

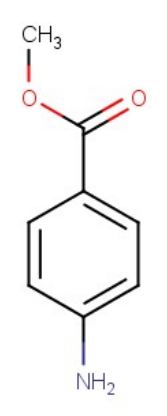
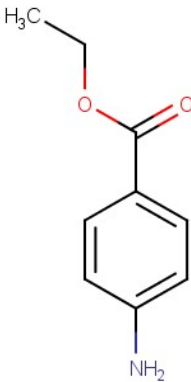
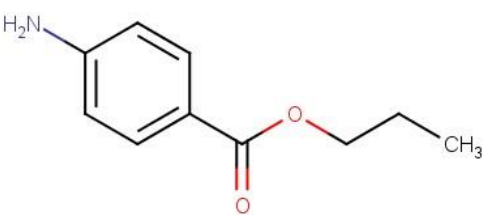
Praktikum z QSAR – zistenie závislosti účinnosti alebo toxicity lokálnych anestetík na hydrofóbnom alebo stérickom štruktúrnom parametri

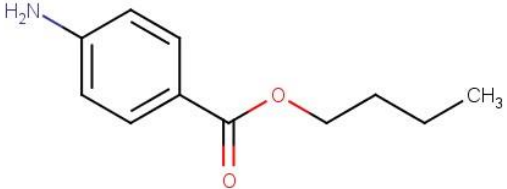
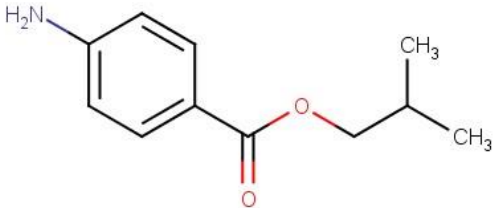
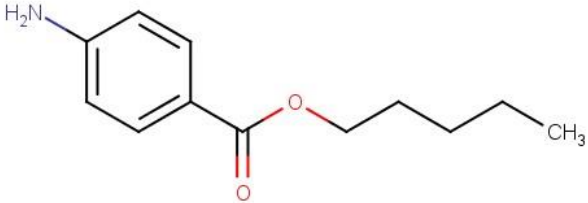
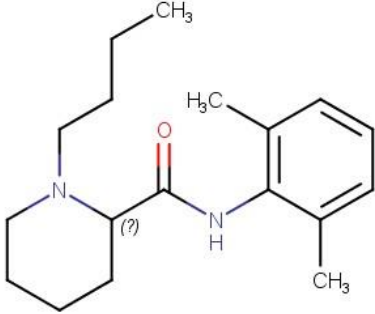
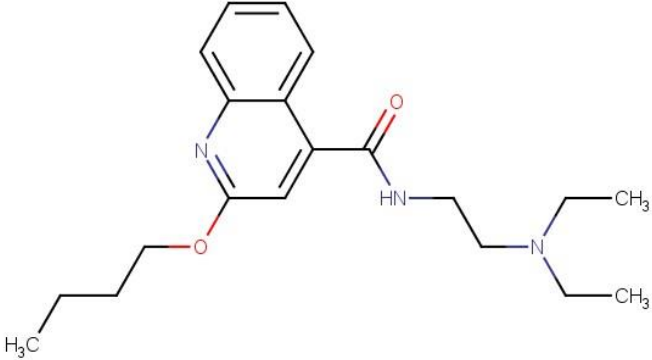
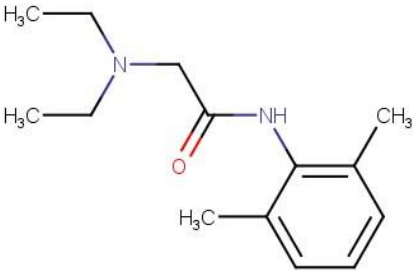
Zuzana Dluhošová

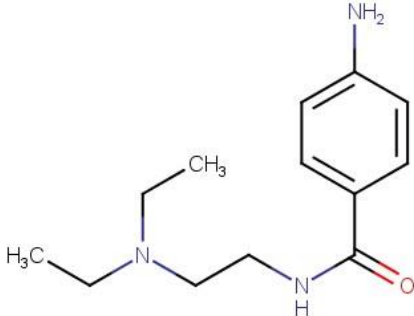
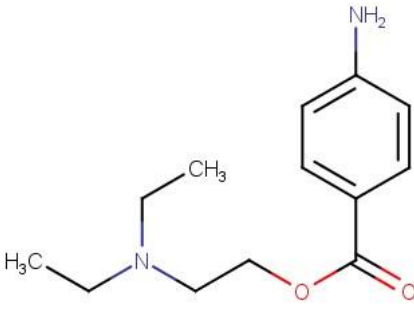

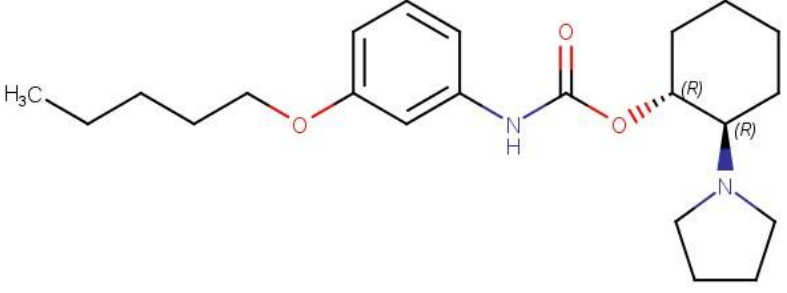
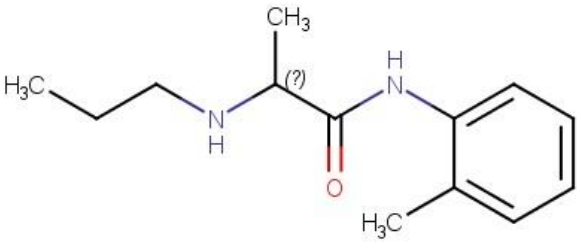
25.4.2020

Úloha:

Korelace toxicity vyjadrené jako LD50 i.p.pro myš s experimentálne stanovenou hodnotou log P(oktanol/voda) pro soubor methyl-4-aminobenzoát, benzokain, propyl-4-aminobenzoát, butyl-4-aminobenzoát, iso-butyl-4-aminobenzoát, pentyl-4-aminobenzoát,bupivakain, cinchokain, lidokain, prokainamid, prokain, tetrakain a trapekain. Pokud se korelace potvrdí ($r \geq 0,6$), vypočtete vypočtete předpokládanou LD50i.p. prilokainu. Pokud LD50 nebude korelovat, zkuste $\log(1/LD50)$.

	log P	LD ₅₀ i.p.	Štruktúry
methyl-4-aminobenzoát	1,63	237	
benzokain	2,15	216	
propyl-4-aminobenzoát	2,82	126	

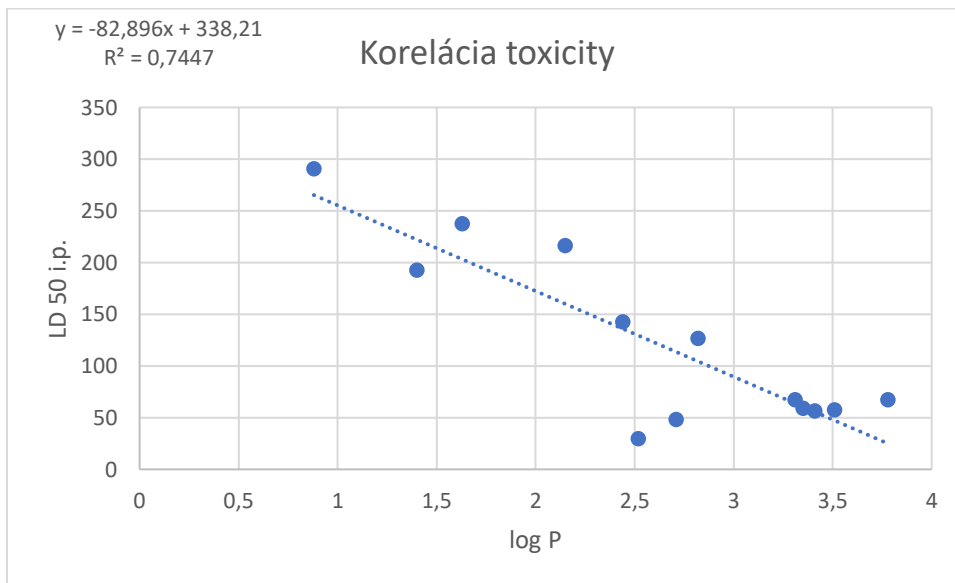
butyl-4-aminobenzoát	3,31	67	
iso-butyl-4-aminobenzoát	2,71	48	
pentyl-4-aminobenzoát	3,78	67	
bupivakain	3,35	58,7	
cinchokain	2,52	29	
lidokain	2,44	142	

prokainamid	0,88	290	
prokain	1,4	192	
tetrakain	3,51	57	
trapekain	3,41	56	
prilokain	1,6	205,5747	

a	-82,89633191	338,2088166	b
	14,63274634	40,18209367	
r²	0,744741899	45,28254427	S_y
F	32,09363725	11	

r = 0,862984298

r ≥ 0,6 – korelácia sa potvrdila



Výpočet pre prilokain:

$$y = -82,896x + 338,21$$

$$y = -82,896 * 1,6 + 338,21 = \underline{\underline{205,5746855}}$$