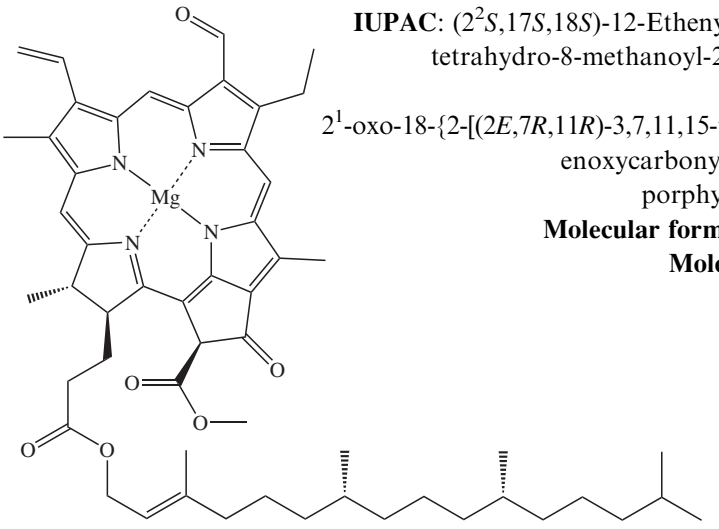


Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	Magnetic sector	906 $[M]^+$ (67), 628 [M-phytyl]$^+$ (100), 569 [M-337]$^+$ (30), 495 [M-60–351]$^+$ (39)	[27]
Remarks	Fluorescence: excitation 453 nm, emission 646 nm (diethyl ether) [26]		

Chlorophyll *b* epimer

Recommended abbreviation: Chl *b*′ (C*b*′)



IUPAC: (2^2*S*,17*S*,18*S*)-12-Ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-8-methanoyl-2^2-(methoxycarbonyl)-3,13,17-trimethyl-2^1-oxo-18-{2-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-enoxycarbonyl]ethyl}cyclopenta[*at*]porphyrinatomagnesium(II)

Molecular formula: $C_{55}H_{70}N_4O_6Mg$

Molecular weight: 907.47

Alteration product of	Chlorophyll *b*; occurs in slightly acidic or basic extracts using polar solvents
Source culture	*Dunaliella tertiolecta* (chlorophyte), *Pycnococcus provasolii* (prasinophyte)
Alteration products	Chl *b*, Phe *b*′, Chl *b*′ allo, Pphe *b*
(Bio)synthetically related to	Chl *b*
Occurs together with	

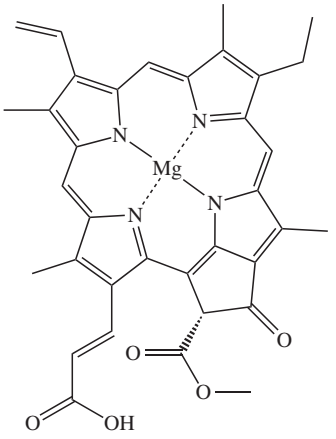
UV-Vis spectra and fluorescence spectra

For all practical purposes, identical with the parent chlorophyll

Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})	Assume identical to Chl *b*

Chlorophyll c_1

Recommended abbreviation: Chl c_1 (Cc_1)

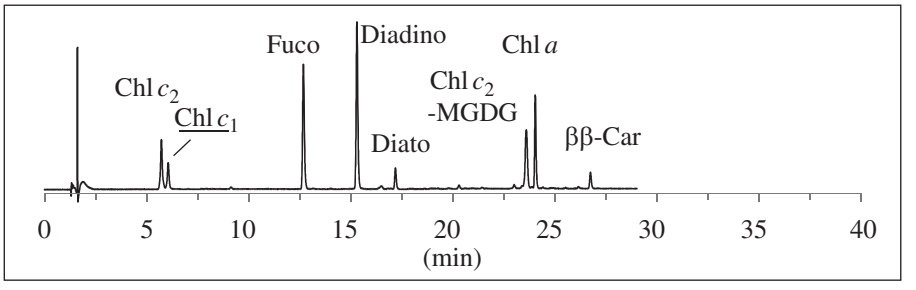


IUPAC: (2^2R,18^1E)-18-(3-Carboxyethenyl)-12-ethenyl-7-ethyl-2^1,2^2-dihydro-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxocyclopenta[*at*]porphyrinatomagnesium(II)

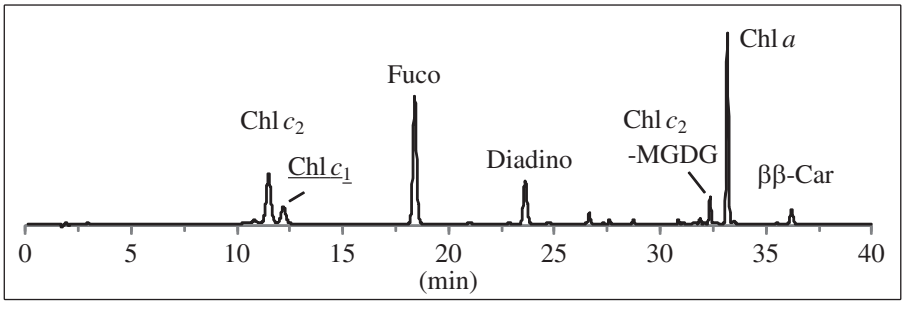
Molecular formula: $C_{35}H_{30}N_4O_5Mg$
Molecular weight: 610.94

Biological occurrence	Minor pigment in most types of algae within the 'red algal lineage' (see Chapter 1, this volume)
Source culture	*Mallomonas papillosa* (synurophyte)
Alteration products	Chl c_1', corresponding pheophorbide and pyro-derivatives
Biosynthetically related to	Chl c_2, MVChl c_3
Occurs together with	Chl c_2, Fuco

HPLC chromatogram of *Pavlova gyrans* (system 1)



HPLC chromatogram of *Isochrysis galbana* (system 2)

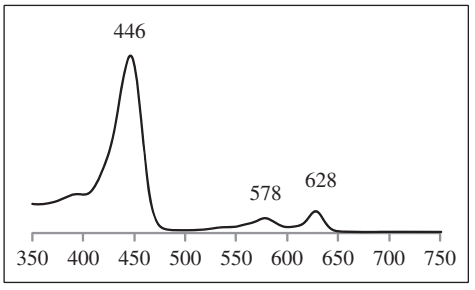


UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*446*, 578, 629	9	[105]
Diethyl ether	*444*, 577, 626	9	[58]
Methanol	*445*, 584, 634	7	[104]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		346 (at 462 nm in pyridine) [105] 318 (at 443 nm, 90% acetone + 1% pyridine) [105]	

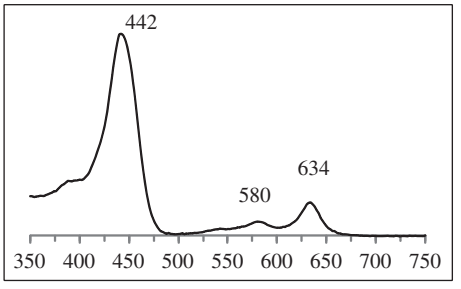
Reference spectra

In acetone

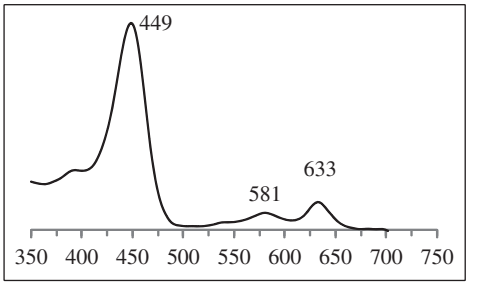


For spectrum in diethyl ether, see [109]

In HPLC solvent system 1



In HPLC solvent system 2

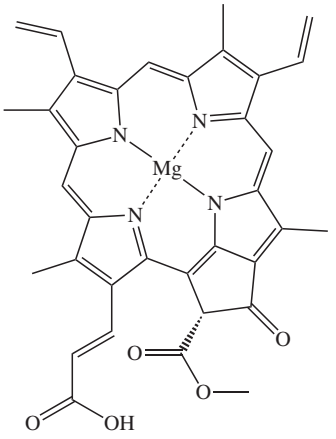


Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
ESI^+	Ion trap	611 $[M+H]^+$; 611 → 593 $[M+H-18]^+$ (100), 567 $[M+H-44]^+$ (20), 551 $[M+H-60]^+$ (63), 534 $[M+H-77]^+$ (15)	[76]
Remarks	Fluorescence: excitation 450 nm, emission peaks at 633, 694 nm (acetone) [105]		

Chlorophyll c_2

Recommended abbreviation: Chl c_2 (Cc_2)

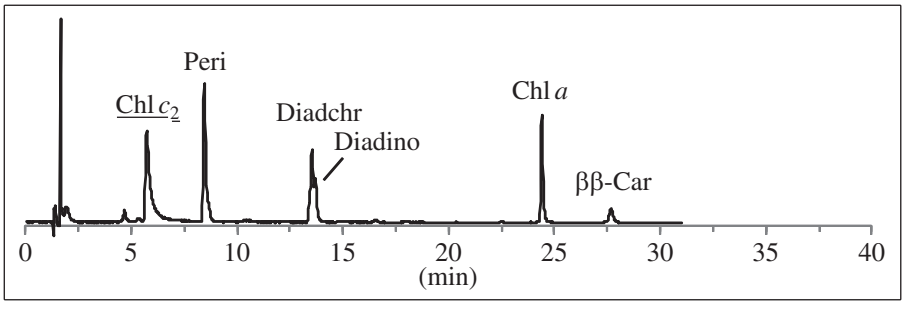


IUPAC: (2^2R,18^1E)-18-(3-Carboxyethenyl)-7,12-diethenyl-2^1,2^2-dihydro-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxocyclopenta[*at*]porphyrinatomagnesium(II)

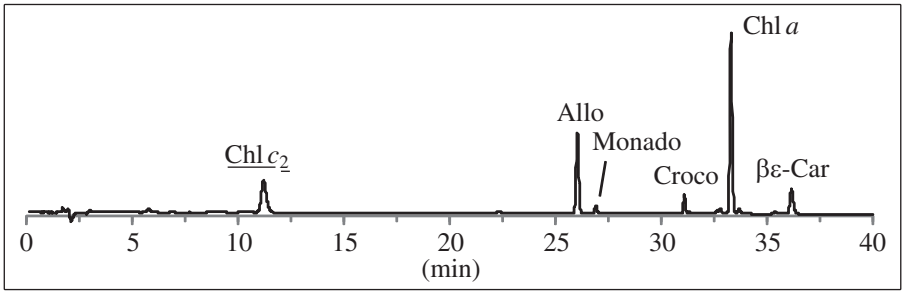
Molecular formula: $C_{35}H_{28}N_4O_5Mg$
Molecular weight: 608.93

Biological occurrence	Minor pigment in most types of algae within the 'red algal lineage' (see Chapter 1, this volume)
Source culture	*Amphidinium carterae* (dinoflagellate)
Alteration products	Chl c_2', corresponding pheophorbide and pyro-derivatives
Biosynthetically related to	Chl c_1, Chl c_3
Occurs together with	Fuco and with Chl c_1 in many cases (see Chapter 1)

HPLC chromatogram of *Gymnodinium catenatum* (system 1)



HPLC chromatogram of *Rhodomonas baltica* (system 2)

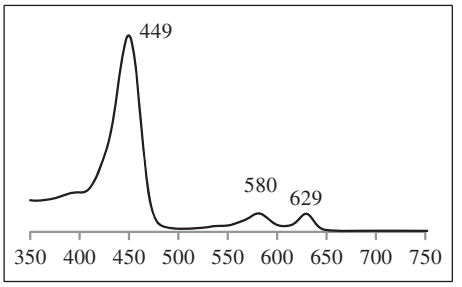


UV-Vis spectra (see also reference spectra below)

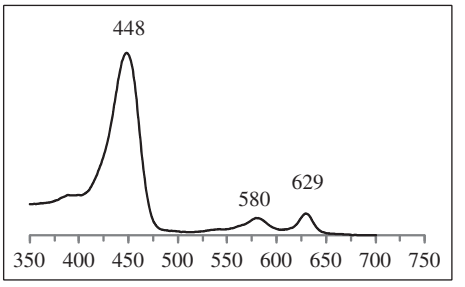
Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*450*, 581, 629	11	[57]
Diethyl ether	*449*, 582, 629	14	[104]
Methanol	*452*, 587, 635	10	[104]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		459 (at 466 nm in pyridine) [105] 374 (at 444 nm in 90% acetone + 1% pyr.) [105]	

Reference spectra

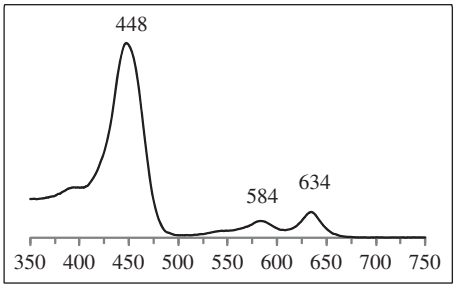
In acetone



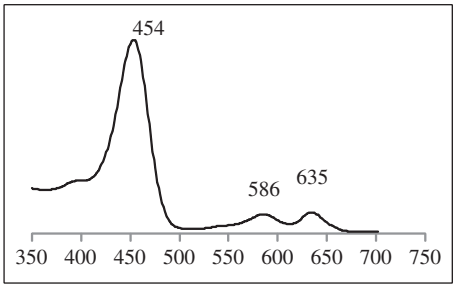
In 90% acetone + 1% pyridine



In HPLC solvent system 1



In HPLC solvent system 2



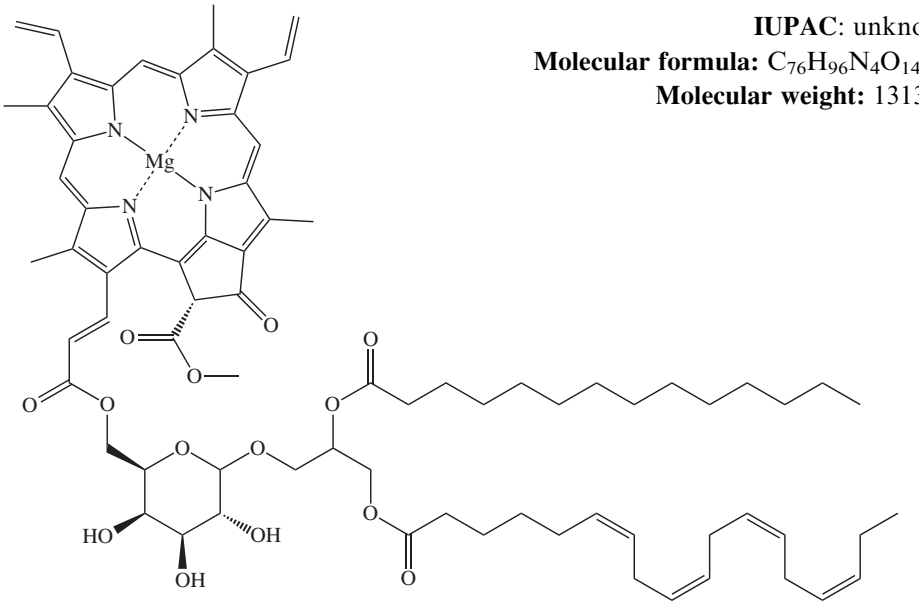
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
ESI^+	Ion trap	609 $[M+H]^+$; 609 → 591 $[M+H\text{-}18]^+$ (33), 565 $[M+H\text{-}44]^+$ (69), 564 $[M+H\text{-}45]^+$ (100), 549 $[M+H\text{-}60]^+$ (53), 532 $[M+H\text{-}77]^+$ (26)	[76]

Remarks Fluorescence: excitation 453 nm, emission 635, 696 nm (acetone) [105]
Several other Chl *c* pigments of unknown structure: see [179]

Chlorophyll c_2-monogalactosyldiacylglyceride ester [18:4/14:0]

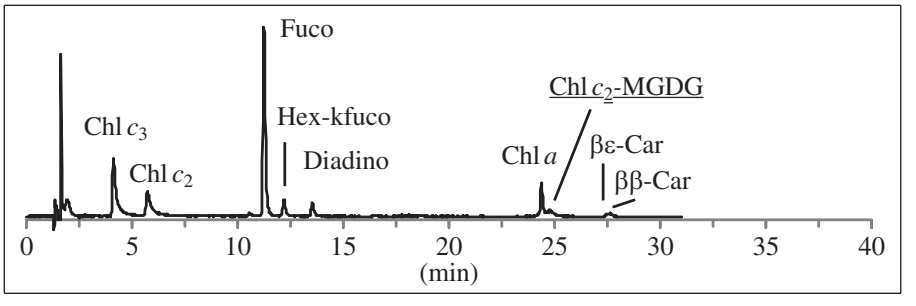
Recommended abbreviation: **Chl c_2-MGDG (Cc_2M)**



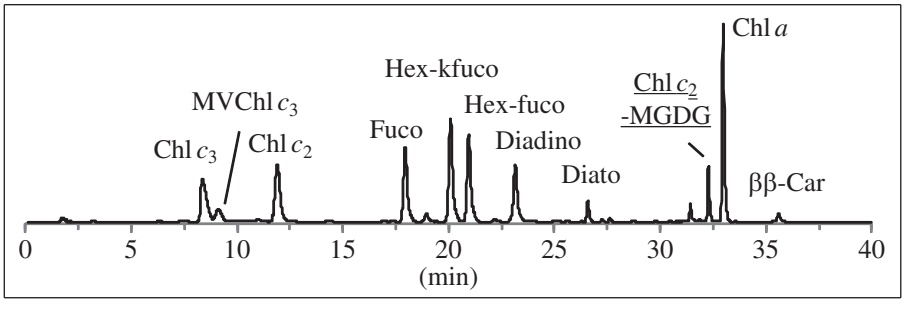
IUPAC: unknown
Molecular formula: $C_{76}H_{96}N_4O_{14}Mg$
Molecular weight: 1313.90

Biological occurrence	Dominant pigment in some haptophytes (see Chapter 1)
Source culture	*Emiliania huxleyi* (coccolithophyte)
Alteration products	Not known, corresponding phytoporphyrins expected
Biosynthetically related to	Chl c_2
Occurs together with	Chl c_2, Fuco, Hex-fuco, Hex-kfuco

HPLC chromatogram of *Chrysochromulina camella* (system 1)



HPLC chromatogram of *Emiliania huxleyi* (system 2)

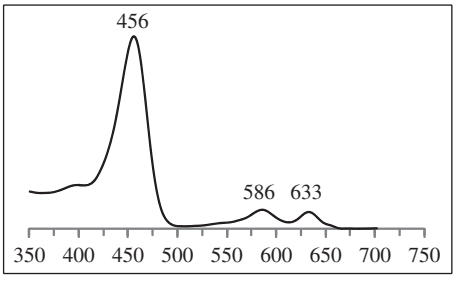


UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*453*, 582, 631	10	[70]
Diethyl ether	*452*, 581, 629	13	[73]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		n.d, see Remarks	

Reference Spectra

In HPLC solvent system 2



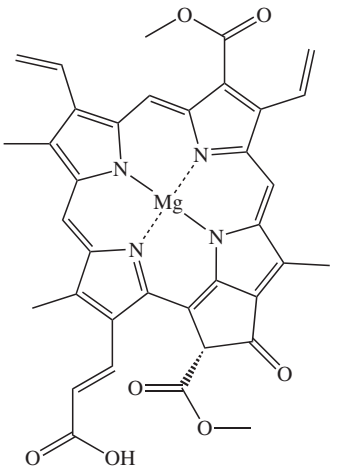
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	Double quadrupole	1312, 1313 $[M, M+1]^+ \rightarrow$ 1085, 1038, 809, 752, 693, 609, 591, 563, 549, 533, 519, 504, 477	[70]

Remarks Fluorescence: excitation 452 nm, emission 634, 695 nm (diethyl ether) [73]
$d = 213\ L\ g^{-1}\ cm^{-1}$ (at 453 nm in acetone; calc. from Chl c_2) is recommended, as no value has been determined for Chl c_2-MGDG [105]. Other fatty acid esters of Chl c_2-MGDG have been reported [179]. Structure not proven by NMR

Chlorophyll c_3

Recommended abbreviation: Chl c_3 (Cc_3)

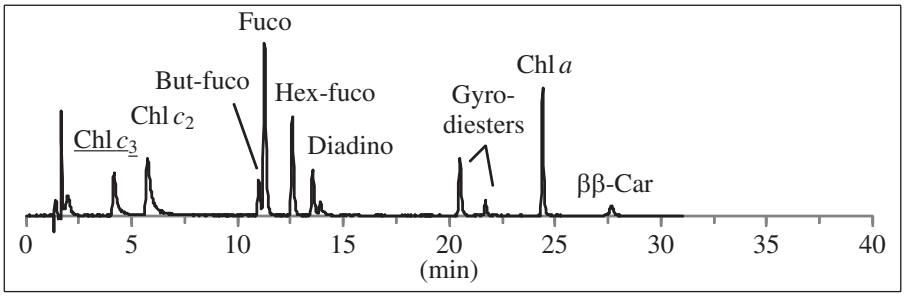


IUPAC: (2^2R,18^1E)-18-(3-Carboxyethenyl)-7,12-diethenyl-2^1,2^2-dihydro-2^2,8-di(methoxycarbonyl)-3,13,17-trimethyl-2^1-oxocyclopenta[*at*]porphyrinatomagnesium(II)

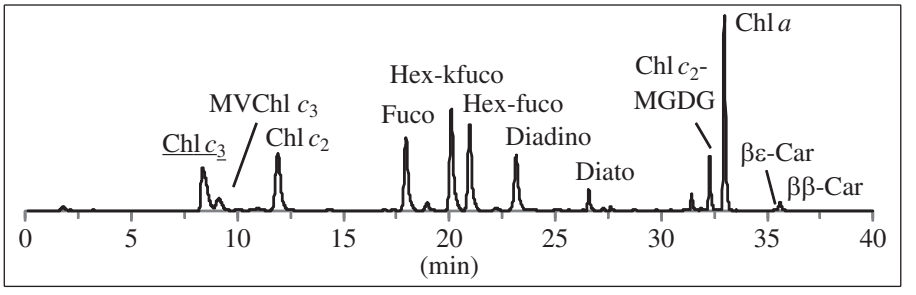
Molecular formula: $C_{36}H_{28}N_4O_7Mg$
Molecular weight: 652.94

Biological occurrence	Dominant pigment in bolidophytes, many diatoms and haptophytes and some dinoflagellates. Occasional in dictyochophytes and pelagophytes
Source culture	*Ochrosphaera neopolitana* [180], strain CS-285 [8]
Alteration products	Chl c_3', corresponding pheophorbide and pyro-derivatives
Biosynthetically related to	Chl c_2, MVChl c_3
Occurs together with	Chl c_2, Diadino, Fuco

HPLC chromatogram of *Karlodinium micrum* (system 1)



HPLC chromatogram of *Emiliania huxleyi* (system 2)



UV-Vis spectra (see also reference spectra below)

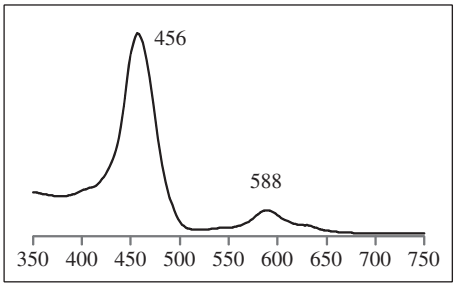
Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*452*, 586, 626	28	[145]
Diethyl ether	*451*, 585, 626	32	[110]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

Reference spectra

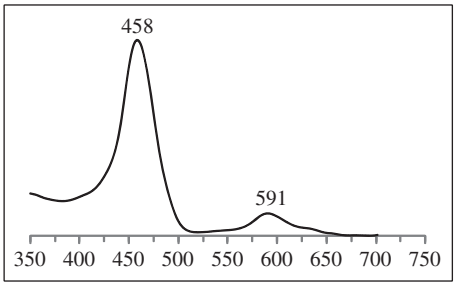
In acetone

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



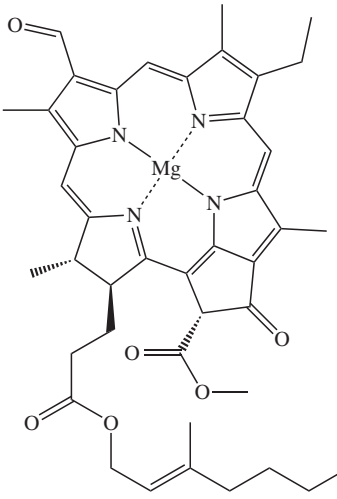
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
ESI^+	Ion trap	653 $[M+H]^+$; 653 → 635 (100), 621 (92), 609 (58), 593 (55)	[76]

Remarks Fluorescence: excitation 452 nm, emission 635, 690 nm (acetone) [145]
$d = 590\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in pyridine) is recommended, as no *d* has been determined for Chl c_3. In 90% acetone + 1% pyridine, use $d = 346\ L\ g^{-1}\ cm^{-1}$ (at 453 nm) (mean of the values for Chl c_1 and c_2 at Soret max.) [109]

Chlorophyll *d*

Recommended abbreviation: Chl *d* (C*d*)



IUPAC: (2^2*R*,17*S*,18*S*)-7-Ethyl-2^1,2^2,17,18-tetrahydro-12-methanoyl-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxo-18-{2-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-oxycarbonyl]ethyl}cyclopenta[*at*]porphyrinatomagnesium(II)

Molecular formula: $C_{54}H_{70}O_6N_4Mg$
Molecular weight: 895.46

Biological occurrence	Major chlorophyll in a few prochlorophytes (Cyano-5, Chapter 1)
Source culture	*Acaryochloris marina* (prochlorophyte/cyanobacteria)
Alteration products	Chlide *d*, Pheide *d*, Phe *d*, Chl *d*′, Chl *d* allo, Pphe *d*
Biosynthetically related to	Chl *a*, MgDVP
Occurs together with	MgDVP, βε-Car, Zea

UV-Vis spectra

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	394, 445, 600, 660, *693*	0.99	[111]
Diethyl ether	392, 447, 595, 643, *688*	0.89	[147]
Methanol	400, 455, 697	n.d.	[129]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		118 (at 687 nm in diethyl ether)	[97]

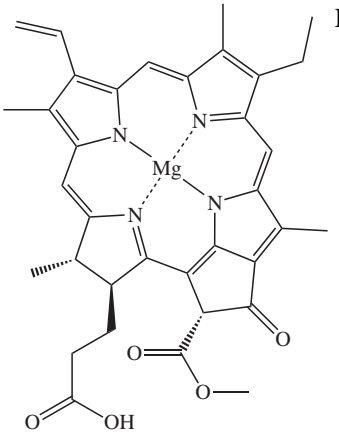
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
MALDI	TOF	894 $[M]^+$, 616; 616 → 557, 543, 530, 515, 494, 483	[161]

Remarks Fluorescence: excitation 696, emission ~752 nm (diethyl ether) [147]

Chlorophyllide *a*

Recommended abbreviation: Chlide *a* (Cd*a*)

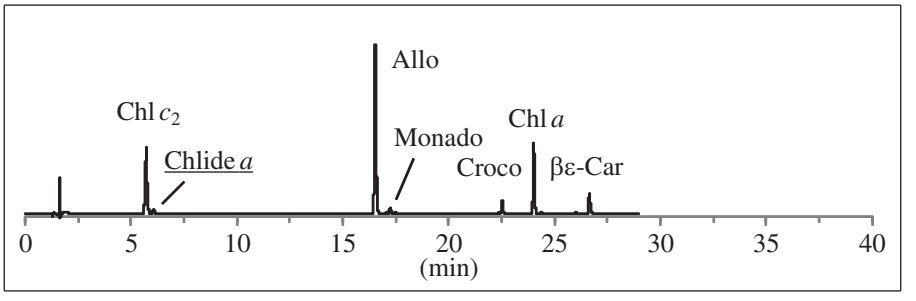


IUPAC: (2^2*R*,17*S*,18*S*)-18-(2-Carboxyethyl)-12-ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxocyclopenta[*at*]porphyrinatomagnesium(II)

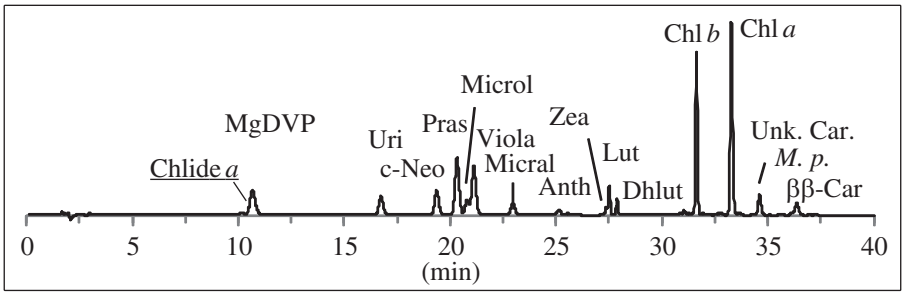
Molecular formula: $C_{35}H_{34}N_4O_5Mg$
Molecular weight: 614.97

Alteration product of	Chlorophyll *a*; occurs in senescent algae, damaged diatoms, zooplankton faecal pellets. Extraction artefact for algae with highly active chlorophyllase enzyme
Source culture	*Chroomonas salina* (cryptophyte)
Alteration products	Pheide *a*
(Bio)synthetically related to	Chl *a*, Pheide *a*
Occurs together with	

HPLC chromatogram of *Guillardia theta* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)



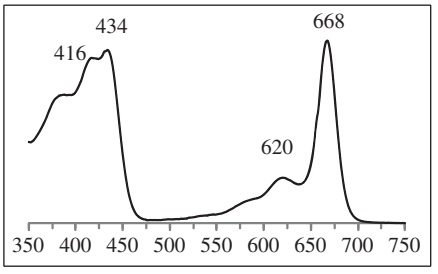
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	412, *431*, 580, 617, 664	1.1	[108]
Diethyl ether	*429*, 661	n.d.	[149]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

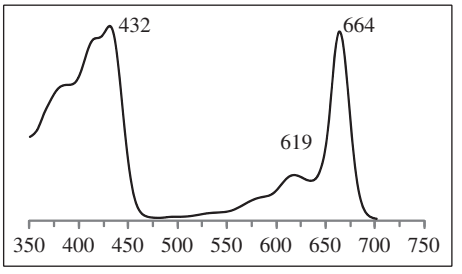
Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



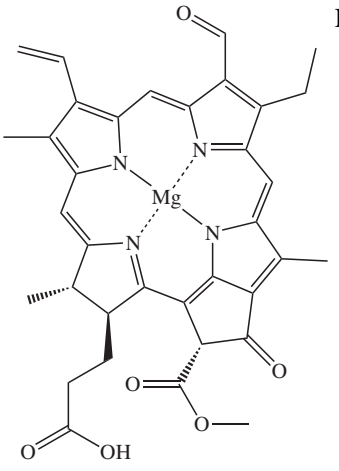
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	Magnetic sector	614 $[M]^+$	[27]

Remarks Fluorescence data: excitation 426 nm, emission 667 nm (acetone) [145]
$d = 187\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in diethyl ether; calc. from Chl *a*) is recommended, as no *d* has been determined for Chlide *a*. In 90% acetone, use $d = 127\ L\ g^{-1}\ cm^{-1}$ (at 664 nm) [124, 109]

Chlorophyllide *b*

Recommended abbreviation: Chlide *b* (Cd*b*)



IUPAC: (2^2*R*,17*S*,18*S*)-18-(2-Carboxyethyl)-12-ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-8-methanoyl-2^2-(methoxycarbonyl)-3,13,17-trimethyl-2^1-oxocyclopenta[*at*]porphyrinatomagnesium(II)

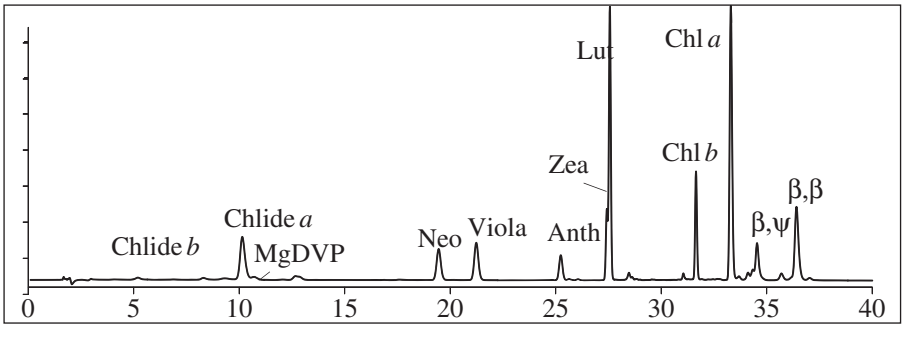
Molecular formula: $C_{35}H_{32}N_4O_6Mg$
Molecular weight: 628.96

Alteration product of	Chlorophyll *b*; occurs in senescent algae, zooplankton fecal pellets
Source culture	*Dunaliella tertiolecta* (chlorophyte), *Pycnococcus provasolii* (prasinophyte)
Alteration products	Pheide *b*
(Bio)synthetically related to	Chl *b*, Pheide *b*
Occurs together with	Chlide *a*

HPLC chromatogram (system 1)

NO DATA AVAILABLE

HPLC chromatogram of *Dunaliella tertiolecta* (system 2)



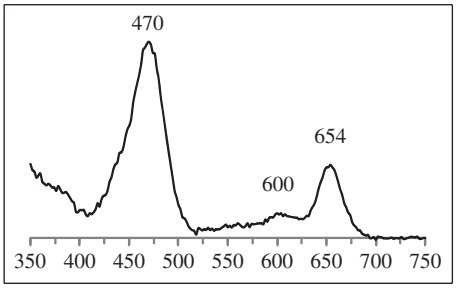
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*458*, 596, 646	2.9	[145]
Diethyl ether	*451*, 642	n.d.	[149]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

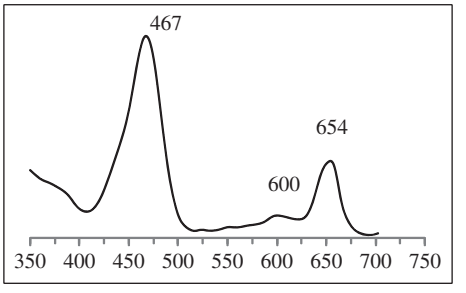
Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



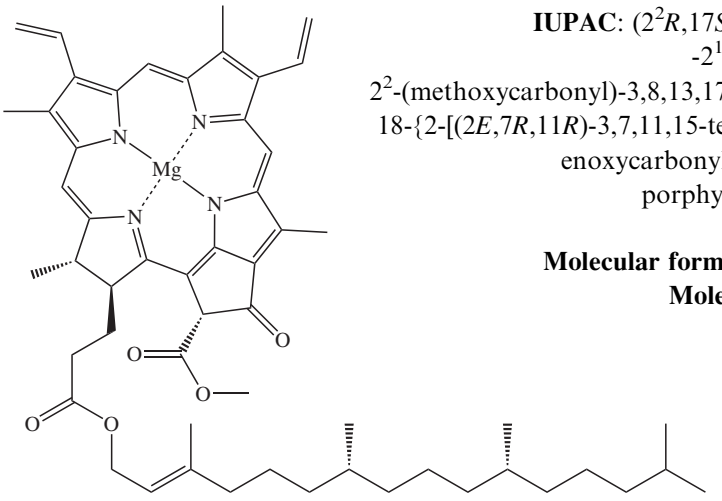
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	Magnetic sector	628 $[M]^+$	[27]

Remarks Fluorescence data: excitation 454 nm, emission 652 nm (acetone) [145]
$d = 254\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in diethyl ether; calc. from Chl *b*) is recommended, as no value has been determined for Chlide *b*. For 90% acetone, use $d = 74.1\ L\ g^{-1}\ cm^{-1}$ (at 645 nm) [124, 109]

Divinyl chlorophyll *a*

Recommended abbreviation: DVChl *a* (DC*a*)

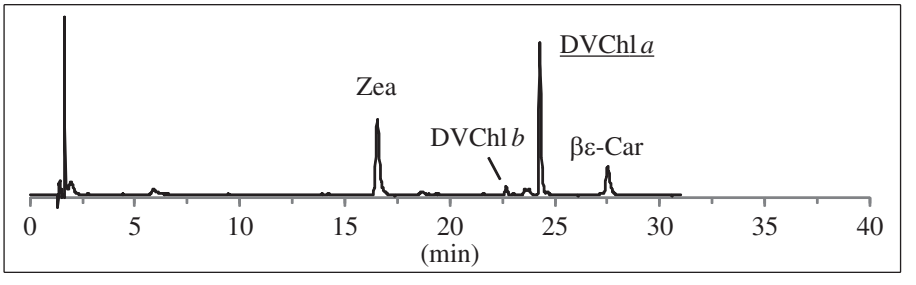


IUPAC: (2^2*R*,17*S*,18*S*)-7,12-Diethenyl-2^1,2^2,17,18-tetrahydro-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxo-18-{2-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-enoxycarbonyl]ethyl}cyclopenta[*at*]porphyrinatomagnesium(II)

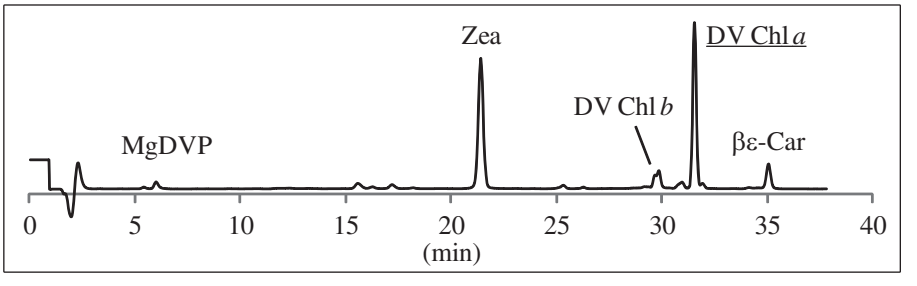
Molecular formula: $C_{55}H_{70}N_4O_5Mg$
Molecular weight: 891.47

Biological occurrence	Dominant chlorophyll in *Prochlorococcus* (prochlorophyte/cyanobacteria) (Cyano-4, Chapter 1)
Source culture	*Prochlorococcus marinus* (prochlorophyte/cyanobacteria)
Alteration products	DVChlide *a*, DVPheide *a*, DVPhe *a*, DVChl *a*′, DVChl *a* allo, DVPphe *a* probable
Biosynthetically related to	DVChl *b*, MgDVP
Occurs together with	DVChl *b*, MgDVP, βε-Car, Zea

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



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



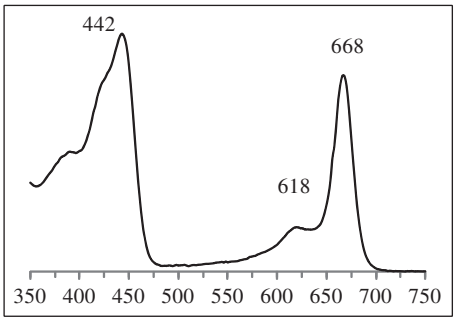
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Diethyl ether	*436*, ≈615, 661	1.3	[74]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

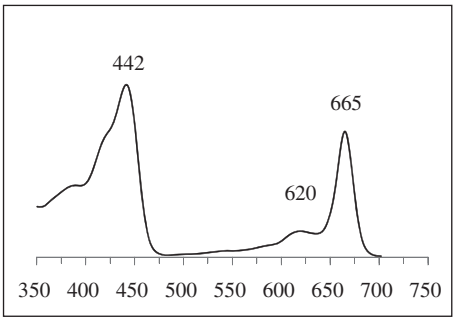
Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



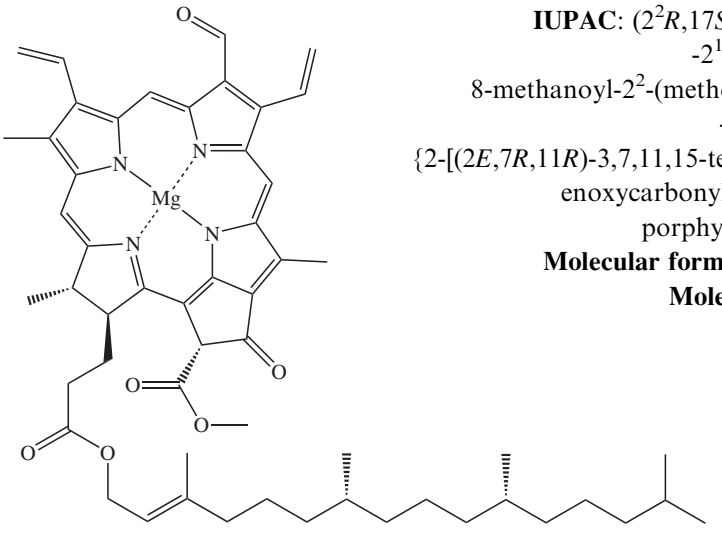
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	magnetic sector	891 $[M+H]^+ \rightarrow$ 613 $[M+H–phytyl]^+$	[13]

Remarks Fluorescence: excitation 439 nm, emission 663, 680 nm (acetone) [11]
$d = 170\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in diethyl ether) is recommended, as no value has been determined for DVChl *a*. For 90% acetone, use $d = 88.3$ (at 663 nm) (calculated from Chl *a* [109])

Divinyl chlorophyll *b*

Recommended abbreviation: DVChl *b* (DC*b*)



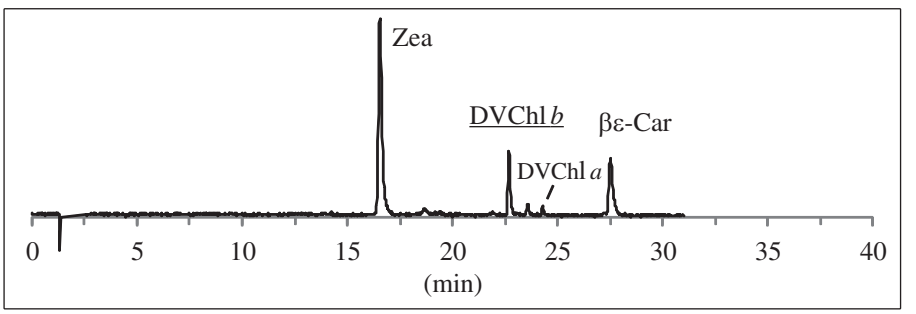
IUPAC: (2^2*R*,17*S*,18*S*)-7,12-Diethenyl-2^1,2^2,17,18-tetrahydro-8-methanoyl-2^2-(methoxycarbonyl)-3,13,17-trimethyl-2^1-oxo-18-{2-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-enoxycarbonyl]ethyl}cyclopenta[*at*]porphyrinatomagnesium(II)

Molecular formula: $C_{55}H_{68}N_4O_6Mg$

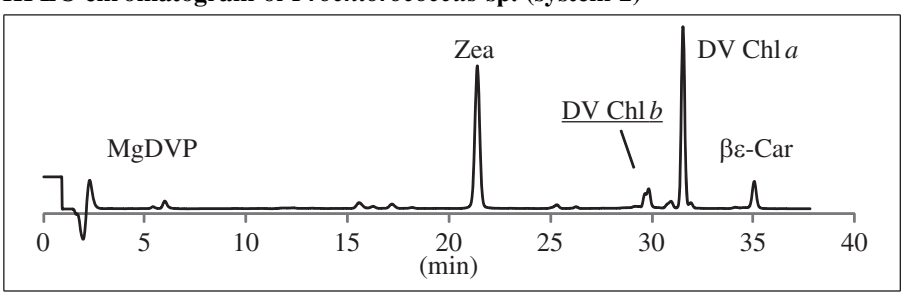
Molecular weight: 905.46

Biological occurrence	Dominant chlorophyll in *Prochlorococcus* (prochlorophyte/cyanobacteria) (Cyano-4, Chapter 1)
Source culture	*Prochlorococcus marinus* (prochlorophyte/cyanobacteria)
Alteration products	DVChlide *b*, DVPheide *b*, DVPhe *b*, DVChl *b*′, DVChl *b* allo, DVPphe *b* probable
Biosynthetically related to	DVChl *a*, MgDVP
Occurs together with	DVChl *a*, MgDVP, βε-Car, Zea

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



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



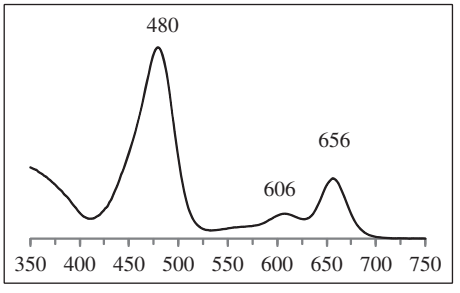
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Diethyl ether	*460*, 595, 644	n.d.	[75]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		n.d., see Remarks	

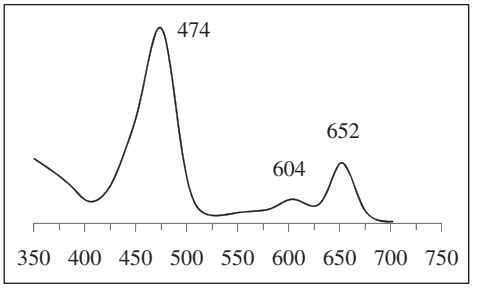
Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2

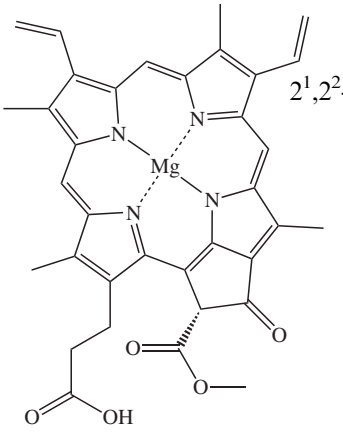


Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	magnetic sector	905 $[M+1]^+$	[29]

Remarks Fluorescence: excitation 462 nm, emission 652 nm (acetone) [11]
$d = 230\ L\ g^{-1} cm^{-1}$ (at λ_{max} in diethyl ether) is recommended, as no value has been determined for DVChl *b*. In 90% acetone, use $d = 51.4$ (at 647 nm) (calculated from Chl *b* [109])

Magnesium 2,4-divinylpheoporphyrin a_5 monomethyl ester

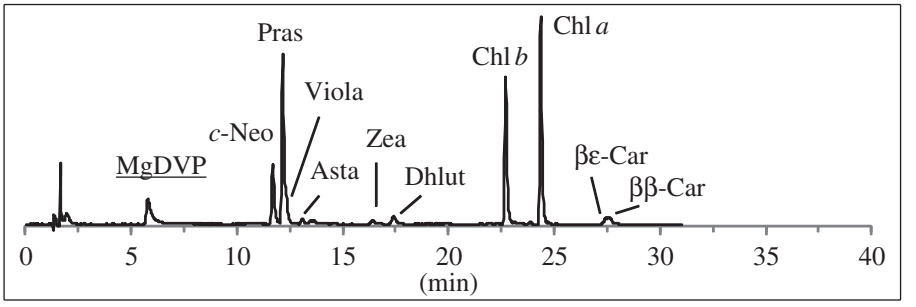


Recommended abbreviation: MgDVP (MD)
IUPAC: (2^2R)-18-(3-Carboxyethenyl)-7,12-diethenyl-2^1,2^2-dihydro-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxocyclopenta[*at*]porphyrinatomagnesium(II)

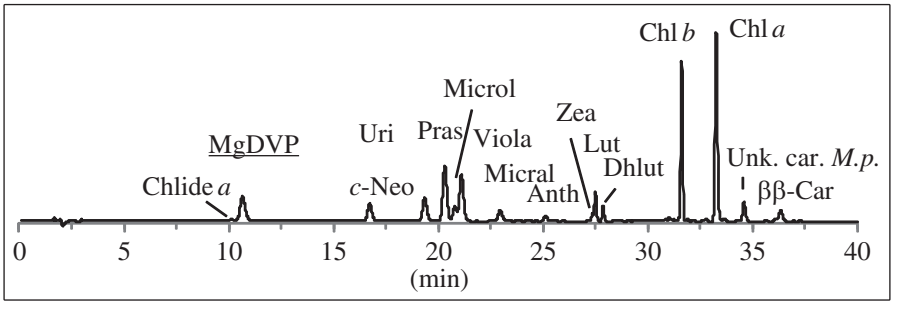
Molecular formula: $C_{35}H_{30}N_4O_5Mg$
Molecular weight: 610.94

Biological occurrence	Dominant pigment in prasinoxanthin-containing algae, trace amounts in most other algal groups (Chapter 1, this volume)
Source culture	*Micromonas pusilla* (prasinophyte)
Alteration products	Corresponding epimer, corresponding pheophorbide and pyro-derivatives
Biosynthetically related to	Precursor of other chlorophylls
Occurs together with	Chl *b*, Micral, *c*-Neo, Pras, Uri, Viola

HPLC chromatogram of *Pycnococcus provasolii* (system 1)



HPLC chromatogram of *Micromonas pusilla* (system 2)



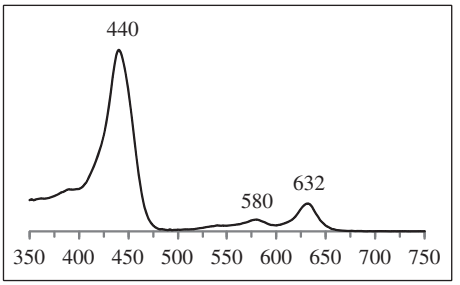
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*438*, 575, 625	9	[145]
Diethyl ether	*437*, 574, 624	10	[110]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		398 (at 456 nm in pyridine) [93] 394 (at 438 nm in 99% acetone + 1% pyridine [93]	

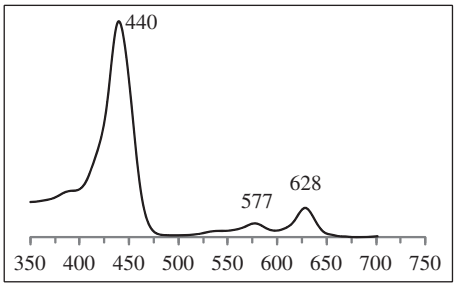
Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2

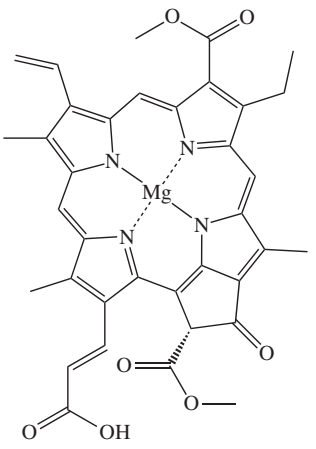


Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
ESI^+	Ion trap	611 $[M+H]^+$; 611 → 551 $[M+H\text{-}60]^+$ → 523 $[M+H\text{-}60\text{–}28]^+$ (29), 522 (36), 509 (44), 505 (81), 495 (100), 494 (98), 492 (30), 453 (22)	[76]

Remarks Fluorescence: excitation 439 nm, emission 625 nm (diethyl ether + 1% pyridine) [93]. Various semisystematic names are given in the scientific literature for this pigment, e.g. magnesium 3,8-divinylpheoporphyrin a_5 monomethyl ester, [3,8-divinyl]protochlorophyllide *a* and [8-vinyl]-protochlorophyllide *a* [93]

Monovinyl chlorophyll c_3 Recommended abbreviation: MVChl c_3 (MC c_3)

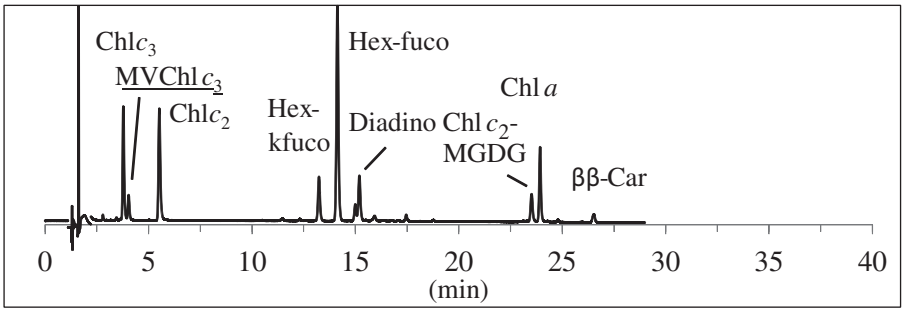


IUPAC: (2^2R,18^1E)-18-(3-Carboxyethenyl)-12-ethenyl-7-ethyl-2^1,2^2-dihydro-2^2,8-di(methoxycarbonyl)-3,13,17-trimethyl-2^1-oxocyclopenta[*at*]porphyrinatomagnesium(II)

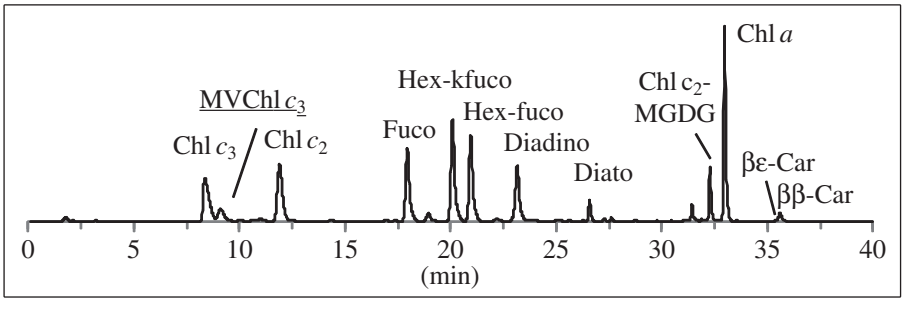
Molecular formula: $C_{35}H_{30}N_4O_7Mg$
Molecular weight: 654.95

Biological occurrence	Minor pigment in haptophytes Pigment Type 6 (see Chapter 1)
Source culture	*Emiliania huxleyi* (coccolithophyte), strain CS-57
Alteration products	MVChl c_3', corresponding pheophorbide and pyro-derivatives
Biosynthetically related to	Chl c_1, Chl c_3
Occurs together with	Chl c_2, Chl c_3, Diadino, Fuco, Hex-fuco, Hex-kfuco

HPLC chromatogram of *Emiliania huxleyi* (system 1)



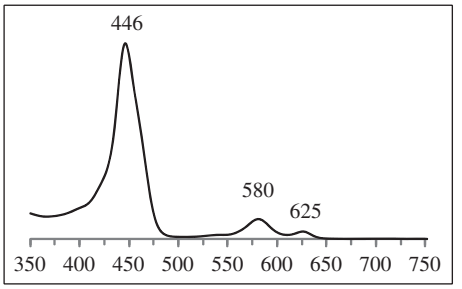
HPLC chromatogram of *Emiliania huxleyi* (system 2)



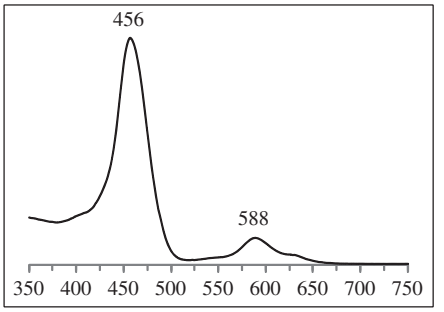
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*446*, 580, 624	25	[72]
Diethyl ether	*447*, 582, 626	24	[73]
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})			n.d., see Remarks

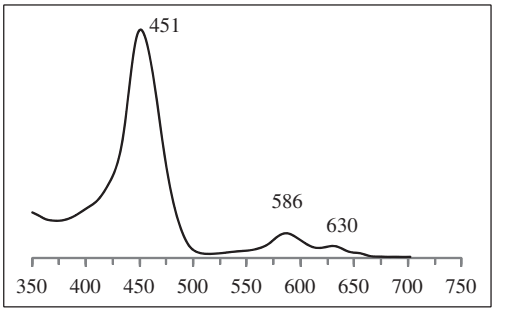
Reference spectra
In acetone



In HPLC solvent system 1



In HPLC solvent system 2



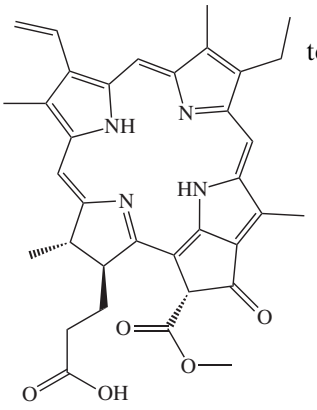
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
ESI^+	Ion trap	655 $[M+H]^+$; 655 → 637 (100), 623 (98), 611 (46), 595 (74)	[76]

Remarks Fluorescence: excitation 445 nm, emission 629, 690 nm (acetone) [73]
$d = 440\ L\ g^{-1}\ cm^{-1}$ (at λ_{max} in pyridine) is recommended, as no value has been determined for MVChl c_3. In 90% acetone + 1% pyridine, use $d = 346$ L g^{-1} cm^{-1} (at 453 nm) [179]. Structure not proven by NMR

Pheophorbide *a*

Recommended abbreviation: Pheide *a* (Pd*a*)

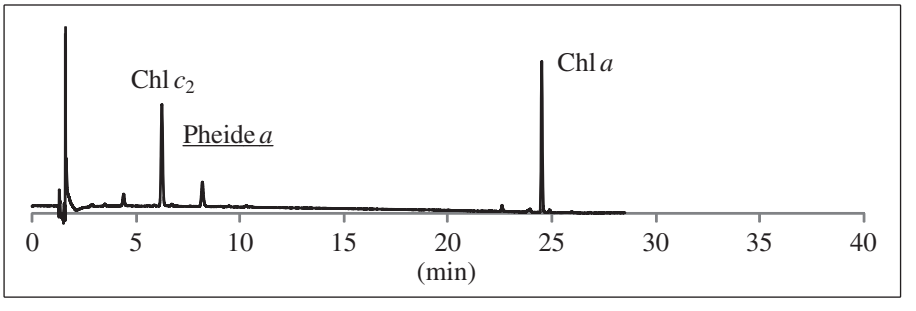


IUPAC: [(2^2*R*,17*S*,18*S*)-12-Ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxocyclopenta[*at*]porphyrin-18-yl]propanoic acid

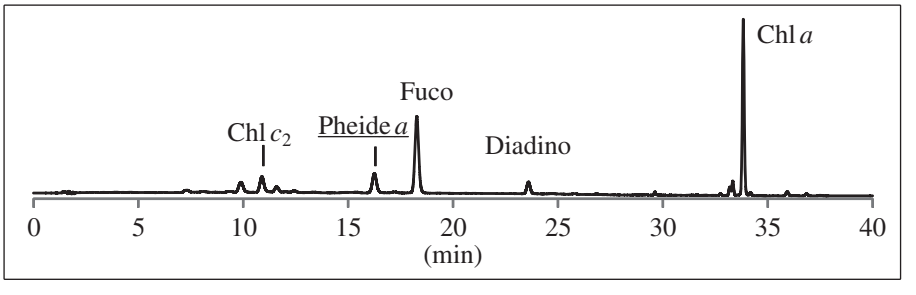
Molecular formula: $C_{35}H_{36}N_4O_5$
Molecular weight: 592.68

Alteration product of	Chlorophyll *a*; occurs in senescent algae, zooplankton fecal pellets and sediments
Source culture	*Chroomonas salina* (cryptophyte)
Alteration products	
Synthetically related to	Chl *a*, Phe *a*
Occurs together with	

HPLC chromatogram of a coastal water sample (system 1)



HPLC chromatogram of a coastal water sample (system 2)



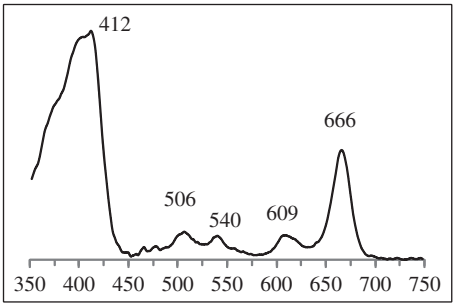
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*410*, 505, 535, 559, 608, 666	2.2	[145]
Diethyl ether	*408*, 467, 504, 533, 560, 610, 667	2.1	[99]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		177 (at 411 nm in tetrahydrofuran)	[101]
		74.2 (at 667 nm in 90% acetone)	[124, 109]

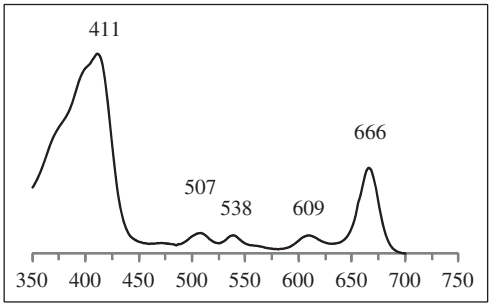
Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2



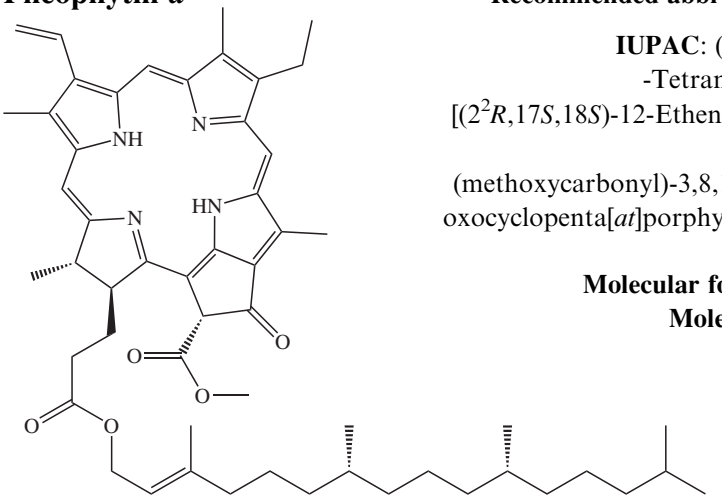
Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	magnetic sector	593 $[M+H]^+ \rightarrow$ 575 $[M+H\text{-}18]^+$	[131]

Remarks Fluorescence: excitation 406 nm, emission 672 nm [145]
Pheopigments are generally easier to detect using fluorescence. Several Phide *a* derivatives often present (e.g. [154]), including cyclic pheophorbide derivatives in fecal pellets and sediment [77, 168]

Pheophytin *a*

Recommended abbreviation: Phe *a* (Ph*a*)

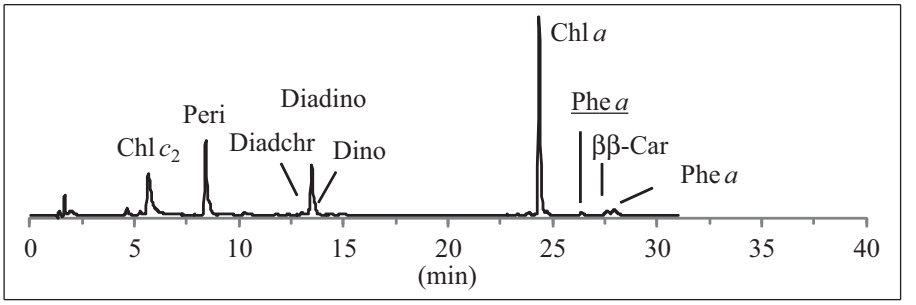


IUPAC: (2*E*,7*R*,11*R*)-3,7,11,15-Tetramethylhexadec-2-enyl [(2^2*R*,17*S*,18*S*)-12-Ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-2^2-(methoxycarbonyl)-3,8,13,17-tetramethyl-2^1-oxocyclopenta[*at*]porphyrin-18-yl]propanoate

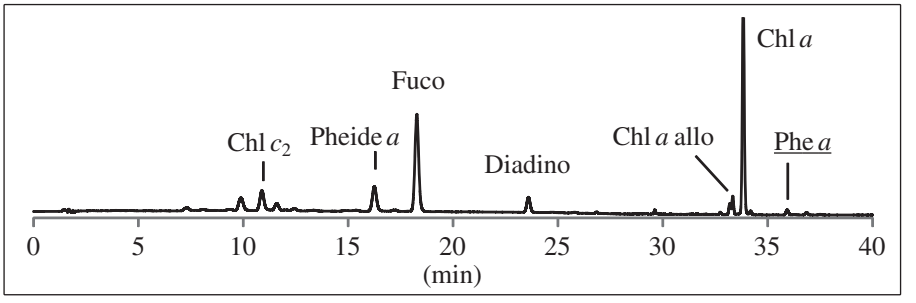
Molecular formula: $C_{55}H_{74}N_4O_5$
Molecular weight: 871.20

Alteration product of	Chlorophyll *a*. Found in zooplankton fecal pellets, senescent algae, sediments. The acid-catalysed demetallation also occurs in slightly acidic extracts, especially in prasinophyte extracts
Source culture	*Chroomonas salina* (cryptophyte)
Alteration products	Epimer, Allomer, Pheide *a*, Pphe *a*
(Bio)synthetically related to	Chl *a*, Pheide *a*, Pphe *a*
Occurs together with	Carotenoid furanoxides

HPLC chromatogram of *Amphidinium carterae* (system 1)



HPLC chromatogram of a coastal marine sample (system 2)



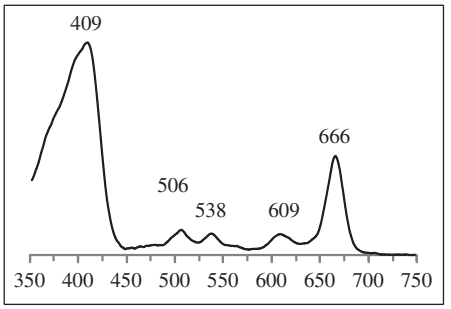
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*410*, 505, 535, 560, 610, 666	2.3	[109]
Diethyl ether	*408*, 505, 534, 610, 667	2.1	[12]
95% Ethanol	*417*, 507, 536, 564, 662	3.3	[121]
Methanol	*417*, 533, 567, 602, 654	4.1	[121]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		139 (at 411 nm in tetrahydrofuran) [125] 51.2 (at 667 nm in 90% acetone) [124, 109]	

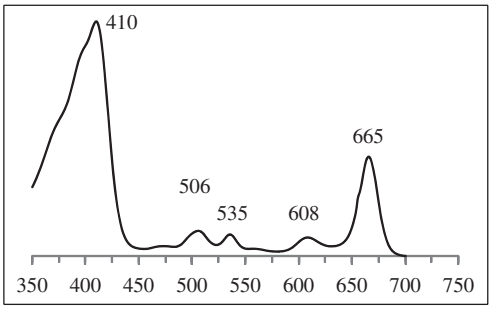
Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2

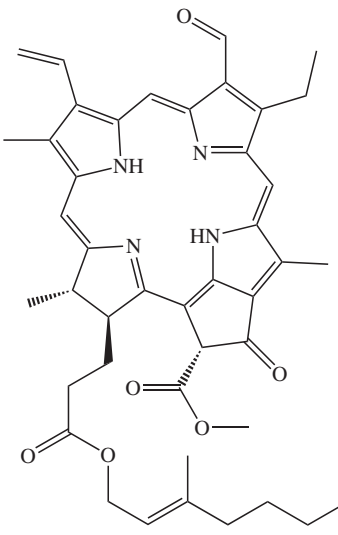


Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	magnetic sector	870 $[M]^+$ (100), 592 $[M\text{-phytyl}]^+$ (53), 533 (41), 520 (36), 459 (83)	[27]
Remarks	Fluorescence: excitation 408 nm, emission 672 nm (diethyl ether) [26] Pheopigments are generally easier to detect using fluorescence		

Pheophytin *b*

Recommended abbreviation: Phe *b* (Ph*b*)

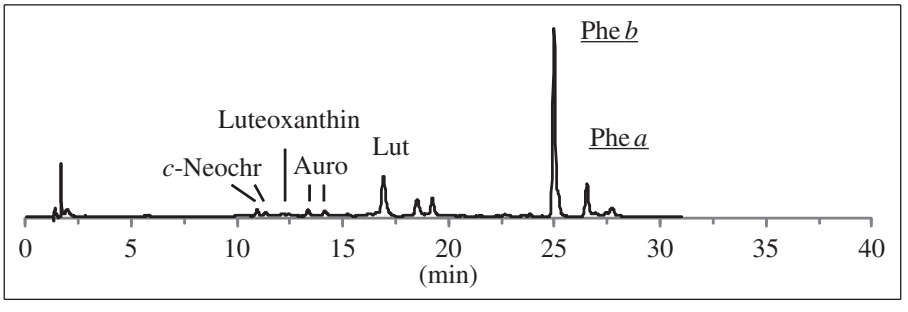


IUPAC: (2*E*,7*R*,11*R*)-3,7,11,15-Tetramethylhexadec-2-enyl [(2^2*R*,17*S*,18*S*)-12-Ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-8-methanoyl-2^2-(methoxycarbonyl)-3,13,17-trimethyl-2^1-oxocyclopenta[*at*]porphyrin-18-yl]propanoate

Molecular formula: $C_{55}H_{72}N_4O_6$
Molecular weight: 885.18

Alteration product of	Chlorophyll *b*. The acid-catalysed demetallation occurs in slightly acidic extracts, especially in prasinophyte extracts. Found in protozoan fecal pellets and terrestrial plant detritus
Source culture	*Dunaliella tertiolecta* (chlorophyte), *Pycnococcus provasolii* (prasinophyte)
Alteration products	Epimer, Allomer, Pheide *b*, Pphe *b*
Synthetically related to	Chl *b*, Pheide *b*, Pphe *b*
Occurs together with	Phe *a*, carotenoid furanoxides

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



HPLC chromatogram (system 2)

NO DATA AVAILABLE

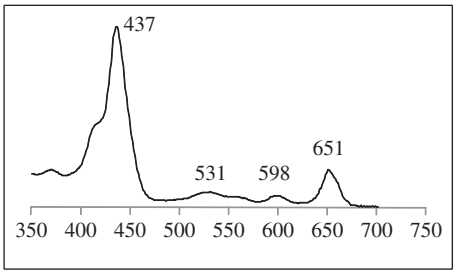
UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*433*, 527, 597, 653	5.1	[121]
Diethyl ether	*433*, 520, 555, 599, 655	5.2	[12]
95% Ethanol	*437*, 528, 599, 654	4.3	[121]
Methanol	*420*, 535, 597, 648	4.9	[121]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		244 (at 435 nm in tetrahydrofuran) [101] 31.8 (at 657 nm in 90% acetone) [109]	

Reference spectra

For spectrum in acetone, see [109]

In HPLC solvent system 1



In HPLC solvent system 2

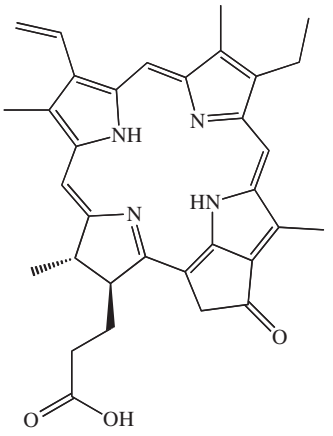
NO DATA AVAILABLE

Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	magnetic sector	884 $[M]^+$ (100), 606 $[M\text{-phytyl}]^+$ (37), 547 (31), 533 (15), 473 (23)	[27]
Remarks	Fluorescence: excitation 434 nm, emission 658 nm (diethyl ether) [26] Pheopigments are generally easier to detect using fluorescence		

Pyropheophorbide *a*

Recommended abbreviation: Pphеide *a* (Pd*a*)



IUPAC: [(17*S*,18*S*)-12-Ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-3,8,13,17-tetramethyl-2^1-oxocyclopenta[*at*]porphyrin-18-yl]propanoic acid

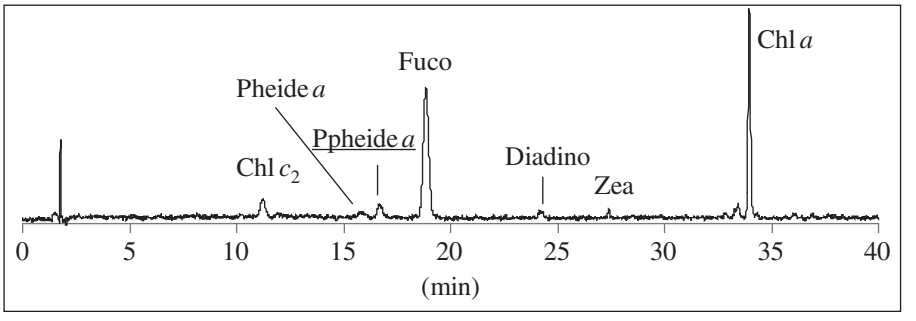
Molecular formula: $C_{33}H_{34}N_4O_3$
Molecular weight: 534.65

Alteration product of	Chlorophyll *a*; occurs in senescent algae and zooplankton fecal pellets
Source culture	*Chroomonas salina* (cryptophyte)
Alteration products	
Synthetically related to	Chl *a*, Pheide *a*, Phe *a*, Pphe *a*
Occurs together with	Pheide *a*, Pphe *a*

HPLC chromatogram (system 1)

NO DATA AVAILABLE

HPLC chromatogram of a coastal marine sample (system 2)



UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
For all practical purposes, identical with pyropheophytin *a*			
Recommended specific absorption coefficient *d* (L g^{-1} cm^{-1})		93.5 (at red maximum in diethyl ether)	[137]

Reference spectra

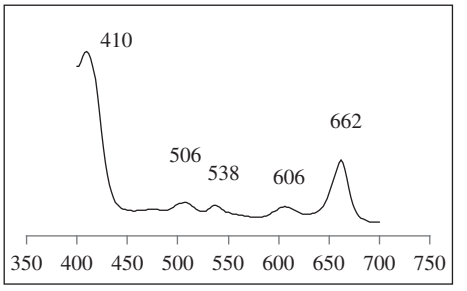
In acetone

For spectrum in acetone, see [109]

In HPLC solvent system 1

NO DATA AVAILABLE

In HPLC solvent system 2

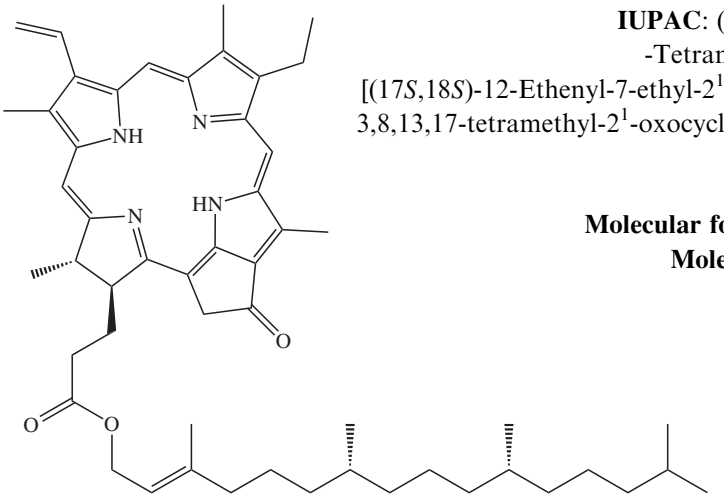


Mass spectra

Ionization technique	Mass analyser type	Diagnostic ions (m/z, rel. intensity)	Ref.
FAB	magnetic sector	534 $[M]^+$; fragments in figure, see ref.	[131]
Remarks	Fluorescence: for all practical purposes, identical with pyropheophytin *a*. Pheopigments are generally easier to detect using fluorescence		

Pyropheophytin *a*

Recommended abbreviation: Pphe *a* (Py*a*)

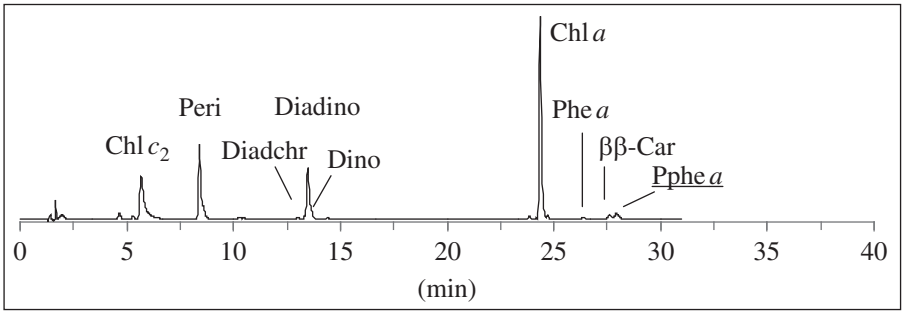


IUPAC: (2*E*,7*R*,11*R*)-3,7,11,15-Tetramethylhexadec-2-enyl [(17*S*,18*S*)-12-Ethenyl-7-ethyl-2^1,2^2,17,18-tetrahydro-3,8,13,17-tetramethyl-2^1-oxocyclopenta[*at*]porphyrin-18-yl]propanoate

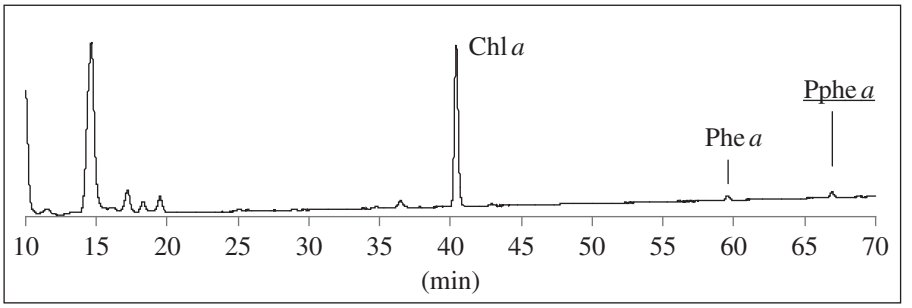
Molecular formula: $C_{53}H_{72}N_4O_3$
Molecular weight: 813.16

Alteration product of	Chlorophyll *a*; occurs in senescent algae and zooplankton fecal pellets
Source culture	*Chroomonas salina* (cryptophyte)
Alteration products	
Synthetically related to	Chl *a*, Phe *a*
Occurs together with	

HPLC chromatogram of *Amphidinium carterae* (system 1)



HPLC chromatogram of a sediment trap sample (system 3)



UV-Vis spectra (see also reference spectra below)

Solvent	λ_{max} (nm)	Band ratio (blue:red ratio)	Ref.
Acetone	*410*, 507, 536, 609, 667	2.3	[145]
Diethyl ether	*409*, 667	2.1	[134]
Recommended specific absorption coefficient *d* ($L\ g^{-1}\ cm^{-1}$)		60.3 (at 667 nm in diethyl ether)	[134]

Reference spectra

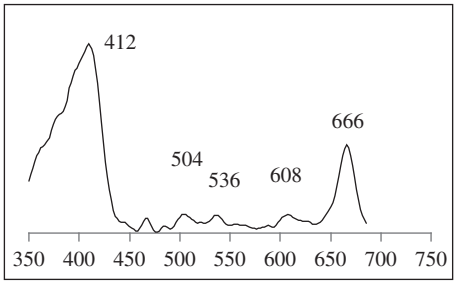
In acetone

For spectrum in acetone, 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.
APCI	Ion trap	813 $[M+H]^+$ MS2: 353, 507	[6]
Remarks	Fluorescence: excitation 407 nm, emission 672 nm (acetone) [145] Pheopigments are generally easier to detect using fluorescence		