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DDMoRe Standalone Execution Environment (SEE) Version 2.0.0 Software Release Note

Project:	DDMoRe
Software Version:	Demonstrator 2.0.0 (Full release for Interoperability Framework and MDL IDE)
Date Of Issue:	19-Aug-2016
Reason for issue:	Release of DDMoRe Demonstrator 2.0.0 to Consortium members and the General Public
Prepared by:	Richard Kaye
Approved by: (Project Management or Company Director)	Jonathan Chard (19-Aug-2016)

Document Approval

Completion of the following signature blocks signifies the approver has read, understands, and agrees with the content of this document.

Name	Job Title or Role	Signature	Date (dd-mmm-yyyy)
The Author is signing to indicate that there is the appropriate technical accuracy and completeness			
Authored by: Richard Kaye	Techical Lead	Authored	18-Aug-2016
Reviewed by: Jonathan Chard	Techical Architect	Reviewed	19-Aug-2016
<<The Technical Lead is signing to indicate that the coverage and completeness of the technical detail is appropriate and that the document has been prepared in accordance with applicable quality processes >>			
Approved by: Richard Kaye	Techical Lead	Approved	19-Aug-2016
<<The Project Manager is signing to confirm that this document has been prepared in accordance with an approved document management process, that content is consistent with the deliverable definition found in the governing Plan, that relevant input from authors has been included and that an appropriate review / editing process has been conducted.>>			
Approved by: Jonathan Chard	Product Director	Approved	19-Aug-2016

Document Revision History

Version	Author	Date	Description
1.0	Richard Kaye	18-Aug-2016	First version for release of Demonstrator 2.0.0. QAT-4161 covers review and approval history.

Table of contents

1   Reference documents

Document Reference	Document Description
[Installation Guide]	SEEInstallationGuide_Demonstrator2.0.0.pdf
[Test Summaries]	See Section 6 Test Summary
[Supported Features]	See http://www.ddmore.eu/timeline/final-public-release-interoperability-framework
[Known Issues]	See http://www.ddmore.eu/timeline/final-public-release-interoperability-framework
[Use-Case Support]	See http://www.ddmore.eu/timeline/final-public-release-interoperability-framework

2   Introduction and overview of the release

This is a Public Release of the MDL IDE and Interoperability Framework. The purpose of the release is to provide DDMoRe Consortium members and the General Public access to the final deliverables of the DDMoRe project, allowing them to assess the deployment, features and usability of the system.

2.1 Scope

This release is being made available to all DDMoRe Consortium members and members of the General Public.

3   Contents of the release

This release contains the following main software artefacts from different providers. Note that the presence of components in *bold italics* will depend on the specific plugins installed:

Location	Description	Provider
\BlackBoxWinBUGS	WinBUGS BlackBox component builder and execution environment	Pavia University
\ConfigureRConsole.R	R script for configuring and initialising the R Console environment	Mango Solutions
\converter-toolbox-distribution	Converter Toolbox distribution including the following converter modules: • MDL-to-PharmML • *PharmML->MLXTRAN* • *PharmML->NM-TRAN* • *PharmML->WinBUGS*	Leiden University Pfizer Inc Lixoft SAS Mango Solutions Pavia University
\docs	Accompanying documentation	Mango Solutions Uppsala University Lixoft SAS
\fis	Framework Integration Service (FIS)	Mango Solutions
\gfortran	*FORTRAN 95 compiler*	GNU
\InstallNonmem.bat	A script for installing the (separately available) NONMEM binaries into the SEE	Mango Solutions
\MDL_IDE	Directory containing MDL IDE products	Leiden University Pfizer Inc
\MDL_IDE\mdl_ide.exe	MDL IDE executable	Leiden University Mango Solutions Pfizer Inc
\MDL_IDE\jre	Java Runtime Environment 64-bit	Oracle
\mif-exec	Mango Interoperability Framework with the following Windows-based connectors: • *Local Monolix execution* • *Local NONMEM execution* • *Local PsN (VPC/SEE/bootstrap) execution* • *Local Simcyp execution* • *Local WinBUGS execution* • Local command-line execution	Lixoft SAS Mango Solutions Uppsala University Simcyp (Certara) Pavia University
\MlxLibrary1.1.0	*MlxLibrary installation 64-bit*	Lixoft SAS
\Monolix432s	*Monolix installation*	Lixoft SAS
\perl	*Perl and PsN installation*	The Perl Foundation Uppsala University

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Location	Description	Provider
\PFIM	*PFIM-related features:* • *R functions* • *PharmML->PFIM converter*	INSERM/UPD Cyprotex
\PopED	*PopED R package initialisation*	Mango Solutions
\R	R Statistical Analysis Environment with preinstalled *DDMoRe* R packages and corresponding dependencies and a selection of other utility packages	R (Mango Solutions) (Pfizer Inc) (Uppsala University)
\README.txt	Text file providing further details and information about the release	Mango Solutions
\SEE_VERSION	Text file providing the version identifier of the release	Mango Solutions
\setup-XXX.bat \setup-XXX.pl	Scripts for configuring the environment for running modelling tools	Mango Solutions Uppsala University Lixoft SAS Simcyp (Certara)
\startup.bat	A script for starting up the FIS, CTS and MIF-EXEC background services	Mango Solutions
\XXX-see-env-setup.bat \XXX-see-env-plugin.info	Scripts for describing and starting up modelling tools and accompanying services	Mango Solutions Uppsala University Lixoft SAS Simcyp (Certara) Pavia University
\WinBugsSO	*Standard-Output generator for WinBUGS executions*	Pavia University

The release also contains the following:

- Documentation
    o See [Installation Guide]
- Installation Qualification
    o See [Installation Guide]
- Release Note
    o This document

4   System requirements for the release

The SEE has been formally validated by DDMoRe Consortium members on the following platform:

- Windows 7 (64-bit) with SP1 or above

Additionally, during ad-hoc testing, DDMoRe Consortium members experienced no adverse effects on the following platforms:

- Windows XP (64-bit)
- Windows 8 (64-bit)
- Windows 10 (64-bit)
- Any non-Windows operating system running a correctly configured Virtual Machine (e.g. VirtualBox) with one of the above Windows versions installed

5   New functionality included in this release

Feature Number	Description
Demonstrator 2.0.0	
1	Support of the latest MDL and PharmML specifications. • See [Supported Features] for further details.
2	Support of additional M&S tools: • WinBUGS, PFIM, PopED
3	Support of further Use-Case models. • See [Use-Case Support] for further details.
4	Additional R scripts provided to demonstrate the capabilities and interoperability features of the framework
5	Multiple bug fixes (see Section 7.1)

6   Test Summary

Testing of this release has been undertaken by various DDMoRe Consortium members.

Reference HTML results of this testing can be found on the DDMoRe Consortium web-site at:

http://www.ddmore.eu/timeline/final-public-release-interoperability-framework

Note that this testing does not cover all possible MDL model forms. The focus has been on the set of Use-Case models that are provided along with the SEE installation. See [Use-Case Support] for further details of these models.

Any issues encountered during this testing are detailed in Section 8.

7   New Features Added/Issues Fixed in this release

7.1 Demonstrator 2.0.0

Key	Description
DDMORE-363	Add support for BUGS translator
DDMORE-484	Deliver Demonstrator 2.0
DDMORE-546	Write TEL execution of 'execute with Simcyp'
DDMORE-606	Build MDL IDE for non-Windows machines
DDMORE-856	Updates to MIF (DDMoRe branch) for platform-independence
DDMORE-915	Review and agree on the licensing and copyright information
DDMORE-1251	Table statement : patab should not be created if no columns are there to add
DDMORE-1313	ErrorStatement and ErrorType restructuring
DDMORE-1400	Add support for Inter Occasion Variability (IOV)
DDMORE-1419	TEL.R Xpose DB - gracefully handle failures for discrete model results
DDMORE-1592	SEE ATH: Post product 4.1 release improvements
DDMORE-1596	Error statement changes
DDMORE-1599	Investigate use of .getMdlInfoFromSO() with what === mdl
DDMORE-1600	Replace getMdlInfoFromSO() calls with getDataObjects() is accessing MDL
DDMORE-1605	Update PharmML version to 0.8
DDMORE-1607	Support the SO Specification v0.3
DDMORE-1610	Upgrade MDL->PharmML converter to PharmML 0.8
DDMORE-1611	Product 5.0 : issue with an omega getting added to theta along with omega block
DDMORE-1612	Upgrade PharmML->NM-TRAN converter to PharmML 0.8
DDMORE-1613	Upgrade Converter-Test-Harness to PharmML 0.8
DDMORE-1621	Make MIF startup service optional
DDMORE-1623	SEE Installer fails to download any of the artifacts from SourceForge
DDMORE-1624	SEE Installer add simcyp plugin support
DDMORE-1627	Test Simcyp integration with SEE
DDMORE-1634	Monolix integration for Product 5: Stage 1 release
DDMORE-1635	Upgrade FIS PharmMLArchiveCreator to PharmML 0.8
DDMORE-1650	R getPopulationParameters - validate all arguments values
DDMORE-1653	Product 5.0 : Pk macros : Add TRANS for respective specific Advans
DDMORE-1655	Deliver Product 5 stage one stable build
DDMORE-1657	Variables with reserved names need to be referred correctly after renaming
DDMORE-1661	Updates to SO structure have resulted in assertions failing
DDMORE-1664	Proper support for categorical covariates
DDMORE-1683	Update MDL<->JSON converter following changes to MDL grammar for Product 5

DDMORE-1685	Expose parameters in estimate function to add extra steps to execution workflow
DDMORE-1686	Add support for Study Design object
DDMORE-1687	Add support for Prior object
DDMORE-1690	Add MDL 8.0.0 support to JSON converter
DDMORE-1693	Add poped, winbugs and pfim see plugins to see installer
DDMORE-1695	MDL IDE workspace upgrade warning on first startup
DDMORE-1699	Demonstrator 2.0 release process
DDMORE-1705	Release Candidate builds and testing
DDMORE-1729	Product 5 : Extend probOnto support for negative binomial
DDMORE-1732	Product 5 : Support for KTR and other pk-macro values
DDMORE-1733	Product 5 : Logit and similar operations need to be supported for unary operations
DDMORE-1734	Product 5.0 : SourceForge ticket #448 : TTE related issues
DDMORE-1735	Product 5.0 : SF#599 : Issue related to Inconsistent order of derivative variable

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8 Known issues with this release

A high-level list of supported/unsupported features and known issues and can be found on the DDMoRe Consortium web-site at:

http://www.ddmore.eu/timeline/final-public-release-interoperability-framework

9 Receiving support for this release

To receive support with the installation and/or use of this software release, please post questions or comments to the relevant DDMoRe Forum:

1. Installation issues/questions/comments:

    http://www.ddmore.eu/forum/product-5-see-installation

2. Usage issues/questions/comments:

    http://www.ddmore.eu/forum/product-5-see-usage