Cortellis Drug Discovery Intelligence
低分子生理活性物質の物理化学特性データ

2021年10月

クラリベイト ライフサイエンス＆ヘルスケア事業部

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-

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Product List | Development Status | Milestones | Overview

物理化学的特性データ

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

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。

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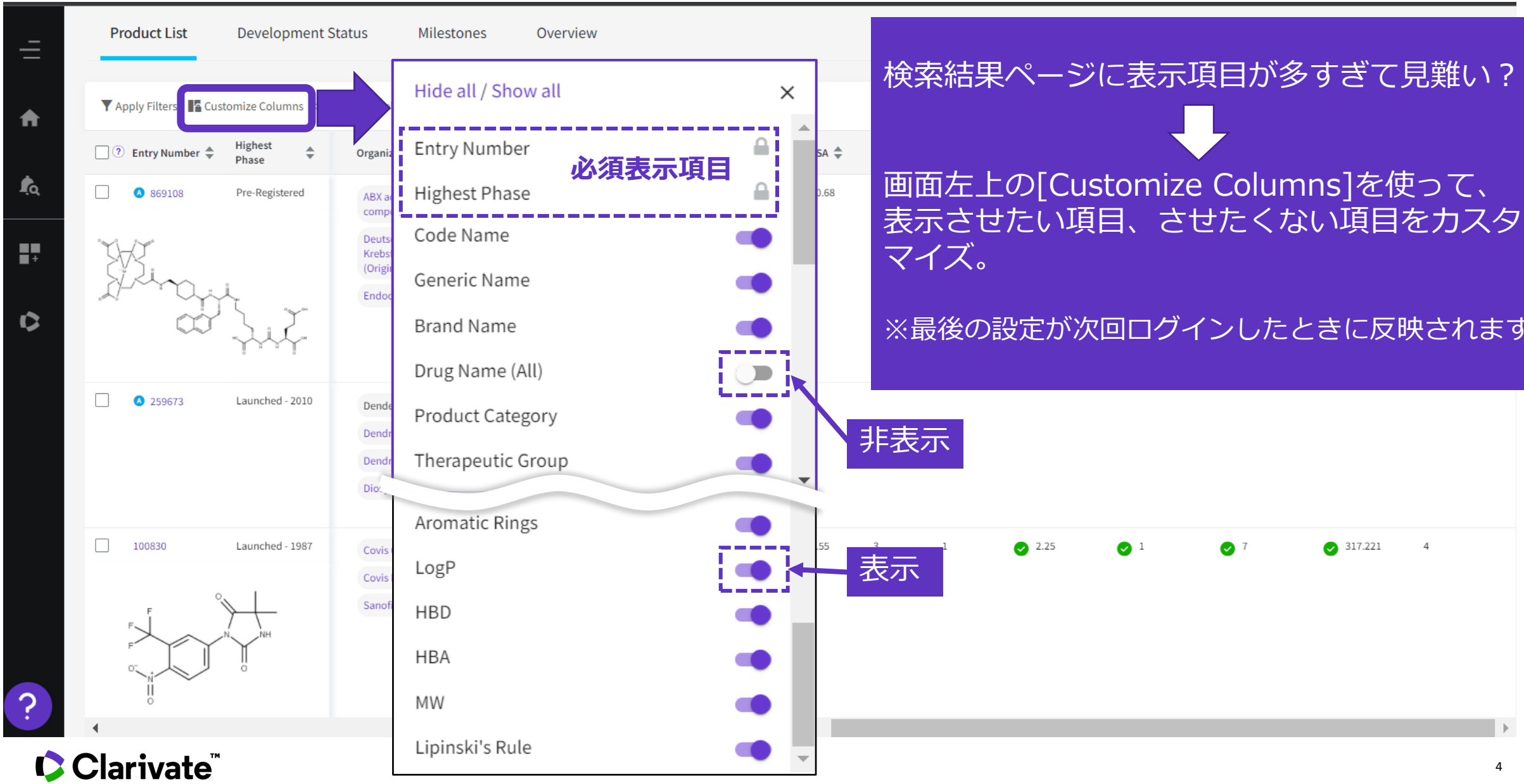

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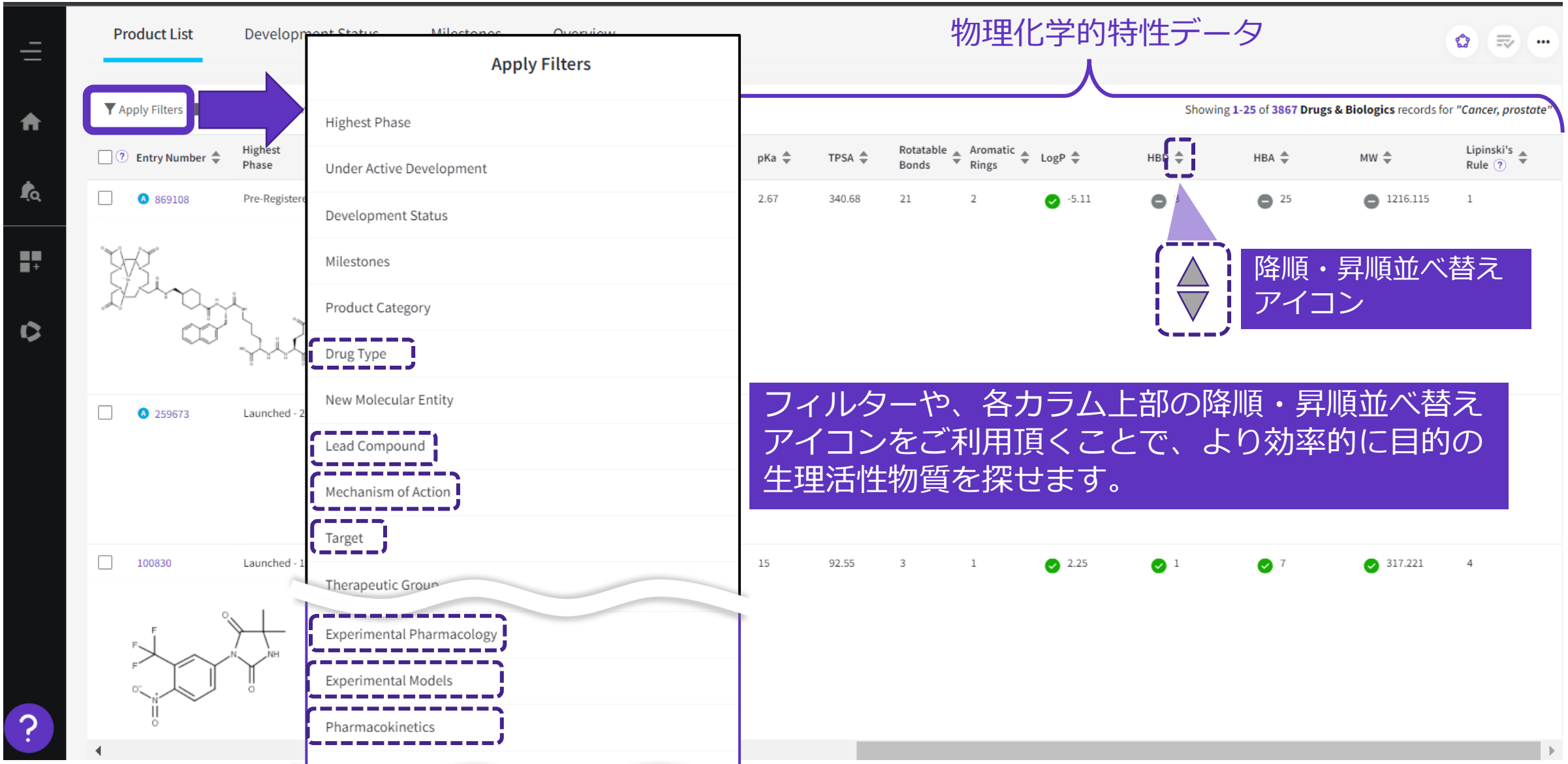

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Property	Description
LogS	Aqueous solubility. Measured as log (solubility measured in mol/l)
LogD	The logarithm of the distribution coefficient is the ratio of the sum of the concentrations of all species of the compound (cation, anion and neutral) 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