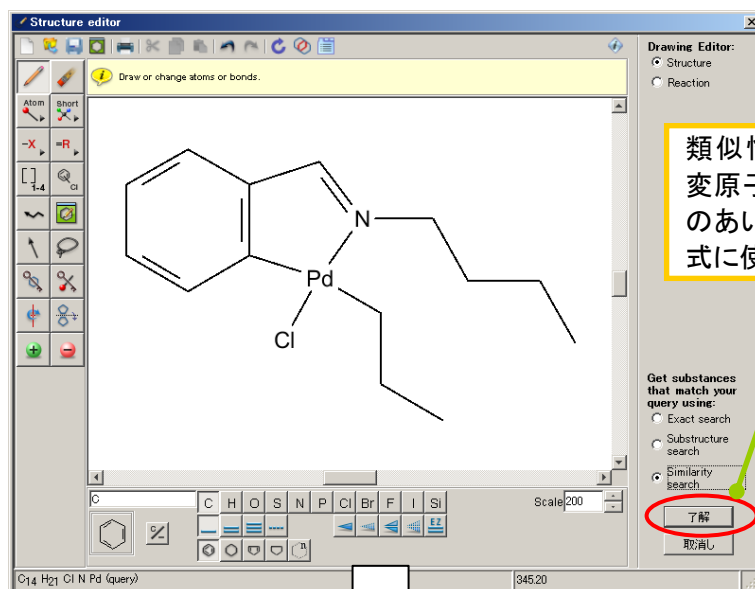


錯体の類似性構造検索

錯体について類似性構造検索を行うと、部分構造検索では得られないような以下の錯体を得られる可能性があります。

- ・ 違う中心金属を持っている
- ・ 似た構造の配位子を持っている

検索例： 下記の構造について類似性構造検索を行う



Explore Substances

Chemical Structure Chemical Structure

Molecular Formula

Substance Identifier

Click image to change structure or view detail

Search type: Exact Structure
 Substructure
 Similarity

Show precision analysis

Characteristic(s)

Single component
 Commercially available
 Included in reference(s)

Class(es)

Alloys
 Coordination compounds
 Incompletely defined
 Mixtures
 Polymers
 Organics, and others not listed

Studies

Analytical
 Biological
 Preparation
 Reactant or reagent

得られる回答を錯体に限定

Similarity Candidates

4 Candidates 4 Selected

Select All Deselect All

Similarity Candidates	Count
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	0
<input type="checkbox"/> 80-84	0
<input checked="" type="checkbox"/> 75-79	4
<input checked="" type="checkbox"/> 70-74	18
<input checked="" type="checkbox"/> 65-69	61
<input checked="" type="checkbox"/> 60-64 (least similar)	175

Tanimoto アルゴリズムに基づいて類似性スコアを計算し、スコアごとの回答件数が表示される

258 件の錯体が得られた。

Substances 258 Substances 0 Selected Keep Selected Remove Selected Save Print Export

Sort by: Similarity Score Answers per Page [15] View: [Icons]

31. Substance Detail 127234-19-9 Score: 69
C11 H16 Cl2 Cu N2
Pyridine, 2-N-pentylformimidoyl-, copper complex (6CI)

32. Substance Detail 127234-20-2 Score: 69
C11 H16 Cl2 Hg N2
Pyridine, 2-N-pentylformimidoyl-, mercury complex (6CI)

33. Substance Detail 127234-21-3 Score: 69
C11 H16 Cl2 N2 Zn
Pyridine, 2-N-pentylformimidoyl-, zinc complex (6CI)

34. Substance Detail 127334-80-9 Score: 69
C10 H14 Br2 Hg N2
Pyridine, 2-(N-butylformimidoyl)-, Hg complex (6CI)

35. Substance Detail 154789-21-6 Score: 69
C14 H20 N4 Pd
Palladium(2+), bis(acetonitrile)[N-(2-pyridinylmethylene)-1-butanamine-N,N']-, (SP-4-3)- (9CI)

36. Substance Detail 154789-22-7 Score: 69
C14 H20 N4 Pd
Palladium(2+), bis(acetonitrile)[N-(2-pyridinylmethylene)-1-butanamine-N,N']-, (SP-4-3)- (9CI)

Analysis Refine
Analyze by: [Dropdown]
Substance Role [Dropdown]
Click bar to view only those substances within the current answer set
Preparation 195
Reactant or Reagent 80
Properties 66
Uses 28
Process 16
Formation, Nonpreparative 5
Biological Study 3
Analytical Study 1
Show More

154789-21-6 C14 H20 N4 Pd
14874-70-5 B F4

Pd だけでなく Cu, Hg などの中心金属を持つ錯体がヒットしている。さらに構成元素で解析することによって、中心金属による分類できる。

Analyze 機能を用いて、構成元素 (Elements) の観点で解析する。

Analysis Refine
Analyze by: [Dropdown]
Elements [Dropdown]
Click bar to view only those substances within the current answer set

C	258
H	258
N	258
Cl	120
O	91
Pd	66
Pt	52
Br	31
Sn	27
Rh	25

Show More

Analysis - Elements [Dropdown]
37 Items 1 Selected Export
Sort by: Frequency [Dropdown]
Select bars to view only those substances within the current answer set.

<input type="checkbox"/>	C	258
<input type="checkbox"/>	H	258
<input type="checkbox"/>	N	258
<input type="checkbox"/>	Cl	120
<input type="checkbox"/>	O	91
<input checked="" type="checkbox"/>	Pd	66
<input type="checkbox"/>	Pt	52
<input type="checkbox"/>	Br	31
<input type="checkbox"/>	Sn	27
<input type="checkbox"/>	Rh	25

Apply Cancel

66 件の Pd (パラジウム原子)を持つ錯体が得られた。

Substances 66 Substances 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All | Sort by: Similarity Score | Answers per Page [15] | View: [Icons]

31. Substance Detail Score: 64
890711-19-0
C9 H10 Cl2 N2 Pd
Palladium, dichloro[N-[(2-pyridinyl-κN)methylene]-2-propen-1-amine-κN], (SP-4-3)-
~2 References
Reactions
Commercial Sources
Regulatory Information
Link

32. Substance Detail Score: 64
942153-56-2
C29 H29 Cl N P Pd
Palladium, [2-[(butylimino-κN)methyl]phenyl-κC]chloro(triphenylphosphine)-, (SP-4-4)-
~1 References
Reactions
Commercial Sources
Regulatory Information
Link

33. Substance Detail Score: 64
1075740-24-7
C12 H21 Cl N2 Pd
Palladium, chloro[2-[(dimethylamino-κN)methyl]phenyl-κC](2-propanamine)-, (SP-4-4)-
~2 References
Reactions
Commercial Sources
Regulatory Information
Link

34. Substance Detail Score: 63
56171-60-9
C9 H12 Cl2 N2 Pd
Palladium, dichloro[N-[(2-pyridinyl-κN)methylene]-2-propen-1-amine-κN], (SP-4-3)-

35. Substance Detail Score: 63
56171-61-0
C8 H10 Cl2 N2 Pd
Palladium, dichloro[N-[(2-pyridinyl-κN)methylene]-2-propen-1-amine-κN], (SP-4-3)-

36. Substance Detail Score: 63
83590-96-9
(Component: 83590-99-2)
C8 H10 Cl2 N2 Pd
Palladium, dichloro[N-[(2-pyridinyl-κN)methylene]-2-propen-1-amine-κN], (SP-4-3)-

Analysis Refine
Analyze by: [Icon]
Elements [Dropdown]
Click bar to view only those substances within the current answer set
C 66
H 66
N 66
Pd 66
Cl 43
O 13
F 11
B 10
P 7
Br 2
Show More

該当の物質が関与する反応を検索

該当の物質を索引している文献を検索

磯崎博士の論文

1. Ultrasound-induced gelation of organic fluids with metalated peptides

By: Isozaki, Katsuhiro; Takaya, Hikaru; Naota, Takeshi

Stable solns. of a palladium ortho-metalated N-dipeptidyl benzaldimine complexes undergo reversible gelation after brief ultrasound irradiation; the sol state may be restored by heating. Palladium complexes [LXPd-1,2-C6H4CH=N-κN-(CH2)nOCOCH2CH2CH(NHFmoc)CONHCH(CONH-Bu)CH2CH2COO(CH2)nN:CHC6H4-1,2-PdXL] (L = PPh3; 1a X = Cl, n = 2; 1b X = NCS, n = 2; 1c X = Cl, n = 5), Fmoc[NH-CH(Y)CONH]mBu (Y = CH2CH2CO2CH2CH2N:CH-1,2-C6H4PdLCl; 2-4; m = 1-4) undergo ultrasound-induced gelation, tentatively explained by extensive H-bond formation. This is the first case of a reversible, remotely controlled, and rapid sol-gel transition by H-bonding aggregates. By adjusting the sonication time, the gelation rates and heat-resistant properties of the aggregates can be controlled.

Indexing
Organometallic and Organometalloidal Compounds (Section 29-13) [Icon]
Section cross-reference(s): 34

Concepts [Icon]
Peptides, preparation
complexes, palladium; ultrasound-induced mechanochem. reversible gelation of palladium benzaldimine-pendant peptide cyclometalated complexes
Physical, engineering or chemical process; Synthetic preparation; Preparation; Process

Metalation
cyclometalation, palladium; ultrasound-induced mechanochem. reversible gelation of palladium benzaldimine-pendant peptide cyclometalated complexes

Transition metal complexes

Substances [Icon]
942153-56-2P

crystal structure, gelation; ultrasound-induced mechanochem. reversible gelation of palladium benzaldimine-pendant peptide cyclometalated complexes
Physical, engineering or chemical process; Properties; Synthetic preparation; Preparation; Process

942153-57-3P

Source
Angewandte Chemie, International Edition
Volume 46
Issue 16
Pages 2855-2857, S2855/1-S2855/31
Journal
2007
CODEN: ACIEF5
ISSN: 1433-7851

Company/Organization
Department of Chemistry
Graduate School of Engineering
Machikaneyama, Toyonaka,
Osaka, Japan 560-8531

Accession Number
2007:473237
CAN 147:95767
CAPLUS

Publisher
Wiley-VCH Verlag GmbH & Co.
KGaA

Language
English

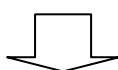
該当物質が原文献中でどのように扱われているかが記載されている

Get Reactions ⓘ

Select a reaction role:

- Product
- Reactant
- Reagent
- Reactant or reagent
- Catalyst
- Solvent
- Any role

該当の物質の合成方法を検索



3 件の反応情報が得られた。

Chemical Structure similarity with limiters > substances (258) > keep analysis "Elements" (66) > get reactions (3)

Reactions ⓘ Get References

3 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] Display: (2 References)

2. ▲2 Hit Reactions in this Reference Similar Reactions NEW

$\text{PdCl}_2(\text{MeCN})_2 + \text{C}_5\text{H}_4\text{N}-\text{CH}=\text{N}-\text{CH}_2-\text{CH}=\text{CH}_2 \xrightarrow{\text{S:Me}_2\text{CO}, 24 \text{ h, rt}}$

NOTE: PdCl₂(COD) and CH₂Cl₂ also used, Schlenck technique used, Reactants: 2, Solvents: 1, Steps: 1, Stages: 1

Functionalized pyridinyl-imine complexes of palladium as catalyst precursors for ethylene polymerization
By Cloete, Jezreel and Mapolie, Selwyn F.
From Journal of Molecular Catalysis A: Chemical, 243(2), 221-225; 2006

3. ▲1 Hit Reaction in this Reference Similar Reactions NEW

$\text{C}_5\text{H}_4\text{N}-\text{CH}=\text{N}-\text{CH}_2-\text{CH}=\text{CH}_2 \xrightarrow{\text{C:91365-07-0}, \text{S:CH}_2\text{Cl}_2, 4 \text{ h, rt}}$

NOTE: Reactants: 1, Catalysts: 1, Solvents: 1, Steps: 1, Stages: 1

生成物・反応物だけでなく、試薬や溶媒、触媒や反応条件なども表示される