

Zpracování dat a vizualizace v chemii

C2150

- Zdeněk Kříž a Martin Prokop
- Co se naučíte
 - Získávání strukturních dat z databází
 - Validace získaných dat
 - Příprava pro molekulové modelování
 - Extrahování dat z modelování
 - Vizualizace dat a tvorba prezentací

Zpracování dat a vizualizace v chemii

C2150

- Jaký software budeme používat
 - Web browser
 - What If
 - Triton
 - VMD
 - Open Office

Jak můžu získat strukturní data o molekule

- Pro malé molekuly:
 - Cambridge Structural Database
 - Glycan Structural Database
 - 3Dchem database
 - Modelování od začátku
- Velké biomolekuly
 - Protein Structural Database – PDB
 - Nucleic Acids Database – NDB
 - Modelování na základě homologie

Jak hledat v databázi

- Znáám název molekuly, nebo její vzorec
- U malých molekul znám jejich SMILES kód (CCO – ethanol, c1CCCCc1 – cyklohexan a pod).
- CSD umí hledat podle funkčních skupin (umožňuje přes grafické rozhraní nakreslit vzorec)
- NDB databáze – hledání podle sekvence bází
- PDB umožňuje několikastupňové prohledávání

Cambridge structural database

- Co ukládá CSD
 - Data o organických molekulách
 - Data o komplexech kovů s organickými molekulami
- Jakými metodami jsou získávána data
 - RTG krystalografie
 - Monokrystalů
 - Prášková difrakce
- Co v CSD nenajdeme
 - Data o polypeptidech, polysacharidech a oligonukleotidech
 - Data o anorganických molekulách

Cambridge structural database

1D Bibliographic Information

TUSJIA

4-(2-chloroethyl)-1-[cyclohex-2-en-1-yl(hydroxy)methyl]

-5-methyl-6-oxa-2-azabicyclo[3.2.0]heptane-3,7-dione

Synonym: Salinosporamide A

Formula: C₁₅ H₂₀ Cl N O₄

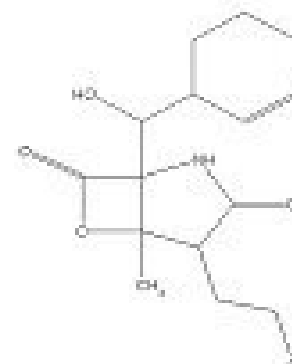
Source: Salinospora strain CNB-392 isolated from heat treated marine sediment

Extra info: absolute configuration; potent cancer cell cytotoxicity through inhibition of the 20S proteasome

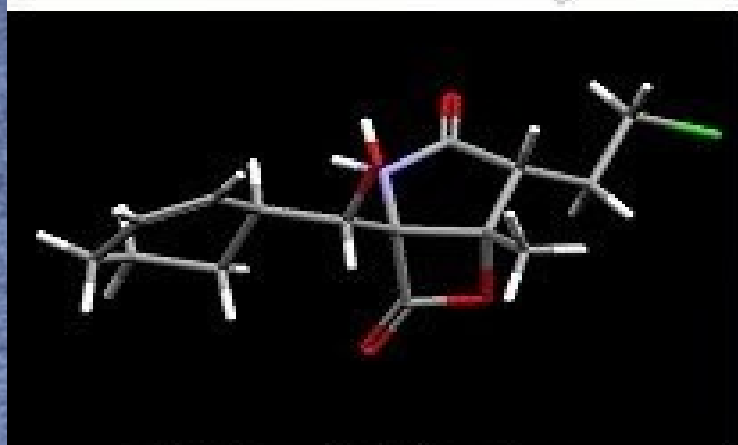
R.H.Feling, G.O.Buchanan, T.J.Mincer, C.A.Kauffman, P.R.Jensen, W.Ferical

Angew.Chem., Int.Ed.Engl., 42, 355, 2003.

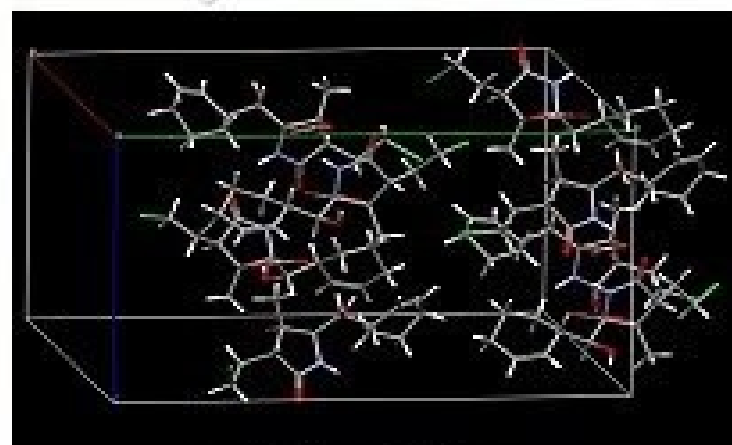
2D Chemical Connectivity



CSD



3D Molecular Structure



3D Crystal Structure

Cambridge structural database

CSD Entries: Summary Statistics (Historical Snapshots) - Mozilla Firefox

File Edit View History Bookmarks ScrapBook Tools Help

http://www.ccdc.cam.ac.uk/products/csd/statistics

	31 Dec 1983		31 Dec 1990		30 Oct 2001		31 Dec 2006	
	Structures	%	Structures	%	Structures	%	Structures	%
Total structures	52 363	100.0	104 380	100.0	251 515	100.0	400 977	100.0
Organic structures	28 995	55.4	52 450	50.3	112 113	44.6	172 583	43.0
Transition metal present	20 439	38.9	45 588	43.7	120 638	48.0	210 700	52.5
Li – Fr or Be – Ra present	2 887	5.5	5 299	5.1	13 471	5.4	21 219	5.3
Main group metal present	2 206	4.2	5 024	4.8	16 171	6.4	25 790	6.4
3D coordinates present	37 318	71.0	83 884	80.4	223 920	89.0	365 075	91.0
Error-free coordinates	35 032	93.9†	80 372	95.8†	219 864	98.2†	357541	97.9†
Neutron studies	567	1.08	786	0.8	1 062	0.4	1 331	0.3
Low/high temp. studies	3 275	6.2	9 943	9.5	55 752	22.2	133 471	33.3
Abs. config. determined	1 330	2.5	2 344	2.2	4 924	2.0	6 291	1.6
Disorder present	4 943	9.4	13 594	13.0	45 728	18.2	81 770	20.4
Polymorphic structures	3 231	6.1	4 618	4.4	7 892	3.1	13 411	3.3
R-factor < 0.100	37 190	70.8	85 389	81.8	227 181	90.3	370 220	92.3
R-factor < 0.075	29 937	57.0	73 424	70.3	202 848	80.7	333 501	83.2
R-factor < 0.050	15 974	30.4	42 996	41.2	125 112	49.7	209 929	52.4
R-factor < 0.030	2 231	4.2	7 150	6.8	22 346	8.9	39 602	9.9
n(atoms)/structure *	44	-	54	-	73	-	74	-
Mb data added in year+	14	-	29	-	86	-	139	-

† Percentage of structures for which coordinates are present in the CSD

Done

ICSD databáze

- http://www.fiz-karlsruhe.de/icsd_content.html
- Co najdeme v ICSD
 - Krystalové struktury prvků
 - Krystalové struktury binárních sloučenin
 - Krystalové struktury složitějších anorganických sloučenin
- ICSD obsahuje více než 108000 záznamů

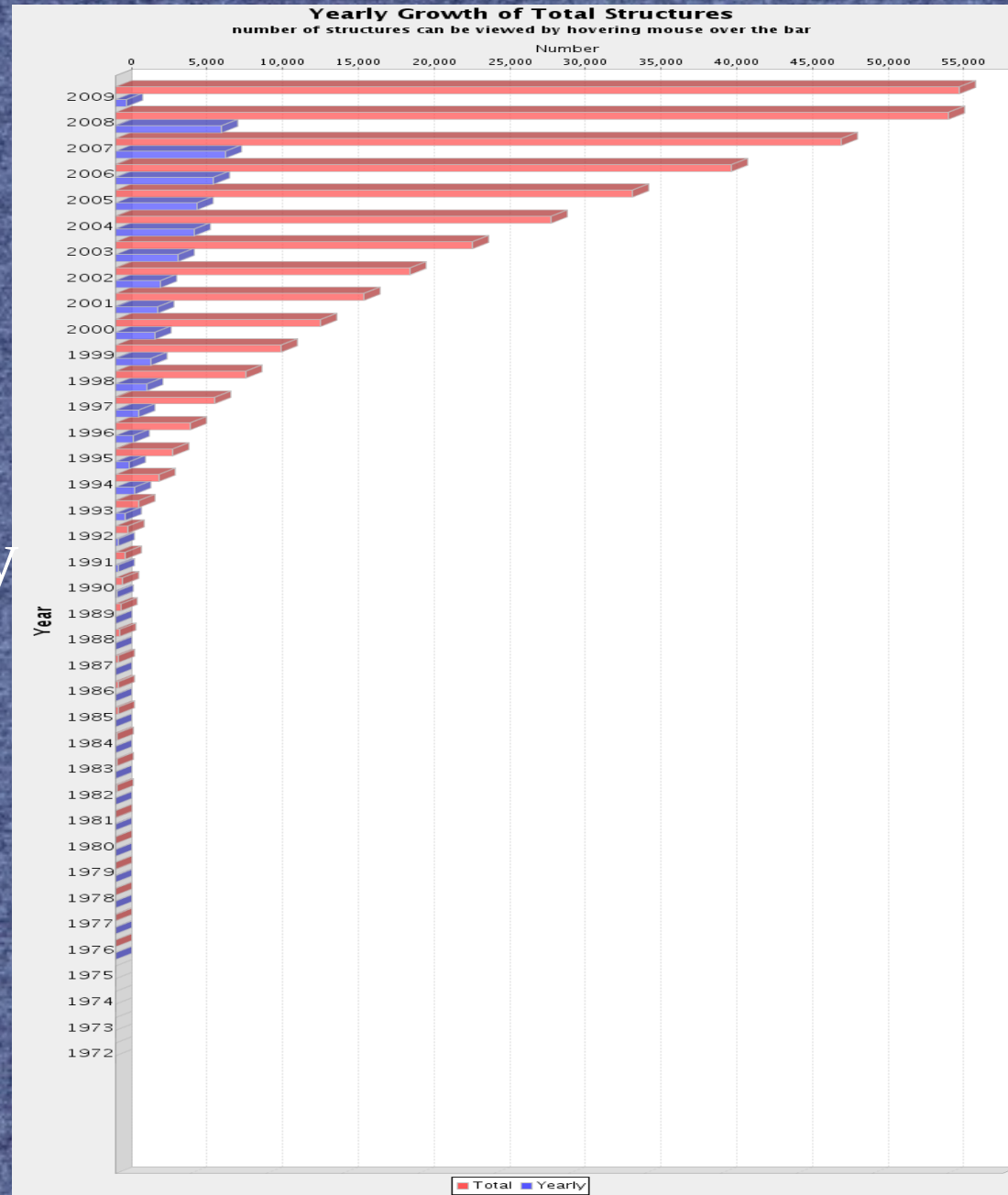
Protein Data Bank - PDB

- <http://www.pdb.org>

The screenshot shows the RCSB Protein Data Bank website in a Mozilla Firefox browser window. The browser's address bar displays the URL <http://www.pdb.org/pdb/home/home.do>. The website header includes the RCSB PDB logo, navigation links for 'CONTACT US | FEEDBACK | HELP | PRINT', and search options for 'PDB ID or keyword' and 'Author'. The main content area features a section titled 'A Resource for Studying Biological Macromolecules' with two featured molecules: 'Molecule of the Month: Auxin and TIR1 Ubiquitin Ligase' and 'PSI Featured Molecule: CBS domain protein TA0289'. A sidebar on the left provides navigation options such as 'Home', 'Getting Started', 'Structural Genomics', 'Download Files', 'Deposit and Validate', 'Dictionaries & File Formats', 'Software Tools', 'General Education', and 'Site Tutorials'. A 'News' section on the right highlights 'Complete News', 'Newsletter', 'Discussion Forum', and 'Job Listings', along with announcements for '10-February-2009 Tools for Education' and '02-December-2008 PDB Archive Version 3.15 to be Released'. The browser's taskbar at the bottom shows the system clock at 15:45 and various application icons.

Protein Data Bank - PDB

- 55795 struktur
 - 47777 – RTG
 - 7696 – NMR
 - 217 – EM
- proteiny/NA/kompleksy
 - 51535 – protein
 - 1173 – DNA
 - 701 – RNA
 - 2255 – kompleksy



Protein Data Bank - PDB

RCSB Protein Data Bank - Mozilla Firefox

File Edit View History Bookmarks ScrapBook Tools Help

http://www.pdb.org/pdb/static.do?p=search/index.html

Most Visited English - Czech Dict... Neviditelný pes Britské listy Seznam Support SunSITE Czech Rep...

RCSB PDB
PROTEIN DATA BANK

A MEMBER OF THE **PDB** MyPDB: [Login](#) | [Register](#)

An Information Portal to Biological Macromolecular Structures

As of Tuesday Feb 10, 2009 there are 55795 Structures | [PDB Statistics](#)

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PDB ID or keyword Author [Site Search](#) | [Advanced Search](#)

Home Search

Search Database

- Advanced Search
- Latest Release
- Sequence
- Ligand Structure
- Ligand Name
- Ligand ID
- Models
- Unreleased Entries
- Structural Genomics Targets
- How to Search

[Browse Database](#)

[Histograms](#)

Quick Tips:

Click [here](#) to see structures released this week.

Searching the RCSB PDB

- Advanced Search:** Allows searches of all types - database fields, browsable ontologies, and text searches
- Latest Release:** Shows the structures loaded this week
- Sequence:** To search using a sequence, or by similarity to the sequence of a given PDB structure
- Ligands:** To search based on ligand or ligand substructure
- Models:** To search for modeled structures (those structures which are NOT experimentally determined)
- Unreleased Entries:** Searches based on structures that are not yet released (minimal data available: ID, title, authors, and possibly sequence)
- Structural Genomics Targets:** Links to TargetDB and a listing of Structural Genomics Target info

Browsing the RCSB PDB

Gene Ontology: The GO Annotation project has mapped PDB IDs and corresponding chain IDs to the GO terms below.


- Biological Process
- Cellular Component
- Molecular Function

- Enzyme Classification:** Browse based on Swiss-Prot/GenBank/KEGG/author specified mapping of the enzyme to EC number

Done

PDB – prohledávání databáze








Search Database

- [Advanced Search](#)
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- [Ligand Structure](#)
- [Ligand Name](#)
- [Ligand ID](#)
- [Models](#)
- [Unreleased Entries](#)
- [Structural Genomics](#)
- [Targets](#)
-  [How to Search](#)

► [Browse Database](#)

► [Histograms](#)

Searching the RCSB PDB

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- [Biological Process](#)
- [Cellular Component](#)
- [Molecular Function](#)

PDB – prohledávání databáze

Search Database

- Advanced Search
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- Ligand Structure
- Ligand Name
- Ligand ID
- Models
- Unreleased Entries
- Structural Genomics
- Targets
- How to Search

[Browse Database](#)

[Histograms](#)

Match of the following conditions:

[Advanced Search Tutorial \(Requires Flash\)](#)

Choose a Query Type:

Choose a Query Type:

ID Search for Structures

- PDB ID(s)
- PubMed ID(s)
- UniProt Accession ID(s)
- Genbank ID(s)
- PIR ID(s)
- PDB Entity ID(s)

Structural Genomics

- Structural Genomics Project

Structure Summary

- Structure Title
- Structure Description
- Molecule Name
- Author Name
- Deposit Date
- Release Date

PDB – prohledávání databáze

▼ **Search Database**

- [Advanced Search](#)
- [Latest Release](#)
- [Sequence](#)
- [Ligand Structure](#)
- [Ligand Name](#)
- [Ligand ID](#)
- [Models](#)
- [Unreleased Entries](#)
- [Structural Genomics](#)
- [Targets](#)
- 🔗 [How to Search](#)

▶ [Browse Database](#)

▶ [Histograms](#)

Match of the following conditions:

[Advanced Search Tutorial \(Requires Flash\)](#)

<input type="text" value="Molecule Name"/>	Molecule Name <input type="text" value="cyclin dependent kinase"/>	31 Structures	Evaluate Subquery	<input type="button" value="-"/> <input type="button" value="+"/>
<input type="text" value="Experimental Method"/>	Experimental Method <input type="text" value="X-RAY"/>		Evaluate Subquery	<input type="button" value="-"/> <input type="button" value="+"/>
	Has Experimental Data <input type="text" value="Yes"/>			

Remove Similar Sequences at Identity


[Clear All](#)

[Evaluate Query](#)

PDB – prohledávání databáze

Molecule Name Search : Molecule Name=cyclin dependent kinase
and


Experimental Method Search : Experimental Method=X-RAY, Has Experimental Data=Y

1 2 3 

- **Results (1-10 of 23)**
- [Results ID List](#)
- [Modify / Refine this Search](#)
- [Select All](#)
- [Deselect All](#)
- [Download Selected](#)

- ▶ [Tabulate](#)
- ▶ [Narrow Query](#)
- ▶ [Sort Results](#)
- ▶ [Results per Page](#)

■ [Show Query Details](#)

 [Results Help](#)

[1w8c](#)    **CO-CRYSTAL STRUCTURE OF 6-CYCLOHEXYLMETHOXY-8-ISOPROPYL-9H-PURIN-2-YLAMINE AND MONOMERIC CDK2**



Characteristics

Release Date: 30-Aug-2006 **Exp. Method:** X Ray Diffraction

Resolution: 2.05 Å

Classification

Transferase

Compound

Polymer: 1 **Molecule:** CELL DIVISION PROTEIN KINASE 2 **Chains:** A **EC no.:** 2.7.1.37 

Authors

Pratt, D.J., Endicott, J.A., Noble, M.E.M.

[1w98](#)    **THE STRUCTURAL BASIS OF CDK2 ACTIVATION BY CYCLIN E**



Characteristics

Release Date: 02-Feb-2005 **Exp. Method:** X Ray Diffraction

Resolution: 2.15 Å

Classification

Transferase

Compound

Polymer: 1 **Molecule:** CELL DIVISION PROTEIN KINASE 2 **Chains:** A **EC no.:** 2.7.1.37  **Other**

Quick Tips:   

Refine this query by

PDB – prohledávání databáze

PROTEIN DATA BANK

As of Tuesday Feb 10, 2009 there are 55795 Structures | PDB Statistics

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PDB ID or keyword Author Site Search Advanced Search

Home Search Structure Results Help Structure Summary Sequence Details Biology & Chemistry Materials & Methods Geometry External Links

Queries

1W98   DOI 10.2210/pdb1w98/pdb

Red - Derived Information

Title	THE STRUCTURAL BASIS OF CDK2 ACTIVATION BY CYCLIN E			
Authors	Lowe, E.D., Honda, R., Dubinina, E., Skamnaki, V., Cook, A., Johnson, L.N.			
Primary Citation	Honda, R., Lowe, E.D., Dubinina, E., Skamnaki, V., Cook, A., Brown, N.R., Johnson, L.N. (2005) The structure of cyclin E1/CDK2: implications for CDK2 activation and CDK2-independent roles. <i>Embo J.</i> 24: 452-463 [Abstract] PubMed			
History	Deposition	2004-10-07	Release	2005-02-02
	Last Modified (REVDAT)	2005-06-15		
Experimental Method	Type	X-RAY DIFFRACTION		Data 
Parameters	Resolution[Å]	R-Value	R-Free	Space Group
	2.15	0.185 (obs.)	0.246	P 4 ₁ 2 ₁ 2
Length[Å]	a	99.62	b	99.62
	c	149.99		

Images and Visualization

<< Biological Molecule >>



Display Options

- KiNG
- Jmol
- WebMol
- MBT SimpleViewer*
- MBT Protein Workshop
- QuickPDB
- All Images

* Capable of displaying biological molecules.

Quick Tips:   

To view **sequence details** of this structure click on the *Sequence Details* tab above the summary page.

PDB – prohledávání databáze

Queries

■ 1W98

▶ Download Files

■ FASTA Sequence

▶ Download Original Files

▶ Display Files

▼ Display Molecule

■ Image Gallery

■ KiNG Viewer

■ Jmol Viewer

■ WebMol Viewer

■ Protein Workshop

■ FirstGlance

■ Rasmol Viewer

(Plugin required)

■ Swiss-PDB Viewer

(Plugin required)

🔗 Molecular Viewers Help

🔗 KiNG Help

🔗 Jmol Help

🔗 WebMol Help

🔗 Protein Workshop Help

🔗 QuickPDB




■ Asymmetric Unit

■ Assumed Biological Molecule 1



PDB – prohledávání databáze

Home Search Structure Results Help Structure Summary Sequence Details Biological Chemistry Materials & Methods Geometry External Links

1w98    DOI 10.2210/pdb1w98/pdb


Red - Derivative information

Title THE STRUCTURAL BASIS OF CDK2 ACTIVATION BY CYCLIN E

Authors Lowe, E.D., Honda, R., Dubinina, E., Skamnaki, V., Cook, A., Johnson, L.N.

Primary Citation Honda, R., Lowe, E.D., Dubinina, E., Skamnaki, V., Cook, A., Brown, N.R., Johnson, L.N. (2005) The structure of cyclin E1/CDK2: implications for CDK2 activation and CDK2-independent roles. *Embo J.* 24: 452-463
[Abstract] PubMed

History Deposition 2004-10-07 Release 2005-02-02
Last Modified (REVDAT) 2005-06-15

Experimental Method Type X-RAY DIFFRACTION Data 


Parameters

Resolution [Å]	R-Value	R-Free	Space Group
2.15	0.185 (obs.)	0.246	P 4 ₁ 2 ₁ 2

Unit Cell

Length [Å]	a	b	c
	99.62	99.62	149.99

Angles [°]	alpha	beta	gamma
	90.00	90.00	90.00

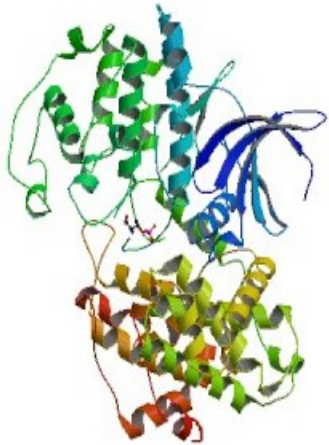
Display Options 

- King
- Jmol
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- QuickPDB
- All Images

* Capable of displaying biological molecules.

Images and Visualization

<< Biological Molecule >>



Download Files

- PDB text
- PDB (Header) text
- PDB gz
- mmCIF text
- mmCIF (Header) text
- mmCIF gz
- PDBML/XML text
- PDBML/XML (Header) text
- PDBML/XML gz
- Structure Factor text
- Structure Factor gz
- Biological Unit gz
- FASTA Sequence

Download Original Files

Display Files

Display Molecule

- Image Gallery
- King Viewer
- Jmol Viewer

Nucleic Acid Database

<http://ndbserver.rutgers.edu>

Nucleic Acid Database (NDB) - Mozilla Firefox

File Edit View History Bookmarks ScrapBook Tools Help

[http://ndbserver.rutgers.edu/](#) NDBDatabase

Most Visited English - Czech Dict... BL Neviditelný pes BL Britské listy S Seznam Support SunSITE Czech Rep...

ndb [Site Index](#)

WELCOME TO THE NUCLEIC ACID DATABASE
a repository of three-dimensional structural information about nucleic acids

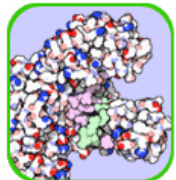
- Atlas
- Deposit Data
- Download Data
- Search
- Reports
- Education
- Standards
- Tools
- Links

Number of Released Structures:
4089 Structures
Last Update: 15-Jan-2009

Search the NDB by ID
Enter an NDB ID or PDB ID

Search for Released Structures

Nucleic Acids Highlight



About NDB

News

The NDB follows the dictionaries and formats used by the Worldwide Protein Data Bank. Please see [www.wwpdb.org](http://www wwpdb.org) for format announcements and documentation.

[Archive of NDB newsletters](#)

The NDB is supported by funds from the [National Science Foundation](#) and the [Department of Energy](#).

In citing the NDB please refer to:
H. M. Berman, W. K. Olson, D. L. Beveridge, J. Westbrook, A. Gelbin, T. Demeny, S.-H. Hsieh, A. R. Srinivasan, and B. Schneider. (1992) The Nucleic Acid Database: A Comprehensive Relational Database of Three

http://ndbserver.rutgers.edu/download_data/index.html

NDB - prohledávání

Search for Released Structures

General Information

NDB ID <input type="text"/>	PDB ID <input type="text"/>	Author <input type="text"/> (ex: Last, F or Last; not Last F or F. Last)
Citation Year (ex: 2002) <input type="text"/>	Released Since <input type="text"/>	

Search

Reset

Experimental Type

Crystal Structure <input type="radio"/> Y <input type="radio"/> N	Structure Factors Available <input type="radio"/> Y <input type="radio"/> N	
Space Group <input type="text"/>	Resolution better than <input type="text" value="2.5"/>	R-factor better than < <input type="text" value="20"/>
NMR <input type="radio"/> Y <input type="radio"/> N	NMR Restraints Available <input type="radio"/> Y <input type="radio"/> N	

Sequence

Nucleic Acid Sequence Pattern <input type="text"/>	Mismatch <input type="radio"/> Y <input type="radio"/> N
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Biomolecule contains

DNA <input type="radio"/> Y <input type="radio"/> N	RNA <input type="radio"/> Y <input type="radio"/> N	Protein <input type="radio"/> Y <input type="radio"/> N	Ligand <input type="radio"/> Y <input type="radio"/> N
--	--	--	---

Nucleic Acid Modification

Base	Sugar	Phosphate
------	-------	-----------

NDB - prohledávání



Results 1 - 20 of 374 records in NDB

Search took 0.595 seconds.

There are 19 pages in total.

[Help](#) [Close](#)

1. Display Dynamically Generated Atlas of

Structures

2. View report of

#	ID	DESCRIPTION
<input type="checkbox"/> All		
<input type="checkbox"/> 1	AD0007	A-DNA DECAMER GCGTA(T23)TACGC WITH INCORPORATED 2'-METHOXY-3'-METHYLENPHOSPHATE-THYMIDINE
<input type="checkbox"/> 2	AD0010	ALTERNATION OF DNA AND SOLVENT LAYERS IN THE A FORM OF D(GGCGCC) OBTAINED BY ETHANOL CRYSTALLIZATION
<input type="checkbox"/> 3	AD0011	1.6 A STRUCTURE OF THE A-DECAMER GCGTATACGC WITH A SINGLE 2'-O-AMINOXYETHYL THYMINE IN PLACE OF T6, BA-FORM
<input type="checkbox"/> 4	AD0012	1.45 A STRUCTURE OF THE A-DECAMER GCGTATACGC WITH A SINGLE 2'-O-FLUOROETHYL THYMINE IN PLACE OF T6, MEDIUM NA-SALT
<input type="checkbox"/> 5	AD0013	1.06 A STRUCTURE OF THE A-DECAMER GCGTATACGC WITH A SINGLE 2'-O-METHYL-3'-METHYLENPHOSPHONATE (T23) THYMINE IN PLACE OF T6, HIGH CS-SALT
<input type="checkbox"/> 6	AD0014	1.05 A STRUCTURE OF THE A-DECAMER GCGTATACGC WITH A SINGLE 2'-O-METHYL-[TRI(OXYETHYL)] THYMINE IN PLACE OF T6, MEDIUM CS-SALT
<input type="checkbox"/> 7	AD0015	1.05 A STRUCTURE OF THE A-DECAMER GCGTATACGC WITH A SINGLE 2'-O-FLUOROETHYL THYMINE IN PLACE OF T6, HIGH RB-SALT
<input type="checkbox"/> 8	AD0016	1.3 A STRUCTURE OF THE A-DECAMER GCGTATACGC WITH A SINGLE 2'-O-METHYL-[TRI(OXYETHYL)] THYMINE IN PLACE OF T6, MEDIUM RB-SALT
<input type="checkbox"/> 9	AD0018	1.3 A STRUCTURE OF THE A-DECAMER GCGTATACGC WITH A SINGLE 2'-O-METHYL-[TRI(OXYETHYL)], MEDIUM K-SALT

NDB - prohledávání

NDB ID: AD0014

[Home](#)

[NMR Atlas](#) [X-Ray Atlas](#)

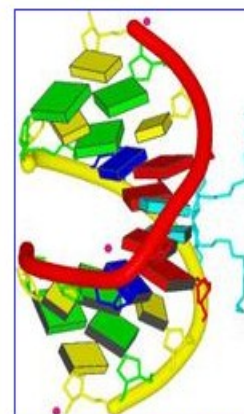
Title: 1.05 Å STRUCTURE OF THE A-DECAMER GCGTATACGC WITH A SINGLE 2'-O-METHYL-[TRI(OXYETHYL)] THYMINE IN PLACE OF T6, MEDIUM CS-SALT

Molecular Description: 5' -D(GpCpGpTpAp(126)pApCpGpC) - 3'

Structural Features: A DOUBLE HELIX

Nucleic Acid Sequence: ChainsA, B: (DG) (DC) (DG) (DT)
(DA) (126) (DA) (DC)
(DG) (DC)

Primary Citation: Tereshko, V., Wilds, C.J., Minasov, G., Prakash, T.P., Maier, M.A., Howard, A., Wawrzak, Z., Manoharan, M., Egli, M. [Detection of alkali metal ions in DNA crystals using state-of-the-art X-ray diffraction experiments.](#) *Nucleic Acids Res.* , **29**, pp. 1208 - 1215, 2001.



Biological Unit 1

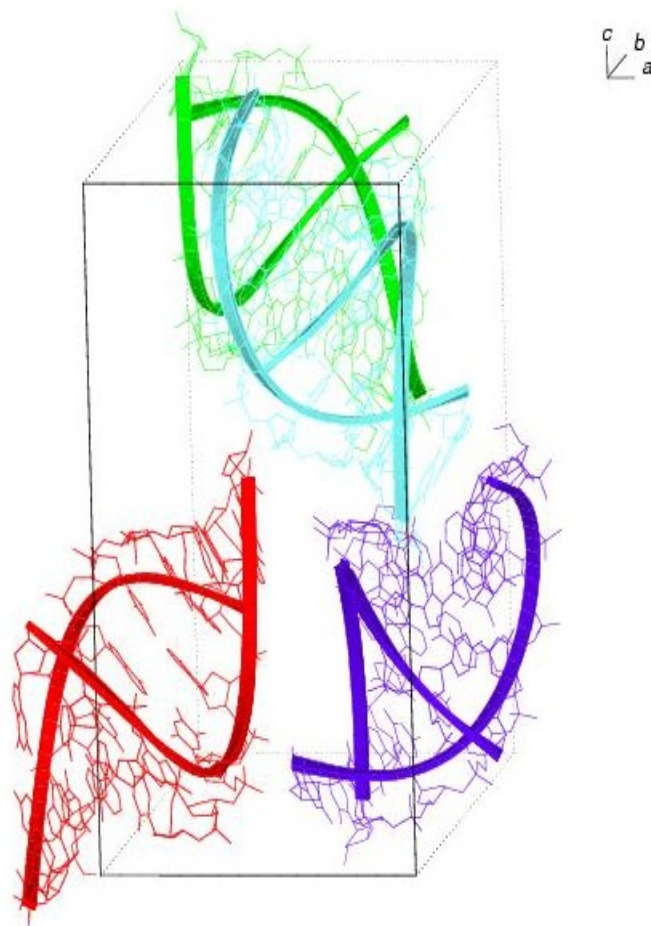
Other Views

[Asymmetric Unit](#)

[Crystal Packing](#)

[Enlarge Biological Unit 1](#)

NDB - prohledávání



Glyco3D databáze

- <http://www.cermav.cnrs.fr/glyco3d/index.php>



Home

- Home page

Databases

- Monosaccharides
- Disaccharides
- Oligosaccharides
- Polysaccharides
- Lectines
- Glycosyltransferases
- Gag binding proteins

Book chapters

- Modeling
- Cellulose
- Starch

Gallery

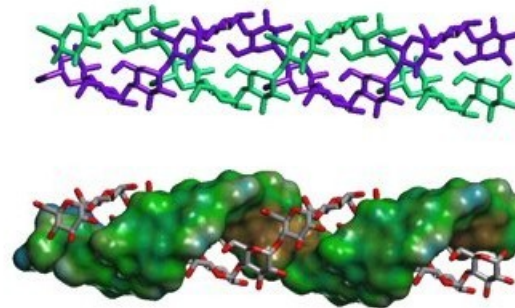
- Models

Tools

- Useful links

GLYCO3D

A site for glycosciences



BP 53 - 38041 Grenoble Cedex 9 - France

Domaine Universitaire - 601 Rue de la Chimie
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Glyco3D databáze

Mozilla Firefox <2>

http://www.cermav.cnrs.fr/cgi-bin/monos/monos.cgi

MONOSACCHARIDES

- ABEQUOSE
- ALTROSE
- APIOSE
- ARABINOSE
 - Alpha
 - a-L-Arabinopyranose**
 - Beta
- FRUCTOSE
- FUCOSE
- GALACTOSE
- GLUCOSE
- GULOSE
- IDOSE
- LYXOSE
- MANNOSE
- MISC
- RHAMNOSE
- RIBOSE
- SIALIC
- TALOSE
- XYLOSE

a-L-Arabinopyranose *Family* : Arabinose
Anomery : Alpha

Carbons : 5

Cycle : Pyranose

Configuration : Levogyre

Comment :

2D view

3D view

Jmol


PDB file

Glyco3D databáze

Mozilla Firefox <2>

http://www.cermav.cnrs.fr/cgi-bin/di/di.cgi

monosaccharide 1 Carbon 1 glycosidic link Carbon 2 monosaccharide 2

Fucose 1  4 Glucose search

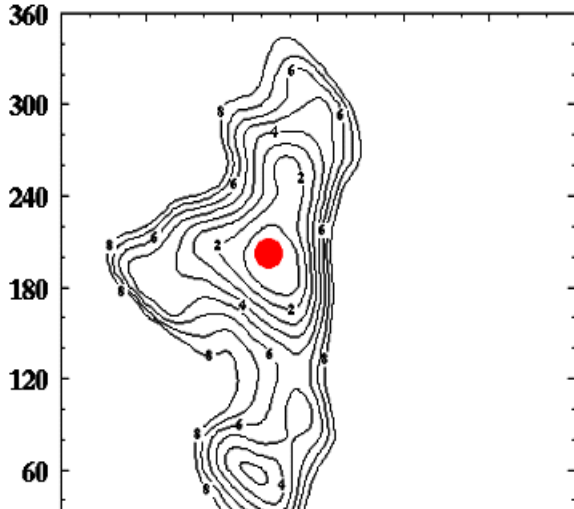
IUPAC name : a-L-Fucopyranose-(1-4)-2-acetamido-2-deoxy-b-D-glucopyranose select

Monomer 1 : a-L-Fucopyranose

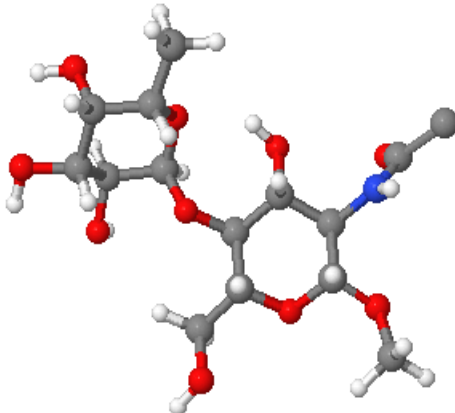
Monomer 2 : 2-Acetamido-2-deoxy-b-D-glucopyranose

Abbreviation : a-L-Fucp(1,4)b-D-GlcpNAc

Iso-potential energy map



3D interactive structure



Jmol

VALUES :

Energy :	29.0400
ϕ :	99.99
Ψ (n+1) :	99.99
Ψ (n-1) :	81.40
Force-field :	MM3(92)
Parameters :	MM3(92)
Dielectric constant :	78.50

Glyco3D databáze

Mozilla Firefox <2>


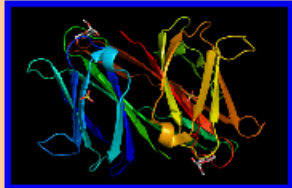
http://www.cermav.cnrs.fr/lectines/

Google

Bacterial lectins - 2-Ca b-sandwich

Burkholderia lectins

PDB code : 2VNV
Species : Burkholderia cenocepacia
Commentaire : Complexed with **aManOMe**
Resolution : 1.70
Reference : Lameignere E, Malinovská L, Sláviková M, Duchaud E, Mitchell EP, Varrot A, Sedo O, Imberty A, Wimmerová M., Structural basis for mannose recognition by a lectin from opportunistic bacteria Burkholderia cenocepacia:, *Biochem. J.*, **411**, 307-318, 2008



Medline

Link to Databases :
[[PDB ENTRY \(RCSB Site\)](#) / [HSSP ENTRY](#) / [SCOP](#) / [RELIBASE](#)]

PDB Files :
([RCSB \(USA CA\)](#) / [Rutgers University \(USA NJ\)](#) / [FRANCE](#) / [SINGAPORE](#) / [UK](#) / [JAPAN](#) / [BRAZIL](#))

Done

Practical structural databases

- <http://xray.bmc.uu.se/embo/structdb/links.html>



The screenshot shows a Mozilla Firefox browser window with the following details:

- Address Bar:** <http://xray.bmc.uu.se/embo/structdb/links.html>
- Page Title:** Practical "Structural Databases" - EMBO Bioinformatics Course - Uppsala 1999/2001 - Mozilla Firefox
- Page Content:**
 - Teal header with two license plate graphics: "STRUCTURAL SOUTH CAROLINA" and "THE FIRST STATE DATABASES DELAWARE".
 - Light blue section with a "Louisiana LINKS SPORTSMAN'S PARADISE" license plate graphic.
 - Orange navigation bar with links: [Primary structural databases](#), [Front-ends](#), [Experimental data](#), [Visualisation](#), [Visualisation software](#), [Structural macro-analysis](#), [Structural micro-analysis](#), [Model validation](#), [Other biomolecules](#), [Small molecules](#), [Specialised & derived databases and servers](#), [Protein-family-specific databases](#), [Sequence databases and resources](#), [Multiple sequence alignment](#), [Literature](#), [Structure prediction & modelling](#), [Structural genomics](#), [Crystallography](#), [NMR spectroscopy](#), [Organisations & institutes](#), [Education](#), [Miscellaneous resources](#).
 - White footer with text: **Please E-mail corrections and additions to [Gerard Kleywegt](#) - thanks !**
You can check the current validity of all links on this page using the [W3C Link Checker](#).