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#### 41 **1. Introduction**

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43 In the enthusiasm that surrounds exciting and novel science it is easy to forget that a 44 unified approach to data management aimed to ensure consistency in data quality, ease of 45 dissemination between collaborators, secure archiving and future utilisation of the data is 46 critical to the success of projects (Lowry *et al*., 2005). This is particularly true of major multi-47 disciplinary and multi-partner programmes. Collection of marine data involves expensive 48 platform operations, such as running research vessels and training of qualified personnel. In 49 addition, because of the inherent difficulties in their collection marine measurements are 50 irreplaceable assets that are both expensive to collect and uniquely document the changing 51 earth system.

52 Over the past two decades the scientific community has become increasingly aware of 53 the importance of time series measurements as baselines for the quantification of changes in 54 the marine environment (Beaugrand, 2002). It is essential that future generations of scientists 55 and research users are able to access environmental data that has been properly managed and 56 preserved, to known standards and formats, together with basic background information on 57 how the data were collected and analysed (metadata). Scientists and funding bodies have also a 58 legal and moral responsibility to make the data and results from publicly funded activities 59 widely available. Moreover, insurance is required against accidental loss and technological 60 redundancy through changes in storage media. Delivering all this requires a dedicated 61 infrastructure of complex relational databases and staff that understand the data and their use as 62 well as information technology.

63 The scarcity and high value of oceanographic data has led increasingly to the 64 development of a culture where long-term data curation and data sharing, through specialised 65 national data centres, has become the norm rather than the exception (Glover *et al* 2006, Seys 66 *et al* 2006). Since its creation in 1979 the British Oceanographic Data Centre (BODC) has 67 provided support to the UK marine science through its data management activities, by 68 delivering fully integrated and quality controlled data for future utilisation by research 69 scientists, the government, industry as well as the wider public. BODC deals with biological, 70 chemical, physical, and geophysical data and its databases contain measurements of nearly 71 15,000 different variables. Its staff includes data scientists from a wide range of scientific 72 disciplines who have direct experience of marine data collection and analysis working 73 alongside information technology specialists developing and maintaining the databases and 74 software infrastructure required to support data management and data distribution systems. One 75 of the key responsibilities of National data centres such as BODC is to provide data 76 management support for the scientific activities of complex multidisciplinary long term 77 research programmes. In the present paper we discuss our experience in managing the data 78 arising from the Atlantic Meridional Transect (AMT) project and provide some guiding 79 principles for the data management of large multi-disciplinary programmes.

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# 81 **2. Overview of the AMT data set**

83 Between 1995 and 2005 AMT has undertaken 18 cruises essentially twice yearly 84 between the UK and the southern Atlantic Ocean which involved 46 international research 85 groups (Table 1; Robinson, *et al.*, 2006). The programme was divided into two phases (i.e. 86 phase I and phase II), separated by two years during which there was no fieldwork.

87 The scientific aims of phase I were to assess mesoscale to basin scale phytoplankton 88 processes, the functional interpretation of bio-optical signatures and the seasonal, regional and 89 latitudinal variations in mesozooplankton dynamics. During phase II, the program was 90 broadened (Figure 1 and Robinson *et al.*, 2006) to address a suite of cross-disciplinary 91 questions concerning ocean plankton ecology and biogeochemistry and their links to 92 atmospheric processes. Broadly, the measurements comprised hydrographic and bio-optical 93 properties, biogeochemistry, aerosol and rainwater composition, plankton community structure 94 and plankton physiology, as summarised in Robinson *et al.* (2006) and Figure 1.

95 The objectives included the determination of how 1) the structure, functional properties 96 and trophic status of the major planktonic ecosystems vary in space and time; 2) physical 97 processes control the rates of nutrient supply, including dissolved organic matter, to the 98 planktonic ecosystem and 3) atmosphere-ocean exchange and photodegradation influence the 99 formation and fate of organic matter. Determinands include temperature, salinity, inorganic 100 nutrients, carbon dioxide, oxygen, nitrous oxide, methane, dimethylsulphide, dissolved and 101 particulate carbon, nitrogen and phosphorus, chlorophyll, phytoplankton pigments and 102 taxonomy, photosynthesis, respiration, new production, nitrogen fixation, calcification, 103 bacterial and microzooplankton abundance and activity, microbial molecular diversity, viral 104 activity, mesozooplankton community structure and physiology (i.e. respiration, copepod egg 105 production rates), atmospheric dust deposition and characterisation, bio-optical properties, and 106 coloured dissolved organic matter (Table 2). An "individual dataset" or "AMT dataset" in the

107 context of this paper is a single or multiple sets of related measurements originating from a 108 single or a team of data originators during a given AMT cruise.

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## 110 **3. Challenges posed by the AMT dataset management: phase I and phase II**

112 The two phases of the AMT project presented BODC with very different challenges. 113 When the formal data management began at the beginning of phase II in 2002 our database 114 system was already designed to deal with the complexity of biological and biogeochemical 115 measurements. However, the number of individual sources of data, the size of the AMT 116 community, each successive cruise often having new scientists and students and the available 117 funding all presented significant challenges for the successful management of the data. The 118 relative importance of these factors varied for each phase.

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## 120 **3.1 Phase I**

121 As no provision had been made for data management during phase I, BODC and the 122 AMT community were essentially involved in a data rescue effort. First additional funding was 123 secured. As a large number of individuals (including temporary staff & PhD students) had been 124 involved in collection, the data were in a varied state of repair. Consequently, the data had been 125 kept in assorted formats on a range of media, there were no authoritative protocols for 126 collection and often there was no definitive version of data sets. Thus, there was considerable 127 potential for: data loss; confusion during analysis and subsequent interpretation; and wasted 128 effort tracking down and re-processing data. The process of acquiring these data was helped 129 considerably as the benefits of a central data management effort were realised during phase II 130 and by the realisation of AMT participants that data from phase I were not readily available.

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## 132 **3.2 Phase II**

133 Phase II presented the opportunity to undertake a more formal and structured approach 134 to the data management. Initially, many scientists were unaccustomed to a culture of integrated 135 data management. Whilst BODC had pioneered such an approach during the NERC North Sea 136 programme in the early 1980's (Lowry *et al*., 2005) and later during other NERC and European 137 projects, a period of organisational upheaval in UK marine science during the late 1990's 138 meant that a number of the guiding principles had to be re-learned. Previously, it had often 139 been the practice that BODC data scientists would accompany cruises to provide direct support 140 on fundamental on-board data management activities (e.g. CTD and underway data 141 processing). Regrettably, space constraints precluded BODC personnel participation during 142 AMT cruises. This situation led to the development and implementation of a more formalised 143 strategy for cruise preparation. This included the writing up of guideline documents of what 144 was expected at the end of a cruise with regards to data and ancillary information associated 145 with CTD and underway continuous measurements and also individual scientist data. 146 Additionally, there was insufficient continuity in shipboard personnel to ensure consistent 147 calibration and quality of the CTD and underway data. Consequently, it proved most efficient 148 for BODC to undertake these tasks for which further resource had to be found. Figure 2 149 illustrates the disparity between the initial estimate of effort required for the data management 150 and that actually expended.

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## 152 **4. How are the data managed by BODC?**  153

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# 154 **4.1 BODC communication and networking culture**

156 BODC's philosophy is that communication lays the foundations to good data 157 management. Data management begins with the exchange of information between the different 158 parties involved in the project (i.e. BODC staff/AMT data manager, scientists and ship 159 personnel) at the planning stage and throughout the fieldwork. Whilst space constraints 160 prevented data scientists from participating on AMT cruises, BODC participated in the AMT 161 planning and science meetings, preparation of newsletter and contributed to reports. As 162 mentioned previously, a number of what should have been standard working practices had to 163 be re-learned to attain the processes described below.

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## 165 **4.2 Initial acquisition of cruise data in liaison with the ship technical personnel & the PI**

167 Before the starts of each cruise BODC liaise closely with the ship's technical personnel 168 based at the National Marine Facility and the Principal Investigator (PI). This enables data 169 scientists to understand the scope of data collection activities and the nature of equipment 170 deployed, but also enables BODC to provide a set of guidelines to assist in good data 171 management practices and the recording of the metadata necessary for the accurate future 172 description of the data. Following the cruise, the PI is required to compile a comprehensive list 173 of the data collected during the cruise into the Cruise Summary Report (CSR, formerly the

174 "ROSCOP") conceived by the Intergovernmental Oceanographic Commission (IOC) in the 175 late 1960s to provide a low level inventory for tracking oceanographic data collected on 176 Research Vessels. It is expected that the PI submits the CSR, within a week of the cruise and a 177 full "Cruise Report" collating the cruise narrative and a description of the methodology of the 178 data sets collected by the scientists on board, within 6 month from the end of a cruise. These 179 documents provide the key information outlining the nature of the data collected and the 180 techniques employed. Alongside this, an electronic version of the CTD and underway 181 navigation data is submitted with the appropriate documentation relating to the calibration and 182 configuration of the scientific instrumentation employed.

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# 184 **4.3 Data tracking and banking**

186 The initial source of information collated by the PI at the end of the AMT cruise is 187 recorded by BODC into a series of inventory tables, one for each data set collected, together 188 with the details of the scientist responsible for the data. The inventory tables are interfaced with 189 the Oracle database to display the AMT data holdings dynamically on the BODC website 190 (http://www.bodc.ac.uk/projects/uk/amt/data\_inventories/). The records contained in the 191 inventory tables are continuously updated following dialogue with data originators and used to 192 keep the AMT participants informed about the availability and the processing status of the 193 data.

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## 195 **4.3.1 Physical security**

196 Clearly, physical security of data is one of BODC's primary concerns and the 197 organisation's approach to this has two components: an 'accession system' and an 'archive 198 system' for long-term preservation of the data. When the data arrive at BODC they are 199 recorded on an electronic accession table and the data copied into the inventory via the Unix 200 operating system. The physical integrity of the data is secured by preservation of the original 201 media together with a copy placed in the BODC data archive and wherever possible, an 202 additional version of the data supplied is saved into ASCII format. The archive system is 203 supported by an accession system containing the metadata record which provide the data 204 submission with a unique identifier and describe its contents and provenance.

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## 207 **4.3.2 Data reformatting and standardisation**

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- 209 Marine data sets cover an unusually wide range of physical, chemical, biological and 210 geological data types. Even a single water sample may be analysed for several hundred 211 parameters. Often, scientists use different words to describe the same type of data. All this 212 means that there can be confusion when seeking data, which may cause errors in reports or 213 misunderstandings between parties. Many organisations also want to be able to provide, search 214 and manipulate data over the internet. To be able to integrate these data into a database and be 215 able to use them reliably there must be no uncertainty surrounding the terms that are used to 216 describe data. Therefore, standardisation of the file format and the parameter defining the data 217 is essential for their professional management.
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# 219 **4.3.2.1 The BODC file format**

220 CTD and underway data are reformatted into the QXF format which is a BODC defined 221 subset of the binary format netCDF. Other data sets relative to discrete measurements are 222 handled in ASCII format prior to loading into a relational database under the Oracle Relational 223 Database Management system. Additionally, each of the data maintained by BODC is held in 224 standard units and it is assigned a parameter code described by the Parameter Dictionary 225 (http://www.bodc.ac.uk/projects/uk/enpardis/).

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## 227 **4.3.2.2 The Parameter Dictionary**

228 To solve the problem of terminology standardization we have established a dictionary 229 of terms which maps directly to dictionaries used by other leading international data 230 management organizations. Containing more than 18,000 terms, the parameter dictionary 231 developed by BODC (http://www.bodc.ac.uk/projects/uk/enpardis/) is a powerful data mark-up 232 tool which uses a single 8-bytes parameter code to associate a data value to its parameter name 233 and methodology through a semantic model. The names of biological entities in the parameter 234 dictionary have been also standardised against the Integrated Taxonomic Information System 235 (ITIS) that further enriches the metadata through access to a biological taxonomy.

- 237 **4.3.3 Data Quality control**
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239 After reformatting and attributing parameter codes, the quality control of many 240 oceanographic data sets is operated through data visualisation. The two main approaches to 241 data quality control are either via screening using bespoke soft-wares or simply via direct 242 visualisation of the data by experienced data scientists:

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# 244 **4.3.3.1 EDSERPLO: the BODC way forward to CTD profile and time series data**  245 **screening**

246 Edserplo (Editing and SERies PLOtting) is the soft-ware developed by BODC for 247 screening 1- and 2-dimensions continuous data series including continuous underway and CTD 248 profile data. This software can be used to visualise multiple parameters and series and it has a 249 quick editing tool which allows the quality control of data through the flagging spikes and 250 suspect data points (Fig 3). Since 2006 EDSERPLO runs on PC computers compared to a 251 previous version, operating on Silicon Graphic stations, allowing a more efficient and faster 252 processing of the data.

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## 254 **4.3.3.2 Quality control of non continuous profiles or time series data**

255 Discrete data measurements measured, for instance, from CTD cast bottles, net hauls or 256 during experiments are also quality controlled through direct visualisation of data points on 257 spreadsheets and graphical plots of the data. After the data are screened, quality controlled and 258 reformatted they become integrated in the databases.

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## 260 **4.4 Integration of AMT data in the databases**

262 Once reformatted and quality controlled, all the data collected during AMT cruises 263 which originates from discrete water column sampling, continuous profilers, tows or benthic 264 sampling, are managed within the BODC databases where they are fully integrated with 265 concomitant oceanographic measurements and associated metadata. The data are stored into 266 the BODC databases into a series of tables linked to each other to various degree of complexity 267 to minimise duplication of information. Figure 4 shows a simplified representation of the 268 BODC databases within the 3 main groups of tables;

270 • The sampling metadata tables consisting of the sampling activity or event 271 description table with links to the fieldwork description table and to the sampling 272 gear code table. 273 274 • The data tables consisting of a series of linkage and data storage tables for each 275 main type of sampling or data collection techniques. 276 277 • The parameter dictionary tables defining the 8-byte parameter codes 278 279 All data storage tables have the same field structure consisting of a unique key linking 280 each record to the linkage tables, a data parameter code, a data value, a data quality control 281 flag, a data originator code and a loading date. The data linkage tables invariably control the 282 one-to-many relationship between the events and the data. Their structure has been adapted 283 differently for each main type of sampling or data collection technique in order to incorporate 284 specific metadata information such as for example bottle depth and bottle type for water

285 collection events, plankton net depth range, mesh size, mouth area for plankton net hauls. The 286 structure of the database is such that it may be easily expanded to include new sampling gear, 287 new methodologies and instrumentation, and new parameters.

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## 289 **5. AMT data policy and data dissemination**

291 The distribution of the AMT data is regulated by the data policy 292 (http://www.bodc.ac.uk/projects/uk/amt/data\_policy/) drawn up by the AMT Scientific 293 Steering Committee (SSC). The policy was developed to ensure an appropriate balance 294 between the protection of data originators' intellectual property rights and the potential benefits 295 that may arise via data use by the programme, the wider research community and other 296 interested parties. According to this policy, when AMT data are transferred to BODC they 297 become available to other investigators within the AMT programme on the condition that the 298 originator is kept informed about how the data are being used and he/she is acknowledged in 299 any exploitation of that data. The AMT data can also be made available to the wider scientific 300 community, immediately upon permission being granted by the data originator and the 301 signature of a licence or after 6 months from the end of the program in April 2006.

302 BODC supplies the AMT data to both internal and external users either directly via 303 email, the ftp system or in the case of the CTD and underway data, via automatic download 304 through the BODC website (http://www.bodc.ac.uk/data/online\_delivery/amt/). Before any of 305 the AMT data can be downloaded, however, users are required to be registered as BODC web 306 users. The data are supplied in a fixed ASCII (CSV) format and they are associated with 307 documentation providing information about sensors, quality control, calibrations and 308 processing status. Each time modifications to data are made by BODC, these files are updated 309 and changes are noted in the documentation.

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#### 311 **6. AMT data requests**  312

313 Requests for AMT data can be made directly to the BODC staff for all data or via the 314 BODC website for CTD and underway data. Data requests and queries made directly to BODC 315 are handled by either the AMT data manager or the BODC requests officer. Data requests and 316 the processing of data sets required by PhD students are given priority over all other requests. 317 When data are lodged at BODC, it is the aim that requests be serviced within 1 to 3 working 318 days. Currently only the CTD and underway cruise data can be downloaded from the BODC 319 website whereas discrete data sets can only be obtained contacting the BODC staff. However, 320 BODC is developing a system for online delivery of its data holding and AMT data will 321 become available alongside all other publicly available data held in its databases.

322 Statistical information on AMT data request is only available from 2002. Since then 323 570 requests for AMT data have been handled (Fig. 5). Figure 5 also shows that data requests 324 have steadily increased from 16 in 2002 to190 in 2005. This increase in data requests reflects 325 both the expansion of the scientific community to approximately 180 scientists from 11 326 countries and the provision of an on-line system for the automatic download of the CTD 327 profiles and the underway data. On the other hand, the slight decrease in 2006 is probably the 328 results of the conclusion of the phase II of the program and the graduation of many of the 329 "AMT PhD students" (who accounted for a significant proportion of the data requests). Since 330 2003 (i.e. after the introduction of the BODC web data delivery system) the proportion of data 331 requests from the web has represented between 47% and 50% of total requests. Interestingly, 332 however, although the number of AMT requests received from external users has also 333 increased, their proportion has remained overall stable over time at around 20 % of the total

334 AMT requests (Fig 5). The largest data request was received from USA scientists followed by 335 that of the UK and French scientific community (Figure 6).

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## 337 **7. Discussion and conclusions**

339 The planning and implementation of research and the efficient management of the 340 resulting data often appear to be two widely separate worlds. This is because, whereas data 341 managers consider data collection, management and dissemination as essential for the effective 342 use of research funds, many researchers consider data management as technical and secondary 343 to publications. As a consequence data management is often insufficiently planned or not 344 planned at all (Seys et al 2006). Perhaps, the realisation by the scientific community, in the 345 1990s, of the importance of long term time series to predict the impact of future changes in the 346 earth system on human activities together with the need to handle increasingly large and 347 complex data sets, has resulted in a change in attitude towards the role of marine data 348 management.

349 A long-term multi-disciplinary international programs such as AMT provide numerous 350 challenges for the managements of the data they produce in terms of their large volume, 351 diversity of measurements, changes in sampling instrumentation and increased sophistication 352 of analytical methods. Increase in diversity and number of variables measured also means 353 increasing demand and needs from the end users for their rational integration. Measurements 354 also need to be supported by a rich metadata if they are to have value for the future. Clearly, 355 when it comes to satisfying the requirements of modern science on the delivery of fully 356 integrated and quality controlled complex data sets, such challenge cannot longer simply be 357 met by individuals or single scientific organisations without large investment of time and 358 resources. BODC through its support to multidisciplinary programs has specialised in handling 359 data sets which are small in volume, but extremely high in complexity covering a wide range 360 of physical, chemical, biological, atmospheric and geological parameters. Progresses in the 361 acquisition and management of AMT data were facilitated by a culture of communication and 362 collaboration between the data scientists and IT specialists with the AMT scientists and ship 363 technical staff. Thanks to this collaboration, BODC has rescued > 90 % of the data collected 364 during the phase I of the project by scientists who have moved on in their careers often loosing 365 contact with the AMT community.

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366 Within modern data management, the role of a National Data Centres such is also 367 evolving from one of data repository to one of active data delivery and redistribution between 368 scientific partner organisations. Such evolution is being fostered and made possible thank to 369 concomitant technological advances in IT soft-wares and the advent of the internet. Although 370 considerable effort has been spent by BODC to ensure the physical security of all data 371 accessed, its primary mission is to guarantee that data may be reused with confidence and 372 without any need for recourse to the data originator no matter how much time has elapsed since 373 the data were submitted. Ensuring this forms the bulk of the work of BODC's data scientists. 374 Thus, another important role played by BODC for the AMT community, and for other large 375 multidisciplinary programs, has been in its ability to manage and disseminate data of 376 increasing complexity through the development of bespoke software and web-portals. The 377 development of the BODC Parameter Dictionary and of screening soft-wares like EDSERPLO, 378 has greatly contributed to the effective data management and dissemination of data. BODC 379 data scientists also use sophisticated software, to extract quickly and efficiently integrated data 380 sets from the databases to satisfy data requests. In addition, the on-line data distribution system 381 has introduced by BODC since 2003 via its website has also allowed the expansion and 382 efficient data delivery within and beyond the AMT community.

383 Finally, it is important to note that the funding initially allocated for the data 384 management of AMT represented considerably less than the minimum required to manage the 385 data of a large multidisciplinary program as estimated by Glover *et al*., (2006). In their review 386 of the data management of the US JGOFS project, they recommended that good data 387 management requires devoted resources to be between 5 - 10 % of the total cost of the 388 programme. Overall, the AMT program received funding by NERC of the order of £2.38 389 millions of which £62k (2.6%) was initially allocated for data management. In the final 390 analysis an additional £140k has been sourced, meaning the total cost of the AMT data 391 management will exceed 8.5% of the total funding.

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## 393 **8. Lessons learnt and recommendations for managing future long term programs**

395 The following recommendations can be drawn from the experience acquired by BODC 396 through the data management of a large multidisciplinary program such as AMT:





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469 **Figure 4:** The BODC database structure detailing the 3 main groups of tables. Sampling 470 metadata tables containing information on sampling activity or event description table with links 471 to the fieldwork description table and to the sampling gear code table. Data tables consisting of a 472 series of data storage tables for each main type of sampling or data collection techniques. 473 Parameter dictionary tables containing the 8-byte parameter codes used in the data tables.

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475 **Figure 5:** Bar chart showing the total AMT data requests handled by BODC between 2002 and 476 2006. Requests for CTD and underway data down-loaded by users from the website (Web) are 477 shown in blue whereas requests handled directly (Direct) by the personnel are shown in red. The 478 solid triangle indicates the relative proportion of requests by non AMT participants.

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480 **Figure 6:** Break-down of external requests for AMT data according to countries**.** 

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491 **Table 2**: Summary of the measurements undertaken during the AMT cruises and protocols 492 (Table redrawn from Robinson et al 2006).









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499 **Figure 2:**  500

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**Figure 3:** 



 

 

 

 









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542 **Figure 6:**





# 545 **Table 1:**

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# 549 **Table 2**:





