

HOW TO ADD NEW CHEMICAL INTO OPEN INVENTORY USING EXCEL SHEET

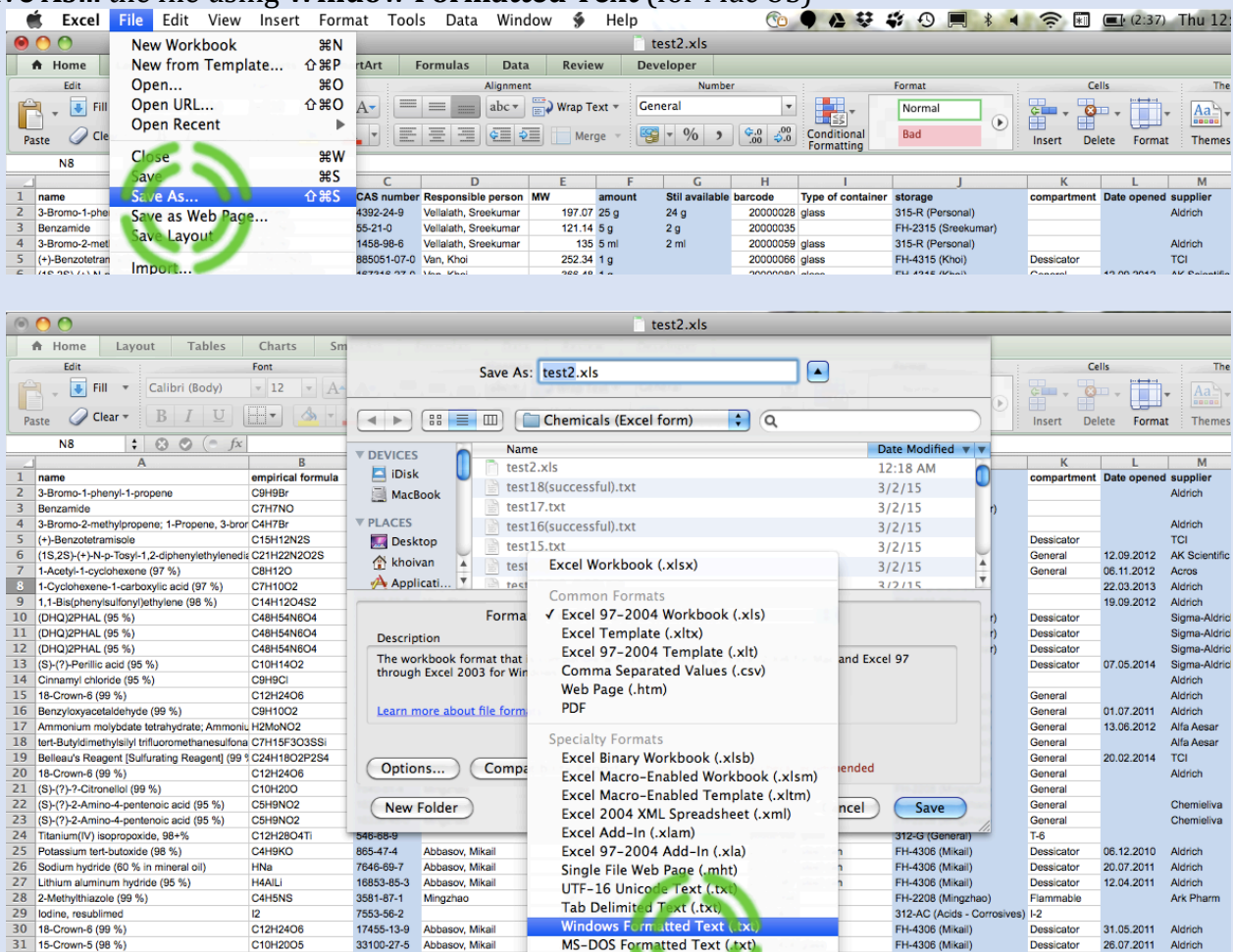
1. Prepare the Excel file, an example might look similar as below. A few important things:
 - Columns that are highlight in blue are important info.
 - You don't need all of the info that show in this example.
 - Empty cells are OK.
 - The amount need to be "xx Y" with xx is the amount and Y is the unit.
 - For unit, it is best to have all in lower case, for example, "ML" should be either "ml" or "mL". It is best to convert all unit to lower case (use lower() command in excel).
 - Double check the CAS number column, Open Inventory uses CAS number as primary source to look up chemical info from the internet.
 - See step 9 for more info about each column in the excel sheet.
 - **Location column: remove all commas (,)** if there is any. Dashes (-) are ok

name	empirical formula	CAS number	Responsible person	MW	amount	Still available	barcode	Type of container	storage	compartment	Date opened	supplier
3-Bromo-1-phenyl-1-propene	C9H9Br	4392-24-9	Vellaiath, Sreekumar	197.07	25 g	24 g	20000028	glass	315-R (Personal)			Aldrich
Benzamide	C7H7NO	55-21-0	Vellaiath, Sreekumar	121.14	5 g	2 g	20000035	glass	FH-2315 (Sreekumar)			
3-Bromo-2-methylpropene; 1-Propene, 3-bromo-	C4H7Br	1458-98-6	Vellaiath, Sreekumar	135	5 ml	2 ml	20000059	glass	315-R (Personal)			Aldrich
(+)-Benzotetramisole	C15H12N2S	885051-07-0	Van, Khoi	252.34	1 g		20000066	glass	FH-4315 (Khoi)	Dessicator		TCI
(1S,2S)-(+)-N-p-Tosyl-1,2-diphenylethylenediamine	C21H22N2O2S	167316-27-0	Van, Khoi	366.48	1 g		20000080	glass	FH-4315 (Khoi)	General	12.09.2012	AK Scientific
1-Acetyl-1-cyclohexene (97 %)	C8H12O	932-66-1	Van, Khoi	124.18	5 g		20000097	glass	FH-4315 (Khoi)	General	06.11.2012	Acros
1-Cyclohexene-1-carboxylic acid (97 %)	C7H10O2	636-82-8	Van, Khoi	126.15	5 g		20000110	glass	315-R (Personal)		22.03.2013	Aldrich
1,1-Bis(phenylsulfonyl)ethylene (98 %)	C14H12O4S2	39082-53-6	Van, Khoi	308.38	1 g		20000127	glass	FH-4315 (Khoi)		19.09.2012	Aldrich
(DHQ)2PHAL (95 %)	C48H54N6O4	140924-50-1	Vellaiath, Sreekumar	778.99	500 mg	200 mg	20000141	glass	FH-2315 (Sreekumar)	Dessicator		Sigma-Aldrich
(DHQ)2PHAL (95 %)	C48H54N6O4	140924-50-1	Vellaiath, Sreekumar	778.99	500 mg		20000158	glass	FH-2315 (Sreekumar)	Dessicator		Sigma-Aldrich
(DHQ)2PHAL (95 %)	C48H54N6O4	140924-50-1	Vellaiath, Sreekumar	778.99	500 mg		20000165	glass	FH-2315 (Sreekumar)	Dessicator		Sigma-Aldrich
(S)-(+)-Pentilic acid (95 %)	C10H14O2	23635-14-5	Morgan	166.22	1 g		20000189	glass	FH-1308 (Morgan)	Dessicator	07.05.2014	Sigma-Aldrich
Cinnamyl chloride (95 %)	C9H9Cl	2687-12-9	Vellaiath, Sreekumar	152.62	5 ml	2.5 ml	20000196	glass	315-R (Personal)			Aldrich
18-Crown-6 (99 %)	C12H24O6	17455-13-9	Mingzhao	264.32	25 g		20000240	glass	FH-2208 (Mingzhao)	General		Aldrich
Benzoyloxycetate/hydrate (99 %)	C9H10O2	60656-87-3	Mingzhao	150.17	5 g		20000257	glass	FH-2208 (Mingzhao)	General	01.07.2011	Aldrich
Ammonium molybdate tetrahydrate; Ammonium H2MoO4	C12H24O6	12054-85-2	Mingzhao	1235.98	25 g		20000284	plastic	FH-2208 (Mingzhao)	General	13.06.2012	Alfa Aesar
tert-Butyl dimethylsilyl trifluoromethanesulfonate	C7H15F3O3SSi	89739-34-0	Mingzhao	264.34	25 g		20000288	glass	FH-2208 (Mingzhao)	General		Alfa Aesar
Bellera's Reagent [Sulfurating Reagent] (99 % 24H18O2P2S4	C12H24O6	88816-02-8	Mingzhao	528.62	5 g		20000295	glass	FH-2208 (Mingzhao)	General	20.02.2014	TCI
18-Crown-6 (99 %)	C12H24O6	17455-13-9	Mingzhao	264.32	25 g		20000301	glass	FH-2208 (Mingzhao)	General		Aldrich
(S)-(+)-Citronellol (99 %)	C10H20O	7540-51-4	Mingzhao	156.27	25 g		20000318	plastic	FH-2208 (Mingzhao)	General		Chemiliva
(S)-(+)-Amino-4-pentenoic acid (95 %)	C5H9NO2	16338-48-0	Mingzhao	115.13	10 g		20000325	glass	FH-2208 (Mingzhao)	General		Chemiliva
(S)-(+)-Amino-4-pentenoic acid (95 %)	C5H9NO2	16338-48-0	Mingzhao	115.13	10 g		20000332	glass	FH-2208 (Mingzhao)	General		Chemiliva
Titanium(IV) isopropoxide, 98+ %	C12H20O4Ti	546-68-9		284.23	250 ml	20 ml	20000358	glass	312-G (General)	T-6		
Potassium tert-butoxide (98 %)	C4H9KO	865-47-4	Abbasov, Mikail	112.21	100 g		20000363	steel can	FH-4306 (Mikail)	Dessicator	06.12.2010	Aldrich
Sodium hydride (60 % in mineral oil)	HNa	7646-69-7	Abbasov, Mikail	24	100 g		20000370	steel can	FH-4306 (Mikail)	Dessicator	20.07.2011	Aldrich
Lithium aluminum hydride (95 %)	H4AlLi	16853-85-3	Abbasov, Mikail	37.95	100 g	90 g	20000387	steel can	FH-4306 (Mikail)	Dessicator	12.04.2011	Aldrich
2-Methylthiazole (99 %)	C4H5NS	3581-87-1	Mingzhao	99.15	10 g		20000394	glass	FH-2208 (Mingzhao)	Flammable		Ark Pharm
Iodine, resublimed	I2	7553-56-2		253.81	100 g		20000400	glass	312-AC (Acids - Corrosives)	I-2		
18-Crown-6 (99 %)	C12H24O6	17455-13-9	Abbasov, Mikail	264.32	25 g		20000417	glass	FH-4306 (Mikail)	Dessicator	31.05.2011	Aldrich
15-Crown-5 (98 %)	C10H20O5	33100-27-5	Abbasov, Mikail	220.28	5 g		20000424	glass	FH-4306 (Mikail)	Dessicator	26.07.2011	Aldrich

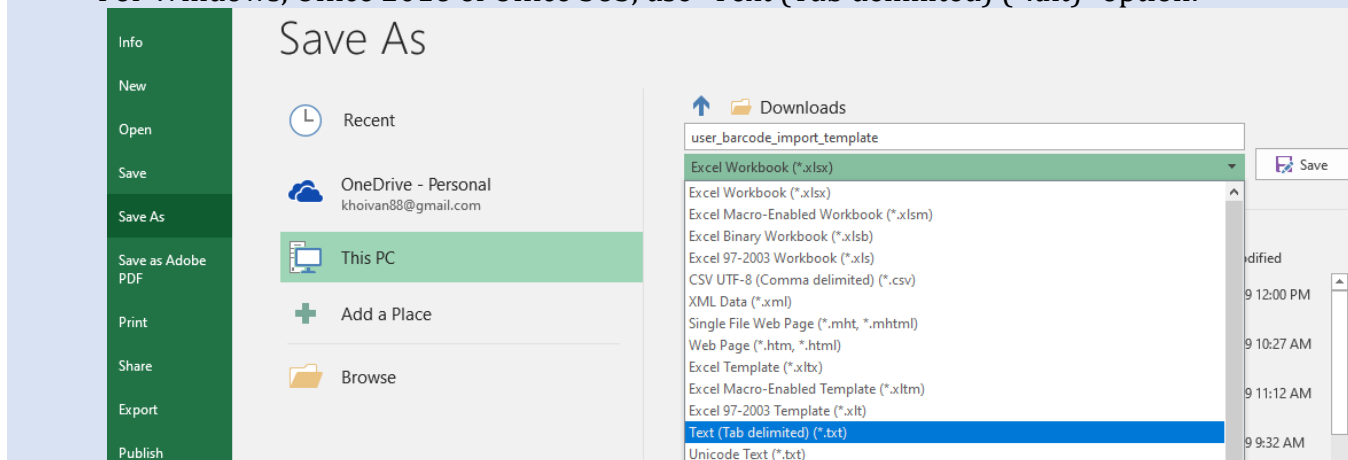
2. **Copy** all of the cells in this file (Ctrl-C for Windows, Cmd-C for Mac) and paste (Ctrl-V for Windows, Cmd-V for Mac) them into Notepad (Windows) or TextEdit (Mac)
3. Save this new file as *your-file-name.txt*. The ".txt" part is important.

Alternatively, instead of step 2 or 3, you can do the following. (Note: in some cases with some chemicals names, Excel has shown to add quotation marks (") around the name when exporting to text file. That is the reason why step 2&3 above is preferred.

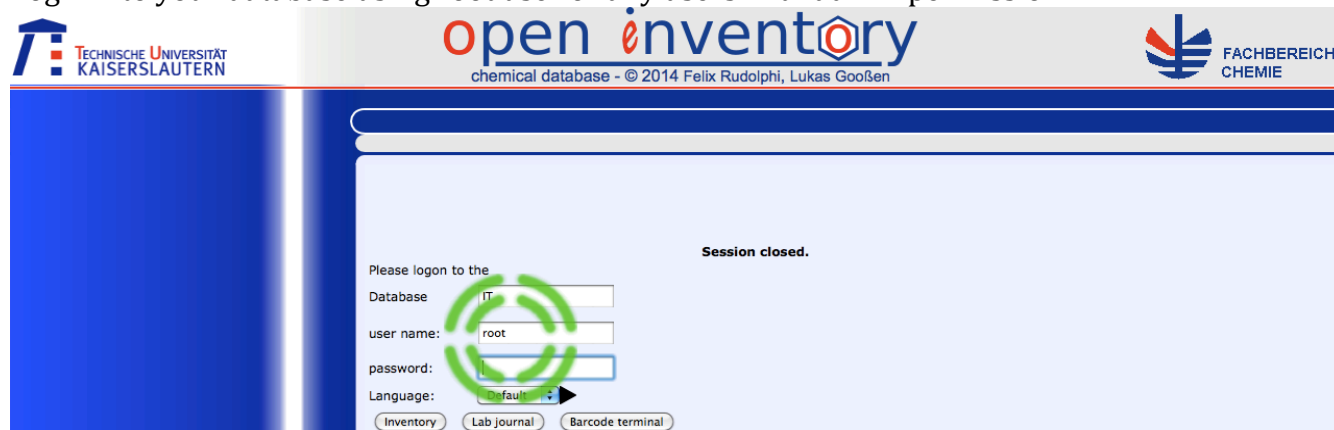
- **Save As...** the file using **Window Formatted Text** (for Mac OS)



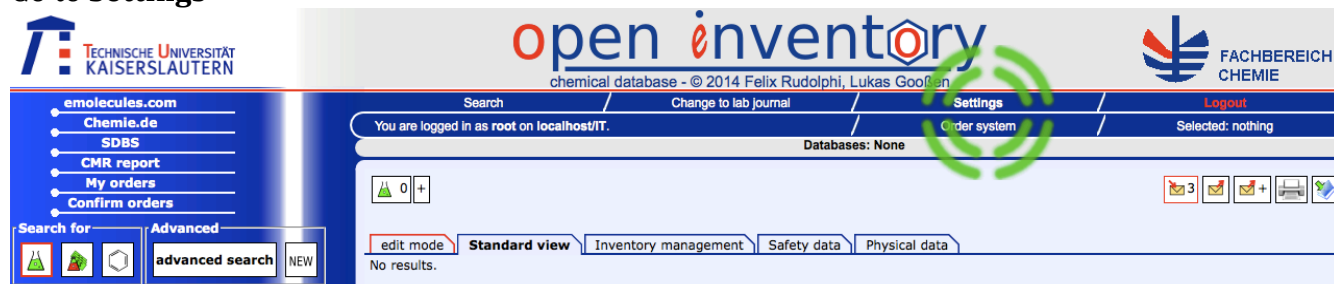
For Windows, Office 2016 or Office 365, use "Text (Tab delimited) (*.txt)" option:



4. Login into your database using root user or any users with admin permission



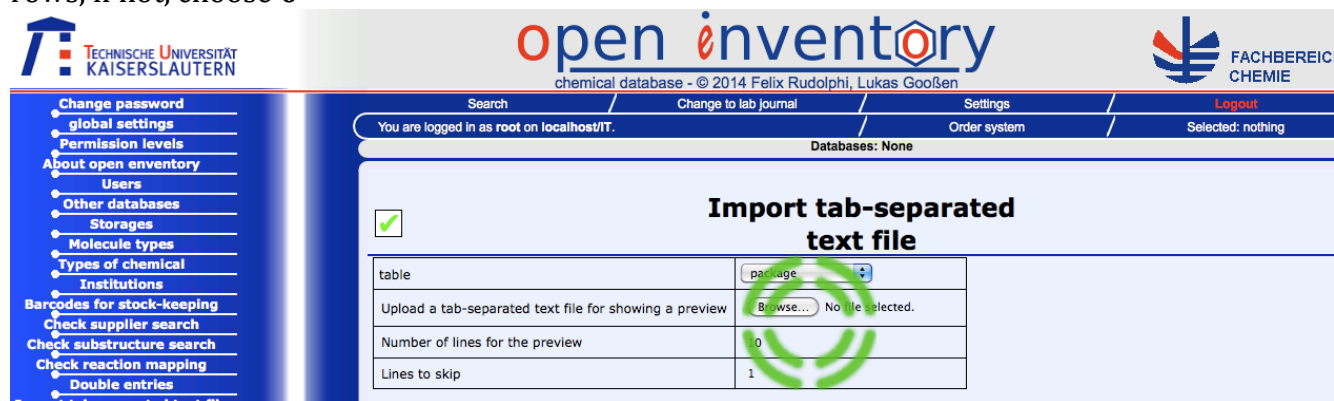
5. Go to **Settings**



6. Go to **Import Tab-separated text file**



7. Choose **Browse...** and choose the exported text file. Note: in *Lines to skip*, put **1** if you have a header rows, if not, choose **0**



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chemical database - © 2014 Felix Rudolphi, Lukas Gooßen

Search | Change to lab journal | Settings | Logout
You are logged in as root on localhost/IT. | Order system | Selected: nothing

Databases: None

Import tab-separated text file

☒

table	package
Upload a tab-separated text file for showing a preview	Browse... test18(successful).txt
Number of lines for the preview	10
Lines to skip	1

8. Click green check mark

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You are logged in as root on localhost/IT. | Order system | Selected: nothing

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Import tab-separated text file

☒

table	package
Upload a tab-separated text file for showing a preview	Browse... test18(successful).txt
Number of lines for the preview	10
Lines to skip	1

9. Screens as below should show up, you can scroll down to see if they show up correctly (info appear correctly in each row)

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You are logged in as root on localhost/IT. | Order system | Selected: nothing

Databases: None

Import tab-separated text file

☒

hazard statements	none	hazard codes	none	column J	multiple equal containers	none
precautionary statements	none	risk statements	none	column K	migrated package identification code	none
safety notes	none	safety statements	none	barcode	comment on chemical	none
WGK	none	density (20°C)	none			


Physical data will also be read from online catalogs
Number of lines: 31

column A	column B	column C	column D	column E	column F	column G	column H	column I	column J	column K	column L	column M
3-Bromo-1-phenyl-1-propene	C9H9Br	4392-24-9	"Vellalath, Sreekumar"	197.07	25 g	24 g	20000028	glass	315-R (Personal)			Aldrich
Benzamide	C7H7NO	55-21-0	"Vellalath, Sreekumar"	121.14	5 g	2 g	20000035	glass	FH-2315 (Sreekumar)			
"3-Bromo-2-methylpropene; 1-Propene, 3-bromo-2-methyl-, 3-Bromo-2-methylpropene,"	C4H7Br	1458-98-6	"Vellalath, Sreekumar"	135	5 ml	2 ml	20000059	glass	315-R (Personal)			Aldrich
(+)-Benzotetramisole	C15H12N2S	885051-07-0	"Van, Khoi"	252.34	1 g		20000066	glass	FH-4315 (Khoi)	Dessicator	12.09.2012	TCI AK Scientific
"(1S,2S)-(+)-N-p-Tosyl-1,2-diphenylethylenediamine (98 %)"	C21H22N2O2S	167316-27-0	"Van, Khoi"	366.48	1 g		20000080	glass	FH-4315 (Khoi)	General	22.03.2013	Aldrich
1-Acetyl-1-cyclohexene (97 %)	C8H12O	932-66-1	"Van, Khoi"	124.18	5 g		20000097	glass	FH-4315 (Khoi)	General	06.11.2012	Acros
1-Cyclohexene-1-carboxylic acid (97 %)	C7H10O2	636-82-8	"Van, Khoi"	126.15	5 g		20000110	glass	315-R (Personal)			Aldrich
"1,1-Bis(phenylsulfonyl)ethylene (98 %)"	C14H12O4S2	39082-53-6	"Van, Khoi"	308.38	1 g		20000127	glass	FH-4315 (Khoi)		19.09.2012	Aldrich
(DHQ)2PHAL (95 %)	C48H54N6O4	140924-50-1	"Vellalath, Sreekumar"	778.99	500 mg	200 mg	20000141	glass	FH-2315 (Sreekumar)	Dessicator		Sigma-Aldrich
(DHQ)2PHAL (95 %)	C48H54N6O4	140924-50-1	"Vellalath, Sreekumar"	778.99	500 mg		20000158	glass	FH-2315 (Sreekumar)	Dessicator		Sigma-Aldrich


10. Choose **Column X** for each content. If you choose **None**, that column will not be imported. You can also add a default value for each column that will apply for ALL items being imported.

Notes:

- CAS number: most important info, OE will use this to look up other info (structures, MW, safety data, etc) from this cas #
- Name: not too important
- Empirical formula: do not import this since OE will use this to find the closest chemicals if CAS# is not present or wrong.
- Amount: = size of the bottle + unit (format should be #+space+unit, for example: 5 g, 125 ml, 1 kg, etc)
- Still available: the amount that left in the bottles (OK is not imported)
- Locations: important. Note: Each location will have its own barcode
- Compartments: = sub-location. Note: each compartment does NOT have its own barcode
- Barcode: if you already have an existing barcode system, add it here.
- Suppliers: = suppliers
- Date open: could be in European style (dd.mm.yyyy) or American style (mm/dd/yy, etc.)



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Search
Change to lab journal
Settings
Logout

You are logged in as root on localhost/IT.
Order system
Selected: nothing

Databases: None


☒

Import tab-separated text file

Lines to skip	1		
Property	column fixed value	Property	column fixed value
name	column A	Storage class	none
additional name	none	carcinogen Cat.	none
CAS number	column C	mutagen Cat.	none
empirical formula	none	teratogen Cat.	none
migrated molecule identification code	none	BtMG (narcotics law) appendix	none
hazard codes (GHS)	none	SprengG appendix III No.	none
hazard statements	none	hazard codes	none
precautionary statements	none	risk statements	none
safety notes	none	safety statements	none
WGK	none	density (20°C)	none
		refractive index (20°C)	none
		melting point	none
		boiling point	none
		amount	column F
		still available	column G
		purity/concentration	none
		(diff. density)	none
		storage name	column J
		in compartment	column K
		barcode	none
		description (e.g. solid support)	none
		supplier	column M
		Catalog no.	none
		Lot no.	none
		price	none
		currency	none USD
		Date opened	column L
		multiple equal containers	none
		migrated package identification code	none
		comment on chemical	none

11. Click green check mark. Screen similar as below should show. Note: line X:... will tell you which lines in the text file is being imported.
Depend of how many chemical containers are imported, this might take a long time, so please be patient.

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 FACHBEREICH CHEMIE

Search Change to lab journal Settings Logout

You are logged in as root on localhost/IT. Order system Selected: nothing

Databases: None

Import tab-separated text file

Lines to skip:

☒

Property	column fixed value
name	<input type="text" value="column A"/>
additional name	<input type="text" value="none"/>
CAS number	<input type="text" value="column C"/>
empirical formula	<input type="text" value="none"/>
migrated molecule identification code	<input type="text" value="none"/>
hazard codes (GHS)	<input type="text" value="none"/>
hazard statements	<input type="text" value="none"/>
precautionary statements	<input type="text" value="none"/>
safety notes	<input type="text" value="none"/>
	<input type="text" value="none"/>

Property	column fixed value	Property	column fixed value	Property	column fixed value
Storage class	<input type="text" value="none"/>	refractive index (20°C)	<input type="text" value="none"/>	description (e.g. solid support)	<input type="text" value="none"/>
carcinogen Cat.	<input type="text" value="none"/>	melting point	<input type="text" value="none"/>	supplier	<input type="text" value="column M"/>
mutagen Cat.	<input type="text" value="none"/>	boiling point	<input type="text" value="none"/>	Catalog no.	<input type="text" value="none"/>
teratogen Cat.	<input type="text" value="none"/>	amount	<input type="text" value="column F"/>	Lot no.	<input type="text" value="none"/>
BtMG (narcotics law) appendix	<input type="text" value="none"/>	still available	<input type="text" value="column G"/>	price	<input type="text" value="none"/>
SprengG appendix III No.	<input type="text" value="none"/>	purity/concentration	<input type="text" value="none"/>	currency	<input type="text" value="none"/>
hazard codes	<input type="text" value="none"/>	(diff. density)	<input type="text" value="none"/>	Date opened	<input type="text" value="column L"/>
risk statements	<input type="text" value="none"/>	storage name	<input type="text" value="column J"/>	multiple equal containers	<input type="text" value="none"/>
safety statements	<input type="text" value="none"/>	in compartment	<input type="text" value="column K"/>	migrated package identification code	<input type="text" value="none"/>
density (20°C)	<input type="text" value="none"/>	barcode	<input type="text" value="none"/>	comment on chemical	<input type="text" value="none"/>

JavaScript:void submitForm("main");

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Search Change to lab journal Settings Logout

You are logged in as root on localhost/IT. Order system Selected: nothing

Databases: None

Import tab-separated text file

Please be patient until the import is complete. Depending on the file size, this process may take several hours. line 1: 4392-24-9

Warning: no language set.: 32
Acros: 43
line 2: 55-21-0
Warning: no language set.: 32
Acros: 43
line 3: 1458-98-6
Warning: no language set.: 32
Acros: 43
line 4: 885051-07-0
Warning: no language set.: 32
Acros: 32
NIST Webbook: 32
Sigma-Aldrich: 34
ChemicalBook: 42
TCI: 42
line 5: 167316-27-0
Warning: no language set.: 32
Acros: 32
NIST Webbook: 32
Sigma-Aldrich: 36
line 6: 932-66-1