

Techniki informatyczne laboratoria komputerowe

**ACD/ChemSketch –
generator**

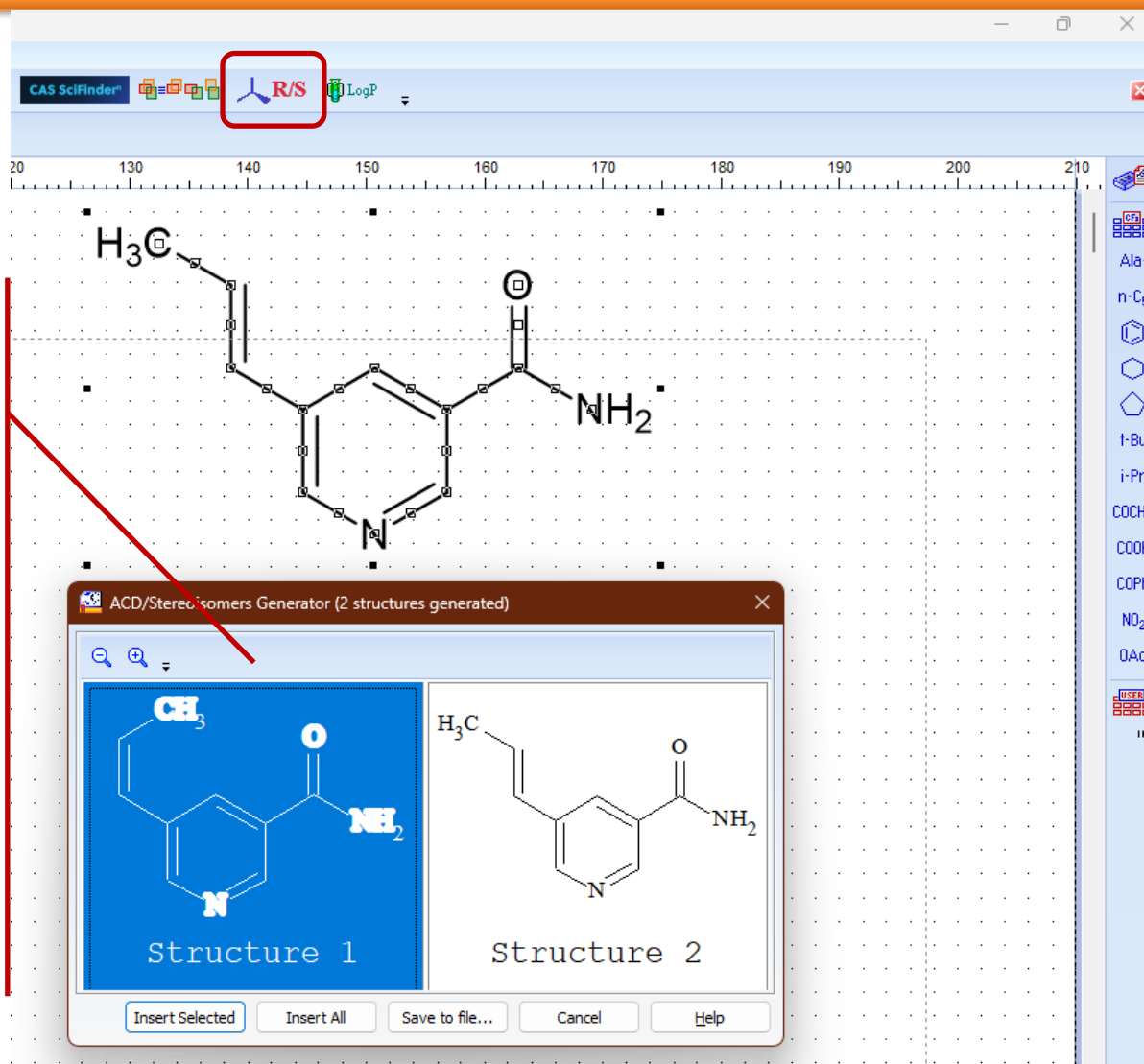
Tomasz Lubera

Enumerate Markush Structure

Narzędzie tworzy wszystkie możliwe cząsteczki odpowiadające strukturze Markusha

The screenshot shows the ChemSketch interface. At the top, there are icons for CAS SciFinder, R/S, and LogP. The main workspace contains a chemical structure of a pyridine ring with a methyl group (H₃C), a chlorine atom (Cl), and an amide group (NH₂). A red circle highlights the chlorine atom, and a red arrow points from a tooltip labeled 'Tworzenie wiązań Markuscha' to it. The tooltip shows icons for creating bonds to various atoms (C, N, O, S, P, M). Below the main workspace, a dialog box titled 'ACD/Enumerate Markush Structures (3 structures generated)' is open, displaying three generated structures: Structure 1 (with Cl at position 4), Structure 2 (with Cl at position 5), and Structure 3 (with Cl at position 6). The dialog box has buttons for 'Insert Selected', 'Insert All', 'Save to file...', 'Cancel', and 'Help'.

Stereoisomers generator



Narzędzie tworzy wszystkie możliwe stereoizomery dla danej substancji

Check tautomeric forms

The screenshot shows the ChemSketch interface. The top toolbar contains various icons, with the 'Check Tautomeric Forms' icon (a double-headed arrow) highlighted by a red box. Below the toolbar, a chemical structure is displayed on a grid background. The structure consists of a pyridine ring with a methyl group (H_3C) at the 2-position and a hydroxyl group (OH) at the 4-position. The hydroxyl group is shown as a neutral OH rather than an ionic O^- . Below the main window, a dialog box titled 'Check Tautomeric Forms' is open. It displays the message '2 possible tautomeric forms were suggested'. The first structure shown in the dialog is the same as the one in the main window, but with the hydroxyl group shown as a neutral OH instead of an ionic O^- . The dialog box includes buttons for 'Replace', 'Copy', 'Copy All', 'Help', '<< Prev.', 'Presumed major form', 'Next >>', and 'Cancel'.

Narzędzie tworzy wszystkie możliwe tautomery dla danej struktury i wskazuje najbardziej prawdopodobną z nich

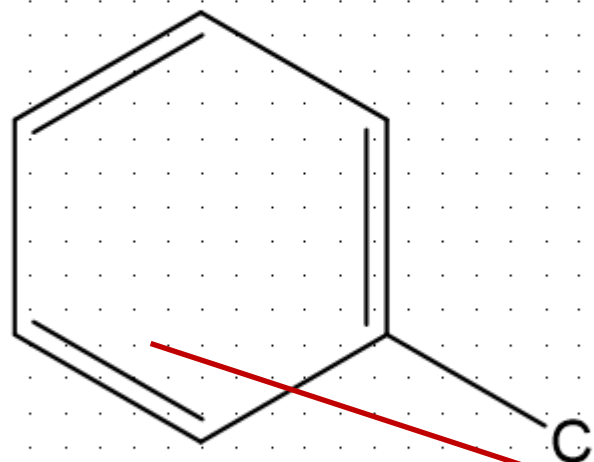
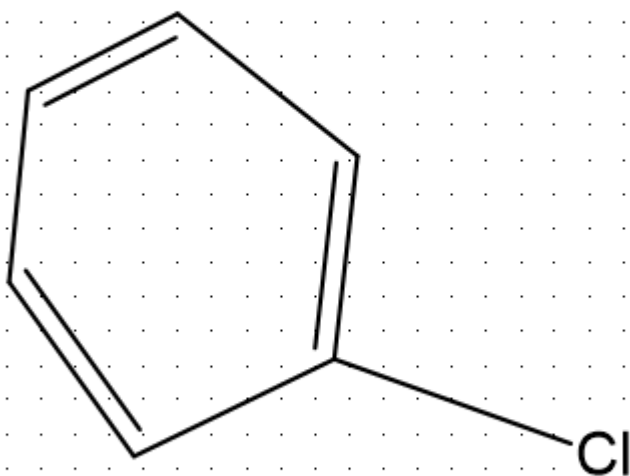
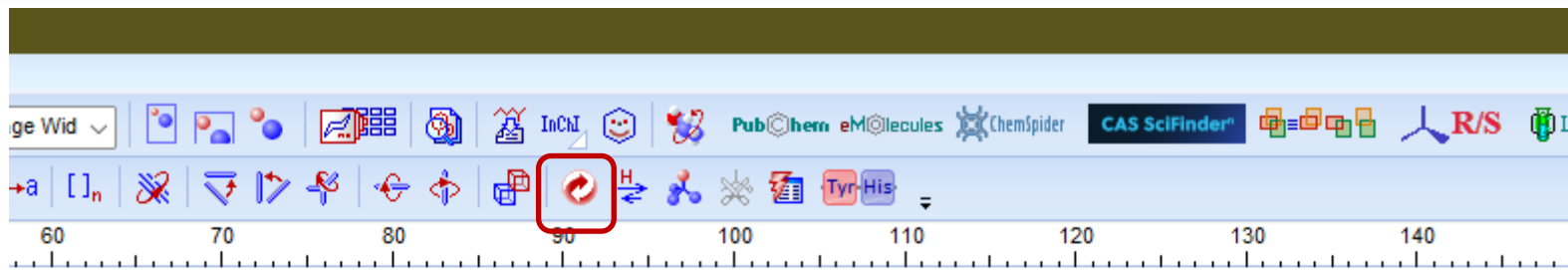
Biosequence Tools

Narzędzie pozwala tworzyć wzory polipeptydów przez wpisywanie symboli (litery lub skrótów 3 literowe) kolejnych aminokwasów.

The screenshot displays the Biosequence Tools interface. At the top, a toolbar contains various icons, with 'Tyr-His' highlighted in a red box. Below the toolbar, a sequence editor shows 'Ala Asp Phe' entered in a purple box. A 'Biosequence Expand Options' dialog box is open, showing '120° Chain' selected. Below the dialog, a 3D ball-and-stick model of the tripeptide Ala-Asp-Phe is shown. The interface includes a list of amino acids (Standard Acids, Non-Standard Acids, Groups, and Linkers) and a structure preview area.

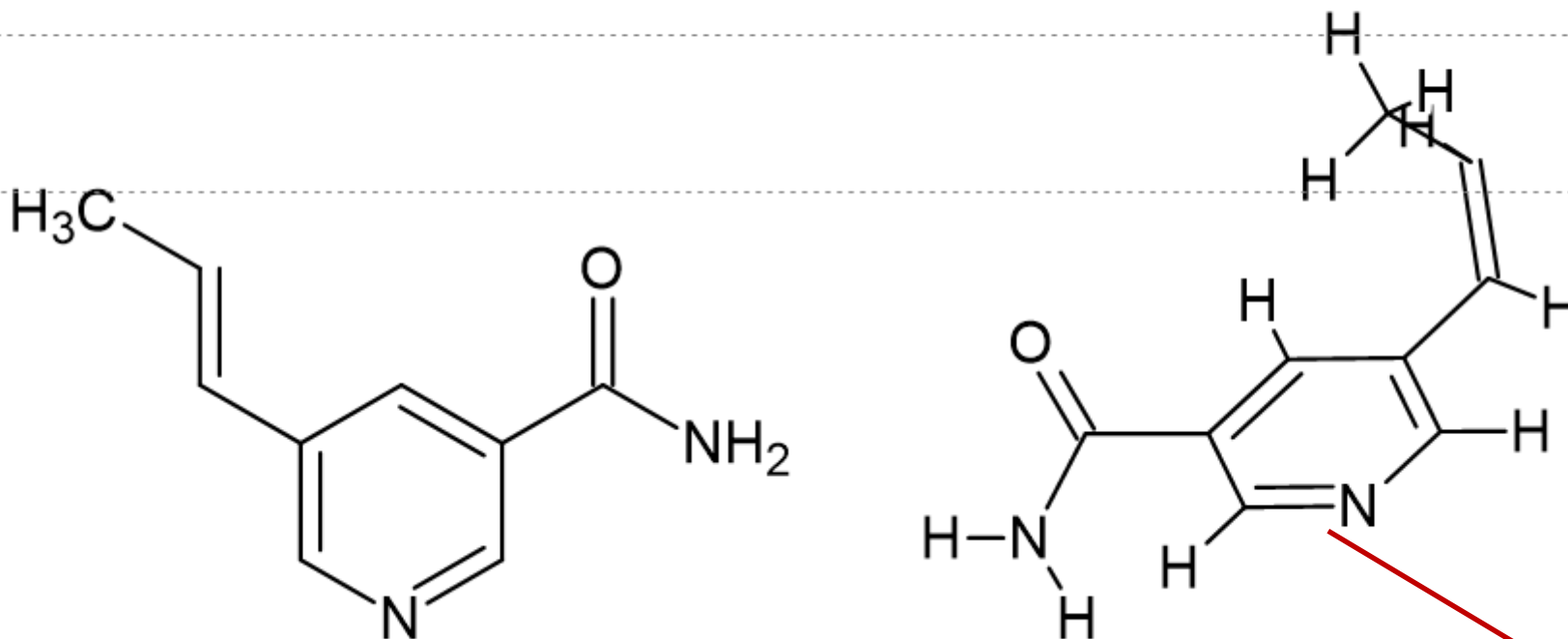
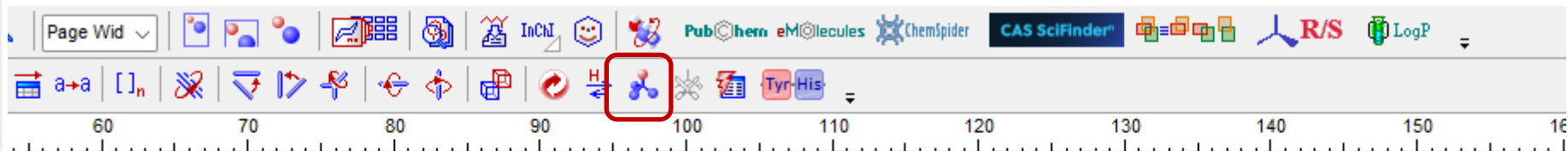
Narzędzie pozwala generować z zapisu liniowego wzór półstrukturalny.

Clean Structure



Narzędzie pozwala oczyścić strukturę poprzez wyrównanie długości wiązań i poprawę kątów.

3D optimization



Narzędzie pozwala zoptymalizować przestrzenny rozkład atomów w zadanej strukturze.

Calculate Selected Properties

The screenshot displays the ChemSketch software interface. At the top, a toolbar contains various icons, with the 'Calculate' icon (a document with a checkmark) highlighted by a red box. Below the toolbar is a ruler and a chemical structure of a pyridine ring substituted with a methyl group (H₃C) and an amide group (NH₂). A 'Calculation Results' dialog box is open in the foreground, displaying the following data:

Calculation Results	
Molecular Formula:	C ₉ H ₁₀ N ₂ O
Formula Weight:	162.192
Composition:	C(66.65%) H(6.21%) N(17.27%) O(9.86%)
Molar Refractivity:	49.16 ± 0.3 cm ³
Molar Volume:	142.3 ± 3.0 cm ³
Parachor:	378.8 ± 4.0 cm ³
Index of Refraction:	1.607 ± 0.02
Surface Tension:	50.1 ± 3.0 dyne/cm
Density:	1.139 ± 0.06 g/cm ³
Dielectric Constant:	Not available

At the bottom of the dialog box, there are four buttons: 'Select Properties', 'Copy To Editor', 'Cancel', and 'Help'.

Narzędzie oblicza wybrane właściwości dla wskazanej struktury

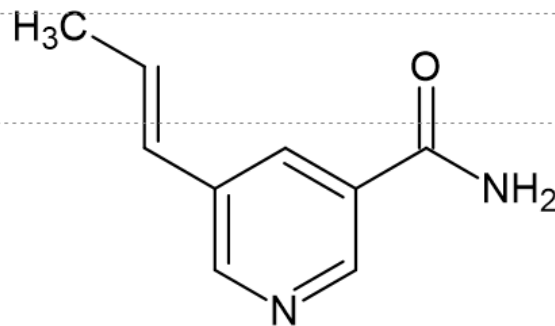
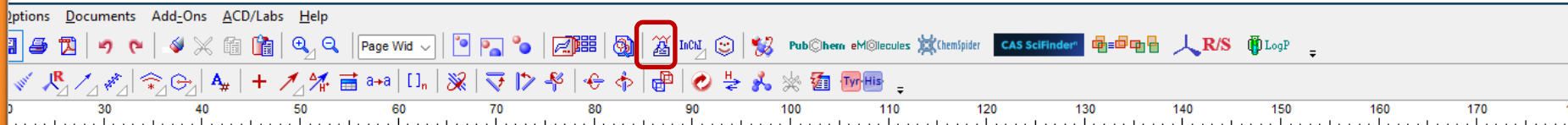
Calculate logP

Log(P) – logarytm dziesiętny ze współczynnika podziału danej substancji pomiędzy oktanol i wodę.

The screenshot shows the ChemSketch interface with the LogP calculation window open. The window title is "LogP (v.14.51)". The "Calculated LogP" is displayed as "1.14+/- 0.25". Below this, there are two informational sections: "Interested how this value was calculated? Want to compare it with experimental data?" with a link to "Learn more about ACD/LogP DB", and "Does your compound contain ionizable groups? You should consider using the pH dependent octanol-water distribution coefficient, logD" with a link to "Learn more about ACD/LogD". At the bottom of the window, it says "Visit our Web site: www.acdlabs.com" and has an "Ok" button. A red arrow points from the "Ok" button to the text below. The chemical structure shown is N-propylbenzamide, with a methyl group (H₃C) at the end of the propyl chain and an amide group (NH₂) attached to the benzene ring.

Narzędzie oblicza log(P) dla wskazanej struktury

Generate name for structure

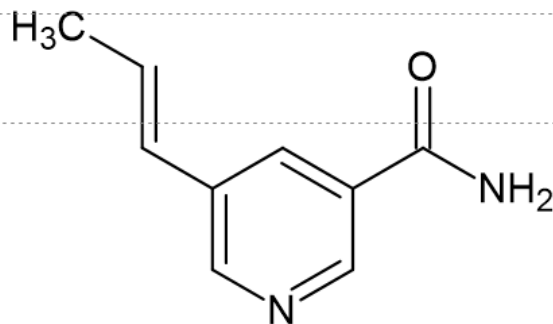


5-[(1*E*)-prop-1-en-1-yl]pyridine-3-carboxamide

Narzędzie tworzy nazwę dla wskazanej struktury

InChI for structure

InChI (ang. International Chemical Identifier) – identyfikator stosowany dla substancji chemicznych, wprowadzony w 2005 roku przez IUPAC.

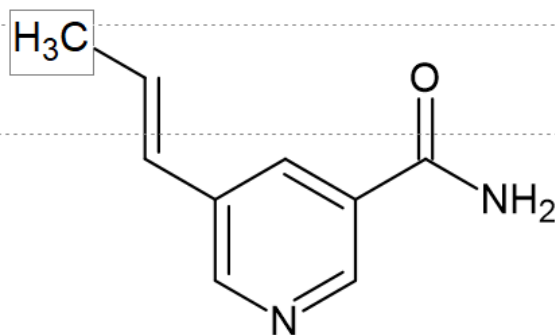
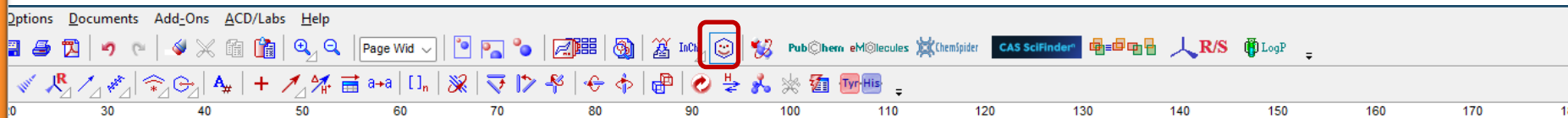


InChI=1S/C9H10N2O/c1-2-3-7-4-8(9(10)12)6-11-5-7/h2-6H,1H3,(H2,10,12)/b3-2+

Narzędzie tworzy InChI dla wskazanej struktury

SMILES notation

SMILES (ang. Simplified Molecular Input Line Entry Specification) – sposób jednoznacznego zapisu struktury cząsteczek związków chemicznych z wykorzystaniem ciągu znaków ASCII.



O=C(N)c1ccc(C)cc1

Narzędzie tworzy zapis SMILES dla wskazanej struktury

Koniec