

ChemTHEATRE MANUAL

(Ver. 2.1.2)

2020.02.27 revised

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1. Introduction

ChemTHEATRE: Chemicals in the THEATRE [Tractable and Heuristic E-Archive for Traceability and Responsible-care Engagement] is the platform to deposit and visualize monitoring data of environmental contaminants more effectively than ever.

You can currently see so many monitoring data of environmental contaminants in scientific journals or reports by public organizations, but unfortunately you can see them in a variety of forms such as texts or excel files. That leads to poor use of such valuable data, which can be input data for the modeling and materials for validation.

To tackle this problem and make use of these valuable data, we first put together such scattered data in one database: ChemTHEATRE, properly and well organized. It will ensure traceability of chemicals and help you simulate the environmental behavior and fate, or assess the risk. Moreover, ChemTHEATRE will make the prediction of global chemical pollution easier in cooperation with external database or other tools in near future.

2. ChemTHEATRE Top page

Chem										Englis
put										
emTHEATRE Wiki			nen	n						
Project Search										
Sample Search				Е				Γ		
Chemical Search		ne to ChemTHEATRE								
	ChemTHEATR ever.	E: Chemicals in the THEATRE [[ractable	and Heuristic E-	Archive for	Traceability and Responsible-care Engageme	ent] is the platform to deposit an	nd visualize monitoring data of environmental conta	minants more effe		English 👻
gister your data: gister@chem-theatre.com										
or inquiry:		in be input data for the modeling and m							la	020050
fo@chem-theatre.com					tered data in one database: ChemTHEATRE, p global chemical pollution easier in cooperatio		II ensure traceability of chemicals and help you sim er tools.	ulate the environm	Ja	panese
f	ChemTHEATR	E was supported through a GrantData o	f Long-range Res	earch Initia	itive (LRI) by Japan Chemical Industry Associa	tion (ICIA).				
CAS RN*	Released	d Entries							Eng	lish≓Japanese
CAS RN* Verified Partner	Sample Top10)			Chemical substance Top10		Contributor Top10			
ite Policy	Sample		#Samples		Chemical	#Data	Submitted by		Swi	tchable!
opyright (C) 2016	Water		2705		Flame retardants PBDEs	9652	Ehime University		Switchabic:	
ChemTHEATRE	Homo sapiens			1585 Organochlorines PCBs		8951	Ministry of the Environment website			
	Sediment		1066		Organochlorines Co-PCBs 6182 National Institute for Environmental Stud		s	9		
		a phocaenoides	216		PAHs	4291	Kagoshima University		5	
	Soil		205		Organochlorines PCDFs	3585	Fisheries Research and Education Agency		4	
	Air		172		Pesticides	3204	Wadsworth Center (New York State Departn	nent of Health)	4	
	Mytilus gallo		169		PPCPs	3147	Hokkaido Research Organization		1	
	Perna viridis		87 0		PPCPs	2853	The University of Tokyo	1	-	
	Katsuwonus				Organochlorines PCDDs	2808	Tokyo University of Agriculture & Technolo			
	Nyctereutes	procyonoides 86 Phenols 2574 Fukuoka Prefecture			1					
	New arri	val project								
	ProjectID	Submitter	ReleaseDate	Date Title				Publication		
	PRA000098	Open data (Ministry of the Environment)	2019/10/18	[MOE_JP]	MOE_JP] The Detailed Environmental Survey in FY2017 (Source: FY2018 Report of Chemicals in the Environment English / Japanese)					
	PRA000097	Open data (Ministry of the Environment)	2019/09/13	[MOE_JP] The Initial Environmental Survey in FY2017 (Source: FY2018 Report of Chemicals in the Environment English / Japanese)						
	PRA000096	PRA000096 Open data 2019/09/02 (Ministry of the Environment)			[MOE_JP] The monitoring of agricultural chemicals in river water in PY2018 (Source: PY2018 (H30)agrichemical monitoring report)					
	PRA000095	Ruriko Tahara (Hokkaido Research Organization)	2019/07/26	[LOC_JP] No. 3 (No		: Environment in Hokkaido (Sou	rce: Report of Institute of Environmental Sciences			
	PRA000094	Takeshi Hano (Fisheries Research and Education Agency)	2019/06/24	Occurren	ce of neonicotinoids and fipronil in estuaries	and their potential risks to aquat	tic invertebrates	10.1016/j.envpol	2019.05.067	
		Open data			The monitoring of agricultural chemicals in r					

2-1. Release Entries and New arrival project

Release Entries	Sample Top 10	The top ten sample groups which are		
		registered in ChemTHEATRE		
	Chemical Substance Top 10	The top ten Chemical groups which are		
		registered in ChemTHEATRE		
	Contributor Top 10	The top ten submitters of monitoring		
		data		
New arrival project	The latest ten projects (Project ID, Submitter, Title, etc.)			

2-2. Menu bar

About	About	Introduction About ChemTHEATRE	
ChemTHEATRE Wiki	ChemTHEATRE Wiki	ChemTHEATRE Wiki	
QProject Search	Project Search	Search by project info. (p.4)	
	Sample Search	Search by sample info. (p.8)	
QSample Search	Chemical Search	Search by chemical info. (p.15)	
QChemical Search	Resister your data: register@chem-theatre.com	Contact address for registration of your data	
Register your data:		or your untu	
register@chem-theatre.com	For inquiry:	Contact address for inquiry	
For inquiry: info@chem-theatre.com	info@chem-theatre.com		
		ChemTHEATRE's Tweeter,	
⊻ f	2	ChemTHEATRE's Facebook	
CAS RN® Verified Partner			
		Indicates that the CAS Registry	
Site Policy	CAS RN [®]	Numbers® of the registered	
Copyright (C) 2016	Verified Partner	chemical substances have been	
ChemTHEATRE	Parcher	confirmed by the Lookup service	
	Site Policy	Terms and conditions of use of	
		ChemTHEATRE	

3. Project Search

<Project search Top>

-	ProjectID			Chemica	l Groups	-		
Sa	mple Type	-	\$	Chemic	al Name	-		
Scien	tific Name	-	\$	Collection	n Region	-		
Tiss	ue / Organ	-	\$	Collection	Country	-		
	Keyword	Project tit	le, Abstract	Collect	tion Year	XXXX	- XXXX	
ow 50 € owing 1 to 5 « 1 2	entries 0 of 96 entries »			Reset				
owing 1 to 5	, 0 of 96 entries		Title 11		Samples	doi 💵	MeasuredData	RegisterDate
owing 1 to 5	,0 of 96 entries	e		urvey in FY2017	Samples Samples	doi 1±	MeasuredData MeasuredData	-

3-1. Search Parameters

-			
Project ID	Project ID which is assigned by ChemTHEATRE		
Sample Type	Select a Sample type from pull-down menu		
	(Biotic \rightarrow Mammals, Birds, Reptiles \cdots Abiotic \rightarrow Water, Sediment \cdots)		
Scientific Name	After selecting a Sample type, pull-down menu of Scientific names		
	categorized in the selected Sample Type shows up. Select one.		
Tissue / Organ After selecting Scientific Name, the pull-down menu of the registered			
	Tissues and Organs shows up.		
Keyword	Search with keywords		
Chemical Groups	Select a Chemical group from pull-down menu		
Chemical Name	After selecting a Chemical Group, the pull-down menu of Chemical		
	Names categorized in the selected Chemical group shows up. Select one.		
Collection Region	Region where the sample was collected. Select one from pull-down		
	menu.		
Collection Country	After selecting Region, the pull-down menu of the Country shows up.		
Collection Year	Year when the sample was collected.		

QSearch

Input parameters and click

. The list of the requested data will appear on the screen.

3 – 2. Project Summary

ProjectID	Submitter 💵	Title li	Samples	doi 💵	MeasuredData	RegisterDate
PRA000002	Kei Nakayama (Ehime University)	Temporal and spatial trends of organotin contamination in the livers of finless porpoises (<i>Neophocaena phocaenoides</i>) and their association with parasitic infection status	Samples	=	MeasuredData	2016/06/27
			Switch	Descen	ding/Ascendi	ng

Project ID	ID which ChemTHEATRE assigns to a paper, report or project
	\rightarrow Click the ID to show the Project Details (p.6)
Submitter	Submitter's name and his/her affiliation name
Title	Project name (Title of his/her paper)
Samples	Link to the list of the samples used for the project
doi	Digital Object Identifier related to the project
	\rightarrow Click the icon to show the original paper
Measured Data	Link to the list of the measured data in the project
Register Date	Register date of the project and its data

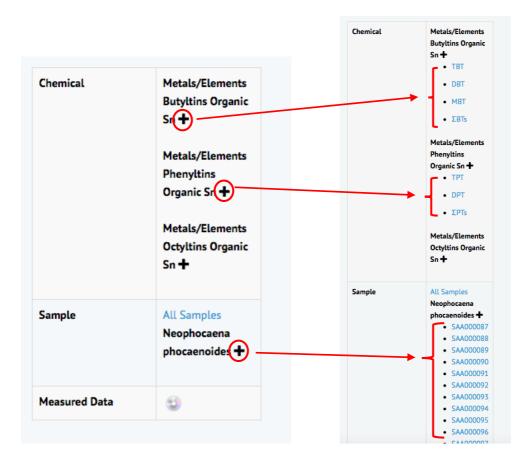
3-3. Project Details

Project Details

Project ID	PRA000002	Chemical	Metals/Elements Butyltins Organic	
Submitter	Ehime University, Kei Nakayama		Sn 🕇	
Corresponding Author			Metals/Elements Phenyltins Organic Sn 🕂	
Release Date	2016/06/27		Metals/Elements	
Title	Temporal and spatial trends of organotin contamination in the livers of finless porpoises (<i>Neophocaena phocaenoides</i>) and their association with parasitic infection status		Octyltins Organic Sn 🕇	
doi	• 10.1016/j.scitotenv.2009.08.043	Sample	All Samples Neophocaena	
Grant	Grants-in-Aid for Scientific Research (S) (No. 20221003) from Japan Society for the Promotion of Science		phocaenoides 🕂	
Register Date	2016/06/27	Measured Data	٢	
Update Date	2016/06/27			

Project ID	ID which ChemTHEATRE assigns to a paper, report or
	project
Submitter	Submitter's name and his/her affiliation name
Corresponding Author	Corresponding author's name and his/her affiliation name
Release Date	Release date in ChemTHEATRE
Title	Project name (title of his/her paper or report)
doi	Digital Object Identifier of the paper related to the project
	\rightarrow Click the doi to show the original paper
Grant	Information on research grant
Register Date	Register date in ChemTHEATRE
Update Date	Date of updating, revising the data in ChemTHEATRE

Chemical	Chemical groups which are measured in the project
	\rightarrow Expand to show the list of chemical names (p.7)
Sample	Scientific names of the samples which are used in the project
	\rightarrow Expand to show the list of samples (p.7)
Measured Data	Click the icon to show the list of measured data



Click "+" to expand

 \downarrow

Chemical names and sample IDs are displayed.

 \downarrow

Click the chemical names or Sample IDs to show the chemical details (p.16) or sample details (p.10).

4. Sample Search

<Sample Search Top>

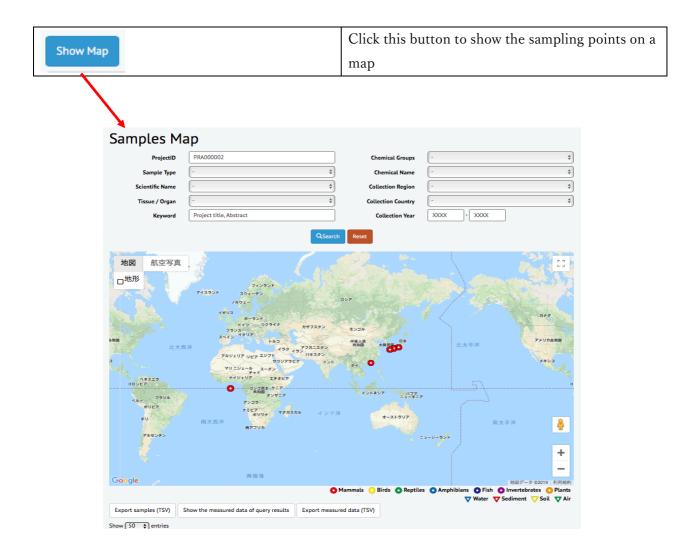
Samples											
ProjectID	PRA000002		Ch	emical Groups	-		\$				
Sample Type	-	\$	c	hemical Name	-		\$				
Scientific Name	-	\$	Col	lection Region			\$				
Tissue / Organ	-	\$	Colle	ection Country		\$					
Keyword	Project title, Abstract		(Collection Year	XXXX - XXXX						
Show Map Export samples (TSV) Show 50 0 entries	Show the sampling points on a map Export samples (TSV) Show the measured data of query results Export measured data (TSV) Show 50 entries Show 50 entries Show 10 for 86 entries										
ProjectID 👔 Samplel	D SampleType	SampleNam	Tissue Ji	Collection Coun	try li Collection Year li	Chemicals 💵	Measured Data				
PRA000002 SAA0000	A000087 Marine Neophocaena phocaenoides mammals - Finless porpoises			Japan	1996	Metals/Elements	٢				
PRA000002 SAA0000	088 Marine mammals	Neophocaena phocaenoides - Finless porpoises	Liver	Japan	1999	Metals/Elements	9				

4-1. Search Parameters

See 3 - 1. (p.4)

4-2. Sample Summary

Project ID	ID which ChemTHEATRE assigns to a paper, report or project
	\rightarrow Click the ID to show the Project Details (p.6)
Sample ID	ID which ChemTHEATRE assigns to a sample used in the project
	\rightarrow Click the ID to show the Sample Details (p.10)
Sample Type	Kinds of sample
	(Biotic→Mammals, Bird, etc. / Abiotic→Water, Sediment, etc.)
Sample Name	Scientific Name and Common Name are shown here.
Tissue	Names of Tissue, organs used in the project
Collection Country	Sampling country
Collection Year	Sampling year
Chemicals	Only chemical groups with measured data are shown here.
Measured Data	Click this icon to show the list of measured data



4-3. Sample Details

Sample ID	SAA000087	Switchable	Projects	 PRA000002 		
Sample Type	Marine mamm	nals	Chemical	Metals/Elements Buty	ltins Organic Sn 🕂	
Taxonomy ID	34892			Metals/Elements Phenyltins Organic Sn +		
Scientific Name	Neophocaena ;	phocaenoides		Metals/Elements Octy		
Common Name	Finless porpoi	ses		Freidig eternents octy	and organic on P	
Collection Year	1996		Measured Data	9		
Collection Month	4		Data			
Collection Day	18					
Collection Region	Asia					
Collection Country	Japan					
Collection Area	Seto Inland Se					
Collection Latitude From	33.61055556	Sampling point is sh	-	•		
Collection Latitude To	33.91	all of latitudes (F		and longitudes		
Collection Longitude From	131.1952778	(From/To) are inpu	t.			
Collection Longitude To	134.6513889					
	127 137 137 137 137	北朝鮮 本時民団 上古町 一部 第二 一部 一部 一部 一部 一部 一部 一部 一部 一部 一部	Projec	this sam →Click the Proj ical Chemica measure	IDs in whic ple is used the ID to show ect details (p.6 al Groups ed by using thi	
Tissue / Organ	Liver	2019 Google, SK telecom 利用規約		sample → Expai	nd to show th	
Weight	5.25				chemical name	
Weight Unit	kg			(p.7)		
Length	72		Measu	-	e icon to show	
Length Unit	cm		Data		asured data c	
Length Type	Body length			this sam		
Uniq Code Type	es-BANK				1 -	
Uniq Code	EW00884					
Register Date	2016/6/27					

General	Sample ID	試料 ID						
info.	Sample Type	試料タイプ (種類)						
Biotic	Taxonomy ID	NCBI 生物分類 ID						
	Scientific Name	学名						
	Common Name	一般名						
	Collection Year	採取年						
	Collection Month	採取月						
	Collection Day	採取日						
	Sampling Time (Start/End)	サンプリング時間(開始時/終了時)						
	Sampling Time (AM PM)	サンプリング時間(午前・午後)						
General	Sampling Duration	サンプリング継続時間						
info.	Weather (Start/End)	天候(開始時/終了時)						
	Temperature (°C) (Start/End)	温度(℃)(開始時/終了時)						
	Collection Region	採取地域						
	Collection Country	採取国						
	Collection Area	採取地						
	Collection Latitude From	採取地の緯度 (From)						
	Collection Latitude To	採取地の緯度 (To)						
	Collection Longitude From	採取地の経度 (From)						
	Collection Longitude To	採取地の経度(To)						
	Maps	マップ						
	Tissue/Organ	組織/臓器						
	Tissue Lipid (%)	脂質含量(%)						
	Tissue Moist (%)	水分含量(%)						
	Sex	性別						
	Weight	重量						
Biotic	Weight Unit	重量単位						
	Length	長さ						
	Length Unit	長さの単位						
	Length Type	長さのタイプ						
	Growth Stage	成長段階						
	Age	年齢						
	Disease	疾病						

	Water Temperature (°C)(Start/End)	水温 (℃) (開始時/終了時)						
	pH	pH						
	DO (mg/L)	溶存酸素量 Dissolved Oxygen (DO)						
	EC (mS/m)	電気伝導率 Electrical Conductivity (EC)						
Water	Salinity	塩分濃度						
	SS (mg/L)	浮遊物質/懸濁物質 Suspended solids /substance (SS)						
	Water Depth (m)	水の深度 (m)						
	Transparency (m)	透明度 (m)						
	Water Color	水の色						
	Sediment Temperature (°C)(Start/End)	底質の温度 (℃) (開始時/終了時)						
	Sediment Depth (m)	底質の深度(m)						
	Sediment Appearance	底質の外観						
	Sediment Color	底質の色						
Sediment	Sediment Surface Color	底質表層の色						
	Sediment Odor	底質の臭気						
	Sediment Impurities	底質中の不純物						
	Sediment Moisture (%)	底質の湿度(%)(採取時/測定時)						
	(On Site / Analysis)							
	Ignition Loss (%) (On Site / Analysis)	強熱減量(%)(採取時/測定時)						
Soil	Soil Depth (m)	土壌の深度(m)						
	Wind Direction (Start / End)	風向(開始時/終了時)						
	Wind Speed (m/s) (Start / End)	風速 (m/s) (開始時/終了時)						
	Flow Rate	流速						
Air	Humidity (%) (Start / End)	湿度(%)(開始時/終了時)						
	Amount Of Collected Air (Start / End)	大気採取量(開始時/終了時)						
	Mean PM10	PM10 平均值						
	Mean Total Suspended Particles	総浮遊粒子 平均值						
	Sample Name	試料名						
	Uniq Code Type	固有コード種						
General	Uniq Code	固有コード						
info.	Remarks	備考						
	Register Date	登録日						
	Update Date	更新日						

4-4. How to export the data you need

Export samples (TSV) Show the meas	ured data of query results Export measured data (TSV)				
Export samples (TSV)	Click this button to export the sample list, after				
	narrowing down the samples to ones you need; an				
	example is below. (p.13) (Tab-separated format)				
Show the measured data of query results	Click this button to show the measured data together				
	with chemicals on the screen; an example is below. (p.14)				
Export measured data (TSV)	Click this button to export the measured data list, after				
	narrowing down the data to ones you need; an example is				
	below. (p.14) (Tab-separated format)				

Export samples (TSV)

=> Sample list (TSV file) exported by clicking this button is as below.

		ы р.	୍ କ୍ କ						📄 samp	les_201910210	133552.tsv										0
ホーム	挿入	ページレ	イアウト 数式		校関	表示														4 * :	共有・
<mark>r - 7</mark>		IS Pゴシッ	ック * 12	• A*	A.	= =	- 2	•	文字列の	折り返し	標準		٣		•		v		∑ - • -	2 ₹	
		BI	<u>u</u> • 🔄 • 🔌	• <u>A</u> •	abc *	= =		•=	🕶 セルを組	合して中央揃え ▼	2 -	% 000	00. 0.¢ 0.¢ 00.	条件付き 書式	テーブルと して書式設				**	<替え/フィルター	
1 ;	\$ ×	$\sqrt{-f_X}$	ProjectID																		
Α	в	C	D E	F	0	н	1	a	к	L M	N	0	Р	0	R	s	т	U	v	w	x
ProjectID	SampleID	SampleType	TaxonomyID UnigCodeT	v UnigCode	SampleNam	e ScientificNar (CommonNarr C	ollectionYe	CollectionMc C	ollectionDa Sampling	Tim Sampling Ti	m SamplingD	w WeatherSta	r CollectionRe	CollectionCc	CollectionAn	CollectionLa C	ollectionLa	CollectionLo	CollectionLo Sex	
PRA000002	SAA000087	ST004	34892 es-BANK	EW00884		Neophocaen F		1996	4	18				Asia			33.6105556		131,195278		
	SAA000088	ST004	34892 os-BANK	EW00812		Neophocaen F		1999	7	19							33,6105556	33.91	131,195278		
	SAA000089		34892 es-BANK	EW00873		Neophocaen F		1995	5	21							33.6105556		131,195278		
PRA000002	SAA000090	ST004	34892 os-BANK	EW04787		Neophogen F	inless nom	2000	9	29				Asia	Japan	Seto Ioland	33 6105556	33.91	131 195278	134.651389	
PRA000002	SAA000091	ST004	34892 es-BANK	EW00867		Neophocaen F		1998	5	7						Seto Inland	33.6105556	33.91	131,195278	134.651389	
PRA000002	SAA000092	ST004	34892 es-BANK	EW00910		Neophocaen F	inless nom	1997	9	8				Asia	Japan	Seto Ioland	33.6105556	33.91	131,195278	134 651389	
	SAA000093		34892 es-BANK	EW04790		Neophocaen F		2001	2	3							33.6105556		131,195278		
	SAA000094		34892 es-BANK	EW00903		Neophocaen F		1997	2	28							33.6105556	33.91	131,195278		
	SAA000095		34892 os-BANK	EW04806		Neophocaen F		2001		14							33.6105556		131.195278		
	SAA000096		34892 es-BANK	EW00911		Neophocaen F		1998		13				Asia			33.6105556	33.91	131,195278		
	SAA000097		34892 es-BANK	EW04703		Neophocaen F		2000	10	19							33.6105556		131,195278		
	SAA000098		34892 es-BANK	EW04595		Neophocaen F		2000	5	18				Asia			33.6105556	33.91	131,195278		
	SAA000099		34892 es-BANK	EW00931		Neophocaen F		1996	4	30							33.6105556		131,195278		
	SAA000100		34892 os-BANK	EW00878		Neophogaen F		1995	7	17				Asia			33.6105556		131.195278		
	SAA000101		34892 es-BANK	EW00929		Neophocaen F		1998	9	12				Asia			33.6105556		131,195278		
	SAA000102		34892 es-BANK	EW04908		Neophocaen F		2002									33.6105556		131,195278		
	SAA000102		34892 es-BANK	EW04883		Neophocaen F		2002	-	11							33.6105556		131.195278		
	SAA000104		34892 es-BANK	EW00934		Neophocaen F		1996		18							33.6105556		131,195278		
	SAA000105		34892 os-BANK	EW00894		Neophocaen F		1996	2	23							33.6105556	33.91	131.195278		
	SAA000105		34892 es-BANK	EW00909		Neophocaen F		1997		20							33.6105556		131.195278		
	SAA000105		34892 es-BANK	EW00909		Neophocaen F		1998	9	25							33.6105556	33.91		134.651389	
	SAA000107 SAA000108		34892 es-BANK	EW04788				2000		25							33.6105556		131.195278		
	SAA000108		34892 es-BANK	EW00921		Neophocaen F		1998	12	12							33.6105556	33.91		134.651389	
	SAA000109 SAA000110		34892 es-BANK 34892 es-BANK	EW00921		Neophocaen F		2002	12	12							33.6105556	33.91	131.195278		
	SAA000110 SAA000111		34892 es-BANK	EW00893		Neophocaen F		1996		23							33.6105556	33.91	131.195278		
	SAA000111 SAA000112		34892 es-BANK 34892 es-BANK	EW00893		Neophocaen P		1996	5	23							33.6105556		131.195278		
	SAA000112 SAA000113			EW04896				2003	2	10							33.6105556				
			34892 es-BANK			Neophocaen F			5	25								33.91	131.195278		
	SAA000114		34892 es-BANK	EW00895 EW00885		Neophocaen F		1996	6	25							33.6105556				
	SAA000115		34892 es-BANK						5								33.6105556	33.91	131.195278		
	SAA000116		34892 es-BANK	EW04866		Neophocaen F		2003	4	21							33.6105556		131.195278		
	SAA000117		34892 os-BANK	EW00925		Neophocaen F		1999	2	15				Asia			33.6105556	33.91	131.195278		
	SAA000118		34892			Neophocaen F		1905	6	25							33.6105556		131.195278		
	SAA000119		34892 os-BANK	EW00904		Neophocaen F	inless porp	1997	4	1				Asia	Japan 1		33.6105556		131.195278		

Show the measured data of query results

=> The measured data displayed on the screen is as below.

Measu	redDa	ta										
	ProjectID	PRA000002		Che	mical Groups -			\$				
s	SampleID			Ch	Chemical Name							
Sam	nple Type	-		¢ Colle	Collection Region							
Scienti	ific Name	-		¢ Colle	ction Country			\$				
Tissue	e / Organ	-		÷ Ca	Collection Year XXXX - XXXX							
	Keyword Project title, Abstract											
Export sample: Show 50 + e Showing 1 to 50	entries	6 7 8 18 1	9 »									
ProjectID 🔒	SampleID 斗	Sample 11	Chemical 11	ExperimentID	MeasuredValue	Unit 👫	Remarks 11	RegisterDate				
PRA000002	SAA000170	Neophocaena phocaenoides	ΣΡΤs	EXA000001	1.68E+1	ng/g wet		2016/7/04				
PRA000002	SAA000170	Neophocaena phocaenoides	DPT	EXA000001	1.41E+0	ng/g wet		2016/7/04				
PRA000002	SAA000170	Neophocaena phocaenoides	трт	EXA000001	1.54E+1	ng/g wet		2016/7/04				
PRA000002	SAA000170	Neophocaena phocaenoides	ΣBTs	EXA000001	2.02E+3	ng/g wet		2016/7/04				
PRA000002	SAA000170	Neophocaena phocaenoides	MBT	EXA000001	1.10E+3	ng/g wet		2016/7/04				
PRA000002	SAA000170	Neophocaena phocaenoides	DBT	EXA000001	7.20E+2	ng/g wet		2016/7/04				
PRA000002	SAA000170	Neophocaena phocaenoides	твт	EXA000001	2.00E+2	ng/g wet		2016/7/04				
PRA000002	SAA000169	Neophocaena phocaenoides	Σoctyltins	EXA000001	-	ng/g wet		2016/7/04				
PRA000002	SAA000169	Neophocaena phocaenoides	мот	EXA000001	<6.00E-1	ng/g wet		2016/7/04				

Export measured data (TSV)

=>Measured data list (TSV file) exported by clicking this button is as below.

	00		ю - б	Ŧ						measured	data_2019	1021033602	.tsv
차	- <u>-</u> _	挿入 ペ-	ージ レイアウ	っト 数式	データ	校閲	表示						
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A1	* *	× v	$f_{\!X}$ Meas	suredID									
	А	в	С	D	E	F	G	н	I	J	к	L	м
1 N	leasuredID	ProjectID	SampleID	ScientificNa	ChemicalID	ChemicalNa	ExperimentII	MeasuredVa	Alternative	Unit	Remarks	RegisterDat	UpdateDat
2		PRA000002		Neophocaen			EXA000001	170		ng/g wet		2016/7/4	2016/8/
3	81	PRA000002	SAA000087	Neophocaen	CH0000155	DBT	EXA000001	220.3591		ng/g wet		2016/7/4	2016/8/
1	82	PRA000002	SAA000087	Neophocaen	CH0000156	MBT	EXA000001	44.5445		ng/g wet		2016/7/4	2016/8/
5	83	PRA000002	SAA000087	Neophocaen	CH0000157	ΣBTs	EXA000001	434.9036		ng/g wet		2016/7/4	2016/8/
3	84	PRA000002	SAA000087	Neophocaen	CH0000158	TPT	EXA000001	12.922		ng/g wet		2016/7/4	2016/8/
7	85	PRA000002	SAA000087	Neophocaen	CH0000159	DPT	EXA000001	0.395		ng/g wet		2016/7/4	2016/8/
3	86	PRA000002	SAA000087	Neophocaen	CH0000160	ΣPTs	EXA000001	13.317		ng/g wet		2016/7/4	2016/8/
9	87	PRA000002	SAA000087	Neophocaen	CH0000161	TOT	EXA000001	0.6	<6.00E-1	ng/g wet		2016/7/4	2018/6/1
0	88	PRA000002	SAA000087	Neophocaen	CH0000162	DOT	EXA000001	1.7	<1.70E+0	ng/g wet		2016/7/4	2018/6/1
1	89	PRA000002	SAA000087	Neophocaen	CH0000163	MOT	EXA000001	1.5092		ng/g wet		2016/7/4	2016/8/
2	90	PRA000002	SAA000087	Neophocaen	CH0000164	Σ octyltins	EXA000001	1.5		ng/g wet		2016/7/4	2016/8/
3	91	PRA000002	SAA000088	Neophocaen	CH0000154	TBT	EXA000001	61.2117		ng/g wet		2016/7/4	2016/8/
4	92	PRA000002	SAA000088	Neophocaen	CH0000155	DBT	EXA000001	120		ng/g wet		2016/7/4	2016/8/
5	93	PRA000002	SAA000088	Neophocaen	CH0000156	MBT	EXA000001	7.2268		ng/g wet		2016/7/4	2016/8/8
6	94	PRA000002	SAA000088	Neophocaen	CH0000157	ΣBTs	EXA000001	188.4385		ng/g wet		2016/7/4	2016/8/
7			SAA000088				EXA000001	8.099		ng/g wet		2016/7/4	2016/8/
8	96	PRA000002	SAA000088	Neophocaen	CH0000159	DPT	EXA000001	0.632		ng/g wet		2016/7/4	2016/8/
9	97	PRA000002	SAA000088	Neophocaen	CH0000160	ΣPTs	EXA000001	8.731		ng/g wet		2016/7/4	2016/8/
0			SAA000088				EXA000001	0.6	<6.00E-1	ng/g wet		2016/7/4	2018/6/13
1				Neophocaen			EXA000001		<1.70E+0	ng/g wet		2016/7/4	2018/6/13

5. Chemical Search

<Chemical Search Top>

Chemic	als						
	ChemicalID	СН000000					
	Chemical Groups						\$
	Chemical	Chemical Name, IUPAC,	Synonyms				
	CAS RN ®	CAS					
Show (50 ¢) en Showing 1 to 50 of « 1 2 ChemicalID 11		23 24		PubChem	CAS RN ®	Synonyms 11	Samples
CH0000001	Organochlorines	2,3,7,8-TCDD	2,3,7,8-tetrachlorodibenzo-p-	15625	1746-01-6	2,3,7,8-Tetrachlorodibenzo-p-	Samples
CHOODOOI	Dioxins PCDDs	2,3,7,8-1000	dioxin	13023	1/40-01-0	dioxin, TCDD, Dioxin	Samptes
СН000002	Organochlorines Dioxins PCDDs	1,2,3,7,8-PentaCDD	1,2,3,7,8-pentachlorodibenzo- p-dioxin	38439	40321-76-4	1,2,3,7,8-pentachlorodibenzo-p- dioxin, PeCDD	Samples

5-1. Search Parameters

Chemical ID	ID which ChemTHEATRE assigns to a chemical
Chemical Group	Select a chemical group from the pull-down menu
	(e.g.) Organochlorines-Dioxins
Chemical	Search with keywords such as chemical names, IUPAC
CAS RN®	Search with CAS Registry Number®

Input parameters and click

. The list of the requested data will appear on the screen.

5-2. Chemicals Summary

QSearch

Chemical ID	ID which ChemTHEATRE assigns to a chemical
	\rightarrow Click the ID to show the Chemical Details. (p.16)
Chemical Group	Chemical group which the chemical is categorized into
Chemical Name	Chemical name
IUPAC	IUPAC name of the chemical
PubChem	PubChem CID and the link to PubChem Compound records
CAS RN®	CAS registry number®
Synonyms	Common names, other names of the chemical
Samples	Click <u>Samples</u> to show the list of Sample IDs used to measure the chemical

5-3. Chemical Details

Chemical

ChemicalID	CH0000001		Projects	• PRA000004
ChemGroup	Organochlorines Dioxins PCDDs	Click "+"		PRA00005 PRA000021 PRA000024 PRA000038
Chemical Name	2,3,7,8-TCDD	Chick		 PRA000058 PRA000059
IUPAC	2,3,7,8-tetrachlorodibenzo-p-dioxin	\downarrow		 PRA000069 PRA000070
Synonyms	2,3,7,8-Tetrachlorodibenzo-p-dioxin, TCDD, Dioxin	Expand		• PRA000071
PubChem	15625	Ļ		 PRA000081 PN-000086
CAS RN ©	1746-01-6	Comple ID-	Samples	Nyctereutes procyonoides +
Remarks	Link to Webkis-plus;	Sample IDs	Junpies	\smile
RegisterDate	2016/8/18	are displayed		Apodemus speciosus 🕂
UpdateDate	2016/8/26	are displayed (See p.7)		Mogera imaizumii 🕇
		(occ p.1)		Phoebastria albatrus 🕂

Chemical ID	ID which ChemTHEATRE assigns to a chemical		
ChemGroup	Chemical group which the chemical is categorized into		
Chemical Name	Chemical name		
IUPAC	IUPAC name of the chemical		
Synonyms	Common names, other names of the chemical		
PubChem	PubChem CID and the link to PubChem Compound		
	records		
CAS RN®	CAS registry number®		
Remarks	Remarks, link to Webkis-Plus		
Register Date	Date of registration to ChemTHEATRE		
Update Date Date last modified			

Projects	Project IDs in which the chemical was measured
	\rightarrow Click the ID to show the Project details (p.6)
Samples	Sample types used to measure the chemical
	\rightarrow Expand to show the sample IDs.
	\rightarrow Click the ID to show the Sample Details (p.10)

6. Measured Data (Chemical concentration)

<Measured Data Top>

Measur	edData								
	ProjectID				Chemical	Groups			
	SampleID				Chemica	al Name		\$	
	Sample Type			\$	Collection	Region		\$	
S	cientific Name	-		\$	Collection	Country	•	\$	
1	Fissue / Organ	-		\$	Collecti	ion Year	XXXX · XXXX		
	Keyword	Project title, Al	ostract						
Export samples Show 50 \$ er Showing 1 to 50 c « 1 2	ntries	neasured data (T		Qsearch	Reset See p.13-14)				
ProjectID	SampleID 1	Sample 💵	Chemical 💵	ExperimentID	MeasuredValue	Unit 👫	Remarks 1	RegisterDate 斗	
PRA000098	SAA006432	Air	Alchol ethoxylate C15EO15	EXA000001	<1.20E-3	µg/L	Quantified using C12EO15 as Standard	2019/10/18	
PRA000098	SAA006350	Water	Alchol ethoxylate C15EO15	EXA000001	<1.20E-3	µg/L	Quantified using C12EO15 as Standard	2019/10/18	

6-1. Search Parameters

See 3-1. (p.4)

6-2. Measured Data Summary

Project ID	ID which ChemTHEATRE assigns to a project
	\rightarrow Click the ID to show the Project Details (p.6)
Sample ID	ID which ChemTHEATRE assigns to a sample used in the project
	\rightarrow Click the ID to show the Sample Details (p.10)
Sample	Sample types are shown. (Mammal, Bird, Water, Sediment, etc.)
Chemical	Chemical name which is measured
	\rightarrow Click the name to show the Chemical Details (p.16)
Experiment ID	Experiment ID which is assigned by ChemTHEATRE
Measured Value	Measured value (chemical concentration)
Unit	Unit (µg/L, ng/g, etc.)
Remarks	Remarks (additional information, etc.)
Register Date	Date of registration to ChemTHEATRE

6-3. How to export the data you need (See 4-4. (p.13-14))

Export samples (TSV)	Click this button to export the sample list, after narrowing down the
	samples to ones you need (Tab-separated format) \rightarrow See p.13
Export measured data	Click this button to export the measured data list, after narrowing down
(TSV)	the data to ones you need. (Tab-separated format) \rightarrow See p.14

7. Ecological Risk Assessment using ChemTHEATRE

~Example for carrying out the risk assessment~

This is an example of step by step procedure to do the risk assessment using ChemTHEATRE.

7-1. How to find and export the measured data you need in ChemTHEATRE

< Narrow down the data by Chemical => Sample type >

① Firstly, select "Perfluoroalkyl and Polyfluoroalkyl substances - PFCAs" from pull-down menu in

Chemical Group column. Then, click ^{Qsearch}. Chemicals categorized into PFCAs are shown on the

screen as below.

Chemic	als							
	ChemicalD CH0000000							
	Chemical Groups Perfluoroalkyl substances - PFCAs \$							
	Chemical	Chemical Name, IUPAC, Synon	yms					
	CAS RN @	CAS						
Show 50 0 ent Showing 1 to 16 of			QSearch Reset					
ChemicalID 1	ChemGroup	ChemicalName	IUPAC IL	PubChem	CAS RN® 11	Synonyms Iž	Samples	
CH0000368	Perfluoroalkyl and polyfluoroalkyl su PFCAs	bstances PFBA	2,2,3,3,4,4,4-heptafluorobutanoic acid	9777	375-22-4	Perfluorobutyric acid	Samples	
CH0000369	Perfluoroalkyl and polyfluoroalkyl su PFCAs	bstances PFPA	2,2,3,3,4,4,5,5,5-nonafluoropentanoic acid	75921	2706-90-3	PFPeA, Perfluoropentanoic acid	Samples	
СН0000370	Perfluoroalkyl and polyfluoroalkyl su PFCAs	bstances PFHxA	2,2,3,3,4,4,5,5,6,6,6-undecafluorohexanoic acid	67542	307-24-4	Perfluorohexanoic acid	Samples	
CH0000371	Perfluoroalkyl and polyfluoroalkyl su PFCAs	bstances PFHpA	2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoroheptanoic acid	67818	375-85-9	Perfluoroheptanoic acid	Samples	
CH0000372	Perfluoroalkyl and polyfluoroalkyl su PFCAs	bstances PFOA	2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanoic acid	9554	335-67-1	Perfluorooctanoic acid	Samples	
CH0000373	Perfluoroalkyl and polyfluoroalkyl su PFCAs	bstances PFNA	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadecafluorononanoic acid	67821	375-95-1	Perfluorononanoic acid	Samples	

② Find "PFOA" and click its Samples to get the list of samples which are used to measure PFOA.

③ Select "Abiotic-Water" from the pull-down menu in Sample Type and click

Samples								
P	ojectID					Chemical Groups	Perfluoroalkyl and polyfluoroalkyl substances - PF	CAs 🗘
Samp	le Type Abiot	ic - Water			>	Chemical Name	PFOA	\$
Scientifi	Name -				\$	Collection Region	-	÷
Tissue	Organ -				\$	Collection Country	-	÷
к	eyword Proje	ct title, Abstract				Collection Year	XXXX - XXXX	
Export samples (TSV) Show 50 c) entries Showing 1 to 50 of 314 er « 1 2 3 4	rries	ed data of query result	Export	measured data (TSV)				
ProjectID	SampleTyp	e SampleName	Tissue J <u>i</u>	Collection Country	Collection Year 1	Chemicals 1		Measured Data
PRA000076 SAA004	34 Surface wa	ater Water - River water		Japan	2016	Organochlorines Flan	ne retardants Perfluoroalkyl and polyfluoroalkyl	
		Kivel water				substances		0
PRA000076 SAA004	33 Surface wa			Japan	2016		ne retardants Perfluoroalkyl and polyfluoroalkyl	0
PRA000076 SAA004 PRA000076 SAA004		ater Water - River water		Japan Japan	2016 2016	Organochlorines Flan substances	ne retardants Perfluoroaikyl and polyfluoroaikyl ne retardants Perfluoroaikyl and polyfluoroaikyl	

(4)Click

Show the measured data of query results

in the above page, and the list of measured data are shown as

below. The same measurement unit " $\mu g/L$ " is used for water.

Measured	dData							
	ProjectID				Chemical Groups	Perfluoroalkyl and	d polyfluoroalkyl subs	tances - PFCAs 🗳
	SampleID				Chemical Name	PFOA		\$
Sa	ample Type Abi	otic - Water		\$	Collection Region			\$
Scier	ntific Name			\$	Collection Country			\$
Tiss	sue / Organ			\$	Collection Year	XXXX - X	XXX	
	Keyword Pro	ject title, Abstract						
Export samples (TSV)) Export measure	ed data (TSV)		QSearch Reset				
Show 50 0 entries Showing 1 to 50 of 218								
Show 50 0 entries Showing 1 to 50 of 218	8 entries	Sample 11	Chemical 11	ExperimentID Iš	MeasuredValue 11	Unit 11	Remarks 11	RegisterDate Ii
Show 50 C entries Showing 1 to 50 of 218 (1 2 3	8 entries	Sample Iš Water	Chemical Li PFOA	ExperimentID IE EXA000001	MeasuredValue I± 3.40E-4	Unit I± µg/L	Remarks Ii	RegisterDate 11 2018/10/05
Show 50 c entries Showing 1 to 50 of 218 « 1 2 3 ProjectID LE	8 entries 4 5 » SampleID 11						Remarks 11	
Show 50 ° entries Showing 1 to 50 of 218 (1 2 3) ProjectID 14 PRA000076	8 entries	Water	PFOA	EXA000001	3.40E-4	µg/L	Remarks Là	2018/10/05
Show 50 c entries Showing 1 to 50 of 218 < 1 2 3 ProjectID Ià PRA000076	8 entries 4 5 > SampleID 11 SAA004234 SAA004233	Water	PFOA PFOA	EXA000001 EXA000001	3.40E-4 4.00E-4	μg/L μg/L	Remarks Iž	2018/10/05 2018/10/05
Show 50 c) entries Showing 1 to 50 of 218 e e 1 2 3 ProjectID I projectID projectID PRA000076 PRA000076 projectID projectID	8 entries 4 5 SampleID 15 SAA004234 SAA004233 SAA004232	Water Water Water	PFOA PFOA PFOA	EXA000001 EXA000001 EXA000001	3.40E-4 4.00E-4 5.60E-4	μg/L μg/L μg/L	Remarks Iš	2018/10/05 2018/10/05 2018/10/05
Show 50 c entries Showing 1 to 50 of 218 1 2 3 ProjectID Iii PRA000076 PRA000076 PRA000076	B entries 4 5 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 > 5 >	Water Water Water Water	PFOA PFOA PFOA	EXA000001 EXA000001 EXA000001 EXA000001	3.40E-4 4.00E-4 5.60E-4 7.60E-4	µg/L µg/L µg/L µg/L	Remarks Iš	2018/10/05 2018/10/05 2018/10/05 2018/10/05

- (5) Click Export measured data (TSV) in the above page, and you can download the list of measured data of the chemical.
- 6 Open the downloaded file in MS excel, and the list below comes up.

•••	E	л <mark>н</mark> го				📄 m	easureddata_2	20190128101828						٢
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1	‡ ⊃	< 🗸 fx	MeasuredID											
A		В	С	D	E	F	G	н	1	J	к	Larrent Larrent	м	N
Measur	redID	ProjectID	SampleID	ScientificName	ChemicalID	ChemicalName	ExperimentID	MeasuredValue	AlternativeData	Unit	Remarks	RegisterDate	UpdateDate	
2	10837	PRA000015	SAA000492	Water	CH0000372	PFOA	EXA000001	0.004712871		μg/L		2016/11/25	2018/6/8	
3	10850	PRA000015	SAA000493	Water	CH0000372	PFOA	EXA000001	0.004524211		μg/L		2016/11/25	2018/6/8	
1	10863	PRA000015	SAA000494	Water	CH0000372	PFOA	EXA000001	0.003318447	,	μg/L		2016/11/25	2018/6/8	
5	10876	PRA000015	SAA000495	Water	CH0000372	PFOA	EXA000001	0.002531313	1	μg/L		2016/11/25	2018/6/8	
5	10889	PRA000015	SAA000496	Water	CH0000372	PFOA	EXA000001	0.005636	1	μg/L		2016/11/25	2018/6/8	
1	10902	PRA000015	SAA000497	Water	CH0000372	PFOA	EXA000001	0.00427	,	μg/L		2016/11/25	2018/6/8	
3	10915	PRA000015	SAA000498	Water	CH0000372	PFOA	EXA000001	0.003063366	1	μg/L		2016/11/25	2018/6/8	
9	10928	PRA000015	SAA000499	Water	CH0000372	PFOA	EXA000001	0.033494		μg/L		2016/11/25	2018/6/8	
0	10941	PRA000015	SAA000500	Water	CH0000372	PFOA	EXA000001	0.034767647	•	μg/L		2016/11/25	2018/6/8	
1	10954	PRA000015	SAA000501	Water	CH0000372	PFOA	EXA000001	0.031275	i l	μg/L		2016/11/25	2018/6/8	
2	10967	PRA000015	SAA000502	Water	CH0000372	PFOA	EXA000001	0.006111111		μg/L		2016/11/25	2018/6/8	
3	10980	PRA000015	SAA000503	Water	CH0000372	PFOA	EXA000001	0.015997087	•	μg/L		2016/11/25	2018/6/8	
4	10993	PRA000015	SAA000504	Water	CH0000372	PFOA	EXA000001	0.01304		μg/L		2016/11/25	2018/6/8	
5	11006	PRA000015	SAA000505	Water	CH0000372	PFOA	EXA000001	0.015504		μg/L		2016/11/25	2018/6/8	
6	11019	PRA000015	SAA000506	Water	CH0000372	PFOA	EXA000001	0.010092157		μg/L		2016/11/25	2018/6/8	
.7	11032	PRA000015	SAA000507	Water	CH0000372	PFOA	EXA000001	0.003322772	1	μg/L		2016/11/25	2018/6/8	
8	11045	PRA000015	SAA000508	Water	CH0000372	PFOA	EXA000001	0.007173267	,	μg/L		2016/11/25	2018/6/8	
9	11058	PRA000015	SAA000509	Water	CH0000372	PFOA	EXA000001	0.004143137		μg/L		2016/11/25	2018/6/8	
0	11071	PRA000015	SAA000510	Water	CH0000372	PFOA	EXA000001	0.003010577		μg/L		2016/11/25	2018/6/8	
1	11084	PRA000015	SAA000511	Water	CH0000372	PFOA	EXA000001	0.002957692	1	μg/L		2016/11/25	2018/6/8	
2	11097	PRA000015	SAA000512	Water	CH0000372	PFOA	EXA000001	0.0014	<1.40E-3	μg/L		2016/11/25	2018/6/13	
3	11110	PRA000015	SAA000513	Water	CH0000372	PFOA	EXA000001	0.00356	i .	μg/L		2016/11/25	2018/6/8	
4	11123	PRA000015	SAA000514	Water	CH0000372	PFOA	EXA000001	0.002913	1	μg/L		2016/11/25	2018/6/8	

 \bigcirc Save only Data ID (e.g. MeasuredID or SampleID) and MeasuredValue as TSV file. This file is read in AIST-MeRAM for exposure assessment and risk assessment.

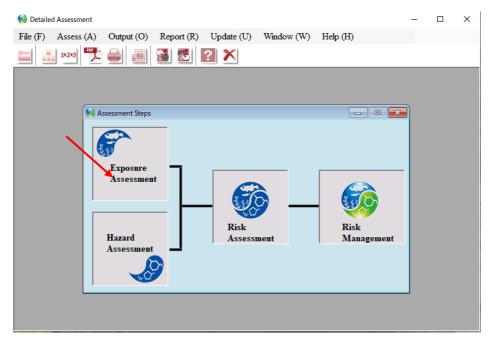
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A1	L _	× √ ƒx San	npleID							
	А	В	С	D	E	F	G	н		J
1	SampleID	MeasuredValue								
2	SAA000492	0.004712871								
3	SAA000493	0.004524211								
4	SAA000494	0.003318447								
5	SAA000495	0.002531313								
6	SAA000496	0.005636								
7	SAA000497	0.00427								
8	SAA000498	0.003063366								
9	SAA000499	0.033494								
10	SAA000500	0.034767647								
11	SAA000501	0.031275								
12	SAA000502	0.006111111								
13	SAA000503	0.015997087								
14	SAA000504	0.01304								
15	SAA000505	0.015504								
16	SAA000506	0.010092157								
17	SAA000507	0.003322772								
18	SAA000508	0.007173267								
19	SAA000509	0.004143137								
20	SAA000510	0.003010577								
21	SAA000511	0.002957692								

7-2. How to import and use the data from ChemTHEATRE in AIST-MeRAM

AIST-MeRAM (AIST-Multi-purpose Ecological Risk Assessment and Management Tool) was developed by National Institute of Advanced Industrial Science and Technology (AIST). It is a free, quasi-artificial intelligence system for ecological risk assessment and management of chemicals substances. For details: https://en-meram.aist-riss.jp

7-2-1. Exposure assessment

① Activate AIST-MeRAM and click "Detailed Evaluation," then the page below comes up. Click "Exposure assessment."

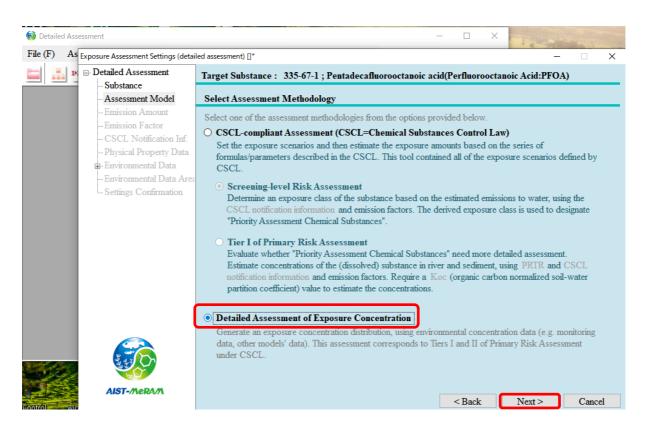


② Select a chemical you want to assess.

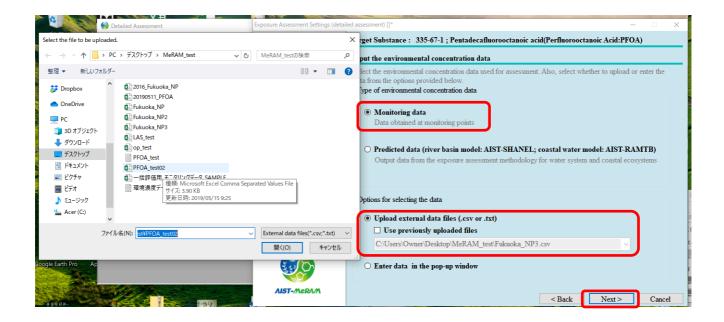
You can search the chemical you want to assess with CAS registry number[®] or chemical name. After choosing PFOA as the target chemical, click "Next."

n Detailed Assessment	- 🗆 X
File (F) As Exposure Assessment Settings (detail	iled assessment) []* — 🗆 🗙
Detailed Assessment	Target Substance : 335-67-1 ; Pentadecafluorooctanoic acid(Perfluorooctanoic Acid:PFOA)
- Substance - Assessment Model - Emission Amount	Select Target Substance
– Emission Amount – Emission Factor – CSCL Notification Inf	Select or enter the target substance name. If you check the box for "Substances Contained in the Tool", the system allows you to search for a substance name or CAS number which resides in its databases.
- Physical Property Data	O Previously-assessed Substances
- Environmental Data	25154-52-3 ; Nonylphenol 🗸
Environmental Data Area	Substances Contained in the Tool CENER ENDER South of "Search by Name", and enter text (partial names/numbers are acceptable) in the search box provided below. Click the "Search" button, and select the target substance from the search results list.
	O Search by CAS Number O Search by Name Search Box PFOA Search Search Results List 335-67-1 ; Pentadecafluorooctanoic acid(Perfluorooctanoic Acid:PFOA)
	O Other Substances Enter the substance name (required) and CAS number (optional).
AIST-MERAM	Substance Name CAS Number Next > Cancel

③ Select "Detailed assessment method of exposure concentration" and move to the next page.



 (4) Select "Monitoring data" => "Upload external data files" =>select the TSV file exported from ChemTHEATRE (See page 20), then import it.

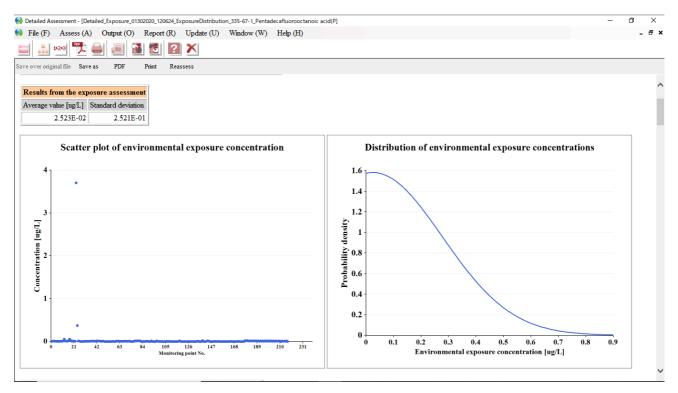


 \bigcirc Once the TSV file is successfully imported, the following screen is displayed.

After that, follow the directions and proceed with the exposure assessment.

n Detailed Assessment	Exposure Assessment Settings (detail	led assessment) []*
File (F) Assess (A) Output (O) Report (R)	Detailed Assessment	Target Substance : 335-67-1 ; Pentadecafluorooctanoic acid(Perfluorooctanoic Acid:PFOA)
🗀 🔝 1229 🚔 进 🔀	- Substance - Assessment Model	Check Uploaded Data and Select One Type of Distribution
	- Env't Concentration Data - Check Data - Settings Confirmation	
Assessment Steps Exposure Assessment Hazard Assessment		SampleID MeasuredValue SAA003568 0.00436 SAA003569 0.01166 SAA003570 0.0118 SAA003572 0.00439 SAA003573 0.00817 SAA003574 0.00673 CAA002575 0.00727 C:Users!Owner/Desktop!MeRAM_test!PFOA_test02.csv Reload
	AIST-/ARRA/A	
1-101		< Back Next > Cancel

(6) The result of exposure assessment is successfully displayed as below. You can download and save the result as PDF file.



1 Keep it open and move to "Hazard assessment."

7-2-2. Hazard assessment

1 Select "Hazard assessment" at the page below.

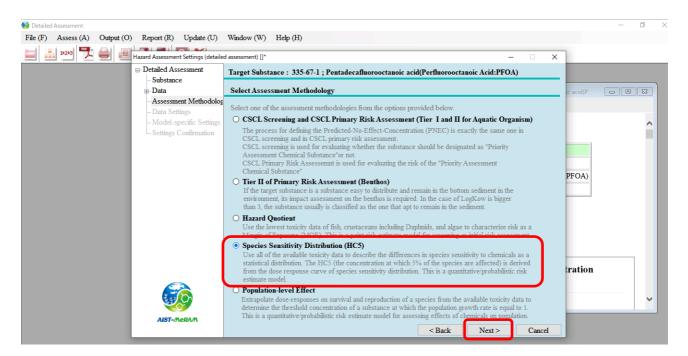
🔯 Detailed Assessment			- 0
File (F) Assess (A) Output (O) Report (R) Update	U) Window (W) Help (H)		
🔚 🚠 🕬 🔁 🗐 🔀 🛃 🗶			
	i Assessment Steps	I I I I I I I I I I I I I I I I I I I	
		eassess	
			~
	Exposure -		
N	Assessment		
		Select Assessment File	
		(Permuorooctanoic Acid.PFOA)	
	Hazard	Create New File	
	Assessment	O Upload Existing File	
		OK	
		Scatter plot of environmental exposure concentration	
		4	~

2 Select a chemical you want to assess.

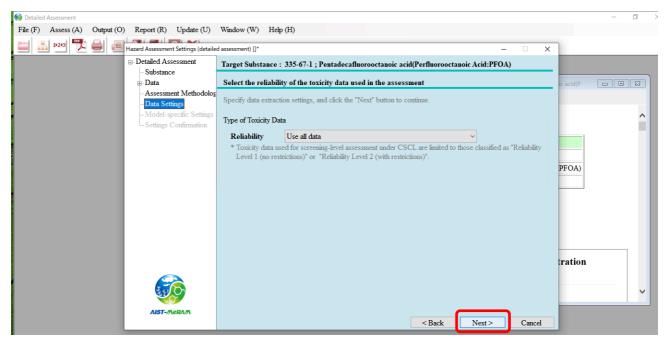
After selecting PFOA as the target chemical, click "Next."

6 Detailed Assessment		- 0
File (F) Assess (A) Output (O) Report (R) Update (U)	Window (W) Help (H)	- 5
		1
Hazard Assessment Settings (detaile	d assessment) []*	
Detailed Assessment Substance	Target Substance : Unchosen	
	Select Target Substance	ic acid(P
– Assessment Methodolog – Data Settings	Select or enter the target substance name. If you check the box for "Substances Contained in the Tool", the system allows you to search for a substance name or CAS number which resides in its databases.	
- Model-specific Settings - Settings Confirmation	Previously-assessed Substances 335-67-1 ; Pentadecafluorooctanoic acid(Perfluorooctanoic Acid1	
	O Substances Contained in the Tool Check either "Search by CAS Number" or "Search by Name", and enter text (partial names/numbers are acceptable) in the search box provided below. Click the "Search" button, and select the target substance from the search results list.	PFOA)
	Search by CAS Number Search by Name	
	Search Box Search	
	Search Results List	
	100-01-6 ; p-Nitroaniline 100-02-7 ; 4-Nitrophenol 100-10-7 ; 4-(Dimethylamino)benzaldehyde	tration
	100-14-1 ; alpha-Chloro-4-nitrotoluene	
	O Other Substances Enter the substance name (required) and CAS number (optional).	
	Substance Name CAS Number	
AIST-//JeRA/A	Next > Cancel	

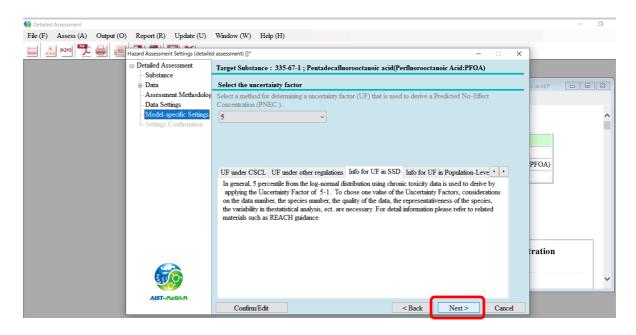
③ Select an assessment methodology and proceed with the hazard assessment. Select "Species Sensitivity Distribution" here.













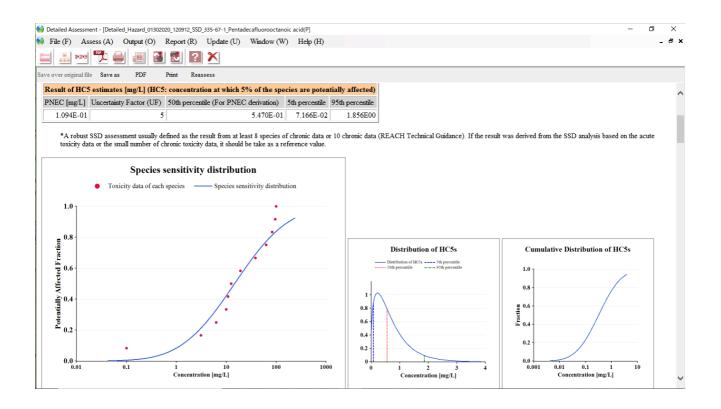
④ Click "Assess"

Detailed Assessment File (F) Assess (A) Output (O) Report (R) Update (U)	Window (W) Help (H)
	window (w) ricip (ii)
📃 📠 🎦 📐 🗐 🛄 Hazard Assessment Settings (detailed	nd assessment) []* X
Detailed Assessment Substance	Target Substance : 335-67-1 ; Pentadecafluorooctanoic acid(Perfluorooctanoic Acid:PFOA)
- Data	Confirm Assessment Settings
– Assessment Methodolog – Data Settings	
Model-specific Settings	Assessment Methodology : Species Sensitivity Distribution (HC5)
	Substance Name : Pentadecafluorooctanoic acid(Perfluorooctanoic Acid:PFOA)
	CAS Number 335-67-1 Option Setting
	Type of Toxicity Data : Chronic PFOA)
	HC5 Estimation Settings Bayesian Settings Log Normal Distribution : Yes <factor> Log Logistic Distribution : Yes Range of Average Values : 5 Maximum Likelihood Estimation of LND : Yes Range of Standard Deviations</factor>
	Maximum Likelihood Estimation of LLD : Yes Lower Limit : 8 Bayesian LND : Yes Upper Limit : 8 Sampling>
	Interval : Equal Sample Average Values : 400 Sample Standard Deviations : 400
AIST-//\eRA/	Confirm/Edit Save Confi < Back Assess Cancel

6 Detailed Assessment		- 0
File (F) Assess (A) Output (O) Report (R) Update (U)	Window (W) Help (H)	
Hazard Assessment Settings (detail	led assessment) []* X	1
- Detailed Assessment - Substance	Target Substance : 335-67-1 ; Pentadecafluorooctanoic acid(Perfluorooctanoic Acid:PFOA)	
Data	Confirm Assessment Settings	ic acid(P 🗖 🖻 🔀
– Assessment Methodolo – Data Settings – Model-specific Settings	or selecting the menu item in the left pane. Otherwise, click the "Assess" button to display the assessment result.	~
Settings Confirmation	Substance Name : Pentadecafluorooctanoic acid(Perfluorooctanoic Acid:PFOA)	
AIS	Substance Name : Pentadecanuorooctanoic acid(Pentuorooctanoic Acid	
	Completed assessment of Log-normal distribution(LND). Completed assessment of Log-logistic distribution(LLD). Completed assessment of Maximum Bichihood estimation of LND. Completed assessment of Bayesian LND. Completed assessment of Bayesian LND.	PFOA)
	OK	
	Log Logistic Distribution : Yes Range of Average Values : 5	
	Maximum Likelihood Estimation of LND : Yes Range of Standard Deviations Maximum Likelihood Estimation of LLD : Yes Lower Limit : 8 Bayesian LND : Yes Upper Limit : 8 Sampline : Yes Sampline	tration
	Interval : Equal Sample Average Values : 400 Sample Standard Deviations : 400	~
AIST-//NERA//	Confirm/Edit Save Confi <back assess="" cancel<="" th=""><th></th></back>	

(5) The results of hazard assessment is displayed as below.

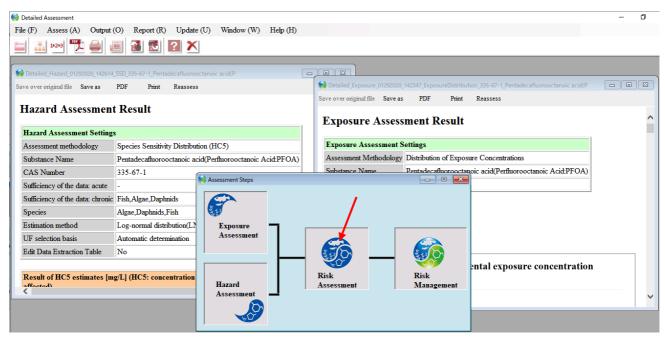
This is an example of the results: The result of Species Sensitivity Distribution (SSD).



6 Keep it open, too. With the above two results: the result of exposure assessment and the result of hazard assessment, proceed with the risk assessment.

7-2-3. Risk assessment

① Click "Risk Assessment" and check the files and click "Assess."

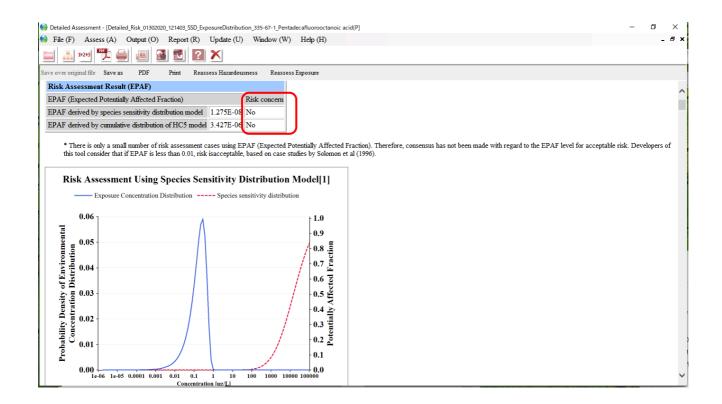




😡 Detailed Assessment	Risk Assessment —	×		- 0	×
File (F) Assess (A) Output (O) Image: Second Seco	Assessment displayed in the combination list will be performed. Combination list and output options Check the combinations of assessment results of hazard and exposure, as well as their file name (editable) for risk assessment result. If you want to delete any combinations from the list, select the row(s), and click the "Delete" button. You can also perform this operation by unchecking the hox in the fact left cohume Also check the curve ristings, and click the "Delete" button.				
Save over original file Save as PE Hazard Assessment H	No Substance Hazard Exposure Risk assessment result (you can change the file name)		pic acid(P		~
Hazard Assessment Settings Assessment methodology SI Substance Name Peters					
CAS Number 33 Sufficiency of the data: acute - Sufficiency of the data: chronic Fi Species A	Delete Delete All To add new combinations to the above output list, firstly display the result sheets of the hazard assessment and/or exposure assessment. Then, press the "Combination" key and the new combinations from the result sheets of the hazard assessment and exposure assessment will automatically chourn in the output list.		PFOA)		
Estimation method Loc UF selection basis A Edit Data Extraction Table N	Hazard assessment result Detailed_Hazard_01292020_142614_SSD_335-67-1_Pentadecafluorooctar > Browse				
Result of HC5 estimates [mg/L efforted)	Add Output setting Output the toxicity data on the results sheet Output the exposure data on the results sheet Output folder Output folder C:Users\Owner Add		tration	,	~

2 The result of risk assessment is displayed as below.

At the top left of the display, it shows the risk concerns. You can download and save the result as PDF file.



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