A Teratological Tour of NCBI

Eric W. Sayers, Ph.D
National Center for Biotechnology Information
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ftp://ftp.ncbi.nih.gov/pub/sayers/Teratology

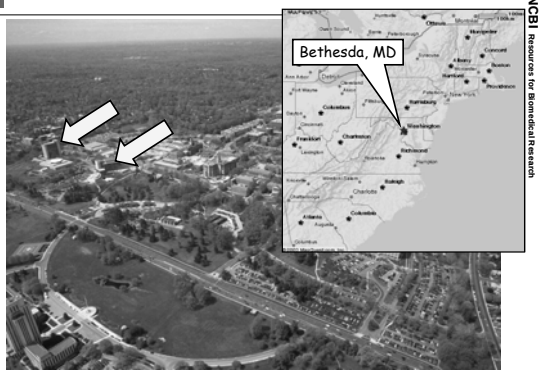
NCBI Resources for Biomedical Research

Course Topics

- Overview of NCBI
- Resources for genetic disorders
  - OMIM: human disease phenotypes
  - From sequences to annotated genes
  - Microarrays and polymorphisms
  - Test case: Muenke syndrome
- Resources for chemical teratogens
  - PubChem datasets
  - Test case: 6-aminonicotinamide

NCBI Resources for Biomedical Research

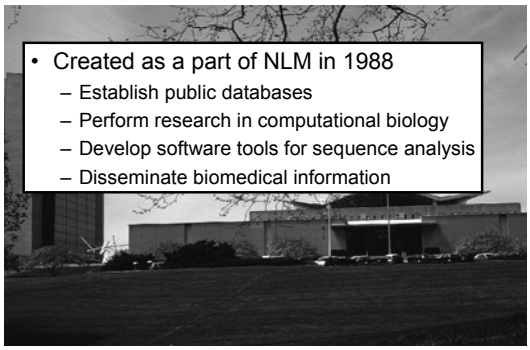
The National Institutes of Health



NCBI Resources for Biomedical Research

The National Center for Biotechnology Information

NCBI Resources for Biomedical Research



- Created as a part of NLM in 1988
  - Establish public databases
  - Perform research in computational biology
  - Develop software tools for sequence analysis
  - Disseminate biomedical information

What does NCBI do?

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- accepts submissions of primary data
- develops tools to analyze these data
- uses these tools to create derivative databases based on the primary data
- provides free search, link, and retrieval of these data, primarily through the Entrez system

Types of Databases

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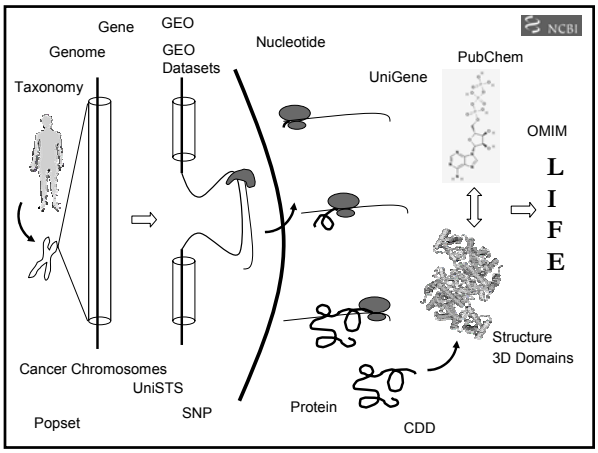
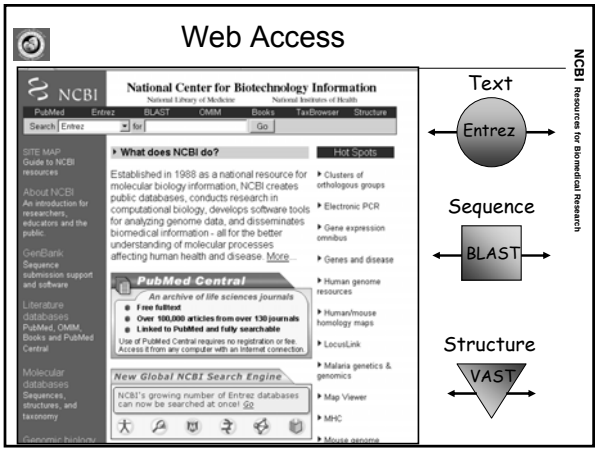
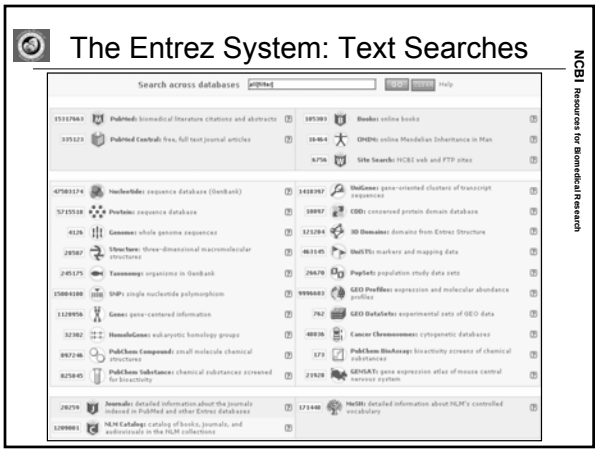
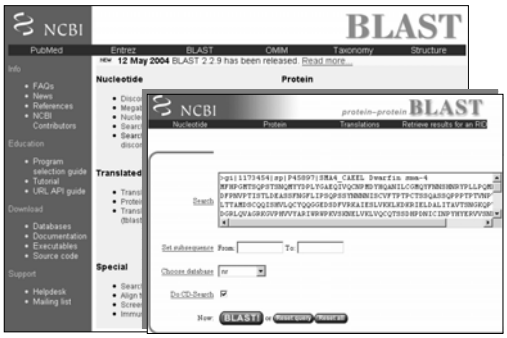
- Primary Databases
  - Original submissions by experimentalists
  - Content controlled by the submitter
- Derivative Databases
  - Built from primary data
  - Content controlled by third party (NCBI)


NCBI
Gene
GEO
Genome
GEO Datasets
Nucleotide
PubChem
UniGene
Taxonomy
OMIM
L
I
F
E
Structure
3D Domains
Cancer Chromosomes
UniSTS
SNP
Protein
Popset
CDD


Web Access
NCBI
National Center for Biotechnology Information
Text
Entrez
Sequence
BLAST
Structure
VAST
NCBI Resources for Biomedical Research

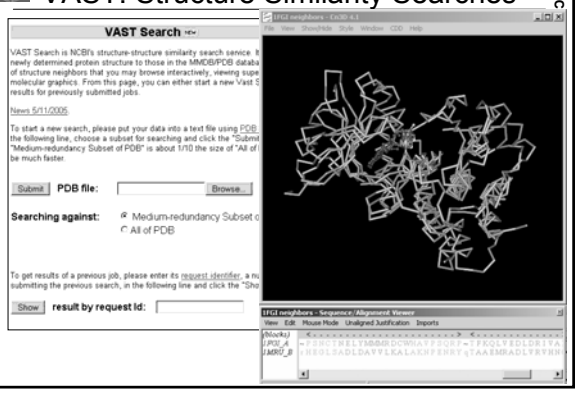

The Entrez System: Text Searches
Search across databases
NCBI Resources for Biomedical Research

BLAST: Sequence Similarity Searches



NCBI Resources for Biomedical Research

VAST: Structure Similarity Searches



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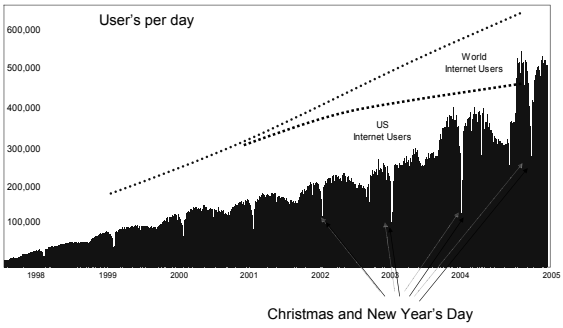
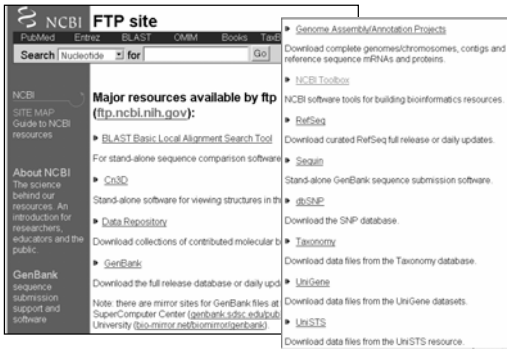
NCBI Web Traffic



NCBI

The NCBI ftp site



NCBI Resources for Biomedical Research

Useful Databases for Teratology

- OMIM (Online Mendelian Inheritance in Man)
  - literature calatog of human disease phenotypes
- Gene
  - curated database of gene loci and associated sequences
- GEO (Gene Expression Omnibus)
  - primary and derivative collections of gene expression data
- SNP (Single Nucleotide Polymorphisms)
  - primary and derivative collections of nucleotide polymorphisms
- PubChem (Substance, Compound, Bioassay)
  - primary and derivative collections of small molecules and their biological activities

NCBI Resources for Biomedical Research

Test Cases: Muenke Syndrome and 6-AN

Muenke syndrome, or Muenke nonsyndromic coronal craniosynostosis, is a developmental disorder characterized by a premature closing of cranial sutures, resulting in deformities in the head and face.

Muenke syndrome is caused by a mutation in the gene for fibroblast growth factor receptor 3, FGFR3.

Mutations in a related gene, fibroblast growth factor receptor 2, cause a similar craniosynostosis called Crouzon syndrome, along with several other related developmental problems.

6-AN, or 6-aminonicotinamide, is an antimetabolite of nicotinic acid (vitamin B-3) and is a known teratogen, causing lesions in the CNS, skin, and digestive tract during embryonic development.

6-AN has been linked to apoptosis in tumors, and is being investigated as a chemotherapeutic agent.

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Searching in OMIM

muenke syndrome

33 records retrieved

`muenke[All Fields] AND syndrome[All Fields]`

"muenke syndrome"

2 records retrieved

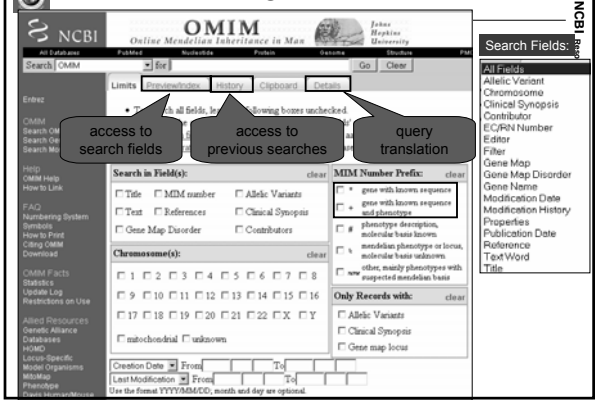
`"muenke syndrome"[All Fields]`

muenke syndrome[title]

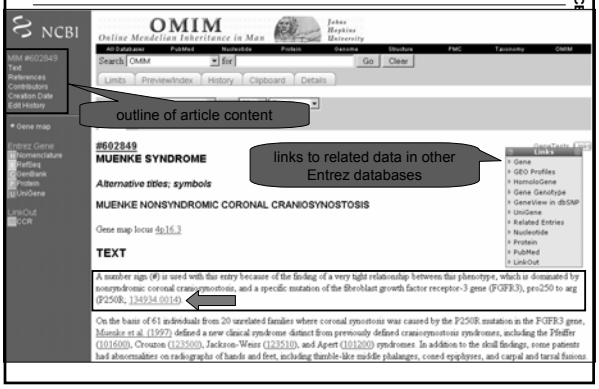
1 record retrieved

`muenke syndrome[title]`

OMIM



An OMIM Record



OMIM Allelic Variant in FGFR3

NCBI

NCBI

MIM *134934
Description
Cloning
Gene Function
Gene Structure
Mapping
Molecular Genetics
Animal Model
Allelic Variants
• View List
References
Contributors
Creation Date
Edit History

• Gene map

Entrez Gene
Nomenclature
RefSeq
GenBank
Protein
UniGene

LinkOut
OCR
HGMD

.0014 MUENKE SYNDROME [FGFR3, PRO250ARG]

SAETHRE-CHOTZEN SYNDROME, INCLUDED
BEARE-STEVENSON SYNDROME-LIKE ANOMALIES, INCLUDED

Reiltat et al. (1996) described a pro250-to-arg (P250R) amino acid substitution in FGFR3 (caused by a C-to-G transversion at position 749 of the coding cDNA sequence) in 10 unrelated patients with nonsyndromic autosomal dominant or sporadic craniosynostosis. This mutation is in the extracellular domain of the FGFR3 protein and occurs precisely at the position within the FGFR3 protein analogous to that of mutations in FGFR1 (P252R; 136350.0001) and FGFR2 (P253R; 176943.0011), previously reported in Pfeiffer (101600) and Apert syndromes, respectively. They pictured the craniofacial and extremity anomalies in some of these cases.

Muenke et al. (1997) provided extensive information on a series of 61 individuals from 20 unrelated families in which coronal craniosynostosis is due to this mutation, defining a new clinical syndrome that is referred to as Muenke nonsyndromic coronal craniosynostosis (602849). At about the same time, Moloney et al. (1997) studied 26 patients with coronal craniosynostosis but no syndromic diagnosis to determine the frequency of the 749C-G (pro250-to-arg) mutation in FGFR3. Heterozygosity for the mutation was found in 8 (31%) of the 26 probands. In 2 cases, the mutation showed autosomal dominant transmission with evidence of variable expressivity, the remaining 6 cases were sporadic. Moloney et al. (1997) pointed out that the 749C nucleotide has one of the highest mutation rates described in the human genome.

Reardon et al. (1997) reported 9 individuals with the P250R mutation. The authors documented a variable clinical presentation and contrasted this with the phenotype produced by the analogous mutation in FGFR1 (P252R; 136350.0001) and FGFR2 (P253R; 176943.0011). In particular, Reardon et al (1997) noted mental retardation in 4 of the 9 cases, which they reported was unrelated to the management of the craniosynostosis. Reardon et al. (1997) suggested that there was a significant overlap between Saethre-Chotzen syndrome (101400), a common autosomal dominant condition of craniosynostosis and limb anomalies, and the phenotype produced by this mutation. They also noted unilateral craniosynostosis in 3 of the 9 cases to emphasize the caution with which the recurrence risks should be approached in craniosynostosis.

OMIM Record for FGFR3

NCB

NCBI

MIM *134934
Description
Cloning
Gene Function
Gene Structure
Mapping
Molecular Genetics
Animal Model
Allelic Variants
• View List
References
Contributors
Creation Date
Edit History

• Gene map

Entrez Gene
Nomenclature
RefSeq
GenBank
Protein
UniGene

LinkOut
OCR
HGMD

***134934**
FIBROBLAST GROWTH FACTOR RECEPTOR 3; FGFR3

***134934**
FIBROBLAST GROWTH FACTOR RECEPTOR 3; FGFR3

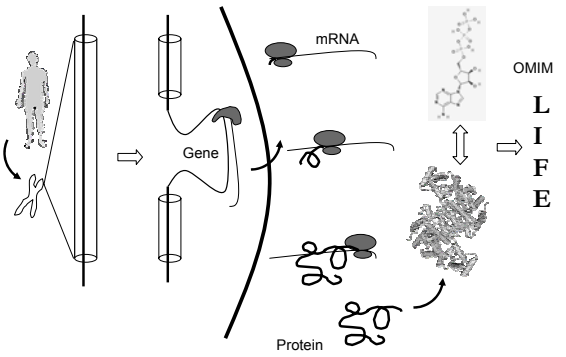
ALLELIC VARIANTS
(selected examples)

- 0001 ACHONDROPLASIA [FGFR3, GLY380ARG, 1138G-A]
- 0002 ACHONDROPLASIA [FGFR3, GLY380ARG, 1138G-C]
- 0003 ACHONDROPLASIA [FGFR3, GLY375CYS]
- 0004 THANATOPHORIC DYSPLASIA, TYPE II [FGFR3, LYS650GLU]
- 0005 THANATOPHORIC DYSPLASIA, TYPE I [FGFR3, ARG248CYS]
- 0006 THANATOPHORIC DYSPLASIA, TYPE I [FGFR3, SER371CYS]
- 0007 THANATOPHORIC DYSPLASIA, TYPE I [FGFR3, TER807GLY]
- 0008 THANATOPHORIC DYSPLASIA, TYPE I [FGFR3, TER807ARG]
- 0009 THANATOPHORIC DYSPLASIA, TYPE I [FGFR3, TER807CYS]
- 0010 HYPOCHONDROPLASIA [FGFR3, ASN540LYS, 1620C-A]
- 0011 CROUZON SYNDROME WITH ACANTHOSIS NIGRICANS [FGFR3, ALA391GLU]
- 0012 HYPOCHONDROPLASIA [FGFR3, ASN540LYS, 1620C-G]
- 0013 THANATOPHORIC DYSPLASIA, TYPE I [FGFR3, SER249CYS]
- 0014 MUENKE SYNDROME [FGFR3, PRO250ARG]
- 0015 SADDAN DYSPLASIA [FGFR3, LYS650MET]
- 0016 THANATOPHORIC DYSPLASIA, TYPE I [FGFR3, TYR373CYS]
- 0017 MULTIPLE MYELOMA, SOMATIC [FGFR3/IGH FUSION]
- 0018 HYPOCHONDROPLASIA [FGFR3, ASN540THR]
- 0019 HYPOCHONDROPLASIA [FGFR3, ILE538VAL]
- 0020 HYPOCHONDROPLASIA [FGFR3, LYS650ASN, 1950G-T]

GeneTests
Links
• Gene
• GEO Profiles
• HomoloGene
• Free in PMC
• Gene Genotype
• GeneView in dbSNP
• UniGene
• Related Entries
• Nucleotide
• Protein
• PubMed
• SNP
• LinkOut

What is a Gene?

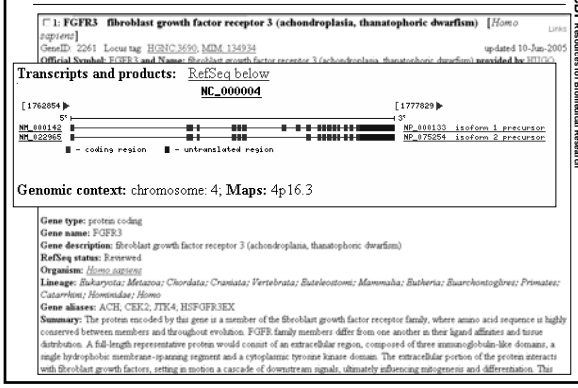
NCBI



OMIM

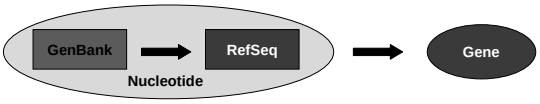
L
I
F
E

Gene Record for FGFR3



NCBI Resources for Biomedical Research

Entrez Gene and RefSeq



- Entrez Gene is the central depository for information about a gene available at NCBI, and often provides links to sites beyond NCBI
- Entrez Gene includes records for organisms that have NCBI Reference Sequences (RefSeqs)
- Entrez Gene records contain RefSeq mRNAs, proteins, and genomic DNA (if known) for a gene locus, plus links to other Entrez databases
- NCBI RefSeqs are based on primary sequence data in GenBank

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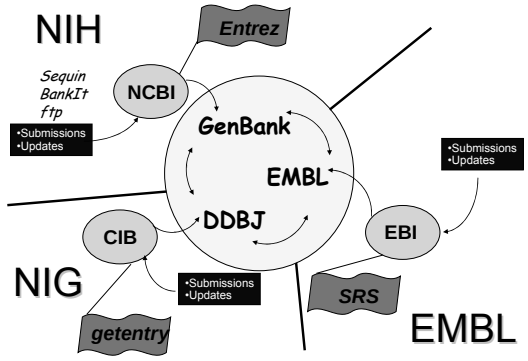
What is GenBank?

NCBI's Primary Sequence Database

- Nucleotide only sequence database
- Archival in nature
- Each record is assigned a stable accession number
- GenBank Data
  - Direct submissions (traditional records)
  - Batch submissions (EST, GSS, STS)
  - ftp accounts (genome data)
- Three collaborating databases
  - GenBank
  - DNA Database of Japan (DDBJ)
  - European Molecular Biology Laboratory (EMBL) Database

NCBI Resources for Biomedical Research

The International Sequence Database Collaboration



NCBI Resources for Biomedical Research

GenBank Releases

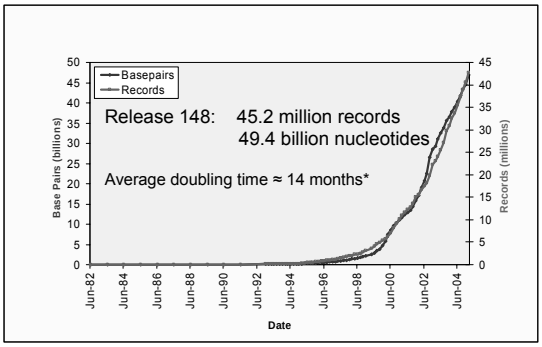
Release 148	June 2005
45,236,251	Records
49,398,852,122	Nucleotides
>140,000	Species
172 Gigabytes	*785 files*

- full release every two months
- incremental and cumulative updates daily
- available only through internet

ftp://ftp.ncbi.nih.gov/genbank/

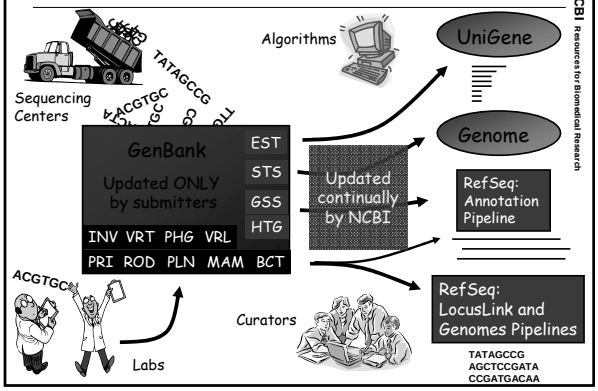
NCBI Resources for Biomedical Research

The Growth of GenBank



NCBI Resources for Biomedical Research

Primary vs. Derivative Databases



NCBI Resources for Biomedical Research

RefSeq: NCBI's Derivative Sequence Database

RefSeq Benefits

- Non-redundant
- Explicitly linked nucleotide and protein sequences
- Updated to reflect current sequence data and biology
- Validated by hand
- Format consistency
- Distinct accession series
- Stewardship by NCBI staff and collaborators

ftp://ftp.ncbi.nih.gov/refseq/release

NCBI Resources for Biomedical Research

RefSeq: NCBI's Derivative Sequence Database

- **Curated transcripts and proteins**
  - **NM_123456 → NP_123456**
  - NR_123456 (non-coding RNA)
- **Model transcripts and proteins**
  - **XM_123456 → XP_123456**
  - XR_123456 (non-coding RNA)
- **Assembled Genomic Regions (contigs)**
  - **NT_123456 (BAC clones)**
  - NW_123456 (WGS)
- **Other Genomic Sequence**
  - NG_123456 (complex regions, pseudogenes)
  - NZ_ABCD12345678 (WGS) → ZP_123456
- **Chromosome records in Entrez Genome**
  - **NC_123456 (chromosome; microbial or organelle genome)**

Nucleotide

Protein

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Entrez Nucleotide

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Primary Data	
DDBJ / EMBL / GenBank	**54,689,634**
Derivative Data	
RefSeq	**1,060,130**
PDB	**5,803**
Third Party Annotation	**4,558**
Total	**55,760,125**

Annotating the Gene

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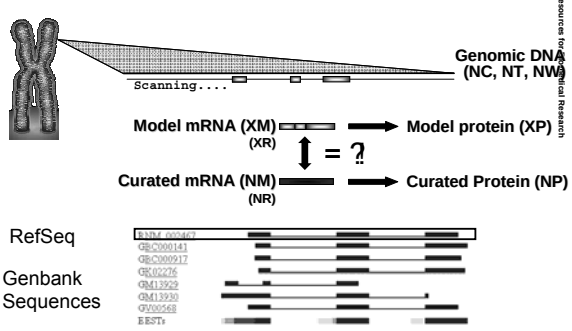
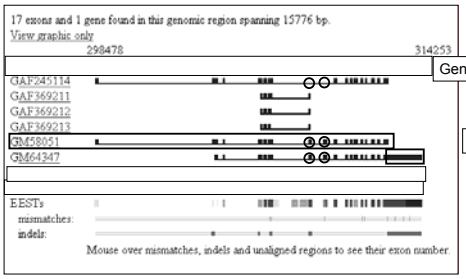


Creating NM Records for FGFR3

NCBI Resources for Biomedical Research



NMs must have cDNA support

NM/NP Records for FGFR3 in Entrez

NCBI Resources for Biomedical Research

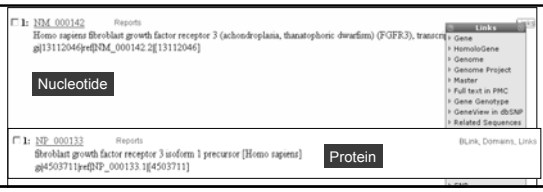
NM_000142: variant 1

```
COMMENT     REVIEWED REFSEQ: This record has been curated by NCBI staff. The
            reference sequence was derived from M58051.1 and M64347.1.
```

mRNA that completes 3' end

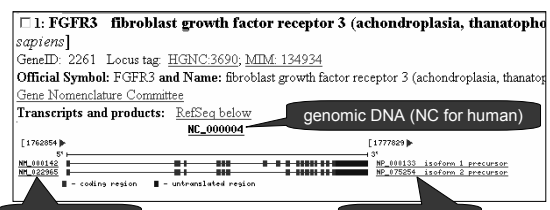
NM_022965: variant 2

```
COMMENT     REVIEWED REFSEQ: This record has been curated by NCBI staff. The
            reference sequence was derived from AF245114.1 and M64347.1.
```



RefSeq Summary for FGFR3

NCBI Resources for Biomedical Research



The RefSeqs for a gene become the basis for feature annotations such as SNPs

```
  1 mgapacalal cvavaivaga sseslgteqr vvgraaevpg pepgqqeqlv fgsgdavels
 61 cpppgggpmg ptvwvkdgtg lvpservlvg pqrlqvlnas hedsgayscr qrltqrvlch
121 fsvrvtdaps sgdde                gvdtga pywtrpermd kkllavpaan tvrfrcpaag
181 nptpsiswlk ngre                klrhqq wslvmesvvp sdrgnytcvv enkfgsirqt
241 ytldvlersp hrpilqaglp anqtavlgsd vefhckvysd aqphiqwlkh vevngskvgp
301 dgtpyvtvlk taganttdke levlslhnvt fedageytcl agnsigfshh sawlvvlpae
361 eelveadeag svyagilsyg vgfflfilvv aavtlcrlrs ppkkglgspt vhkisrfplk
```

P250

Searching in Gene

NCBI Resources for Biomedical Research

muenke syndrome

1 record retrieved

⇓

`muenke[All Fields] AND syndrome[All Fields] AND alive[prop]`

fgfr3	➡	`fgfr3[All Fields]`	19 records retrieved
fgfr3[gene name]	➡	`fgfr3[gene name]`	8 records retrieved

fgfr3[gene name] AND human[orgn]

1 record retrieved

⇓

`fgfr3[gene name] AND "Homo sapiens"[Organism] AND alive[prop]`

Gene Expression Omnibus

NCBI Resources for Biomedical Research

Submitted by Experimentalists

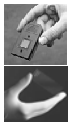
Curated by NCBI

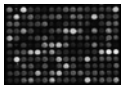
GPL
Platform descriptions

GSM
Raw/processed spot intensities from a single slide/chip

GSE
Grouping of slide/chip data "a single experiment"

GDS
Grouping of experiments



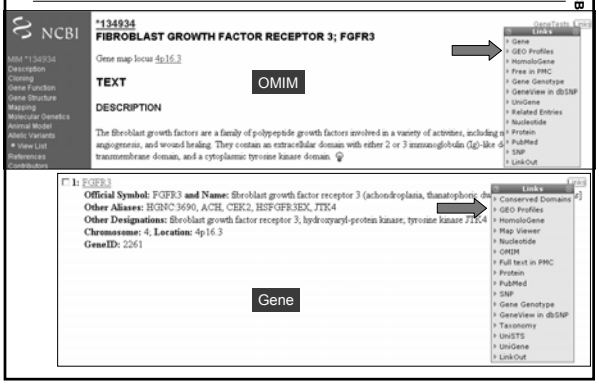


Entrez GEO Profiles

Entrez GEO Datasets

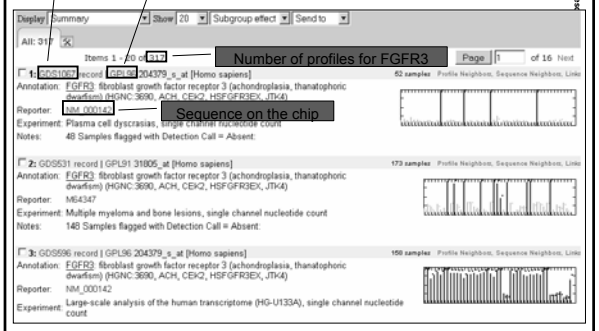
Linking to GEO Profiles

NCBI

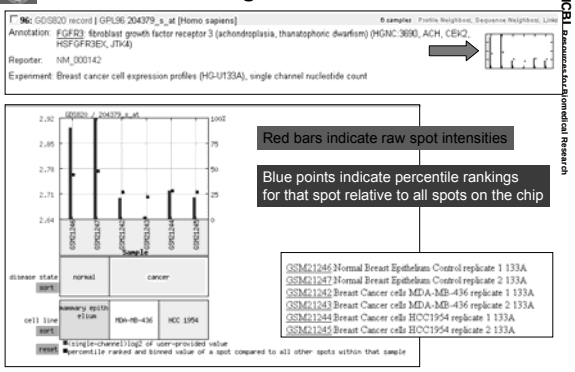


GEO Profiles for FGFR3

NCBI

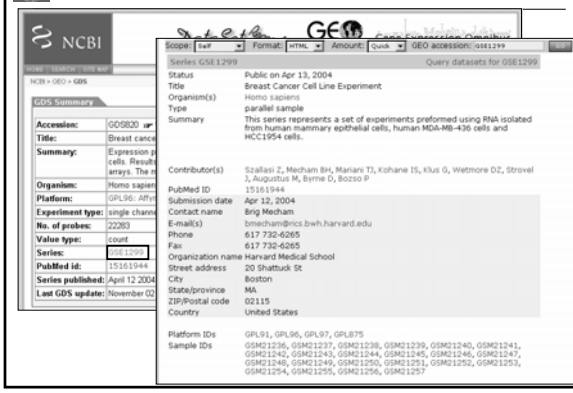


Viewing a GEO Profile



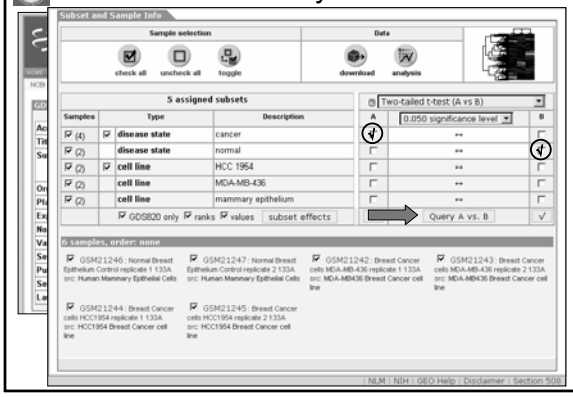
NCBI Resources for Biomedical Research

Viewing the GDS and GSE Records



NCBI Re

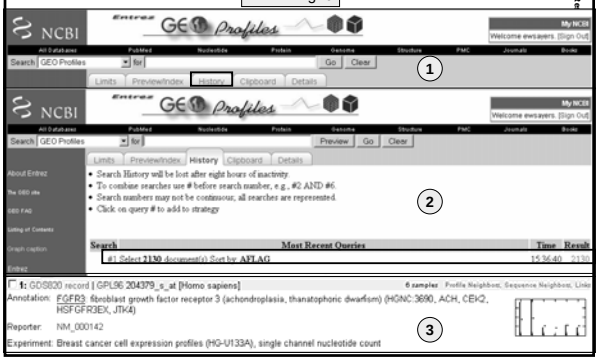
GEO Analysis Tools



NCBI Resources for Biomedical Research

Limit Results to FGFR3 with Entrez

#1 AND fgfr3



Sequence Polymorphisms

OMIM

Human Phenotypes

- Clinical literature database
- Curated at Johns Hopkins Univ
- Links human genes and genetic disorders to human disease
- Lists allelic variants that have clinical consequences

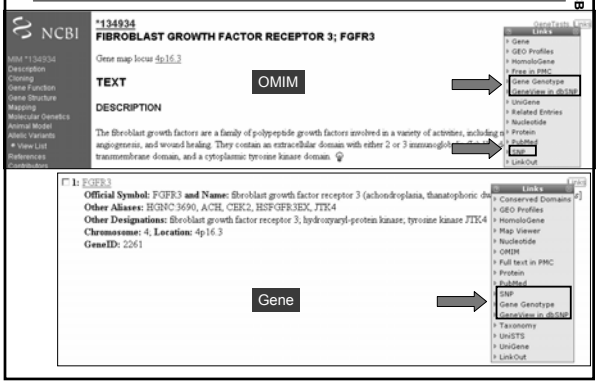
SNP

General Polymorphisms

- Primary database of submitted SNPs
- Curated database of reference SNPs
- Contains more than just SNPs:
  - True SNPs
  - MNP (multiple nucleotide)
  - Insertions
  - Deletions
  - Microsatellites
  - Mixed
  - No variation (constant)

Variations in SNP are not necessarily in OMIM, and vice versa!

Linking to SNP



SNP Links

NCBI Resources for Biomedical Research

SNP	List of all SNPs associated with the given record
GeneView in dbSNP	Graphical view of all SNPs associated with the given gene locus
Gene Genotype	List of populations and statistics of observed SNPs associated with the given record

SNP Links for FGFR3

NCBI Resources for Biomedical Re

Number of SNPs in FGFR3

non-coding region

nonsynonymous, 3D, OMIM

synonymous

SNP rs4647924

NCBI Resources for Biomedical Research

NCBI Resource Links

Submitter-Referenced Accessions:
GenBank: AC016773

dbSNP Blast Analysis:
NCBI RefSeq NM (mRNA): NM_000142.2 NM_022965.1
GenBank HTGS Finished: AC016773.8

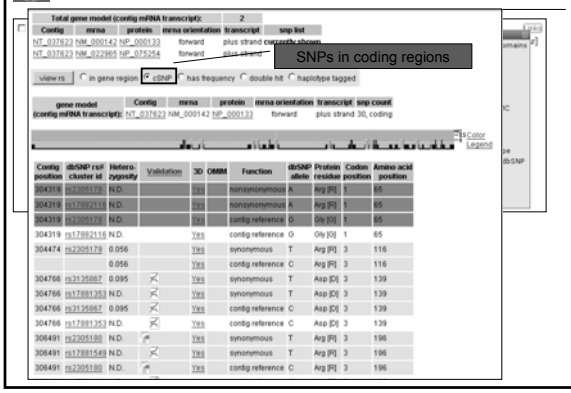
UniGene transcribed sequence cluster:
UniGene Cluster ID: 1420

3D structure mapping:
Hits to proteins with structure available: NP_000133

P250R

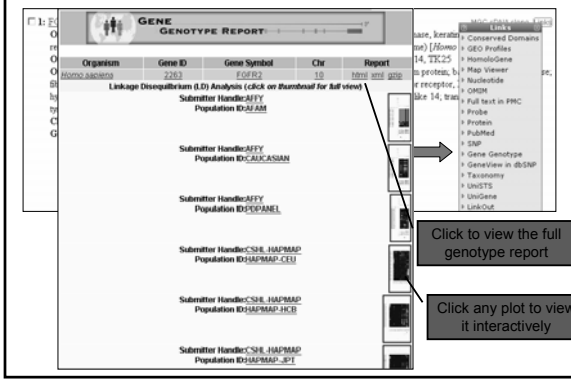
Contig accession	Contig position	mRNA accession	mRNA orientation	Protein accession	Function	dbSNP allele	Protein residue	Codon position	Amino acid position
NT_037623	306826	NM_000142	forward	NP_000133	nonsynonymous	G	Arg [R]	2	250
					contig reference	C	Pro [P]	2	250

GeneView in dbSNP



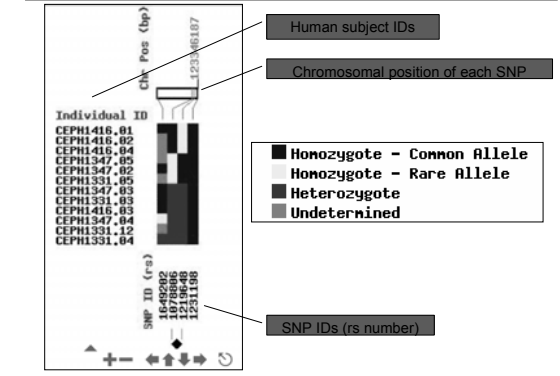
NCBI Resources for Biomedical Research

Gene Genotype for FGFR2



NCBI Resources for Biomedical Research

Linkage Disequilibrium Plots



NCBI Resources for Biomedical Research

Genotype Detail

NCBI Resources for Biomedical Research

Genotypes on Human *Homo sapiens* Subjects

+TSC-CSHL-SC_12_A

+TSC-CSHL-SC_12_AA

r2 =TSC-CSHL-SC_12_C

Click to view the pedigree chart

Plot of pairwise r squared values:

Individual Group	dbSNP Pedigree	Individual	Sex	Mother	Father	rs1649202	rs1078806	rs1219648	rs1231198
European	95	CEPH1331.03	F	CEPH1331.02	CEPH1331.01	T/T	C/T	A/G	N/N
European	95	CEPH1331.04	M	CEPH1331.02	CEPH1331.01	C/T	C/T	A/G	T/T
European	95	CEPH1331.05	F	CEPH1331.02	CEPH1331.01	N/N	C/C	G/G	T/T
European	95	CEPH1331.12	M	0	0	N/N	C/T	A/G	T/T
European	84	CEPH1347.02	F	CEPH1347.15	CEPH1347.14	T/T	C/C	G/G	T/T
European	84	CEPH1347.03	F	CEPH1347.02	CEPH1347.01	T/T	C/T	A/G	T/T
European	84	CEPH1347.04	M	CEPH1347.02	CEPH1347.01	C/C	C/T	A/G	T/T
European	84	CEPH1347.05	M	CEPH1347.02	CEPH1347.01	N/N	C/C	G/G	T/T
European	70	CEPH1416.01	M	CEPH1416.12	CEPH1416.11	T/T	T/T	A/A	T/T
European	70	CEPH1416.02	F	CEPH1416.14	CEPH1416.13	N/N	T/T	A/A	T/T
European	70	CEPH1416.03	M	CEPH1416.02	CEPH1416.01	T/T	C/T	A/G	T/T
European	70	CEPH1416.04	M	CEPH1416.02	CEPH1416.01	N/N	T/T	A/A	T/T

Colors: green-consistent with, or red-inconsistent with another submission

Pedigree Chart

NCBI

dbSNP Pedigree Table
Pedigree: CEPH 1347

male

female

G/G A/G A/G G/G

12 13 14 15

01 02 G/G

A/G A/G G/G

03 04 06 08 10 11 16 05

Finding Genotype Data for a SNP

NCBI Resources for Biomedical Research

NCBI ENTREZ SNP

All Databases | PubMed | Nucleotide | Protein | Genome | Structure | Popset

Search SNP for Go Clear

Limits | Preview/Index | History | Clipboard | Details

```
fgfr2[gene name] AND human[orgn] AND coding nonsynon[func]
AND true[genotype]
```

Nonsynonymous SNPs with genotype data in human FGFR2

All: 2

Items 1 - 2 of 2

One page.

1: rs3750819 [Homo sapiens]

Links YUSUKE

GGTGACCACGACCAGGCAGATGAAA[C/G]GACCCCAGCTGACCATGGTTACGGT

2: rs755793 [Homo sapiens]

Links TSC-CSHL

CGCTGCCCAGCCGGGGGGAACCCAA[C/T]GCCAACCATGCGGTGGCTGAAAAAC

Population Data for rs755793

NCBI Resources for Biomedical Research

Variation Summary:

Assay sample size (number of chromosomes):	132
Population data sample size (number of chromosomes):	352
Total number of populations with frequency data:	3
Total number of individuals with genotype data:	71
Hardy-weinberg Probability:	Pr(chiSq= 7.591,df=1) = 0.010
Average estimated heterozygosity	0.191

Average Allele Frequency:

T	0.893
C	0.107

Genotype Detail NEW

Click to access genotype detail and pedigree charts

1: rs755793 [Homo sapiens]

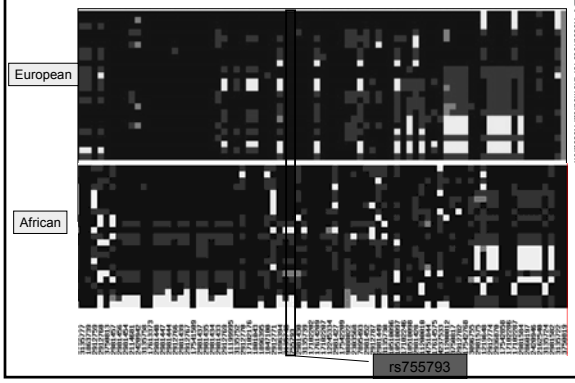
Genotypes on Human *Homo sapiens* Subjects

- PERLEGEN-AFD_EUR_PANEL — European
- PERLEGEN-AFD_AFR_PANEL — African
- PERLEGEN-AFD_CHN_PANEL — Asian

SNP Detail

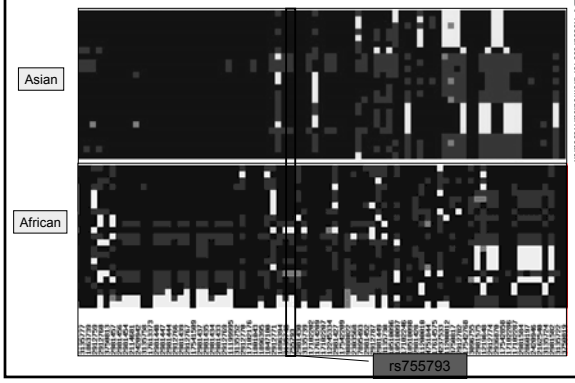
LD Plots for FGFR2

NCBI Resources for Biomedical Research



LD Plots for FGFR2

NCBI Resources for Biomedical Research



Genotype Detail for rs755793

NCBI Resources for Biomedical Research

1: rs755793

Genot

+PERL

+PERL

+PERL

+SNI

SNP Detail

rs755793

Assembly	Chromosome	Start	Gene	SNP Type	Orientation	Genotype Freq
35:reference	10	123300861		2	rev	C/C 0.043
35:Celera	10	116525980		2	rev	C/T 0.129
						T/T 0.829

ss110143 **Submitter's Id** TSC0148329 **Orientation to rs** fwd

Handle-Population Id	2n Allele Freq	Genotype Freq	Hardy-Weinberg
TSC-CSHL-TSC_42_C	84 T 1	N/A	N/A
TSC-CSHL-TSC_42_A	84 T 1	N/A	N/A
SEQUENOM-CEPH	92 C 0 T 1	N/A	N/A

ss23605078 **Submitter's Id** af42312054 **Orientation to rs** rev

Handle-Population Id	2n Allele Freq	Genotype Freq	Hardy-Weinberg
PERLEGEN-AFD_EUR_PANEL	48 A 1	A/A 1	N/A
PERLEGEN-AFD_AFR_PANEL	44 G 0.25 A 0.75	G/G 0.136 A/G 0.227 A/A 0.636	Chi Square 3.414
PERLEGEN-AFD_CHN_PANEL	48 G 0.083 A 0.917	A/G 0.167 A/A 0.833	Chi Square 0.198

Entrez PubChem

NCBI Resources for Biomedical Research

PC Substance

Primary database of chemical samples

PC Compound

Derived database of known chemicals from PC Substance records

PC BioAssay

Primary database of bioactivity screens of samples in PC Substance

PC Substance

855,201

PC Compound

656,659

PC BioAssay

173 (NCI)

NCBI PubChem National Library of Medicine NLM

HOME | SEARCH | SITE MAP | PubMed | Entrez | Structure | GenBank | PubChem | Help

PubChem Text Search

PubChem Substance GO!

PubChem contains the chemical structures of small organic molecules and information on their biological activities.

PubChem Substance: Search PubChem/Substance using text, e.g. substance name, keyword, synonym, external ID, formula, SID, etc.

PubChem Compound: Search PubChem/Compound using text terms including name, synonym, keyword, external ID, CID, formula, etc.

PubChem BioAssay: Search PubChem/BioActivity database using text terms such as cell name, protocol keyword, etc.

PubChem Structure Search: Search PubChem/Compound using chemical structure. Structure may be specified using SMILES, MOL file, molecular formula, etc.

Search for a Teratogen: 6-AN

NCBI Resources for Biomedical Research

6-aminonicotinamide

NCBI PubChem National Library of Medicine NLM

HOME | SEARCH | SITE MAP | PubMed | Entrez | Structure | GenBank | PubChem | Help

PubChem Text Search

PubChem Substance 6-aminonicotinamide GO!

Results from PC Substance

A redundant set with multiple records per compound

NIST

ChemIDplus

DTP/NCI

NIAID

NCBI Resources for Biomedical Research

Results from PC Compound

A non-redundant set with one record per compound

Links
- PubChem BioAssay
- PubChem BioAssay, Active
- PubChem BioAssay, Inactive
- PubChem Substance
- Full text in PMC
- PubMed via MeSH
- Similar Compound

NCBI Resources for Biomedical Research

CID (Compound ID) 9500

Compound Summary:

Redundant Substances

Bioassays

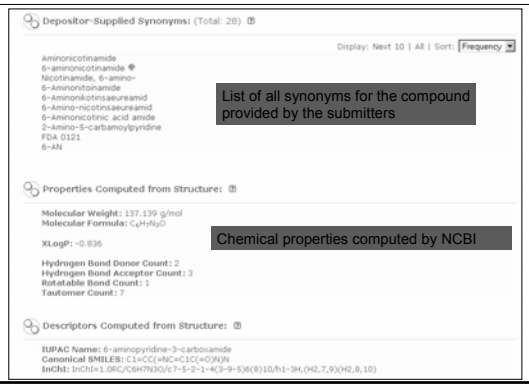
Similar compounds

Search by structure

Links to MeSH

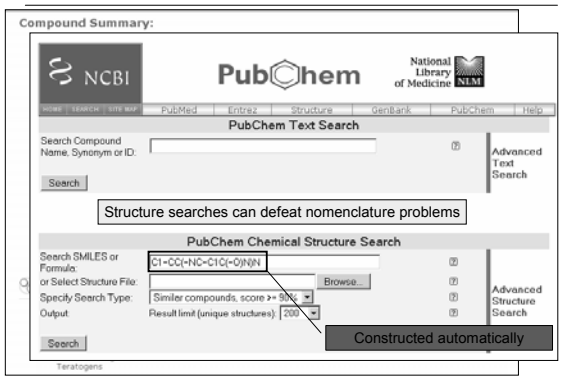
NCBI Resources for Biomedical Research

Compound Details



NCBI Resources for Biomedical Research

Search by Structure

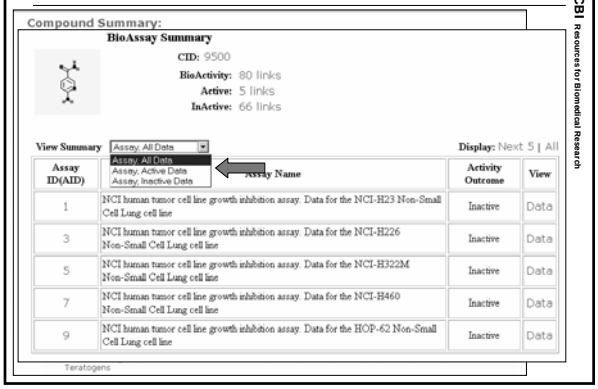


NCBI Resources for Biomedical Research

Similar Structures

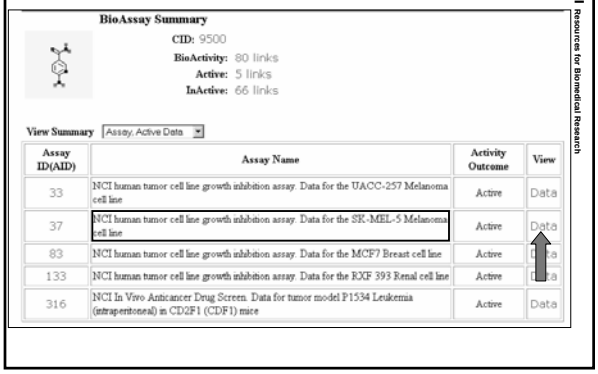
NCBI Resources for Biomedical Research

Linking to BioAssays



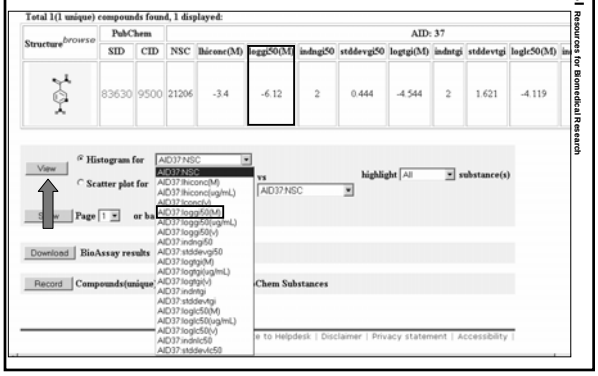
NCBI Resources for Biomedical Research

Bioassays with Active 6-AN



NCBI Resources for Biomedical Research

Detailed Assay Results for 6-AN



NCBI Resources for Biomedical Research

Histogram of Activity Data

NCBI Resources for Biomedical Research

Bin	From	To	Count Active	Count Inactive	Count Inconclusive
# 1	-13.30	-11.88	9	0	0
# 2	-11.88	-10.45	13	0	0
# 3	-10.45	-9.03	100	0	0
# 4	-9.03	-7.60	833	0	0
# 5	-7.60	-6.17	1453	0	0
# 6	-6.17	-4.75	360	10912	13
# 7	-4.75	-3.32	6	27069	16
# 8	-3.32	-1.90	1	95	0
# 9	-1.90	-0.47	0	5	0
# 10	-0.47	0.95	0	1	0

Count: 25000, 20000, 15000, 10000, 5000, 0

1 # 2 # 3 # 4 # 5 # 7 # 8 # 9 # 10

Bin

Active substances; Inactive substances; Inconclusive assay result substances

Links
- Zoom in
- Display result
- Display result - active
- Display result - inactive

Show Data table

Active Compounds in Bin #5

NCBI Resources for Biomedical Research

BioAssay Results

BioAssay ID(AID): 37

Source: DTP/NCI (NCI human tumor cell line growth inhibition assay. Data for the SK-MEL-5 Melanoma cell line)

Name: NCI human tumor cell line growth inhibition assay. Data for the SK-MEL-5 Melanoma cell line

PubMed Links: 3

Displayed substances have log GI50(M) from -7.60 to -6.17

** This page displays the PubChem BioAssay results you have selected. These may be downloaded in text format using the box at bottom. Note that the PubChem Substances you have selected via this search may be recorded for use in subsequent query refinement using the Entrez PubChem Substances. These results may be combined, for example, with PubChem Substances searches based on chemical properties or similarity to selected compounds. To use this feature select "Record" to send list of substances to Entrez, query will appear in the PubChem Substances "History" pulldown, identified by the number of selected substances as show at the top of this page.

Total 1453(1354 unique) compounds found, 20 displayed:

Structure browse	PubChem		AID: 37	
	SID	CID	loggi50(M)	Outcome
	510217	379156	-6.175	Active
	524069	392762	-6.176	Active

Substance IDs

Compound IDs

log GI50 (M)

Transferring Data to Entrez

NCBI Resources for Biomedical Research

BioAssay Results

BioAssay ID(AID): 37

Source: DTP/NCI (NCI human tumor cell line growth inhibition assay. Data for the SK-MEL-5 Melanoma cell line)

Name: NCI human tumor cell line growth inhibition assay. Data for the SK-MEL-5 Melanoma cell line

PubMed Links: 3

** This page displays the PubChem BioAssay results you have selected. These may be downloaded in text format using the box at bottom. Note that the PubChem Substances you have selected via this search may be recorded for use in subsequent query refinement using the Entrez PubChem Substances. These results may be combined, for example, with PubChem Substances searches based on chemical properties or similarity to selected compounds. To use this feature select "Record" to send list of substances to Entrez, query will appear in the PubChem Substances "History" pulldown, identified by the number of selected substances as show at the top of this page.

Total 1453(1354 unique) compounds found, 20 displayed:

View

Histogram for AID37:NSC

Scatter plot for AID37:NSC vs AID37:NSC

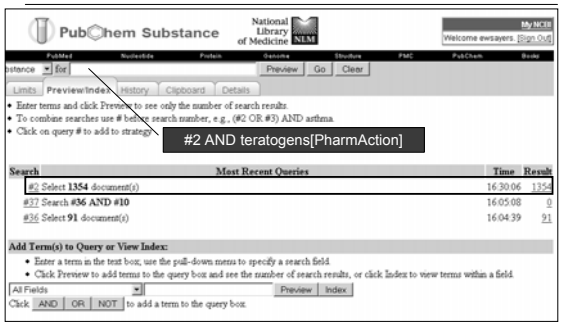
highlight All substance(s)

Show Page 1 or back to summary

Download BioAssay results

Record Compounds(unique) to Entrez history in PubChem Substances

Finding Teratogens in the Active List



NCBI Resources for Biomedical Research

A More Active Teratogen

NCBI Resources for Biomedical Research

For More Information…

E-mail addresses

· General Help	info@ncbi.nlm.nih.gov
· BLAST	blast-help@ncbi.nlm.nih.gov

The (free!) NCBI Newsletter

http://www.ncbi.nih.gov/About/newsletter.html

The NCBI Handbook

Follow the link from the NCBI Home Page

The NCBI Education Page

http://www.ncbi.nih.gov/Education/index.html

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