2022.7 CAS SciFinderⁿ新增功能与使用技巧

- ✓ 标亮显示来自 CAS Lexicon 的检索词(P1-3)
- ✔ 筛选序列长度(P4-6)
- ✓ 显示实验属性中混合溶剂的比例 (P7-8)

CAS SciFinderⁿ 使用技巧|标亮显示来自 CAS Lexicon 的 检索词

选择 CAS SciFinder[®]中 References 选项后,点击 Launch CAS Lexicon,可以在 CAS 科学家创建 的词库层级中浏览概念词(Concept)和物质。在检索的文献结果中,命中的概念词 (Concept)和物质会被标亮显示。

1. 在 CAS SciFinderⁿ的 References 检索页面,点击页面中间的 Launch CAS Lexicon 打开 CAS 词库,选择目标词语进行文献检索。

Searching for	References		
S All	Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn More		
⊖ Substances	Enter a query	Draw	Q,
A Reactions	Author Name - Enter last name, first name middle name.	×	
References	Example: Sch	hubert, J A	
🚬 Suppliers	+ Add Advanced Search Field Learn more about SciFinder ⁿ Ad	lvanced Search.	
	Launch CAS Lexicon enables you to browse the CAS General Thesaurus to find index substances to build a Reference query with up to 1,000 indexed search term	ked concepts and ls.	
Retrosynthesis			

在 CAS 词库中输入感兴趣的词,例如 vaccines。并在层级中选择同义词、上下位词或相关词,然后点击 Add Terms 将目标词语加入右侧的 Query 中。点击右下角放大镜开始检索。

iccines	Search Concept	Your Query You may include up to 1,000 terms in a search.	Clear A
Preferred Term	A	Vaccines	×
Vaccines		Vaccines - Narrower Terms (23 Concepts)	×
This will search synonyms: Vaccin: Vaccine: Vaccins		Biopharmaceuticals	×
 A Broader Terms (1) 	Select All		
Biopharmaceuticals			
 Narrower Terms (23) 	Select All		
ACW 135XY			
ACW 135Y			

获得使用来自 CAS 词库的词语进行检索的文献结果,点击文献标题可查看文献详情。文献详情中命中的 Concepts(概念词)和物质会被标亮显示。

References search for	25 CAS Lexicon Terms			
♀ Substances ▾ ▲ Reactions ▾	66 Citing -			L Save and Alert
Filter Behavior	0 169,155 Results		Sort: Relevance 👻 N	/iew: Partial Abstract 🔹
Filter by Exclude	□ 1			
 Document Type Journal (108K) Patent (54K) Review (32K) Biography (22) Book (392) View All 	Vaccine formulations comprisi By: Sangareddy. Veerapandu: Burki, Raje India, IN201841027285 A 2020-01-24 Li The present invention relates to vaccine relates to preservative systems for vaccin one other preservative selected from m- PatentPak - Full Text -	ng preservative system ndar; Sriraman, Rajan; Matur, Ramesh anguage: English, Database: CAplus formulations comprising preservative : he formulations which is free of thiome cresol, benzyl alc., phenol and benzoic Q Substances (6)	Venkat; Mantena, Narender De systems. More particularly, the ţ ersal, and comprising 2-phenoxy acid. Reactions (0)	v; Datla, Mahima present invention rethanol and at least ⑦ Citation Map
 Substance Role 	2			
Biological Study (2) Vaccine formulations comprising preservative system Biological Study (2) By: Sangareddy, Veerapandu; Burki, Rajendar; Sriraman, Rajan; Matur, Ramesh Venkat; Mantena, Narender Dev; Datla, M World Intellectual Property Organization, WO2020021416 A1 2020-01-30 Language: English, Database: CAplus The present invention relates to vaccine formulations comprising preservative systems. More particularly, the present in relates to preservative systems for vaccine formulations which is free of thiomersal, and comprising 2-phenoxyethanol - or other presentitive calcular of form mulations and in the present and particular study for more core of home and homeries and				
 Language English (131K) 	PatentPak Full Text	Q Substances (6)	Reactions (0) 66 Citing (0)	 Citation Map

← Return to Results						← Prev	(1 of 169,155)	Next →
Vaccine formulations comprising preservative system								
O Substances (6) A Reaction	ons (0) 66 Citing (0)						⊻ ■	Save
PATENT	PATENT By: Sangareddy, Veerapandu; Burki, Rajendar; Sriraman, Rajan; Matur, Ramesh Venkat; Mantena, Narender Dev; Datla, Mahima							а
Patent Number IN201841027285 Publication Date	The present invention relates to vaccine formulations comprising preservative systems. More particularly, the present invention relates to preservative systems for vaccine formulations which is free of thiomersal, and comprising 2-phenoxyethanol and at least one other preservative selected from m-cresol, benzyl alc., phenol and benzoic acid.							
Application Number IN2018-41027285	PatentPak View	ver Get Pi	rior Art Analys	sis Full Text -				
Application Date	Application Date Patent Family							
2018-07-21	Patent	Language	Kind Code	PatentPak Options	Publication Date	Application Num	ber Applicat	ion Date
Kind Code A	IN201841027285	English	А	PDF PDF+ Viewer	2020-01-24	IN2018-41027285	2018-07-	-21
Assignee	WO2020021416	English	A1	PDF PDF+ Viewer	2020-01-30	WO2019-IB56202	2019-07-	-19
Biological E Limited. India	CN112469435	Chinoso	٨	Phe	2021 03 09	CN2019 800/876	5 2010.07	10

1	 IPC Data 			
	 Concepts 			
	Antigens Role: Therapeutic Use	Hepatitis B virus proteins Role: Biological Study, Unclassified; Therapeutic Use	Corynebacterium diphtheriae Modifier: antigens	Proteins, conjugates Role: Therapeutic Use
	Bordetella pertussis Modifier: antigens	Hepatitis C antigens Role: Biological Study, Unclassified; Therapeutic Use	Diphtheria toxoids Role: Therapeutic Use	Salmonella enterica paratyphi Modifier: antigens
	Closerdium tetani	Modifier: antigens Neisseria meningitidis	Enterovirus C Modifier: antigens	Salmonella typhi Modifier: antigens
	Modifier: antigens Combination vaccine DTaP-Hib	Modifier: antigens Pertussis toxoids Role: Therapeutic Use	Haemophilus influenzae Modifier: antigens	Streptococcus pneumoniae Modifier: antigens
	Combination vaccine DTwP-HepB Role: Biological Study, Unclassified; Therapeutic Use	Pharmaceutical carriers	Hepatitis A virus	Tetanus toxoids Modifier: antigens
	Combination vaccine DTwP-IPV Role: Biological Study, Unclassified; Therapeutic Use	Pneumococcal vaccines Preservatives		Role: Therapeutic Use
L	Combination vaccines			racentes

 Substances 		
Substances (6)		
2375119-26-7 Image Not Available	122-99-6 HO	108-95-2 OH
ACW 135Y Role: Biological Study, Unclassified,	C ₈ H ₁₀ O ₂ Phenoxyethanol PatentPak	C ₆ H ₆ O Phenol PatentPak
Therapeutic Use, Biological Study, Uses	Role: Therapeutic Use, Biological Study, Uses	Role: Therapeutic Use, Biological Study, Uses

CAS SciFinderⁿ使用技巧|筛选序列长度

在 CAS SciFinder[®] 的 Biosequences 检索结果中,可以浏览目标序列的长度分布区间,也可以筛 选特定长度或长度范围内的目标序列。

 在 CAS SciFinderⁿ的 Biosequences 检索结果页面,通过左侧 Filter by 选项下的 Sequence Length 可以查看目标序列的长度分布区间。如果检索的是肽或蛋白,序列结果 中 Sequence Length 下呈现的是目标序列中氨基酸的数量分布(此例中显示的是 447-1367 个氨基酸)。

References		⊥
otif Search Details	Query Details > Seq 1: 1 QVQLVQSGGGVVQPGRSLRLSCKASGYTFTRYTMHWVRQAPGKGLEWIGYINPSRGYTNYNQKVKD	RFTISRD View Mo
equence Type: Protein CBI Included: Yes	127 Results Sort: E-Vall	ue 👻 View: Expand
uery Coverage: 90% Value: 10	1 Ali	gnment Identity: 1009
oscape Analysis	Query (1) (449)	
sually explore sequence milarity with a new tool. earn more about Bioscape.		Matches: 44 Mismatches:
Create Bioscape Analysis	View Less ~	
ter by	Alignment Subject Pafarances	References
E-Value	Algument Subject References	
Query Coverage %	Alignment Data BLAST Score: 3398	
Subject Coverage %	E-Value: 0	
Alignment Identity %	Q 1 QVQLVQSGGG VVQPGRSLRL SCKASGYTFT RYTMHWVRQA PGKGLEWIGY INPSRGYTNY NQKVKDRFTI	70
·0	S 1 QVQLVQSGGG VVQPGRSLRL SCKASGYTFT RYTMHWVRQA PGKGLEWIGY INPSRGYTNY NQKVKDRFTI	70
to	Q 71 SRDNSKNTAF LQMDSLRPED TGVYFCARYY DDHYCLDYWG QGTPVTVSSA STKGPSVFPL APSSKSTSGG	140
00		140
	0 141 TAALIGCI VKD YEPEPVTVSW NSGALTSGVH TEPAVLOSSG I YSLSSVVTV PSSSI GTOTY TCIMUHKPSN	210
Sequence Length		
0	S 141 TAALGCLVKD YFPEPVTVSW NSGALTSGVH TFPAVLQSSG LYSLSSVVTV PSSSLGTQTY ICNVNHKPSN	210 🔻
47 to		
367	2 Ali	gnment Identity: 100
	Query (1) (449)	

如果检索的是 DNA 或 RNA,序列结果中 Sequence Length 下呈现的是目标序列中核苷酸碱基数量的分布(此例中呈现的是 48-51 个碱基)。

Biosequences sea	rch for your query
References	
BLAST Search Details	Query Details CTGAGCTGGCTGGCTGAGACTGCTGAACACCTACATCTGCAACGTGAACCAC View More
Sequence Type: Nucleotide Search Within: Nucleotides	3 Results Sort: E-Value - View: Expanded
BLAST Algorithm: BLASTn NCBI Included: Yes	1 Alignment Identity: 100%
Alignment Identity: 80% Query Coverage: 90% E-Value: 10 Match with Gaps?: No	Query (1) (51) Matches: 51
Gap Costs: Existence 5 Extension 2 Word Size: 11	Subject (1)
Bioscape Analysis	View Less ~
Visually explore sequence similarity with a new tool. Learn more about Bioscape. Create Bioscape Analysis	Alignment Subject References Alignment Data BLAST Score: 102 E-Value: 3,50452e-18
Filter by	Q 1 CTGAGCTGGC TGCTGAGACT GCTGAACACC TACATCTGCA ACGTGAACCA C 51
✓ E-Value	S 1 CTGAGCTGGC TGCTGAGACT GCTGAACACC TACATCTGCA ACGTGAACCA C 51
 Query Coverage % 	
 Subject Coverage % 	2 Alignment Identity: 86.96%
 Alignment Identity % Sequence Length 	Query 1 51 Matches: 40
48 to	Subject 1 49
	View Less 🗸
Apply Reset Filters	Alignment Subject References

2. 在 Sequence Length 下的输入框中,输入感兴趣的目标序列长度或长度区间,点击 Apply,即可获得精炼后的目标序列。例如,此例中限定目标序列长度为 449,精炼结果中的目标序列都含有 449 个氨基酸。

References		⊥
otif Search Details	Query Details > Seq 1: 1 QVQLVQSGGGVVQPGRSLRLSCKASGYTFTRYTMHWVRQAPGKGLEWIGYINPSRGY	TNYNQKVKDRFTISRD View Mo
quence Type: Protein EBI Included: Yes	38 Results	Sort: E-Value 👻 View: Expand
uery Coverage: 90% Value: 10	1	Alignment Identity: 100
oscape Analysis	Query (1) (449)
sually explore sequence milarity with a new tool. arn more about Bioscape.		Matches: 44 Mismatches:
Create Bioscape Analysis	View Less ~)
ter by	Alignment Subject References	References
E-Value	Aighneit Subject References	
Query Coverage %	Alignment Data	
Subject Coverage %	E-Value: 0	
Alignment Identity %	Q 1 QVQLVQSGGG VVQPGRSLRL SCKASGYTFT RYTMHWVRQA PGKGLEWIGY INPSRGYTNY NQI	KVKDRFTI 70
, 	S 1 QVQLVQSGGG VVQPGRSLRL SCKASGYTFT RYTMHWVRQA PGKGLEWIGY INPSRGYTNY NQ	(VKDRFTI 70
10	Q 71 SRDNSKNTAF LQMDSLRPED TGVYFCARYY DDHYCLDYWG QGTPVTVSSA STKGPSVFPL AP	55KST5GG 140
00	S 71 SRDNSKNTAF LQMDSLRPED TGVYFCARYY DDHYCLDYWG QGTPVTVSSA STKGPSVFPL AP	SSKSTSGG 140
Sequence Length	Q 141 TAALGCLVKD YFPEPVTVSW NSGALTSGVH TFPAVLQSSG LYSLSSVVTV PSSSLGTQTY IC	NVNHKPSN 210
	S 141 TAALGCLVKD YFPEPVTVSW NSGALTSGVH TFPAVLQSSG LYSLSSVVTV PSSSLGTQTY IC	NVNHKPSN 210 -
49 to		
49	2	Alignment Identity: 99.55
		\ \
Apply Reset Filters	Query () (449)

CAS SciFinderⁿ 使用技巧 显示实验属性中混合溶剂的比例

在 CAS SciFinder[®]物质属性(熔点、核磁等)信息中,如有涉及混合溶剂的条件,则增加了混合 溶剂的用量比例信息。

 在物质的熔点测试条件中,如有涉及混合溶剂(例如此例中的石油醚和苯),则会提供各 种溶剂的用量比例。

🔾 CAS Registry Number: 10002-82-	-1	
References (11)		
	O (S) (S) (S) (S) (S) H Absolute stereochem	(S) (R) (R) (R) (R) (R) (R) (R) (R) (R) (R
C ₂₃ H ₃₆ O ₃ Pregnan-20-one, 3-(acetyloxy)-, (3β,5α,14β,17α)- (9CI)	Value	Condition
Molecular Weight	360.53	-
Melting Point (Experimental)	95-100 °C	Solvent: Ligroine; Benzene (4:1)
Boiling Point (Predicted)	443.7±18.0 °C	Press: 760 Torr
Density (Predicted)	1.07±0.1 g/cm ³	Temp: 20 °C; Press: 760 Torr
Experimental Properties		

 在物质的核磁谱图测试条件中,如有涉及混合溶剂(例如此例中的 DMSO-d6 和水),则 会提供各种溶剂的用量比例。

