



# Cortellis Drug Discovery Intelligence

## 低分子生理活性物質の物理化学特性データ

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# Cortellis Drug Discovery Intelligence

-Drugs&Biologicsの検索結果画面に低分子生理活性物質の物理化学特性を追加-

物理化学的特性データ

Showing 1-25 of 3867 Drugs & Biologics records for "Cancer, prostate"

物理化学的特性データを見るには、画面下のスクロールバーを右へ。

LogS	LogD	pKa	TPSA	Rotatable Bonds	Aromatic Rings
1.71	-10.52	2.67	340.68	21	2

LogP	HBD	HBA	MW	Lipinski's Rule
✓ -5.11	8	25	1216.115	1

Rule of fiveに当てはまる : ✓  
Rule of fiveに当てはまらない : -

4つのうちいくつ当てはまったか？

物理化学的特性データを見るには、画面下のスクロールバーを右へ。

?

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## -Drugs&Biologicsの検索結果画面に低分子生理活性物質の物理化学特性を追加-

Product List Development Status Milestones Overview

物理化学的特性データ

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Entry Number Highest Phase Organization LogS LogD pKa TPSA Rotatable Bonds Aromatic Rings LogP HBD HBA MW Lipinski's Rule

Entry Number	Highest Phase	Organization	LogS	LogD	pKa	TPSA	Rotatable Bonds	Aromatic Rings	LogP	HBD	HBA	MW	Lipinski's Rule
869108	Pre-Registered	ABX advanced biochemical compounds Deutsches Krebsforschungszentrum (DKFZ) (Originator) Endocyte (Novartis) Novartis	1.71	-10.52	2.67	340.68	21	2	-5.11	8	25	1216.115	1
259673	Launched - 2010	Denderah Pharm Dendreon (Dendreon Pharmaceuticals) Dendreon Pharmaceuticals (Originator) Diosynth (FUJIFILM)											
100830	Launched - 1987	Covis Group Covis Pharma (Covis Group) Sanofi (Originator)	-3.7	2.25	15	92.55	3	1	2.25	1	7	317.221	4

この生理活性物質は組換え融合タンパクなので「物理化学的特性データ」がありません。

# Cortellis Drug Discovery Intelligence

## -Drugs&Biologicsの検索結果画面に低分子生理活性物質の物理化学特性を追加-

The screenshot shows the Cortellis Drug Discovery Intelligence interface. On the left, there's a sidebar with icons for Home, Help, and Clarivate. The main area has tabs for Product List, Development Status, Milestones, and Overview. In the Product List tab, there are two rows of drug entries. The first entry is for '869108' (Pre-Registered) with a chemical structure. The second entry is for '259673' (Launched - 2010) with a chemical structure. A purple arrow points from the 'Customize Columns' button in the top-left corner of the main area to a detailed customization modal window.

**Hide all / Show all**

**必須表示項目**

**非表示**

**表示**

**検索結果ページに表示項目が多すぎて見難い？**

画面左上の[Customize Columns]を使って、表示させたい項目、させたくない項目をカスタマイズ。

※最後の設定が次回ログインしたときに反映されます。

The modal window contains a 'Hide all / Show all' button at the top. Below it is a list of columns with toggle switches. The first two columns, 'Entry Number' and 'Highest Phase', are highlighted with a dashed blue border and labeled '必須表示項目' (Must Show Item). The last column, 'Lipinski's Rule', is also highlighted with a dashed blue border and labeled '表示' (Show). Other columns include 'Code Name', 'Generic Name', 'Brand Name', 'Drug Name (All)', 'Product Category', 'Therapeutic Group', 'Aromatic Rings', 'LogP', 'HBD', 'HBA', 'MW', and 'SA'. Some columns have a lock icon next to their names.

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-Drugs&Biologicsの検索結果画面に低分子生理活性物質の物理化学特性を追加-

Product List Development Status Milestones Overview

Apply Filters

Highest Phase Under Active Development Development Status Milestones Product Category

Drug Type

New Molecular Entity Lead Compound Mechanism of Action Target

Therapeutic Group

Experimental Pharmacology Experimental Models Pharmacokinetics Metabolism

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## 物理化学的特性データ

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pKa	TPSA	Rotatable Bonds	Aromatic Rings	LogP	HBP	HBA	MW	Lipinski's Rule
2.67	340.68	21	2	-5.11	3	25	1216.115	1
15	92.55	3	1	2.25	1	7	317.221	4

降順・昇順並べ替えアイコン

フィルターと、各カラム上部の降順・昇順並べ替えアイコンをご利用頂くことで、より効率的に目的の生理活性物質を探せます。

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## -Drugs&Biologicsの検索結果画面に低分子生理活性物質の物理化学特性を追加-

Property	Description
LogS	Aqueous solubility. Measured as log (solubility measured in mol/l)
LogD	The logarithm of the distribution coefficient is the ratio of the sum of the concentrations of all species of the compound (cation, anion and neutral) in octanol to the sum of the concentrations of all species of the compound in water
pKa	Equilibrium constant between the protonated and deprotonated forms of the compound, based on it's partial charge distribution at pH7.4
TPSA	Topological Polar Surface Area; formed by polarized atoms of the compound. Shows good correlation with passive molecular transport through membranes and useful to estimate the transport properties of drugs.
Rotatable Bonds	Number of rotatable bonds in the compound. One of the topological descriptors
Aromatic Rings	Number of aromatic rings in the compound. One of the topological descriptors
LogP	The logarithm of the partition coefficient is the ratio of the concentration of the compound in octanol to its concentration in water. This is a measure of its lipophilicity and is useful to help predict the penetration of drugs through biological membranes
HBD	Hydrogen Bond Donor; the sum of atoms in the molecule which have hydrogen donor properties
HBA	Hydrogen Bond Acceptor; the sum of atoms in the molecule which have hydrogen acceptor properties
MW	Molecular Weight