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Supplement of

Data compilation on the biological response to ocean acidification: an update

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1 Guidelines for reporting ocean acidification data in scientific journals

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3 These guidelines were prepared by J.-P. Gattuso (gattuso@obs-vlfr.fr), H. Garcia
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8 This document was prepared in the framework of the data management activity of the Ocean
9 Acidification International Coordination Centre of the International Atomic Energy Agency
10 (OAICC; www.iaea.org/ocean-acidification). Please contact the first author (gattuso@obs-
11 vlfr.fr) in case of any error or omission. It is primarily based on Dickson et al. (2007),
12 Dickson (2010), Nisumaa et al. (2010), Pesant et al. (2010), Pörtner et al. (2010) and Orr et al.
13 (2015).

14 To ensure reproducibility, it is critical to report at least two variables of the carbonate system
15 of seawater as well as salinity, temperature, and the hydrostatic pressure (if the measurements
16 were not performed at atmospheric pressure). In addition, authors should report
17 concentrations of total dissolved inorganic phosphorus as well as total dissolved inorganic
18 silicon (in $\mu\text{mol kg}^{-1}$) whenever possible. Furthermore,

- 19 - Authors should carefully report how the parameters were measured and, if
20 applicable, which protocol they followed.
- 21 - The use of Certified Reference Materials, source, and batch numbers must be
22 mentioned.
- 23 - At least two of the following carbonate system parameters should be measured and
24 reported (note the preferred acronyms and units):
- 25 - Dissolved inorganic carbon (C_T ; $\mu\text{mol kg}^{-1}$)
 - 26 - Total alkalinity (A_T ; $\mu\text{mol kg}^{-1}$)
 - 27 - pH (it is critical to mention its scale; see below)
 - 28 - Partial pressure of carbon dioxide ($p\text{CO}_2$; μatm)
 - 29 - Fugacity of carbon dioxide ($f\text{CO}_2$; μatm)
 - 30 - Carbonate ion concentration (CO_3^{2-} ; $\mu\text{mol kg}^{-1}$)

- 31 - The pH scale (NBS, free, total, or seawater) must be mentioned prominently in the
32 manuscript.
- 33 - If more than one pH scale is used in a given manuscript, the pH should always be
34 given with the associated scale as a subscript:
- 35 - on the National Bureau of Standards scale (pH_{NBS})
 - 36 - on the seawater scale (pH_{SWS})
 - 37 - on the free scale (pH_{F})
 - 38 - on the total scale (pH_{T})
- 39 - The temperature at the time of sampling and at the time of measurement should both
40 be mentioned, if they differ.
- 41 - Salinity is needed (note that it is unitless).
- 42 - The formulations used to calculate the following variables should be mentioned:
- 43 - Concentrations of total boron
 - 44 - CO_2 solubility (K_0)
 - 45 - Dissociation constants of carbonic acid (K_1 and K_2), boric acid (K_b), water
46 (K_w), phosphoric acid (K_{p1} , K_{p2} , K_{p3}), silicic acid (K_{Si}), hydrogen fluoride
47 (K_f), and bisulfate (K_s)
 - 48 - Solubility products of calcite (K_{spc}) and aragonite (K_{spa})
- 49 - The software package used to calculate the carbonate chemistry, along with its
50 version number, and any associated options must all be mentioned.
- 51 - Average reproducibility of the performed measurements (with number of
52 measurements) should be mentioned.
- 53 - Finally, it is strongly recommended that the chemistry and biological data are either
54 archived in an on-line database (preferred) or provided along with the paper as
55 supplementary information.

56

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