化學家在做什麼?

以有機化學家為例

11/15/2016

部分內容來自:

展望化學的未來: An Era of Reimagining and Reinventing

趙奕姈

中央研究院化學所

Science:

Knowledge about the world, especially based on **examining, testing** and **proving** facts.

Chemistry:

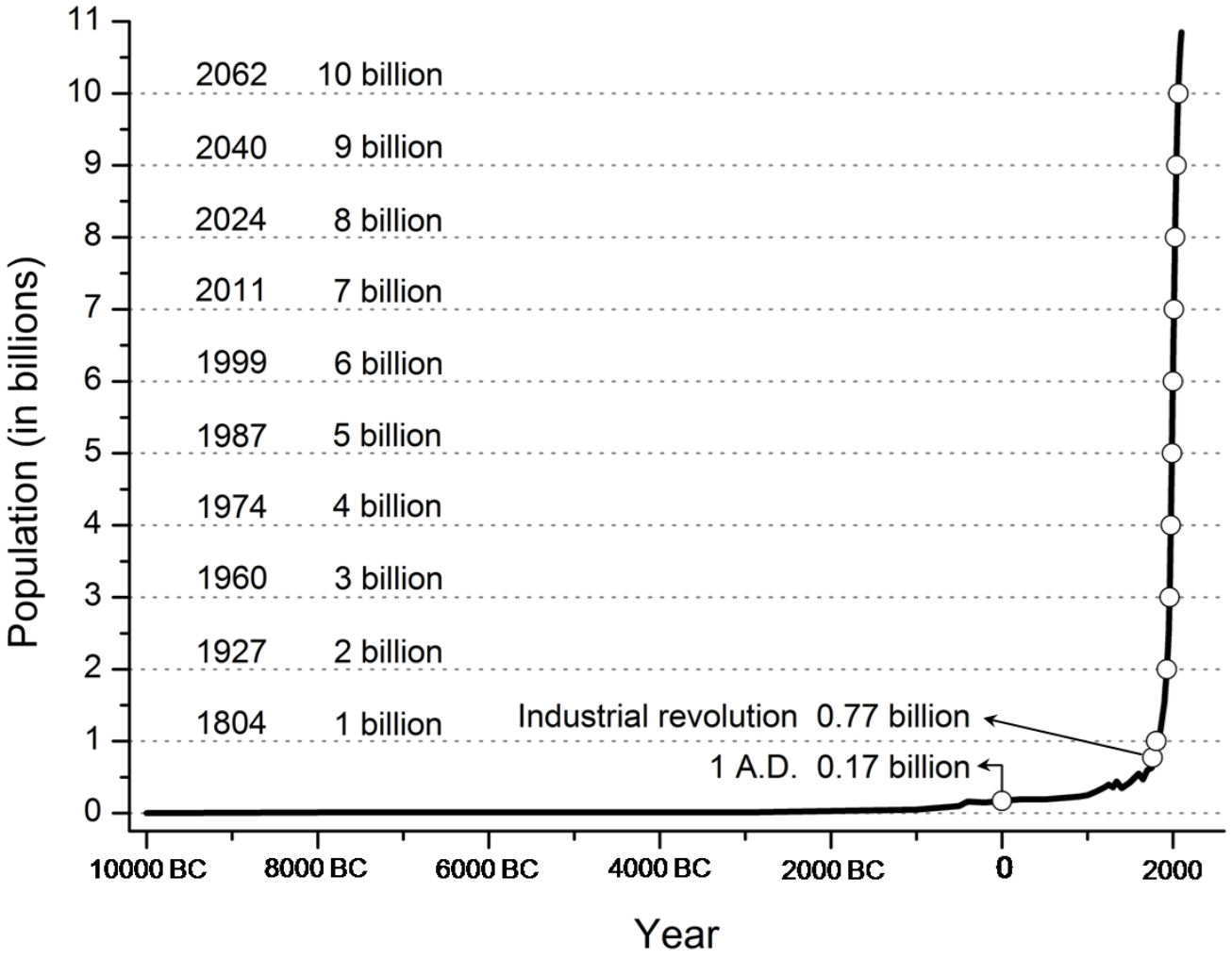
The **science** that is concerned with studying the ***structure*** of **substances** and the way that they ***change*** or ***combine*** with each other.

Longman Dictionary

現況與需求?

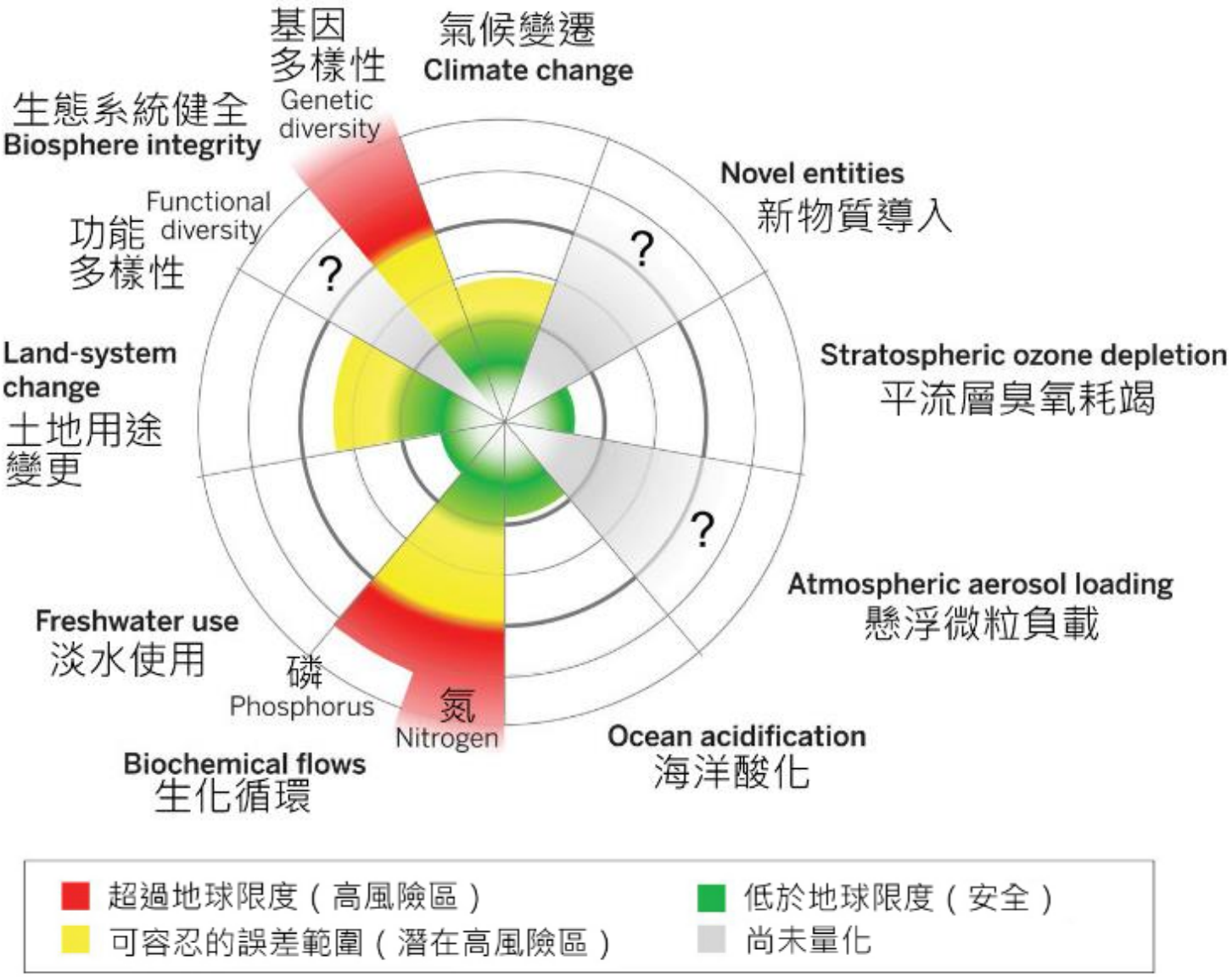
機器人會取代化學家嗎？

World Population



- Food/water enough when 30% more people?

Data before 1940: http://www.census.gov/population/international/data/worldpop/table_history.php
Data after 1940: http://esa.un.org/unpd/wpp/Excel-Data/population.htm Graph prepared by Hung-Yu Huang



中文翻譯：Impact Hub Taipei

資料來源：Will Steffen ▪ 2015 ▪ Planetary boundaries: Guiding human development on a changing planet ▪ Science

http://npost.tw/archives/24609

聯合國永續發展目標2016~2030 (Agenda 30)

※ 此表由CSRone永續報告平台翻譯與製作

√ Chemistry related

http://globalgoals.org/

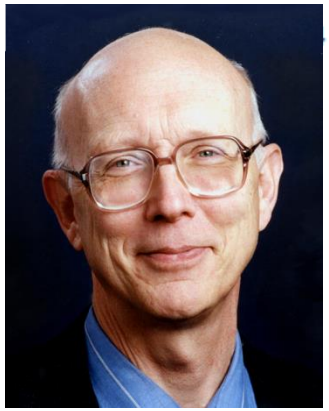
http://www.un.org/apps/news/story.asp?NewsID=51968#.Vhxtyfmqqko

Angewandte Essays

Future of Chemistry | Special Issue 150 Years of BASF

Reinventing Chemistry

*George M. Whitesides**



change · chemistry · science

The End of One Era and the Beginning of Another

Nothing goes on forever. The years following World War II were very kind to chemistry. The research universities and the chemical industry—one of the most beneficial partner-

ment, whatever—"chemical" or not? Any simple definition of the field of chemistry—or at least any definition as simple as "atoms, molecules, and reactions"—no longer seems to fit its potential, its obligations to society, or the complexity of the challenges it faces.

Abstract

"Chemistry may now be the most important of the sciences in its potential to impact society."

Chemistry is in a period of change, from an era focused on molecules and reactions, to one in which manipulations of systems of molecules and reactions will be essential parts of controlling larger systems. This Essay traces paths from the past to possible futures.

可以不要化學工業嗎？ PET vs. Wool

Land-Use Intensification in Manufacturing Fiber

Figure 2.11 Fleece made from recycled synthetic PET fibre. Image copyright O. Akhøj.

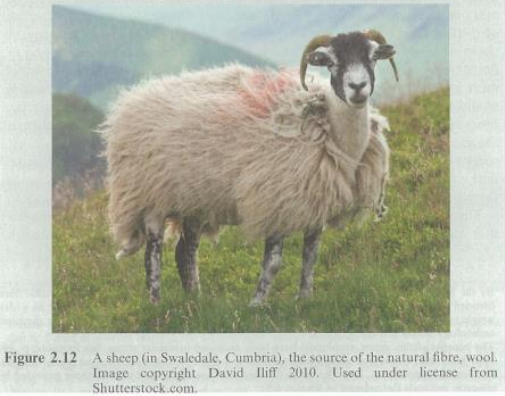


Figure 2.12 A sheep (in Swaledale, Cumbria), the source of the natural fibre, wool. Image copyright David Iliff 2010. Used under license from Shutterstock.com.

PET

- A 4-hectare plant produces 0.5 million tonnes per year

Wool

- To obtain 0.5 million tonnes per year; 25 sheep/hectare . Need 4×10^6 ha of pasture. **(Size of the Netherlands)**

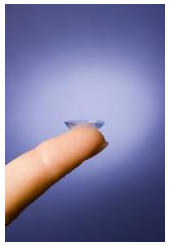
Land use ratio!! = $4 \times 10^6/4 = 10^6$!!

If 39 million tonnes of wool needed per year. **Size of India!!**

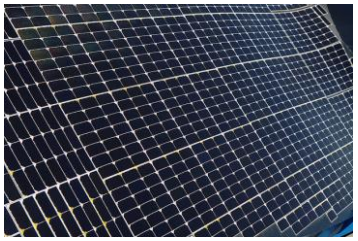
Chemistry for Sustainable Technologies: A Foundation (Neil Winterton; RSC) Chap. 2, section 2.7, Box 2.1

化學化工--現代社會的支柱

延長壽命 改變世(視)界!






化學 帶來工作機會

歐洲 雇用一百二十萬人

美國 雇用八十萬人

台灣

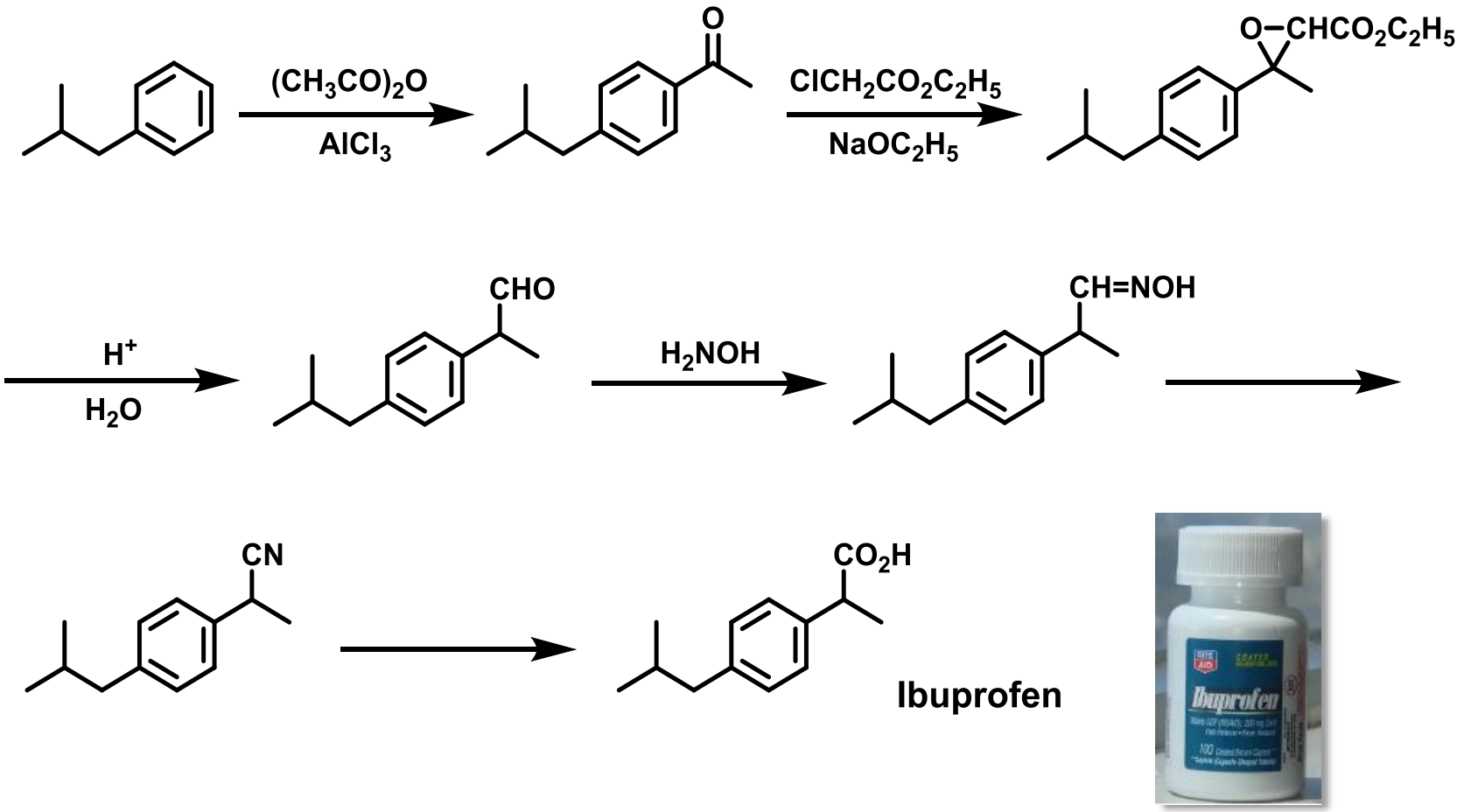
製造業分為四大產業；分別為金屬機械、**資訊電子**、**化學工業**與民生工業

- 2000年生產產值比例依序為24.68%、**37.39%**、**22.84%**(1.92兆)與15.09%
- 2008年生產產值比例依序為27.96%、**31.94%**、**30.36%**(3.03兆)與9.75%
- 2012年生產產值比例依序為26.08%、**32.74%**、**31.34%**(3.13兆)與9.85%

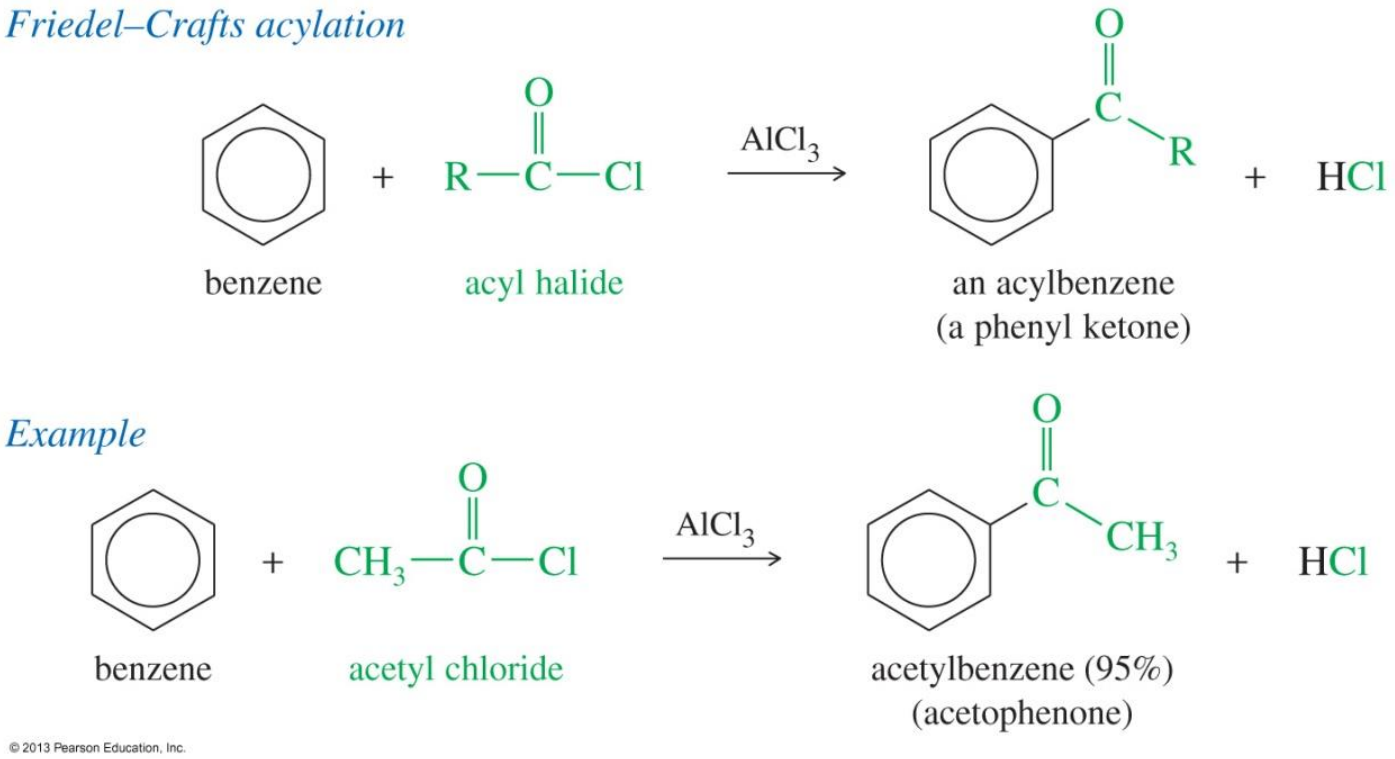
資訊電子與化學工業近年來分佔第一、二位，且差距小

Success Story about Ibuprofen

- UK market for ibuprofen is about 3,000,000 kg per year
- Old synthetic route (6 steps; atom economy = 40%)



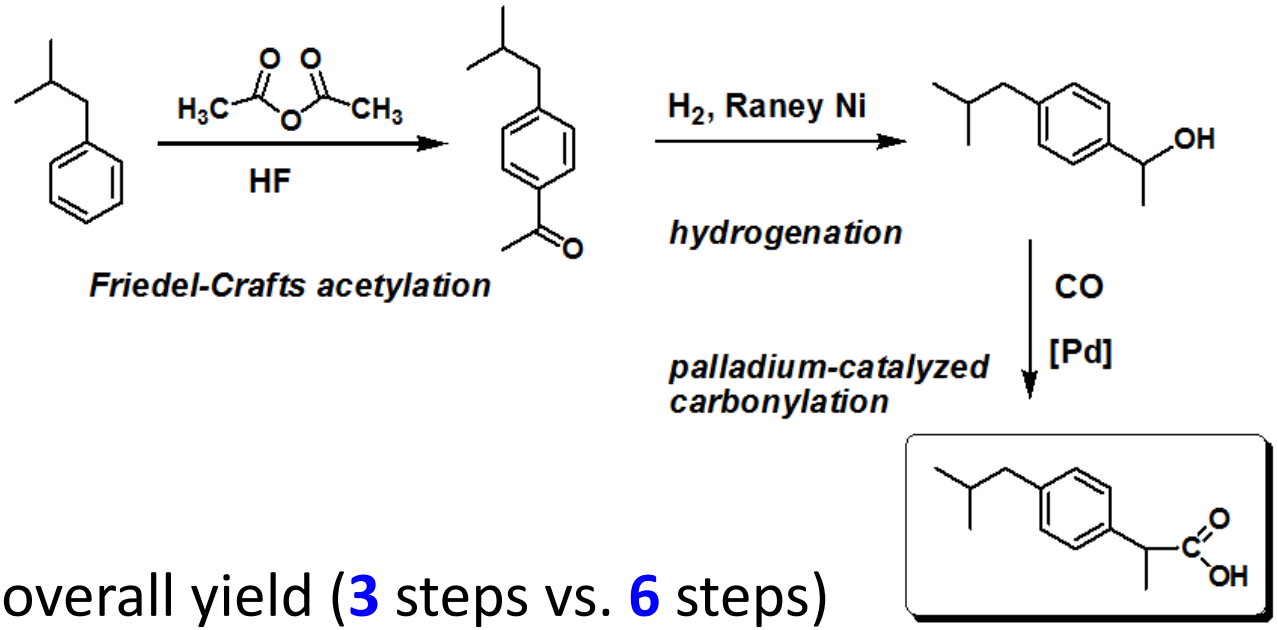
In Organic Chemistry textbook
Friedel–Crafts Acylation



- Acyl chloride is used in place of alkyl chloride.
- The product is a phenyl ketone that is less reactive than benzene.

Green Synthesis of Ibuprofen

SCST-2016

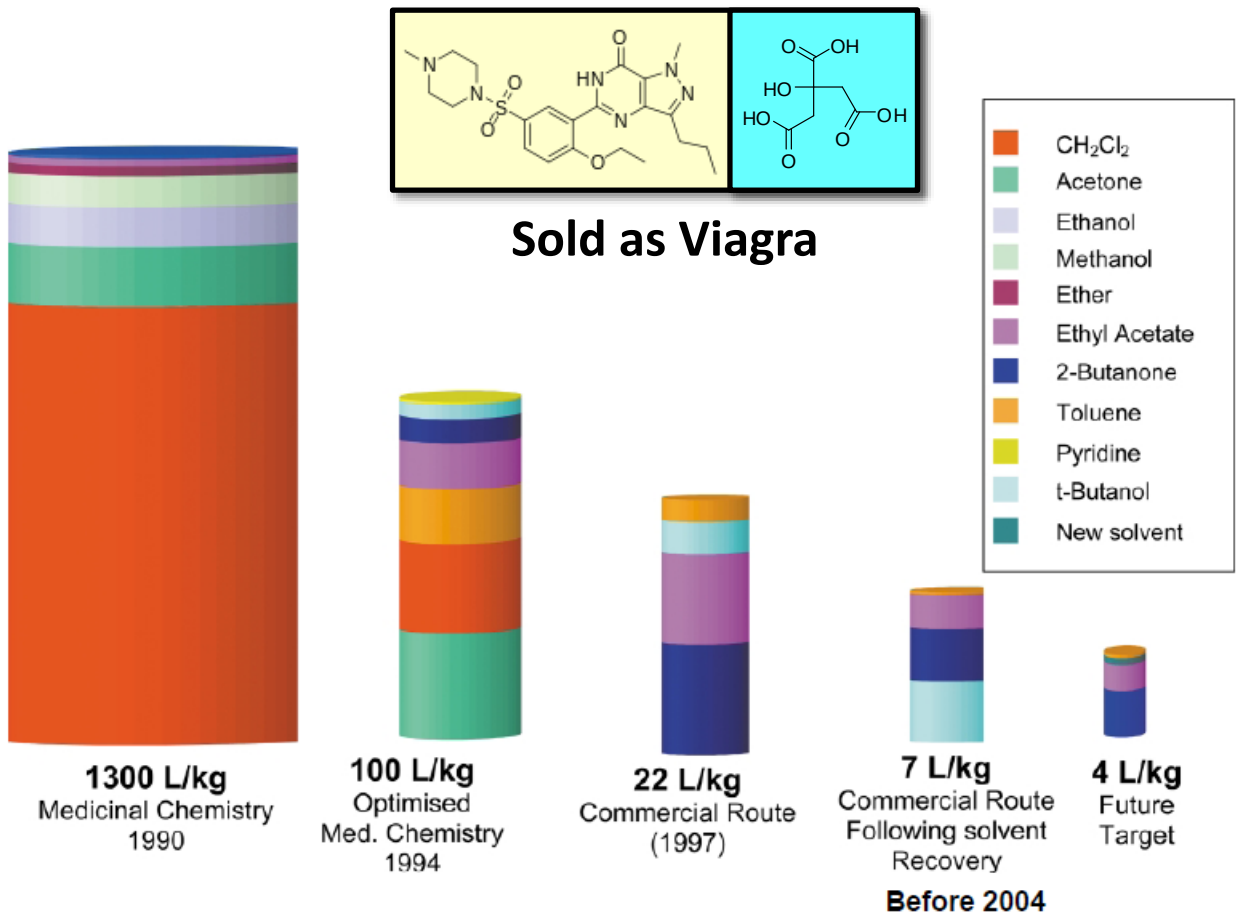


- Greater overall yield (**3** steps vs. **6** steps)
- Greater atom economy (**77%** vs. **40%** atom economy)
- Fewer auxiliary substances (products and solvents separation agents)
- **Less waste:** greater atom economy, catalytic vs. stoichiometric reagents, recovery of byproducts and reagents, recycling, and reuse, lower disposal costs.

Presidential Green Chemistry Challenge Awards

Greener Synthetic Pathways Award in 1997

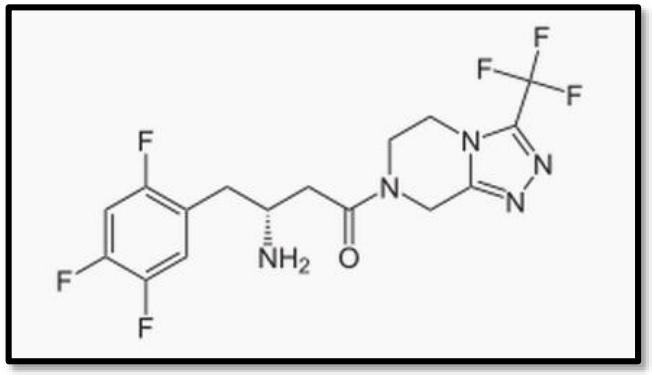
The Sildenafil Citrate Process: Reduction of Solvent Usage



2003 CRTSTAL Faraday Award

Green Chem. **2004**, *6*, 43; *Org. Proc. Res. Dev*. **2005**, *9*, 88.

Green Synthesis of Sitagliptin: Biocatalysis



Active ingredient in Januvia for treating of type 2 diabetes

- Enzymatic process affording chiral amine
- Eliminate the use of a rare metal catalyst
- Remove the use of high pressure condition
- Increase yield
- **Less waste:** compared to original catalytic synthesis, the enzymatic process creates **99.8 kg less waste for each kg** of sitagliptin produced.

Presidential Green Chemistry Challenge Award

Greener Reaction Conditions Award in 2010

Science **2010**, *329*, 305.

Prospects of Chemists

The Economist | World politics | Business & finance | Economics | Science & technology | Culture

The future of jobs

The onrushing wave

Previous technological innovation has always delivered more long-run employment, not less. But things can change

Jan 18th 2014 | From the print edition | Timekeeper | Like 6.9k

A bright future ahead for chemists and chemical engineers in a world of computerisation!

Bring on the personal trainers

Probability that computerisation will lead to job losses within the next two decades, 2013 (1=certain)

Job	Probability
Recreational therapists	0.003
Dentists	0.004
Athletic trainers	0.007
Clergy	0.008
Chemical engineers	0.02
Editors	0.06
Firefighters	0.17
Actors	0.37
Health technologists	0.40
Economists	0.43
Commercial pilots	0.55
Machinists	0.65
Word processors and typists	0.81
Real estate sales agents	0.86
Technical writers	0.89
Retail salespersons	0.92
Accountants and auditors	0.94
Telemarketers	0.99

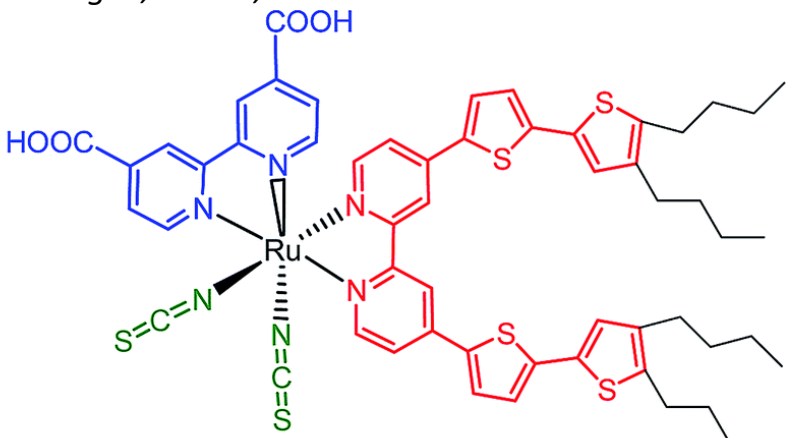
Source: "The Future of Employment: How Susceptible are Jobs to Computerisation?" by C.Frey and M.Osborne (2013)

17

Structural design of ruthenium sensitizer compatible with cobalt electrolyte for a dye-sensitized solar cell†

Chia Li , Shi-Jhang Wu and Chun-Guey Wu *

Department of Chemistry and Research Center for New Generation Photovoltaics, National Central University, Jhong-Li, 32001, Taiwan.

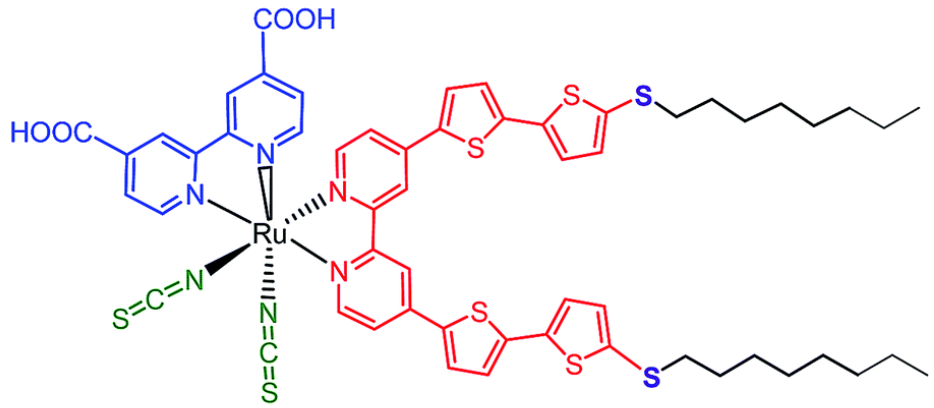


SJW-B18

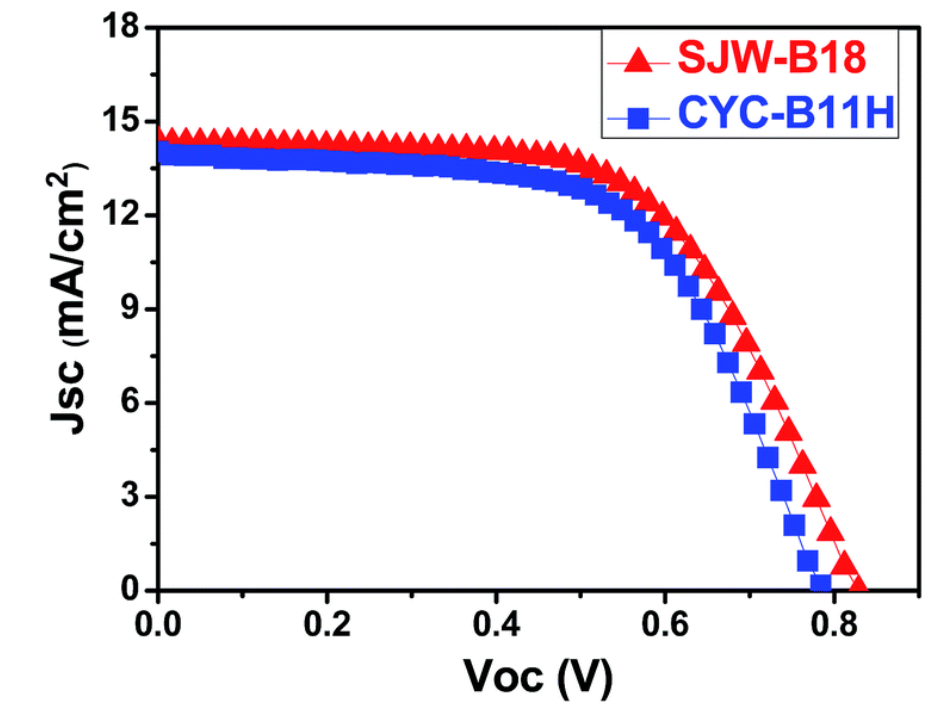
DOI: 10.1039/C4TA01750A

J. Mater. Chem. A, 2014, **2**, 17551-17560

功能(function)導向的合成化學



CYC-B11H



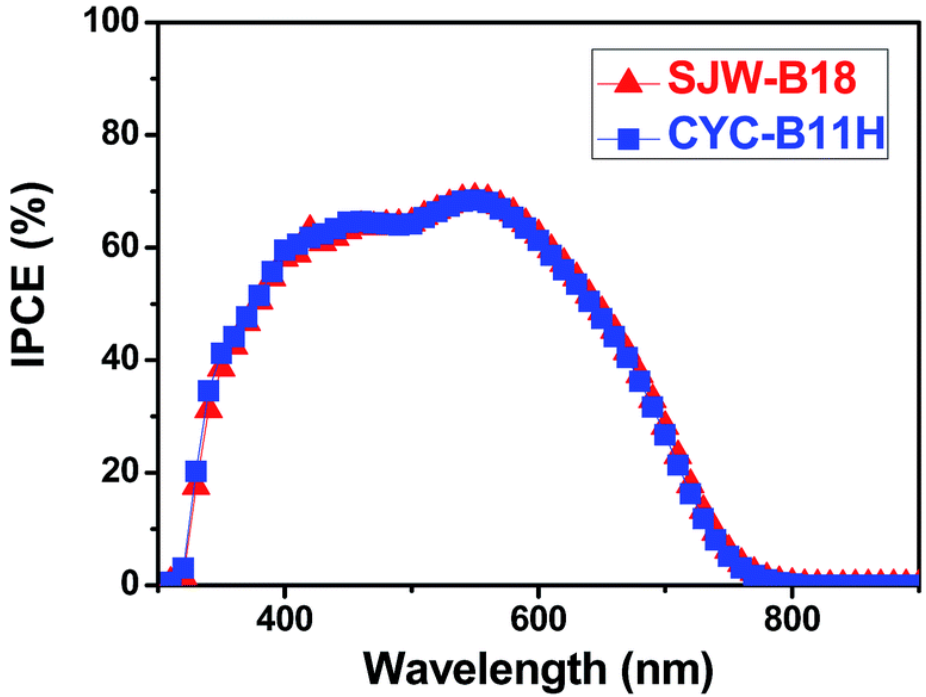
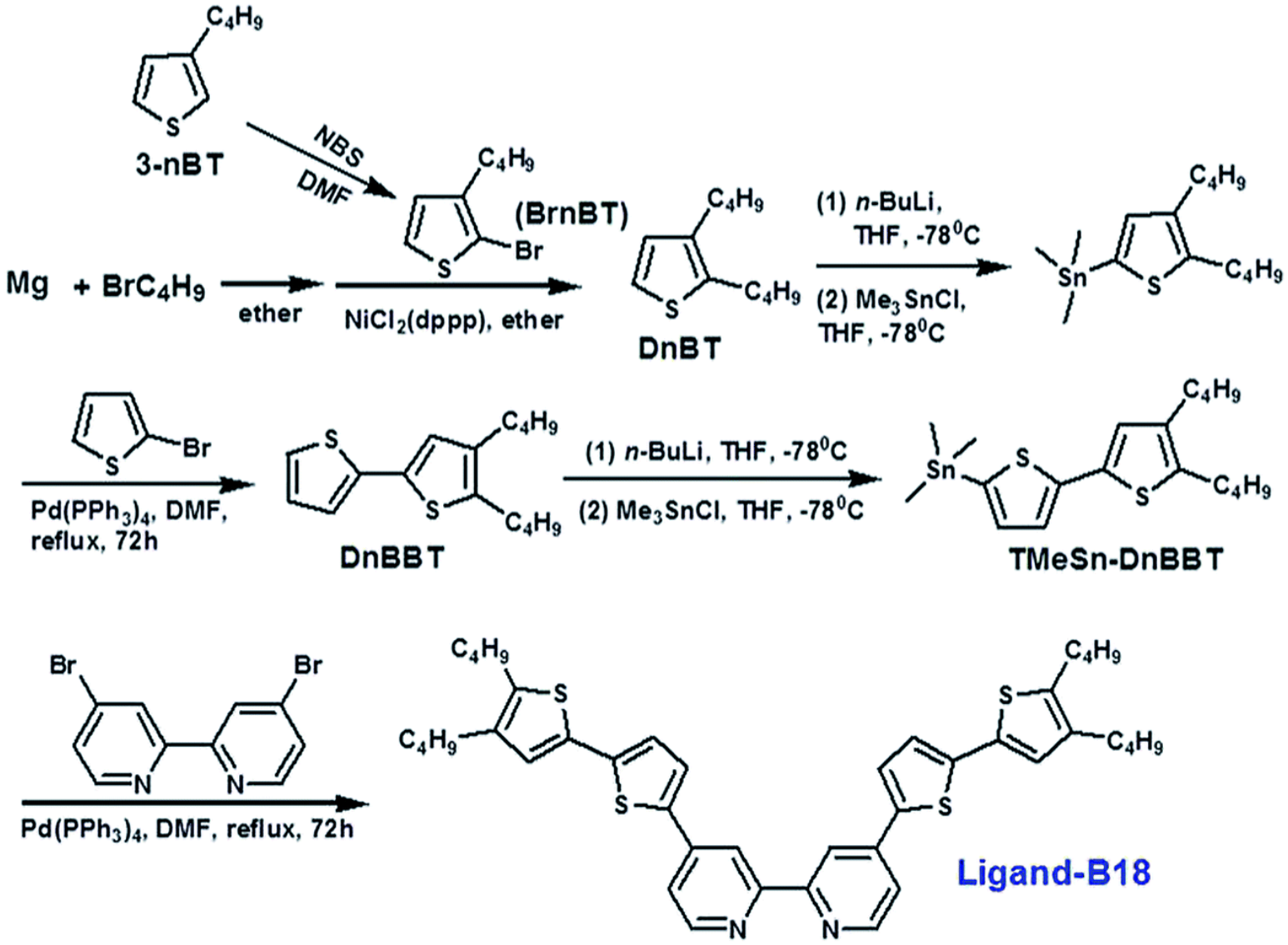
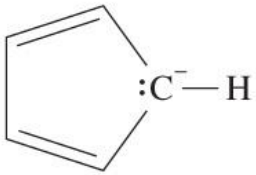


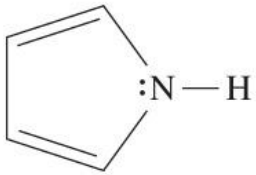
Fig. 6 Photocurrent density–voltage (*I*–*V*) and IPCE curves for device E and F sensitized with **SJW-B18** and **CYC-B11H**, respectively, measured under AM 1.5G simulated sunlight illumination (100 mW cm^{-2}). Thickness of TiO_2 film: 4 + 4 μm.


3-nBT
NBS
DMF
(BrnBT)
Mg + BrC4H9
ether
NiCl2(dppp), ether
DnBT
(1) n-BuLi, THF, -78°C
(2) Me3SnCl, THF, -78°C
Pd(PPh3)4, DMF, reflux, 72h
DnBBT
(1) n-BuLi, THF, -78°C
(2) Me3SnCl, THF, -78°C
TMeSn-DnBBT
Pd(PPh3)4, DMF, reflux, 72h
Ligand-B18

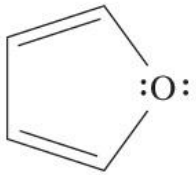
In Organic Chemistry textbook….



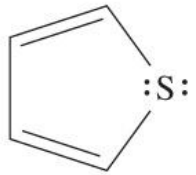
cyclopentadienyl anion



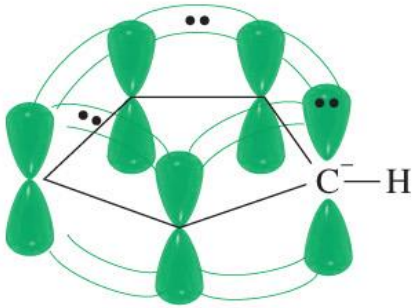
pyrrole



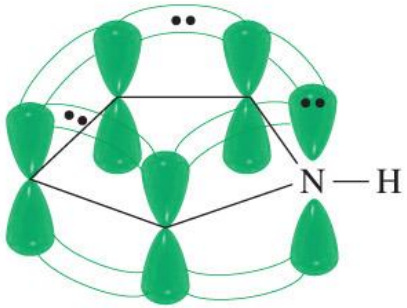
furan



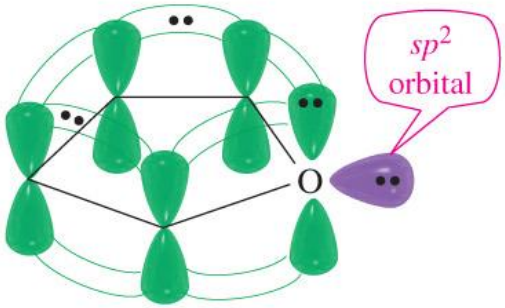
thiophene



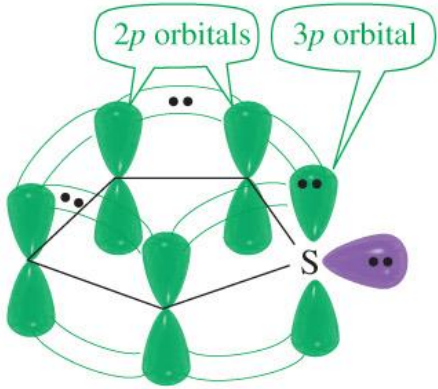
six pi electrons



six pi electrons

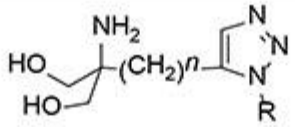


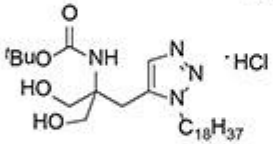
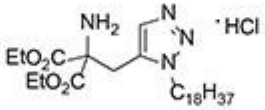
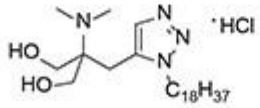
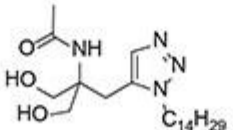
six pi electrons



six pi electrons

Non-immunosuppressive triazole-based small molecule induces anticancer activity against human hormone-refractory prostate cancers: the role in inhibition of PI3K/AKT/mTOR and c-Myc signaling pathways

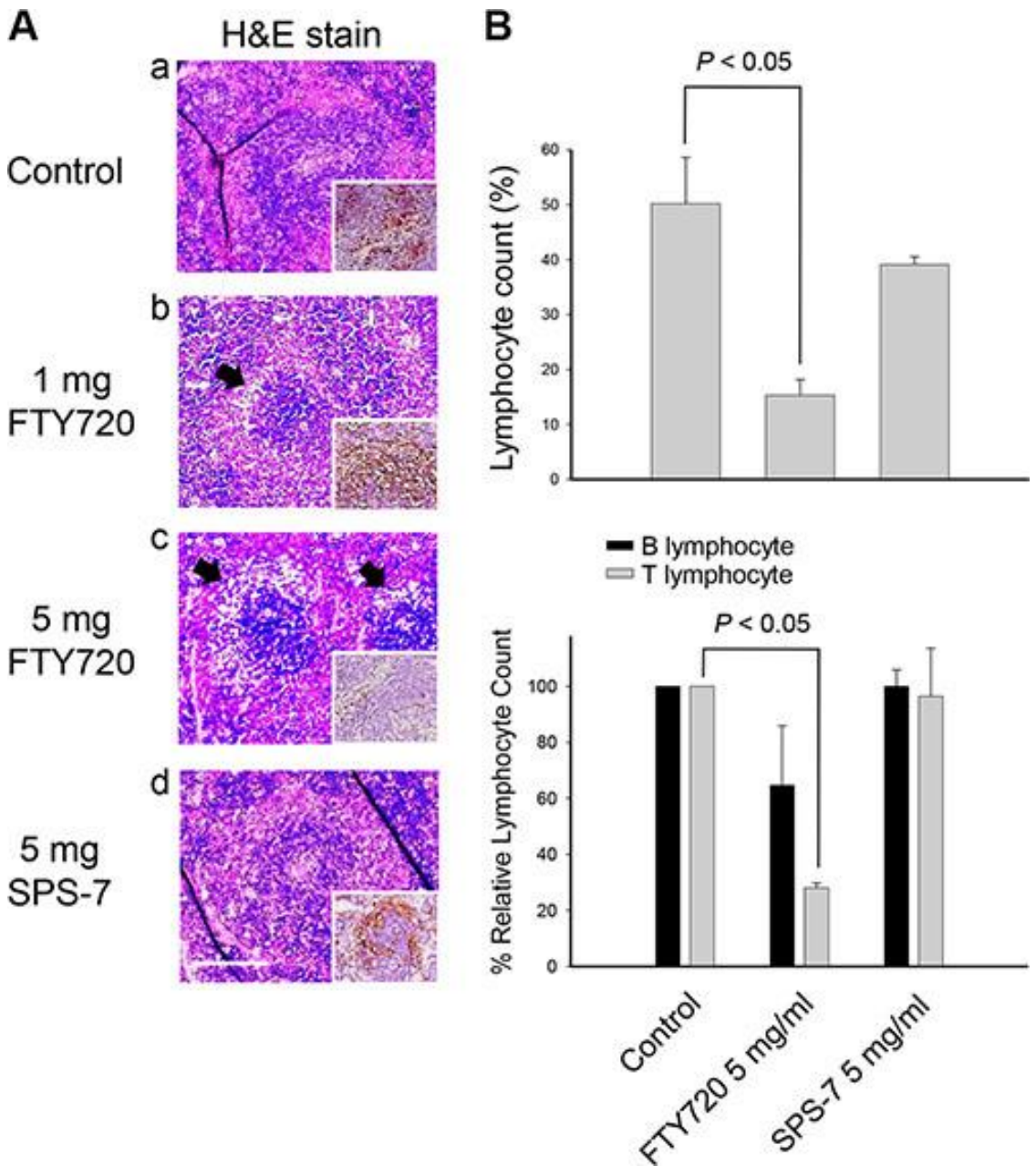


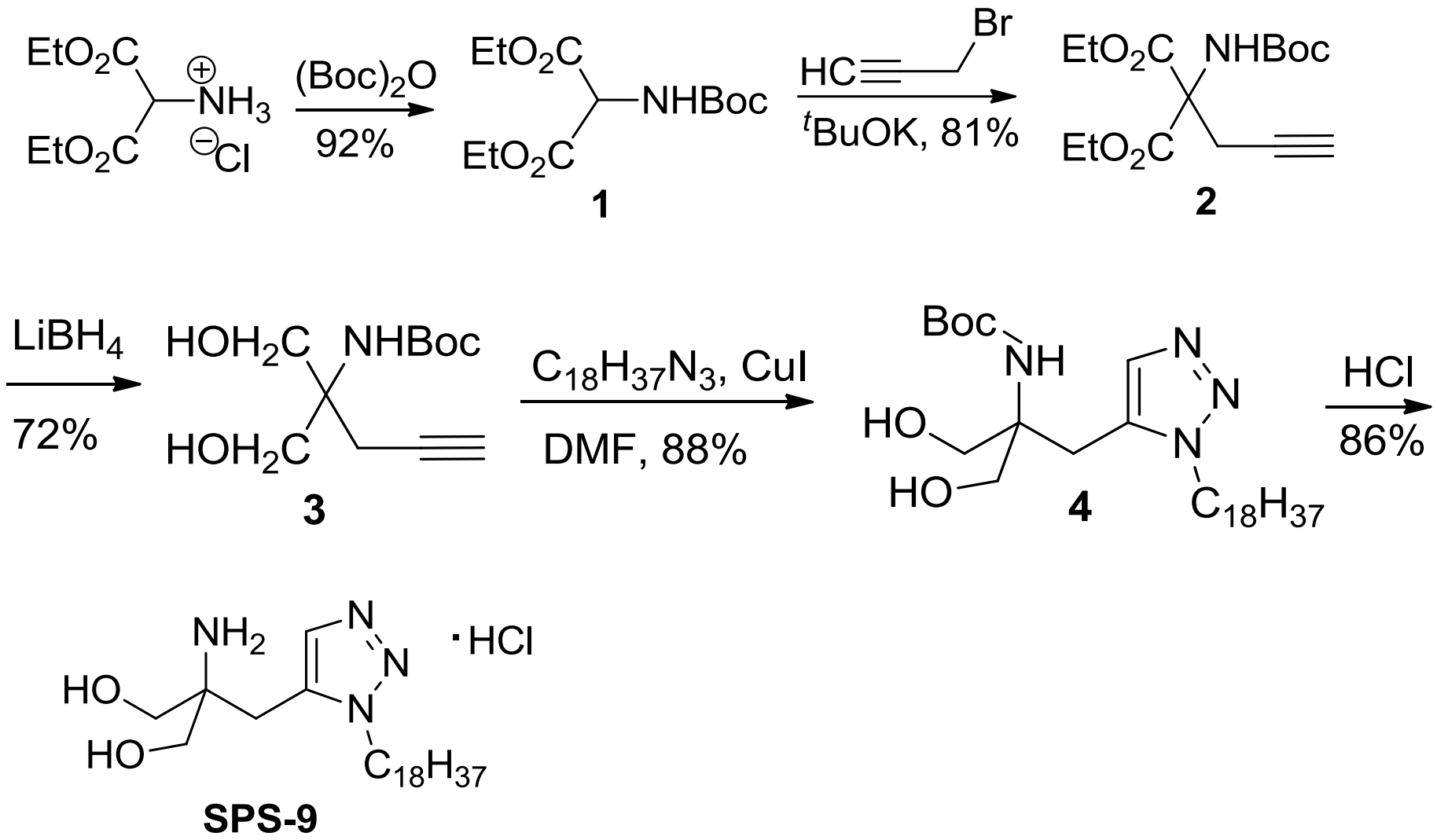
	n	R	PC-3 (IC_{50}, μM)	DU-145 (IC_{50}, μM)
SPS-1	1	C_6H_{13}	>10	>10
SPS-2	1	C_8H_{17}	>10	>10
SPS-3	1	$C_{10}H_{21}$	>10	9.7
SPS-4	1	$C_{12}H_{25}$	>10	>10
SPS-5	1	$C_{14}H_{29}$	4.9	4.7
SPS-6	1	$C_{16}H_{33}$	3.3	5.3
SPS-7	1	$C_{18}H_{37}$	3.0	4.6
SPS-8	1	$C_{20}H_{41}$	3.8	6.2
SPS-9	2	$C_{16}H_{33}$	6.2	nd
SPS-10	2	$C_{14}H_{29}$	>10	nd
SPS-11	3	$C_{14}H_{29}$	4.2	5.4
SPS-12	4	$C_{13}H_{27}$	9.0	6.6
SPS-13			>10	>10
SPS-14			7.9	> 10
SPS-15			> 10	> 10
SPS-16			> 10	> 10

DOI: 10.18632/oncotarget.12765
Metrics:PDF *127 views* | HTML *27 views?*

Wohn-Jenn Leu[1,*], Sharada Prasanna Swain[2,*], She-Hung Chan[1], Jui-Ling Hsu[1], Shih-Ping Liu[3], Mei-Ling Chan[1], Chia-Chun Yu[1], Lih-Ching Hsu[1], Yen-Lin Chou[2], Wei-Ling Chang[1], Duen-Ren Hou[2], Jih-Hwa Guh[1]

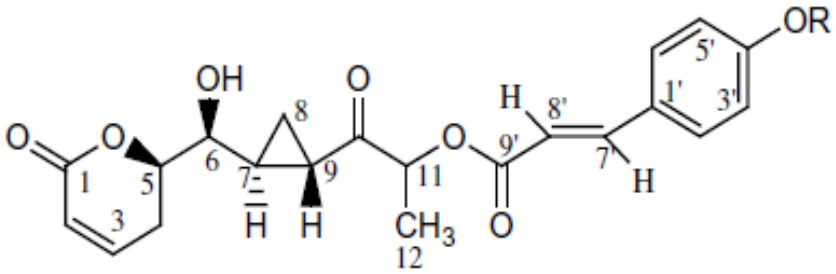
[1]School of Pharmacy, National Taiwan University, Taipei, Taiwan
[2]Department of Chemistry, National Central University, Jhong-li, Taoyuan, Taiwan
[3]Department of Urology, National Taiwan University Hospital, Taipei, Taiwan


A
H&E stain
a
Control
b
1 mg
FTY720
c
5 mg
FTY720
d
5 mg
SPS-7
B
P < 0.05
Lymphocyte count (%)
60
50
40
30
20
10
0
B lymphocyte
T lymphocyte
P < 0.05
% Relative Lymphocyte Count
100
80
60
40
20
0
Control
FTY720 5 mg/ml
SPS-7 5 mg/ml


EtO2C
NH3
EtO2C
Cl
(Boc)2O
92%
EtO2C
NHBoc
EtO2C
1
Br
HC
tBuOK, 81%
EtO2C
NHBoc
EtO2C
2
LiBH4
72%
HOH2C
NHBoc
HOH2C
3
C18H37N3, CuI
DMF, 88%
Boc
NH
HO
HO
N
N
N
C18H37
4
HCl
86%
NH2
HO
HO
N
N
N
C18H37
· HCl
SPS-9

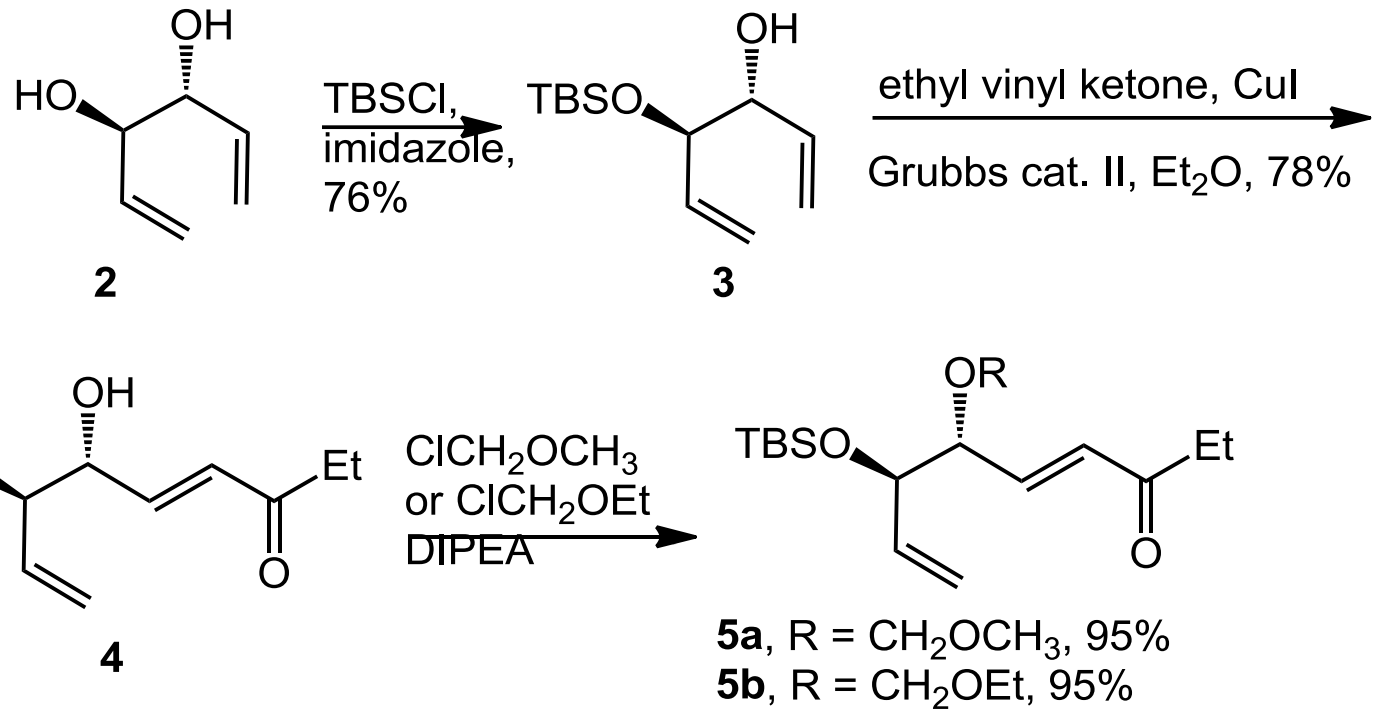
目標導向的合成 (target oriented synthesis)

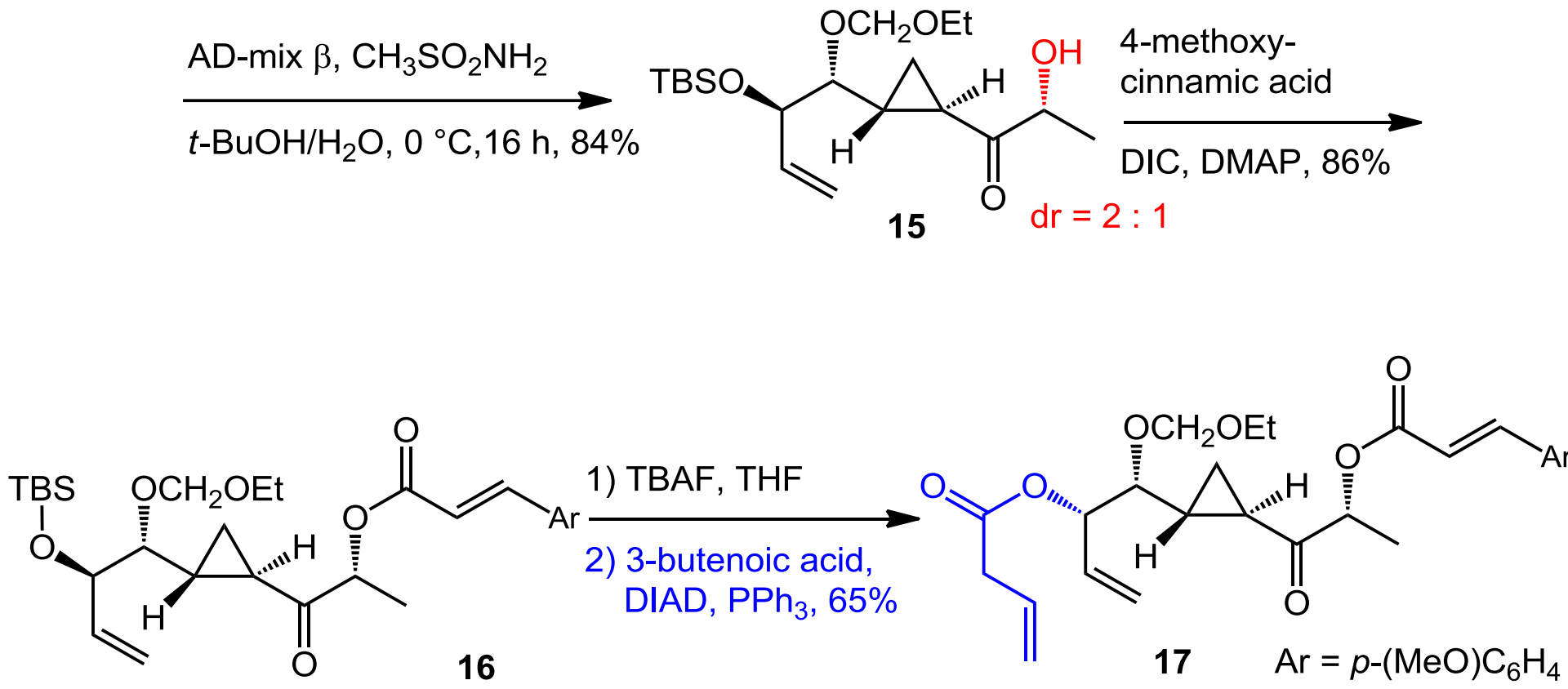
Brevipolides

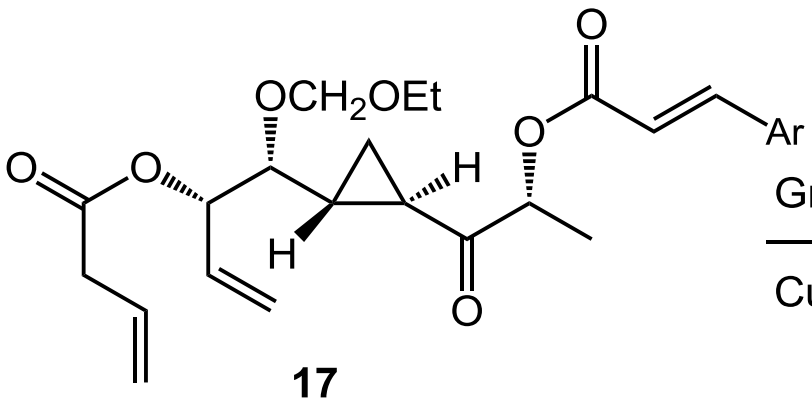


1. R = -CH_3
3. R = -H

http://taibnet.sinica.edu.tw/chi/taibnet_addpicture3.php?name_code=203489&id=9919


OH
HO
TBSCl,
imidazole,
76%
TBSO
ethyl vinyl ketone, CuI
Grubbs cat. II, Et2O, 78%
2
3
4
ClCH2OCH3
or ClCH2OEt
DIPEA
OR
Et
O
5a, R = CH2OCH3, 95%
5b, R = CH2OEt, 95%
RO
H
Me3S(O)I
NaH, DMF/THF
10a, R = CH2OCH3, 54%
10b, R = CH2OEt, 79%
TBSOTf, LHMDS
-78 °C, 1 h, 86%
OCH2OEt
OTBS
14
Z > 99%

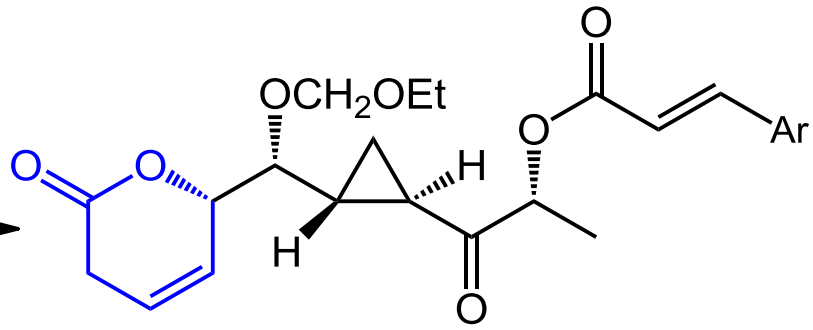

AD-mix β, CH3SO2NH2
t-BuOH/H2O, 0 °C,16 h, 84%
OCH2OEt
TBSO
OH
H
H
O
15
dr = 2 : 1
4-methoxy-
cinnamic acid
DIC, DMAP, 86%
TBS
O
OCH2OEt
H
O
O
Ar
16
1) TBAF, THF
2) 3-butenoic acid,
DIAD, PPh3, 65%
O
O
OCH2OEt
H
H
O
O
O
Ar
17
Ar = p-(MeO)C6H4



17

Grubbs cat. II

CuI, Et_2O, 88%

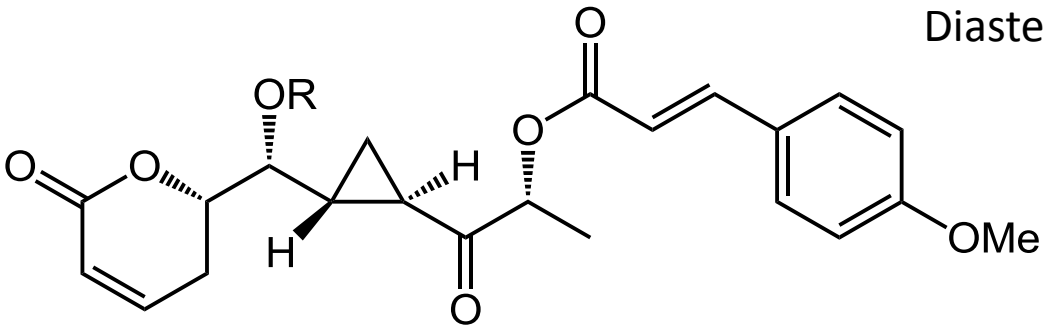


18 Ar = *p*-(MeO)C_6H_4

Diastereomers separated here.

DBU, CH_2Cl_2

0 °C, 97%



19, R = CH_2OEt

20, R = H, *ent*-**brevipolide H**

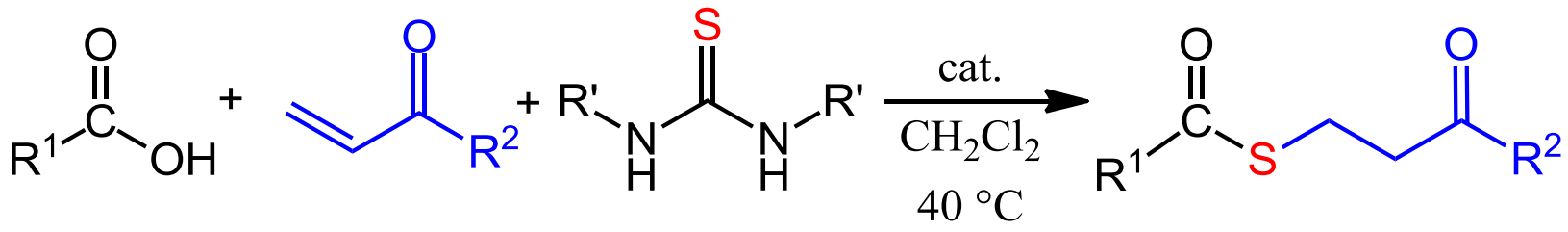
$HCl_{(aq)}$

THF, 95%

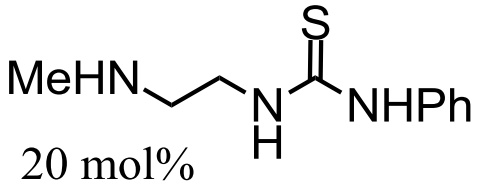
ent-Brevipolide H showed a comparable bioactivity (IC_{50}: **7.7** *versus* **13.5** µM of natural analogue, against the cell proliferation of human hormone-refractory prostate cancer cell line (PC-3).

Org. Lett. **2014**, *16*, 5328

意外的發現



R^1 = aryl alkyl　　R^2 = Et, Ph, OEt　　R' = Me, Ph



20 mol%

給學生的建議

- 對趨勢好奇
- 珍惜跨領域的機會
- 培養自己的思考能力

What we know? Why we know it?
Why should we care?

What? So what? Now what?

"**Research universities: in principle, the organizations with the greatest flexibility**. Universities should, ideally, lead in changing the structure of chemistry, not because they are more competent than industry or government, but because they are less constrained, and because one of their jobs is education, and education is the future."

"Many useful types of change would be (in principle) easily accomplished: combining different departments (chemistry, biochemistry, chemical engineering, materials science), broadening education, and changing the criteria for tenure to give credit for collaborative research are among them."

Angew. Chem. Int. Ed. **2015**, *54*, 3196.

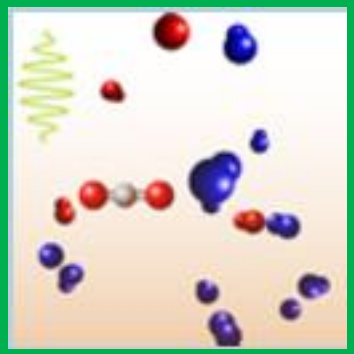
Context-Based Learning

Context-Based Learning

VC3 Visualizing the Chemistry of Climate Change

Welcome to the Visualizing the Chemistry of Climate Change (VC3) portal. Here you will find resources for teaching and learning 1st year chemistry through the rich context of climate science.

Isotope



Gases

Acid/Base

Thermo-chemistry

http://www.kcvs.ca/vc3/Lessons/

Context-Based Learning

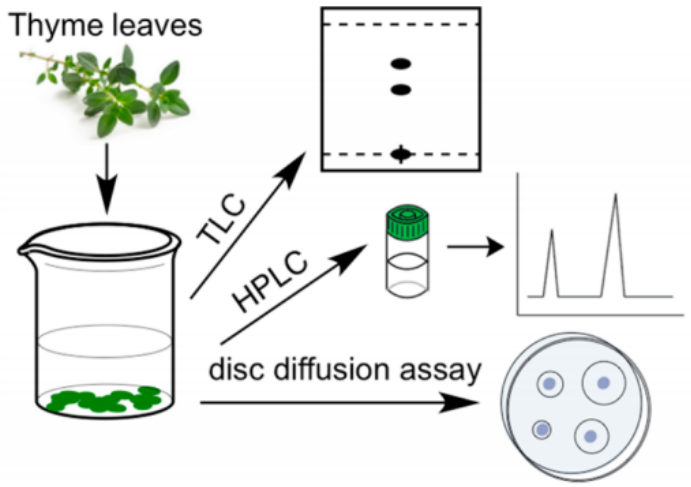
Extraction and Antibacterial Properties of Thyme Leaf Extracts: Authentic Practice of Green Chemistry

Sean C. Purcell, Prithvi Pande, Yingxin Lin, Ernesto J. Rivera, Latisha Paw U, Luisa M. Smallwood, Geri A. Kerstiens, Laura B. Armstrong, MaryAnn T. Robak, Anne M. Baranger, and Michelle C. Douskey*

Department of Chemistry, University of California, Berkeley, Berkeley, California 94720, United States

Supporting Information

ABSTRACT: In this undergraduate analytical chemistry experiment, students quantitatively assess the antibacterial activity of essential oils found in thyme leaves (*Thymus vulgaris*) in an authentic, research-like environment. This multiweek experiment aims to instill green chemistry principles as intrinsic to chemical problem solving. Students progress through various techniques including extraction, chromatography (TLC and HPLC), culturing bacteria, and disk diffusion via a process of guided exploration that emphasizes green experimental design. Approximately 600 undergraduate students carried out the experiment and self-reported substantial learning gains.



KEYWORDS: *First-Year Undergraduate/General, Green Chemistry, HPLC, Biochemistry, Laboratory Instruction, Inquiry-Based/Discovery Learning, Problem Solving/Decision Making, Natural Products, Quantitative Analysis, Thin Layer Chromatography*

J. Chem. Educ. **2016**, *93*, 1422

"Today, most students who want to change the world end up being activists. How many 18-year-olds who care about the planet say, 'I'm going to go be a chemist'? But now they can go to the lab and invent something that can save the world. "

by John Warner