



1 **Floodwater Impact on Galveston Bay Phytoplankton Taxonomy, Pigment Composition and Photo-**  
2 **Physiological State following Hurricane Harvey from Field and Ocean Color (Sentinel-3A OLCI)**  
3 **Observations**

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14 **Abstract**

15 Phytoplankton taxonomy, pigment composition and photo-physiological state were studied in Galveston  
16 Bay (GB), Texas (USA) following the extreme flooding associated with Hurricane Harvey (August 25–29,  
17 2017) using field and satellite ocean color observations. Percentage of chlorophyll a (Chl a) in different  
18 phytoplankton groups were determined from a semi-analytical IOP (inherent optical property) inversion  
19 algorithm. The IOP inversion algorithm revealed the dominance of freshwater species (cyanobacteria and  
20 green algae) in the bay following the hurricane passage (September 29, 2017) under low salinity  
21 conditions associated with the discharge of floodwaters into GB; 2 months after the hurricane (October  
22 29–30, 2017), under more seasonal salinity conditions, the phytoplankton community transitioned to an  
23 increase in small sized groups such as haptophyte and prochlorophyte. Sentinel-3A OLCI-derived Chl a  
24 obtained using a red/NIR band ratio algorithm for the turbid estuarine waters was highly correlated ( $R^2 >$   
25 0.90) to HPLC-derived Chl a concentrations. A Non-Negative Least Square (NNLS) inversion model was  
26 then applied to OLCI-derived Chl a maps of GB to obtain spatiotemporal distributions of phytoplankton  
27 diagnostic pigments; results appeared consistent with extracted phytoplankton taxonomic composition  
28 derived from the IOP inversion algorithm. OLCI-derived diagnostic pigment distributions also exhibited  
29 good agreement with HPLC measurements, with mean  $R^2$  ranging from 0.39 for violaxanthin to 0.98 for  
30 Chl a. Environmental factors (e.g. floodwaters) combined with phytoplankton taxonomy also strongly  
31 modulated phytoplankton physiology in the bay as indicated by measurements of photosynthetic  
32 parameters with a Fluorescence Induction and Relaxation (FIRE) system. Phytoplankton in well-mixed  
33 waters (mid-bay area) exhibited maximum PSII photochemical efficiency ( $F_V/F_M$ ) and low effective  
34 absorption cross section ( $\sigma_{PSII}$ ), while the areas adjacent to the shelf (likely nutrient-limited) showed low  
35  $F_V/F_M$  and elevated  $\sigma_{PSII}$  values. Overall, the approach using field and ocean color data combined with  
36 inversion models allowed, for the first time, an assessment of phytoplankton response to a large  
37 hurricane-related floodwater perturbation in a turbid estuarine environment based on its taxonomy,  
38 pigment composition and physiological state.

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45 **Key words:** Galveston Bay, phytoplankton taxonomy, pigment composition, physiology, ocean color,  
46 chlorophyll a, Sentinel-3A OLCI



## 49 1. Introduction

50 Phytoplankton, which form the basis of the aquatic food web, are crucial to marine ecosystems and play a  
51 strong role in marine biogeochemical cycling and climate change. Phytoplankton contributes  
52 approximately half of the total primary production on Earth, fixing ~50 GT of carbon into organic matter  
53 per year through photosynthesis; however, various phytoplankton taxa affect differently the carbon  
54 fixation and export (Sathyendranath et al., 2014). Chlorophyll a (Chl a), an essential phytoplankton  
55 photosynthetic pigment, has been considered a reliable indicator of phytoplankton biomass and primary  
56 productivity in aquatic systems (Bracher et al., 2015). Phytoplankton also contain several accessory  
57 pigments such as chlorophyll-b (Chl b), chlorophyll-c (Chl c), photosynthetic carotenoids (PSC) and  
58 photo-protective carotenoids (PPC) that are either involved in light harvesting, or in protecting Chl a and  
59 other sensitive pigments from photo-damage (Fishwick et al., 2006). Some of PSCs and PPCs are taxa-  
60 specific and have been considered as bio-marker pigments: e.g., fucoxanthin (PSC) for diatoms, peridinin  
61 (PPC) for certain dinoflagellates, alloxanthin (PPC) for cryptophytes, zeaxanthin (PPC) for prokaryotes  
62 (e.g. cyanobacteria), and the degradation products of Chl a, namely, divinyl Chl a and divinyl-Chl b for  
63 prochlorophyte (Jeffrey and Vest, 1997). High-Performance Liquid Chromatography (HPLC) which can  
64 efficiently detect and quantify several chemo-taxonomically significant chlorophylls and carotenoids,  
65 when coupled with these taxa-specific pigment ratios, allow phytoplankton taxonomic composition to be  
66 quantified based on a pigment concentration diagnostic procedures such as CHEMTAX (Mackey et al.,  
67 1996). Furthermore, phytoplankton pigments with distinct absorption characteristics strongly influence  
68 the light absorption by phytoplankton (Bidigare et al., 1990; Ciotti et al., 2002; Bricaud et al., 2004). As  
69 such, phytoplankton absorption spectra has been used to infer underlying pigments and also  
70 phytoplankton taxonomy by Gaussian-decomposition of (Hoepffner and Sathyendranath, 1991; Lohrenz  
71 et al., 2003; Ficek et al., 2004; Chase et al., 2013; Moisan et al., 2013; Wang et al., 2016; Moisan et al.,  
72 2017). More importantly, phytoplankton optical properties (absorption and backscattering) bearing the  
73 imprints of different pigments and cell-size, are important contributors to reflectance in a waterbody  
74 (Gordon et al., 1988). Morel and Prieur, (1977) first reported the feasibility of calculating the  
75 phytoplankton absorption coefficients and other inherent optical properties (IOPs) from measured  
76 subsurface irradiance reflectance based on the simplified radiative transfer equation. Improvements in  
77 semi-analytical inversion algorithms to derive IOPs from in-situ and remotely sensed reflectance spectra  
78 have been reported (Roesler and Perry, 1995; Hoge and Lyon, 1996; Lee et al., 1996; Garver and Siegel,  
79 1997; Carder et al., 1999; Maritorena et al., 2002; Roesler and Boss, 2003; Chase et al., 2017). Roesler et  
80 al. (2003) further modified an earlier IOP inversion algorithm used in Roesler and Perry, (1995) by  
81 adding a set of 5 species-specific phytoplankton absorption spectra, and derived phytoplankton taxonomic  
82 composition from the field measured remote sensing reflectance.

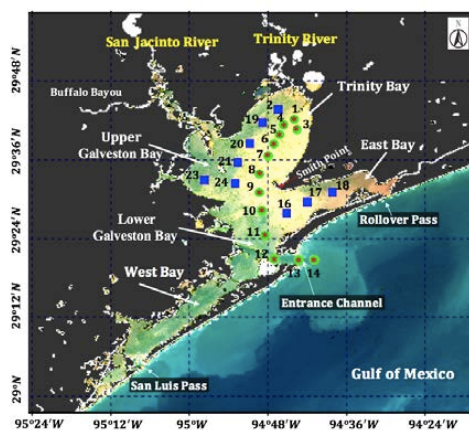
83 Phytoplankton pigment composition varies not only between taxonomic groups but also with photo-  
84 physiological state of cells and environmental stress (e.g., light, nutrients, temperature, salinity,  
85 turbulence and stratification) (Suggett et al., 2009). The photosynthetic pigment field is an important  
86 factor influencing the magnitude of fluorescence emitted by phytoplankton, with active fluorometry  
87 commonly used to obtain estimates of phytoplankton biomass (D'Sa et al., 1997). Advanced active  
88 fluorometry termed as fast repetition rate (FRR; (Kolber et al., 1998)) and analogous techniques such as  
89 the fluorescence induction and relaxation (FIRE; (Suggett et al., 2008)) allows for the simultaneous  
90 measurements of the maximum PSII photochemical efficiency ( $F_v/F_m$ ; where  $F_m$  and  $F_o$  is maximum and  
91 minimum fluorescence yield and  $F_v$  is variable fluorescence obtained by subtracting  $F_o$  from  $F_m$ ) and the  
92 effective absorption cross section ( $\sigma_{PSII}$ ) of a phytoplankton population; these have been used as  
93 diagnostic indicators for the rapid assessment of phytoplankton health and photo-physiological state  
94 linked to environmental stressors. Considerable effort has been invested to achieve a deeper  
95 understanding of the impacts of environmental factors and phytoplankton taxonomy on photosynthetic  
96 performance of natural communities from field and laboratory fluorescence measurements (Kolber et al.,  
97 1988; Geider et al., 1993; Schittler et al., 1997; Behrenfeld and Kolber, 1999; D'Sa and Lohrenz, 1999;



98 Holmboe et al., 1999; Moore et al., 2003). Furthermore, knowledge of photo-physiological responses of  
99 phytoplankton in combination with information on phytoplankton taxonomic composition could provide  
100 additional insights on regional environmental conditions.

101 Synoptic mapping of aquatic ecosystems using satellite remote sensing has revolutionized our  
102 understanding of phytoplankton dynamics at various spatial and temporal scales in response to  
103 environmental variabilities and climate change. It has also provided greater understanding of biological  
104 response to large events such as hurricanes in oceanic and coastal waters (Babin et al. 2004; Acker et al.  
105 2009; D'Sa 2014; Farfan et al. 2014; Hu and Feng, 2016). Although the primary focus of ocean color  
106 sensors has been to determine the Chl a concentration and related estimates of phytoplankton primary  
107 production (Mitchell, 1994; Behrenfeld and Falkowski, 1997), more recently, several approaches have  
108 been developed based on phytoplankton optical signatures to derive spatial distributions of phytoplankton  
109 functional types (PFTs) (Alvain et al., 2005; Nair et al., 2008; Hirata et al., 2011), phytoplankton size  
110 classification (Ciotti et al., 2002; Hirata et al., 2008; Brewin et al., 2010; Devred et al., 2011), and  
111 phytoplankton accessory pigments (Pan et al., 2010; Pan et al., 2011; Moisan et al., 2013; Moisan et al.,  
112 2017; Sun et al., 2017). The basis of these satellite-based remote sensing algorithms have relied on  
113 distinct spectral contributions from phytoplankton community composition (e.g., taxonomy, size structure)  
114 to remote sensing reflectance ( $R_{rs}$ ,  $sr^{-1}$ ); however, these studies have all been confined to open ocean and  
115 shelf waters. In contrast, satellite studies of phytoplankton pigments have been limited in the optically  
116 complex estuarine waters where the influence from wetlands, rivers, and coastal ocean make  
117 phytoplankton communities highly variable and complex.

118 In this study, field bio-optical measurements and ocean color remote sensing data (Sentinel-3A OLCI)  
119 acquired in Galveston Bay, a shallow estuary along the Gulf coast (Texas, USA; Fig. 1), are used to  
120 investigate the spatial distribution of phytoplankton pigments, taxonomic composition, and their photo-  
121 physiological state following the extreme flooding of the Houston Metropolitan and surrounding areas  
122 due to Hurricane Harvey and the consequent biological impact of the floodwater discharge into the bay.  
123 The paper is organized as follows: section 2 describes the field data acquisition, laboratory processing,  
124 and the algorithms and methods used to distinguish phytoplankton groups, retrieve spatial distribution of  
125 pigments, and calibrate phytoplankton physiological parameters. Results and discussion (sections 3 and 4),  
126 and conclusions (section 5) addresses the main contributions and findings of this paper.



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128 **Figure 1.** Sentinel-3A OLCI RGB image (October 29, 2017) with locations of sampling sites in  
129 Galveston Bay acquired on September 29 (red asterisk), October 29 (green circles) and October 30 (blue  
130 solid squares), 2017, respectively.



## 131 2. Data and Methods

### 132 2.1 Study area

133 Galveston Bay (GB), a shallow water estuary (~2.1 m average depth), encompasses two major sub-  
134 estuaries: San Jacinto Estuary (also divided as Upper GB and Lower GB), and Trinity Estuary (Trinity  
135 Bay) (Fig. 1). It is located adjacent to the heavily urbanized and industrialized metropolitan areas of  
136 Houston, Texas (Dorado et al., 2015). A deep (~14 m) narrow Houston Ship Channel connects the bay to  
137 the northern Gulf of Mexico (nGoM) through a narrow entrance, the Bolivar Roads Pass. Tidal exchange  
138 between GB and the nGoM occurs through the entrance channel with diurnal tides ranging from ~0.15 to  
139 ~0.5 m. The major freshwater sources to GB are the Trinity River (55%), the San Jacinto River (16%),  
140 and Buffalo Bayou (12%) (Guthrie et al., 2012). The San Jacinto River was frequently observed to  
141 transport greater amounts of dissolved nutrients into GB than the Trinity River (Quigg, 2011). The  
142 catastrophic flooding of Houston and surrounding areas associated with Hurricane Harvey resulted in  
143 strong freshwater inflows into GB from the San Jacinto River ( $>3300 \text{ m}^3 \text{ s}^{-1}$ ; USGS 8068090) on August  
144 29, 2017 and the Trinity River ( $>2500 \text{ m}^3 \text{ s}^{-1}$ ; USGS 08066500 site at Romayor, Texas) on August 30,  
145 2017, respectively. Although the discharge from the two rivers in the upstream returned to normal  
146 conditions ( $\sim 50\text{--}120 \text{ m}^3 \text{ s}^{-1}$ ) in about 2 weeks after the Hurricane passage, salinity remained low for over a  
147 month following the hurricane passage (D'Sa et al., 2018).

### 148 2.2 Sampling and Data Collection

149 Surface water samples were collected at a total of 34 stations during two surveys on September 29 and  
150 October 29–30, 2017 (Fig. 1). Samples at stations 1 to 14 (red asterisk on top of green circle; Fig. 1)  
151 along the Trinity River transect were collected repetitively on September 29 and October 29, 2017,  
152 respectively. Additional 9 sampling sites (blue squares; Fig. 1) around the upper bay and in the East Bay  
153 were sampled on October 30, 2017. The surface water samples were stored in coolers and filtered on the  
154 same day. The filter pads were immediately frozen and stored in liquid nitrogen for laboratory absorption  
155 spectroscopic and HPLC measurements of the samples. An optical package equipped with a conductivity-  
156 temperature-depth recorder (Sea-Bird SBE) and a Fluorescence Induction and Relaxation System (FIRE;  
157 Satlantic Inc) was used to obtain profiles of salinity, temperature, pressure, and phytoplankton  
158 physiological parameters ( $F_V/F_M$  and  $\sigma_{PSII}$ ). Measurements of backscattering were also made at each  
159 station using a WETLabs VSF-3 (470, 530, 670 nm) backscattering sensor (D'Sa et al. 2006; Naik et al.  
160 2013). Included in the optical package was also a hyperspectral downwelling spectral irradiance meter  
161 (HyperOCR, Satlantic). The irradiance data from HyperOCR were processed using Prosoft 7.7.14 and the  
162 Photosynthetically Active Radiation (PAR) were estimated from the irradiance measurements. The above-  
163 water reflectance measurements were collected using a GER 1500 512iHR spectroradiometer in the 350-  
164 1050 nm spectral range. At each station, sky radiance, plate radiance, and water radiance were recorded  
165 (each repeated three times) and processed to obtain above-water remote sensing reflectance (Joshi et al.,  
166 2017). Sentinel-3A OLCI full resolution mode, cloud free level-1 images were obtained for September 29,  
167 October 29 and 30, 2017 over GB from the European Organization for Meteorological Satellites  
168 (EUMESAT) website and pre-processed using Sentinel-3 Toolbox Kit Module (S3TBX) version 5.0.1 in  
169 Sentinel Application Platform (SNAP). These OLCI data were further atmospherically corrected to obtain  
170 remote sensing reflectance ( $R_{rs,OLCI}$ ,  $\text{sr}^{-1}$ ) using Case-2 Regional Coast Color (C2RCC) module version  
171 0.15 (Doerffer and Schiller, 2007).

### 172 2.3 Absorption Spectroscopy

173 Surface water samples were filtered through 0.2- $\mu\text{m}$  nuclepore membrane filters and the colored dissolved  
174 organic matter (CDOM) absorbance ( $A_{CDOM}$ ) were obtained using a 1-cm path length quartz cuvette on a



175 Perkin Elmer Lambda-850 UV/VIS spectrophotometer equipped with an integrating sphere. The  
 176 Quantitative Filter Technique (QFT) with 0.7- $\mu\text{m}$  GF/F filters were used to measure absorbance of  
 177 particles ( $A_{\text{total}}$ ) and non-algal particles ( $A_{\text{NAP}}$ ) inside an integrating sphere at 1 nm intervals from 300 to  
 178 800 nm. The absorption coefficients of CDOM ( $a_{\text{CDOM}}$ ), NAP ( $a_{\text{NAP}}$ ), particles ( $a_{\text{total}}$ ) and phytoplankton  
 179 ( $a_{\text{PHY}}$ ) were calculated using the following equations:

$$180 \quad a_{\text{CDOM}}(\lambda) = 2.303 \times \frac{A_{\text{CDOM}}(\lambda)}{L} \quad \dots\dots (1)$$

181 where  $L$  is the path length in meters. The  $a_{\text{CDOM}}$  were corrected for scattering, temperature, and baseline  
 182 drift by subtracting an average value of absorption between 700-750 nm for each spectrum (Joshi and  
 183 D'Sa, 2015).

$$184 \quad a_{\text{total}}(\lambda) = 2.303 \times \frac{A_{\text{total}}(\lambda)}{V_{\text{filtered}}/S_{\text{filter}}} \quad \dots\dots (2)$$

$$185 \quad a_{\text{NAP}}(\lambda) = 2.303 \times \frac{A_{\text{NAP}}(\lambda)}{V_{\text{filtered}}/S_{\text{filter}}} \quad \dots\dots (3)$$

$$186 \quad a_{\text{PHY}}(\lambda) = a_{\text{total}} - a_{\text{NAP}} \quad \dots\dots (4)$$

187 where  $V_{\text{filtered}}$  is the filtered volume of sample,  $S_{\text{filter}}$  is the area of filter pads and the path length  
 188 correction for filter pad was applied according to (Stramski et al., 2015).

## 189 2.4 Pigment Absorption Spectra

190 The water samples were filtered with 0.7- $\mu\text{m}$  GF/F filter. The filter pads were stored in liquid nitrogen  
 191 until transferred into 30 ml vials containing 10 ml cold 96% ethanol (Ritchie, 2006). The vials were spun  
 192 evenly to ensure full exposure of the filter pad to the ethanol and then kept in the refrigerator (in the dark)  
 193 overnight. The pigment solutions at room-temperature were poured off from vials into 1 cm cuvette and  
 194 measured on a Perkin Elmer Lambda-850 UV/VIS spectrophotometer to obtain pigment absorbance  
 195 spectra ( $A_{\text{pig}}$ ), while, 90% ethanol was used as a blank (Thrane et al., 2015). The total absorption  
 196 coefficients of pigments  $a_{\text{pig}}(\lambda)$  were calculated as follow:

$$197 \quad a_{\text{pig}}(\lambda) = 2.303 \times \frac{A_{\text{pig}}(\lambda)}{L} \times \left(\frac{V_{\text{ethanol}}}{V_{\text{filtered}}}\right) \quad \dots\dots (5)$$

198 where  $L$  is the path length in meters,  $V_{\text{ethanol}}$  is the volume of ethanol, and  $V_{\text{filtered}}$  is the filtered volume of  
 199 the water samples.

## 200 2.5 HPLC Measurements

201 Water samples were filtered through 0.7- $\mu\text{m}$  GF/F filters and immediately frozen in liquid nitrogen for  
 202 HPLC analysis using the methods reported by Barlow et al. (1997). The detected pigments along with  
 203 their abbreviations are listed in Table 1. Diagnostic biomarker pigments are marked in bold letters (Table  
 204 1).

205 **Table 1.** Pigments information acquired from HPLC samples in Galveston Bay.

Variable	Primary Pigment (PPig)	Calculation
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Chlorophylls		
[TChl a]	Total chlorophyll a (TChl a)	[Chlide a]+[DVChl a]+[Chl a]
[TChl b]	Total chlorophyll b (TChl b)	[DVChl b]+[Chl b]
[TChl c]	Total chlorophyll c (TChl c)	[Chl c <sub>1</sub> ]+[Chl c <sub>2</sub> ]+[Chl c <sub>3</sub> ]
Carotenoids		
[Caro]	Carotenes†	[ββ-Car]+[βε-Car]
[Allo]	<b>Alloxanthin</b>	
[Buta]	<b>19'-Butanoyloxyfucoxanthin</b>	
[Diadino]	Diadinoxanthin	
[Diatol]	Diatoxanthin	
[Fuco]	<b>Fucoxanthin</b>	
[Hexa]	<b>19'-Hexanoyloxyfucoxanthin</b>	
[Peri]	<b>Peridinin</b>	
[Zea]	<b>Zeaxanthin</b>	
[Neo]	Neoxanthin	
[Lut]	Lutein	
[Viola]	Violaxanthin	
[Pras]	Prasinolaxanthin	
[Anthera]	Antheraxanthin	
Note: (1) [Chl b], [Allo], [Fuco], [Peri], [Zea], [Buta] and [Hexa] are considered as diagnostic pigments for PFTs (Moisan et al., 2017).		
Variable	Pigment Sum	Calculation
[TChl]	Total Chlorophyll (TChl)	[TChl a]+[TChl b]+[TChl c]
[PPC]	Photoprotective Carotenoids (PPC)	[Allo]+[Diadino]+[Diatol]+[Zea]+[Caro]+[Viola]
[PSC]	Photosynthetic Carotenoids (PSC)	[Buta]+[Fuco]+[Hexa]+[Peri]+[Lut]+[Pras]
[PSP]	Photosynthetic Pigments (PSP)	[PSC]+[TChl]
[AP]	Total Accessory Pigments (AP)	[PPC]+[PSC]+[TChl b]+[TChl c]
[TP]	Total Pigments (TP)	[AP]+[TChl a]
[DP]	Total Diagnostic Pigments (DP)	[PSC]+[Allo]+[Zea]+[T Chl b]

## 206 2.6 FIRE Measurements

207 An in-situ Fluorescence Induction and Relaxation System (FIRE, Satlantic Inc.) was used to characterize  
 208 phytoplankton photosynthetic physiology during the two surveys in GB. The FIRE is based on  
 209 illuminating a sample with an intense flash of light to instantaneously saturate the reaction centers of  
 210 photosystem II (PSII); under these light conditions, reaction centers do not accept electrons and most of  
 211 the absorbed light energy is dissipated as fluorescence. The fundamental parameter measured by FIRE is  
 212 fluorescence yield  $F(t)$ , which is the emitted fluorescence divided by the irradiance intensity (no unit). In  
 213 contrast to strong flashes, dark adaption enables all reaction centers of PSII to be open with least  
 214 fluorescence emitted, thus, resulting in minimal fluorescence yield ( $F_0$ ). Maximum fluorescence yield ( $F_m$ )  
 215 can be obtained after sufficient irradiation when all reaction centers are closed. Maximum photochemical  
 216 efficiency, which quantify the potential of converting light to chemical energy for the PSII reaction  
 217 centers (Moore et al., 2006), was calculated as  $(F_m - F_0) / F_m = F_v / F_m$ . The functional absorption cross  
 218 section  $\sigma_{PSII}$  ( $\text{\AA}^2 \text{quantum}^{-1}$ ) measures the capability of reaction centers to absorb light from the ambient  
 219 environment. The FIRE was deployed at a slow descent rate, with 12 and 20 vertical profiles obtained  
 220 during the first and second surveys, respectively. All measurements were programmed using standard



221 protocols of single saturating turn-over (ST) flash saturation of PSII (Kolber et al., 1998). Flashes were  
 222 generated from highly uniform blue LEDs at 455 nm with approximately 30 nm half-bandwidth. Chl a  
 223 fluorescence was stimulated using saturating sequence of 80 1.1  $\mu$ s flashes applied at 1  $\mu$ s intervals, 8  
 224 sequences were averaged per acquisition, and the fluorescence signal was detected at 668 nm. All data  
 225 were processed using standard FIRECom software (Satlantic). In addition, samples of 0.2- $\mu$ m filtered sea  
 226 water at each station were used as ‘blank’ to remove the background fluorescence signals (Cullen and  
 227 Davis, 2003); in this step, the fluorescence from the filtered samples (without phytoplankton) were  
 228 subtracted from in-situ fluorescence signals to get more accurate values of  $F_v/F_m$ .

## 229 2.7 Retrieving Phytoplankton Groups from above-water $R_{rs}$

230 A fundamental relationship that links sub-surface remote-sensing reflectance ( $r_{rs}$ ) and the IOPs was  
 231 expressed using a quadratic function developed by (Gordon et al., 1988):

$$232 \quad r_{rs} = g_1 * u(\lambda) + g_2 * u(\lambda)^2; \quad u(\lambda) = \frac{b_b}{a_{total} + b_b} \quad \dots\dots (6)$$

233 where, the parameters  $g_1$  (~0.0788) and  $g_2$  (~0.2379) are values for turbid estuarine waters (Joshi and  
 234 D'Sa, 2018);  $r_{rs}$  is the sub-surface remote sensing reflectance that were obtained from above-water remote  
 235 sensing reflectance ( $R_{rs}$ ) using (Lee et al., 2002):

$$236 \quad r_{rs} = \frac{R_{rs}}{0.52 + 1.7 * R_{rs}} \quad \dots\dots (7)$$

237 The total backscattering coefficient  $b_b$  is comprised of water ( $b_{bw}$ ) and particulates including both organic  
 238 and inorganic particles ( $b_{bp}$ ), while the total absorption coefficients ( $a_{total}$ ) can be further separated into  
 239 four sub-constituents (Roesler and Perry, 1995) as indicated by:

$$240 \quad b_b = b_{bw} + b_{bp}; \quad a_{total} = a_w + a_{phy} + a_{CDOM} + a_{NAP} \quad \dots\dots (8)$$

241 where  $a_w$ ,  $a_{phy}$ ,  $a_{CDOM}$ , and  $a_{NAP}$  represent the absorption coefficients of pure water, phytoplankton,  
 242 colored dissolved organic matter and non-algal particles, respectively.

243 The IOP inversion algorithm for retrieving IOPs from  $R_{rs}$  require known spectral shape (eigenvector) of  
 244 each component in Eq. (8) to estimate the magnitude (eigenvalue) of each component (Table 2). The  
 245 spectral shape can be adjusted by changing the values of slope based on characteristics of the study area.  
 246 It is worth noting that a single averaged phytoplankton eigenvector does not provide species information  
 247 whereas a set of several species-specific phytoplankton eigenvectors allow estimates of species  
 248 composition. IOPs inversion algorithm applied in this study makes use of mass-specific phytoplankton  
 249 absorption spectra of 10 groups namely, dinoflagellate, diatom, chlorophyte, cryptophyte, haptophyte,  
 250 prochlorophyte, raphidophyte, rhodophyte, red cyanobacteria (*Synechococcus*) and blue cyanobacteria  
 251 (*Trichodesmium*); these were obtained from Dierssen et al. (2006) and Dutkiewicz et al. (2015) as eigen  
 252 vectors rather than using one average  $a_{phy}(\lambda)$  spectrum. Subsequently, the inversion algorithm iterates  
 253 repeatedly to minimize the difference between modeled  $R_{rs}$  and in-situ measured  $R_{rs}$  ( $R_{rs\_insitu}$ ) until a best  
 254 fit is achieved while allowing for alterations of all parameters listed in Table 2 (Chase et al., 2017). The  
 255 absolute percent errors between modeled and measured values of  $R_{rs}$ ,  $a_{phy}$ ,  $a_{CDOM}$ ,  $a_{NAP}$  and  $b_{bp}$  were  
 256 calculated as:

$$257 \quad \%error = \left| \frac{X_{modeled} - X_{measured}}{X_{measured}} \right| \times 100 \quad \dots\dots (9)$$



258 **Table 2.** Parameters and eigenvectors used in the semi-analytical inversion algorithm.

Parameter	Equation	Slope	Eigenvalue
$a_{\text{CDOM}}(\lambda)$	$a_{\text{CDOM}}(\lambda) = M_{\text{CDOM}} \times \exp^{-S_{\text{CDOM}} \times (\lambda - \lambda_0)}$ ; $\lambda_0 = 443$	$S_{\text{CDOM}}$	$M_{\text{CDOM}}$
$a_{\text{NAP}}(\lambda)$	$a_{\text{NAP}}(\lambda) = M_{\text{NAP}} \times \exp^{-S_{\text{NAP}} \times (\lambda - \lambda_0)}$ ; $\lambda_0 = 443$	$S_{\text{NAP}}$	$M_{\text{NAP}}$
$a_{\text{phy}}(\lambda)$	$a_{\text{phy}}(\lambda) = \sum \text{Chl } a_i \times a_{\text{phi}}^*$ ; $a_{\text{phi}}^*$ is the spectral shape of each phytoplankton group.		Chl $a_i$
$b_{\text{bp}}(\lambda)$	$b_{\text{bp}}(\lambda) = B_{\text{bp}} \times (\lambda_0/\lambda)^{S_{\text{bp}}}$ ; $\lambda_0 = 443$	$S_{\text{bp}}$	$B_{\text{bp}}$

Note:  $a_{\text{phi}}^*(\lambda)$  for 10 different groups of phytoplankton used in this study were extracted from (Dierssen et al., 2006) and Dutkiewicz et al., (2015).

259 **2.8 Retrieving Pigments from Sentinel 3-OLCI  $R_{rs}$**

260 **2.8.1 Reconstruction of Pigment Absorption Spectrum by Multiple Linear Regression**

261 Total pigment absorption spectra  $a_{\text{pig}}(\lambda)$  obtained during both surveys (Eq. 5), were modeled as a third  
 262 order function of HPLC measured Chl a (Chl  $a_{\text{HPLC}}$ ) concentration at each station as (Moisan et al., 2017):

263 
$$a_{\text{pig}}(\lambda) = C_3 \times (\text{Chl } a_{\text{HPLC}})^3 + C_2 \times (\text{Chl } a_{\text{HPLC}})^2 + C_1 \times \text{Chl } a_{\text{HPLC}} + C_0 \quad \dots\dots (11)$$

264 where  $C=[C_3, C_2, C_1, C_0]$ , is the wavelength-dependent vector coefficient ranging from 400 to 700 nm at  
 265 1 nm interval; these were further applied to Sentinel-3A OLCI Chl a to calculate  $a_{\text{pig\_OLCI}}$  at each pixel as:

266 
$$a_{\text{pig\_OLCI}}(\lambda) = C_3 \times (\text{Chl } a_{\text{OLCI}})^3 + C_2 \times (\text{Chl } a_{\text{OLCI}})^2 + C_1 \times \text{Chl } a_{\text{OLCI}} + C_0 \quad \dots\dots (12)$$

267 where Chl  $a_{\text{OLCI}}$  is Sentinel-3A OLCI derived Chl a concentration (259×224 pixels); the obtained image  
 268 represents the value of  $a_{\text{pig\_OLCI}}$  at a certain wavelength and 301 images of  $a_{\text{pig\_OLCI}}$  can be obtained in  
 269 the 400-700 nm wavelength range at 1 nm interval.

270 **2.8.2 Satellite Retrieval of Pigments using Non-Negative Least Square (NNLS) Inversion Model**

271 The  $a_{\text{pig\_OLCI}}$  is a mixture of n pigments with known absorption spectra  $a_i(\lambda)$ ,  $i = 1, 2, \dots, n$  at wavelength  
 272  $\lambda$  (nm); thus,  $a_{\text{pig\_OLCI}}(\lambda)$  can be considered as a weighted sum of individual component spectrum  
 273 (Thrane et al., 2015) at each image point as:

274  
 275 
$$a_{\text{pig\_OLCI}}(\lambda) = x_1 \times a_1(\lambda) + x_2 \times a_2(\lambda) + \dots x_n \times a_n(\lambda) \quad \dots\dots (13)$$

276  
 277 where  $A(\lambda) = [a_1(\lambda), a_2(\lambda), \dots a_n(\lambda)]$  are the spectra of 16 pigments (Chl a, Chl b, Chl  $c_1$ , Chl  $c_2$ ,  
 278 pheophytin-a, pheophytin-b, peridinin, fucoxanthin, neoxanthin, lutein, violaxanthin, alloxanthin,  
 279 diadinoxanthin, diatoxanthin, zeaxanthin, and  $\beta$ -carotenoid) extracted from supplementary R scripts of  
 280 Thrane et al. (2015). All these 16 spectra are normalized to unit maximum peak absorbing value. The  
 281 vector coefficient  $[x_1, x_2, \dots x_n]$  correspond to the weights of these distinct pigments; note that X cannot be  
 282 negative, therefore, non-negative least squares (NNLS) was used to guarantee positive solutions of X  
 283 (Moisan et al., 2013; Thrane et al., 2015). Eq. 13 can be further expressed as:





284

$$\begin{bmatrix} a_{\text{pig}}(400)_{\text{OLCI}} \\ a_{\text{pig}}(401)_{\text{OLCI}} \\ \vdots \\ a_{\text{pig}}(700)_{\text{OLCI}} \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \times \begin{bmatrix} a_1(400), a_2(400), \dots, a_n(400) \\ a_1(401), a_2(401), \dots, a_n(401) \\ \vdots \\ a_1(700), a_2(700), \dots, a_n(700) \end{bmatrix} \quad \dots (14)$$

286

287 where  $n=16$  is the number of pigment components included in the NNLS inversion model and  $x_n$  is the  
 288 weight mentioned above for the  $n^{\text{th}}$  pigment. Note:  $x_n$  is not the concentration of each pigment component;  
 289 the concentration of pigments ( $C_n, \mu\text{g L}^{-1}$ ) were further calculated by dividing the pigment's weight-  
 290 specific absorption coefficient ( $U_n, \text{L g}^{-1}\text{cm}^{-1}$ ) at maximum peak wavelength (Thrane et al., 2015) as:

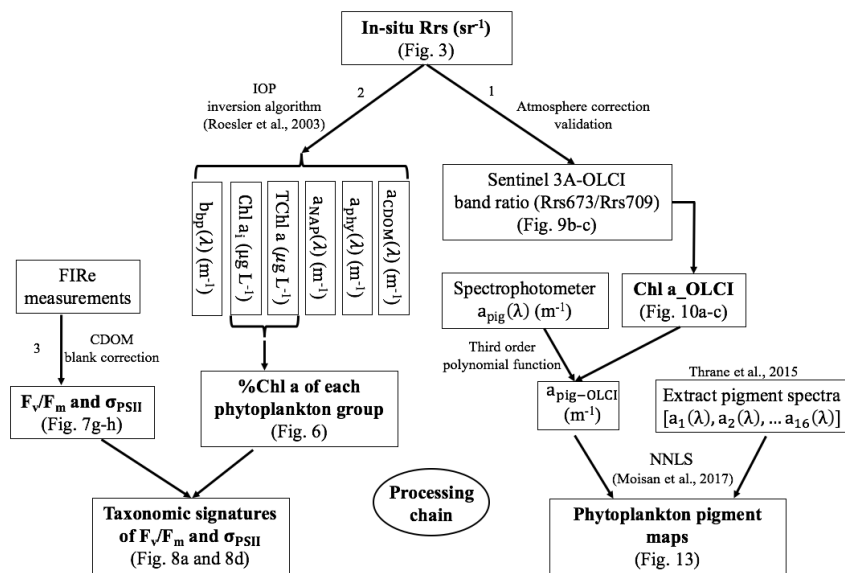
291

$$C_n = 10000 \times \left( \frac{x_n}{U_n} \right) \quad \dots (15)$$

## 292 2.9 Processing Approach

293 Sentinel 3A-OLCI pigment maps were generated using the processing pathway 1 (Fig. 2) that includes the  
 294 following: 1) developing empirical relationships between HPLC-measured Chl a and  $R_{rs\_in\text{-}situ}$  band ratio  
 295 for Sentinel 3A-OLCI band 9 (673 nm) and band 11 (709 nm) to generate Sentinel 3A-OLCI Chl a maps,  
 296 2) converting Chl a concentration to  $a_{\text{pig\_OLCI}}(\lambda)$  maps, and subsequently decomposing  $a_{\text{pig\_OLCI}}(\lambda)$  into  
 297 individual pigment spectra to generate phytoplankton pigment maps for GB. In processing pathway 2,  
 298 phytoplankton taxonomic composition at each sampling station was obtained from a 10-species IOP  
 299 inversion model, which take  $R_{rs\_in\text{-}situ}$  as input and estimates Chl a concentration of each phytoplankton  
 300 group (Fig. 2). Finally, CDOM-corrected FIRE measurements of  $F_v/F_m$  and  $\sigma_{\text{PSII}}$  were combined with  
 301 phytoplankton taxonomy to assess photosynthetic physiology of different phytoplankton groups.

302



303 **Figure 2.** Flowchart showing the three processing steps for: (1) retrieving pigments spatial distribution  
 304 maps from OLCI, (2) distinguishing phytoplankton groups, and (3) assessing phytoplankton physiological  
 305 parameters and their linkages to taxonomic groups.

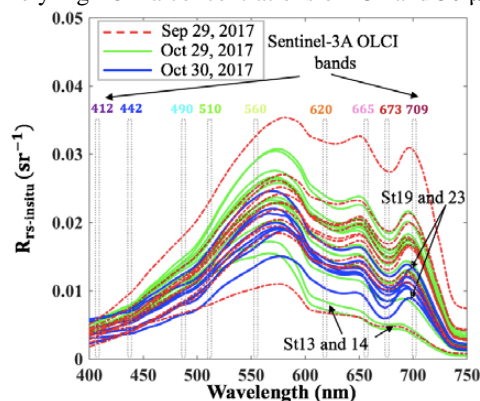


306 3. Results

307 3.1 Phytoplankton Taxonomy and Physiological State from Field Observations

308 3.1.1 Measurements of Above Water Remote Sensing Reflectance

309 Above-water remote sensing reflectances ( $R_{rs\_insitu}$ ) from the two surveys (Fig. 3) reflect the influence of  
 310 the absorbing and scattering features of water constituents. Low reflectance ( $\sim 675$  nm) caused by Chl a  
 311 red light absorption and maximum reflectance at green wavelength ( $\sim 550$  nm) were observed. Obvious  
 312 dips at  $\sim 625$  nm versus reflectance peaks  $\sim 650$  nm were observed in spectra during both surveys, which  
 313 could be attributed to cyanobacteria (*Trichodesmium*) modulation of the spectra (Hu et al., 2010). The  
 314 reflectance peak around 690–700 nm was obvious at most sampling sites except at stations 13 and 14  
 315 adjacent to the nGOM and were likely due to the suspended sediment scattering and effect of Chl a  
 316 fluorescence (Gitelson, 1992). The peak position at stations with lower Chl a concentration ( $\sim 5 \mu\text{g L}^{-1}$ )  
 317 were observed at 690–693 nm; however, the peaks shifted to longer wavelengths of 705 and 710 nm for  
 318 station 23 and 19 with extremely high Chl a concentrations of  $\sim 31$  and  $50 \mu\text{g L}^{-1}$ , respectively (Fig. 3).



319  
 320 **Figure 3.**  $R_{rs\_insitu}$  spectra at stations in GB on September 29, and October 29–30, 2017; vertical bars  
 321 represent Sentinel-3A OLCI spectral bands.

322 3.1.2 Performance of IOP Inversion Algorithm

323 The IOP inversion algorithm was applied to  $R_{rs\_insitu}$  data (Fig. 3) obtained during the two surveys in GB.  
 324 The mean errors for modeled  $a_{CDOM}$ ,  $a_{NAP}$ ,  $a_{phy}$  and  $b_{bp\_470}$  at all wavelengths for the 34 stations were  
 325 5.86%, 6.83%, 12.19% and 10.79%, respectively (Table 3). A total of 8 phytoplankton groups  
 326 (dinoflagellate, diatom, chlorophyte, cryptophyte, haptophyte, prochlorophyte, raphidophyte, and blue  
 327 cyanobacteria) were spectrally detected from the IOP inversion algorithm. The sum of 8 eigenvalues of  
 328  $Chl_i$  (Table 2) represents the modeled total Chl a (TChl  $a_{mod}$ ) of the whole phytoplankton community.  
 329 The TChl  $a_{mod}$  is better correlated with HPLC-measured total Chl a (TChl  $a_{HPLC}$ ) for survey 2 (green  
 330 circle; Fig. 4a) with  $R^2 \sim 0.92$ , compared to survey 1 (red color; Fig. 4a). In addition, the TChl  $a_{mod}$   
 331 appear to be slightly higher than TChl  $a_{HPLC}$  for survey 2. The modeled  $a_{CDOM}$  ( $a_{CDOM\_mod}$ ) are in close  
 332 agreement with spectrophotometrically measured  $a_{CDOM}$  at 412 nm (Fig. 4b), with  $a_{CDOM}$  obtained on  
 333 September 29, 2017 much higher than that on October 29–30, 2017. The modeled  $b_{bp}$  ( $b_{bp\_mod}$ ) are well  
 334 correlated with in-situ  $b_{bp}$  ( $b_{bp\_insitu}$ ) at 470 nm (Fig. 4c) with higher  $R^2$  (0.81) observed on September 29,  
 335 2017. In addition, both modeled and field-measured  $b_{bp}$  showed stronger backscattering at most stations  
 336 on September 29, 2017 than those on October 29–30, 2017.  
 337

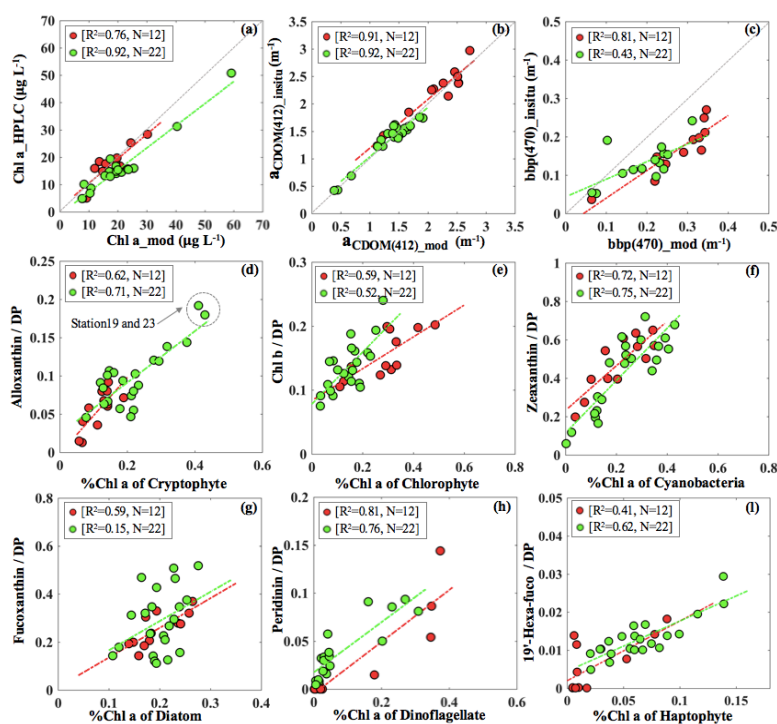


338 **Table 3.** Error statistics over all wavelengths and sampling stations ( $N=301 \times 34=10234$ ; 12 and 22  
 339 stations on Sep 29 and Oct 29-30, 2017) from semi-analytical IOP inversion algorithm.  
 340

Parameter	Min. error (%)	Max. error (%)	Mean error (%)	R <sup>2</sup> (Sep)	R <sup>2</sup> (Oct)
$R_{rs} \lambda \in [400,700]$	0.005	40.12	18.71	0.90	0.89
$a_{CDOM}(\lambda), \lambda \in [400,700]$	0.042	11.20	5.86	0.92	0.94
$a_{NAP}(\lambda), \lambda \in [400,700]$	0.001	11.46	6.73	0.90	0.91
$a_{PHY}(\lambda), \lambda \in [400,700]$	0.001	36.42	12.19	0.84	0.85
$b_{bp}(\lambda), \lambda = 470 \text{ nm}$	0.057	40.22	10.79	0.81	0.43

341

342 The Chl a percentage (%Chl a), which is  $Chl_i/TChl a$ , were also compared with diagnostic pigment  
 343 percentage (%DP), which is specific DP for each phytoplankton group over the sum of DP ( $\sum DP$ ). The  
 344 DP for diatom (fucoxanthin), dinoflagellate (peridinin), cryptophytes (alloxanthin), chlorophyte (Chl b),  
 345 haptophyte (19'-hexanoxyfucoxanthin), and cyanobacteria (zeaxanthin) referred in (Moisan et al.,  
 346 2017) were used in this study. The R<sup>2</sup> between %Chl a and %DP for different phytoplankton groups range  
 347 from 0.15 to 0.81 (Fig. 4). The %Chl a of cryptophyte is between 5%-42% and well correlated with  
 348 alloxanthin/ $\sum DP$  ( $R^2 \sim 0.62$ - $0.72$ ; Fig. 4d) for both surveys. In addition, the cryptophyte %Chl a at station  
 349 19 and 23 on October 30, 2017 was highest ( $\sim 40\%$ ) in coincidence with the highest value of alloxanthin/  
 350  $\sum DP$  (Fig. 4d). Furthermore, relationship between chlorophyte %Chl a and  $Chl b/\sum DP$  ( $R^2 \sim 0.55$ ; Fig. 4e)  
 351 showed that chlorophyte during survey 1 contributed higher fraction to the whole phytoplankton  
 352 community compared to survey 2. The %Chl a of cyanobacteria highly correlated with zeaxanthin/ $\sum DP$   
 353 with R<sup>2</sup> larger than 0.7 (Fig. 4f) for both surveys. Low %Chl a of dinoflagellate in coincidence with low  
 354 peridinin/ $\sum DP$  ( $R^2 \sim 0.78$ ) were observed at stations along the transect, however, increased contribution  
 355 of dinoflagellate appeared adjacent to the entrance during both surveys (Fig. 4g).



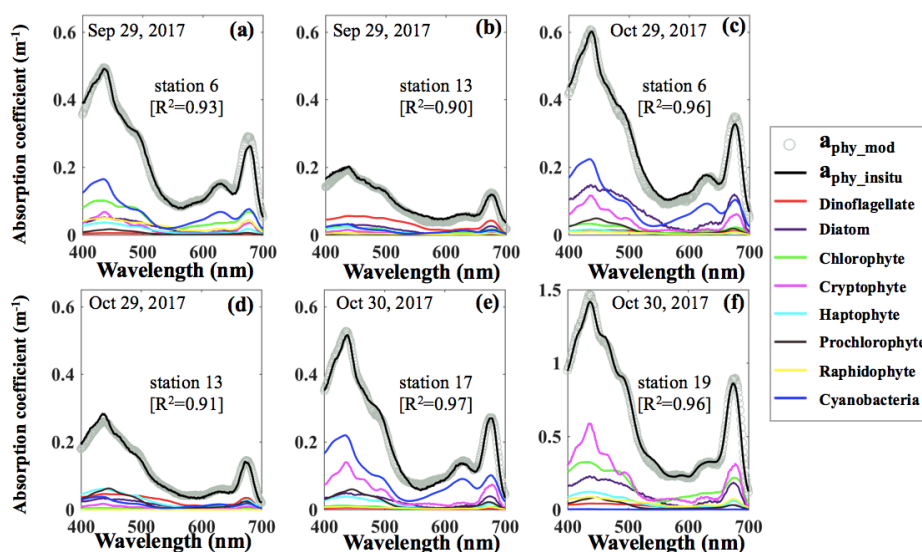
356



357 **Figure 4.** (a) Validation of TChl  $a_{mod}$  via HPLC-measured TChl  $a$ ; individual %Chl  $a$  of each detected  
 358 taxa versus corresponding %DP shown with (d) cryptophyte, (e) chlorophyte, (f) cyanobacteria, (g)  
 359 diatom, (h) dinoflagellate, and (i) haptophyte; red and green dots indicate the samples on September 29  
 360 and October 29-30, 2017, respectively. Comparison between in-situ measurements and modeled results  
 361 with (b)  $a_{CDOM}(412)$  and (c)  $b_{bp}(470)$ .

### 362 3.1.3 Variations in Phytoplankton Community Structure

363 Reconstruction of the phytoplankton absorption coefficients spectra revealed variations in phytoplankton  
 364 community structure (Fig. 5) even several weeks after Hurricane Harvey. The modeled  $a_{phy}$  spectra  
 365 ( $a_{phy\_mod}$ ) at stations 6, 13, 17 and 19 (Fig. 5a-f) yielded spatiotemporal differences of phytoplankton  
 366 taxonomic composition in GB. The strong absorption peak around 625 nm induced by cyanobacteria was  
 367 observed at most of the stations for both modeled results and in-situ measurements (Fig. 5a, 5c and 5e)  
 368 except at stations adjacent to the entrance (Fig. 5b and d). The  $a_{phy\_mod}$  at station 6 was primarily  
 369 dominated by group of cyanobacteria (blue line) and chlorophyte (green line) on September 29, 2017 (Fig.  
 370 5a); in contrast, the spectrum of chlorophyte contributed very little at station 6 on October 29, 2017  
 371 (green line; Fig. 5c). Furthermore, the shape of spectra for samples obtained at station 13 showed strong  
 372 dinoflagellate-modulation versus extremely low cyanobacteria contribution during survey 1 (red line; Fig.  
 373 5b). However, small-size group like haptophyte and prochlorophyte displayed increasing proportions at  
 374 station 13 on October 29, 2017 (Fig. 5d). Station 17 in the East Bay was dominated by cyanobacteria  
 375 (blue line; Fig. 5e) and cryptophyte (pink line; Fig. 5e) absorption spectra, whereas, on October 30, 2017,  
 376 the main spectral features at station 19 in the upper GB was from cryptophyte (pink line) and chlorophyte  
 377 (green line; Fig. 5f).

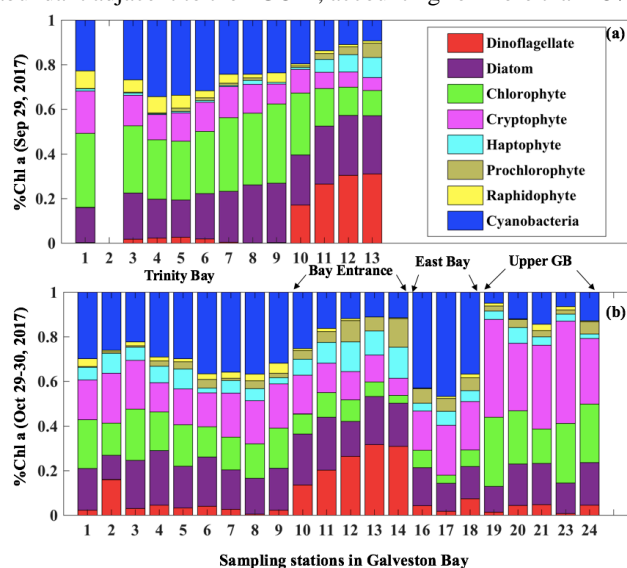


378 **Figure 5.** Reconstruction of phytoplankton absorption coefficients spectra at station 6 (a) and 13 (b) on  
 379 September 29, 2017, at station 6 (c) and 13 (d) on October 29, 2017 and at 17(e), and 19 (f) on October  
 380 30, 2017 based on the mass specific absorption spectra of different phytoplankton groups including  
 381 diatom, chlorophyte, dinoflagellate, cryptophyte, cyanobacteria (blue), haptophyte, prochlorophyte and  
 382 raphidophyte presented using different colors.  
 383

384  
 385 The corresponding taxa-specific %Chl  $a$  derived from IOPs inversion algorithm for the two surveys on  
 386 September 29 and October 29-30, 2017 are shown in Figure 6a and 6b, respectively. Cyanobacteria (blue



387 bars) and chlorophyte (green bars) constituted over 55% of the phytoplankton communities during survey  
 388 1 (September 29, 2017; Fig. 6a). In addition, chlorophyte, known to proliferate in freshwater  
 389 environments, showed higher fraction than that observed in survey 2 (green color; Fig. 6). Also,  
 390 chlorophyte together with diatoms (purple color; Fig. 6a) accounted for ~ 60% of TChl a<sub>mod</sub> at stations  
 391 (e.g., station 7, 8 and 9) with a well-mixed water column (inferred from salinity profiles; not shown) on  
 392 September 29, 2017. Cryptophyte, haptophyte and raphidophyte became a minor component of the  
 393 community and accounted in total to ~25% of TChl a<sub>mod</sub> (Fig. 6a). Furthermore, dinoflagellate group had  
 394 low contributions to TChl a<sub>mod</sub> inside the bay, but showed increasing %Chl a (~30%) in higher salinity  
 395 waters adjacent to the nGOM (red color; Fig. 6a). Cyanobacteria (blue color; Fig. 7) exhibited a slightly  
 396 elevated percentage during survey 2 (~60 days after hurricane passage, October 29-30, 2017) and were  
 397 quite abundant at station 16, 17 and 18 in East Bay where the water was calm and stratified as observed  
 398 from salinity profiles. In addition, cyanobacteria were not prevailing adjacent to the nGOM (Station 12,  
 399 13 and 14) and close to San Jacinto (station 19, 20, 21, 23 and 24), where cryptophyte (pink color) and  
 400 chlorophyte (green color) showed dominance (Fig. 6b). The %Chl a of chlorophyte obtained at stations  
 401 along the Trinity River transect decreased by ~10% on October 29-30, 2017 compared to that on  
 402 September 29, 2017. Small size groups like haptophyte and prochlorophyte increased on October 29-30,  
 403 2017 and were more abundant adjacent to the nGOM, accounting for more than 25% of the TChl a<sub>mod</sub>.



404  
 405 **Figure 6.** Phytoplankton taxonomic compositions detected from IOP inversion algorithm on September  
 406 29 and October 29-30, 2017 in Galveston Bay; phytoplankton groups are represented in different colors as  
 407 shown in the legend.

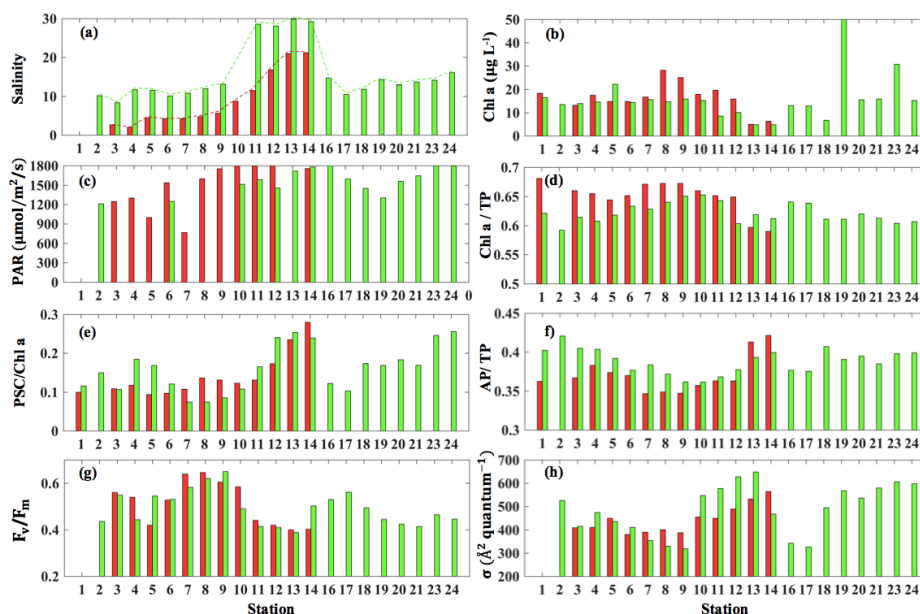
### 408 3.1.4 Environmental Conditions and Physiological State of Phytoplankton Community

409 The surface salinity presented a pronounced seaward increasing gradient along the transect (station 3-14)  
 410 during both the surveys (Fig. 7a) with primarily lower salinity throughout the bay during survey 1 in  
 411 comparison to survey 2, which indicated the freshening impact was still ongoing even 4 weeks after  
 412 Hurricane Harvey. The salinity was ~15 at station 16 and decreasing when going further into East Bay  
 413 (~10 at station 17 and 18; Fig. 7a). In upper GB, salinity at station 19-24 did not vary significantly (~15),  
 414 increasing along with the distance away from the San Jacinto River mouth with highest value (~17.5) at  
 415 station 24. During both surveys, lowest Chl a (Fig. 7b) were observed adjacent to the nGOM, and the  
 416 highest Chl a were closest to the river mouth. The Photosynthetically Active Radiation (PAR) which were



417 calculated from down-welling irradiance (not shown) decreased significantly with depth, but surface PAR  
 418 (Fig. 7c) were similar in magnitude at all stations. Pigment ratios including TChl a/TP (0.58-0.68),  
 419 PSC/Chl a (0.07-0.26) and AP/TP (0.34-0.42) were obtained from HPLC measurements and shown in  
 420 Figure 7d, 7e and 7f, respectively.

421 The CDOM calibrated and 0-0.5m depth averaged photosynthetic parameters  $F_V/F_M$  varied from 0.41 to  
 422 0.64 (Fig. 7g), while  $\sigma_{PSII}$  was in the range of 329-668  $\text{\AA}^2 \text{quantum}^{-1}$  (Fig. 7h). The highest  $\sigma_{PSII}$  and  
 423 lowest  $F_V/F_M$  appeared adjacent to the nGOM (station 12-14). Conversely, values of  $F_V/F_M$  at stations 7-  
 424 9 with a well-mixed water column were high with low values of  $\sigma_{PSII}$ . Both  $F_V/F_M$  and  $\sigma_{PSII}$  did not  
 425 directly correlate with Chl a, (e.g., high Chl a  $\sim 51 \mu\text{g L}^{-1}$  at station 19 corresponded to a relatively low  
 426 level of  $F_V/F_M \sim 0.45$ , versus high  $\sigma_{PSII} \sim 550 \text{\AA}^2 \text{quantum}^{-1}$ ). However, the stations with high  $F_V/F_M$   
 427 coincided with the high fraction of Chl a (Chl a/TP) and low fraction of AP (AP/TP) (Fig. 7d and 7f). In  
 428 contrast,  $\sigma_{PSII}$  showed an overall positive relationship with AP/TP, but altered negatively with Chl a/TP  
 429 during both surveys. The lowest (highest) value of  $\sigma_{PSII}$  ( $F_V/F_M$ ) were observed at station 9  
 430 corresponding to the highest Chl a/TP value ( $\sim 0.64$ ) on October 29, 2017. The highest AP/TP and  
 431 PSC/Chl a were obtained from stations adjacent to the nGOM.



432

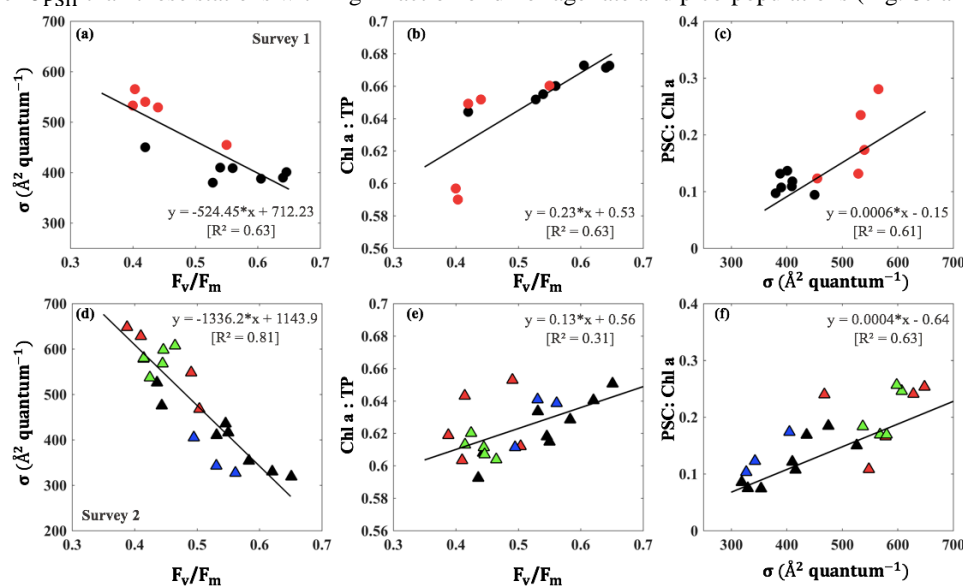
433 **Figure 7.** Environmental conditions (salinity, light field), pigment composition and physiological state in  
 434 GB surface waters (red bars indicating samples from September 29, 2017 and blue bars representing  
 435 samples from October 29 and 30, 2017). (a) Salinity, (b) Chl-a concentration, (c) PAR, (d) Chl a/TP, (e)  
 436 PSC/Chl a, (f) AP/TP, (g)  $F_V/F_M$ , and (h)  $\sigma_{PSII}$ .

### 437 3.1.5 $F_V/F_M$ and $\sigma_{PSII}$ Taxonomic Signatures

438 Distinct pigments housed within phytoplankton light-harvesting antennae can strongly influence PSII  
 439 light-harvesting capability and the photosynthetic quantum efficiency of phytoplankton (Lutz et al., 2001).  
 440 In this study, we observed an inverse relationship ( $R^2 \sim 0.63-0.81$ ; Fig. 8a and d) between the  $F_V/F_M$  and  
 441  $\sigma_{PSII}$ , that appeared related to taxonomic signals during surveys 1 and 2 in GB. Stations 1-9 along the



442 transect were considered as well-mixed group with no dominance by any particular group (black circles;  
 443 Fig. 8a-c); stations 10-14 close to the entrance were however, strongly dominated by dinoflagellate and  
 444 haptophyte (red symbol; Fig. 8a-c) during survey 1. This well-mixed group displayed low values of  $\sigma_{PSII}$   
 445 ( $\sim 390\text{--}439 \text{ \AA}^2 \text{ quantum}^{-1}$ ), and high levels of  $F_V/F_M$  ( $\sim 0.42\text{--}0.65$ ) with  $F_V/F_M$  approaching 0.65 at  
 446 station 9 on September 29, 2017 (Fig. 8a). However, enhanced contributions of dinoflagellate and  
 447 haptophyte around the entrance corresponded to a decline of  $F_V/F_M$  ( $0.3\text{--}0.4$ ) against an increase of  $\sigma_{PSII}$   
 448 ( $500\text{--}600 \text{ \AA}^2 \text{ quantum}^{-1}$ ) during survey 1. Furthermore, samples obtained from survey 2 at station 1-9,  
 449 station 10-14, station 16-18 and station 19-24 were considered as well-mixed (black), dinoflagellate-  
 450 haptophyte dominated (red), cyanobacteria dominated (blue) and cryptophyte-chlorophyte dominated  
 451 (green), respectively. Stations 16-17 dominated by cyanobacteria (blue triangles; Fig. 8d) showed high  
 452 level of  $F_V/F_M$  ( $0.5\text{--}0.6$ ) and relatively low values of  $\sigma_{PSII}$  ( $300\text{--}400 \text{ \AA}^2 \text{ quantum}^{-1}$ ). The  $F_V/F_M$  and  
 453  $\sigma_{PSII}$  of cryptophyte-chlorophyte dominated stations showed a moderate level of  $F_V/F_M$  ( $0.4\text{--}0.5$ ) and  
 454  $\sigma_{PSII}$  ( $580\text{--}680 \text{ \AA}^2 \text{ quantum}^{-1}$ ). More importantly, tight positive relationships existed between  
 455 measurements of  $F_V/F_M$  and Chl a/TP ( $R^2\sim 0.31\text{--}0.63$ ; Fig. 8b and e). On the other hand,  $\sigma_{PSII}$  were  
 456 positively correlated with PSC/Chl a with  $R^2\sim 0.6$  (Fig. 8c and f). The PSC/Chl a of cyanobacteria  
 457 dominated group (blue symbols), and well mixed group (brown symbols) were relatively low. Highest  
 458 PSC/Chl a and lowest Chl a/TP was observed for the dinoflagellate-haptophyte dominated group,  
 459 corresponding to the lowest  $\sigma_{PSII}$  and highest  $F_V/F_M$ . In addition, cryptophyte-chlorophyte dominated  
 460 group had high levels of PSC/TChl a ( $\sim 0.18\text{--}0.26$ ) and slightly higher Chl a/TP compared to  
 461 dinoflagellate-haptophyte dominated group. Overall, well-mixed groups with high proportion of large-  
 462 size phytoplankton (e.g., diatoms and chlorophyte) showed higher Chl a/TP along with larger  $F_V/F_M$  and  
 463 smaller  $\sigma_{PSII}$  than those stations with high fraction of dinoflagellate and pico-populations (Fig. 8c and f).



464  
 465 **Figure 8.** a, d)  $\sigma_{PSII}$  against  $F_V/F_M$ ; b, e)  $F_V/F_M$  versus Chl a/TP; and c, f)  $\sigma_{PSII}$  versus PSC/Chl a on  
 466 September 29 and October 29-30, 2017 respectively. The data points identified by dominant taxa with  
 467 black, red, green and blue symbols denoting well-mixed, dinoflagellate-haptophyte dominated,  
 468 cryptophyte-chlorophyte dominated, and cyanobacteria dominated groups, respectively.

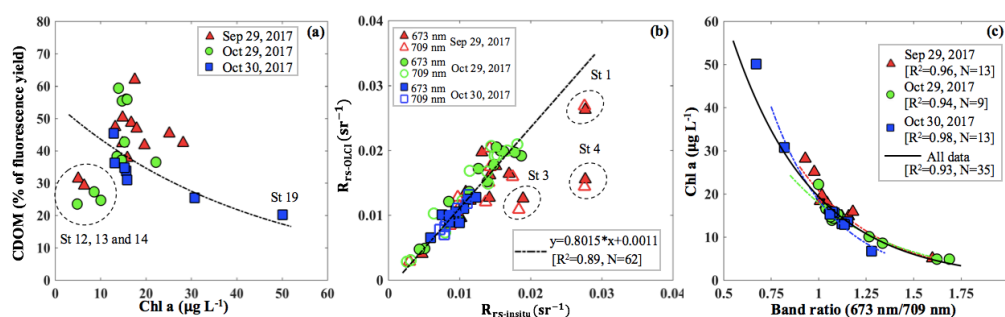
## 469 3.2 Satellite Observations of Phytoplankton Pigments

### 470 3.2.1 An OLCI Chl a Algorithm and its Validation



471 Blue to green band ratio algorithms have been widely used to study Chl a in the open ocean and shelf  
 472 waters (D'Sa et al., 2006; Blondeau-Patissier et al., 2014); however, these bands generally fail in  
 473 estuarine waters due to strong blue absorption by the high levels of CDOM and suspended particulate  
 474 matter, especially after flooding events associated with hurricanes (D'Sa et al., 2011; D'Sa et al., 2018;  
 475 Joshi and D'Sa, 2018). The percentage contribution by CDOM fluorescence (blank) to maximum  
 476 fluorescence yield ( $F_m$ ) obtained from in-situ FIRE (Fig. 9a) demonstrated that Chl a fluorescence was  
 477 strongly influenced by high amounts of CDOM fluorescence in GB, especially during the first survey  
 478 (September 29, 2017), when the bay was under strong floodwater influence (red triangles; Fig. 9a). The  
 479 CDOM fluorescence signal constituted ~ 25 % in the region adjacent to the nGOM (stations 12-14),  
 480 between 25%-50% in the upper GB, and up to ~65% in Trinity Bay, which implied that blue and even  
 481 green band are highly contaminated by CDOM and might not be the most suitable bands for estimating  
 482 Chl a in GB. However, an increase in peak height near 700 nm and its shift towards longer wavelength  
 483 (Fig. 3) can be used as a proxy to estimate Chl a concentration.

484



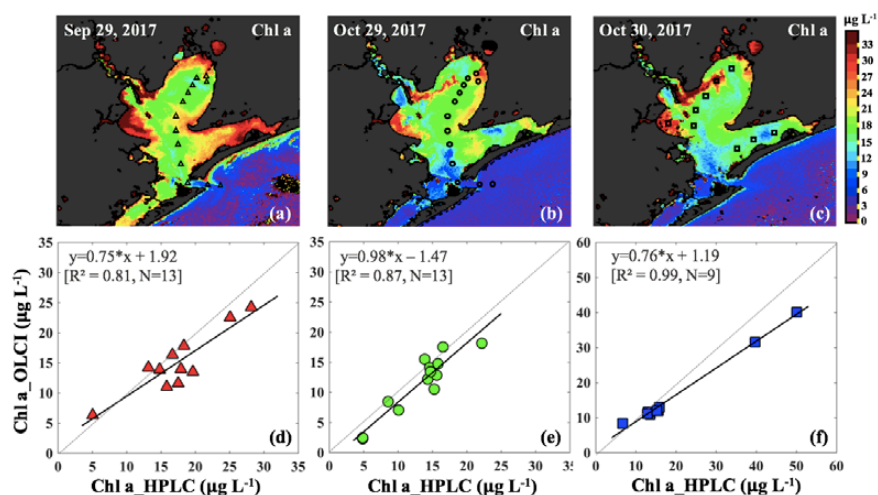
485 **Figure 9.** (a) Relationship between the percentage of the fluorescence yield of CDOM measured by FIRE  
 486 against HPLC measured Chl a concentration. (b) Comparisons between  $R_{rs\_in situ}$  and  $R_{rs\_OLCI}$  at band 9  
 487 (673 nm) and band 11 (709 nm). (c) Exponential relationships between HPLC-measured Chl a  
 488 concentrations and  $R_{rs\_in situ}$  band ratio (673 nm/709 nm) in GB on September 29 ( $R^2=0.89$ ), October 29  
 489 ( $R^2=0.93$ ) and October 30 ( $R^2=0.97$ ). Red, green and blue lines and symbols indicate data sets obtained on  
 490 September 29, October 29 and 30, 2017, respectively.

491 The C2RCC atmospheric-corrected  $R_{rs\_OLCI}$  at each of the sampling sites were further averaged (3×3  
 492 pixels) and compared with  $R_{rs\_in situ}$  (Fig. 3) at phytoplankton red absorption (~673 nm) and Chl a  
 493 fluorescence (~700 nm) bands (Fig. 9b). The C2RCC performed overall better for the second survey on  
 494 October 29-30, 2017 (green and blue symbols; Fig. 9b) than the first survey on September 29, 2017 (red  
 495 triangles; Fig. 9b) when stations 1, 3 and 4 (circled triangles; Fig. 9c) adjacent to the Trinity River mouth  
 496 were included; these stations were the last sampling sites in the afternoon (~4:30 pm) and under  
 497 somewhat cloudy conditions. The time difference between satellite pass and in-situ measurements, sky  
 498 conditions and shallow water depth also likely introduced more errors at these locations. The  $R^2$  between  
 499  $R_{rs\_OLCI}$  and  $R_{rs\_in situ}$  at red and near infrared (NIR) bands was 0.89 when the data from station 3 and 4 were  
 500 excluded, suggesting good usability of these two bands for Chl a empirical algorithms in GB. Thus, the  
 501 higher the Chl a concentration, the stronger the red light absorption, resulting in higher reflectance at 709  
 502 nm; consequently, negative correlations were observed between Red/NIR band ratio and Chl a. The ratio  
 503 of Red (~673 nm) and NIR (709 nm) reflectance bands from in-situ measurements were overall highly  
 504 correlated with HPLC-measured Chl a with  $R^2 \sim 0.96, 0.94$  and  $0.98$  on September 29, October 29 and  
 505 October 30, 2017, respectively (Fig. 9c). The Sentinel-3A OLCI Chl a maps (Fig. 10a-c) were generated  
 506 for all data based on the relationship between Chl a and the Red and NIR band ratio as:

507

$$\text{Chl a } (\mu\text{g L}^{-1}) = 216.38 \times \exp(-2.399 \times \frac{R_{rs}(673)}{R_{rs}(709)}) \quad [\text{All data}] \quad \dots (16)$$





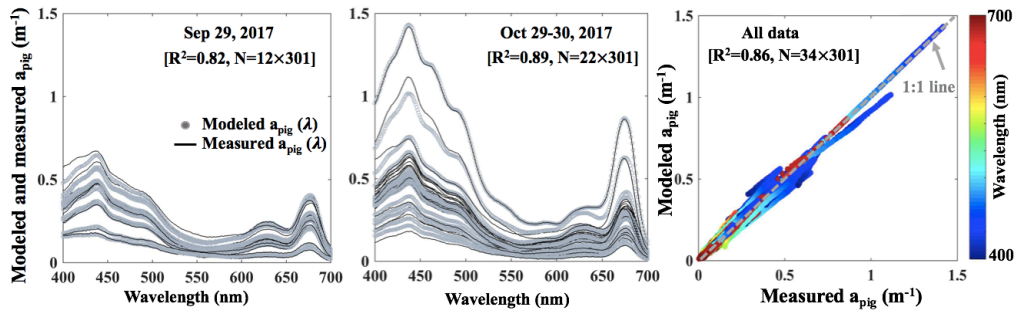
508

509 **Figure 10.** Chl a concentration generated based on in-situ band ratio ( $R_{rs673}/R_{rs709}$ ) algorithm with (a),  
 510 (b) and (c) representing Chl a distribution on September 29, October 29 and October 30, 2017,  
 511 respectively; (c), (d) and (f) show the validation between HPLC-measured Chl a and OLCI-derived Chl a  
 512 on September 29, October 29 and October 30, 2017, respectively.

513 The OLCI-derived Chl a (Fig. 10a-c) showed a good spatial agreement with Chl a<sub>HPLC</sub> (Fig. 10d-f). The  
 514 Chl a concentration on September 29, 2017 was overall higher than that on October 29-30, 2017 through  
 515 the entire bay. East Bay displayed very high Chl a concentration, with highest value ( $>30 \mu\text{g L}^{-1}$ )  
 516 observed on September 29, 2017 (Fig. 10a). The narrow shape and shallow topography of East Bay  
 517 results in relatively higher water residence time (Rayson et al. 2016); thus, the reduced exchange with  
 518 shelf waters likely lends the East Bay vulnerable to eutrophication. The average Chl a concentration on  
 519 October 29-30, 2017 were  $\sim 15 \mu\text{g L}^{-1}$  along the transect (station 1-11) and  $\sim 4\text{-}6 \mu\text{g/L}$  (station 12-14)  
 520 close the entrance of GB. In addition, Chl a adjacent to San Jacinto River mouth ( $>16 \mu\text{g L}^{-1}$ ) was higher  
 521 than that in Trinity Bay, which might suggest that San Jacinto inflow had higher nutrient concentrations  
 522 than Trinity as also previously reported (Quigg et al., 2010). Furthermore, the OLCI-Chl a maps on  
 523 October 29 and 30, 2017 showed extremely high Chl a in a narrow area adjacent to the San Jacinto River  
 524 mouth, with Chl a approaching  $\sim 40 \mu\text{g L}^{-1}$  at station 19 (Fig. 10c).

### 525 3.2.2 Reconstruction of Total Pigment Absorption Spectra from OLCI-derived Chl a

526 The reconstructed  $a_{\text{pig}}(\lambda)$  based on the third order function of Chl a<sub>HPLC</sub> (gray lines; Fig. 11a and b)  
 527 agreed well with the spectrophotometrically measured  $a_{\text{pig}}(\lambda)$  (black lines; Fig. 11a and b) during both  
 528 surveys ( $R^2=0.86$ ; Fig. 11c). The  $R^2$  for modeled versus measured  $a_{\text{pig}}(\lambda)$  are between 0.76 and 1.00 from  
 529 400 to 700 nm with averaged  $R^2$  of whole spectra reaching  $\sim 0.82$  on September 29, 2017 and  $\sim 0.89$  on  
 530 October 29-30, 2017, respectively. The vector coefficients  $C = [C_3, C_2, C_1, C_0]$  obtained from Eq. (11)  
 531 were further applied to Eq. (12) to generate  $a_{\text{pig\_OLCI}}(\lambda)$  based on OLCI-derived Chl a images (Fig. 10a-c),  
 532 which contained  $259 \times 224$  pixels in each image. The  $a_{\text{pig\_OLCI}}(\lambda)$  at each pixel was retrieved at 1 nm  
 533 interval, and thus 301 images of  $a_{\text{pig\_OLCI}}(\lambda)$  representing each wavelength were obtained over GB.

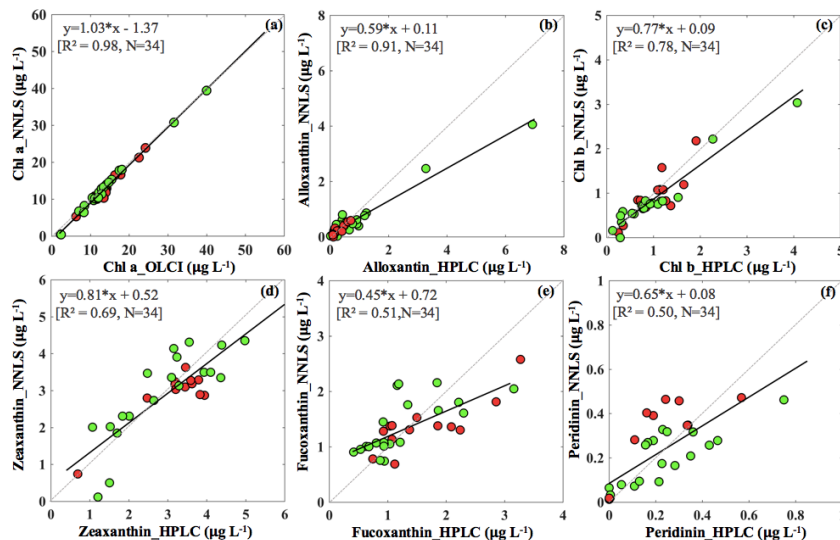


534

535 **Figure 11.** Spectrophotometrically measured and multi-regression fitted  $a_{pig}(\lambda)$  spectra acquired on (a)  
 536 September 29 and (b) October 29-30, 2017 in GB. Gray and black lines represent modeled and measured  
 537 results, respectively. (c) Comparison between modeled and spectrophotometrically measured  $a_{pig}(\lambda)$  for  
 538 all data with color representing wavelength.

### 539 3.2.3 Accuracy of phytoplankton pigment retrievals from Sentinel 3A-OLCI

540 The reconstructed  $a_{pig\_OLCI}(\lambda)$  was spectrally decomposed into 16 individual pigment spectra at each pixel  
 541 based on Eq. (14). A comparison of HPLC-measured pigments to averaged NNLS inversion model  
 542 retrieved pigments showed  $R^2$  ranging from a low of 0.39 for violaxanthin to 0.98 for Chl a (Table 4). The  
 543 NNLS-modeled Chl a also correlated well with OLCI-derived Chl a ( $R^2=0.98$ ; Fig. 12a), with each  
 544 exhibiting similar quantitative and spatial patterns. For the other 15 simultaneously simulated pigments,  
 545 only 7 pigments averaged  $R^2$  value greater than 0.65 (Table 4). Five NNLS-derived versus HPLC  
 546 measured diagnostic pigments including alloxanthin, Chl b, zeaxanthin, fucoxanthin and peridinin are  
 547 shown in Figure 12. The  $R^2$  between NNLS-derived and HPLC-measured pigments for surveys 1 and 2  
 548 was highest for alloxanthin (0.91; Fig. 12b). For the other pigments  $R^2$  was 0.78 for Chl b (Fig. 12c),  
 549 0.69 for zeaxanthin (Fig. 12d), 0.51 for fucoxanthin (Fig. 12e) and 0.50 for peridinin (Fig. 12f),  
 550 respectively.



551



552 **Figure 12.** Sentinel-3A OLCI derived pigment concentration against HPLC measured pigment  
 553 concentration in Galveston Bay; **a)** Chl a, **b)** alloxanthin, **c)** Chl-b, **d)** zeaxanthin, **e)** fucoxanthin, and **f)**  
 554 peridinin.

555 **Table 4.** Correlation between HPLC-measured pigment concentration with NNLS-modeled pigments.  
 556

Pigments	Sep 29, 2017	Oct 29, 2017	Oct 30, 2017	Averaged R <sup>2</sup>
Chl a	0.95	0.97	0.98	0.97
Chl b	0.76	0.77	0.95	0.82
Chl c <sub>1</sub>	0.56	0.42	0.79	0.59
Chl c <sub>2</sub>	0.49	0.45	0.74	0.56
Pheophythin a	0.76	0.79	0.72	0.75
Pheophythin b	0.75	0.88	0.76	0.79
Peridinin	0.65	0.48	0.51	0.54
Fucoxanthin	0.65	0.45	0.85	0.60
Neoxanthin	0.55	0.63	0.79	0.65
Lutein	0.61	0.78	0.72	0.70
Violaxanthin	0.43	0.34	0.39	0.39
Alloxanthin	0.81	0.40	0.91	0.72
Diadinoxanthin	0.69	0.40	0.89	0.66
Diatoxanthin	0.49	0.43	0.49	0.47
Zeaxanthin	0.76	0.65	0.78	0.73
β-carotenoid	0.41	0.42	0.82	0.55

### 557 3.3.1 Spatial Distributions of Diagnostic Pigments

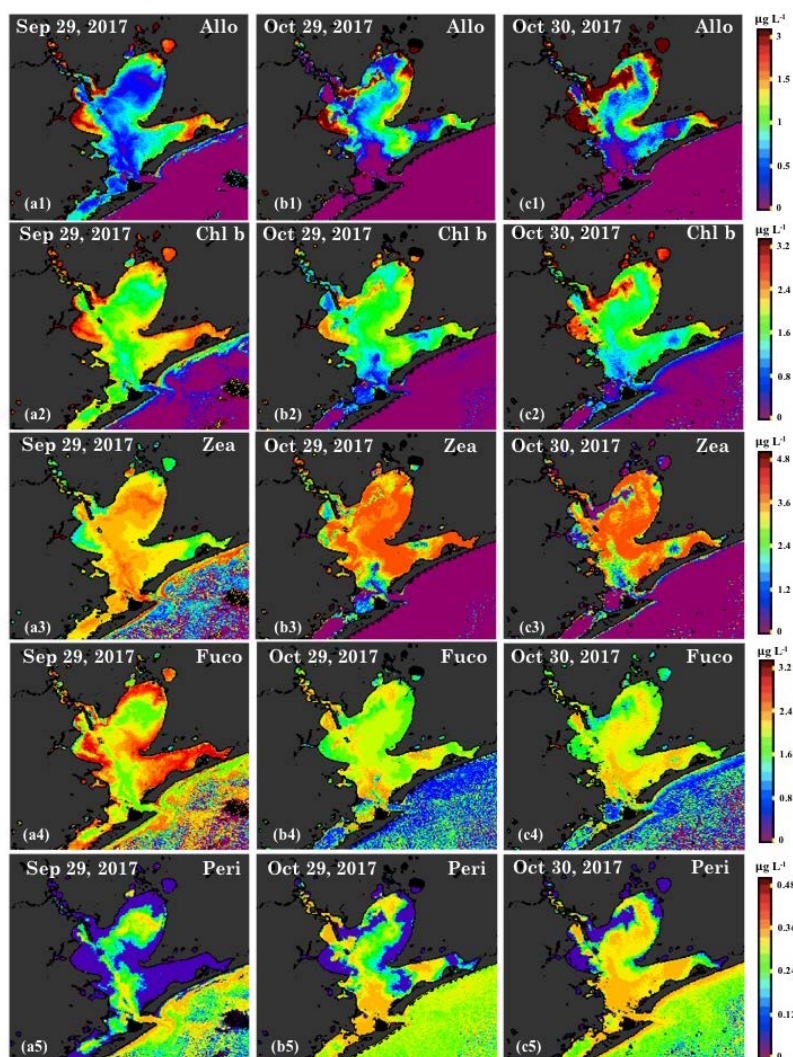
558 Alloxanthin which is unique to cryptophytes (Wright and Jeffrey, 2006) exhibited spatial distributions  
 559 patterns (Fig. 13a<sub>1</sub>-c<sub>1</sub>) that correlated reasonably well with Chl a distribution (Fig. 10a-c) during both  
 560 surveys. Alloxanthin was especially low (~ 0.7 μg L<sup>-1</sup>, Fig. 13a<sub>1</sub>) in the major basin area on September 29,  
 561 2017. However, alloxanthin showed very high concentrations (~ 3.5 μg L<sup>-1</sup>, Fig. 13a<sub>1</sub>-c<sub>1</sub>) adjacent to San  
 562 Jacinto River mouth, which coincided with the high %Chl a of cryptophyte at stations 19 and 23 (Fig. 6b).  
 563 The bloom with high concentration of alloxanthin on October 29, 2017 (~3.5 μg L<sup>-1</sup>; Fig. 13b<sub>1</sub>) then  
 564 extended to a broader area on October 30, 2017 (Fig. 13c<sub>1</sub>).  
 565

566 Chl b is abundant in the group of chlorophyte (green algae) (Hirata et al., 2011) and the spatial  
 567 distributions of Chl b (Fig. 13a<sub>2</sub>-c<sub>2</sub>) as well showed strong correlations with Chl a (Fig. 10a-c) for both  
 568 surveys. The NNLS-derived Chl b exhibited overall elevated concentrations throughout bay and were  
 569 higher in northern part of the bay than the area adjacent to the nGOM. Chl b concentrations observed on  
 570 September 29, 2017 were higher than that on October 29-30, 2017, which corresponded to a decline of  
 571 chlorophyte percentage derived from the IOP inversion algorithm for survey 2 (Fig. 6). Furthermore, Chl  
 572 b concentrations approached ~2.8 μg L<sup>-1</sup> in the bloom area and the corresponding green discoloration of  
 573 water was also observed during the field survey on October 30, 2017.  
 574

575 Zeaxanthin was considered as taxa-specific pigment for prokaryotes (cyanobacteria) (Moisan et al., 2017)  
 576 and NNLS-derived zeaxanthin maps revealed higher concentrations during survey 2 compared to survey 1.  
 577 Zeaxanthin distributions (Fig. 12a<sub>3</sub>-c<sub>3</sub>) displayed significantly different patterns than Chl a and exhibited  
 578 relatively lower concentration in the mid-bay (around Smith Point) on September 29, 2017. Zeaxanthin  
 579 also displayed especially low concentrations in the bloom area during survey 2; furthermore, low %Chl a  
 580 of cyanobacteria was also observed at stations 19-24 (Fig. 6), thus indicating that this localized algal  
 581 bloom event was not associated with cyanobacteria.  
 582



583 Fucoxanthin is a major carotenoid found in diatoms (Hirata et al., 2011; Moisan et al. 2017) and the  
584 NNLS-derived fucoxanthin maps (Fig. 12a<sub>4</sub>-c<sub>4</sub>) showed highly similar distribution patterns with Chl a  
585 maps on September 29, 2017, but distributions differed on October 29-30, 2017. More interestingly, maps  
586 of fucoxanthin showed low concentrations around Smith Point on October 29-30, which also  
587 corresponded to the relatively low %Chl a of diatom derived from IOP inversion algorithm at station 7, 8  
588 and 9. In addition, relatively low concentration of fucoxanthin was observed in the bloom area for survey  
589 2. Overall, fucoxanthin concentration in GB was relatively higher for survey 1, which corresponded to the  
590 higher %Chl a of diatom (Fig. 6) compared to survey 2.  
591



592  
593 **Figure 13.** Sentinel-3 OLCI derived maps of diagnostic pigments for Galveston Bay. Simulated **a1-c1)**  
594 alloxanthin, **a2-c2)** Chl b, **a3-c3)** zeaxanthin, **a4-c4)** fucoxanthin, and **a5-c5)** peridinin concentrations. a,  
595 b and c represent columns (maps for 29 September, 29 and 30 October 2017) and 1-5 represent rows  
596 (pigments), respectively.  
597



598 Peridinin is a primary bio-marker pigment for certain dinoflagellates (Örnólfsson et al., 2003). Peridinin  
599 concentrations were lowest in GB compared to other diagnostic pigments ( $0.001\text{--}0.05\ \mu\text{g L}^{-1}$ ), implying  
600 that dinoflagellate was not the dominant species during both surveys. Maps of peridinin (Fig. 12a<sub>5</sub>–c<sub>5</sub>)  
601 presented higher concentration ( $\sim 0.3\ \mu\text{g L}^{-1}$ ) in higher salinity waters adjacent to the bay entrance, which  
602 agreed well with the increasing fraction of dinoflagellate at station 10–14 detected from IOP inversion  
603 model (Fig. 6). Furthermore, the areas with high concentrations of peridinin generally corresponded to  
604 lower Chl a concentrations during both surveys, this was especially obvious in the center of Trinity Bay  
605 and the entrance of GB on September 29, 2017, and bloom area on October 29–30, 2017. In addition, both  
606 fucoxanthin and peridinin pigments showed high concentrations along the Houston Ship Channel during  
607 survey 2.  
608

## 609 4 Discussion

### 610 4.1 Performance of the Semi-Analytical IOP Inversion Algorithm

611 The residuals between  $R_{rs\_insitu}$  and  $R_{rs\_mod}$  on September 29 and October 29–30, 2017, are negative in the  
612 blue (400–450 nm) and red (610–630 nm) spectral range at most stations, whilst keeping positive  $\sim 700\text{ nm}$ ,  
613 which could be attributed to a number of factors. First, the underestimation near  $700\text{ nm}$  by the IOP  
614 inversion model is possibly induced by the absence of a fluorescence component in the IOP inversion  
615 model; thus,  $R_{rs\_insitu}$  containing fluorescence signals were generally higher than  $R_{rs\_mod}$  near  $700\text{ nm}$ .  
616 Second, in the range of 610–630 nm, the absorption was overestimated at most of the stations; in this  
617 spectral range, the shape of spectra was strongly modulated by cyanobacteria absorption. Thus this  
618 overestimation  $\sim 620\text{ nm}$  is likely introduced by the input absorption spectrum (eigenvector) for  
619 cyanobacteria since all of input  $a_{phi}^*(\lambda)$  are general absorption spectral shapes for different phytoplankton  
620 groups. However, the spectra of  $a_{phi}^*(\lambda)$  can vary in magnitude and shape associated with package effects  
621 under different environmental conditions (e.g. nutrient, light and temperature) even for the same species  
622 (Bricaud et al., 2004). More detailed absorption spectra of phytoplankton under different conditions (e.g.  
623 high/low light and nutrient) could improve the performance of the IOP algorithm. Furthermore, the role of  
624 scattering might be another key factor to explain differences between  $R_{rs\_insitu}$  and  $R_{rs\_mod}$  for the whole  
625 spectra. The quantity and composition of suspended materials including phytoplankton, sediment and  
626 minerals will collaboratively determine  $b_{bp}(\lambda)$  in both shape and magnitude. However, the input  
627 eigenvector of  $b_{bp}(\lambda)$  in the present study was not divided into detailed sub-constituents and was a sum  
628 spectrum based on a power law function (Table 2). In reality,  $b_{bp}(\lambda)$  spectra are not smooth and regular,  
629 and thus, the  $b_{bp}(\lambda)$  value of phytoplankton and sediment might introduce errors to the whole spectrum  
630 due to their own scattering characteristics.

### 631 4.2 Distributions of NNLS-Retrieved Phytoplankton Pigments from Sentinel-3A OLCI

632 The derived maps of phytoplankton diagnostic pigments appeared to be reasonably correlated with  
633 HPLC-measured diagnostic pigments and showed overall agreement with extracted phytoplankton  
634 taxonomic compositions detected from the IOP inversion algorithm. The retrieved diatom-specific  
635 fucoxanthin maps however, showed high concentrations compared to other pigments adjacent to the  
636 entrance (Fig. 13b<sub>4</sub> and c<sub>4</sub>), which contradicted with diatom %Chl a calculated from IOP inversion  
637 algorithm that Chl a fraction of diatom was relatively uniform at stations 12–14 (Fig. 6b). (Nair et al.,  
638 2008) concluded that fucoxanthin can occur in other phytoplankton types (e.g. raphidophyte and  
639 haptophyte). Fucoxanthin and/or fucoxanthin derivatives such as 19'-hexanoyloxyfucoxanthin can also  
640 replace peridinin as the major carotenoid in some dinoflagellates (e.g., *Karenia brevis*; Jeffrey and Vest,  
641 1997). The elevated contributions from groups of dinoflagellate, haptophyte and prochlorophyte adjacent  
642 to the entrance (stations 10–14; Fig. 6b) along with high concentrations of fucoxanthin likely suggest the



643 presence of elevated fractions of haptophyte and dinoflagellate, and further implies that fucoxanthin is an  
644 ambiguous marker pigment for diatoms. This could also explain the poor correlation between  
645 inverted %Chl a and %DP observed for the groups of diatom and haptophyte (Fig. 4g and l). These results  
646 also further suggest the inherent limitations of using DP-type comparison between major biomarker  
647 pigments and phytoplankton groups because the major assumption for DP-type methods is that diagnostic  
648 pigment of distinct phytoplankton groups are uncorrelated to each other. This assumption is invalid in that  
649 concentrations of major biomarker pigments are significantly correlated with each other and also may  
650 vary in time and space under some external environmental stress (e.g., temperature, salinity, mixing, light  
651 and nutrient) (Latasa and Bidigare, 1998).

652 Chl a concentration is another crucial factor that influences the accuracy of retrieved pigments. The goal  
653 of the empirical Chl a algorithm for Sentinel 3A-OLCI is to obtain more accurate estimation of surface  
654 Chl a concentration, which is better for retrieving other accessory pigments. However, the primary  
655 limitation of Chl a empirical algorithms in this study was that the derived relationships between Red/NIR  
656 and Chl a in GB may only be valid within a specific time period due to temporally-limited field  
657 observations versus highly dynamic estuarine environments. Therefore, a Chl a empirical algorithm that is  
658 more broadly applicable over a longer time period will largely improve the accuracy of retrieved  
659 pigments over a series of remote sensing images and can be more useful for spatiotemporal studies of  
660 phytoplankton functional diversity. In addition, the similarity of many carotenoid absorption spectra  
661 could as well introduce errors when applying spectral decomposition techniques. Thus, the 16 input  
662 pigment spectra used in this study were selected from (Thrane et al., 2015), which were correctly  
663 identified from unknown phytoplankton community structure with low error rate reported from Monte  
664 Carlo tests to minimize the potential effects of aliasing the spectra.

#### 665 **4.3 Response of Phytoplankton Taxonomic Composition to Environmental Conditions**

666 Previous studies showed phytoplankton community in GB to be primarily dominated by  
667 diatoms/dinoflagellates during winter/spring, corresponding to the period of high fresh water discharge  
668 and nutrient concentrations (Dorado et al., 2015), while, cyanobacteria were the dominant species during  
669 the warmer months (Jun-Aug) (Roelke et al., 2013). However, perturbations following Hurricane Harvey  
670 affected the phytoplankton taxonomic composition with alterations in phytoplankton community structure  
671 were observed as GB system transitioned from marine to freshwater then to marine system. The decline  
672 of Chl a during survey 2 likely resulted from the depletion of nutrients associated with floodwaters.  
673 Higher fractions of diatom, cyanobacteria, and chlorophyte observed during survey 1 to some extent  
674 agreed well with measurements of Steichen et al., 2018 two weeks following Hurricane Harvey wherein,  
675 the phytoplankton community which was dominated by estuarine and marine diatoms and dinoflagellates  
676 pre-Hurricane Harvey, then transitioned to primarily freshwater species (cyanobacteria and green algae)  
677 immediately following the flooding event. The results of high cyanobacteria %Chl a accompanied by high  
678 concentration of zeaxanthin further confirmed that cyanobacteria biomass could probably be enhanced by  
679 high discharge of phosphorus-rich floodwaters (Schindler, 1977). In addition, the relatively higher  
680 fraction of diatom observed during survey 1 in comparison to survey 2 was likely associated with the  
681 rapid nutrient uptake rate of diatoms under high nutrient loading conditions after the freshwater inflows  
682 (Örnólfsson et al., 2004). The decline of diatoms and chlorophyte versus slightly increased  
683 cyanobacteria observed during survey 2 could be due to the more rapid depletion of nutrients after the  
684 flooding event. Some cyanobacteria species are nitrogen (N<sub>2</sub>) fixers, which could succeed in low nitrogen  
685 (N) waters (Howarth et al., 1988), and thus likely outcompeted diatoms and chlorophytes under more  
686 seasonal conditions during survey 2. Further, the presence of green algae and cyanobacteria could as well  
687 as be explained by the clarity and turbidity gradient of water. Quigg et al. (2010) reported that when  
688 turbidity was relatively high, chlorophyte dominated over cyanobacteria with biomass ratio of  
689 chlorophyte/cyanobacteria larger than 2, which supported our observations that chlorophyte dropped off



690 whilst cyanobacteria increased during survey 2. Highest cyanobacteria percentage in East Bay also  
691 suggest that calm and stratified waters may accelerate cyanobacteria growth as the buoyancy regulation  
692 mechanism of cyanobacteria is possibly restricted by water mixing. Dinoflagellates increased during  
693 survey 2 and showed overall preference for high-salinity waters. Previous Imaging FlowCytobot (IFCB)  
694 observations from Biological and Chemical Oceanography Data Management Office (BCO-DMO)  
695 showed that algal blooms after hurricanes in the nGOM were initially dominated by diatoms, and  
696 subsequently transitioned to blooms of dinoflagellates, likely associated with nutrient ratios and chemical  
697 forms of nutrient supplied by the flood waters and rainfall. Generally, silica (Si) is essential for the  
698 growth and reproduction of diatoms, whereas dinoflagellates show preference of higher phosphorus (P)  
699 compared to some other groups (Heisler et al., 2008). In this study, distribution of fucoxanthin and  
700 diatom %Chl a decreased from survey 1 to 2; in contrast, peridinin and dinoflagellate %Chl a showed  
701 overall increased elevation during survey 2. Nutrient supply ratio with low N:P or Si:P could be a  
702 contributor for shifting diatom-dominated community to dinoflagellates (Smayda et al., 1997). In addition,  
703 high concentrations of fucoxanthin and peridinin observed along the Houston Ship Channel, which was  
704 also shown in Steichen et al. (2018), might provide evidence that the ballast water addition from shipping  
705 vessels likely promote harmful species of dinoflagellates and diatoms (Steichen et al., 2015).

706 The localized cryptophyte-chlorophyte bloom that occurred ~60d after Hurricane Harvey, was captured  
707 by both satellite and in-situ measurements. This bloom might not be associated with the flooding events  
708 of Hurricane Harvey, and could be linked to nutrient-rich runoff flowing into GB, reflecting sensitivity  
709 and rapid response of phytoplankton community to nutrient input in GB. In shallow and turbid estuaries,  
710 human activities are altering the environment and causing phytoplankton changes in diversity and  
711 biomass to occur more frequently. Dugdale et al. (2012) reported that variations of phytoplankton  
712 community in San Francisco estuary could be attributed to anthropogenically-elevated concentration of  
713 ammonium, which restrain the uptake of nitrate, thus reducing the growth and reproduction of larger  
714 diatoms and shifting towards smaller species (e.g., cryptophyte and green flagellate). Furthermore, 'pink  
715 oyster' events related to alloxanthin of cryptophyte in GB occurred more frequently in recent years (Paerl  
716 et al., 2003). The eastern side of Houston Ship Channel in mid bay region was reported as the area most  
717 heavily impacted by the intense 'pink oyster' events. Previous studies and present observations both  
718 suggest that this cryptophyte-chlorophyte dominated bloom could be promoted by the nutrient-driven  
719 eutrophication from Houston Ship Channel, urbanization and industrialization along the upper San Jacinto  
720 River complex.

#### 721 **4.4 Photo-Physiological State of Natural Phytoplankton Community**

722 In this study, the CDOM-corrected  $F_v/F_M$  and  $\sigma_{PSII}$  likely represented a composite of both phytoplankton  
723 taxonomy and physiological stress (e.g., nutrient and mixing). Typically, lowest N and P concentrations  
724 were measured closest to the nGOM (Quigg et al., 2009). Phytoplankton community living close to  
725 nGOM were usually in poor nutrient conditions and would be expected to maximize their light harvesting  
726 (increase in  $\sigma_{PSII}$ ) due to nutrient stress. Simultaneously, phytoplankton cells might experience a decline  
727 of functional proportion of reaction centers of PSII (RCII), which means decrease in  $F_v/F_M$ . The observed  
728 low levels of  $F_v/F_M$  and Chl a/TP versus high values of  $\sigma_{PSII}$  and AP/TP adjacent to the nGOM showed  
729 agreement with previous studies that the fraction of carotenoids to be higher for nutrient-poor cultures  
730 (Schittler et al., 1997; Holmboe et al., 1999). In contrast, phytoplankton in well-mixed waters (station 7-9)  
731 might experience abundant nutrients due to the resuspension associated with the cyclonic gyre around  
732 Smith Points; as such, their photosynthetic machinery were likely healthier. Aiken et al. (2004)  
733 documented that the Chl a/TP ratio was relatively higher when plants were in good growing conditions,  
734 which is similar to the observations in this study that phytoplankton have higher fraction of Chl a  
735 accompanying higher rate of photosynthetic efficiency ( $F_v/F_M$ ) under nutrient replete conditions. Overall,  
736 the spatial pattern of  $F_v/F_M$  and  $\sigma_{PSII}$  in GB could be mainly attributed to physiological stress of nutrient



737 and hydrodynamics conditions since the light availability (PAR) during the sampling period did not vary  
738 much spatially at the surface. Furthermore, F<sub>IRE</sub> measurements ( $F_v/F_m$  and  $\sigma_{PSII}$ ) also presented a  
739 taxonomic signal super-imposed upon environmental factors. Each cluster with different dominant taxa  
740 (well mixed group, chlorophyte & cryptophyte, cyanobacteria, and dinoflagellate & haptophyte)  
741 displayed different physiological characteristics. The taxonomic sequence of eukaryotic groups from high  
742  $F_v/F_m$ , low  $\sigma_{PSII}$  to low  $F_v/F_m$ , high  $\sigma_{PSII}$  in the present observations showed potential effects of  
743 phytoplankton cell size corresponding to diatoms, chlorophyte, and cryptophyte, dinoflagellate and  
744 haptophyte. The prokaryote (cyanobacteria) had relatively high values of  $F_v/F_m$  and low values of  $\sigma_{PSII}$ ;  
745 this agreed with  $F_v/F_m$  for some species of nitrogen-fixing cyanobacteria that can range from 0.6 to 0.65  
746 (Berman-Frank et al., 2007). Yet, it is difficult to separate the contributions from environmental factors  
747 and taxonomic variations to the changes of F<sub>IRE</sub> fluorescence signals since all these parameters are inter-  
748 related. Different phytoplankton groups/sizes will display distinct physiological traits ( $F_v/F_m$  and  $\sigma_{PSII}$ )  
749 when experiencing considerable environmental pressures. Thus, effects of physiological stress on  
750  $F_v/F_m$  and  $\sigma_{PSII}$  variations for natural samples can only be determined when taxonomic composition can  
751 be excluded as a contributor (Suggett et al., 2009).

## 752 5 Conclusions

753 Field measurements (salinity, pigments, optical properties and physiological parameters) and ocean color  
754 observations from Sentinel-3A OLCI were used to study the effects of extreme flooding associated with  
755 Hurricane Harvey on the phytoplankton community structures, pigment distributions and their  
756 physiological state in GB. Flooding effects made the entire GB transition from saline to freshwater then  
757 back to a more marine influenced system. The band ratio (Red/NIR) of  $R_{rs\_in situ}$  were negatively correlated  
758 with HPLC-measured Chl a in an exponential relationship ( $R^2 > 0.93$ ). The satellite-retrieved Chl a maps  
759 yielded much higher Chl a concentration on September 29, 2017 compared to October 29-30, 2017 with  
760 lowest Chl a observed adjacent to the shelf waters. Phytoplankton taxonomic composition was further  
761 retrieved from  $R_{rs\_in situ}$  using a 10-species IOP inversion algorithm. Phytoplankton community generally  
762 dominated by estuarine marine diatoms/dinoflagellates before flood events, was altered to freshwater  
763 species of green algae (chlorophyte) and cyanobacteria during survey 1. It also showed an increase of  
764 small-size species including cryptophyte, haptophyte, prochlorophyte and cyanobacteria accompanied by  
765 a decline of chlorophyte and diatoms during survey 2.

766 Phytoplankton diagnostic pigments which were retrieved using an NNLS inversion model based on  
767 Sentinel-3A OLCI Chl a maps also confirmed spatiotemporal variations of phytoplankton taxonomy. The  
768 NNLS-retrieved diagnostic pigment maps showed overall spatiotemporal agreement with HPLC  
769 measurements with  $R^2$  ranging from 0.39 (violaxanthin) to 0.98 (Chl a). Chl b showed overall higher  
770 concentrations during survey 1 compared to survey 2, and its distribution displayed highly similar  
771 patterns with Chl a. Alloxanthin showed especially low concentration in the main basin area but very high  
772 concentration in a localized bloom area adjacent to the San Jacinto River mouth. Zeaxanthin presented  
773 significantly different patterns with other pigments during both the surveys. Concentration of peridinin  
774 was overall low inside of GB, and generally displayed high concentrations in areas where Chl a was low.

775 Finally, the retrieved phytoplankton taxonomic compositions from the IOP inversion algorithm were  
776 linked with F<sub>IRE</sub>-measured photosynthetic parameters ( $F_v/F_m$  and  $\sigma_{PSII}$ ) to assess the effects of  
777 physiological stress and taxonomic contributions on phytoplankton photosynthetic performance. An  
778 inverse relationship between the  $F_v/F_m$  and  $\sigma_{PSII}$  were observed during both surveys. Phytoplankton  
779 community in well-mixed waters (around Smith Point) showed high  $F_v/F_m$  against low  $\sigma_{PSII}$ ; in contrast,  
780 the area with poor nutrient conditions (adjacent to the shelf waters), showed low  $F_v/F_m$  and elevated  
781  $\sigma_{PSII}$ . Taxonomic signatures of  $F_v/F_m$  and  $\sigma_{PSII}$  revealed diverse physiological characteristics with  
782 dinoflagellate-haptophyte group showing the lowest  $F_v/F_m$  versus the highest  $\sigma_{PSII}$ , whereas prokaryote





783 of cyanobacteria-dominated group showed high values of  $F_v/F_M$  and low values of  $\sigma_{PSII}$ . Overall, this  
784 study using field and ocean color data combined with inversion algorithms provided novel insights on  
785 phytoplankton response to an extreme flood perturbation in a turbid estuarine environment based on  
786 taxonomy, pigment composition and physiological state of phytoplankton.

787

788 *Data availability.* Data from field measurements are available upon request from the corresponding  
789 author.

790

791 *Author contributions.* BL and ED conceived and designed the research; BL, ED and IJ collected and  
792 processed the data; BL analyzed the data and all authors contributed to writing the paper.

793

794 *Competing interests.* The authors declare that they have no conflict of interest.

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