Revvity Signals Spotfire Lead Discovery Premium Biotech Bundle on the AWS Cloud

Quick Start Reference Deployment

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This Quick Start was created by Revvity Signals Software, Inc. in collaboration with Amazon Web Services (AWS). Quick Starts are automated reference deployments that use AWS CloudFormation templates to deploy key technologies on AWS, following AWS best practices.

Overview

This guide provides instructions for deploying the Spotfire Lead Discovery Premium Quick Start reference architecture on the AWS Cloud.

This Quick Start is for teams and individuals responsible for managing informatics infrastructure for a biotech company. It covers how to deploy an support a scientific data analysis platform based on Spotfire and Revvity Lead Discovery Premium.

The Biotech Bundle CloudFormation script is for **new installations ONLY**. For upgrades, customers will need to create a new deployment and then follow standard database and configuration migration (see ‘Data Migration’ section of this user guide).

Revvity Signals Spotfire Lead Discovery Premium Biotech Bundle on AWS

The Revvity Signals Spotfire Lead Discovery Premium Biotech Bundle provides advanced scientific data analysis tools essential for developing both small molecule and biologics-based therapies. Revvity extends the core capabilities of Spotfire with innovative data visualization and guided analysis workflows that enable scientists to elucidate the correlations of chemical structure and biological sequence variations to desired therapeutic activities. It is the essential tool used by pharmaceutical and biotechnology companies for progressing from Lead compounds to viable drug candidates.

For the first time this advanced technology stack widely deployed at global pharmaceutical companies is now available in a cost effective and easy to deploy and maintain Amazon Web Services Quick Start. This guide will detail the steps to deploy the Revvity Spotfire Lead Discovery Premium Biotech Bundle following AWS best practices. It is intended for teams or individuals who are responsible for managing and maintaining chem and bio informatics solutions at a

biotechnology company. It will accelerate the deployment for companies that are new to the Amazon cloud. Revvity's biotech bundle includes the following components:

- Spotfire Server
- Spotfire Analyst
- Spotfire Web Player Service
- Lead Discovery Premium

The deployment is performed via a CloudFormation template that creates and configures:

1. A Windows Server EC2 instance to host the Spotfire Server and Web Player
2. An RDS (PostgreSQL) instance to host the Spotfire Server Database

As this solution is intended for small scientific teams in startup environments, it is designed for maximum simplicity and minimum cost. The resources are non-redundant and deployed on a single region and availability zone. The RDS instance can optionally be replicated across two availability zones. However, Revvity Signals professional services can help scale out the environment as companies grow and require higher availability, performance, and resiliency.

Additional databases or data sources to host the scientific data under analysis are out of the scope of this deployment.

AWS costs

You are responsible for the cost of the AWS services and any third-party licenses used while running this Quick Start. There is no additional cost for using the Quick Start.

The AWS CloudFormation templates for Quick Starts include configuration parameters that you can customize. Some of the settings, such as the instance type, affect the cost of deployment. For cost estimates, see the pricing pages for each AWS service you use. Prices are subject to change.

After you deploy the Quick Start, create AWS Cost and Usage Reports to deliver billing metrics to an Amazon Simple Storage Service (Amazon S3) bucket in your account. These reports provide cost estimates based on usage throughout each month and aggregate the data at the end of the month. For more information, see What are AWS Cost and Usage Reports?

Software licenses

This Quick Start requires a license for Spotfire Lead Discovery Premium prior to deployment. Discounted licenses are issued for a fixed number of users with a minimum of 5 and a maximum of 25. Biotech Bundle discount does not apply to larger orders. Please contact Revvity via BiotechBundle@revvity.com or by calling +1 (800) 315-7300 before deployment. Your AWS account will be whitelisted to allow execution of the Quick Start upon completion of a license order from Revvity.

Deploying this Quick Start without ensuring that Revvity has whitelisted your AWS account will result in the creation of the infrastructure (EC2 and RDS instances) without any Spotfire software installed. In order for the script to complete the software installation, the customer's Amazon account must be white-listed by Revvity so that it can access a pre-configured product image from Revvity's AWS account. The order must include the customer's AWS account number and desired AWS Region in order to be processed. The script will only work for customers that have been white-listed.

Architecture

This Quick Start deploys Revvity Biotech Bundle into a new or existing virtual private cloud (VPC) in the AWS Cloud. You can create your own VPC or use an existing VPC in your AWS account. However, we recommend that you set up the VPC environment shown in Figure 1.

This environment is automatically configured for identity management, access control, encryption key management, network configuration, logging, alarms, partitioned environments (for example, to separate production, development, and management processes), and built-in compliance auditing, to help meet your security and compliance requirements.

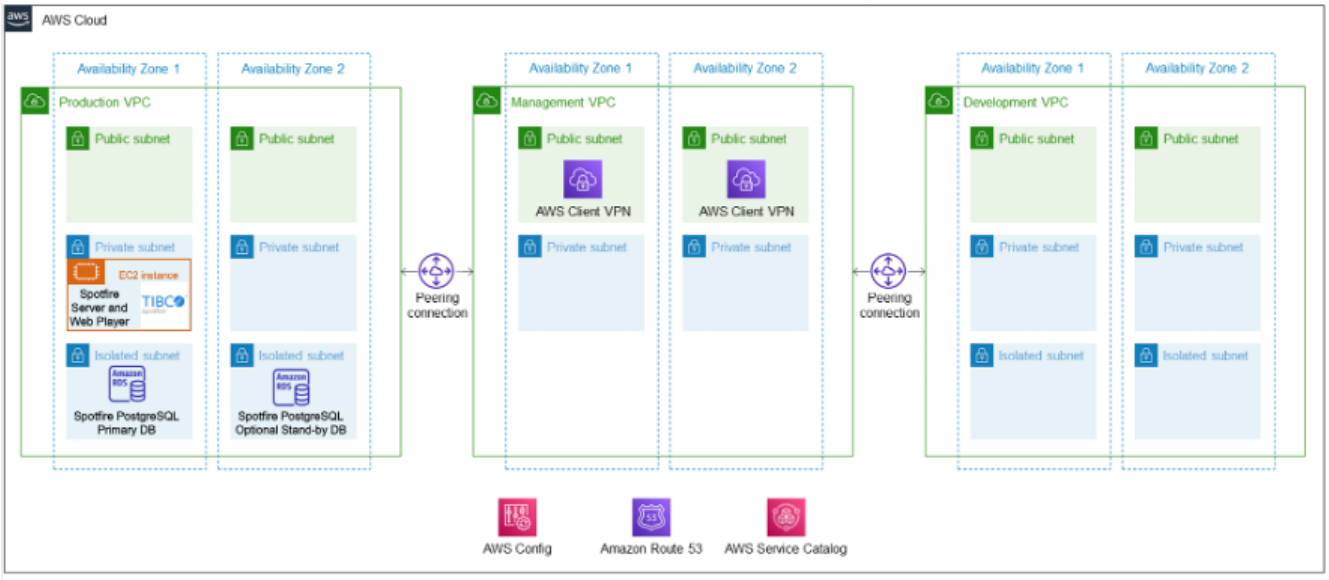


Figure 1. Quick Start architecture for Spotfire Lead Discovery Premium on AWS

As shown in Figure 1, the Quick Start sets up the following resources in the target VPC:

- In a private application subnet, a Windows Server EC2 instance with Spotfire Server, Web Player service with Revvity Lead Discovery Premium software installed and configured.
- In a private isolated database subnet, an RDS (PostgreSQL) database instance with Spotfire database and server configuration. The RDS instance may be optionally deployed as Multi-AZ for enhanced availability and durability.

The Spotfire application services are deployed in a private subnet and do not include https configuration. TLS/SSL termination if desired could be provided via an ingress load balancer, or subsequently configured on the Spotfire Server.

All customer data, including Spotfire analysis templates and Information Designs are persisted to the RDS service. All RDS data is encrypted at rest as well as in transit to the optional stand-by replica.

Planning the deployment

Specialized knowledge

This deployment requires a moderate level of familiarity with AWS services. If you're new to AWS, see Getting Started Resource Center and AWS Training and Certification. These sites provide materials for learning how to design, deploy, and operate your infrastructure and applications on the AWS Cloud.

The following links are relevant for the resources and services deployed by this Quick Start:

- AWS Cloud Formation
- Amazon Elastic Compute Cloud (Amazon EC2)
- Amazon Relational Database Service (Amazon RDS)
- Amazon Route 53
- Amazon Virtual Private Cloud (Amazon VPC)

You will need to obtain software licenses for the Revvity Signals Spotfire Lead Discovery Premium Biotech Bundle prior to deployment. Discounted licenses are issued for a fixed number of users with a minimum of 5 and a maximum of 25. Biotech Bundle discount does not apply to larger orders. Please contact Revvity Signals Software, Inc. via BiotechBundle@revvity.com or by calling +1 (800) 315-7300 before deployment. Upon completion of an order from Revvity Signals Software, Inc., your AWS account will be whitelisted to enable the installation of the software. Note that if you launch the Revvity Signals Spotfire Lead Discovery Premium Biotech Bundle CloudFormation template without confirming that your account has been whitelisted by Revvity Signals Software, Inc., the AWS resources (EC2 instance and RDS database) will be created, but they will not include the Revvity Signals Software, Inc. or Spotfire software products.

AWS account

If you don't already have an AWS account, create one at https://aws.amazon.com by following the on-screen instructions. Part of the sign-up process involves receiving a phone call and entering a PIN using the phone keypad.

Your AWS account is automatically signed up for all AWS services. You are charged only for the services you use.

Technical requirements

Before you launch the Quick Start, review the following information and ensure that your account is properly configured. Otherwise, deployment might fail.

Resource quotas

If necessary, request service quota increases for the following resources. You might need to request increases if your existing deployment currently uses these resources and if this Quick Start deployment could result in exceeding the default quotas. The Service Quotas console displays your usage and quotas for some aspects of some services. For more information, see What is Service Quotas? and AWS service quotas.

Resource	This deployment uses
EC2 Instance	1 r4.2xlarge(default)
RDS PostgreSQL	1 db.m5.2xlarge(default)
Security groups	2
AWS Identity and Access Management (IAM) roles	1
AIM Instance Profile	1

Supported AWS Regions

This Quick Start supports all AWS Regions:

Full list: https://docs.aws.amazon.com/general/latest/gr/rande.html

Certain Regions are available on an opt-in basis. For more information, see Managing AWS Regions.

IAM permissions

Before launching the Quick Start, you must sign in to the AWS Management Console with IAM permissions for the resources that the templates deploy. The *AdministratorAccess* managed policy within IAM provides sufficient permissions, although your organization may choose to use a custom policy with more restrictions. For more information, see AWS managed policies for job functions.

EC2 Key Pairs

Make sure that at least one Amazon EC2 key pair exists in your AWS account in the Region where you plan to deploy the Quick Start. Make note of the key pair name. You need it during deployment. To create a key pair, follow the instructions in the AWS documentation.

For testing or proof-of-concept purposes, we recommend creating a new key pair instead of using one that's already being used by a production instance.

Deployment options

We strongly recommend that you set up the Revvity Signals Spotfire Lead Discovery Premium Biotech Bundle on top of the based on the Figure 1 which follows industry best practices for high availability, security and regulatory compliance.

This Quick Start provides three deployment options:

- Option 1: Deploy on Figure 1
- Option 2: Deploy on an existing VPC
- Option 3: Deploy on a newly created VPC

All configuration, data, and analysis templates managed by the Spotfire Server are stored in the PostgreSQL RDS database. Amazon provides convenient and cost-effective approaches to backup and restore all your data. Refer to Amazon RDS Backup and Restore documentation for full details. By default, the Revvity Signals Spotfire Lead Discovery Premium Biotech Bundle Quick Start configures the RDS instance for automated backup of data and transaction logs with a retention time of 7 days. You can modify the retention time during deployment. You can also make modify any aspect of RDS backup after deployment as described in the above backup and restore documentation.

Deployment steps

Confirm your AWS account configuration

1. Sign in to your AWS account at https://aws.amazon.com with an IAM user role that has the necessary permissions. For details, see Planning the deployment earlier in this guide.
2. Ensure that your AWS account is configured correctly, as discussed in the Technical requirements section.

Network verification or setup

This Quick Start requires preexisting virtual network resources on which to deploy the application and database server instances. It is strongly recommended that you deploy on top of the based on the Figure 1 as it creates all the VPC and subnets required by this Quick Start using best practices for network isolation and security.

If you choose to deploy without Figure 1, then you must ensure that your target environment meets the following requirements:

1. At least one VPC is available to deploy EC2 and RDS resources
2. The VPC must have at least 2 subnets each in a different availability zone
3. The subnet chosen to deploy the EC2 instance must have outbound access to the public internet in order to download installation assets

4. It is highly recommended that the EC2 and RDS resources be deployed onto internal subnets. The security group setup by this Quick Start allows inbound traffic on port 80 (http) and 3389 (RDP) for all IP addresses routable to the subnet.
5. You must make provisions for the EC2 instance to be accessible to administrators and end users. This main involve creating internet gateways, load balancers, or VPN tunnels to route traffic the internal subnet.

Note that the application server is by default configured without an SSL/TLS certificate for https access. As such, it is recommended that you deploy the server onto an internal subnet and/or configure https access on or in front of the application server.

Launch the Quick Start

Ensure that you have met the network requirements described in the previous subsection of this document.

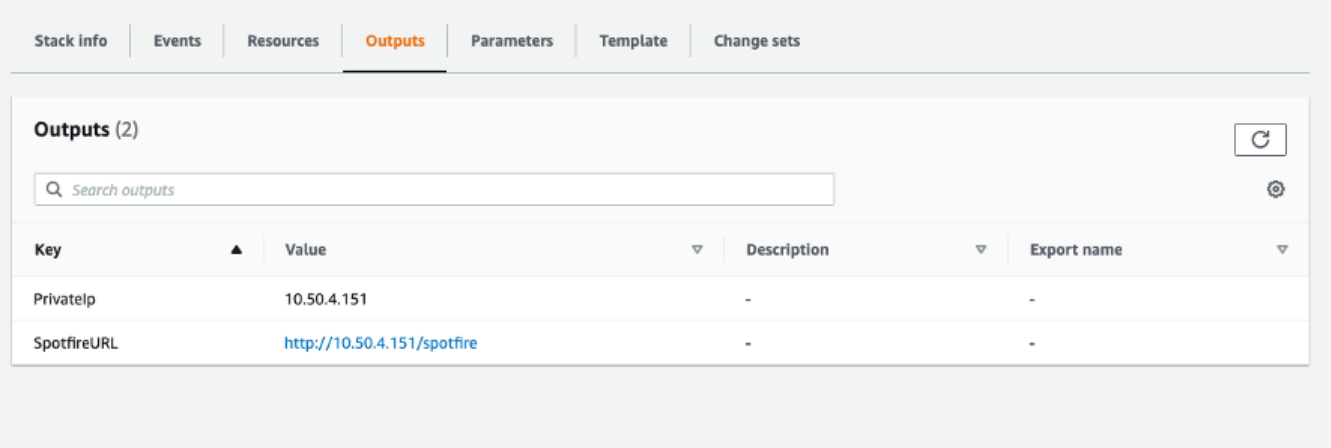
Each deployment takes about 30 minutes to complete.

1. Sign in to your AWS account and launch the CloudFormation service
2. Click the "Create Stack" button
3. Select the "upload a template file" option
4. Upload the CloudFormation yaml template provided by Revvity and click Next
5. Check the AWS Region that’s displayed in the upper-right corner of the navigation bar, and change it if necessary. This Region is where you build the network infrastructure. The template is launched in the us-east-1 Region by default. For other choices, see Supported AWS Regions earlier in this guide.
6. On the **Create stack** page, keep the default setting for the template URL, and then choose **Next**.
7. On the **Specify stack details** page, change the stack name if needed. Review the parameters for the template. Provide values for the parameters that require input. For all other parameters, review the default settings and customize them as necessary. For details on each parameter, see the Parameter reference section of this guide. When you finish reviewing and customizing the parameters, choose **Next**.
8. On the **Configure stack options** page, you can specify tags (key-value pairs) for resources in your stack and set advanced options. When you finish, choose **Next**.
9. On the **Review** page, review and confirm the template settings. Under **Capabilities**, select the two check boxes to acknowledge that the template creates IAM resources and might require the ability to automatically expand macros.
10. Choose **Create stack** to deploy the stack.
11. Monitor the status of the stack. When the status is **CREATE_COMPLETE**, the Spotfire Lead Discovery Premium deployment is ready.
12. To view the created resources, see the values displayed in the **Outputs** tab for the stack.

The Spotfire installation and configuration process begins after the stack creation completes. Please allow 10-15 additional minutes before testing the deployment.

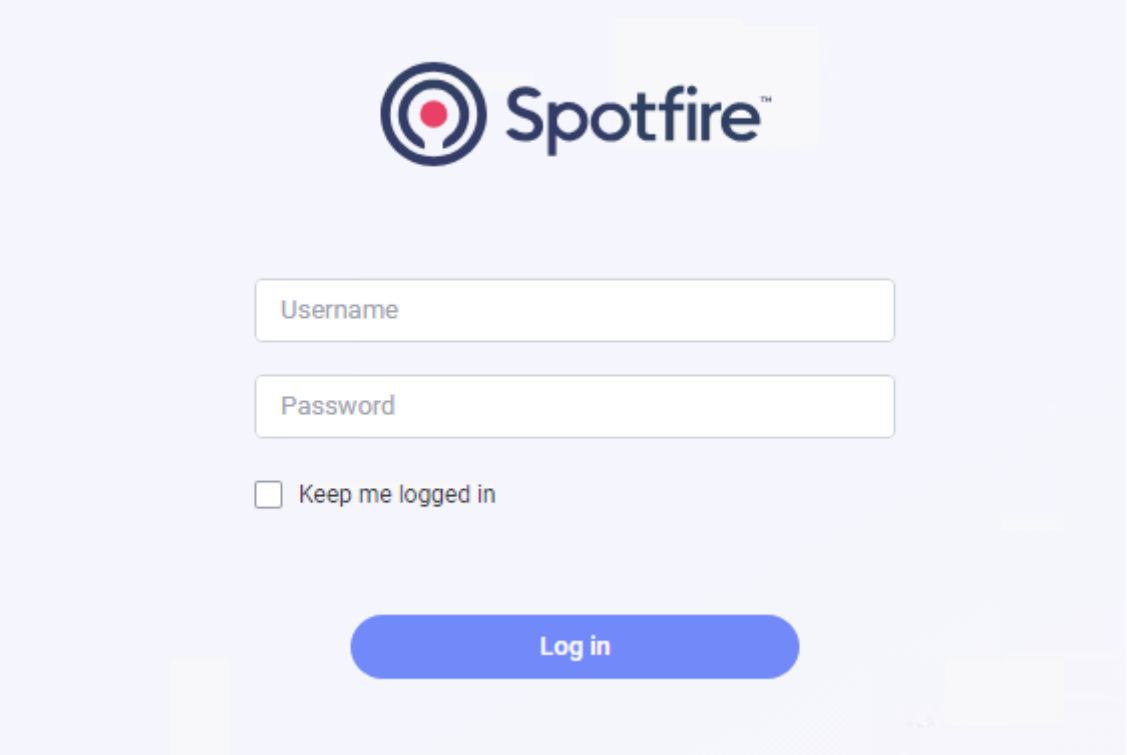
Test the deployment

- The web address to access the Spotfire Server can be found in the SpotfireURL key in the Cloud Formation Stack **output tab**:



- Allow **10-15 minutes after stack creation** before testing the Spotfire Server installation.
- Ensure that the client system you are testing from has network access to the IP of the Spotfire server. This may require connecting via a VPN client or deploying a load balancer to forward traffic from a public IP to the Spotfire server.
- You may optionally setup DNS A record within your domain to define a user-friendly host name for the Spotfire IP or external ELB address.

The Spotfire server should be accessible on port 80 via **http://<SpotfireIP>/spotfire** or **http://<hostname>/spotifre** and display the login screen:



- Login using the Spotfire Admin User and Password provided in the Stack parameters to access the administration dashboard:

Refer to the Spotfire Server Administration Documentation for details on managing the server.

Post-deployment steps

Users who wish the download and install the Spotfire Analyst client can download the installer from the Spotfire server via the following link: **http://<SpotfireIP>/client** if a host entry has been created in DNS.

- Click the **Download** button in the page to get the installer zip file:

Spotfire Analyst Client Installation Notes:

- Spotfire Analyst installer must be launched "as Administrator"
- After installation, launch the Analyst via right-click on the Desktop shortcut to elevate to Administrator privileges
- After initial login, allow the client to install updates from the server
- After second login allow the installation of Microsoft Visual C++ redistributables and ChemDraw ActiveX components required by Lead Discovery Premium

Data Migration

Please find below options to migrate data to your new server:

- You can export library content and then import it into the new server. This can be done manually from the Analyst client via the Library Administration tool or programmatically via the command line tool: Command-based library administration tasks. In either case, you will need access to the Spotfire Server either to run the command line tool or to copy/paste the file exported/imported. You will also need to have a user & password that is in the Library Administrator group. E.g.

```
cd <server installation dir>/tomcat/spotfire-bin
rem export-library-content
config export-library-content --tool-password=<user_password> --file
-path=<path_to_export> --user=<username> --item-type=all_items --library-path=/
rem import-library-content
config import-library-content --tool-password=<user_password> --file
-path=<path_to_import> --conflict-resolution-mode=KEEP_BOTH --user=<username>
--library-path=/
```

- You may also wish to export/import the user and group information from the old server to the

new one. Again this can be done manually from the Analyst client using the Import/Export tabs in the Administration Manager tool or via command line:

    - export-users
    - import-users
    - export-groups
    - import-groups

- For more migration options, please refer to Spotfire® Server: Backup and restore

Currently, it is not possible to migrate preferences.

Product Documentation

- Spotfire User Guide is accessible from the Spotfire Analyst Client via the Help menu
- Lead Discovery Premium User Guides are available from the Spotfire Analyst Client via the Help > Additional Help menu
- Spotfire Administration Guide and other resources are available on the Spotfire Documentation Site

Tehcnical Support

Your license to Revvity Signals Spotfire Lead Discovery Premium Biotech Bundle provides you access to technical support from Revvity Signals Software, Inc.. You can open a support ticket at:

```
https://support.revvitysignals.com/
```

Please provide as much detail as possible within the support ticket and ensure to include any deployment or Spotfire logs collected during the troubleshooting steps described below. Because the software is deployed in your Amazon account, Revvity Signals Software, Inc. support personnel will not have direct access to troubleshoot the issue. They may need to arrange for a remote session to review and correct reported issues.

FAQ

Q. I encountered a **CREATE_FAILED** error when I launched the Quick Start.

A. If AWS CloudFormation fails to create the stack, relaunch the template with **Rollback on failure** set to **Disabled**. This setting is under **Advanced** in the AWS CloudFormation console on the **Configure stack options** page. With this setting, the stack's state is retained, and the instance keeps running so that you can troubleshoot the issue. (For Windows, look at the log files in `%ProgramFiles%\Amazon\EC2ConfigService` and `C:\cfn\log`.)

When you set **Rollback on failure** to **Disabled**, you continue to incur AWS charges

> for this stack. Delete the stack when you finish troubleshooting.

For more information, see Troubleshooting AWS CloudFormation.

Q. I encountered a size-limitation error when I deployed the AWS CloudFormation templates.

A. Launch the Quick Start templates from the links in this guide or from another S3 bucket. If you deploy the templates from a local copy on your computer or from a location other than an S3 bucket, you might encounter template-size limitations. For more information, see AWS CloudFormation quotas.

Troubleshooting

If the Spotfire service cannot be reached at the **SpotfireURL** displayed in the Stack creation output tab:

- Check that the client machine used for testing has network connectivity to the that internal subnet. Gaining access may require additional steps like establishing a VPN connection, configuring access via a publicly available ELB, or accessing from a jumpbox via remote desktop.

If the application server EC2 instance is accessible, but the Spotfire server does not respond or responds with errors:

- Access the EC2 instance via Remote Desktop connection on port 3389
- Capture and/or review the contents of C:\logs for failures during server installation and configuration
- Check the Windows Services control panel to ensure that the Spotfire Service is running
- Capture and/or review Spotfire Server Logs at C:\spotfire\spotfireserver\14.0.2\tomcat\logs
- Check that the Spotfire Server configuration and database access by using Configure Spotfire Server 14.0.2LTS application.
- Ensure that the tool can connect to the RDS database by entering the configuration tool password which you provided during Stack creation.
- If necessary, create a new bootstrap file using the hostname and credentials for your RDS database.
- Review and save the Spotfire Server configuration to the database
- Restart the Spotfire Service using the Windows Services control panel

If the SpotfireURL responds, but you are unable to login using the username and password you provided during Stack creation:

- Access the EC2 instance via Remote Desktop connection on port 3389
- Launch the Configure Spotfire Server 14.0.2LTS application.
- Enter the configuration tool password which you provided during Stack creation

- Use the Administration tab in the Configuration tool to verify the expected admin user exists and/or create a new administrative user before attempting to login again

If during troubleshooting, you are unable to gain access to the Configuration tool because the bootstrap file does not exist or you don't have the correct Tool password:

- Create a new bootstrap file to connect the Spotfire Service to your RDS instance
- Review and save the Spotfire Server configuration to the database
- Restart the Spotfire Service using the Windows Services control panel

Customer responsibility

After you successfully deploy this Quick Start, confirm that your resources and services are updated and configured — including any required patches — to meet your security and other needs. For more information, see the AWS Shared Responsibility Model.

Parameter reference

Unless you are customizing the Quick Start templates for your own deployment projects, keep the default settings for the parameters labeled **Quick Start S3 bucket name**, **Quick Start S3 bucket Region**, and **Quick Start S3 key prefix**. Changing these parameter settings automatically updates code references to point to a new Quick Start location. For more information, see the AWS Quick Start Contributor's Guide.

Launch into an existing VPC

Table 1. AWS Quick Start Configuration

Parameter label (name)	Default value	Description
Quick Start S3 bucket name (`QSS3BucketName`)	`aws-quickstart`	S3 bucket name for the Quick Start assets. Quick Start bucket name can include numbers, lowercase letters, uppercase letters, and hyphens (-). It cannot start or end with a hyphen (-).
Quick Start S3 key prefix (`QSS3KeyPrefix`)	`ldp-biotech-bundle/`	S3 key prefix for the Quick Start assets. Quick Start key prefix can include numbers, lowercase letters, uppercase letters, hyphens (-), and forward slash (/).

Table 2. Network Configuration

Parameter label (name)	Default value	Description
VPC ID (VpcId)	**Requires input**	The VPC on which resources will be created
Application Subnet (AppSubnet)	**Requires input**	Subnet ID for App
DB Subnet A (DBSubnetA)	**Requires input**	Subnet ID for primary DB instance.
DB Subnet B (DBSubnetB)	**Requires input**	Subnet ID for secondary DB instance.

Table 3. Database Configuration

Parameter label (name)	Default value	Description
DB Instance Type(DBInstanceClass)	db.m5.2xlarge	NO_DESCRIPTION
DB Instance Id(DBInstanceId)	spotfire	The name of the RDS instance. Ensure it does not conflict with an existing postgresql RDS database identifier. — default is spotfire.
DB Instance Engine Version(DBInstanceEngineVersion)	15.7	The name of the RDS instance engine version. For detailed information about postgresql versions, please refer to https://docs.aws.amazon.com/AmazonRDS/latest/PostgreSQLReleaseNotes/postgresql-versions.html
Main DB User Name(DBUserName)	postgres	The name of the main database user. — default is postgres and not changeable.
Main DB Password(DBUserPassword)	**Requires input**	The main password for the database instance. Must be between 8 and 32 characters containing letters, numbers and symbols
Spotfire DB Name(ServerDBName)	spotfiredb	The name of the spotfire server database. — default is spotfiredb.
Spotfire DB User(ServerDBUser)	spotfire	The name of the user that connects to Spotfire Server database. — default is spotfire.
Spotfire DB Password(ServerDBUserPassword)	**Requires input**	The password for the user that connects to Spotfire Server database. Must be between 8 and 32 characters containing letters, numbers and symbols

Parameter label (name)	Default value	Description
DB Multi-AZ Replication(`DBMultiAZ`)	`false`	Whether RDS is setup with Multi-AZ replication. true/false — default is false.
DB Disk Storage(`DBAllocatedStorage`)	`100`	The disk space (GiB) allocated to the database (between 5 and 65536 GiB)
DB Backup Retention(`DBBackupRetentionPeriod`)	`7`	The number of days for which automated backups are retained (between 0 and 35)

Table 4. EC2 Configuration

Parameter label (name)	Default value	Description
EC2 Instance Type (`EC2InstanceClass`)	`r4.2xlarge`	Amazon EC2 Instance Type
Windows Image (`LatestAmiId`)	**`Requires input`**	The ID of AMI shared by the Revvity for your deployment region
SSL Key Name (`KeyPair`)	**`Requires input`**	EC2 key pair for creating/accessing the instance
EC2 Admin User (`EC2InstanceUserName`)	**`Requires input`**	Name for admin user on EC2 instance
EC2 Admin User Password (`EC2InstanceUserPassword`)	**`Requires input`**	Password for admin user on EC2 instance. Must be between 8 and 32 characters containing letters, numbers and symbols

Table 5. Spotfire Configuration

Parameter label (name)	Default value	Description
Sotfire Admin User (`SpotfireAdminUser`)	`spotfireadmin`	Name for admin user on Spotfire service

Parameter label (name)	Default value	Description
Spotfire Admin Password (`SpotfireAdminUserPassword`)	**`Requires input`**	Password for admin user. Must be between 8 and 32 characters containing letters, numbers and symbols
Spotfire Config Tool Password (`SpotfireToolPassword`)	**`Requires input`**	Password for the Spotfire configuration tool. Must be between 8 and 32 characters containing letters, numbers and symbols

Quick Start reference deployments

See the AWS Quick Start home page.

Notices