

Marine

Microbial Biodiversity, Bioinformatics & Biotechnology



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Deliverable 3.2

Plan for supporting data management for Tara-Oceans cruise

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Summary

The present deliverable is part of Task 3.3. It outlines the data generated by Tara Oceans, its data management system, and the work plan to ensure access to relevant Tara-Oceans data via Micro B3's Information System during the lifetime of the project. The work plan was coordinated and agreed with the executive group to Tara-Oceans and will be carried into the Tara Oceans community. The work plan addresses three aspects of data management: (1) Development of standard protocols and vocabularies; (2) Development of oceanographic services; and (3) Evaluation of oceanographic services.

The Tara Oceans expedition is a unique sampling programme encompassing optical and genomic methods to describe viruses, bacteria, archaea, protists and metazoans in their physico-chemical environment. The goal is to generate open access datasets to be used in probing the morphological and molecular makeup, diversity, evolution, ecology and global impacts of plankton on the Earth system. The sampling strategy, sample/data analysis and data management have been carefully tailored and integrated toward this overarching goal. A key component for integration is the Tara Oceans Sample Registry that will link samples (e.g. jars and tubes), data archived in a distributed network of databases, and metadata about sampling and analysis methodology. This component and the manual curation of all metadata from Tara-Oceans are under the responsibility of PANGAEA/UniHB who is also involved in Micro B3 WPs 2-6.

Micro B3 will support the data management of Tara Oceans through an active participation of UniHB in (1) WP4 activities towards the development of the Oceans Sampling Handbook; (2) WP5 activities to make rapid progress with Tara-Oceans' sample registry and to tailor its web-service to the requirements of MB3-IS; and (3) WP6 activities to provide environmental data management skills (Task 3.3) and propose methods to evaluate the oceanographic services and vocabularies. How the web-service of Tara-Oceans will feed into MicroB3-IS is to be defined in deliverable D3.3.

Context of the deliverable

There is a recent revival of global scale expeditions to explore biodiversity in the world oceans, using a combination of classical analysis methods and genomics. The following examples are particularly relevant to Micro B3 since they all targeted microorganisms: (1) the Sorcerer II expedition (2004-2006) focused on genomic of microbial life and more specifically prokaryotes (Gross, 2007); (2) the Malaspina expedition (2010-2011) focused on twilight zones of the oceans; and (3) the Tara Oceans expedition (2009-2012), focused on the photic layer of the world oceans (Karsenti *et al.*, 2011). The ability to access and integrate data generated by these expeditions is therefore an important proof of concept for the Information System of Micro B3. In order to complement the public data on planktonic prokaryotes from the Sorcerer II expedition, the DOW of Micro B3 includes resources to support the data management of the Tara Oceans expedition, which investigated both planktonic prokaryotes and eukaryotes. The present deliverable outlines the data generated by Tara Oceans, its data management system, and the plan to ensure access to relevant Tara Oceans data via Micro B3's Information System during the lifetime of the project.

Overview of Tara Oceans Data

The Tara Oceans project was launched in September 2009 for a 3-year study of the global ocean ecosystem aboard the ship Tara. A unique sampling programme encompassing optical and genomic methods to describe viruses, bacteria, archaea, protists and metazoans in their physico-chemical environment has been implemented. The goal is to generate open access datasets to be used in probing the morphological and molecular makeup, diversity, evolution, ecology and global impacts of plankton on the Earth system. The sampling strategy, sample/data analysis and data management have been carefully tailored and integrated toward this overarching goal.

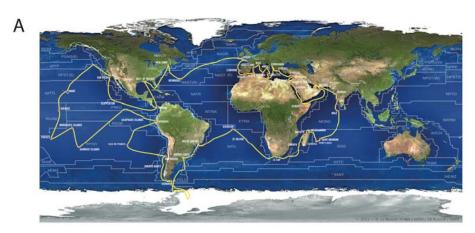


Figure 1. The *Tara-Oceans* expedition; Red dots are stop-overs; A total of 154 stations were sampled along the yellow path of Tara (map credits to Noan Le bescot & Fabrice Not/EPPO/SB Roscoff/CNRS).

The different groups of organisms targeted by Tara Oceans were separated based on their size, using various meshes on the sampling instruments or on filtration units onboard (Figure 2). Viruses, giruses and bacteria were collected with a large volume peristaltic pump or Niskin bottles, corresponding to sampling volumes in the order of a few hundreds of liters, and were subsequently size-fractionated on filtration ramps using membranes of appropriate mesh size. The relatively larger-in-size and less-abundant organisms such metazoans and protists required greater sampling volumes in the order of 10 to 100 hundreds of litres. They were therefore targeted using sampling nets of specified mesh size (i.e. 5, 20 and 180 μ m) and then further separated into more specific size-fractions using gravity filtration on sieves and membranes of appropriate mesh size. Details of the sampling procedures and sample treatments onboard will be published in a Methods paper (Not *et al.*, in prep).

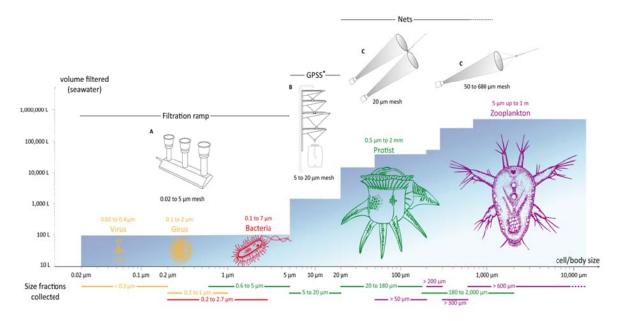


Figure 2. A partial summary of sampling instruments and targeted organisms (Karsenti et al. 2011)

Environmental conditions at each sampling location were determined onboard using sensors deployed on the meteorology station (i.e. continuous time series), rosette system (i.e. vertical profiles from 0-1000 m), large volume pumping system (i.e. time series at discrete sampling depths), underway system (i.e. continuous time series at 5 m), and occasionally on surface drifters and gliders (Table 1). Additionally, the oceanographic context at each station is characterized using remote sensing products such as ocean colour, SST and SSH to determine meso- to large-scale features and variability in key parameters such as surface temperature, salinity, chlorophyll a, currents and mixed layer depth.

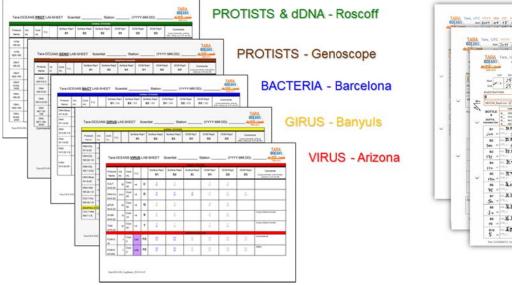
Table 1. Summary of parameters obtained by sensors on the different sampling systems

Parameter	Rosette	Pumping system	Underway	Stand alone
Parameter	system	Pullipling system	system	systems
Lat., Long. position and	✓(GPS)	✓(GPS)	√(GPS)	√(provbio,
time	V (GF 3)	* (GF3)	· (GF3)	glider, TSRB)
Pressure (depth)	✓(CTD)	✓(Ecotriplet)	✓(fixed @	√(Provbio,
Pressure (deptil)		(Ecotifiet)	5m)	glider)
Conductivity (salinity)	✓(CTD)	√(Ecotriplet)	✓(TSG)	✓(Provbio,

				glider)
Temperature (water)	✓(CTD)	✓(Ecotriplet)	✓(TSG)	√(Provbio, glider)
Fluorescence (Chl a)	✓(WET Labs)	✓(WET Labs)	✓(WET Labs)	√(Provbio, glider)
Nitrate	✓(ISUS)			
CDOM	✓(CSTAR)			
Transmissiometer	✓(CSTAR)			
Backscatter	✓(CSTAR)			
Zooplankton > 500μm image	✓(UVP5)			
Particle size spectrum	✓(UVP5)		✓(ACs)	
Absorption			✓(ACs)	
Attenuation			✓(ACs)	
Photosynthetic activity			✓(FRRF)	
Upwelling Radiance				√(TSRB)
Surface Irradiance				√(TSRB)

Tara Oceans Data Management

On average, Tara Oceans generated about 300 samples per station corresponding to over 12 sampling protocols and over 30 onboard treatment protocols, and being shipped to 8 laboratories in Europe and America. In order to identify and track all samples, a system of unique identifiers (i.e. barcodes), colour-coded stickers and logsheets was organised (see Appendix I). An electronic logbook version of the logsheets could not be successfully implemented as originally planned and thus, considerable efforts were required to manually extract metadata from the logsheets and match these to sample barcodes. Barcodes on logsheets were semi-automatically assigned to specific protocols and sampling depths based on their positions on the logsheets. In parallel, laboratories have manually assigned protocols to samples based on the information written by hand on the barcode stickers, i.e. station number, protocol code and sampling depth.





UniHB (PANGAEA) is currently cross-checking the central sample registry (i.e. based on logsheets) with registries of samples stored at the different laboratories, and filling the occasional, but still numerous gaps and mismatches in the metadata. The central sample registry depicted in red on figure 3 is the key to linking samples (e.g. jars and tubes), data archived in a distributed network of databases, and metadata about sampling and analysis methodology.

UniHB (PANGAEA) is currently setting up a web-service that will allow users to search for unique sample identifiers based on sampling date, time, location, depth, protocol name, size fraction etc., and to fetch the corresponding detailed metadata about all onboard protocols used to generate each sample. The sample unique identifiers will also be the reference to link and access additional metadata from the laboratories about the location and state of samples stored on land (e.g. jars and tubes) and about analyses performed on each sample. Finally, the sample unique identifiers will allow linking images, sequences and environmental data from a distributed network of databases (Figure 3).

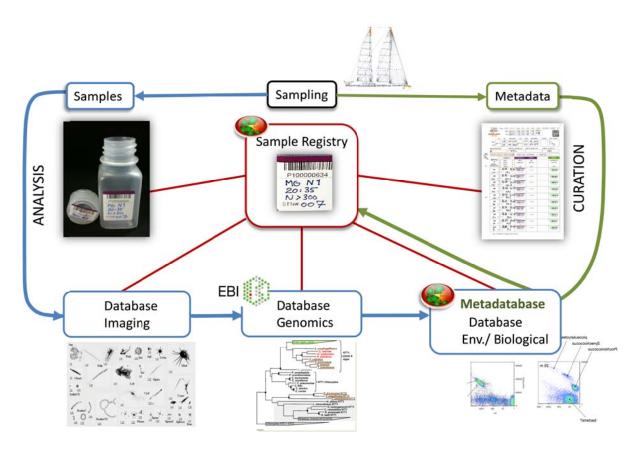


Figure 3. Summary of the data management workflow showing data analysis and safeguarding in blue, metadata curation in green and the central sample registry in red, which is the key to linking samples (e.g. jars and tubes), data archived in a distributed network of databases, and metadata about sampling and analysis methodology.

In addition to the central sample registry and distributed databases (permanent archives) described above in the data management workflow (Figure 3 & blue boxes in Figure 4), data generated by Tara Oceans are stored locally in the different labs and mirrored in a central FTP data repository (green boxes in Figure 4). The FTP repository is for temporary and internal use of validated and unvalidated data for the purpose of working up publications. Another important component of the Tara Oceans data management infrastructure is the Integration System (orange box in figure 4). The Integration System is equivalent in scope to the Micro B3 Information System, and it will be developed as part of the currently funded project OCEANOMICS, starting in 2013. The parallel development of the two Information Systems should be stimulating and lead to innovations on both sides. In both systems the integration of data generated by the Tara Oceans expedition will rely on the central sample registry described above in Figure 3.

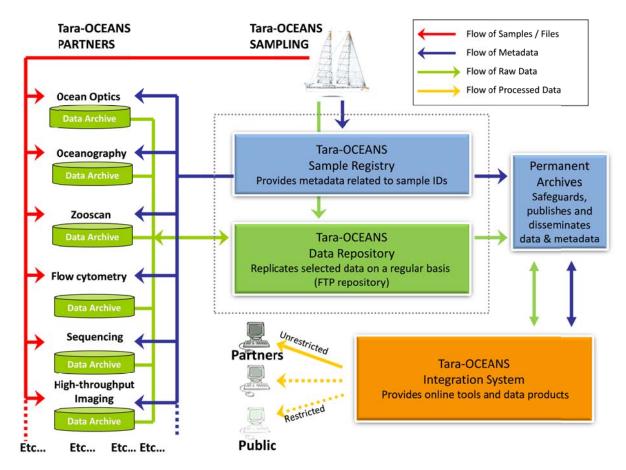


Figure 4. Summary of the data management infrastructure showing: in blue the central sample registry and Permanent archives (also shown in Figure 3); in green local databases and the FTP data repository; and in orange the Tara Oceans data Integration System.

Micro B3's plan to support Tara Oceans data management

A work plan was devised to ensure that a subset of Tara Oceans data can be used within the lifetime of Micro B3 as proof of concept for its Information System (MB3-IS). The spirit of the work plan is to set win-win collaborations between Micro B3 and Tara-Oceans projects. This is of course facilitated by the simple fact that several individuals/institutes are partners of both Tara Oceans and Micro B3 consortia. Notably, UniHB is responsible for data management in Tara-Oceans and contributes actively to activities of Micro B3's WPs 2-6. The work plan was coordinated and agreed with the executive group to Tara-Oceans and will be carried into the Tara Oceans community. The work plan addresses three aspects of data management:

- DEVELOPMENT OF STANDARD PROTOCOLS and VOCABULARIES;
- DEVELOPMENT OF OCEANOGRAPHIC SERVICES;
- EVALUATION OF OCEANOGRAPHIC SERVICES.

DEVELOPMENT OF STANDARD PROTOCOLS and VOCABULARIES

Tara-Oceans and Micro B3 have almost identical requirements for standard protocols and vocabularies, with the particularity that Tara-Oceans focuses on a finite number of sampling and analysis protocols and thus develops information components and vocabularies for a finite number of parameters. Nevertheless, these parameters cover the full spectrum of organisms addressed in Micro B3 and thus constitute an excellent case study for Micro B3. Tara-Oceans will therefore provide Micro B3 with a detailed set of protocols, information components and vocabularies to be reviewed by WP4. While Micro B3 will build upon this knowledge, Tara-Oceans will follow the recommendations of WP4 in order to improve their metadata and bring them in the context of a broader community. Examples of information components developed so far by Tara-Oceans to describe sampling Events and Samples are listed in Appendix II.

Collaboration has already started with the participation of UniHB to two Micro B3 WP4 workshops (April & July 2012) and one Tara-Oceans workshop (May 2012) aimed at defining which metadata and parameters are required to describe the environmental context for genomics data. UniHB is co-author on a publication (Not et al., in prep) that describes in details the standard sampling protocols of Tara-Oceans, which will be submitted before the end of 2012. UniHB will also have completed its sample registry before the end of 2012. The work plan to support this aspect of data management is to maintain an active participation of UniHB in WP4 activities towards the development of the Oceans Sampling Handbook (D4.3), due for month 18 (June 2013).

DEVELOPMENT OF OCEANOGRAPHIC SERVICES

As with vocabularies, Tara-Oceans and Micro B3 have almost identical requirements for oceanographic services, with the particularity that environmental data and the registry of

samples collected during the Tara-Oceans expedition are archived and managed centrally at PANGAEA. The oceanographic services developed for Tara-Oceans are therefore provided by a single World Data Centre. In contrast, oceanographic services for Micro B3 will involve the SeaDataNet infrastructure and several European and international data centres, including ICES, PANGAEA, VLIZ and National Oceanographic Data Centres. These services will be described in Deliverable D3.3 which is planned for end 2012. It is therefore not decided yet how oceanographic services from PANGAEA will be connected to other oceanographic services in Micro B3, but in the case of data from the Tara-Oceans expedition, the PANGAEA sample registry will be the key web-service to access extensive metadata and to link related datasets. The work plan to support this aspect of data management is for UniHB to continue his work as part of WP5 to make rapid progress with the sample registry and to tailor its web-service to the requirements of MB3-IS.

EVALUATION OF OCEANOGRAPHIC SERVICES

One proof of concept for MB3-IS is for WP6 partners to integrate and analyse a subset of Tara-Oceans environmental and genomic data. As mentioned before, several beneficiaries of WP6 are partners of Tara-Oceans. The extent of Tara-Oceans data to be used by WP6 needs to be determined within the intellectual property and confidentiality agreements of the two consortia. For now, the intention is to integrate environmental and diversity data based on 16S and 18S sequences from prokaryotes and eukaryotes, respectively, together with diagnostic sequences from viruses and giruses. WP6 partners will therefore evaluate the oceanographic services, information components and vocabularies used to discover data and will thus report on their clarity and usefulness. The work plan for this aspect of data management is for UniHB to provide environmental data management skills to WP6 (Task 3.3) and propose methods to evaluate the oceanographic services, information components and vocabularies. UniHB will attend the next WP6 meeting in December 2012.

Reference list

Gross L (2007) Untapped Bounty: Sampling the Seas to Survey Microbial Biodiversity. PLoS Biol 5(3): e85. doi:10.1371/journal.pbio.0050085

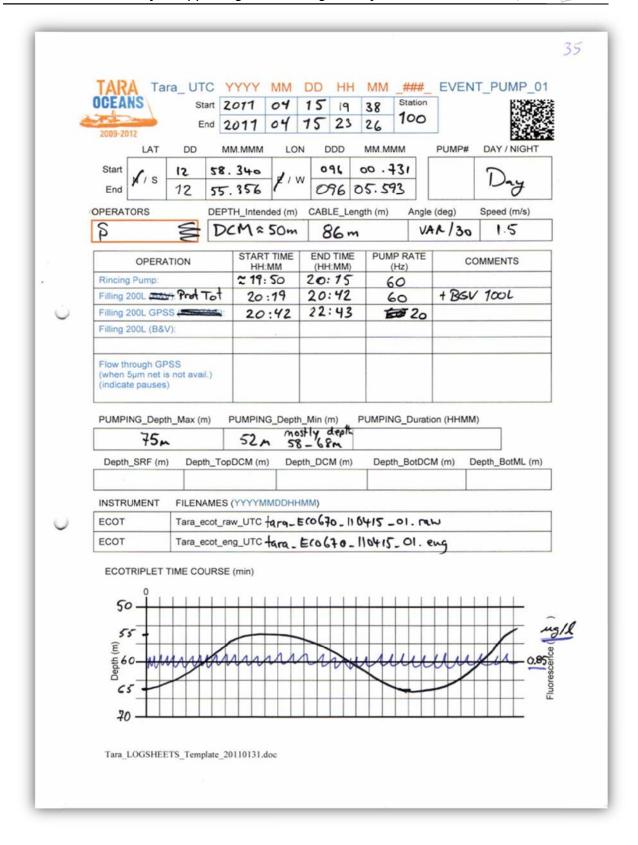
Karsenti E, Acinas SG, Bork P, Bowler C, De Vargas C, et al. (2011) A Holistic Approach to Marine Ecosystems Biology. PLoS Biol 9(10): e1001177. doi:10.1371/journal.pbio.1001177

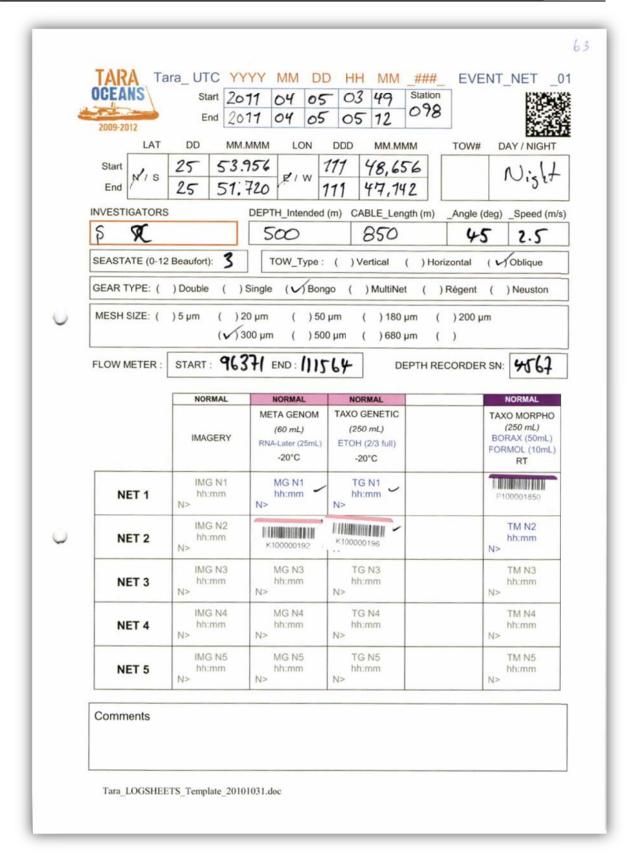
Not F, Le Bescot N, Pesant S, Kandels-Lewis S, Picheral M, et al. (in prep) Tara Oceans expedition: Plankton Sampling Strategy & Methods. PLoS Biol or Nature Methods

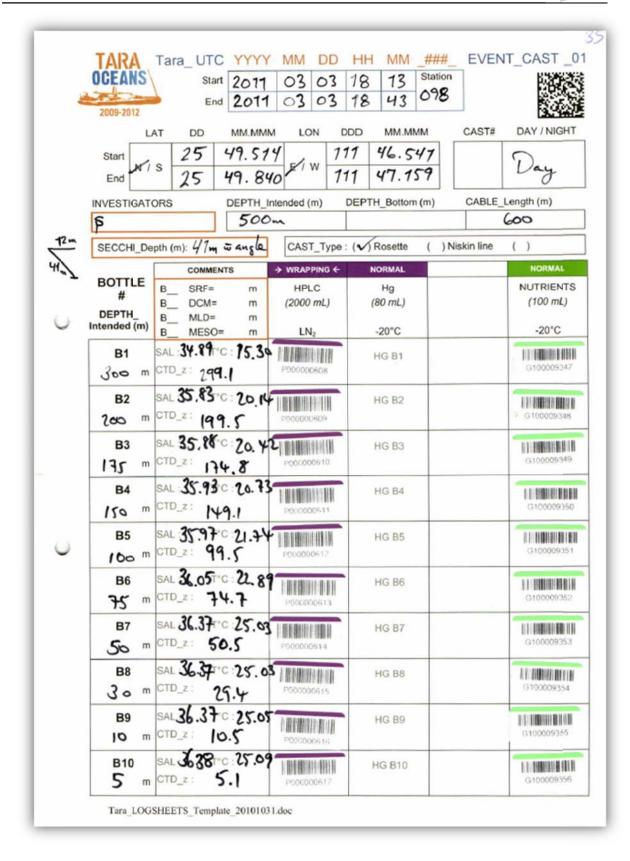
Та	ra_STATIO	N_PLAN_ST	N###_UTC	YYYY	MM	DD	НН	MM
TAR	A		Start:	2011	04	09	13	45
OCEA	NS	STN099	End:	2011	04	10	00	30
2009-20	12							
CHIEF SC	CIENTIST		LAT	DDD	MM.MMM	LON	DDD	MM.MMM
S. PE	CANT	Start:	South	021	08.758	West	104	47.220
3. PE	SANT	End:	South	021	06.254	West	104	48.045
00:15	LT=UTC+	-8						
JTC TIME	FWD STA	RBOARD	AFT A-FRAME		DEPTH	AFT CRANE		DEPTH
13:30	BREA	KFAST	BREAKFAST			BREAK	KFAST	
13:45	PREPA	RATION	START					
14:00	PUMF	_SRF	PREPAI	RATION				
14:15	PUMP	_SRF	CAST_R	OSETTE	1000m			
14:30	PREPA	RATION	CAST_ROSETTE					
14:45	PUMF	_SRF	CAST_R	OSETTE				
15:00	PUMF	SRF	PREPARATION					
15:15	PREPA	RATION	REGENT_	680µm_dz	500m	PREPAR	RATION	
15:30	PUMF	PUMP_SRF REG		REGENT_680µm_dz		DOUBLE_2	20µm_SRF	SRF
15:45	PUMF	_SRF	REGENT_	680µm_dz		PREPAR	RATION	
16:00	PREPA	RATION	PREPARATION					
16:15	PUMF	SRF	WPII_200µm_dz		100m			
16:30	PUMF	SRF	PREPARATION			PREPARATION		
16:45	PREPA	RATION	WPII_50µm_dz		100m	DOUBLE_20µm_SRF		SRF
17:00			PREPARATION			DOUBLE_20µm_SRF		
17:15			WPII_50µm_dz		100m	DOUBLE_20µm_SRF		
17:30			WPII_50µm_dz			PREPAR	RATION	
17:45			PREPAI	RATION				
18:00			TS	RB				
18:15	LUN	NCH	LUN			LUN	-	
18:30		NCH	LUN			LUN		
18:45		NCH	LUNCH			LUN	Color Color	
19:00	LUN	NCH	LUN			LUN	ICH	
19:15			PREPAI					
19:30			CAST_R		500m	SEC	CHI	
19:45			CAST_ROSETTE					
20:00			PREPARATION					
20:15			NEUSTON		SRF			
20:30			PREPAI	0.0000000000000000000000000000000000000	G. 12/2000	PREPARATION		
20:45			BONGO_300µm_dz		500m	DOUBLE_180µm_SRF		SRF

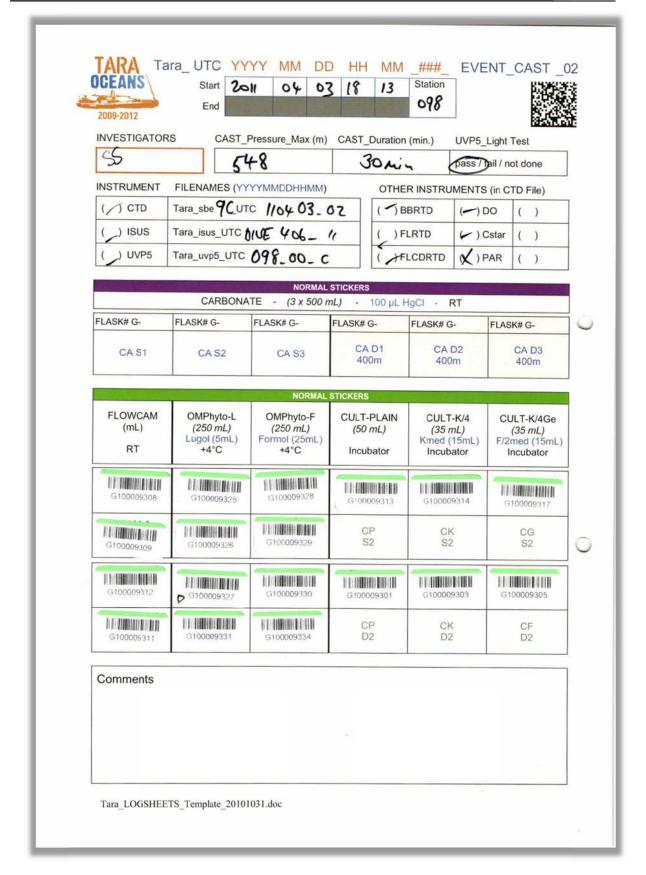












APPENDIX II Example of information components used to describe sampling Events and Samples from Tara-Oceans

```
EVENT ID
EVENT LABEL
EVENT LABEL_Alternative
EVENT DATETIME_Start
EVENT DATETIME_End
EVENT LATITUDE_Start
EVENT LATITUDE_End
EVENT LONGITUDE_Start
EVENT LONGITUDE_End
EVENT AREA_ID
EVENT CAMPAIGN_ID
EVENT DEVICE_ID
EVENT LOGSHEET_Filename_(URI)
EVENT COMMENT
EVENT COMMENT_by_Curator
EVENT COMMENT by Engineer
EVENT COMMENT_on_Logsheet
EVENT STATION_Label
EVENT OPERATOR(s)
EVENT TIME_of_the_Day
EVENT DEPTH_Intended_Max_(m)
EVENT DEPTH_Intented_Nominal
EVENT DEPTH Pressure Max (m)
EVENT DEPTH_Pressure_Min_(m)
EVENT CABLE_Angle_(deg)
EVENT CABLE_length_(m)
EVENT CABLE_Speed_(m/s)
EVENT DURATION_(min)
EVENT SAMPLING Method
EVENT SAMPLING Sequence (#)
EVENT SENSOR_CAMERA_Filename_(URI)
EVENT SENSOR_CTD_Filename_(URI)
EVENT SENSOR DepthRecorder Filename (URI)
EVENT SENSOR_DepthRecorder_Label
EVENT SENSOR_ECO_Filename_(URI)
```

```
EVENT
EVENT
SENSOR_Flowmeter_Start
EVENT
SENSOR_ISUS_Filename_(URI)
EVENT
SENSOR_Other_Filename_(URI)
EVENT
SENSOR_TSRB_Filename_(URI)
EVENT
SENSOR_UVP5_Filename_(URI)
EVENT
ENVIRONMENT_Bathymetry_(m)
EVENT
ENVIRONMENT_Secchi_(m)
EVENT
ENVIRONMENT_SeaState_(Beaufort)
EVENT
EVENT
ENVIRONMENT_Wave_Height_(m)
EVENT
EVENT
ENVIRONMENT_Wind_Direction_from
EVENT
EVENT
ENVIRONMENT_Wind_Speed_(knots)
EVENT
EVENT
ENVIRONMENT_Cloud_(0-8)
EVENT
ENVIRONMENT_Blueness_(D-M-L)
EVENT
EVENT
EVENT
```

```
SAMPLE ID
SAMPLE Label
SAMPLE Label_Barcode
SAMPLE Label Alternative
SAMPLE Label_Comment
SAMPLE EVENT_ID
SAMPLE DEVICE_ID
SAMPLE SAMPLING Container Type
SAMPLE SAMPLING_Container Number
SAMPLE SAMPLING_Volume_(m^3)
SAMPLE ID(s)_of_Replicates
SAMPLE DEPTH_(m)
SAMPLE DEPTH_Nominal
SAMPLE DEPTH Nominal Alternative
SAMPLE DEPTH_Pressure_Max_(m)
SAMPLE DEPTH_Pressure_Min_(m)
SAMPLE OPERATOR(s)
SAMPLE COMMENT
SAMPLE COMMENT_by_Curator
SAMPLE COMMENT_by_Laboratory
```

	COMMENT_on_Logsheet
SAMPLE	METHOD_ID
SAMPLE	PROTOCOL_Label
SAMPLE	PROTOCOL_Systematics_Group
SAMPLE	PROTOCOL_for_Onland_Analysis_Name
SAMPLE	PROTOCOL_for_Onland_Analysis_Name_Short
SAMPLE	PROTOCOL_Filtering_Filter_Description
SAMPLE	PROTOCOL_Filtering_Filter_Retention_Size_(μm)
SAMPLE	PROTOCOL_Filtering_Time_(min)
SAMPLE	PROTOCOL_Filtering_Volume_(mL)
SAMPLE	PROTOCOL_Filtering_Pre-Filter_Description
SAMPLE	PROTOCOL_Filtering_Pre-Filter_is_PROTOCOL_Label
SAMPLE	PROTOCOL_Filtering_Pre-Filter_is_SAMPLE_ID
SAMPLE	PROTOCOL_Filtering_Pre-Filter_Retention_Size_(μm)
SAMPLE	PROTOCOL_Filtering_Filtrate_
SAMPLE	PROTOCOL_Filtering_Filtrate_is_PROTOCOL_Label
SAMPLE	PROTOCOL_Filtering_Filtrate_is_SAMPLE_ID
SAMPLE	PROTOCOL_Chemical_Added_Amount_(mL or #)
SAMPLE	PROTOCOL_Chemical_Added_Description
SAMPLE	PROTOCOL_Chemical_Added_Name
SAMPLE	CONTAINER_Description
SAMPLE	CONTAINER_Type
SAMPLE	CONTAINER_Amount_(mL or #)
	CONTENT_Description
	CONTENT_Type
	CONTENT_Amount_(mL or #)
	PROTOCOL_FlashFreezing_(Y/N)
	STORAGE_Onboard_Temperature_(degC)
	STORAGE_Onboard_Comment
	SHIPPING_Date
	SHIPPING_Comment
SAMPLE	SHIPPING_Destination