



Find and exchange digital research data

Dr. Felix Rudolphi
Sciformation Consulting GmbH

Publication platform: why?

"Typical results
are shown."

The best results
are shown.

"Correct within an order of magnitude."
Wrong.

"Three of the samples were chosen
for detailed study."
The results on the others didn't
make sense and were ignored.

"In my experience..." = Once.
"In case after case..." = Twice.
"In a series of cases..." = Thrice.

Publication platform: why?

- Only a selection of experiments and data is published
- Limited searchability
- Access limited or costly
- „Supporting information“ is text and images, but no original data
- The percentage of failed experiments is too high
- Where can I search for reaction parameters like „< 80 °C“?
- ChemRxiv is a nice approach, but offers only full text search
- Original data should be published together with a paper

sciflection

- Publish lab notebook entries with a few clicks
- Search for structures, parameters, keywords, etc.
- Free at <https://sciflection.com>

Filter by various criteria

Search for a dataset

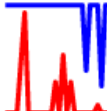
Search criteria

Quick search

Choose the search criteria here


A→B


Lab notebook entry


Analytical data

[isol. %](#)
[Y_{ana} \(%\)](#)
[T \(°C\)](#)
[Dur. \(h\)](#)
[Solv.](#)
[Amount \(ml\)](#)
[Reaction equation](#)
[Parts of the reaction equation](#)

[Score](#)
[Analytics type](#)
[Analytical device](#)
[Method](#)
[Tags](#)
[Signal search in analytical data](#)
[13C NMR peaks \(ppm\)](#)
[1H NMR peaks \(ppm\)](#)

Search


Show all

Advanced

Search criteria

Lab notebook entry

Reaction equation



Lab notebook entry

isol. %

☒ from-to ☐ is not set

>5

Lab notebook entry

Score

☒ ≥ ☐ ≤

★

★

★

★

★

★

☒ Unrated

July 2020

sciformation

4

Search results like in the lab notebook

Search for a dataset		Search criteria	26 results	Quick search	
26 experiments		1 / 3	Detail mode 10 lines Columns Print Quick search	Login Register	A→B
Lab notebook	Title	Reaction equation	Yisol (%)	Yana (%)	Score
Ruhr-Universität Bochum/RI			97.46%	79.92% 13.57% 3.9%	 0
			1 : - : -	20.5 : 3.48 : 1	
Ruhr-Universität Bochum/RI			82.62%	74.89% 9.63% 6.81%	 0
			1 : - : -	11 : 1.41 : 1	
Ruhr-Universität Bochum/RI			56.75%	41.37% 22.95% 0%	 0
			1 : - : -	1.8 : 1 : 0	
Ruhr-Universität Bochum/RI			95.01%	80.23% 22.53% 0%	 0
			1 : - : -	3.56 : 1 : 0	

Importing an experiment

Search for a dataset Search criteria **1171 results**

/ 1171
 [List mode](#)
 [Print](#)
 [Quick search](#)
 [Login](#)
 [Register](#)
 [0 comments](#)
 [»](#)

Quick search

Score: ★★★★★

Carried out by: Felix Rudolphi

Ruhr-Universität Bochum/RUD-037

Publication confirmed

Click to copy permalink

[UUID: 3ecfa5d9-dbab-4e1e-b1b8-d8f1570ad51a](#)
 Copied URL to clipboard
 CC-BY 3.0-DE
 [Go to article](#)

Project: [Phenyllessigsäure](#)

Tags:

Experiment type: Chemical reaction

Metadata

Procedure Additional files (0) Analytical data (2) Diagrams (0) Literature (0) Advanced All

Reference amount	<input type="text" value="1"/>	mmol	T (°C)	<input type="text" value="70"/>	Dur. (h)	<input type="text" value="16"/>
<input type="checkbox"/> Product retained	Solv.	<input type="text" value="THF"/>		Amount (ml)	<input type="text" value="2"/>	

Reactants

#	eq	Structure	Substance names / Package	Formula / CAS No.	MW	n [mmol]	c [%]	m [mg]	p	V [ml]	Comment Rem. (%)	Hazard codes	H P
A	1		4-Bromtoluol 100 (25) ml, Schrank, B	C7H7Br CAS No.	171.04	1	c	171	1.39	0.123	Comment Rem. (%)	MSDS	Hazard statements Precautionary statements
B	1.2		Meldrum's Acid 100 g, Kühlfach, Schlenk	C6H8O4 CAS No.	144.13	1.2	c	173	p	V	Comment Rem. (%)	MSDS	Hazard statements Precautionary statements
C	0.01		Palladium(II)-acetat 1 (0.1) g, Schrank, P3	C4H6O4Pd CAS No.	224.51	0.01	c	2.25	p	V	Comment Rem. (%)	MSDS	Hazard statements Precautionary statements
D	0.022		2-(Di-tert-butylphosphino)-2'-methylbiphenyl Glasflasche, 1 (1) g, Kühlfach, Phosphine	C21H29P CAS No.	312.44	0.022	c	6.87	p	V	Comment Rem. (%)	MSDS	Hazard statements Precautionary statements

Paste link or GUID here

July 2020

Importing an experiment

TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

Sciflection URL DOI+

18 / 18 RUD 18

Reaction setup Results Custom list mode Search

Start over!

RUD 18

project none

Type none

status: planned

title

date of reaction start 09.07.2020 00:00:00

carried out by rudolphi

Reaction setup

A B C D E 1
 solv. THF Amount (ml) T (°C) 70 p (bar) dur. (h) 16 Reference amount 0.001

reactants

	eq	structure	Compound barcode	formula CAS number	MW	n [mmol]	c [%]	m [mg]	p	V [ml]
A	1		benzene, 1-bromo-4-methyl- (hartwig: 1) gl. (hartwig) 20007775	C7H7Br 106-38-7	171.03	0.001	100	0.171	1.39	0.123
B	1.2		1,3-dioxane-4,6-dione, 2,2-... (hartwig: 1) gl. (hartwig) 20007676	C6H8O4 2033-24-1	144.13	0.0012	100	0.173		
C	0.01		palladium(ii) acetate (1) 2 g, C 3.042 20014353	C4H6O4Pd 3375-31-3	224.51	1	100	0.00225		

sciformation ELN is even better or support this project with a donation?

Uploading your experiments

The screenshot displays the sciformation ELN web interface. At the top, a navigation bar includes the university logo (Technische Universität Kaiserslautern) and a search bar containing the text "Present your research topics - at sciflection.com". Below the navigation bar, there are tabs for "edit mode" and "list mode". The left sidebar contains a search filter section with dropdown menus for "Database" (own database), "User" (rudolphi), "Project" (any), "lab journal" (RUD), "carried out by" (any), "status" (any), "date of reaction start" (any), and "Order by" (Lab journal entry). Below these filters is a "Result list" section with a "New search" button. The main content area shows "No results." and a blue box with the text "Prerequisite: connect your database with Sciflection.com". The bottom of the sidebar features a list of links: "Change to Inventory", "My projects", "Projects", "Lab journals", "Data publications" (highlighted with a red box), "Literature", "My orders", "Confirm orders", "Settings", and "Logout". The sciformation ELN logo is at the bottom left of the sidebar.

Technische Universität Kaiserslautern

Present your research topics - at sciflection.com

edit mode list mode

No results.

Database: own database X

User: rudolphi X

Project: any

lab journal: RUD X

carried out by: any

status: any

date of reaction start: any

Order by: Lab journal entry

Selected items only

Result list: New search

list mode edit mode

Change to Inventory

My projects

Projects

Lab journals

Data publications

Literature

My orders

Confirm orders

Settings

Logout

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Prerequisite: connect your database with Sciflection.com

Database X

User X

Project

lab journal X

carried out by

status

date of reaction start

Order by

☐ Selected items only

Result list

☒ list mode
☐ edit mode

- Change to Inventory
- My projects
- Projects
- Lab journals
- Data publications
- Literature
- My orders
- Confirm orders
- Settings
- Logout

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is even better

or support this project with a donation?

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Begriffe

Dienst:

Die Website sciflection.com sowie jegliche Unterseiten und Aliasnamen. Der Dienst bietet *Nutzern* bis auf Widerruf die Möglichkeit, Forschungsdaten anderen Nutzern zugänglich zu machen.

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 - Nutzer schädigen können (Malware),
 - die Rechte Dritter verletzen (z.B. Geheimhaltungsregeln, Exklusivverträge, Marken-, Patent- oder sonstige Schutzrechte)

institution	TU Kaiserslautern-Goossen
user name	tu_kaiserslautern_goossen
email	rudolphi@chemie.uni-kl.de
	
Please enter the text above, unless you are a robot.	<input type="text" value="VHSYI"/> <input type="button" value="refresh"/>

☒ Yes, I accept the terms and conditions and want to create an account at sciflection.com

Uploading your experiments



TECHNISCHE UNIVERSITÄT
KAISERSLAUTERN

Join sciflection.com - it's free

Settings saved.

Database: own database ▾

User: rudolphi ▾

Project: any ▾

lab journal: RUD ▾

carried out by: any ▾

status: any ▾

date of reaction start: any ▾

Order by: Lab journal entry ▾

☐ Selected Items only

Result list: New search ▾

☒ list mode
☐ edit mode

- Change to Inventory
- My projects
- Projects
- Lab journals
- Data publications
- Literature
- My orders

TBD: some explanations
guiding users

Uploading your experiments

TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

Database: own database ☒ X
 User: rudolphi ☒ X
 Project: any ☐
 lab journal: RUD ☒ X
 carried out by: any ☐
 status: any ☐
 date of reaction start: any ☐
 Order by: Lab journal entry ☐
☐ Selected items only
 Result list: New search ☐
☒ list mode
☐ edit mode
 Change to inventory
 My projects
 Projects
 Lab journals

edit mode | list mode

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New

Edit Project

project name: rudolphi privat
 date of project start: 09.05.2009
 status: in progress
 description: Die Reaktionen in diesem Projekt können nur von rudolphi angesehen werden.
 assigned persons: rudolphi
☒ Reactions visible for members only

citation	Title	DOI
Alan Armstrong, James C. Collins, <i>Angew. Chem. Int. Ed.</i> 2010 , 49 (13), 2282-2285.	Direct Azole Amination: C-H Functionalization as a New Approach to Biologically Important Heterocycles	10.1002/anie.200906750 ANGE

Create a new "data publication" and add

- single experiments
- lab notebooks
- whole projects

DOI: 10.1002/anie.200906750

n: C-H Functionalization as a Biologically Important Heterocycles**

Alan Armstrong* and James C. Collins

Uploading your experiments

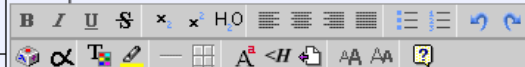


Add Data publication

Name	My test publication
License	CC-BY 4.0
DOI	
Destination	sciflection.com
<p>After upload, the data publication will be available under the following address:</p> <p>citation:</p> <p>rud</p> <p>rudolphi_privat +</p> <p>A→B RUD 1 +</p> <p>A→B RUD 2 +</p> <p>A→B RUD 3 +</p> <p>A→B RUD 4 +</p>	

Enter a name

Description



Optionally: link with a literature citation

Add more reactions or spectra if required

Assigned experiments

code	carried out by	date of reaction start	Comment
TESTC106	rudolphi	2010-01-23 00:00:00	
TESTC119	rudolphi	2010-04-04 00:00:00	

Assigned analytical data

Identifier	type name	device name	method name	code	measured by		Comment
				TESTC119		2010-05-31 21:53:27	
A-butandiol.raw	GC	PEtest	A-butandiol.raw	TESTC119		2010-05-31 22:21:05	
rud48.SMS	GC-MS	VarianTest	Lukas.mth	TESTC119		2010-05-31 22:27:31	
blaag68	HPLC	Shimadzu Test	Lukas.met	TESTC119		2010-05-31 22:21:30	
rudua131.sp	IR	TestIR		TESTC119		2010-05-31 22:19:03	

Uploading your experiments

1
 /1

0

 +

edit mode | **list mode**

Edit Data publication

Name:	My test publication
License:	CC-BY 4.0
Destination:	sciflection.com
After upload, the data publication will be available under the following address:	http://127.0.0.1:8080/startUseCase?useCase=performSearch&viewMode=1&table=EInReaction&UUID=0095cb44-bee2-11ea-8f2f-d8253080f23e
citation:	none

Options:

- wait and collect more entries
- check that you upload the right entries and confirm

Assigned experiments					Assigned analytical data								
code	carried out by	date of reaction start	Comment		Identifier	type name	device name	method name	code	measured by		Comment	
RUD1	rudolphi	2010-08-14 00:00:00							TESTC119		2010-05-31 21:53:27		
TESTC106	rudolphi	2010-01-23 00:00:00			A-butandiol.raw	GC	PEtest	A-butandiol.raw	TESTC119		2010-05-31 22:21:05		
TESTC119	rudolphi	2010-04-04 00:00:00			rud48.SMS	GC-MS	VarianTest	Lukas.mth	TESTC119		2010-05-31 22:27:31		
					blaag68	HPLC	Shimadzu Test	Lukas.met	TESTC119		2010-05-31 22:21:30		
					rudua131.sp	IR	TestIR		TESTC119		2010-05-31 22:19:03		
					rudua252.sp	IR	TestIR		TESTC119		2010-05-31 22:20:09		

Created by: rudolphi 09.07.2020 16:09:20
Last change by: rudolphi 09.07.2020 16:09:20

Uploading your experiments

Technische Universität Kaiserslautern

Database: own database
User: rudolphi
Project: any
lab journal: RUD
carried out by: any
status: any
date of reaction start: any
Order by: Lab journal entry

Reaction setup

project: none
status: planned
date of reaction start: 09.07.2020 00:00:00
carried out by: rudolphi

Reaction setup

solv.: THF T (°C): 70 dur. (h): 16

reactants

	eq	structure	Compound barcode	formula CAS number	MW	n [mmol]	c [%]	m [mg]	p	V [ml]	H P
A	1		benzene, 1-bromo-4-methyl- gl., (hartwig) 20007775	C ₇ H ₇ Br 106-38-7	171.03	0.001	100	0.171	1.39	0.123	302-315 264-270-273-280-301+312+330-302+350-305+351+338-332+313-337+313-362-391-501
B	1.2		1,3-dioxane-4,6-dione, 2,2-dimethyl- gl., (hartwig) 20007676	C ₆ H ₈ O ₄ 2033-24-1	144.13	0.0012	100	0.173			
C	0.01		palladium(II) acetate 2.g., C 3.042 20014353	C ₄ H ₆ O ₄ Pd 3375-31-3	224.51	1	100	0.00225			318 280-305+351+338
D	0.022		2-(Di-tert-butylphosphino)- 2'-methylbiphenyl	C ₂₁ H ₂₉ P	312.44	2.2	100	0.00687			
E			tripotassium orthophosphate 250.g., C 3.042 20013516	K ₃ O ₄ P 7778-53-2	212.27	0.00238	100	0.505	2.564		315-318 280-305+351+338

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Uploading your experiments

The screenshot shows the 'Edit Data publication' interface in the sciformation system. At the top, there is a toolbar with icons for editing, deleting, publishing, and other actions. Below the toolbar, there are tabs for 'edit mode' and 'list mode'. The 'edit mode' tab is active, showing a form for editing a publication. The form includes fields for Name, License, Destination, and a URL for the data after upload. A confirmation dialog is displayed in the center, asking for confirmation to release experiments and measurements under the CC-BY 4.0 license. The dialog has 'Abbrechen' and 'OK' buttons. Below the dialog, there is a table of assigned experiments.

Edit Data publication

Name: My test publication

License: CC-BY 4.0

Destination: sciflection.com

After upload, the data publication will be available under the following address: <http://127.0.0.1:8080/startUseCase?useCase=performSearch&viewMode=1&table=ElNReaction&UUID=0095cb44-bee2-11ea-8f2f-d8253080f23e>

citation: none

Assigned experiments

code	carried out by	date of reac	Comment
RUD1	rudolphi	2010-08-14 0	
TESTC106	rudolphi	2010-01-23 0	
TESTC119	rudolphi	2010-04-04 0	

Are you sure that you want to release 3 experiments and 6 analytical measurements irrevocably under the terms of the CC-BY 4.0 license and publish them using the account "sciflection.com" at <http://127.0.0.1:8080>? By clicking "OK", you declare that all copyright holders have approved and that the content is in accordance with applicable laws.

Abbrechen OK

code	carried out by	date of reac	Comment				
blaag68	HPLC	Shimadzu Test	Lukas.met	TESTC119		2010-05-31 22:21:30	
rudua131.sp	IR	TestIR		TESTC119		2010-05-31 22:19:03	
rudua252.sp	IR	TestIR		TESTC119		2010-05-31 22:20:09	

Created by: rudolphi 09.07.2020 16:09:20
Last change by: rudolphi 09.07.2020 16:09:20

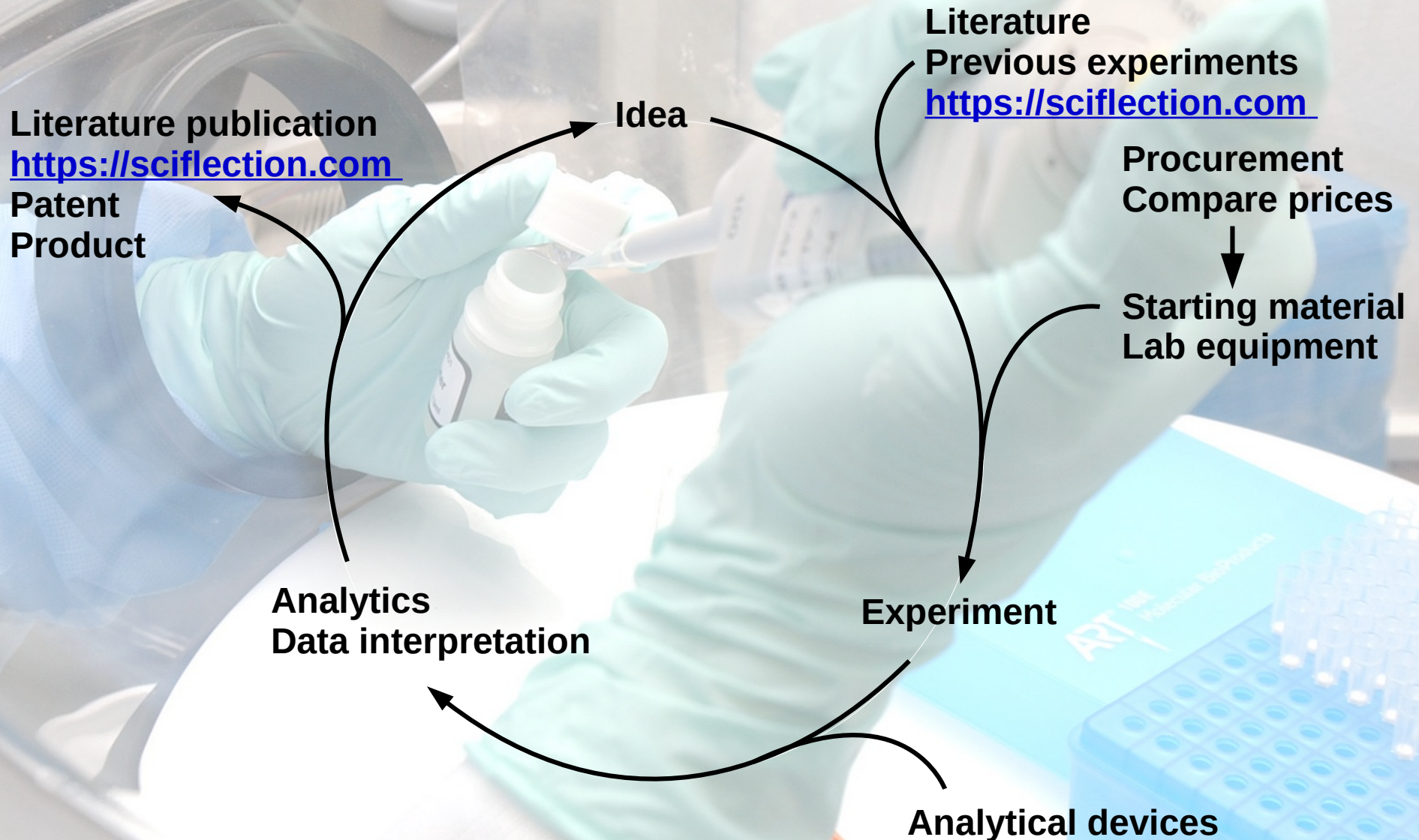
sciflection

- Signup only required to rate and comment (free)
- Connection from Sciformation ELN or open enventory with about three clicks
- Content under CC-BY licenses (Attribution)
- Every entry can be referenced using a GUID
- Import experiments into Sciformation ELN or open enventory
- API open for other products

<https://sciflection.com>

sciformation

Closing the circle



Advantages of going digital

Save time

Save money

Work more safely

**Explore
new horizons**

**Calculation
of amounts**

**Purchase starting
material if you
cannot find it**

Risk assessment

**Use existing
data better**

**Find the starting
material**

**Avoid unnecessary
repetitions**

Avoid mistakes

**Better team
coordination**

**Searching for
spectra**

**Quality of
documentation**

Users of

sciformation

ELN



Fluorescent Labels and Dyes



July 2020

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Thanks for your attention



https://sciformaion-demo.eu/intern/2007Sciflection/sciflection_short_v.1.pdf