

# Open PHACTS

## Milestone 3

### First working release demonstrate use, associate partners enlisted and integrated

Prepared by UNIMAN, Janssen, HLU, VUA, ConnDisc, Pfizer, SIB,  
RSC, UNIVIE

Approved by Steering Committee

April 2012  
Version 1.0

Project title: An open, integrated and sustainable chemistry, biology and pharmacology  
knowledge resource for drug discovery

Instrument: IMI JU

Contract no: 115191

Start date: 01 March 2011

Duration: 3 years

<b>Nature of the Deliverable</b>	
Report	<b>x</b>
Prototype	
Other	
<b>Dissemination level</b>	
Public dissemination level	<b>x</b>
For internal use only	

<b>Open PHACTS</b>	Milestone: First working release demonstrate use, associate partners enlisted and integrated	Milestone: M3	
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## Definitions

- Partners of the Open PHACTS Consortium are referred to herein according to the following codes:

**Pfizer** – Pfizer limited – **Coordinator**

**UNIVIE** – Universität Wien – **Managing entity of IMI JU funding**

**DTU** – Technical University of Denmark – DTU

**UHAM** – University of Hamburg, Center for Bioinformatics

**BIT** – BioSolveIT GmbH

**PSMAR** – Consorci Mar Parc de Salut de Barcelona

**LUMC** – Leiden University Medical Centre

**RSC** – Royal Society of Chemistry

**VUA** – Vrije Universiteit Amsterdam

**CNIO** – Spanish National Cancer Research Centre

**UNIMAN** – University of Manchester

**UM** – University of Maastricht

**ACK** – ACKnowledge

**USC** – University of Santiago de Compostela

**UBO** – Rheinische Friedrich-Wilhelms-Universität Bonn

**AZ** – AstraZeneca

**GSK** – GlaxoSmithKline

**Esteve** – Laboratorios del Dr. Esteve, S.A.

**Novartis** – Novartis

**ME** – Merck Serono

**HLU** – H. Lundbeck A/S

**E.Lilly** – Eli Lilly

- Grant Agreement:** The agreement signed between the beneficiaries and the IMI JU for the undertaking of the Open PHACTS project.
- Project:** The sum of all activities carried out in the framework of the Grant Agreement.
- Work plan:** Schedule of tasks, deliverables, efforts, dates and responsibilities corresponding to the work to be carried, out as specified in the Grant Agreement.
- Consortium:** The Open PHACTS Consortium composed of the above-mentioned legal entities.
- Project Agreement:** Agreement concluded amongst Open PHACTS participants for the implementation of the Grant Agreement. Such an agreement shall not affect the parties' obligations to the Community and/or to one another arising from the Grant Agreement.

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## 1 Introduction

The Open PHACTS project proposal defines a major technical milestone at the end of Month 12, specifically a working version of the Open PHACTS system with the milestone verified by "Prototype delivered within the consortium and running". This document describes how this was achieved. This software was designated "Version 0.2" (or v0.2 for short) and this is used in the remainder of this document.

We have set up a process for adding Associated Partners and we successfully go along with enlisting and integrating them in the project.

## 2 Verification

Version 0.2 of the Open PHACTS Core platform and GUI was released within the consortium on March 30, 2012. The Milestone of delivery of a pilot version of the Open PHACTS platform and core GUI to the consortium was achieved. The system is now being used by the members of the Open PHACTS consortium, led by the user testing team and a process of gathering bugs, feedback and future needs is now in operation.

The process of adding associate partners was officially approved at the Steering Committee Meeting in Stevenage on February 7-8, 2012.

## 3 Prototype delivered within the consortium and running

### 3.1 Release Timeline

- Software coding ceased and the final package was delivered on the 2<sup>nd</sup> March 2012
- An acknowledgement was sent to the ExCo and PMU to notify the milestone had been met
- There then followed a period of technical and scientific testing until 16<sup>th</sup> March, followed by rapid bug-fixing before more wider release
- Full scientific testing and phased rollout began w/c 19<sup>th</sup> March, with email and webinars presenting the software
- A full release note guidance document was created and made available to all members of the consortium

### 3.2 Datasets in this release

- Enzyme: Necessary for the enzyme classifications
- ChEMBL v2: Essential SAR database
- Drugbank v3: Provides additional information on known drugs
- These are connected through ConceptWiki IDs (which contains Uniprot mappings) and ChemSpider Ids

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### 3.3 Scientific Functionality

The following queries are possible:

- Query pharmacology data by target (via target name search)
- Query pharmacology data by compound (via compound name search)
- Query pharmacology data by target family (via Enzyme hierarchy)
- Structure searches to identify compounds in the system (which can then be used in pharmacology searches)
- Text search to identify targets/proteins

### 3.4 Functionality Details

- Text search now uses ConceptWiki. The interface has “Google-like” auto-complete functionality to aid entry. The identifier resolution service takes care of mapping the input concept to the required database identifiers in the system
- A more integrated view across targets is now available; protein identifiers in the different databases are now fully connected
- The system now enables pharmacology queries over the full ChEMBLdatabase
- Many interface enhancements and bug fixes, including pagination, table resizing and presentation enhancements (better labels etc.)
- More robust chemical structure searching via the ChemSpider API has now been implemented

### 3.5 Technical Achievements

- Sourced required data, converting to RDF or adjusting RDF as required (much of the existing RDF requiring modification to work correctly in Open PHACTS)
- Loaded approximately 70 million triples into the semantic data cache
- Dynamic identifier mapping is facilitated via the Identity Mapping Service using 7 linksets and providing 3,149,260 mappings that relate the core datasets. Additional non-critical mappings are ready to load once we are sure they will not affect system performance
- Created a real-time text to concept API using ConceptWiki and synonyms sourced from multiple databases, including validated synonyms from ChemSpider
- Data integration across the different databases is demonstrated,
- Chemistry normalisation and mapping through a ChemSpider pipeline is in place
- Created the Open PHACTS API which delivers results of optimised queries over the platform
- Demonstrated integration with “external” web services (ChemSpider) is a critical element of the system

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- Created a pharmacology-oriented interface using real data, seeded by the Lundbeck LSP platform and querying the semantic data cache
- Deployed the GUI widget framework now in full use within the platform, and successfully used by multiple groups on the project

### 3.6 Known Limitations

- Currently the pharmacology data is ChEMBL02 source from the Chem2Bio2RDF project. This means that users cannot compare data to that at the ChEMBL website, which is currently version 13. We are planning to update the OPS platform to ChEMBL 13 as soon as possible.
- For target-based pharmacology, the user must currently select the specific species of protein (f.e. “mouse”) and will only return pharmacology data for that species. We are working on the next iteration of this, whereby data can be retrieved for all species and then filtered as required
- There will be duplicate rows present in the pharmacology data. These will be distinct ChEMBL records but often covering the same compound-target relationship. We will look for guidance from the STF as to how to de-duplicate once the system is available
- The user may be able to select targets or compounds that are not associated with any pharmacological data. These selections will return no results.
- Filtering, export and sorting of pharmacology records will only take place on the records currently loaded into the interface. We are working on a solution such that these operations can take place on the entire dataset

### 3.7 APIs available

These methods are documented at [https://wiki.openphacts.org/index.php/Core\\_API](https://wiki.openphacts.org/index.php/Core_API).

### 3.8 Testing

It is critical that scientific software be tested before providing to users, who will expect that the results they obtain result from a tested system. While the v0.2 of the software was intended as an internal “demonstrator” release it still, nevertheless, required considerable testing. Within Open PHACTS our testing is split roughly into two separate elements – technical testing where we ensure the platform is robust and eliminate software bugs; and scientific testing, where we assess the scientific accuracy and coverage of the results obtained. In reality there is overlap between the two test data sets which is used to ensure technical algorithms are working correctly. Over the coming months WP5/6 will develop a barrage of scientific use-cases and tests that will be used to validate future versions of this platform. For the v0.2 release the tests covered the core components and major areas of functionality. Using the OPS GUI an initial set of queries were performed and graded into

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pass/fail. The results of this testing are provided in document 1 in the Appendix. Each failure was analysed and changes were made to the system to remove the issue. Testing was also performed on components such as ChemSpider (Document 2) which provides much of the compound-structure based support inside OPS. Automated unit tests were also performed on components such as the IMS and Query Expander systems (Documents 3/4). Thus, a series of tests across the system confirmed it was operating correctly and the system could be released to project members.

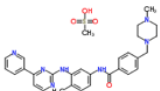
### 3.9 Figures showing v0.2 in action

Compound by name x

Hint: Type in compound name. E.g. "Aspirin"

Compound name:

Compound by Name search results



## Gleevec

Imatinib is a drug used to treat certain types of cancer. It is currently marketed by Novartis as Gleevec (USA) or Gleevec (Europe/Australia) as its mesylate salt, imatinib mesilate (INN). It is occasionally referred to as CGP57148B or ST1571 (especially in older publications). It is used in treating chronic myelogenous leukemia (CML), gastrointestinal stromal tumors (GISTs) and a number of other malignancies. It is the first member of a new class of agents that act by inhibiting particular tyrosine kinase enzymes, instead of non-specifically inhibiting rapidly dividing cells.

Primarily hepatic via CYP3A4. Other cytochrome P450 enzymes, such as CYP1A2, CYP2D6, CYP2C9, and CYP2C19, play a minor role in its metabolism. The main circulating active metabolite in humans is the N-demethylated piperazine derivative, formed predominantly by CYP3A4.

ChemSpider ID: [5101](#)

Molecular Formula: C29 H31 N7 O

SMILES: Cc1ccc(cc1Nc2nccc(n2)c3ccnc3)NC(=O)c4ccc(cc4)CN5CCN(CC5)C

Standard InChI: InChI=1S/C29H31N7O/c1-21-5-10-25(18-27(21)34-29-31-13-11-26(33-29)24-4-3-12-30-19-24)32-28(37)23-8-6-22(7-9-23)20-36-16-14-35(2)15-17-36/h3-13,18-19H,14-17,20H2,1-2H3,(H,32,37)(H,31,33,34)

Standard InChIKey: KTUFNOKKBVMGRW-UHFFFAOYSA-N

Affected Organism: Humans and other mammals

Indication: For the treatment of newly diagnosed adult patients with Philadelphia chromosome positive chronic myeloid leukemia (CML). Also indicated for the treatment of pediatric patients with Ph+ chronic phase CML whose disease has recurred after stem cell transplant or who are resistant to interferon-alpha therapy. Also indicated with unresectable and/or metastatic malignant gastrointestinal stromal tumors (GIST).

Protein Binding: Very high (95%)

Toxicity: Side effects include nausea, vomiting, diarrhea, loss of appetite, dry skin, hair loss, swelling (especially in the legs or around the eyes) and muscle cramps

Melting Point: 226 oC (mesylate salt)

ALogP:	# H-Bond Receptors:	# H-Bond Donors:	Mol Weight:	MW Freebase:	# Rule of 5 Violations:
2.583	7	2	482.612	482.603	0

Figure 1: Compound Information. As the user types, ConceptWiki uses ChemSpider validated synonyms to map text entry to a Concept. This is then linked to a Chemspider ID which is used to retrieve data from both ChemSpider and the DrugBank database

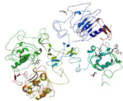
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Compound by name  Target by name

Hint: Start typing in protein name and species. E.g. "Adenosine receptor A2a (Homo sapiens)"

Protein name:

**Target Data**

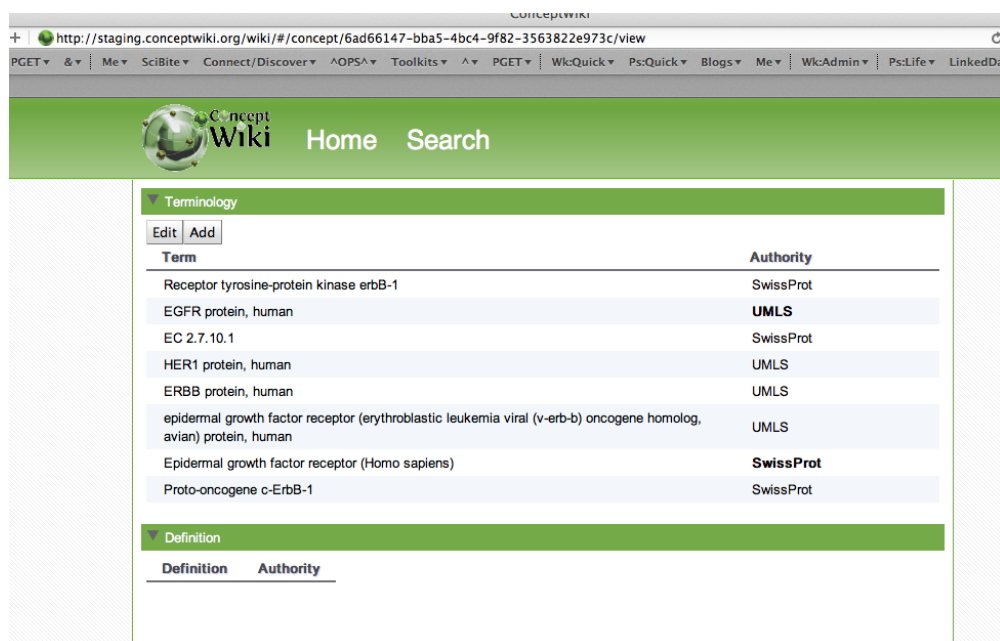


### Epidermal growth factor receptor (Homo sapiens)

Target Type: PROTEIN  
Organism: *Homo sapiens*  
Description: Epidermal growth factor receptor  
Synonyms: Epidermal growth factor receptor Receptor tyrosine-protein kinase ErbB-1  
Specific Function: Isoform 2/truncated isoform may act as an antagonist  
Cellular Location: single-passTypeI MembraneProtein.Isoform2:secretedProtein  
Keywords: 3D-structure Alternative splicing ATP-binding Cell membrane Complete proteome Direct protein sequencing Disease mutation Disulfide bond Glycoprotein Isopeptide bond Kinase Membrane Nucleotide-binding Phosphoprotein Polymorphism Receptor Repeat Secreted Signal Transferase Transmembrane Tumor suppressor Tyrosine-protein kinase Ubi conjugation  
PDB Entry: [1WQ](#)

Molecular Weight: 134279      Number of Residues: 1230      Theoretical PI: 6.67

Figure 2: Target Information. As with compounds, ConceptWiki is used to translate entered text to an OPS Concept, using Uniprot as the main protein information system.



http://staging.conceptwiki.org/wiki/#/concept/6ad66147-bba5-4bc4-9f82-3563822e973c/view

PGET & Me SciBite Connect/Discover AOPS Toolkits PGET WkQuick Ps:Quick Blogs Me WkAdmin Ps:Life LinkedDa

Concept Wiki Home Search

**Terminology**

Edit Add

Term	Authority
Receptor tyrosine-protein kinase erbB-1	SwissProt
EGFR protein, human	UMLS
EC 2.7.10.1	SwissProt
HER1 protein, human	UMLS
ERBB protein, human	UMLS
epidermal growth factor receptor (erythroblastic leukemia viral (v-erb-b) oncogene homolog, avian) protein, human	UMLS
Epidermal growth factor receptor (Homo sapiens)	SwissProt
Proto-oncogene c-ErbB-1	SwissProt

**Definition**

Definition	Authority
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Figure 3: Compounds and targets can be community edited via ConceptWiki by clicking on the "Definition" link in the main OPS interface

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Protein name:  Search...

Pharmacology by Target name search results - Records loaded: 100

Structure	Target name	Compound name	Smiles	Inchi	Inchikey	Molweight	Num ro5 violations	Std type
	Beta-2 adrenergic recepto...	(1R,7aS)-hexahydro-1H-py...	O=C(O)C[C@H]1CCN2C...	InChI=1/C16H19N3O2/c2...	D1PQWJKTULKTC-FZM2J...	285.345	0	IC50
	Beta-2 adrenergic recepto...	(1R)-2-((2-(4-(2-cyclopent...	O)C(C)H)1CNCCO1ccc(c...	InChI=1/C23H27N3O2S/c...	ISJPANQFRQZLQ-QFIPX...	409.551	0	Intrinsic activit
	Beta-2 adrenergic recepto...	N-(3-Chloro-4-(2-hydroxy...	CC(C)C)NCC(O)C1ccc(c...	InChI=1/C18H23ClN3O2S...	WBEJBAFWFWVTG-UHFF...	382.91	0	ID50
	Beta-2 adrenergic recepto...	ethanesulfonamide, N-[3-...	Oc1ccc(CNCCCN(=O)O)...	InChI=1/C23H29N3O5S2/...	XLFAMOWBQDIE-UHFFF...	479.619	0	Beta2 duration

Figure 4: Pharmacology search for the B2-adrenergic receptor

Pharmacology by Target name search results - Records loaded: 100

Retrieve next 100 records | Download CSV-file | SD-File 8% ready | Download SD-file

Structure	Target name	Compound name	Sn
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Figure 5: Pharmacology control bar. Here, SDFile export is progressing in the background and the “Download SD File” button will be activated once complete

A.

Std type: IC50

Relation:

- Sort Ascending
- Sort Descending
- Columns
- Group By This Field**
- Show in Groups
- Filters

Intrinsic activity



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B.

Structure	Target name	Compound name	Smiles	Inchi	Inchikey
<b>Group: Activity (1 Item)</b>					
<b>Group: Affinity constant (1 Item)</b>					
<b>Group: Beta2 duration (6 Items)</b>					
<b>Group: EC50 (13 Items)</b>					
9	Beta-2 adrenergic recepto...	N-{4-[(6,7-dihydroxy-1,2,3...	CCCCCNC(=O)Nc1ccc(cc...	InChI=1/C29H36M055(c...	YSNYDDH4ZGWFH4
10	Beta-2 adrenergic recepto...	N-{4-(2-[(2S)-2-Hydroxy...	O[C@@H](CNCCc1ccc(NC...	InChI=1/C24H27N3O4(c2...	FSACXLYORFFJK4
11	Beta-2 adrenergic recepto...	4-[(2R)-2-[(2R)-2-Hydrox...	C[C@H](Cc1ccc(cc1)c2ccc...	InChI=1/C23H24N2O3(c1...	OTLVQMFMEFVEFP4

Figure 6 Grouping data records based on some column property.

Std unites	Assay organism

Context Menu:

- Sort Ascending
- Sort Descending
- Columns
- Group By This Field
- Show in Groups
- Filters
  - Felis catus
    - < Enter Number...
    - > Enter Number...
    - = Enter Number...

Figure 7: Filtering data based on column values

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## 4 Associated partners enlisted and integrated

### 4.1 How to get involved in the project

Open systems need an engaged community, to grow, develop and sustain. We actively manage our partners, and the wider community. We term this the Open PHACTS Waiting Room, managed by a Gatekeeper (Bryn Williams-Jones)

- Our relationships with all partners are visible: what we are doing together and why
- Opportunities to engage and develop are open and are based on project needs

We hold regular community workshops and events

- Learn more about Open PHACTS and the Open Pharmacological Space
- Participate in new ideas and functions
- Engage in development of new use cases, help us answer new questions
- Contribute to development, and engage in plans for sustaining the Open Pharmacological Space

There are different degrees of involvement of an organization with the Open PHACTS project (shown in Figure 8):

- **Associated Partners:** We have a Memorandum of Understanding (MoU) ready for institutions to sign for mutual support and exchange of ideas, data or technology. Associated Partners will be the first to hear about the latest developments in the Open PHACTS project and will also have the opportunity to present ideas and use cases to the core Open PHACTS team.
- **Development Partnerships:** Once an institution is an Associated Partner and want to do some more specific development work together with us (e.g. develop APIs, new data, algorithms etc), they can enter a Development Partnership with the Open PHACTS project. This will give them greater access to the core of the project. Development Partnerships are focused on defined pieces of work of mutual interest and an agreed collaborative annex is added to the MoU.
- **Joining the consortium:** If an institution would like to become an integral part of the project, it might be worth to consider the option to join the Open PHACTS consortium.

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## Associated partners

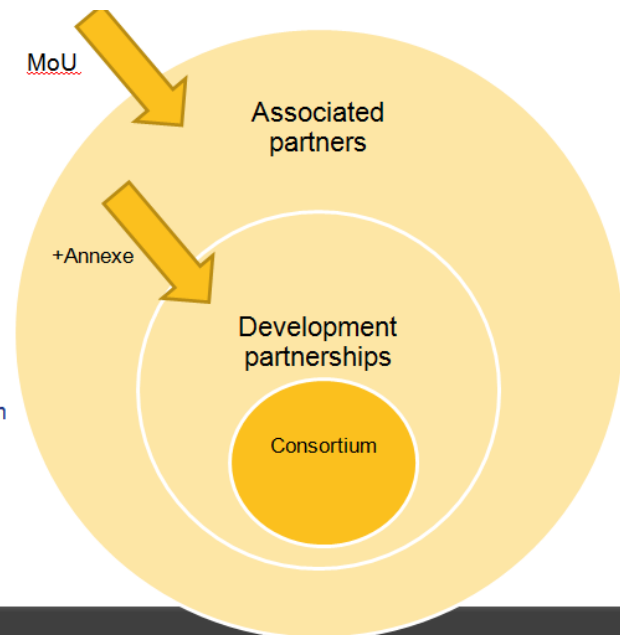
Organisations, most will join here  
 Support, information  
 Exchange of ideas, data, technology  
 Opportunities to demo at community webinars  
 Need [MoU](#)

## Development partnerships

Influence on API developments  
 Opportunities to demo ideas & use cases to core team  
 Need [MoU](#) and [annexe](#)

## Consortium

22 current members



# Open PHACTS and the scientific community

Figure 8: Different degrees of involvement of an organization with the Open PHACTS project

## 4.2 Process of adding Associated Partners

To become an Associated Partner a Memorandum of Understanding (MoU – document 6 in the Appendix) has to be signed. We agreed on the following process:

1. Internal sponsor proposes an Associated Partner by filling the “Associated Partner Details Form” (document 7 in the Appendix) including a short justification why it will be of benefit to the Open PHACTS project if the proposed institution becomes an Associated Partner. This will be the basis for deciding whether or not an Associated Partner proposal is accepted or not.
2. Discussion and decision in the Management Task Force (WPs 7-9).
3. Information about proposed Associated Partner will be sent out with the Friday PMU message. If there is no objection from the consortium within one week, we can sign the MoU.
4. Internal sponsor organizes the signature and logo of potential Associated Partner and sends it to the gatekeeper Bryn Williams-Jones.

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### 4.3 List of Associated Partners

At the moment we have 4 Associated Partners enlisted:

- Aureus Sciences
- Code-N Computing
- GVK Bio
- Thomson Reuters

Further potential Associated Partners are in the process of being added at the moment.

The up-to-date list of our Associated Partners can be found on our website:

[http://www.openphacts.org/index.php?option=com\\_content&view=article&id=64&Itemid=73](http://www.openphacts.org/index.php?option=com_content&view=article&id=64&Itemid=73)

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## 5 Appendix

**Document 1:** Initial GUI Analysis.



GUI Analysis.docx

**Document 2:** ChemSpider testing results



ChemSpider Web Services  
- Test results.

**Document 3/4:** IMS test results, see:

<https://universityofvienna1.basecamphq.com/projects/6361646/file/117610170/ims-test-coveraga.tar.gz>

<https://github.com/openphacts/OpsPlatform/tree/master/ops-platform/larkc-plugins/plugin.imsSgarqlExpand/src/test/java/eu/ops/plugin>

**Document 5:** LarkC core test results

For LarkC, stress testing was performed: 20 parallel threads which chose an API method at random and fired 20 requests without waiting for a response. This takes 94s to complete, and the platform responds as normal afterwards. Additional LarkC unit testing was performed and is reported in the code repository,

<https://larkc.svn.sourceforge.net/svnroot/larkc/trunk/platform/src/main/test/eu/larkc/core/>

**Document 6:** Memorandum of Understanding



OPS\_MoU

**Document 7:** Associated Partner details form



OPS\_AP details form