Why transition to WebIDQ

Content

1   Why WebIDQ

1.1   What is WebIDQ

WebIDQ is the next evolution of biocrates' workflow management and data processing software. As an essential companion to the biocrates metabolomics kits, WebIDQ guides users from sample registration and plate layout customization, through metabolite quantification, data normalization, and exporting the results in various file formats. It features state-of-the-art security protocols and integration with My biocrates portal.

1.2   WebIDQ features

WebIDQ accelerates research and takes biocrates' metabolomics technology to the cloud. Building on the proven functionality of the MetIDQ software, WebIDQ is redesigned from the ground up for ease of use. New features (described below) including the new MetaboINDICATOR extension lighten your workload and make WebIDQ the go-to companion for quantitative metabolomics.

Advanced features streamline sample analysis and give confidence in metabolomics results:

− **Automated peak picking**

  The new automated peak picking feature, based on machine learning, increases reproducibility, simplifies peak integration, and speeds up metabolite quantification.

− **Improved performance assessment**

  New validation and monitoring features enhance performance assessment, providing a higher confidence in the analytical quality of the data. Accuracies and coefficients of variation (CVs) are calculated across quality control replicates within each plate and across plates.

− **Easy user management**

  WebIDQ is accessible through the My biocrates portal where users, roles, and rights can be managed. A WebIDQ subscription allows multiple concurrent users to collaborate across projects and groups more efficiently within an organization.

− **More flexibility**

  WebIDQ cloud software is accessible from any computer with internet access at any time.

− **Worry-free cloud-based service (cloud version only)**

  Database backups and maintenance are performed by biocrates. Software updates go live immediately, and users always have access to the latest version.

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2 New WebIDQ key features

WebIDQ has all essential functions of MetIDQ plus many new features.

Feature	MetIDQ	WebIDQ
Integrated user manual	✖	✔
Sample and project administration	✔	✔
Layout and worklist generation/export	✔	✔
Support SCIEX OS software	✖	✔
Quantification of FIA data across all kit products	✔	✔
Quantification of LC data across all kit products	✖	✔
AI-based automated peak picking and integration	✖	✔
Technical validation	✔	✔
New integration and validation features	✖	✔
MetaboINDICATOR for all kits	✖	✔

3 WebIDQ versions and service options

To provide the best support, security, and ongoing development, WebIDQ is available as a subscription service model separate from the kits and other service products.

WebIDQ is available as a cloud or on-premises subscription. WebIDQ cloud is designed to take full advantage of the cloud-based infrastructure, offering new features and improved performance.

An on-premises version is available for institutions with restrictive policies. With a WebIDQ on-premises version all measurement data is stored locally and only user management and authentication take place in the cloud. This version does not offer all features.

biocrates highly recommends the cloud-based option, as it has powerful advantages compared to on-premises (see section 3.1 and 3.2).

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3.1   Key features cloud vs. on-premises

Feature	WebIDQ cloud	WebIDQ on-premises
MetIDQ functions	✓	✓
New and improved features	✓	✓
MetaboINDICATOR	✓	✓
Automatic backups and updates	✓	✗
Access from anywhere via browser	✓	✗
Instant security patches and bug fixes	✓	✗

3.2   Technical differences between cloud and on-premises version

| Feature	WebIDQ cloud	WebIDQ on-premises
Server setup	Quick start – No server installation required (Easy and secure access)	Database and WebIDQ installation on a central server on the local network (comparable to MetIDQ)
Database system	Worry-free cloud-based service. biocrates is responsible for infrastructure, maintenance, and backups	PostgreSQL User responsible for database upkeep
Software updates	Automated updates and immediate access to new features	Manual installation of updates on the server is required
Performance	Improved performance – All computations performed in the cloud	Limited by local hardware – All computations performed on the local server
Customer support	Priority support (including database issues)	Standard support (not including database issues)
Storage	Pay what you need. Different storage plans available	Limited by local hardware and database type

3.3 Cloud infrastructure and security

biocrates' infrastructure is designed with several layers of protection to help ensure data security during transmission, storage, and processing. Protections include industry standard encryption and security protocols. Our information security team continuously implements new security controls and monitors all services for malicious activity across physical data centers, networks, and IT devices. WebIDQ's infrastructure is secured by routine backups and recovery procedures for restoring services in case of unforeseen events.

4 MetIDQ-WebIDQ transition for existing customers

4.1 Timelines

MetIDQ support will continue until April 30th, 2024, while new kit and service products along with future updates will be exclusive to WebIDQ. MetIDQ support may be extended on case-by-case for users with ongoing studies. The transition scheme and timelines are below.
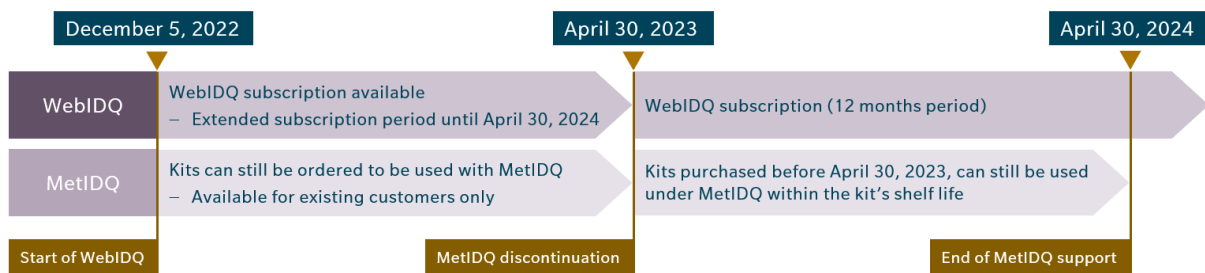
Please note

− There will be no more MetIDQ updates. Future updates, i.e. new QC batches, will only be available for WebIDQ.

− We strongly encourage users to perform the software update and to migrate the MetIDQ database before starting a new project.

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4.2 Transition and database migration

WebIDQ has built-in tools to migrate existing MetIDQ databases to the cloud. Below is a step-by-step guide for accessing the new WebIDQ software and migrating (cloud) or updating (on-premises) your existing database.

4.2.1 Cloud version

Step	Description
1. Account creation	Create a biocrates account for subscription and user management, authentication, and webshop access
2. Purchase subscription	Purchase a WebIDQ cloud subscription via webshop or business development representative
3. Database backup	Create a MetIDQ database backup prior to migration
4. Database migration	Use the WebIDQ migration wizard to transfer your local data to the cloud

4.2.2 On-premises version

Step	Description
1. Account creation	Create a biocrates account for subscription and user management, authentication, and webshop access
2. Purchase subscription	Purchase a WebIDQ on-premises subscription via webshop or business development representative
3. Database backup	Create a MetIDQ database backup prior to migration
4. Installation	Download WebIDQ and install on your local WebIDQ and database server
5. Database migration	Migrate your MetIDQ database

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5 FAQ

5.1 Can I continue to purchase biocrates kits with MetIDQ?

All kits (except MxP® Quant 500 XL) purchased by April 30, 2023, can be used with MetIDQ. After April 30, 2023, MetIDQ will be discontinued, but support will continue until April 30, 2024. All biocrates kits purchased after April 30, 2023 will require a WebIDQ subscription. **Please note that the new MxP® Quant 500 XL kit is not compatible with MetIDQ and requires WebIDQ.**

5.2 Can I migrate my MetIDQ data to WebIDQ?

Yes, WebIDQ includes a migration wizard and online instructions that help to easily move MetIDQ data to WebIDQ. Our customer support team will be there for you should you need any assistance.

5.3 Can I use MetIDQ and WebIDQ in parallel?

No, MetIDQ and WebIDQ cannot be used in parallel. We strongly recommend fully migrating your MetIDQ data to WebIDQ before you start using WebIDQ. During the migration process, the WebIDQ database will be overwritten by the MetIDQ database.

5.4 Can I migrate from MetIDQ to WebIDQ in the middle of a project? Is the data comparable?

The data processed under WebIDQ aligns with the data processed under MetIDQ. Comparability is further ensured through data normalization in WebIDQ, which corrects for deviations in accuracy and batch effects. When publishing results, all data should have been processed with the same software to avoid confusion for the reviewer and reader. To minimize complications and maintain a consistent workflow, we recommend updating the software after completion of an ongoing project. As of May 1st, 2024, MetIDQ will become obsolete and will no longer be supported. Please contact support@biocrates.com for any assistance.

5.5 What are the recommended system requirements for WebIDQ?

Please refer to our latest specifications:
https://shop.biocrates.com/faq/What-are-the-system-requirements-for-WebIDQ

5.6 Does WebIDQ need to communicate with the Mass Spectrometry (MS) vendor software?

No, WebIDQ works independently from the MS software. The MS data files can be processed in WebIDQ without the need for the MS software.

5.7 Can I have multiple users from my organization in WebIDQ?

Yes, multiple users can work concurrently in WebIDQ.

5.8   What happens to my data if I don't renew my subscription?

This depends on the type of subscription.

WebIDQ cloud subscription: In case of subscription expiration, WebIDQ changes to a read-only mode. Read-only access to WebIDQ lasts for 30 days during which a subscription can be renewed, and results can and should be easily downloaded to your local computer or network. After the read-only period, the account is marked for deletion. Data will be deleted once a quarter.

On-premises subscription: After the expiration of the subscription, WebIDQ changes to a read-only mode. Read-only access to WebIDQ lasts for 30 days during which results can and should be easily downloaded to your local computer. Data backup and retention depends on the local database server. biocrates will not delete any data.

5.9   I would like to choose the cloud version, but my IT administrator does not like it, or our internal rules do not permit cloud versions

There is a general market transition from local to cloud-based applications. Many leading software providers have shifted their services to the cloud (e.g. Microsoft, Oracle, Google) as benefits exceed the disadvantages. In case your institutional restrictions apply, you may use the on-premises subscription. You can always migrate from on-premises to cloud-based subscription any time. Many organizations tend to change positions over time and may allow exceptions. Please reach out to us with any questions or concerns.

5.10   Where is the data residence of biocrates cloud applications?

All data of biocrates cloud applications, i.e. biocrates webshop, My biocrates, WebIDQ cloud and QMDB, are stored in an European data center.

5.11   Is my data in the cloud safe

biocrates is committed to protecting and honoring your privacy rights. We fully comply with the GDPR regulations. Each organization gets their own secure and unique database instance assigned for their data. It is not possible to access other organizations' data. All client-to-service communication is encrypted (SSL protection). Access within the organization is managed by user role management through the organizations' administrators. biocrates may use anonymized data for error handling and to improve the application. For details, please refer to our privacy policy and terms and conditions.

> **i**   Please check our **support FAQ** for solutions to common performance issues and technical questions or contact us: **support@biocrates.com**.