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KATEの操作説明

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KATEの操作説明 全体の構成

1.生態毒性QSARと「KATE」の紹介

- 生態毒性QSAR・KATEの概要

2.KATEによる予測の流れ

- 実際に一構造を予測

3.Verify QSAR画面

- 予測結果画面の確認・操作方法

4.その他

- 今回操作してお見せできなかった機能等

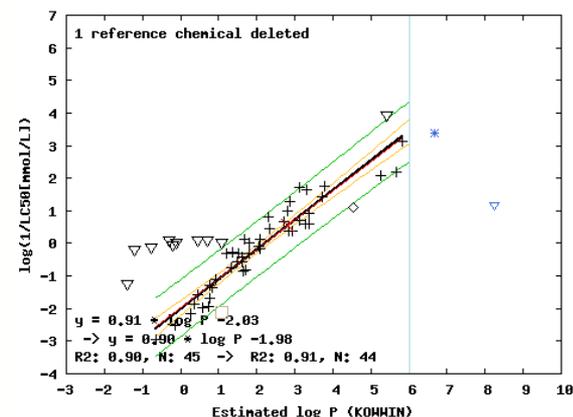
1. 生態毒性のQSAR と「KATE」の紹介



National
Institute for
Environmental
Studies, Japan

QSAR (定量的構造活性相関)
Quantitative Structure-Activity Relationship

- 化学物質の**構造上の特徴**（物理化学的なパラメータを含む）と**生物学的活性**（毒性や薬効など）との間に成り立つ関係のこと
- 定性的な関係の場合： SAR
定量的な関係の場合： QSAR
両者をあわせて(Q)SARと表記する場合があります



「KATE」(ケイト)とは

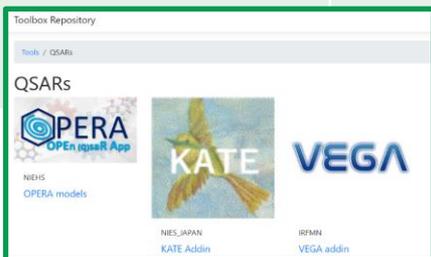
- KATE (KAshinhou Tool for Ecotoxicology)
環境省の請負業務として、国立研究開発法人 国立環境研究所 環境リスク・健康研究領域において、研究・開発されている生態毒性QSARシステムです。
- KATEを構築している参照物質データは、環境省が実施した生態影響試験*結果（魚類、ミジンコ、藻類）及び米国環境保護庁(USEPA)のファットヘッドミノール・データベースの魚類急性毒性試験結果です。

* 環境省試験は、OECDの定めたテストガイドラインに準拠した方法により、環境省の優良試験所基準 (GLP: Good Laboratory Practice)に適合している試験施設において実施されています。

<https://www.env.go.jp/chemi/sesaku/seitai.html>

生態毒性予測に関するQSARソフトの例

名称	開発元	記述子	予測する毒性の種類	その他
KATE	環境省、国立環境研究所環境リスク・健康領域	logP (オクタノール/水分配係数)	藻類・ミジンコ・魚類の急性毒性と慢性毒性 (2020 ver4.1)	・適用領域の判定：構造、logP(記述子)
ECOSAR	米国環境保護庁 (USEPA)	主にlogP	魚類・甲殻類・藻類急性毒性 魚類・甲殻類・藻類慢性毒性(NOECとLOECの幾何平均(ChV))	・適用領域の判定：log P (記述子)
TIMES	ブルガリアブルガス大学	logBCFto _x , LUMO等	魚類・甲殻類急性毒性等	・適用領域の判定：構造、記述子 ・有償
(参考) OECD QSAR Toolbox	OECD、EU	任意 (ユーザーが選択)	任意	・適用領域：ユーザーが判断 ・ユーザーがQSAR式を構築することも可能



←KATEをAddinとしてOECD QSAR Toolboxに組み込むこともできます。

KATE2020で予測可能な毒性の種類

生物群 急性/慢性	生物種	試験	試験期間	毒性指標
魚類急性	メダカ (<i>Oryzias latipes</i>) および フアットヘッドミノー (<i>Pimephales promelas</i>)	魚類急性毒性試験 (OECDテ ストガイドライン203)	96-hr	LC50
ミジンコ急性	オオミジンコ (<i>Daphnia magna</i>)	ミジンコ遊泳阻害試験 (OECDテストガイドライン 202)	48-hr	EC50
藻類急性	<i>Pseudokirchneriella subcapitata</i> *2	藻類生長阻害試験 (OECDテ ストガイドライン201)	72-hr	EC50
魚類慢性	メダカ (<i>Oryzias latipes</i>)	魚類初期生活段階毒性試験 (OECDテストガイドライン 210)	-*1	NOEC
ミジンコ慢性	オオミジンコ (<i>Daphnia magna</i>)	ミジンコ繁殖試験 (OECDテ ストガイドライン211)	21-day	NOEC
藻類慢性	<i>Pseudokirchneriella subcapitata</i> *2	藻類生長阻害試験 (OECDテ ストガイドライン201)	72-hr	NOEC

*1 魚類初期生活段階試験は魚種やふ化日数によって試験期間が異なります

*2 ムレミカヅキモ (*Raphidocelis subcapitata*)の旧名

2. KATEによる予測 の流れ



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1.KATEによる予測の流れ①資料の凡例

注目してほしい項目

説明のポイント

KATEに接続できる方は
実際に操作してみてください

1.KATEによる予測の流れ①KATEへの接続

- KATE(英語)
 - <https://kate.nies.go.jp/>
- KATE(日本語)
 - <https://kate.nies.go.jp/index.html>

注) ホーム画面は英語と日本語版がありますが、予測セッションはいずれも英語です。

1.KATEによる予測の流れ①KATEモデルの選択

The screenshot shows the KATE website interface. At the top, there is a header with the KATE logo and the text "KAshinhou Tool for Ecotoxicity prediction system". Below the header, there is a navigation bar with several buttons: "KATE2020", "KATE on PAS 2011 Japanese", "KATE on NET 2011 Japanese", "Change Log", "Site Policy", and "FAQ". The "KATE2020" button is highlighted with a red box. A green callout bubble points to this button with the text "①KATE2020 を選ぶ". Below the navigation bar, there is a section titled "HOME > KATE2020". Underneath, there is a "KATE2020 login" button, also highlighted with a red box. A green callout bubble points to this button with the text "②予測ページ はここから". Below the login button, there is a section titled "How to use" which contains a paragraph of text and a list of links. The first link in the list, "KATE2020 login (version 4.1)", is highlighted with a red box. Below the "How to use" section, there is a section titled "About KATE2020" which contains a paragraph of text and a list of features.

現在公開しているKATEは
3バージョンです

①KATE2020
を選ぶ

②予測ページ
はここから

KATE2020 login (version 4.1)

KATE2020 login (version 4.1)

KATE2020 Operating manual (PDF 4.6MB)

KATE2020 Technical Document (PDF 1.2MB)

QMR (PDF 0.8MB)

KATE2020 is an updated version of KATE2017 on NET.
For the main changes from "KATE2017 on NET", please see the [Change Log](#).

■ Features

- Prediction of toxicity values for an input chemical (Acute)
 - 50% lethal concentration (LC₅₀) in the fish acute toxicity test (OECD TG 203)

1.KATEによる予測の流れ

①'ユーザー登録が不要になりました

NIES > HERD > KATE > KATE2020
Index

国立研究開発法人
国立環境研究所
National Institute for Environmental Studies

KAshinhou Tool for Ecotoxicity

KATE2020 version 4.1

Terms of Agreement

KOWWIN v1.69 (April 2015)

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KOWWIN is owned by the U.S. Environmental Protection Agency and is protected by copyright throughout the world.

Permission is granted for individuals to download and use the software on their personal and business computers.

Users may not alter, modify, merge, adapt or prepare derivative works from the software. Users may not remove or obscure copyright, tradename, or proprietary notices on the program or related documentation.

KOWWIN contained therein is a tradename owned by the U.S. Environmental Protection Agency.

チェックを
入れて
スタート

I agree to and accept the terms of agreement above.

Start the session

1. KATEによる予測の流れ②Input

Input - login:

The KATE system can predict ecotoxicity of only organic chemicals except for some inorganic nitrogen compounds such as hydrazine.

KATE2020 cannot predict ecotoxicity of chemicals represented as following types of SMILES:

- i. SMILES which does not contain carbon or nitrogen atoms.
- ii. SMILES which includes elements other than H, C, N, O, F, Si, P, S, Cl, As, Br, Sn, and I.
- iii. SMILES which includes ions other than ammonium [N+] or [n+].
- iv. SMILES which includes ".", i.e. SMILES which expresses a mixture.

The strings such as [Na], [K], [Li], [Na+], [K+] and [Li+] in SMILES should be replaced by the protonated forms. For example, "c1ccccc1O[Na]" needs to be replaced by "c1ccccc1O".

Glossary is [here](#).

Thanks to [Chemical Identifier Resolver Service](#) provided by NCI/CADD Group.

Output from <https://cactus.nci.nih.gov> may be shown here.

SMILES
入力規則

物質検索

Input SMILES of your chemical

CAS to SMILES, IUPAC Name Name to SMILES, CAS SMILES to CAS, IUPAC Name

CAS Name

• SMILES * Required

SMILES can be generated by using molecular editor [JSME Editor](#).

log P Optional

When any error occurs in log P calculation by KOWWIN, you can skip KOWWIN Calculation.

Skip KOWWIN Calculation

SMILES
入力

logP入力

物質リスト
の入力

Prediction of Multiple Chemicals

• SMILES List

1.KATEによる予測の流れ②Input

①ペンタンの
SMILES
「CCCCC(大文字の
Cを5つ)」を入力

CAS to SMILES, IUPAC Name Name to SMILES, CAS SMILES to CAS, IUPAC Name

CAS Name

• SMILES * Required

Predict

②クリック

SMILES can be generated by using molecular editor [JSME Editor](#) .

log P Optional

When any error occurs in log P calculation by KOWWIN, you can skip KOWWIN Calculation.

Skip KOWWIN Calculation

1.KATEによる予測の流れ③Results

NIES > HERD > KATE > KATE2020
Index > Input > Results

下の表に表示する項目の選択

User Input Value	
Estimated Value by KOWWIN	2.80
Measured Value in KOWWIN Database	3.39

予測結果のVerifyQSAR画面へ移動

Include (Acute): Fish Daphnid Alga
 Include (Chronic): Fish Daphnid Alga
 Exclude (): R² < 0.7 Q² < 0.5 n < 5

QSAR Results

Print Detail	QSAR Class Name*1 <small>Click the class name to see the QSAR details</small>	Type of Predicted Toxicity*2		Predicted Toxicity [mg/L]	95% Prediction Interval	Statistics of QSAR Class								
		Organism	Acute or Chronic			R ²	Q ²	RMSE	n*5					
<input checked="" type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X			9.2	[1.5, 58]	0.73	0.68	0.36	21(4)					
<input checked="" type="checkbox"/>	narcotic group Fish Acute	Fish	Acute	15	[2.1, 100]	2.80	Estimated	in	[-0.63, 5.88]	in	0.87	0.87	0.43	154(31)
<input type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X	Daphnid	Acute	2.9	[0.28, 30]	0.66	0.51	0.42	15(3)					
<input checked="" type="checkbox"/>	narcotic group Daphnid Acute	Daphnid	Acute	4.0	[0.54, 30]	0.71	0.70	0.43	83(22)					
<input type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X	Alga	Acute	26	[0.64, 1100]	0.66	0.38	0.47	6(12)					
<input checked="" type="checkbox"/>	narcotic group Alga Acute	Alga	Acute			0.76	0.74	0.43	52(48)					

結果一覧出力項目の選択

結果一覧出力

Create Print Format

*1 The query chemical may be classified into multiple QSAR classes.

1.KATEによる予測の流れ③Results

CAS RN*		
Chemical Name		
SMILES	COCCC	
Molecular Weight	72.15	
log P	User Input Value	
	Estimated Value by KOWWIN	2.80
	Measured Value in KOWWIN Database	3.39

Include(Acute): Fish Daphnid Alga
 Include(Chronic): Fish Daphnid Alga
 Exclude(): R² < 0.7 Q² < 0.5 n < 5

QSAR Results

Print Detail	QSAR Class Name	Type of Predicted Toxicity*2		Predicted Toxicity [mg/L]	95% Prediction Interval
		Organism	Acute or Chronic		
<input checked="" type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X	Fish	Acute	9.2	[1.5, 58]
<input checked="" type="checkbox"/>	narcotic group Fish Acute	Fish	Acute	15	[2.1, 100]
<input checked="" type="checkbox"/>	narcotic group Daphnid Acute	Daphnid	Acute	4.0	[0.54, 30]
<input checked="" type="checkbox"/>	narcotic group Alga Acute	Alga	Acute	11	[1.5, 84]
<input checked="" type="checkbox"/>	C_X hydrocarbon unreactive	Fish	Chronic	0.36	[0.033, 3.9]
<input checked="" type="checkbox"/>	Cnos_X unreactive Fish Chronic	Fish	Chronic	0.33	[0.030, 3.7]
<input checked="" type="checkbox"/>	narcotic group Fish Chronic	Fish	Chronic	0.36	[0.036, 3.5]
<input checked="" type="checkbox"/>	narcotic group Daphnid Chronic	Daphnid	Chronic	0.43	[0.037, 4.9]

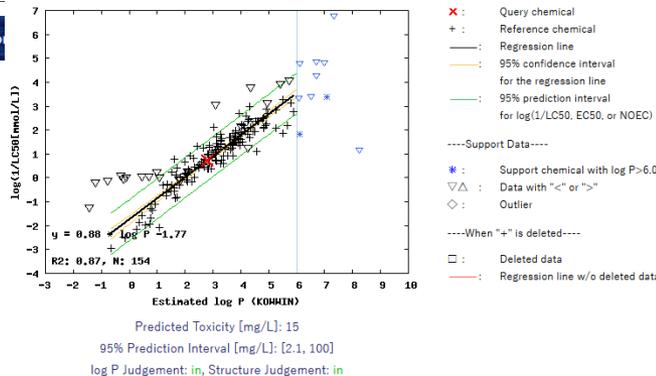
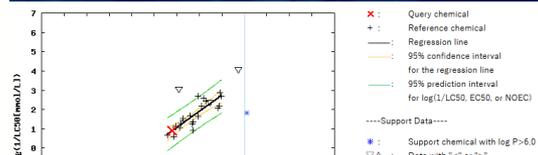
Structural Judgement:

Judgement	FragID	S
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Print Detailにチェックを入れたクラスの予測結果一覧とグラフ情報、参照物質一覧をまとめた頁が作成される

Type: **Fish (acute)** Structure Class ID: GF_28999 QSAR Class Name: narcotic group Fish Acute

Type: **Fish (acute)** Structure Class ID: G1_21203 QSAR Class Name: C_X hydrocarbon



Equation	Number of Chemicals used for Regression	Number of Support Chemicals	Applicable Range of log P	R ²	Q ²	RMSE
y = 0.88 * log P - 1.77	154	31	[-0.63, 5.88]	0.87	0.87	0.43

Reference Chemicals:

CAS No.	Chemical Name	SMILES	Structure Formula	Similarity	Molecular Weight	Estimated log P	Measured Toxicity Data			
							LC50 [mg/L]	log(1/LC50) [mmol/L]	Reference	Note
100-40-3	4-Vinylcyclohexene	C=CC1CCC=CC1		0.290	108.18	3.73	4.6	1.37	MOE 2000	
100-41-4	Ethylbenzene	CCc1ccccc1		0.185	106.17	3.03	10.5	1.00	USEPA	

1.KATEによる予測の流れ③Results

NIES > HERD > KATE > KATE2020

Index > Input > Results

Results

CAS RN [®]		
Chemical Name		
SMILES	CCCC	
Molecular Weight	72.15	
log P	User Input Value	
	Estimated Value by KOWWIN	2.80
	Measured Value in KOWWIN Database	3.39

Include(Acute): Fish Daphnid Alga
 Include(Chronic): Fish Daphnid Alga
 Exclude(): R² < 0.7 Q² < 0.5 n < 5

ドメイン判定結果
(in:内挿、out of:
外挿)

QSAR式統計情報

QSAR Results

Print Detail	QSAR Class Name* ¹ <small>Click the class name to see the QSAR details</small>	Type of Predicted Toxicity* ²		Predicted Toxicity [mg/L]	95% Prediction Interval	log P		Applicability Domain Judgement			Statistics of QSAR Class			
		Organism	Acute or Chronic			Value	Type	log P* ³ [Range]	Structure	R ²	Q ²	RMSE	n* ⁵	
<input checked="" type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X	Fish	Acute	9.2	[1.5, 58]	2.80	Estimated	in	[2.58, 4.98]	in	0.73	0.68	0.36	21(4)
<input checked="" type="checkbox"/>	narcotic group Fish Acute	Fish	Acute	15	[2.1, 100]	2.80	Estimated	in	[-0.63, 5.88]	in	0.87	0.87	0.43	154(31)
<input type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X	Daphnid	Acute	2.9	[0.28, 30]	2.80	Estimated	in	[2.58, 5.74]	in	0.66	0.51	0.42	15(3)
<input checked="" type="checkbox"/>	narcotic group Daphnid Acute	Daphnid	Acute	4.0	[0.54, 30]	2.80	Estimated	in	[1.08, 5.88]	in	0.71	0.70	0.43	83(22)
<input type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X	Alga	Acute	26	[0.64, 1100]	2.80	Estimated	in	[2.58, 4.08]	in	0.66	0.38	0.47	6(12)
<input checked="" type="checkbox"/>	narcotic group Alga Acute	Alga	Acute	11	[1.5, 84]	2.80	Estimated	in	[1.08, 5.26]	in	0.76	0.74	0.43	52(48)

Create Print Format

*1 The query chemical may be classified into multiple QSAR classes.

2.KATEによる予測の流れ③Results

NIES > HERD > KATE > KATE2020

Index > Input > Results

Results

① Include(Acute)のみにチェックが入った状態にしてUpdate

CAS RN®		
Chemical Name		
SMILES	CCCCC	
Molecular Weight	72.15	
log P	User Input Value	
	Estimated Value by KOWWIN	2.80
	Measured Value in KOWWIN Database	3.39

Include(Acute): Fish Daphnid Alga
 Include(Chronic): Fish Daphnid Alga
 Exclude(): R² < 0.7 Q² < 0.5 n < 5

Update

QSAR Results

Print Detail	QSAR Class Name*1 <small>Click the class name to see the QSAR details</small>	Type of Predicted Toxicity*2		Predicted Toxicity [mg/L]	95% Prediction									
		Organism	Acute or Chronic											
<input checked="" type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X	Fish	Acute	9.2	[1.5, 58]	2.80	Estimated	in	[-0.63, 5.88]	in	0.87	0.87	0.43	154(31)
<input checked="" type="checkbox"/>	narcotic group Fish Acute	Fish	Acute	15	[2.1, 100]	2.80	Estimated	in	[-0.63, 5.88]	in	0.87	0.87	0.43	154(31)
<input type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X	Daphnid	Acute	2.9	[0.28, 30]	2.80	Estimated	in	[2.58, 5.74]	in	0.66	0.51	0.42	15(3)
<input checked="" type="checkbox"/>	narcotic group Daphnid Acute	Daphnid	Acute	4.0	[0.54, 30]	2.80	Estimated	in	[1.08, 5.88]	in	0.71	0.70	0.43	83(22)
<input type="checkbox"/>	C_X hydrocarbon unreactive aliphatic w/o X	Alga	Acute	26	[0.64, 1100]	2.80	Estimated	in	[2.58, 4.08]	in	0.66	0.38	0.47	6(12)
<input checked="" type="checkbox"/>	narcotic group Alga Acute	Alga	Acute	11	[1.5, 84]	2.80	Estimated	in	[1.08, 5.26]	in	0.76	0.74	0.43	52(48)

② C_X hydrocarbon unreactive aliphatic w/o Xをクリック

Create Print Format

*1 The query chemical may be classified into multiple QSAR classes.

3. Verify QSAR画面



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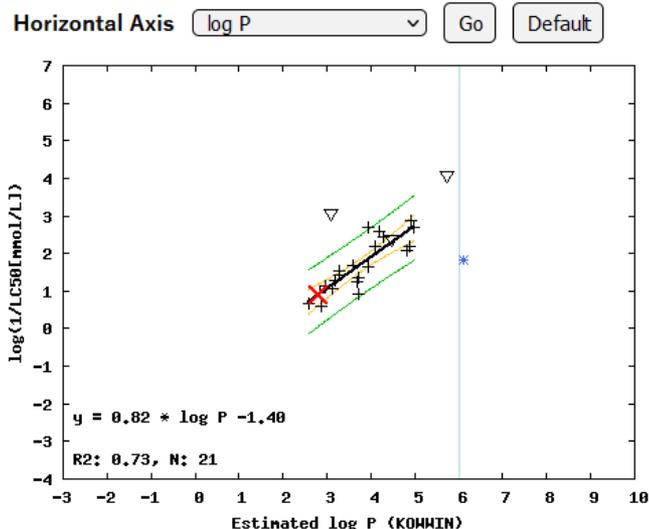
3. Verify QSAR画面①グラフの見方

NIES > HERD > KATE > KATE2020
Index > Input > Results > Verify QSAR

Verify QSAR

Type: Fish (acute) Structure Class ID: G1_21203 QSAR Class Name: C_X hydrocarbon unrea

グラフの凡例



- ✕ : Query chemical
- + : Reference chemical
- : Regression line
- : 95% confidence interval for the regression line
- : 95% prediction interval for log(1/LC50, EC50, or NOEC)
- Support Data---
- * : Support chemical with log P>6.0
- ▽△ : Data with "<" or ">"
- ◇ : Outlier
- When "+" is deleted---
- : Deleted data
- : Regression line w/o deleted data

Query Chemical

SMILES	CCCCC
Chemical Name (User Input)	
CAS RN (User Input)	

Predicted Toxicity [mg/L]: 9.2

95% Prediction Interval [mg/L]: [1.5, 58]

log P Judgement: in, Structure Judgement: in

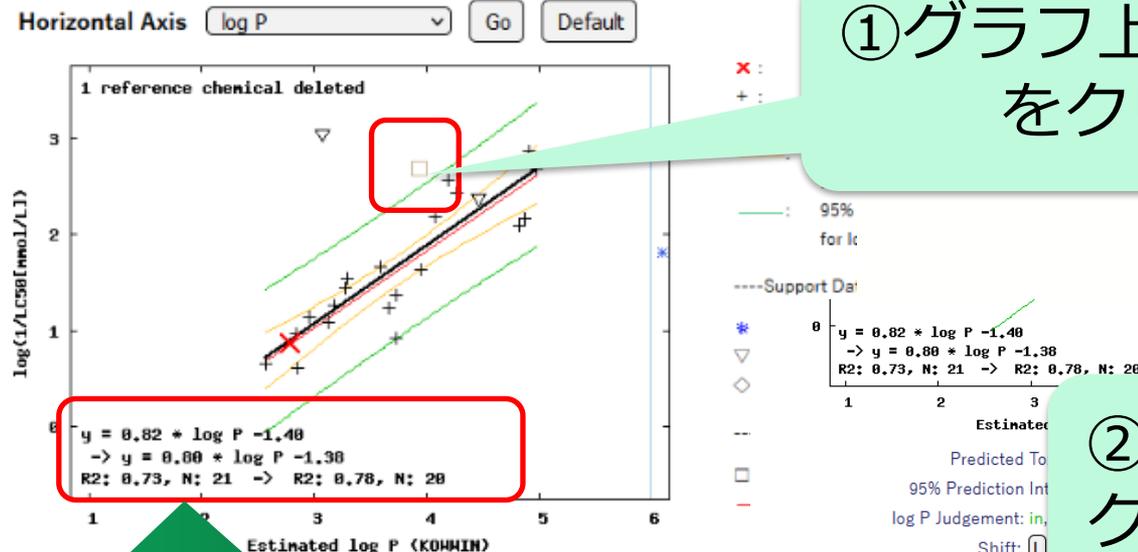
Shift:
Zoom: X: Y:

シフトやズームを操作し、
グラフを見やすい大きさに調整してください
(おすすめはZoomの「+」を4回クリック)

Equation	Number of Chemicals used for Regression	Number of Support Chemicals	Applicable Range of log P
$y = 0.82 * \log P - 1.40$	21	4	[2.58, 4.98]

3. Verify QSAR画面②グラフ上の参照物質の確認

① グラフ上の参照物質をクリック



② もう一度参照物質をクリックして選択解除

選択した参照物質を除いたQSAR式の情報

Equation	Number of Chemicals used for Regression	Number of Support Chemicals	Applicable Range of log P
$y = 0.82 * \log P - 1.40$	21	4	[2.58, 4.98]

Chemical Clicked Last



SMILES: C1C2CC3CC1CC(C2)C3
 CAS: 281-23-2
 Name: Adamantane
 (X, Y): (3.94, 2.69)
 Square of Residual: 0.75
 Molecular Weight: 136.24
 Measured Toxicity Value Data:
 LC50 [mg/L]: 0.28, Species: Pimephales promelas, Reference: USEPA

選択した参照物質の情報

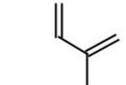
3. Verify QSAR画面③参照物質からグラフを確認

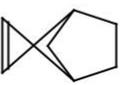
- Chemical List

sort by X-axis with ascending order Update

The value below chemical structure represents the similarity (Tanimoto coefficient with Pub
The figures in parentheses represent the coordinate values (x, y) of the chemical in the

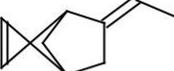
- Reference Chemicals


0.429
(2.58, 0.66)


0.273
(2.85, 0.97)


0.474
(2.86, 0.61)


0.360
(2.96, 1.15)

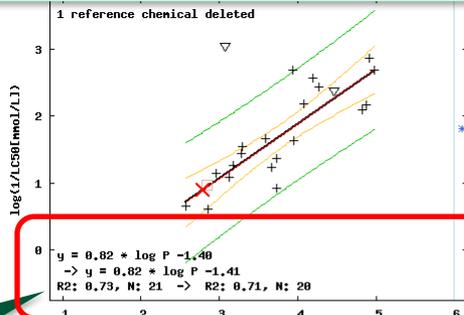

0.286
(3.0, 0.66)


0.320
(3.0, 0.66)


0.290
(3.0, 0.66)


0.321
(3.0, 0.66)

Reference Chemicals
中の構造をクリック



$y = 0.82 * \log P - 1.40$
 $\rightarrow y = 0.82 * \log P - 1.41$
 $R2: 0.73, N: 21 \rightarrow R2: 0.71, N: 20$

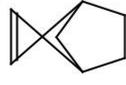
Predicted Toxicity [mg/L]: 9.2
 95% Prediction Interval [mg/L]: [1.5, 58]
 log P Judgement: in, Structure Judgement: in
 Shift: L Dn Up R
 Zoom: - + X: - + Y: - + Default

Equation	Number of Chemicals used for Regression	Number of Support Chemicals	Applicable Range of log P
$y = 0.82 * \log P - 1.40$	21	4	[2.58, 4.98]

選択した参照物質
を除いたQSAR式の
情報

選択した参照物質
の情報

Chemical Clicked Last



SMILES: C1CC2CC1C=C2

CAS: 498-66-8

Name: Norbornylene

(X, Y): (2.85, 0.97)

Square of Residual: 0.00

Molecular Weight: 94.16

Measured Toxicity Value Data:
LC50 [mg/L]: 10, Species: Pimephales promelas, Reference: USA

- Chemical List

3. Verify QSAR画面④構造類似物質の確認

- Chemical List

sort by **X-axis** with **ascending order**

The value below chemical structure represents the similarity (Tanimoto coefficient with Pubchem Fingerprints) to the query chemical structure.

The figures in parentheses represent the coordinate values (x, y) of the chemical in the log(1/LC50, EC50) plane.

Ref Square of Residual
Similarity

- Chemical List

sort by **X-axis** with **ascending order**

The value below chemical structure represents the similarity (Tanimoto coefficient with Pubchem Fingerprints) to the query chemical structure.

The figures in parentheses represent the coordinate values (x, y) of the chemical in the log(1/LC50, EC50) plane.

- Reference Chemicals

0.429 (2.58, 0.66)

0.286 (3.67, 1.23)

0.429 (2.58, 0.66)

0.273 (2.85, 0.97)

0.474 (2.86, 0.61)

0.360 (2.99, 1.17)

0.286

0.320

0.290

① Similarityを選択

② descending orderを選択

③ Update

- Chemical List

sort by **Similarity** with **descending order**

The value below chemical structure represents the similarity (Tanimoto coefficient with Pubchem Fingerprints) to the query chemical structure.

The figures in parentheses represent the coordinate values (x, y) of the chemical in the log(1/LC50, EC50) plane.

- Reference Chemicals

0.909 (3.29, 1.54)

0.692 (3.18, 1.27)

0.667 (4.27, 2.43)

0.526 (3.59, 1.67)

0.474 (2.86, 0.61)

0.474 (3.13, 1.08)

物質が類似度順に並ぶ

4. その他



National
Institute for
Environmental
Studies, Japan

4. その他① 構造判定結果の確認

+ Chemical Data

+ Definition of Structure Class (ID: GA_22075)

- Substructures of the Query Chemical

+ Substructures used only for Structural Classification

- Substructures used for the Judgement of Structure Classification

構造判定結果を構造 (SMARTS)で確認

(参考: 一例として紹介)
 SMARTS可視化サービス SMARTS PLUS(ハンブルク大学)
<https://smarts.plus/>

Hide SMARTS

Judgement*1	TagID	Substructure Name	Count	SMARTS
in	5007	Nitrogen [N,n]	4	[#7]
out of	5084	protein binding 9	1	[!\$(C=C):!(C#C)]C(=[O,SX1,N])[O,S,N][CX4,O,S][\$(C=O).a.\$(C=C).\$(C#C).\$(C=N).\$(C#N)]
out of	5136	IRAC 4 nicotinic AChR agonist	1	nccC[S&\$\$(S(=N)(=O)C).N&X3&!\$(NC=[S,O])]

*1 The "Judgement" result.

in:

in (conditionally)

out of:

農薬や反応性を有する構造の確認も可能

ent result.

gement" extracted from the reference chemicals in the QSAR class.

structure is found in "substructures for structure judgement" extracted from the reference chemicals (conditionally)", that is, the substructure is found in neither the "substructures for structure judgement" extracted from the reference chemicals in the QSAR class.

4. その他②Batch Mode

User Login > Input > Results (batch mode)

Results - login:

Include: Fish (acute) Daphnid (acute) Alga (acute) Fish (chronic) Daphnid (chronic) Alga (chronic)

Exclude: R² < 0.7 Q² < 0.5 n < 5

複数物質(上限100)まで予測可能。
予め物質リスト(.txtファイル)作成の必要あり

表示結果のInclude、Exclude操作

クラス名をクリックしてVerify QSAR画面へ移動

	Molecular Weight	Estimated log P	Structural Formula	QSAR Class Name*1 <small>Click the name to see details of the QSAR model</small>	Type of Predicted Toxicity*2		Predicted Toxicity [mg/L]	95% Prediction Interval
					Organism	Acute or Chronic		
	104.15	2.90		C_X unreactive aromatic w/o X, fused R=0 narcotic group Fish Acute C_X unreactive aromatic w/o X, fused R=0 narcotic group Daphnid Acute narcotic group Alga Acute C_X HC unreactive Cnos_X unreactive Fish Chronic narcotic group Fish Chronic C_X unreactive aromatic w/o X, fused R=0	Fish Fish Daphnid Daphnid Alga Fish Fish Daphnid	Acute Acute Acute Acute Acute Chronic Chronic Chronic	13 16 3.3 4.9 13 0.44 0.41 0.45 1.0	[3.1, 53] [2.5, 110] [0.90, 12] [0.74, 33] [1.6, 110] [0.031, 6.2] [0.030, 5.5] [0.036, 5.5] [0.20, 5.5]
2 2	128.17	2.20						No applicable results
3 3								No applicable results
4 4				ester reactive methacrylate COS_X methacrylate ester reactive methacrylate ester reactive methacrylate COS_X methacrylate ester reactive methacrylate	Fish Fish Daphnid Fish Fish Daphnid	Acute Acute Acute Acute Acute Acute	9.7 11 22 95 150 190	[1.2, 79] [1.7, 68] [0.62, 760] [9.3, 970] [18, 1200] [3.9, 9200]
5 5								No applicable results
6 6								No applicable results
7 7								No applicable results
8 8				narcotic group Fish Acute narcotic group Daphnid Acute CNO_X ester unreactive CNO_X ester unreactive CNO_X ester unreactive Daphnid	Fish Daphnid Fish Daphnid Daphnid	Acute Acute Acute Acute Acute	1.2 0.72 23 51 54	[0.17, 7.7] [0.11, 4.8] [2.9, 190] [6.8, 380] [6.1, 470]
9 9								No applicable results

ご清聴ありがとうございました。

KATEの操作方法に対するご質問、
KATEに対するご意見・ご感想等ございましたら
以下のメールアドレスまでご連絡ください。

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