

ACD ChemSketch

Факультет Биоинженерии и Биоинформатики

I семестр, 2009

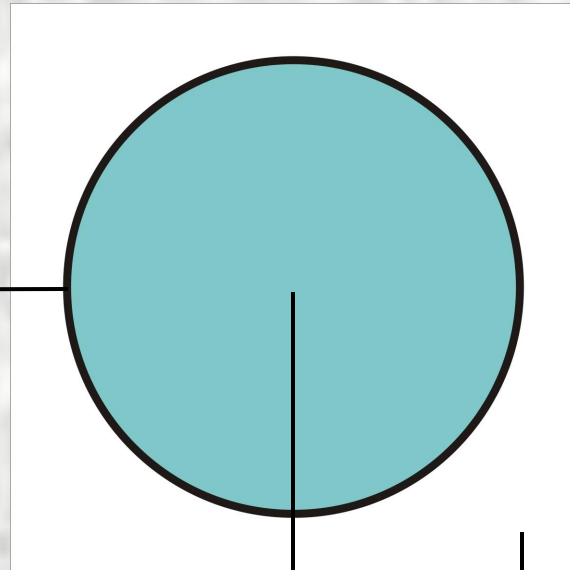
ACD ChemSketch

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

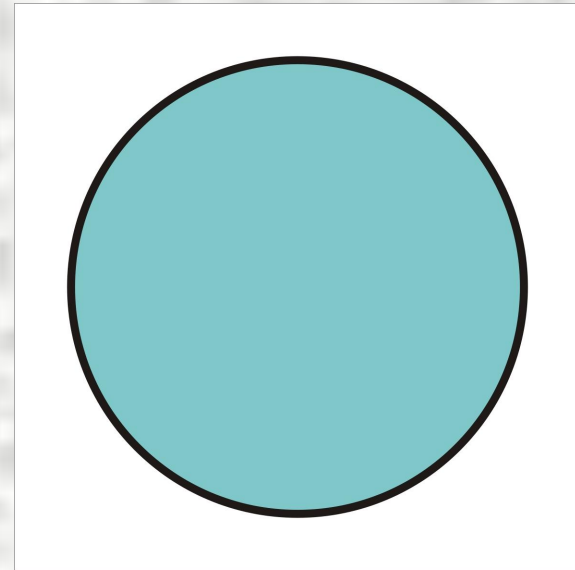


(50;50) цвет: #00FFFF

(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

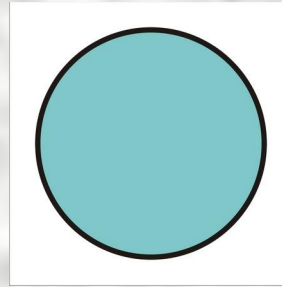
цвет заливки: #00FFFF

цвет линии: #000000

Растровая графика

Векторная графика

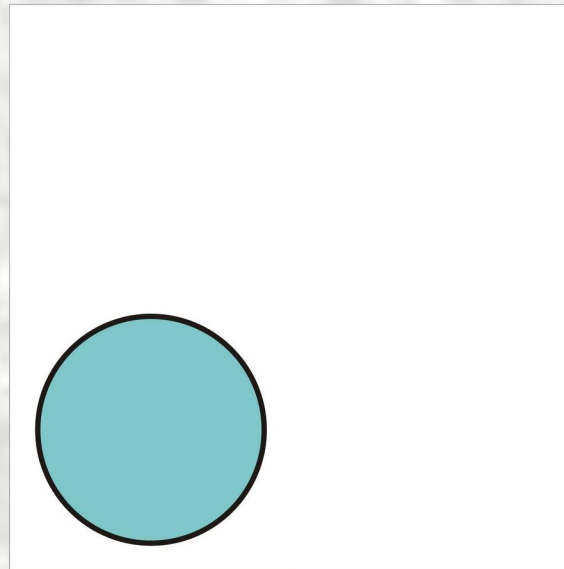
N байт



M байт

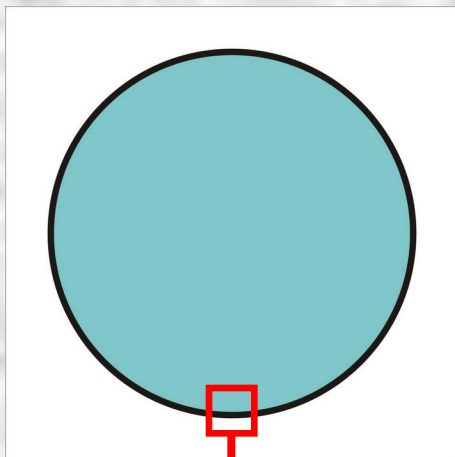


4N байт

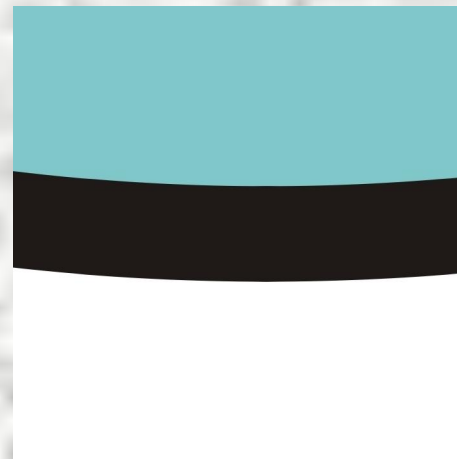
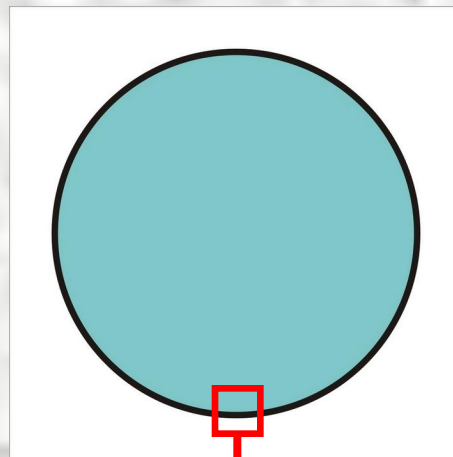


~ M байт

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 three tabs: '1-ChemSketch', '2-Copy to 3D', and '3-3D View'.

Список листов файла

ПереклЮчение между программами

Рабочее окно ACD/ChemSketch

The screenshot displays the ACD/3D Viewer window with the following components:

- Menu Bar:** File, Edit, Pages, Tools, Templates, Options, Documents, Add-Ons, I-Lab, ACD/Labs, Help.
- Structure Toolbar:** Contains icons for file operations (Open, Save, Print, etc.), editing (Undo, Redo, Copy, Paste), and viewing (Zoom, Rotate, etc.).
- Scale Bar:** A horizontal ruler at the top of the workspace, ranging from 0 to 210 mm.
- Chemical Structure:** A 2D structure of a substituted benzene ring with a hydroxyl group (-OH), a methylammonium group (-NH₃⁺), and a propionic acid side chain (-CH₂-CH₂-COOH).
- Right Panel:** A vertical toolbar containing various chemical fragments and functional groups such as -Bu, -Pr, COCH₃, COOH, COPh, NO₂, OAc, SO₂H, and PO₂H₂.
- Bottom Bar:** Includes a color calibration strip, a status bar with text like "ACD/Labs RSS Feed", "I-Lab Login", and "Page 1/1", and a tabbed interface with "1-ChemSketch", "2-Copy to 3D", and "3-3D View".

Three red arrows point to specific toolbars with the following labels:

- Кнопки для работы с файлами** (Buttons for file work) - points to the top toolbar.
- Кнопки для редактирования** (Buttons for editing) - points to the middle toolbar.
- Кнопки для изменения масштаба** (Buttons for scale change) - points to the right toolbar.

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 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 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, one to the 'Edit' icon, and one to the 'View' icon.

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 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 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 the atom list. Another red arrow points from the text 'Часто используемые атомы' to the highlighted atoms. A third red arrow points from the text 'Дополнительные атомы (последние использованные)' to the atoms Br, Ac, and Mg. To the right of the atom list is a chemical structure of a molecule: a benzene ring with a hydroxyl group (HO-) attached, connected to a chain of three carbons. The second carbon in the chain has an ammonium group (-NH₃⁺) attached, and the third carbon has a carbonyl group (=O) attached.

Периодическая таблица

Часто используемые атомы

Дополнительные атомы
(последние использованные)

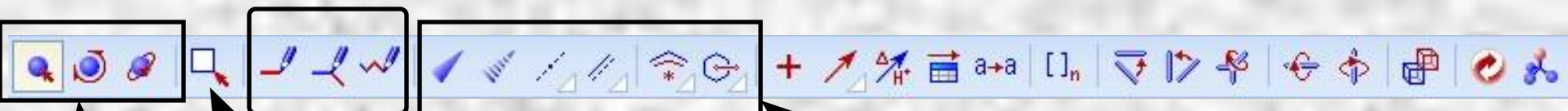
Работа с атомами

Periodic Table of Elements

1											18							
H											He							
2											13	14	15	16	17	18		
Li	Be											B	C	N	O	F	Ne	
3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18			
Na	Mg	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
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

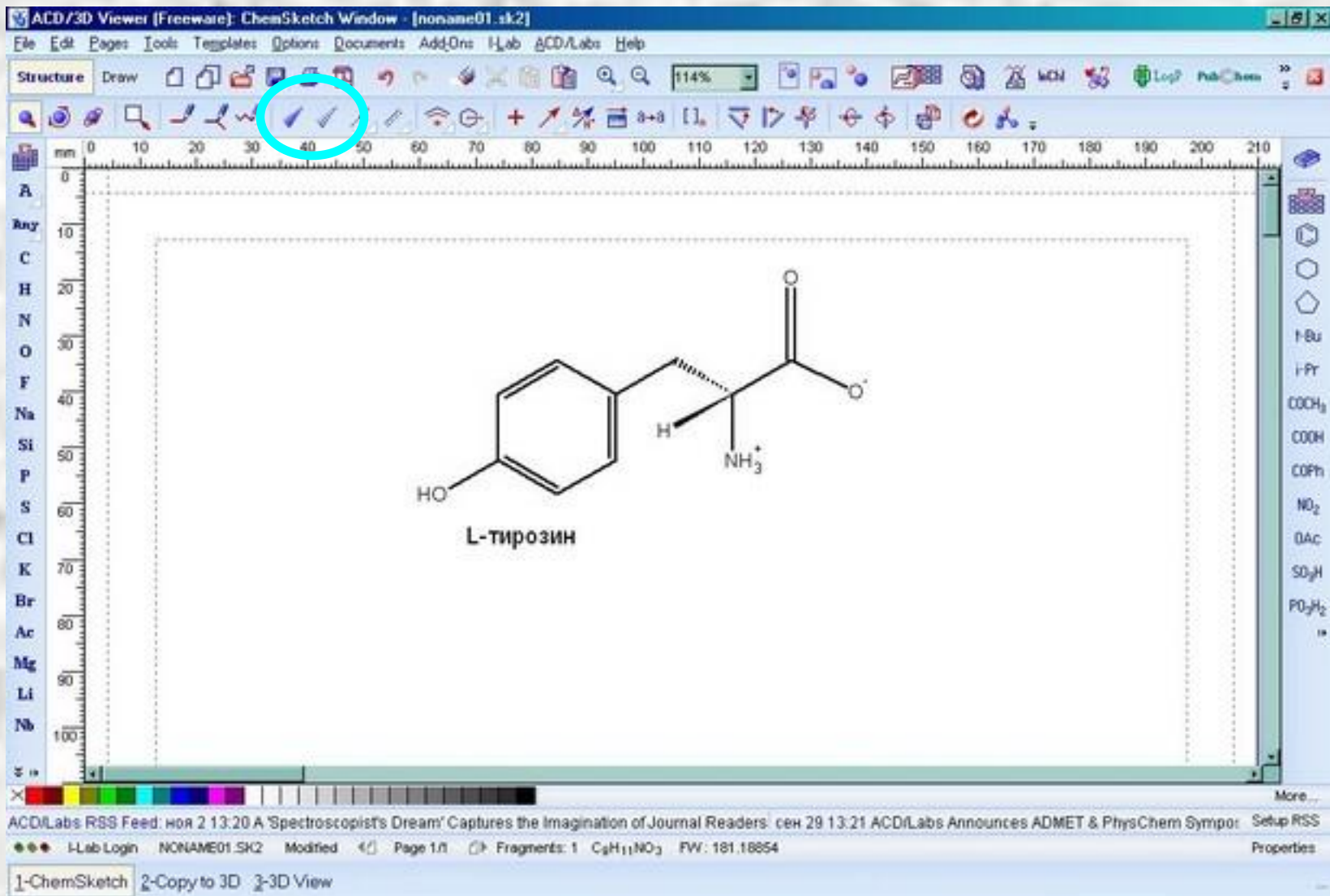
The screenshot displays the ACD/3D Viewer software window. The main workspace shows the chemical structure of Tyrosine (Tyr; Y), which consists of a benzene ring with a hydroxyl group (-OH) at the para position, a methylene group (-CH₂-), an amino group (-NH₃⁺), and a carboxylate group (-COO⁻). The structure 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 circles. A blue arrow points from the text "Кнопки для создания новых объектов" to this toolbar.

Below the structure, the text "Тирозин (Тур; Y)" is displayed. At the bottom of the window, there is a status bar with information about the software version and user login.

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 ethylammonium side chain (-CH2-CH(NH3+)COO-) at the other para position. 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 3D view icon circled in green. A vertical list of chemical groups is visible on the right side. The status bar at the bottom shows the current document name, date, time, and page information, along with a blue arrow pointing to the "3-3D View" button.

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

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

Structure Draw

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

0
10
20
30
40
50
60
70
80
90
100

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

L-тирозин

COOCH₃
COOH
COPh
NO₂
OAc
SO₂H
PO₂H₂

сен 29 13:21 ACD/Labs Ann... nces 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 NOV... K2 Modified Page 1.0 Fragments: 1 C₉H₁₁NO₃ FW: 181.18854 Properties

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

Построение трехмерных структур

