

**Meno:** Miriama Chmúriková, F17039

**Predmet:** Molekulárne základy vývoja liečiv

**Šk. rok:** 2019/2020

**Zistenie závislosti účinnosti a  
stérickom štruktúrnom paran**

Hľadáme závislosť  $A = f(v)$  tvare

**ZADANIE:**

Korelácia toxicity vyjadrenej a  
 $\log P$  (oktanol/voda) pre súbo  
lidokain, trimekain, prilokain,  
korelácia potvrdí ( $r > 0,6$ ), vyř  
Pokiaľ LD50 nebude korelovať

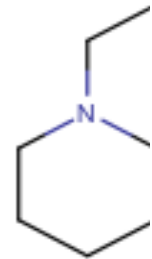
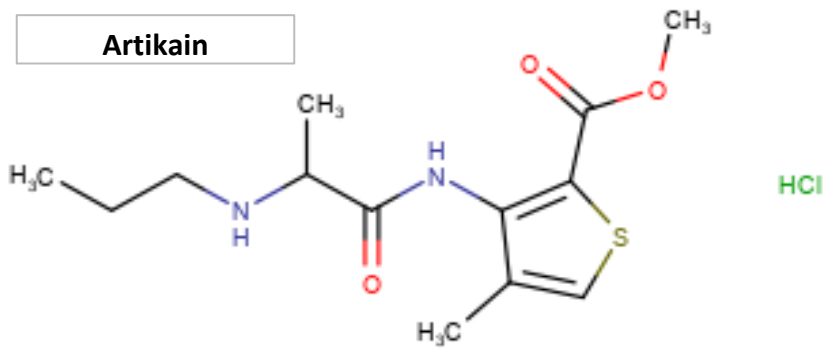
## **PRAKTIKUM Z QSAR**

**lebo toxicity lokálnych anestetík na hydrofóbnom čí  
netri**

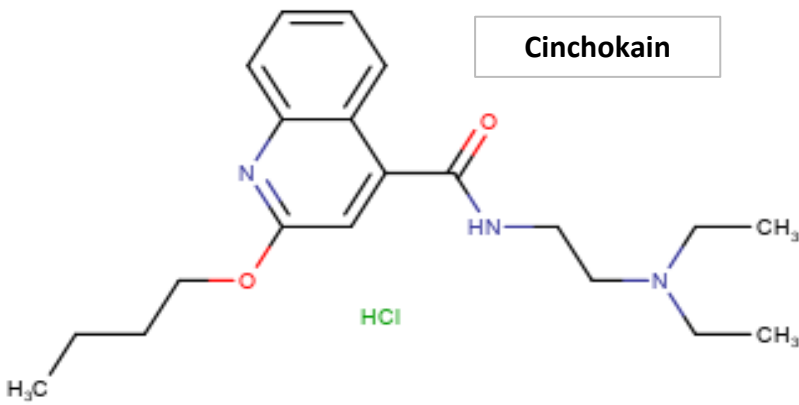
**$\epsilon$  A= a1 x+ b** alebo v tvare  **$A= a1 x^2 + a2 x + b$**

iko LD50 i.v. pre myš s experimentálne stanovenou hodnotou  
r artikain, bupivakain, ropivakain, cinchokain, kokain,  
prokainamid, prokain, tetrakain, trapenkain. Pokiaľ sa  
počítajte predpokladanú LD50 i.v. propyl-4-aminobenzoátu.  
ť, skúste  $\log(1/ LD50)$ .

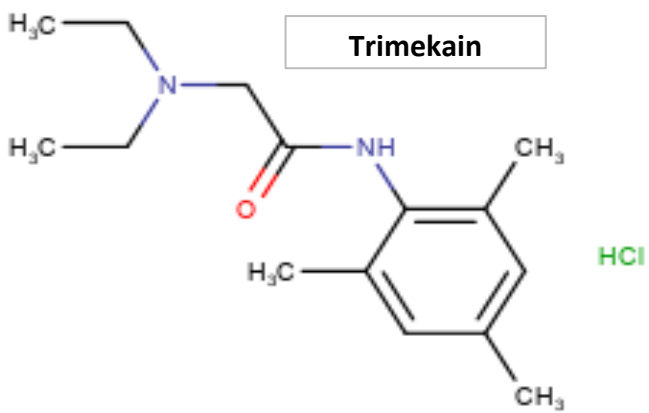
Artikain



Cinchokain



Trimekain

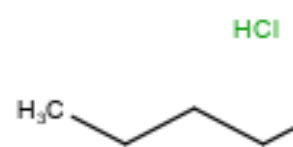
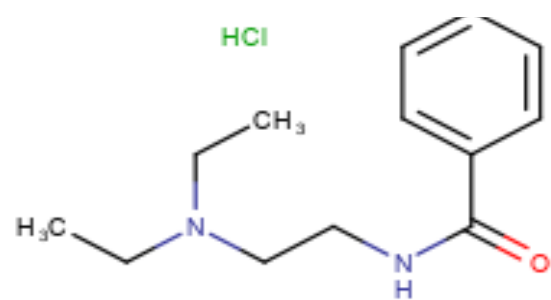


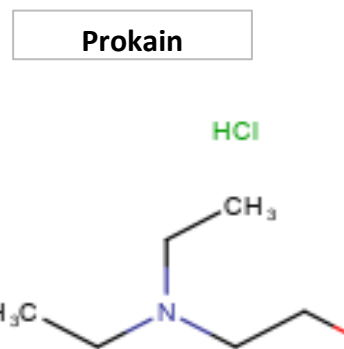
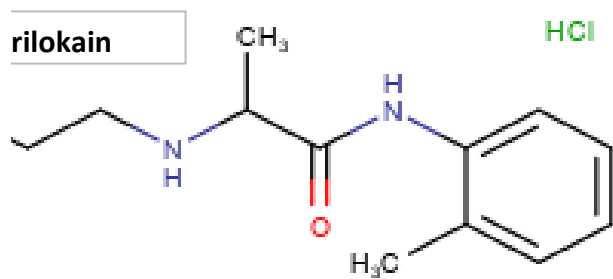
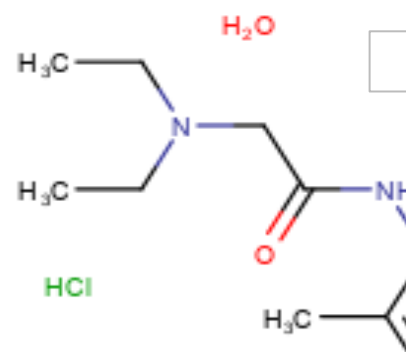
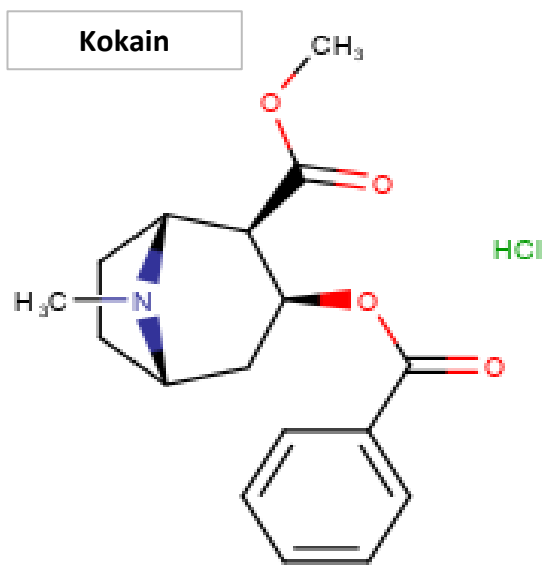
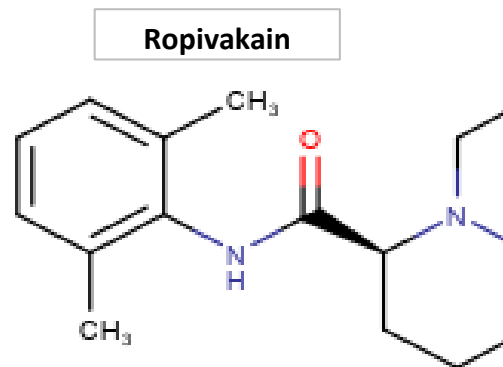
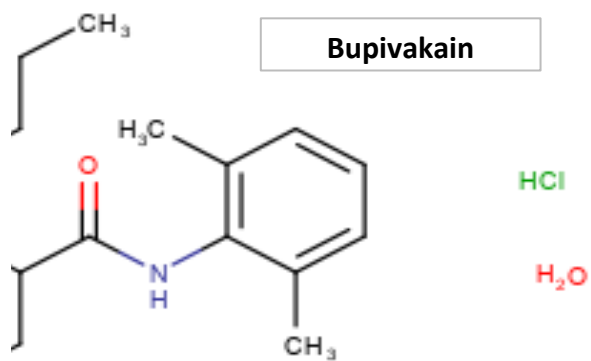
Pi

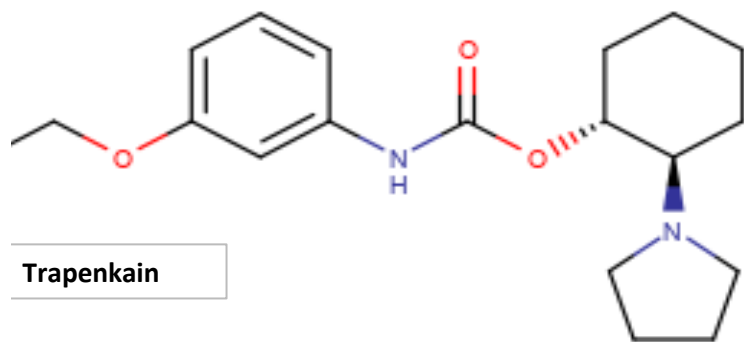
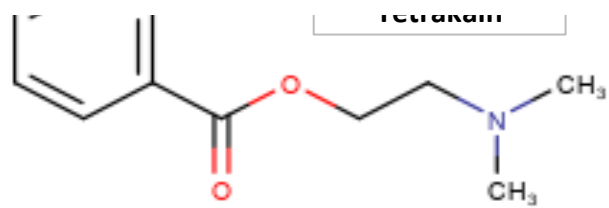


Prokainamid







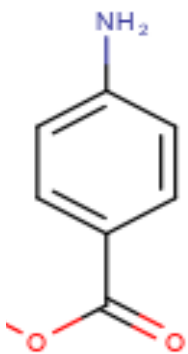
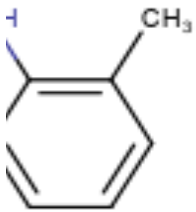




HCl



Lidokain



## VSTUPNÉ DÁTA:

	x	y
	HYDROFÓBNY PARAMETER	AKTIVITA
Názov látky	log P	log (1/LD50)
prokainamid	0.88	-1.98
prilokain	1.4	-1.74
artikain	1.7	-1.57
prokain	2.03	-1.72
kokain	2.3	-1.18
lidokain	2.44	-1.36
cinchokain	2.52	-0.58
ropivakain	2.9	-1.13
trimekain	3.13	-1.7
bupivakain	3.35	-0.79
trapekain	3.41	-1.18
tetrakain	3.51	-1.79



**VÝPOČET:**

a	0.231378538	-1.963488615
smodch a	0.143656577	0.372577932
r <sup>2</sup>	0.205980568	0.402533103
Fisher-Snedecorov test	2.594150208	10
r	0.4539	

**ROVNICA:**  $y = 0,2314x - 1,9635$

**ZÁVER:**

Výpočtom sa nepodarilo preukázať koreláciu log (1/ LD50) s experimentálne stanovenou hodnotou log P (oktanol/voda). Hodnota lineárneho korelačného koeficientu je rovná 0,4539, čo nepredstavuje hodnotu potvrdzujúcu koreláciu ( $r > 0,6$ ).

GRAF:

b  
smoch b  
smoch y  
stupne volnosti df

