

Representação das Moléculas Visualização

Ignez Caracelli



Julio Zukerman Schpector

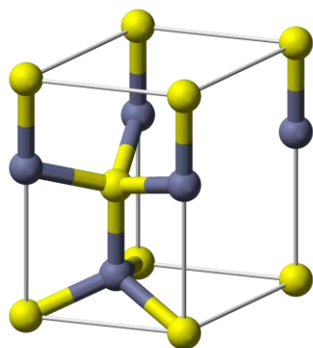


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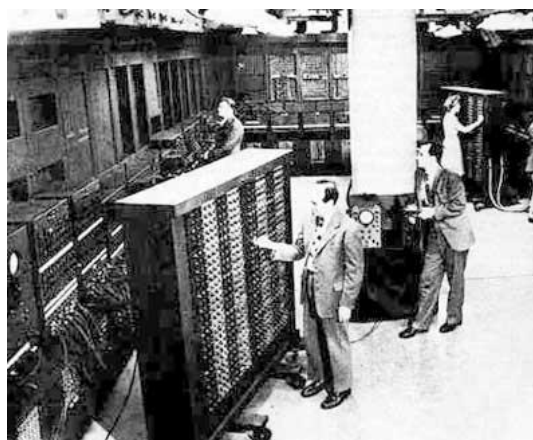
1

O início



primeiras estruturas: 1912-1920

Wurtzite unit cell. The gray balls represent sulfur or selenium atoms, and yellow balls represent metal atoms.



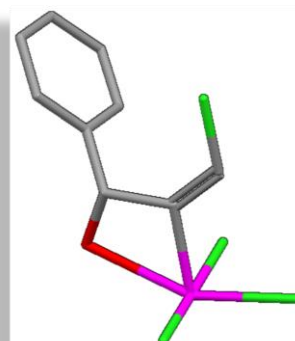
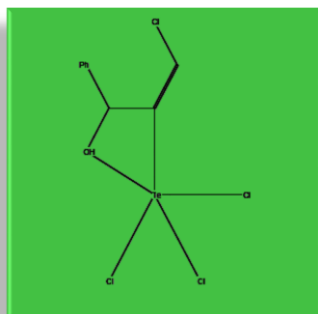
primeiros computadores: 1946



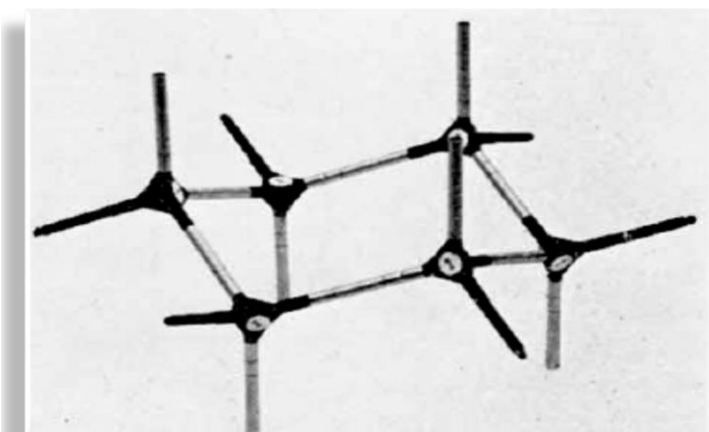
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Moléculas e representação



Modelo de Dreiding



Modelo de Dreiding para o ciclohexano (Fieser, 1963)

Os modelos de Dreiding, apresentados em 1958, foram um avanço na representação de moléculas, permitindo demonstrar a estereoquímica (o modo como os átomos de uma molécula estão arranjados no espaço tridimensional).

Estes modelos pré-fabricados tinham peças diferentes para representar os diferentes estados de hibridização de um átomo e permitiram a visualização das moléculas de modo mais realista.



Dorothy Crowfoot Hodgkin

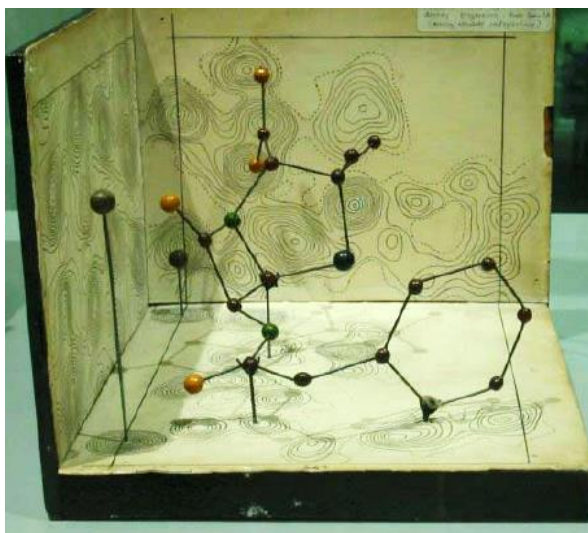
Royal Society Oxford University
Oxford, Great Britain

1910 - 1994



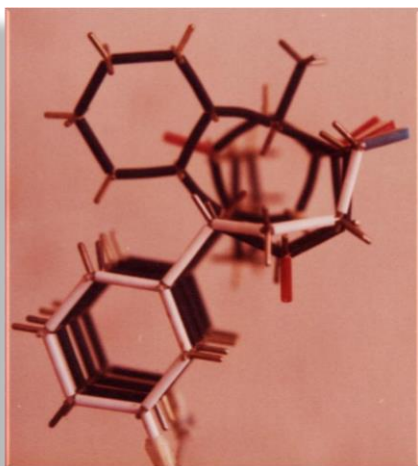
The Nobel Prize in Chemistry 1964

"for her determinations by X-ray techniques of the structures of important biochemical substances"



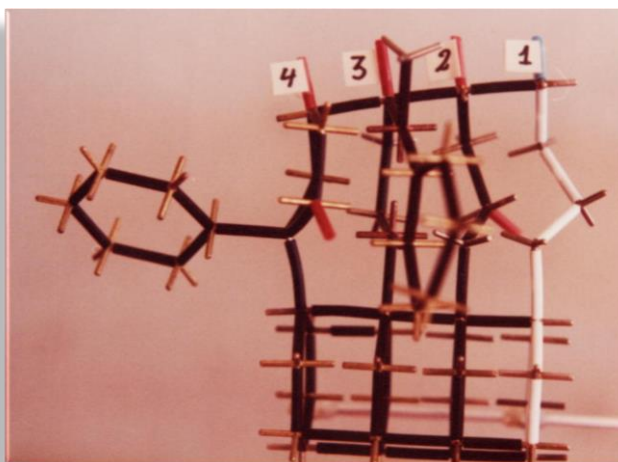
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Zukerman-Schpector,
Tese de Doutorado

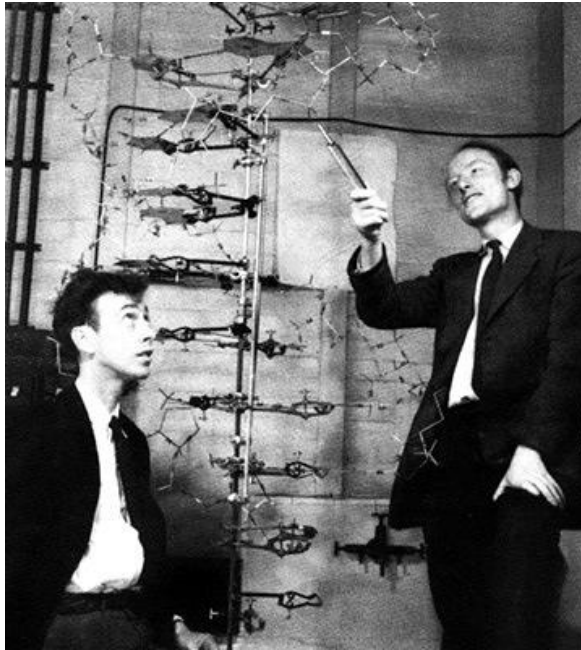
Modelo de Dreiding



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6



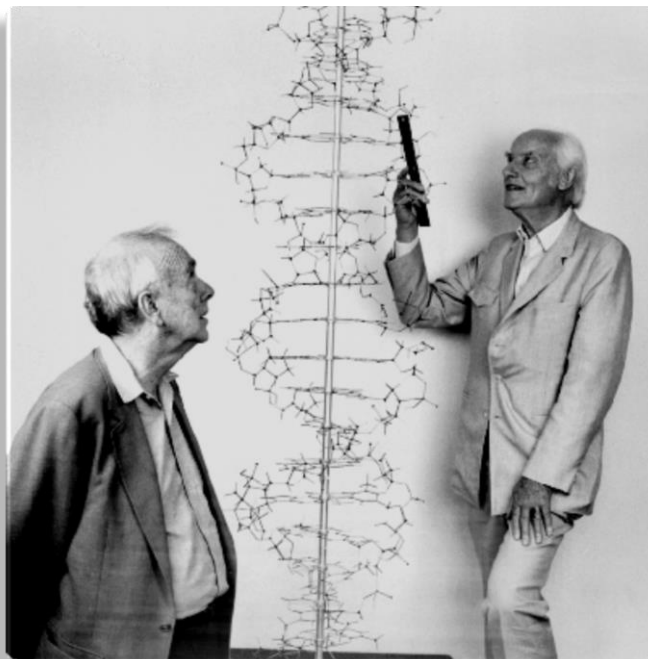
DNA

Watson & Crick
1953



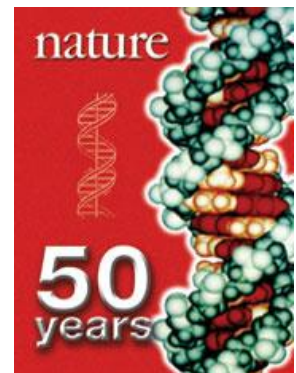
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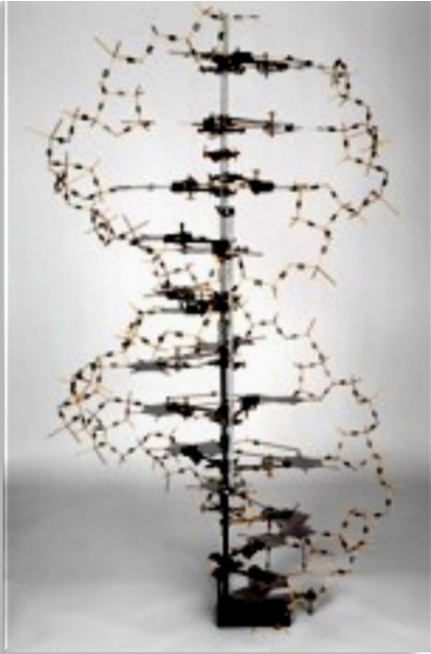
DNA

Watson & Crick
2003



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DNA

Reproduction of Watson & Crick's 1953 skeletal model

Built by Roger Lucke and Claudio Villa, LMB workshop, for the '**DNA: 50 years of the double helix**' exhibition, Cambridge, 2003
H200cm x W120cm x D120cm

On display at the Museum of Archaeology & Anthropology, Cambridge, until December 2010

DNA



Base plate from the Watson and Crick 1953 model
Signed by Francis Crick and Jim Watson



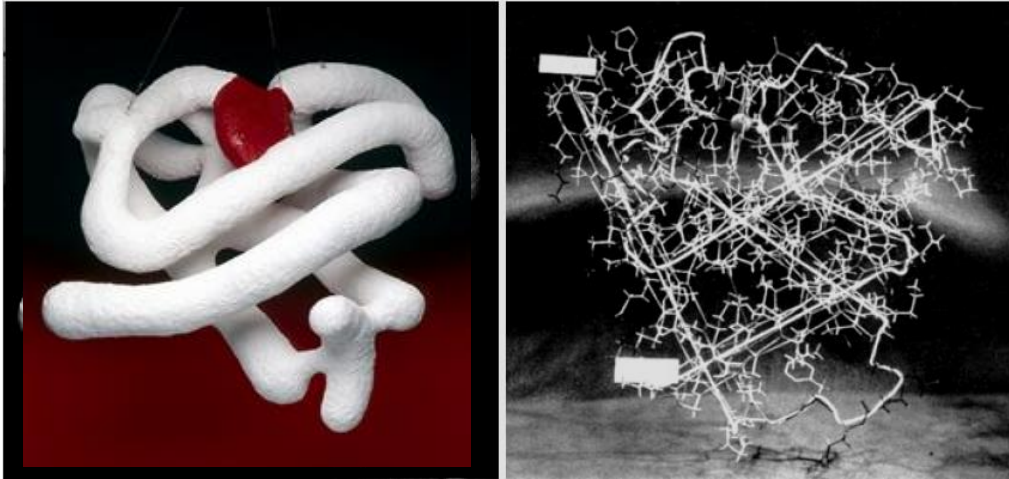
Primeira Proteína

Forma das moléculas –
Kendrew & Mioglobina

Kendrew & Mioglobina: Modelo de Dreiding



Kendrew & Mioglobina



1^{as} Estruturas 3D

Perutz ⇨
Hemoglobina

Orientador:
Bernal

Estudantes:
Francis Crick



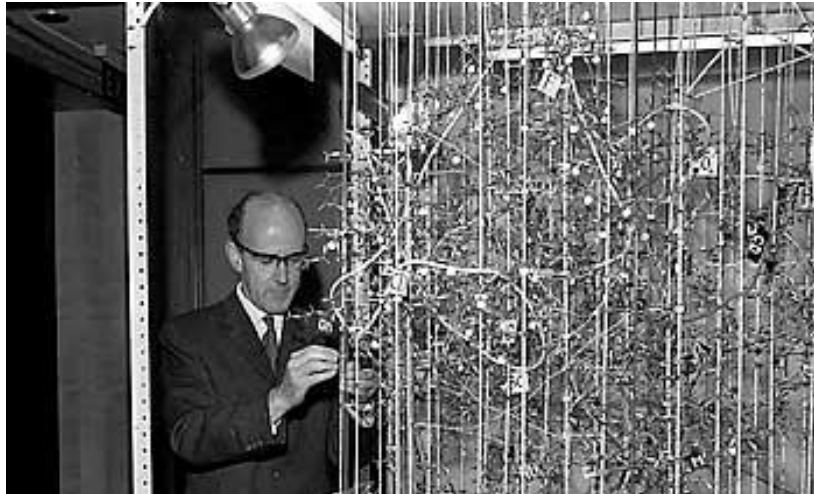
Kendrew ⇨
Mioglobina

Orientador:
Perutz

Prêmio Nobel em 1962.

Estrutura 3D Hemoglobina: 1º modelo

Perutz

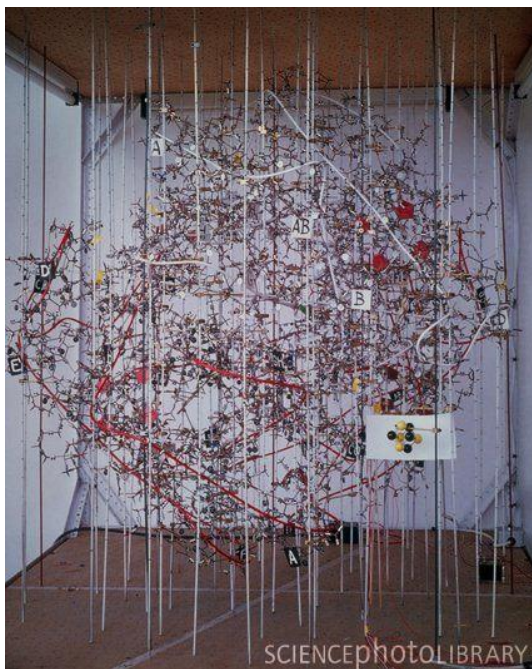


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<http://www.sciencephoto.com/media/304606/enlarge>

Model showing structure of haemoglobin molecule

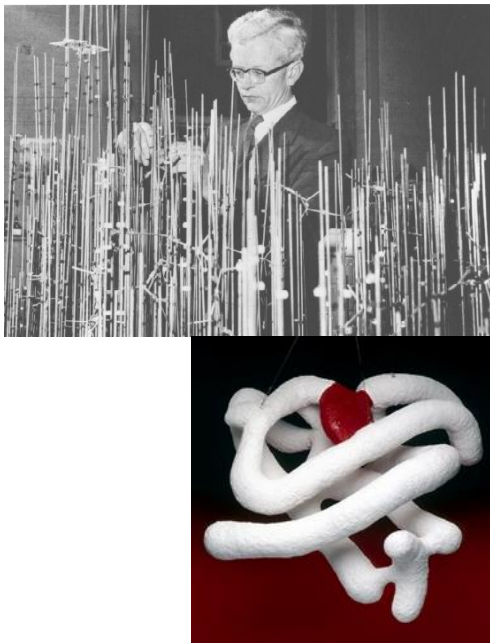


Estrutura 3D Hemoglobina: 1º modelo

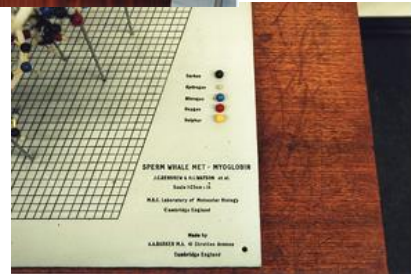
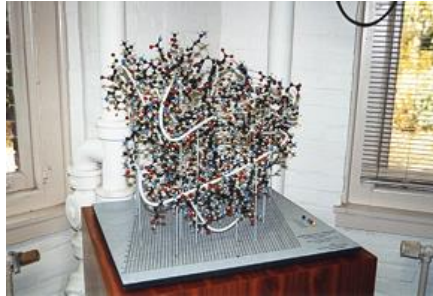


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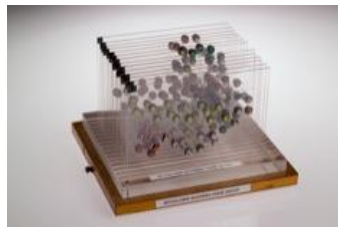
Modelos: Representações Físicas



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Modelos: Representações Físicas



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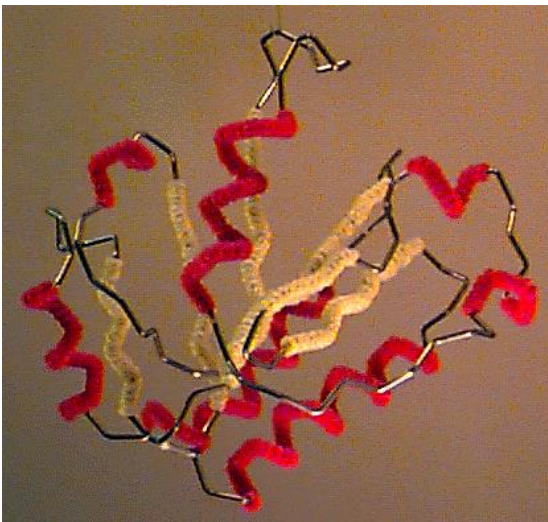
Modelos: Representações Físicas & Arte



'DNA Double Helix'
Bronze by Robin Holliday



Modelos: Representações Físicas



Wire model of the backbone trace of the I domain of CD11a (from 1LFA.PDB), an alpha/beta domain of a leukocyte integrin adhesion molecule. Alpha helices are decorated with red pipecleaner, while beta strands are decorated yellow. Model generously constructed by Tim Herman in 1997.

Modelos: Representações Físicas



Sculpture of human neutrophil collagenase by Byron Rubin on permanent exhibition at the

Smithsonian Institution, Washington DC USA. Image copyright © 2001, Byron H. Rubin, with permission. Height: 11 inches.

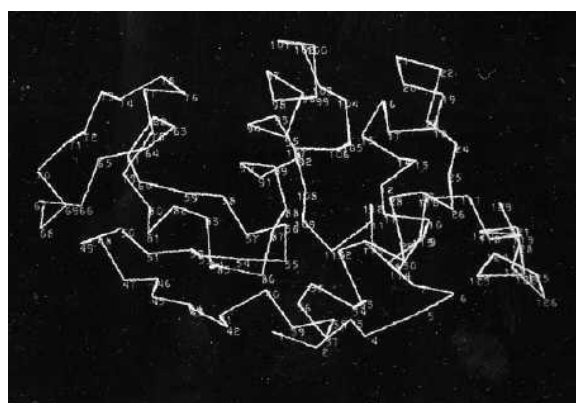


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Modelos: Representações Computacionais

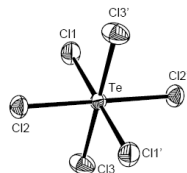
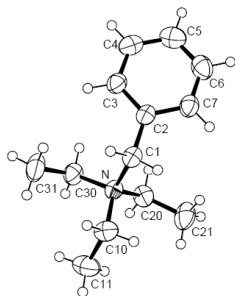
As early as 1964, Cyrus Levinthal and his colleagues at MIT had developed a system that displayed, on an oscilloscope, rotating "wireframe" representations of macromolecular structures.



http://www.umass.edu/molvis/frontoedus/levinthal/lev_index.html#animation

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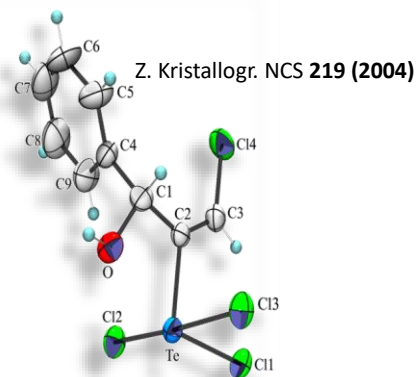
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Modelos: Representações Computacionais

In 1965, Carroll K. Johnson, of Oak Ridge National Laboratory, released **ORTEP**, a program to produce stereoscopic drawings of molecular and crystal structures with a pen-plotter. See the **ORTEP** page for more details.

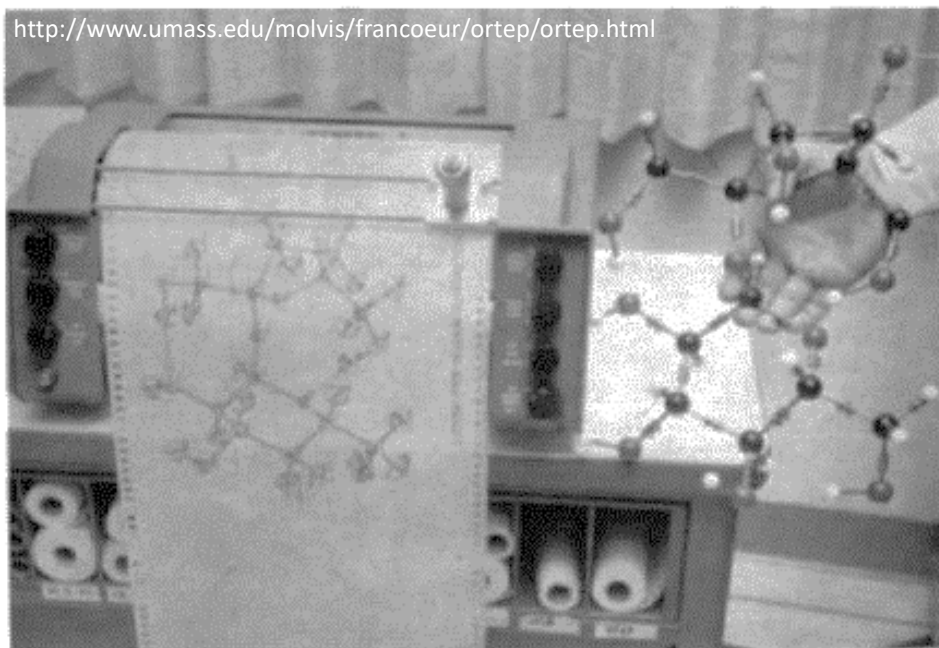
Created in FORTRAN by Carroll K. Johnson, of the Oak Ridge National Laboratory (ORNL), and first released in 1965, ORTEP (Oak Ridge Thermal-Ellipsoid Plot Program) rapidly became a favorite of crystallographers and protein crystallographers to produce illustrations of structures for conference presentations and publications.



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<http://www.umass.edu/molvis/francoeur/ortep/ortep.html>



Modelos:
Representações
Computacionais



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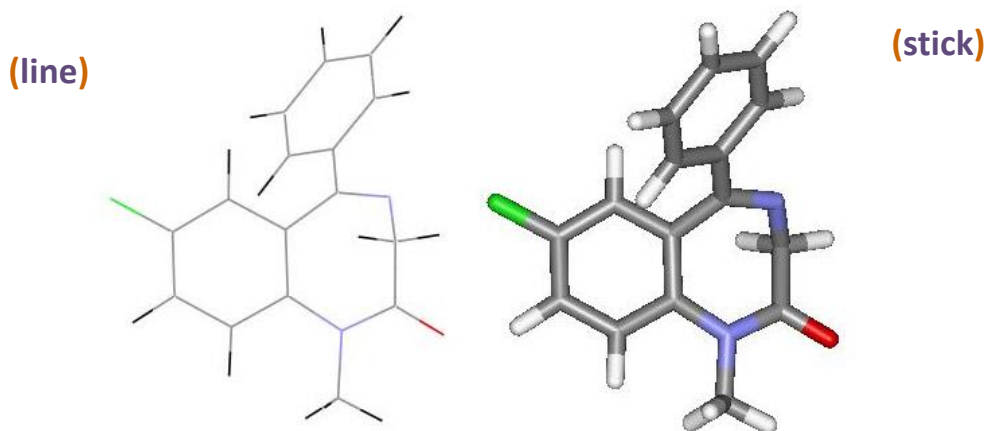
Diferentes formas de representar moléculas

Graficamente

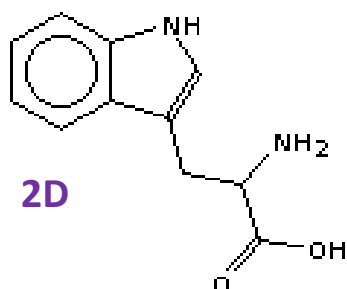
- Modelo de varetas **stick**
- Modelo de varetas e bolas **ball and stick**
- Modelos CPK (Corey-Pauling-Koltun) **CPK**
- Superfícies pontilhadas, de van der Waals, de Connolly
- Modelos Ribbons

Diferentes formas de representar moléculas

Modelo de varetas (line ou stick)



Diferentes formas de representar moléculas



Vantagens:

Mostra a estrutura completa
Fácil reconhecimento de padrões

Desvantagens:

Torna impossível a comparação espacial das estruturas



Vantagens:

Disponibiliza a informação estrutural
Entendimento de formas

Desvantagens:

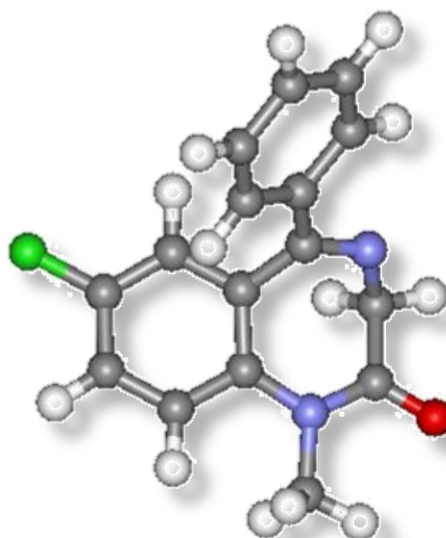
Limita a visualização de parte da estrutura
Dificulta comparações rápidas

Diferentes formas de representar moléculas

Modelo de varetas e bolas

(ball and stick)

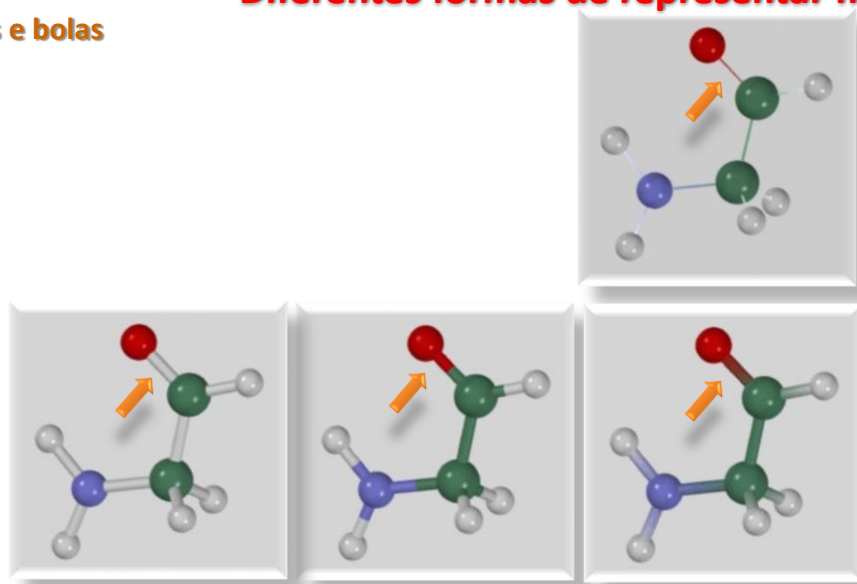
The original function of physical ball and stick models were the support of measurements of structure angles and bonds lengths, leaving the real structure representation to space filling models.



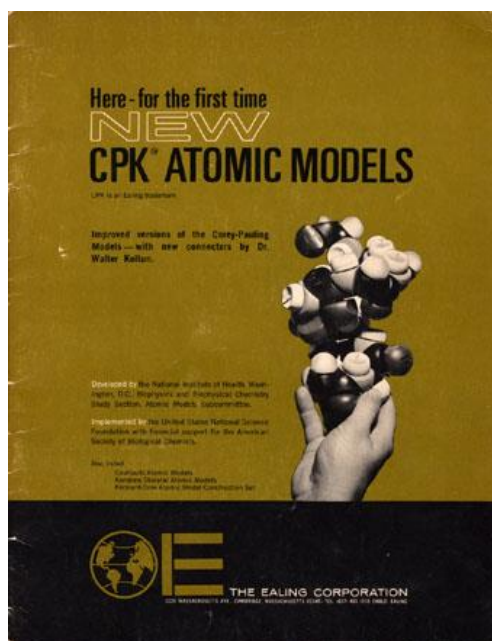
Diferentes formas de representar moléculas

Modelo de varetas e bolas

(ball and stick)



Modelos: Representações Físicas



1966 Molecular Model Catalogue

Before molecular graphics and modeling became affordable and widely available in the 1980s, physical molecular models were the primary tool to model and visualise the structure of biological macromolecules.

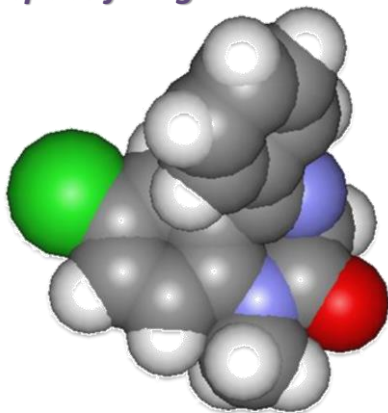
This 1966 catalogue from the Ealing Corporation is the first to describe the **Corey-Pauling-Koltun** space-filling models (or **CPK** models, for short).

<http://www.umass.edu/molvis/francoeur/ealing/ealing.html>

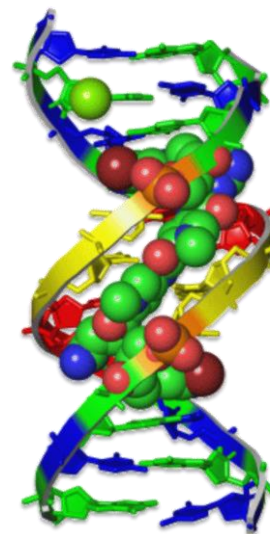
Diferentes formas de representar moléculas

Modelo CPK

space filling

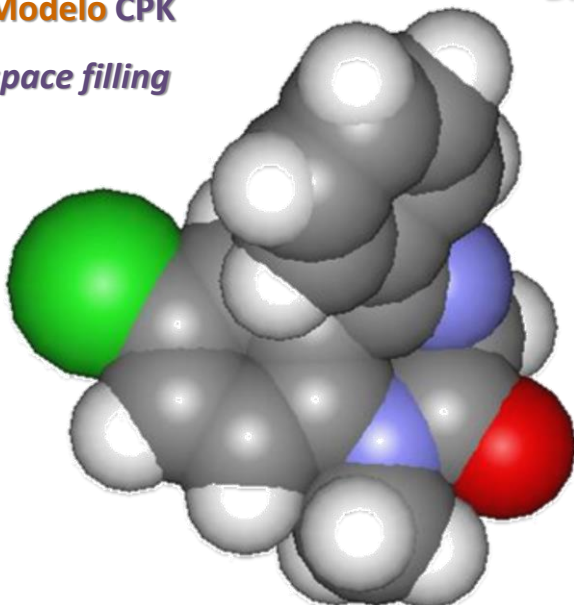


- idéia da superfície externa
- originalmente visualização de impedimento estérico "*steric hindrance*"



Modelo CPK

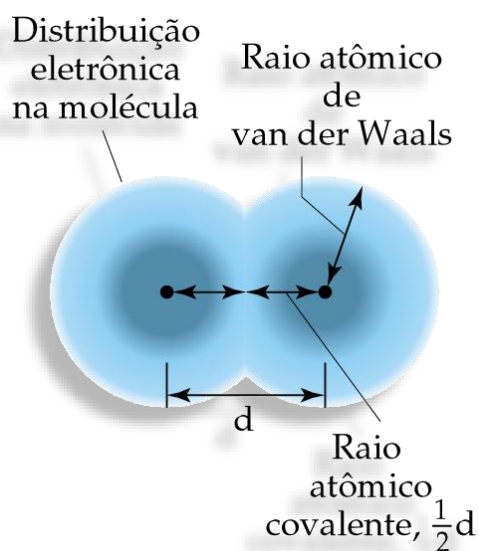
space filling



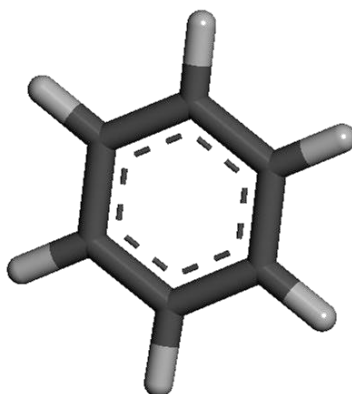
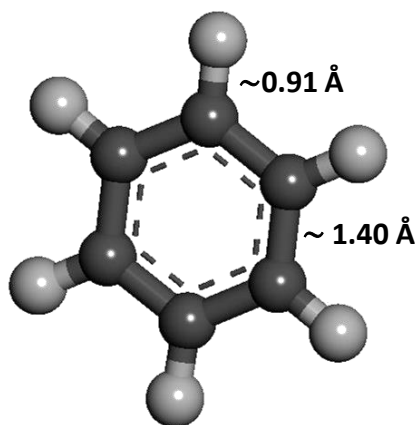
Diferentes formas de representar moléculas

- esferas com raios = raios de van der Waals
- O **raio de van der Waals** é o raio de uma esfera sólida imaginária empregada para representar um átomo. (obs: MQ → átomos não são esferas rígidas)
- O raio de **van der Waals** define o volume e superfície de um átomo ou molécula

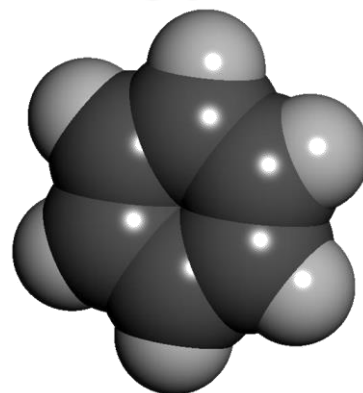
Raio Covalente



A distância entre os dois núcleos é denominada de **comprimento de ligação**.



Ligação Covalente



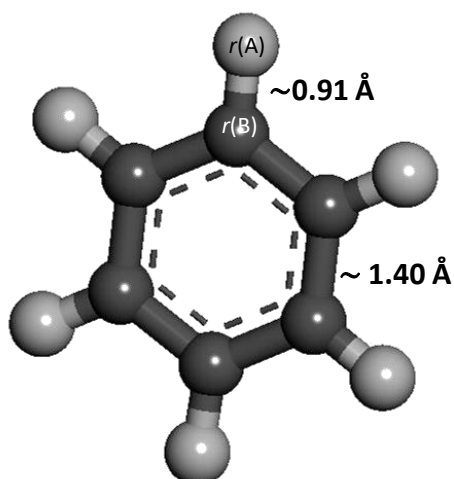
Ligação entre átomos ou interação?

raio de van der Waals

raio covalente

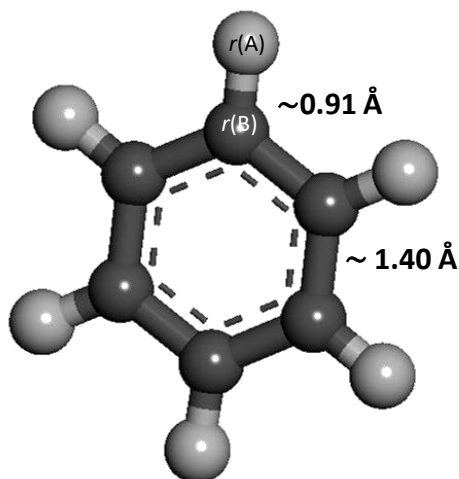
element	raio de van der Waals (Å)	element	raio covalente(Å)
H	1.20	H	0.23
C	1.70	C	0.68
N	1.55	N	0.68
O	1.52	O	0.68
F	1.47	F	0.64
P	1.80	P	1.05
S	1.80	S	1.02
Cl	1.89	Cl	0.99

Ligações ou não



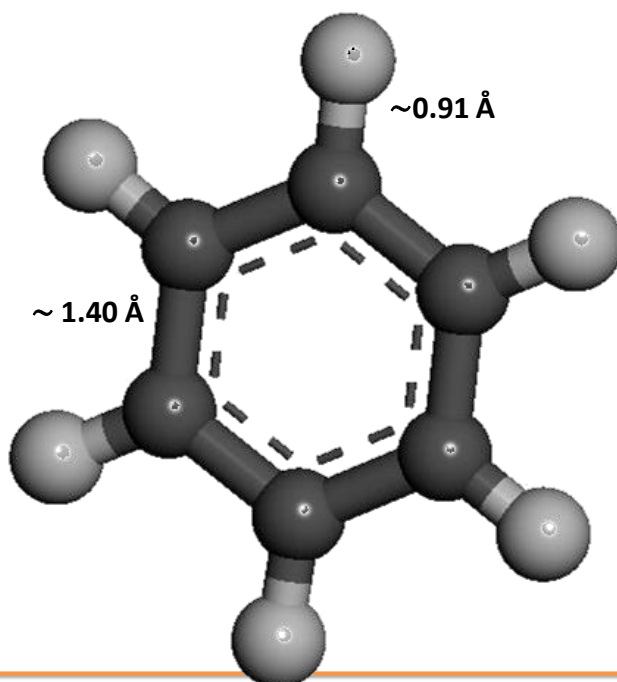
a soma dos raios covalentes
 $R(AB)$ deveria ser igual à soma

$$R(AB) = r(A) + r(B)$$

Como sabemos?

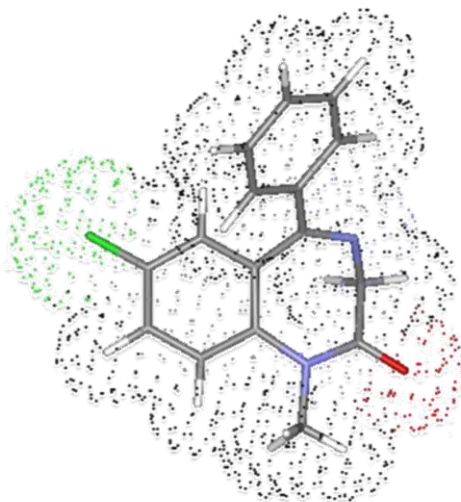
difração de raios X
difração de nêutrons
espectroscopia rotacional

[Cambridge Crystallographic Database](#) CSD

Ligações ou não

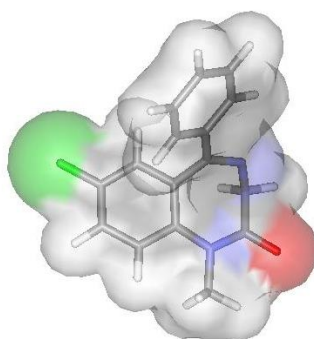
Diferentes formas de representar moléculas

Superfície pontilhada



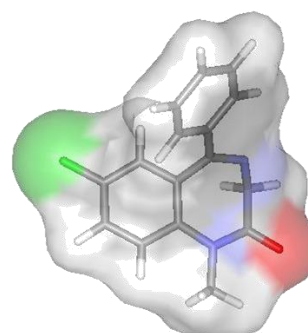
Diferentes formas de representar moléculas

Superfícies transparentes



A

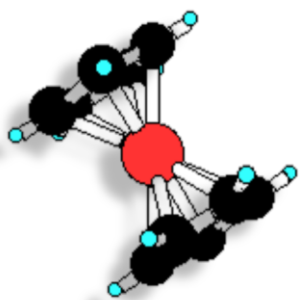
Superfície de van der Waals



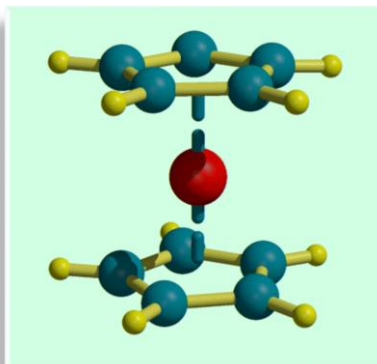
B

Superfície de Connolly (raio 1.4 Å)

Diferentes formas de representar moléculas



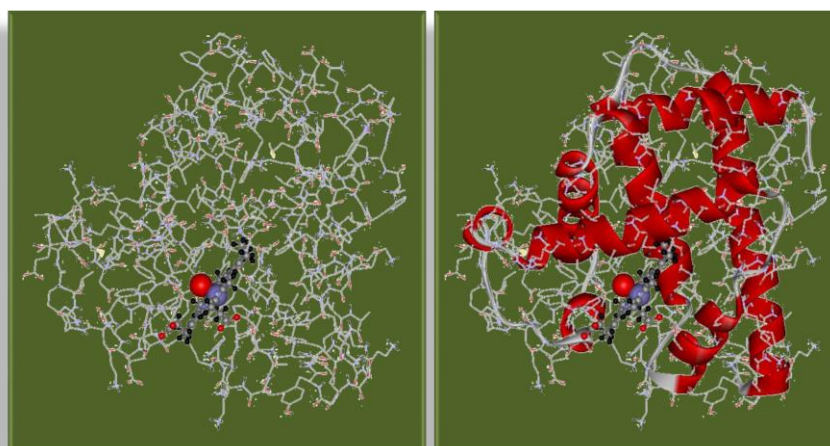
ferrocene, $\text{Fe}(\text{C}_5\text{H}_5)_2$



The discovery and characterisation of the structure of ferrocene, $\text{Fe}(\text{C}_5\text{H}_5)_2$ in the early 1950's, led to an explosion of interest in *d*-block metal carbon bonds and brought about development and the now flourishing study of organometallic chemistry.

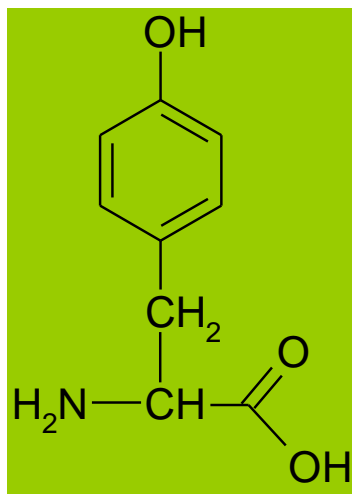
Diferentes formas de representar moléculas

Modelo Ribbons



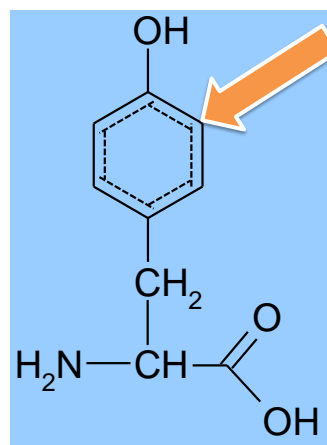
Representando uma estrutura química

- Quanta informação queremos incluir?
 - **átomos presentes**
 - **conexões entre átomos**
 - **tipos de ligações**
 - configuração estereoquímica
 - cargas
 - isótopos
 - coordenadas-3D dos átomos



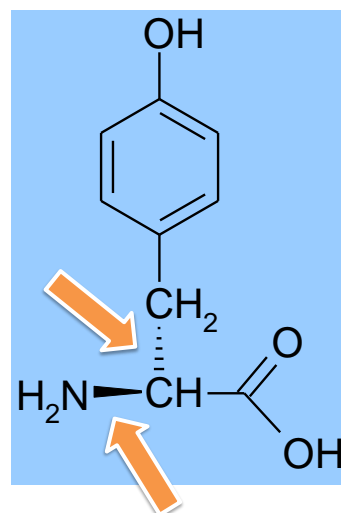
Representando uma estrutura química

- Quanta informação queremos incluir?
 - átomos presentes
 - conexões entre átomos
 - **tipos de ligações**
(identificação do anel aromático)
 - configuração estereoquímica
 - cargas
 - isótopos
 - coordenadas-3D dos átomos



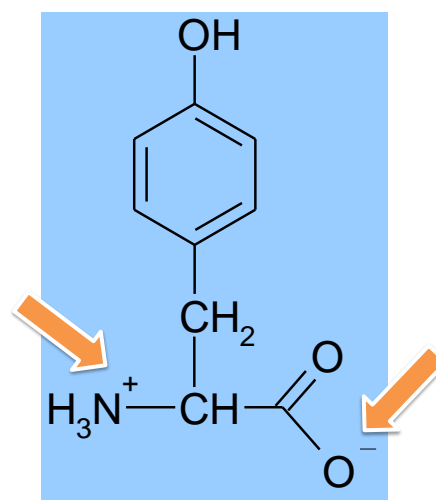
Representando uma estrutura química

- Quanta informação queremos incluir?
 - átomos presentes
 - conexões entre átomos
 - tipos de ligações
 - **configuração estereoquímica**
 - cargas
 - isótopos
 - coordenadas-3D dos átomos



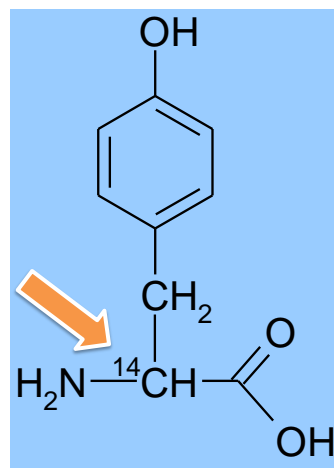
Representando uma estrutura química

- Quanta informação queremos incluir?
 - átomos presentes
 - conexões entre átomos
 - tipos de ligações
 - configuração estereoquímica
 - **cargas**
 - isótopos
 - coordenadas-3D dos átomos



Representando uma estrutura química

- Quanta informação queremos incluir?
 - átomos presentes
 - conexões entre átomos
 - tipos de ligações
 - configuração estereoquímica
 - cargas
 - **isótopos**
 - coordenadas-3D dos átomos

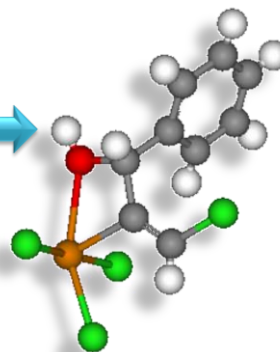


Formato (texto) × Programa × Visualização

informações:
átomos,
ligações, etc.

arquivo texto
(mol2, pdb, cif,
etc.)

Mercury
Jmol
Rasmol
DSVisualizer
O
PyMol
VMD
outros



PDB: texto

deposição

enzima HEADER OXIDOREDUCTASE 15-DEC-92 1GRE
 TITLE SUBSTRATE BINDING AND CATALYSIS BY GLUTATHIONE REDUCTASE AS DERIVED
 TITLE 2 FROM REFINED ENZYME: SUBSTRATE CRYSTAL STRUCTURES AT 2 ANGSTROMS
 TITLE 3 RESOLUTION
 COMPND MOL_ID: 1;

enzima COMPND 2 MOLECULE: GLUTATHIONE REDUCTASE;
 COMPND 3 CHAIN: A;
 COMPND 4 EC: 1.6.4.2;
 COMPND 5 **ENGINEERED: YES**
 SOURCE MOL_ID: 1;

fonte SOURCE 2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
 SOURCE 3 ORGANISM_COMMON: HUMAN;
 SOURCE 4 ORGANISM_TAXID: 9606
 KEYWDS OXIDOREDUCTASE(FLAVOENZYME), OXIDOREDUCTASE
 EXPDTA X-RAY DIFFRACTION **método experimental**

autor AUTHOR P.A.KARPLUS,G.E.SCHULZ

REVDAT 4 13-JUL-11 1GRE 1 VERSN
 REVDAT 3 24-FEB-09 1GRE 1 VERSN
 REVDAT 2 01-APR-03 1GRE 1 JRNL
 REVDAT 1 31-JAN-94 1GRE 0

PDB: texto

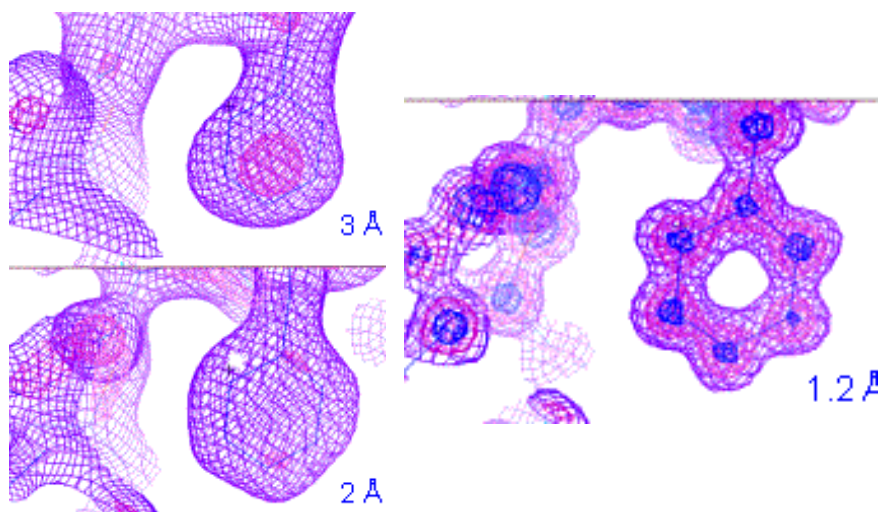
REMARK 1
 REMARK 1 REFERENCE 1
 REMARK 1 AUTH P.A.KARPLUS,R.L.KRAUTH-SIEGEL,R.H.SCHIRMER,G.E.SCHULZ
 REMARK 1 TITL INHIBITION OF HUMAN GLUTATHIONE REDUCTASE BY THE NITROSOUREA
 REMARK 1 TITL 2 DRUGS 1,3-BIS(2-CHLOROETHYL)-1-NITROSOUREA AND
 REMARK 1 TITL 3 1-(2-CHLOROETHYL)-3-(2-HYDROXYETHYL)-1-NITROSOUREA
 REMARK 1 REF EUR.J.BIOCHEM. V. 171 193 1988
 REMARK 1 REFN ISSN 0014-2956
 REMARK 1 REFERENCE 2
 REMARK 1 AUTH P.A.KARPLUS,G.E.SCHULZ
 REMARK 1 TITL REFINED STRUCTURE OF GLUTATHIONE REDUCTASE AT 1.54 ANGSTROMS
 REMARK 1 TITL 2 RESOLUTION
 REMARK 1 REF J.MOL.BIOL. V. 195 701 1987
 REMARK 1 REFN ISSN 0022-2836
 REMARK 1 REFERENCE 3
 REMARK 1 AUTH M.BILZER,R.L.KRAUTH-SIEGEL,R.H.SCHIRMER,T.P.M.AKERBOOM,
 REMARK 1 AUTH 2 H.SIES,G.E.SCHULZ
 REMARK 1 TITL INTERACTION OF A GLUTATHIONE S-CONJUGATE WITH GLUTATHIONE
 REMARK 1 TITL 2 REDUCTASE. KINETIC AND X-RAY CRYSTALLOGRAPHIC STUDIES
 REMARK 1 REF EUR.J.BIOCHEM. V. 138 373 1984
 REMARK 1 REFN ISSN 0014-2956
 REMARK 1 REFERENCE 4
 REMARK 1 AUTH R.K.WIERENGA,J.DRENTH,G.E.SCHULZ
 REMARK 1 TITL COMPARISON OF THE THREE-DIMENSIONAL PROTEIN AND NUCLEOTIDE
 REMARK 1 TITL 2 STRUCTURE OF THE FAD-BINDING DOMAIN OF P-HYDROXYBENZOATE

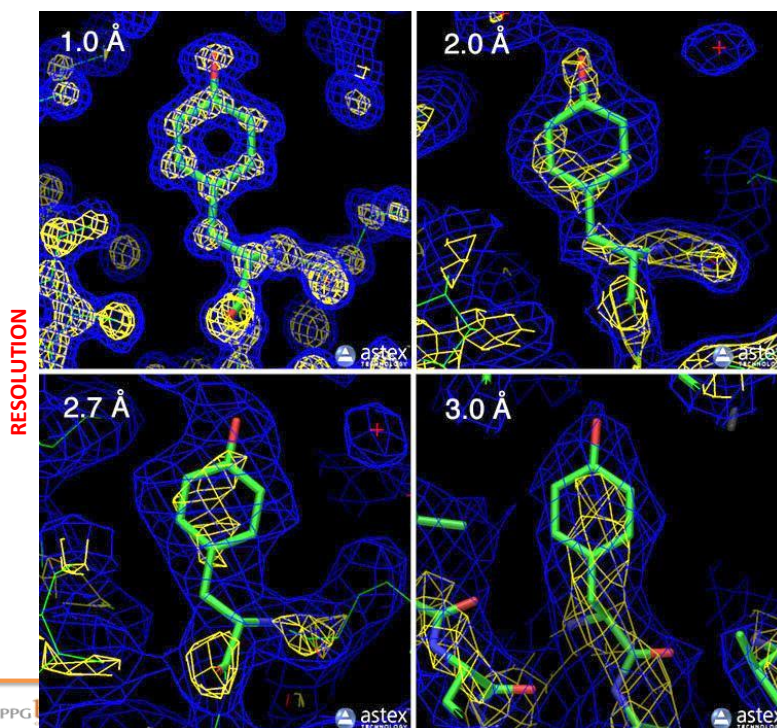
REMARK 2 **RESOLUTION. 2.00 ANGSTROMS.**
 REMARK 3
 REMARK 3 REFINEMENT.
 REMARK 3 PROGRAM : TNT
 REMARK 3 AUTHORS : TRONRUD,TEN EYCK,MATTHEWS
 REMARK 3
 REMARK 3 DATA USED IN REFINEMENT.
 REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.00
 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 10.00
 REMARK 3 DATA CUTOFF (SIGMA(F)) : 0.000
 REMARK 3 COMPLETENESS FOR RANGE (%) : NULL
 REMARK 3 NUMBER OF REFLECTIONS : 36365
 REMARK 3
 REMARK 3 USING DATA ABOVE SIGMA CUTOFF.
 REMARK 3 CROSS-VALIDATION METHOD : NULL
 REMARK 3 FREE R VALUE TEST SET SELECTION : NULL
 REMARK 3 R VALUE (WORKING + TEST SET) : 0.155
 REMARK 3 R VALUE (WORKING SET) : NULL
 REMARK 3 FREE R VALUE : NULL
 REMARK 3 FREE R VALUE TEST SET SIZE (%) : NULL
 REMARK 3 FREE R VALUE TEST SET COUNT : NULL
 REMARK 3
 REMARK 3 USING ALL DATA, NO SIGMA CUTOFF.
 REMARK 3 R VALUE (WORKING + TEST SET, NO CUTOFF) : NULL

dados experimentais

PDB: texto

RESOLUTION. 2.00 ANGSTROMS





http://www.pdb.org/pdb/home/hy/pdb/static.do?p=education_discussion_looking-at-Structures/resolution.html

PDB: texto

dados da molecula

REMARK 3
 REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
 REMARK 3 PROTEIN ATOMS : 3499
 REMARK 3 NUCLEIC ACID ATOMS : 0
 REMARK 3 HETEROGEN ATOMS : 98
 REMARK 3 SOLVENT ATOMS : 529
 REMARK 3
 REMARK 3 .

ATOM	3497	NH1	ARG	A	478	104.439	39.423	30.809	1.00	33.06	N
ATOM	3498	NH2	ARG	A	478	104.176	38.995	33.062	1.00	47.81	N
ATOM	3499	OXT	ARG	A	478	99.944	44.814	28.780	1.00	44.37	O
TER	3500		ARG	A	478						
HETATM	3501	P	PO4	A	480	78.187	65.140	18.209	0.82	40.06	P
HETATM	3502	O1	PO4	A	480	78.093	66.255	19.210	0.39	33.10	O
HETATM	3503	O2	PO4	A	480	78.647	65.636	16.866	0.87	37.44	O
HETATM	3504	O3	PO4	A	480	79.151	64.099	18.695	0.22	37.14	O
HETATM	3505	O4	PO4	A	480	76.825	64.527	18.050	0.42	44.67	O
HETATM	3506	PA	FAD	A	479	58.831	50.946	20.012	1.00	16.10	P
HETATM	3507	O1A	FAD	A	479	58.971	52.128	19.218	1.00	14.50	O

PDB: texto

sequência de aminoácidos: parte proteica

```

DBREF 1GRE A 1 478 UNP P00390 GSHR_HUMAN 1 478
SEQRES 1 A 478 ALA CYS ARG GLN GLU PRO GLN PRO GLN GLY PRO PRO PRO
SEQRES 2 A 478 ALA ALA GLY ALA VAL ALA SER TYR ASP TYR LEU VAL ILE
SEQRES 3 A 478 GLY GLY GLY SER GLY GLY LEU ALA SER ALA ARG ARG ALA
SEQRES 4 A 478 ALA GLU LEU GLY ALA ARG ALA ALA VAL VAL GLU SER HIS
SEQRES 5 A 478 LYS LEU GLY GLY THR CYS VAL ASN VAL GLY CYS VAL PRO
SEQRES 6 A 478 LYS LYS VAL MET TRP ASN THR ALA VAL HIS SER GLU PHE
SEQRES 7 A 478 MET HIS ASP HIS ALA ASP TYR GLY PHE PRO SER CYS GLU
SEQRES 8 A 478 GLY LYS PHE ASN TRP ARG VAL ILE LYS GLU LYS ARG ASP
SEQRES 9 A 478 ALA TYR VAL SER ARG LEU ASN ALA ILE TYR GLN ASN ASN
SEQRES 10 A 478 LEU THR LYS SER HIS ILE GLU ILE ILE ARG GLY HIS ALA

SEQRES 22 A 478 PRO VAL MET THR MET ILE PRO ASP VAL ASP CYS LEU LEU
SEQRES 23 A 478 TRP ALA ILE GLY ARG VAL PRO ASN THR LYS ASP LEU SER
SEQRES 24 A 478 LEU ASN LYS LEU GLY ILE GLN THR ASP ASP LYS GLY HIS
SEQRES 25 A 478 ILE ILE VAL ASP GLU PHE GLN ASN THR ASN VAL LYS GLY
SEQRES 26 A 478 ILE TYR ALA VAL GLY ASP VAL CYS GLY LYS ALA LEU LEU
SEQRES 27 A 478 THR PRO VAL ALA ILE ALA ALA GLY ARG LYS LEU ALA HIS
SEQRES 28 A 478 ARG LEU PHE GLU TYR LYS GLU ASP SER LYS LEU ASP TYR
SEQRES 29 A 478 ASN ASN ILE PRO THR VAL VAL PHE SER HIS PRO PRO ILE
SEQRES 30 A 478 GLY THR VAL GLY LEU THR GLU ASP GLU ALA ILE HIS LYS
SEQRES 31 A 478 TYR GLY ILE GLU ASN VAL LYS THR TYR SER THR SER PHE
SEQRES 32 A 478 THR PRO MET TYR HIS ALA VAL THR LYS ARG LYS THR LYS
SEQRES 33 A 478 CYS VAL MET LYS MET VAL CYS ALA ASN LYS GLU GLU LYS
SEQRES 34 A 478 VAL VAL GLY ILE HIS MET GLN GLY LEU GLY CYS ASP GLU
SEQRES 35 A 478 MET LEU GLN GLY PHE ALA VAL ALA VAL LYS MET GLY ALA
SEQRES 36 A 478 THR LYS ALA ASP PHE ASP ASN THR VAL ALA ILE ALA PRO
SEQRES 37 A 478 THR SER SER GLU GLU LEU VAL THR LEU ARG

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PDB: texto

heteroátomos: parte não-proteica

```

HET PO4 A 480 5
HET FAD A 479 53
HET GSH A 481 20
HET GSH A 482 20
HETNAM PO4 PHOSPHATE ION
HETNAM FAD FLAVIN-ADENINE DINUCLEOTIDE
HETNAM GSH GLUTATHIONE
FORMUL 2 PO4 O4 P 3-
FORMUL 3 FAD C27 H33 N9 O15 P2
FORMUL 4 GSH 2(C10 H17 N3 O6 S)
FORMUL 6 HOH *529(H2 O)

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parte proteica: estrutura secundária
hélices

PDB: texto

HELIX	1	H1	GLY A	29	GLY A	43	1RES 43 IN 3/10 CONFORMATION	15
HELIX	2	H2	GLY A	56	GLY A	86	1RES 80-86 3/10 CONFORMATION	31
HELIX	3	H3	TRP A	96	HIS A	122	1RES 121-122 3/10 CONFORMATN	27
HELIX	4	H4	GLY A	170	GLY A	174	5	5
HELIX	5	H5	SER A	177	LEU A	183	5	7
HELIX	6	H6	GLY A	196	LEU A	209	1	14
HELIX	7	H7	ASP A	227	GLY A	242	1RES 242 IN 3/10 CONFORMATION	16
HELIX	8	H8	SER A	299	GLY A	304	5	6
HELIX	9	H9	GLY A	330	GLY A	334	5	5
HELIX	10	H10	LEU A	338	PHE A	354	1	17
HELIX	11	H11	THR A	383	GLY A	392	1	10
HELIX	12	H12	PRO A	405	ALA A	409	5	5
HELIX	13	H13	LEU A	444	MET A	453	1	10
HELIX	14	H14	THR A	456	ASN A	462	1	7
HELIX	15	H15	SER A	470	THR A	476	5	7

parte proteica: estrutura secundária
fitas β e folhas β

PDB: texto

SHEET	1	A 8	GLU A	124	GLY A	128	0
SHEET	2	A 8	ARG A	45	GLU A	50	1
SHEET	3	A 8	ASP A	22	GLY A	27	1
SHEET	4	A 8	HIS A	151	ALA A	155	1
SHEET	5	A 8	GLY A	325	VAL A	329	1
SHEET	6	A 8	GLN A	319	VAL A	323	-1
SHEET	7	A 8	GLY A	311	ILE A	314	-1
SHEET	8	A 8	GLN A	306	ASP A	308	-1
SHEET	1	B 4	ALA A	19	TYR A	21	0
SHEET	2	B 4	LYS A	145	THR A	148	1
SHEET	3	B 4	THR A	139	VAL A	142	-1
SHEET	4	B 4	ALA A	131	THR A	133	-1
SHEET	1	C 5	ILE A	175	ILE A	175	0
SHEET	2	C 5	ASP A	283	ALA A	288	1
SHEET	3	C 5	GLY A	188	GLY A	194	1
SHEET	4	C 5	LYS A	212	ILE A	217	1
SHEET	5	C 5	GLU A	244	SER A	249	1
SHEET	1	D 4	PRO A	169	PRO A	169	0
SHEET	2	D 4	PHE A	248	THR A	257	1
SHEET	3	D 4	GLY A	260	ALA A	268	-1

PDB: texto**parte proteica: ligação dissulfeto (covalente)**

SSBOND	1	CYS A	90	CYS B	90		
1555	2665	1.80					
LINK		SG	CYS A	58		SG2	GSH A 481
1555	1555	2.07					

coordenadas: posição de todos os átomos **PDB: texto**

a ordem e formatação permite aos programas de visualização o desenho das moléculas

ATOM	1	N	VAL A	18	33.094	50.904	30.111	1.00	43.51
ATOM	2	CA	VAL A	18	34.520	50.904	30.464	1.00	45.08
ATOM	3	C	VAL A	18	34.962	49.489	30.799	1.00	30.38
ATOM	4	O	VAL A	18	34.660	48.923	31.862	1.00	42.44
ATOM	5	CB	VAL A	18	34.972	51.857	31.589	1.00	32.03
ATOM	6	CG1	VAL A	18	36.500	51.898	31.647	1.00	27.14

coordenadas: posição de todos os átomos **PDB: texto**

átomos

ATOM	1	N	VAL	A	18	33.094	50.904	30.111	1.00	43.51
ATOM	2	CA	VAL	A	18	34.520	50.904	30.464	1.00	45.08
ATOM	3	C	VAL	A	18	34.962	49.489	30.799	1.00	30.38
ATOM	4	O	VAL	A	18	34.660	48.923	31.862	1.00	42.44
ATOM	5	CB	VAL	A	18	34.972	51.857	31.589	1.00	32.03
ATOM	6	CG1	VAL	A	18	36.500	51.898	31.647	1.00	27.14

coordenadas: posição de todos os átomos **PDB: texto**

numeração
dos átomos
sequencial

ATOM	1	N	VAL	A	18	33.094	50.904	30.111	1.00	43.51
ATOM	2	CA	VAL	A	18	34.520	50.904	30.464	1.00	45.08
ATOM	3	C	VAL	A	18	34.962	49.489	30.799	1.00	30.38
ATOM	4	O	VAL	A	18	34.660	48.923	31.862	1.00	42.44
ATOM	5	CB	VAL	A	18	34.972	51.857	31.589	1.00	32.03
ATOM	6	CG1	VAL	A	18	36.500	51.898	31.647	1.00	27.14

coordenadas: posição de todos os átomos **PDB: texto**

átomos N, C, O, S

ATOM	1	N	VAL	A	18	33.094	50.904	30.111	1.00	43.51
ATOM	2	CA	VAL	A	18	34.520	50.904	30.464	1.00	45.08
ATOM	3	C	VAL	A	18	34.962	49.489	30.799	1.00	30.38
ATOM	4	O	VAL	A	18	34.660	48.923	31.862	1.00	42.44
ATOM	5	CB	VAL	A	18	34.972	51.857	31.589	1.00	32.03
ATOM	6	CG1	VAL	A	18	36.500	51.898	31.647	1.00	27.14

coordenadas: posição de todos os átomos **PDB: texto**

nome dos aminoácidos

ATOM	1	N	VAL	A	18	33.094	50.904	30.111	1.00	43.51
ATOM	2	CA	VAL	A	18	34.520	50.904	30.464	1.00	45.08
ATOM	3	C	VAL	A	18	34.962	49.489	30.799	1.00	30.38
ATOM	4	O	VAL	A	18	34.660	48.923	31.862	1.00	42.44
ATOM	5	CB	VAL	A	18	34.972	51.857	31.589	1.00	32.03
ATOM	6	CG1	VAL	A	18	36.500	51.898	31.647	1.00	27.14

coordenadas: posição de todos os átomos **PDB: texto**

cadeia A

ATOM	1	N	VAL	A	18	33.094	50.904	30.111	1.00	43.51
ATOM	2	CA	VAL	A	18	34.520	50.904	30.464	1.00	45.08
ATOM	3	C	VAL	A	18	34.962	49.489	30.799	1.00	30.38
ATOM	4	O	VAL	A	18	34.660	48.923	31.862	1.00	42.44
ATOM	5	CB	VAL	A	18	34.972	51.857	31.589	1.00	32.03
ATOM	6	CG1	VAL	A	18	36.500	51.898	31.647	1.00	27.14

coordenadas: posição de todos os átomos **PDB: texto**

numeração sequencial
dos aminoácidos

ATOM	1	N	VAL	A	18	33.094	50.904	30.111	1.00	43.51
ATOM	2	CA	VAL	A	18	34.520	50.904	30.464	1.00	45.08
ATOM	3	C	VAL	A	18	34.962	49.489	30.799	1.00	30.38
ATOM	4	O	VAL	A	18	34.660	48.923	31.862	1.00	42.44
ATOM	5	CB	VAL	A	18	34.972	51.857	31.589	1.00	32.03
ATOM	6	CG1	VAL	A	18	36.500	51.898	31.647	1.00	27.14

coordenadas: posição de todos os átomos **PDB: texto**



ATOM	1	N	VAL	A	18	33.094	50.904	30.111	1.00	43.51
ATOM	2	CA	VAL	A	18	34.520	50.904	30.464	1.00	45.08
ATOM	3	C	VAL	A	18	34.962	49.489	30.799	1.00	30.38
ATOM	4	O	VAL	A	18	34.660	48.923	31.862	1.00	42.44
ATOM	5	CB	VAL	A	18	34.972	51.857	31.589	1.00	32.03
ATOM	6	CG1	VAL	A	18	36.500	51.898	31.647	1.00	27.14

coordenadas: posição de todos os átomos **PDB: texto**



ATOM	1	N	VAL	A	18	33.094	50.904	30.111	1.00	43.51
ATOM	2	CA	VAL	A	18	34.520	50.904	30.464	1.00	45.08
ATOM	3	C	VAL	A	18	34.962	49.489	30.799	1.00	30.38
ATOM	4	O	VAL	A	18	34.660	48.923	31.862	1.00	42.44
ATOM	5	CB	VAL	A	18	34.972	51.857	31.589	1.00	32.03
ATOM	6	CG1	VAL	A	18	36.500	51.898	31.647	1.00	27.14

ATOM	7	CG2	VAL	A	18	34.427	53.276	31.397	1.00	33.25
ATOM	8	N	ALA	A	19	35.703	48.921	29.875	1.00	26.95
ATOM	9	CA	ALA	A	19	36.239	47.598	30.077	1.00	17.30
ATOM	10	C	ALA	A	19	37.488	47.658	30.953	1.00	28.02
ATOM	11	O	ALA	A	19	38.397	48.475	30.766	1.00	20.25
ATOM	12	CB	ALA	A	19	36.498	46.982	28.714	1.00	22.55
ATOM	13	N	SER	A	20	37.509	46.806	31.955	1.00	13.05
ATOM	14	CA	SER	A	20	38.584	46.794	32.893	1.00	9.82
ATOM	15	C	SER	A	20	39.483	45.587	32.693	1.00	29.27
ATOM	16	O	SER	A	20	39.010	44.530	32.276	1.00	25.05
ATOM	17	CB	SER	A	20	38.006	46.852	34.283	1.00	11.19
ATOM	18	OG	SER	A	20	39.057	47.137	35.182	1.00	53.49
ATOM	19	N	TYR	A	21	40.793	45.793	32.920	1.00	18.02
ATOM	20	CA	TYR	A	21	41.810	44.747	32.805	1.00	18.42
ATOM	21	C	TYR	A	21	42.700	44.855	34.016	1.00	12.52
ATOM	22	O	TYR	A	21	42.562	45.822	34.767	1.00	22.57
ATOM	23	CB	TYR	A	21	42.725	44.891	31.564	1.00	20.54
ATOM	24	CG	TYR	A	21	42.032	44.625	30.273	1.00	14.61
ATOM	25	CD1	TYR	A	21	41.300	45.658	29.688	1.00	16.50
ATOM	26	CD2	TYR	A	21	42.042	43.354	29.674	1.00	13.27
ATOM	27	CE1	TYR	A	21	40.581	45.442	28.524	1.00	33.82
ATOM	28	CE2	TYR	A	21	41.305	43.132	28.506	1.00	19.90
ATOM	29	CZ	TYR	A	21	40.590	44.171	27.923	1.00	23.16
ATOM	30	OH	TYR	A	21	39.897	44.011	26.744	1.00	33.73
ATOM	31	N	ASP	A	22	43.619	43.884	34.192	1.00	22.48



Bioinformática I

Julia Zukerman
Ignacio Corbelli

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TER	3500		ARG	A	478					
HETATM	3501	P	PO4	A	480	78.187	65.140	18.209	0.82	40.06
HETATM	3502	O1	PO4	A	480	78.093	66.255	19.210	0.39	33.10
HETATM	3503	O2	PO4	A	480	78.647	65.636	16.866	0.87	37.44
HETATM	3504	O3	PO4	A	480	79.151	64.099	18.695	0.22	37.14
HETATM	3505	O4	PO4	A	480	76.825	64.527	18.050	0.42	44.67
HETATM	3506	PA	FAD	A	479	58.831	50.946	20.012	1.00	16.10
HETATM	3507	O1A	FAD	A	479	58.971	52.128	19.218	1.00	14.50
HETATM	3508	O2A	FAD	A	479	59.474	49.618	19.687	1.00	15.08
HETATM	3509	O5B	FAD	A	479	57.361	50.663	20.227	1.00	15.72
HETATM	3510	C5B	FAD	A	479	56.376	51.833	20.301	1.00	17.98
HETATM	3511	C4B	FAD	A	479	55.092	51.221	19.742	1.00	10.80
HETATM	3512	O4B	FAD	A	479	53.940	51.971	20.295	1.00	13.46
HETATM	3513	C3B	FAD	A	479	54.963	51.228	18.226	1.00	13.69
HETATM	3514	O3B	FAD	A	479	54.620	50.008	17.649	1.00	14.78
HETATM	3515	C2B	FAD	A	479	54.008	52.405	18.027	1.00	8.15
HETATM	3516	O2B	FAD	A	479	53.329	52.198	16.797	1.00	13.80
HETATM	3517	C1B	FAD	A	479	53.039	52.193	19.170	1.00	18.61
HETATM	3518	N9A	FAD	A	479	52.344	53.408	19.639	1.00	15.10
HETATM	3519	C8A	FAD	A	479	52.921	54.647	19.897	1.00	16.11
HETATM	3520	N7A	FAD	A	479	52.036	55.494	20.397	1.00	21.59
HETATM	3521	C5A	FAD	A	479	50.864	54.805	20.467	1.00	20.59
HETATM	3522	C6A	FAD	A	479	49.532	55.198	20.907	1.00	16.60
HETATM	3523	N6A	FAD	A	479	49.233	56.388	21.269	1.00	14.48
HETATM	3524	N1A	FAD	A	479	48.581	54.222	20.771	1.00	14.86



Bioinformática I

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Ignacio Corbelli

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HETATM	3562	O11	GSH	A	481	63.334	36.432	25.048	1.00	35.23
HETATM	3563	O12	GSH	A	481	64.503	38.281	25.590	1.00	22.73
HETATM	3564	CB1	GSH	A	481	64.041	38.827	22.636	1.00	17.95
HETATM	3565	CG1	GSH	A	481	64.228	38.880	21.092	1.00	24.48
HETATM	3566	CD1	GSH	A	481	63.809	40.306	20.698	1.00	26.51
HETATM	3567	OE1	GSH	A	481	64.475	41.247	21.111	1.00	14.27
HETATM	3568	N2	GSH	A	481	62.686	40.468	20.011	1.00	23.17
HETATM	3569	CA2	GSH	A	481	62.178	41.821	19.748	1.00	15.79
HETATM	3570	C2	GSH	A	481	61.011	42.125	20.666	1.00	26.84
HETATM	3571	O2	GSH	A	481	60.376	43.175	20.574	1.00	39.73
HETATM	3572	CB2	GSH	A	481	61.698	42.016	18.309	1.00	24.83
HETATM	3573	SG2	GSH	A	481	62.931	42.714	17.179	1.00	22.88
HETATM	3574	N3	GSH	A	481	60.693	41.129	21.489	1.00	23.93
HETATM	3575	CA3	GSH	A	481	59.574	41.244	22.389	1.00	22.27
HETATM	3576	C3	GSH	A	481	59.401	39.911	23.089	1.00	31.11
HETATM	3577	O31	GSH	A	481	58.469	39.793	23.890	1.00	26.36
HETATM	3578	O32	GSH	A	481	60.202	38.972	22.888	1.00	26.68
HETATM	3579	N1	GSH	A	482	68.796	36.360	18.363	1.00	19.48
HETATM	3580	CA1	GSH	A	482	69.043	35.408	17.267	1.00	34.01
HETATM	3581	C1	GSH	A	482	69.696	36.032	16.047	1.00	37.29
HETATM	3582	O11	GSH	A	482	69.738	37.261	15.967	1.00	31.58
HETATM	3583	O12	GSH	A	482	70.088	35.167	15.126	1.00	25.33
HETATM	3584	CB1	GSH	A	482	67.767	34.679	16.821	1.00	32.45
HETATM	3585	CG1	GSH	A	482	66.942	35.652	15.951	1.00	34.08
HETATM	3586	CD1	GSH	A	482	65.876	36.452	16.733	1.00	26.47



Bioinformática I

Julio Zukerman
Ignes Caracelli

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HETATM	3599	O	HOH	A	483	77.894	39.601	21.811	1.00	9.38
HETATM	3600	O	HOH	A	484	58.802	53.242	24.949	0.95	9.34
HETATM	3601	O	HOH	A	485	71.847	45.784	24.545	1.00	11.16
HETATM	3602	O	HOH	A	486	56.475	48.948	23.248	0.97	7.80
HETATM	3603	O	HOH	A	487	64.462	51.085	24.951	1.00	12.33

HETATM	4125	O	HOH	A1009		63.748	69.165	30.831	1.00	39.18
HETATM	4126	O	HOH	A1010		61.234	36.028	22.997	0.43	39.41
HETATM	4127	O	HOH	A1011		57.696	64.941	21.669	1.00	47.83
CONECT	279	3573								

CONECT 3595 3594 3596
 CONECT 3596 3595 3597 3598
 CONECT 3597 3596
 CONECT 3598 3596
 MASTER 462 1 4 15 28 0 22 6 4126 1 99 37
 END



Bioinformática I

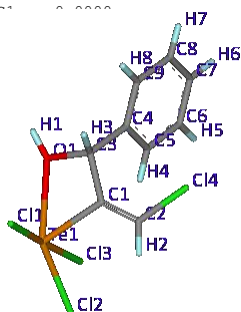
Julio Zukerman
Ignes Caracelli

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Formato mol2

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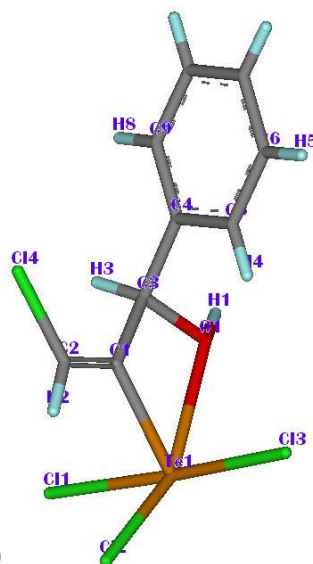
1	Te1	5.2600	0.8060	12.0298	Te	1	RES1	0.0000
2	C11	3.1368	2.1115	12.2513	C1	1	RES1	0.0000
3	C12	4.0776	-1.1283	12.5514	C1	1	RES1	0.0000
4	C13	7.3573	-0.5627	12.0078	C1	1	RES1	0.0000
5	C14	5.6229	1.0364	16.6760	C1			
6	O1	6.6012	2.8134	12.5780	O.3			
7	H1	6.7671	3.6286	12.4026	H			
8	C1	5.6881	1.3360	14.0355	C.2			
9	C2	5.3076	0.5761	15.0543	C.2			
10	H2	4.8592	-0.2212	14.8859	H			
11	C3	6.3705	2.6681	13.9888	C.3			
12	H3	5.7455	3.3612	14.2859	H			
13	C4	7.6547	2.7806	14.7840	C.ar			
14	C5	8.5963	1.7571	14.7401	C.ar			
15	H4	8.4286	0.9901	14.2421	H			
16	C6	9.7837	1.8818	15.4377	C.ar			
17	H5	10.4126	1.1984	15.4109	H			
18	C7	10.0337	3.0204	16.1750	C.ar	1	RES1	0.0000
19	H6	10.8383	3.1059	16.6334	H	1	RES1	0.0000
20	C8	9.1222	4.0067	16.2344	C.ar	1	RES1	0.0000
21	H7	9.2931	4.7608	16.7509	H	1	RES1	0.0000
22	C9	7.9105	3.9090	15.5212	C.ar	1	RES1	0.0000
23	H8	7.2909	4.6020	15.5509	H	1	RES1	0.0000



Formato mol2

@<TRIPOS>BOND

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3	4	1	1
4	5	9	1
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6	7	6	1
7	8	1	1
8	9	8	2
9	10	9	1
10	11	6	1
11	12	11	1
12	13	11	1
13	14	13	ar
14	15	14	1
15	16	14	ar
16	17	16	1
17	18	16	ar
18	19	18	1
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21	22	13	ar
22	23	22	1
23	8	11	1
24	20	22	ar

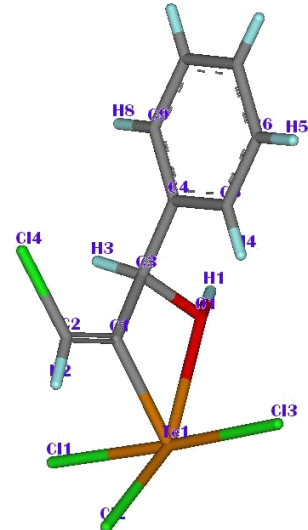


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HEADER      CSD ENTRY WERWUM
COMPND      UNNAMED
AUTHOR      GENERATED BY CONQUEST
CRYST1      14.441    6.429    14.755    90.00 106.46    90.00 P 21/c    4
ATOM        1  Te1  UNK  0    1      5.260    0.806    12.030    1.00  0.00
ATOM        2  C11  UNK  0    1      3.137    2.111    12.251    1.00  0.00
ATOM        3  C12  UNK  0    1      4.078   -1.128    12.551    1.00  0.00
ATOM        4  C13  UNK  0    1      7.357   -0.563    12.008    1.00  0.00
ATOM        5  C14  UNK  0    1      5.623    1.036    16.676    1.00  0.00
ATOM        6  O1   UNK  0    1      6.601    2.813    12.578    1.00  0.00
ATOM        7  H1   UNK  0    1      6.767    3.629    12.403    1.00  0.00
ATOM        8  C1   UNK  0    1      5.688    1.336    14.035    1.00  0.00
ATOM        9  C2   UNK  0    1      5.308    0.576    15.054    1.00  0.00
ATOM       10  H2   UNK  0    1      4.859   -0.221    14.886    1.00  0.00
ATOM       11  C3   UNK  0    1      6.371    2.668    13.989    1.00  0.00
ATOM       12  H3   UNK  0    1      5.746    3.361    14.286    1.00  0.00
ATOM       13  C4   UNK  0    1      7.655    2.781    14.784    1.00  0.00
ATOM       14  C5   UNK  0    1      8.596    1.757    14.740    1.00  0.00
ATOM       15  H4   UNK  0    1      8.429    0.990    14.242    1.00  0.00
ATOM       16  C6   UNK  0    1      9.784    1.882    15.438    1.00  0.00
ATOM       17  H5   UNK  0    1     10.413    1.198    15.411    1.00  0.00
ATOM       18  C7   UNK  0    1     10.034    3.020    16.175    1.00  0.00
ATOM       19  H6   UNK  0    1     10.838    3.106    16.633    1.00  0.00
ATOM       20  C8   UNK  0    1      9.122    4.007    16.234    1.00  0.00
ATOM       21  H7   UNK  0    1      9.293    4.761    16.751    1.00  0.00
ATOM       22  C9   UNK  0    1      7.911    3.909    15.521    1.00  0.00
ATOM       23  H8   UNK  0    1      7.291    4.602    15.551    1.00  0.00

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Formato pdb

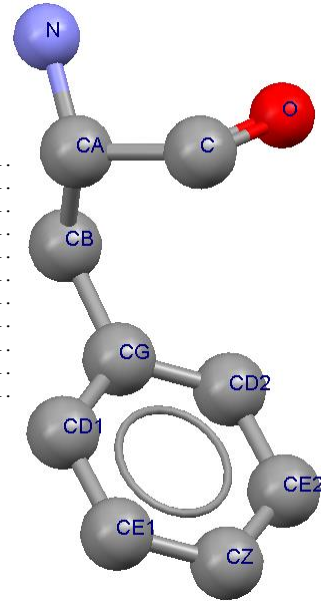


Aminoácidos & proteínas

ATOM	1084	N	XXX	A	138	3.800	20.200	9.600	1.00	0.00	N
ATOM	1085	CA	XXX	A	138	4.500	21.400	9.300	1.00	0.00	C
ATOM	1086	C	XXX	A	138	4.200	21.700	7.800	1.00	0.00	C
ATOM	1087	O	XXX	A	138	3.900	22.800	7.400	1.00	0.00	O
ATOM	1088	CB	XXX	A	138	5.900	21.100	9.900	1.00	0.00	C
ATOM	1089	CG	XXX	A	138	7.000	21.900	9.300	1.00	0.00	C
ATOM	1090	CD1	XXX	A	138	7.500	21.600	8.100	1.00	0.00	C
ATOM	1091	CD2	XXX	A	138	7.400	23.100	9.900	1.00	0.00	C
ATOM	1092	CE1	XXX	A	138	8.600	22.300	7.500	1.00	0.00	C
ATOM	1093	CE2	XXX	A	138	8.400	23.900	9.200	1.00	0.00	C
ATOM	1094	CZ	XXX	A	138	9.000	23.500	8.100	1.00	0.00	C

Qual o aminoácido?

ATOM	1084	N	PHE A 138	3.800	20.200	9.600	1.
ATOM	1085	CA	PHE A 138	4.500	21.400	9.300	1.
ATOM	1086	C	PHE A 138	4.200	21.700	7.800	1.
ATOM	1087	O	PHE A 138	3.900	22.800	7.400	1.
ATOM	1088	CB	PHE A 138	5.900	21.100	9.900	1.
ATOM	1089	CG	PHE A 138	7.000	21.900	9.300	1.
ATOM	1090	CD1	PHE A 138	7.500	21.600	8.100	1.
ATOM	1091	CD2	PHE A 138	7.400	23.100	9.900	1.
ATOM	1092	CE1	PHE A 138	8.600	22.300	7.500	1.
ATOM	1093	CE2	PHE A 138	8.400	23.900	9.200	1.
ATOM	1094	CZ	PHE A 138	9.000	23.500	8.100	1.



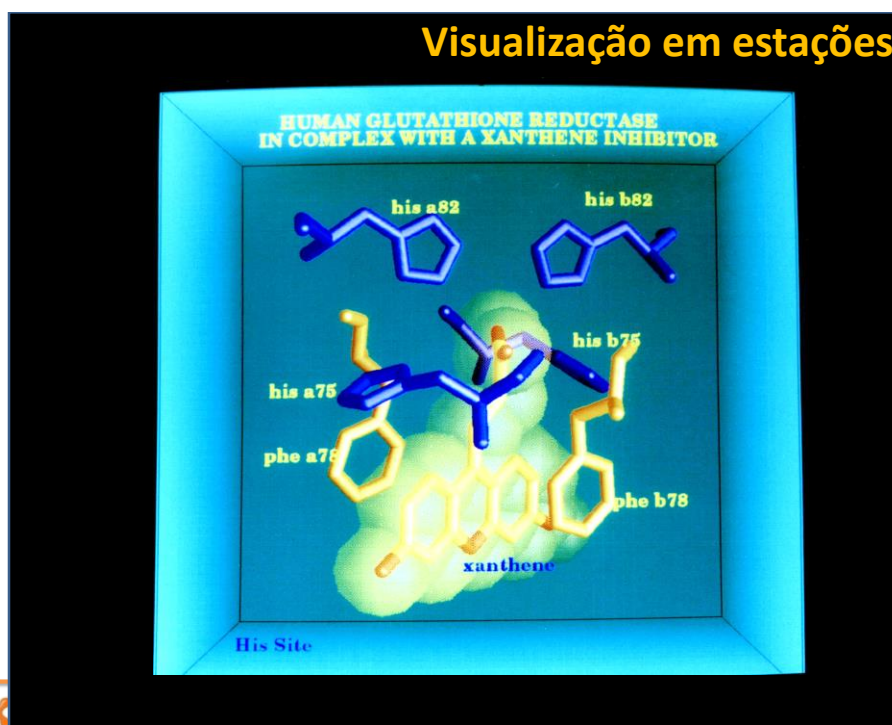
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2 C5* 19.8040 33.4500 23.8900 C.3 1 C1 0.0000
3 C4* 20.7420 32.2660 23.7840 C.3 1 C1 0.0000
4 O4* 20.1040 31.1230 24.3850 O.3 1 C1 0.0000
5 C3* 21.1090 31.8590 22.3660 C.3 1 C1 0.0000
6 O3* 22.4850 31.5070 22.2970 O.3 1 C1 0.0000
7 C2* 20.2030 30.6900 22.0780 C.3 1 C1 0.0000
8 C1* 20.0650 30.0510 23.4480 C.3 1 C1 0.0000
9 N1 18.8070 29.3710 23.7540 N.am 1 C1 0.0000
10 C2 18.8970 28.1030 24.3540 C.2 1 C1 0.0000
11 O2 20.0330 27.6540 24.5710 O.2 1 C1 0.0000
12 N3 17.7580 27.4450 24.6530 N.2 1 C1 0.0000
13 C4 16.5680 28.0020 24.3830 C.2 1 C1 0.0000
14 N4 15.4730 27.3020 24.7020 N.p13 1 C1 0.0000
15 C5 16.4490 29.2900 23.7790 C.2 1 C1 0.0000
16 C6 17.5920 29.9240 23.4900 C.2 1 C1 0.0000
17 H5* 19.9800 35.3860 23.7600 H 1 C1 0.0000
18 H5*1 18.9360 33.3750 23.1940 H 1 C1 0.0000
19 H5*2 19.4030 33.4720 24.9300 H 1 C1 0.0000
20 H4* 21.6770 32.4950 24.3470 H 1 C1 0.0000
21 H3* 20.8920 32.6940 21.6600 H 1 C1 0.0000
22 H2*1 19.2400 30.9510 21.5800 H 1 C1 0.0000
23 H2*2 20.7530 29.9790 21.4180 H 1 C1 0.0000
24 H1* 20.9210 29.3600 23.6300 H 1 C1 0.0000
25 H41 15.5580 26.3820 25.1340 H 1 C1 0.0000
26 H42 14.5490 27.6910 24.5130 H 1 C1 0.0000
27 H5 15.4660 29.7400 23.5620 H 1 C1 0.0000
28 H6 17.5480 30.9230 23.0250 H 1 C1 0.0000
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DNA

1vzk: arquivo texto de coordenadas

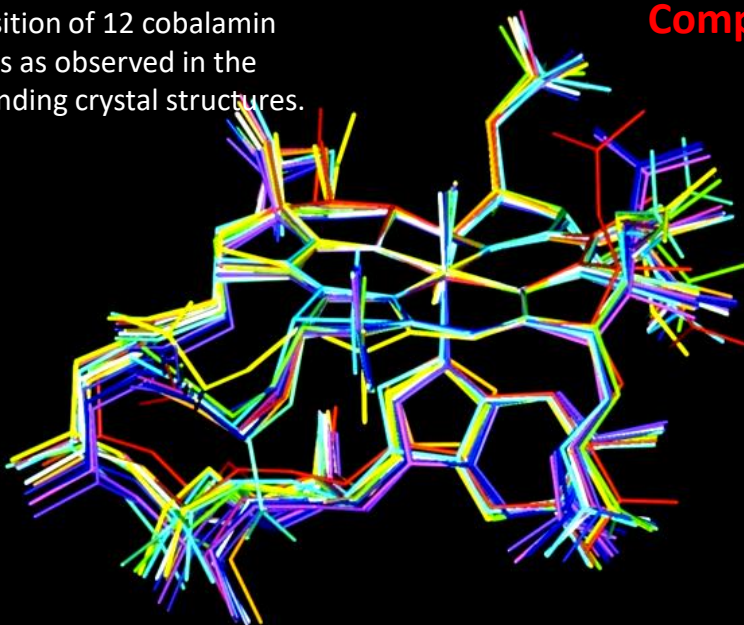
ATOM	39	P	DC	A	3	25.585	25.276	18.534	1.00	30.62	P
ATOM	40	OP1	DC	A	3	27.060	25.288	18.677	1.00	37.04	O
ATOM	41	OP2	DC	A	3	24.889	25.966	17.423	1.00	33.38	O
ATOM	42	O5'	DC	A	3	25.081	23.755	18.538	1.00	28.67	O
ATOM	43	C5'	DC	A	3	25.162	22.978	19.736	1.00	23.94	C
ATOM	44	C4'	DC	A	3	24.072	21.936	19.787	1.00	23.50	C
ATOM	45	O4'	DC	A	3	22.800	22.540	20.100	1.00	23.10	O
ATOM	46	C3'	DC	A	3	23.820	21.202	18.477	1.00	25.60	C
ATOM	47	O3'	DC	A	3	24.686	20.071	18.379	1.00	32.06	O
ATOM	48	C2'	DC	A	3	22.367	20.817	18.534	1.00	26.01	C
ATOM	49	C1'	DC	A	3	21.762	21.715	19.594	1.00	24.49	C
ATOM	50	N1	DC	A	3	20.727	22.632	19.093	1.00	22.43	N
ATOM	51	C2	DC	A	3	19.390	22.374	19.389	1.00	22.08	C
ATOM	52	O2	DC	A	3	19.100	21.374	20.073	1.00	23.13	O
ATOM	53	N3	DC	A	3	18.457	23.230	18.918	1.00	24.96	N
ATOM	54	C4	DC	A	3	18.829	24.290	18.187	1.00	30.21	C
ATOM	55	N4	DC	A	3	17.888	25.125	17.730	1.00	34.79	N
ATOM	56	C5	DC	A	3	20.191	24.574	17.870	1.00	27.52	C
ATOM	57	C6	DC	A	3	21.097	23.716	18.346	1.00	26.15	C

Visualização em estações gráficas

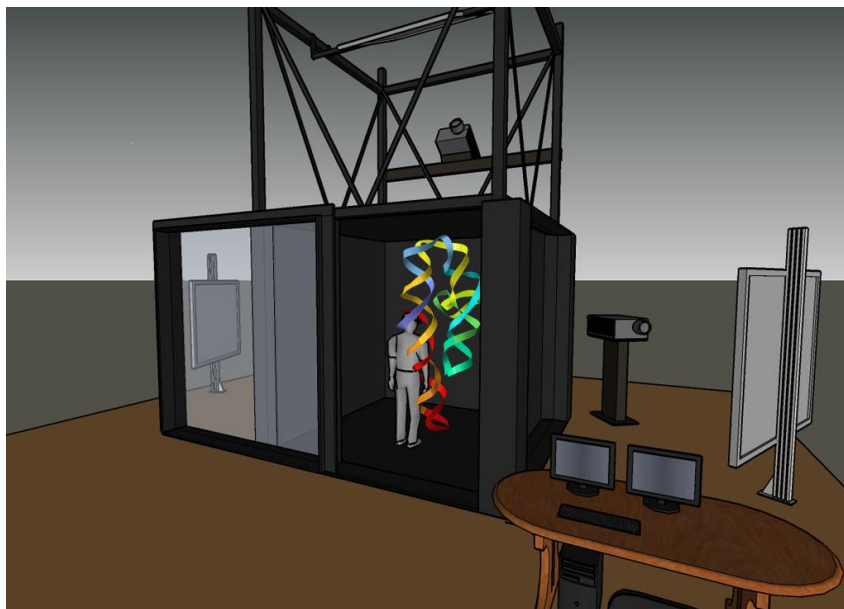


Superposition of 12 cobalamin molecules as observed in the corresponding crystal structures.

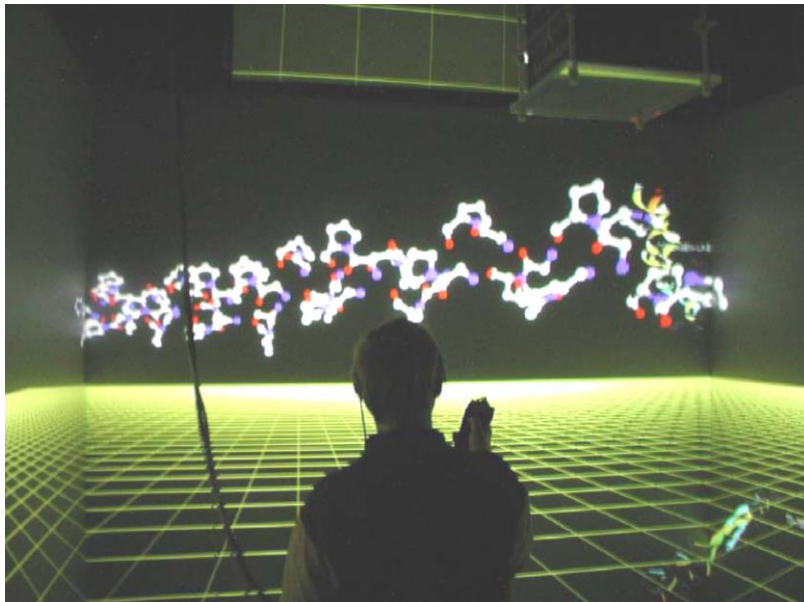
Comparação de Estruturas



Salas de visualização



Salas de visualização



Bioinformática I

Julio Zukerman
Ignez Caracelli

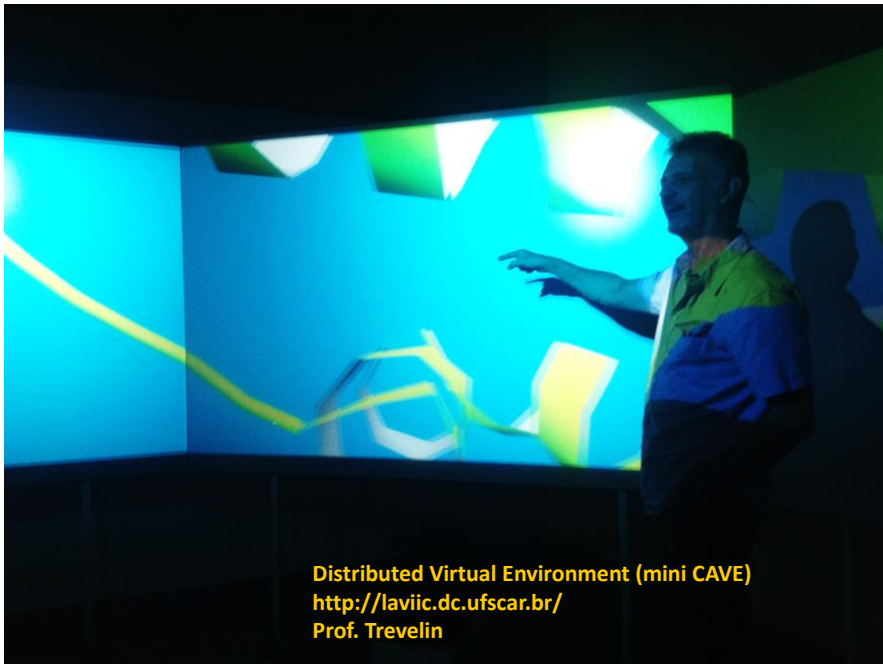
Salas de visualização



Bioinformática I

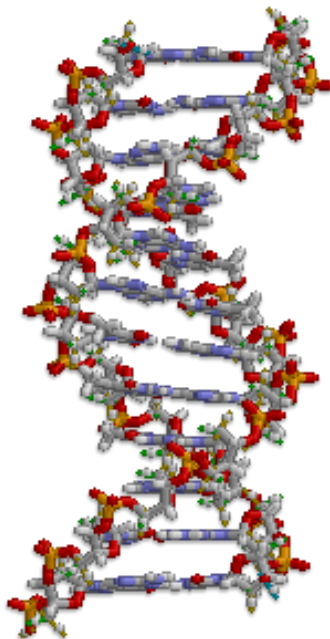
Julio Zukerman
Ignez Caracelli

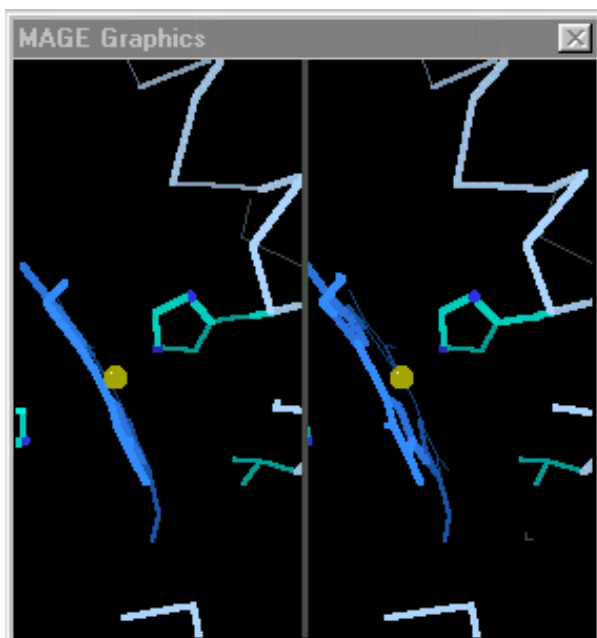
Salas de visualização



Distributed Virtual Environment (mini CAVE)
<http://laviic.dc.ufscar.br/>
 Prof. Trevelin

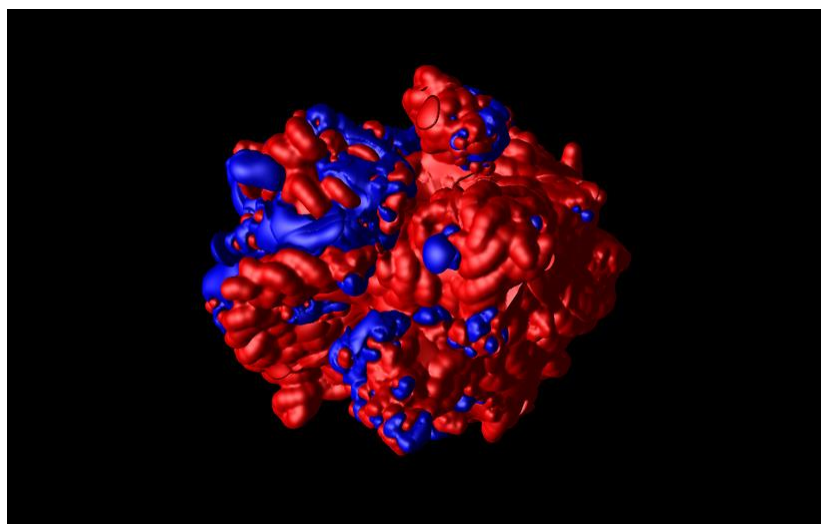
Movimento



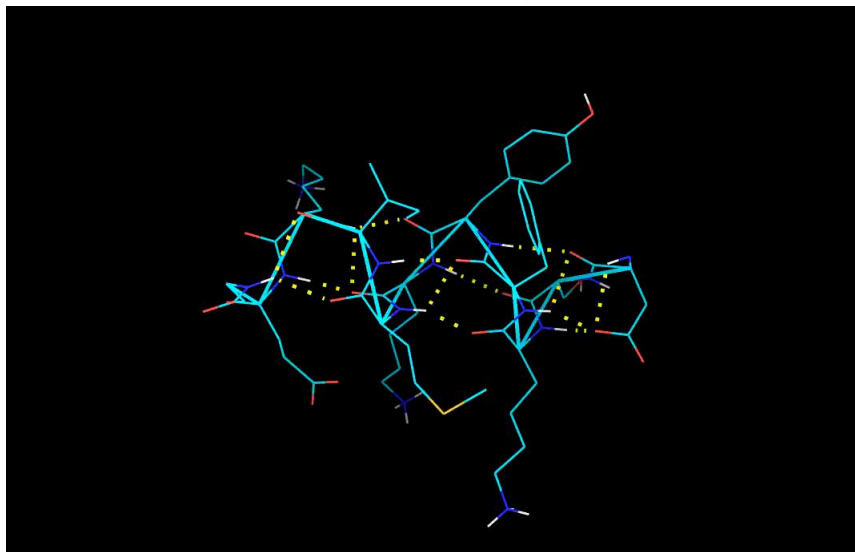


Visualização de dados dependente do tempo

Visualização de dados dependente do tempo



Visualização de dados dependente do tempo



Visualização de dados dependente do tempo

THEORETICAL AND COMPUTATIONAL BIOPHYSICS GROUP

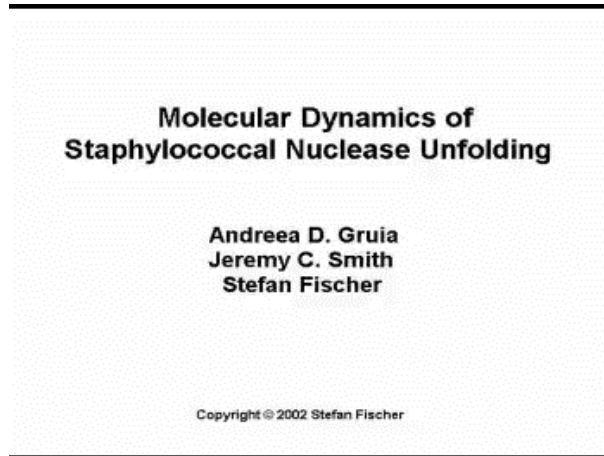
NIH Center for Macromolecular Modeling and Bioinformatics
www.ks.uiuc.edu

presents

Six Microseconds of Protein Folding

<https://www.youtube.com/watch?v=sD6vyfTtE4U>

Visualização de dados dependente do tempo



Gruia, Fischer and Smith, (2003). Proteins, 50: 507–515. doi: 10.1002/prot.10312

<http://spider.iwr.uni-heidelberg.de/fischer/>