2021 INTERNATIONAL QA CONFERENCE

3RD–5TH NOVEMBER 2021

LONG TERM DATA READABILITY AND GXP COMPLIANCE SESSION

4TH NOVEMBER 2021

Implementation of the OECD/MHRA guidance on legacy software management in virtual environments

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INTACT DIGITAL

Software use for data readability

Long-term access to archived data and reliable reconstruction of research studies from raw data

Organisation for Economic Co-operation and Development

6.16 Archive.

When legacy systems can no longer be supported, consideration should be given to the importance of the data, and if required, to maintaining the software for data accessibility purposes. This may be achieved by maintaining software in a virtual environment.

OECD SERIES ON PRINCIPLES OF GOOD LABORATORY PRACTICE AND COMPLIANCE MONITORING, Number 22. Advisory Document of the Working Party on Good Laboratory Practice on GLP Data.

Regulations on data integrity

ALCOA+ Data integrity requirements

Attributable
Document must clearly identify who has created and contributed to them, and be protected against falsification or forgery of those details

Legible
Stored documentation must be legible and easy to read

Contemporaneous
Documentation should demonstrate and support contemporaneous record-keeping

Original
Storing original copies of documentation guarantees accuracy and confidentiality

Accurate
The processes and procedures by which companies record and keep their documentation up to date must ensure accuracy and reliability

+Complete
All documentation must have an audit trail to show no data has been deleted or lost

+Consistent
Documentation must be date and time stamped and stored in such a way to prove it has been assembled in the expected sequence

+Enduring
Data must be available for as long as the regulation requires

+Available

- Archived study data in electronic form must remain immutable, readable and 'dynamic', i.e., interactive
- Reproducibility of study results requires software to remain functional and usable.

Challenges

- Software is subject to rapid obsolescence if not regularly updated
- Updated software cannot guarantee the same functionality and output as the original software version.

Digital preservation perspective

- Entire archived study is a ‘digital object’ to be preserved
  - Raw digital data and derived information
  - Study reports and documentation.
- **Significant properties** of the digital object are intrinsically tied to the data types and representation that results from the software use.

Preservation principles considered **sufficient to preserve significant properties of archived studies**:

Data integrity – verified through checksum of electronic data files

Software integrity – verified functionality of the legacy software.

Compliance considerations

DATA INTEGRITY

Extent to which data is complete, consistent and accurate throughout the data lifecycle from data collection to analysis and archiving

- ☑ **Complete**
  All the required data needs to be collected and stored
- ☑ **Unaltered**
  Data must not be changed
- ☑ **Secure**
  Data must not be destroyed
- ☑ **Confidential**
  Data must not be disclosed to unauthorised individuals
- ☑ **Usable**
  Study metadata needs to provide context for experts reproducing study results

SOFTWARE INTEGRITY

Extent to which a software installation is functional, reliable, and usable throughout its lifecycle from operational use to archived study reproducibility.

- ☑ **Functional**
  Software installation must stay operational
- ☑ **Unaltered**
  Software must not be changed
- ☑ **Secure**
  Software installation must not present risks from cyber attacks and confidentiality breaches
- ☑ **Accessible**
  Software installation needs to be easily accessed for repeated use

Requirements: Human factors

ARCHIVIST	Study records and raw data are stored and preserved by archivists, following the instructions of scientists.
RESEARCHER	Studies are reconstructed by scientists. Use of the specialty software is outside the scope of archivists' competences.
IT SPECIALIST	Software installation and management is a matter for IT specialists, particularly use of legacy operating systems that present security risks.

How to achieve preservation and reliable use of archived research study, considering

- Long-term retention of knowledge and skill-sets
- Separation of concerns and competencies among three types of specialists.

About software virtualization

- Why is software important for digital content use?
- Why do we need legacy software?
- Why does the software become obsolete?

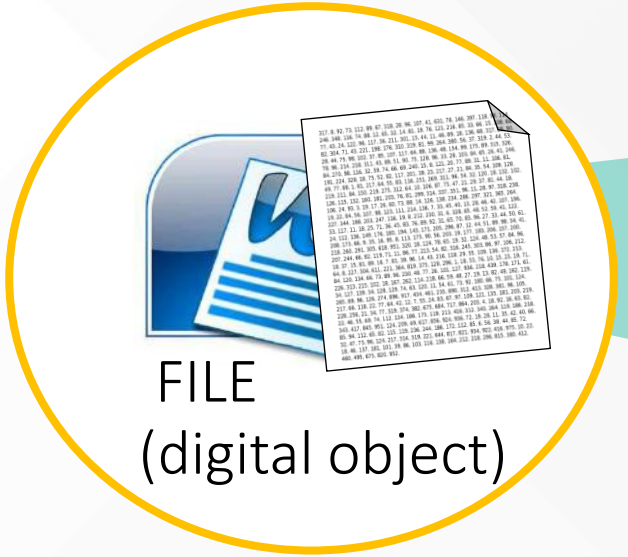
- What is virtualization and virtual machines?
- How can virtualization help with long term data access?
- What do we need to consider in order to use virtualization for GXP compliance?

Digital depends on software

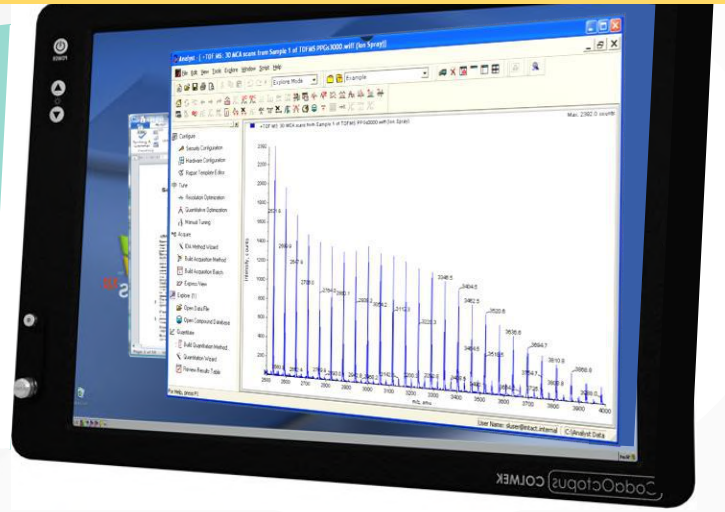
Digital content cannot be used without software that can ‘play’ it.

- Digital data and content are persisted as computer files
- Software is needed to process the files and represent digital encoding in a human readable form
- For consistent presentation of data, **integrity of both data files and software must be ensured.**

DIGITAL ‘ARTEFACT’



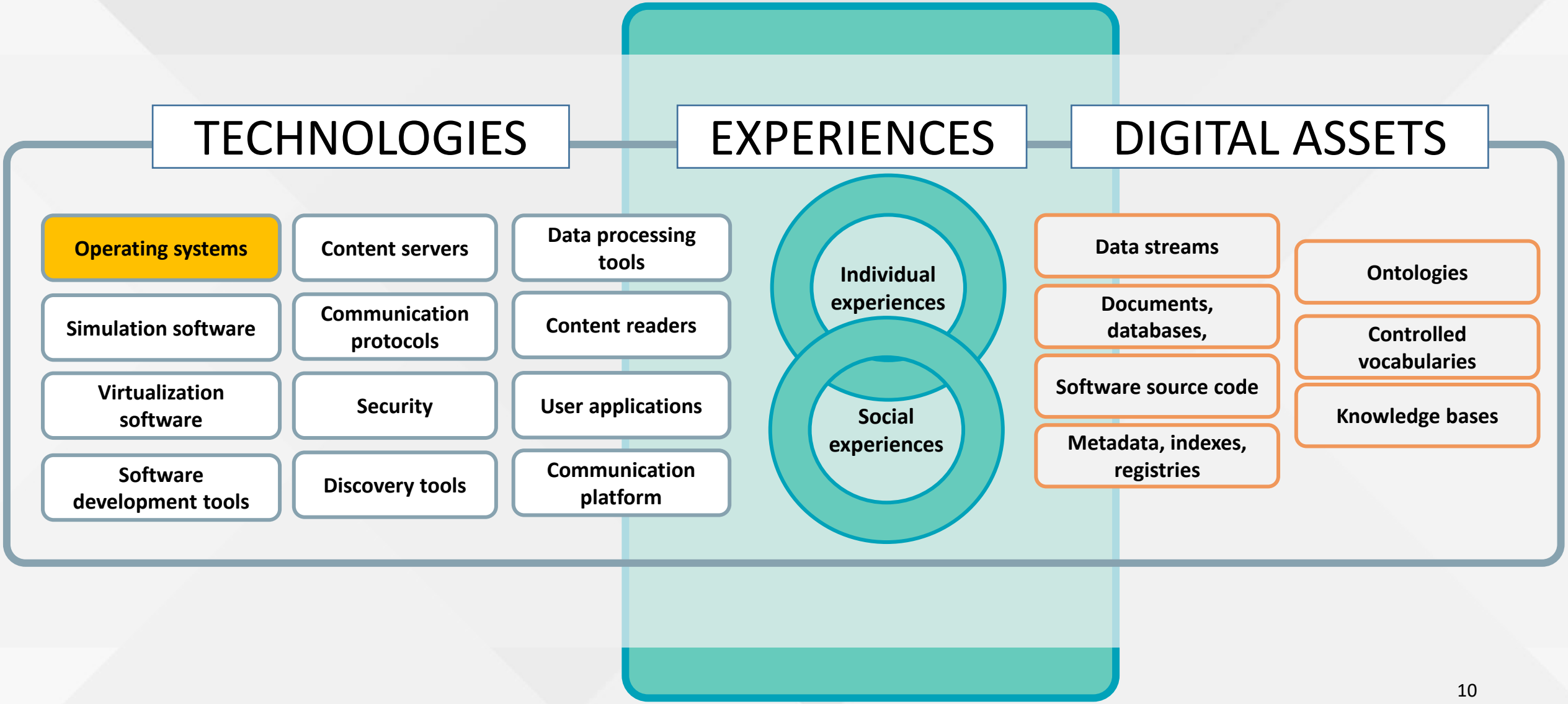
SOFTWARE
(file decoder)



Persisted part of the digital artefact

Hardware to process and display

Digital Ecosystem



Impact of OS obsolescence

	Windows xp	Windows Vista	Windows 7	Windows 8.1	Windows 10
End of Extented Support	2014-04-08	2017-04-11	2020-01-14	2023-01-10	2026-01-16

	Windows Server 2003	Windows Server 2008	Windows Server 2012	Windows Server 2016
End of Extented Support	2015-07-14	2020-01-14	2023-10-10	2027-01-11

Microsoft Windows

Released for sale:
2001

End of extended support:
2014

Released for sale:
2009

End of extended support:
2020

SARS Epidemic 2002-2004

Started 16 Nov 2002

Severe Acute Respiratory Syndrome Coronavirus

SARS-CoV or SARS-CoV-1

Access and validation of all studies since 2001 are now affected.

Quality by agility
REFLECT | CHALLENGE | INNOVATE

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Legacy software in a Lab environment

Current practice: Keep the operational system

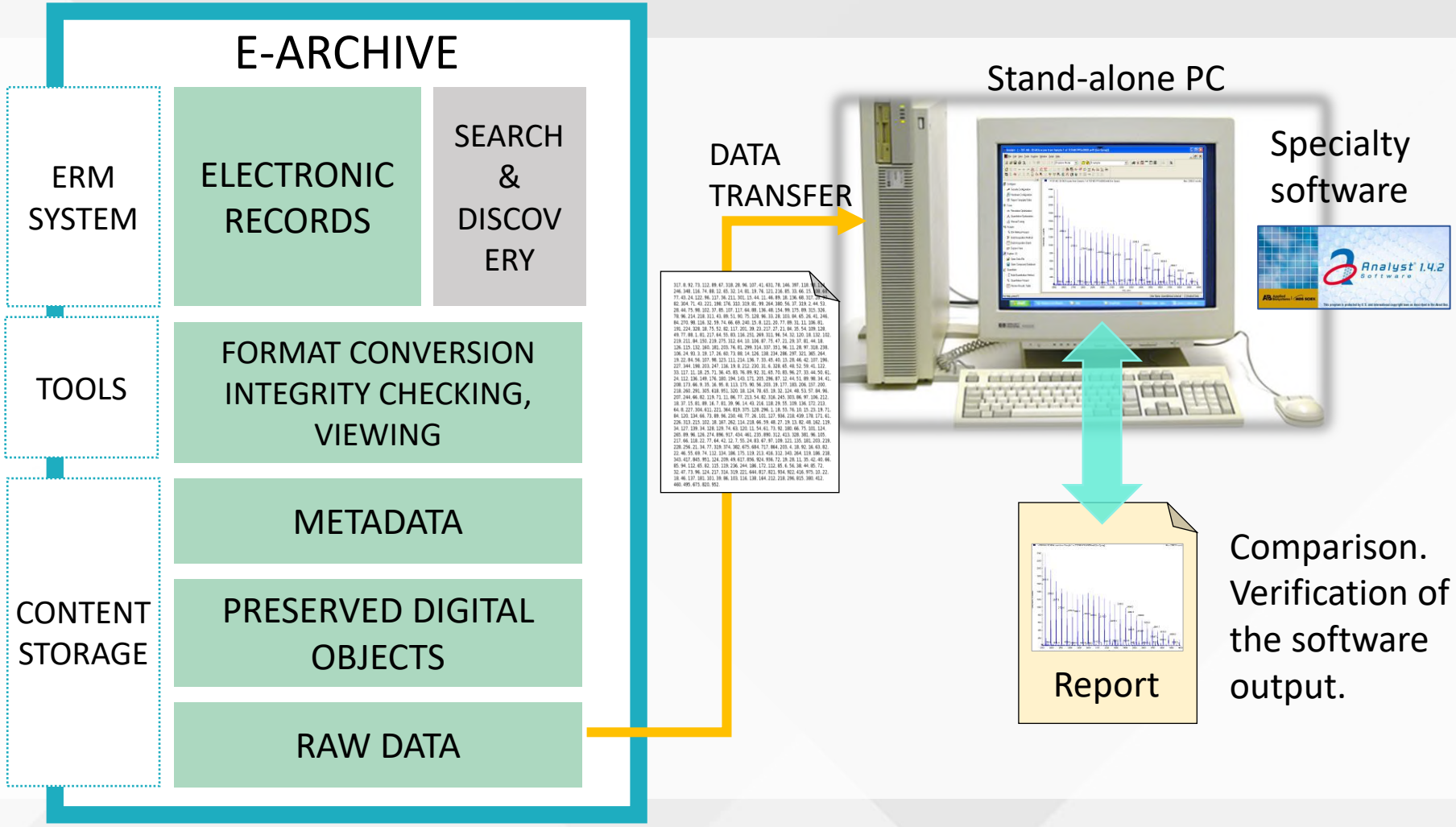
E-ARCHIVE

ERM SYSTEM	ELECTRONIC RECORDS	SEARCH & DISCOVERY
TOOLS	FORMAT CONVERSION INTEGRITY CHECKING, VIEWING	
CONTENT STORAGE	METADATA	
	PRESERVED DIGITAL OBJECTS	
	RAW DATA	

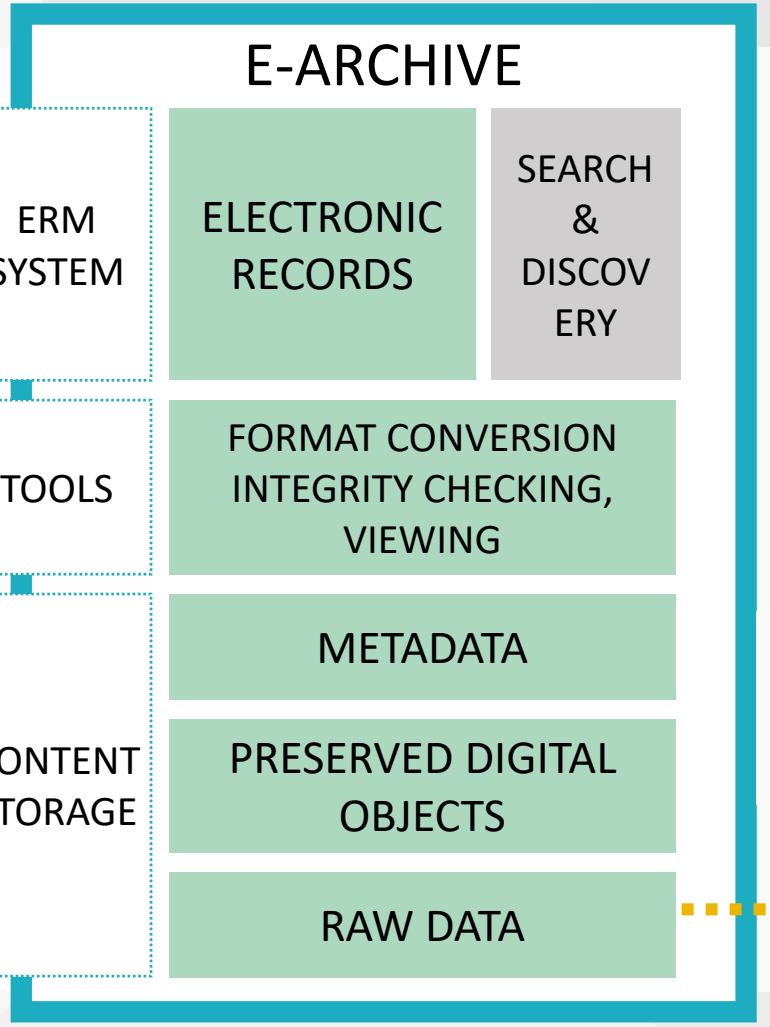
Stand-alone PC

Specialty software

Current practice: Transfer data to a local PC



Technology obsolescence impact



PHYSICAL DATA TRANSFER

System isolation, to mediate security risks

If hardware fails, re-install software.

Technology obsolescence

- Unsupported PC hardware
- Unsupported operating system (Windows XP, Windows 7)
- Unsupported application
- Compatible software may not be available.

Re-install software in virtual machines

E-ARCHIVE

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	RAW DATA	

Stand-alone PC

VIRTUALIZATION

SOFTWARE LIBRARY

Virtualized software

- Software hosting with no risk from hardware obsolescence
- Validated software installations
- Remote access through Virtual Desktops (in standard browsers).

Re-install software in virtual machines

E-ARCHIVE

ERM SYSTEM	ELECTRONIC RECORDS	SEARCH & DISCOVERY
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Stand-alone PC

VIRTUALIZATION

SECURE DATA TRANSFER

- Data is transferred secure for study reconstruction
- Data is removed from the Software Library once the task is completed.

SOFTWARE LIBRARY

Virtualized software

- Software hosting with no risk from hardware obsolescence
- Validated software installations
- Remote access through Virtual Desktops (in standard browsers).

Study reconstruction

E-ARCHIVE

ERM SYSTEM	ELECTRONIC RECORDS	SEARCH & DISCOVERY
TOOLS	FORMAT CONVERSION INTEGRITY CHECKING, VIEWING	
CONTENT STORAGE	METADATA	
	PRESERVED DIGITAL OBJECTS	
	RAW DATA	

SOFTWARE LIBRARY

Virtualized software

Data Transfer Desktop

Study reconstruction

E-ARCHIVE

ERM SYSTEM

TOOLS

CONTENT STORAGE

ELECTRONIC RECORDS

SEARCH & DISCOVERY

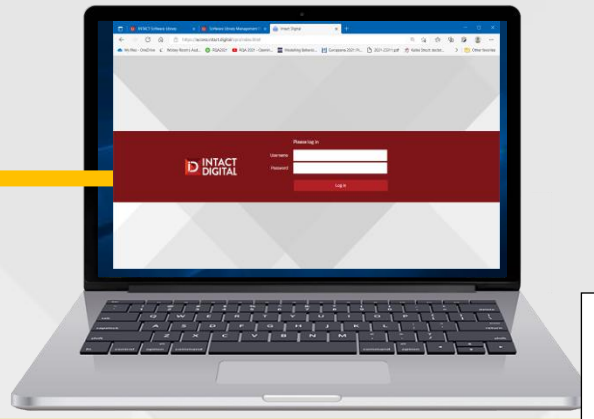
FORMAT CONVERSION INTEGRITY CHECKING, VIEWING

METADATA

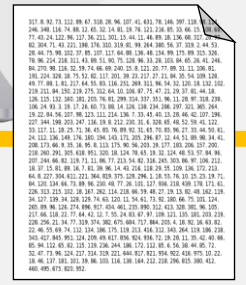
PRESERVED DIGITAL OBJECTS

RAW DATA

Virtual Desktop



Secure transfer of raw data

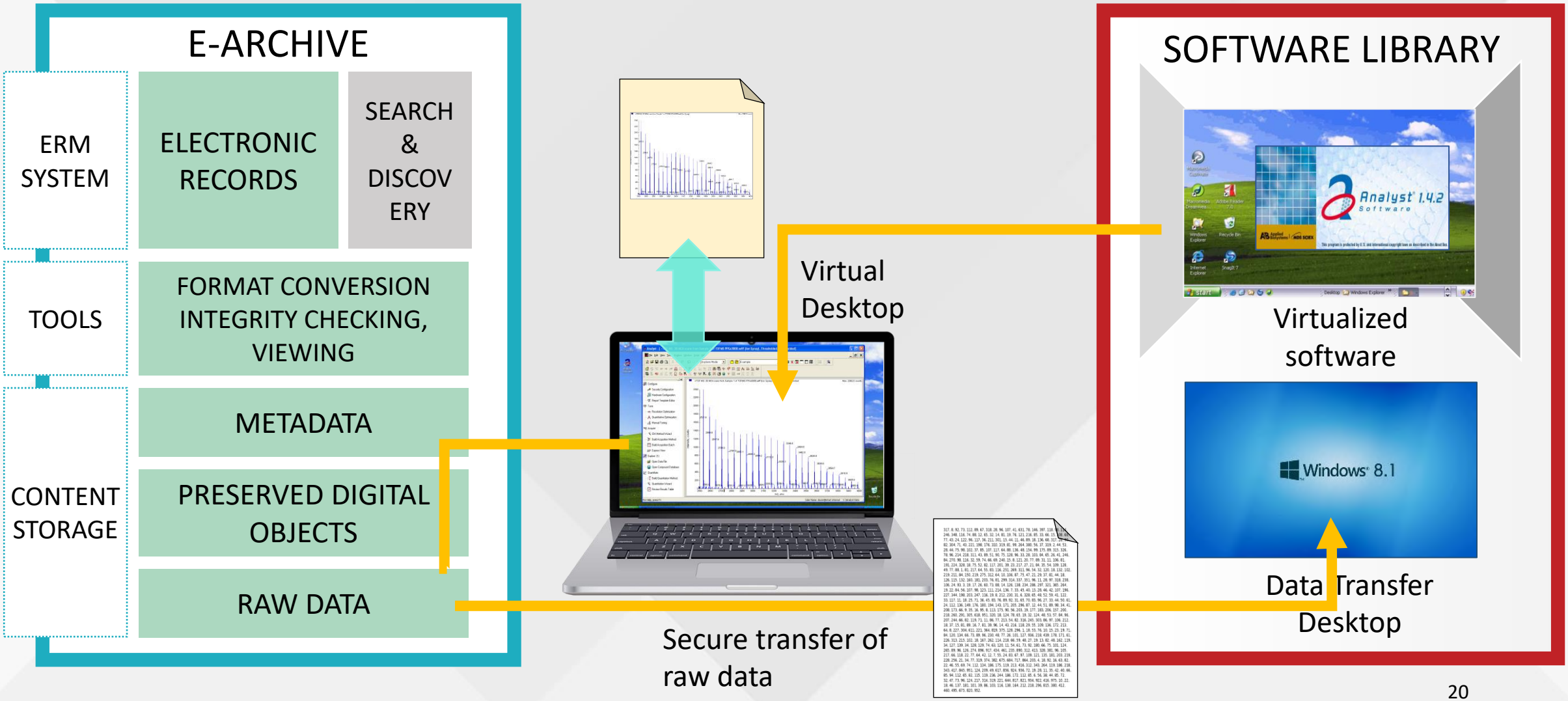


SOFTWARE LIBRARY

Virtualized software

Data Transfer Desktop

Study reconstruction



What is virtualization? How does it work?

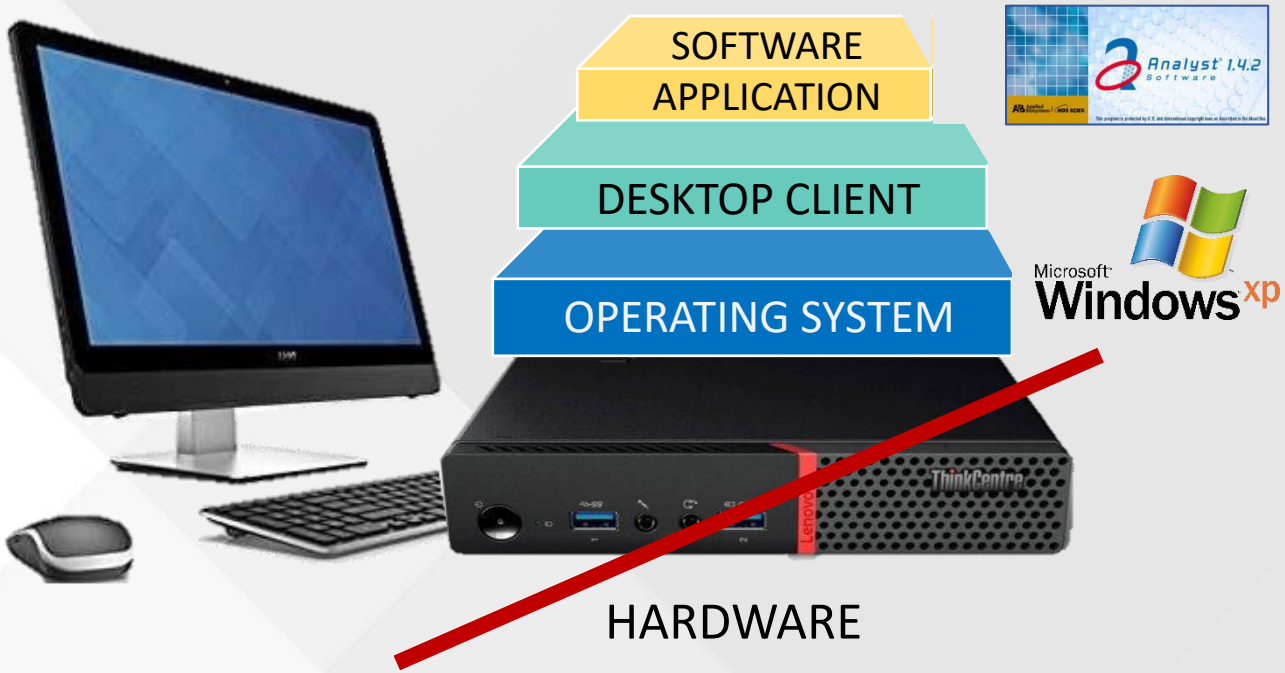
Physical computer

A physical computer has

- Hardware
- Operating system
- Desktop
- Software applications

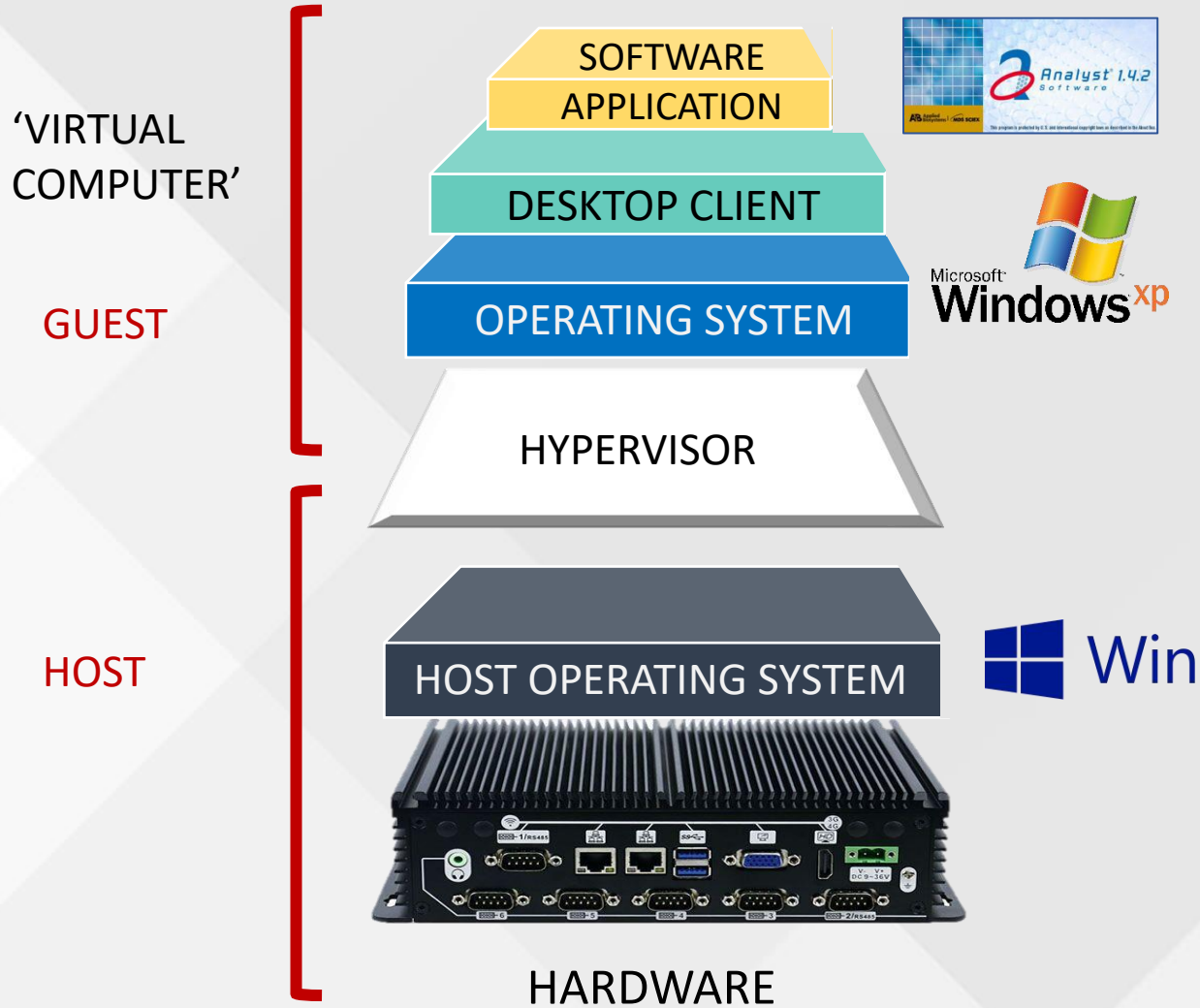
Operating system is a collection of programs that manage hardware, user interaction with he desktop and execution of the applications.

Physical computer: Obsolescence



- Hardware needs to be changed
- Operating system has to be shielded.

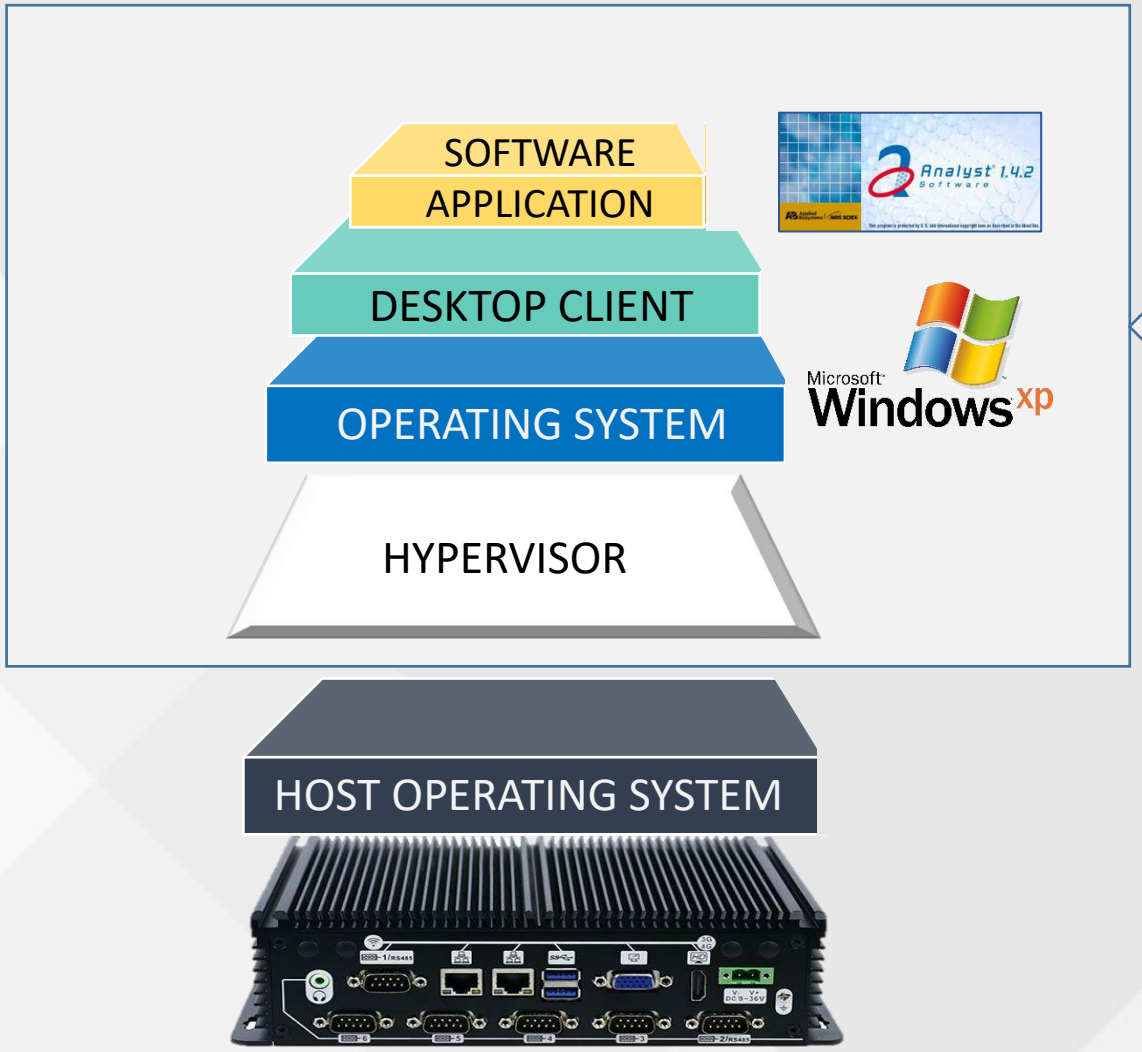
Virtualized computing environment



Legacy operating system runs as a 'GUEST' on a modern 'HOST' computing system.

Hypervisor 'translates' the GUEST operations so that they can be executed on the HOST.

Virtualized computing environment

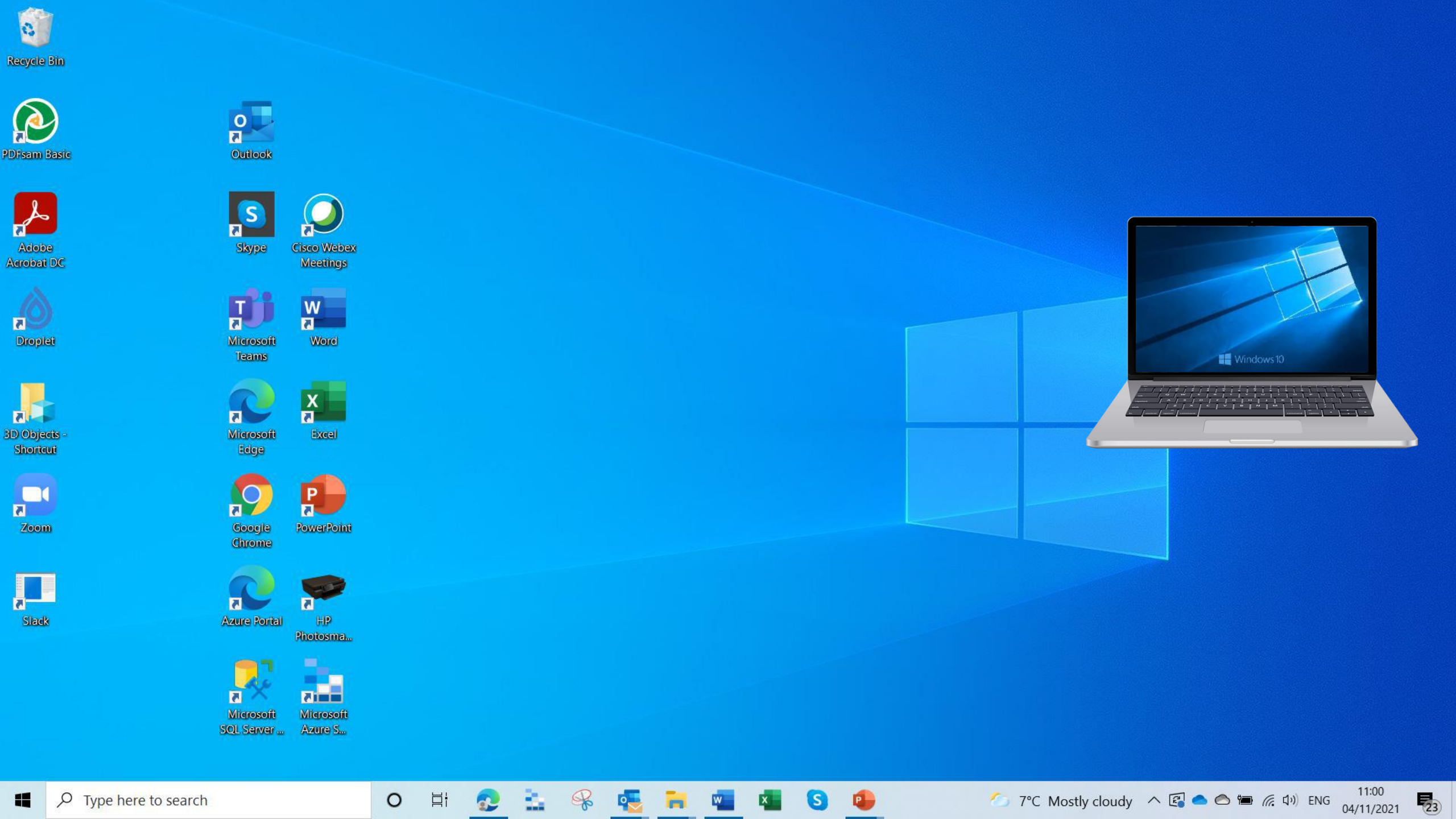


Remote access enables

- Secure access to the virtual machines
- Passing the mouse and typing instructions to the VMs
- Display of the outcomes on the user screen.

Example

- Virtual environment with installed software in virtual machines
- Remote access from a secure personal laptop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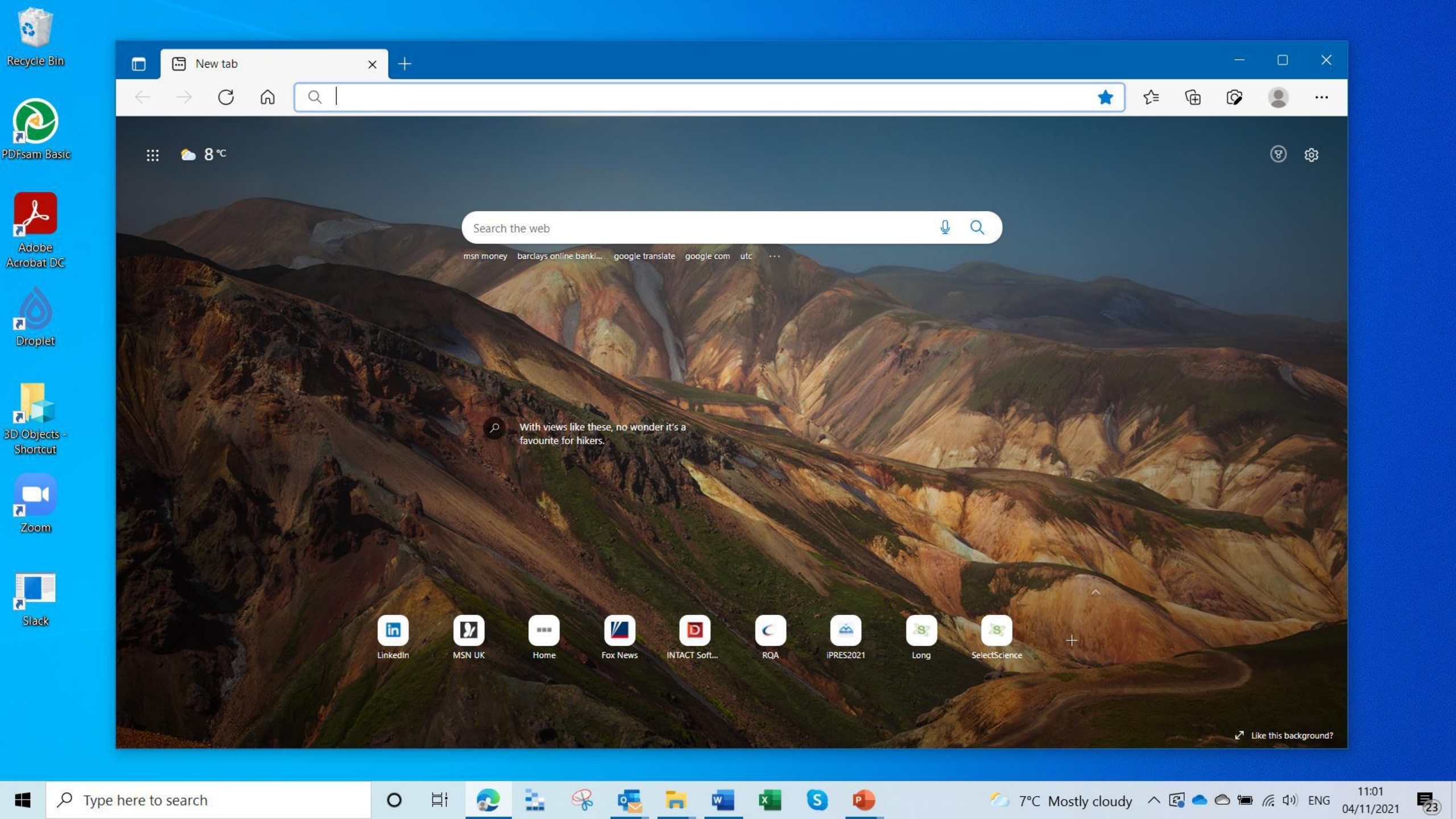
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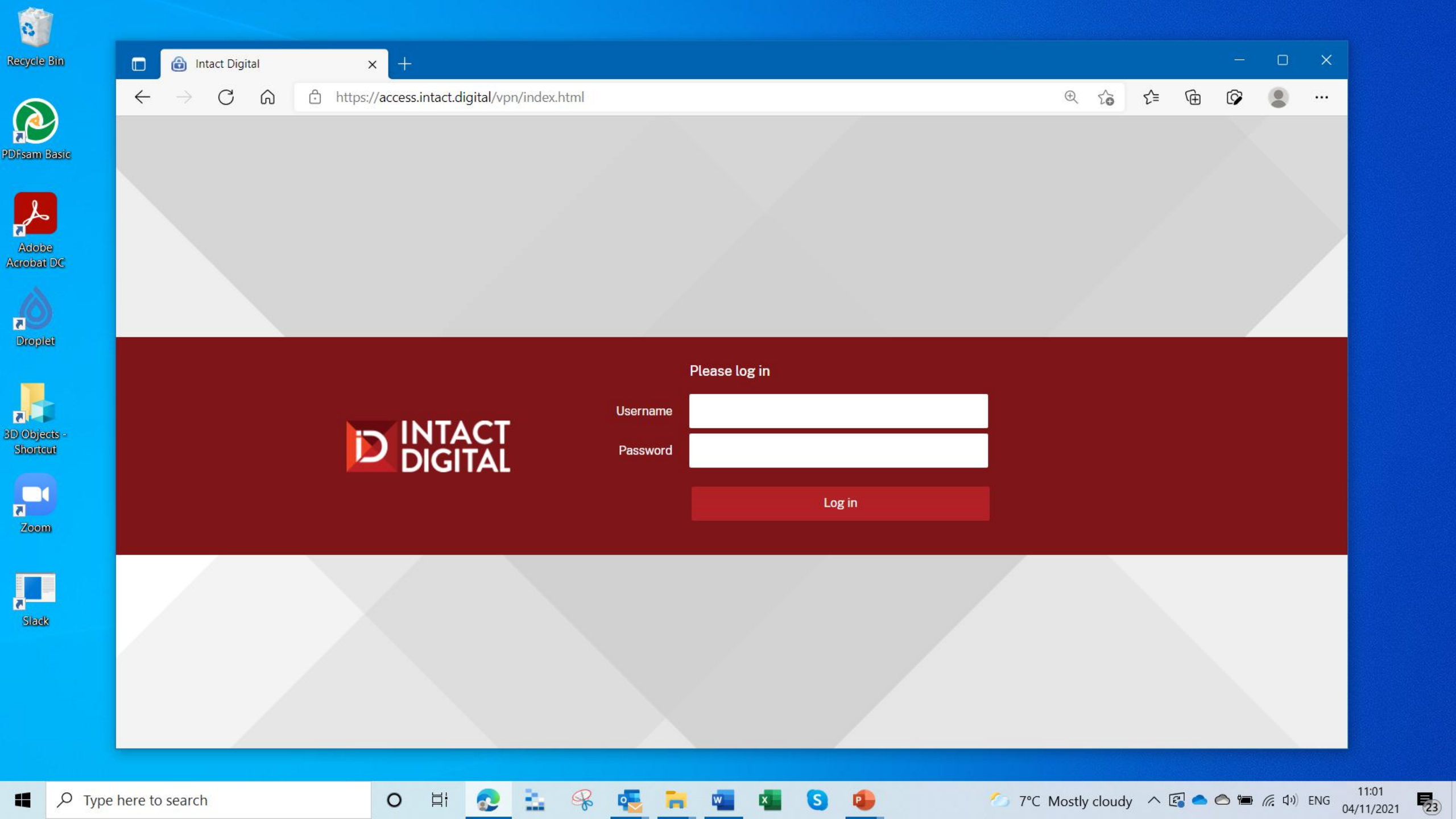
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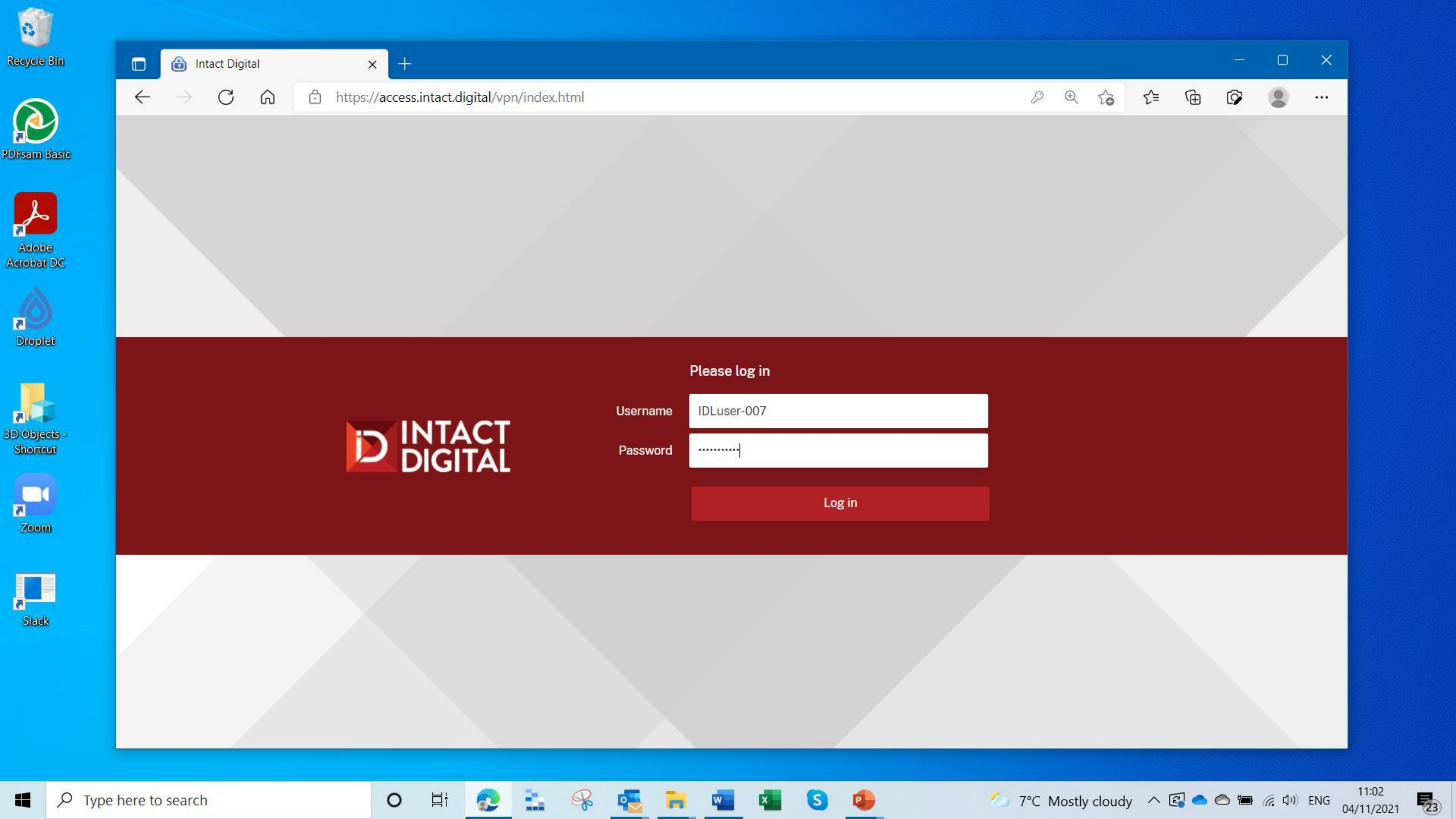
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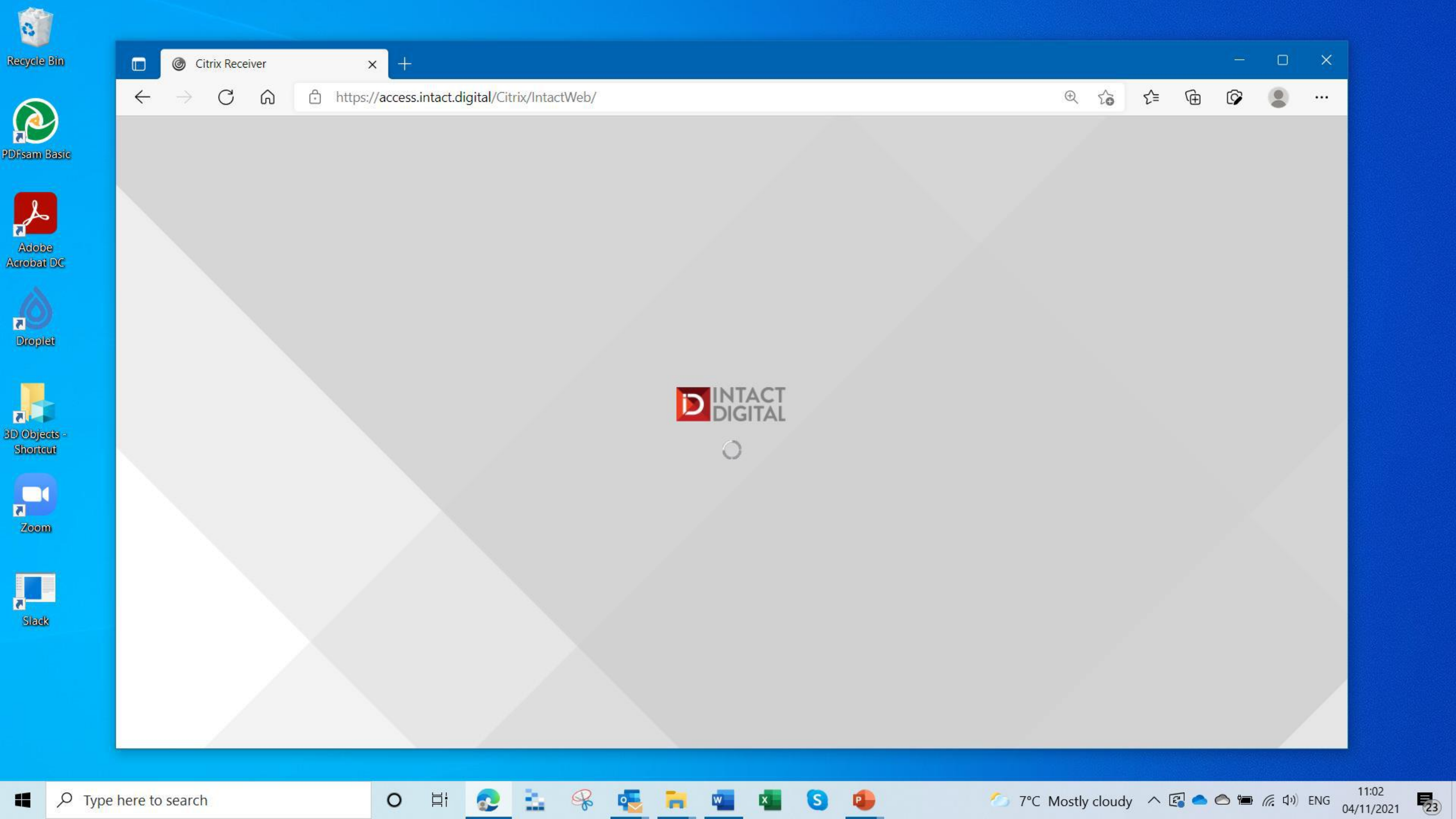
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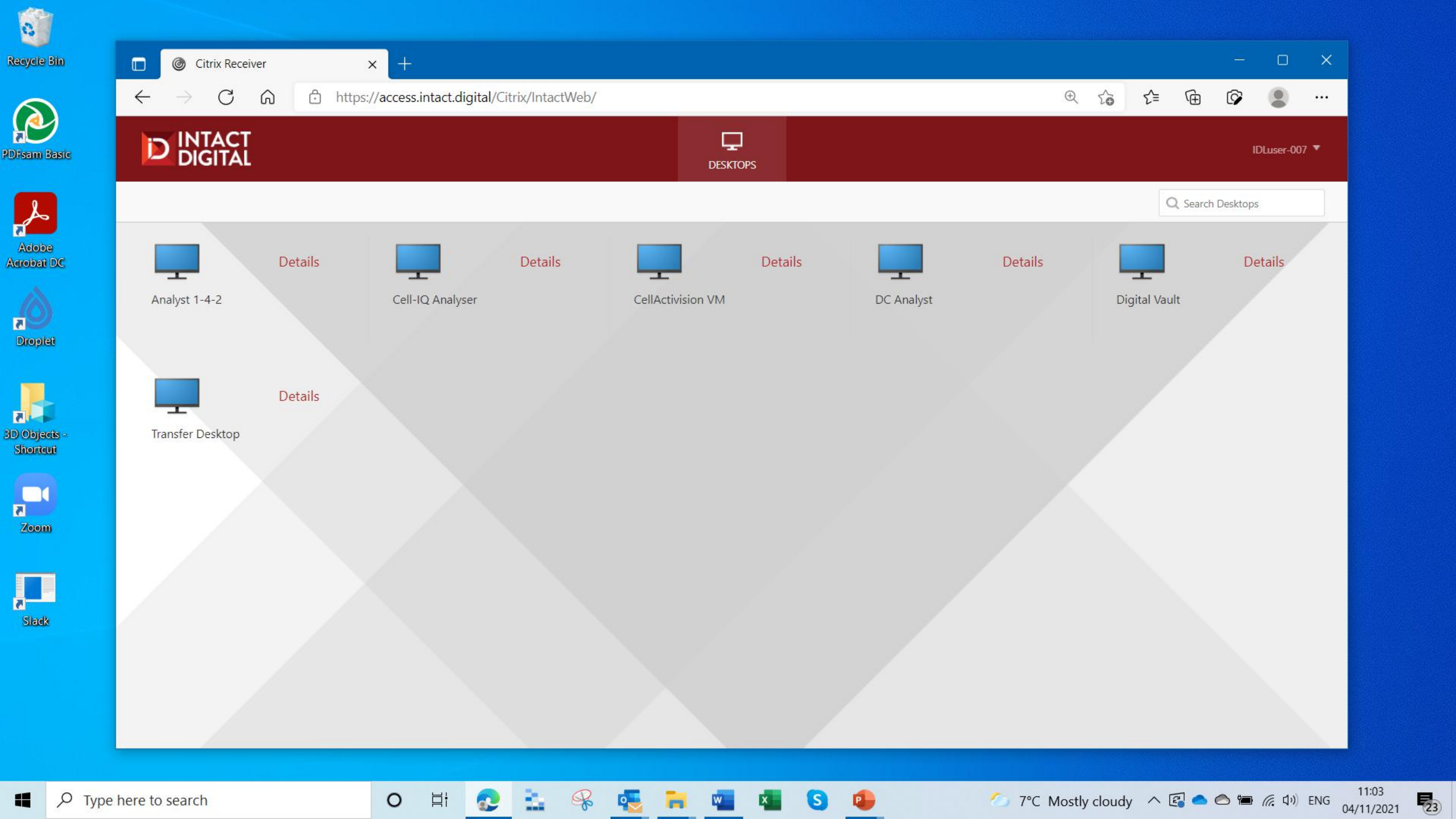
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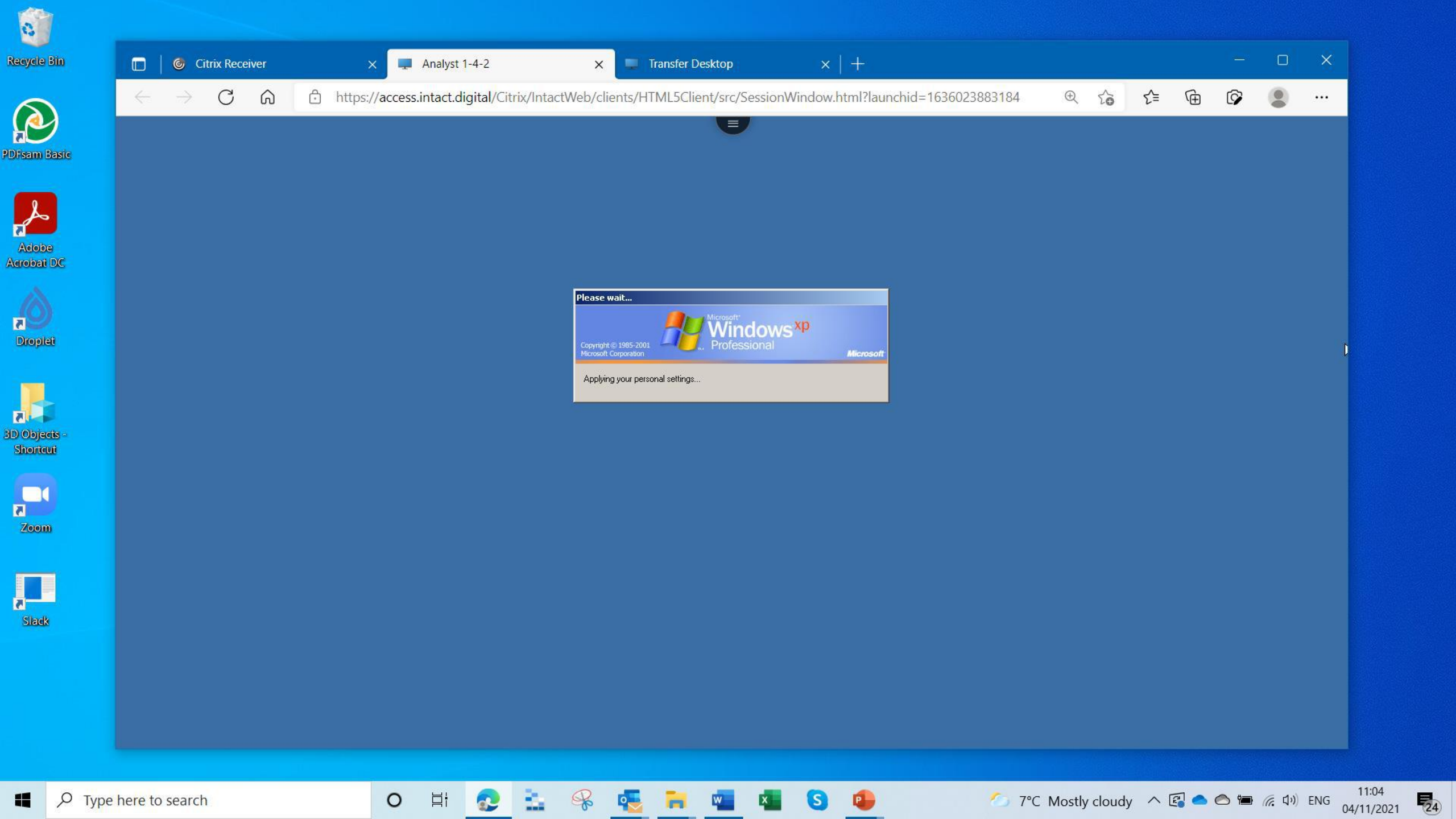
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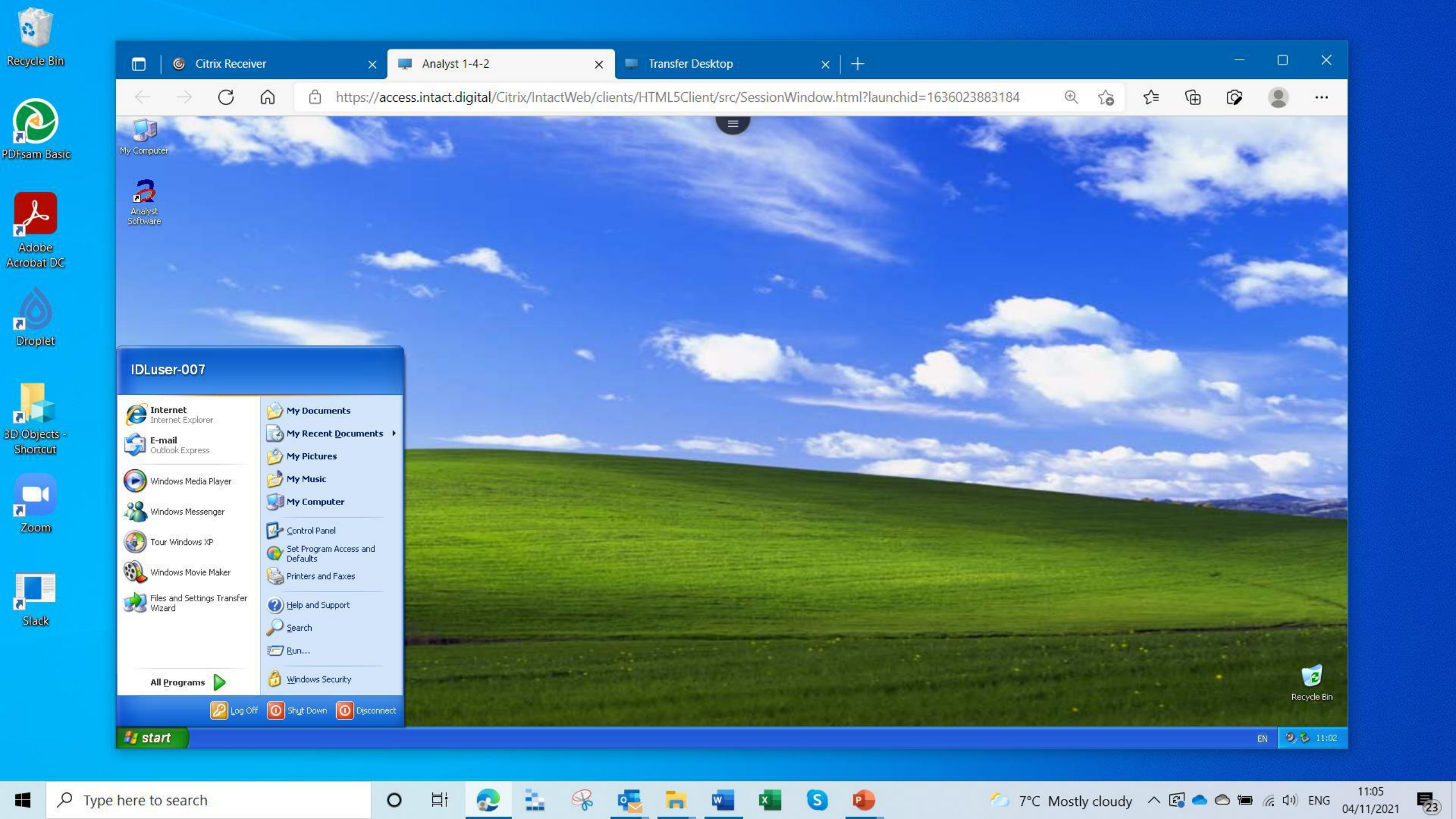
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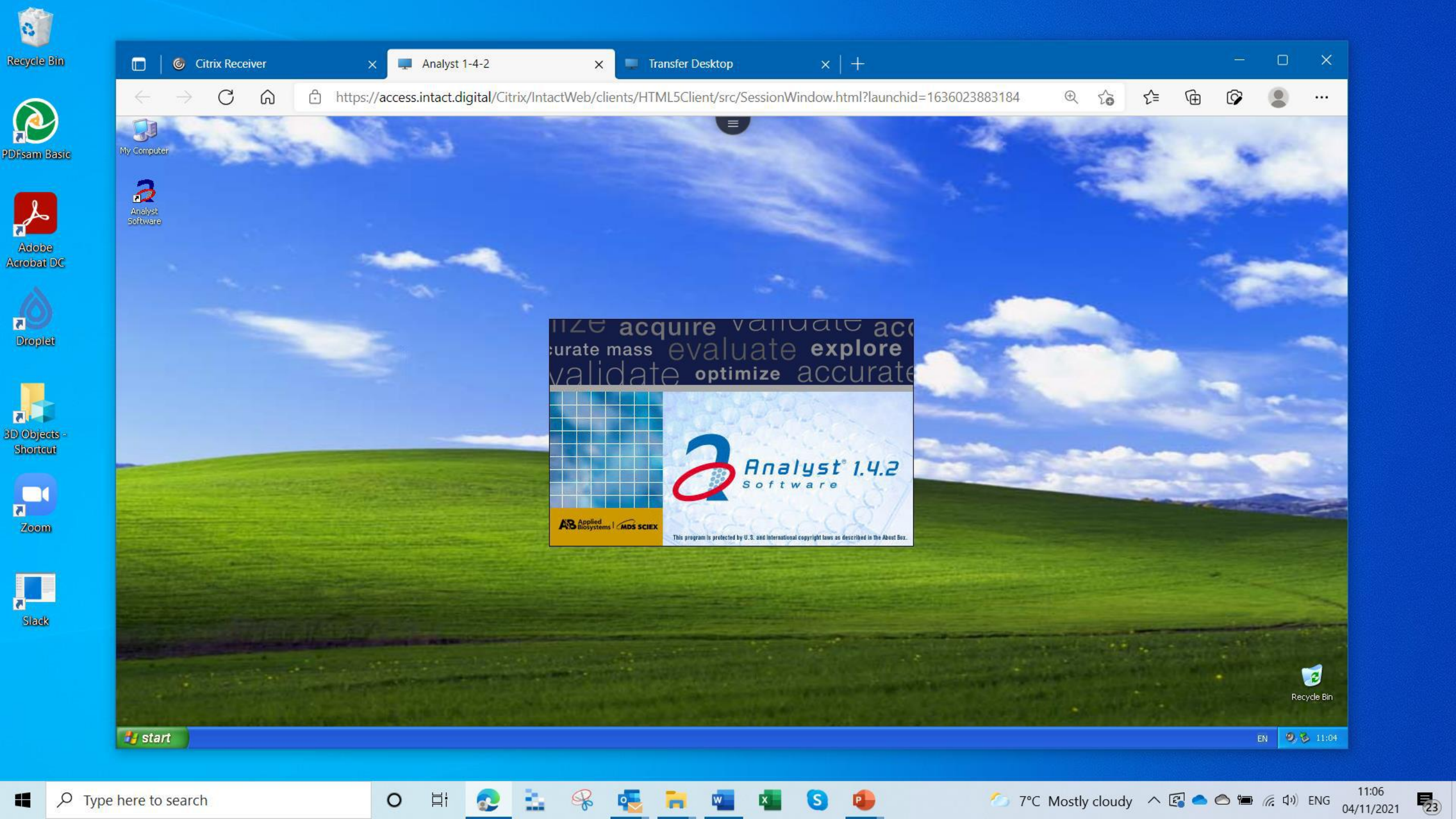
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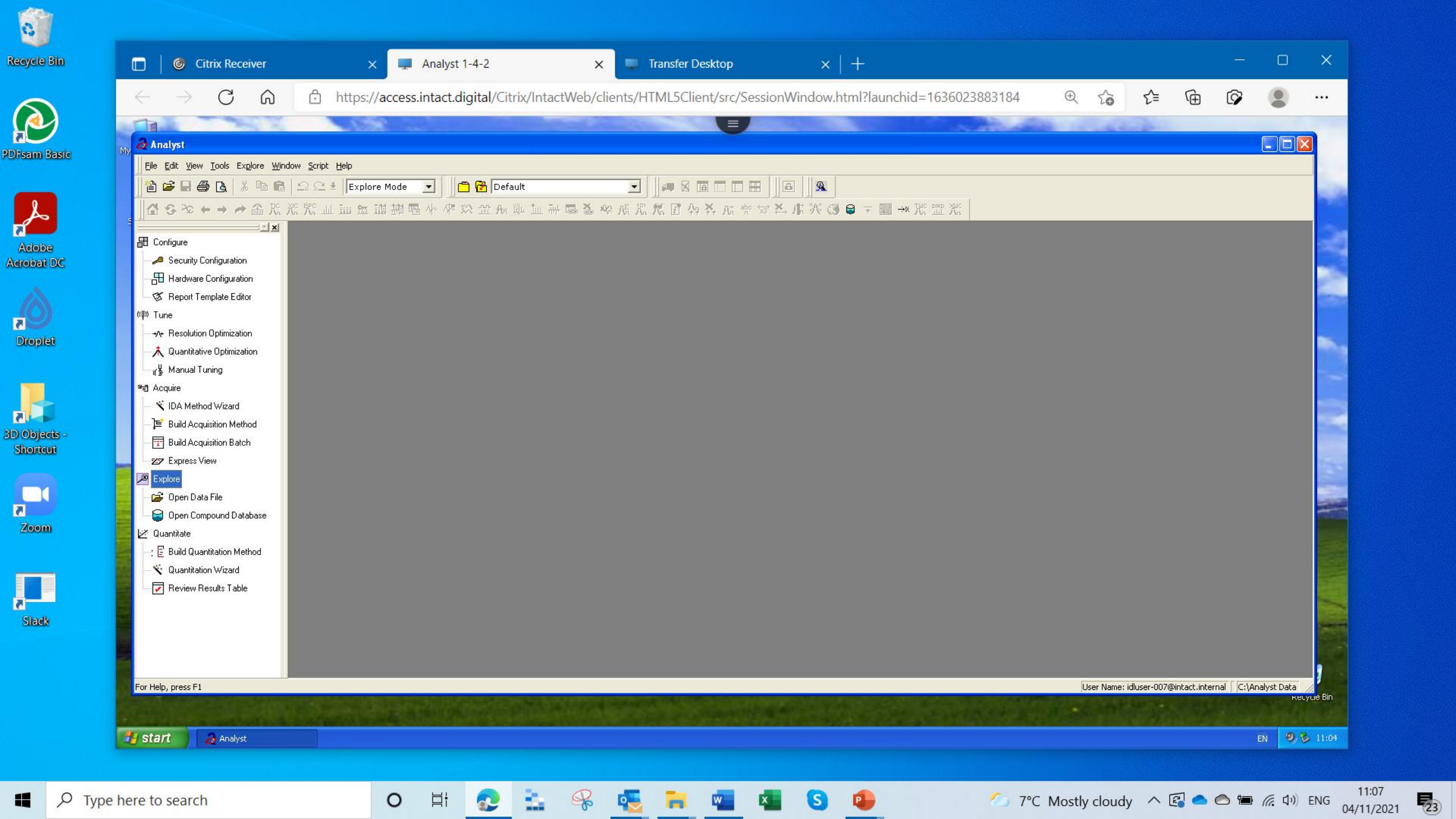
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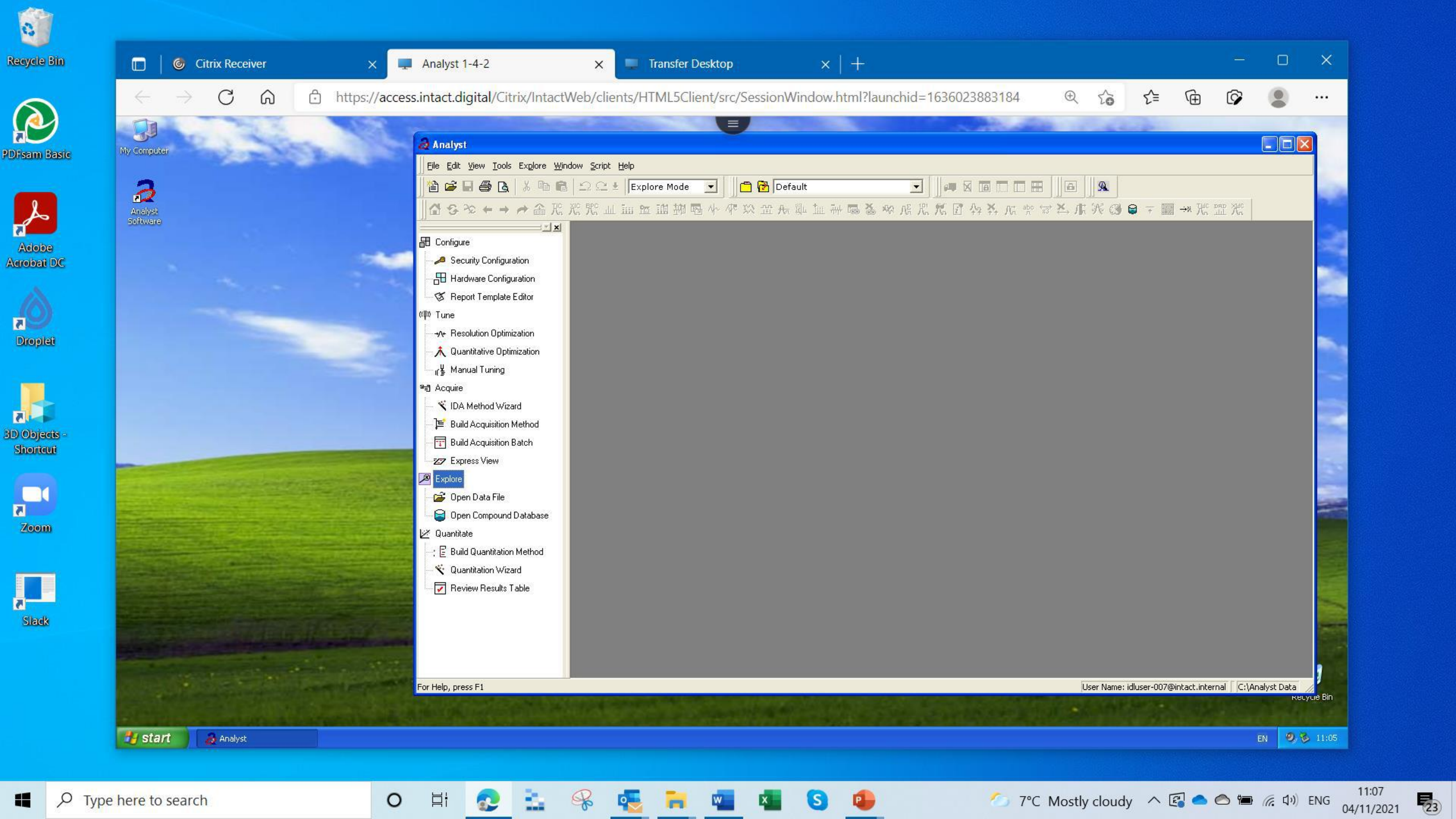
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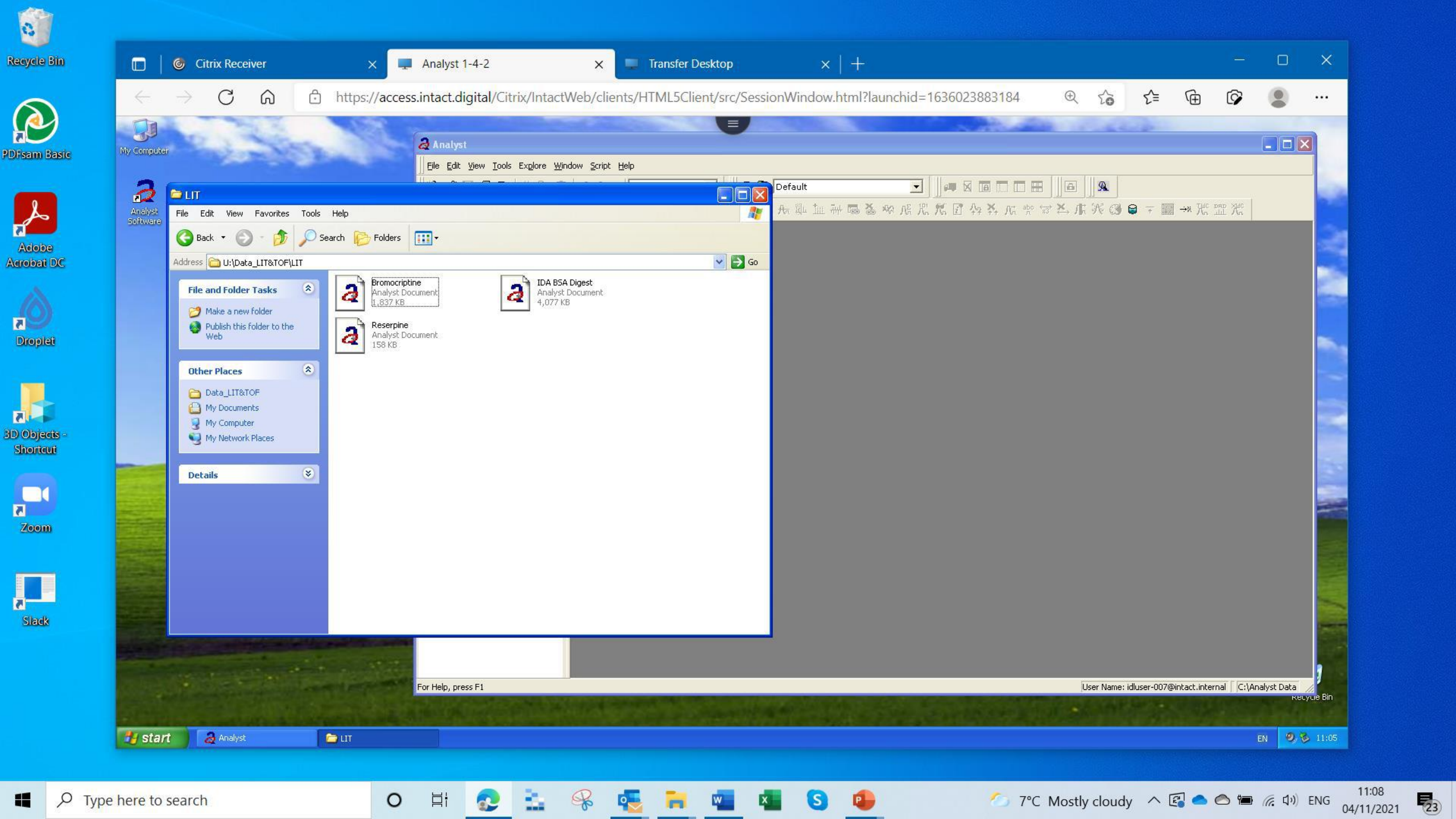
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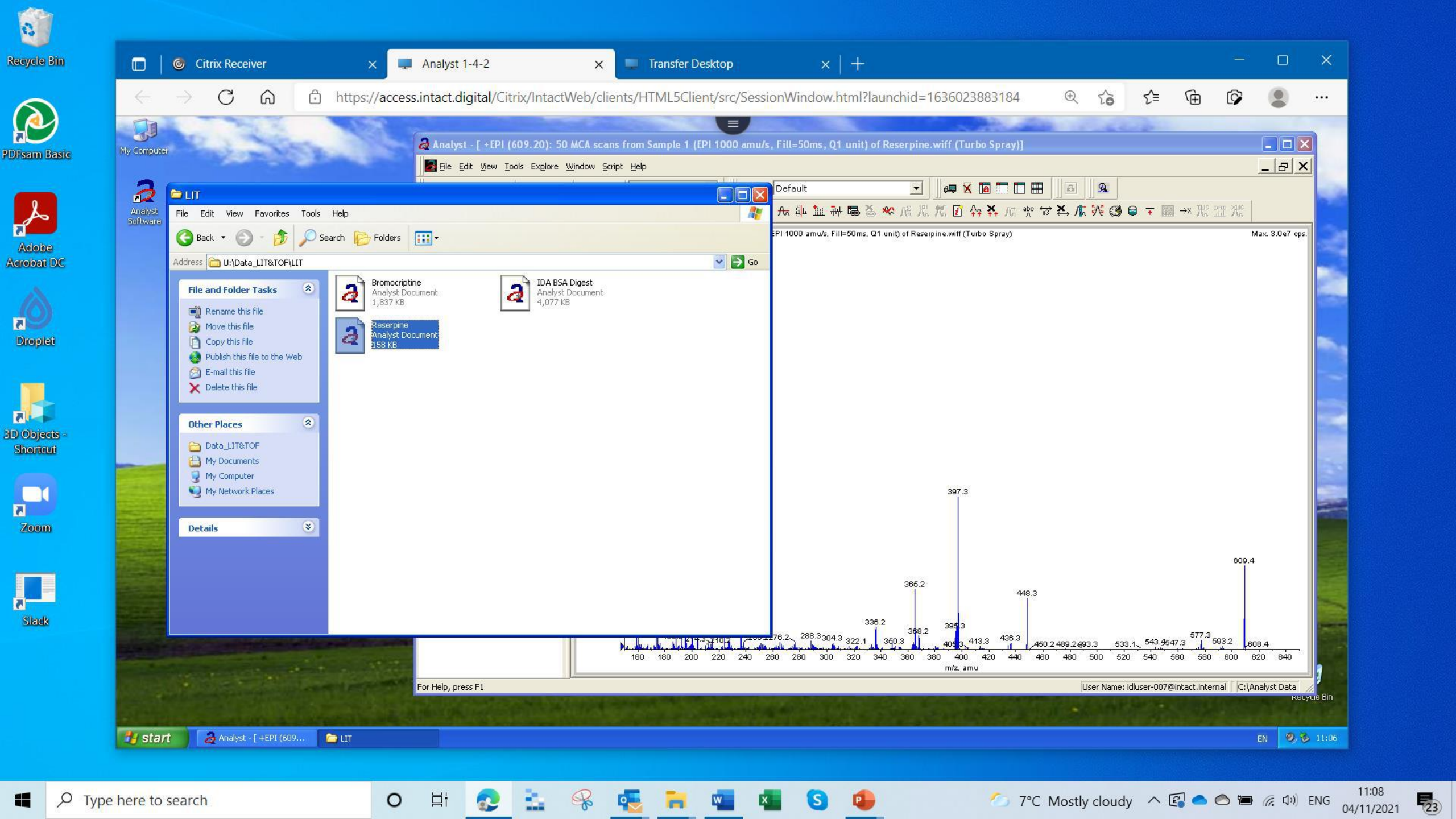
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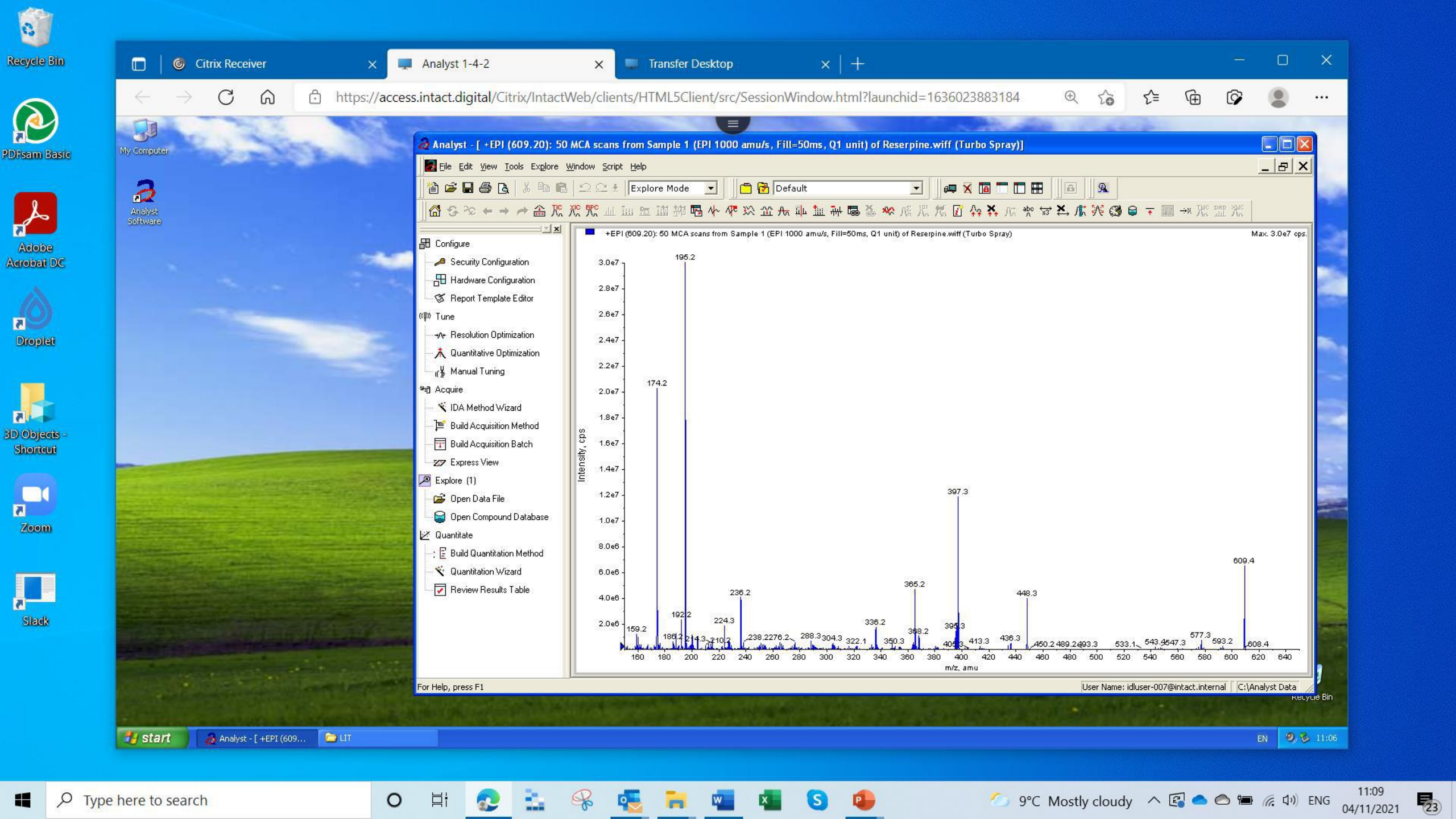
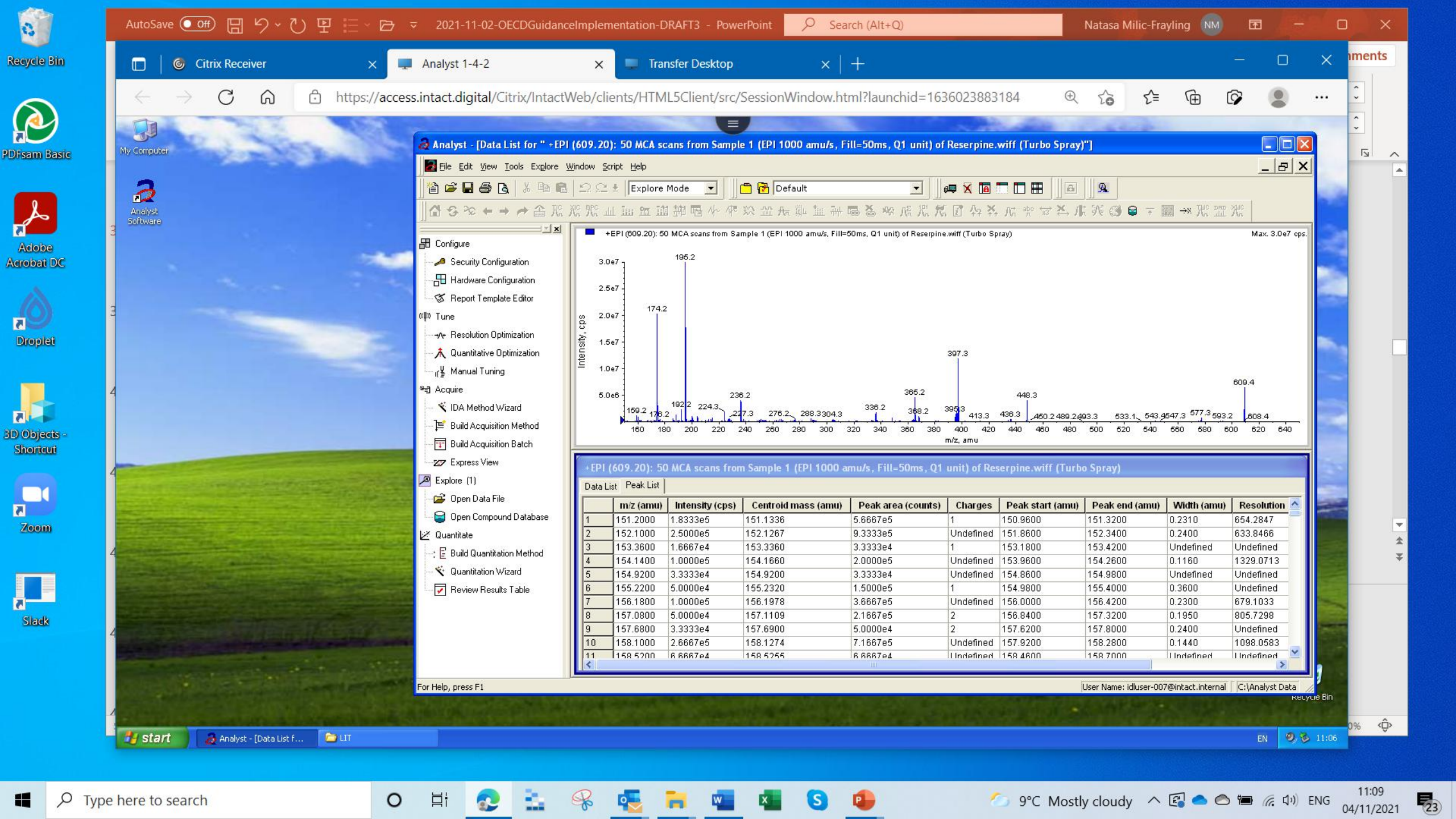
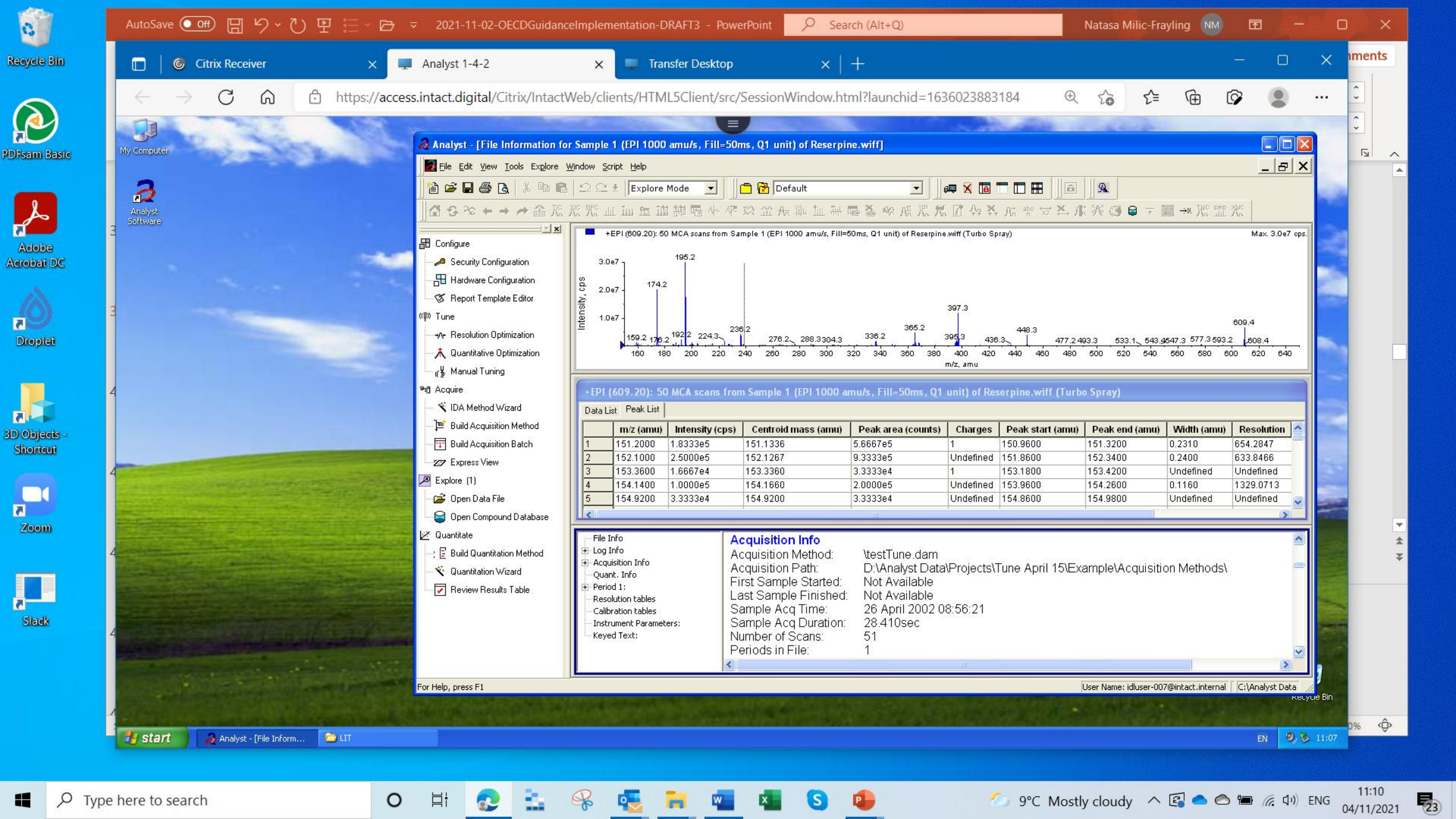
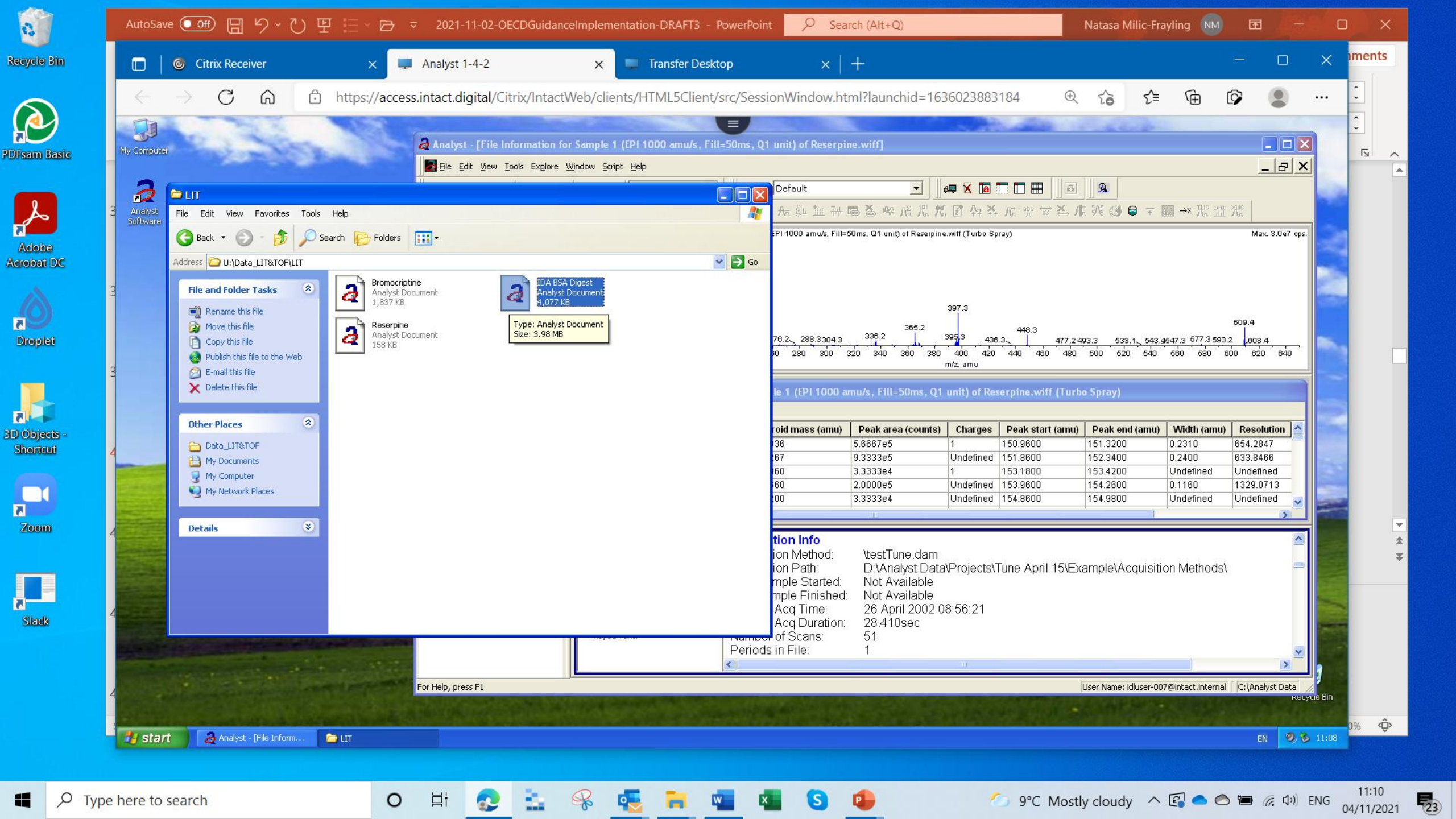
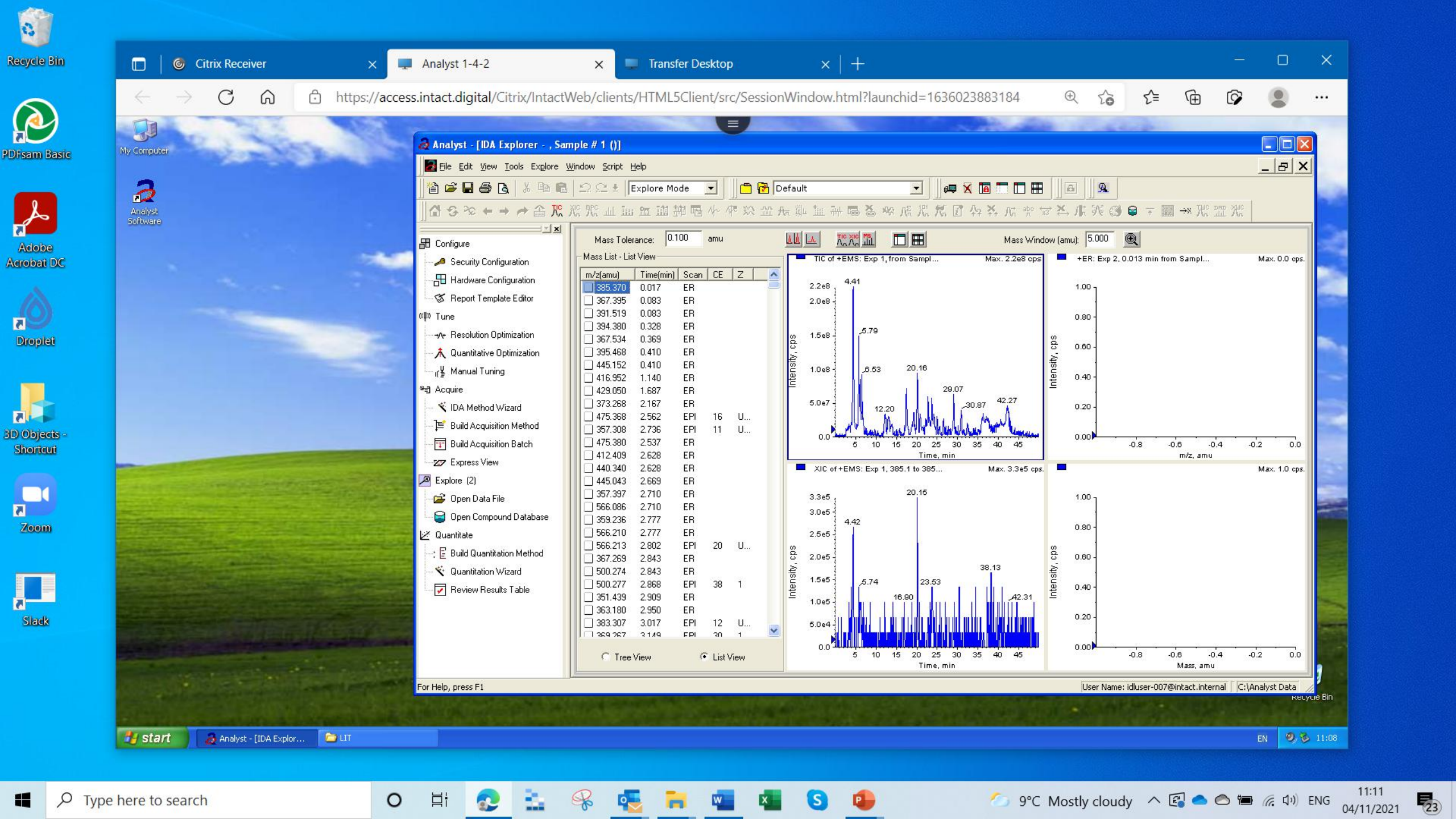
File Edit View Tools Explore Window Script Help
Default
EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)
Max. 3.0e7 cps.
397.3
609.4
365.2
448.3
336.2
368.2
395.3
m/z, amu
For Help, press F1
User Name: idluser-007@intact.internal
C:\Analyst Data
start
Analyst - [+EPI (609...
LIT
EN
11:06
Type here to search
7°C Mostly cloudy
ENG
11:08
04/11/2021

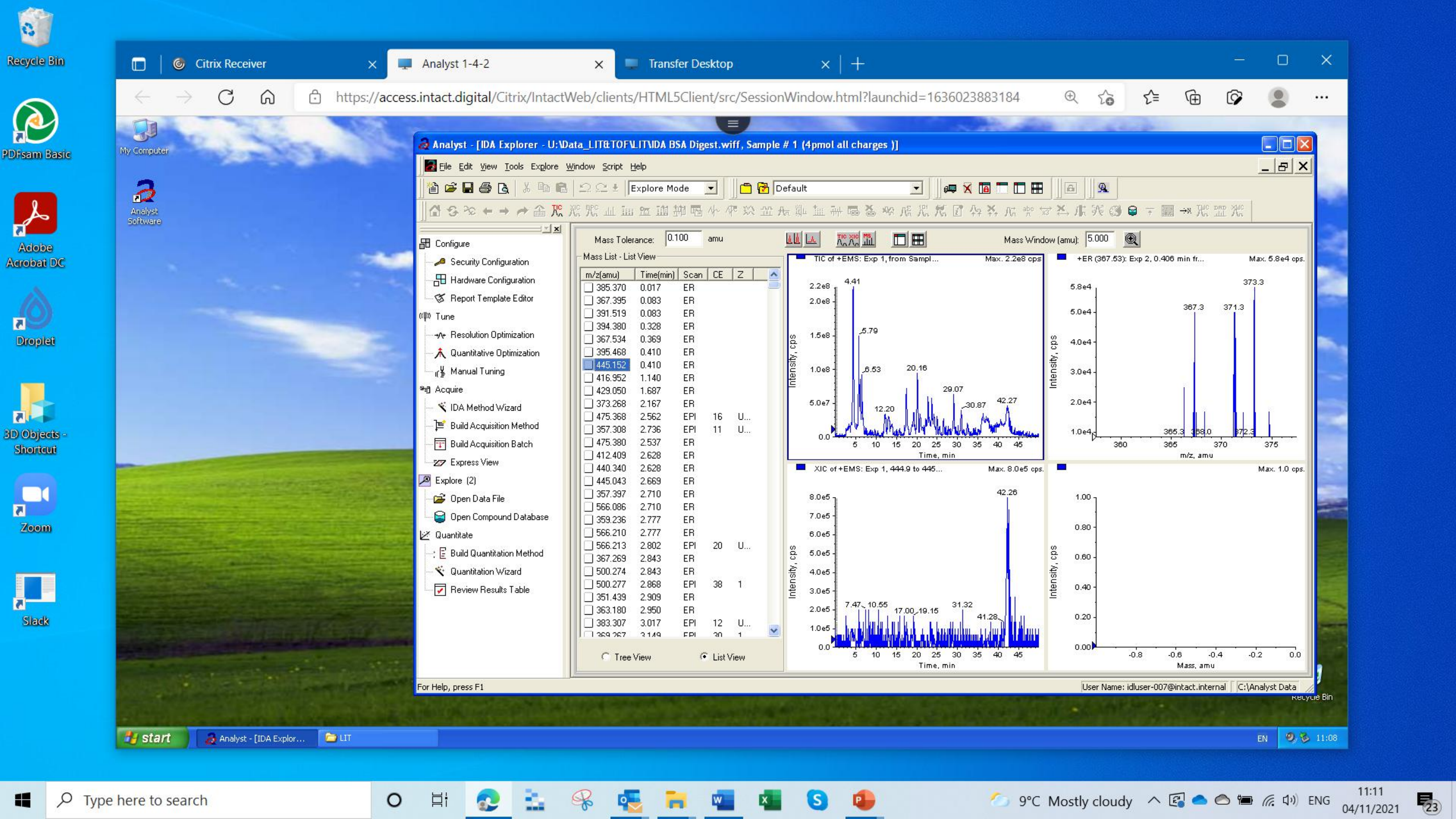

Recycle Bin
PDFsam Basic
Adobe Acrobat DC
Droplet
3D Objects - Shortcut
Zoom
Slack
Citrix Receiver
Analyst 1-4-2
Transfer Desktop
https://access.intact.digital/Citrix/IntactWeb/clients/HTML5Client/src/SessionWindow.html?launchid=1636023883184
My Computer
Analyst Software
Analyst - [+EPI (609.20): 50 MCA scans from Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)]
File Edit View Tools Explore Window Script Help
Explore Mode
Default
Configure
Security Configuration
Hardware Configuration
Report Template Editor
Tune
Resolution Optimization
Quantitative Optimization
Manual Tuning
Acquire
IDA Method Wizard
Build Acquisition Method
Build Acquisition Batch
Express View
Explore (1)
Open Data File
Open Compound Database
Quantitate
Build Quantitation Method
Quantitation Wizard
Review Results Table
+EPI (609.20): 50 MCA scans from Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)
Max. 3.0e7 cps.
Intensity, cps
m/z, amu
195.2
174.2
397.3
609.4
365.2
236.2
448.3
For Help, press F1
User Name: idluser-007@intact.internal
C:\Analyst Data
start
Analyst - [+EPI (609...
LIT
EN
11:06
Type here to search
9°C Mostly cloudy
ENG
11:09
04/11/2021

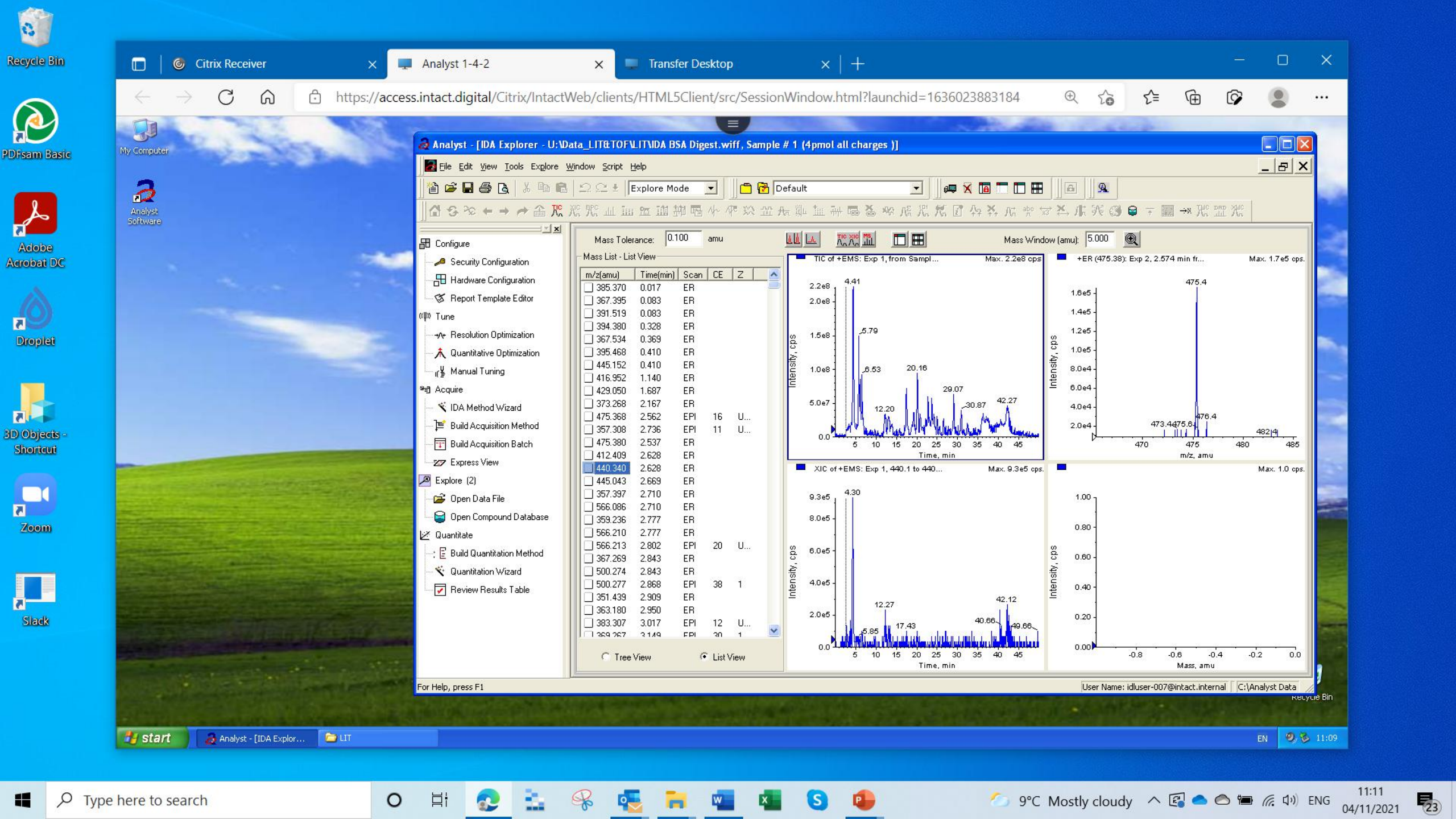

Analyst - [Data List for " +EPI (609.20): 50 MCA scans from Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)"]
+EPI (609.20): 50 MCA scans from Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)
Max. 3.0e7 cps.
Intensity, cps
m/z, amu
Data List
Peak List
m/z (amu) | Intensity (cps) | Centroid mass (amu) | Peak area (counts) | Charges | Peak start (amu) | Peak end (amu) | Width (amu) | Resolution
1 | 151.2000 | 1.8333e5 | 151.1336 | 5.6667e5 | 1 | 150.9600 | 151.3200 | 0.2310 | 654.2847
2 | 152.1000 | 2.5000e5 | 152.1267 | 9.3333e5 | Undefined | 151.8600 | 152.3400 | 0.2400 | 633.8466
3 | 153.3600 | 1.6667e4 | 153.3360 | 3.3333e4 | 1 | 153.1800 | 153.4200 | Undefined | Undefined
4 | 154.1400 | 1.0000e5 | 154.1660 | 2.0000e5 | Undefined | 153.9600 | 154.2600 | 0.1160 | 1329.0713
5 | 154.9200 | 3.3333e4 | 154.9200 | 3.3333e4 | Undefined | 154.8600 | 154.9800 | Undefined | Undefined
6 | 155.2200 | 5.0000e4 | 155.2320 | 1.5000e5 | 1 | 154.9800 | 155.4000 | 0.3600 | Undefined
7 | 156.1800 | 1.0000e5 | 156.1978 | 3.6667e5 | Undefined | 156.0000 | 156.4200 | 0.2300 | 679.1033
8 | 157.0800 | 5.0000e4 | 157.1109 | 2.1667e5 | 2 | 156.8400 | 157.3200 | 0.1950 | 805.7298
9 | 157.6800 | 3.3333e4 | 157.6900 | 5.0000e4 | 2 | 157.6200 | 157.8000 | 0.2400 | Undefined
10 | 158.1000 | 2.6667e5 | 158.1274 | 7.1667e5 | Undefined | 157.9200 | 158.2800 | 0.1440 | 1098.0583
For Help, press F1
User Name: idluser-007@intact.internal
C:\Analyst Data

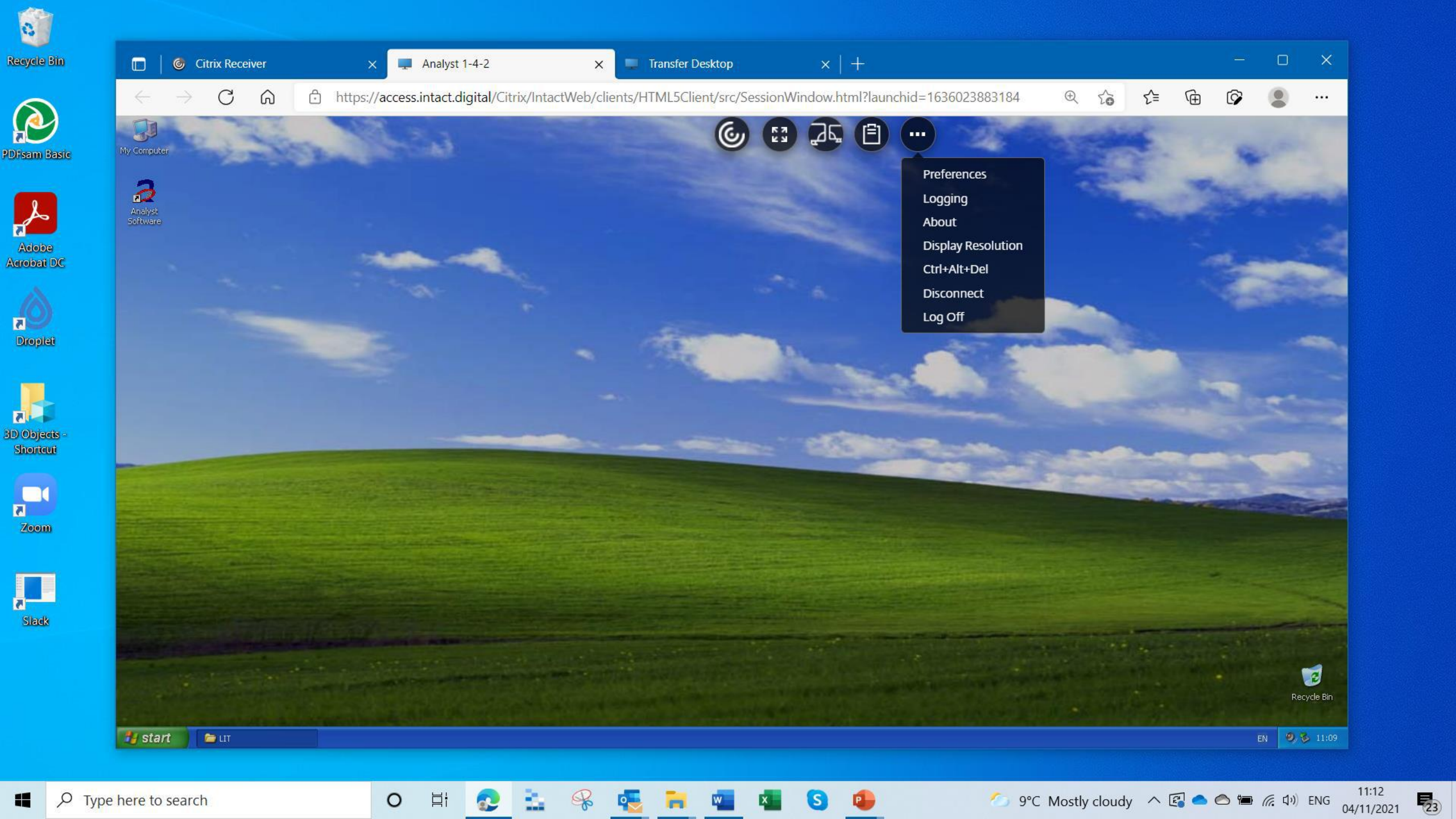

AutoSave Off
2021-11-02-OECDGuidanceImplementation-DRAFT3 - PowerPoint
Search (Alt+Q)
Natasa Milic-Frayling
Citrix Receiver
Analyst 1-4-2
Transfer Desktop
https://access.intact.digital/Citrix/IntactWeb/clients/HTML5Client/src/SessionWindow.html?launchid=1636023883184
Analyst - [File Information for Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff]
File Edit View Tools Explore Window Script Help
Explore Mode
Default
Configure
Security Configuration
Hardware Configuration
Report Template Editor
Tune
Resolution Optimization
Quantitative Optimization
Manual Tuning
Acquire
IDA Method Wizard
Build Acquisition Method
Build Acquisition Batch
Express View
Explore (1)
Open Data File
Open Compound Database
Quantitate
Build Quantitation Method
Quantitation Wizard
Review Results Table
+EPI (609.20): 50 MCA scans from Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)
Max. 3.0e7 cps.
Intensity, cps
m/z, amu
Data List
Peak List
m/z (amu) | Intensity (cps) | Centroid mass (amu) | Peak area (counts) | Charges | Peak start (amu) | Peak end (amu) | Width (amu) | Resolution
1 | 151.2000 | 1.8333e5 | 151.1336 | 5.6667e5 | 1 | 150.9600 | 151.3200 | 0.2310 | 654.2847
2 | 152.1000 | 2.5000e5 | 152.1267 | 9.3333e5 | Undefined | 151.8600 | 152.3400 | 0.2400 | 633.8466
3 | 153.3600 | 1.6667e4 | 153.3360 | 3.3333e4 | 1 | 153.1800 | 153.4200 | Undefined | Undefined
4 | 154.1400 | 1.0000e5 | 154.1660 | 2.0000e5 | Undefined | 153.9600 | 154.2600 | 0.1160 | 1329.0713
5 | 154.9200 | 3.3333e4 | 154.9200 | 3.3333e4 | Undefined | 154.8600 | 154.9800 | Undefined | Undefined
File Info
Log Info
Acquisition Info
Quant. Info
Period 1:
Resolution tables
Calibration tables
Instrument Parameters:
Keyed Text:
Acquisition Info
Acquisition Method: \testTune.dam
Acquisition Path: D:\Analyst Data\Projects\Tune April 15\Example\Acquisition Methods\
First Sample Started: Not Available
Last Sample Finished: Not Available
Sample Acq Time: 26 April 2002 08:56:21
Sample Acq Duration: 28.410sec
Number of Scans: 51
Periods in File: 1
For Help, press F1
User Name: idluser-007@intact.internal
C:\Analyst Data
start
Analyst - [File Inform...
LIT
EN
11:07
Type here to search
9°C Mostly cloudy
ENG
11:10
04/11/2021

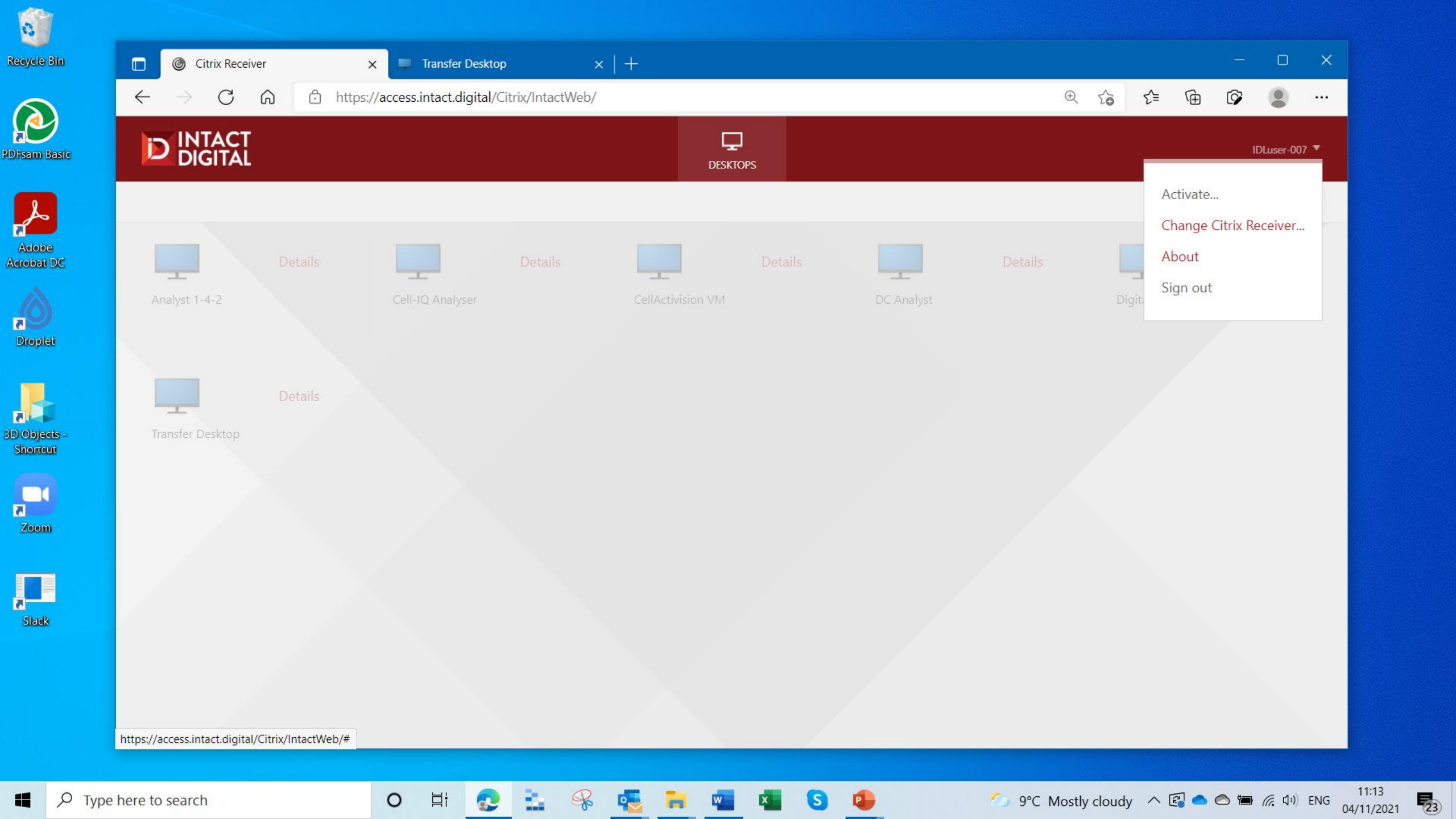

AutoSave Off
2021-11-02-OECDGuidanceImplementation-DRAFT3 - PowerPoint
Search (Alt+Q)
Natasa Milic-Frayling
Citrix Receiver
Analyst 1-4-2
Transfer Desktop
https://access.intact.digital/Citrix/IntactWeb/clients/HTML5Client/src/SessionWindow.html?launchid=1636023883184
Recycle Bin
PDFsam Basic
Adobe Acrobat DC
Droplet
3D Objects - Shortcut
Zoom
Slack
My Computer
Analyst Software
Analyst - [File Information for Sample 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff]
File Edit View Tools Explore Window Script Help
LIT
File Edit View Favorites Tools Help
Back Search Folders
Address U:\Data_LIT&TOF\LIT
Go
File and Folder Tasks
Rename this file
Move this file
Copy this file
Publish this file to the Web
E-mail this file
Delete this file
Other Places
Data_LIT&TOF
My Documents
My Computer
My Network Places
Details
Bromocriptine
Analyst Document
1,837 KB
Reserpine
Analyst Document
158 KB
IDA BSA Digest
Analyst Document
4,077 KB
Type: Analyst Document
Size: 3.98 MB
Default
EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)
Max. 3.0e7 cps.
397.3
365.2
448.3
609.4
m/z, amu
le 1 (EPI 1000 amu/s, Fill=50ms, Q1 unit) of Reserpine.wiff (Turbo Spray)
oid mass (amu) | Peak area (counts) | Charges | Peak start (amu) | Peak end (amu) | Width (amu) | Resolution
36 | 5.6667e5 | 1 | 150.9600 | 151.3200 | 0.2310 | 654.2847
67 | 9.3333e5 | Undefined | 151.8600 | 152.3400 | 0.2400 | 633.8466
60 | 3.3333e4 | 1 | 153.1800 | 153.4200 | Undefined | Undefined
60 | 2.0000e5 | Undefined | 153.9600 | 154.2600 | 0.1160 | 1329.0713
00 | 3.3333e4 | Undefined | 154.8600 | 154.9800 | Undefined | Undefined
tion Info
ion Method: \testTune.dam
ion Path: D:\Analyst Data\Projects\Tune April 15\Example\Acquisition Methods\
mple Started: Not Available
mple Finished: Not Available
Acq Time: 26 April 2002 08:56:21
Acq Duration: 28.410sec
of Scans: 51
Periods in File: 1
For Help, press F1
User Name: idluser-007@intact.internal
C:\Analyst Data
start
Analyst - [File Inform...
LIT
EN
11:08
Type here to search
9°C Mostly cloudy
ENG
11:10
04/11/2021


Recycle Bin
Citrix Receiver
Analyst 1-4-2
Transfer Desktop
https://access.intact.digital/Citrix/IntactWeb/clients/HTML5Client/src/SessionWindow.html?launchid=1636023883184
PDFsam Basic
My Computer
Analyst Software
Adobe Acrobat DC
Droplet
3D Objects - Shortcut
Zoom
Slack
Analyst - [IDA Explorer - , Sample # 1 ()]
File Edit View Tools Explore Window Script Help
Explore Mode
Default
Configure
Security Configuration
Hardware Configuration
Report Template Editor
Tune
Resolution Optimization
Quantitative Optimization
Manual Tuning
Acquire
IDA Method Wizard
Build Acquisition Method
Build Acquisition Batch
Express View
Explore (2)
Open Data File
Open Compound Database
Quantitate
Build Quantitation Method
Quantitation Wizard
Review Results Table
Mass Tolerance: 0.100 amu
Mass Window (amu): 5.000
Mass List - List View
m/z(amu) Time(min) Scan CE Z
385.370 0.017 ER
367.395 0.083 ER
391.519 0.083 ER
394.380 0.328 ER
367.534 0.369 ER
395.468 0.410 ER
445.152 0.410 ER
416.952 1.140 ER
429.050 1.687 ER
373.268 2.167 ER
475.368 2.562 EPI 16 U...
357.308 2.736 EPI 11 U...
475.380 2.537 ER
412.409 2.628 ER
440.340 2.628 ER
445.043 2.669 ER
357.397 2.710 ER
566.086 2.710 ER
359.236 2.777 ER
566.210 2.777 ER
566.213 2.802 EPI 20 U...
367.269 2.843 ER
500.274 2.843 ER
500.277 2.868 EPI 38 1
351.439 2.909 ER
363.180 2.950 ER
383.307 3.017 EPI 12 U...
Tree View
List View
TIC of +EMS: Exp 1, from Sampl... Max. 2.2e8 cps
+ER: Exp 2, 0.013 min from Sampl... Max. 0.0 cps.
XIC of +EMS: Exp 1, 385.1 to 385... Max. 3.3e5 cps.
Max. 1.0 cps.
Intensity, cps
Time, min
m/z, amu
Mass, amu
For Help, press F1
User Name: idluser-007@intact.internal
C:\Analyst Data
start
Analyst - [IDA Explor...
LIT
EN
11:08
Type here to search
9°C Mostly cloudy
ENG
11:11
04/11/2021


Recycle Bin
PDFsam Basic
Adobe Acrobat DC
Droplet
3D Objects - Shortcut
Zoom
Slack
Citrix Receiver
Analyst 1-4-2
Transfer Desktop
https://access.intact.digital/Citrix/IntactWeb/clients/HTML5Client/src/SessionWindow.html?launchid=1636023883184
My Computer
Analyst Software
Analyst - [IDA Explorer - U:\Data_LIT&TOF\LIT\IDA BSA Digest.wiff, Sample # 1 (4pmol all charges)]
File Edit View Tools Explore Window Script Help
Explore Mode
Default
Configure
Security Configuration
Hardware Configuration
Report Template Editor
Tune
Resolution Optimization
Quantitative Optimization
Manual Tuning
Acquire
IDA Method Wizard
Build Acquisition Method
Build Acquisition Batch
Express View
Explore (2)
Open Data File
Open Compound Database
Quantitate
Build Quantitation Method
Quantitation Wizard
Review Results Table
Mass Tolerance: 0.100 amu
Mass Window (amu): 5.000
Mass List - List View
m/z(amu) Time(min) Scan CE Z
385.370 0.017 ER
367.395 0.083 ER
391.519 0.083 ER
394.380 0.328 ER
367.534 0.369 ER
395.468 0.410 ER
445.152 0.410 ER
416.952 1.140 ER
429.050 1.687 ER
373.268 2.167 ER
475.368 2.562 EPI 16 U...
357.308 2.736 EPI 11 U...
475.380 2.537 ER
412.409 2.628 ER
440.340 2.628 ER
445.043 2.669 ER
357.397 2.710 ER
566.086 2.710 ER
359.236 2.777 ER
566.210 2.777 ER
566.213 2.802 EPI 20 U...
367.269 2.843 ER
500.274 2.843 ER
500.277 2.868 EPI 38 1
351.439 2.909 ER
363.180 2.950 ER
383.307 3.017 EPI 12 U...
Tree View
List View
TIC of +EMS: Exp 1, from Sampl... Max. 2.2e8 cps
+ER (367.53): Exp 2, 0.406 min fr... Max. 5.8e4 cps.
XIC of +EMS: Exp 1, 444.9 to 445... Max. 8.0e5 cps.
Max. 1.0 cps.
Intensity, cps
Time, min
m/z, amu
Mass, amu
For Help, press F1
User Name: idluser-007@intact.internal
C:\Analyst Data
start
Analyst - [IDA Explor...
LIT
EN
11:08
Type here to search
9°C Mostly cloudy
ENG
11:11
04/11/2021


Recycle Bin
PDFsam Basic
Adobe Acrobat DC
Droplet
3D Objects - Shortcut
Zoom
Slack
Citrix Receiver
Analyst 1-4-2
Transfer Desktop
https://access.intact.digital/Citrix/IntactWeb/clients/HTML5Client/src/SessionWindow.html?launchid=1636023883184
My Computer
Analyst Software
Analyst - [IDA Explorer - U:\Data_LIT&TOF\LIT\IDA BSA Digest.wiff, Sample # 1 (4pmol all charges)]
File Edit View Tools Explore Window Script Help
Explore Mode
Default
Configure
Security Configuration
Hardware Configuration
Report Template Editor
Tune
Resolution Optimization
Quantitative Optimization
Manual Tuning
Acquire
IDA Method Wizard
Build Acquisition Method
Build Acquisition Batch
Express View
Explore (2)
Open Data File
Open Compound Database
Quantitate
Build Quantitation Method
Quantitation Wizard
Review Results Table
Mass Tolerance: 0.100 amu
Mass Window (amu): 5.000
Mass List - List View
m/z(amu) Time(min) Scan CE Z
385.370 0.017 ER
367.395 0.083 ER
391.519 0.083 ER
394.380 0.328 ER
367.534 0.369 ER
395.468 0.410 ER
445.152 0.410 ER
416.952 1.140 ER
429.050 1.687 ER
373.268 2.167 ER
475.368 2.562 EPI 16 U...
357.308 2.736 EPI 11 U...
475.380 2.537 ER
412.409 2.628 ER
440.340 2.628 ER
445.043 2.669 ER
357.397 2.710 ER
566.086 2.710 ER
359.236 2.777 ER
566.210 2.777 ER
566.213 2.802 EPI 20 U...
367.269 2.843 ER
500.274 2.843 ER
500.277 2.868 EPI 38 1
351.439 2.909 ER
363.180 2.950 ER
383.307 3.017 EPI 12 U...
Tree View
List View
TIC of +EMS: Exp 1, from Sampl... Max. 2.2e8 cps
+ER (475.38): Exp 2, 2.574 min fr... Max. 1.7e5 cps.
XIC of +EMS: Exp 1, 440.1 to 440... Max. 9.3e5 cps.
Max. 1.0 cps.
Intensity, cps
Time, min
m/z, amu
Mass, amu
For Help, press F1
User Name: idluser-007@intact.internal
C:\Analyst Data
start
Analyst - [IDA Explor...
LIT
EN
11:09
Type here to search
9°C Mostly cloudy
ENG
11:11
04/11/2021


Recycle Bin
PDFsam Basic
Adobe Acrobat DC
Droplet
3D Objects - Shortcut
Zoom
Slack
Citrix Receiver
Analyst 1-4-2
Transfer Desktop
https://access.intact.digital/Citrix/IntactWeb/clients/HTML5Client/src/SessionWindow.html?launchid=1636023883184
My Computer
Analyst Software
Preferences
Logging
About
Display Resolution
Ctrl+Alt+Del
Disconnect
Log Off
Recycle Bin
start
LIT
EN
11:09
Type here to search
9°C Mostly cloudy
ENG
11:12
04/11/2021

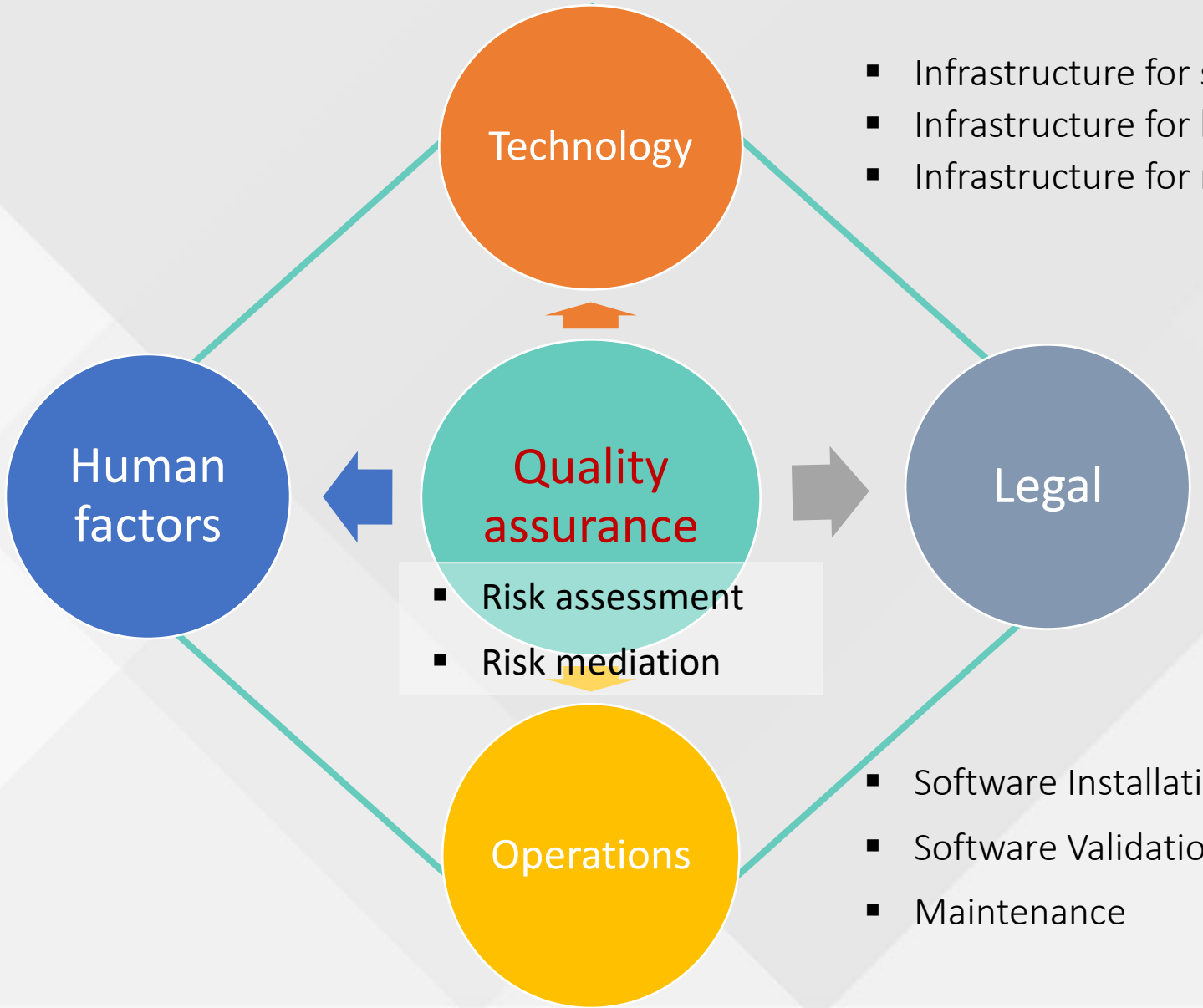

Recycle Bin
PDFsam Basic
Adobe Acrobat DC
Droplet
3D Objects - Shortcut
Zoom
Slack
Citrix Receiver
Transfer Desktop
https://access.intact.digital/Citrix/IntactWeb/
INTACT DIGITAL
DESKTOPS
IDLuser-007
Activate...
Change Citrix Receiver...
About
Sign out
Analyst 1-4-2
Details
Cell-IQ Analyser
Details
CellActivision VM
Details
DC Analyst
Details
Transfer Desktop
Details
https://access.intact.digital/Citrix/IntactWeb/#
Type here to search
9°C Mostly cloudy
ENG
11:13
04/11/2021

Quality by agility
REFLECT | CHALLENGE | INNOVATE

INTACT DIGITAL

Compliance considerations

Long-term software management



- Infrastructure for storing software assets
- Infrastructure for hosting validated software installations
- Infrastructure for remote access

- User training
- Technical staff training

- Licenses for the operating systems, hypervisors and remote access
- Addressing DRM issues that present barriers to software re-installation

- Software Installations
- Software Validation
- Maintenance

Procedures: Installation management

INSTALLATION QUALIFICATION (IQ → SL-IQ)

- IT — Create a sandboxed VM environment for software installation
- IT — Upload of software and software installation documentation
- IT — **Document the process of installing the software in the VM**
  - Follow the original **Installation Qualification** (IQ) used to create installations in the Lab.
  - Create **Software Library IQ** (SL-IQ) for the specific software.

OPERATIONAL QUALIFICATION (OQ → SL-OQ)

- IT — Configure Virtual Desktops (VD) to support data transfer and software use.
- RS — Review the Operational Qualification (OQ) of the original software installed in the Lab
- RS — **Document the testing of the virtualized software installation**
  - Select and test software features that support the study reconstruction task
  - Document the operational qualification process SL-OQ for virtualized software installations.

Roles

- IT — IT Specialist
- RS — Researcher
- AR — Archivist

Procedures: Software integrity checks

PERFORMANCE QUALIFICATION (PQ → SL-PQ)

RS Create a **Performance Qualification (PQ)** test and select representative test data

- Select a minimal set of steps to establish the **software integrity**
- Perform the test with the original software (in the Lab) and virtualized software

RS **Document the PQ procedure for the virtualized installation to create SL-PQ**

- Apply SL-PQ test before importing the study data.

STUDY RECONSTRUCTION

AR Use Transfer Desktop to transfer data into the Software Library environment

- Data is accessible to all the VMs available to the user

RS Activate the desktop with specific software and gain access to data

- Move the data to the VM if it needs to be used locally by the software

AR Access the study documentation and reconstruction process.

RS Reproduce the results and document the study reconstruction process.

Roles

- IT IT Specialist
- RS Researcher
- AR Archivist

Vision: Software assurance

Work with vendors on **safe deposit of released software** for archival use

- At the time of software deployment
  - Service agreement for operational software
  - Assurance agreement to access virtualized software installations in the VMs
  - Identical copy of software is validated and running in the isolated/archival environment.

BENEFITS

- Data archive is always in sync with installed software
- The community has a common standard for managing data integrity
- Regulators can confirm and approve specific software installation practice
- The ecosystem is stable and innovation is not affected by software obsolescence.

Thank you!

Natasa Milic-Frayling

natasamf@intact.digital

www.intact.digital

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