

Introdução a Bioquímica: Biomoléculas

Aula 1

Introdução ao Curso Representação das Moléculas Aminoácidos

Ignéz Caracelli



Julio Zukerman Schpector



São Carlos, 9 de agosto de 2010.

- Seminário em grupo (**S**)
 - alunos de **mestrado**: 1 seminário
 - alunos de **doutorado**: 2 seminários ou 1 mais elaborado
- Prova individual (**P**)
- Atividades em grupo e individuais (**A**)
- Média (**M**)

$$M = 0,4 S + 0,6 P + A$$

Avaliação - Conceitos

$$M = 0,4 S + 0,6 P + A$$

$6,5 \leq M \leq 7,8 \rightarrow$ conceito C

$7,9 \leq M \leq 8,9 \rightarrow$ conceito B

$9,0 \leq M \leq 11,0 \rightarrow$ conceito A

bit.603@gmail.com → envio e entrega de material e exercícios

(exercício1-fulano de tal)

nunca fazer reply

urgente:

ignez@ufscar.br

julio@power.ufscar.br

(disponibilizacao de material)

www.quimica.ufscar.br

ou

www.ignez.com → disciplinas → BIT603

- proteínas (enzimas, ...)
- ácidos nucleicos.
- lipídeos e membranas.
- açúcares.
- o que está acontecendo...

bioquímica



bioquímica
estrutural

- programas de visualização gráfica
- bancos de dados
- conhecimentos de química ↑
- conhecimentos de bioquímica ↑
- conhecimentos de interações, ligações ↑

Referência

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Julio Zukerman-Schpector

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Série

Apontamentos

Ignez Caracelli

Julio Zukerman-Schpector

INTRODUÇÃO À BIOFÍSICA ESTRUTURAL



Universidade Federal de São Carlos



EdUFSCar

Aluno: _____

Principais Referências

- Lehninger
- Voet & Voet
- Voet, Voet & Pratt



PDB

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



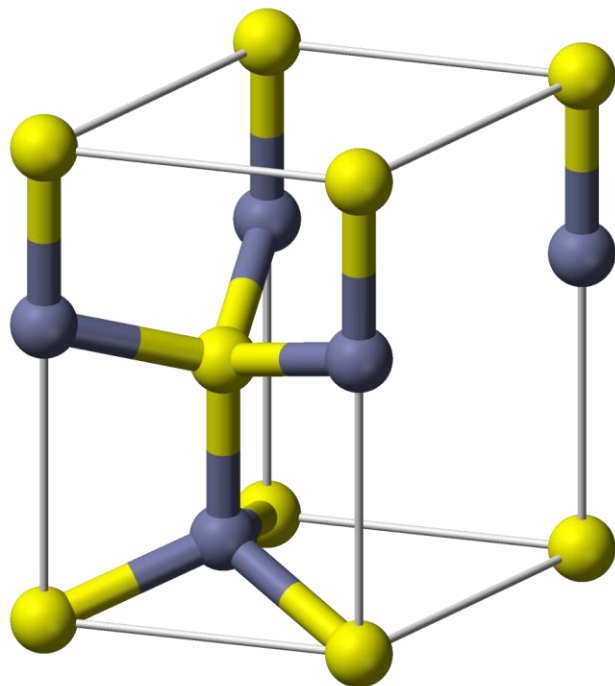
PDBSum

<http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/>



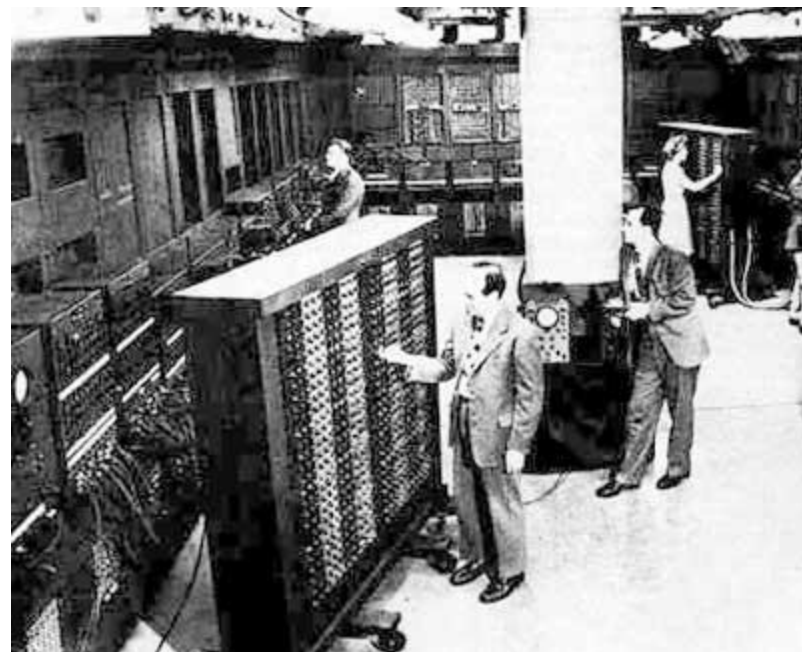
NDB

<http://ndbserver.rutgers.edu/NDB/structure-finder/index.html>

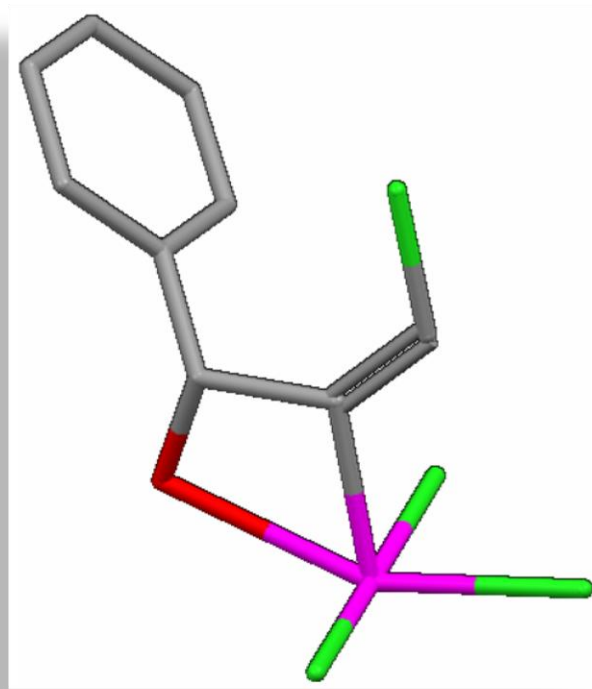
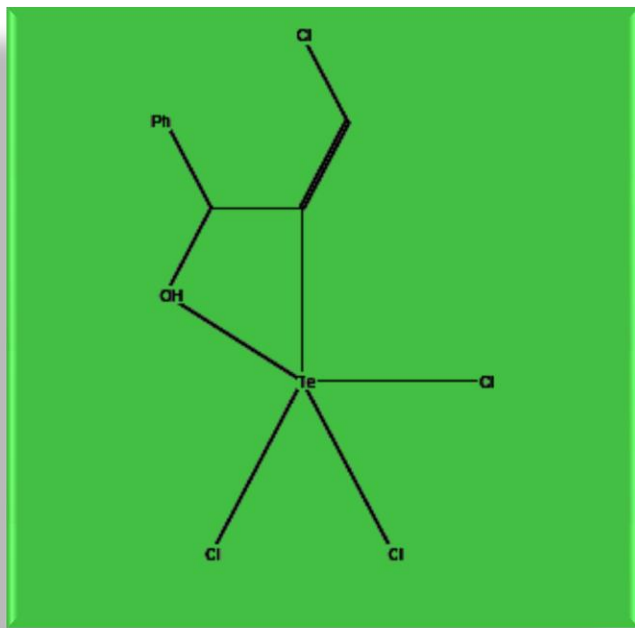


primeiras estruturas: 1912-1920

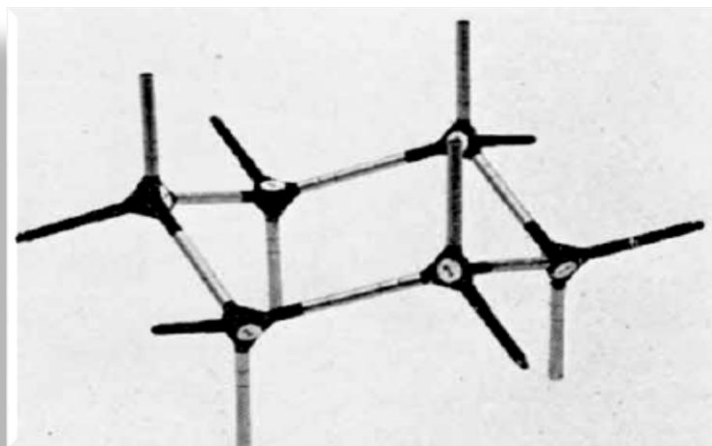
Wurtzite unit cell. The gray balls represent sulfur or selenium atoms, and yellow balls represent metal atoms.



primeiros computadores: 1946



Modelo de Dreiding

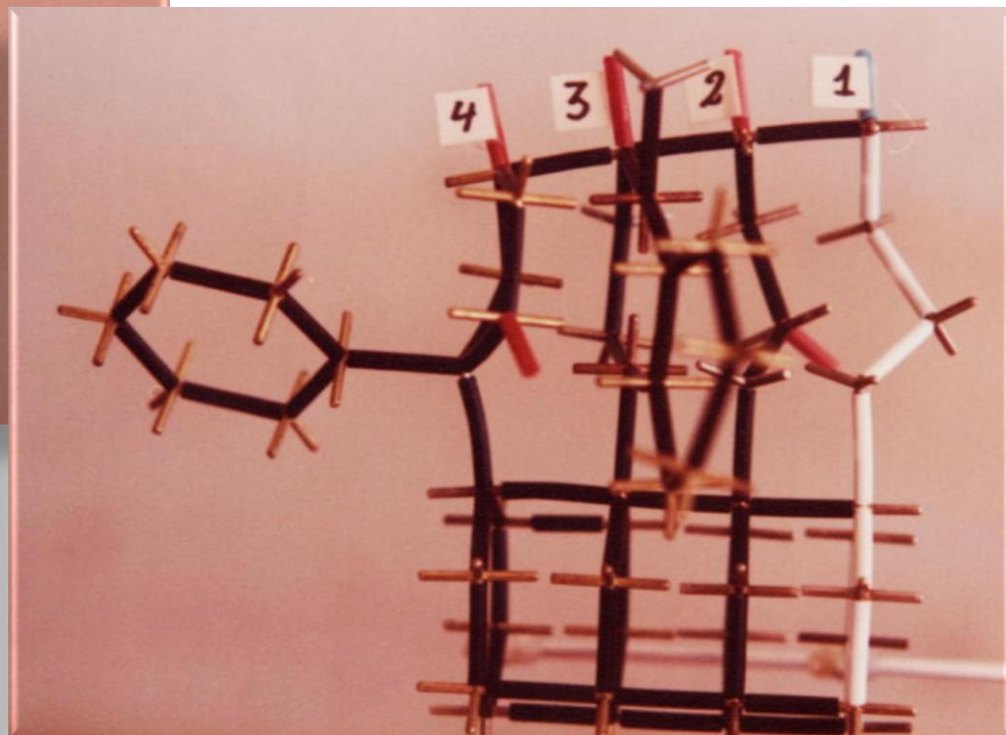
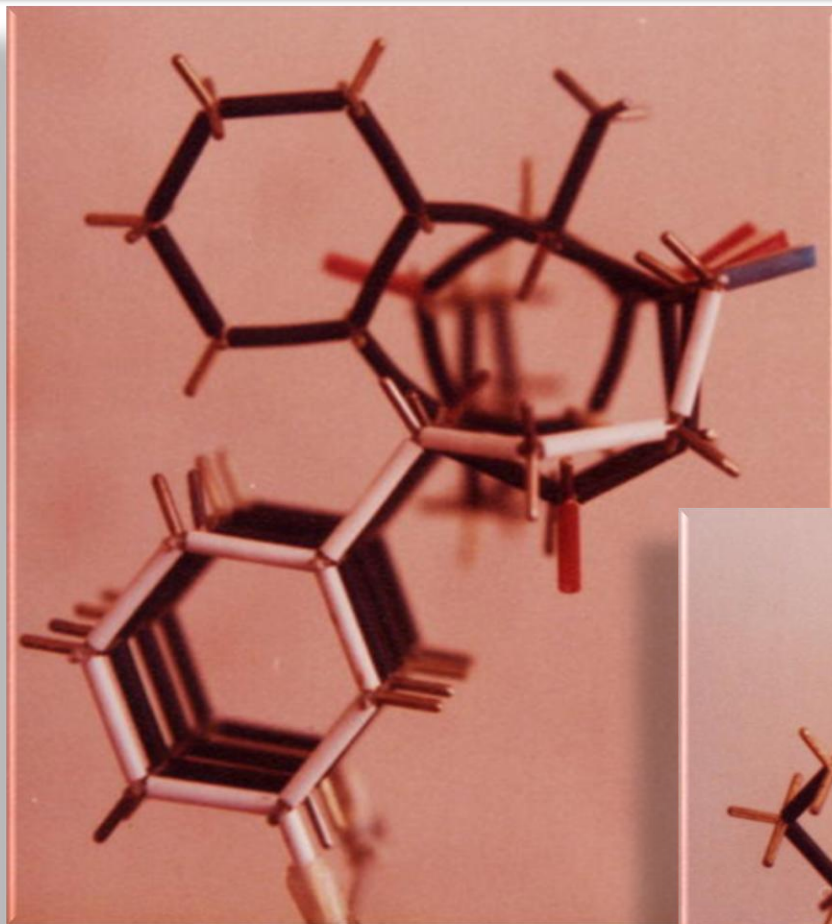


Modelo de Dreiding para o ciclohexano (Fieser, 1963)

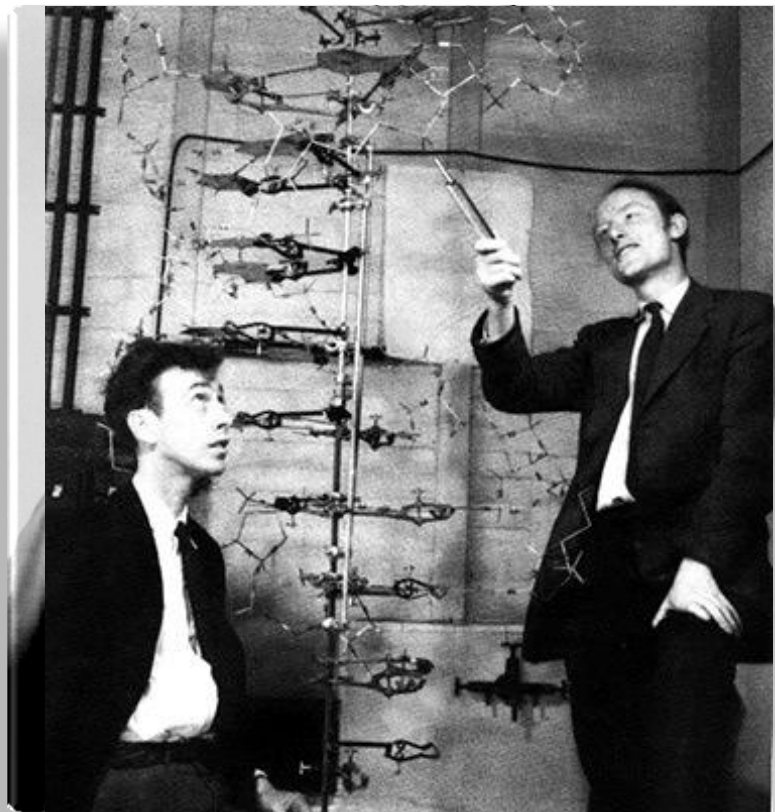
Os modelos de Dreiding, apresentados em 1958, foram um avanço na representação de moléculas, permitindo demonstrar a estereoquímica (o modo como os átomos de uma molécula estão arranjados no espaço tridimensional).

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.

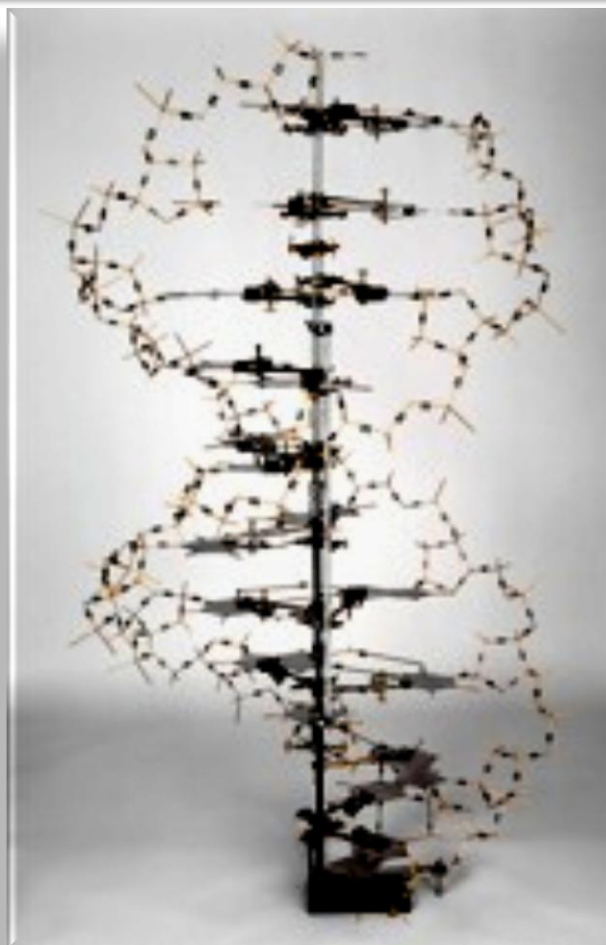
Modelo de Dreiding



Zukerman-Schpector,
Tese de Doutorado



Watson & Crick
2003



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



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

Forma das moléculas – Kendrew & Mioglobina

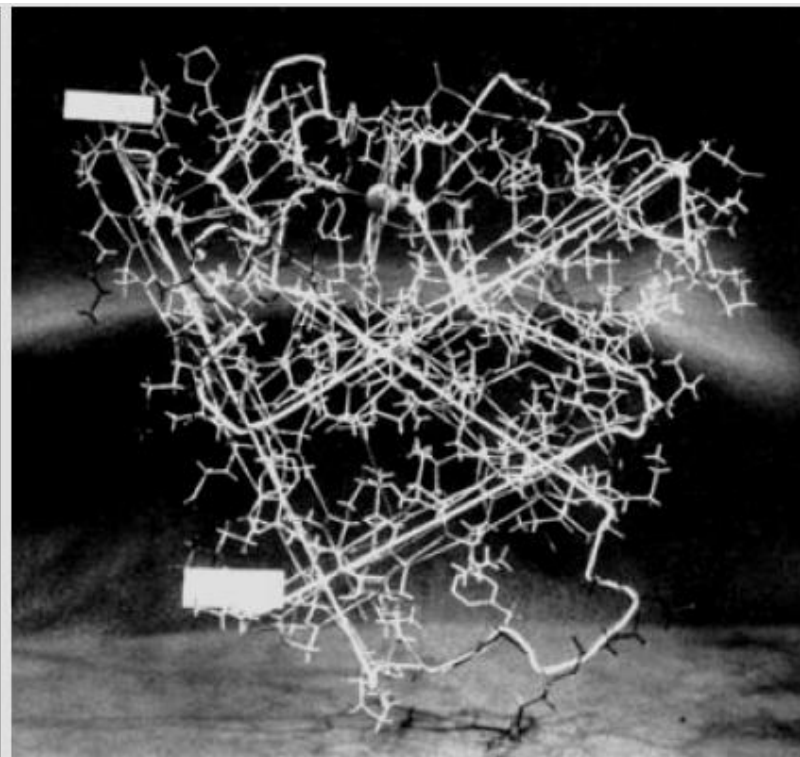


Kendrew & Mioglobina: Modelo de Dreiding

Bioquímica: BIT603 & BIT903

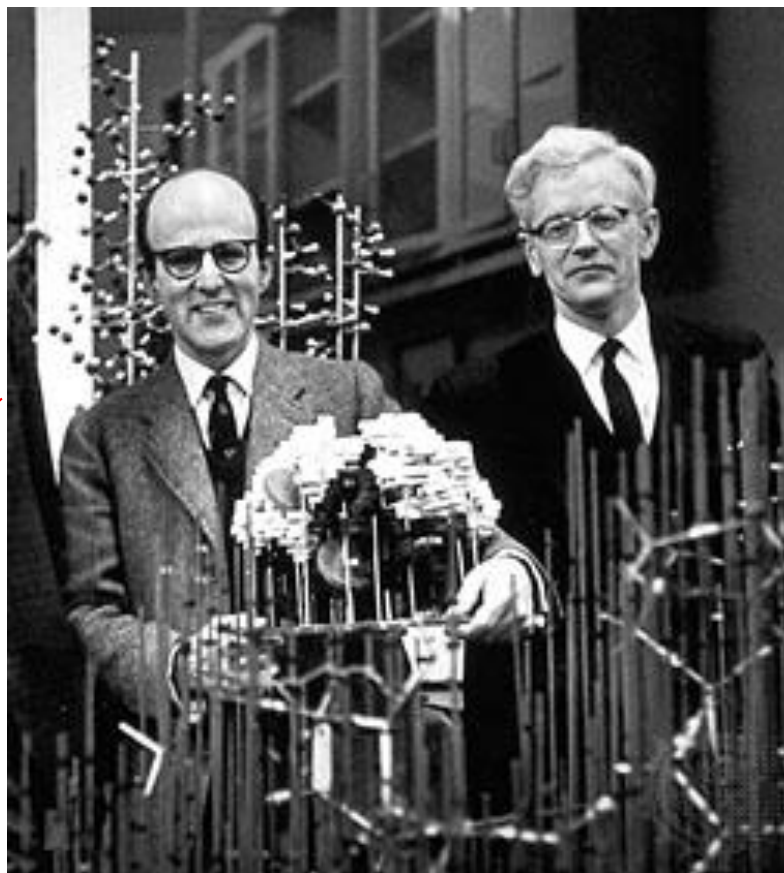


Kendrew & Mioglobina



1^{as} Estruturas 3D

Perutz ⇒
Hemoglobina



Kendrew ⇒
Mioglobina

Prêmio Nobel em 1962.

Estrutura 3D Hemoglobina: 1º modelo



Perutz

Bioquímica: BIT603 & BIT903

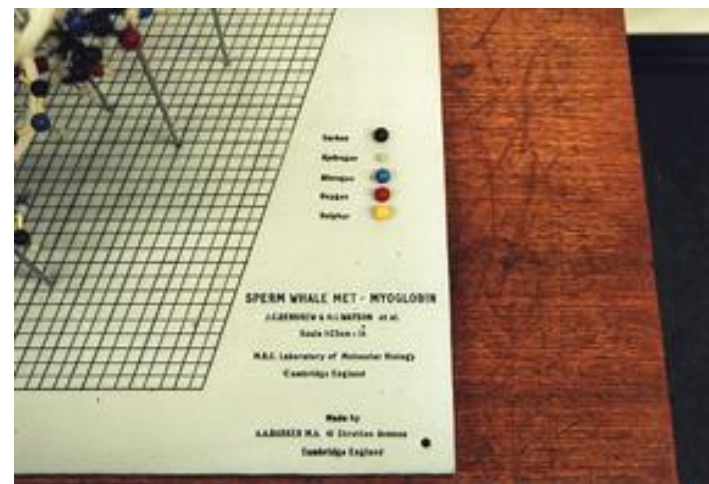
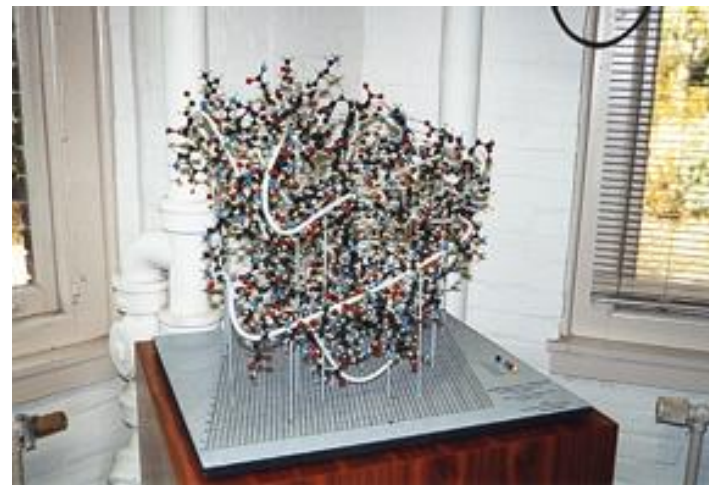
PPG biotec
conhecimento para a vida



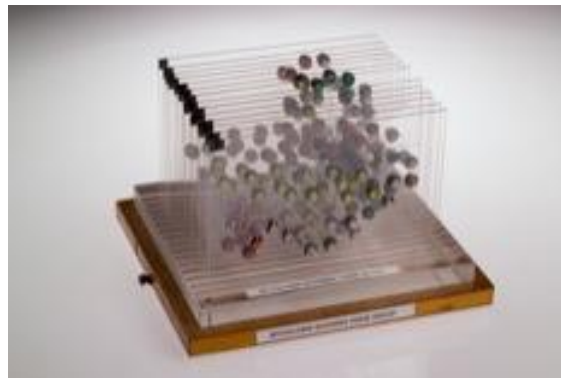
40
ANOS



Modelos: Representações Físicas



Modelos: Representações Físicas



Modelos: Representações Físicas & Arte

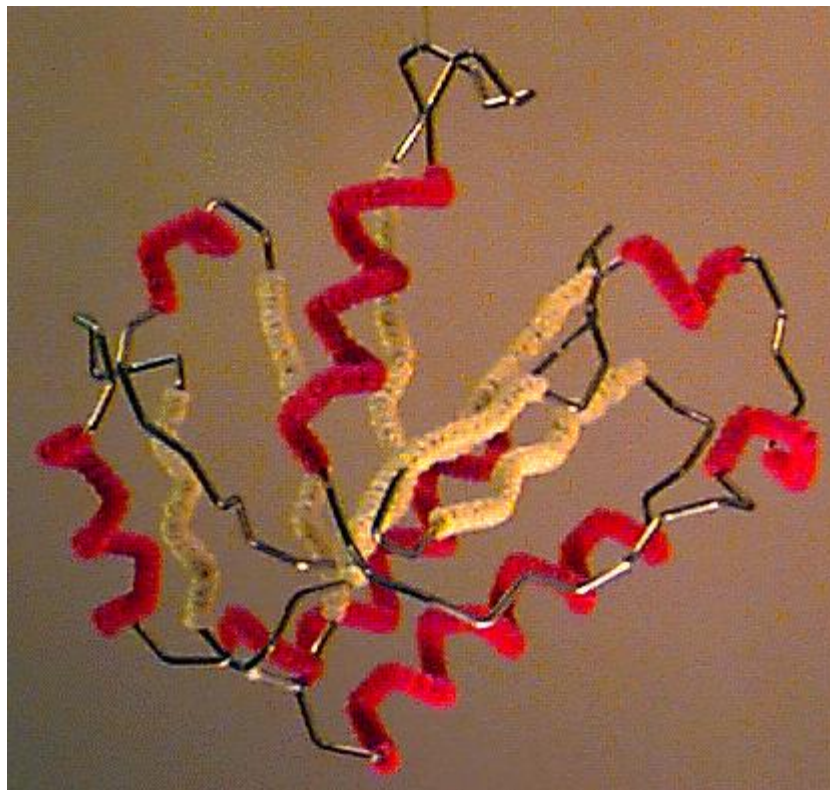


'DNA Double Helix'
Bronze by Robin Holliday



'The Trio and the Double Helix'
Francis Crick, James Watson and Rosalind
Franklin
By Professor Sir Roy Calne, 2003





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.

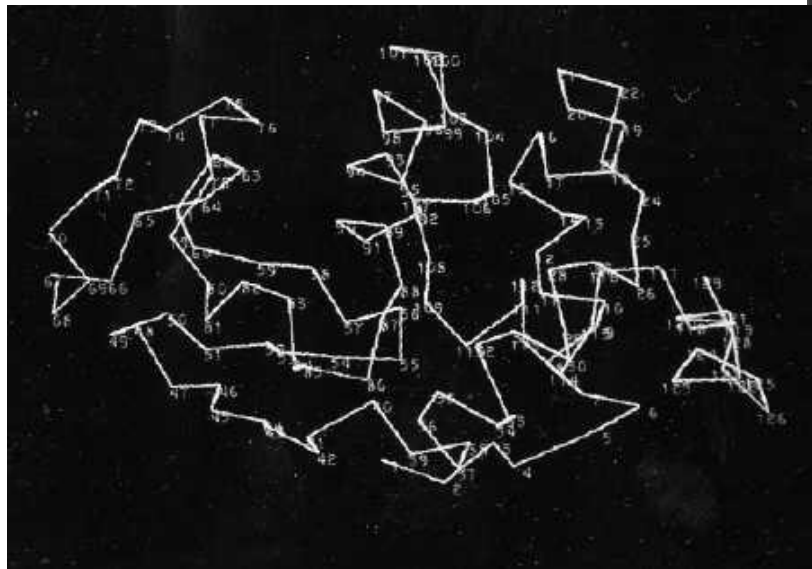
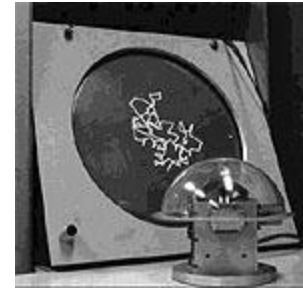
Modelos: Representações Físicas



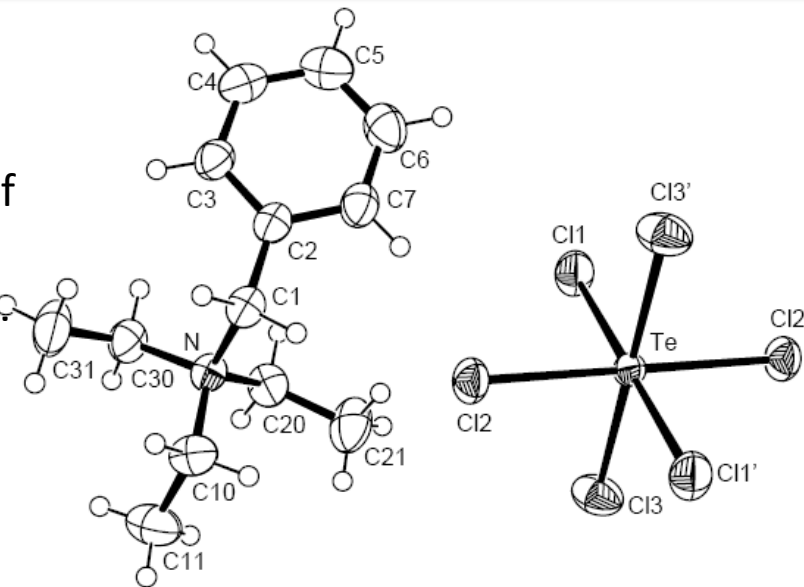
Sculpture of human neutrophil collagenase by [Byron Rubin](#) on permanent exhibition at the Smithsonian Institution, Washington DC USA. Image copyright © 2001, Byron H. Rubin, with permission. Height: 11 inches.

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.

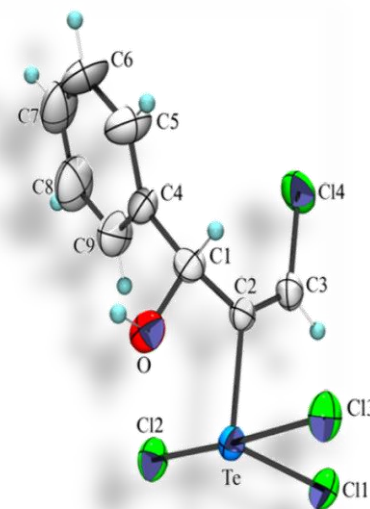


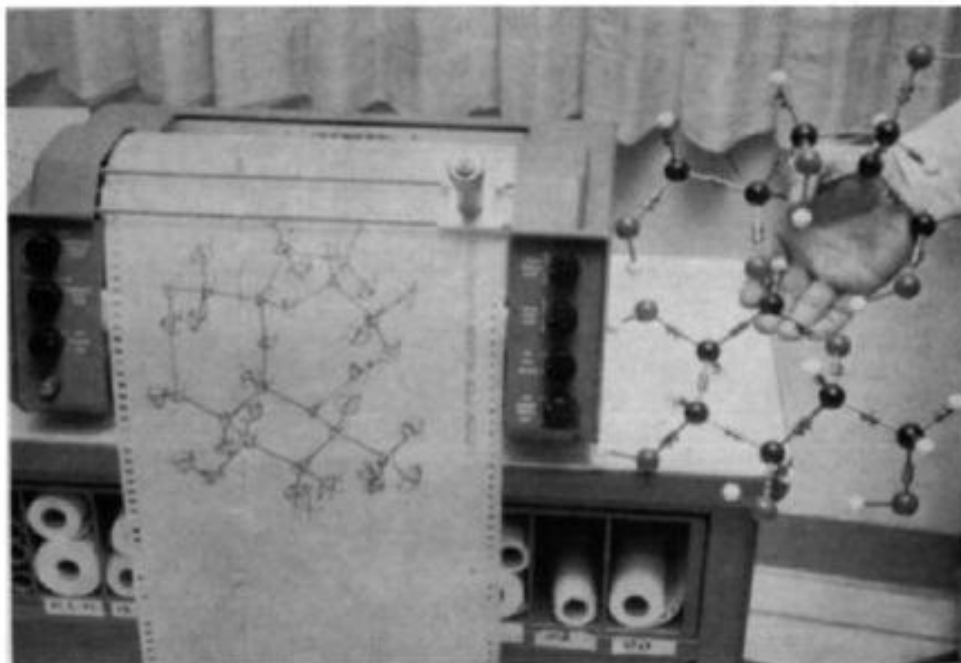
In 1965, Carroll K. Johnson, of Oak Ridge National Laboratory, released **ORTEP**, a program to produce stereoscopic drawings of molecular and crystal structures with a pen-plotter. See the [ORTEP](#) page for more details.



Z. Kristallogr. NCS **219** (2004)

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.



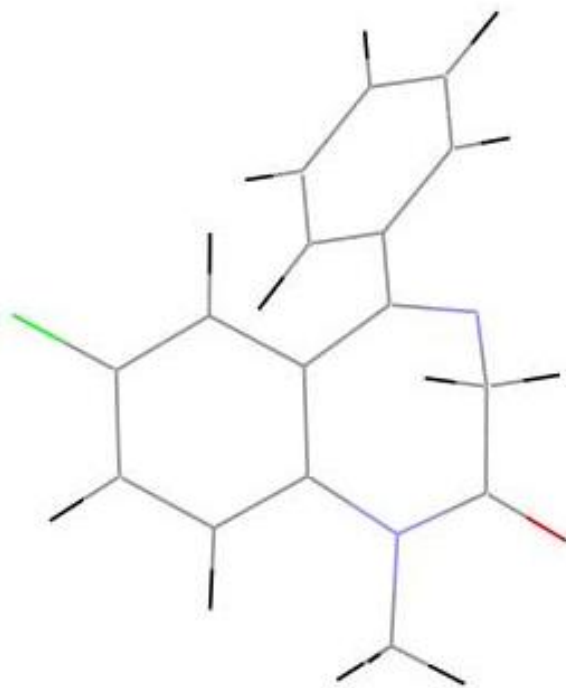


THIS CLOSEUP shows the CalComp X-Y plotter and a perspective line drawing it just produced (left). This computer-drawn illustration shows the molecular configurations and thermal-motion ellipsoids of common table sugar (sucrose). The stereo-mate to this illustration would be plotted next and the pair reduced photographically for stereoscopic (three dimensional) viewing. A conventional ball and stick three-dimensional model of the same material is held beside the plotter for comparison.

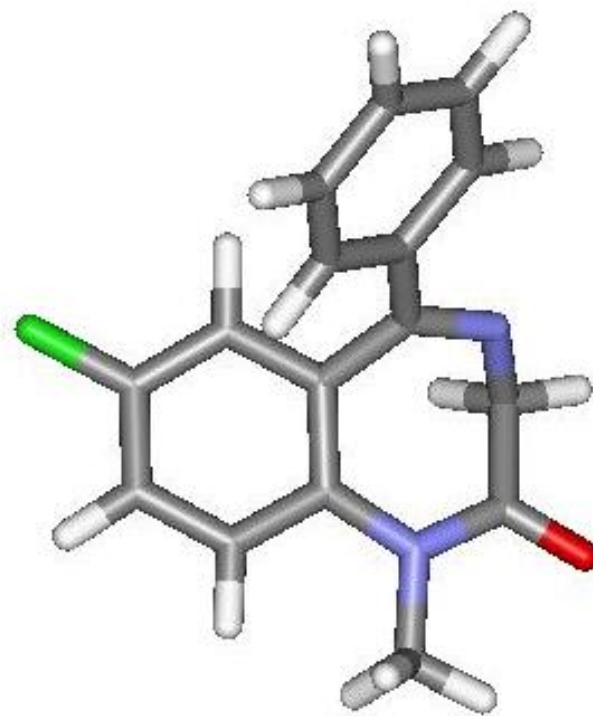
Graficamente

- 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

Modelo de varetas (line ou stick)

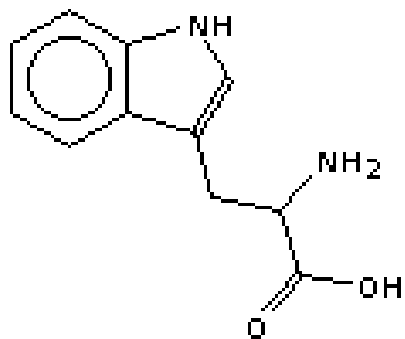


(line)



(stick)

Diferentes formas de representar moléculas



2D

Vantagens:

Mostra a estrutura completa
Fácil reconhecimento de padrões

Desvantagens:

Torna impossível a comparação espacial das estruturas



3D

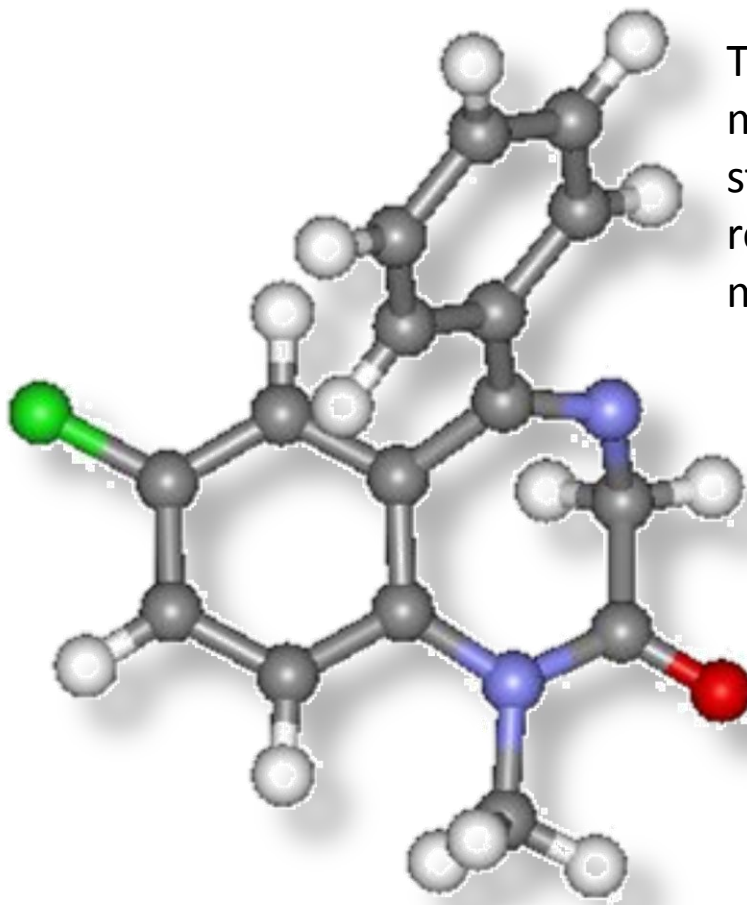
Vantagens:

Disponibiliza a informação estrutural
Entendimento de formas

Desvantagens:

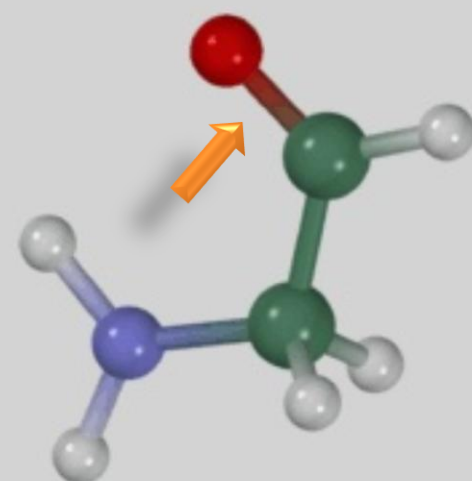
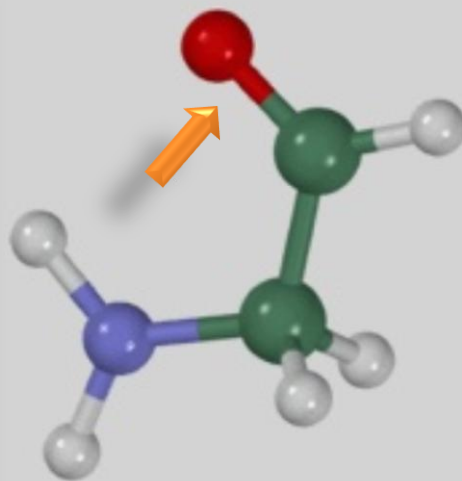
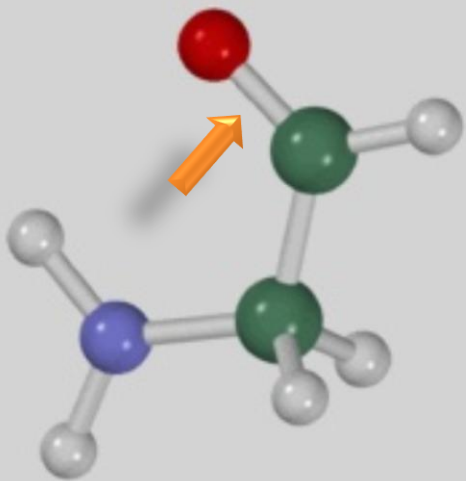
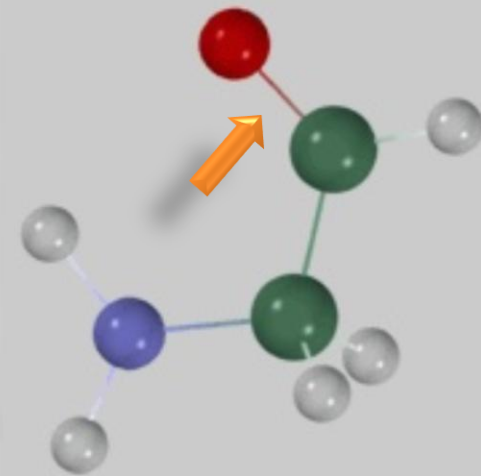
Limita a visualização de parte da estrutura
Dificulta comparações rápidas

Modelo de varetas e bolas *(ball and stick)*

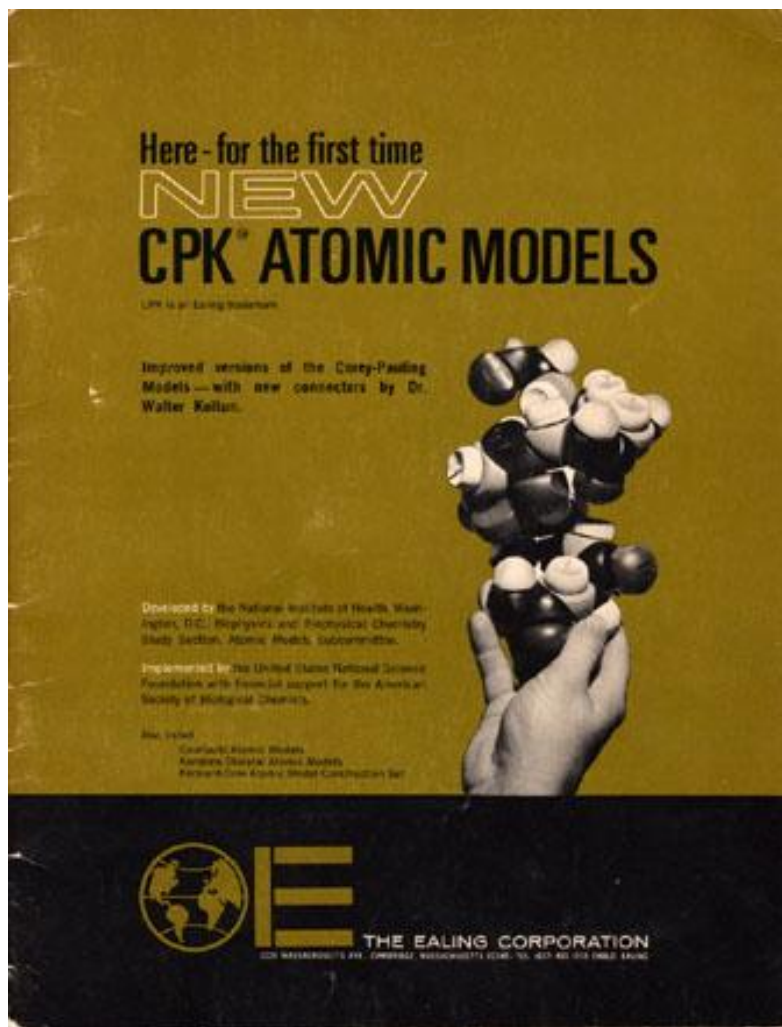


The original function of physical ball and stick models were the support of measurements of structure angles and bonds lengths, leaving the real structure representation to space filling models.

Modelo de varetas e bolas *(ball and stick)*



Modelos: Representações Físicas



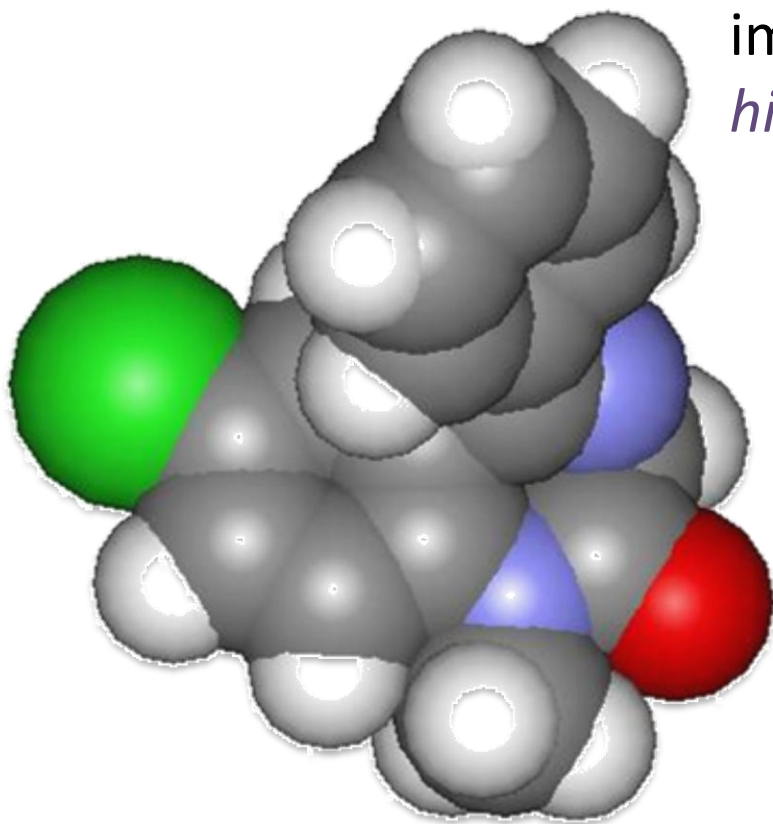
1966 Molecular Model Catalogue

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).

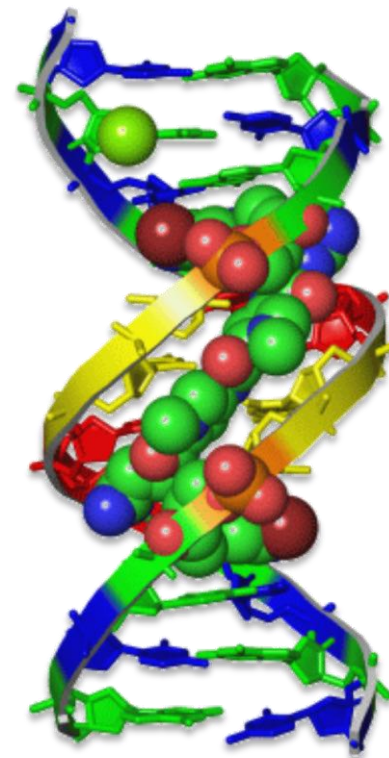
<http://www.umass.edu/molvis/francoeur/ealing/ealing.html>

Modelo CPK

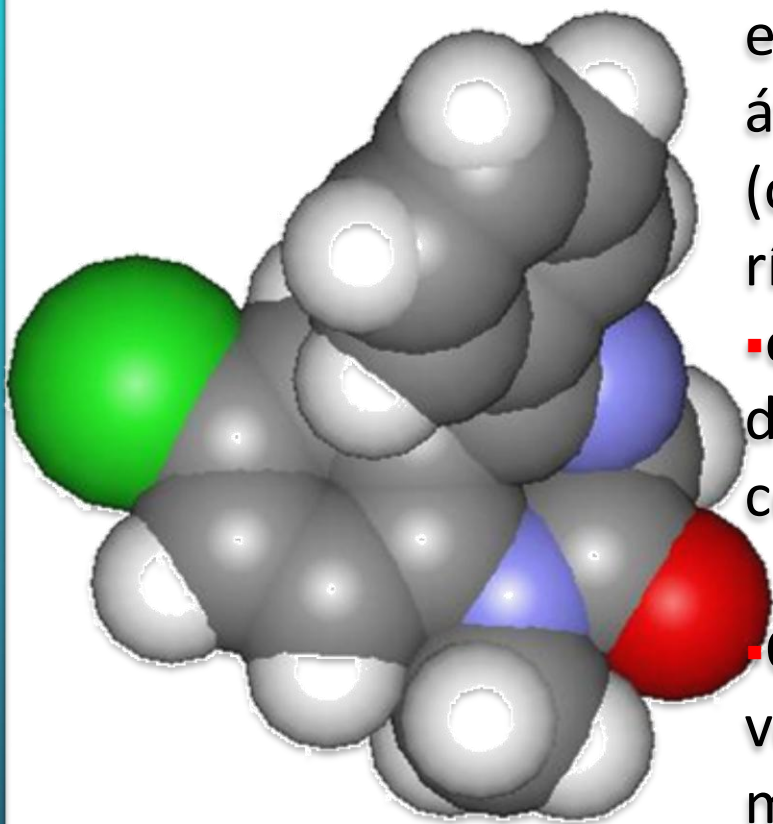
space filling



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



Modelo CPK *space filling*



- 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)
- os raios de **van der Waals** são determinados a partir de distâncias de contato de átomos não-ligados
- O raio de **van der Waals** define o volume e superfície de um átomo ou molécula

raio de van der Waals

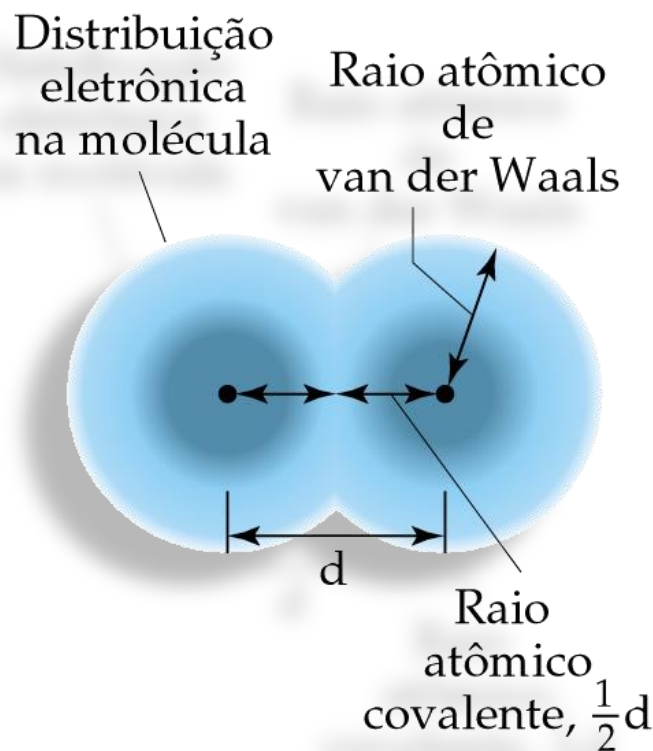
element	raio de van der Waals (Å)
H	1.20
C	1.70
N	1.55
O	1.52
F	1.47
P	1.80
S	1.80
Cl	1.89

- 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)
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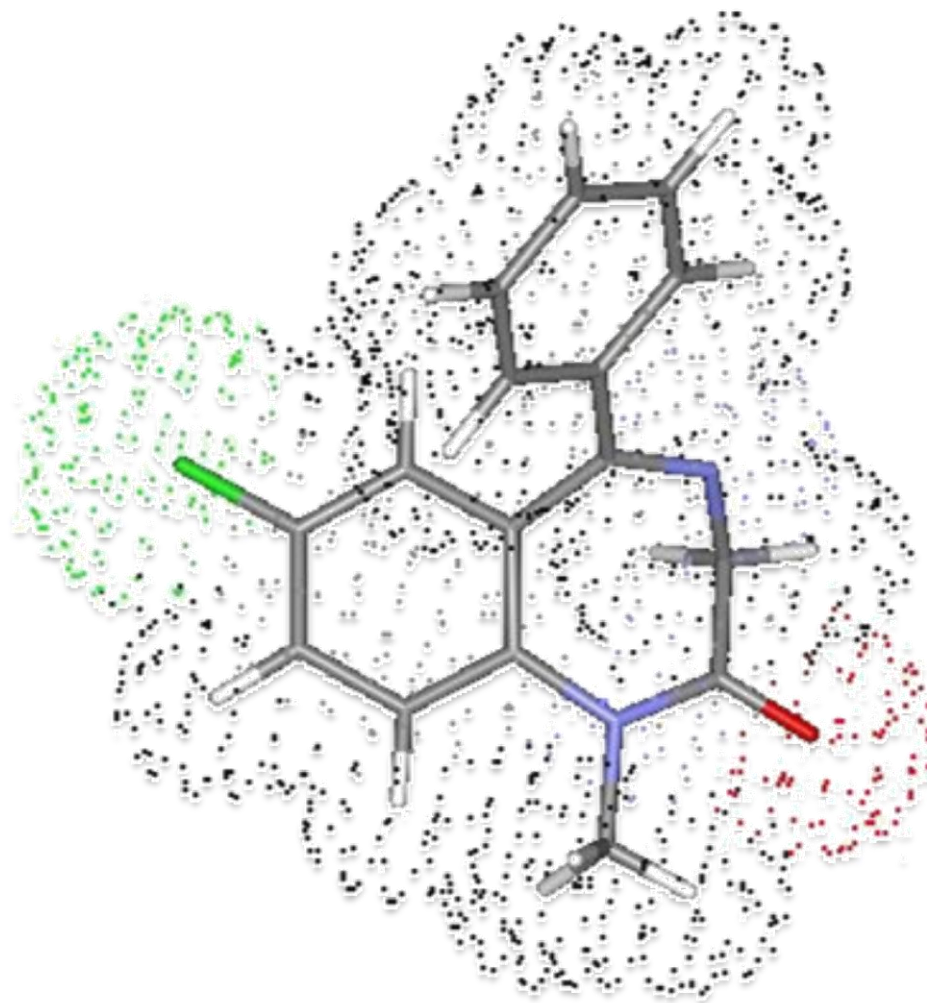
raio de van der Waals

element	raio de van der Waals (Å)
H	1.20
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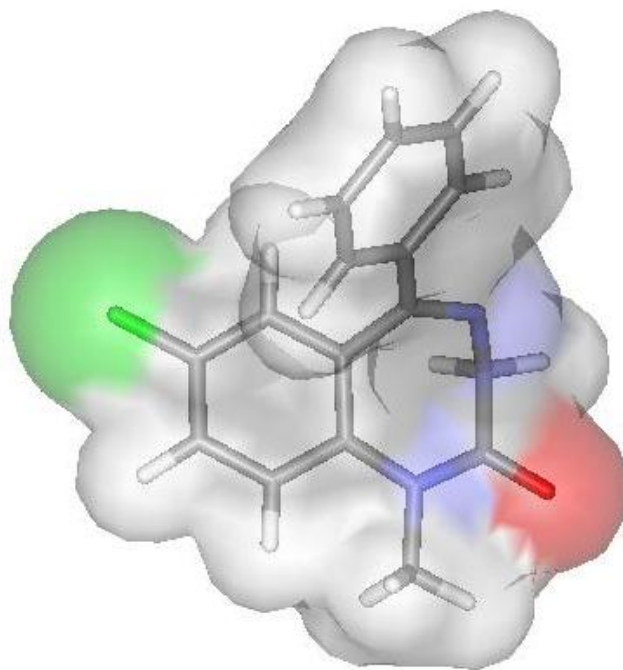
- A distância entre os dois núcleos é denominada distância de ligação.
- Se os dois átomos que formam a molécula são os mesmos, metade da distância de ligação é denominada raio covalente do átomo.



Superfície pontilhada

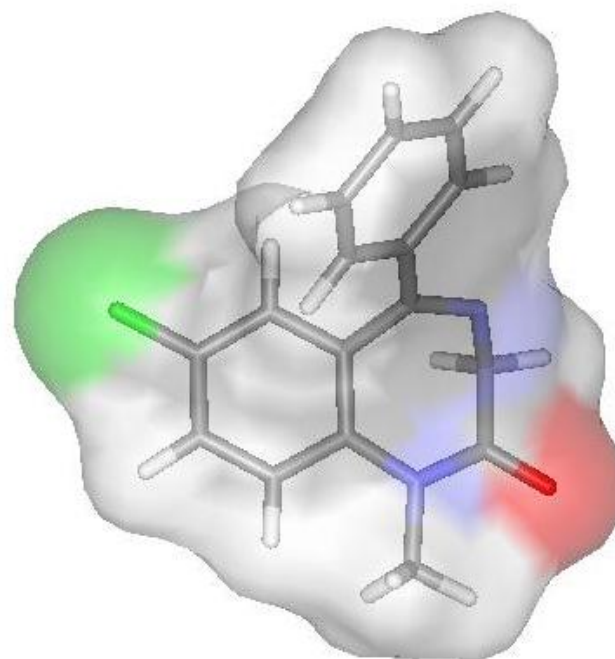


Superfícies transparentes



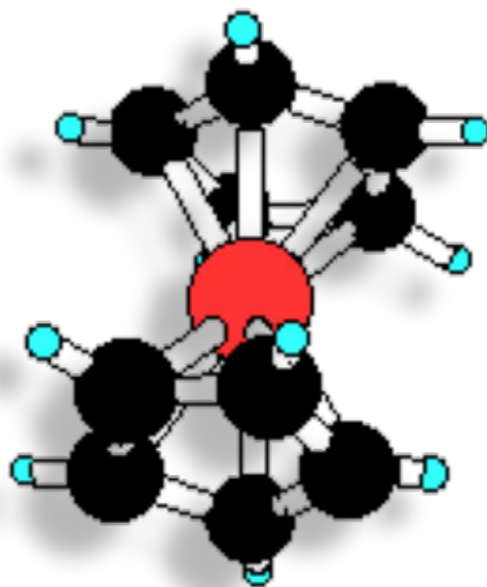
A

Superfície de van der Waals



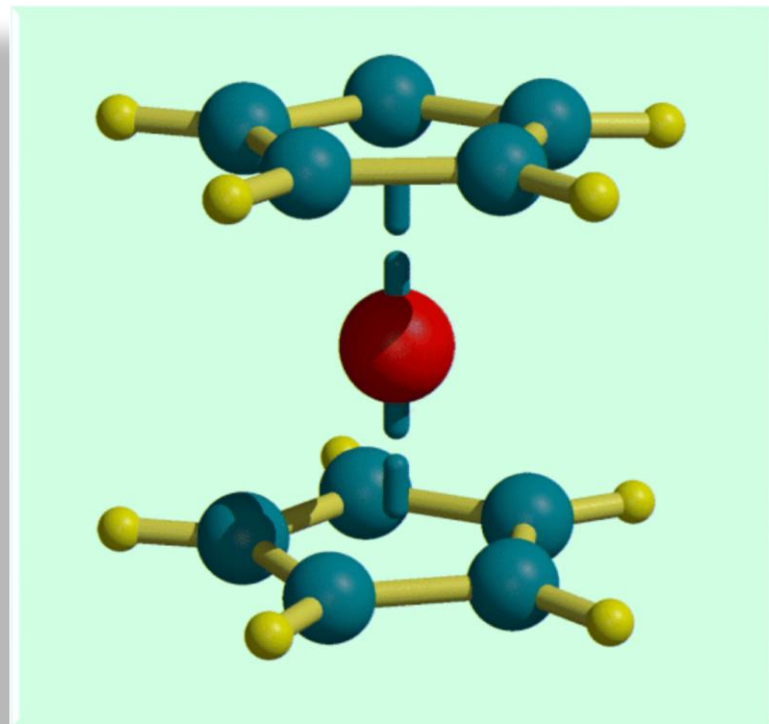
B

Superfície de Connolly (raio 1.4 Å)

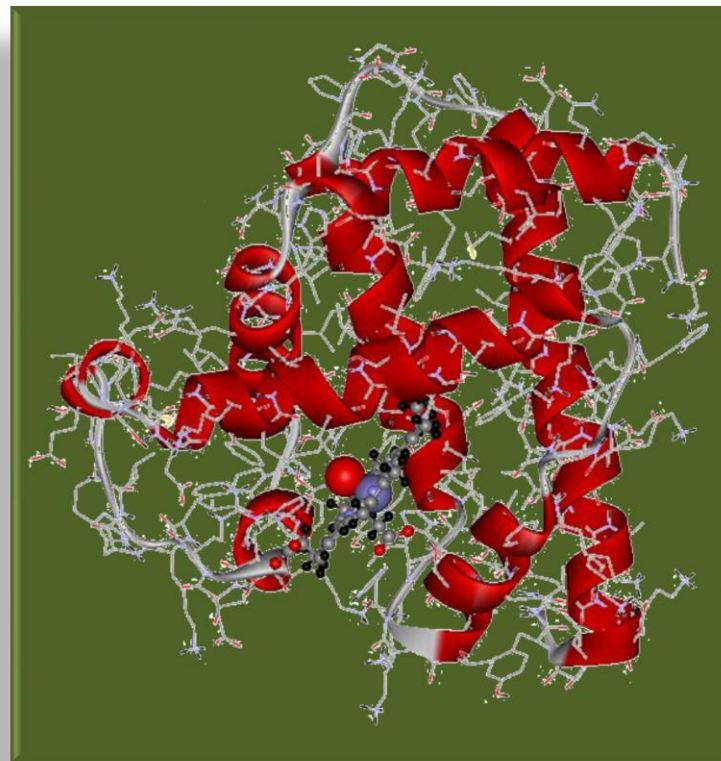
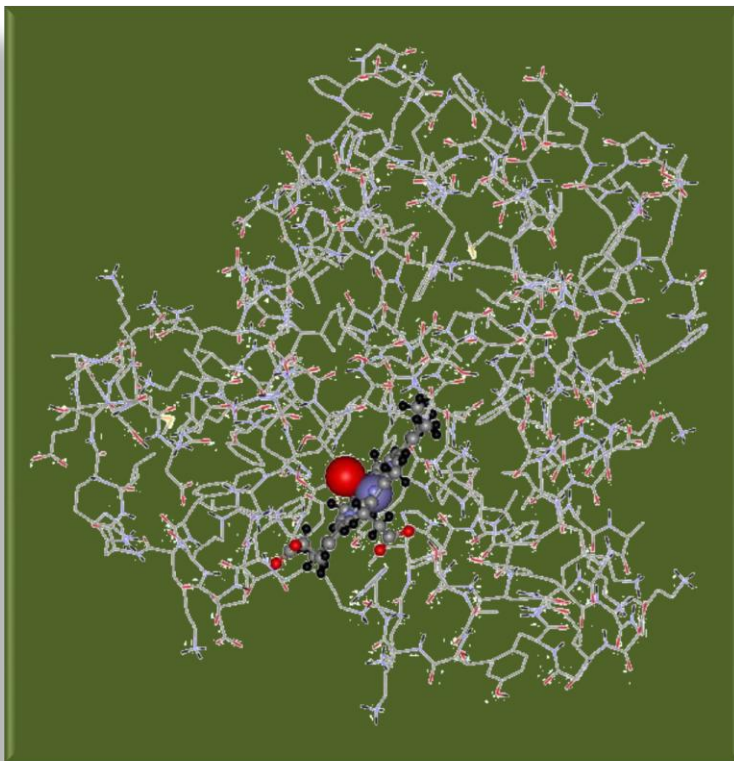


ferrocene, $\text{Fe}(\text{C}_5\text{H}_5)_2$

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.

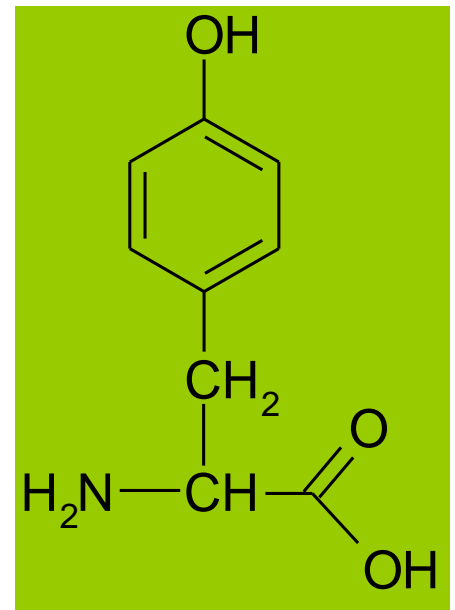


Modelo Ribbon

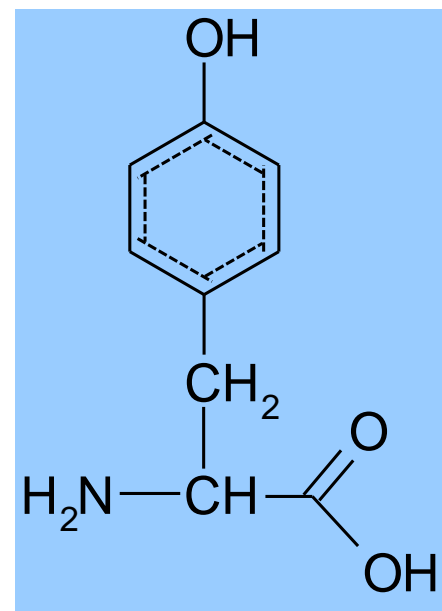


Representando uma estrutura química

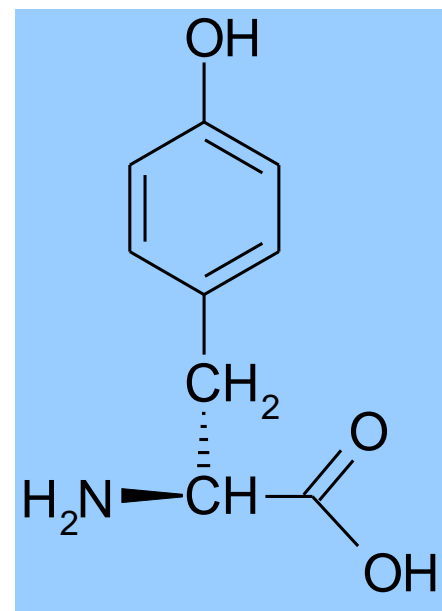
- Quanta informação queremos incluir?
 - átomos presentes
 - conexões entre átomos
 - tipos de ligações
 - configuração estereoquímica
 - cargas
 - isótopos
 - coordenadas-3D dos átomos



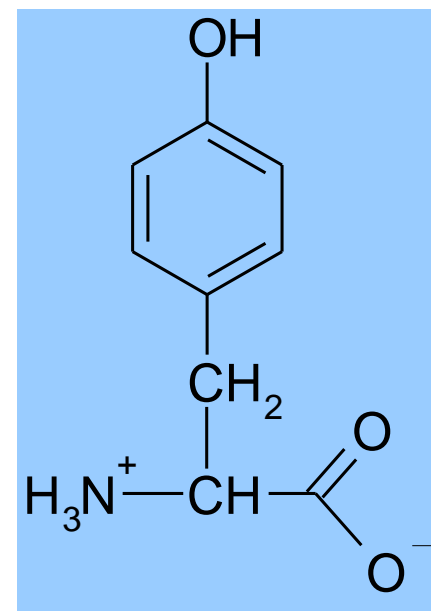
- Quanta informação queremos incluir?
 - átomos presentes
 - conexões entre átomos
 - tipos de ligações
(identificação do anel aromático)
 - configuração estereoquímica
 - cargas
 - isótopos
 - coordenadas-3D dos átomos



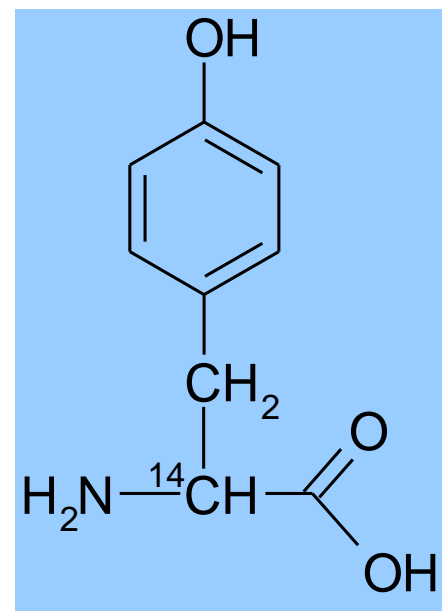
- Quanta informação queremos incluir?
 - átomos presentes
 - conexões entre átomos
 - tipos de ligações
 - **configuração estereoquímica**
 - cargas
 - isótopos
 - coordenadas-3D dos átomos



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



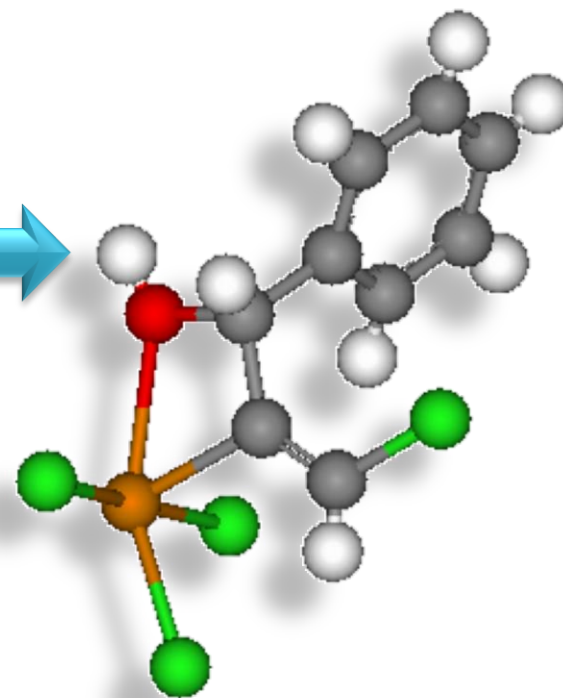
- Quanta informação queremos incluir?
 - átomos presentes
 - conexões entre átomos
 - tipos de ligações
 - configuração estereoquímica
 - cargas
 - isótopos
 - coordenadas-3D dos átomos



informações:
átomos, ligações,
etc.

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

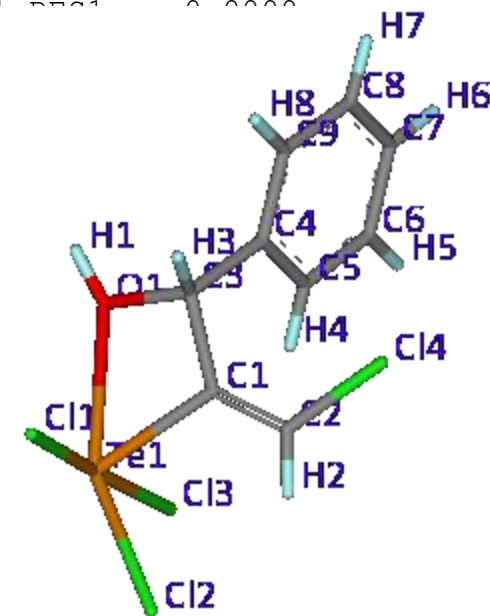
Jmol
Rasmol
DSVisualizer
O
PyMol
VMD
outros



Formato mol2

@<TRIPOS>ATOM

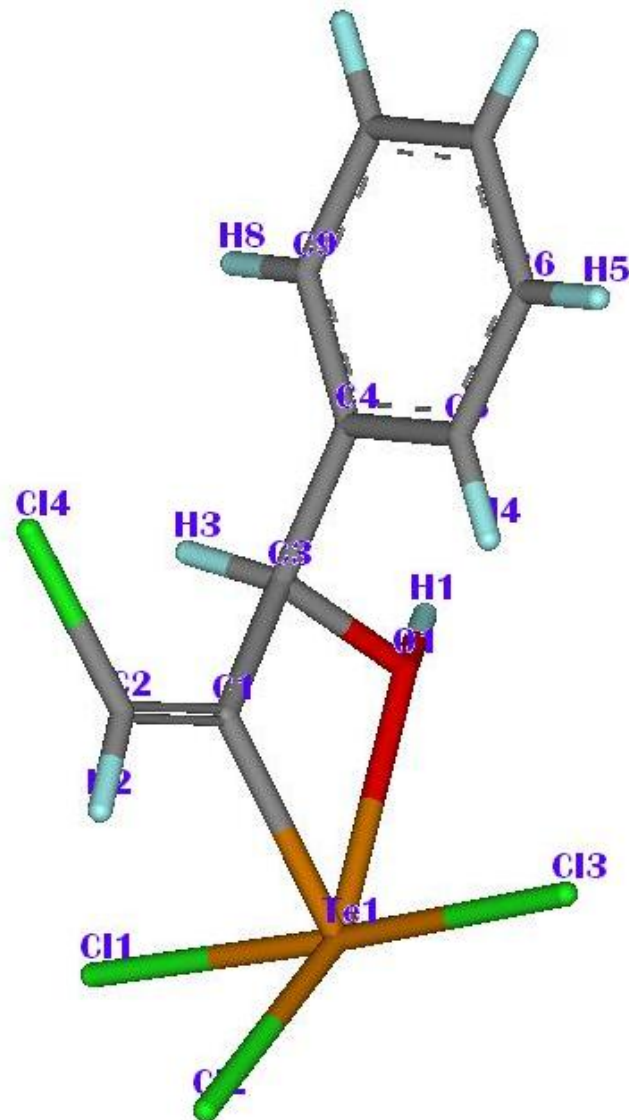
1	Te1	5.2600	0.8060	12.0298	Te	1	RES1	0.0000
2	C11	3.1368	2.1115	12.2513	C1	1	RES1	0.0000
3	C12	4.0776	-1.1283	12.5514	C1	1	RES1	0.0000
4	C13	7.3573	-0.5627	12.0078	C1	1	RES1	0.0000
5	C14	5.6229	1.0364	16.6760	C1			
6	O1	6.6012	2.8134	12.5780	O.3			
7	H1	6.7671	3.6286	12.4026	H			
8	C1	5.6881	1.3360	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

1	1	2	1
2	3	1	1
3	4	1	1
4	5	9	1
5	6	1	1
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
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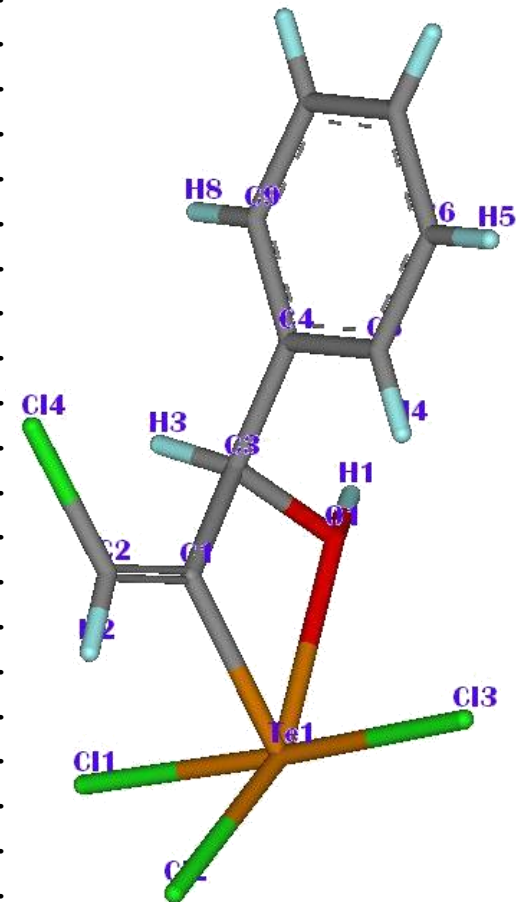


Formato pdb

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COMPND          UNNAMED
AUTHOR          GENERATED BY CONQUEST
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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
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ATOM           5  C14  UNK  0    1          5.623    1.036   16.         .
ATOM           6   O1  UNK  0    1          6.601    2.813   12.         .
ATOM           7   H1  UNK  0    1          6.767    3.629   12.         .
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ATOM           9   C2  UNK  0    1          5.308    0.576   15.         .
ATOM          10   H2  UNK  0    1          4.859   -0.221   14.         .
ATOM          11   C3  UNK  0    1          6.371    2.668   13.         .
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ATOM          14   C5  UNK  0    1          8.596    1.757   14.         .
ATOM          15   H4  UNK  0    1          8.429    0.990   14.         .
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ATOM          21   H7  UNK  0    1          9.293    4.761   16.         .
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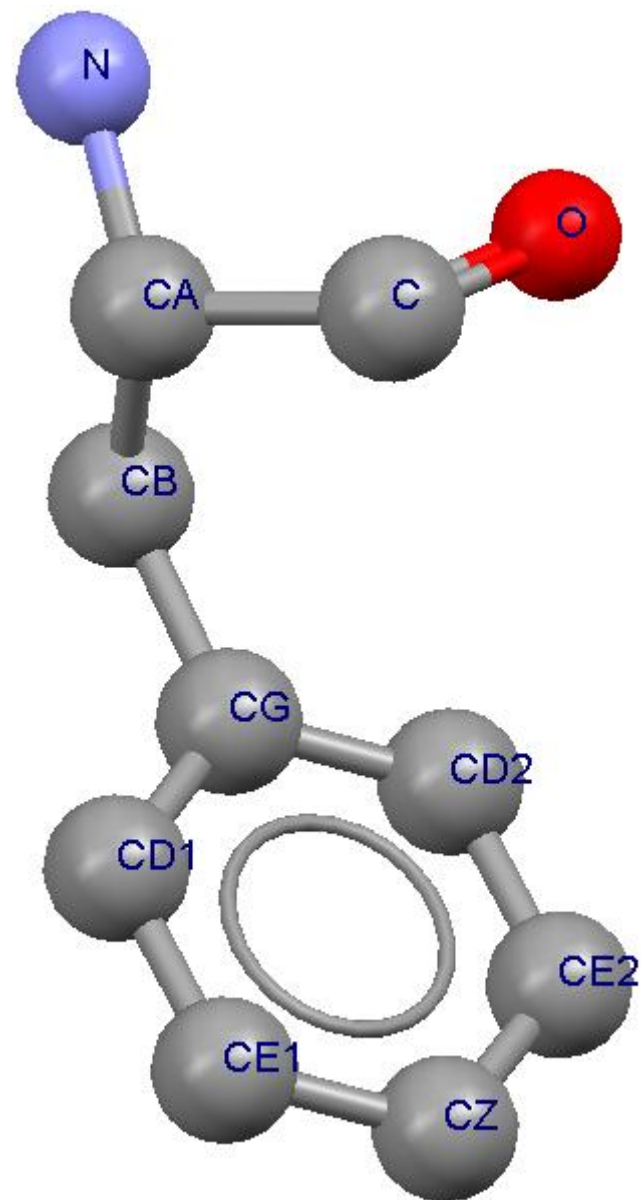


Aminoácidos & proteínas

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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
ATOM	1085	CA	PHE A 138	4.500	21.400	9.300
ATOM	1086	C	PHE A 138	4.200	21.700	7.800
ATOM	1087	O	PHE A 138	3.900	22.800	7.400
ATOM	1088	CB	PHE A 138	5.900	21.100	9.900
ATOM	1089	CG	PHE A 138	7.000	21.900	9.300
ATOM	1090	CD1	PHE A 138	7.500	21.600	8.100
ATOM	1091	CD2	PHE A 138	7.400	23.100	9.900
ATOM	1092	CE1	PHE A 138	8.600	22.300	7.500
ATOM	1093	CE2	PHE A 138	8.400	23.900	9.200
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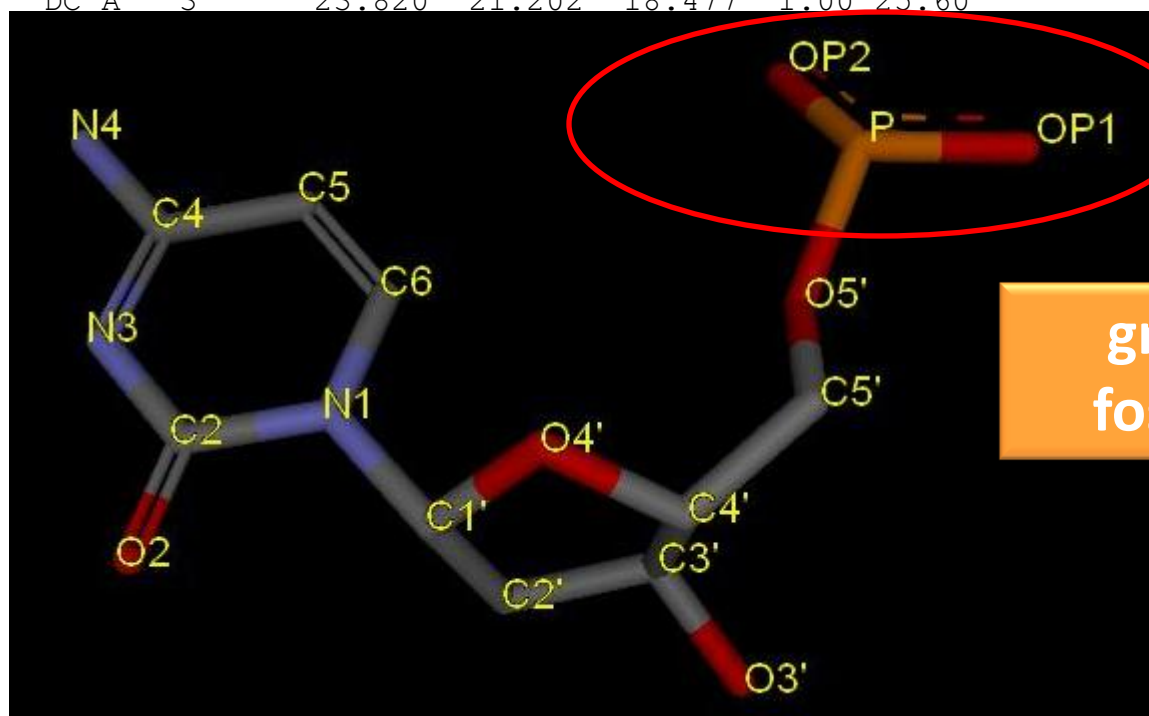
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3	C4*	20.7420	32.2660	23.7840	C.3	1	C1	0.0000
4	O4*	20.1040	31.1230	24.3850	O.3	1	C1	0.0000
5	C3*	21.1090	31.8590	22.3660	C.3	1	C1	0.0000
6	O3*	22.4850	31.5070	22.2970	O.3	1	C1	0.0000
7	C2*	20.2030	30.6900	22.0780	C.3	1	C1	0.0000
8	C1*	20.0650	30.0510	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

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
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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
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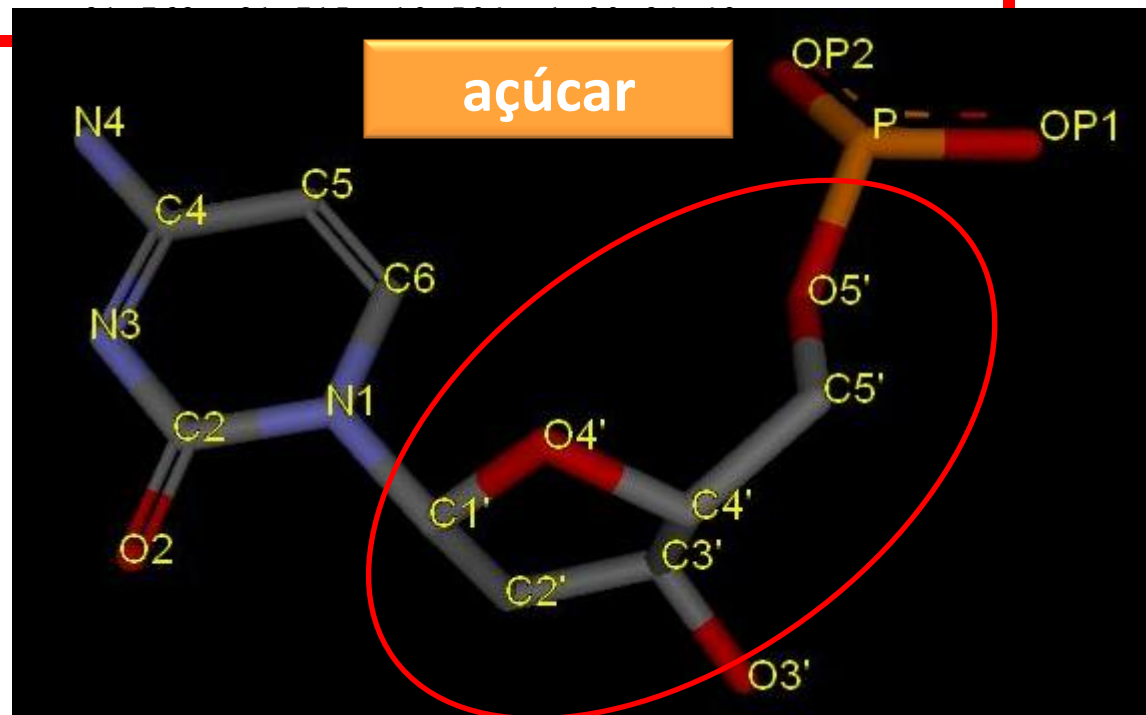
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ATOM	41	OP2	DC	A	3	24.889	25.966	17.423	1.00	33.38	O
ATOM	42	O5'	DC	A	3	25.081	23.755	18.538	1.00	28.67	O
ATOM	43	C5'	DC	A	3	25.162	22.978	19.736	1.00	23.94	C
ATOM	44	C4'	DC	A	3	24.072	21.936	19.787	1.00	23.50	C
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ATOM	47	O3'									O
ATOM	48	C2'									C
ATOM	49	C1'									C
ATOM	50	N1									N
ATOM	51	C2									C
ATOM	52	O2									O
ATOM	53	N3									N
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grupo
fosfato

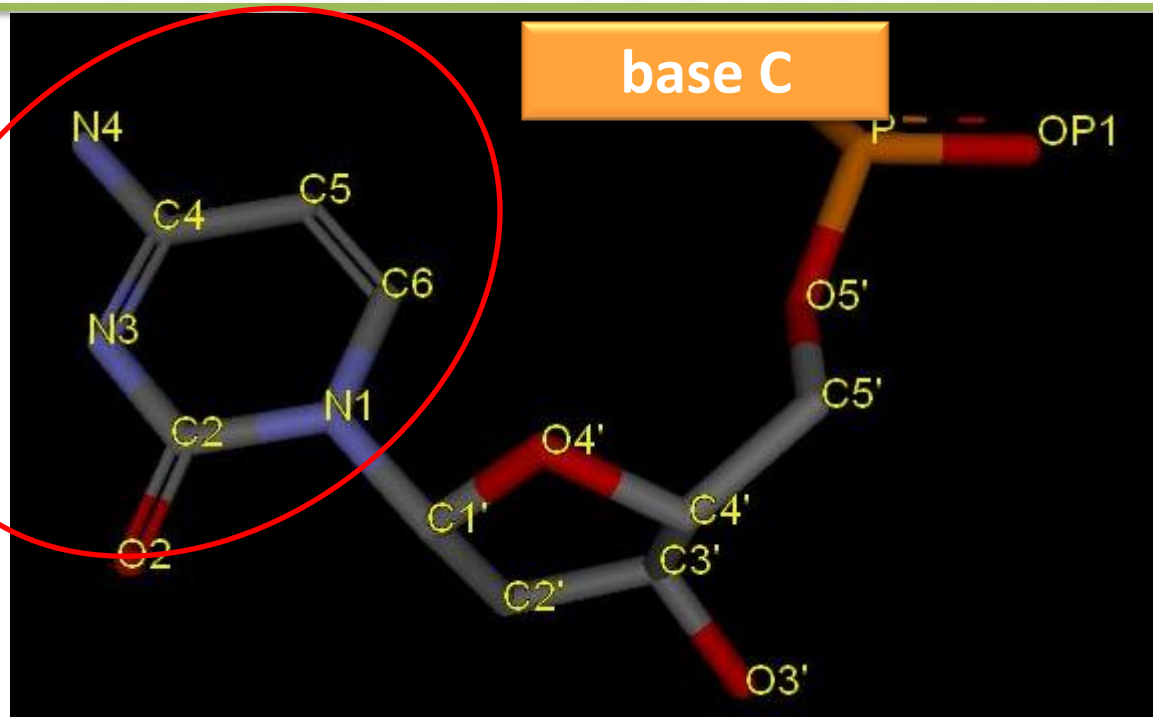
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ATOM	40	OP1	DC A	3	27.060	25.288	18.677	1.00	37.04	O
ATOM	41	OP2	DC A	3	24.889	25.966	17.423	1.00	33.38	O
ATOM	42	O5'	DC A	3	25.081	23.755	18.538	1.00	28.67	O
ATOM	43	C5'	DC A	3	25.162	22.978	19.736	1.00	23.94	C
ATOM	44	C4'	DC A	3	24.072	21.936	19.787	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
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1vzk: arquivo texto de coordenadas

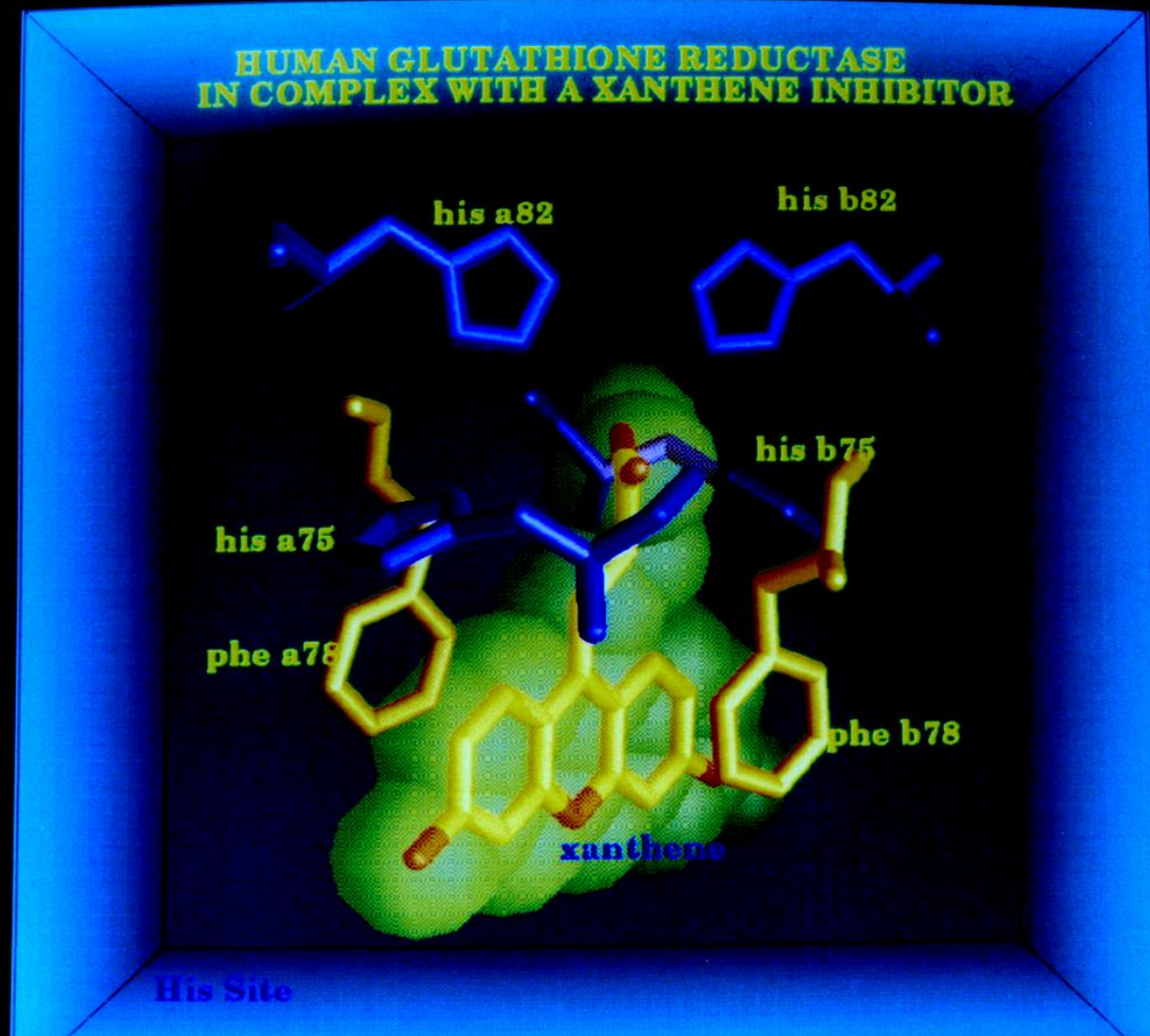
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ATOM	54	C4	DC	A	3
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ATOM	56	C5	DC	A	3
ATOM	57	C6	DC	A	3



24.686	20.071	18.379	1.00	32.06	O
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21.762	21.715	19.594	1.00	24.49	C
20.727	22.632	19.093	1.00	22.43	N
19.390	22.374	19.389	1.00	22.08	C
19.100	21.374	20.073	1.00	23.13	O
18.457	23.230	18.918	1.00	24.96	N
18.829	24.290	18.187	1.00	30.21	C
17.888	25.125	17.730	1.00	34.79	N
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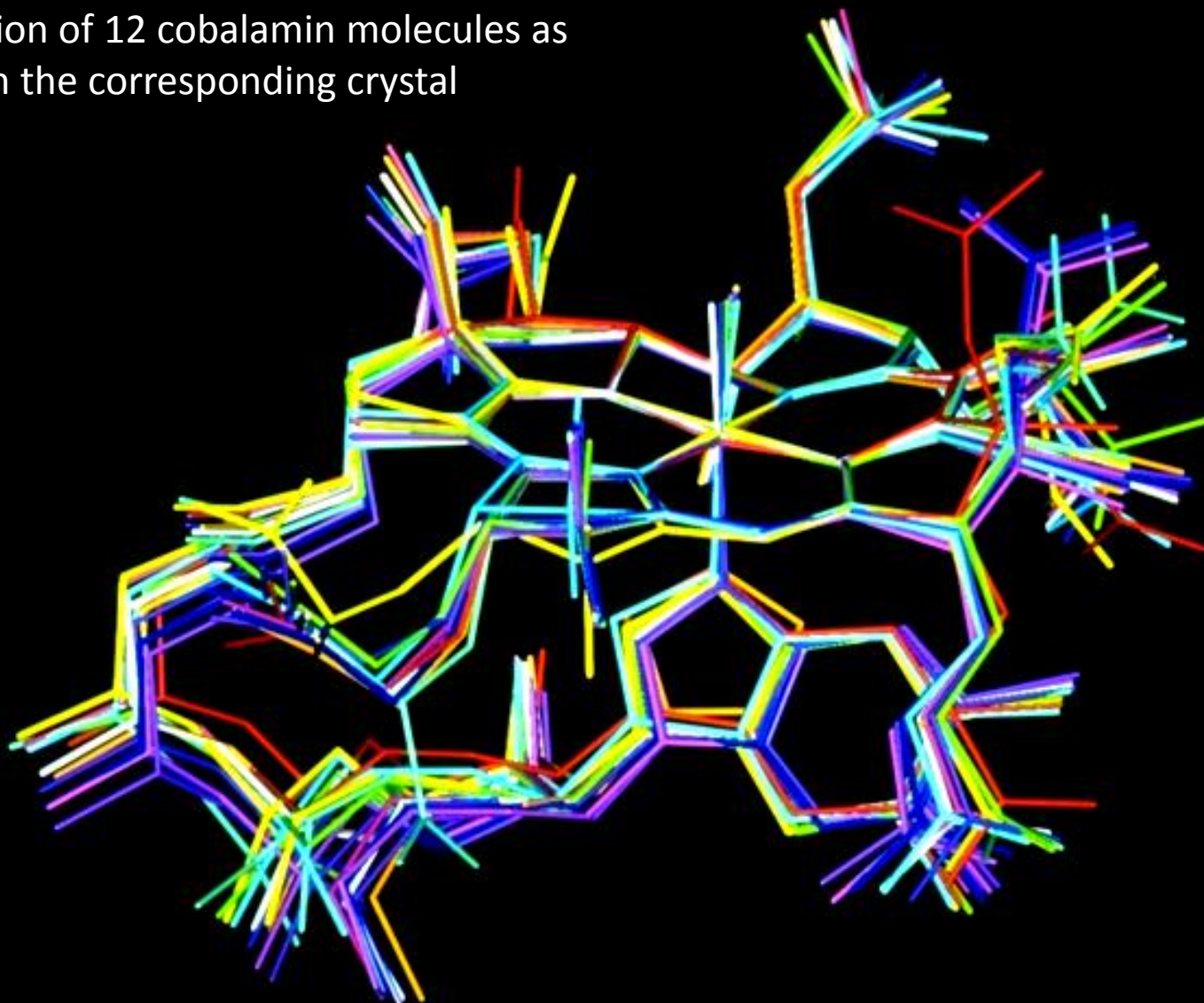
Visualização em estações gráficas

Bioquímica: BIT603 & BIT903

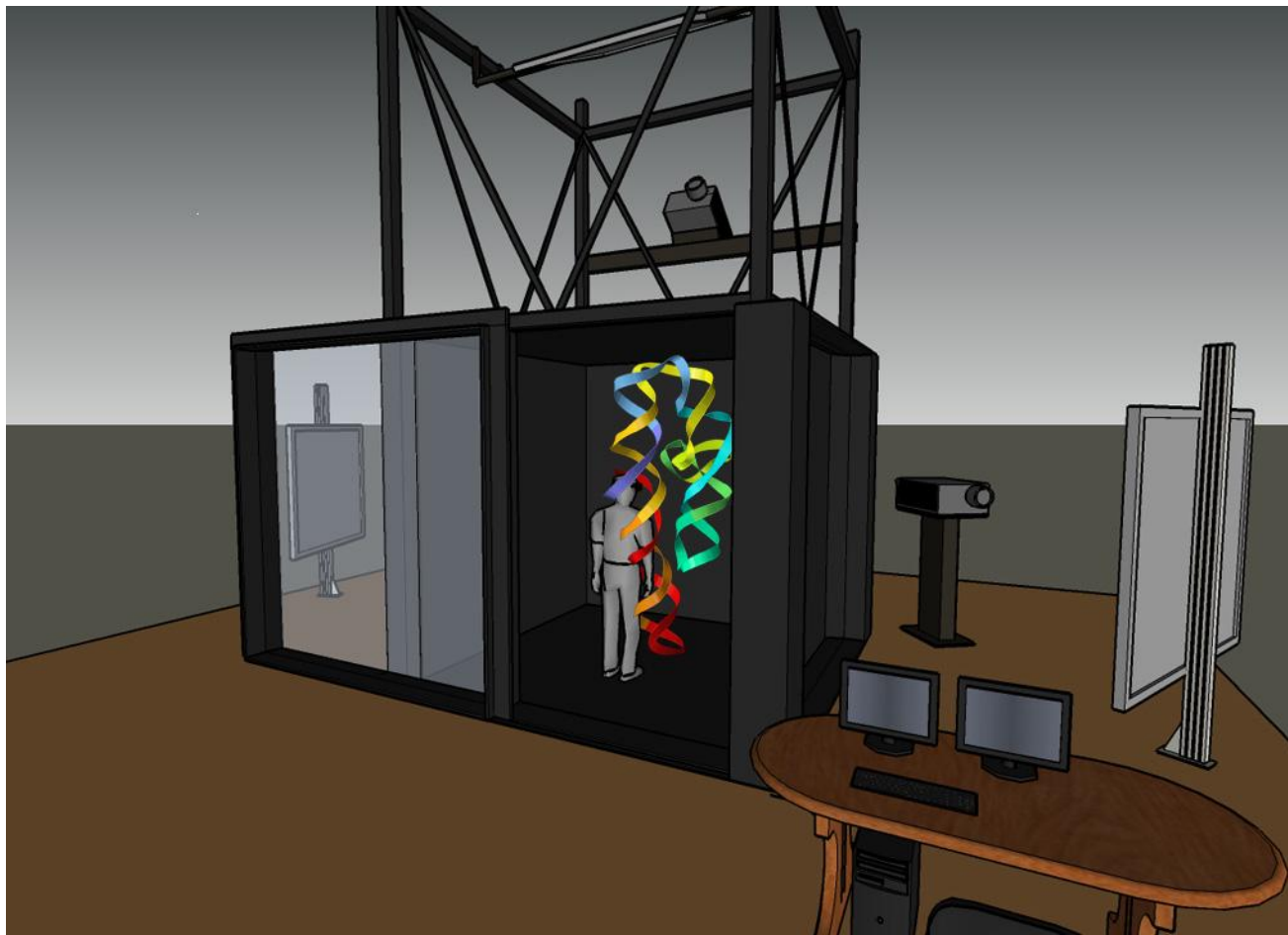


Comparação de Estruturas

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

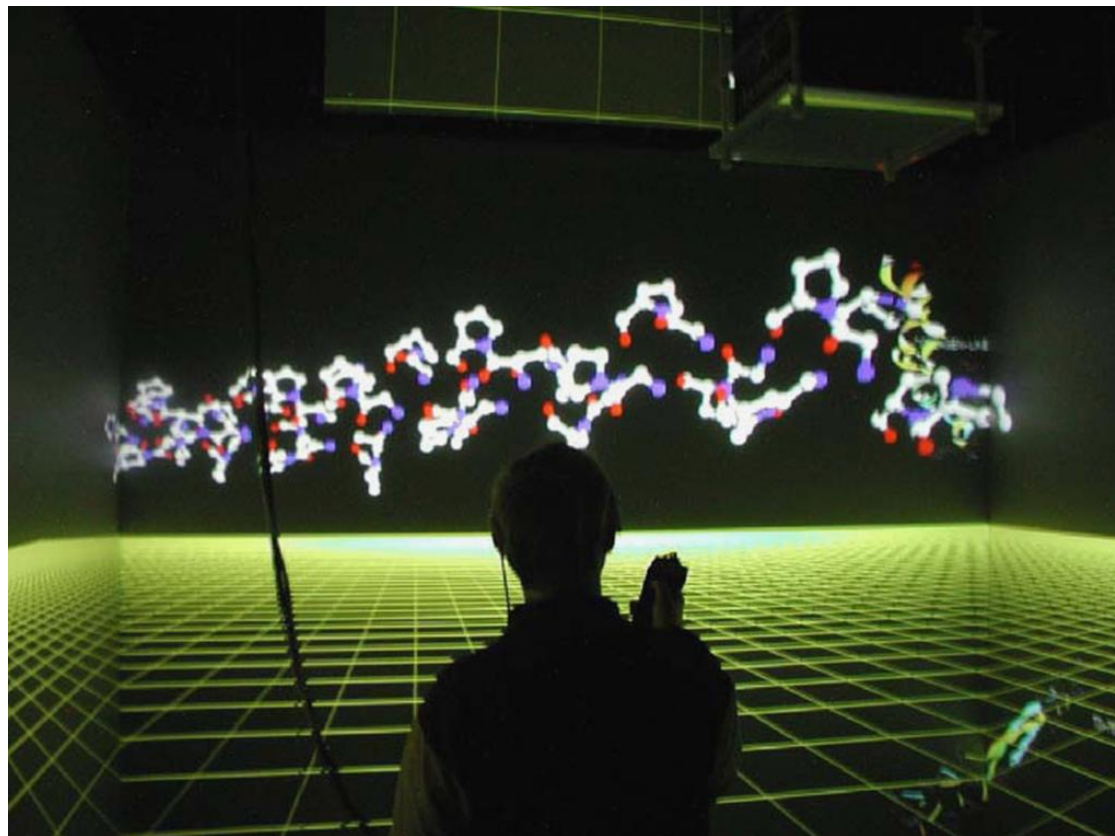


Salas de visualização

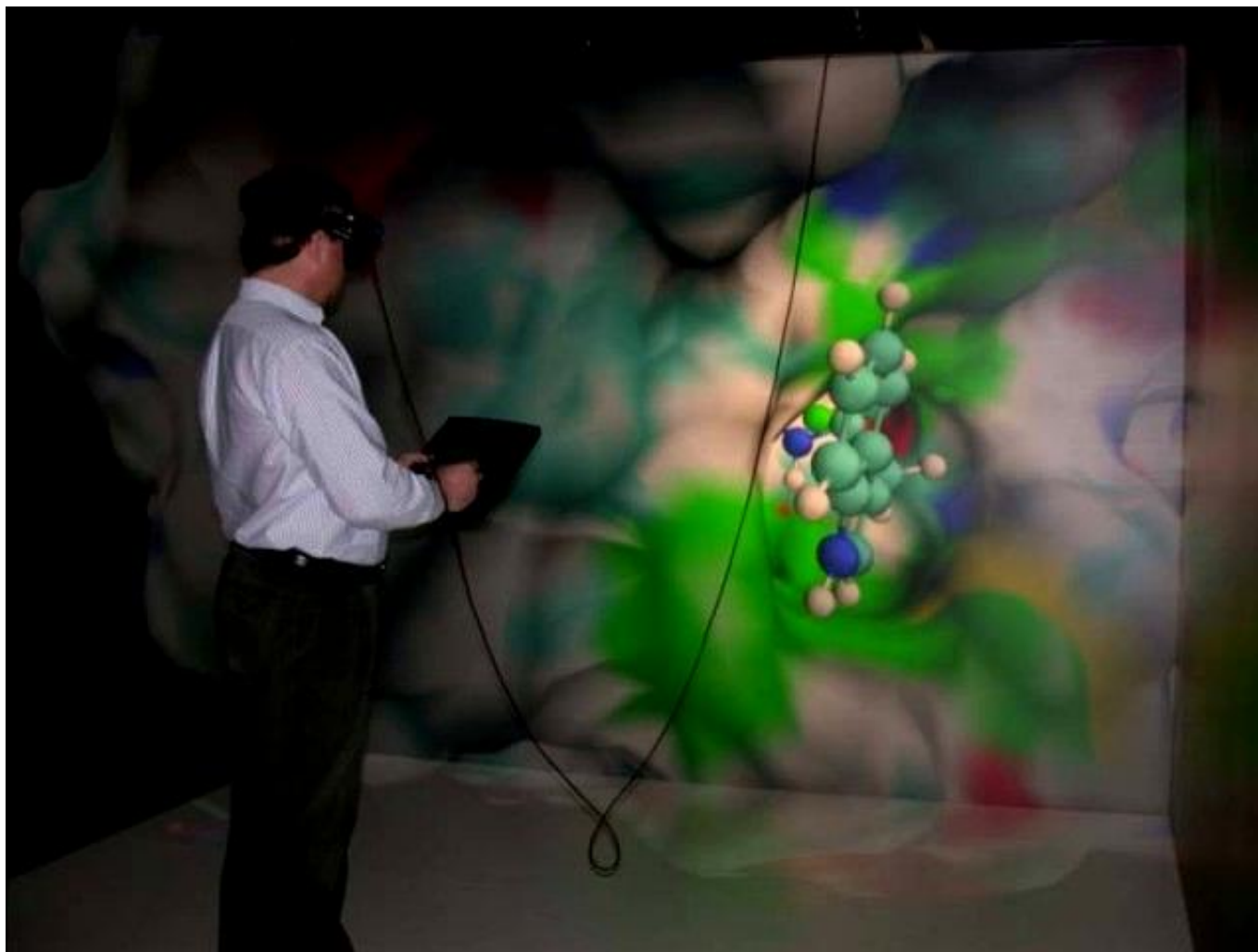


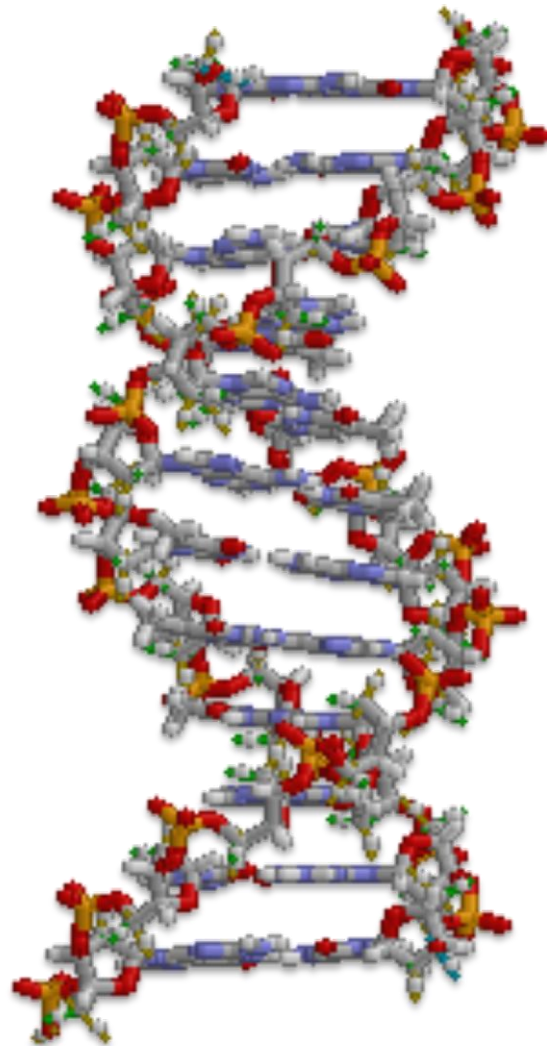


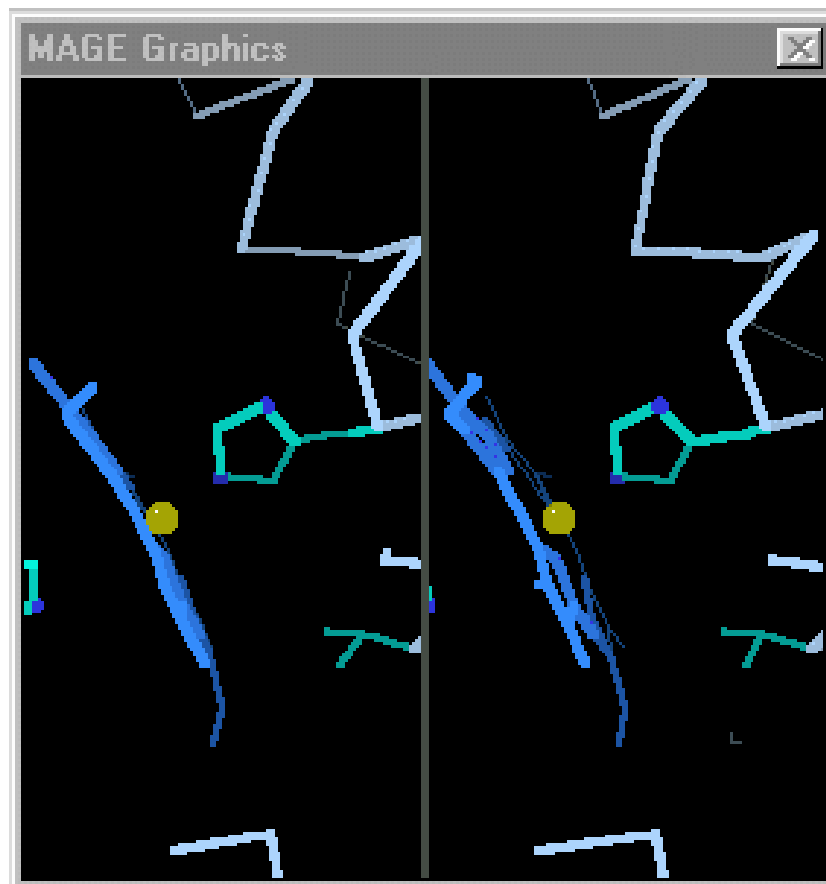
Salas de visualização



Salas de visualização







Visualização de dados dependente do tempo

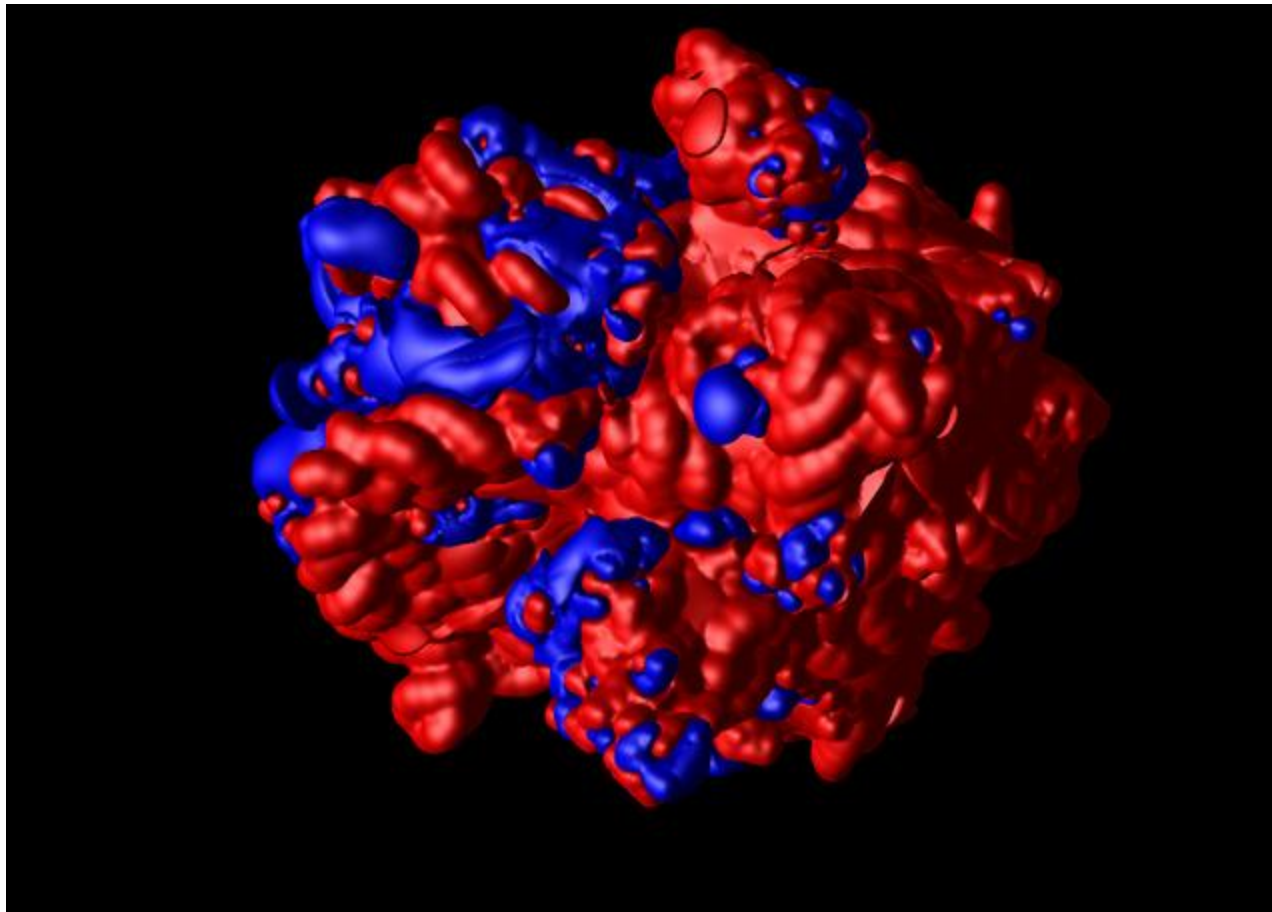
Molecular Dynamics of Staphylococcal Nuclease Unfolding

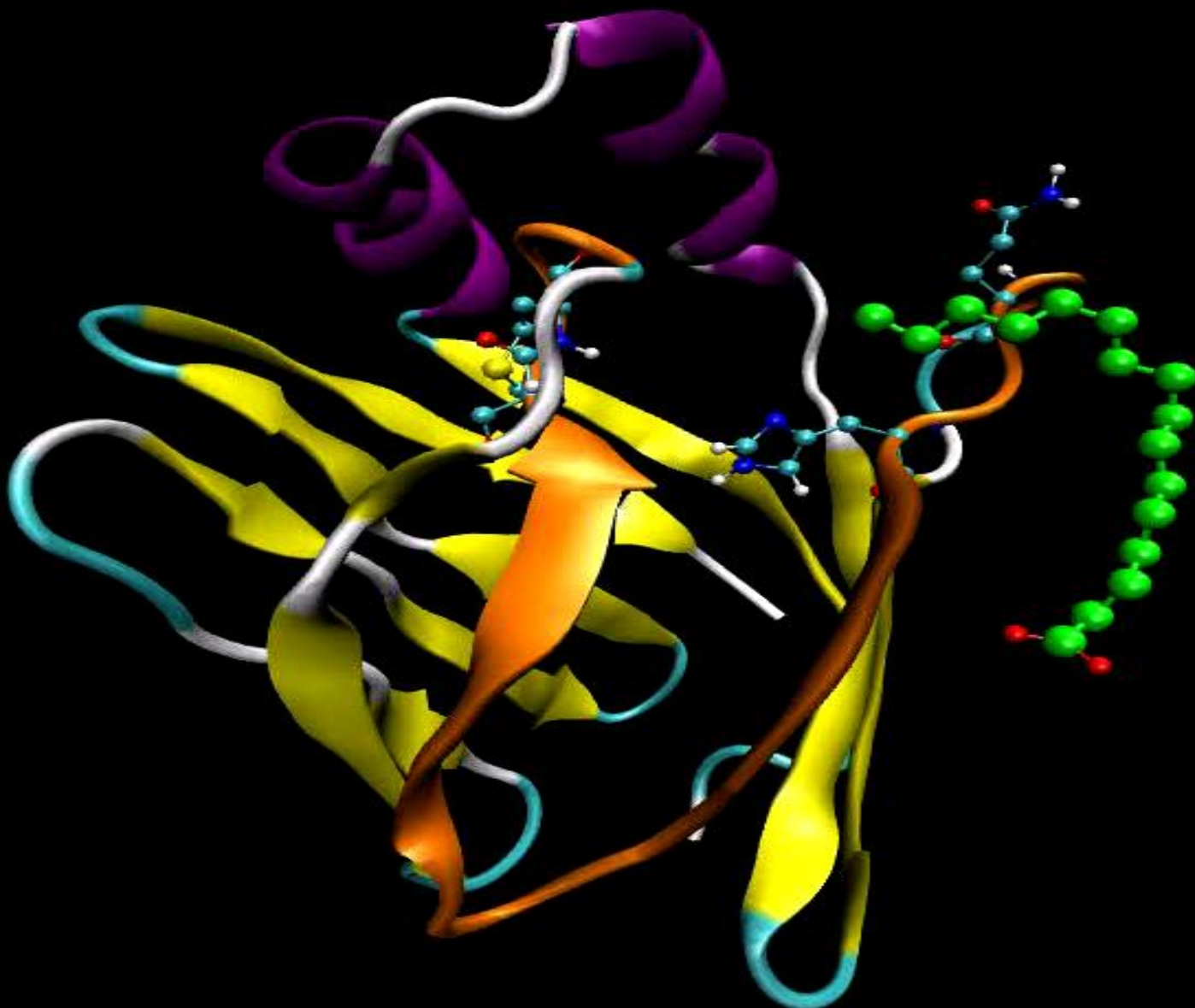
Andreea D. Gruia
Jeremy C. Smith
Stefan Fischer

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Visualização de dados dependente do tempo

Bioquímica: BIT603 & BIT903





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Para instalar:

- a) descompacte
- b) troque por **txe** por **exe**

<http://accelrys.com/products/discovery-studio/visualization-download.php>