

# Inhalt

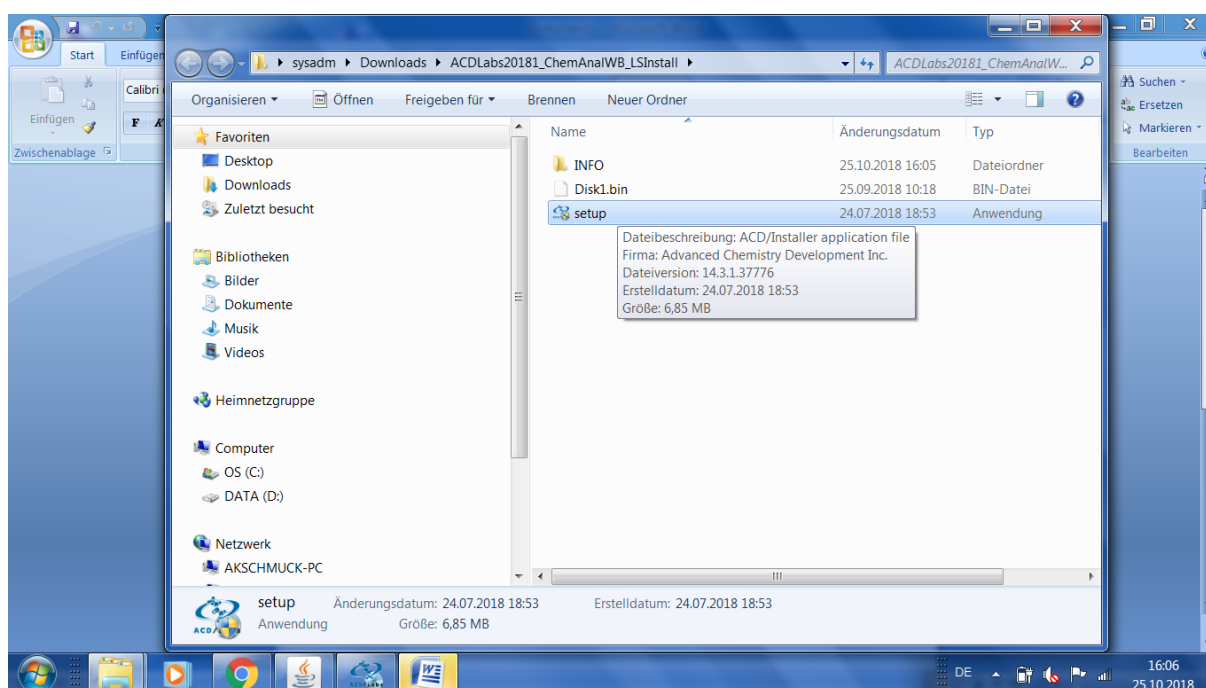
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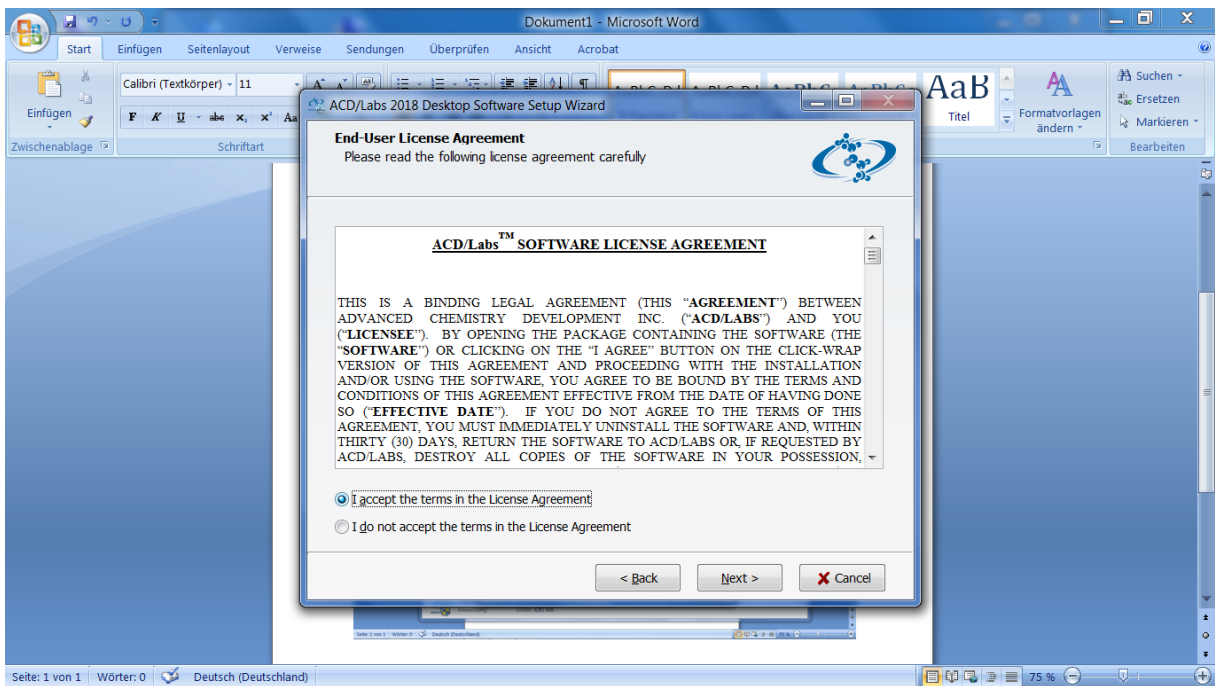
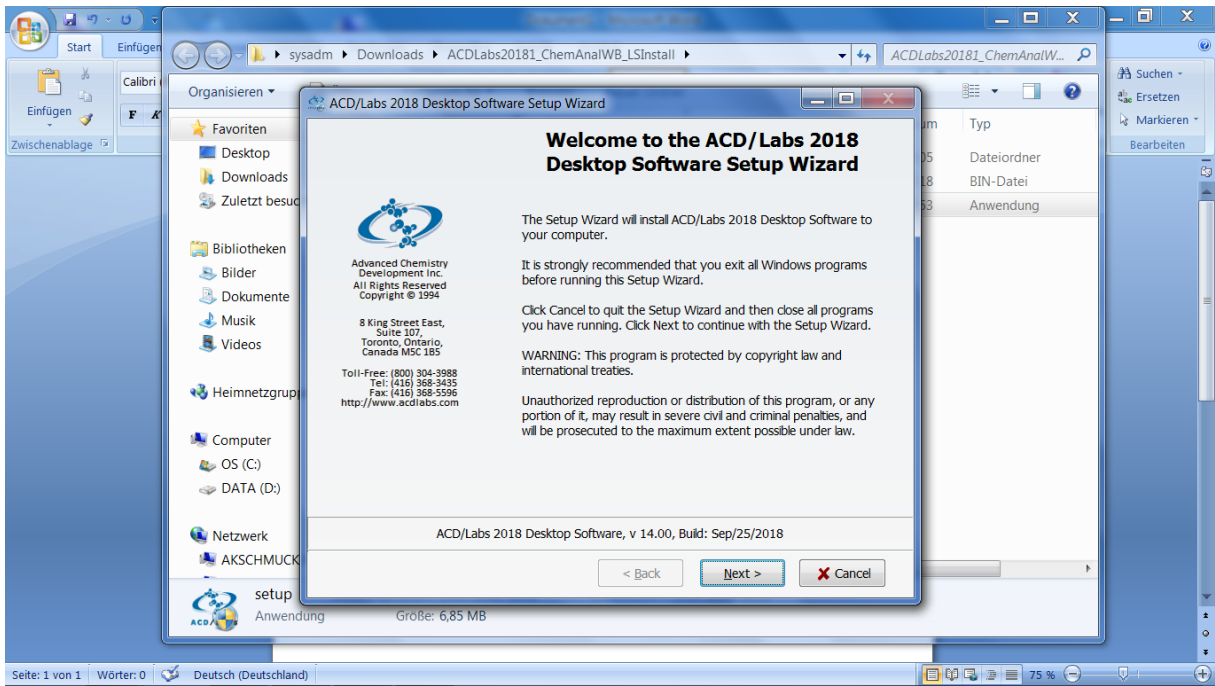
## Deutsche Version

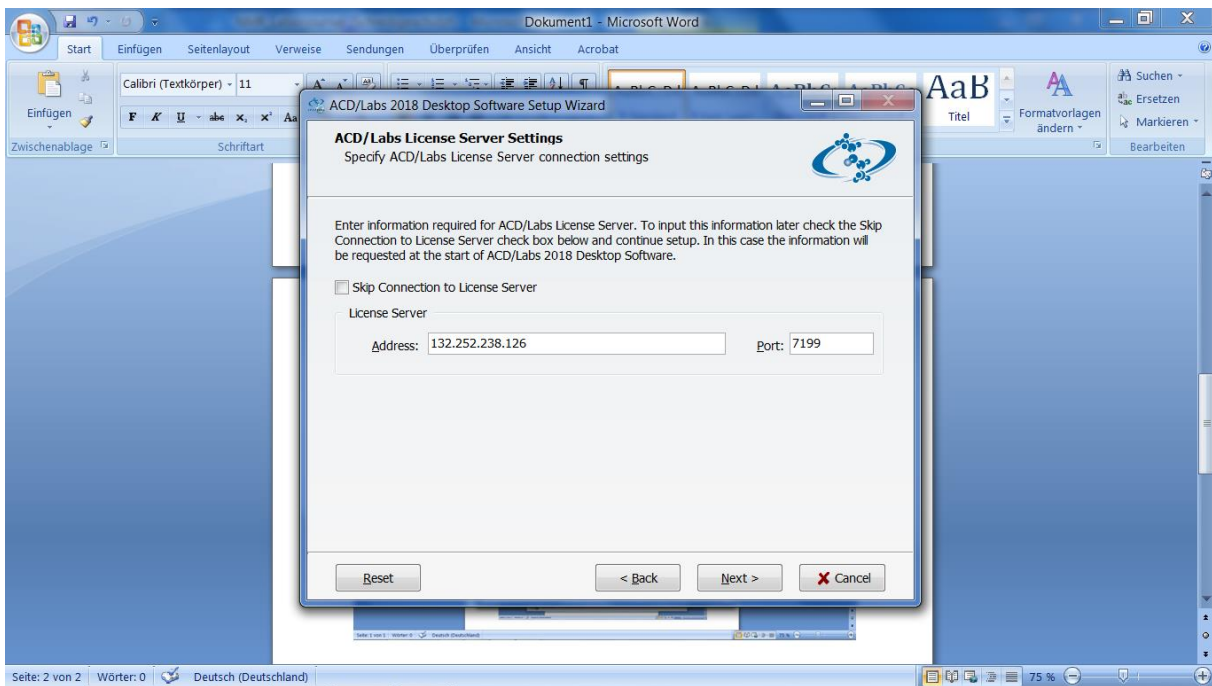
Download des Installationsarchives:

<https://uni-duisburg-essen.sciebo.de/s/IGplnfcTud6Mfe4/download>

Benötigt wird das ChemAnalytical Workbook. Dieses entpacken:

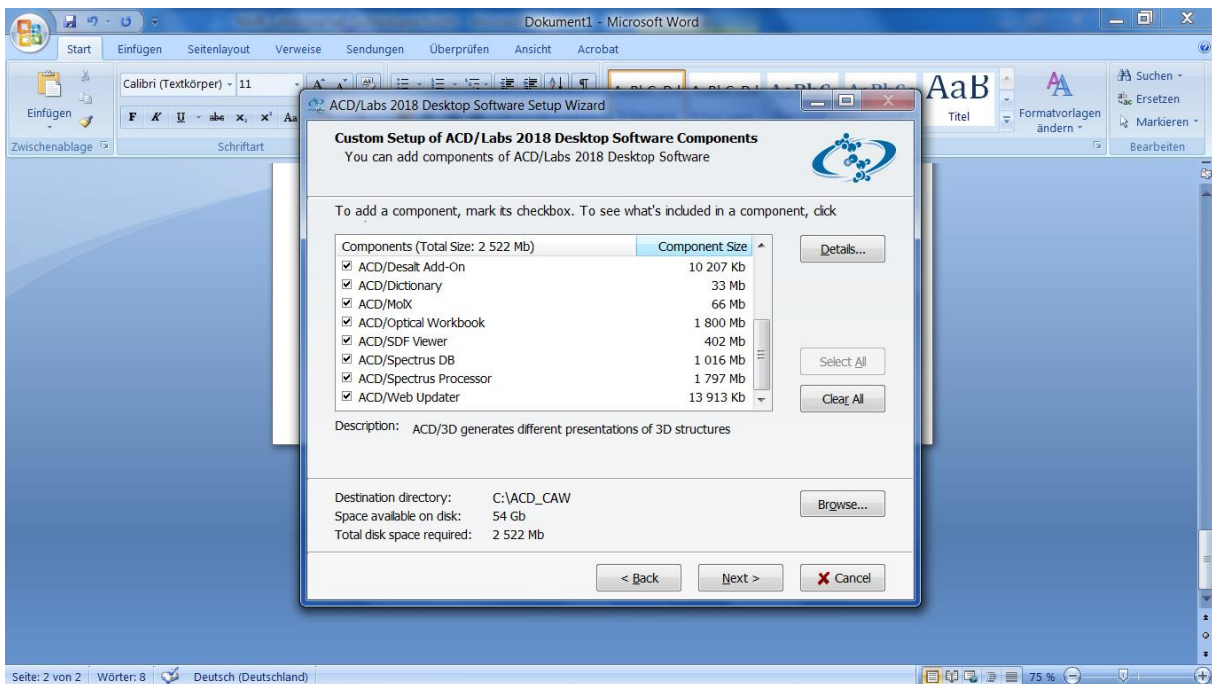


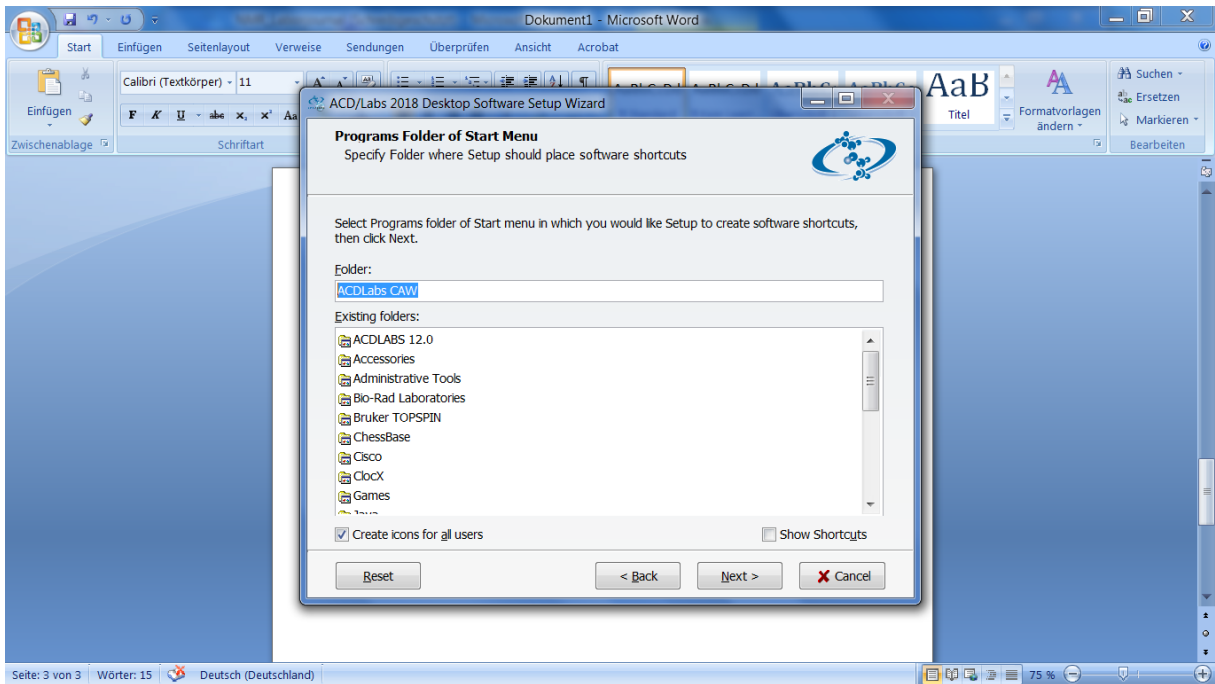




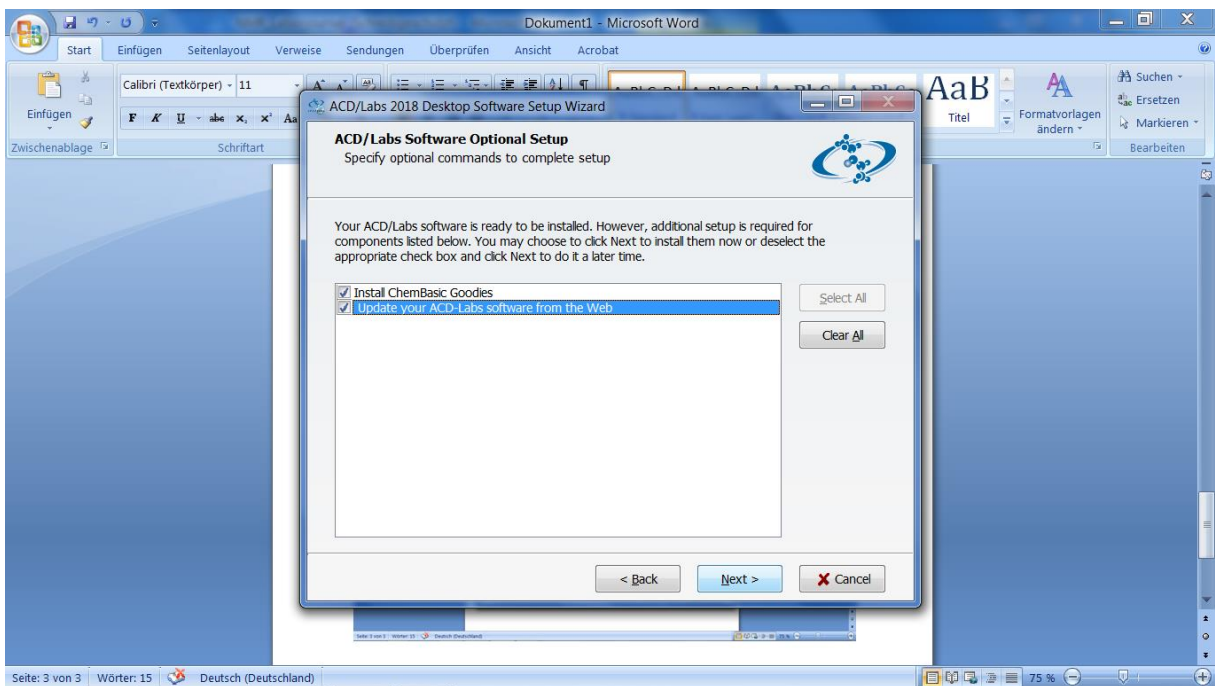
Lizenzserver-Adresse: **acd-labs.win.uni-due.de**

Installationspfad (Empfehlung v. Herrn Rheinwald (Hersteller-Support)) C:\ACD\_CAW, kann aber auch auf Standard belassen werden: C:\Program Files\ACD64LSM

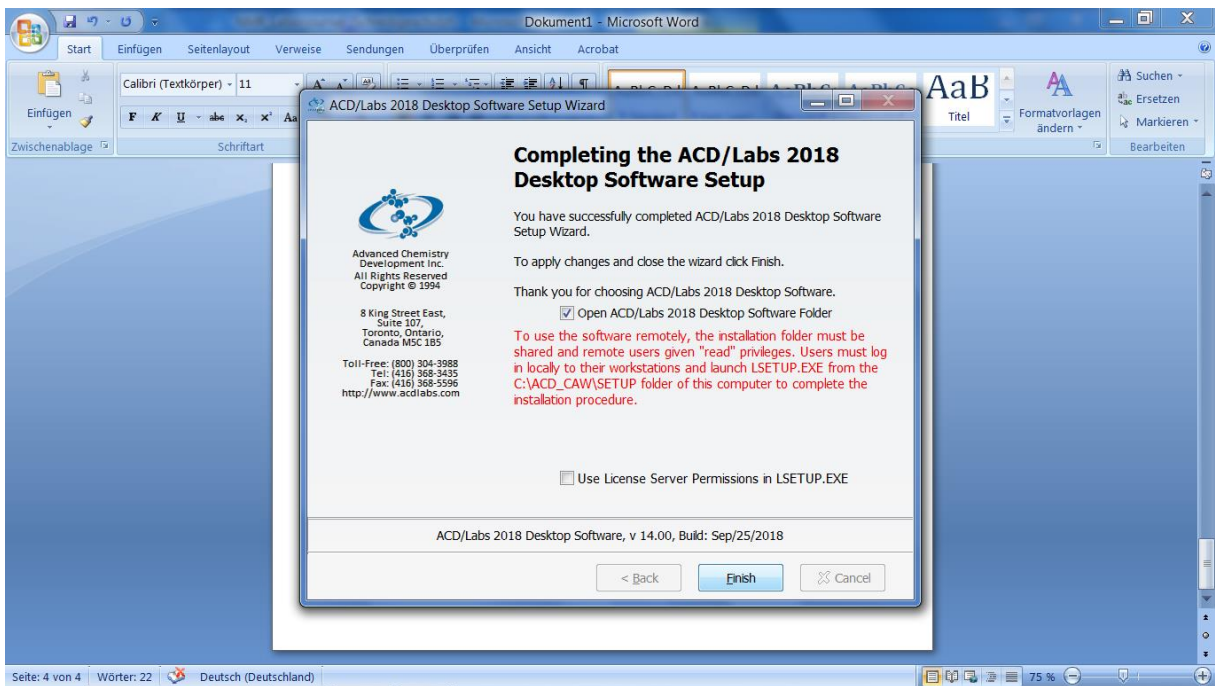
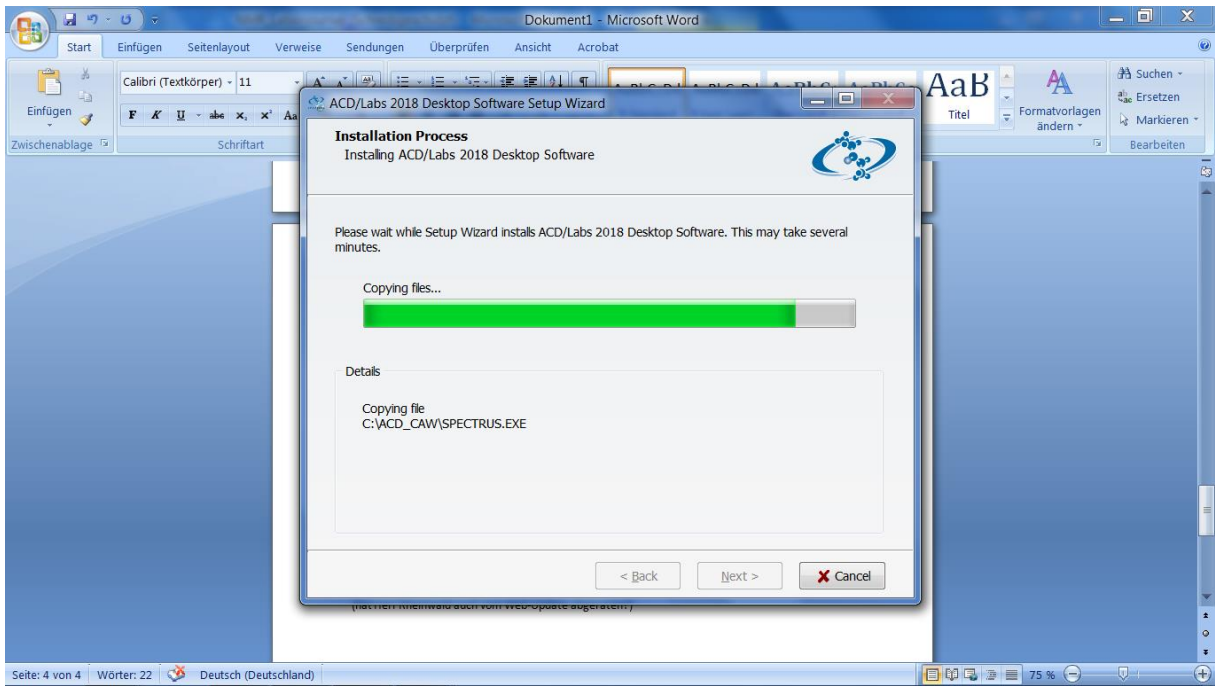




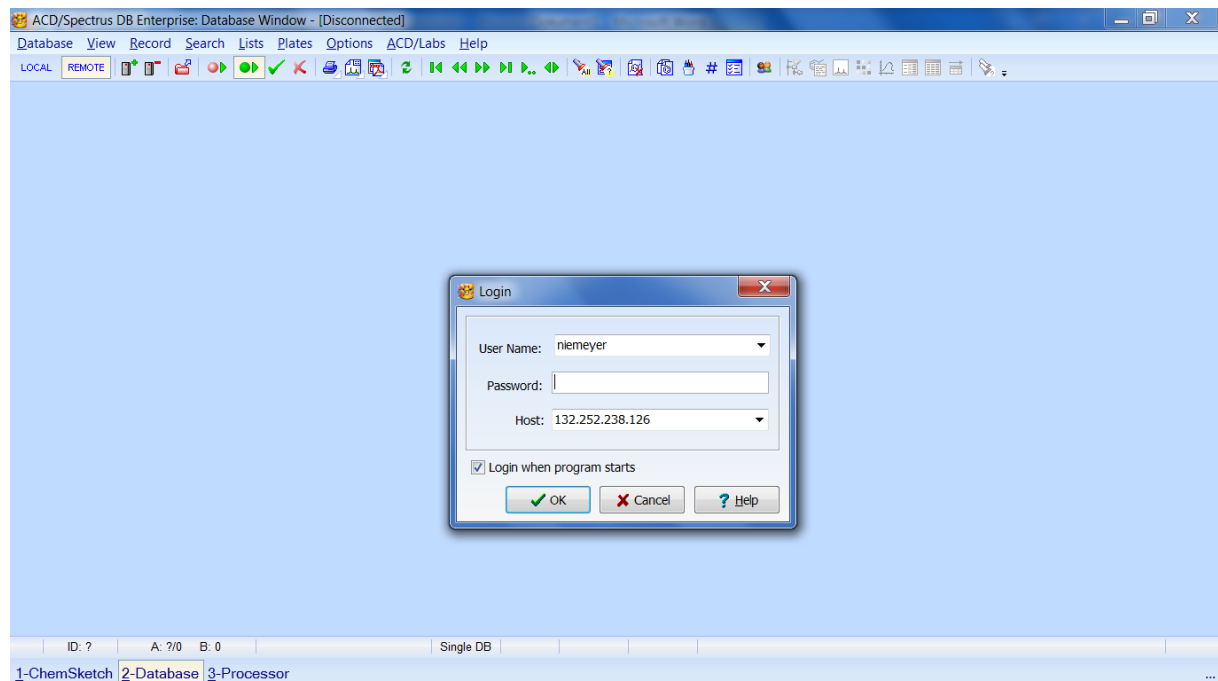
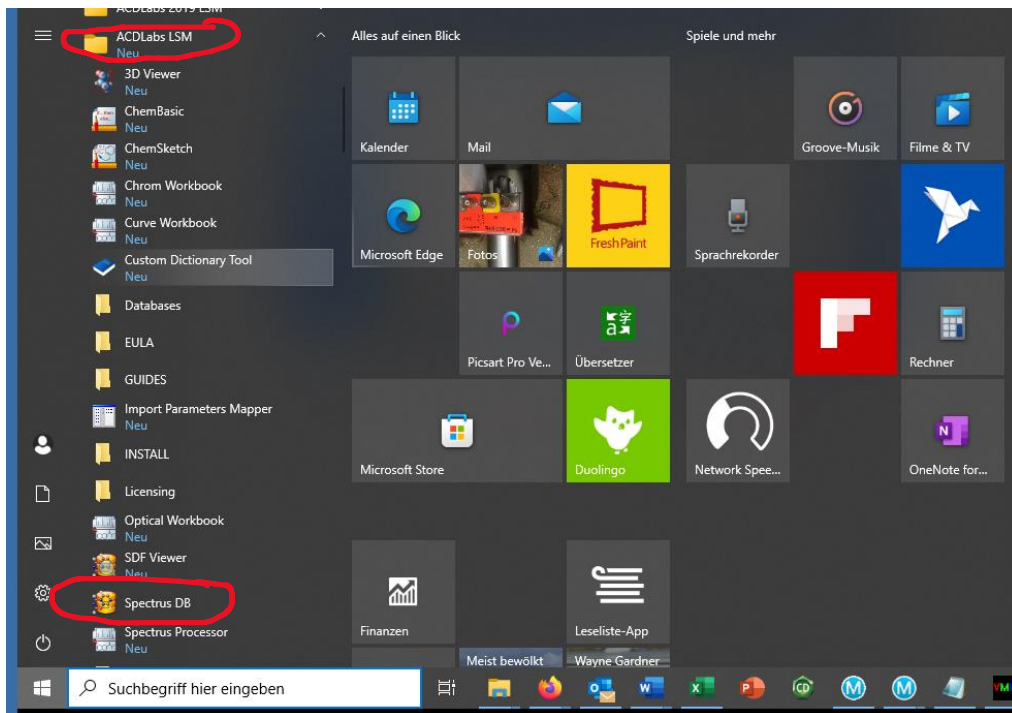
Ordner kann auf Standard belassen werden



Web-Update erst später durchführen, wenn es Updates geben sollte.



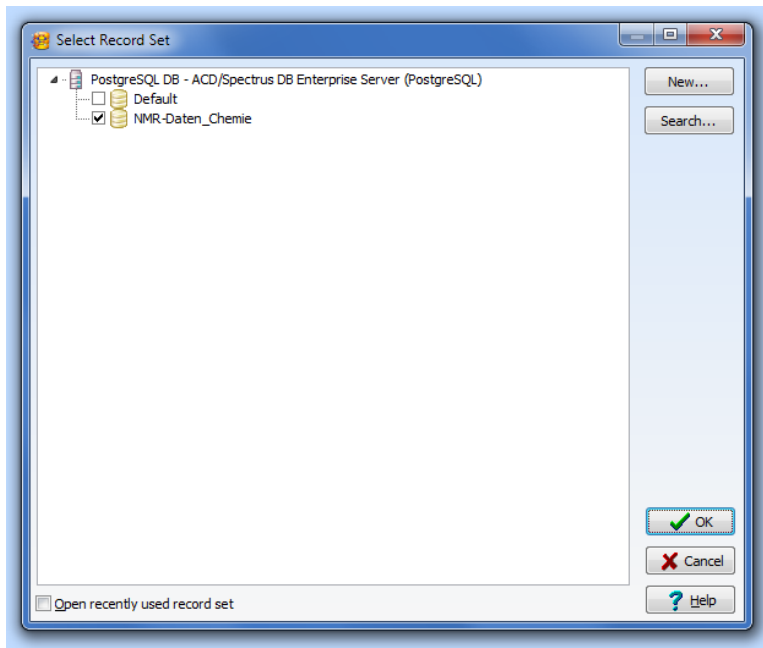
Unter Programme findet man nun ACDLabs LSM und darin das Programm Spectrus DB



Adresse: [acd-labs.win.uni-due.de](http://acd-labs.win.uni-due.de)

Passwort und Nutzer legen wir an. Diese entsprechen den bisherigen Accounts.





Nun die Datenbank NMR-Daten\_Chemie auswählen.

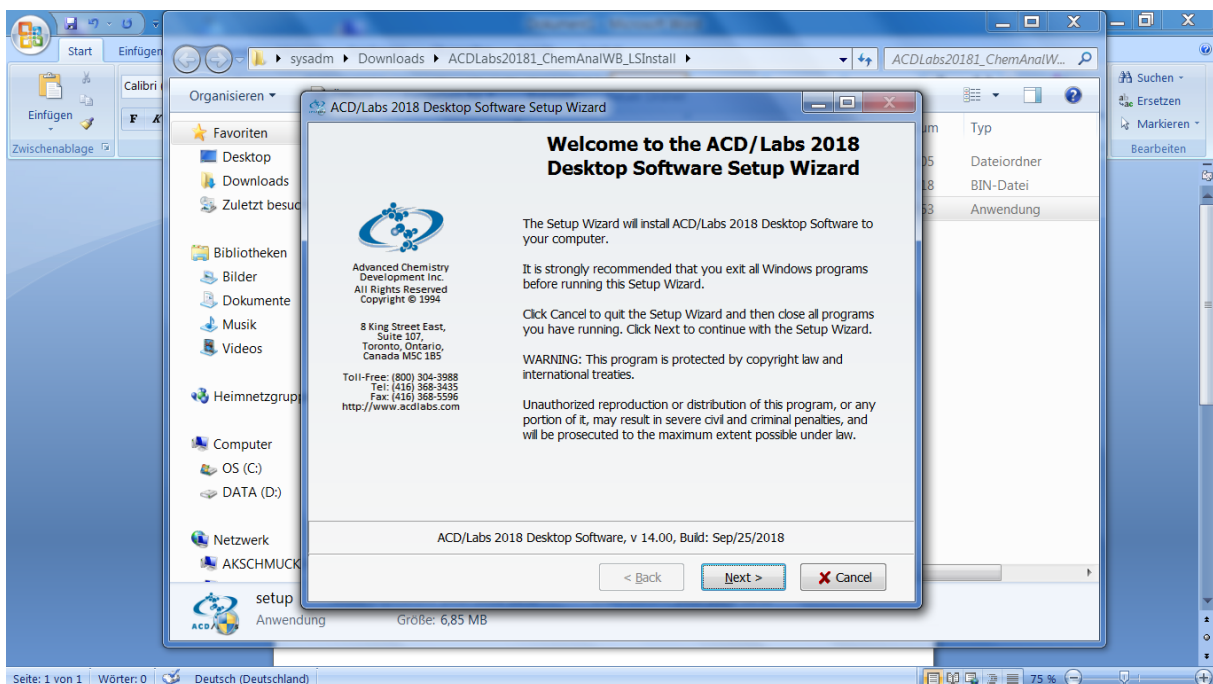
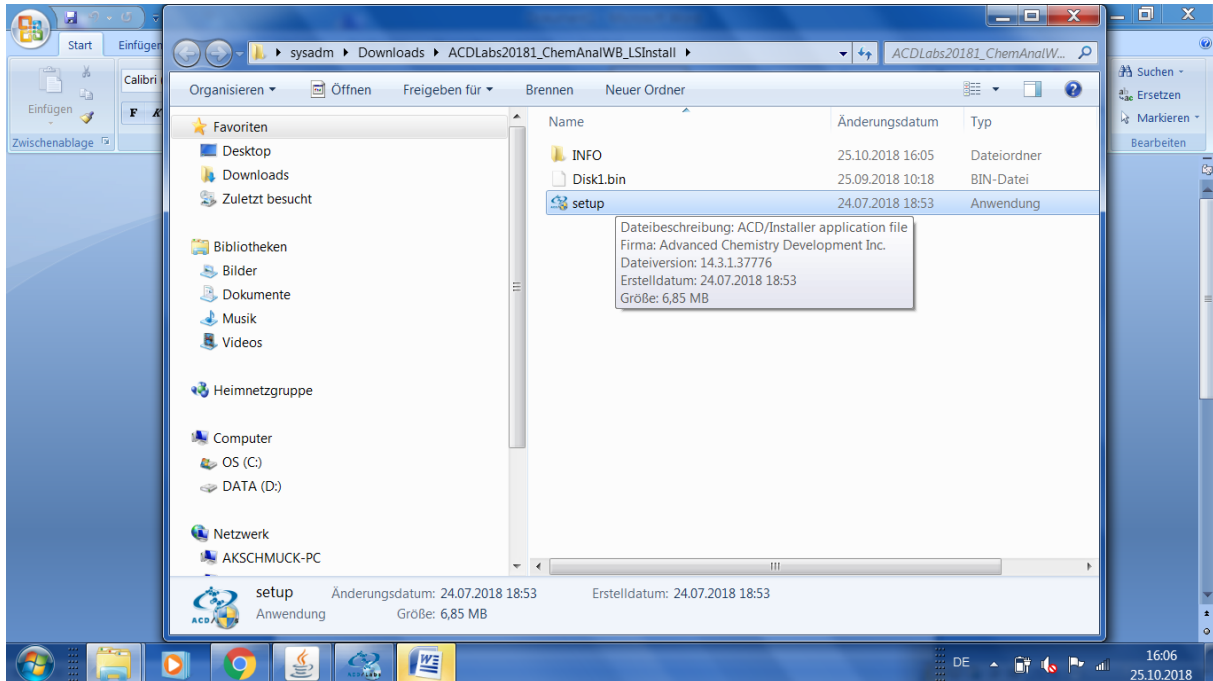
Es öffnet sich eine Ansicht, die an den Probenzettel angelehnt ist.

## English Version

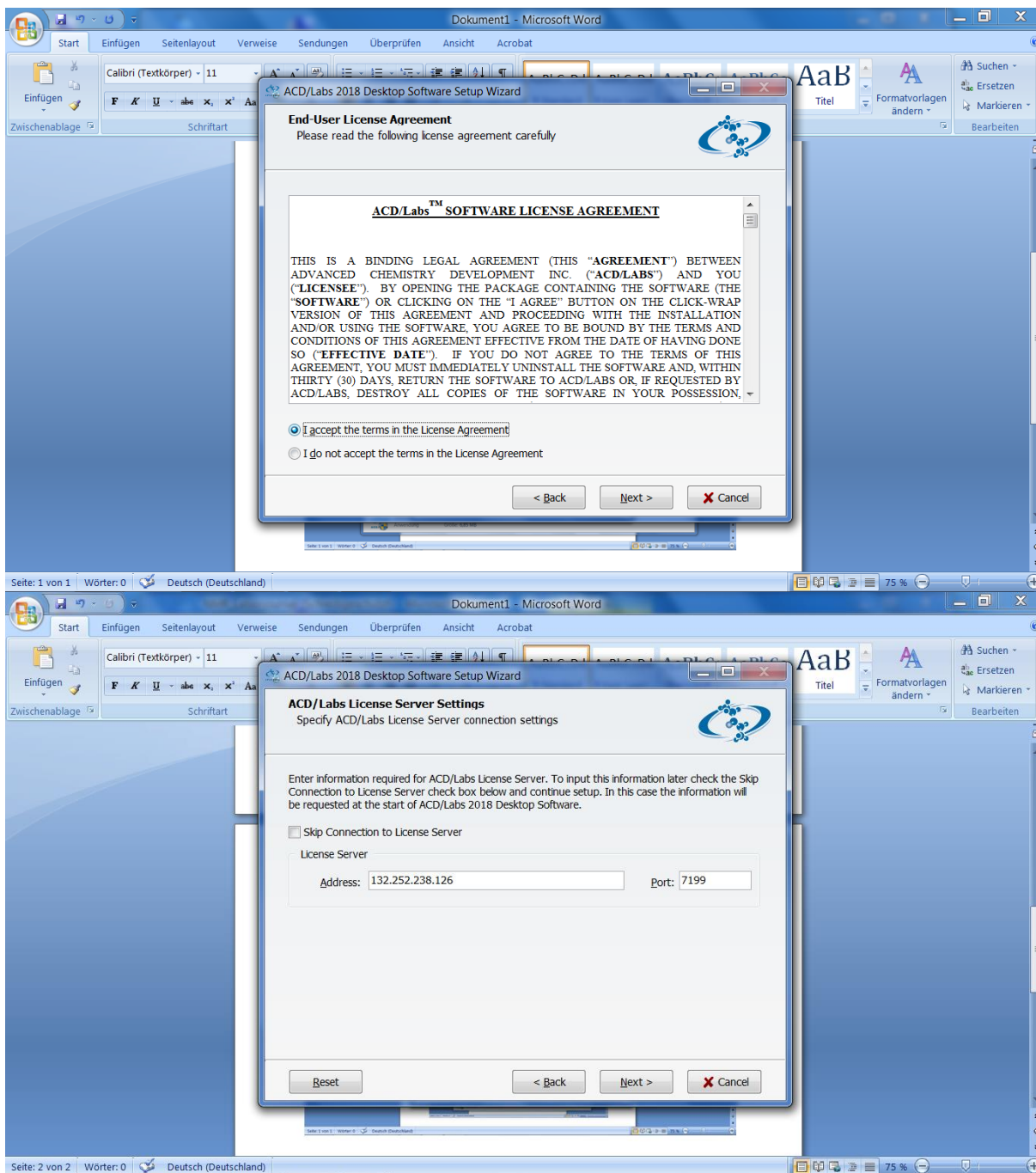
Download the installation archive:

<https://uni-duisburg-essen.sciebo.de/s/IGpInfcTud6Mfe4/download>

The ChemAnalytical Workbook is required. Unpack it:

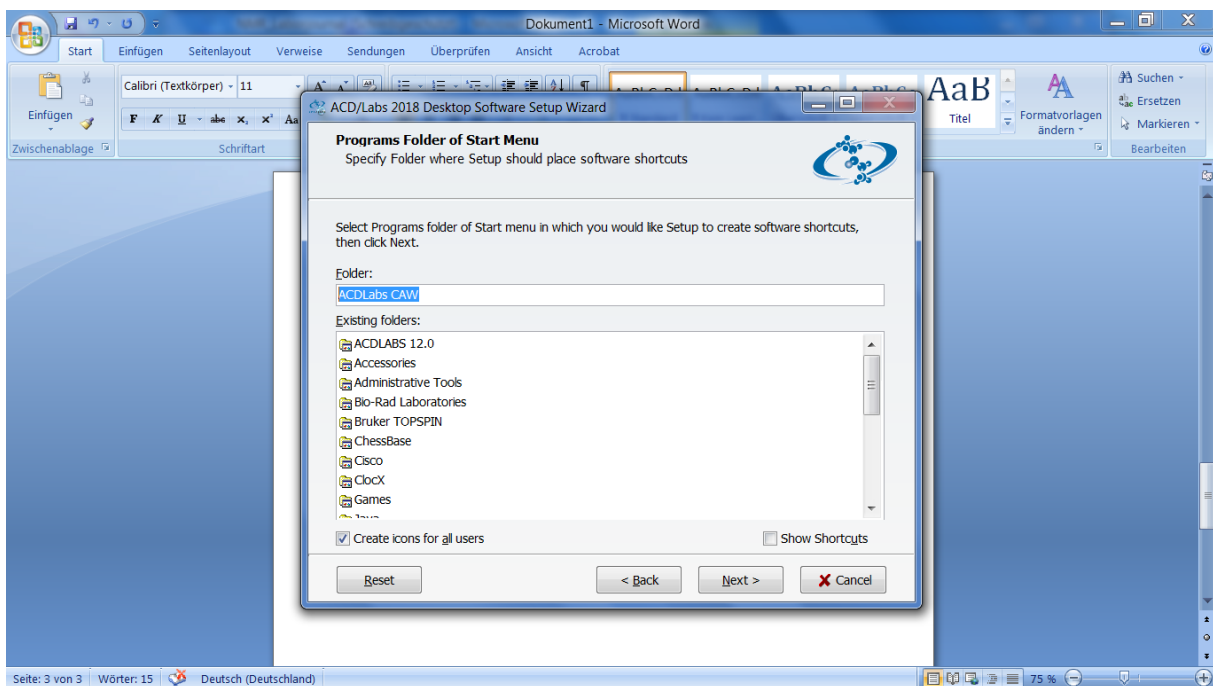
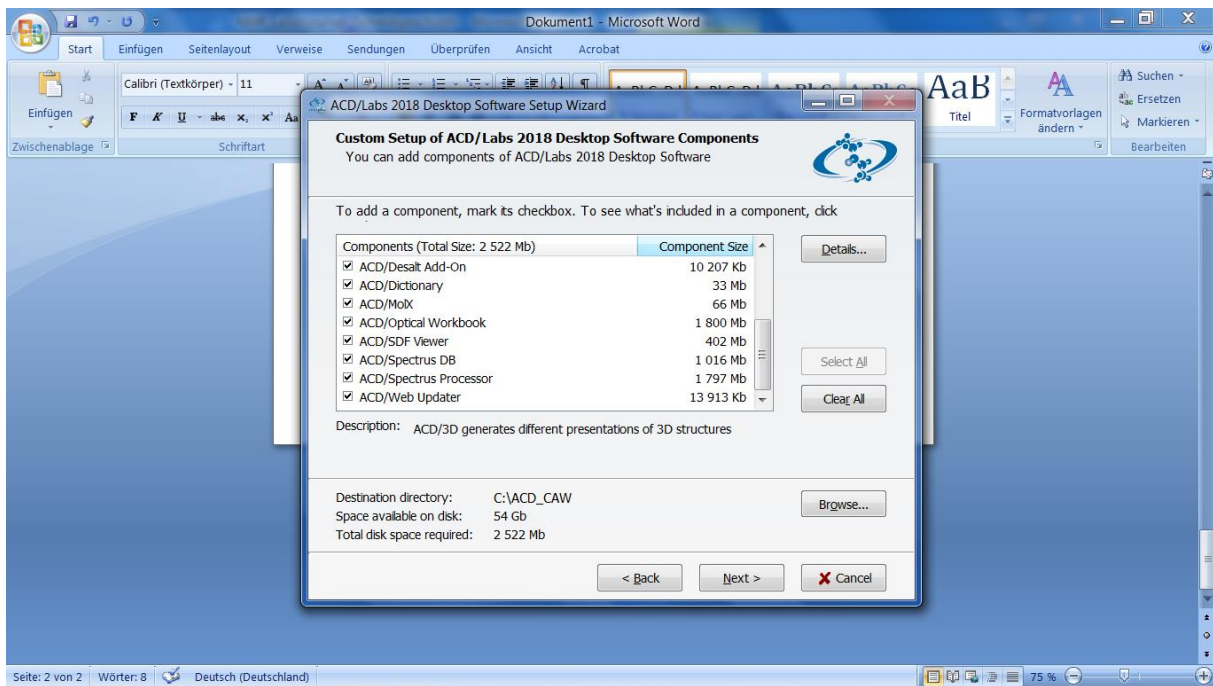




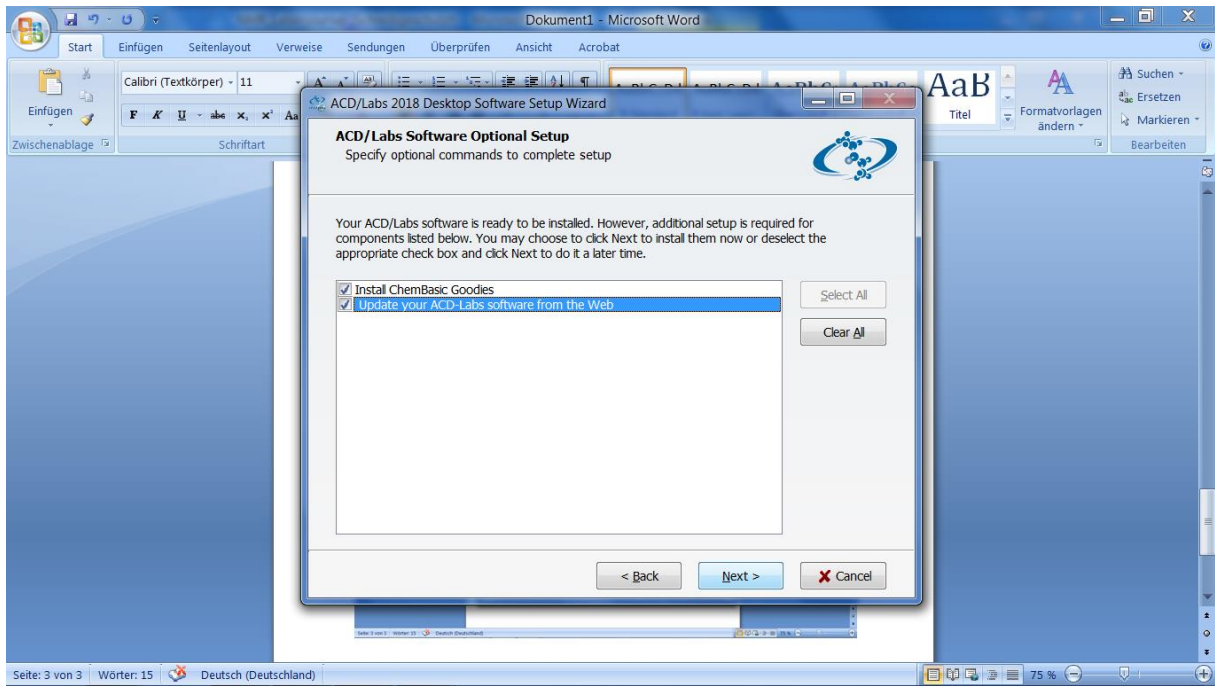


Licence server address: **acd-labs.win.uni-due.de**

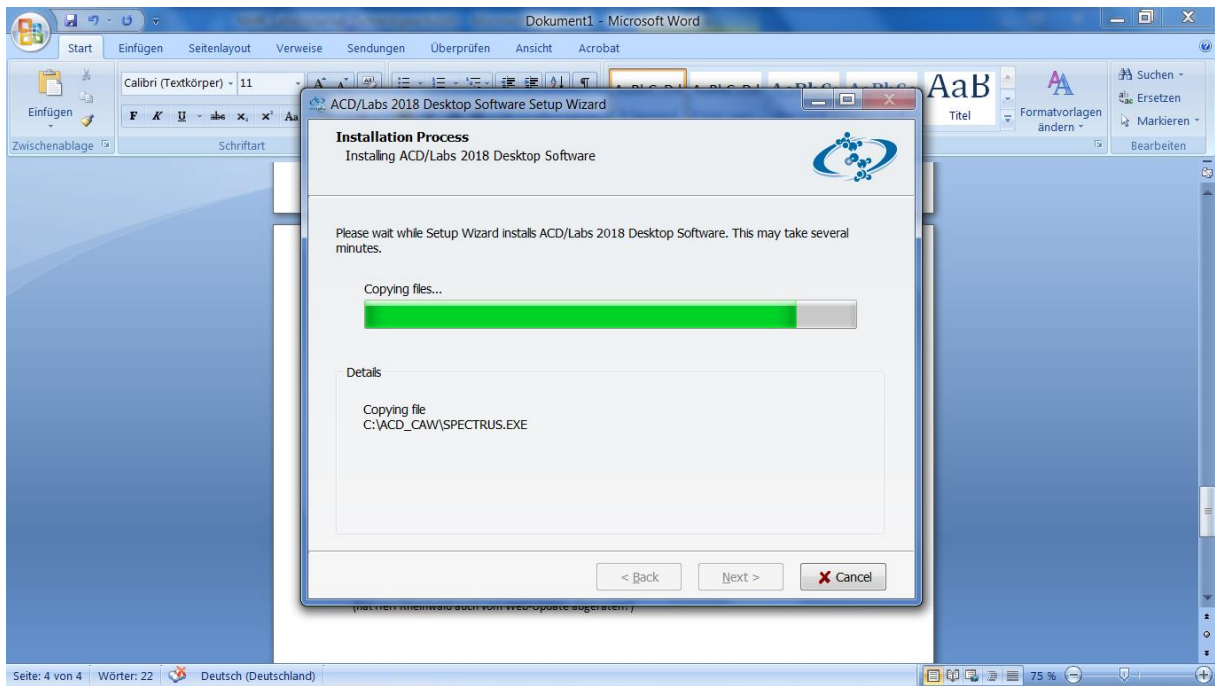
Installation path (recommended by Mr. Rheinwald (manufacturer support)) C:\ACD\_CAW, but can also be left at default: C:\Program Files\ACD64LSM

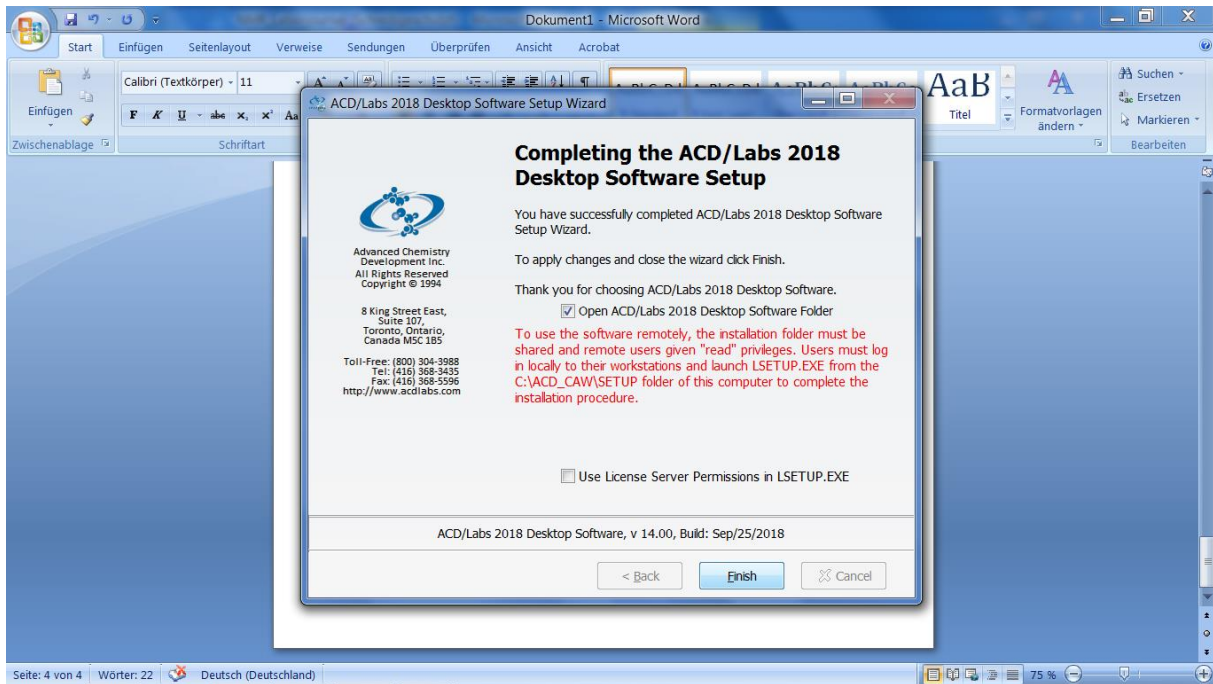


Folder can be left at default

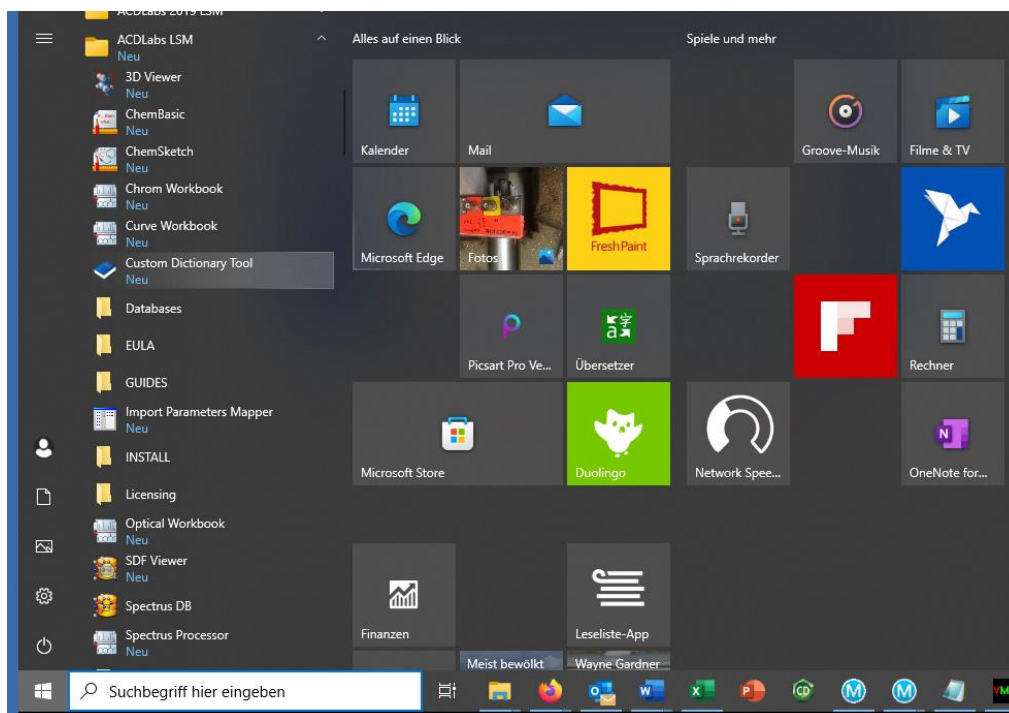


Do not perform the web update until later, when there should be updates.



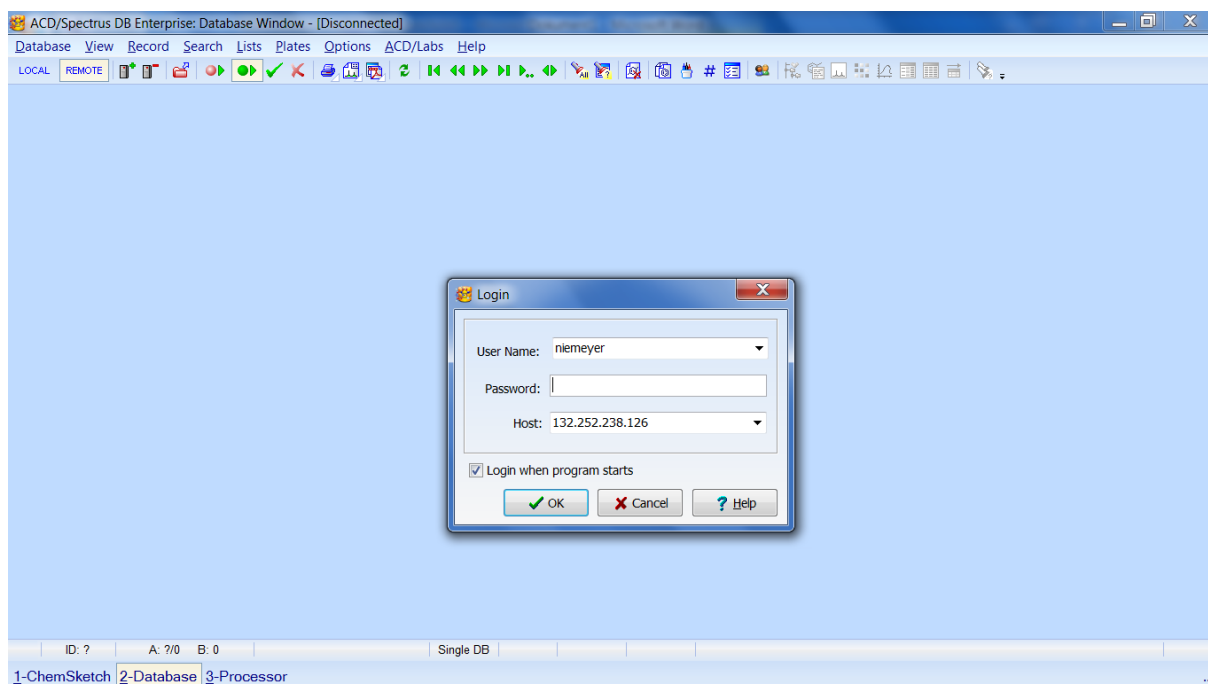


Under Programs you will now find ACDLabs LSM and in it the programme Spectrus DB.

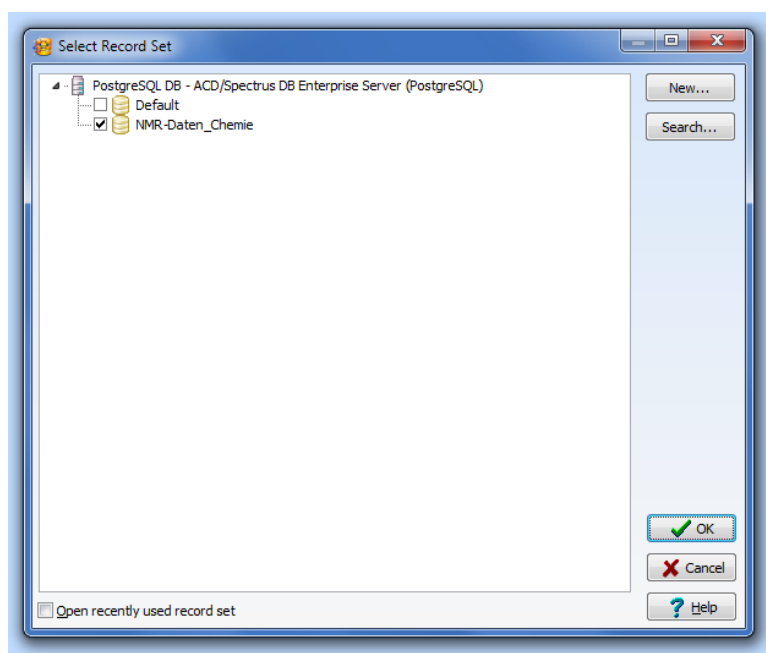


Address: C:\Program Files\ACD64LSM

We create a password and user. These correspond to the existing accounts.



Now select the database NMR-Daten\_Chemie.



A view opens that is based on the sample form.

ACD/Spectrus DB Enterprise: Database Window - [niemeyer is now connected to PostgreSQL... 132.252.238.126 <NMR-Daten\_Haberhauer>]

Database View Record Search Lists Plates Options ACD/Labs Help

LOCAL REMOTE

File Table Default (One Record) Status Probenabgabe Statusänderung

### Bruker Avance DRX500/Avance HD 600 Uni DUISBURG-ESSEN - NMR Auftrag - Übersicht und Bearbeitungsstatus

Filters: JobID

- Job Submitted: Probenbeze...
- Job Rejected
- Analysis Completed
- Job Reported

Probeninfo | Spektren

Datum: 11/10/2018 Telefon: \_\_\_\_\_

Name, Vorname: Liese, David

Arbeitskreis: Haberhauer

NMR Messungen

<input checked="" type="checkbox"/> 1H	<input checked="" type="checkbox"/> HMBC
<input checked="" type="checkbox"/> 13C CPD	<input type="checkbox"/> NOESY
<input type="checkbox"/> 13C DEPT135	<input type="checkbox"/> ROESY
<input type="checkbox"/> 13C DEPT90	<input type="checkbox"/> H,H-TOCSY
<input checked="" type="checkbox"/> H,H-COSY	<input type="checkbox"/> 19F
<input checked="" type="checkbox"/> HSQC mult. edited	<input type="checkbox"/> 31P CPD

Andere Experimente o. Kerne

Temperatur (°C): 25 No. of Samples: 1 Probenrückgabe:  Nein  Ja

Allgemeine Hinweise für den Operator

Probenbez: KS243-B\_6

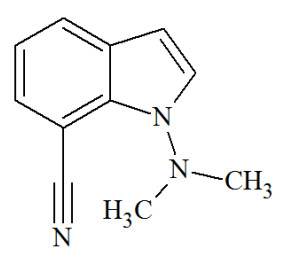
Solvent: CDCl3

Molarität: 0.02mM

Reinheit: \_\_\_\_\_

Methoden

- NMR
- GC-MS
- LC/MS
- IR
- Therm
- Chron
- Wet C

CN1C=CN2C=CC=C(C=C2N1)C#N

ID: 62834 A: 1/13 B: 13 Single DB Owners: o3lie

1-ChemSketch 2-Database 3-Processor