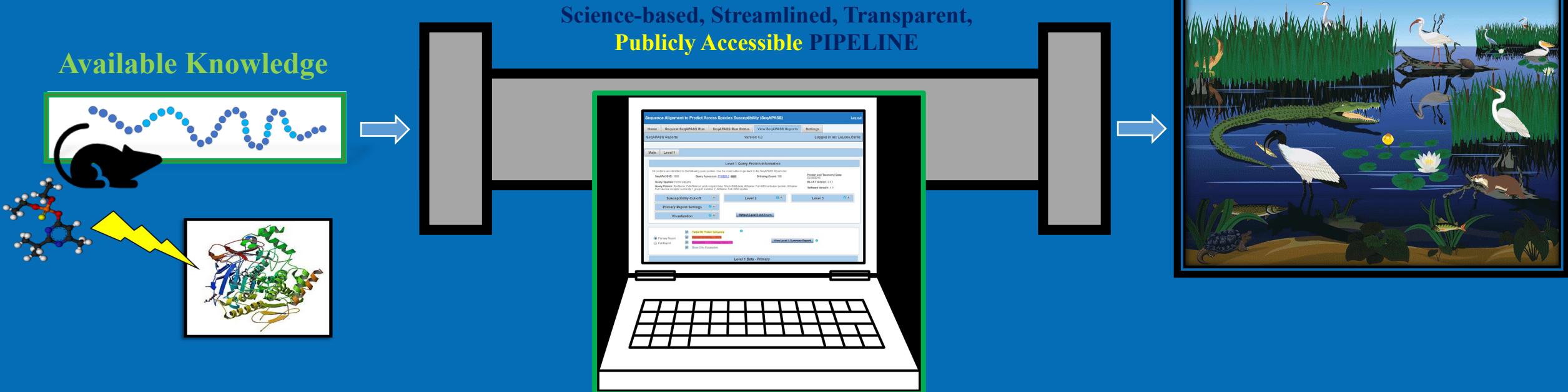
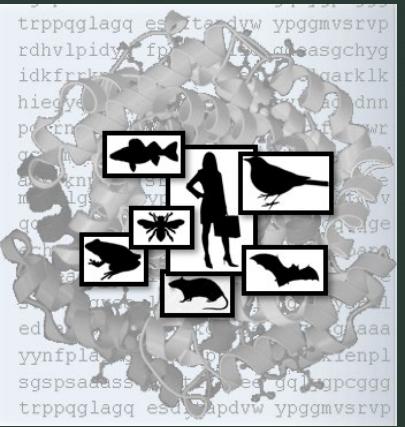


Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS) Demo

Carlie A. LaLone, Ph.D.
Research Bioinformaticist

Predict Susceptibility





<https://seqapass.epa.gov/seqapass/>

Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS)



SOT | Society of Toxicology
www.toxsci.oxfordjournals.org

TOXICOLOGICAL SCIENCES, 153(2), 2016, 228–245

doi: 10.1093/toxsci/kfw119
Advance Access Publication Date: June 30, 2016
Research article

Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS): A Web-Based Tool for Addressing the Challenges of Cross-Species Extrapolation of Chemical Toxicity

Carlie A. LaLone,^{*,1} Daniel L. Villeneuve,^{*} David Lyons,[†] Henry W. Helgen,[‡] Serina L. Robinson,^{§,2} Joseph A. Swintek,[¶] Travis W. Saari,^{*} and Gerald T. Ankley^{*}



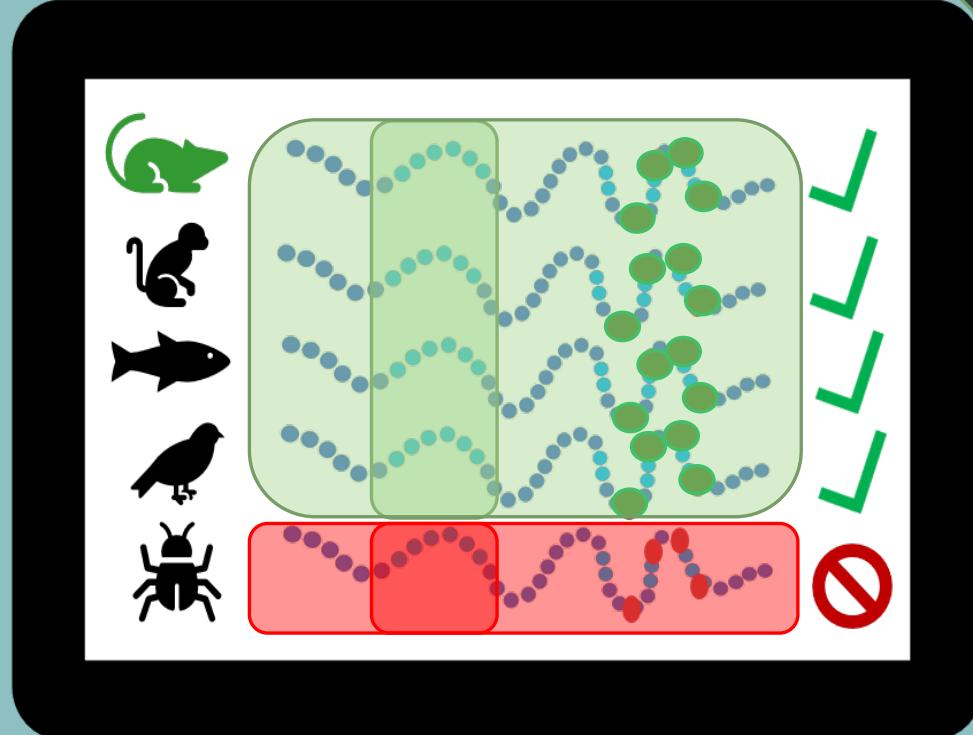
Flexible Analysis Based On Available Data

Level 1 Primary Amino Acid Sequence Alignments

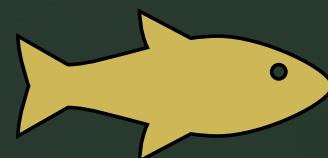
Level 2 Conserved Functional Domain Alignments

Level 3 Critical (Close Contact) Amino Acid Conservation

seqapass.epa.gov/seqapass/



Gather Lines of Evidence Toward Protein Conservation



Androgen Receptor (AR), Homo Sapiens

- NCBI Protein Accession: P10275.3
- PDB: 1E3G (metribolone (R1881), 2.4 Å)
- Critical amino acids used for SeqAPASS and DUET are as follows; N706, Q712, R753, T878
- Note that amino acid position numbering was updated in 2014, therefore literature and analysis performed before this time will use positions -1 from current. For example, A878 is reported at A877 in papers older than 2014.

Reference	Method Used	Ligand	Ligand-Amino Acid Interaction	Amino Acid (hAR)
Pereira et al. 2006	Protien Crystal Structure	TES, DHT, THG	Hydrogen Bond	N706, T878, Q712, R753
Marhefka et al. 2000	Homology modeling	TES	Hydrogen Bond	N706, T878, Q712, R753
Wang 2006	Protien Crystal Structure	R1181, LGD2226	Hydrogen Bond	N706, T878, Q712, R753
Sack et al. 2001	Protien Crystal Structure	DHT	Hydrogen Bond	N706, T878, Q712, R753

TES= Testosterone; DHT= Dihydrotestosterone; THG= tetrahydrogestrione; R1181= model synthetic androgen; LGD2226= investigational synthetic androgen

Related Topics: [SeqAPASS](#)

Contact Us

Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS)



New to SeqAPASS Version 5 (See [user guide](#) for more details)

- SeqAPASS Level 3 individual amino acid comparisons across species now have a customizable heat map visualization for rapid data interpretation and prediction of chemical susceptibility. The heat map can be downloaded for use in publication and presentation.
- In order to rapidly synthesize SeqAPASS results (i.e., data tables and visualizations) across all Levels (1, 2, and 3) of the SeqAPASS evaluation, a customizable Decision Summary Report has been created. Users can now push SeqAPASS results to a final downloadable (.pdf) summary report.

[Log In to SeqAPASS](#)

Version 5.0



Welcome to SeqAPASS

[Login](#)

For optimal SeqAPASS performance use Chrome [i](#)

Want an account? Click [here](#) for instructions.

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Identify a Protein Target

SeqAPASS is designed to predict cross species chemical susceptibility based on a protein molecular target. The following resources have been identified to guide the user to an appropriate protein target based on the chemical, adverse outcome pathway (AOP), or high-throughput screening (HTS) assay target of interest. Click the help buttons below for descriptions of how to find relevant protein target information from these resources.

All links will open in a new tab.

The following links exit the site [EXIT](#)

▶ Pharmaceutical protein targets:

▶ Pesticides and other chemical protein targets:

▶ AOP chemical initiators:

▶ ToxCast HTS results by chemical:

Identify a Protein Target

SeqAPASS is designed to predict cross species chemical susceptibility based on a protein molecular target. The following resources have been identified to guide the user to an appropriate protein target based on the chemical, adverse outcome pathway (AOP), or high-throughput screening (HTS) assay target of interest. Click the help buttons below for descriptions of how to find relevant protein target information from these resources.

All links will open in a new tab.

The following links exit the site [EXIT](#)

▶ Pharmaceutical protein targets:

▶ Pesticides and other chemical protein targets:

▼ AOP chemical initiators:

Adverse Outcome Pathway Wiki

Adverse Outcome Pathway Wiki is the central repository for all AOPs.

- Click the Stressors link on the top of the page. Use the search stressors Search function to search for a chemical of interest or scroll through the stressors presented in the Listing Stressors table. Click on chemical name. On Stressor Overview page, view the Events Including This Stressor section for Event Names associated with the molecular target. Click on the Event Name to learn more about the event. Scroll to Taxonomic Applicability. If species are listed these are the species for which there is evidence to link them to the event. This information provides the SeqAPASS user with the molecular target in the form of the event and the target species from the Taxonomic Applicability information.

<https://aopwiki.org>



▼ ToxCast HTS results by chemical:

<https://comptox.epa.gov/dashboard>



Compare Primary Amino Acid Sequences



Select Search: By Species
 By Accession

Query Species Selection



Query Species Search:

[NCBI Taxonomy Database](#)

Query Species:

fathead minnow (Taxid:90988)

Query Protein Selection



Query Protein Search:

[NCBI Protein Database](#)

Query Proteins:

[CAC38767.1] cytochrome P450 aromatase
[AAG00590.1] aromatase, partial

SeqAPASS Submission



Final Query Protein(s)

[CAC38767.1] cytochrome P450 aromatase



Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS)

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SeqAPASS Reports

Version 4.0

Logged in as: LaLone,Carlie

 Partial Protein Sequence[Request Selected Report](#)[Refresh Available Reports](#) View Report Save Report(s)

Available Reports

Search:

	SeqAPASS Run Id	Data Version	Ortholog Count	Level 1 Query Accession	Query Protein Name	NCBI Taxonomy ID	Query Species Name	Query Common Name	
<input type="radio"/>	1631	4	305	CAC38767.1	cytochrome P450 aromatase	90988	Pimephales promelas	Fathead minnow	
<input type="radio"/>	1630	4	648	ABF74729.1	retinoid X receptor-like protein	35525	Daphnia magna	Common water fleas	
<input type="radio"/>	1629	4	470	NP_001097670.1	neverland	7227	Drosophila melanogaster	Fruit fly	
<input type="radio"/>	1628	4	152	BAM83853.1	Methoprene-tolerant	6689	Daphnia pulex	Common water flea	
<input type="radio"/>	1627	4	90	NP_524143.2	ftz transcription factor 1, isoform B	7227	Drosophila melanogaster	Fruit fly	
<input type="radio"/>	1626	4	215	BAF49033.1	ecdysone receptor B	35525	Daphnia magna	Common water fleas	
<input type="radio"/>	1625	4	14	XP_011493380.2	ecdysone-inducible protein E75 isoform X2	7159	Aedes aegypti	Yellow fever mosquito	
<input type="radio"/>	1624	4	48	ALC49375.1	Cyp18a1	30019	Drosophila busckii	Fruit flies	
<input type="radio"/>	1623	4	116	NP_001011578.1	vitellogenin precursor	7480	Apis mellifera	Honey bee	
<input type="radio"/>	1622	4	269	NP_001314895.1	methyl farnesoate epoxidase precursor	7480	Apis mellifera	Honey bee	

(1 of 578)

 [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#) [10](#)

10

Download Table:

[Home](#)[Request SeqAPASS Run](#)[SeqAPASS Run Status](#)[View SeqAPASS Reports](#)[Settings](#)

SeqAPASS Reports

Version 4.0

Logged in as: LaLone,Carlie

[Main](#)[Level 1](#)

Level 1 Query Protein Information

Hit proteins are identified for the following query protein. Use the main button to go back to the SeqAPASS Reports list.

SeqAPASS ID: 1631

Query Accession: [CAC38767.1](#) [EXIT](#)

Ortholog Count: 305

Protein and Taxonomy Data: 02/28/2019

Query Species: Pimephales promelas

BLAST Version: 2.8.1

Query Protein: cytochrome P450 aromatase

Software Version: 4.0

[Susceptibility Cut-off](#)[Level 2](#)[Level 3](#)[Primary Report Settings](#)[Visualization](#)[Refresh Level 2 and 3 runs](#)

Primary Report
 Full Report

- Partial Hit Protein Sequence
- Percent Similarity > 100%
- Susceptible = Y, Ortholog Count = 0
- Show Only Eukaryotes

[View Level 1 Summary Report](#)

Level 1 Data - Primary

The following links exit the site [EXIT](#)[Download Current Level 1 Report Settings](#)Search:

	Data Version	NCBI Accession 	Protein Count 	Species Tax ID 	Taxonomic Group 	Filtered Taxonomic Group 	Scientific Name 	Common Name 	Protein Name 
<input type="checkbox"/>	4	CAC38767.1	495	90988	Actinopteri	Actinopteri	Pimephales promelas	Fathead minnow	cytochrome P450 aromatase
<input type="checkbox"/>	4	BAD91038.1	786	48668	Actinopteri	Actinopteri	Rutilus rutilus	Roach minnow	brain-type aromatase
<input type="checkbox"/>	4	AMK51587.1	61	291482	Actinopteri	Actinopteri	Chanodichthys ilishaeformis	Teleost fishes	cytochrome p450 aromatase

Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS)

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SeqAPASS Reports

Version 4.0

Logged in as: LaLone,Carlie

[Main](#) [Level 1](#)

Level 1 Query Protein Information

Hit proteins are identified for the following query protein. Use the main button to go back to the SeqAPASS Reports list.

SeqAPASS ID: 1631

Query Accession: [CAC38767.1](#) [EXIT](#)

Ortholog Count: 305

Protein and Taxonomy Data: 02/28/2019

Query Species: Pimephales promelas

BLAST Version: 2.8.1

Query Protein: cytochrome P450 aromatase

Software Version: 4.0

[Susceptibility Cut-off](#)  [Primary Report Settings](#)  [Visualization](#)  [Visualize Data](#)

This will open in a separate tab.

[Level 2](#)  [Level 3](#)  [Refresh Level 2 and 3 runs](#)

Interactive Data Visualization

100-
Query species/sensitive species

Susceptible: Yes

Level 1 Data - Primary

Search: Enter keyword

	Common Name	Protein Name	BLASTp Bitscore	Ortholog Candidate	Ortholog Count	Cut-off	Percent Similarity	Susceptibility Prediction	Analysis Completed	Eukaryote
	Human	estrogen receptor isoform 1	1241.87	Y	348	27.98	100.00	Y	2019 05 16 11:04:08	Y
	Western gorilla	estrogen receptor alpha	1229.54	Y	348	27.98	99.01	Y	2019 05 16 11:04:08	Y
	Chimpanzee	estrogen receptor isoform X2	1229.54	Y	348	27.98	99.01	Y	2019 05 16 11:04:08	Y
	Western lowland gorilla	PREDICTED: estrogen receptor isoform X2	1228.77	Y	348	27.98	98.95	Y	2019 05 16 11:04:08	Y
	Pygmy chimpanzee	estrogen receptor isoform X2	1228.00	Y	348	27.98	98.88	Y	2019 05 16 11:04:08	Y
	Sumatran orangutan	estrogen receptor isoform X2	1227.62	Y	348	27.98	98.85	Y	2019 05 16 11:04:08	Y
	Bornean orangutan	estrogen receptor alpha	1227.62	Y	348	27.98	98.85	Y	2019 05 16 11:04:08	Y
	Pig-tailed macaque	estrogen receptor isoform X2	1227.23	Y	348	27.98	98.82	Y	2019 05 16 11:04:08	Y
	Rhesus monkey	PREDICTED: estrogen receptor isoform X2	1227.23	Y	348	27.98	98.82	Y	2019 05 16 11:04:08	Y
	Sooty mangabey	PREDICTED: estrogen receptor isoform X2	1227.23	Y	348	27.98	98.82	Y	2019 05 16 11:04:08	Y

(1 of 94)

1 2 3 4 5 6 7 8 9 10 > >>

10

<

Download Table: 

Taxonomic group: Class

Mammali	Testudine	Ave	Crocodili	Lepidosauri	Amphibi	Chondrichye	Ceratodontimorph	Coelacanthiforme	Actinopte	Cladisti	Petromyzontiforme	Myxiniforme	Enteropneust	Gastropod	Bivalvi	Branchiostomida	Cephalopod	Priapulida	Ascidiae	Linguat	Polychaet	Arachnid	Malacostrac	Insect	Collembol	Maxillopod	Enopl	Branchiopod	Echinoide	Merostomat	Ciliat	Liliopsid	Eutardigrad	Monogonont	Rhopalurida	Anthozo	Asterioide	Appendiculari	Hydrozo	Scyphozo	Trichopla	Chilopod	Cuboza	Peripatopsisda	Tricladid	Chromadore	Enopie	Macrostomid	Trematod	Cestod	Diplopod	Anopl
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Taxon

Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS)

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SeqAPASS Reports

Version 4.0

Logged in as: LaLone,Carlie

[Main](#) [Level 1](#)

Level 1 Query Protein Information

Hit proteins are identified for the following query protein. Use the main button to go back to the SeqAPASS Reports list.

SeqAPASS ID: 1631

Query Accession: [CAC38767.1](#) [EXIT](#)

Ortholog Count: 305

Protein and Taxonomy Data: 02/28/2019

Query Species: Pimephales promelas

BLAST Version: 2.8.1

Query Protein: cytochrome P450 aromatase

Software Version: 4.0

[Susceptibility Cut-off](#)[Primary Report Settings](#)[Visualization](#)[Visualize Data](#)

This will open in a separate tab.

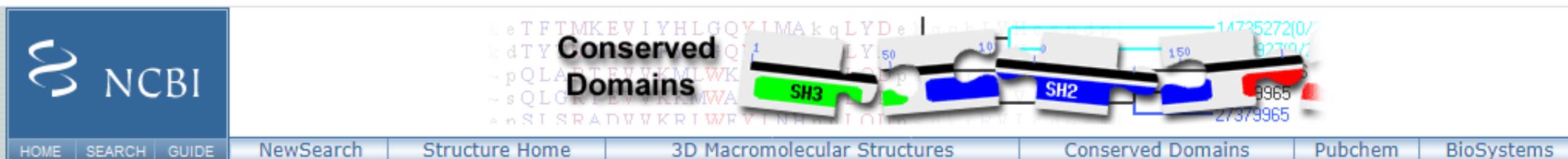
[Level 2](#)[Level 2 Query Domain](#)[NCBI Conserved Domain Database](#) [EXIT](#) [?](#)

Functional Domains

[-Select Domain -](#)[Request Domain Run](#)[View Level 2 Data](#)

Choose Domain to View

[-Select Completed Domain -](#)[View Level 2 Data](#)[Level 3](#)[Refresh Level 2 and 3 runs](#)



Conserved domains on [gi|14041612|emb|CAC38767|]

View Concise Results 

cytochrome P450 aromatase [Pimephales promelas]

Protein Classification



cytochrome P450 (domain architecture ID 10441782)

cytochrome P450 catalyzes the oxidation of organic species by molecular oxygen, by the oxidative addition of atomic oxygen into an unactivated C-H or C-C bond

Graphical summary

Zoom to residue level

[show extra options >](#)



[Search for similar domain architectures](#)  [Refine search](#) 

List of domain hits



Name	Accession	Description	Interval	E-value
[+] p450	pfam00067	Cytochrome P450; Cytochrome P450s are haem-thiolate proteins involved in the oxidative ...	47-463	8.82e-95

References:

-  Marchler-Bauer A et al. (2017), "CDD/SPARCLE: functional classification of proteins via subfamily domain architectures.", **Nucleic Acids Res.** **45**(D)200-3.
-  Marchler-Bauer A et al. (2015), "CDD: NCBI's conserved domain database.", **Nucleic Acids Res.** **43**(D)222-6.
-  Marchler-Bauer A et al. (2011), "CDD: a Conserved Domain Database for the functional annotation of proteins.", **Nucleic Acids Res.** **39**(D)225-9.
-  Marchler-Bauer A, Bryant SH (2004), "CD-Search: protein domain annotations on the fly.", **Nucleic Acids Res.** **32**(W)327-331.

Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS)

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SeqAPASS Reports

Version 4.0

Logged in as: LaLone,Carlie

Main [Level 1](#)

Level 1 Query Protein Information

Hit proteins are identified for the following query protein. Use the main button to go back to the SeqAPASS Reports list.

SeqAPASS ID: 1631

Query Accession: [CAC38767.1](#) [EXIT](#)

Ortholog Count: 305

Protein and Taxonomy Data: 02/28/2019

Query Species: Pimephales promelas

BLAST Version: 2.8.1

Query Protein: cytochrome P450 aromatase

Software Version: 4.0

Susceptibility Cut-off [+](#)

Primary Report Settings [+/-](#)

Visualization [+/-](#)

[Visualize Data](#)

This will open in a separate tab.

Level 2 [+/-](#)

NCBI Conserved Domain Database [EXIT](#) [+/-](#)

Functional Domains

-Select Domain -

(295) PLN03195, PLN03195, fatty acid omega-hydroxylase; Provisional

(80) PLN03234, PLN03234, cytochrome P450 83B1; Provisional

(296) PTZ00404, PTZ00404, cytochrome P450; Provisional

(349) TIGR04458, putative_cytochrome_P450, 4-nitrotryptophan

(149) TIGR04538, P450_cycloAA_1, cytochrome P450, cyclodipeptidyl

(47) pfam00067, p450, Cytochrome P450

Level 3 [+/-](#)

[Refresh Level 2 and 3 runs](#)



United States
Environmental Protection
Agency

Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS)

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SeqAPASS Reports

[Main](#) [Level 1](#) [Level 2](#)

Level 2 Query

Hit domains are identified for the following query domain. Use the main button to go back to the SeqAPASS Reports list.

SeqAPASS ID: 1631

Query Accession: [CAC38767.1](#) [EXIT](#)

Ortholog Count: 348

Query Species: Pimephales promelas

Query Domain: (47) [pfam00067](#) [EXIT](#) . p450 , Cytochrome P450

Query Protein: cytochrome P450 aromatase

Susceptibility Cut-off

Visualization

Primary Report
 Full Report

- Partial Hit Protein Sequence
- Percent Similarity > 100%
- Susceptible = Y, Ortholog Count = 0
- Show Only Eukaryotes

[View Level 2 Summary Report](#)

Level 2 Data - Primary

The following links exit the site [EXIT](#)

[Download Current Level 2 Report Settings](#)

Search:

Data Version	NCBI Accession	Protein Count	Species Tax ID	Taxonomic Group	Filtered Taxonomic Group	Scientific Name	Common Name	Protein Name
4	CAC38767.1	495	90988	Actinopteri	Actinopteri	Pimephales.promelas	Fathead minnow	cytochrome P450 aromatase
4	BAD91038.1	786	48688	Actinopteri	Actinopteri	Rutilus.rutilus	Roach minnow	brain-type aromatase
4	AMK51587.1	61	291482	Actinopteri	Actinopteri	Chondrichthys.ilishaeformis	Teleost fishes	cytochrome p450 aromatase
4	ADB44832.1	343	143808	Actinopteri	Actinopteri	Gobiocypris.rarus	Teleost fishes	cytochrome P450 aromatase
4	ROI37052.1	23922	495550	Actinopteri	Actinopteri	Anabarilius.grahami	Teleost fishes	Brain aromatase
4	XP_016324429.1	68487	1806454	Actinopteri	Actinopteri	Sinocyclocheilus.anshuiensis	Teleost fishes	PREDICTED: brain aromatase isoform X1
4	ACB12198.1	117439	7982	Actinopteri	Actinopteri	Cyprinus.carpio	Common carp	aromatase
4	AAK00642.1	87698	7955	Actinopteri	Actinopteri	Danio.rerio	Zebrafish	cytochrome P450 aromatase
4	AVY53511.1	784	210638	Actinopteri	Actinopteri	Tor.putitora	Golden mahseer	cytochrome P450 aromatase
4	AXG24156.1	68	145923	Actinopteri	Actinopteri	Carassius.auratus.grandoculis	Goldfish	cytochrome P450 19A1B

(1 of 131)

1 2 3 4 5 6 7 8 9 10

10

Download Table:

Level Two Summary Report

Taxonomic Group	Filtered Taxonomic Group	Number of Species	Mean Percent Similarity	Median Percent Similarity	Susceptibility Prediction
Actinopteri	Actinopteri	228	58.06	66.03	Y
Chondrichthyes	Chondrichthyes	5	55.61	58.82	Y
Aves	Aves	87	56.35	60.94	Y
Crocodylia	Crocodylia	4	60.05	60.01	Y
Amphibia	Amphibia	18	41.71	37.92	Y
Mammalia	Mammalia	149	51.96	59.03	Y
Testudines	Testudines	10	50.68	60.20	Y
Lepidosauria	Lepidosauria	14	45.24	56.22	Y
Ceratodontimorpha	Ceratodontimorpha	1	54.47	54.47	Y
Coelacanthiformes	Coelacanthiformes	1	50.04	50.04	Y

(1 of 11)

1 2 3 4 5 6 7 8 9 10 Download

Table:

Primary Report
 Full Report

- Partial Hit Protein Sequence i
- Percent Similarity > 100% i
- Susceptible = Y, Ortholog Count = 0 i
- Show Only Eukaryotes

[View Level 1 Summary Report](#) i

Level 1 Data - Primary

The following links exit the site [EXIT](#)

[Download Current Level 1 Report Settings](#) i

Search: i

Protein Name ▼	BLASTp Bitscore ▼	Ortholog Candidate ▼	Ortholog Count	Cut-off ▼	Percent Similarity ▼	Susceptibility Prediction ▼	Analysis Completed ▼	Eukaryote ▼	ECOTOX
PREDICTED: fatty_acid-binding_protein_liver	236.11	N	62	39.23	93.59	Y	2019 05 24 14:31:09	Y	-
PREDICTED: fatty_acid-binding_protein_liver	235.73	N	62	39.23	93.43	Y	2019 05 24 14:31:09	Y	-
PREDICTED: fatty_acid-binding_protein_liver	235.73	N	62	39.23	93.43	Y	2019 05 24 14:31:09	Y	Explore in ECOTOX
fatty_acid-binding_protein_liver	235.73	N	62	39.23	93.43	Y	2019 05 24 14:31:09	Y	-
liver_fatty_acid_binding_protein	234.96	Y	62	39.23	93.13	Y	2019 05 24 14:31:09	Y	Explore in ECOTOX
PREDICTED: fatty_acid-binding_protein_liver	234.96	N	62	39.23	93.13	Y	2019 05 24 14:31:09	Y	-
fatty_acid-binding_protein_liver	234.96	N	62	39.23	93.13	Y	2019 05 24 14:31:09	Y	-
fatty_acid-binding_protein_liver	234.96	N	62	39.23	93.13	Y	2019 05 24 14:31:09	Y	Explore in ECOTOX
fatty_acid-binding_protein_liver	234.19	N	62	39.23	92.82	Y	2019 05 24 14:31:09	Y	-
fatty_acid-binding_protein_liver	234.19	N	62	39.23	92.82	Y	2019 05 24 14:31:09	Y	Explore in ECOTOX

(3 of 35)

ECOTOX Knowledgebase

[Home](#)[Search](#)[Explore](#)[Help](#)[Contact Us](#) [Explore](#) | Species | Custom Group Aquatic Terrestrial[Group Summary](#)[Records](#)[Plot View](#) [Send Query Filters to Search](#)

Query Filters

Select one or more of each filter to reduce the records.

Chemical Group (2)

All

Chemicals (10)

All

Class (1)

1 Species

Species are ordered by **Scientific Name (A-Z)**.

Showing all 1 species from *Mustela putorius ssp.*

SCIENTIFIC NAME	COMMON NAME
-----------------	-------------

type to filter...

...

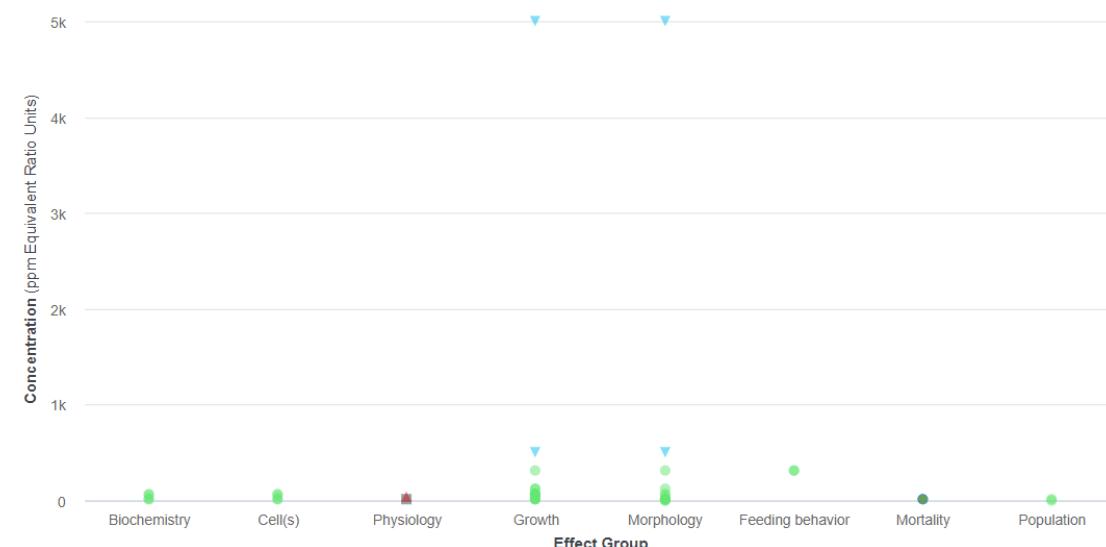
Mustela putorius ssp. furo	European Ferret
----------------------------	-----------------

Rows per page: 20

[Effect x Chem](#) [Dur x Chem](#) [Dur x Endpt](#)

Y-axis scale: Linear Logarithmic

Click and drag to zoom in. Hold down shift key to pan.



Level One Summary Report

Taxonomic Group ▾	Filtered Taxonomic Group ▾	Number of Species ▾	Mean Percent Similarity ▾	Median Percent Similarity ▾	Susceptibility Prediction ▾
Mammalia	Mammalia	122	87.15	88.78	Y
Aves	Aves	78	75.84	77.33	Y
Lepidosauria	Lepidosauria	10	52.36	45.72	Y
Testudines	Testudines	4	76.53	76.64	Y
Crocodylia	Crocodylia	4	74.81	75.11	Y
Amphibia	Amphibia	6	63.71	69.08	Y
Actinopteri	Actinopteri	75	61.49	65.19	Y
Chondrichthyes	Chondrichthyes	3	56.54	63.51	Y
Ceratodontimorpha	Ceratodontimorpha	1	37.40	37.40	N
Branchiopoda	Branchiopoda	1	27.32	27.32	N

(1 of 3)



1

2

3

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10 ▾

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Level 3

i -

Reference Explorer i

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fatty acid-binding protein
liver

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Google Scholar

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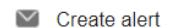
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The **crystal structure** of the recombinant form of rat **liver fatty acid-binding protein** was completed to 2.3 Å and refined to an R factor of 19.0%. The structural solution was obtained by molecular replacement using superimposed polyalanine coordinates of six intracellular ...
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Crystal structure of rat intestinal fatty-acid-binding protein: Refinement and analysis of the Escherichia coli-derived protein with bound palmitate
JC Sacchettini, JL Gordon, LJ Banaszak - Journal of molecular biology, 1989 - Elsevier
Rat intestinal **fatty-acid-binding protein** (I-FABP) is a small (15,124 M r) cytoplasmic polypeptide that binds long-chain **fatty** acids in a non-covalent fashion. I-FABP is a member of a family of intracellular binding proteins that are thought to participate in the uptake ...
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GK Balendiran, F Schnütgen, G Scapin... - Journal of Biological ..., 2000 - ASBMB
Expression of brain **fatty acid-binding protein** (B-FABP) is spatially and temporally correlated with neuronal differentiation during brain development. Isothermal titration calorimetry demonstrates that recombinant human B-FABP clearly exhibits high affinity for the ...
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Crystal structure of human serum albumin complexed with fatty acid reveals an asymmetric distribution of binding sites
S Curry, H Mandelkow, P Brick, N Franks - Nature Structural & Molecular ..., 1998 - nature.com
... III is in accordance with our structural results, although the difficulty in distinguishing between disorder and occupancy in **crystal structure** determinations makes it ... Although most iLBP proteins bind only a single long-chain **fatty** acid, rat **liver fatty acid binding protein** can hold two ...
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SeqAPASS ID: 1290

Query Accession: [NP_000116.2](#) [EXIT](#)

Ortholog Count: 348

Protein and Taxonomy Data: 02/28/2019

Level 3 Run Name: Actinopteri

BLAST Version: 2.8.1

Template Species: Homo sapiens

Cobalt Data: 07/09/2010

Template Protein: [NP_000116.2] estrogen receptor isoform 1

Cobalt Version: 2.1.0

Query Residues: No Residues Selected

Software Version: 3.2

[Show Amino Acid Info...](#)

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Enter Amino Acid Residue Positions

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1M
2T
3M
4T
5L
6H
7T
8K
9A

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Data Version	NCBI Accession ?	Protein Count ?	Species Tax ID ?	Taxonomic Group ?	Scientific Name ?	Common Name ?	Protein Name ?	Analysis Completed ?	Similar Susceptibility as Template ?
4	NP_000116.2	1265506	9606	Mammalia	Homo sapiens	Human	estrogen receptor isoform 1	2019 08 29 14:55:59	TBD
4	AAU87498.1	495	90988	Actinopteri	Pimephales promelas	Fathead minnow	estrogen receptor alpha	2019 08 29 14:55:59	TBD
4	XP_014061037.1	112166	8030	Actinopteri	Salmo salar	Atlantic salmon	PREDICTED: estrogen receptor isoform X2	2019 08 29 14:55:59	TBD
4	XP_020570152.1	47555	8090	Actinopteri	Oryzias latipes	Japanese medaka	estrogen receptor	2019 08 29 14:55:59	TBD
4	XP_021454037.1	124397	8022	Actinopteri	Oncorhynchus mykiss	Rainbow trout	estrogen receptor isoform X3	2019 08 29 14:55:59	TBD
4	AAI62466.1	87698	7955	Actinopteri	Danio rerio	Zebrafish	Estrogen receptor 1	2019 08 29 14:55:59	TBD

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10

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SeqAPASS ID: 1290

Query Accession: NP_000116.2 [EXIT](#)

Ortholog Count: 348

Level 3 Run Name: Actinopteri

Template Species: Homo sapiens

Template Protein: [NP_000116.2] estrogen receptor isoform 1

Query Residues: No Residues Selected

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1M
2T
3M
4T
5L
6H
7T
8K
9A
10S

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Protein and Taxonomy Data: 02/28/2019

BLAST Version: 2.8.1

Cobalt Data: 07/09/2010

Cobalt Version: 2.1.0

Software Version: 3.2

Amino Acid info

ID	Name	Side Chain	Size
A	Alanine	Aliphatic	89.094
C	Cysteine	Sulfur-Containing	121.154
D	Aspartic Acid	Acidic	133.104
E	Glutamic Acid	Acidic	147.131
F	Phenylalanine	Aromatic	165.192
G	Glycine	Aliphatic	75.067
H	Histidine	Basic	155.156
I	Isoleucine	Aliphatic	131.175
K	Lysine	Basic	146.189
L	Leucine	Aliphatic	131.175
M	Methionine	Sulfur-Containing	149.208
N	Asparagine	Amidic	132.119
P	Proline	Aliphatic	115.132
Q	Glutamine	Amidic	146.146
R	Arginine	Basic	174.203
S	Serine	Hydroxylic	105.093
T	Threonine	Hydroxylic	119.119
U	Seleno-cysteine	Sulfur-Containing	168.064
V	Valine	Aliphatic	117.148
W	Tryptophan	Aromatic	204.228
X	Unknown	Unknown	-
Y	Tyrosine	Aromatic	181.191

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Data Version	NCBI Accession	Protein Count	Species Tax ID	Taxonomic Group	Scientific Name	Common Name	Protein Name	
4	NP_000116.2	1265506	9606	Mammalia	Homo sapiens	Human	estrogen receptor isoform 1	
4	AAU87498.1	495	90988	Actinopteri	Pimephales promelas	Fathead minnow	estrogen receptor alpha	



Common Name	Amino Acid 1	Amino Acid 2	Amino Acid 3	Amino Acid 4
Human	32K	46S	55P	64A
Diamondback terrapin	32K	46S	55P	64T
Western painted turtle	32K	46S	55P	64T
Chinese soft-shelled turtle	32K	46S	55P	64T
Terrapins	32K	46S	55P	64T
Goode's thornscrub tortoise	32K	46S	55P	64T
Pacific ridley	32K	46S	55P	64T
Painted turtle	32K	46S	55P	64T
Green sea turtle	32K	46S	55P	64T
Three-toed box turtle	61K	75S	84P	93T

Common Name	Similar Susceptibility	Amino Acid 1	Amino Acid 2	Amino Acid 3	Amino Acid 4
Human	Y	133E	135E	137S	584I
Western painted turtle	Y	127E	129D	131S	577V
Lappet-faced vulture	N	125E	127E	129G	575I
Nile crocodile	Y	127E	129D	131S	575I
Split-tongued squamates	Y	127E	129E	131N	576V
Japanese giant salamander	N	126E	128E	130G	573L
West African lungfish	Y	131E	133E	135S	580G

- Total Match
- Partial Match
- Not a Match

Common Name	Similar Susceptibility	Amino Acid 1	Side Chain 1	MW 1	Total Match 1	Amino Acid 2	Side Chain 2	MW 2	Total Match 2	Amino Acid 3	Side Chain 3	MW 3	Total Match 3
Human	Y	274G	Aliphatic	75.067	Y	275E	Acidic	147.131	Y	276G	Aliphatic	75.067	Y
Western painted turtle	N	268Q	Amidic	146.146	N	269D	Acidic	133.104	Y	270A	Aliphatic	89.094	Y
Nile crocodile	N	268Q	Amidic	146.146	N	269D	Acidic	133.104	Y	270A	Aliphatic	89.094	Y
Split-tongued squamates	N	268Q	Amidic	146.146	N	269D	Acidic	133.104	Y	270S	Hydroxylic	105.093	N
Japanese giant salamander	N	267P	Aliphatic	115.132	Y	268D	Acidic	133.104	Y	269Q	Amidic	146.146	N

 Match

 Not a Match

Acknowledgements

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