

Adding TLC Plates to a Reaction Database

ACD/ChemFolder
Version 8.0

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Introduction

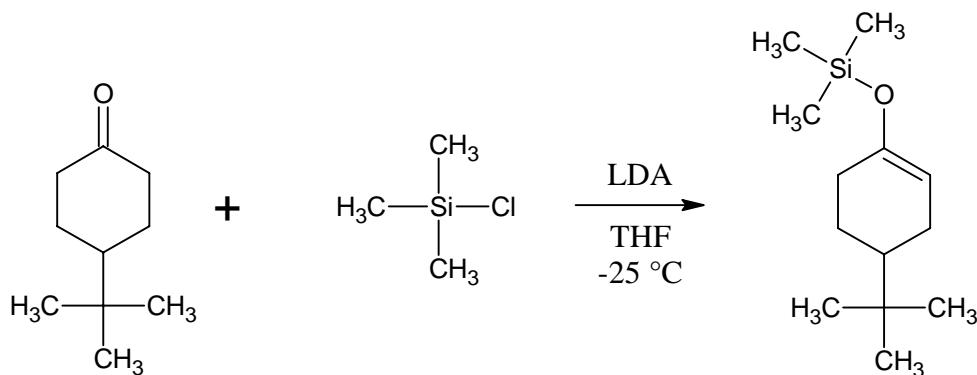
Hands-on organic chemists are all too familiar with running Thin Layer Chromatography (TLC) plates to monitor their reactions. However, storage of the plates that capture reaction dynamics is often a challenge. Not only do the plates deteriorate over time, but they can also add extra bulk and weight to a notebook. When it comes to reporting your findings, a hand drawn sketch of the plate or a photocopy image is often used. Is there a better way?


In another technical note, we've outlined software capabilities that allow for easy creation of TLC images using [ACD/ChemSketch](#) [1]. The addition of TLC information to an [ACD/ChemFolder](#) [2] reaction database can help make reaction information more complete. This document shows how to improve the storage and retrieval of data stored on a TLC plate using the ChemFolder chemical databasing software.

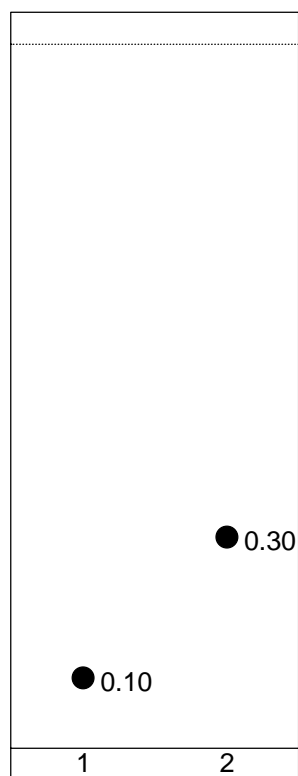
Procedure

This document outlines steps on how to add the TLC Plate image and R_f information into a ChemFolder database.

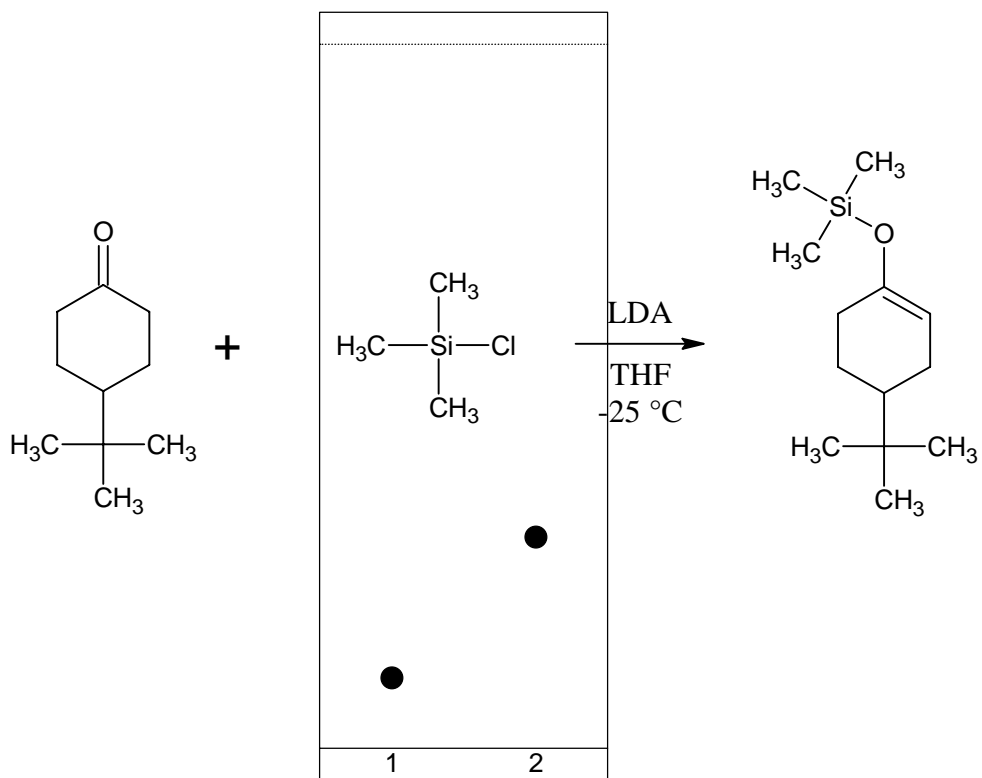
1. Create or open a ChemFolder database.
2. Draw the reaction.



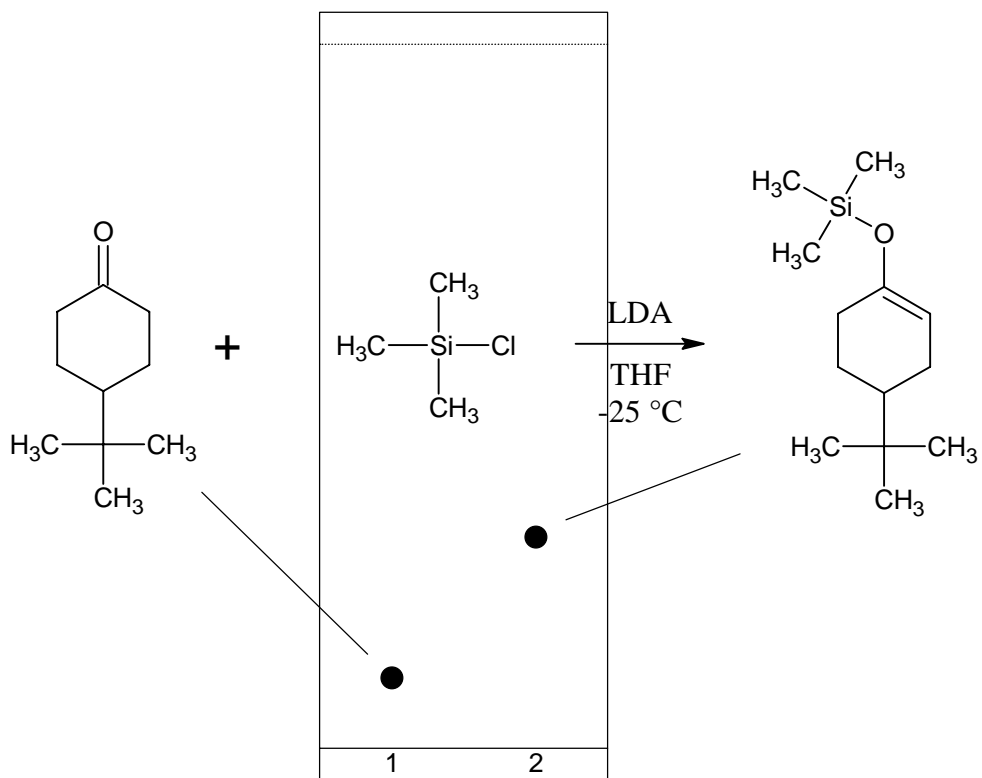
3. Generate the corresponding TLC plate with the **TLC Plate Tool** . Please refer to the TLC Plate Drawing Tool technical note [3] for instructions.



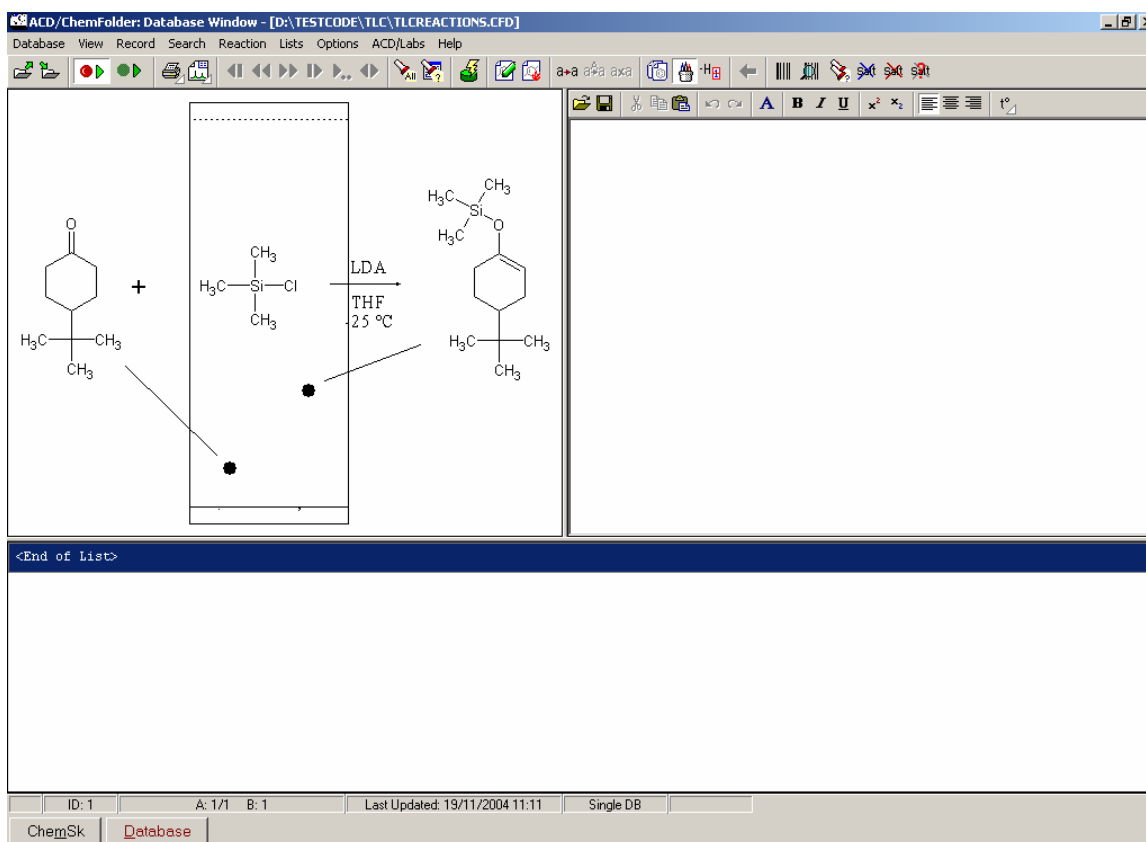
4. Copy the TLC plate onto the given page with the reaction and center it over the reaction. Remove the R_f labels if necessary to tidy up the display.



5. Add lines or other symbols to match structures with TLC spots if desired.



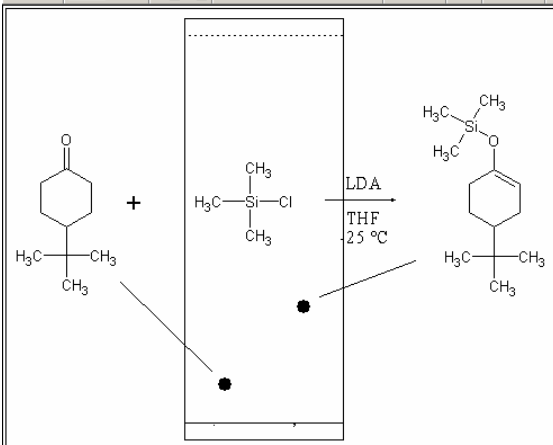
6. Make sure you are in **DRAW** mode and then click **Add Picture** . The reaction and the TLC plate will be transferred into ChemFolder.



7. On the **View** menu, point to **Screen Forms**, and then choose **Default with Reaction Table**.

ACD/ChemFolder: Database Window - [D:\TESTCODE\TLC\TLCREACTIONS.CFD]


Database View Record Search Reaction Lists Options ACD/Labs Help



Reactant	Formula	FW	Name	K	n	C	m	V	d	Yield
1	C ₁₀ H ₁₈ O	154.2493	-	1	-	-	-	-	-	-
2	C ₃ H ₉ ClSi	108.6421	-	1	-	-	-	-	-	-
Product										
1	C ₁₃ H ₂₆ OSi	226.4304	-	1	-	-	-	-	-	-

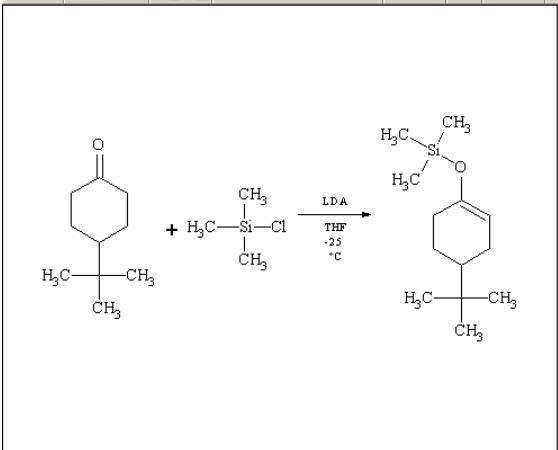
ID: 1 A: 1/1 B: 1 Last Updated: 19/11/2004 11:11 Single DB

ChemSk Database

8. To hide the TLC plate for a clearer view of the reaction, click **Show Pictures On/Off** .

ACD/ChemFolder: Database Window - [D:\TESTCODE\TLC\TLCREACTIONS.CFD]

Database View Record Search Reaction Lists Options ACD/Labs Help

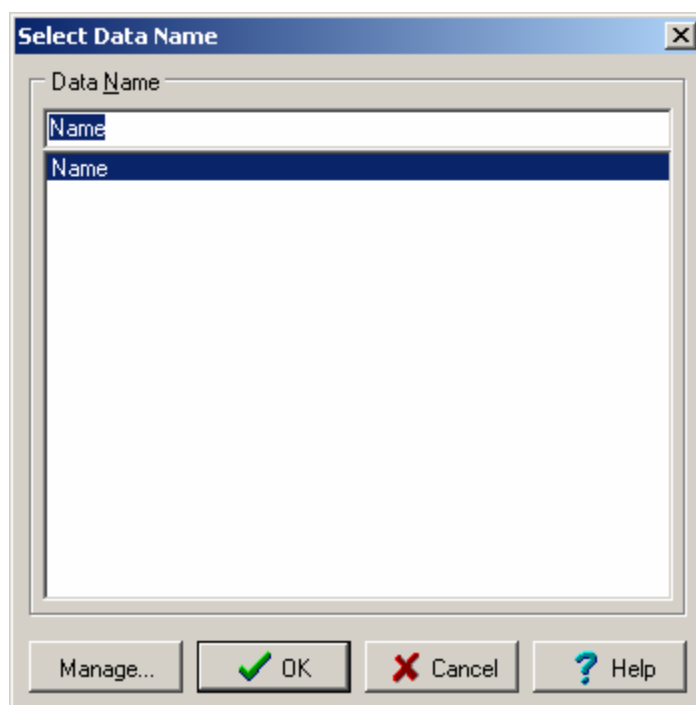


Reactant	Formula	FW	Name	K	n	C	m	V	d	Yield
1	C ₁₀ H ₁₈ O	154.2493	-	1	-	-	-	-	-	-
2	C ₃ H ₉ ClSi	108.6421	-	1	-	-	-	-	-	-
Product										
1	C ₁₃ H ₂₆ OSi	226.4304	-	1	-	-	-	-	-	-

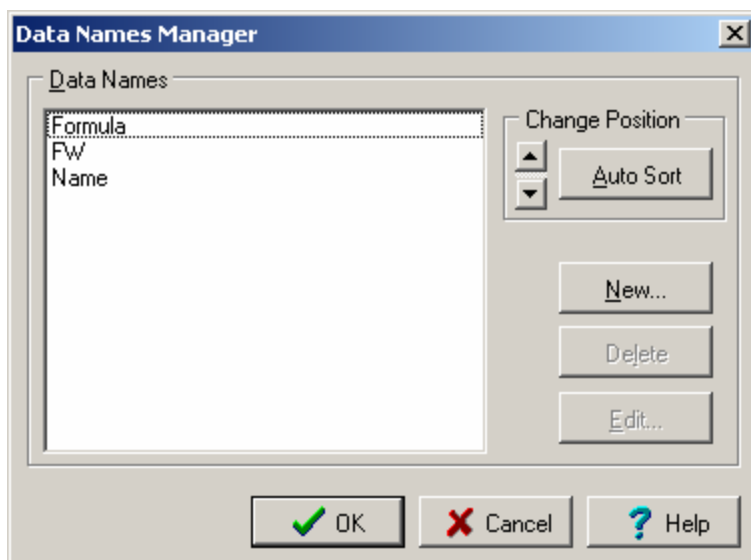
ID: 1 A: 1/1 B: 1 Last Updated: 19/11/2004 11:11 Single DB

ChemSk Database

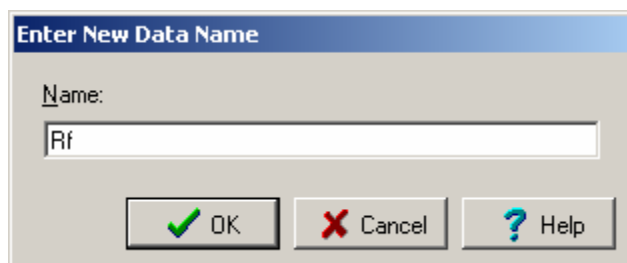
9. On the **View** menu, point to **Screen Forms**, and then choose **Default with User Data**.
10. Select one of the structures. The User Data should only list the **Formula** and **FW** fields. Double-click on **<End Of List>** to bring up the following dialog box.



11. Click **Manage** to open the **Data Names Manager** dialog box.



12. Click **New** and enter “R_f” in the **Enter New Data Name** dialog box.



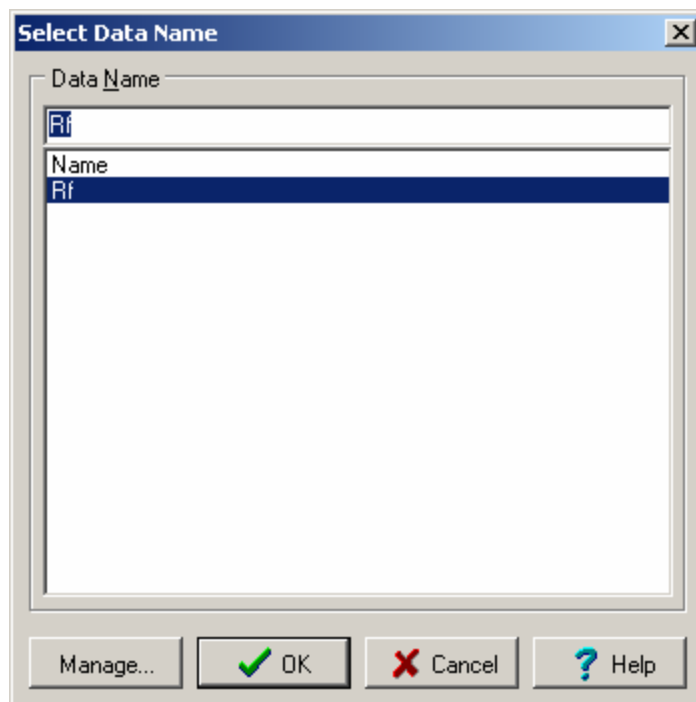
Enter New Data Name

Name:

Rf

OK Cancel Help

13. Click **OK** and then click **OK** to close the **Data Names Manager** dialog box.
14. In the **Select Data Name** dialog box, click **R_f** and click **OK**.



Select Data Name

Data Name

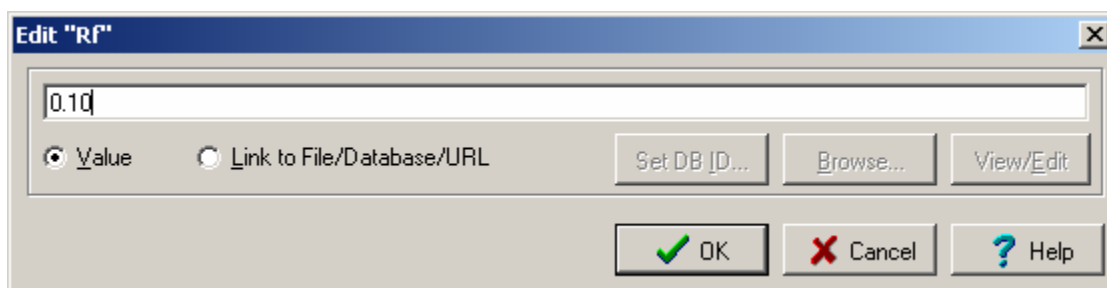
Rf

Name

Rf

Manage... OK Cancel Help

15. In the **Edit "R_f"** dialog box, click **Value** and enter the R_f value for the selected structure.



Edit "Rf"

0.10

Value Link to File/Database/URL

Set DB ID... Browse... View/Edit

OK Cancel Help

16. Click **OK**. The new **R_f** field and the value entered will now appear in the **User Data** window.

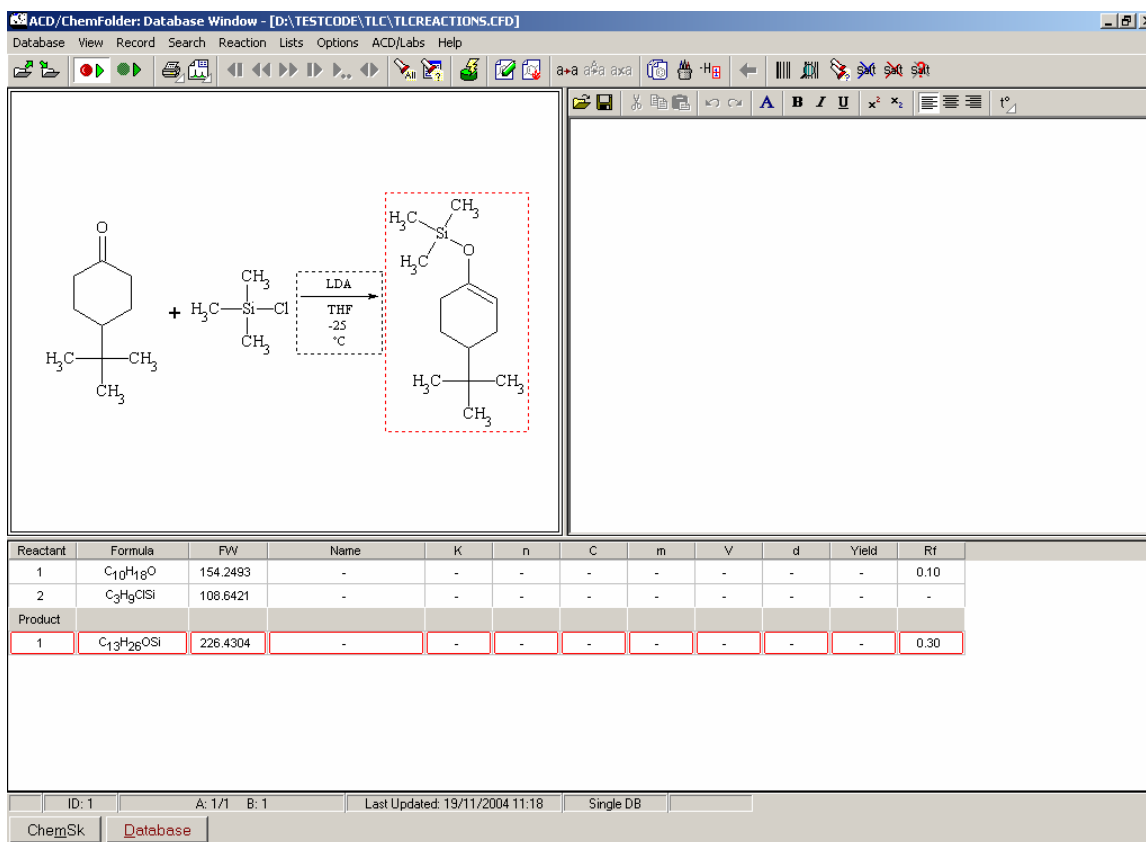
Formula: C₁₀H₁₈O

FW: 154.2493

R_f: 0.10

<End of List>

17. On the **View** menu, point to **Screen Forms**, and then choose **Default with Reaction Table**. The reaction table should now include the R_f field.



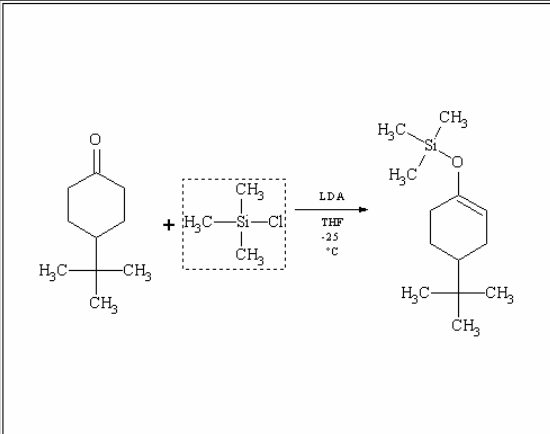
Reactant	Formula	FW	Name	K	n	C	m	V	d	Yield	R _f
1	C ₁₀ H ₁₈ O	154.2493	-	-	-	-	-	-	-	-	0.10
2	C ₃ H ₇ ClSi	108.6421	-	-	-	-	-	-	-	-	-
Product											
1	C ₁₃ H ₂₆ OSi	226.4304	-	-	-	-	-	-	-	-	0.30

Note If the R_f field is not listed, right-click within the reaction table area and from the pop-up menu choose **Select/Setup Columns**. Make sure that in the **Setup Table** dialog box, the **Selected Columns** list contains the R_f field.

18. Populate the rest of the reaction table data as necessary.

ACD/ChemFolder: Database Window - [D:\TESTCODE\TLC\TLCREACTIONS.CFD]

Database View Record Search Reaction Lists Options ACD/Labs Help



Reactant	Formula	FW	Name	K	n	C	m	V	d	Yield	Rf
1	C ₁₀ H ₁₈ O	154.2493	-	1	0.0032 mo	-	0.5 g	-	-	Based on	0.10
2	C ₃ H ₇ ClSi	108.6421	-	1	0.0079 mo	-	0.856 g	1 mL	0.856 g/mL	-	-
3	C ₆ H ₁₄ NLi	107.126	LDA	1	0.005 mol	1 M	-	5 mL	-	-	-
Product											
1	C ₁₃ H ₂₆ OSi	226.4304	-	1	0.0025 mo	-	0.566 g	-	-	78.1 %	0.30
Solvent											
1	C ₄ H ₈ O	72.107	Tetrahydrofuran	1	0.308 mol	-	22.2 g	25 mL	0.889 g/mL	-	-

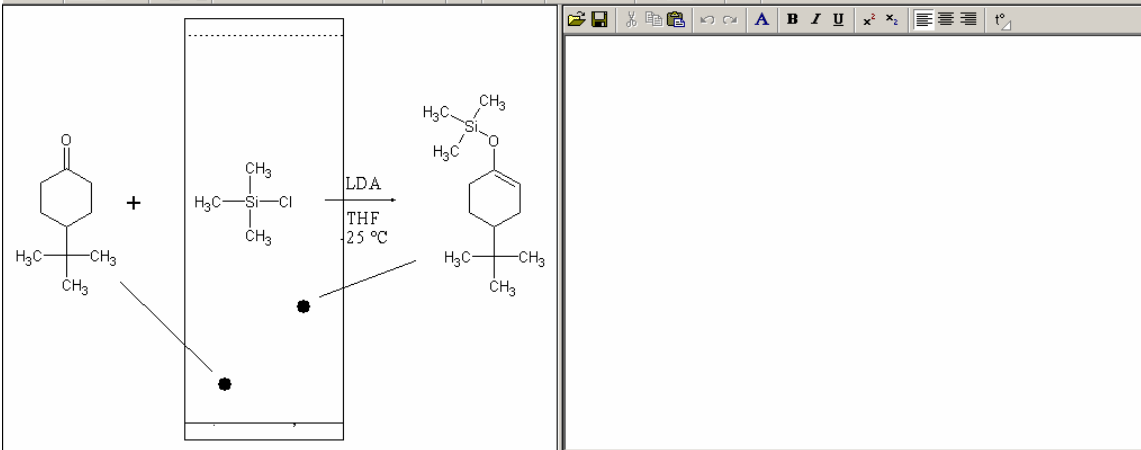
ID: 1 A: 1/1 B: 1 Last Updated: 19/11/2004 11:34 Single DB

ChemSk Database

19. Click **Show Pictures On/Off**  to show the TLC plate over the reaction.

ACD/ChemFolder: Database Window - [D:\TESTCODE\TLC\TLCREACTIONS.CFD]

Database View Record Search Reaction Lists Options ACD/Labs Help



Reactant	Formula	FW	Name	K	n	C	m	V	d	Yield	Rf
1	C ₁₀ H ₁₈ O	154.2493	-	1	0.0032 mo	-	0.5 g	-	-	Based on	0.10
2	C ₃ H ₇ ClSi	108.6421	-	1	0.0079 mo	-	0.856 g	1 mL	0.856 g/mL	-	-
3	C ₆ H ₁₄ NLi	107.126	LDA	-	0.005 mol	1 M	-	5 mL	-	-	-
Product											
1	C ₁₃ H ₂₆ OSi	226.4304	-	1	0.0025 mo	-	0.566 g	-	-	78.1 %	0.30
Solvent											
1	C ₄ H ₈ O	72.107	Tetrahydrofuran	1	0.308 mol	-	22.2 g	25 mL	0.889 g/mL	-	-

ID: 1 A: 1/1 B: 1 Last Updated: 19/11/2004 11:36 Single DB

ChemSk Database

Note The database containing these TLC images remains completely structure/substructure searchable as long as the images and reactions are added to the database as described in this document.

Conclusion

In this technical note, we have reviewed steps on how to store chromatographic results captured from a TLC plate together into an ACD/ChemFolder record. Chemical structures from the particular reaction can also be associated with the TLC spots to improve storage and retrieval of chemical information, as well as to facilitate reporting and data mining.

References

1. ACD/ChemSketch. <http://www.acdlabs.com/chemsketch/>, February 11, 2005.
2. ACD/ChemFolder. <http://www.acdlabs.com/chemfolder/>. February 11, 2005.

3. ACD/Technical Note, "TLC Plate Drawing Tool"
http://www.acdlabs.com/download/technotes/80/draw_db/tlc_plate.pdf