



New Reaxys 2.0 User Training

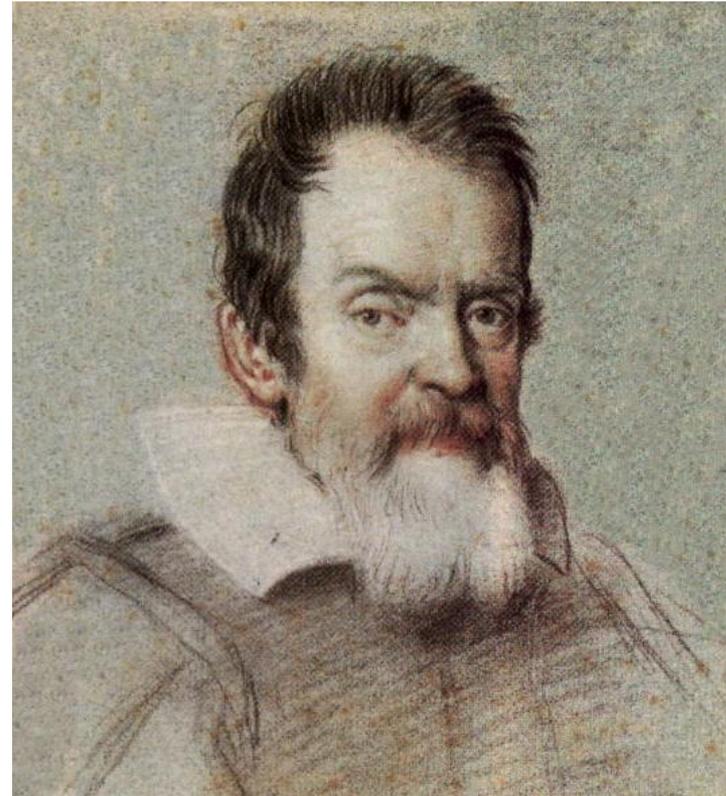
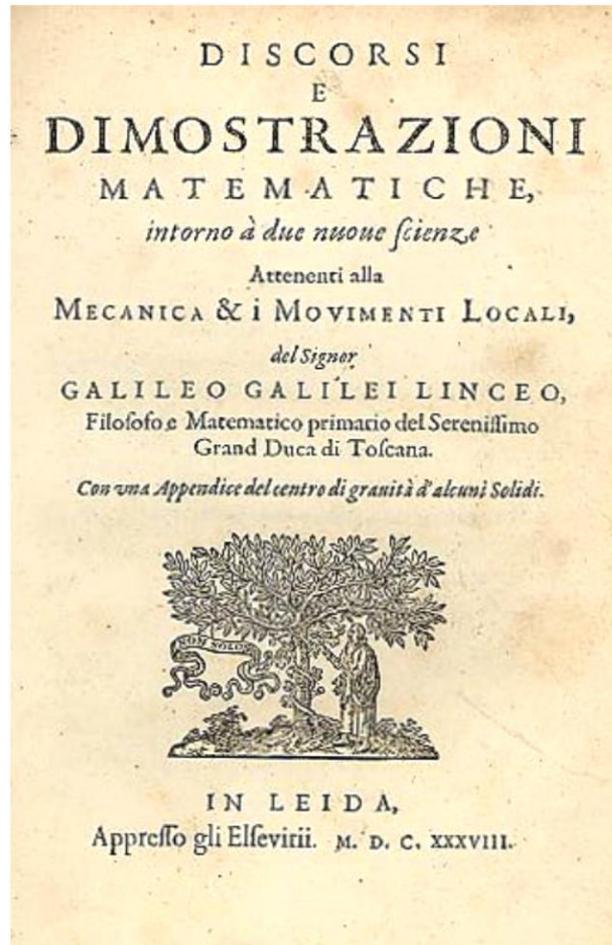
김세진 Customer Consultant, 엘스비어 한국지사,



ELSEVIER

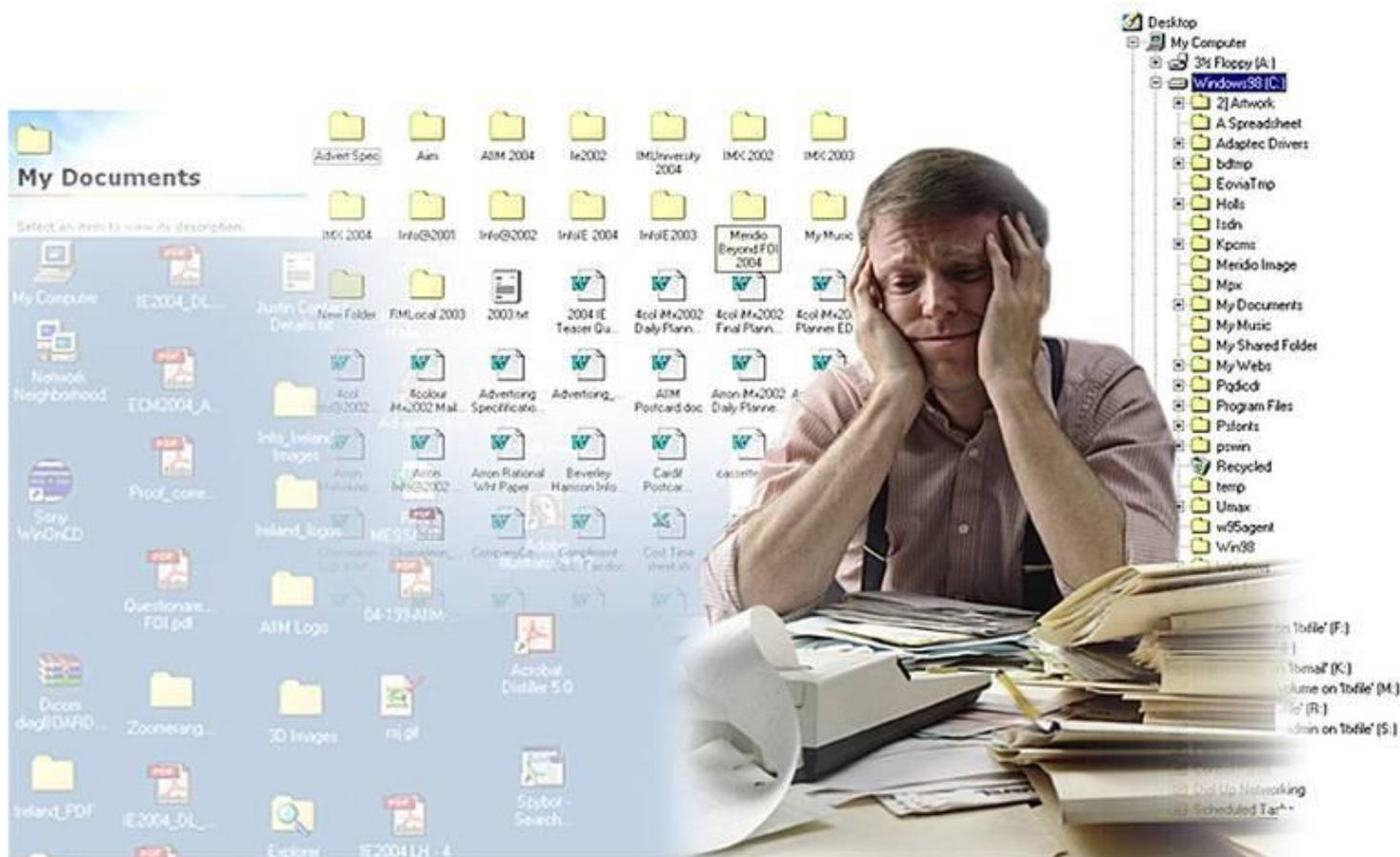
Elsevier B.V. (Dutch pronunciation: [ˈɛlzəviːr]) is an academic publishing company that publishes medical and scientific literature. It is a part of the Reed **Elsevier** group. Based in Amsterdam.

Founded	1880
Headquarters	Amsterdam , Netherlands (headquarters)



갈릴레오 갈릴레이도 엘스비어의 고객

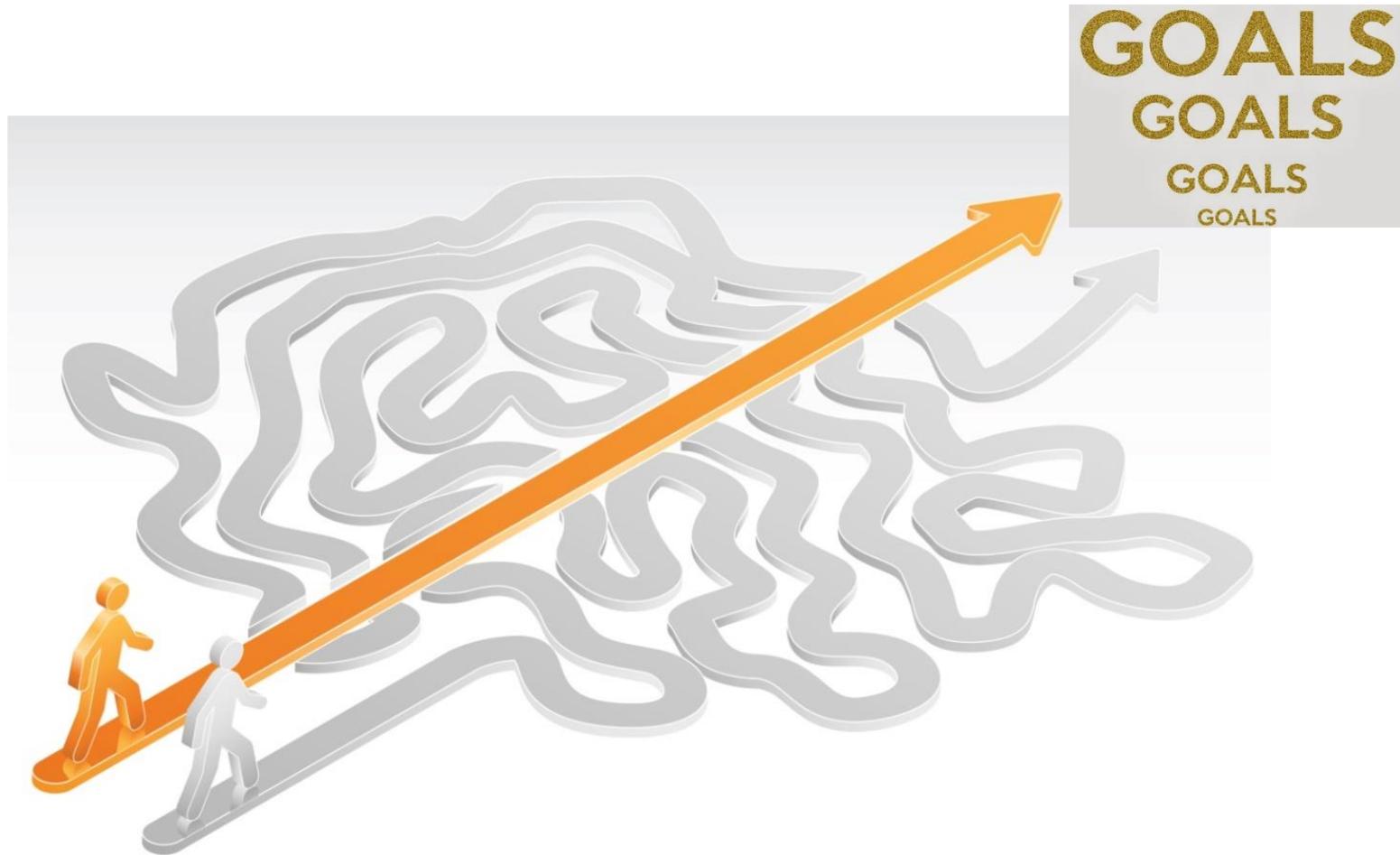
Information overload!



“Information that’s hard to find will remain information that’s hardly found”

– *Information Architecture Institute*

Right content, right time, right context



Elsevier Life Science Portfolios

Pathway Studio®

Reaxys Medicinal Chemistry

Reaxys®

PharmaPendium®

Embase®



Pathway Studio®



신약 개발 초기 단계의 질병경로를 확인할 수 있는 생물학적 Pathway 정보 제공
 새로운 질병 마커 식별, 분자간 상호 작용(Binding), 유전자 발견제어, 대사경로, 문헌
 중 생물학적 상호작용 정보, protein interaction maps, protein 과 물질의 상호작용
 정보를 맵으로 구현.

Reaxys®

Quick search Query builder Results Synthesis planner History

Search substances, reactions, documents and bioactivity data
 in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, LabNetwork and SigmaAldrich

Q Substance Properties, e.g. melting point of xylitol

AND

Create Structure or Reaction Drawing

신약 후보 물질에 대한 Validation & Evaluation

유기화학 및 반응 정보를 제공하는 Beilstein(발스타인)과 유기 금속 및 무기화합물 정보를 제공하는 Gmelin(그멜린)의 정보를 토대로 만들어진 세계 최대의 화학 부문 반응·화합물·문헌정보 데이터베이스.

유기화학을 비롯하여 무기화학, 유기금속, 착체 화학까지 폭넓게 정보 제공. 물질 합성 정보, 화학 관련 구조, 물리화학 정보, 분광학, 타겟에 따른 물질의 바이오 액티비티값, 생체 독성정보검색 가능.

Elsevier Life Science Portfolios

Pathway Studio®

Reaxys Medicinal Chemistry

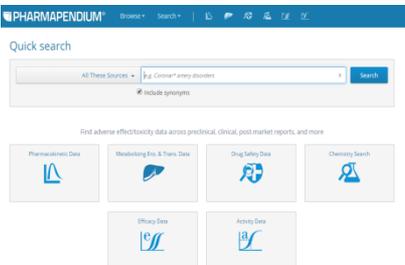
Reaxys®

PharmaPendium®

Embase®



PharmaPendium®

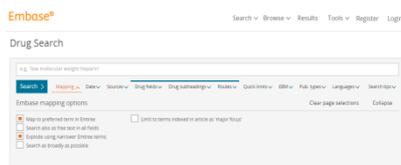


비임상 및 임상 분야 연구를 위한 FDA,EMA의 승인약물 자료

FDA와 EMA의 승인문서의 전문 검색이 가능하며, 독성, 부작용, 약물동태, 제형정보, 약효약리, 치료방법, 임상시험결과등의 정보 수집 가능.

또한 모든 자료를 인덱싱 하였으며, 비임상, 임상, 시판후로 구분하여 데이터 비교 한번에 확인 가능.

Embase®



Bio, Medical 분야 Drug 문헌 검색 DB

최신의 의학관련 저널에 대한 최대의 정보를 제공하며, 세계적인 의학 전문 학술지에 게재된 광범위하고, 신뢰할 수 있는 질병 및 의약품, 의료장비 관련 문헌 검색 기능을 제공하여, 의약품에 대한 최신 정보 및 시판후 사례에 대한 정보를 빠르게 수집 가능.

Reaxys 는 문헌을 검색 (Get), 검토(Read), 비교 (Compare) 하는 시간을 줄여줍니다.

WITHOUT Reaxys[®]

화학정보를
1차 검색 틀에서
검색한다면



문헌검색



문헌 검토



정보비교 검토



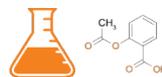
결과

WITH Reaxys[®]

화학정보를
Reaxys에서
검색한다면

→ Reaxys[®] →

문헌검색
구조 검색
데이터 검색



결과



Time saving

shortest path to answer



Technical requirements for Reaxys?

- Reaxys is a **Java-free application.**
- Mac and Windows 에서 이용 가능
- Firefox (version 49 or higher)
- **Chrome (version 53 or higher)**
- Edge (version 14 or higher)
- Safari (version 9)
- **Internet Explorer (version 11)**

사용자 개인 ID/PW 등록 안내

Reaxys[®][Quick search](#)[Query builder](#)[Results](#)[Synthesis planner](#)[History](#)[Sign in](#)

Sign in Institution sign in **Register**

Your IP: 198.176.85.34 ✕

Sign in

With your Reaxys Account

Username or Email

Password

Remember me on this computer

Sign in >

[Sign in via your institution](#)
[Forgot your password?](#)

Your IP: 198.176.85.34 ✕

Register

by registering your details on Reaxys you can log in and customize the user interface, **Create Alerts** and **Save Searches**. This will also give you a longer session timeout (6 hours compared to 30 minutes).

First Name Last Name

Username

Email address

Password

Confirm password

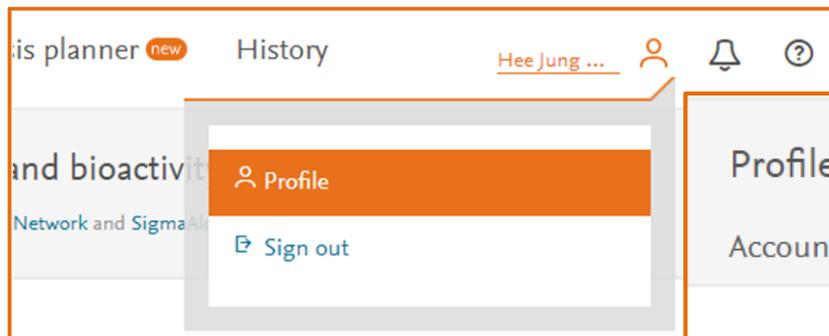
Stay informed about Elsevier products and services

I have read and agree to the [Registered User Agreement](#)

Register >

[Privacy Policy](#) [Terms and Conditions](#)

Quick Tip : 개인 로그인시, Profile을 통해 보여지는 화면 조정을 할 수 있습니다.



A screenshot of the Reaxys 'Profile' settings page. The page is titled 'Profile' and has three tabs: 'Account', 'Profile', and 'Preferences'. The 'Preferences' tab is selected. The page is divided into two main sections: 'Default structure/reaction editor settings' and 'Autoplan'.
Default structure/reaction editor settings
Search structure as: As drawn (with an edit icon)
Preferences: Include Stereo, Include Additional ring closures, Include Salts, Include Mixtures, Include Isotopes, Include Charges, Include Radicals (with an edit icon)
Autoplan
Default settings: Number of plans to create = 10, Max. alternative branches = 5, Max. number of steps = 5, Stop searching if starting material is commercially available (with an edit icon)



ELSEVIER

What's New Reaxys 2.0



Contents lists available at ScienceDirect

European Polymer Journal

journal homepage: www.elsevier.com/locate/europolj

Synthesis, drug release and targeting behaviors of Novel Folated Pluronic F87/poly(lactic acid) block copolymer



Xiang Yuan Xiong*, Xiang Qin, Zi Ling Li, Yan Chun Gong, Yu Ping Li

School of Life Science, Jangsi Science and Technology Normal University, Nanchang 330013, China

ARTICLE INFO

Article history:

Received 26 March 2015

Received in revised form 23 April 2015

Accepted 5 May 2015

Available online 6 May 2015

Keywords:

Targeted drug delivery

Folic acid

Pluronic

Poly(lactic acid)

Nanoparticle

ABSTRACT

Novel Folated Pluronic F87/poly(lactic acid) block copolymer (FA-F87-PLA) was synthesized by two step reactions. The self-assembling behavior of FA-F87-PLA block copolymer in aqueous solutions was examined by fluorescence measurement, Dynamic light Scattering (DLS) and Transmission Electron Microscopic (TEM) techniques. The morphology of FA-F87-PLA nanoparticles was found to be spherical micelles. Paclitaxel (PTX) loaded in FA-F87-PLA nanoparticles shows an initial burst release in the first 11 h and followed by a slow release. The in vitro targeting behavior of FA-F87-PLA nanoparticles against OVCAR-3 (folate receptor positive) was investigated by 3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT) tests. MTT results show that the anticancer effect of PTX in FA-F87-PLA nanoparticle over OVCAR-3 cells was stronger than that of PTX in non-targeted PLA-F87-PLA nanoparticle under the specific targeting interaction between folate groups on the surface of FA-F87-PLA nanoparticles and folate receptor on the surface of OVCAR-3 cells. The targeting behaviors of FA-F87-PLA nanoparticles were further confirmed by fluorescence microscopy (FM) technique. The intracellular distribution of FA-F87-PLA nanoparticles was also studied using a triple-labeling method. It was observed that FA-F87-PLA nanoparticles are mainly localized within the cytoplasm of OVCAR-3 cells.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

Amphiphilic block copolymers have been widely studied in the past few decades for their application in drug delivery systems because they are able to self-assemble into nanoparticles containing a hydrophobic core and a hydrophilic shell [1–5]. Hydrophobic poly(lactic acid) (PLA) are well-known biodegradable and biocompatible polyester [6–9]. Pluronic block copolymers are one of the very few synthetic polymeric materials approved by the U.S. Food and Drug Administration for use as food additives and pharmaceutical ingredients. The biocompatible amphiphilic block copolymers PLA-Pluronic-PLA have been synthesized previously and their application in drug delivery systems have been studied in detail by us [10–14].

There has always been a strong impetus to the development of polymeric nanoparticles with targeting ligands, which are able to increase the selectivity and efficiency of drug delivery to the target cells, leading to a better therapeutic efficacy as

2. Materials and methods

2.1. Materials

Pluronic F87 was kindly supplied by BASF Corporation. ϵ -lactide was purchased from Sigma-Aldrich and recrystallized twice from ethyl acetate (EtAc). The purified ϵ -lactide was stored at 4–5 °C under argon environment. Dichloromethane (CH_2Cl_2) and dimethyl sulfoxide (DMSO) was purified by distillation over CaH_2 . Folic acid (FA), stannous octoate [$\text{Sn}(\text{Oct})_2$] and sodium phosphotungstate were purchased from Sigma-Aldrich and used as received. Pyrene was purchased from Acros and used as received. N,N' -Dicyclohexylcarbodiimide (DCC), 4-Dimethylaminopyridine (DMAP) was purchased from J&K Chemica and used as received. Paclitaxel (PTX) was kindly supplied by Fujian South Pharmaceutical Co., Ltd. PTX injections was purchased from Sichuan Shenhe Pharmaceutical Co., Ltd. Tetramethylrhodamine-5-carbonyl azide (TMRC-A) was purchased from Invitrogen. 3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide (MTT) was purchased from Solarbio and used as received. Dulbecco's Modified Eagle's Medium (DMEM) was purchased from Gibco and used as received. All other chemicals were of reagent grade. Human ovarian cancer cells OVCAR-3 and human lung carcinoma cells A549 were purchased from CICAMS, Beijing.

2.2. Synthesis of FA-F87-OH

Pluronic F87 (20 g, 2.6 mmol) was dissolved in 100 mL of dry CH_2Cl_2 . A solution of FA (0.83 g, 1.9 mmol) and DMAP (0.19 g, 1.56 mmol) in anhydrous DMSO was then added to the reaction flask under stirring. After cooling of the above solution to 0 °C, DCC (0.36 g, 1.75 mmol) was added dropwise via a dropping funnel over 30 min and then the reaction was carried out for 48 h at room temperature. The reaction mixture was then extracted with 10% NaHCO_3 solution to remove unreacted FA. After this step, the organic phase was frozen overnight and the insoluble substances were removed by filtration. The organic solution was then precipitated twice in cold diethyl ether. The polymers were filtered and dried overnight under vacuum.

2.3. Synthesis of FA-F87-PLA block copolymer

PLA segment was attached to one end of Pluronic F87 by ring-opening polymerization to obtain FA-F87-PLA amphiphilic block copolymer. FA-F87-OH (2.5 g) was distilled by azeotropic distillation under argon. LA (2.5 g) was added at room temperature under argon and was followed by the addition of stannous octoate (about 0.1 wt% of LA). The mixture was stirred at 120 °C for 6 h. After cooling to room temperature, the reaction mixture was dissolved in CH_2Cl_2 and then precipitated into cold ethyl ether. Following this, the product was dissolved in methylene chloride, and precipitated in cold methanol. The white product was then filtered and dried overnight under vacuum.

2.4. Fluorescence measurements

The critical micellization concentration (CMC) of FA-F87-PLA nanoparticles in PBS solutions was determined by fluorescence measurements (HITACHI F2700) using pyrene as a fluorescence probe [27,28]. The pyrene stock solution in acetone (5 μl) was added into a series of test tubes respectively and the acetone was evaporated. Following this, the FA-F87-PLA solutions (5 mL) were added to each test tube and then sonicated for 2 h. The final concentration of pyrene in the solutions was 6×10^{-7} M. For the measurement of pyrene excitation spectra, the slit widths for both excitation and emission sides were maintained at 2.5 nm, and the emission wavelength used was 390 nm.

2.5. Preparation of PTX-loaded FA-F87-PLA and PTX free nanoparticles

FA-F87-PLA block copolymer (25 mg) and hydrophobic drug PTX (15 mg) were dissolved in DMSO (15 mL). The solution with polymer and PTX was added drop-wise to distilled water (90 g) under gentle stirring. The drug loaded polymer aggregates in water were centrifuged and the supernatant was dialyzed against distilled water using a dialysis membrane (molec-

3. Results and discussion

3.1. Synthesis and characterization of FA-F87-PLA block copolymer

FA-F87-PLA block copolymer was synthesized by two steps. Pluronic F87 block copolymer was firstly modified by folic acid to obtain FA-F87-OH. FA-F87-PLA block copolymer was then synthesized by ring opening polymerization of the monomer ϵ -lactide using FA-F87-OH as the initiator and stannous octoate [Sn(Oct)₂] as the catalyst (Scheme 1). The possible byproduct FA-F87-FA generated in the first step can be removed by methanol in the second step.

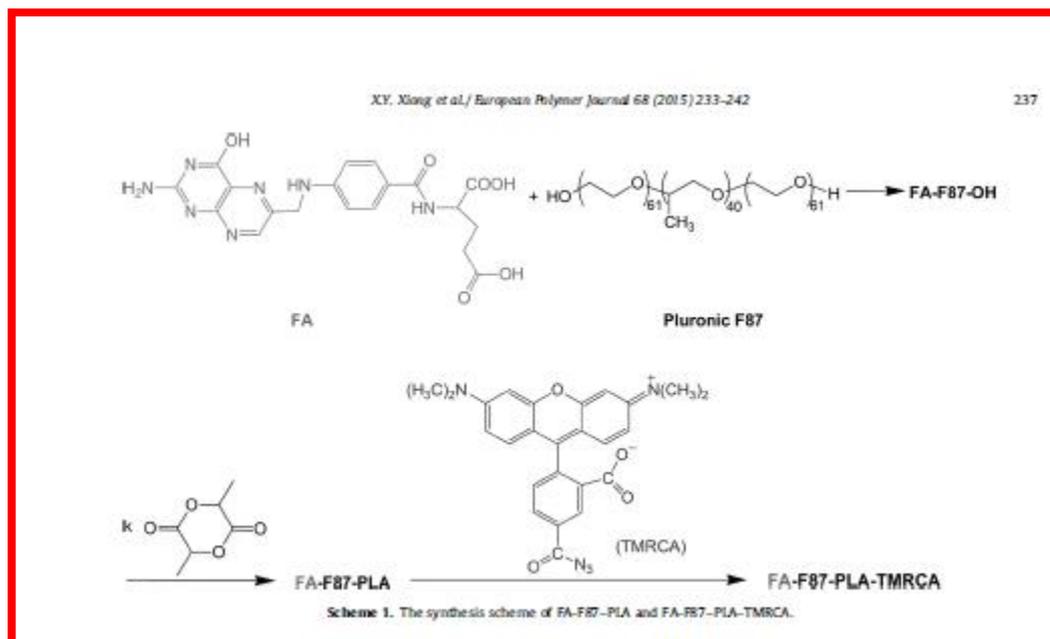
The polymer composition, structure and molecular weight were characterized by NMR and GPC techniques. Fig. 1(A) shows a ¹H NMR spectrum of FA-F87-PLA block copolymer in CDCl₃. ¹H NMR (400 MHz, CDCl₃, TMS), δ (ppm): 1.13–1.15 (m, -OCH₂-CH(CH₃)-), 1.41–1.75 (m, -O-CH(CH₃)-CO- and HO-CH(CH₃)-CO-), 3.40–3.65 (m, -OCH₂-CH₂- and -OCH₂-CH(CH₃)-), 4.3–4.4 (m, HO-CH(CH₃)-CO- and -CO-OCH₂-CH₂-O-), 5.13–5.18 (m, -O-CH(CH₃)-CO-). The small peak at δ of 4.35 ppm belongs to methylene protons of PLA-CO-OCH₂-CH₂-O-PEO- segment, indicating the successful synthesis of FA-F87-PLA block copolymer. The absence of a peak at δ of 4.9–5.0 ppm which could have been contributed by the methine proton of the PLA-O-CH(CH₃)-COOH group, suggests that there was negligible or no PLA homopolymer in the FA-F87-PLA block copolymer. The peaks belonging to FA group were hard to see in Fig. 1(A) due to the high molecular weight of FA-F87-PLA block copolymer.

The degree of polymerization (*n*) of PLA in FA-F87-PLA copolymer was calculated from the peak intensity ratio of methyl protons of PLA (O-CH(CH₃)-CO-; δ = 1.58 ppm) and methyl protons of Pluronic (-OCH₂-CH(CH₃)-; δ = 1.14 ppm). The number-average molecular weight (\overline{M}_n) of the FA-F87-PLA_k copolymer was obtained by using the following expression:

$$\overline{M}_n = \overline{M}_n(\text{F87}) + 72k + 423$$

The molecular weight of FA-F87-PLA copolymer was calculated to be 24,800 and the weight fraction of PLA block was calculated to be 67%.

The amount of -OH groups of FA-F87-PLA copolymer functionalized by FA was determined by UV-vis spectrum. It was shown in Fig. 1(B) that both characteristic peaks belonging to folate groups at 285 and 362 nm are all detected for FA-F87-



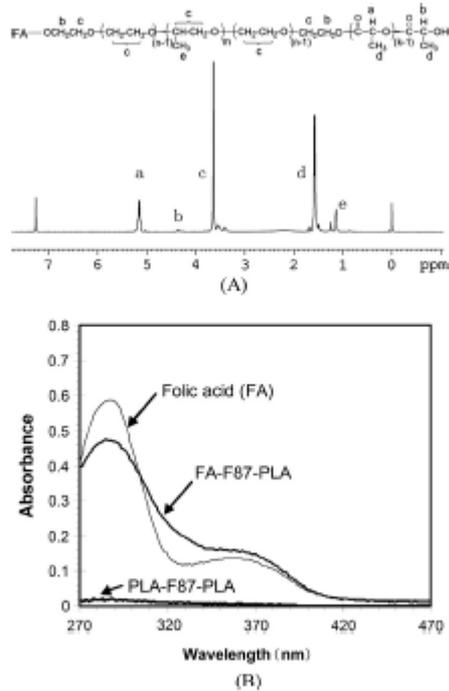


Fig. 1. (A) ¹H NMR spectra of FA-F87-PLA block copolymer (CDCl₃), (B) UV-vis spectra of FA-F87-PLA copolymer at

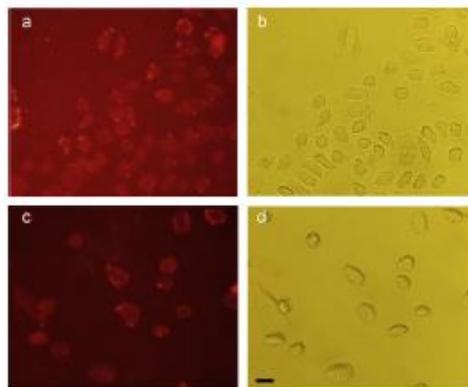
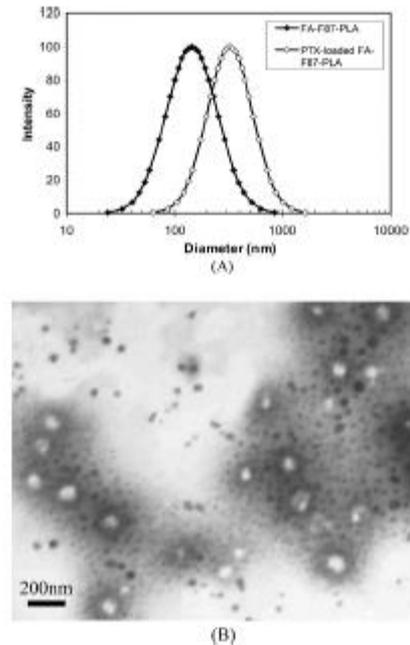


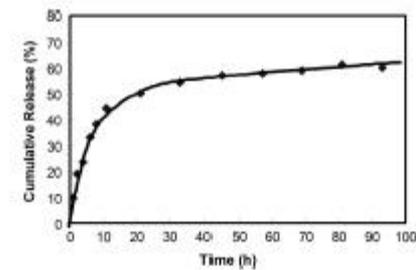
Fig. 6. Internalization of nanoparticles to cancer cells. Fluorescent images for two kinds of cells incubated with FA-F87-PLA-TMRCa nanoparticles. (a) nanoparticles incubated in OVCA8-3 cells for 2 h; (c) nanoparticles incubated in A549 cells for 2 h; (b) and (d) are the corresponding phase-contrast photographs of (a) and (c). Scale bar, 20 μm.

for imaging. The synthesis scheme is shown in Scheme 1. The acyl azide group of TMRCa was first rearranged into isocyanate. Then the hydroxyl end group in the PLA block of FA-F87-PLA reacted the isocyanate group to form a urethane [29,30,36].

X.Y. Xiang et al. / European Polymer Journal 68 (2015) 233–242



A) Size distributions for FA-F87-PLA and PTX-loaded FA-F87-PLA nanoparticles. (B) TEM picture of FA-F87-PLA nanoparticles.



4. Conclusions

In the present study, FA-Pluronic F87-PLA block copolymer was synthesized by two step reactions. The self-assembling behaviors of FA-F87-PLA block copolymer in aqueous solutions were examined. The CMC of FA-F87-PLA block copolymer is pretty low, indicating the good stability of FA-F87-PLA nanoparticles. The morphology of FA-F87-PLA nanoparticles is spherical micelles. The release of PTX loaded in FA-F87-PLA nanoparticles shows an initial burst release in the first 11 h and followed by a pretty slow release. The *in vitro* targeting properties of FA-F87-PLA nanoparticles over OVCAR-3 and A549 cancer cells were investigated by MTT assays and FM technique. Results from MTT tests show that FA-F87-PLA nanoparticles were delivered more effectively to OVCAR-3 cells (folate receptor positive) than PLA-F87-PLA nanoparticles did, indicating the targeting property of FA-F87-PLA nanoparticles. These results were confirmed by FM through labeling a dye to the PLA end of FA-F87-PLA block copolymers. The intracellular fate of FA-F87-PLA nanoparticles was also studied using a triple-labeling method by FM. It was observed that FA-F87-PLA-TMRCA nanoparticles are mainly localized within the cytoplasm of OVCAR-3 cells.

Acknowledgements

The authors would like to acknowledge the financial support from the National Natural Science Foundation of China (Nos. 21264009 and 31360376), the Natural Science Foundation of Jiangxi Province (No. 20132BAB206034), and the Scientific and Technological Landing Project of Higher Education of Jiangxi Province (No. KJLD13071).

References

- [1] Z.L. Tyrrell, Y.Q. Shen, M. Radosz, *Prog. Polym. Sci.* 35 (2010) 1128–1143.
- [2] G. Gaucher, R.H. Marchessault, J.C. Leiroux, *J. Control. Release* 143 (2010) 2–12.
- [3] J.H. Park, S. Lee, J.H. Kim, K. Park, K. Kim, I.C. Kwon, *Prog. Polym. Sci.* 33 (2008) 113–137.
- [4] E.M. Pridgen, R. Langer, O.C. Farokhzad, *Nanomedicine* 2 (2007) 669–680.
- [5] L.Y. Qiu, Y.H. Bae, *Pharm. Res.* 23 (2006) 1–30.
- [6] Y. Mi, J. Zhao, S.-S. Feng, *J. Control. Release* 169 (2013) 185–192.
- [7] Y. Mi, X. Liu, J. Zhao, J. Ding, S.-S. Feng, *Biomaterials* 33 (2012) 7519–7529.
- [8] R. Hashide, K. Yoshida, Y. Hasebe, S. Takahashi, K. Sato, J.-I. Anzai, *Colloid Surf. B* 89 (2012) 242–247.
- [9] Y.F. Tan, P. Chandrasekharan, D. Maitly, C.X. Yong, K.-H. Chuang, Y. Zhao, S. Wang, J. Ding, S.-S. Feng, *Biomaterials* 32 (2011) 2969–2978.
- [10] X.Y. Xiong, K.C. Tam, L.H. Gan, *J. Control. Release* 108 (2005) 269–270.
- [11] X.Y. Xiong, K.C. Tam, L.H. Gan, *J. Control. Release* 103 (2005) 73–82.
- [12] X.Y. Xiong, K.C. Tam, L.H. Gan, *Polymer* 46 (2005) 1841–1850.
- [13] X.Y. Xiong, K.C. Tam, L.H. Gan, *Macromolecules* 37 (2004) 3425–3430.

16k 저널/ 7개 특허 원문에서 정보 색인

- ✓ 실제 화합물
- ✓ 광범위한 반응정보
- ✓ 정확한 물질 정보와 연구 결과
- ✓ 광범위한 실험 데이터 및 결과

Scientific topic, author

Can be searched in full text, but difficult to find the right search term

Abstract

Dimers constituting differing porphyrin basicities undergo selective demetalation or protonation of one unit of the dimer. The efficiency of singlet excited energy transfer from neutral free-base/zinc(II) porphyrin to diprotonated porphyrin unit could be fine tuned by varying acidity in the covalently linked dimers. © 1998 Elsevier Science B.V. All rights reserved.

1. Introduction

Covalently linked porphyrin dimers have furnished important models to elucidate mechanisms of excitation energy transfer and photoinduced electron transfer in natural photosynthetic processes [1–8]. In addition, some of these models are potentially important materials for use in molecular-scale electronic devices [9–11]. Recently, a molecular optoelectronic gate consisting of an array of porphyrins has been reported [12]. Two basic photochemical properties have been exploited in the design of molecular devices, (i) singlet–singlet energy transfer and (ii) photoinduced electron transfer. We made use of the differential basicity of the inner imino nitrogens of the meso-fluoroarylporphyrin and meso-tetraarylporphyrin to construct simple dimeric porphyrins wherein absorption of a photon of visible light by a neutral porphyrin leads to an emission of a photon from diprotonated porphyrin with very high efficiency (> 95%). The occurrence of such processes can be easily tuned by the acidity of the medium, fundamentals of which could be used in the construction of artificial photonic devices.

The substitution of pentafluoroaryl groups in the meso positions of the porphyrin confers unique inertness of the inner imino nitrogens towards protonation and metallation reactions. The fluoroarylporphyrins exhibit interesting optical and electrochemical properties [13]. We synthesised porphyrin dimers (Fig. 1) comprising of meso-fluoroarylporphyrin and meso-tetraarylporphyrin with an ethylenedioic covalent bridge to accomplish selective protonation and demetalation of the meso-tetraarylporphyrin moiety in the dimer. We demonstrate here that the dicationic porphyrin dimer exhibits efficient intramolecular singlet excitation energy transfer (eet) from

* Corresponding author. Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India. E-mail: vkrishna@ipc.iisc.ernet.in

Chemical structure

Cannot be searched by text terms in full text

Chemical reactions

Cannot be searched by text terms in full text

Fig. 2. Schematic representation of different processes of dimer porphyrins.

Chemical spectra

Cannot be searched by text terms in full text

Fig. 3. The fluorescence emission spectra (λ_{exc} at 260 nm) of excited intermediates ZnF5-ZnH5 (1), ZnF5-H4+2H5 DM (2), and H2F6-H4+2H5 DM (3) in CH2Cl2. Inset shows the comparison of the corrected emission spectrum (solid line) and absorption spectrum (dotted line) of the (a) intermolecular mixture of ZnF5OCH3 and ZnH5OCH3, and (b) ZnF5-ZnH5 DM.

2. Experimental

Covalently linked porphyrin dimer was synthesised by the method of Little [14]. We have used 5-(4-methoxyphenyl)-10,15,20-triphenylporphyrin ($H_2H_5OCH_3$) and 5-(4-methoxyphenyl)-10,15,20-tri(pentafluoro)phenylporphyrin ($H_2F_6OCH_3$) as reference compounds for comparison studies. Hereafter these two porphyrins are referred to as meso-tetraarylporphyrin and meso-fluoroarylporphyrin, respectively.

Can be searched in full text, but you don't want to read the whole paper in you are interested only by this section!

Experimental procedures

Substances and their physicochemical properties

Compound	λ_{abs} (nm; log ϵ) ^a	λ_{em} (nm) ^b
$H_2F_6OCH_3$	415(5.45), 509(4.28), 543(3.60), 584(3.82), 640(3.23)	644, 707

Table 1
Optical

^a 1.1 (10⁻⁴ M/NaOAc, v/v).

^b 1.1 (10⁻⁴ M/NaOAc, v/v). λ_{exc} values were 303 and 580 nm for the free base porphyrin and free base dimer, respectively.

^c Electrochemical redox data of the porphyrins in CH2Cl2 solution containing 0.1 M TBAPF6. Potential values are referenced to internal Fc+/Fc couple. All the potentials observed involve one electron redox, reduction processes unless otherwise mentioned.

^d Presence of TFA acid.

^e Numbers in parentheses are electron transfer rates.

원문에서 발췌한 표준화되고, 잘 정리된 화학 데이터 제공

Arbutin *에* 관련된
1,588 문헌과 특허

arbutin
C₁₂H₁₆O₇ 272.255

Identification
Druglikeness

arbutin

^ Identification

Reaxys ID:	89673
Chemical Names:	arbutin, hydroquinone glucopyranoside, 4-hydroxyphenyl β-D-glucopyranoside
CAS Registry Number(s):	497-76-7
Molecular Formula:	C ₁₂ H ₁₆ O ₇
Molecular Weight:	272.255
InChIKey:	B1RNKVDFDLYUGJ-RM

^ Patent-Specific Data - 2

^ Related Structure - 2

^ Derivative - 3

^ Physical Data - 60

- ^ Melting Point - 19
- ^ Association (MCS) - 5
- ^ Chromatographic Data - 5
- ^ Crystal Property Description - 3
- ^ Dissociation Exponent - 1
- ^ Electrochemical Behaviour - 1
- ^ Electrochemical Characteristics - 1
- ^ Further Information - 2
- ^ Liquid/Liquid Systems (MCS) - 5
- ^ Liquid/Solid Systems (MCS) - 1
- ^ Magnetic Susceptibility - 1
- ^ Optical Rotatory Power - 13
- ^ Partition octan-1-ol/water (MCS) - 1
- ^ Solubility (MCS) - 1
- ^ Transport Phenomena (MCS) - 1

^ Other Data - 299

- ^ Biodegradation - 1
- ^ Use - 222
- ^ Isolation from Natural Product - 76

^ Bioactivity (All)

- ^ In vitro: Efficacy - 481
- ^ In vivo: Animal Model - 13
- ^ Metabolism - 3
- ^ Toxicity/Safety Pharmacology - 68

^ Spectra - 112

- ^ NMR Spectroscopy - 52
- ^ IR Spectroscopy - 6
- ^ Mass Spectrometry - 24
- ^ UV/VIS Spectroscopy - 28
- ^ Fluorescence Spectroscopy - 2

All relevant data are accessible for a common point and tabulated for direct use.

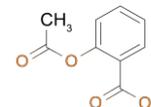
2018 Reaxys 2.0 콘텐츠



문헌서지·특허

>53.5 million records
(from ~16,000 journal titles plus records
from key patent organisations)

화합물정보



> 105 million substances (total)
~ 87 million substances (unique) (from
~13,000 journal titles plus
records from key patent organisations)

Reaxys
2018



화학반응

> 43.5 million single- and multi-
step reactions

물성



> 500 million experimental properties
in > 500 fields in > 130 subject areas

Quick Search (간편검색)



1) 검색 모드
간편/ 고급 검색

Reaxys®

Quick search Query builder Results Synthesis planner History

Markus Bussen

Search substances, reactions, citations and bioactivity data

Reaxys

2) 텍스트 입력/물성 (properties)

예) CAS#, melting point, density, Enthalpy of Formation, concepts

3) 구조 검색

Substance CAS Registry Number, e.g. 102625-70-7

AND

Create Structure or Reaction Drawing

> 95% user
→ Keyword + Structure

Query Builder – 고급 통합검색

Find more specific answer by combined multi fields

The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, Query builder (selected), Results, Synthesis planner, and History. A 'Sign in' button is in the top right. Below the navigation, there is a search bar with a dropdown menu currently set to 'Search Substances'. To the left of the search bar are icons for Import, Save, Reset form, and Delete. Below the search bar, there are four search field options: Structure, Molecular Formula, CAS RN, and Doc. Index. A large central area contains the text 'Drag & Drop to build a new query'. On the right side, there is a 'Search properties' section with tabs for Fields, Forms, and History. Below these tabs is a list of search sources: Reaxys, PubChem, eMolecules, and LabNetwork. At the bottom right, there is a 'Feedback' button.

Annotation 1: 검색 (Search) - points to the search bar.

Annotation 2: > 400여 검색 창 (More than 400 search windows) - points to the search bar dropdown.

Annotation 3: 가장 자주 이용되는 검색 창 (Most frequently used search window) - points to the search field options.

Annotation 4: FIELD : 범주 별로 모든 필드를 검색 (FIELD: Search all fields by category), FORMS : 자주 사용되는 필드 (FORMS: Frequently used fields), HISTORY: 검색 기록 (HISTORY: Search history) - points to the search properties tabs.

Part1. 문헌, 특허, 연구동향검색

문헌 내 색인용어 (Index term)

특허 문헌 내 정보 둘러보기 – Abstract 확인, 원문바로보기 링크

문헌/특허 내 물질, 반응 바로 확인하기

문헌을 검색할 때는?

Query Builder – 고급 통합검색 활용 할 것!

- 자동 완성 기능
- 유사 검색어 추가 용이
- 단어 조합 용이

Non-small Cell lung cancer, EGFR inhibitor

◇ Document Basic Index ×

is ▼ Document Basic Index
non-small cell lung cancer;non-small cell lung cancer (nsc 🔍

AND

◇ Document Basic Index ×

is ▼ Document Basic Index
egfr inhibitors;egfr inhibitor 🔍

6,615 Documents with 8,351 Substances, 18,025 Reactions, 1,482 Targets

결과에서 저널/ 특허 문헌 by publication type, by journal title

Document Type		Count
<input type="checkbox"/> article	4,207	
<input type="checkbox"/> review	1,572	
<input type="checkbox"/> conference paper	121	
<input type="checkbox"/> note	73	
<input type="checkbox"/> short survey	61	
<input type="checkbox"/> letter	55	
<input type="checkbox"/> editorial	51	
<input type="checkbox"/> patent	24	
<input type="checkbox"/> erratum	9	
<input type="checkbox"/> article in press	7	
<input type="checkbox"/> book	2	
<input type="checkbox"/> retracted article	1	
<input type="checkbox"/> chapter	1	
<input type="checkbox"/> book review / secondary ref.	1	

Journal Title		Count
<input type="checkbox"/> lung cancer	298	
<input type="checkbox"/> journal of thoracic ...	218	
<input type="checkbox"/> clinical cancer rese...	160	
<input type="checkbox"/> oncotarget	147	
<input type="checkbox"/> chinese journal of l...	140	
<input type="checkbox"/> plos one	135	
<input type="checkbox"/> clinical lung cancer	113	
<input type="checkbox"/> cancer research	96	
<input type="checkbox"/> journal of clinical o...	87	
<input type="checkbox"/> cancer chemothera...	69	
<input type="checkbox"/> anticancer research	69	
<input type="checkbox"/> molecular cancer t...	68	
<input type="checkbox"/> annals of oncology	56	
<input type="checkbox"/> oncology reports	54	
<input type="checkbox"/> british journal of ca...	54	
<input type="checkbox"/> translational lung c...	53	
<input type="checkbox"/> oncotargets and th...	51	
<input type="checkbox"/> the lancet oncology	50	
<input type="checkbox"/> oncologist	49	
<input type="checkbox"/> oncogene	49	

나의 논문을 발표할 상위 저널에 대한 정보를 얻을 수 있어요.

결과에서 연도별, 최신 연구키워드, 추가 연구동향 확인

Publication Year ^

<input type="checkbox"/> 2015	803
<input type="checkbox"/> 2014	745
<input type="checkbox"/> 2016	703
<input type="checkbox"/> 2017	112

Index Terms (List) Clear selected x ↓ ↑ Sort by Occurrence v x

<input type="checkbox"/> protein tyrosine kin...	877	<input type="checkbox"/> maximum tolerate...	50	<input type="checkbox"/> ablation	28
<input type="checkbox"/> toxicity	283	<input type="checkbox"/> magnetic resonance	48	<input type="checkbox"/> hydrogen bond	27
<input type="checkbox"/> phosphorylation	222	<input type="checkbox"/> growth factor	45	<input type="checkbox"/> pharmacological pr...	26
<input type="checkbox"/> phosphotransferas...	147	<input type="checkbox"/> drug	45	<input type="checkbox"/> hydrophobic surface	26
<input type="checkbox"/> chain reaction	131	<input type="checkbox"/> adjuvant	39	<input type="checkbox"/> dimerization	26
<input type="checkbox"/> fluorescence	126	<input type="checkbox"/> plasma concentrati...	38	<input type="checkbox"/> separation method	24
<input type="checkbox"/> ic50	124	<input type="checkbox"/> area under the curve	32	<input type="checkbox"/> clearance	24
<input type="checkbox"/> biological marker	90	<input type="checkbox"/> steric hindrance	30	<input type="checkbox"/> heat shock protein ...	21
<input type="checkbox"/> antineoplastic agent	66	<input type="checkbox"/> crystal structure	30	<input type="checkbox"/> reaction kinetics	20
<input type="checkbox"/> pharmacokinetics	62	<input type="checkbox"/> permeability	28	<input type="checkbox"/> methylation	19

JAK2 inhibition sensitizes kinase inhibitors
 2 Gao, Sizhi P.; Chang, Qing; Mao, N

Abstract v Index Terms ^ Substances v Full Text ↗

Index terms

EMTREE drug term: 5 chloro n2 [1 (5 fluoro 2 pyrimidinyl) growth factor receptor, erlotinib, gefitinib, Janus kinase 2, pyrimidinyl]oxy]phenyl]acrylamide, STAT3 protein, suppressor of cytokine signaling

EMTREE medical term: animal cell, Article, cell growth, controlled study, drug potentiation, enzyme inhibition, IC50, immunohistochemistry, in vitro study, in vivo study, lung adenocarcinoma, lung cancer cell line, mouse, non small cell lung cancer, nonhuman, priority journal, signal transduction, tumor volume, Western blotting, wild typ

Reaxys Index Terms: heterodimerization, protein tyrosine kinase inhibitor

분야별로 원문에 많이 사용된 용어들을 참고하여 키워드를 추가로 검색을 진행할 수 있고, 최신연구 관련 동향 정보 수집에도 활용할 수 있습니다.

Abstract 확인, 원문보기 링크

A decade of EGFR inhibition in EGFR-mutated non small cell lung cancer (NSCLC): Old successes and future perspectives Cited 35 times

Russo, Alessandro; Franchina, Tindara; Ricciardi, Giuseppina Rosaria Rita; +6 others - Oncotarget, 2015, vol. 6, # 29, p. 26814 - 26825

Abstract Index Terms Substances Full Text

Abstract

The discovery of Epidermal Growth Factor Receptor (EGFR) mutations launched the era of personalized medicine in advanced NSCLC, leading to a dramatic shift in the therapeutic landscape of this disease. After ten years from the individuation of a domain of the EGFR in NSCLC patients responding to the EGFR tyrosine kinase inhibitor (TKI) Gefitinib, several progresses have been done and first line treatment with EGFR TKIs is a firmly established option in advanced EGFR-mutated NSCLC patients. During the last decade, different EGFR TKIs have been approved so far in these selected patients. However, despite great breakthroughs have been made, treatment of these molecularly selected patients poses novel therapeutic challenges, such as emerging of acquired resistance, brain metastases development or the need to translate these treatments in earlier clinical settings, such as adjuvant therapy. The aim of this paper is to provide a comprehensive review of the major progresses reported so far in the EGFR inhibition in this molecularly-selected subgroup of NSCLC patients, from the early successes with first generation EGFR TKIs, Erlotinib and Gefitinib, to the novel irreversible and mutant-selective inhibitors and ultimately the emerging challenges that we, in the next future, are called to deal with.

Online ISSN: 1949-2553

Oncotarget

Reviews:

A decade of EGFR inhibition in EGFR-mutated non small cell lung cancer (NSCLC): Old successes and future perspectives

[PDF](#) | [HTML](#) | [Order a Reprint](#)

Oncotarget. 2015; 6:26814-26825. doi: 10.18632/oncotarget.4254

Metrics: PDF **1189 views** | HTML **644 views**

Alessandro Russo¹, Tindara Franchina¹, Giuseppina Rosaria Rita Ricciardi¹, Antonio Picone¹, Giuseppa Ferraro¹, Mariangela Zanghi², Giuseppe Toscano¹, Antonio Giordano², Vincenzo Adamo¹

¹Medical Oncology Unit AOOR Papardo-Piemonte & Department of Human Pathology, University of Messina, Messina, Italy
²Sbarro Institute for Cancer Research and Molecular Medicine, Center for Biotechnology, Temple University, Philadelphia, Pennsylvania, USA

Correspondence to:
 Vincenzo Adamo, e-mail: vadam@unime.it

Keywords: *EGFR mutations, third generation EGFR TKIs, non small cell lung cancer, tyrosine kinase inhibitors, targeted therapy*

Received: **April 25, 2015** Accepted: **June 01, 2015** Published: **June 12, 2015**

ABSTRACT

The discovery of Epidermal Growth Factor Receptor (EGFR) mutations in Non Small Cell Lung Cancer (NSCLC) launched the era of personalized medicine in advanced NSCLC, leading to a dramatic shift in the therapeutic landscape of this disease. After ten years from the individuation of activating mutations in the tyrosine kinase domain of the EGFR in NSCLC patients responding to the EGFR tyrosine kinase inhibitor (TKI) Gefitinib, several progresses have been done and first line treatment with EGFR TKIs is a firmly established option in advanced EGFR-mutated NSCLC patients. During the last decade, different EGFR TKIs have been approved and three inhibitors have been approved so far in these selected patients. However, despite great breakthroughs have been made, treatment of these molecularly selected patients poses novel therapeutic challenges, such as emerging of acquired resistance, brain metastases development or the need to translate these treatments in earlier clinical settings, such as adjuvant therapy. The aim of this paper is to provide a comprehensive review of the major progresses reported so far in the EGFR inhibition in this molecularly-selected subgroup of NSCLC patients, from the early successes with first generation EGFR TKIs, Erlotinib and Gefitinib, to the novel irreversible and mutant-selective inhibitors and ultimately the emerging challenges that we, in the next future, are called to deal with.

문헌 내의 물질, 반응정보 확인하기

원문 내의 반응이나 물질정보 바로 보기로 원문을 확인하기 전에 화학정보 확인이 용인합니다.

□ A decade of EGFR inhibition in EGFR-mutated non small cell lung cancer (NSCLC): Old successes and future perspectives Cited 35 times
 5 [Russo, Alessandro; Franchina, Tindara; Ricciardi, Giuseppina Rosaria Rita; +6 others](#) - *Oncotarget*, 2015, vol. 6, # 29, p. 26814 - 26825

Abstract ▾ Index Terms ▾

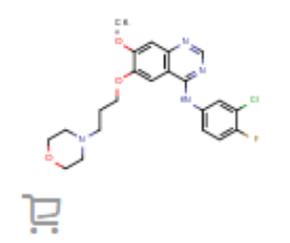
Substances ▲

Options ×

- > Find Similar
- > View details
- > Copy structure to query

물질정보로 이동
 물질구조- 구조검색으로
 바로 붙이기

Substances

	erlotinib	epidermal growth factor receptor
--	-----------	----------------------------------

Synthesize >

합성하기로
 바로 가기

특허문헌 정보 둘러보기

Publication Year	▼
Document Type	▲
<input type="checkbox"/> patent	24

비 영어권 (한국어, 유럽, 일본, 중국, 대만)
특허에 대해 번역 색인된 특허 현황 확인가능,
원문으로 링크

5 COMBINATION THERAPY FOR NON-SMALL CELL LUNG CANCER POSITIVE FOR EGFR MUTATION

MEDIMMUNE LIMITED; DAR, Mohammed, M; KARAKUNNEL, Joyson, J; [+2 others](#) - WO2016/170157, 2016, A1
Patent Family Members: WO2016/170157 A1

[Abstract](#) ▲ [Front Page Info](#) ▼ [Substances](#) ▼ [Full Text](#) ↗

Abstract

The present invention features methods of treating lung cancer (e.g., NSCLC) with an anti-PD-L1 antibody and a tyrosine kinase inhibitor in a subject identified as having an EGFR mutation-positive tumor.

특허문헌 – 특허현황정보(Front page info)

Publication Year ▼

Document Type ▲

patent 24

Front page info			Inventors (Authors)		
Assignees			Inventors (Authors)		
ISOFOL MEDICAL AB; GUSTAVSSON, Bengt; CARLSSON, Björn			GUSTAVSSON, Bengt; CARLSSON, Björn		
Patent No	Kind Code	Publ. Date	Application No	Filing Date	Indexed Patent
EP2617421	A1	2013/07/24	EP2012-151993	2012/01/20	
WO2013/107883	A1	2013/07/25	WO2013-EP50973	2013/01/18	yes
CA2860889	A1	2013/07/25	CA2860889	2013/01/18	

청구항, 특허 Application, 패밀리특허 확인

Priority No	Priority Date
EP2012-151993	2012/01/20
EP2012-15199	2012/01/20

Patent Classification	
Main IPC	A61K 31/519
Secondary IPC	A61K 39/395; A61K 45/06; A61P 35/00

특허문헌 -특허 내 물질정보확인

Publication Year ▼

Document Type ▲

patent ▬ 24

5 COMBINATION THERAPY FOR NON-SMALL CELL LUNG CANCER POSITIVE FOR EGFR MUTATION

MEDIMMUNE LIMITED; DAR, Mohammed, M; KARAKUNNEL, Joyson, J; [+2 others](#) - WO2016/170157, 2016, A1

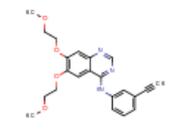
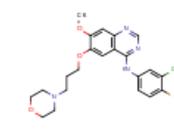
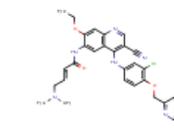
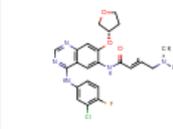
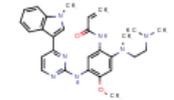
Patent Family Members: WO2016/170157 A1

Abstract ▲ Front Page Info ▼ **Substances ▼** Full Text ➤

Abstract

The present invention features a combination of a tyrosine kinase inhibitor in a sub

Substances

			
	anti-PD-L1 antibody BMS-936559	anti-PD-L1 antibody MEDI4736	anti-PD-L1 antibody MPDL3280A

특허 원문 내 물질의 원문 페이지 정보 표시

non-small cell lung cancer (NSCLC)

Page/Page column title page; 30-33

MEDIMMUNE LIMITED; DAR, Mohammed, M; KARAKUNNEL, Joyson, J; [+2 others](#) - WO2016/170157, 2016, A1

Full Text ➤ Show details >

원문보기

특허 원문보기

COMBINATION THERAPY FOR NON-SMALL CELL LUNG CANCER POSITIVE FOR EGFR MUTATION

MEDIMMUNE LIMITED; DAR, Mohammed, M; KARAKUNNEL, Joyson, J; [+2 others](#) - WO2016/170157, 2016, A1

Patent Family Members: WO2016/170157 A1

Abstract ^ Front Page Info v Substances v **Full Text ↗ 원문보기 클릭**

<p>non-small cell lung cancer (NSCLC)</p> <p>특허 원문 내 물질의 원문 페이지 정보 표시</p>	<p>Page/Page column title page; 30-33</p> <p>원문보기 클릭</p>	<p>MEDIMMUNE LIMITED; DAR, Mohammed, M; KARAKUNNEL, Joyson, J; +2 others - WO2016/170157, 2016, A1</p> <p>Full Text ↗ Show details ></p>
--	---	--

<p>Pharmaceuticals</p>	<p>Page/Page column title page</p> <ul style="list-style-type: none"> WO2016170157 (A1) Bibliographic data Description Claims Mosaics Original document Cited documents Citing documents INPADOC legal status INPADOC patent family
------------------------	--

The following document

Patent Number	WO2016/170157
Patent Kind Code	A1
Publication Date	2016

can be obtained from:

Espacenet 원문보기 클릭

Please click the hyperlink of the preferred vendor to get the p

Original document: WO2016170157 (A1) — 2016-10-27

★ In my patents list EP Register Report data error Print

COMBINATION THERAPY FOR NON-SMALL CELL LUNG CANCER POSITIVE FOR EGFR MUTATION

Page 1/38 Abstract Bibliography Maximise Download

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)
 (19) World Intellectual Property Organization
 International Bureau

(43) International Publication Date
 27 October 2016 (27.10.2016) **WIPO | PCT**

(10) International Publication Number
WO 2016/170157 A1

(51) International Patent Classification:
 A61K 39/395 (2006.01) A61P 35/00 (2006.01)
 A61K 31/517 (2006.01)

(74) Agent: WINTER, CHRISTOPHER, SPENCER;
 MEDIMMUNE LIMITED, Milstein Building, Granta Park, Cambridge Cambridgeshire CB21 6GH (GB).

(21) International Application Number:
 PCT/EP2016/059083

(22) International Filing Date:
 22 April 2016 (22.04.2016)

(25) Filing Language:
 English

(26) Publication Language:
 English

(30) Priority Data:
 62/151.739 23 April 2015 (23.04.2015) US

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JP, KE, KG, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN,

문헌찾기

대두(Soybean) 의 알려진 성분(Phytochemical) 에 관련된 문헌을 찾고 싶습니다.

Query builder로 단어 조합으로 문헌을 찾아보시고 몇 개의 문헌이 나오는지

말해주세요.

Part2. 물질 검색

물질의 물성데이터 확인 (실험측정데이터, USE/ Application, 스펙트라 정보 등)
물질의 구매여부 확인
물질의 합성법 바로보기

※ Unknown compound 검색하기 / 특정물성을 가진 물질 찾기

※ Functional group의 종류와 위치의 변화의 따른 물성 변화 검색

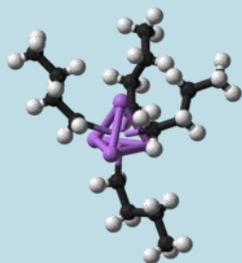
화합물 클래스

REAXYS SUBSTANCE RECORDS 에서 검색

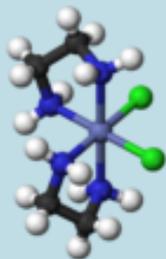
REAXYS 서지 레코드의 키워드 검색



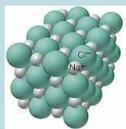
CLASSIC ORGANICS



ORGANOMETALLICS
COORDINATION
COMPOUNDS



CLASSIC
INORGANICS

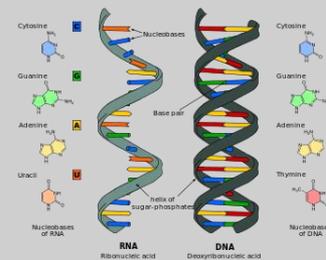
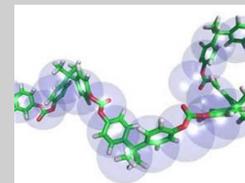


ALLOYS & METALS

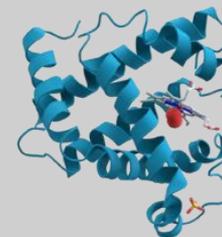
CERAMICS



POLYMERS



NUCLEIC ACIDS &
PROTEINS



물질/반응 검색을 통해 검색
(Search Substances)

문헌검색을 통해 검색
Search Literature

Query Builder 활용- Unknown compound/ 특정물성 화합물 찾기

“Identify an unknown antimicrobial compound isolated from a natural product. Experimental results indicate that the substance has 30 carbon atoms and an optical rotation of 75-85°.”

①

Molecular Formula

eg. C₆H₅COOH
C₃₀*

Look up

②

Optical Rotatory Power

is Type (Optical Rotatory Power)

is Concentration (Optical Rotatory Power)

= Length of Path, cm

is Solvent (Optical Rotatory Power)

= Optical Rotatory Power, deg
75-85

= Wavelength (Optical Rotatory Power), nm

= Temperature (Optical Rotatory Power), °C

③

Effect (PharmData)

is Effect (PharmData)
antimicrobial;antimicrobial activity

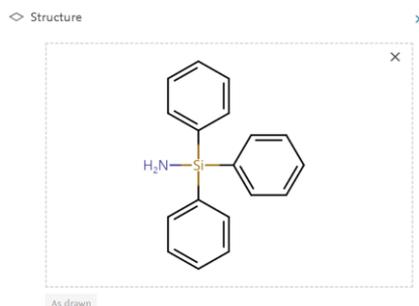
④

Available data 1

<input type="checkbox"/>	Pharmacological Data	4
<input type="checkbox"/>	Mass Spectrometry	4
<input type="checkbox"/>	IR Spectroscopy	4
<input type="checkbox"/>	NMR Spectroscopy	4
<input type="checkbox"/>	Optical Rotatory Power	4
<input type="checkbox"/>	Melting Point	4
<input checked="" type="checkbox"/>	Isolation from Natural Product	4

물질 검색을 위한 다양한 검색 창

1 Structure 구조검색



2 Mol. Formula

Molecular Formula search interface showing the input 'is' and the resulting formula C[10-18]H[10-17]*Si*N.

OR

Chemical Name search interface showing the input 'is' and the resulting name TPSA.

3 Chemical Nam

4 Keyword

Plus Many More!

- NMR Spectroscopy
- IR Spectroscopy
- Mass Spectrometry
- UV/VIS Spectroscopy
- Raman Spectroscopy
- ESR Spectroscopy
- NQR Spectroscopy
- Rotational Spectroscopy
- Luminescence Spectroscopy
- Fluorescence Spectroscopy
- Phosphorescence Spectroscopy
- Other Spectroscopic Methods

Query builder를 활용한 여러 조건 통합검색- 용매 찾기

☰ Substance Basic Index 🗑️

is 🔍

AND

☰ Boiling Point Exist 🗑️

= 🔍

= 🔍

AND

☰ Structure

As drawn

실습

Part 3. 반응 검색

반응검색 입력

반응검색 필터 활용하기 (수득율, 시약, 촉매, 용매, 문헌종류, 1-step/ multi-step 반응 등)

반응실험과정 참고하기

Synthesis planner 에서 반응식 직접 설계하기

※ 생성물/반응물로 검색이 안될 때 – 반응정보 확인하는 법

Marvin JS 를 얼마나 잘 활용하는가?

Reaxys® New Features[Quick search](#) [Query builder](#) [Results](#) [Synthesis planner](#) [History](#)

Structure editor

Create structure template from name >

Search this structure as:

- As drawn
- As substructure
- Similar

- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

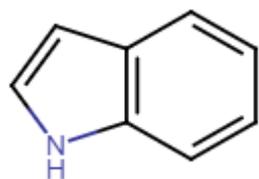
[+ More options](#)

Marvin JS
by ChemAxon

Clear 

Cancel ×

[Transfer to query >](#)



indole

Search this structure as:

- As drawn
- As substructure
- Similar

Search this structure as:

- As drawn
- As substructure
 - On all atoms
 - On heteroatoms

Search this structure as:

- As drawn
- As substructure
 - On all atoms
 - On heteroatoms

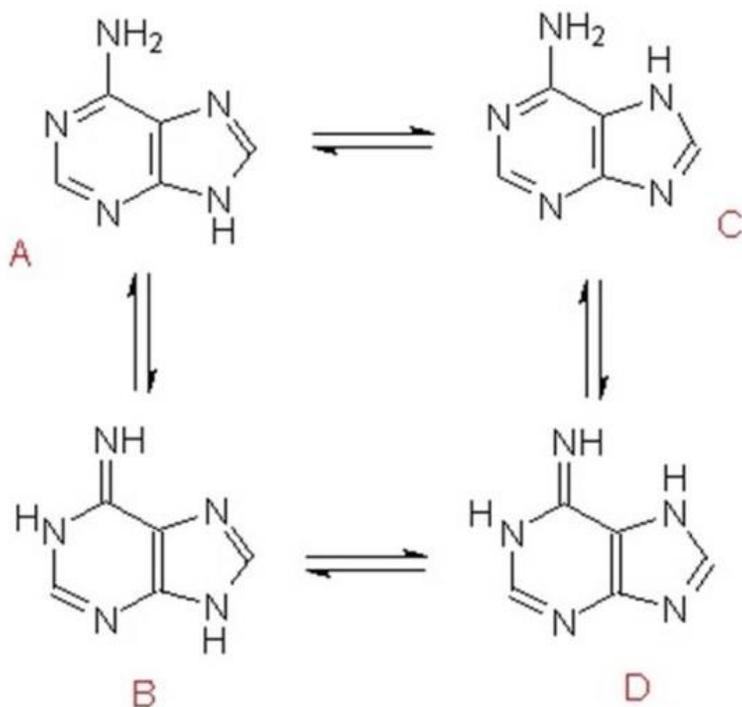
336	Substances	Structure : as drawn; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals	Preview Results <input type="button" value="View Results >"/>
3,970	Substances	Structure : average similarity; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals	Preview Results <input type="button" value="View Results >"/>
805	Reactions	Product(s) : as drawn; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals	Preview Results <input type="button" value="View Results >"/>

1,080,310	Substances	Structure : substructure; included: only absolute stereo, additional ring closures allowed, salts, mixture radicals	
14,731	Targets	Structure : substructure; included: only absolute stereo, additional ring cl radicals	
1,680,157	Reactions	Product(s) : additional ring cl radicals	

7,451	Substances	Structure : substructure on heteroatoms; included: only absolute stereo, additional ring closures allowed, salts, mixtures isotopes, charges, radicals Edit in Query Builder Create Alert	Preview Results <input type="button" value="View Results >"/>
892	Targets	Structure : substructure on heteroatoms; included: only absolute stereo, additional ring closures allowed, salts, mixtures isotopes, charges, radicals	
13,009	Reactions	Product(s) : substructure on heteroatoms; included: on absolute stereo, additional ring closures allowed, salts, mixture isotopes, charges, radicals	

*Tautomers

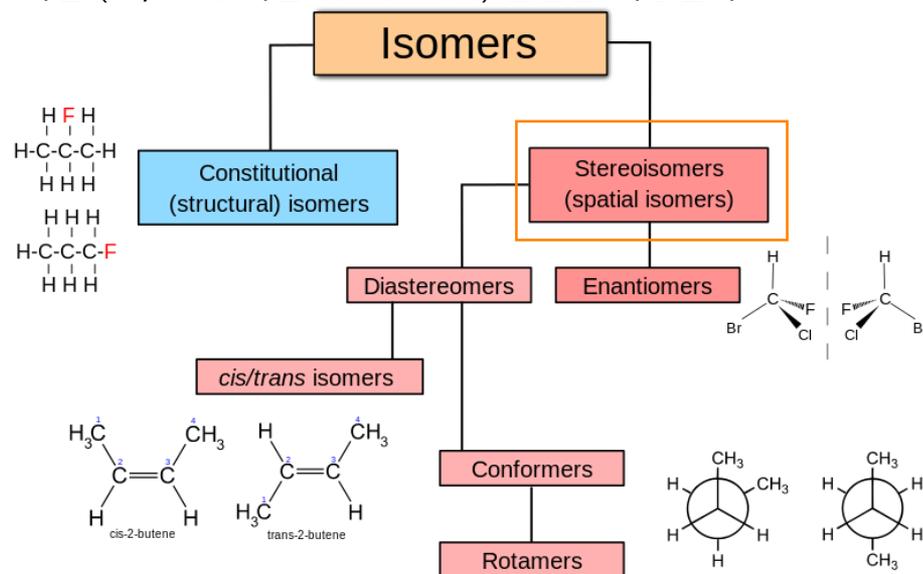
호변이성질체(tautomers)는 유기화합물의 구조이성질체로서 단일결합과 이중결합의 여부에 따라 수소의 위치가 바뀌는 관계가 되는 이성질체입니다. 대표적인 구조는 아데닌(Adenine)이 있습니다. 즉 Reaxys에서 검색시, Tautomers에 표기하게 되면, 호변이성질체까지 결과에 제공합니다.



- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

*Stereo

입체이성질체 - 거울로 사물을 보았을 때 대칭적이나 방향이 다르거나(Enantiomers), 화합물의 molecular는 같지만 위치가 다른 (cis/trans 혹은 conformers) 물질을 제공한다.

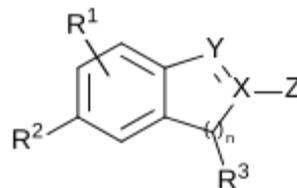


*Additional ring closures

반응이 일어날수 있는 곳(free sites)에 원자나 그룹이 합쳐서 링을 만든 결과를 제공합니다.

*Related Markush

Markush structure는 어떤화합물에 대한 그룹을 나타내는데 사용됩니다. 주로 특허와 관련이 있고, 어떤 화학구조에 치환기를 R 그룹, R1 그룹 등으로 설정해 두고, 여러가지 화합물을 R이나 R1등에 포함 시킬 수 있습니다.



- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

*Salt

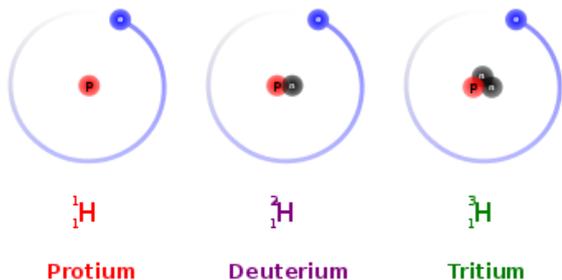
Multi-fragment 화합물, salt나 charge-transfer 같은 물질이 결과에 제공됩니다.

*Mixtures

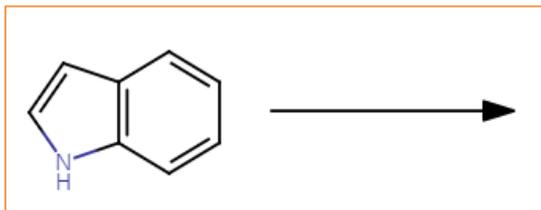
혼합물(고분자도 포함)

*Isotopes

동위원소 -예를 들어 수소의 isotopes는 아래와 같다.



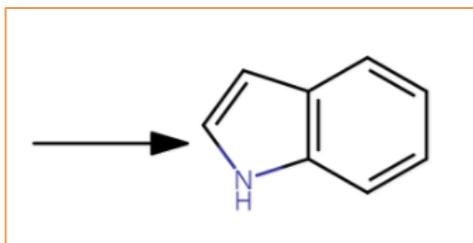
Indole



인돌로부터 합성할 수 있는 물질 찾기

Reaction ID: 1560417

63 Conditions Find Similar



인돌을 만드는 방법 찾기

805 Reactions out of 787 Documents containing 961 Substances, 1,140 Targets

1 selected Limit To Exclude Export Syn-Plan

Reaction ID: 4668689

17 Conditions Find Similar

Yield	Conditions	References
100%	With methanol; magnesium for 0.333333h; sonication: 35 kHz, 120-240 W;	Nyasse, Barthelemy; Grehn, Leif; Ragnarsson, Ulf - Chemical Communications, 1997, # 11, p. 1017 - 1018 Full Text Cited 121 times Details Abstract
97%	With naphthalene; tetraethylammonium bromide In N,N-dimethylformamide at 0°C; Inert atmosphere; Electrolysis;	Senboku, Hisanori; Nakahara, Kazuo; Fukuhara, Tsuyoshi; Hara, Shoji - Tetrahedron Letters, 2010, vol. 51, # 2, p. 435 - 438 Full Text Cited 24 times Details Abstract
91%	With dimethyl(phenyl)silyl lithium In tetrahydrofuran for 6h;	Fleming, Ian; Frackenpohl, Jens; Ila, Hiriyakkanavar - Journal of the Chemical Society - Perkin Transactions 1, 1998, # 7, p. 1229 - 1235 Full Text Cited 40 times Details Abstract

+ Show all conditions

Your export is ready

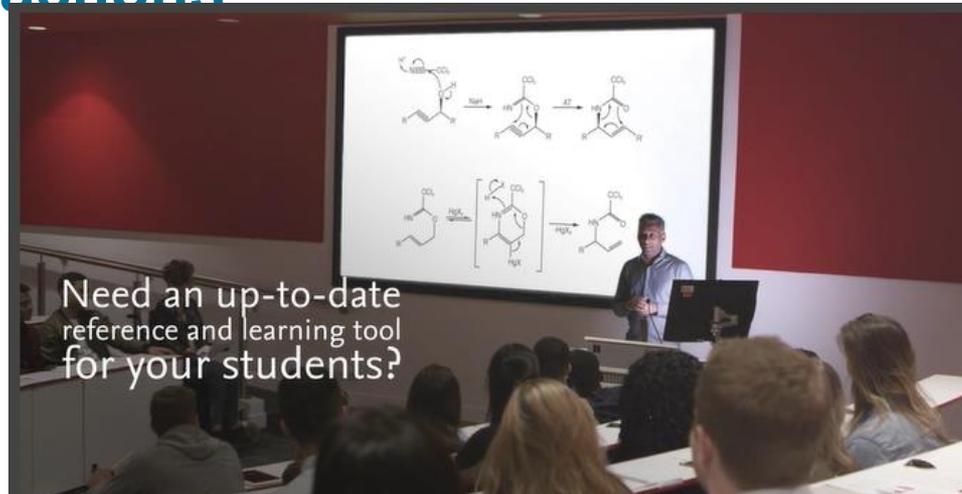
Download

Cancel

Exports Feedback

ReactionFlash Gives Details for 600+ Named Reactions

Now available for Android as well as iPhone



Need to check named reaction during group meeting?

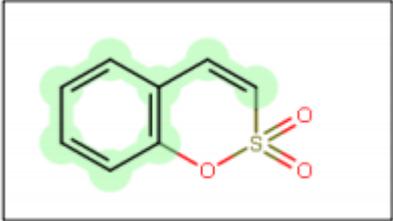


ReactionFlash
by Reaxys[®]

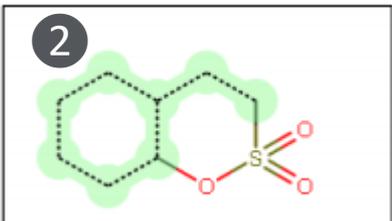
여러 기능기와 물성간의 관계 검색

I am interested in sulfocoumarins (1,2-benzoxathiine 2,2-dioxide). I'd like to retrieve *sulfocoumarins with various substituents* and then quickly analyze the results to see *any relationships between functional groups and various properties*.

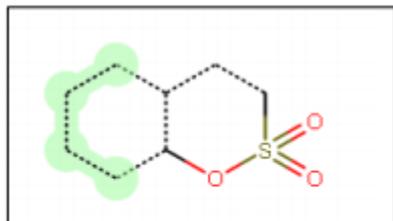
1



2



3



4



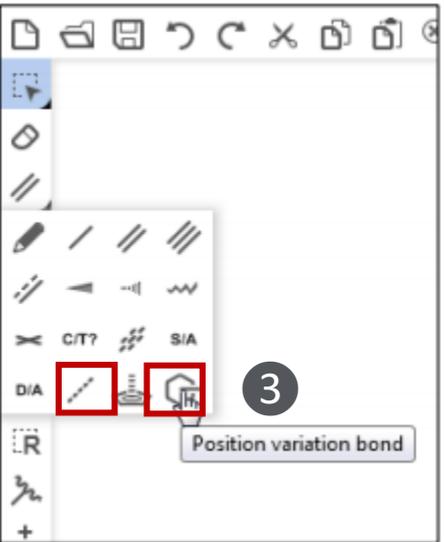
1. 선택 툴을 사용해 구조 선택

2. Any bond 툴 선택

3. Position variation bond 툴로 위치 지정

4. Generic group tool 에서 G 선택

5. Atom property에서 치환 허용개수 설정

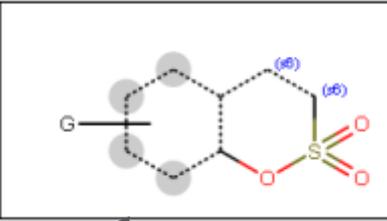


3



실습2

5



반응검색 - 구조 + synthesis or preparation

Search Reaxys

Q synthesis ①

AND

②

As drawn

5

Reactions

Reaction Query :  as drawn; included: only absolute stereo, salts, mixtures, isotopes, charges, radicals

[Preview Results](#) ▾[View Results](#) >

반응검색 결과 - 왼쪽 필터 활용하여 검색 결과 내 검색

Yield ^

<input type="checkbox"/> >95 - 100	<div style="width: 100%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	5
<input type="checkbox"/> >90 - 95	<div style="width: 80%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	3
<input type="checkbox"/> >85 - 90	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	1
<input type="checkbox"/> >80 - 85	<div style="width: 70%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	2
<input type="checkbox"/> >65 - 70	<div style="width: 50%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	1
<input type="checkbox"/> >30 - 35	<div style="width: 40%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	1
<input type="checkbox"/> >25 - 30	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	3

[+ More](#)

Reagent/Catalyst ^

<input type="checkbox"/> hydrogenchloride	<div style="width: 100%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	63
<input type="checkbox"/> water	<div style="width: 90%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	52
<input type="checkbox"/> zinc(ii) chloride	<div style="width: 70%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	20
<input type="checkbox"/> sodium carbonate	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	15
<input type="checkbox"/> calcium chloride	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	15
<input type="checkbox"/> ammonium chloride	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	15
<input type="checkbox"/> na2moo4	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	14

[+ More](#)

Solvent ^

<input type="checkbox"/> water	<div style="width: 100%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	43
<input type="checkbox"/> methanol	<div style="width: 80%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	12
<input type="checkbox"/> various solvent(s)	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	9
<input type="checkbox"/> water-d2	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	7
<input type="checkbox"/> dichloromethane	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	6
<input type="checkbox"/> hydrogenchloride	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	5
<input type="checkbox"/> aq. phosphate buffer	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	5

[+ More](#)

Catalyst Classes

<input checked="" type="checkbox"/> active center	<div style="width: 100%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	34
<input type="checkbox"/> organism / enzymes	<div style="width: 80%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	15
<input type="checkbox"/> heterogeneous	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	2

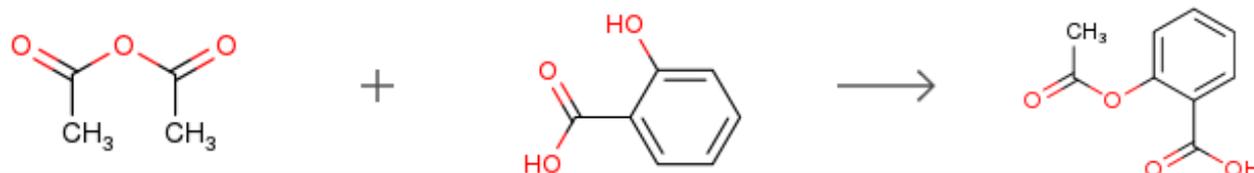
<input checked="" type="checkbox"/> Zn	<div style="width: 100%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	20
<input checked="" type="checkbox"/> Mo	<div style="width: 90%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	18
<input checked="" type="checkbox"/> Fe	<div style="width: 80%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	14
<input checked="" type="checkbox"/> Pd	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	6
<input checked="" type="checkbox"/> Ni	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	3
<input checked="" type="checkbox"/> B	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	2
<input checked="" type="checkbox"/> Si	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	1

Document Type ^

<input type="checkbox"/> article	<div style="width: 100%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	179
<input type="checkbox"/> patent	<div style="width: 80%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	7
<input type="checkbox"/> book review / secondary ref.	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	2
<input type="checkbox"/> conference paper	<div style="width: 60%; height: 10px; background: linear-gradient(to right, black 50%, grey 50%);"></div>	1

Single step reactions only

결과 : 반응정보 / 실험과정 정보 찾기



Yield	Conditions	Reference
100%	In neat (no solvent) ;Molecular sieve;Microwave irradiationGreen chemistry Experimental Procedure ^	Oliverio, Manuela; Costanzo, Paola; Nardi, Monica; +3 others - Beilstein Journal of Organic Chemistry, 2016, vol. 12, p. 2222 - 2233 Full Text ↗ Show details >

Optimized MW-assisted peracetylation

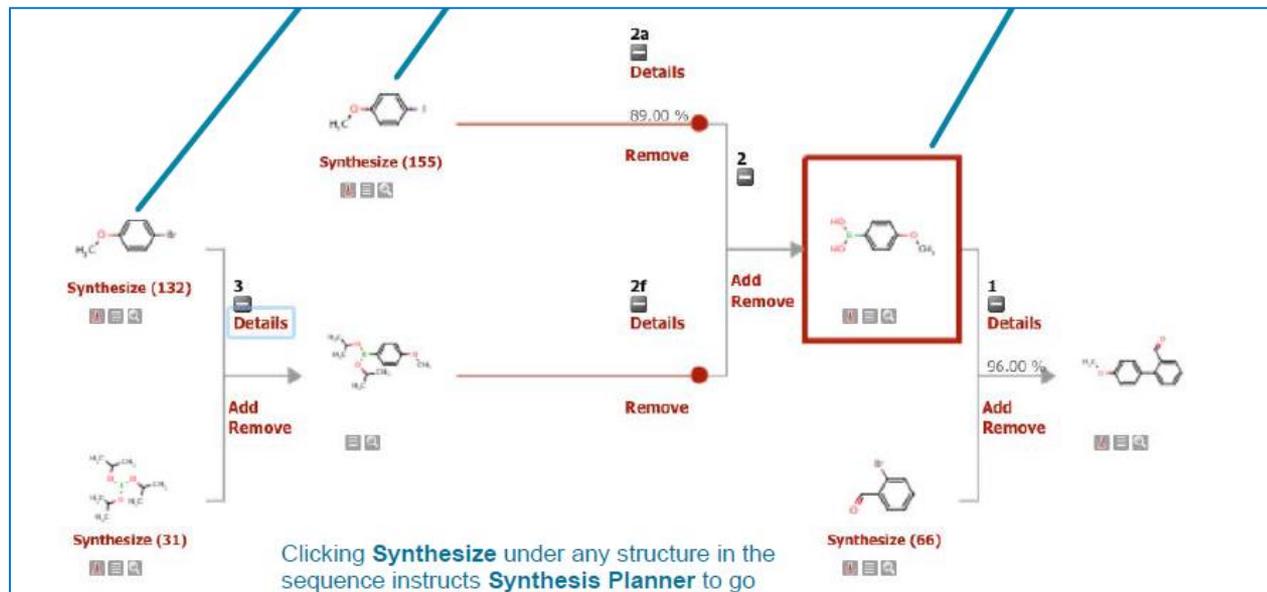
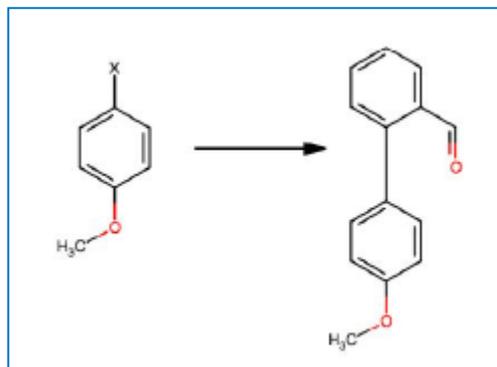
General procedure: The substrate belonging to one of the subset reported in Table 1(NTC, TC, CP, DGNP) (0.1 mmol) was left to react under MW heating (Synthos 3000, Anton Paar) with dry acetic anhydride (1 mL, 10 mmol) in a 3 mL vial (Rotor 64MG5), equipped with a magnetic stirrer in the presence of molecular sieves (10 percent w/w). The microwave, equipped with IR sensor for external temperature control (IR limit calculated as follows: $T_{\text{internal}} = 1.214 \times T_{\text{IR}}$), has been set with the power programs provided for its subset as described in Table 1. At the end of the reaction, the mixture was filtered, diluted with ethanol (2 mL) and left under vigorous stirring for 30 minutes at 50 °C. The mixture was then evaporated under reduced pressure and a small amount of a saturated solution of sodium bicarbonate (3.8 mL, 10 mmol NaHCO_3) was added. After the evolution of CO_2 , the precipitation of the peracetylated product was observed. The products were separated by simple decantation. For compounds which do not precipitate upon addition of NaHCO_3 , an extraction with AcOEt was needed. The organic phase, after drying with Na_2SO_4 , filtration and evaporation, gave the reaction crude.

Synthesis Planner 활용- 합성설계하기

반응 검색 구조식으로 검색 시 대부분의 반응레코드는 single-step reaction (A => B)으로 검색 결과를 보여주며, 문헌에 있는 반응과 직접적으로 관련이 있는 sequences (A =>C=> B) 검색 결과에서 빠질 수 있습니다.

Synthesis planner를 활용하면 여러 단계의 합성경로를 캔버스에서 직접 단계 단계 설계가 가능합니다.

예: Reaction records for single-step reactions from halo-anisoles to the biphenyl derivative.

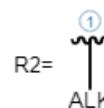
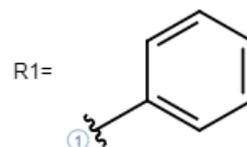
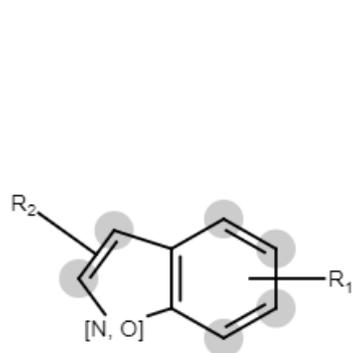


Indole의 합성 검색-Query Builder에서 Reaction으로 검색

Reaxys®

[Quick search](#) [Query builder](#) [Results](#) [Synthesis planner](#) [History](#)[Sign in](#)Structure editor ?

Create structure template from name >

**R**

Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

[+ More options](#)

실습3

결과

Reaxys®

Quick search Query builder Results Synthesis planner ⓘ History

Sign in ⓘ

49

Filters and Analysis

- By Structure ▾
- Yield ▾
- Reagent/Catalyst ▾
- Solvent ▾
- Catalyst Classes ▾
- Solvent Classes ▾
- Product Availability ▾
- Reactant Availability ▾
- Reaction Classes ▾
- Document Type ▾
- Publication Year ▾

Single step reactions only

49 Reactions out of 17 Documents containing 59 Substances, 0 Targets

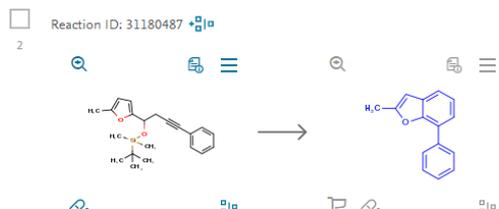
0 selected Limit To Exclude Export Syn-Plan Sort by Reaxys Ranking ▾



1 Conditions ^ Find Similar >

Yield	Conditions	References
90%	With palladium on activated charcoal; hydrogen In methanol for 4h;	Gritzalis, Dimitrios; Park, Jaeok; Chiu, Wei; Cho, Hyungjun; Lin, Yih-Shyan; De Schutter, Joris W.; Lacbay, Cyrus M.; Zielinski, Michal; Berghuis, Albert M.; Tsantrizos, Youla S. - Bioorganic and Medicinal Chemistry Letters, 2015, vol. 25, # 5, p. 1117 - 1123
Experimental Procedure ▾		Full Text Cited 3 times Details Abstract >

1 out of 1



Feedback ⓘ



Thank You!

s.kim.2@elsevier.com