

ACD ChemSketch

Факультет Биоинженерии и Биоинформатики

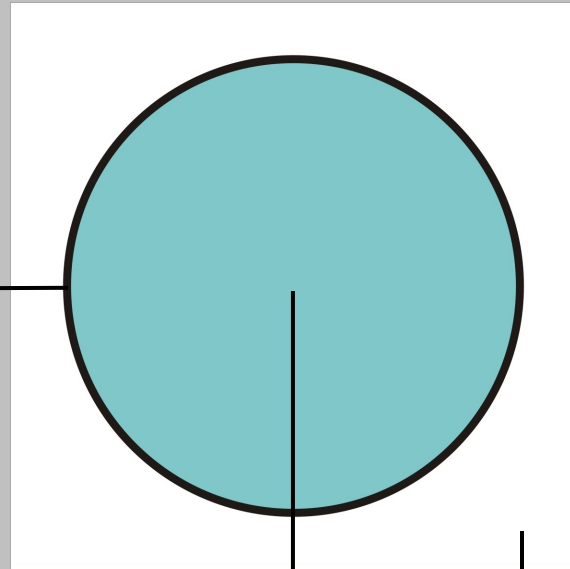
I семестр

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



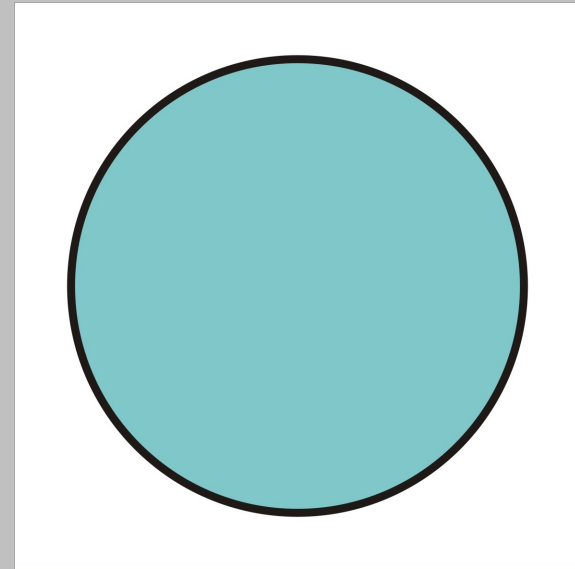
(50;50) цвет: #00FFFF

(10;50) цвет: #000000

(10;50) цвет: #FFFFFF

И так – для каждой точки

Векторная графика



объект: эллипс

центр: (50;50)

ширина: 80

высота: 80

толщина линии: 2

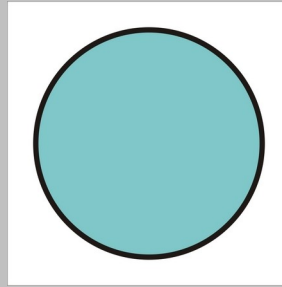
цвет заливки: #00FFFF

цвет линии: #000000

Растровая графика

Векторная графика

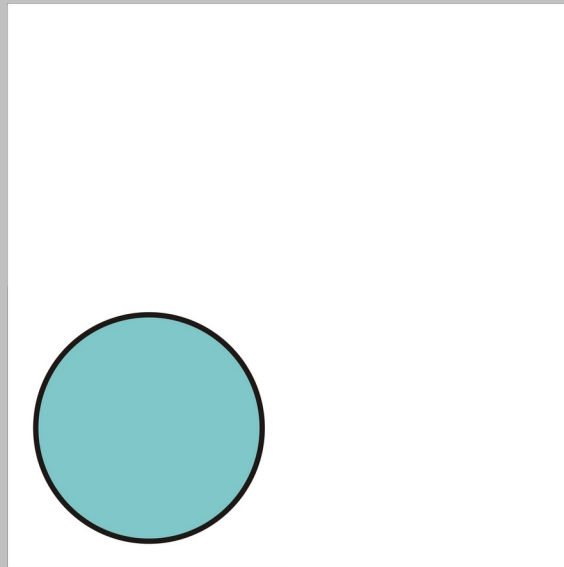
N байт



M байт

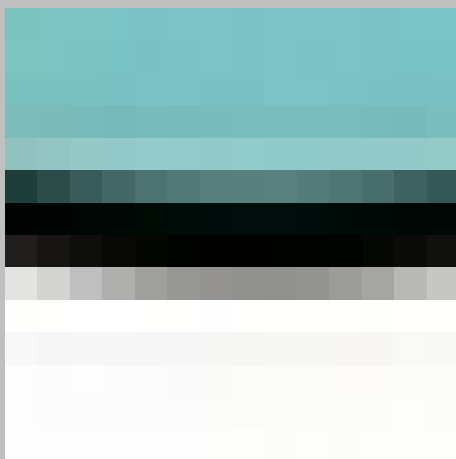
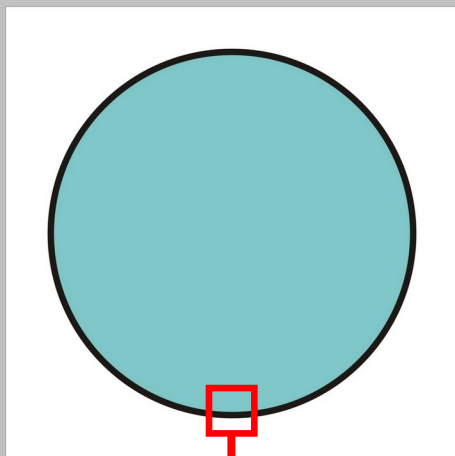


4N байт

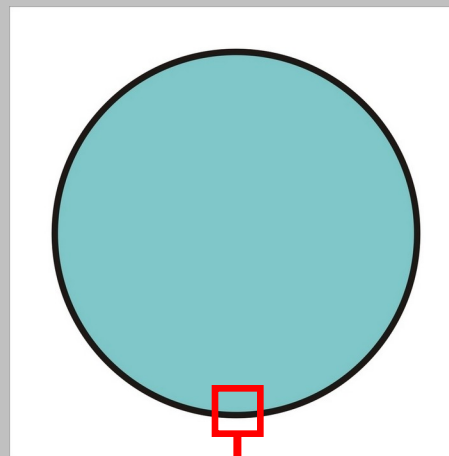


~ M байт

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 pre-defined 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 C₉H₁₁NO₃ 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 methylammonium group, and a propionic acid side chain. 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 a status bar at the bottom provides information about the current document and fragments.

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

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 with magnifying glass), one to the 'Erase' icon (eraser), and one to the 'Zoom' icon (magnifying glass with plus sign).

Кнопки для работы с файлами

Кнопки для редактирования

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

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

Панель инструментов

Кнопки для работы с атомами

HO

NH₃⁺

COO⁻

More...

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

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 chemical symbols: A, Any, C, H, N, O, F, Na, Si, P, S, Cl, K, Br, Ac, Mg. A red oval highlights the symbols C, H, N, O, F, Na, Si, P, S, Cl, K. A red arrow points from the text 'Периодическая таблица' to the top of this list. Another red arrow points from the text 'Дополнительные атомы (последние использованные)' to the symbols Ac and Mg. In the center-right, a chemical structure is shown: a benzene ring with a hydroxyl group (HO-) at the para position, a propyl chain attached to the ring, and a primary amine group (-NH₃⁺) at the end of the propyl chain. The text 'Часто используемые атомы' is placed to the left of this structure.

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	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

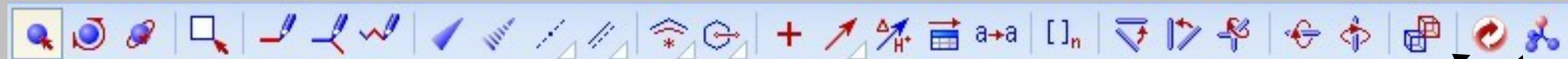
Полимеры

Изменение положения
связей в пространстве

Вращение молекулы
относительно связи

«Клонирование»
структуры

Панель инструментов



Плоская
оптимизация
структуры

Объемная
оптимизация
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 (-NH₃⁺) and a carboxylate group (-COO⁻).

Кнопки для редактирования объектов

Кнопки для создания новых объектов

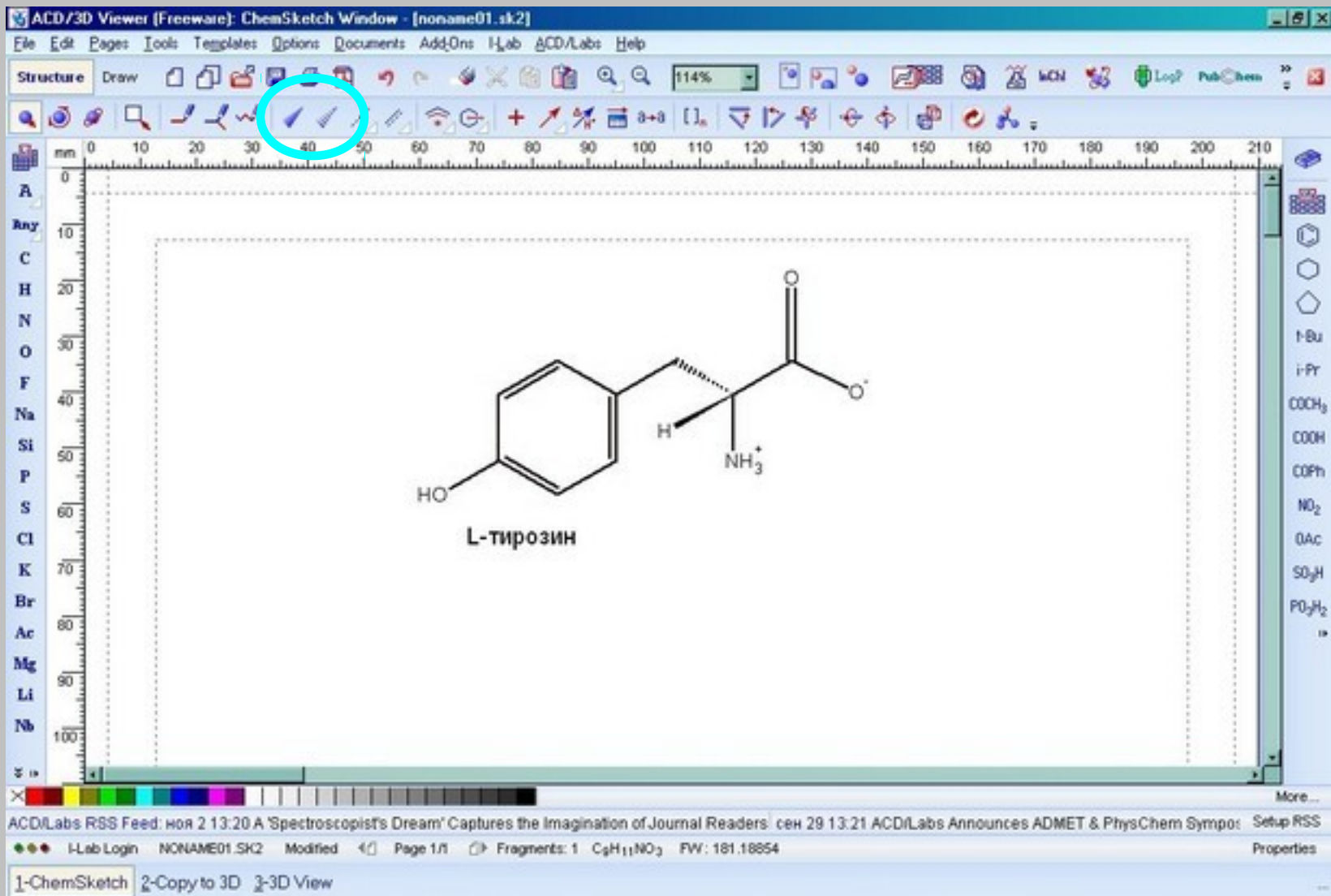
Тирозин (Тур; Y)

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

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 is a benzene ring with a hydroxyl group at the para position and an ethylamine side chain at the other para position. The side chain consists of a methylene group attached to a chiral carbon, which is also bonded to an amino group (NH₃⁺) and a carboxylate group (COO⁻). The stereochemistry is indicated with wedged and dashed bonds. The software 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 list of chemical groups on the right side. A blue arrow points to the "3D View" button in the bottom status bar.

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

Инструменты: Draw, Structure, 3D View (circled in green)

Вертикальный список групп: C, H, N, O, F, Na, Si, P, S, Cl, K, Br, Ac, Mg, Li, Nb, COCH₃, COOH, COPh, NO₂, OAc, SO₂H, PO₃H₂

Статусная строка: 1-ChemSketch 2-Copy to 3D 3-3D View

Построение трехмерных структур

