

Reaxys User Guide

Elsevier Life Science Solution Team



1. 접속방법

i) IP 접속으로 <u>www.reaxys.com접속시</u> 바로 접속 ii) ID 와 PW로 접속 가능- IP 대역에서 개인계정 만드는법은 다음 페이지 참고

2. 접속 후 보여지는 첫화면



1. 접속후 개인 계정 만드는법

i) IP 접속으로 <u>www.reaxys.com</u>접속후 화면 오른쪽 상단의 Register 클릭 ii) 팝업되는 창에 이름과 이메일(아이디), 비밀번호를 설정.

이때 이메일은 앞으로 사용할 아이디이며, 비밀 번호는 소문자, 대문자, 특수기호 1개이상씩 총 8문자 이상되어야함.

6		rch substances, reactions, documents and bioactivity
Reaxys Quick search Query builder Results Synthesis planner History Search substances reactions documents and bioactivity data	Register > Sign in O	n Re Your IP: 198.176.125.2 🗙 no
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User name에 이메일 주소, 그리고 미민들 콩고 도그인	Username a.hong@elsevier.com Password	☞ Register > 위해 체크 필요.
번을 잊었을 때 Sign In 팝업창에 "Forgot your password 업되는 창에 이메일 주소를 넣으면 메일로 새롭게 번을 세팅할 수 있는 URL이 발송 됨.		Privacy Policy Terms and Conditions
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Query builder 고급검색 창에서는 여러 조건의 검색 조건을 조합하여 검색이 가능합니다.



Reaxys Contents



문헌 검색 방법 : Quick Search

예로 「Supramolecular chemistry fluorescent sensing」키워드를 검색합니다. 형광분자센서는 의학적 진단, 생리학적 이미지, 생화학, 화학적 분석 및 모니터링 시스템 등 다양한 분야에 적용 가능합니다.

Quick search Query builder Results Synthesis planner Hi	istory Aleri	ts	1. Reaxys의 첫 화면에서, Search Reaxys에 "supramolecular chemistry fluorescent sensing"를 입력합니다. (단어들간의 검색 연관성을 높이기 의해 도 단어 이상의 경우 "fluorescent sensing" 과 같이 잡은 따온표					
Search for Supramolecular chemistry fluorescer	nt sensing	ţ	혹은 큰 따옴표를 사용하면 보다 정확한 검색결과를 표시합니다.)					
Search Reaxys <u>Supramolecular</u> chemistry fluorescent sensing	×F	ind >						
Substance Properties, e.g. ferroelectric materials AND	Results f	for "supramole	Quick search Query builder Results Retrosynthesis History Register > lecular chemistry fluorescent sensing" Preview Result 에서는 가장 신뢰도 높은 3개의 결과를 미리 볼수 있습니다. New O Edit @					
2. 결과에서는 "Supramolecular chemistry" 그리고 "Fluorescent sensing"이 들어가 있는 29개의 문헌과	P	29	Documents Titles, Abstracts, Keywords : "supramolecular chemistry", "fluores- cent sensing" Edit in Query Builder 🔗 Create Alert 🗘					
각각의 검색어(Supramolecular chemistr와 Fluorescent sensing)검색 결과가 각각 제공됩니다.	ß	30,201	Documents Titles, Abstracts, Keywords : "supramolecular chemistry" Preview Results View Results > Edit in Query Builder 🖉 Create Alert 🗘					
	ß	1,539	Documents Titles, Abstracts, Keywords : "fluorescent sensing" Preview Results View Results > Edit in Query Builder 🖉 Create Alert 📮					

문헌 검색 방법 : Quick Search → View Result 클릭 시 결과

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Filters	ude >	29	Documents with 188 Substances, 45 Reactions, 0 Targets Imit To Exclude Export Imit To Exclude Export	Heatmap 🖽
Publication Year Document Type Authors Patent Assignee	~ ~ ~		Synthesis, structure and property of boron-based metal-organic materials Xia, Qingchun; Zhang, Jie; Chen, Xuenian; Cheng; Chu, Dandan; Tang, Xianhui; Li, Haiyang; Cui, Yong [Coord views. 2021. vol. 435. art. no. 213783] Ibstract ~ Index Terms ~ Substances 22 ~ Full Text ; Abstract hit: {chemistry and supramolecular chemistry. Among which, boron-based metal-orga	2는 = 있으 로 연 ✓
Patent Office Journal Title	× ×	2	Naphthotubes: Macrocyclic Hosts with a Biomimetic Cavity Feature Cited 29 times Yang, Liu-Pan; Wang, Xiaoping; Yao, Huan; Jiang, Wei [Accounts of Chemical Research, 2020, vol. 53, # 1, p. 198 - 208] Abstract V Index Terms V Substances (9) V Full Text 7	
Substance Classes Reaction Classes Index Terms (List) 1 필터를 이용하 다 색 범위를 좁힐	、 、 、 や さ ざ	3	Abstract hit: {used in supramolecular chemistry because they can recognize other small molecules through non-covalent} Unusual Fluorescence Quenching-Based Al ³⁺ Sensing by an Imidazolylpiperazine Derivative. β-Cyclodextrin En- capsulation-Assisted Augmented Sensing Kaliyamoorthi, Kiruthiga; Maniraj, Sumithra; Govindaraj, Tamil Selvan; Ramasamy, Sivaraj; Paulraj, Mosae Selvakumar; Enoch, Israel Vmv; Melchior, Andrea [Journal of Fluorescence, 2020, vol. 30, # 3, p. 445 - 453] Abstract \checkmark Index Terms \checkmark Substances (8) \checkmark Reactions (4) \checkmark Full Text 7	~
' 있습니다.			Abstract hit: {fluorescence. The fluorescent sensing of metal ions by a new ligand prepared (L} Index Terms hit: {2-D NMR, Fluorescent sensing, Lower limit of detections}	× ×
		4	Cucurbit[6]uril-based supramolecular assemblies incorporating metal complexes with multiaromatic ligands as <u>Cited 25 times</u> structure-directing agent for detection of aromatic amines and nitroaromatic compounds	Feedback 🖵

문헌 검색 방법 : Query Builder

동일 키워드 검색을 Query Builder로 검색 시 좀더 세심한 검색을 할 수 있습니다. 1. TI, AB&KW 아이콘을 두번 클릭하면, 아래와 같이 검색 조건에 2개의 Ti,AB&KW가 생깁니다. 2. 그곳에 각각 supramolecular chemistry와 fluorescent sensing 를 And 조건 혹은 or 조건으로 검색이 가능합니다.

Reaxys Quick search Query builder Results Synthesis planner History Alerts Hee Jung Hong 👌 💿 Reactions > Targets > Substances > Documents > Search in: Search fields Q 俞 5 0 0 # \mathbf{z} Fields Forms History Import Save Reset form Delete all Structure Molecular Formula CAS RN TI, AB & KW Reaxys **^** Topics and Keywords V ✓ supramolecular chemistry is E X Identification V → Titles Abstracts & K... fluorescent sensing is E X Physical Properties V OR AND Spectra V NOT MedChem \sim NEAR NEXT Other V PROXIMITY Reactions \sim Bibliography V PubChem V eMolecules 🗸

문헌 검색 방법 : Query Builder

	Search in: Reactions	> Targets > Substances > Documents >	Search fields Q chromatog ×
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♦ Structure		×	
	Create Structure / Reaction Drawing		
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밑에 나타난 해당 폴더를 클릭하면 오른쪽 검색 창에 추가가 됩니다. 문헌, 특허 검색 예 Query builder에서 "TI,AB&KW" 그리고 "Structure"에 검색어 Remdesivir를 넣고 Documents를 클릭 합니다.

leaxys	Quick search Query builder Results Synth	hesis planner History Alerts
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문헌, 특허 검색 예 결과 4,286개의 문헌에서 특허만 확인하고 싶을때는 오른쪽 필터에서 Document Type 선택 후 Patents 선택후 Limit to를 클릭합니다.

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4.29 K IIII Query	Filters Limit to > Exclude >	4,2 □	 86 Documents with 4,915 Substances, 3,357 Reactions, 82 Targets 0 selected	Sort by Publication Year 🔸 🗸	Heatmap 🎛
	Publication Year Document Type 1 article 2,035 review 1,381		Identification of chymotrypsin-like protease inhibitors of SARS-CoV-2 via integrated computational approach Khan, Salman Ali; Zia, Komal; Ashraf, Sajda; Uddin, Reaz; UI-Haq, Zaheer [Journal of Biomolecular Structure and Dynamics, 2021, vol. 39, # 7, p. 2607 - 2616] Abstract V Index Terms V Full Text 2	Cited 152 times	
	letter 316		Abstract hit: {approved drugs (Remdesivir, Saquinavir and Darunavir) and two natural compounds (. flavone and}		~
	note 209		Index Terms hit: {MD simulation, remdesivir, SARS-CoV-2}		~
	patent 59 short survey 38 View more	 ↓ 2 	The impact of coronavirus infectious disease 19 (COVID-19) on oral health <u>Dziedzic, Arkadiusz; Wojtyczka, Robert</u> [Oral Diseases, 2021, vol. 27, # S3, p. 703 - 706] Abstract V Index Terms V Full Text 7	Cited 30 times	
	Authors 🗸		Index Terms hit: {lopinavir, remdesivir, ritonavir}		\sim
	Patent Assignee \checkmark Patent Office \checkmark	3	SARS-CoV-2 RNA dependent RNA polymerase (RdRp) targeting: an in silico perspective Elfiky, Abdo A. [Journal of Biomolecular Structure and Dynamics, 2021, vol. 39, # 9, p. 3204 - 3212] Abstract V Index Terms V Full Text 7	Cited 87 times	
	Journal Title 🗸 🗸		Abstract hit: {Ribavirin, Galidesivir, Remdesivir, Favipiravir, Cefuroxime, Tenofovir, and Hydroxychloroquine, in binding to SA	RS-CoV-2 RdRp}	\sim
	Substance Classes 🗸 🗸		Perspective: SARS-CoV-2, COVID-19 and Haematologists	Cited 5 times	
	Reaction Classes 🗸 🗸	4	Gale, Robert Peter [Acta Haematologica, 2021, vol. 144, # 2, p. 117 - 120]		
	🗸 Index Terms (List) 🗸 🗸				Feedback 💭

문헌, 특허 검색 예 7개의 특허가 결과로 나옵니다.

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	Publication Year Document Type patent	~ 59		ANTI-CD154 ANTIBODIES AND USES THEREOF TONIX PHARMA HOLDINGS LIMITED; LEDERMAN, Seth - WO2021/1458, 2021, A1 Patent Family Members: WO2021/1458 A1 Abstract Index Terms Claims Front Page Info Full Text ㅋ Abstract Index Terms Claims Front Page Info Full Text ㅋ Abstract Index Terms Claims Front Page Info Full Text ㅋ Abstract Index Terms Claims Front Page Info Full Text ㅋ	= ₽. ext
	Authors	~		Claims hit: {GS-44-524 and remdesivir.99. A method of inducing hematopoietic chimerism in a transplant recipient,}	~
	Patent Assignee	\sim	2	Application of tannic acid in preparation of anti-coronavirus medicine	
	Patent Office	× •		Author Information pending - CN111759851, 2021, B Patent Family Members: CN111759851 A; CN111759851 B Abstract 🗸 Index Terms 🗸 Claims 🗸 Front Page Info 🗸 Full Text 🧃	
	Substance Classes	~		Abstract hit: {that of Remdesivir, the curative effect is exact, and the tannic acid has}	~
	Reaction Classes	~	3	PEPTIDOMIMETICS FOR THE TREATMENT OF CORONAVIRUS AND PICORNAVIRUS INFECTIONS Emory University - US2021/8150, 2021, A1	
	Index Terms (List)	~		Patent Family Members: US2021/8150 A1 Abstract 🗸 Index Terms 🗸 Claims 🗸 Front Page Info 🗸 Full Text 🧃	
	Index Terms (ReaxysTree)	~		Claims hit: {agents comprise remdesivir, GS-441524, N-hydroxy cytidine, Jakafi, Tofacitinib, Baricitinib, or a pharmaceutically-acceptable salt}	\checkmark
	Manually processed content only		4	Method and composition for the reduction of viral replication, duration and spread of the COVID-19 and the Flu	
				Martin, Alain - US2021/8105, 2021, A1 Patent Family Members: US2021/8105 A1	Feedback 🖵

Reaxys^{*}

물질정보



물질정보

Substances out of 7 Documents	s, containing 36 Reactions, 0 Targets			Reaxys - 4	\sim
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	(2S)-2-ethylbutyl 2-(((S)-(((2R,3S,4R,5R)-5-(4 (phenoxy)phosphoryl)amino)propanoate C ₂₇ H ₃₅ N ₆ O ₈ P 602.584 29506468	-aminopyrrolo[2,1-f][1,2,4]triazin-7-yl)	-5-cyano-3,4-dihydroxytetrahydro	furan-2-yl)methoxy)	
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	Druglikeness F	Physical Data - 11	Other Data - 34	Reactions - 36	>
				Documents - 7	>
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	Physical Data - 5	제공합니다.	물다만 데이너를 포하		
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간편검색가이드 2022 version1



Reaxys^{*}

반응정보 반응 정보를 보기위해 구조 편집기 활용이 필요합니다.





반응정보



Reaxys^{*}







1→1



1→1

반응정보 Smail

Smax와 Slock 설명



반응정보

R group을 활용하면 원하는 위치에 여러 치환기를 설정하여 붙일 수 있습니다. R group attachment 기능은 붙이려는 치환기에서 어디에 붙일지 활성화 해 주는 역할입니다.



반응정보 응용 실습

Reaxys

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



반응정보 Manual Mapping은 반응시 Atom 대 Atom을 매명하여 고정해 주는 역할을 합니다.	Reaxys		간편검색가이드 2022 version1
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반응정보



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[C, N, O]	



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- Atom list 클릭후 C,N,O를 선택하고 OK 클릭
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Thank you

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사용하다가 궁금하신 부분은 언제든 메일로 문의주세요.

