

# CrISP - Cross Species In-Silico Platform

CrISP report vers 1.5

Produced by Moleculomics Ltd on 15-01-2019

## Report on Flupenthixol Pubchem id: 5281881

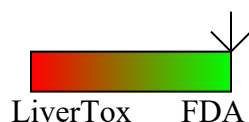
### Toxicity estimation

The CRISP toxicity estimation is based on a 'similarity profile' technique, comparing the docking results across all Human proteins to the profile for a set of FDA-approved drugs and compounds in the LiverTox database.

This is not a direct prediction of toxicity, just an expression of resemblance to a known compound set.

A percentage similarity to each group is given as an indicator of whether the compound in question behaves like other members of that group.

LiverTox: 0% - FDA 100%



### Human proteins with the top 6 docking scores

Docking analysis against a panel of Human liver proteins indicates potential interactions with the following proteins, in docking affinity order:

Uniprot	Gene	Affinity	Similarity - Mouse	Similarity - Rat
P49638	TTPA	-10.76	3.5 : <b>Good</b>	3.5 : <b>Good</b>
P35790	CHKA	-10.74	3.0 : <b>Good</b>	3.5 : <b>Good</b>
Q96RT1	ERBIN	-9.95	1.0 : <b>Poor</b>	0.0 : <b>Poor</b>
Q16236	NF2L2	-9.77	1.0 : <b>Poor</b>	1.0 : <b>Poor</b>
Q9HAW9	UD18	-9.7	6.0 : <b>Good</b>	10.5 : <b>Good</b>
Q92925	SMRD2	-9.68	2.5 : <b>Good</b>	1.0 : <b>Good</b>

A good similarity for a specific protein may be all that is needed if only a specific pathway is under consideration. If a general view is required, a good similarity across several proteins will be necessary.

### Overall species similarity:

Human:Mouse overall score: 17.0 **Good**

Human:Rat overall score: 19.5 **Good**

## Per-protein information

For each Human protein with a potential interaction, similar proteins have been found in other species. Similarity is assessed on sequence, structural, and ligand docking similarity.

NOTE: These similarity metrics have been displayed with a 'traffic light' indicator. These should be progressed through in sequence, as later measures of similarity are only meaningful if earlier measures are similar.

Keep going through the traffic lights while they are green, and stop when they are red (proceed with caution when amber).

Sequence similarity is the simplest definition, and is measured as percentage sequence identity.

Structural similarity is assessed by performing a structural alignment between the two proteins and reporting the percentage of residues that match within 2 Angstroms, and then the overall RMS distance between residues over the whole sequence (to indicate the similarity of the remaining un-matched residues).

Docking similarity is assessed in two ways. This is only meaningful if the proteins are similar on a structural level.

A 3D alignment of the docked structures is performed, and the RMS distance between the docked ligands is reported, to assess if ligands are docked in the same location (pocket) in both proteins. If the ligand docks in a similar location, the docking affinity can be compared, to assess energetic similarity.

Database searches for pathways involving the each protein are also reported.

## Information on protein P49638: TTPA, *Alpha-tocopherol*

### Indicated Pathways for Human P49638 : TTPA

Reactome:





	ReactomeID	PathwayName
0	R-HSA-1430728	Metabolism
1	R-HSA-196854	Metabolism of vitamins and cofactors
2	R-HSA-6806667	Metabolism of fat-soluble vitamins
3	R-HSA-8877627	Vitamin E

KEGG:

### Top 6 most similar proteins found

Human:Mouse similarity score for P49638: 3.5 Good

Human:Rat similarity score P49638: 3.5 Good

MOUSE	RAT
<i>HUMAN</i> P49638: <b>TTPA</b> Similar to <i>MOUSE</i> Q8BWP5: <b>TTPA</b>	<i>HUMAN</i> P49638: <b>TTPA</b> Similar to <i>RAT</i> P41034: <b>TTPA</b>
 Protein sequence identity <b>89.2%</b>	 Protein sequence identity <b>88.8%</b>
 Structural similarity - <b>94.6%</b> of structure matches to ( 263 out of 278 ) to RMS 0.61 Å	 Structural similarity - <b>94.2%</b> of structure matches to ( 262 out of 278 ) to RMS 0.76 Å

- Whole protein RMSD: **1.63 Å**
- Docking pose RMS distance: **5.53 Å**
- Docking affinity difference: **1.81** : HUMAN affinity=-10.7632 vs. MOUSE affinity=-8.95687

#### Indicated Pathways for *MOUSE* Q8BWP5:TTPA

Reactome:

	ReactomeID	PathwayName
0	R-MMU-1430728	Metabolism
1	R-MMU-196854	Metabolism of vitamins and cofactors
2	R-MMU-6806667	Metabolism of fat-soluble vitamins
3	R-MMU-8877627	Vitamin E

KEGG:

MOUSE

*HUMAN* P49638:TTPA Similar to *MOUSE* P62843:RS15

- Protein sequence identity **22.5%**
- Structural similarity - **23.4%** of structure matches to ( 11 out of 47 ) to RMS 1.01 Å
- Whole protein RMSD: **9.78 Å**
- Docking pose RMS distance: **24.03 Å**
- Docking affinity difference: **4.39** : HUMAN affinity=-10.7632 vs. MOUSE affinity=-6.37745

#### Indicated Pathways for *MOUSE* P62843:RS15

Reactome:

KEGG:

	KeggPathID	PathwayName
0	mmu03010	Ribosome - Mus musculus (mouse)
1	mmu03010	Ribosome - Mus musculus (mouse)

MOUSE

*HUMAN* P49638:TTPA Similar to *MOUSE* P49722:PSA2

- Protein sequence identity **21.8%**
- Structural similarity - **3.1%** of structure matches to ( 5 out of 161 ) to RMS 1.06 Å
- Whole protein RMSD: **21.24 Å**
- Docking pose RMS distance: **25.84 Å**

- Whole protein RMSD: **3.09 Å**
- Docking pose RMS distance: **9.67 Å**
- Docking affinity difference: **2.89** : HUMAN affinity=-10.7632 vs. RAT affinity=-7.87116

#### Indicated Pathways for *RAT* P41034:TTPA

Reactome:

	ReactomeID	PathwayName
0	R-RNO-1430728	Metabolism
1	R-RNO-196854	Metabolism of vitamins and cofactors
2	R-RNO-6806667	Metabolism of fat-soluble vitamins
3	R-RNO-8877627	Vitamin E

KEGG:

RAT

*HUMAN* P49638:TTPA Similar to *RAT* P62845:RS15

- Protein sequence identity **22.5%**
- Structural similarity - **23.4%** of structure matches to ( 11 out of 47 ) to RMS 1.01 Å
- Whole protein RMSD: **9.78 Å**
- Docking pose RMS distance: **23.58 Å**
- Docking affinity difference: **4.32** : HUMAN affinity=-10.7632 vs. RAT affinity=-6.44206

#### Indicated Pathways for *RAT* P62845:RS15

Reactome:

KEGG:

	KeggPathID	PathwayName
0	rno03010	Ribosome - Rattus norvegicus (rat)
1	rno03010	Ribosome - Rattus norvegicus (rat)

RAT

*HUMAN* P49638:TTPA Similar to *RAT* P17220:PSA2

- Protein sequence identity **21.8%**
- Structural similarity - **3.1%** of structure matches to ( 5 out of 161 ) to RMS 1.06 Å
- Whole protein RMSD: **21.24 Å**
- Docking pose RMS distance: **24.94 Å**

● Docking affinity difference: **4.48** : HUMAN affinity=-10.7632 vs. MOUSE affinity=-6.27994

● Docking affinity difference: **5.03** : HUMAN affinity=-10.7632 vs. RAT affinity=-5.72968

**Indicated Pathways for *MOUSE* P49722:PSA2**

Reactome:

KEGG:

	<b>KeggPathID</b>	<b>PathwayName</b>
<b>0</b>	mmu03050	Proteasome - Mus musculus (mouse)
<b>1</b>	mmu03050	Proteasome - Mus musculus (mouse)

**Indicated Pathways for *RAT* P17220:PSA2**

Reactome:

KEGG:

	<b>KeggPathID</b>	<b>PathwayName</b>
<b>0</b>	rno03050	Proteasome - Rattus norvegicus (rat)
<b>1</b>	rno03050	Proteasome - Rattus norvegicus (rat)

**Information on protein P35790: CHKA, *Choline***

**Indicated Pathways for Human P35790 : CHKA**

Reactome:

	<b>ReactomeID</b>	<b>PathwayName</b>
<b>0</b>	R-HSA-1430728	Metabolism
<b>1</b>	R-HSA-1483191	Synthesis of PC
<b>2</b>	R-HSA-1483206	Glycerophospholipid biosynthesis
<b>3</b>	R-HSA-1483213	Synthesis of PE
<b>4</b>	R-HSA-1483257	Phospholipid metabolism
<b>5</b>	R-HSA-556833	Metabolism of lipids

KEGG:

	<b>KeggPathID</b>	<b>PathwayName</b>
<b>0</b>	hsa00564	Glycerophospholipid metabolism - Homo sapiens ...
<b>1</b>	hsa01100	Metabolic pathways - Homo sapiens (human)
<b>2</b>	hsa05231	Choline metabolism in cancer - Homo sapiens (h...
<b>3</b>	hsa00564	Glycerophospholipid metabolism - Homo sapiens ...
<b>4</b>	hsa01100	Metabolic pathways - Homo sapiens (human)
<b>5</b>	hsa05231	Choline metabolism in cancer - Homo sapiens (h...

**Top 6 most similar proteins found**

Human:Mouse similarity score for P35790: 3 Good

Human:Rat similarity score P35790: 3.5 Good

<b>MOUSE</b>	<b>RAT</b>
<i>HUMAN</i> P35790: <b>CHKA</b> Similar to <i>MOUSE</i> O54804: <b>CHKA</b>	<i>HUMAN</i> P35790: <b>CHKA</b> Similar to <i>RAT</i> Q01134: <b>CHKA</b>

- Protein sequence identity **87.8%**
- Structural similarity - **79.0%** of structure matches to ( 358 out of 453 ) to RMS 0.71 Å
- Whole protein RMSD: **6.58 Å**
- Docking pose RMS distance: **27.2 Å**
- Docking affinity difference: **5.92** : HUMAN affinity=-10.745 vs. MOUSE affinity=-4.82764

**Indicated Pathways for *MOUSE* O54804:CHKA**

Reactome:

	ReactomeID	PathwayName
0	R-MMU-1430728	Metabolism
1	R-MMU-1483191	Synthesis of PC
2	R-MMU-1483206	Glycerophospholipid biosynthesis
3	R-MMU-1483213	Synthesis of PE
4	R-MMU-1483257	Phospholipid metabolism
5	R-MMU-556833	Metabolism of lipids

KEGG:

	KeggPathID	PathwayName
0	mmu00564	Glycerophospholipid metabolism - Mus musculus ...
1	mmu01100	Metabolic pathways - Mus musculus (mouse)
2	mmu05231	Choline metabolism in cancer - Mus musculus (m...
3	mmu00564	Glycerophospholipid metabolism - Mus musculus ...
4	mmu01100	Metabolic pathways - Mus musculus (mouse)
5	mmu05231	Choline metabolism in cancer - Mus musculus (m...

MOUSE No matching gene.

- Protein sequence identity **89.3%**
- Structural similarity - **78.6%** of structure matches to ( 356 out of 453 ) to RMS 0.73 Å
- Whole protein RMSD: **6.74 Å**
- Docking pose RMS distance: **6.38 Å**
- Docking affinity difference: **1.39** : HUMAN affinity=-10.745 vs. RAT affinity=-9.35991

**Indicated Pathways for *RAT* Q01134:CHKA**

Reactome:

	ReactomeID	PathwayName
0	R-RNO-1430728	Metabolism
1	R-RNO-1483191	Synthesis of PC
2	R-RNO-1483206	Glycerophospholipid biosynthesis
3	R-RNO-1483213	Synthesis of PE
4	R-RNO-1483257	Phospholipid metabolism
5	R-RNO-556833	Metabolism of lipids

KEGG:

	KeggPathID	PathwayName
0	rno00564	Glycerophospholipid metabolism - Rattus norveg...
1	rno01100	Metabolic pathways - Rattus norvegicus (rat)
2	rno05231	Choline metabolism in cancer - Rattus norvegic...
3	rno00564	Glycerophospholipid metabolism - Rattus norveg...
4	rno01100	Metabolic pathways - Rattus norvegicus (rat)
5	rno05231	Choline metabolism in cancer - Rattus norvegic...

RAT

*HUMAN* P35790:**CHKA** Similar to *RAT* P05544:**SPA3L**

- Protein sequence identity **20.2%**
- Structural similarity - **22.7%** of structure matches to ( 20 out of 88 ) to RMS 0.73 Å
- Whole protein RMSD: **13.51 Å**
- Docking pose RMS distance: **36.02 Å**
- Docking affinity difference: **4.83** : HUMAN affinity=-10.745 vs. RAT affinity=-5.91494

**Indicated Pathways for *RAT* P05544:SPA3L**

Reactome:

KEGG:

MOUSE

*HUMAN* P35790:**CHKA** Similar to *MOUSE*

P50429:**ARSB**

- Protein sequence identity **20.2%**
- Structural similarity - **3.3%** of structure matches to ( 6 out of 182 ) to RMS 1.22 Å
- Whole protein RMSD: **24.25 Å**
- Docking pose RMS distance: **22.44 Å**
- Docking affinity difference: **3.8** : HUMAN affinity=-10.745 vs. MOUSE affinity=-6.94502

**Indicated Pathways for *MOUSE* P50429:ARSB**

Reactome:

KEGG:

KeggPathID	PathwayName
0 mmu00531	Glycosaminoglycan degradation - Mus musculus (...)
1 mmu01100	Metabolic pathways - Mus musculus (mouse)
2 mmu04142	Lysosome - Mus musculus (mouse)
3 mmu00531	Glycosaminoglycan degradation - Mus musculus (...)
4 mmu01100	Metabolic pathways - Mus musculus (mouse)
5 mmu04142	Lysosome - Mus musculus (mouse)

RAT No matching gene.

MOUSE No matching gene.

RAT

*HUMAN* P35790:**CHKA** Similar to *RAT*

P21643:**T230**

- Protein sequence identity **20.1%**
- Structural similarity - **3.7%** of structure matches to ( 10 out of 268 ) to RMS 1.39 Å
- Whole protein RMSD: **35.77 Å**
- Docking pose RMS distance: **33.62 Å**
- Docking affinity difference: **4.95** : HUMAN affinity=-10.745 vs. RAT affinity=-5.79438

**Indicated Pathways for *RAT* P21643:T230**

Reactome:

ReactomeID	PathwayName
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	ReactomeID	PathwayName
	0 R-RNO-1430728	Metabolism
	1 R-RNO-6788656	Histidine, lysine, phenylalanine, tyrosine, pr...
	2 R-RNO-71240	Tryptophan catabolism
	3 R-RNO-71291	Metabolism of amino acids and derivatives
	KEGG:	
	KeggPathID	PathwayName
	0 rno00380	Tryptophan metabolism - Rattus norvegicus (rat)
	1 rno01100	Metabolic pathways - Rattus norvegicus (rat)
	2 rno00380	Tryptophan metabolism - Rattus norvegicus (rat)
	3 rno01100	Metabolic pathways - Rattus norvegicus (rat)
MOUSE No matching gene.	<p>RAT</p> <p><i>HUMAN</i> P35790:<b>CHKA</b> Similar to <i>RAT</i> Q05343:<b>RXRA</b></p> <ul style="list-style-type: none"> <li>● Protein sequence identity <b>20.1%</b></li> <li>● Structural similarity - <b>1.7%</b> of structure matches to ( 6 out of 362 ) to RMS 1.12 Å</li> <li>● Whole protein RMSD: <b>31.37 Å</b></li> <li>● Docking pose RMS distance: <b>32.27 Å</b></li> <li>● Docking affinity difference: <b>3.6</b> : HUMAN affinity=-10.745 vs. RAT affinity=-7.1457</li> </ul> <p><b>Indicated Pathways for <i>RAT</i> Q05343:RXRA</b></p> <p>Reactome:</p> <p>KEGG:</p>	

## Information on protein Q96RT1: ERBIN, *Erbin*

### Indicated Pathways for Human Q96RT1 : ERBIN

Reactome:

	ReactomeID	PathwayName
	0 R-HSA-1227986	Signaling by ERBB2
	1 R-HSA-162582	Signal Transduction
	2 R-HSA-8863795	Downregulation of ERBB2 signaling

	ReactomeID	PathwayName
3	R-HSA-9006934	Signaling by Receptor Tyrosine Kinases

KEGG:

	KeggPathID	PathwayName
0	hsa04621	NOD-like receptor signaling pathway - Homo sap...
1	hsa04621	NOD-like receptor signaling pathway - Homo sap...

### Top 6 most similar proteins found

Human:Mouse similarity score for Q96RT1: 1 Poor

Human:Rat similarity score Q96RT1: 0 Poor

MOUSE

*HUMAN* Q96RT1:**ERBIN** Similar to *MOUSE*

Q80TH2:**ERBIN**

- Protein sequence identity **88.8%**
- Structural similarity - **36.1%** of structure matches to ( 506 out of 1401 ) to RMS 1.13 Å
- Whole protein RMSD: **62.17 Å**
- Docking pose RMS distance: **42.91 Å**
- Docking affinity difference: **2.06** : HUMAN affinity=-9.95092 vs. MOUSE affinity=-7.89205

**Indicated Pathways for *MOUSE* Q80TH2:ERBIN**

Reactome:

	ReactomeID	PathwayName
0	R-MMU-1227986	Signaling by ERBB2
1	R-MMU-162582	Signal Transduction
2	R-MMU-8863795	Downregulation of ERBB2 signaling
3	R-MMU-9006934	Signaling by Receptor Tyrosine Kinases

KEGG:

	KeggPathID	PathwayName
0	mmu04621	NOD-like receptor signaling pathway - Mus musc...
1	mmu04621	NOD-like receptor signaling pathway - Mus musc...

RAT No matching gene.

MOUSE

*HUMAN* Q96RT1:**ERBIN** Similar to *MOUSE*

Q62417:**SRBS1**

- Protein sequence identity **18.6%**
- Structural similarity - **0.5%** of structure matches to

RAT No matching gene.



( 5 out of 1055 ) to RMS 1.12 Å

- Whole protein RMSD: **83.33** Å
- Docking pose RMS distance: **199.32** Å
- Docking affinity difference: **2.34** : HUMAN affinity=-9.95092 vs. MOUSE affinity=-7.608

**Indicated Pathways for *MOUSE* Q62417:SRBS1**

Reactome:

KEGG:

KeggPathID	PathwayName
0 mmu03320	PPAR signaling pathway - Mus musculus (mouse)
1 mmu04520	Adherens junction - Mus musculus (mouse)
2 mmu04910	Insulin signaling pathway - Mus musculus (mouse)
3 mmu03320	PPAR signaling pathway - Mus musculus (mouse)
4 mmu04520	Adherens junction - Mus musculus (mouse)
5 mmu04910	Insulin signaling pathway - Mus musculus (mouse)

MOUSE

*HUMAN* Q96RT1:**ERBIN** Similar to *MOUSE* Q69ZB8:**ZCHC2**

- Protein sequence identity **18.6%**
- Structural similarity - **13.3%** of structure matches to ( 131 out of 984 ) to RMS 1.1 Å
- Whole protein RMSD: **13.03** Å
- Docking pose RMS distance: **51.73** Å
- Docking affinity difference: **0.69** : HUMAN affinity=-9.95092 vs. MOUSE affinity=-9.25973

**Indicated Pathways for *MOUSE* Q69ZB8:ZCHC2**

Reactome:

KEGG:



MOUSE No matching gene.

RAT No matching gene.

RAT

*HUMAN* Q96RT1:**ERBIN** Similar to *RAT* Q7TP36:**SHRM2**

- Protein sequence identity **18.5%**
- Structural similarity - **0.7%** of structure matches to ( 8 out of 1164 ) to RMS 1.24 Å
- Whole protein RMSD: **106.48** Å

 Docking pose RMS distance: **174.95 Å**  
 Docking affinity difference: **4.46** : HUMAN affinity=-9.95092 vs. RAT affinity=-5.4864

**Indicated Pathways for *RAT* Q7TP36:SHRM2**






Reactome:

KEGG:

MOUSE No matching gene.

RAT

*HUMAN* Q96RT1:**ERBIN** Similar to *RAT* Q64535:**ATP7B**

 Protein sequence identity **18.3%**  
 Structural similarity - **0.5%** of structure matches to ( 5 out of 1092 ) to RMS 0.96 Å  
 Whole protein RMSD: **77.81 Å**  
 Docking pose RMS distance: **93.66 Å**  
 Docking affinity difference: **2.94** : HUMAN affinity=-9.95092 vs. RAT affinity=-7.01484






**Indicated Pathways for *RAT* Q64535:ATP7B**

Reactome:

KEGG:

MOUSE

*HUMAN* Q96RT1:**ERBIN** Similar to *MOUSE* Q9QY30:**ABCBB**

 Protein sequence identity **18.1%**  
 Structural similarity - **10.4%** of structure matches to ( 13 out of 125 ) to RMS 1.19 Å  
 Whole protein RMSD: **28.26 Å**  
 Docking pose RMS distance: **46.61 Å**  
 Docking affinity difference: **1.91** : HUMAN affinity=-9.95092 vs. MOUSE affinity=-8.04051

**Indicated Pathways for *MOUSE* Q9QY30:ABCBB**

Reactome:

ReactomeID	PathwayName
0 R-MMU-1430728	Metabolism

RAT No matching gene.

	ReactomeID	PathwayName
1	R-MMU-159418	Recycling of bile acids and salts
2	R-MMU-192105	Synthesis of bile acids and bile salts
3	R-MMU-193368	Synthesis of bile acids and bile salts via 7al...
4	R-MMU-194068	Bile acid and bile salt metabolism
5	R-MMU-556833	Metabolism of lipids
6	R-MMU-8957322	Metabolism of steroids

KEGG:

	KeggPathID	PathwayName
0	mmu01522	Endocrine resistance - Mus musculus (mouse)
1	mmu02010	ABC transporters - Mus musculus (mouse)
2	mmu04976	Bile secretion - Mus musculus (mouse)
3	mmu04979	Cholesterol metabolism - Mus musculus (mouse)
4	mmu01522	Endocrine resistance - Mus musculus (mouse)
5	mmu02010	ABC transporters - Mus musculus (mouse)
6	mmu04976	Bile secretion - Mus musculus (mouse)
7	mmu04979	Cholesterol metabolism - Mus musculus (mouse)

## Information on protein Q16236: NF2L2, Nuclear

### Indicated Pathways for Human Q16236 : NF2L2

Reactome:

KEGG:

	KeggPathID	PathwayName
0	hsa04141	Protein processing in endoplasmic reticulum - ...
1	hsa05200	Pathways in cancer - Homo sapiens (human)
2	hsa05225	Hepatocellular carcinoma - Homo sapiens (human)
3	hsa05418	Fluid shear stress and atherosclerosis - Homo ...
4	hsa04141	Protein processing in endoplasmic reticulum - ...
5	hsa05200	Pathways in cancer - Homo sapiens (human)
6	hsa05225	Hepatocellular carcinoma - Homo sapiens (human)
7	hsa05418	Fluid shear stress and atherosclerosis - Homo ...

### Top 6 most similar proteins found

Human:Mouse similarity score for Q16236: 1 Poor

Human:Rat similarity score Q16236: 1 Poor

MOUSE	RAT
<i>HUMAN</i> Q16236: <b>NF2L2</b> Similar to <i>MOUSE</i> Q60795: <b>NF2L2</b>	<i>HUMAN</i> Q16236: <b>NF2L2</b> Similar to <i>RAT</i> O54968: <b>NF2L2</b>

- Protein sequence identity **80.9%**
- Structural similarity - **1.5%** of structure matches to ( 9 out of 595 ) to RMS 1.19 Å
- Whole protein RMSD: **43.77 Å**
- Docking pose RMS distance: **28.54 Å**
- Docking affinity difference: **2.36** : HUMAN affinity=-9.77281 vs. MOUSE affinity=-7.40934

**Indicated Pathways for *MOUSE* Q60795:NF2L2**

Reactome:

KEGG:

KeggPathID	PathwayName
0 mmu04141	Protein processing in endoplasmic reticulum - ...
1 mmu05200	Pathways in cancer - Mus musculus (mouse)
2 mmu05225	Hepatocellular carcinoma - Mus musculus (mouse)
3 mmu05418	Fluid shear stress and atherosclerosis - Mus m...
4 mmu04141	Protein processing in endoplasmic reticulum - ...
5 mmu05200	Pathways in cancer - Mus musculus (mouse)
6 mmu05225	Hepatocellular carcinoma - Mus musculus (mouse)
7 mmu05418	Fluid shear stress and atherosclerosis - Mus m...

MOUSE

*HUMAN* Q16236:NF2L2 Similar to *MOUSE* P07724:ALBU

- Protein sequence identity **20.2%**
- Structural similarity - **3.3%** of structure matches to ( 5 out of 153 ) to RMS 0.98 Å
- Whole protein RMSD: **26.0 Å**
- Docking pose RMS distance: **40.09 Å**
- Docking affinity difference: **2.07** : HUMAN affinity=-9.77281 vs. MOUSE affinity=-7.70668

**Indicated Pathways for *MOUSE* P07724:ALBU**

Reactome:

ReactomeID	PathwayName
0 R-MMU-109582	Hemostasis

- Protein sequence identity **82.5%**
- Structural similarity - **2.0%** of structure matches to ( 12 out of 602 ) to RMS 1.25 Å
- Whole protein RMSD: **58.05 Å**
- Docking pose RMS distance: **61.67 Å**
- Docking affinity difference: **2.45** : HUMAN affinity=-9.77281 vs. RAT affinity=-7.32749

**Indicated Pathways for *RAT* O54968:NF2L2**

Reactome:

KEGG:

KeggPathID	PathwayName
0 rno04141	Protein processing in endoplasmic reticulum - ...
1 rno05200	Pathways in cancer - Rattus norvegicus (rat)
2 rno05225	Hepatocellular carcinoma - Rattus norvegicus (...)
3 rno05418	Fluid shear stress and atherosclerosis - Rattu...
4 rno04141	Protein processing in endoplasmic reticulum - ...
5 rno05200	Pathways in cancer - Rattus norvegicus (rat)
6 rno05225	Hepatocellular carcinoma - Rattus norvegicus (...)
7 rno05418	Fluid shear stress and atherosclerosis - Rattu...

RAT No matching gene.

	<b>ReactomeID</b>	<b>PathwayName</b>
1	R-MMU-114608	Platelet degranulation
2	R-MMU-1430728	Metabolism
3	R-MMU-159418	Recycling of bile acids and salts
4	R-MMU-174824	Plasma lipoprotein assembly, remodeling, and c...
5	R-MMU-194068	Bile acid and bile salt metabolism
6	R-MMU-2168880	Scavenging of heme from plasma
7	R-MMU-2173782	Binding and Uptake of Ligands by Scavenger Rec...
8	R-MMU-381426	Regulation of Insulin-like Growth Factor (IGF)...
9	R-MMU-382551	Transport of small molecules
10	R-MMU-392499	Metabolism of proteins
11	R-MMU-425397	Transport of vitamins, nucleosides, and relate...
12	R-MMU-425407	SLC-mediated transmembrane transport
13	R-MMU-556833	Metabolism of lipids
14	R-MMU-5653656	Vesicle-mediated transport
15	R-MMU-597592	Post-translational protein modification
16	R-MMU-76002	Platelet activation, signaling and aggregation
17	R-MMU-76005	Response to elevated platelet cytosolic Ca <sup>2+</sup>
18	R-MMU-879518	Transport of organic anions
19	R-MMU-8957275	Post-translational protein phosphorylation
20	R-MMU-8957322	Metabolism of steroids
21	R-MMU-8963899	Plasma lipoprotein remodeling
22	R-MMU-8964058	HDL remodeling

KEGG:

	<b>KeggPathID</b>	<b>PathwayName</b>
0	mmu04918	Thyroid hormone synthesis - Mus musculus (mouse)
1	mmu04918	Thyroid hormone synthesis - Mus musculus (mouse)

MOUSE

RAT No matching gene.

*HUMAN* Q16236:**NF2L2** Similar to *MOUSE* Q9D0I9:**SYRC**

- Protein sequence identity **19.9%**
- Structural similarity - **1.2%** of structure matches to ( 5 out of 400 ) to RMS 0.68 Å
- Whole protein RMSD: **40.16 Å**
- Docking pose RMS distance: **43.03 Å**
- Docking affinity difference: **2.58** : HUMAN affinity=-9.77281 vs. MOUSE affinity=-7.19706

**Indicated Pathways for *MOUSE* Q9D0I9:SYRC**

Reactome:

KEGG:

KeggPathID	PathwayName
0 mmu00970	Aminoacyl-tRNA biosynthesis - Mus musculus (mo...
1 mmu00970	Aminoacyl-tRNA biosynthesis - Mus musculus (mo...

MOUSE No matching gene.

RAT

*HUMAN* Q16236:**NF2L2** Similar to *RAT* Q569C4:**HDA10**

- Protein sequence identity **19.7%**
- Structural similarity - **1.9%** of structure matches to ( 8 out of 416 ) to RMS 1.32 Å
- Whole protein RMSD: **36.36 Å**
- Docking pose RMS distance: **28.78 Å**
- Docking affinity difference: **1.23** : HUMAN affinity=-9.77281 vs. RAT affinity=-8.53975

**Indicated Pathways for *RAT* Q569C4:HDA10**

Reactome:

KEGG:

KeggPathID	PathwayName
0 rno05034	Alcoholism - Rattus norvegicus (rat)
1 rno05165	Human papillomavirus infection - Rattus norveg...
2 rno05203	Viral carcinogenesis - Rattus norvegicus (rat)
3 rno05034	Alcoholism - Rattus norvegicus (rat)
4 rno05165	Human papillomavirus infection - Rattus norveg...

	KeggPathID	PathwayName
	5 rno05203	Viral carcinogenesis - Rattus norvegicus (rat)
MOUSE No matching gene.	RAT	<p><i>HUMAN</i> Q16236:NF2L2 Similar to <i>RAT</i> Q5FVG8:GRM2B</p> <ul style="list-style-type: none"> <li>● Protein sequence identity <b>19.6%</b></li> <li>● Structural similarity - <b>1.4%</b> of structure matches to ( 5 out of 349 ) to RMS 1.34 Å</li> <li>● Whole protein RMSD: <b>47.97 Å</b></li> <li>● Docking pose RMS distance: <b>35.63 Å</b></li> <li>● Docking affinity difference: <b>3.21</b> : HUMAN affinity=-9.77281 vs. RAT affinity=-6.56242</li> </ul> <p><b>Indicated Pathways for <i>RAT</i> Q5FVG8:GRM2B</b></p> <p>Reactome:</p> <p>KEGG:</p>

## Information on protein Q9HAW9: UD18, *UDP-glucuronosyltransferase*

### Indicated Pathways for Human Q9HAW9 : UD18

Reactome:

	ReactomeID	PathwayName
0	R-HSA-1430728	Metabolism
1	R-HSA-156580	Phase II - Conjugation of compounds
2	R-HSA-156588	Glucuronidation
3	R-HSA-211859	Biological oxidations

KEGG:

	KeggPathID	PathwayName
0	hsa00040	Pentose and glucuronate interconversions - Hom...
1	hsa00053	Ascorbate and aldarate metabolism - Homo sapie...
2	hsa00140	Steroid hormone biosynthesis - Homo sapiens (h...
3	hsa00830	Retinol metabolism - Homo sapiens (human)
4	hsa00860	Porphyryn and chlorophyll metabolism - Homo sa...
5	hsa00980	Metabolism of xenobiotics by cytochrome P450 -...
6	hsa00982	Drug metabolism - cytochrome P450 - Homo sapie...
7	hsa00983	Drug metabolism - other enzymes - Homo sapiens...

	<b>KeggPathID</b>	<b>PathwayName</b>
8	hsa01100	Metabolic pathways - Homo sapiens (human)
9	hsa05204	Chemical carcinogenesis - Homo sapiens (human)
10	hsa00040	Pentose and glucuronate interconversions - Hom...
11	hsa00053	Ascorbate and aldarate metabolism - Homo sapie...
12	hsa00140	Steroid hormone biosynthesis - Homo sapiens (h...
13	hsa00830	Retinol metabolism - Homo sapiens (human)
14	hsa00860	Porphyrin and chlorophyll metabolism - Homo sa...
15	hsa00980	Metabolism of xenobiotics by cytochrome P450 -...
16	hsa00982	Drug metabolism - cytochrome P450 - Homo sapie...
17	hsa00983	Drug metabolism - other enzymes - Homo sapiens...
18	hsa01100	Metabolic pathways - Homo sapiens (human)
19	hsa05204	Chemical carcinogenesis - Homo sapiens (human)

### Top 6 most similar proteins found

Human:Mouse similarity score for Q9HAW9: 6.0 Good

Human:Rat similarity score Q9HAW9: 10.5 Good

MOUSE	RAT																											
<p>MOUSE</p> <p><i>HUMAN</i> Q9HAW9:UD18 Similar to <i>MOUSE</i> Q62452:UD19</p> <ul style="list-style-type: none"> <li><span style="color: green;">●</span> Protein sequence identity <b>79.4%</b></li> <li><span style="color: yellow;">●</span> Structural similarity - <b>59.7%</b> of structure matches to ( 315 out of 528 ) to RMS 1.03 Å</li> <li><span style="color: green;">●</span> Whole protein RMSD: <b>9.89 Å</b></li> <li><span style="color: yellow;">●</span> Docking pose RMS distance: <b>9.43 Å</b></li> <li><span style="color: red;">●</span> Docking affinity difference: <b>2.34</b> : HUMAN affinity=-9.69582 vs. MOUSE affinity=-7.35743</li> </ul> <p><b>Indicated Pathways for <i>MOUSE</i> Q62452:UD19</b></p> <p>Reactome:</p> <table border="1"> <thead> <tr> <th></th> <th><b>ReactomeID</b></th> <th><b>PathwayName</b></th> </tr> </thead> <tbody> <tr> <td>0</td> <td>R-MMU-1430728</td> <td>Metabolism</td> </tr> <tr> <td>1</td> <td>R-MMU-156580</td> <td>Phase II - Conjugation of compounds</td> </tr> <tr> <td>2</td> <td>R-MMU-156588</td> <td>Glucuronidation</td> </tr> <tr> <td>3</td> <td>R-MMU-211859</td> <td>Biological oxidations</td> </tr> </tbody> </table> <p>KEGG:</p> <table border="1"> <thead> <tr> <th></th> <th><b>KeggPathID</b></th> <th><b>PathwayName</b></th> </tr> </thead> <tbody> <tr> <td>0</td> <td>mmu00040</td> <td>Pentose and glucuronate interconversions - Mus...</td> </tr> <tr> <td>1</td> <td>mmu00053</td> <td>Ascorbate and aldarate metabolism - Mus muscul...</td> </tr> <tr> <td>2</td> <td>mmu00140</td> <td></td> </tr> </tbody> </table>		<b>ReactomeID</b>	<b>PathwayName</b>	0	R-MMU-1430728	Metabolism	1	R-MMU-156580	Phase II - Conjugation of compounds	2	R-MMU-156588	Glucuronidation	3	R-MMU-211859	Biological oxidations		<b>KeggPathID</b>	<b>PathwayName</b>	0	mmu00040	Pentose and glucuronate interconversions - Mus...	1	mmu00053	Ascorbate and aldarate metabolism - Mus muscul...	2	mmu00140		<p>RAT No matching gene.</p>
	<b>ReactomeID</b>	<b>PathwayName</b>																										
0	R-MMU-1430728	Metabolism																										
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0	mmu00040	Pentose and glucuronate interconversions - Mus...																										
1	mmu00053	Ascorbate and aldarate metabolism - Mus muscul...																										
2	mmu00140																											








KeggPathID	PathwayName
	Steroid hormone biosynthesis - Mus musculus (m...
3 mmu00830	Retinol metabolism - Mus musculus (mouse)
4 mmu00860	Porphyrin and chlorophyll metabolism - Mus mus...
5 mmu00980	Metabolism of xenobiotics by cytochrome P450 - ...
6 mmu00982	Drug metabolism - cytochrome P450 - Mus muscul...
7 mmu00983	Drug metabolism - other enzymes - Mus musculus...
8 mmu01100	Metabolic pathways - Mus musculus (mouse)
9 mmu05204	Chemical carcinogenesis - Mus musculus (mouse)
10 mmu00040	Pentose and glucuronate interconversions - Mus...
11 mmu00053	Ascorbate and aldarate metabolism - Mus muscul...
12 mmu00140	Steroid hormone biosynthesis - Mus musculus (m...
13 mmu00830	Retinol metabolism - Mus musculus (mouse)
14 mmu00860	Porphyrin and chlorophyll metabolism - Mus mus...
15 mmu00980	Metabolism of xenobiotics by cytochrome P450 - ...
16 mmu00982	Drug metabolism - cytochrome P450 - Mus muscul...
17 mmu00983	Drug metabolism - other enzymes - Mus musculus...
18 mmu01100	Metabolic pathways - Mus musculus (mouse)
19 mmu05204	Chemical carcinogenesis - Mus musculus (mouse)

MOUSE No matching gene.

RAT

*HUMAN* Q9HAW9:UD18 Similar to *RAT* Q64634:UD18

-  Protein sequence identity **78.1%**
-  Structural similarity - **60.2%** of structure matches to ( 319 out of 530 ) to RMS 0.94 Å
-  Whole protein RMSD: **7.57 Å**
-  Docking pose RMS distance: **20.04 Å**
-  Docking affinity difference: **2.06** :  
HUMAN affinity=-9.69582 vs. RAT affinity=-7.63332

**Indicated Pathways for *RAT* Q64634:UD18**

Reactome:

KEGG:

MOUSE No matching gene.

RAT

*HUMAN* Q9HAW9:UD18 Similar to *RAT* Q64633:UD17

- Protein sequence identity **77.8%**
- Structural similarity - **52.3%** of structure matches to ( 277 out of 530 ) to RMS 1.03 Å
- Whole protein RMSD: **7.63 Å**
- Docking pose RMS distance: **17.97 Å**
- Docking affinity difference: **2.4** : HUMAN affinity=-9.69582 vs. RAT affinity=-7.29093

**Indicated Pathways for *RAT* Q64633:UD17**

Reactome:

KEGG:

MOUSE

*HUMAN* Q9HAW9:UD18 Similar to *MOUSE* P70691:UD12

- Protein sequence identity **62.8%**
- Structural similarity - **45.6%** of structure matches to ( 236 out of 517 ) to RMS 1.08 Å
- Whole protein RMSD: **7.76 Å**
- Docking pose RMS distance: **10.27 Å**
- Docking affinity difference: **2.26** : HUMAN affinity=-9.69582 vs. MOUSE affinity=-7.43579

**Indicated Pathways for *MOUSE* P70691:UD12**

Reactome:

	ReactomeID	PathwayName
0	R-MMU-1430728	Metabolism
1	R-MMU-156580	Phase II - Conjugation of compounds
2	R-MMU-156588	Glucuronidation
3	R-MMU-189445	Metabolism of porphyrins
4	R-MMU-189483	Heme degradation
5	R-MMU-211859	Biological oxidations

KEGG:

	KeggPathID	PathwayName
0	mmu00040	Pentose and glucuronate interconversions - Mus...
1	mmu00053	Ascorbate and aldarate metabolism - Mus muscul...

RAT

*HUMAN* Q9HAW9:UD18 Similar to *RAT* P20720:UD12

- Protein sequence identity **63.6%**
- Structural similarity - **46.8%** of structure matches to ( 247 out of 528 ) to RMS 1.16 Å
- Whole protein RMSD: **8.59 Å**
- Docking pose RMS distance: **36.82 Å**
- Docking affinity difference: **3.49** : HUMAN affinity=-9.69582 vs. RAT affinity=-6.20279

**Indicated Pathways for *RAT* P20720:UD12**

Reactome:


KEGG:


KeggPathID	PathwayName
2 mmu00140	Steroid hormone biosynthesis - Mus musculus (m...
3 mmu00830	Retinol metabolism - Mus musculus (mouse)
4 mmu00860	Porphyrin and chlorophyll metabolism - Mus mus...
5 mmu00980	Metabolism of xenobiotics by cytochrome P450 - ...
6 mmu00982	Drug metabolism - cytochrome P450 - Mus muscul...
7 mmu00983	Drug metabolism - other enzymes - Mus musculus...
8 mmu01100	Metabolic pathways - Mus musculus (mouse)
9 mmu05204	Chemical carcinogenesis - Mus musculus (mouse)
10 mmu00040	Pentose and glucuronate interconversions - Mus...
11 mmu00053	Ascorbate and aldarate metabolism - Mus muscul...
12 mmu00140	Steroid hormone biosynthesis - Mus musculus (m...
13 mmu00830	Retinol metabolism - Mus musculus (mouse)
14 mmu00860	Porphyrin and chlorophyll metabolism - Mus mus...
15 mmu00980	Metabolism of xenobiotics by cytochrome P450 - ...
16 mmu00982	Drug metabolism - cytochrome P450 - Mus muscul...
17 mmu00983	Drug metabolism - other enzymes - Mus musculus...
18 mmu01100	Metabolic pathways - Mus musculus (mouse)
19 mmu05204	Chemical carcinogenesis - Mus musculus (mouse)

MOUSE No matching gene.

RAT


*HUMAN* Q9HAW9:UD18 Similar to *RAT* Q64638:UD15

 Protein sequence identity **61.6%**

 Structural similarity - **57.1%** of structure matches to ( 298 out of 522 ) to RMS 0.99 Å

 Whole protein RMSD: **7.82 Å**

 Docking pose RMS distance: **27.6 Å**

 Docking affinity difference: **2.4** : *HUMAN* affinity=-9.69582 vs. *RAT* affinity=-7.29766

**Indicated Pathways for *RAT* Q64638:UD15**

Reactome:

KEGG:

## Information on protein Q92925: SMRD2, *SWI*

### Indicated Pathways for Human Q92925 : SMRD2

Reactome:

	ReactomeID	PathwayName
0	R-HSA-212436	Generic Transcription Pathway
1	R-HSA-3214858	RMTs methylate histone arginines
2	R-HSA-3247509	Chromatin modifying enzymes
3	R-HSA-4839726	Chromatin organization
4	R-HSA-73857	RNA Polymerase II Transcription
5	R-HSA-74160	Gene expression (Transcription)
6	R-HSA-8878171	Transcriptional regulation by RUNX1
7	R-HSA-8939243	RUNX1 interacts with co-factors whose precise ...

KEGG:

	KeggPathID	PathwayName
0	hsa04714	Thermogenesis - Homo sapiens (human)
1	hsa05225	Hepatocellular carcinoma - Homo sapiens (human)
2	hsa04714	Thermogenesis - Homo sapiens (human)
3	hsa05225	Hepatocellular carcinoma - Homo sapiens (human)

### Top 6 most similar proteins found

Human:Mouse similarity score for Q92925: 2.5 Good

Human:Rat similarity score Q92925: 1 Poor

MOUSE	RAT				
<p><i>HUMAN</i> Q92925:<b>SMRD2</b> Similar to <i>MOUSE</i> Q99JR8:<b>SMRD2</b></p> <ul style="list-style-type: none"> <li><span style="color: green;">●</span> Protein sequence identity <b>98.1%</b></li> <li><span style="color: yellow;">●</span> Structural similarity - <b>55.4%</b> of structure matches to ( 294 out of 531 ) to RMS 1.26 Å</li> <li><span style="color: green;">●</span> Whole protein RMSD: <b>2.78 Å</b></li> <li><span style="color: red;">●</span> Docking pose RMS distance: <b>25.95 Å</b></li> <li><span style="color: yellow;">●</span> Docking affinity difference: <b>0.51</b> : HUMAN affinity=-9.68458 vs. MOUSE affinity=-10.191</li> </ul> <p><b>Indicated Pathways for <i>MOUSE</i> Q99JR8:SMRD2</b></p> <p>Reactome:</p> <table border="1"> <thead> <tr> <th>ReactomeID</th> <th>PathwayName</th> </tr> </thead> <tbody> </tbody> </table>	ReactomeID	PathwayName	<p><i>HUMAN</i> Q92925:<b>SMRD2</b> Similar to <i>RAT</i> O54772:<b>SMRD2</b></p> <ul style="list-style-type: none"> <li><span style="color: green;">●</span> Protein sequence identity <b>97.9%</b></li> <li><span style="color: red;">●</span> Structural similarity - <b>18.6%</b> of structure matches to ( 99 out of 531 ) to RMS 1.43 Å</li> <li><span style="color: green;">●</span> Whole protein RMSD: <b>7.53 Å</b></li> <li><span style="color: red;">●</span> Docking pose RMS distance: <b>30.89 Å</b></li> <li><span style="color: red;">●</span> Docking affinity difference: <b>1.7</b> : HUMAN affinity=-9.68458 vs. RAT affinity=-7.98802</li> </ul> <p><b>Indicated Pathways for <i>RAT</i> O54772:SMRD2</b></p> <p>Reactome:</p> <table border="1"> <thead> <tr> <th>ReactomeID</th> <th>PathwayName</th> </tr> </thead> <tbody> </tbody> </table>	ReactomeID	PathwayName
ReactomeID	PathwayName				
ReactomeID	PathwayName				

ReactomeID	PathwayName	ReactomeID	PathwayName
0 R-MMU-212436	Generic Transcription Pathway	0 R-RNO-212436	Generic Transcription Pathway
1 R-MMU-3214858	RMTs methylate histone arginines	1 R-RNO-3214858	RMTs methylate histone arginines
2 R-MMU-3247509	Chromatin modifying enzymes	2 R-RNO-3247509	Chromatin modifying enzymes
3 R-MMU-4839726	Chromatin organization	3 R-RNO-4839726	Chromatin organization
4 R-MMU-73857	RNA Polymerase II Transcription	4 R-RNO-73857	RNA Polymerase II Transcription
5 R-MMU-74160	Gene expression (Transcription)	5 R-RNO-74160	Gene expression (Transcription)
6 R-MMU-8878171	Transcriptional regulation by RUNX1	6 R-RNO-8878171	Transcriptional regulation by RUNX1
7 R-MMU-8939243	RUNX1 interacts with co-factors whose precise ...	7 R-RNO-8939243	RUNX1 interacts with co-factors whose precise ...
KEGG:		KEGG:	
KeggPathID	PathwayName	KeggPathID	PathwayName
0 mmu04714	Thermogenesis - Mus musculus (mouse)	0 rno04714	Thermogenesis - Rattus norvegicus (rat)
1 mmu05225	Hepatocellular carcinoma - Mus musculus (mouse)	1 rno05225	Hepatocellular carcinoma - Rattus norvegicus (...)
2 mmu04714	Thermogenesis - Mus musculus (mouse)	2 rno04714	Thermogenesis - Rattus norvegicus (rat)
3 mmu05225	Hepatocellular carcinoma - Mus musculus (mouse)	3 rno05225	Hepatocellular carcinoma - Rattus norvegicus (...)
MOUSE		RAT	
<i>HUMAN</i> Q92925: <b>SMRD2</b> Similar to <i>MOUSE</i> Q91YE2: <b>EGLN2</b>		<i>HUMAN</i> Q92925: <b>SMRD2</b> Similar to <i>RAT</i> Q6AYU4: <b>EGLN2</b>	
● Protein sequence identity <b>20.7%</b>		● Protein sequence identity <b>20.6%</b>	
● Structural similarity - <b>2.9%</b> of structure matches to ( 7 out of 238 ) to RMS 1.38 Å		● Structural similarity - <b>5.2%</b> of structure matches to ( 12 out of 233 ) to RMS 0.31 Å	
● Whole protein RMSD: <b>27.24 Å</b>		● Whole protein RMSD: <b>27.55 Å</b>	
● Docking pose RMS distance: <b>17.77 Å</b>		● Docking pose RMS distance: <b>24.57 Å</b>	
● Docking affinity difference: <b>1.36</b> : HUMAN affinity=-9.68458 vs. MOUSE affinity=-8.32316		● Docking affinity difference: <b>3.2</b> : HUMAN affinity=-9.68458 vs. RAT affinity=-6.48653	
Indicated Pathways for <i>MOUSE</i> Q91YE2: <b>EGLN2</b>		Indicated Pathways for <i>RAT</i> Q6AYU4: <b>EGLN2</b>	
Reactome:		Reactome:	
ReactomeID	PathwayName	ReactomeID	PathwayName
0 R-MMU-1234174	Regulation of Hypoxia-inducible Factor (HIF) b...	0 R-RNO-1234174	Regulation of Hypoxia-inducible Factor (HIF) b...
1 R-MMU-1234176	Oxygen-dependent proline hydroxylation of Hypo...	1 R-RNO-1234176	Oxygen-dependent proline hydroxylation of Hypo...
2 R-MMU-2262749	Cellular response to hypoxia	2 R-RNO-2262749	Cellular response to hypoxia
3 R-MMU-2262752	Cellular responses to stress	3 R-RNO-2262752	Cellular responses to stress
4 R-MMU-8953897	Cellular responses to external stimuli	4 R-RNO-8953897	Cellular responses to external stimuli

KEGG:

	KeggPathID	PathwayName
0	mmu04066	HIF-1 signaling pathway - Mus musculus (mouse)
1	mmu05200	Pathways in cancer - Mus musculus (mouse)
2	mmu05211	Renal cell carcinoma - Mus musculus (mouse)
3	mmu04066	HIF-1 signaling pathway - Mus musculus (mouse)
4	mmu05200	Pathways in cancer - Mus musculus (mouse)
5	mmu05211	Renal cell carcinoma - Mus musculus (mouse)

MOUSE

*HUMAN* Q92925:**SMRD2** Similar to *MOUSE* Q9DBG1:**CP27A**

- Protein sequence identity **20.2%**
- Structural similarity - **4.6%** of structure matches to ( 14 out of 302 ) to RMS 1.06 Å
- Whole protein RMSD: **34.33 Å**
- Docking pose RMS distance: **16.6 Å**
- Docking affinity difference: **0.95** : HUMAN affinity=-9.68458 vs. MOUSE affinity=-8.7372

**Indicated Pathways for *MOUSE* Q9DBG1:CP27A**

Reactome:

	ReactomeID	PathwayName
0	R-MMU-1430728	Metabolism
1	R-MMU-192105	Synthesis of bile acids and bile salts
2	R-MMU-193368	Synthesis of bile acids and bile salts via 7al...
3	R-MMU-193775	Synthesis of bile acids and bile salts via 24-...
4	R-MMU-193807	Synthesis of bile acids and bile salts via 27-...
5	R-MMU-194068	Bile acid and bile salt metabolism
6	R-MMU-211859	Biological oxidations
7	R-MMU-211897	Cytochrome P450 - arranged by substrate type
8	R-MMU-211945	Phase I - Functionalization of compounds
9	R-MMU-211976	Endogenous sterols
10	R-MMU-556833	Metabolism of lipids
11	R-MMU-8957322	Metabolism of steroids

KEGG:

KEGG:

	KeggPathID	PathwayName
0	rno04066	HIF-1 signaling pathway - Rattus norvegicus (rat)
1	rno05200	Pathways in cancer - Rattus norvegicus (rat)
2	rno05211	Renal cell carcinoma - Rattus norvegicus (rat)
3	rno04066	HIF-1 signaling pathway - Rattus norvegicus (rat)
4	rno05200	Pathways in cancer - Rattus norvegicus (rat)
5	rno05211	Renal cell carcinoma - Rattus norvegicus (rat)

RAT No matching gene.

KeggPathID	PathwayName
0 mmu00120	Primary bile acid biosynthesis - Mus musculus ...
1 mmu01100	Metabolic pathways - Mus musculus (mouse)
2 mmu03320	PPAR signaling pathway - Mus musculus (mouse)
3 mmu04979	Cholesterol metabolism - Mus musculus (mouse)
4 mmu00120	Primary bile acid biosynthesis - Mus musculus ...
5 mmu01100	Metabolic pathways - Mus musculus (mouse)
6 mmu03320	PPAR signaling pathway - Mus musculus (mouse)
7 mmu04979	Cholesterol metabolism - Mus musculus (mouse)

## MOUSE

*HUMAN* Q92925:SMRD2 Similar to *MOUSE*

Q91XD4:FTCD

- Protein sequence identity **20.0%**
- Structural similarity - **3.1%** of structure matches to ( 6 out of 193 ) to RMS 1.38 Å
- Whole protein RMSD: **23.11 Å**
- Docking pose RMS distance: **23.35 Å**
- Docking affinity difference: **2.18** : HUMAN affinity=-9.68458 vs. MOUSE affinity=-7.50237

### Indicated Pathways for *MOUSE* Q91XD4:FTCD

Reactome:

ReactomeID	PathwayName
0 R-MMU-1430728	Metabolism
1 R-MMU-6788656	Histidine, lysine, phenylalanine, tyrosine, pr...
2 R-MMU-70921	Histidine catabolism
3 R-MMU-71291	Metabolism of amino acids and derivatives

KEGG:

KeggPathID	PathwayName
0 mmu00340	Histidine metabolism - Mus musculus (mouse)
1 mmu00670	One carbon pool by folate - Mus musculus (mouse)
2 mmu01100	Metabolic pathways - Mus musculus (mouse)
3 mmu00340	Histidine metabolism - Mus musculus (mouse)
4 mmu00670	One carbon pool by folate - Mus musculus (mouse)
5 mmu01100	Metabolic pathways - Mus musculus (mouse)

RAT No matching gene.

