

ACD ChemSketch

Факультет Биоинженерии и Биоинформатики

I семестр, 2009

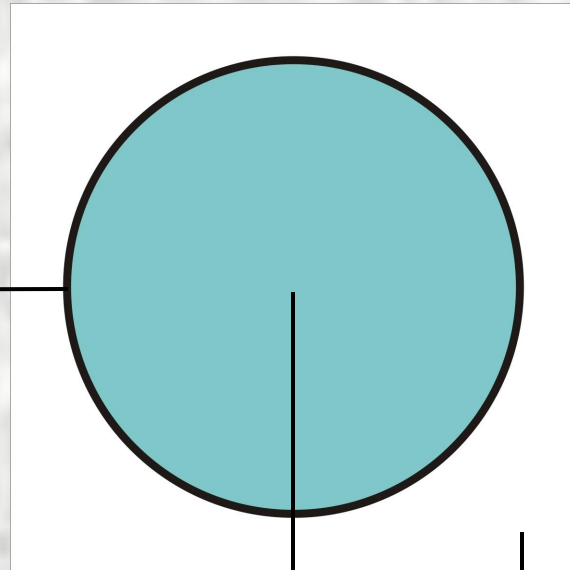
ACD ChemSketch

Графический редактор:

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

Растровая графика

Векторная графика

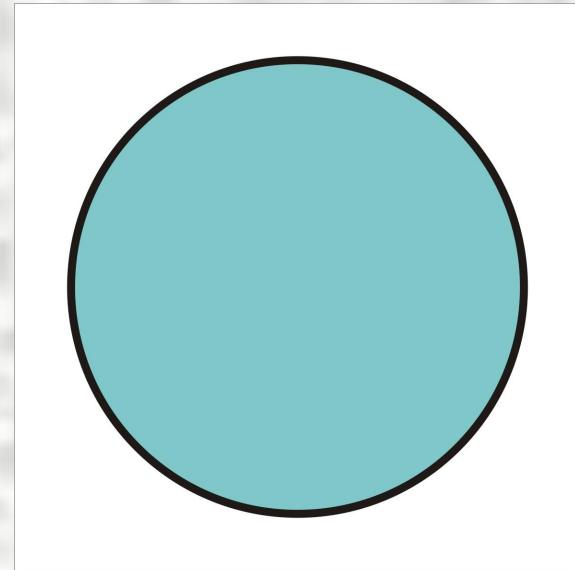


(50;50) цвет: #00FFFF

(10;50) цвет: #000000

(10;50) цвет: #FFFFFF

И так – для каждой точки



объект: эллипс

центр: (50;50)

ширина: 80

высота: 80

толщина линии: 2

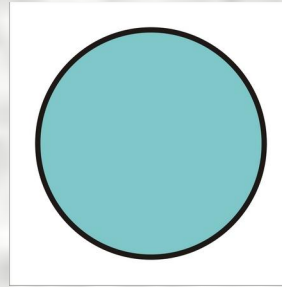
цвет заливки: #00FFFF

цвет линии: #000000

Растровая графика

Векторная графика

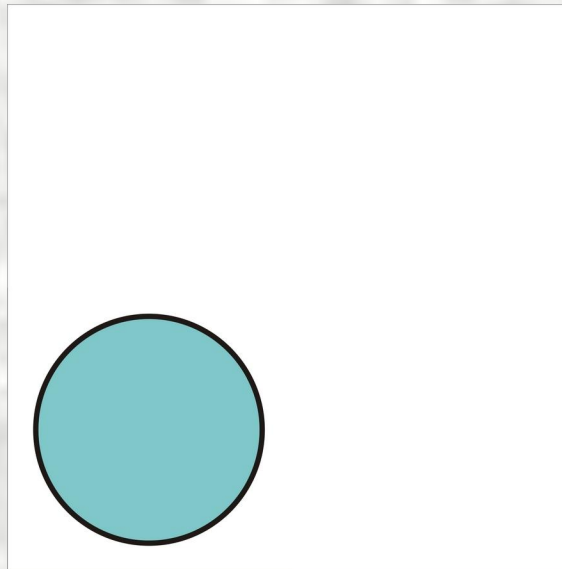
N байт



M байт

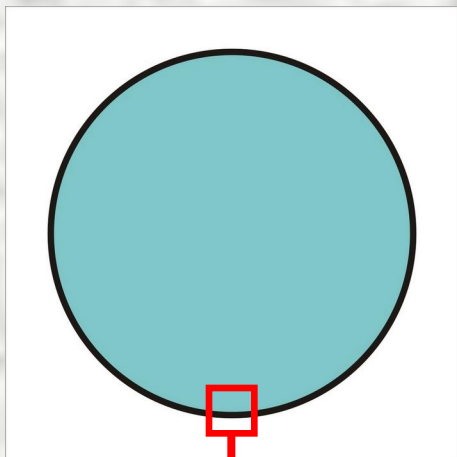


4N байт

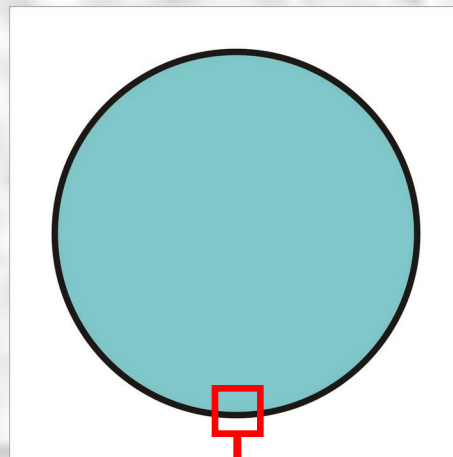


~ M байт

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 list of chemical fragments on the right. At the bottom, there is a status bar with file information and a tab bar with buttons for '1-ChemSketch', '2-Copy to 3D', and '3-3D View'.

Список листов файла

Переключение между программами

Рабочее окно ACD/ChemSketch

The image shows the ACD/ChemSketch software interface. The main window displays 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 various drawing and editing tools, and a vertical toolbar on the right with pre-defined chemical fragments. A ruler is visible at the top of the workspace. Three red arrows point to specific tool icons: one to the 'Open' icon (file work), one to the 'Erase' icon (editing), and one to the 'Zoom' icon (scaling).

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 C₉H₁₁NO₃ FW: 181.18854 Properties

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

Рабочее окно ACD/ChemSketch

The image displays the ACD/ChemSketch software interface. The main window shows a chemical structure of a substituted benzene ring with a hydroxyl group, a methyl group, and a side chain containing an ammonium group and a carbonyl group. The interface includes a menu bar (File, Edit, Pages, Tools, Templates, Options, Documents, Add-Ons, I-Lab, ACD/Labs, Help), a toolbar with various drawing and editing tools, and a vertical toolbar on the right with pre-defined chemical fragments. A ruler is visible at the top of the workspace. Three red arrows point to specific tool icons: one to the 'File' icon (top left), one to the 'Edit' icon (top center), and one to the 'View' icon (top right).

Кнопки для работы с файлами

Кнопки для редактирования

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

Рабочее окно ACD/ChemSketch

The screenshot displays the ACD/3D Viewer software window. 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 (File, Edit, Pages, Tools, Templates, Options, Documents, Add-Ons, I-Lab, ACD/Labs, Help), a toolbar with various drawing and editing tools, and a vertical toolbar on the right with pre-defined fragments. A ruler is visible at the top and left. Two red arrows point to specific areas: one to the drawing toolbar and another to the vertical fragment toolbar.

Панель 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 Sympor. Setup RSS

●●● I-Lab Login NONAME01.SK2 Modified Page 1/1 Fragments: 1 C₉H₁₁NO₃ FW: 181.18854 Properties

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 list of atoms: A, Any, C, H, N, O, F, Na, Si, P, S, Cl, K, Br, Ac, Mg. A red oval highlights the atoms C, H, N, O, F, Na, Si, P, S, Cl, and K. A red arrow points from the text 'Периодическая таблица' to the top of this list. Another red arrow points from the text 'Часто используемые атомы' to the middle of the list. A third red arrow points from the text 'Дополнительные атомы (последние использованные)' to the bottom of the list. To the right of the atom list is a chemical structure of a molecule: CC(=O)C(N)CCc1ccc(O)cc1. The structure consists of a benzene ring with a hydroxyl group (-OH) and a propyl chain attached. The propyl chain has an ammonium group (-NH₃⁺) and a methyl group (-CH₃) at the end.

Периодическая таблица

Часто используемые атомы

Дополнительные атомы
(последние использованные)

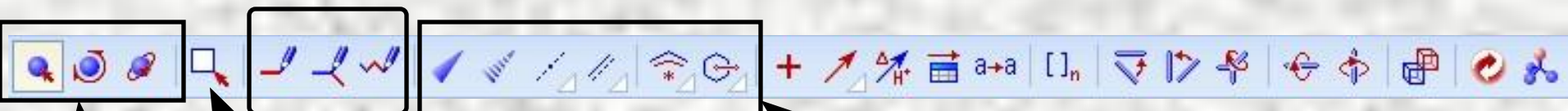
Работа с атомами

Periodic Table of Elements

1																	18	
H																	He	
Li	Be											B	C	N	O	F	Ne	
Na	Mg											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**

Панель инструментов



**Плоская
оптимизация
структуры**

**Объемная
оптимизация
структуры**

Работа с графическими объектами

The screenshot displays the ACD/3D Viewer software window. The main workspace shows the chemical structure of Tyrosine (Tyr; Y), which consists of a benzene ring with a hydroxyl group (-OH) at the para position, a methylene group (-CH₂-), an amino group (-NH₃⁺), and a carboxylate group (-COO⁻). The structure is rendered in a 3D perspective view.

Two toolbars are highlighted with red and blue boxes:

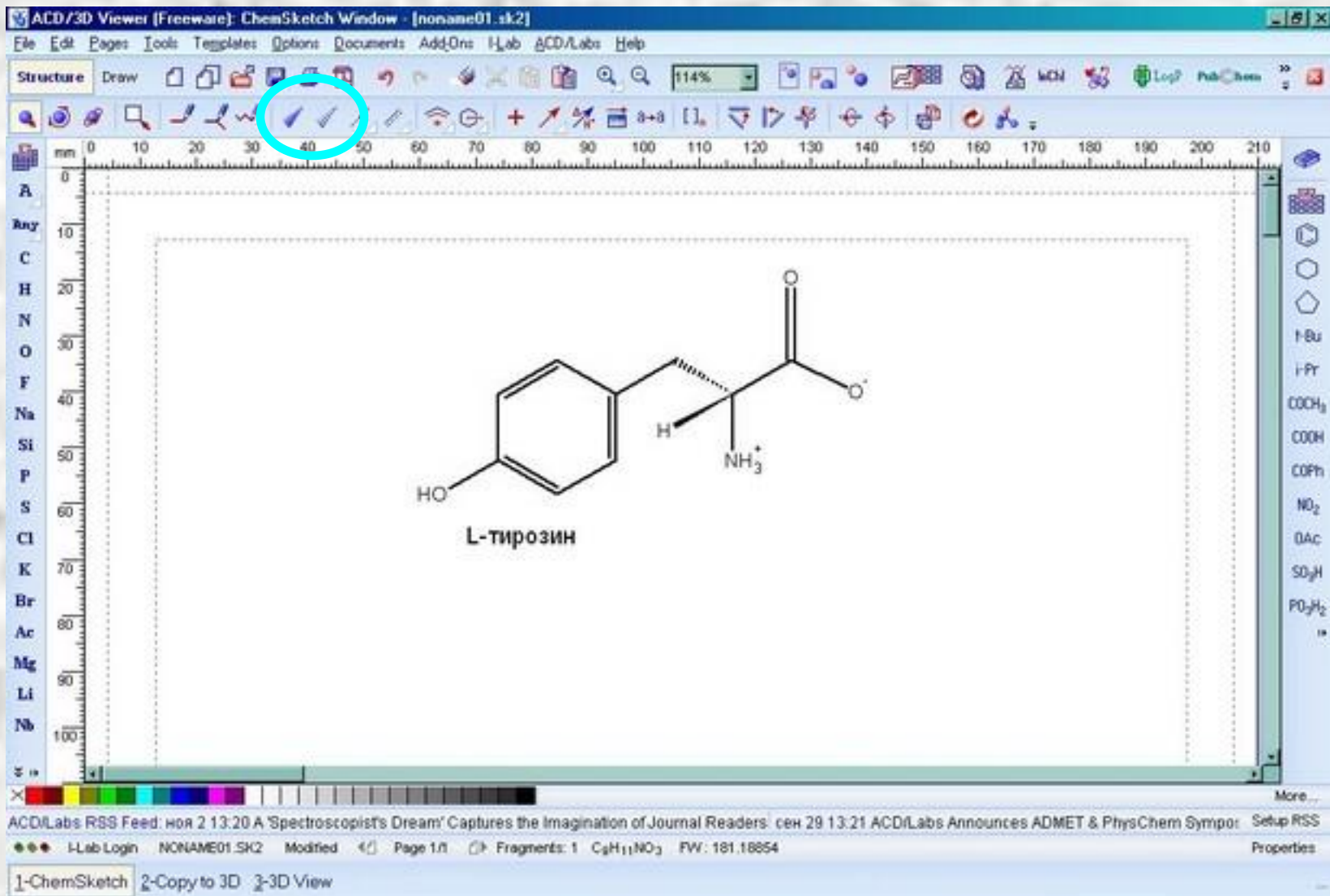
- The top toolbar, outlined in red, contains various editing tools such as delete, copy, paste, and zoom. A red arrow points from the text "Кнопки для редактирования объектов" to this toolbar.
- The left toolbar, outlined in blue, contains tools for creating new objects, including lines, polygons, and text. A blue arrow points from the text "Кнопки для создания новых объектов" to this toolbar.

The text "Кнопки для редактирования объектов" is written in red, and "Кнопки для создания новых объектов" is written in blue. The chemical structure is labeled "Тирозин (Тур; Y)".

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

Построение трехмерных структур



Построение трехмерных структур

The screenshot displays the ACD/3D Viewer software interface. The main window shows the 2D chemical structure of L-tyrosine, labeled "L-тирозин". The structure consists of a benzene ring with a hydroxyl group (-OH) at the para position and an ethylamine side chain (-CH2-CH(NH3+)COO-). The software interface includes a menu bar (File, Edit, Pages, Tools, Templates, Options, Documents, Add-Ons, Lab, ACD/Labs, Help), a toolbar with various drawing and editing tools, and a vertical list of chemical groups on the right side. A blue arrow points to the "3D View" button in the bottom status bar.

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

File Edit Pages Tools Templates Options Documents Add-Ons 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

Ang

C

H

N

O

F

Na

Si

P

S

Cl

K

Br

Ac

Mg

Li

Nb

I-Bu

I-Pr

COCH₃

COOH

COPh

NO₂

OAc

SO₂H

PO₂H₂

L-тирозин

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

1-Lab Login Modified Page 1.0 Fragments: 1 C₉H₁₁NO₃ FW: 181.18854 Properties

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

Построение трехмерных структур

