

# ACD ChemSketch

*Факультет Биоинженерии и Биоинформатики*

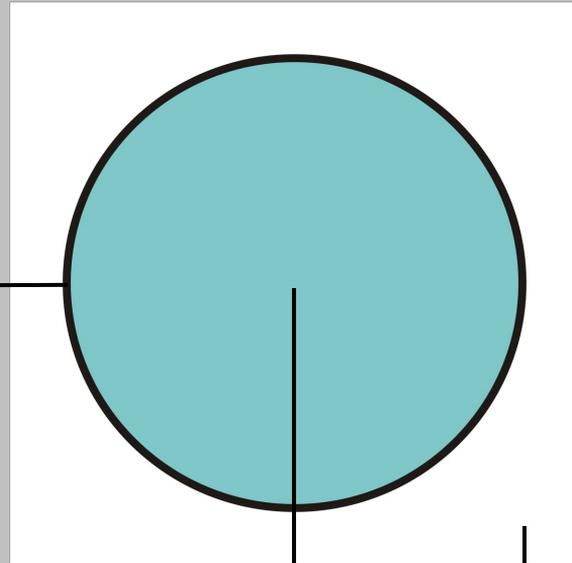
**I семестр**

# ACD ChemSketch

## Графический редактор:

- 🌐 **Векторная графика**
- 🌐 **Стандартные функции** (линии, геометрические фигуры, текст...)
- 🌐 **Химические формулы**
- 🌐 **Структурные формулы структуры**
- 🌐 **Химические реакции**
- 🌐 **Другие объекты** (орбитали, проекции...)

# Растровая графика



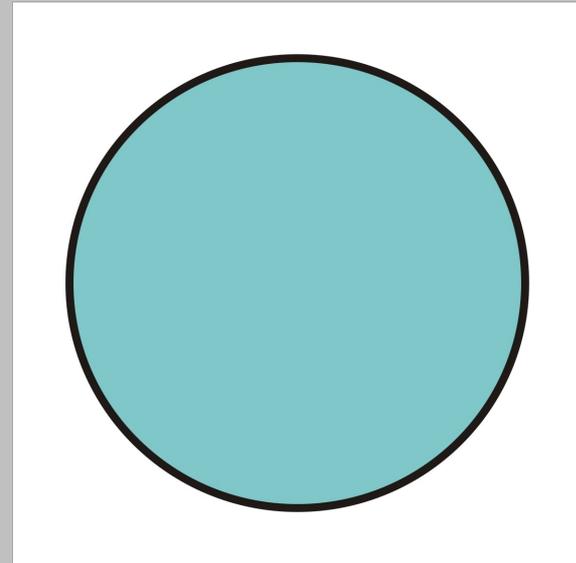
(10;50) цвет: #000000

(50;50) цвет: #00FFFF

(10;50) цвет: #FFFFFF

**И так – для каждой точки**

# Векторная графика



**объект: эллипс**

**центр: (50;50)**

**ширина: 80**

**высота: 80**

**толщина линии: 2**

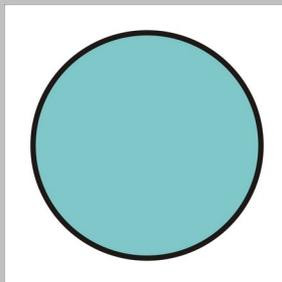
**цвет заливки: #00FFFF**

**цвет линии: #000000**

# Растровая графика

# Векторная графика

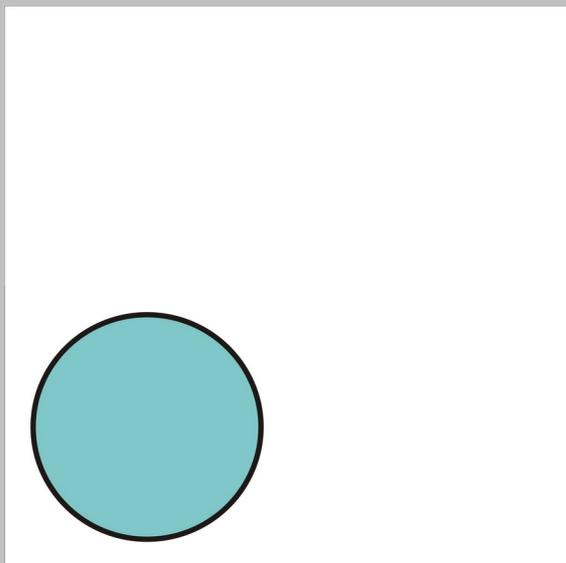
*N байт*



*M байт*

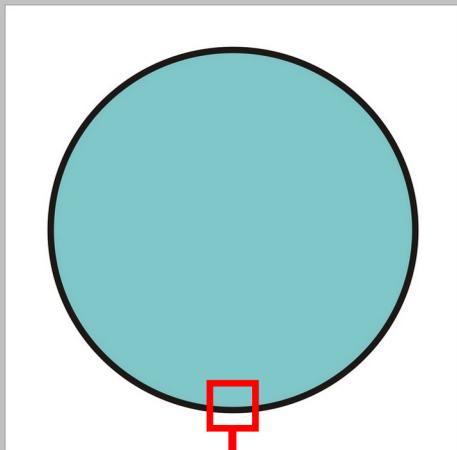


*4N байт*

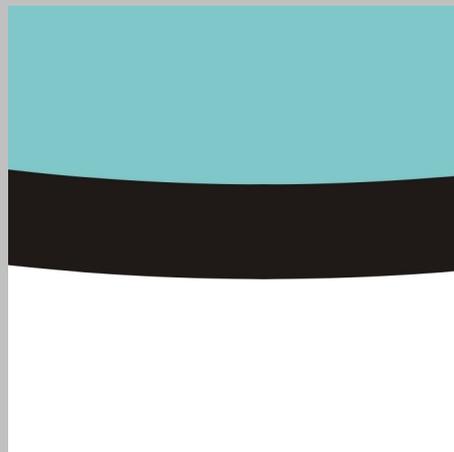
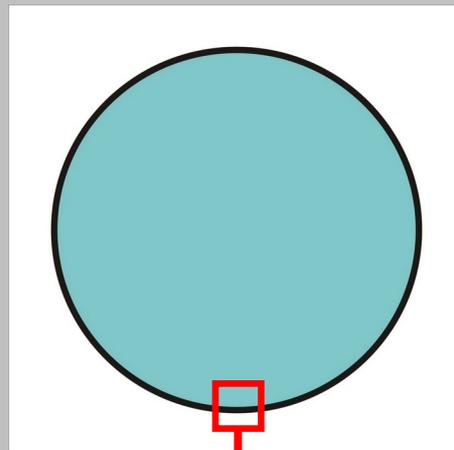


*~ M байт*

# Растровая графика



# Векторная графика



# Рабочее окно ACD/ChemSketch

Строка меню

The screenshot displays the ACD/3D Viewer window for ChemSketch. The main workspace shows a chemical structure of a substituted benzene ring with a hydroxyl group, a methylene group, a methylammonium group, and a carboxylate group. The interface includes a menu bar at the top, a toolbar with various drawing and editing tools, a ruler at the top and left, and a vertical toolbar on the right with various chemical fragments. The status bar at the bottom shows the current file name, page number, and chemical formula.

ACD/Labs RSS Feed: ноя 2 13:20 A 'Spectroscopist's Dream' Captures the Imagination of Journal Readers: сен 29 13:21 ACD/Labs Announces ADMET & PhysChem Sympo: Setup RSS  
●●● I-Lab Login NONAME01.SK2 Modified Page 1/1 Fragments: 1 C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub> FW: 181.18854 Properties

1-ChemSketch 2-Copy to 3D 3-3D View

Список листов файла

Переключение между программами

# Рабочее окно ACD/ChemSketch

The screenshot displays the ACD/3D Viewer (Freeware) interface for ChemSketch. The main window shows a chemical structure of a substituted benzene ring with a hydroxyl group, a methyl group, and a propyl chain ending in an ammonium group. The interface includes a menu bar (File, Edit, Pages, Tools, Templates, Options, Documents, Add-Ons, I-Lab, ACD/Labs, Help), a toolbar with icons for drawing and editing, and a vertical toolbar on the right with various chemical fragments. A ruler is visible at the top and left. Three red arrows point to specific icons in the top toolbar: one to the 'Open' icon (labeled 'Кнопки для работы с файлами'), one to the 'Erase' icon (labeled 'Кнопки для редактирования'), and one to the 'Zoom' icon (labeled 'Кнопки для изменения масштаба').

Кнопки для работы с файлами

Кнопки для редактирования

Кнопки для изменения масштаба

ACD/Labs RSS Feed: ноя 2 13:20 A 'Spectroscopist's Dream' Captures the Imagination of Journal Readers: сен 29 13:21 ACD/Labs Announces ADMET & PhysChem Sympo: Setup RSS  
I-Lab Login NONAME01.SK2 Modified Page 1/1 Fragments: 1 C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub> FW: 181.18854 Properties  
1-ChemSketch 2-Copy to 3D 3-3D View

# Рабочее окно ACD/ChemSketch

The screenshot displays the ACD/3D Viewer (Freeware) interface for ChemSketch. The main window shows a chemical structure of a substituted benzene ring with a hydroxyl group, a propyl chain, and a protonated amine group. The interface includes a menu bar (File, Edit, Pages, Tools, Templates, Options, Documents, Add-Ons, I-Lab, ACD/Labs, Help), a toolbar with icons for drawing and editing, and a vertical toolbar on the right with various chemical fragments. A ruler is visible at the top and left. Three red arrows point to specific icons in the top toolbar: one to the 'Open' icon (labeled 'Кнопки для работы с файлами'), one to the 'Erase' icon (labeled 'Кнопки для редактирования'), and one to the 'Zoom' icon (labeled 'Кнопки для изменения масштаба').

Кнопки для работы с файлами

Кнопки для редактирования

Кнопки для изменения масштаба

ACD/Labs RSS Feed: ноя 2 13:20 A 'Spectroscopist's Dream' Captures the Imagination of Journal Readers: сен 29 13:21 ACD/Labs Announces ADMET & PhysChem Sympo: Setup RSS  
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1-ChemSketch 2-Copy to 3D 3-3D View

# Рабочее окно ACD/ChemSketch

ACD/3D Viewer (Freeware): ChemSketch Window - [noname01.sk2]

File Edit Pages Tools Templates Options Documents Add-Ons I-Lab ACD/Labs Help

Structure Draw

114%

mm 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210

A  
Any  
C  
H  
N  
O  
F  
Na  
Si  
P  
S  
Cl  
K  
Br  
HF  
Mg  
Li  
Nb

HO

NH<sub>3</sub><sup>+</sup>

Panel  
инструментов

Кнопки для работы  
с атомами

ACD/Labs RSS Feed: ноя 2 13:20 A 'Spectroscopist's Dream' Captures the Imagination of Journal Readers: сен 29 13:21 ACD/Labs Announces ADMET & PhysChem Sympo: Setup RSS

I-Lab Login NONAME01.SK2 Modified Page 1/1 Fragments: 1 C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub> FW: 181.18854

1-ChemSketch 2-Copy to 3D 3-3D View

# Работа с атомами

The image shows a software interface for working with atoms. At the top is a toolbar with various drawing tools. Below it is a horizontal ruler in millimeters (0 to 130). On the left is a vertical periodic table with a ruler (0 to 80). The periodic table is divided into three sections:

- Периодическая таблица** (Periodic table): The top section, indicated by a red arrow pointing to the grid icon.
- Часто используемые атомы** (Commonly used atoms): The middle section, containing a red oval around the elements C, H, N, O, F, Na, Si, P, S, Cl, K.
- Дополнительные атомы (последние использованные)** (Additional atoms (last used)): The bottom section, containing Br, Ac, and Mg, with a red arrow pointing to the Ac icon.

In the center-right, a chemical structure is displayed, featuring a benzene ring with a hydroxyl group (HO) and a side chain containing a primary amine group (NH<sub>3</sub><sup>+</sup>) and a carbonyl group (C=O).

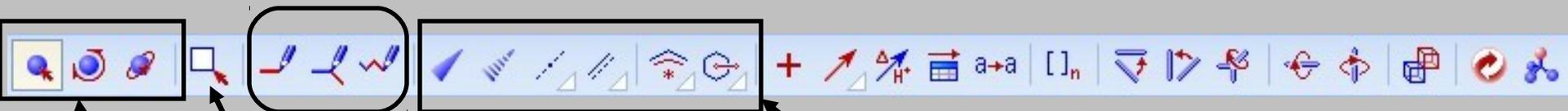
# Работа с атомами

Periodic Table of Elements

1											18							
H												He						
2																		
Li	Be											B	C	N	O	F	Ne	
Na	Mg	3	4	5	6	7	8	9	10	11	12	Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg								
		*	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	D
		**	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	T

OK Cancel Help

# Панель инструментов



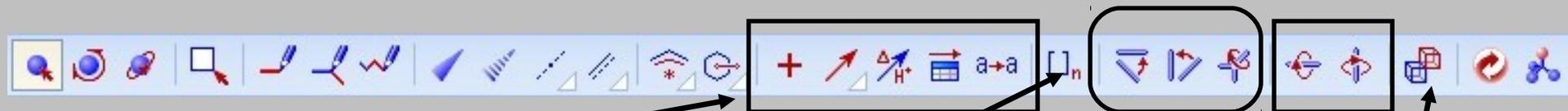
Перемещение и  
вращение атомов

Выделение  
атомов

Рисование  
связей

Изменение  
связей

# Панель инструментов



Рисование  
реакций

Полимеры

Изменение положения  
связей в пространстве

Вращение молекулы  
относительно связи

«Клонирование»  
структуры



# Работа с графическими объектами

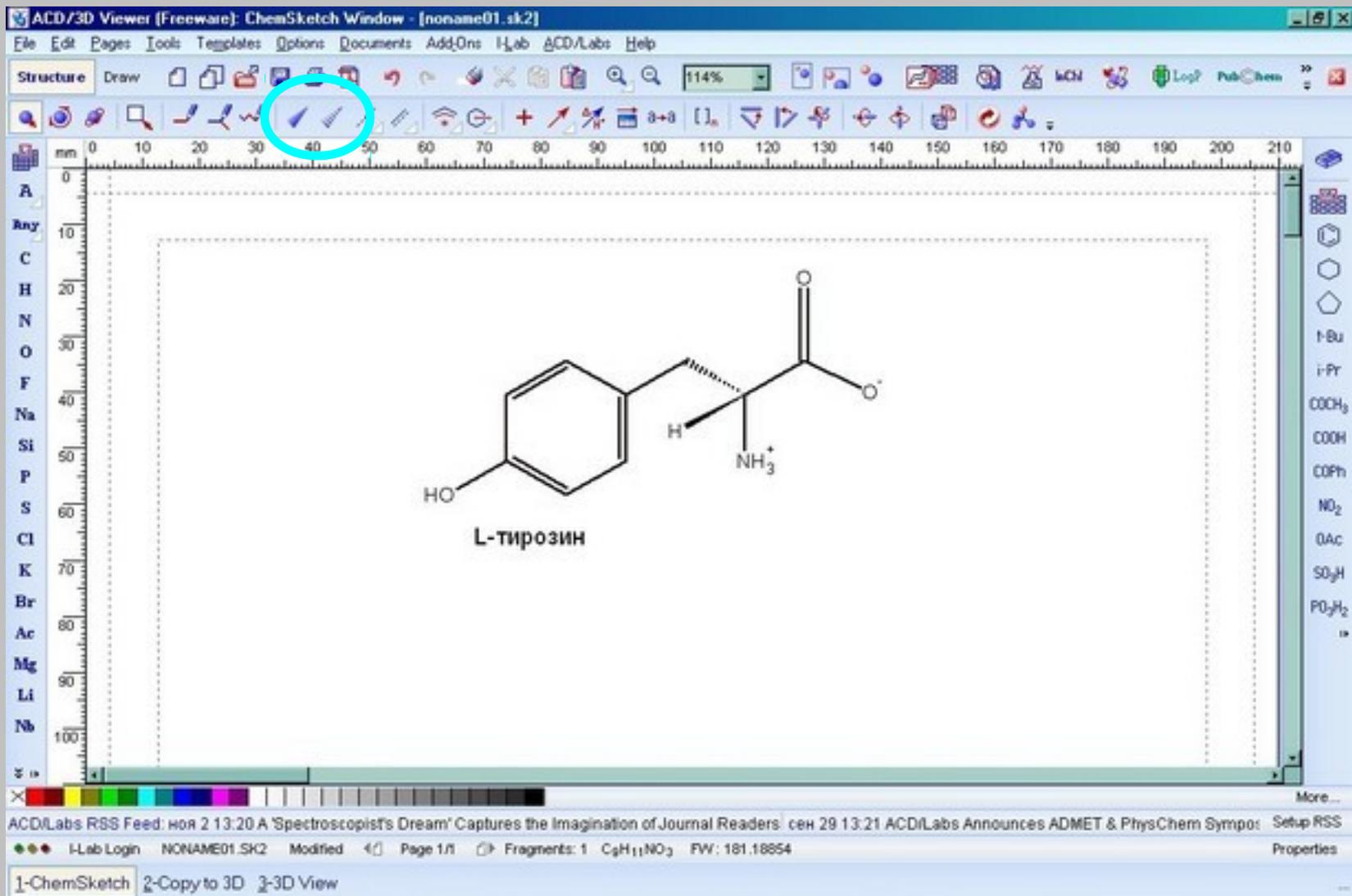
The image shows a screenshot of the ChemSketch software interface. The title bar reads "ACD/3D (Freeware): ChemSketch Window - [noname01.sk2]". The menu bar includes "File", "Edit", "Page", "Tools", "Object", "Templates", "Options", "Documents", "Add-Ons", "I-Lab", "ACD/Labs", and "Help". The "Draw" toolbar is highlighted with a red box and contains various icons for drawing and editing. A blue arrow points to the "Draw" button in the menu bar. A red arrow points to the "Draw" toolbar, and a blue arrow points to the left-hand toolbar. The main workspace displays the chemical structure of Tyrosine (Tyr; Y) with the text "Тирозин (Тур; Y)" below it. The structure is a benzene ring with a hydroxyl group (-OH) and a side chain containing an amino group (-NH<sub>3</sub><sup>+</sup>) and a carboxylate group (-COO<sup>-</sup>). The bottom status bar shows "ACD/Labs RSS Feed: ноя 2 13:20 A 'Spectroscopist's Dream' Captures the Imagination of Journal Readers: сен 29 13:21 ACD/Labs Announces ADMET & PhysChem Sympo: Setup RSS" and "I-Lab Login NONAME01.SK2 Modified Page 1/1".

**Кнопки для редактирования объектов**

**Кнопки для создания новых объектов**

Тирозин (Тур; Y)

# Построение трехмерных структур



# Построение трехмерных структур

ACD/3D Viewer (Freeware): ChemSketch Window - [noname01.sk2]

File Edit Pages Tools Templates Options Documents Add-Ons I-Lab ACD/Labs Help

Structure Draw [114%]

mm 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210

A  
Br  
C  
H  
N  
O  
F  
Na  
Si  
P  
S  
Cl  
K  
Br  
Ac  
Mg  
Li  
Nb

L-тирозин

COCH<sub>3</sub>  
COOH  
COPh  
NO<sub>2</sub>  
OAc  
SO<sub>2</sub>H  
PO<sub>3</sub>H<sub>2</sub>

сен 29 13:21 ACD/Labs A... es ADMET & PhysChem Symposium сен 1 13:23 ACD/Labs Incorporates New Company to Serve Germany, Austria, Switzerland ноя 2 11:4... Setup RSS

I-Lab Login Modified Page 1/1 Fragments: 1 C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub> FW: 181.18854 Properties

1-ChemSketch 2-Copy to 3D 3-3D View

# Построение трехмерных структур

