LabJ License and Usage Conditions
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The LabJ is usable for the "chemistry community" free of charge by anybody for any commercial, non-commercial or purely in-house purpose, but it is not yet completely true GPL/GNU program.*) Nevertheless you may adapt the functionality of the program to your local needs and redistribute copies of the package. If you add a valuable feature, or hunt down a bug, you are welcome to contact the author by email and the fix or feature will be most certainly integrated into the official release of LabJ.

However the LabJ package cannot be distributed as part of another program package. Particularly the author strictly forbid the MDL Information Systems, Inc. and its affiliated companies to include a LabJ package as a part of any product. If anybody is interested in providing the LabJ as integrated part of another package, this must be negotiated.

The author assumes no responsibility for errors or malfunctions, or for damages resulting from the use of the programs.

*) LabJ requires use of proprietary software programs ISIS(tm)/Draw and ISIS(tm)/Base from MDL Information Systems, Inc. ("MDL"), which are available under the appropriate licensing agreements from MDL from http://www.mdli.com. MDL and its affiliated companies are in no way associated with, nor do any of them endorse LabJ, nor does your use of ISIS/Draw and/or ISIS/Base imply any such association or endorsement.



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# User's Manual

## Electronic Laboratory Notebook


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## Table of Contents

# Introduction

LabJ (Laboratory Journal, electronic laboratory notebook, ELN) stores chemical information and assists in planning chemical reactions. It calculates information such as molecular weights, moles, reactant amounts and volumes, percent yields and more. Notes (procedures, results, references, comments, graphics, etc.) can be attached to the LabJ records. LabJ can be also used to store various data of synthesized compounds, such as melting and boiling points, spectral data as well as unlimited number of custom fields for your specific needs.

LabJ is realized as a database file (*labj.db*) for MDL ISIS/Base™ program. Reaction drawings and (sub)structure searches use the ISIS/Draw™ module.

## Description

Following is a brief overview of the most prominent features of LabJ:

- LabJ is a calculations and database program (a.k.a electronic laboratory notebook, ELN) for organic chemists. It can be used, *e.g.* in:
  - ✴ classical organic synthesis (incl. total synthesis)
  - ✴ screening for catalysts, optimization, *etc.*
  - ✴ parallel and automated synthesis
  - ✴ solid support synthesis
- Chemical reactions can be easily introduced graphically by drawing them in ISIS/Draw™ module.
- LabJ eliminates most of the tedious work of calculating chemical reaction data such as molecular formulas and weights of reactants and products, amounts and volumes of the reactants and yields of products. Calculations are based on graphical reaction and choosed scale, stoichiometry and purity of reagents. Volumes of reactants are calculated based on either reagents' density or molarity (*M* [mol/L]).
- Because LabJ uses ISIS/Base™ program as a "database engine" all records can be easily stored and searched. If you want to re-examine or scale-up a reaction simply retrieve an existing record, duplicate it, change one or more values (incl. reagents), and everything is recalculated.
- All records in a LabJ database are sequenced in numeric order based on reaction number (e.g. KG-1023). Simillary, all products (and fractions) can be logically labelled based on reaction number (e.g. KG-1023-1-3).
- You can browse through the database page by page or

search for a record by reaction number, reaction scheme, (sub)structure, analytical data, procedure, keywords and much more. This search tool generates a list that can be browsed, printed (as separated pages or in tabular form) or saved as a new LabJ database.
- LabJ prints records in a form of Reaction Page, Report Page, Tabular Form, and various Analytical Forms (e.g. for IR, NMR and MS departments), as well as virtually unlimited number of custom forms for your specific needs.

### Bugs

LabJ was originally written for my own use and a lot of it is messy, so ideas on how to clean it up would be great. You are welcome to read the database structure (source code of LabJ) and to try to modify it and save as your own LabJ Database. Please send bug descriptions, suggestions, new LabJ files or successful stories to `grela@technologist.com` (cf. Copyright)

### Copyright



## Installation

### System Requirements

For using LabJ program the ISIS/Desktop™ (ISIS/Base™ and ISIS/Draw™) software package is needed. Please contact MDL Information Systems, Inc. for more information.
Currently, you can use LabJ with ISIS/Base™ 1.x and 2.x (recommended) for Microsoft Windows 3.x, 95, 98, 2000 and NT, Apple Macintosh and IRIX SGI. It is also possible to use LabJ under Linux with Microsoft Windows emulator, such as WABI™ and Win4Lin™.

### Download

The newest version of the package can be downloaded from http://zinc.ichf.edu.pl/labj/.

## Installation

- Get "*labj1x.zip*" (for ISIS/Base 1.x) or "*labj2x.zip*" (for ISIS/Base 2.x) from http://zinc.ichf.edu.pl/labj/.
- Use "`unzip *.zip`" command (DOS) to extract the "*labj.db*" file from the archive. Alternatively you can use any GUI program, like *WinZip* (Windows) to extract the archive file.
- Start ISIS/Base program and open the "*labj.db*" file.

# Using LabJ

## A Brief Lesson

This chapter explains how to use LabJ on your computer:

- Opening the *labj.db* file.
- Retrieving existing records
- Browsing records
- Retrieving forms

Use this procedure to open LabJ:

- Start ISIS/Base.
- Choose File > Open Database.
- Change to the directory (Mac=folder) where the *labj.db* file is located.
- Click the name of the *labj.db* (Mac=*labj*) file to open.
- Click OK (Mac=Open).

You will see a default form in the ISIS/Base window. A form is required for searching or to register data in the database. In LabJ electronic notebook a form called "DATA INPUT — MMOLS" is used as a default form. Consult APPENDIX A for a detailed description of fields in "DATA INPUT" form.

- Choose Search > Retrieve All to retrieve all existing records. LabJ database contains five sample reactions. Click the [←] [→] buttons or use Up and Down cursor keys to move between records.

For browsing and printing records a separate form is provided, called "DATA BROWSE". Consult APPENDIX B for a detailed description of fields in "DATA BROWSE" form. To retrieve a form:

- Choose File > Open Form.
- Click the name of an appropriate form for data entry.

- (Optional) To make this form the default form you see when you open the current database, click Set Default Form.
- Click OK. You see the selected form in the window.

## Registration of Reaction

This chapter shows you how to register new records or edit existing records in the laboratory notebook.

To register a new reaction or changes to an existing record in a LabJ database, you typically complete the following steps in the order shown:

***Hint**: Regularly make backups of your LabJ database.*

### ⌘ Opening the LabJ database

- Start ISIS/Base.
- Open the LabJ database: Choose File > Open Database.
- Click *labj.db* (Mac=*labj*). The database opens. You see the default data-entry form in the LabJ database window.
- Choose Search > Retrieve All to retrieve all existing records
- Use  button to display the last record.

### ⌘ Creating a new record

Before you enter data onto a form, you must create a new record:


- Click the Update button.
- Choose Edit > New Record. ISIS/Base assigns a new record number that appears in the "ID" box (cf. Figure 1). The ID Number is a unique number that ISIS/Base automatically assigns when it creates a new record. You can change the ID number before the record is registered but not after. For LabJ typical use, do not change the default ID number.
- According to the **scale** of the planned reaction use default form "DATA INPUT MMOLS" (for reactions of scale <0.1 mol) or open a form called "DATA INPUT MOLS" if reaction scale ≥0.1 mol. See page 3 for how to open forms.

### ⌘ Entering a reaction onto the form

In this example, you will calculate the reaction between one equivalent of phenol and one equivalent of NaH and a slight excess of allyl bromide (1:1:1.2), producing one equivalent of corresponding ether in a scale of 1 mmol.

To enter the reaction onto the form:

- Select the box that is connected to the reaction field. It is the large box on the top, called "REACTION" (Figure 1).
-  Click the ISIS/Draw Transfer icon at the top of the ISIS/Base toolbar to start ISIS/Draw. Alternatively, you can double-click inside the "REACTION" box.
- Draw the reaction scheme in ISIS/Draw.

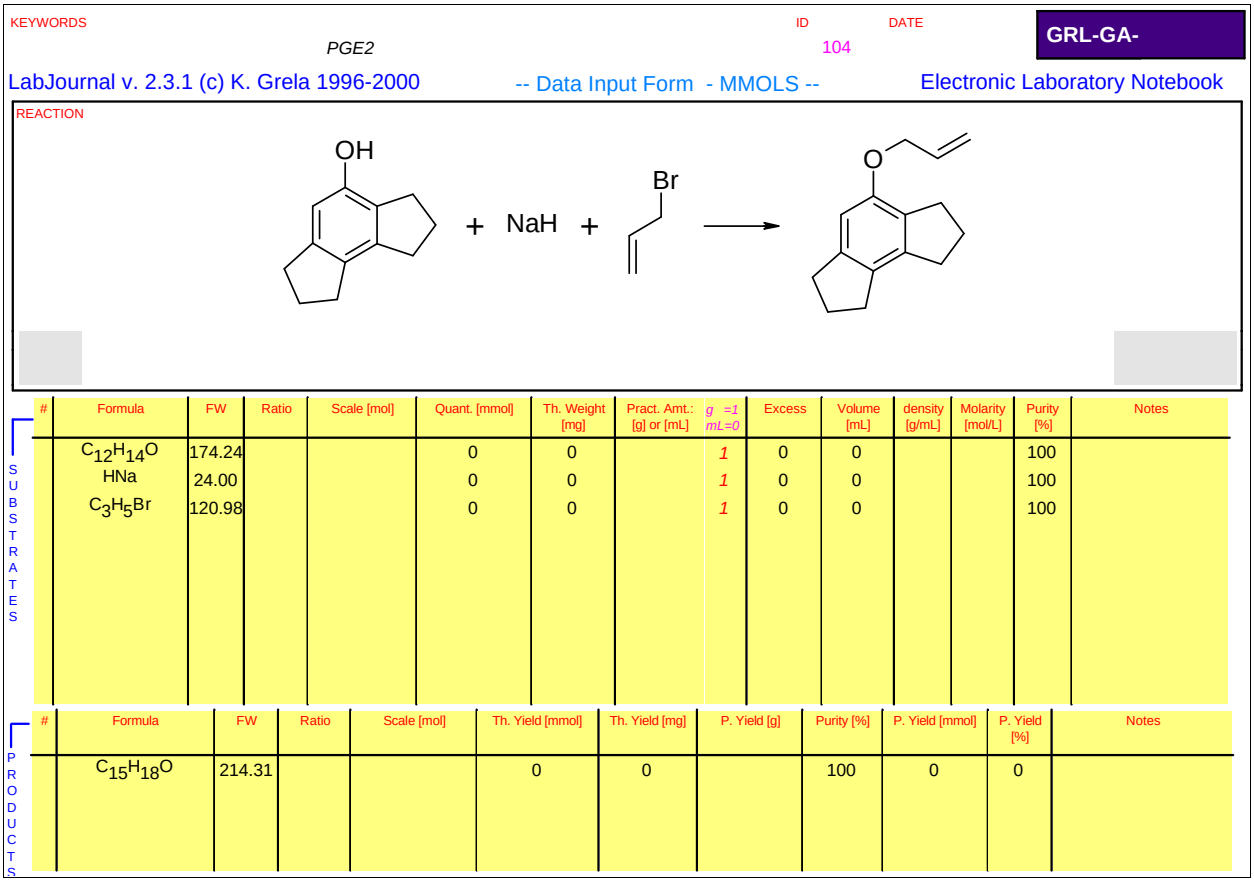
***Hint**: To learn how to speed-up drawing process consult* Help > ISIS/Draw Contents > QUICK START. *See page 12 for details.*

-  Click the ISIS/Base Transfer icon at the top of the ISIS/Draw toolbar to transfer the reaction into the structure box in the ISIS/Base form.
- Choose Database > End Update to register the new record.

You will see a reaction scheme and reagents' formulas and formula weights in the ISIS/Base window (Figure 1).

### ⌘ Calculating stoichiometry of the reaction

- Select the spreadsheet that is connected to the stoichiometry of the **reagents**. It is the first big yellow table, called "SUBSTRATES" (Figure 1).
- Click the first cell in the column called "RATIO". Type `1` in the first cell of the "RATIO" column. Enter `1` and `1.2` in the second and third cell in this column.
- In this example, you calculate the reaction in a scale of 1 mmol. Click the first cell in the column called "SCALE". Type `0.001` in the first cell of the "SCALE" column. Usually the values used in this column are the same for all substrates and products and are equal to the scale of the reaction. Therefore type `0.001` in the second and third cell in this column.




SUBSTRATES

| # | Formula | FW | Ratio | Scale [mol] | Quant. [mmol] | Th. Weight [mg] | Pract. Amt.: [g] or [mL] | g =1 mL=0 | Excess | Volume [mL] | density [g/mL] | Molarity [mol/L] | Purity [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{12}H_{14}O$ | 174.24 | | | 0 | 0 | | 1 | 0 | 0 | | | 100 | |
| | HNa | 24.00 | | | 0 | 0 | | 1 | 0 | 0 | | | 100 | |
| | $C_3H_5Br$ | 120.98 | | | 0 | 0 | | 1 | 0 | 0 | | | 100 | |

PRODUCTS

| # | Formula | FW | Ratio | Scale [mol] | Th. Yield [mmol] | Th. Yield [mg] | P. Yield [g] | Purity [%] | P. Yield [mmol] | P. Yield [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{15}H_{18}O$ | 214.31 | | | 0 | 0 | | 100 | 0 | 0 | |

Figure 1.

***Hint.*** *To speed-up typing you can use* Edit > Copy *and* Paste *from the menu, or* [Ctrl+C], [Ctrl+V] *from the keyboard.*

- Select the spreadsheet connected to the stoichiometry of the **products**. It is the second yellow table, called "PRODUCTS" (Figure 1).
- Click the first cell in the column called "RATIO". Type `1`.
- Select the first cell in the column called "SCALE". Type `0.001`
- Choose Database > End Update to update the new data into the LabJ.

You will see amounts of reagents and product(s) in the "QUANT." (= calculated amounts in millimols), "TH. WEIGHT" (= calculated amounts in milligrams), and "TH. YIELD" (= yield of theory) columns (Figure 2).

SUBSTRATES

| # | Formula | FW | Ratio | Scale [mol] | Quant. [mmol] | Th. Weight [mg] | Pract. Amt.: [g] or [mL] | g =1 mL=0 | Excess | Volume [mL] | density [g/mL] | Molarity [mol/L] | Purity [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{12}H_{14}O$ | 174.24 | 1.000 | 0.001000000 | 1.00000 | 174.24 | | 1 | 0 | 0 | | | 100 | |
| | HNa | 24.00 | 1.000 | 0.001000000 | 1.00000 | 24.00 | | 1 | 0 | 0 | | | 100 | |
| | $C_3H_5Br$ | 120.98 | 1.200 | 0.001000000 | 1.20000 | 145.18 | | 1 | 0 | 0 | | | 100 | |

PRODUCTS

| # | Formula | FW | Ratio | Scale [mol] | Th. Yield [mmol] | Th. Yield [mg] | P. Yield [g] | Purity [%] | P. Yield [mmol] | P. Yield [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{15}H_{18}O$ | 214.31 | 1.000 | 0.0010000000 | 1.00000 | 214.31 | | 100 | 0 | 0 | |

Figure 2.

## ⌘ Calculating amounts of the reagents (incl. reagents volumes)

- Select the "SUBSTRATES" table.
- Click the second cell in the column called "PURITY". In this example, the NaH is used as a 40 wt.% suspension in mineral oil. Therefore type `40` in this cell.
- Click the third cell in the column called "DENSITY". Type `1.398` (the density of allyl bromide).
- Choose Database > End Update to update the new data into the LabJ.

You will see new weight of NaH suspension in the "TH. WEIGHT" cell and a volume (in mL) of allylbromide in the "VOLUME" cell (Figure 3).

- Review all of the data for the "DATA INPUT" form and correct any mistakes. To correct mistakes, click in the box that contains the error (double-click in case of the "REACTION" box).

## ⌘ Executing the reaction

Weigh out the reagents and start the reaction. In the event, you use different amounts of reagents than you calculated before, you should input the real amounts of reagents used.

SUBSTRATES

| # | Formula | FW | Ratio | Scale [mol] | Quant. [mmol] | Th. Weight [mg] | Pract. Amt.: [g] or [mL] | g =1 mL=0 | Excess | Volume [mL] | density [g/mL] | Molarity [mol/L] | Purity [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{12}H_{14}O$ | 174.24 | 1.000 | 0.001000000 | 1.00000 | 174.24 | | 1 | 0 | 0 | | | 100 | |
| | HNa | 24.00 | 1.000 | 0.001000000 | 1.00000 | 60.00 | | 1 | 0 | 0 | | | 40.0 | Fluka, 40% wt. |
| | $C_3H_5Br$ | 120.98 | 1.200 | 0.001000000 | 1.20000 | 145.18 | | 1 | 0 | 0.104 | 1.398 | | 100 | Aldrich |

PRODUCTS

| # | Formula | FW | Ratio | Scale [mol] | Th. Yield [mmol] | Th. Yield [mg] | P. Yield [g] | Purity [%] | P. Yield [mmol] | P. Yield [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{15}H_{18}O$ | 214.31 | 1.000 | 0.0010000000 | 1.00000 | 214.31 | | 100 | 0 | 0 | |

Figure 3.

- Select the "SUBSTRATES" table.
- Click the cell in the column called "PRACT. AMT.". In this example, type `0.175` in the first cell. That means that you have used exactly the calculated amount of phenol.
- Click the second cell in the column called "PRACT. AMT." Type `0.0650` (you have added a slight excess of sodium hydride).
- Click the third cell in the column called "PRACT. AMT." Type `0.1` (allylbromide was added neat by a micro-syringe). Because the value of `0.1` corresponds to the volume of allylbromide, you have to change the number in the next column from `1` to `0` (1=g, 0=mL).
- Choose Database > End Update to update the new data into the LabJ.

You will see the calculated excess of the reagents in the "EXCESS" column (Figure 4).

### ⌘ Finishing the reaction

- Select the box connected to the description of of the reaction. It is the big box, called "PROCEDURE" (APPENDIX A). Note the reaction conditions, additions of reagents, temperature etc. Describe the work-up procedure and the isolation and purification of product(s).
- Choose Database > End Update to update the new data into the LabJ.

SUBSTRATES

| # | Formula | FW | Ratio | Scale [mol] | Quant. [mmol] | Th. Weight [mg] | Pract. Amt.: [g] or [mL] | g =1 mL=0 | Excess | Volume [mL] | density [g/mL] | Molarity [mol/L] | Purity [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{12}H_{14}O$ | 174.24 | 1.000 | 0.001000000 | 1.00000 | 174.24 | 0.17500 | 1 | 1.004 | 0 | | | 100 | |
| | HNa | 24.00 | 1.000 | 0.001000000 | 1.00000 | 60.00 | 0.06500 | 1 | 1.083 | 0 | | | 40.0 | Fluka, 40% wt. |
| | $C_3H_5Br$ | 120.98 | 1.200 | 0.001000000 | 1.20000 | 145.18 | 0.10000 | 0 | 0.962 | 0.104 | 1.398 | | 100 | Aldrich |

PRODUCTS

| # | Formula | FW | Ratio | Scale [mol] | Th. Yield [mmol] | Th. Yield [mg] | P. Yield [g] | Purity [%] | P. Yield [mmol] | P. Yield [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{15}H_{18}O$ | 214.31 | 1.000 | 0.0010000000 | 1.00000 | 214.31 | | 100 | 0 | 0 | |

Figure 4.

## ⌘ Calculating the yield of product(s) (incl. product purity)

- Select the "PRODUCTS" table.
- Click the cell in the "P. YIELD" column. In this example, the yield of an analytically pure product is 198 mg. Therefore, type `0.198` in this cell.
- Choose Database > End Update to calculate the yield.

You will see the yield of product (calculated as mmols and % of theory) in the "P. YIELD" cells (Figure 5).

## ⌘ Tracking the fractions/samples

To describe different fractions obtained during product isolation and purification you can fill a special table. You can also use this table to track sample flow (Figure 6).

- Select the box that is connected to the FRACTIONS field. It is the large table on the bottom, called "FR. #" (cf. APPENDIX A and B).
- Choose Edit > New Record. ISIS/Base creates a new sub-record (row) that appears in the "FR. #" table.
- Select the newly created row in this table and type fraction number and weight, fraction description, *etc*.
- Repeat above steps for each sample/fraction.
- Choose Database > End Update to register the new record (Figure 6).

SUBSTRATES

| # | Formula | FW | Ratio | Scale [mol] | Quant. [mmol] | Th. Weight [mg] | Pract. Amt.: [g] or [mL] | g =1 mL=0 | Excess | Volume [mL] | density [g/mL] | Molarity [mol/L] | Purity [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{12}H_{14}O$ | 174.24 | 1.000 | 0.001000000 | 1.00000 | 174.24 | 0.17500 | 1 | 1.004 | 0 | | | 100 | |
| | HNa | 24.00 | 1.000 | 0.001000000 | 1.00000 | 60.00 | 0.06500 | 1 | 1.083 | 0 | | | 40.0 | Fluka, 40% wt. |
| | $C_3H_5Br$ | 120.98 | 1.200 | 0.001000000 | 1.20000 | 145.18 | 0.10000 | 0 | 0.962 | 0.104 | 1.398 | | 100 | Aldrich |

PRODUCTS

| # | Formula | FW | Ratio | Scale [mol] | Th. Yield [mmol] | Th. Yield [mg] | P. Yield [g] | Purity [%] | P. Yield [mmol] | P. Yield [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | $C_{15}H_{18}O$ | 214.31 | 1.000 | 0.0010000000 | 1.00000 | 214.31 | 0.1980 | 100 | 0.923895 | 92 | |

Figure 5.

*Hint*: You can delete a existing row in the "FR. #" table:

- Click the row you want to delete.
- Choose Edit > Delete Record. ISIS/Base deletes one sub-record (row).
- Choose Database > End Update to update changes.

### ⌘ Inserting additional data

In the sample forms used in the LabJ notebook, each form box has a label that describes the type of data to enter. To enter additional data (chemist's and experiment code, keywords, date, conditions, and notes) see APPENDIX A and B.

### ⌘ Registering the record into the LabJ database

When you complete the data entry for one reaction, you can finally register the record into the database.

- Choose Database > End Update. The data is registered as a new record that can be retrieved in a search.
- (Optional) to close the database, choose File > Close Database.

| Fr. # | Quant. | Descripton | Anal. Data, Identification |
|---|---|---|---|
| **1** | 0.198g | Fractions 22-29 in column chrom. (hexan:EtOAc 9:1). Pure product. | TLC, NMR, MS |
| **SR** | 50mg | GRL-GA-104-01 -> to Sample Repository of MPI | |
| **BY** | 10mg | GRL-GA-104-01 -> to Bayer GmbH (Wuppertal) | bio |

Figure 6.

## Advanced

***Caution**: Make a backup of your LabJ database before you begin.*

***Hint**: Logging Database Transactions.*
Activate the database journal to log transactions for a database during registration. When you register new records during data entry, ISIS/Base creates the log file using the name of the database with a *.log* file extension. The log file is saved in the same directory (Mac=folder) as the database. Each transaction is added to the end of the log file until you delete the file. View or print the log file using a word processor.
The ISIS/Base transaction log records database transactions that occur during registration. The log is a text (ASCII) file that you can view or print later. The log file records:

- Registration of new records
- Updating of existing records
- Deletion of existing records
- Date and time each operation occurred.

Use this procedure to instruct ISIS/Base to log database transactions that occur during registration for the LabJ database:

- If the LabJ database is open, close the database. To do so, choose File > Close Database.
- Choose File > Configure Database. The File Open dialog box appears.
- Double-click the name *"labj.db"* (Mac="*labj"*).

- Ensure that the Log database transactions setting is *On*.
- Click OK.

Backup and delete the transaction-log file after you view or print the transactions. Each time that you register data for the database, information is appended to the end of the file and it can quickly increase in file size.

***Note**: Data types.*
Each field in the LabJ database has restrictions on the type of data it stores. If you enter the wrong type of data for a field, a warning message appears. For example, if you enter text for a field that expects a number, you see the message "*Error in data format, a (n) Real value was expected*." To view the database fields and their field types, choose Database > View Definition.

***Note**: Formula and Molecular Weight.*
LabJ automatically calculates data for the "FORMULA" and Formula Weight ("FW") boxes when you register the reaction. For future reference, you can enter a molecular weight instead of having the program calculate it for you, but you cannot enter a formula.

## Getting Help

The ISIS/Desktop online help has detailed examples and step-by-step instructions to help you complete your tasks in the LabJ program:

- **To use the ISIS/Desktop online help.** To access Help, choose Help > ISIS/Desktop Contents. Then, choose How to Use ISIS/Desktop Help. This gives you full details on using the ISIS/Desktop online help.
- **To learn how to draw.** To quickly learn how to draw structures, reactions, objects, and text for use as search queries, records in a database, or to insert in a document, see Help > ISIS/Draw Contents > QUICK START.
- **To learn how to search.** To see a complete list of all the searches that you can do in ISIS/Base, see Help > ISIS/Base Search Types.
- **To learn about creating and editing forms.** To learn how to create or edit forms to view search results or to enter data into a form to register as new records in a database, choose Help > ISIS/Base Contents > Creating and Editing FORMS.

- **To find out more about ISIS applications.** To find out more about the following ISIS applications: File-format conversion, ISIS Reaction Database Access System, SAR Table, or the Add-in Manager, choose Help > ISIS/Desktop Contents > ISIS Overview and Documentation.

## Searching LabJ

With LabJ you can search for a record by reaction number, reaction scheme, (sub)structure, analytical data, procedure, keywords and much more. To see a complete list of all the searches that you can do in ISIS/Base, see Help > ISIS/Base Search Types.

Example (searching by reaction/structure):


- Click the Query button (if not highlighted).
- (Optional) To remove all data from the form, choose Edit > Clear Data > Form.
- Select the "REACTION" box (if not highlighted).
- Do one of the following:
  * Draw a new query.
  * Import a query from a *rxnfile*.*)
  * Restore a query that you previously saved as an object in the database.*)

*) see Help > ISIS/Base Search Types for details (page 12).

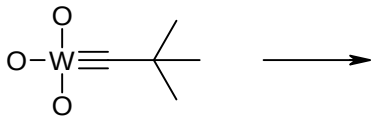
To draw a new query:

- Transfer to ISIS/Draw. Select the "REACTION" box. Click the ISIS/Draw Transfer icon at the top of the ISIS/Base toolbar to start ISIS/Draw. Alternatively, you can double-click inside the "REACTION" box.
- Draw the query in ISIS/Draw.

***Hint**: To learn how to speed-up drawing process consult* Help > ISIS/Draw Contents > QUICK START. *See page 12 for details.*

- Click the ISIS/Base Transfer icon at the top of the ISIS/Draw toolbar to transfer the molecule into the reaction box in the ISIS/Base form.
- Choose Search > Current Rxn.

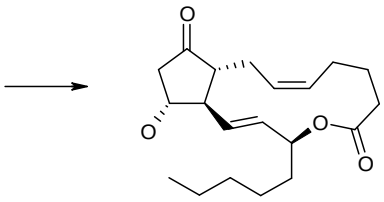

- Click the Browse mode (if not highlighted). You see the first record displayed on the boxes and tables in your form.
- To see how many records you retrieved, click the "REACTION" box (if not selected) and check the status bar.
- Use [⬅] and [➡] buttons to display the record that you want to view.



*sample query*

This search tool generates *a list* that can be saved, browsed, printed (as separated pages or in tabular form) or exported as a new LabJ database.

- Click the Browse mode (if not highlighted).
- Choose List > Save.
- Click the List Name box and enter a name for the list (without a file-name extension).
- (Optional) To save the query with the same name as the list name, you require this setting: Save query under the same name.
- Do one of the following:
  * To store the list as a permanent database object, you require this setting: ☒ Permanent.
  * To delete the list when you close the database, you require this setting: ☐ Permanent.
- Click OK.



*sample query*

## Editing Existing Records

This chapter shows you how to edit or delete existing records in the LabJ laboratory notebook.

To change an existing record in a LabJ database, you typically complete the following steps in the order shown:

***Hint**: Regularly make backups of your LabJ database.*

### ⌘ Locating a record to change

- Start ISIS/Base.
- Open the LabJ database: Choose File > Open Database.
- Click *labj.db* (Mac=*labj*). The database opens. You see the default data-entry form in the LabJ database window.

- Do one of the following:
  * (Optional) choose Search > Retrieve All to retrieve all existing records, and then select a record you want to change using navigation bar.
  * (Optional) search for records to change by a specific reaction, (sub)structure, keywords *etc*. (see page 13 for reference). To see a complete list of all the searches that you can do in ISIS/Base, see Help > ISIS/Base Search Types.

### ⌘ Editing a record


- Click the Update button.
- To change a data, click in the box that contains the data (double-click in case of the "REACTION" box). See chapter "Registration of Reaction", page 4, for more information.
- Choose Database > End Update to update the new record.

### ⌘ Deleting a record

***Caution**: Make a backup of your LabJ database before you begin.*

- Click the Update button.
- Select the "REACTION" box.
- Choose Edit > Delete Record. ISIS/Base deletes one record of your LabJ notebook.

### ⌘ Editing a reaction manually

When you draw a reaction LabJ automatically registers all substrates and products into the appropriate tables. You can also manually add or delete a reagent in the "SUBSTRATES" spreadsheet. Similarly you can manually add or delete products in the "PRODUCTS" spreadsheet. You will see changes only in "SUBSTRATES" or "PRODUCTS" tables, but not in the "REACTION" box.

***Caution**: Make a backup of your LabJ database before you begin.*

To add a new reagent or product:

- Select the row **after** which you want to add a new sub-record in the "SUBSTRATES" or "PRODUCTS" spreadsheet.
- Choose Edit > New Record. ISIS/Base creates a new sub-record (row) that appears in the table.
- Select the newly created row and type a Formula Weight (but **not** a Formula!), ratio, scale, *etc*. See chapter "Registration of Reaction", page 4, for more information.
- Choose Database > End Update to update the new record.

To delete an existing reagent or product:

- Click the row you want to delete in the "SUBSTRATES" or "PRODUCTS" spreadsheet.
- Choose Edit > Delete Record. ISIS/Base deletes one sub-record (row).
- Choose Database > End Update to update changes.

***Hint***: You can also add or delete rows in the "FR. #" table. See chapter "Registration of Reaction", page 4, for more information.

### ⌘ Updating the changed record into the LabJ

When you complete data entry for one reaction you can update the record into the database.

- Choose Database > End Update.
- (Optional) to close the database, choose File > Close Database.

## Modifying LabJ

LabJ can display or print records in a form of Reaction Page, Report Page, Tabular Form, and various Analytical Forms (e.g. for IR, NMR and MS departments), as well as virtually unlimited number of custom forms for your specific needs.

To learn how to create or edit forms to view search results or to enter data into a database, choose Help > ISIS/Base Contents > Creating and Editing FORMS.

## Creating and Editing Forms

This procedure will show you how to create or edit a form.

***Hint**: You can Undo many of the changes that you make when you edit a form.*

***Caution**: Make a backup of your LabJ database before you begin.*


- Click the Forms button.
- Do one of the following:
  - (Optional) create display/ new box, create a new table, or create a new column in an existing table.
  - (Optional) change the field that is connected to a box or column.
  - (Optional) edit one of the following:
    - Boxes, or Columns, or Tables
    - Box labels or column headings
    - Chemical display of structures
    - Text or numeric data display
    - Lines or Text
    - Entire form
- Do one of the following:
  - To save a new form or an existing form under the same name, choose File > Save Form. For new forms only, enter a name and an optional description for the form.
  - To save an existing form under a new name, choose File > Save Form As. Enter a name and an optional description for the form.
- Click OK. The form is saved inside the database and you will not see it as a separate form file on disk.


Figure 7.

Example.

In this example you will change the default chemist's code (*e.g.* "GRL-GA-", Figure 7). Use this procedure to set a default string for this code.

- Click the Forms button.
- Select a box that is connected to a chemist's code (field "Name"). It is a blue box on the right top of the default form (see APPENDIX A and B).
- Choose Object > Box Properties, and then click the Function tab.

- Click the Default data box, and choose String.
- Type a new chemist's code, *e.g.* "PRR-PA-"
- Click OK.
- Choose File > Save Form.

## Anatomy of LabJ

You are welcome to read the database structure (source code of LabJ) and to try to modify it and save as your own LabJ Database. To find out more about the ISIS/Base features choose Help > ISIS/Desktop Contents > ISIS Overview and Documentation.

Table 1. The LabJ database structure.

| | | |
|---|---|---|
| 0 | RXN | Parent |
| 1 | RXNREGNO | Integer |
| 2 | RXNSTRUCTURE | Reaction |
| 3 | VARIATION | Parent |
| 4 | VARIATION_NO | Integer |
| 5 | REACTANT | Parent |
| 6 | REACTANT_NO | Integer |
| 7 | LIST_OF_REACTANTS | Integer |
| 8 | PRODUCT | Parent |
| 9 | PRODUCT_NO | Integer |
| 10 | LIST_OF_PRODUCTS | Integer |
| 11 | REACTANT_LINK | Parent |
| 12 | LIST_OF_REACTANTS | Integer |
| 13 | REACTANT_NO | Integer |
| 14 | MOL | Parent |
| 15 | REF_REAGNT | Real |
| 16 | MOLREGNO | Integer |
| 17 | MOLSTRUCTURE | Structure |
| 18 | *fmla_MOLSTRUCTURE | Formula |
| 19 | *mol.weight_MOLSTRUCTURE | Real |
| 20 | CORP_ID[20] | Fixed Text |
| 21 | REACT_EQ | Real |
| 22 | REACT_n | Real |
| 23 | REACT_m | Real |
| 24 | REACT_V | Real |
| 25 | REACT_d | Real |
| 26 | REACT_P | Real |
| 59 | REACT_DESC[64] | Fixed Text |
| 60 | REACT_Molarity | Real |
| 62 | REACT_mP | Real |
| 63 | REACT_Exs | Real |
| 79 | REACT_Exs_Unit | Integer |
| 27 | PRODUCT_LINK | Parent |
| 28 | LIST_OF_PRODUCTS | Integer |
| 29 | PRODUCT_NO | Integer |
| 30 | MOL | Parent |
| 31 | MOLREGNO | Integer |
| 32 | MOLSTRUCTURE | Structure |
| 33 | *fmla_MOLSTRUCTURE | Formula |
| 34 | *mol.weight_MOLSTRUCTURE | Real |
| 35 | CORP_ID[20] | Fixed Text |
| 36 | PROD_EQ | Real |
| 37 | PROD_nT | Real |
| 38 | PROD_mT | Real |
| 39 | PROD_mP | Real |
| 40 | PROD_nP | Real |
| 41 | PROD_YIELD | Real |
| 42 | PROD_DESC | Variable Text |
| 43 | REF_PRODUCT | Real |

| | | |
|---|---|---|
| 44 | PROD_PP | Real |
| 64 | PROD_ANAL | Variable Text |
| 77 | PROD_NAME | Variable Text |
| 45 | DATE[10] | Fixed Text |
| 46 | GDH# | Integer |
| 47 | PROC | Variable Text |
| 48 | ANAL | Parent |
| 49 | FRACTION_NO | Variable Text |
| 74 | FRACTION_DESCR | Variable Text |
| 75 | FRACTION_QUANT | Variable Text |
| 76 | FRACTION_ANAL | Variable Text |
| 54 | RESULTS | Variable Text |
| 55 | RXNCOND | Variable Text |
| 56 | RXNCOND# | Variable Text |
| 57 | RESULTS_SKETCH | Sketch |
| 58 | KEYWORDS | Variable Text |
| 61 | YIELD[10] | Fixed Text |
| 78 | NAME[07] | Fixed Text |

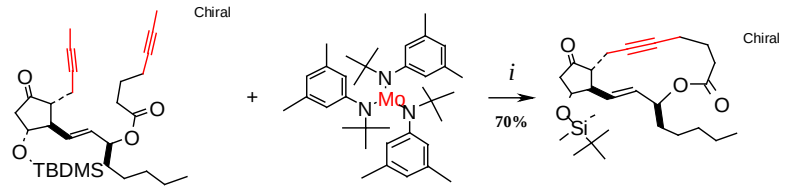
# Appendix 1

KEYWORDS: *C26H42O4Si : PGE2LA , RCM, Mo, chiral*

ID: 41 | DATE: 1999.09.29 | **GRL-GA-041**

LabJournal v. 2.3.0 (c) K. Grela 1996-2000 -- Data Input Form - MMOLS -- Max-Planck-Institut für Kohlenforschung

REACTION




*i*

*i) PhMe/CH2Cl2 (c[A]=0.01M), 16h, 80°C*

*70%*

SUBSTRATES

| # | Formula | FW | Ratio | Scale [mol] | Quant. [mmol] | Th. Weight [mg] | Pract. Amt.: [g] or [mL] | g =1 mL=0 | Excess | Volume [mL] | density [g/mL] | Molarity [mol/L] | Purity [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | $C_{30}H_{48}O_4Si$ | 500.80 | 1.000 | 0.000100000 | 0.10000 | 50.08 | 0.05280 | 1 | 1.054 | 0 | | | 100 | GRL-GA-039-02 |
| B | $C_{36}H_{54}MoN_3$ | 624.79 | 0.075 | 0.000100000 | 0.00750 | 4.69 | 0.00500 | 1 | 1.066 | 0 | | | 100 | |

PRODUCTS

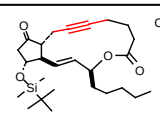
| # | Formula | FW | Ratio | Scale [mol] | Th. Yield [mmol] | Th. Yield [mg] | P. Yield [g] | Purity [%] | P. Yield [mmol] | P. Yield [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $C_{26}H_{42}O_4Si$ | 446.71 | 1.054 | 0.0001000000 | 0.10540 | 47.08 | 0.0328 | 100 | 0.073426 | 70 | |

A mixture of A, B and CHCl2 (dry, 2 mL) in toluene (dry, 10 mL, c[1]= 0.01M) was stirred at 80°C (t/o 85°) for 5 hr under argon atmosphere. Then the mixture was evaporated, and the residue was subjected to the CC (EH 7.5%).

PROCEDURE

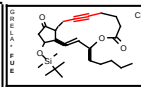
| Fr. # | Quant. | Descripton | Anal. Data, Identification |
|---|---|---|---|
| 1 | .0328 | fr. 32-56 | 1: TLC, NMR |

GRELA-FUE




**GRL-GA-**

$C_{26}H_{42}O_4Si$ = 446.71




GRL-GA-

GRL-GA-

GRL-GA-

GRL-GA-

REF: #24, #25

OK

RESUL

viscous colorless oil

[a]20/D : -188.2° (0.78, CHCl3)

TLC

NMR

MS

HRMS

IR

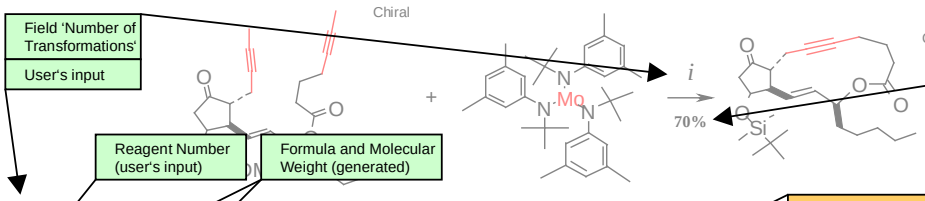
Anal. Data

KEYWORDS: C26H42O4Si : PGE2LA , RCM, Mo, chiral

ID: 41 | DATE: 1999.09.29 | **GRL-GA-041**

LabJournal v. 2.3.0 (c) K. Grela 1996-2000 -- Data Input Form - MMOLS -- Max-Planck-Institut für Kohlenforschung

REACTION




Field 'Number of Transformations' — User's input

Chemist and Reaction Code (user's input)

Final Yield (user's input)

Reagent Number (user's input)

Formula and Molecular Weight (generated)

*i) PhMe/CH2Cl2 (c[A]=0.01M), 16h, 80°C*

Conditions (user's input)

SUBSTRATES

| # | Formula | FW | Ratio | Scale [mol] | Quant. [mmol] | Th. Weight [mg] | Pract. Amt.: [g] or [mL] | g =1 mL=0 | Excess | Volume [mL] | density [g/mL] | Molarity [mol/L] | Purity [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | $C_{30}H_{48}O_4Si$ | 500.80 | 1.000 | 0.000100000 | 0.10000 | 50.08 | 0.05280 | 1 | 1.054 | 0 | | | 100 | GRL-GA-039-02 |
| B | $C_{36}H_{54}MoN_3$ | 624.79 | 0.075 | 0.000100000 | 0.00750 | 4.69 | 0.00500 | 1 | 1.066 | 0 | | | 100 | |

Scale of Reaction (user's input)

Amount of Reagent (calculated)

Amount of Reagent Used (user's input)

Units (grams or mL) (user's input)

Excess of Reagent Used (calculated)

Volume of Reagent based on density or molarity [M] (calculated)

Density **or** Molarity and Purity of Reagent (user's input)

PRODUCTS

| # | Formula | FW | Ratio | Scale [mol] | Th. Yield [mmol] | Th. Yield [mg] | P. Yield [g] | Purity [%] | P. Yield [mmol] | P. Yield [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $C_{26}H_{42}O_4Si$ | 446.71 | 1.054 | 0.0001000000 | 0.10540 | 47.08 | 0.0328 | 100 | 0.073426 | 70 | |

Formula and Molecular Weight (generated)

Ratio of Products (user's input)

Scale of Reaction (user's input)

Amount and Purity of Product Obtained (user's input)

Amount in (m)mols and Yield of Product (calculated)

Additional Notes (user's input)

Product Number (user's input)

Theorethical Amount of Product (calculated)

A mixture of A, B and CHCl2 (dry, 2 mL) in toluene (dry, 10 mL, c[1]= 0.01M) v... Then the mixture was evaporated, a...

Experimental (Description of Reaction) (user's input)

PROCEDURE

| Fr. # | Quant. | Descripton | Anal. Data, Identification |
|---|---|---|---|
| 1 | .0328 | fr. 32-56 | 1: TLC, NMR |

Description (tubes collected, fraction in recrystallization, etc. User's input)

Amount of Fraction/ Product (user's input)

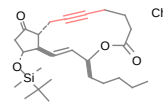
Add. Info (*e.g.* method of identification. User's input)

Number of Fraction/ Product (user's input)

Labels for samples (generated)

Cf. Browse Form for this fields

GRELA-FUE




**GRL-GA-**

$C_{26}H_{42}O_4Si$ = 446.71

GRL-GA-

GRL-GA-

GRL-GA-

GRL-GA-

GRL-GA-

REF: #24, #25

OK

NOTE: Acc. to TLC during GC conversion is near 90-100% (only traces of A,B)

RESULT

viscous colorless oil

[a]20/D : -188.2° (0.78, CHCl3)

TLC

NMR

MS

HRMS

IR

Anal. Data

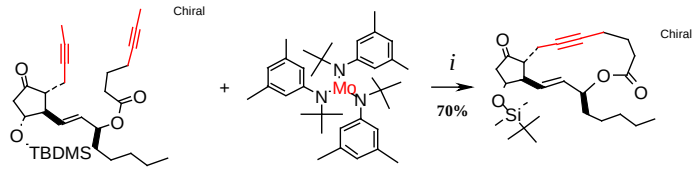
# Appendix 2

KEYWORDS: *C26H42O4Si : PGE2LA , RCM, Mo, chiral*

ID: 41 | DATE: 1999.09.29 | **GRL-GA-041**

LabJournal v. 2.3.0 (c) K. Grela 1996-1999 -- Data Browse Form - mmols -- Max-Planck-Institut für Kohlenforschung

REACTION




i) PhMe/CH2Cl2 (c[A]=0.01M), 16h, 80°C

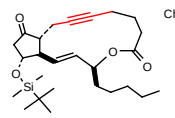
REF: #24, #25
OK
NOTE: Acc. to TLC during CC conversion is near 90-100% (only traces of A are detected)

RESULTS

Sketch

| Fr. # | Quant. | Descripton | Anal. Data, Identification |
|---|---|---|---|
| 1 | .0328 | fr. 32-56 | 1: TLC, NMR |

$C_{26}H_{42}O_4Si$ 446.71




viscous colorless oil
[a]20/D : -188.2° (0.78, CHCl3)
TLC
NMR
MS
HRMS
IR

(3S,11aR,14R,14aR)-14-{[1-(tert-butyl)-1,1-dimethylsilyl]oxy}-3-pentyl-9,10-didehydro-6,7,8,11,11a,13,14,14a-octahydro-3H-cyclopenta[e]oxacyclotridecine-5,12-dione

A mixture of A, B and CHCl2 (dry, 2 mL) in toluene (dry, 10 mL, c[1]= 0.01M) was stirred at 80°C (t/o 85°) for 5 hr under argon atmosphere. Then the mixture was evaporated, and the residue was subjected to the CC (EH 7.5%).

PROCEDURE

SUBSTRATES

| # | Formula | FW | Ratio | Scale [mol] | Quant. [mmol] | Th. Weight [mg] | Pract. Amt.: [g] or [mL] | g =1 mL=0 | Excess | Volume [mL] | density [g/mL] | Molarity [mol/L] | Purity [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | $C_{30}H_{48}O_4Si$ | 500.80 | 1.000 | 0.000100000 | 0.10000 | 50.08 | 0.05280 | 1 | 1.054 | 0 | | | 100 | GRL-GA-039-02 |
| B | $C_{36}H_{54}MoN_3$ | 624.79 | 0.075 | 0.000100000 | 0.00750 | 4.69 | 0.00500 | 1 | 1.066 | 0 | | | 100 | |

PRODUCTS

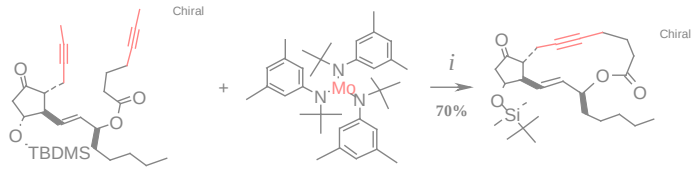
| # | Formula | FW | Ratio | Scale [mol] | Th. Yield [mmol] | Th. Yield [mg] | P. Yield [g] | Purity [%] | P. Yield [mmol] | P. Yield [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $C_{26}H_{42}O_4Si$ | 446.71 | 1.054 | 0.0001000000 | 0.10540 | 47.08 | 0.0328 | 100 | 0.073426 | 70 | |

KEYWORDS: *C26H42O4Si : PGE2LA , RCM, Mo, chiral*

ID: 41 | DATE: 1999.09.29 | **GRL-GA-041**

LabJournal v. 2.3.0 (c) K. Grela 1996-1999 -- Data Browse Form - mmols -- Max-Planck-Institut für Kohlenforschung

REACTION




i) PhMe/CH2Cl2 (c[A]=0.01M), 16h, 80°C

Place for graphical comment (*e.g* drawning of equippment used. User's input. Double-click in this field to open ISIS/Draw)

REF: #24, #25
OK
NOTE: Acc. to TLC during CC conversion is near 90-100% (only traces of A are detected)

RESULTS

Sketch

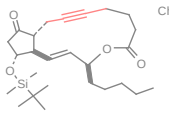
| Fr. # | Quant. | Descripton | Anal. Data, Identification |
|---|---|---|---|
| 1 | .0328 | | 1: TLC, NMR |

Place for textual comment (*e.g.* references, notes. User's input)

Name of Product (user's input)

Summary of Analytycal Data (user's input)

$C_{26}H_{42}O_4Si$ 446.71




viscous colorless oil
[a]20/D : -188.2° (0.78, CHCl3)
TLC
NMR
MS
HRMS
IR

(3S,11aR,14R,14aR)-14-{[1-(tert-butyl)-1,1-dimethylsilyl]oxy}-3-pentyl-9,10-didehydro-6,7,8,11,11a,13,14,14a-octahydro-3H-cyclopenta[e]oxacyclotridecine-5,12-dione

A mixture of A, B and CHCl2 (dry, 2 mL) in toluene (dry, 10 mL, c[1]= 0.01M) was stirred at 80°C (t/o 85°) for 5 hr under argon atmosphere. Then the mixture was evaporated, and the residue was subjected to the CC (EH 7.5%).

Produtc Structure, as drawn on the reaction scheme. If you have more than one product, use Up/Down buttons to swicht beetween products (*generated*)

PROCEDURE

SUBSTRATES

| # | Formula | FW | Ratio | Scale [mol] | Quant. [mmol] | Th. Weight [mg] | Pract. Amt.: [g] or [mL] | *g =1 mL=0* | Excess | Volume [mL] | density [g/mL] | Molarity [mol/L] | Purity [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | $C_{30}H_{48}O_4Si$ | 500.80 | 1.000 | 0.000100000 | 0.10000 | 50.08 | 0.05280 | *1* | 1.054 | 0 | | | 100 | GRL-GA-039-02 |
| B | $C_{36}H_{54}MoN_3$ | 624.79 | 0.075 | 0.000100000 | 0.00750 | 4.69 | 0.00500 | *1* | 1.066 | 0 | | | 100 | |

PRODUCTS

| # | Formula | FW | Ratio | Scale [mol] | Th. Yield [mmol] | Th. Yield [mg] | P. Yield [g] | Purity [%] | P. Yield [mmol] | P. Yield [%] | Notes |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | $C_{26}H_{42}O_4Si$ | 446.71 | 1.054 | 0.0001000000 | 0.10540 | 47.08 | 0.0328 | 100 | 0.073426 | 70 | |