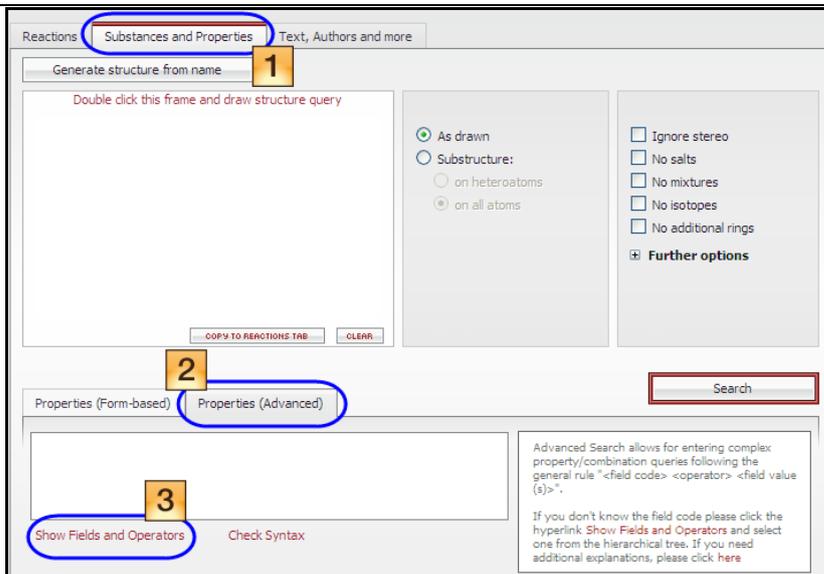
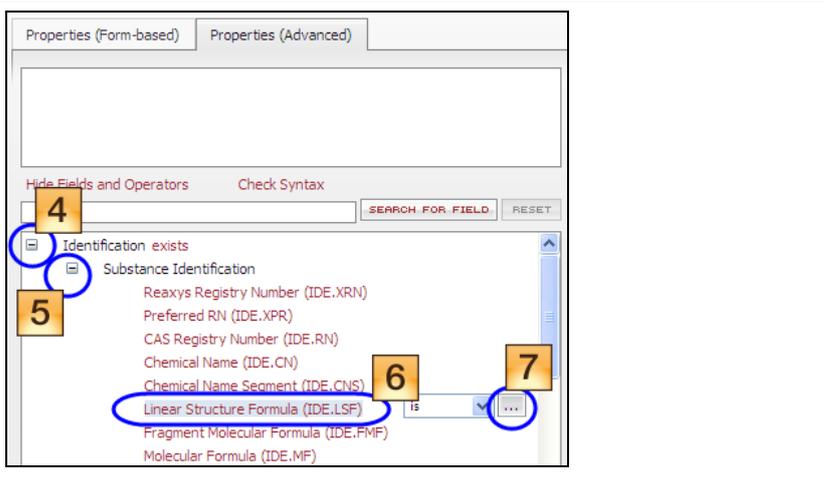


示性式から検索する方法

Question : 化合物を示性式から検索する方法はありますか？

Answer : Advanced Search で Linear Structure Formula を指定することで検索できます。

検索例 : ZNO/TiO₂ (酸化チタン/酸化亜鉛の複合体) の物性値を検索する

<p>Step 1 – 3</p> <p>「Substances and Properties」タブを選択し、「Properties (Advanced)」 → 「Show Fields and Operators」の順にクリックする。</p>	 <p>Reactions Substances and Properties Text, Authors and more</p> <p>Generate structure from name 1</p> <p>Double click this frame and draw structure query</p> <p>As drawn Substructure: <input type="radio"/> on heteroatoms <input checked="" type="radio"/> on all atoms</p> <p>Ignore stereo No salts No mixtures No isotopes No additional rings <input checked="" type="checkbox"/> Further options</p> <p>Properties (Form-based) Properties (Advanced) Search</p> <p>3 Show Fields and Operators Check Syntax</p> <p>Advanced Search allows for entering complex property/combination queries following the general rule "<field code> <operator> <field value (s)>". If you don't know the field code please click the hyperlink Show Fields and Operators and select one from the hierarchical tree. If you need additional explanations, please click here</p>
<p>Step 4 – 7</p> <p>「Identification」→「Substance Identification」→「Linear Structure Formula (IDE.LSF)」の順に選択し、「…」ボタンをクリックする。</p>	 <p>Properties (Form-based) Properties (Advanced)</p> <p>Hide Fields and Operators Check Syntax</p> <p>4 Identification exists</p> <p>5 Substance Identification</p> <p>Reaxys Registry Number (IDE.XRN) Preferred RN (IDE.XPR) CAS Registry Number (IDE.RN) Chemical Name (IDE.CN) Chemical Name Segment (IDE.CNS) 6</p> <p>7 Linear Structure Formula (IDE.LSF) ...</p> <p>Fragment Molecular Formula (IDE.FMF) Molecular Formula (IDE.MF)</p>

Step 8 - 10

入力欄に「zno」と入力し、表示された候補リストの一番上の「ZNO(21)」を選択して「Transfer」ボタンをクリックする。

Step 11

表示された検索式を、手入力で「IDE.LSF = 'zno*tio2」と修正する。

Step 12

「Search」をクリックすると検索結果が表示される。

Structure	Chemical Name	N° of preparations All Preps All Reactions	Available Data	N° of ref.
mixture (composition partially given) ; Titanium(IV) oxide zinc oxide 	titanium oxide doped zinc oxide	1 prep out of 1 reactions.	Physical Data (5) Spectra (3) Use/Application (9)	6

Structure/Compound Data

Reaxys Registry Number: 11381866
 Type of Substance: mixture (composition partially given)

▲ **Composition**

Titanium(IV) oxide	zinc oxide
O_2Ti Synthesize	OZn Synthesize

▲ **Physical Data**

▲ **Crystal Phase (1)**

Description	Comment	Reference
Crystal growth forms	from Gmelin	Chung, Jeng-Lin; Chen, Jyh-Chen; Tseng, Chung-Jen Journal of Physics and Chemistry of Solids, 2008, vol. 69, p. 535 - 539 Title/Abstract Full Text View citing articles Show Details

▲ **Electrical Data (2)**

Description	Comment	Reference
Electronic band structure	from Google	Turkina, L. I.; Sychev, M. M.; Sudakas, L. G. Journal of Applied Chemistry USSR (English Translation), 1981, vol. 5