

## Which ocean colour algorithm for MERIS in North West European waters?

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### Abstract :

Chlorophyll-a (Chl a) is a key parameter for the assessment of water quality in coastal and shelf environments. The availability of satellite ocean colour offers the potential of monitoring these regions at unprecedented spatial and temporal scales, as long as a high level of accuracy can be achieved. To use satellite derived Chl a to monitor these environments, it is imperative that rigorous accuracy assessments are undertaken to select the most accurate ocean colour algorithm(s).

To this end, the accuracy of a range of ocean colour Chl a algorithms for use with Medium Imaging Resolution Spectrometer (MERIS) Level 2 (L2) Remote Sensing Reflectance (Rrs), using two different atmospheric correction (AC) processors (COASTCOLOUR and MERIS Ground Segment processor version 8.0 – MEGS8.0), were assessed in North West European waters. A total of 594 measurements of Rrs( $\lambda$ ) and/or Chl a were made in the North Sea, Mediterranean Sea, along the Portuguese Coast, English Channel and Celtic Sea between June 2001 and March 2012, where Chl a varied from 0.2 to 35 mg m<sup>-3</sup>. The following algorithms were compared: MERIS Case 1 water Chl a algorithm OC4Me, the MERIS Case 2 algorithm Algal Pigment 2 (AP2), the MODIS-Aqua Case 1 Chl a algorithm OC3 adapted for MERIS (OC3Me), the MODIS-Aqua Garver-Siegel-Maritorena algorithm (GSM) adapted for MERIS and the Gohin et al. (2002) algorithm for MERIS (OC5Me). For both COASTCOLOUR and MEGS8.0 processors, OC5Me was the most accurate Chl a algorithm, which was within ~ 25% of in situ values in these coastal and shelf waters. The uncertainty in MEGS8.0 Rrs(442) (~ 17%) was slightly higher compared to COASTCOLOUR (~ 12%) from 0.3 to 7 mg m<sup>-3</sup> Chl a, but for Rrs(560) the uncertainty was lower for MEGS8.0 (~ 10%) compared to COASTCOLOUR (~ 13%), which meant that MEGS8.0 Chl a was more accurate than COASTCOLOUR for all of the Chl a algorithms tested. Compared to OC5Me, OC4Me tended to over-estimate Chl a, which was caused by non-algal SPM especially at values > 14 g m<sup>-3</sup>. GSM also over-estimated Chl a, which was caused by variations in absorption

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coefficient of coloured dissolved organic matter at 442 nm ( $a_{CDOM}(442)$ ). AP2 consistently underestimated Chl *a*, especially when non-algal SPM was  $> 4 \text{ g m}^{-3}$ .

### Highlights

► Accuracy of MERIS ocean colour algorithms was assessed in NW European waters. ► Both COASTCOLOUR and MEGS8.0 processors were compared for computation of Chl *a*. ► MEGS8.0 OC5Me was the most accurate algorithm; OC4 & AP2 over-estimated Chl *a*. ► Computation of uncertainties in MERIS  $R_{rs}$  over the range in Chl *a* was conducted.

**Keywords** : Case 2 waters, Coastal waters, Shelf waters, Chlorophyll-a, North Sea, Ocean colour, Remote sensing, MERIS, English Channel, Mediterranean coast, Portuguese coast

## 55 1. Introduction.

56 Information on marine environmental parameters, such as chlorophyll-*a* (Chl *a*), is  
57 fundamental for monitoring water quality, eutrophication and climate change ([Birk et al.](#)  
58 [2012](#); [Boyce et al. 2010](#); [Ferreira et al. 2011](#)). Large scale spatial and temporal information  
59 on these parameters can be obtained by means of satellite remote sensing, which can aid our  
60 understanding of biogeochemical cycles ([Chang et al. 2015](#); [Siegel et al. 2014](#)).

61 Monitoring the water quality of coastal and shelf waters is an integral part of water  
62 resource management, which allows tracking the effects of anthropogenic pollutants in the  
63 marine environment. Through the Urban Waste Water Treatment, Nitrate and Water  
64 Framework Directives, the European Union provided a general definition of ‘good ecological  
65 status’ for coastal waters based on 19 key parameters, which includes microbiological and  
66 physico-chemical variables. One of these parameters is Chl *a*, which is the photo-  
67 synthetically active pigment of phytoplankton, and can be measured indirectly from satellite  
68 ocean colour. In open ocean waters, a range of satellite ocean colour products have been  
69 developed, which have proven successful in areas where the principal optically active  
70 material in the water column is phytoplankton. It is however, more difficult to accurately  
71 determine Chl *a* from satellite in optically complex coastal and shelf regions ([IOCCG 2000](#)).  
72 Coastal areas only account for ~7% of the world ocean’s surface, yet play a globally  
73 important role in ameliorating human impacts on the marine ecosystem. Anthropogenic  
74 discharge of nutrients is advantageous for micro-phytoplankton such as diatoms and  
75 dinoflagellates, which potentially could result in increases in planktonic food web

76 productivity in global coastal and shelf zones, and in turn may enhance annual carbon  
77 sequestration in marginal seas (Calbet et al. 2014). Coastal and shelf areas of Europe are  
78 commercially important for fishing and tourism, yet are subject to the increasingly adverse  
79 effects of harmful algal blooms (Baez et al. 2014; Glibert et al. 2014), eutrophication  
80 (Grizzetti et al. 2012; Romero et al. 2013) and climate change (Andersson et al. 2013;  
81 McQuatters-Gollop et al. 2007). In these regions, the presence of Coloured Dissolved  
82 Organic Material (CDOM) and mineral SPM as well as Chl *a* modify the light field (IOCCG  
83 2000), which makes accurate estimation of Chl *a* from satellite data in these regions, difficult.  
84 It is therefore necessary to develop and validate the accuracy of Chl *a* algorithms in coastal  
85 and shelf regions to facilitate monitoring of these environments.

86         The availability of data from the satellite sensor MERIS (2002-2012), which had  
87 more spectral bands and a higher spatial resolution compared to SeaWiFS (1997-2010) plus  
88 novel atmospheric correction (AC) models, has enabled the development of new products for  
89 optically complex waters. These include an algorithm that retrieves inherent optical  
90 properties (IOP) and biogeochemical parameters from Case 2 waters (Doerffer and Schiller  
91 2007). Directional water leaving radiance is input to the algorithm and it outputs Chl *a*, Total  
92 Suspended Matter (SPM) and the absorption coefficient of detrital material and gelbstoff ( $a_{dg}$ )  
93 based on the conversion of scattering and absorption coefficients using non-linear multiple  
94 inversion solutions and regional conversion factors to give concentrations. This algorithm has  
95 been shown to be accurate in some (Doerffer and Schiller 2007; Schiller and Doerffer 2005),  
96 but not all Case 2 coastal (Cui et al. 2014; Melin et al. 2007; Tilstone et al. 2012), estuarine  
97 (Ambarwulan et al. 2010), lakes (Binding et al. 2011; Palmer et al. 2015) and other highly  
98 absorbing water bodies (Beltran-Abaunza et al. 2014; Folkestad et al. 2007; Ohde et al.  
99 2007). As a consequence, a number of alternative algorithms have been proposed (Beltran-  
100 Abaunza et al. 2014; Hokedal et al. 2005; Peters et al. 2005; Tilstone et al. 2012; van der

101 [Woerd and Pasterkamp 2004; Zibordi et al. 2009a](#)) . To improve satellite ocean colour  
102 algorithms, it is fundamental to improve the input satellite  $R_{rs}$  that are used to calculate Chl  $a$ .  
103 To this end, ESA funded a number of initiatives to improve the AC scheme for MERIS which  
104 included improvements in the neural network (NN) AC model for coastal waters  
105 (COASTCOLOUR), and re-processing of the MERIS archive using the MEGS8.0 processor  
106 which uses both a bright pixel correction for highly scattering waters and a clear water AC  
107 model ([Lerebourg et al. 2011](#)). It is important to test these and to select the most accurate  
108 algorithm for remotely sensed Chl  $a$  in European coastal and shelf seas to coincide with the  
109 launch of the Copernicus new generation satellite Sentinel-3 ([Donlon et al. 2012](#)).

110 In this paper we validate a range of MERIS Chl  $a$  products, using both MEGS8.0 and  
111 COASTCOLOUR processors, for the North West European regions of the North Sea, Celtic  
112 Sea, English Channel, South and Western Iberian Peninsula and Mediterranean Sea. Five  
113 ocean colour algorithms were compared and the choice of the algorithms was based on their  
114 availability to the user community as standard products for MERIS and MODIS-Aqua.

115

## 116 **2. Methods.**

### 117 *2.1. Study area characteristics and sampling regime*

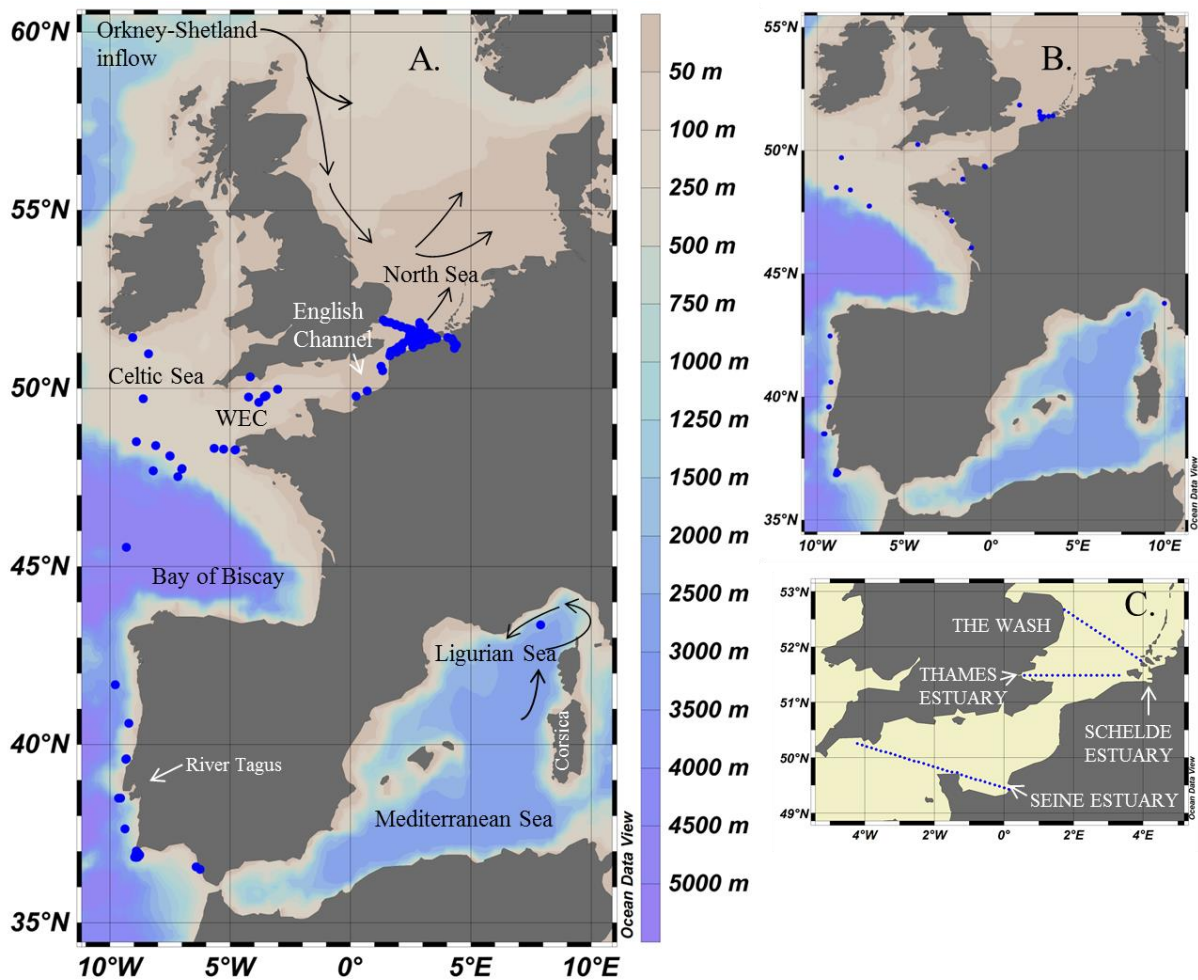
118 Remote Sensing Reflectance ( $R_{rs}(\lambda)$ ) and / or Chl  $a$  were measured at 594 stations between  
119 April 2001 and March 2012 in the North Sea, English Channel and Celtic Sea (from here on  
120 referred to as English Channel), Mediterranean Sea and along the Iberian coast ([Fig. 1A](#)).

121 These data are available from ESA's MERMAID and CCOASTCOLOUR data sets ([Nechad  
122 et al. 2015](#)).

123 The North Sea is characterized by the entrance of warm, high saline water through the  
124 Orkney-Shetland inflow (off NE Scotland) and through the English Channel-Straits of Dover  
125 in the south ([Fig. 1A](#)), which drives a cyclonic pattern of circulation, which can cause re-

126 suspension of sediment over the shallow North Sea shelf (Reid et al. 1988). The Portuguese  
 127 coast is affected by seasonal upwelling from March to September and the poleward current  
 128 during the winter months (Fiuza et al. 1982). In addition, the coastal waters close to Lisbon  
 129 are strongly affected by the River Tagus, which elevates the CDOM and SPM on the shelf  
 130 break (Sa et al. 2015). The Mediterranean Sea stations are in the central Ligurian Sea which  
 131 is characterised by a cyclonic circulation that causes strong flows close to the coast which  
 132 circulate north of the Island of Corsica and return in a south west direction (Fig. 1A) to  
 133 establish a front between the coastal shelf and the deeper offshore water (Antoine et al.  
 134 2008).

135



136

137 **Figure 1.** Location of sampling stations for (A.) *in situ* measurements of  $R_{rs}$  and Chl  $a$  (B.)  
138 match-ups between *in situ* and MERIS MEGS8.0 & COASTCOLOUR  $R_{rs}$  and Chl  $a$ , (C.)  
139 Transects from which MEGS8.0 Chl  $a$  processed using OC5Me, OC4Me, AP2 and non-algal  
140 SPM were extracted. The colour scale indicates the bathymetry depth. In (A.), the arrows  
141 represent the predominant currents to illustrate the inflow of Atlantic water through the  
142 Orkney-Shetland channel in the North and the English Channel in the South and the flow of  
143 the Mediterranean Sea current around Corsica Island.

144

145 North Sea and English Channel coastal areas have high absorption and scattering  
146 properties (Hommersom et al. 2009), which are optically variable due to different regional  
147 and seasonal contributions of  $a_{CDOM}$ ,  $a_{NAP}$  and  $b_{bp}$  (Babin et al. 2003a; Babin et al. 2003b) and  
148 can therefore switch between case 1 and 2 water types (Groom et al. 2009). There are three  
149 main groups of specific-absorption properties in the North Sea, English Channel and Celtic  
150 Sea with low  $a_{ph}^*$  ( $<0.03 \text{ mg m}^{-2}$ ), high  $a_{NAP}^*$  ( $>0.04 \text{ g m}^{-2}$ ) and  $a_{CDOM}$  ( $>0.4 \text{ m}^{-1}$ ) close to the  
151 coast; medium  $a_{ph}^*$  ( $>0.03, <0.05 \text{ mg m}^{-2}$ ),  $a_{NAP}^*$  ( $>0.02, <0.04 \text{ g m}^{-2}$ ) and  $a_{CDOM}$  ( $>0.1, <0.4$   
152  $\text{m}^{-1}$ ) over the shelf; and high  $a_{ph}^*$  ( $>0.05 \text{ mg m}^{-2}$ ), low  $a_{NAP}^*$  ( $<0.02 \text{ g m}^{-2}$ ) and  $a_{CDOM}$  ( $<0.1 \text{ m}^{-1}$ )  
153 further offshore (Tilstone et al. 2012). Portuguese coastal waters are dominated by  $a_{ph}$ ,  
154 though  $a_{CDOM}$  can account for between 33 and 60% of the total absorption between bloom  
155 and non-bloom conditions (Goela et al. 2015). The principal satellite validation station in the  
156 Mediterranean Sea is BOUSSOLE, which is a deep clear water site where the dominant  
157 optically substance is phytoplankton. Other stations are sampled closer to the coast on the  
158 monthly transect to BOUSSOLE, which can be affected by other optically active substances  
159 (Antoine et al. 2008).

160

161 2.2. Measurement of normalized water leaving radiance and Remote Sensing Reflectance.

162 Measurements of normalized water leaving radiance ( $nL_w$ ) were performed by the Royal  
 163 Belgian Institute of Natural Sciences (RBINS), CIMA and Laboratoire d’Oceanographie de  
 164 Villefranche (LOV). RBINS used three TriOS-RAMSES hyperspectral spectro-radiometers,  
 165 two measuring radiance and one measuring downwelling irradiance, mounted on a steel  
 166 frame fixed to the bow of the ship, facing forward to minimize ship shadow and reflection, so  
 167 that zenith angles of the sea and sky viewing radiance sensors were  $40^\circ$  as in (Ruddick et al.  
 168 (2006). To reduce sun glint and bidirectional reflectance effects, the ship was maneuvered on  
 169 station to point the radiance sensors at a relative azimuth angle of  $135^\circ$  away from the sun.  
 170 The spectro-radiometers were calibrated before and after the cruise consistent with SeaWiFS  
 171 protocols (Mueller 2000). Water-leaving reflectance ( $\rho_w$ ) was calculated from simultaneous  
 172 above-water measurements of downwelling irradiance ( $E_d^{0+}$ ), total upwelling radiance ( $L_{sea}^{0+}$ )  
 173 and sky radiance ( $L_{sky}^{0+}$ ) (in the direction of the region of sky that reflects into the sea viewing  
 174 sensor), from:

$$175 \quad \rho_w(\lambda) = \pi \frac{L_{sea}^{0+}(\lambda) - \rho_{sky} L_{sky}^{0+}(\lambda)}{E_d^{0+}(\lambda)} \quad (\text{Equation 1})$$

176 where  $\rho_{sky}$  is the air-water interface reflection coefficient for radiance. In the case of a flat sea  
 177 surface  $\rho_{sky}$  is equal to the Fresnel reflection coefficient and is assumed to be 0.02 for clear  
 178 skies for satellite ‘match-ups’ (Ruddick et al. 2006). Residual skylight was removed using  
 179 baseline correction following Mobley (1999). The normalized water leaving radiance ( $nL_w$ )  
 180 was calculated from:

$$181 \quad nL_w(\lambda) = \frac{\rho_w(\lambda)}{\pi} \times f_0(\lambda) \quad (\text{in mW cm}^{-2} \mu\text{m}^{-1} \text{sr}^{-1}) \quad (\text{Equation 2})$$

182

183 where  $f_0(\lambda)$  is the mean solar flux above the earth’s atmosphere.  $R_{rs}(\lambda)$  ( $\text{sr}^{-1}$ ) was then

184 calculated from:



185 
$$R_{rs}(\lambda) = \frac{L_w(\lambda)}{E_s(\lambda, 0^+)} \quad (\text{Equation 3}),$$

186 where  $E_s(\lambda, 0^+)$  is the above surface downwelling spectral irradiance ( $\text{W m}^{-2} \text{ nm}^{-1}$ ) and  
187  $L_w(\lambda)$  is the water leaving radiance ( $\text{W m}^{-2} \text{ nm}^{-1} \text{ sr}^{-1}$ ). NASA ocean optics protocols were  
188 used to compute of  $L_w(\lambda)$ ,  $nL_w(\lambda)$  and  $R_{rs}(\lambda)$  (Mueller 2000). Surface downwelling irradiance  
189 ( $E_s(\lambda, 0^+)$ ) was calculated from:

190 
$$E_s(\lambda, 0^+) = (1 + \alpha) E_d(\lambda, 0^-) \quad (\text{Equation 4}),$$

191 where  $\alpha$  is the Fresnel reflection albedo from air + sky ( $\sim 0.043$ ), and  $E_d(\lambda, 0^-)$  is extrapolated  
192 from the  $E_d(\lambda, z)$  profile.

193 CIMA collected *in situ* radiometric measurements at three sampling stations off South  
194 West Portugal, following MERIS protocols (Barker 2011; Doerffer 2002). Measurements of  
195  $\rho_w$  were acquired with a Satlantic tethered attenuation coefficient chain sensor (TACCS),  
196 which consists of a floating buoy encasing a hyperspectral surface irradiance sensor ( $E_s(\lambda)$ )  
197 and a subsurface radiance sensor ( $L_u(\lambda)$ ) located 0.62 m below the surface and a tethered  
198 attenuation chain supporting four subsurface irradiance sensors  $E_d(z)$  at 2, 4, 8, and 16 m.  
199 Further details of the processing of  $E_s$ ,  $L_u$  and  $E_d$  are given in (Cristina et al. 2014; Cristina et  
200 al. 2009). The  $\rho_w$  acquired by the TACCS was calculated from:

201 
$$\rho_w(\lambda) = \pi \frac{L_w(\lambda)}{E_s(\lambda)} \quad (\text{Equation 5}),$$

202 where  $\rho_w$  is equivalent to  $R_{rs}$  (equation 3) when scaling by a factor of  $\pi$  (i.e.  $R_{rs} = \rho_w / \pi$ ).

203 Measurements taken by LOV were obtained from the radiometric data buoy

204 BOUSSOLE using the methods described in Antoine et al. (2008).

205

### 206 2.3. Measurement of Chlorophyll-a

207 On all cruises, surface water samples were collected using 10 L Niskin bottles and

208 between 0.25 and 2 L of seawater were filtered onto 0.7 µm GF/F filters. PML, MARE and  
209 CIMA used High Performance Liquid Chromatography (HPLC) to determine Chl *a*. PML  
210 extracted phytoplankton pigments into 2 mL 100% acetone containing an internal standard  
211 (apocarotenoate; Sigma) using an ultrasonic probe (35 s, 50 W). Extracts were centrifuged to  
212 remove filter and cell debris (3 min at 20 x g) and analyzed by HPLC using a reversed phase  
213 C8 column and gradient elution (Barlow et al. 1997) on an Agilent 1100 Series system with  
214 chilled autosampler (4°C) and photodiode array detection (Agilent Technologies). CIMA  
215 extracted the pigments in 90% acetone for 4-6 hours in a refrigerator (-4°C) and using an  
216 ultrasonic probe for 20 s before and after refrigeration. Extracts were centrifuged and then  
217 analysed either on a Waters 600E HPLC system with diode array detector and a C8 Thermo  
218 Hypersil-Keystone (ODS-2) column or on an Agilent HPLC with diode array using a C8  
219 Alltech Altima column following Goela et al. (2014). MARE extracted pigments with 2–5 ml  
220 of 95% cold-buffered methanol (2% ammonium acetate) for 30 min to 1 h at -20 °C, in the  
221 dark. Pigment extracts were analysed using a Shimadzu HPLC comprising a solvent delivery  
222 module (LC-10ADVP) with system controller (SCL-10AVP), a photodiode array (SPD-  
223 M10ADVP), and a fluorescence detector (RF-10AXL). Chromatographic separation was  
224 carried out with a C8 column, following Kraay et al. (1992) and adapted by Brotas and  
225 PlanteCuny (1996). PML, CIMA and MARE calibrated the HPLC system using a suite of  
226 standards (DHI) and pigments in samples identified from retention time and spectral match  
227 using photodiode array spectroscopy (Jeffrey et al. 1997). Chl *a* concentration was calculated  
228 using response factors generated from calibration using a Chl *a* standard (DHI Water and  
229 Environment, Denmark). Samples taken by IFREMER along the North France coast were  
230 measured by spectrophotometry using the methods outlined in Lorenzen (1967).

231

232 *2.4. Measurement of Suspended Particulate Material (SPM)*

233 All laboratories filtered between 0.5 and 3 L of seawater onto 47 mm, 0.7  $\mu\text{m}$  GF/F filters in  
234 triplicate. The filters were ashed at 450°C, washed for 5 mins in 0.5 L of MilliQ, and then  
235 dried in a hot air oven at 75°C for one hour, pre-weighed and stored in desiccators ([Van der](#)  
236 [Linde 1998](#)). Seawater samples were filtered in triplicate onto the pre-prepared filters which  
237 were then washed (including the rim) three times with 0.05 L MilliQ to remove residual salt.  
238 Blank filters were also washed with MilliQ to quantify any potential error due to incomplete  
239 drying. The filters were then dried at 75°C for 24 hrs and weighed on microbalances  
240 (detection limit 10  $\mu\text{g}$ ). SPM concentrations were determined from the difference between  
241 blank and sample filters and the volume of seawater filtered.

242

#### 243 *2.5. Measurement of CDOM absorption coefficients ( $a_{CDOM}(\lambda)$ ).*

244 All laboratories filtered replicate seawater samples through 0.2  $\mu\text{m}$  Whatman Nuclepore  
245 membrane filters into acid cleaned glassware. The first two 0.25 L of the filtered seawater  
246 were discarded.  $a_{CDOM}(\lambda)$  was determined using the third sample in a 10 cm quartz cuvette  
247 from 350 to 750 nm relative to a bi-distilled MilliQ reference blank and was calculated from  
248 the optical density of the sample and the cuvette path length following the protocols given in  
249 [Tilstone et al. \(2004\)](#).

250

#### 251 *2.6. Satellite data and algorithms.*

252 MERIS full resolution (300 m) COASTCOLOUR v2013 and reduced resolution (1  
253 km) MEGS8.0 data were downloaded from Brockman Consult and extracted using Beam  
254 v4.8. Both MEGS8.0 and COASTCOLOUR L2  $R_{rs}$  were used to process five Chl  $a$   
255 algorithms. MEGS8.0 processor has a two-step approach to atmospheric correction; if there is  
256 any signal in the NIR due to backscattering by sediment or coccolithophores, the Bright Pixel  
257 AC ([Moore and Lavender 2010](#)) is triggered ([Lerebourg et al. 2011](#)). If this is not triggered,

258 the Clear Water Atmospheric Correction model is implemented (Antoine and Morel 1997).  
259 The COASTCOLOUR AC is an NN based inversion technique that implements a forward  
260 model configured with a set of regional, coastal aerosol optical properties (Brockmann 2011)  
261 collected from the global aeronet network (Zibordi et al. 2009b).

262 The following MERIS quality flags were used to eliminate erroneous data generated  
263 from the processors: cloud flag over ocean (CLOUD), land (LAND), no glint correction  
264 applied – accuracy uncertain (HIGH\_GLINT), reflectance corrected for medium glint –  
265 accuracy maybe degraded (MEDIUM\_GLINT), highly absorbing aerosols (AODB), low sun  
266 angle (LOW\_SUN), low confidence flag for water leaving or surface reflectance (PCD1\_13)  
267 and reflectance out of range (PCD\_15). The MERIS L2 products were extracted from a 3 x 3  
268 pixel box, within  $\pm 0.5$  hrs of MERIS overpasses. The functional form of each of the Chl *a*  
269 algorithms tested is given in Table 1 and described in brief below.

270 The first Chl *a* algorithm tested was the standard Case 2 MERIS Chl *a* product (AP2)  
271 (Doerffer and Schiller 2007; Schiller and Doerffer 2005), which uses an NN to derive the  
272 absorption coefficient of phytoplankton ( $a_{ph}$ ) and the particulate scattering coefficient ( $b_p$ ),  
273 and through empirical bio-optical relationships, Chl *a*, SPM and  $a_{dg}$  are computed. An inverse  
274 model solves the IOPs from  $R_{rs}(\lambda)$  using a look up table. The total absorption coefficient ( $a_{tot}$ )  
275 is then apportioned into  $a_{ph}$  and  $a_{dg}$  and empirical solutions are used to convert  $a_{ph}$  to Chl *a*  
276 and the particulate backscatter coefficient ( $b_{bp}$ ) to SPM. The AP2 algorithm was calibrated  
277 using a global dataset, which included a large IOP data set from North Sea coastal waters of  
278 the German Bight. AP2 solves Chl *a* from  $a_{ph}$  as follows;  $Chl\ a = 21.0 * a_{ph}(442)^{1.04}$  (Table 1).

279 The second algorithm tested is the default MERIS Case 1 Chl *a* algorithm (AP1; also  
280 known as OC4Me). OC4Me is a fourth-order polynomial original designed for use with  
281 SeaWiFs (O'Reilly et al. 1998), that has been adapted for MERIS (Morel and Antoine 2011).  
282 It uses the maximum remote sensing reflectance ratio from:  $R_{rs}\ 442/560$ ,  $R_{rs}\ 490/560$  or

Algorithm	Reference	Functional form
AP2	Doerffer & Schiller (2007)	$Chla = 21.0 * a_{ph} (442)^{1.04}$
OC4Me	Morel & Antoine (2011)	$Chl\_a = 10^{(a+bR+cR^2+dR^5+eR^4)}$ $R = \log_{10} \left\{ \max \left[ \left( \frac{R_{rs} 443}{R_{rs} 560} \right), \left( \frac{R_{rs} 490}{R_{rs} 560} \right), \left( \frac{R_{rs} 510}{R_{rs} 560} \right) \right] \right\}$ <p>a = 0.4502748; b = -3.259491; c = 3.52271; d = -3.359422; e = 0.949586.</p>
OC3Me	O'Reilly et al. (2000)	$Chl\_a = 10^{(a+bR+cR^2+dR^5+eR^4)}$ $R = \log_{10} \left\{ \max \left[ \left( \frac{R_{rs} 442}{R_{rs} 560} \right), \left( \frac{R_{rs} 490}{R_{rs} 560} \right) \right] \right\}$ <p>a = 0.40657; b = -3.6303; c = 5.44357; d = 0.0015; e = -1.228.</p>
GSM	Maritorena et al. (2002)	$L_{wN}(\lambda) = \frac{tF_0(\lambda)}{n_w^2} \sum_{i=1}^2 g_i \left\{ \frac{[b_{bw}(\lambda) + b_{bp}(442)(\lambda/442)^{-1.0337}]}{[b_{bw}(\lambda) + b_{bp}(442)(\lambda/442)^{-1.0337}] + [a_w(\lambda) + Chl\_a \times a_{ph}^*(\lambda) + a_{CDOM}(442) \times e^{-0.020\alpha(\lambda-442)}]} \right\}^i$
OC5Me	Gohin et al. (2002)	$Chl\ a = R, nLw(412), nLw(555)$ triplet – based on Look Up Table

285 510/560. The switch between  $R_{rs}$  442/560 and  $R_{rs}$  490/560 theoretically occurs at a Chl  $a$   
286 concentration of  $0.534 \text{ mg m}^{-3}$  and between  $R_{rs}$  490/560 and  $R_{rs}$  510/560 at  $2.23 \text{ mg m}^{-3}$ . Chl  
287  $a$  was estimated using the equation given in Table 1, where  $\rho$  is the maximum  $R_{rs}(\lambda)/560$   
288 ratio.

289 OC3Me is a fourth-order band ratio algorithm that uses one of two  $R_{rs}(\lambda)/R_{rs}(560)$   
290 ratios; either  $R_{rs}(442)/R_{rs}(560)$  or  $R_{rs}(490)/R_{rs}(560)$ , depending on the reflectance  
291 characteristics of the water type (O'Reilly et al. 2000). It is the default Case 1 water algorithm  
292 for MODIS-Aqua and has been adapted for MERIS using the maximum remote sensing  
293 reflectance ratio from:  $R_{rs}$  442/560 or  $R_{rs}$  490/560 and the coefficients for OC4Me given in  
294 Table 1.

295 OC5Me is a modified version of OC4Me, which includes an empirical  
296 parameterisation of 412 and 560 nm channels for MERIS related to the absorption of CDOM  
297 and scattering of SPM (Novoa et al. 2012; Saulquin et al. 2011). Chl  $a$  concentration is  
298 determined from the triplet values of OC4Me maximum band ratio,  $nL_w(412)$  and  $nL_w(560)$ ,  
299 from a Look Up Table (LUT), based on the relationships between measured Chl  $a$  and  
300 satellite  $R_{rs}(\lambda)$  from observations in the English Channel and Bay of Biscay (Gohin et al.  
301 2002). The method has also been extended to the Mediterranean Sea and applied to MODIS-  
302 Aqua and MERIS (Gohin 2011). OC5 satellite images using both MODIS-Aqua and MERIS  
303 are available from <https://www.neodaas.ac.uk/multiview/pa/>

304 The GSM is an optimized semi-analytical algorithm that simultaneously retrieves Chl  
305  $a$ ,  $a_{dg}$  and  $b_{bp}$  at 442 nm, from spectral measurements of  $nL_w(\lambda)$ . The parameters for the  
306 model were obtained through simulated annealing which is a global optimization technique  
307 (Maritorena et al. 2002). The model was originally parameterised for SeaWiFS and in this  
308 paper has been adapted for MERIS using the amoeba implementation from SeaDAS with an

309 update of the absorption spectrum values for pure water (Pope and Fry 1997) to (Kou et al.  
310 1993) which extend the spectrum beyond 700 nm to 709, 753 & 778 nm for MERIS.

311 The concentration of non-algal SPM (the inorganic component of SPM that is not  
312 related to phytoplankton) was derived using the method developed in Gohin et al. (2005).  
313 Once Chl *a* has been determined using OC5Me, non-algal SPM is estimated from  $nL_w(560)$   
314 or  $nL_w(670)$  by inverting the semi-analytic model.  $nL_w(560)$  is used in clear or moderately  
315 turbid waters (where non-algal SPM  $<4 \text{ g m}^{-3}$ ) and  $nL_w(670)$  for highly turbid waters (Gohin  
316 2011).

317

### 318 2.7. Algorithm Performance.

319 The performance of the Chl *a* algorithms was assessed in four ways: (1.) using 482  
320 coincident *in situ* measurements of  $R_{rs}(\lambda)$  and Chl *a*; the *in situ*  $R_{rs}(\lambda)$  were used to run the  
321 algorithms and the resulting Chl *a* values were compared against the *in situ* Chl *a* (Fig. 2,  
322 Table 2). (2.) A data base of 594 *in situ* HPLC and fluorometric Chl *a* (which includes the  
323 482 coincident *in situ*  $R_{rs}(\lambda)$  and Chl *a*, plus additional Chl *a* measurements) comprising data  
324 from the Celtic Sea (PML), Eastern English Channel (IFREMER), Iberian Peninsula (CIMA

325 **Table 2.** Performance indices for relative errors between *in situ* and modelled Chl *a* from  
326 AP2, GSM, OC3Me, OC4Me and OC5Me using *in situ*, COASTCOLOUR and MEGS8.0  
327  $R_{rs}(\lambda)$ . Percentage variance explained ( $R^2$ ), intercept and slope and log-difference errors in  
328 measured and satellite Chl *a* ratio ( $r$ ) as Mean ( $M$ ), Standard deviation ( $S$ ), root-mean square  
329 ( $\text{Log}_{10}$ -RMS) and root-mean square error (RMS-E). The geometric mean and one-sigma  
330 range of the ratio ( $F = \text{Value}_{\text{alg}}/\text{Value}_{\text{meas}}$ ) are given by  $F_{\text{med}}$ ,  $F_{\text{min}}$ , and  $F_{\text{max}}$ , respectively;  
331 values closer to 1 are more accurate. RPD is the relative percentage difference. The algorithm  
332 with the highest Chl *a* accuracy is highlighted in bold.  
333

$R_{rs}(\lambda)$	$R^2$	Slope	Intercept	$r$	RPD	$\text{Log}_{10}$ -RMS	M	S	$F_{\text{med}}$	$F_{\text{max}}$	$F_{\text{min}}$	RMS-E
<b><i>in situ</i> N=482.</b> (North Sea, N = 384; Portugal, N = 87; Med, N = 12).												
OC3Me	0.41	0.23	3.07	<b>0.92</b>	<b>-9</b>	<b>0.23</b>	-0.03	<b>0.23</b>	0.93	1.57	0.55	<b>4.97</b>
OC4Me	<b>0.50</b>	0.24	2.54	0.76	24	0.24	<b>-0.02</b>	0.24	<b>0.95</b>	1.66	0.55	5.77
GSM	0.47	<b>1.34</b>	6.41	1.13	-61	0.43	0.29	0.31	1.96	4.01	<b>0.96</b>	27.20
OC5Me	0.38	0.32	<b>1.54</b>	0.80	104	0.33	-0.11	0.28	0.78	<b>1.49</b>	0.41	5.90
<b>COASTCOLOUR N=113</b> (North Sea, N = 18; WEC, N = 16; Portugal, N = 66; Med, N = 13).												
AP2	0.61	0.71	0.61	<b>1.42</b>	83	0.44	<b>0.03</b>	0.43	<b>1.07</b>	2.92	0.39	2.46
OC3Me	0.65	0.72	0.26	2.05	64	0.42	0.05	0.42	1.12	2.92	0.43	2.10
OC4Me	0.67	0.76	0.46	<b>0.68</b>	<b>20</b>	0.43	-0.09	0.42	0.81	<b>2.14</b>	0.31	2.04
GSM <sup>a</sup>	0.61	<b>0.99</b>	<b>0.10</b>	2.42	105	0.40	0.05	0.54	1.13	3.89	0.33	<b>2.01</b>
OC5Me	<b>0.75</b>	0.65	0.26	1.58	63	<b>0.39</b>	0.06	<b>0.39</b>	1.14	2.79	<b>0.44</b>	2.14
<b>MEGS8.0 N = 88</b> (North Sea, N = 18; WEC, N = 9; Portugal, N = 45; Med, N = 16).												
AP2	0.31	0.42	0.72	1.42	103	0.47	0.09	0.46	1.24	3.56	0.43	2.41
OC3Me	0.51	0.64	0.48	1.32	42	0.32	<b>0.04</b>	0.32	1.11	2.29	0.54	1.98
OC4Me	0.55	<b>0.83</b>	0.63	0.62	<b>25</b>	0.32	-0.09	0.31	<b>0.81</b>	1.65	0.40	2.14
GSM <sup>b</sup>	0.58	0.60	0.40	1.51	84	0.36	0.11	0.34	1.30	2.85	0.59	2.54
OC5Me	<b>0.87</b>	0.62	<b>0.18</b>	<b>1.05</b>	46	<b>0.27</b>	0.10	<b>0.25</b>	1.25	2.21	<b>0.71</b>	<b>1.61</b>

334 <sup>a</sup>For GSM Chl *a* calculated using COASTCOLOUR  $R_{rs}$ , N=89 match-ups were available  
335 (North Sea, N = 11; WEC, N = 0; Portugal, N = 65; Med, N = 13).

336 <sup>b</sup>For GSM Chl *a* calculated using MEGS8.0  $R_{rs}$ , N=81 match-ups were available (North Sea,  
337 N = 18; WEC, N = 2; Portugal, N = 45; Med, N = 16).



338 & MARE), North Sea (RBINS & PML), Mediterranean Sea (LOV) and Western English  
339 Channel (PML) (Fig. 1B), were compared against Chl *a* match-ups from MERIS overpasses  
340 using COASTCOLOUR (Fig. 3, Table 2) and MEGS 8.0 (Fig. 4, Table 2) data. MERIS  
341 match-ups  $\pm 0.5$  hr between *in situ* sampling and MERIS data from a  $3 \times 3$  pixel array around  
342 the sampling station were extracted to compare against *in situ* Chl *a* following the procedures  
343 outlined in (Bailey and Werdell 2006). The Chl *a* algorithms yielded a varying number of  
344 match-ups depending on the input  $R_{rs}(\lambda)$  used and the associated quality flags raised. To  
345 facilitate statistical comparison, common returns for OC5Me, OC4Me, OC3Me & AP2 were  
346 used. (3.) MERIS MEGS 8.0 Chl *a* values from AP2, OC4Me and OC5Me were compared  
347 along transects in the North Sea from the Thames Estuary in the UK (51.47 °N, 0.59 °E) to  
348 the Schelde Estuary in the Netherlands (51.49 °N, 3.31 °E) and from the Schelde Estuary  
349 (51.49 °N, 4.13 °E) to The Wash in the UK (52.67 °N, 2.01 °E). Chl *a* values were extracted  
350 at every 10 km along each transect from daily images between March and September from  
351 2003 to 2007 (Fig. 5). (4.) monthly composite images from AP2, OC4Me, GSM and OC5Me  
352 using MERIS MEGS 8.0 Chl *a* were compared for the months of April 2010 and July 2011  
353 (Fig. 6, 7). Additional data were extracted from a transect from the UK coast in the Western  
354 English Channel (50.25 °N, 4.21 °W) to the River Seine on the French coast (49.42 °N, 0.14  
355 °E) at every 10 km to evaluate spatial differences in algorithm performance for these images  
356 (Fig. 8).

357 To assess algorithm performance, the following statistical metrics were used: The  
358 mean (M), standard deviation (S), and  $\log_{10}$ -root-mean square ( $\log_{10}$  RMS) of the difference  
359 error (r) between measured and MERIS Chl *a* at each station following the methods described  
360 in Campbell et al. (2002). The geometric mean and one-sigma range of the inverse  
361 transformed ratio between satellite and measured values are given by M ( $F_{\text{med}}$ ), M-S ( $F_{\text{min}}$ ),  
362 M+S ( $F_{\text{max}}$ ) and were used as algorithm performance indices. The relative percentage

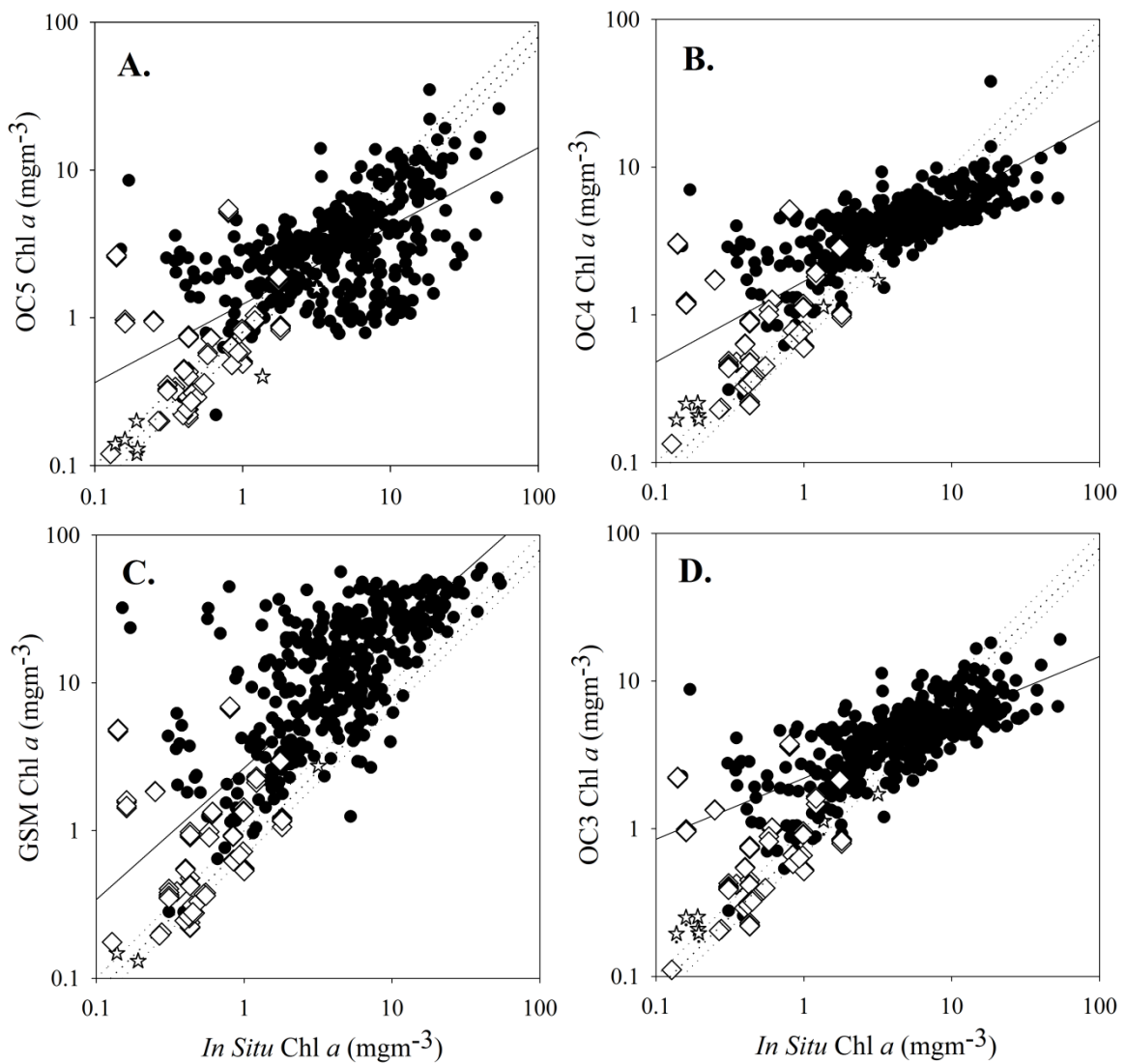
363 difference (RPD) was calculated following Antoine et al. (2008). The uncertainty in  
364 MEGS8.0 and COASTCOLOUR  $R_{rs}(\lambda)$  were assessed against *in situ*  $R_{rs}(\lambda)$  at match-up  
365 stations. The relative difference between *in situ* and satellite  $R_{rs}(\lambda)$  was calculated following  
366 Hu et al. (2013) and expressed as percentage uncertainty over the range in *in situ* Chl *a* and  
367 SPM (Fig. 11).

368

### 369 3. Results

370 3.1. Accuracy assessment of ocean colour algorithms for MERIS in North West European  
371 waters using *in situ*  $R_{rs}(\lambda)$ .

372 Firstly we assessed the accuracy of the algorithms using *in situ*  $R_{rs}$  to calculate Chl *a* (Fig. 2,  
373 Table 2) measured at the stations given in Figure 1A. The majority of *in situ*  $R_{rs}$  used to  
374 compute algorithm Chl *a* values were from the North Sea, which comprised 80% of the  
375 dataset. *In situ*  $R_{rs}$  from the Portuguese coast and Mediterranean Sea constituted 20% of the  
376 data set. The log-RMS, RMS-E bias and random error were smallest for OC4Me and  
377 OC3Me. The percentage variance explained ( $R^2$ ) was greatest for OC4Me and OC3Me had  
378 the lowest RPD, which was within 24 and 9 % of *in situ* Chl *a*, respectively (Fig. 2B, D,  
379 Table 2). The linear regression slope and  $F_{\min}$  for GSM were closest to 1, indicating that the  
380 GSM is more accurate at the lower range of Chl *a* values when using *in situ*  $R_{rs}$ . The GSM  
381 however, had the highest log-RMS, RMS-E,  $F_{\max}$ ,  $F_{\text{med}}$  and intercept (Fig. 2C, Table 2),  
382 which suggests that it may not be suitable for these coastal waters. By comparison, OC5 had  
383 the lowest intercept and  $F_{\max}$  closest to 1, indicating that it is more accurate at the higher  
384 range Chl *a* values when using these *in situ*  $R_{rs}$  data (Fig. 2A, Table 2). The processing of  
385 AP2 using *in situ*  $R_{rs}$  was not possible as the atmospheric correction is embedded within the  
386 standard AP2 processor such that any other input source of  $R_{rs}$  other than MERIS  $R_{rs}$ , is not  
387 feasible.



388  
 389 **Figure 2.** Comparison of *in situ* Chl *a* and *in situ*  $R_{rs}$  derived Chl *a* for (A.) OC5, (B.) OC4,  
 390 (C.) GSM, (D.) OC3. Faint dotted lines are the 1:1 line, upper and lower 20% quartiles. Solid  
 391 line is the regression line. Filled circles are North Sea, open stars are Portuguese waters, open  
 392 diamonds are Mediterranean Sea. All data points are from coastal and shelf waters, except for  
 393 one station in the Mediterranean Sea and five stations off the Portuguese Shelf (see [Figure](#)  
 394 [1A](#)).

395

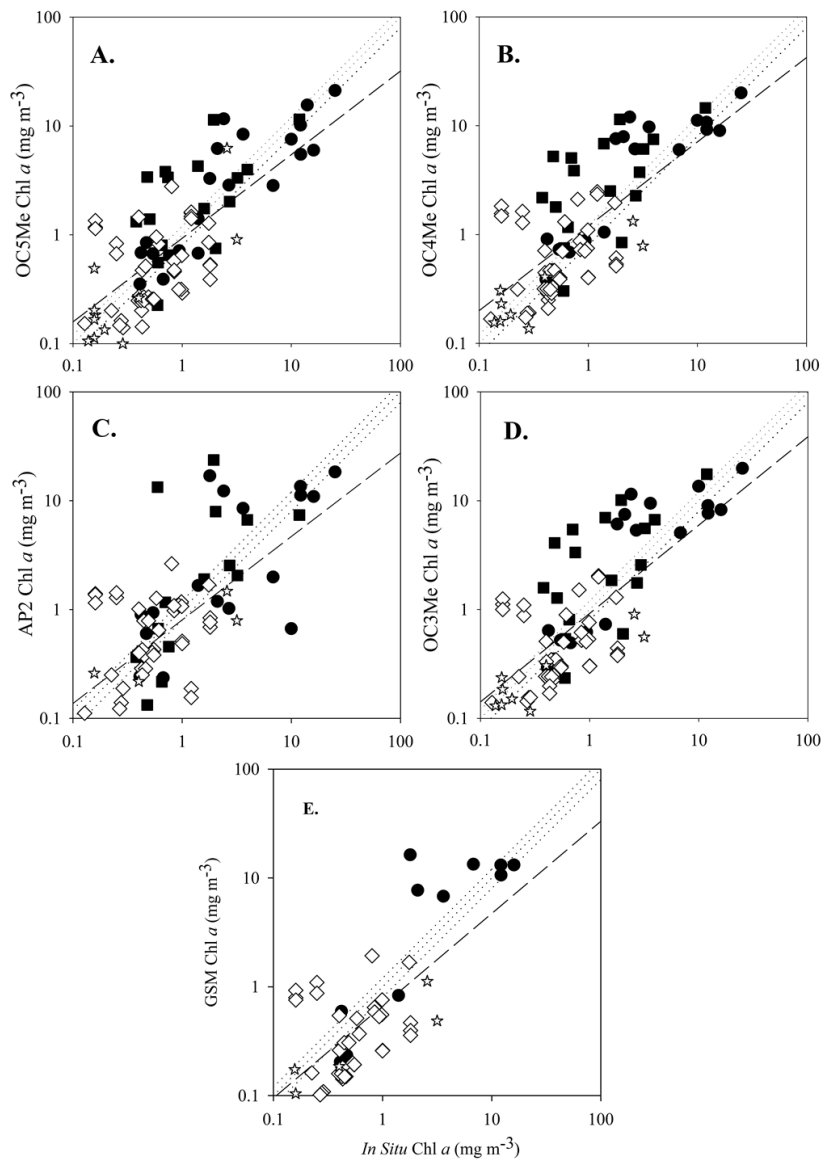
396 *3.2. Accuracy assessment of MERIS MEGS8.0 and COASTCOLOUR Chl a products in North*  
 397 *West European waters.*

398 Using COASTCOLOUR L2  $R_{rs}$ , OC4Me had the lowest RPD and  $r$  and  $F_{max}$  closest to 1.  
399 The GSM had the lowest intercept and RMS-E and slope closest to 1, though fewer match-  
400 ups were available using the GSM, since the algorithm did not converge at some stations in  
401 the North Sea and at all of the English Channel stations (Table 2). OC5Me had the lowest  
402  $\log_{10}$ -RMS,  $M$  and  $S$  and  $R^2$  and  $F_{min}$  closest to 1. OC5Me with COASTCOLOUR L2  $R_{rs}$  had  
403 a similarly low intercept, random error and RMS-E and  $F_{med}$  compared to the GSM and AP2.  
404 Of the algorithms tested using COASTCOLOUR L2  $R_{rs}$ , AP2 was the least accurate (Table 2,  
405 Fig. 3).

406 Similarly using MEGS8.0 L2  $R_{rs}$ , OC4Me had the lowest RPD and OC3Me had the  
407 lowest random error (Table 2, Fig. 4B, D). OC5Me had the lowest  $\log_{10}$ -RMS, RMS-E,  
408 intercept and bias, the highest  $R^2$  and the slope,  $r$ , and  $F_{min}$  closest to 1 and was the most  
409 accurate algorithm in 7 out of the 12 statistical tests performed (Table 2, Fig. 4A). GSM also  
410 had  $F_{min}$  close to 1 whereas  $F_{max}$  was high, indicating that it is more accurate at lower rather  
411 than at higher Chl  $a$  concentrations (Table 2, Fig. 4E). For GSM with MEGS8.0 L2  $R_{rs}$ , there  
412 were only four data points that exhibited high scatter from the 1:1 line, and in the absence of  
413 these, this algorithm would have been accurate for these coastal waters. Where the other  
414 algorithms returned data, the GSM did not converge at some stations in the English Channel  
415 however, questioning its suitability for providing contiguous satellite imagery. AP2 was the  
416 least accurate across all statistical tests (Table 2, Fig. 4C). Of the MEGS8.0 and  
417 COASTCOLOUR match-ups, 17% were from the North Sea, 13% from the English Channel,  
418 55% were from the Portuguese coast and 15% from the Mediterranean. Comparing MEGS8.0  
419 and COASTCOLOUR OC5Me Chl  $a$  against *in situ* Chl  $a$  and using the same number of  
420 match-ups (figure not shown), MEGS8.0 OC5Me had a lower bias and log-RMS and a higher  
421 percentage variance explained compared to COASTCOLOUR OC5Me, indicating that

422 OC5Me Chl  $a$  is slightly more accurate using MEGS8.0 compared to COASTCOLOUR  $R_{rs}$

423 (Table 2, Fig. 3A, Fig. 4A).



424

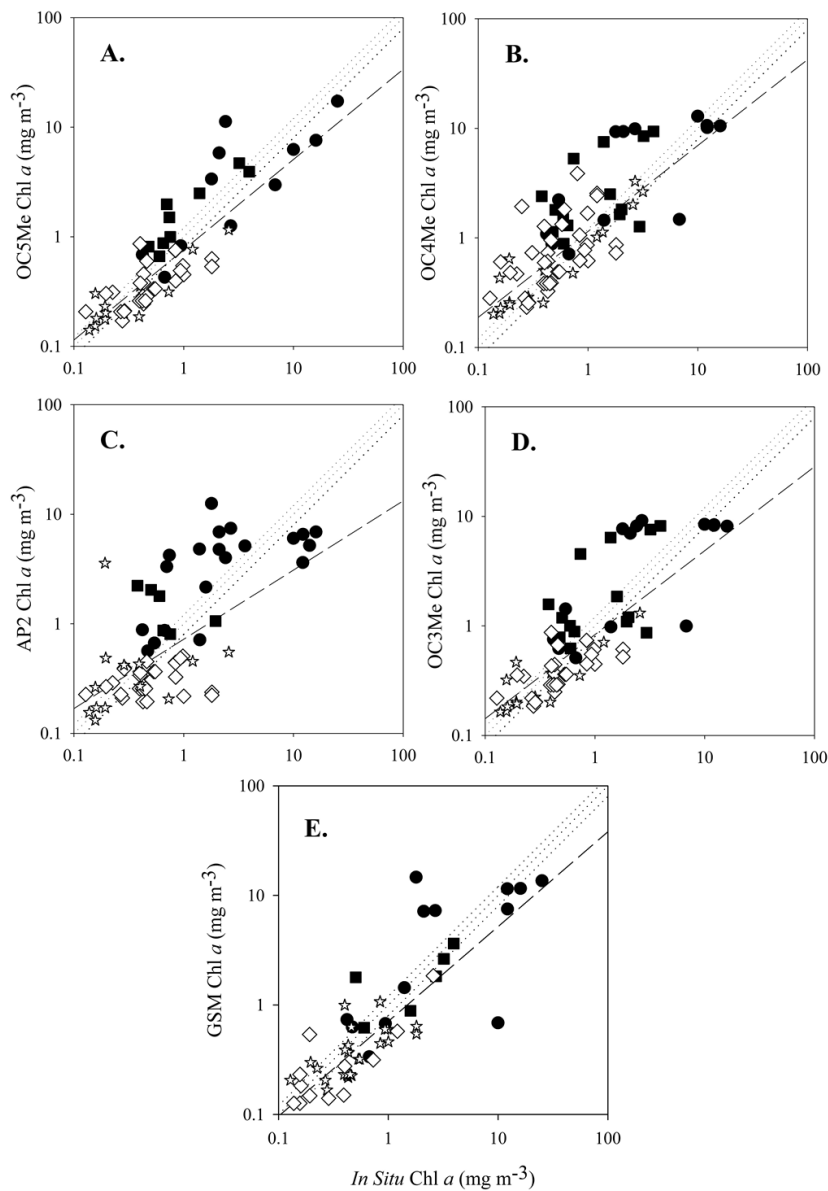
425 **Figure 3.** Comparison of *in situ* Chl  $a$  and COASTCOLOUR L2  $R_{rs}$  derived Chl  $a$  for (A.)

426 OC5Me, (B.) OC4Me, (C.) AP2, (D.) OC3Me and (E.) GSM. Faint dotted lines are the 1:1

427 line, upper and lower 20% quartiles. Dashed line is the regression line. Filled circles are data

428 from the North Sea, filled squares are from the Western English Channel, open diamonds are

429 from the Portuguese Shelf, open stars are the Mediterranean Sea.



430

431 **Figure 4.** Comparison of *in situ* Chl *a* and MEGS8.0 L2  $R_{rs}$  derived Chl *a* for (A.) OC5Me,  
 432 (B.) OC4Me, (C.) AP2, (D.) OC3Me and (E.) GSM. Faint dotted lines are the 1:1 line, upper  
 433 and lower 20% quartiles. Dashed line is the regression line. Filled circles are data from the  
 434 North Sea, filled squares are from the Western English Channel, open diamonds are from the  
 435 Portuguese Shelf, open stars are the Mediterranean Sea.

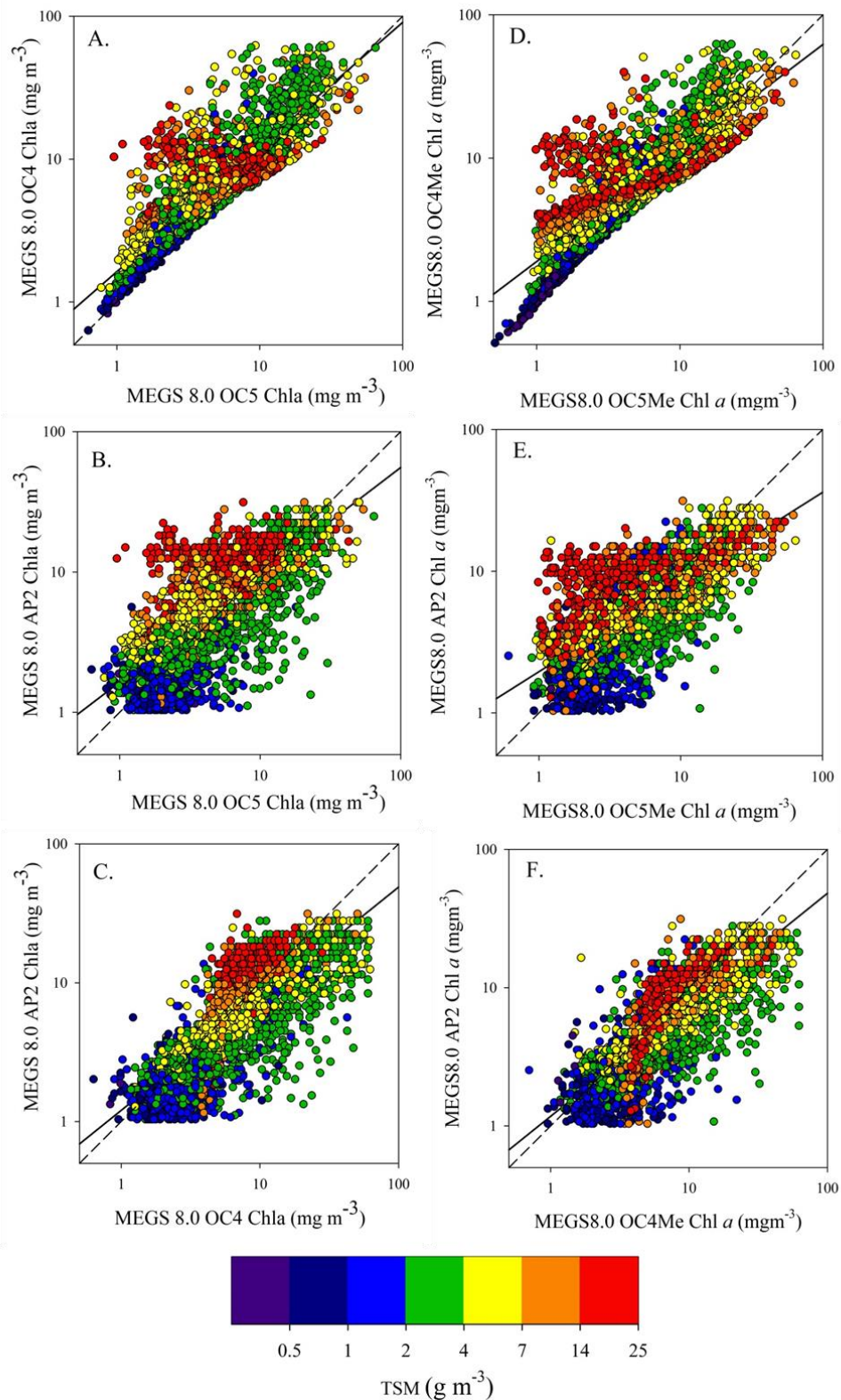
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437 *3.3. Spatial comparison between MERIS Ocean Colour algorithms in the North Sea.*

438 A comparison of Chl *a* from MERIS algorithms along two transects from the Schelde Estuary

439 and to the Wash on the SE UK coast and from the Schelde to the River Thames estuary  
440 across the Southern Bight of the North Sea using data from January 2003 to December 2007  
441 (Fig. 1C, 5). For these two transects over the 6 yr period, there were 68,332 data points; for  
442 coincident OC5Me, OC4Me AP2 and non-algal SPM data there were 7,776 data. Comparison  
443 between OC4Me and OC5Me explained 58% of the variance in the data with a slope close to  
444 1, but a high intercept (Table 3). OC4Me tended to over-estimate at Chl *a* >1 mg m<sup>-3</sup> OC5Me  
445 and the corresponding OC4Me Chl *a* was ~10 mg m<sup>-3</sup> (Fig. 5A, D). At OC5Me Chl *a*  
446 between 1 and 10 mg m<sup>-3</sup>, the over-estimate in OC4Me Chl *a* was related to high non-algal  
447 SPM >14 g m<sup>-3</sup>. At OC5Me Chl *a* >10 mg m<sup>-3</sup>, the over-estimate in OC4Me was not related  
448 to SPM which was between 2 and 8 g m<sup>-3</sup>. The offset between OC5Me and OC4Me was  
449 worse on the Thames compared to the Wash transects due to an increase in SPM adjacent to  
450 the Thames estuary. For OC5Me and AP2, 51% of the variance between the two algorithms  
451 was explained, the slope was low (~0.58), the intercept was high (Table 3) and there was a  
452 large offset between the algorithms at both low and high Chl *a* concentrations (Fig. 5B, E).  
453 There was a large error in AP2 Chl *a* between 1 to 20 mg m<sup>-3</sup> at both high (>14 g m<sup>-3</sup>) and  
454 low (2-3 g m<sup>-3</sup>) non-algal SPM. The slope was lower on the Thames transect but the scatter  
455 was higher on the Wash transect (Fig. 5B, E, Table 3). Above 10 mg m<sup>-3</sup> Chl *a*, the scatter  
456 between OC5Me and AP2 was reduced. Similarly, for OC4Me and AP2, 45 % of the variance  
457 was explained, the slope was low and the intercept was high (Table 3) and there was a large  
458 scatter between the two algorithms over the entire OC4 Chl *a* range from 0.6-65.0 mg m<sup>-3</sup>.  
459 The offset and scatter between the algorithms was similar on both transects (Fig. 5C, F). The  
460 spatial and temporal differences between the algorithms are illustrated in satellite images  
461 during two different periods in spring (April 2010; Fig. 6) and summer (July 2011; Fig. 7). In  
462 coastal waters during both periods, OC5Me Chl *a* < OC4Me Chl *a*, whereas in open ocean  
463 waters OC5Me and OC4Me were similar (Fig. 6) except in July 2011 when OC4Me > OC5





464  
 465 **Figure 5.** Comparison of OC5Me, OC4Me and AP2 processed using MEGS8.0  $R_{rs}$  along  
 466 transects from the Schelde estuary to The Wash; (A.) OC4Me versus OC5 Me, (B.) AP2  
 467 versus OC5Me and (C.) AP2 versus OC4Me; and from the Thames to the Schelde estuaries;  
 468 (D.) OC4Me versus OC5Me, (E.) AP2 versus OC5Me and (F.) AP2 versus OC4Me.



469 Me (Fig. 7).

470

471 **Table 3.** Percentage variance explained ( $R^2$ ), intercept and slope from linear regression

472 between OC5Me, OC4Me and AP2 Chl *a* along transects from the Schelde estuary to The Wash

473 and the Thames to the Schelde estuaries (see Fig. 1C for details of transects).

	$R^2$	Slope	Intercept	$R^2$	Slope	Intercept
	The Wash-Schelde Estuary N=3734			Thames-Schelde Estuaries N=4042		
<b>OC5Me v OC4Me</b>	0.60	1.13	1.36	0.57	0.87	2.27
<b>OC5Me v AP2</b>	0.49	0.64	2.77	0.50	0.53	3.00
<b>OC4Me v AP2</b>	0.44	0.42	3.09	0.47	0.43	2.85

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475

476 By contrast, AP2 exhibited the lowest Chl *a* in coastal regions of the North Sea and English

477 Channel and did not yield data at all in some coastal and shelf areas (Fig. 6C, 7C). For GSM,

478 in the coastal regions off Denmark, Holland, Belgium, northern France and the UK, Chl *a*

479 was higher than for OC5Me and OC4Me (Fig. 6D, 7D). In some offshore areas of the North

480 Sea and Celtic Sea off SW England and southern Ireland, GSM Chl *a* was lower, but in

481 spring in the Bay of Biscay, off the west Irish Coast and central North Sea, GSM Chl *a* was

482 also higher. To highlight the spatial variability in the satellite images between the algorithms,

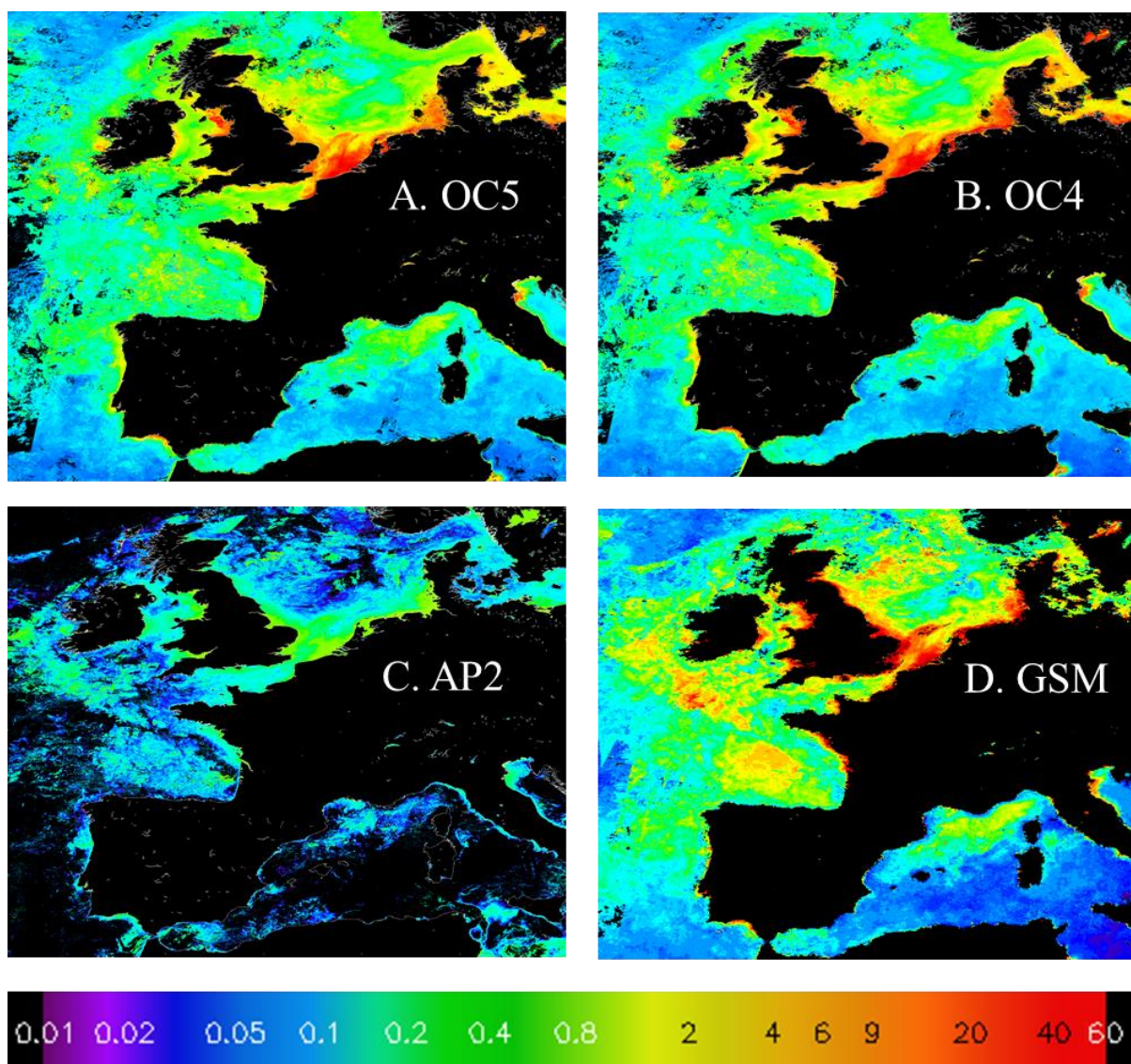
483 Chl *a* were extracted from the April 2010 images (Fig. 6) at every 10 km along transects from

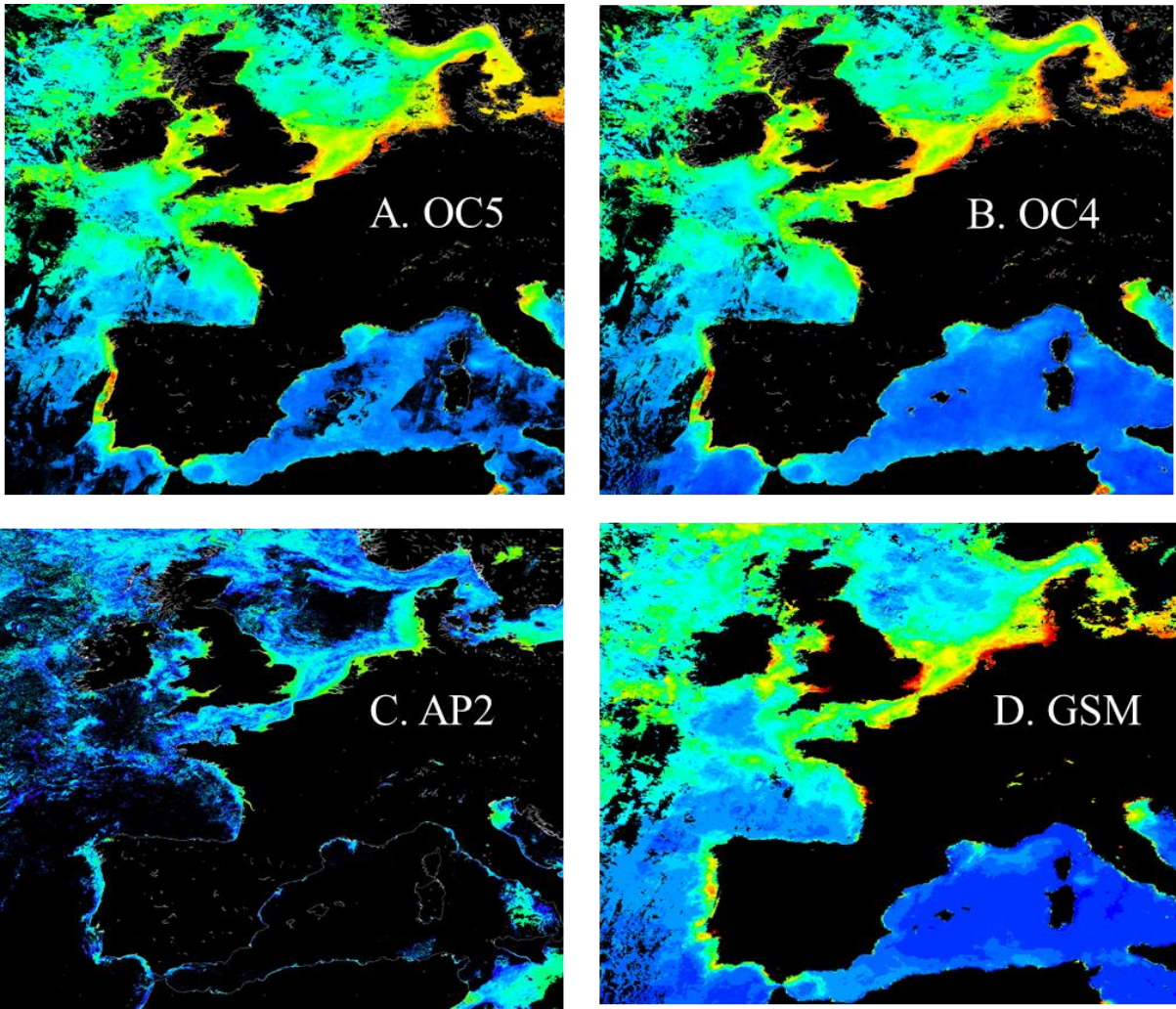
484 the Wash to the Schelde Estuary and from the English Channel to the Seine Estuary on the

485 French coast (Fig. 1C). At the ends of the transects near to the UK coast, OC4Me Chl *a* was 2

486 to 6 times higher than OC5Me (Fig. 8A, B, E, F). AP2 under-estimated Chl *a* across the

487 entire transect (Fig. 8C, G). GSM generally over-estimated Chl *a* but the spatial trends were





492

493 **Figure 7.** Comparison of MERIS MEGS8.0 Chl *a* monthly composites for July 2011 using  
 494 (A.) OC5Me, (B.) OC4Me, (C.) AP2, (D.) GSM.

495

496 erratic with large oscillations between high and low Chl *a* values over small spatial scales  
 497 (Fig. 8D, H).

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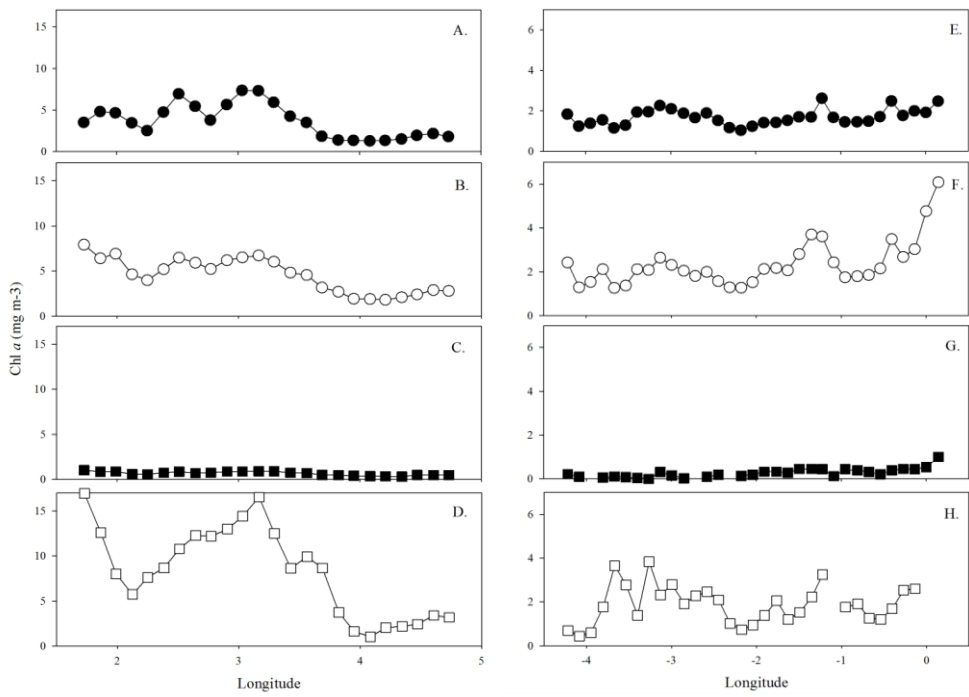
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**Figure 8.** Comparison of MERIS MEGS8.0 Chl *a* from the monthly composite of April 2010 (given in Fig. 6) along Longitudinal transects from the Wash to the Schelde for (A.) OC5Me, (B.) OC4Me, (C.) AP2, (D.) GSM and from the western English Channel to the River Seine for (E.) OC5Me, (F.) OC4Me, (G.) AP2, (H.) GSM. The location of the transects are given in Figure 1C.

517

#### 4. Discussion.

518

##### 4.1. MERIS ocean colour algorithm accuracy assessment.

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The principal objective of this study was to assess the performance of Chl *a* algorithms, that are widely available to end users, using two different MERIS AC processors for use in North West European waters. *In situ*  $R_{rs}$  were firstly used to test the algorithms in the absence of the MERIS AC model to indicate potential errors in the Chl *a* algorithm alone rather than combined errors arising from the input MERIS  $R_{rs}$  and the Chl *a* algorithm. Using *in situ*  $R_{rs}$ , OC5Me, OC4Me and OC3Me had a similar slope, but OC5Me showed a higher scatter, illustrated by the higher S and M values compared to OC4Me and OC3Me (Table 2). This

527 suggests that with *in situ*  $R_{rs}$ , OC4Me and OC3Me are the most accurate algorithms for the  
528 NW European region (Fig. 2B, D). The slope for GSM was closer to 1, but the scatter from  
529 0.5 to 20 mg m<sup>-3</sup> was high (Fig. 2C) and this algorithm was the least accurate using *in situ*  
530  $R_{rs}$ . It was not possible to run AP2 with just *in situ*  $R_{rs}$ , since the AC is an integral part of the  
531 AP2 NN processor and is not available without the AC component of the model.

532 Secondly, both COASTCOLOUR and MEGS8.0  $R_{rs}$  were used to test the algorithms.  
533 We found that AP2 was the least accurate in these regions (Figs. 3C, 4C); AP2 had a large  
534 bias using both processors at low and high Chl *a* concentrations, which is reflected in the  
535 high log<sub>10</sub>-RMS, S, F<sub>min</sub> and F<sub>max</sub> values (Table 2). When AP2 was processed as MEGS8.0  
536 monthly composite images for European coastal regions, there were a large number of pixel  
537 drop-outs caused by none convergence in the NN (Fig. 6C, 7C). In addition, AP2 Chl *a*  
538 values in both coastal and open ocean areas of the North Sea and Atlantic Ocean were  
539 significantly lower than those obtained from OC4Me and OC5Me (Fig. 6, 7, 8), which is  
540 reflected by the tendency to under-estimate Chl *a* shown in Figures 3C, 4C.

541 The AP2 NN has been shown to be accurate in the North Sea (Doerffer and Schiller  
542 2007), but is not as accurate in the Adriatic (Zibordi et al. 2006a), Baltic (Attila et al. 2013),  
543 Mediterranean (Antoine et al. 2008) Seas, South African coastal and shelf waters (Smith et al.  
544 2013), Siberian Arctic coastal and shelf waters (Heim et al. 2014), US coastal regions  
545 (Mishra and Mishra 2012) and tropical coastal regions (Ambarwulan et al. 2010), especially  
546 when compared against standard MODIS-Aqua or SeaWiFS ocean colour products. In a  
547 number of studies the MERIS AP2 NN has been modified to account for the regional  
548 variation in IOPs which has improved it's performance (Attila et al. 2013; Smith et al. 2013).  
549 Alternative algorithms have been proposed for MERIS that have proven to be more accurate  
550 for the North Sea (Tilstone et al. 2012; Van der Woerd and Pasterkamp 2008) and Iberian  
551 Peninsula (Gonzalez Vilas et al. 2011; Sa et al. 2015), but these are not widely available to

552 end users. There is a tendency for MERIS AP2 in some coastal waters to under-estimate Chl  
553 *a* in the range  $<1 \text{ mg m}^{-3}$  and to over-estimate Chl *a* at values  $>6 \text{ mg m}^{-3}$  (Tilstone et al.  
554 2012). Knowing this bias in the algorithm, MERIS AP2 has undergone several rounds of re-  
555 calibration, which has resulted in re-processing the MERIS archive (Bourg et al. 2011). One  
556 of the problems experienced with the AP2 NN is that adding further training data can lead to  
557 ‘over-training’ which offers the algorithm further multiple possible solutions to retrieving  
558 IOPs, which may not necessarily result in accurate IOP spectra (IOCCG 2006). From our  
559 analyses, the scatter plots indicated that COASTCOLOUR AP2 under- and over-estimates  
560 Chl *a* in all regions tested and that MEGS8.0 AP2 under- and over-estimates Chl *a* in the  
561 North Sea and English Channel, and under-estimates in the Mediterranean Sea and off the  
562 Portuguese coast (Fig. 3C, 4C). Analysis of the satellite imagery indicated that AP2  
563 consistently under-estimated Chl *a* in all regions (Fig. 6C, 7C, 8C, G).

564 By comparison, OC4Me was designed for global applications over optically deep  
565 ocean waters (Morel and Antoine 2011). The retrieval accuracy of Chl *a* by satellite ocean  
566 color sensors is expected to be within  $\pm 35\%$  in oceanic waters (Bailey and Werdell 2006;  
567 Blondeau-Patissier et al. 2014). This may not always be the case (Hu et al. 2000; Moore et al.  
568 2009) and therefore may not be sufficient for the purpose of monitoring phytoplankton  
569 biomass in the coastal zone. In the coastal waters tested, OC4Me consistently over-estimated  
570 Chl *a* at values  $>1 \text{ mg m}^{-3}$  (Fig. 3B, 4B), though for the few match-ups with Chl *a*  $>10 \text{ mg m}^{-3}$ ,  
571 the retrieval accuracy improved. The use of these blue : blue–green band-ratios often leads  
572 to erroneous retrievals in coastal waters, where the optical complexity is highly variable  
573 (Blondeau-Patissier et al. 2004). The blue band can be affected by both the absorption of  
574 CDOM and scattering from SPM (Dierssen 2010) and in turbid waters the blue-green band  
575 can be related to SPM more than to phytoplankton. Absorbing aerosols and the absorption  
576 coefficient of coloured dissolved material ( $a_{CDOM}$ ) can propagate as negative  $nL_w$  at short

577 wavelengths, which can result in an over-estimate of Chl *a*, as observed in coastal regions of  
578 the Bay of Bengal (Tilstone et al. 2011), United States (Cannizzaro et al. 2013; Le et al.  
579 2013a), the Bering Sea (Naik et al. 2013), South-East Asia (Ahn and Shanmugam 2006), the  
580 North Sea and Kattegat (Jorgensen 2004). OC4 is often applied indiscriminately in some  
581 coastal waters (Dupouy et al. 2010), without a proper understanding of the potential errors  
582 that can be incurred in these waters. For the coastal and shelf environments tested in this  
583 study however, the relative difference between the *in situ* measurements and OC4Me over the  
584 entire Chl *a* range was ~25%, and therefore within the accepted tolerance for Case 1 waters.  
585 OC4Me tended over-estimate Chl *a* in coastal areas of the North Sea, English Channel and  
586 Portuguese coast (Fig 3B, 4B, 8B, F).

587 The performance of OC3Me was similar to OC4Me, with the advantage of omitting  
588 the  $R_{rs}(412)$  band where the error is greatest (see Section 4.2). For OC3Me, of the ~90  
589 satellite-*in situ* Chl *a* match ups obtained with MEGS8.0 (Fig. 4D), 83 % of these used the  
590  $R_{rs}(490) : R_{rs}(560)$  ratio. The  $R_{rs}(442) : R_{rs}(560)$  ratio was used to calculate Chl *a* at stations  
591 predominantly from the Portuguese coast and Mediterranean Sea, which relate to those points  
592 below the 1:1 in Figure 4D, where the under-estimate in  $R_{rs}(442)$  (see Section 4.2) led to  
593 lower Chl *a* concentrations. The high scatter in OC3Me Chl *a* in the North Sea were  
594 predominantly at stations in the southern North Sea off the coast of France, principally due to  
595 an under-estimate in  $R_{rs}(490)$  (see Section 4.2), which led to higher Chl *a* values (Figs. 3D &  
596 4D).

597 The GSM algorithm had a slope close to 1 and a low intercept though there was a  
598 very high scatter for some of the match-up points, which resulted in high log-RMS and RPD  
599 (Fig 3E, 4E). This was also reflected in the composite images from April 2010 (Fig. 6) and  
600 July 2011 (Fig. 7), which showed that GSM Chl *a* was consistently higher in coastal regions  
601 and both lower and higher offshore compared with OC5Me and OC4Me. The GSM Chl *a*

602 extracted from transects in April 2010 in the North Sea and English Channel (Fig 8D, H)  
603 indicate that the outliers in the scatter plot represent large areas of the image where GSM  
604 consistently over-estimate Chl *a* (Fig. 8). The GSM is semi-analytical and was calibrated  
605 using the SeaBAM dataset (Maritorena et al. 2002) and like OC4, was originally developed  
606 for Case 1 waters. The GSM uses  $R_{rs}(442)$  to partition the absorption  $a_{dg}(442)$  and  $b_{bp}(442)$   
607 and is calibrated using a simulated annealing procedure to retrieve  $a_{ph}^*(\lambda)$  at 412, 443, 488,  
608 530 and 555 nm. It solves  $a_{ph}(\lambda)$  in the presence of SPM and  $a_{CDOM}(\lambda)$  by using a constant  
609 exponential slope of CDOM ( $S_{CDOM}$ ) of  $0.0206 \text{ m}^{-1}\text{nm}^{-1}$ , a power-law exponent for particulate  
610 backscattering ( $\eta=1.03373$ ) expressed as a function of Chl *a* (Morel and Maritorena 2001),  
611 and an optimized Chl *a* specific  $a_{ph}$  ( $a_{ph}^*$ ) as a fixed value [ $a_{ph}^*(443)=0.05582$ ]. This IOP  
612 parameterisation may not be appropriate for these European coastal waters;  $S_{CDOM}$  used for  
613 calibrating the GSM is too high for the North Sea;  $S_{CDOM}$  of  $0.0101$  and  $0.0232 \text{ m}^{-1}\text{nm}^{-1}$  have  
614 been reported for this area (Astoreca et al. 2009) and therefore  $0.0206 \text{ m}^{-1}\text{nm}^{-1}$  is towards the  
615 upper limit for these waters. Similarly the assigned  $a_{ph}^*(\lambda)$  is too low for the Celtic Sea and  
616 the English Channel which have mean values of between  $0.07$  &  $0.09 \text{ mg m}^{-2}$ , respectively  
617 (Tilstone et al. 2012). With MEGS 8.0, the under-estimate in  $R_{rs}(442)$  (Fig. 10B) particularly  
618 at low values, this error will propagate into the partitioning of  $a_{dg}(442)$  and  $b_{bp}(442)$  and then  
619 to estimating  $a_{ph}^*(442)$ , which will result in an over-estimate in Chl *a* (Fig. 4E). This was  
620 observed over the entire region particularly in coastal and shelf regions of the North Sea and  
621 English Channel in spring (Fig. 6D, 8D, H).

622 OC5 was initially developed to provide realistic maps of Chl *a* for the turbid waters of  
623 the English Channel and the Bay of Biscay for validating biogeochemical model outputs  
624 (Menesguen et al. 2007). The first SeaWiFS OC4v4 products showed blooms in January  
625 1998 in the English Channel, which never occur and therefore prevented the use of these  
626 products being used for model assessment. High SeaWiFS  $R_{rs}$  in blue and green bands for



627 this region during winter, due to an increase in scattering from SPM, caused the over-estimate  
628 OC4v4 Chl *a*. The rationale for developing OC5 was therefore to provide more accurate  
629 estimates of Chl *a* in turbid waters and to be as close as possible to OC4 Chl *a* in Case 1  
630 waters. By construction, OC5 Chl *a* is always lower than OC4 Chl *a*, which makes its  
631 application in Case 1 waters less reliable (Marrec et al. 2015). In the shelf waters of the Celtic  
632 and North Seas for example, OC5Me was similar, but slightly lower than OC4Me (e.g. Figs.  
633 6, 7, 8). Since OC5 is empirical and is calibrated using level 2  $R_{rs}(\lambda)$ , when data from a  
634 specific satellite sensor or mission, reprocessing may be required before applying OC5 to  
635 different data sources (Morozov et al. 2010). This implies that when using  $nL_w(\lambda)$  from  
636 MODIS, MERIS, merged MERIS-MODIS-SeaWiFS, Sentinel-3 or any variant of these with  
637 a different atmospheric correction model or with *in situ*  $R_{rs}$  (as illustrated in Fig. 2A), OC5  
638 would require a full re-parameterization. The necessity to re-parameterize OC5Me when  
639 using a different  $nL_w(\lambda)$  source is illustrated in Figure 2. Since the LUT for OC5Me was  
640 parameterized using MERIS  $R_{rs}(\lambda)$ , using *in situ*  $R_{rs}(\lambda)$  to run the algorithm resulted in a high  
641 scatter at Chl *a*  $>1 \text{ mg m}^{-3}$  in the North Sea (Fig. 2A) and was the third most accurate  
642 algorithm after OC3Me and OC4Me. Despite these limitations, OC5 has proven to be  
643 accurate in a range of different coastal waters including the Ganges Delta in the Bay of  
644 Bengal (Tilstone et al. 2011), the Bay of Biscay (Novoa et al. 2012) and the Ligurian and  
645 Tyrrhenian Seas (Lapucci et al. 2012). In NW European waters OC5Me was the most  
646 accurate algorithm using both COASTCOLOUR and MEGS8.0  $R_{rs}(\lambda)$  over the range of 0.1  
647 to  $35.0 \text{ mg m}^{-3}$  Chl *a*. OC5Me was parameterised using the OC4Me maximum band ratio and  
648  $nL_w(412)$  and  $nL_w(560)$  bands from MERIS data in the English Channel and Bay of Biscay,  
649 where Chl *a* is 0.05 to  $15 \text{ mg m}^{-3}$ , SPM are 0.1 to  $10 \text{ g m}^{-3}$  (Gohin et al. 2002) and  
650  $a_{CDOM}(375)$  is 0.02 -  $1.76 \text{ m}^{-1}$  (Vantrepotte et al. 2007). The range in Chl *a*, SPM and  $a_{dg}(442)$   
651 in North Sea, Mediterranean Sea, Western English Channel and Portuguese waters was 0.13 –

652 25.13 mg m<sup>-3</sup> Chl *a*; 0.001 – 27.02 g m<sup>-3</sup> SPM; 0.22 – 1.80 m<sup>-1</sup>  $a_{dg}(442)$ , which covers the  
653 OC5 parameterisation range. Since OC5 was originally parameterised using *in situ* data from  
654 the English Channel and the neighbouring Bay of Biscay, it is perhaps not surprising that  
655 OC5Me performed so well. Further testing of OC5Me in other coastal and shelf seas is  
656 necessary to assess the applicability of this algorithm globally and whether further  
657 parameterisation may be necessary for other water types. Other empirical algorithms such as  
658 red : NIR, red : green, fluorescent line height and normalised difference Chl *a* index  
659 algorithms have been shown to be accurate with MERIS  $R_{rs}$  in optically complex waters at  
660 Chl *a* >10 mg m<sup>-3</sup> (Gower et al. 2005; Le et al. 2013b; Mishra and Mishra 2012; Moses et al.  
661 2012), including freshwater Lakes (Binding et al. 2011; Gilerson et al. 2010). In future  
662 studies, it may be interesting to compare these algorithms against OC5Me for coastal and  
663 shelf environments.

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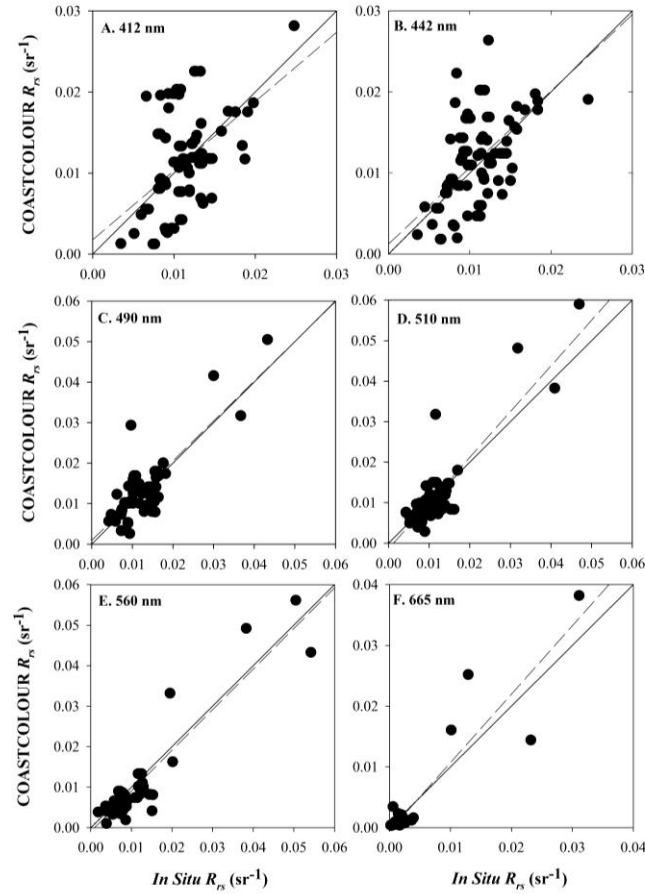
#### 665 4.2. Causes of differences between MERIS Ocean colour algorithms.

666 To assess the performance of MERIS Chl *a* algorithms in NW European waters, we  
667 firstly addressed the question; what is the accuracy of MERIS  $R_{rs}(\lambda)$  derived from different  
668 AC processors? MEGS8.0 was designed for use in Case 1 and 2 waters and  
669 COASTCOLOUR was designed specifically for use Case 2 waters. We were therefore also  
670 able to address the question of whether AC algorithms developed for global water types are  
671 more accurate than those developed specifically for Case 2 waters? In Figures 9 & 10 *in situ*  
672 and COASTCOLOUR and MEGS8.0  $R_{rs}(\lambda)$  are compared at MERIS bands. In Figure 11 the  
673 error between  $R_{rs}(442)$  and  $R_{rs}(560)$  for COASTCOLOUR and MEGS8.0 is compared and  
674 the uncertainty in these bands over the range of *in situ* Chl *a* concentrations is given. The  
675 difference between *in situ* and COASTCOLOUR  $R_{rs}(442)$  over the match-up dataset was 5%  
676 and 8% for MEGS8.0 (Fig. 9, 10; Table 4).

677 **Table 4.** Performance indices for relative errors between *in situ* and COASTCOLOUR and MEGS8.0  $R_{rs}(\lambda)$  at visible wavebands. Percentage  
678 variance explained ( $R^2$ ), intercept and slope and log-difference errors in measured and satellite Chla ratio as Mean ( $M$ ), Standard deviation ( $S$ )  
679 and root-mean square ( $\text{Log}_{10}$ -RMS).  
680

$\lambda$	N	$R^2$	Slope	Intercept	R	RPD	$\text{Log}_{10}$ - RMS	M	S	$F_{\text{med}}$	$F_{\text{max}}$	$F_{\text{min}}$	RMS- E
<b>COASTCOLOUR</b>													
412	98	0.53	1.14	-0.004	1.02	0.67	0.25	0.05	0.25	1.11	1.98	0.62	0.005
442	103	0.72	1.02	-0.003	1.00	5.33	0.19	0.01	0.20	1.02	1.60	0.65	0.004
490	101	0.65	0.98	0.0009	0.99	0.19	0.15	-0.01	0.15	0.97	1.36	0.69	0.004
510	101	0.61	1.23	-0.002	1.01	16.98	0.13	0.01	0.13	1.03	1.39	0.77	0.004
560	100	0.86	0.86	0.002	1.03	69.06	0.16	0.07	0.14	1.17	1.63	0.84	0.003
665	91	0.76	1.28	0.0006	1.06	132.66	0.26	0.19	0.17	1.54	2.30	1.04	0.001
<b>MEGS8.0</b>													
412	68	0.41	0.49	0.004	1.05	-9.2	0.14	0.09	0.11	1.22	1.58	0.94	0.0005
442	70	0.46	0.54	0.003	1.06	-8.3	0.20	0.11	0.16	1.29	1.87	0.89	0.004
490	94	0.63	0.78	0.0006	1.05	-6.8	0.14	0.09	0.11	1.23	1.58	0.96	0.0007
510	94	0.75	0.91	-0.0008	1.05	2.8	0.14	0.09	0.10	1.23	1.56	0.98	0.001
560	88	0.89	1.12	0.0009	1.05	32.5	0.15	0.11	0.10	1.27	1.62	1.00	0.0006
665	18	0.99	1.05	-0.0007	1.07	84.1	0.25	0.18	0.14	1.53	2.11	1.11	0.0003

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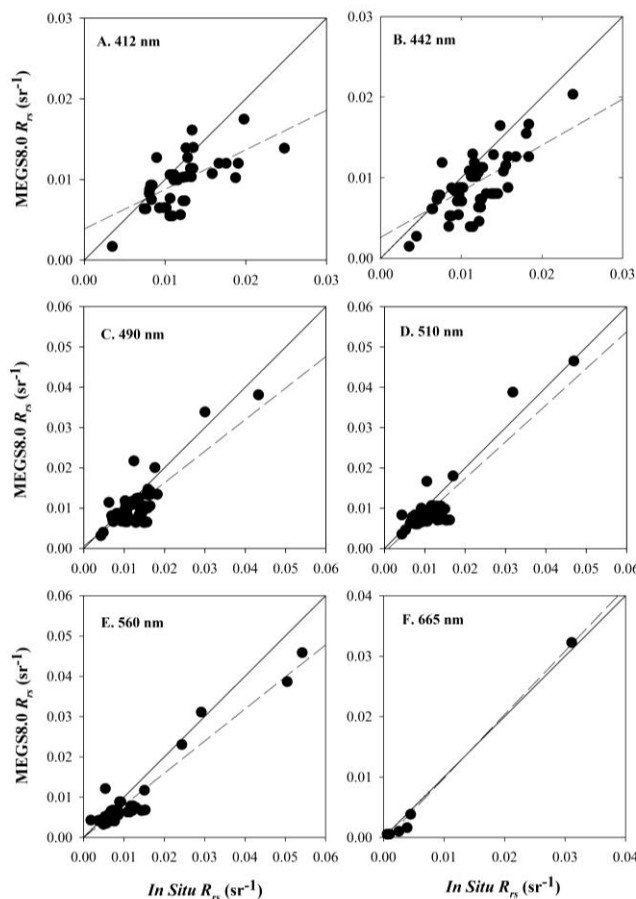


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**Figure 9.** Scatter plots of *in situ*  $R_{rs}(\lambda)$  against COASTCOLOUR  $R_{rs}(\lambda)$  for (A.) 412, (B.) 442, (C.) 490, (D.) 510, (E.) 560 and (F.) 665 nm. Solid line is the 1:1; dashed line is the regression line.

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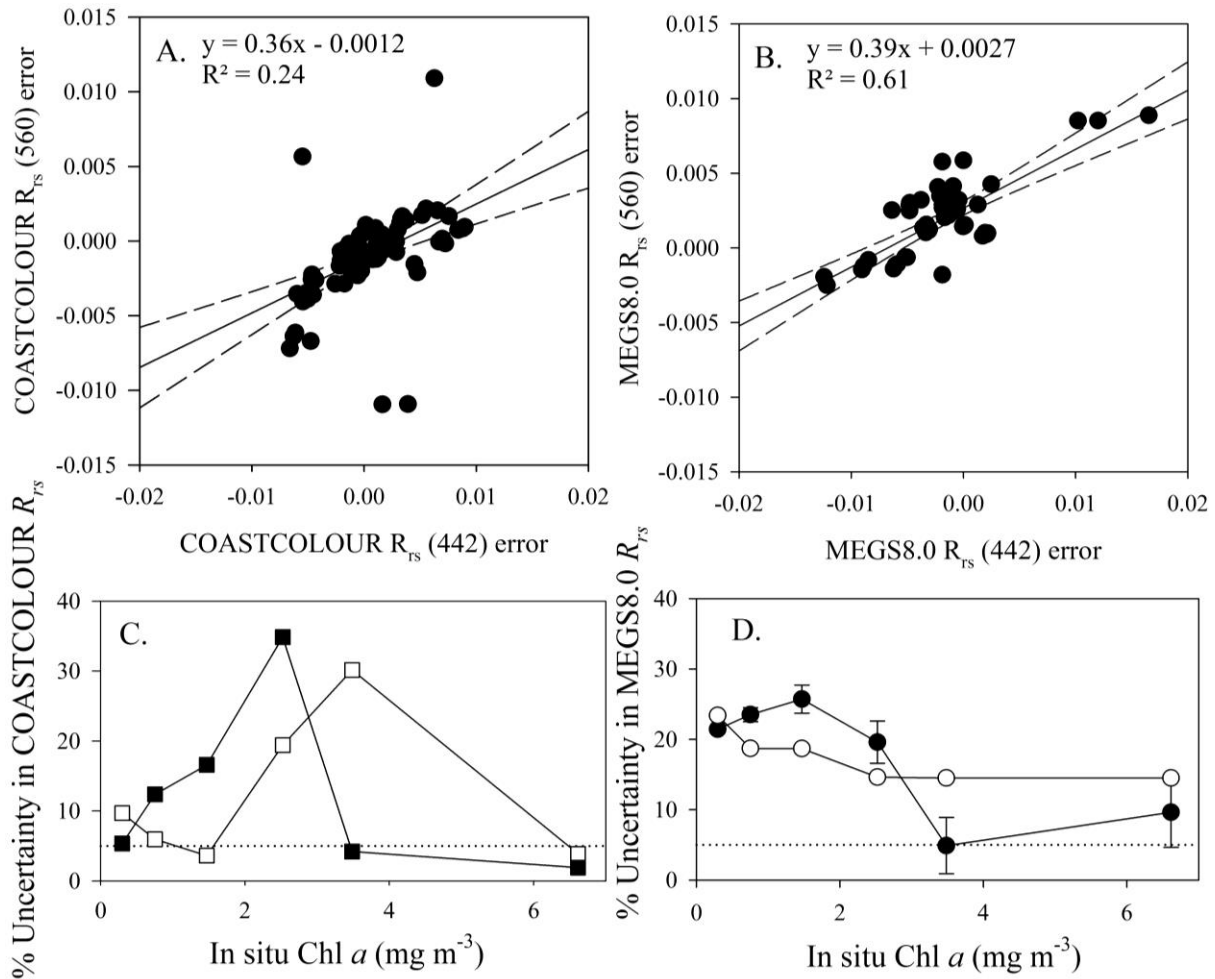
Recent studies based on continuous *in situ* measurement acquisition from towers or buoys have shown that MERIS over-estimates  $nL_w(442)$  globally by 44% (Maritorena et al. 2010) and at coastal sites in the Adriatic-Baltic by 39% (Zibordi et al. 2009a; Zibordi et al. 2006b), in the Mediterranean by 36% (Antoine et al. 2008) and in the Skagerrak by 40% (Sorensen et al. 2007), which suggest that both of these MERIS AC processors improve  $R_{rs}(442)$  in NW European waters. At least 65% of the stations in the validation data set had  $SPM > 3.0 \text{ g m}^{-3}$ , which theoretically should not affect these AC processors since both the COASTCOLOUR NN and MEGS8.0 BP AC are optimized for turbid, highly scattering waters. At  $R_{rs}$  490, 510, and 560 nm, the difference between *in situ* and MEGS8.0 and COASTCOLOUR  $R_{rs}(\lambda)$  decreased and MEGS8.0  $R_{rs}(560)$  and the NN COASTCOLOUR processor showed a similar



698  
 699 **Figure 10.** Scatter plots of *in situ*  $R_{rs}(\lambda)$  against MEGS8.0  $R_{rs}(\lambda)$  for (A.) 412, (B.) 442, (C.)  
 700 490, (D.) 510, (E.) 560 and (F.) 665 nm. Solid line is the 1:1; dashed line is the regression  
 701 line.  
 702

703 accuracy (Fig. 9, 10; Table 4). Though the slope was closer to 1 for COASTCOLOUR  
 704  $R_{rs}(412)$ ,  $R_{rs}(442)$ ,  $R_{rs}(490)$  and  $R_{rs}(510)$ , compared to MEGS8.0, the scatter was higher  
 705 which increased the bias and random error (Table 4). Similarly, Goyens et al. (2013) found  
 706 that MODIS-Aqua with a NN AC model, performed better at blue bands in water masses  
 707 influenced by SPM, compared to the standard MODIS-Aqua AC. For  $R_{rs}(560)$ , MEGS8.0  
 708 was more accurate than COASTCOLOUR. For  $R_{rs}(665)$ , the RPD for both MEGS8.0 and  
 709 COASTCOLOUR in these waters were higher than those reported both globally (~125%), in  
 710 the Baltic and Adriatic (~47%), the Mediterranean (~70%) and in the Skagerrak (~ 40%)  
 711 (Antoine et al. 2008; Zibordi et al. 2006a), though for MEGS8.0 there were fewer points due  
 712 to a high number of error flags raised. Figure 11 shows the relationship between the error in

713  $R_{rs}$  (calculated as the difference between MEGS8.0 or COASTCOLOUR  $R_{rs}(\lambda)$  and *in situ*  
714  $R_{rs}(\lambda)$ ) at  $R_{rs}(560)$  and  $R_{rs}(442)$ . For MEGS8.0, the error in  $R_{rs}(560)$  varied by  $>0.009 \text{ sr}^{-1}$ , and  
715 for COASTCOLOUR the error was  $>0.015 \text{ sr}^{-1}$ , which is  $\sim 4$  times higher than that reported  
716 for the global open ocean (Hu et al. 2013). By comparison, the error in  $R_{rs}(442)$  was lower for  
717 COASTCOLOUR compared to MEGS8.0, though for both processors this was  $>0.02 \text{ sr}^{-1}$   
718 (Fig. 11A, B). The potential error from atmospheric correction is estimated as  $<\pm 0.0006 \text{ Sr}^{-1}$   
719 for  $R_{rs}(443)$  in the global open ocean (Gordon et al. 1997). The error in  $R_{rs}(\lambda)$  was therefore  
720 over an order of magnitude greater than the nominal error due to AC, indicating that other  
721 environmental effects (e.g. non-algal SPM backscattering, high absorption by CDOM, sun  
722 glint) contribute more to the errors in both MEGS8.0 and COASTCOLOUR  $R_{rs}(442)$  (Fig.  
723 11A, B). High uncertainty in  $R_{rs}(\lambda)$  may be attributed to errors in the standard aerosol model  
724 of optical thickness used (Aznay and Santer 2009) or failure in the correction at cloud borders  
725 (Gomez-Chova et al. 2007). The errors between COASTCOLOUR and MEGS8.0  $R_{rs}(560)$   
726 and  $R_{rs}(442)$  were correlated especially for MEGS8.0 (Fig. 11A, B), suggesting that it could  
727 be possible to predict the errors between these bands and systematically correct for them. For  
728 both COASTCOLOUR and MEGS8.0, the error in the  $R_{rs}(560)$  band was less than half of the  
729 error at  $R_{rs}(442)$  (Fig. 11A, B). The differences reported in Table 4 provide an average  
730 uncertainty over the entire  $R_{rs}(\lambda)$  match-up data set. The errors in ocean colour Chl *a*  
731 however, may not always be uniform (Lee et al. 2010). For example, for SeaWiFS and



732

733 **Figure 11.** Spectral relationships between  $R_{rs}$  errors for (A.) MEGS8.0  $R_{rs}(442)$  and  
 734  $R_{rs}(560)$  and (B.) COASTCOLOUR  $R_{rs}(442)$  and  $R_{rs}(560)$ . The errors are determined as the  
 735 relative difference between MERIS and *in situ*  $R_{rs}$ . Percentage uncertainty in (C.)  
 736 COASTCOLOUR  $R_{rs}(442)$  (open squares) and  $R_{rs}(560)$  (filled squares) and (D.) MEGS8.0  
 737  $R_{rs}(442)$  (open circles) and  $R_{rs}(560)$  (filled circles) as a function of Chl *a*. In (A.) and (B.),  
 738 the solid line is the regression and the dashed lines are the 95% confidence intervals. In (C.)  
 739 and (D.), the dashed line is the 5% uncertainty limit.

740

741 MODIS-Aqua in oligotrophic regions of the Atlantic and Pacific Oceans over a Chl *a* range

742 of 0.05 to 0.2  $\text{mg m}^{-3}$ , Hu et al. (2013) reported an absolute accuracy of <5% for  $R_{rs}(\lambda)$  at

743 blue bands for repeat satellite passes. For green and red bands the accuracy was >5% and the

744 uncertainty in both SeaWiFS and MODIS-Aqua  $R_{rs}(\lambda)$  tended to increase with increasing Chl

745 *a*. From MERIS match-ups with *in situ*  $R_{rs}(\lambda)$ , we found that the uncertainty in MEGS8.0

746  $R_{rs}(442)$  (~17%) was slightly higher than COASTCOLOUR (~12%) over a Chl *a* range of 0.3

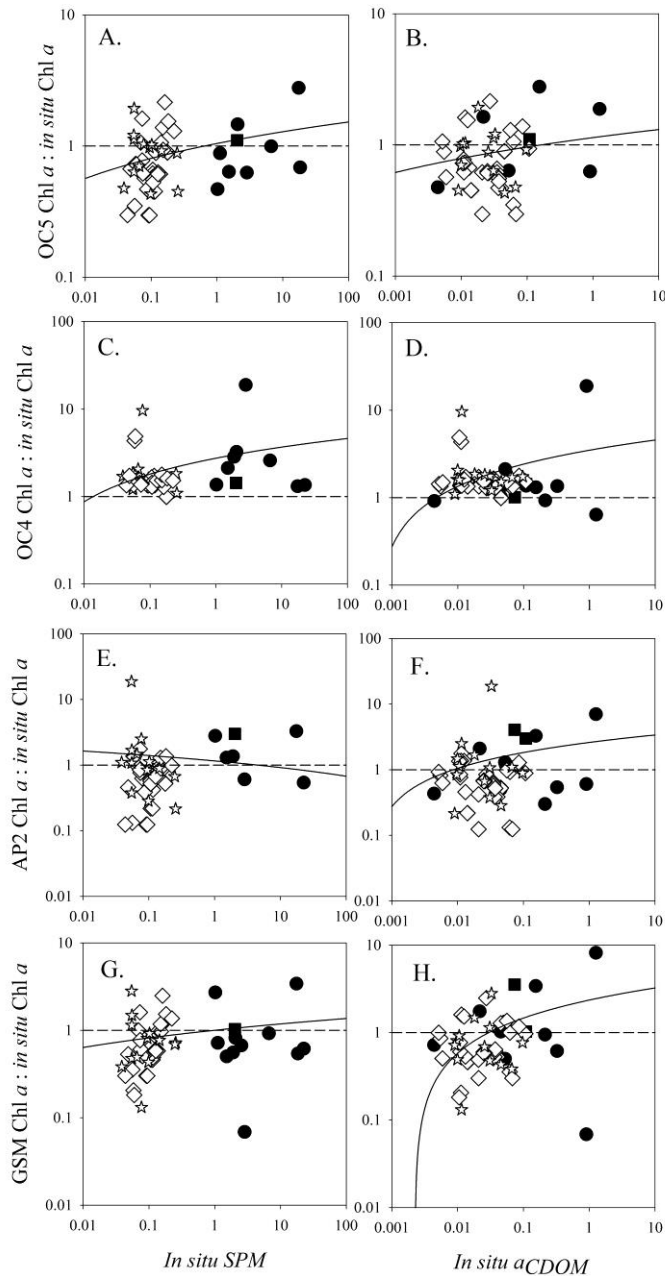
747 to 7  $\text{mg m}^{-3}$  (Fig. 11D). At specific Chl *a* concentrations however, there were large variations

748 between the processors. Whilst the uncertainty for MEGS8.0  $R_{rs}(442)$  was fairly constant  
749 with increasing Chl  $a$ , for COASTCOLOUR  $R_{rs}(442)$  the uncertainty was low from 0.3 to 1.5  
750  $\text{mg m}^{-3}$  and at  $6.5 \text{ mg m}^{-3}$ , but then increased sharply between 2 to  $4 \text{ mg m}^{-3}$  Chl  $a$  (Fig. 11D),  
751 reflecting the high scatter at the mid to upper range of  $R_{rs}(442)$  values (Fig. 9B). For  $R_{rs}(560)$ ,  
752 both MEGS8.0 and COASTCOLOUR processors exhibited a similar pattern, with low  
753 uncertainty at low and high Chl  $a$  concentrations, which for COASTCOLOUR were within  
754 the mission goal of absolute accuracy of  $<5\%$  (Fig. 11D). By comparison, the uncertainty in  
755 MEGS8.0  $R_{rs}(560)$  was  $\sim 20\%$  from 0 to  $2.5 \text{ mg m}^{-3}$  and  $<5\%$  at Chl  $a > 2.5 \text{ mg m}^{-3}$ . The net  
756 effect of these differences between AC processors is that when they are applied to a range of  
757 Chl  $a$  algorithms, MEGS8.0 proved to be slightly more accurate than COASTCOLOUR.  
758 Though the majority of the match-ups points were close to the coast (Fig. 1B), they  
759 potentially represent a mix of Case 1 waters along the Portugese coast, Celtic and  
760 Meditteranean seas and Case 2 waters of the English Channel and North Sea. The ability of  
761 the MEGS8.0 processor to switch between the bright pixel and clear water AC models, means  
762 that it can be applied to a diverse range of water types typical of NW Europe from the coastal  
763 Atlantic Ocean and North Sea. By comparison, the COASTCOLOUR AC showed a higher  
764 scatter than MEGS8.0 at coastal Atlantic, Meditteranean and English Channel stations (Fig.  
765 3, 4). Using MEGS8.0 OC5Me in these NW European waters, the target error tolerance for  
766 Chl  $a$  is met (Table 2). These results have implications for the Sentinel-3 Ocean Colour Land  
767 Instrument (OLCI); the improved signal-to-noise ratio, long term radiometric stability and  
768 mitigation of sunglint and improvements in the AC for turbid and highly absorbing waters for  
769 OLCI, due to an increase in the number and position of spectral bands (Donlon et al. 2012),  
770 suggest that the accuracy of OC5 with OLCI could be improved further. Sentinel-3 OLCI will  
771 use the same or similar AC models that have been used for COASTCOLOUR and MEGS8.0



772 ([Antoine 2010](#); [Doerffer 2010](#); [Moore and Lavender 2010](#)). Based on these results for  
773 MERIS, OC5 warrants further investigation with Sentinel-3 OLCI data.

774 Previous studies with SeaWiFS also found that accurate ocean colour estimates for the  
775 North Sea and English Channel can be achieved using the bright pixel AC in conjunction  
776 with band ratio Chl *a* algorithms ([Blondeau-Patissier et al. 2004](#); [Tilstone et al. 2013](#)). This is  
777 facilitated by the use of the  $R_{rs}(490) : R_{rs}(560)$  ratio to derive Chl *a* ([Tilstone et al. 2013](#)),  
778 since these bands are less affected by errors in the AC or due to high  $a_{CDOM}(\lambda)$  absorption in  
779 the blue portion of the spectrum. Moore et al. ([2009](#)) assessed the uncertainty in Chl *a* in  
780 eight optical water types classified on the shape of  $R_{rs}(\lambda)$ , and found that only in clear waters  
781 was the 35% mission error met. In turbid high sediment water types, the relative error  
782 increased to >100%. By comparison with MODIS-Aqua, the largest errors were encountered  
783 for water types dominated by phytoplankton and  $a_{CDOM}$  ([Goyens et al. 2013](#)). Lee et al.  
784 ([2010](#)) used the theory of error propagation to derive the uncertainties in the inversion of  
785 inherent optical properties from  $R_{rs}(\lambda)$  using the quasi analytical algorithm QAA ([Werdell et](#)  
786 [al. 2013](#)) with a simulated data set and found that the error in  $a(440)$  was 13 to 37 % over



787  
 788 **Figure 12.** Ratio of MERIS MEGS8.0 Chl *a* : in situ Chl *a* versus SPM for (A.) OC5Me, (C.)  
 789 OC4Me, (E.) AP2, (G.) GSM and versus  $a_{CDOM}(442)$  for (B.) OC5Me, (D.) OC4Me, (F.)  
 790 AP2, (H.) GSM. Dotted line represents when MERIS Chl *a* = in situ Chl *a*. Solid regression  
 791 line is the regression line in log- space. Filled circles are data from the North Sea, filled  
 792 squares are from the English Channel, open diamonds are from the Portuguese Shelf, open  
 793 stars are the Mediterranean Sea.

794  
 795 a range of  $a_{CDOM}(440)$  from 0 to 2  $m^{-1}$ . We therefore also addressed the question; what is the  
 796 effect of  $a_{CDOM}(442)$  and non-algal SPM on the Chl *a* algorithms? To assess this we plot *in*  
 797 *situ* SPM and  $a_{CDOM}(442)$  against the MEGS8.0 Chl *a* : *in situ* Chl *a* ratio for OC5Me,  
 798 OC4Me, AP2 and GSM (Figure 12). The vertical dotted line represents where the algorithm

799 Chl *a* equals *in situ* Chl *a* and data points above this line represent an over-estimate in  
800 algorithm Chl *a*, and points below the dotted line represent an under-estimate in Chl *a*. A  
801 significant correlation with SPM or  $a_{CDOM}(442)$  would suggest that the under- or over-  
802 estimate in the Chl *a* algorithm could be partially accounted for by these variables. For  
803 OC5Me there was a significant positive correlation with non-algal SPM ( $F_{1,69} = 6.91$ ,  $P =$   
804  $0.011$ ,  $R^2 = 0.08$ ; Figs. 12A), suggesting that with MEGS8.0 the over-estimate in Chl *a*  
805 observed for this algorithm (Figs. 3A, 4A) was due to non-algal SPM. For GSM, there was a  
806 significant positive correlation between  $a_{CDOM}(442)$  and algorithm : *in situ* Chl *a* (GSM -  $F_{1,72}$   
807  $= 34.40$ ,  $P < 0.0001$   $R^2 = 0.32$ ; Figs. 12H), suggesting that the over-estimate in Chl *a* (Fig.  
808 4E) is due to  $a_{CDOM}(442)$ . For OC4Me, the over-estimate in Chl *a* at  $<10.0 \text{ mg m}^{-3}$  (Fig. 4E)  
809 is due to non-algal SPM (Fig. 5A, D). The over-estimate in OC4Me at Chl *a*  $>10.0 \text{ mg m}^{-3}$   
810 could be due to  $a_{CDOM}(442)$ , though there were not sufficient data points in Fig. 12D to verify  
811 this. There was no significant correlation between AP2 and SPM or  $a_{CDOM}(442)$  suggesting  
812 that under- and over-estimate in AP2 Chl *a* is due to random error in the algorithm.

813

## 814 5. Conclusions.

815 An accuracy assessment of MERIS Chl *a* in NW European waters, was conducted using  
816 MEGS8.0 and COASTCOLOUR processors with ocean colour algorithms that are widely  
817 available from the European Space Agency and NASA. OC5Me Chl *a* was more accurate  
818 than OC3Me, OC4Me, GSM and AP2 Chl *a* using both COASTCOLOUR and MEGS8.0  
819 processors, and MEGS8.0 OC5Me was slightly more accurate than COASTCOLOUR.  
820 Satellite images processed using MEGS8.0  $R_{rs}(\lambda)$  illustrated that OC4Me was 5 to 10 fold  
821 higher than OC5Me in coastal regions of the North Sea and English Channel, which was  
822 principally caused by errors in OC4Me that co-varied with SPM. The GSM was  $>10$  times

823 higher than OC5Me in these regions, which was caused by variations in  $a_{CDOM}$ (442). AP2  
824 was the least accurate algorithm in these waters.

825 The error and uncertainty in both MEGS8.0 and COASTCOLOUR  $R_{rs}$ (442) and  $R_{rs}$ (560)  
826 over a Chl  $a$  range of 0.3 to 7 mg m<sup>-3</sup>, were higher than the mission goal of 5% for the global  
827 ocean. The lower uncertainty in MEGS8.0  $R_{rs}$ (560) and the higher error in COASTCOLOUR  
828  $R_{rs}$ (560) led to slightly more accurate Chl  $a$  for the ocean colour algorithms tested with  
829 MEGS8.0. The performance of OC5 with MERIS data warrants further investigation with  
830 Sentinel-3 OLCI data for NW European and similar coastal and shelf waters.

831

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847

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1329 **Figure Legends.**

1330 **Figure 1.** Location of sampling stations for (A.) *in situ* measurements of  $R_{rs}$  and Chl *a* (B.)  
1331 match-ups between *in situ* and MERIS MEGS8.0 & COASTCOLOUR  $R_{rs}$  and Chl *a*, (C.)  
1332 Transects from which MEGS8.0 Chl *a* processed using OC5Me, OC4Me, AP2 and non-algal  
1333 SPM were extracted. The colour scale indicates the bathymetry depth. In (A.), the arrows  
1334 represent the predominant currents and illustrate the inflow of Atlantic water through the

1335 Orkney-Shetland channel in the North and the English Channel in the South and the flow of  
1336 the Mediterranean Sea current around Corsica Island.

1337

1338 **Figure 2.** Comparison of *in situ* Chl *a* and COASTCOLOUR L2  $R_{rs}$  derived Chl *a* for (A.)  
1339 OC5Me, (B.) OC4Me, (C.) AP2, (D.) OC3Me and (E.) GSM. Faint dotted lines are the 1:1  
1340 line, upper and lower 20% quartiles. Dashed line is the regression line. Filled circles are data  
1341 from the North Sea, filled squares are from the English Channel, open diamonds are from the  
1342 Portuguese Shelf, open stars are the Mediterranean Sea.

1343

1344 **Figure 3.** Comparison of *in situ* Chl *a* and COASTCOLOUR L2  $R_{rs}$  derived Chl *a* for (A.)  
1345 OC5Me, (B.) OC4Me, (C.) AP2, (D.) OC3Me and (E.) GSM. Faint dotted lines are the 1:1  
1346 line, upper and lower 20% quartiles. Dashed line is the regression line. Filled circles are data  
1347 from the North Sea, filled squares are from the English Channel, open diamonds are from the  
1348 Portuguese Shelf, open stars are the Mediterranean Sea.

1349

1350 **Figure 4.** Comparison of *in situ* Chl *a* and MEGS8.0 L2  $R_{rs}$  derived Chl *a* for (A.) OC5Me,  
1351 (B.) OC4Me, (C.) AP2, (D.) OC3Me and (E.) GSM. Faint dotted lines are the 1:1 line, upper  
1352 and lower 20% quartiles. Dashed line is the regression line. Filled circles are data from the  
1353 North Sea, filled squares are from the English Channel, open diamonds are from the  
1354 Portuguese Shelf, open stars are the Mediterranean Sea.

1355

1356 **Figure 5.** Comparison of OC5Me, OC4Me and AP2 processed using MEGS8.0  $R_{rs}$  along  
1357 transects from the Schelde estuary to The Wash; (A.) OC4Me versus OC5 Me, (B.) AP2  
1358 versus OC5Me and (C.) AP2 versus OC4Me; and from the Thames to the Schelde estuaries;  
1359 (D.) OC4Me versus OC5Me, (E.) AP2 versus OC5Me and (F.) AP2 versus OC4Me.

1360 Coloured circles indicate non-algal SPM concentration ( $\text{g m}^{-3}$ ) estimated using the [Gohin](#)  
1361 [\(2011\)](#) algorithm.

1362

1363 **Figure 6.** Comparison of MERIS MEGS8.0 Chl *a* monthly composites for April 2010 using  
1364 (A.) OC5Me, (B.) OC4Me, (C.) AP2, (D.) GSM.

1365

1366 **Figure 7.** Comparison of MERIS MEGS8.0 Chl *a* monthly composites of July 2011 using  
1367 (A.) OC5Me, (B.) OC4Me, (C.) AP2, (D.) GSM.

1368

1369 **Figure 8.** Comparison of MERIS MEGS8.0 Chl *a* from the monthly composite of April 2010  
1370 (given in [Fig. 6](#)) along Longitudinal transects from the Wash to the Schelde for (A.) OC5Me,  
1371 (B.) OC4Me, (C.) AP2, (D.) GSM and from the western English Channel to the River Seine  
1372 for (E.) OC5Me, (F.) OC4Me, (G.) AP2, (H.) GSM. The location of the transects are given in  
1373 [Figure 1C](#).

1374

1375 **Figure 9.** Scatter plots of *in situ*  $R_{rs}(\lambda)$  against COASTCOLOUR  $R_{rs}(\lambda)$  for (A.) 412, (B.)  
1376 442, (C.) 490, (D.) 510, (E.) 560 and (F.) 665 nm. Solid line is the 1:1; dashed line is the  
1377 regression line.

1378

1379 **Figure 10.** Scatter plots of *in situ*  $R_{rs}(\lambda)$  against MEGS8.0  $R_{rs}(\lambda)$  for (A.) 412, (B.) 442, (C.)  
1380 490, (D.) 510, (E.) 560 and (F.) 665 nm. Solid line is the 1:1; dashed line is the regression  
1381 line.

1382



1383 **Figure 11.** Spectral relationships between Rrs errors for (A.) MEGS8.0  $R_{rs}(442)$  and  
1384  $R_{rs}(560)$  and (B.) COASTCOLOUR  $R_{rs}(442)$  and  $R_{rs}(560)$ . The errors are determined as the  
1385 relative difference between MERIS and *in situ*  $R_{rs}$ . Percentage uncertainty in (C.)  
1386 COASTCOLOUR  $R_{rs}(442)$  (open squares) and  $R_{rs}(560)$  (filled squares) and (D.) MEGS8.0  
1387  $R_{rs}(442)$  (open circles) and  $R_{rs}(560)$  (filled circles) as a function of Chl  $a$ . In (A.) and (B.),  
1388 the solid line is the regression and the dashed lines are the 95% confidence intervals. In (C.)  
1389 and (D.), the dashed line is the 5% uncertainty limit.

1390

1391 **Figure 12.** Ratio of MERIS MEGS8.0 Chl  $a$  : *in situ* Chl  $a$  versus SPM for (A.) OC5Me, (C.)  
1392 OC4Me, (E.) AP2, (G.) GSM and versus  $a_{CDOM}(442)$  for (B.) OC5Me, (D.) OC4Me, (F.)  
1393 AP2, (H.) GSM. Dotted line represents when MERIS Chl  $a$  = *in situ* Chl  $a$ . Solid regression  
1394 line is the regression line in log- space. Filled circles are data from the North Sea, filled  
1395 squares are from the English Channel, open diamonds are from the Portuguese Shelf, open  
1396 stars are the Mediterranean Sea.