



Sveučilište u Zagrebu  
Prirodoslovno-matematički fakultet  
Kemijski odsjek



# SELEKTIVNA OKSIDACIJA BENZILNOG ALKOHOLA I NJEGOVIH DERIVATA UZ PRIMJENU RAZLIČITIH KATALIZATORA



Kemijski seminar 1

Izrađen prema radu:

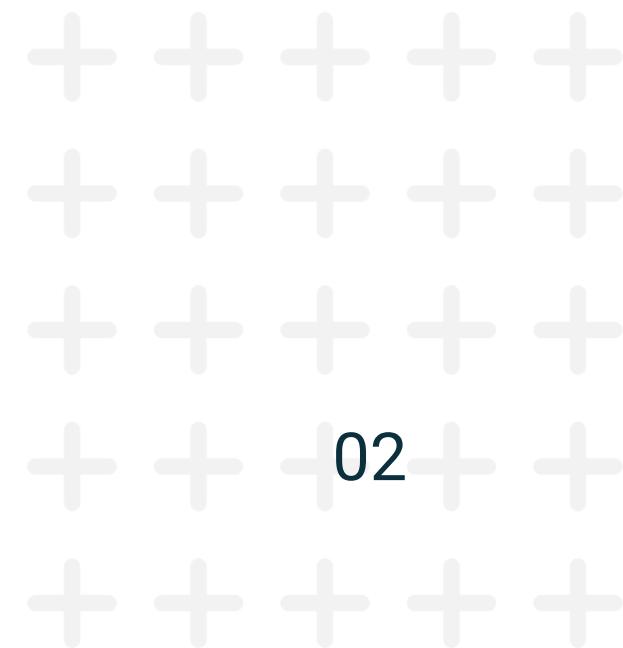
M. M. Heravi, N. Ghalavand, E. Hashemi, *Chemistry* **2** (2020) 101–178.

Josipa Sarjanović

Doktorski studij Kemija - Anorganska i struktturna kemija

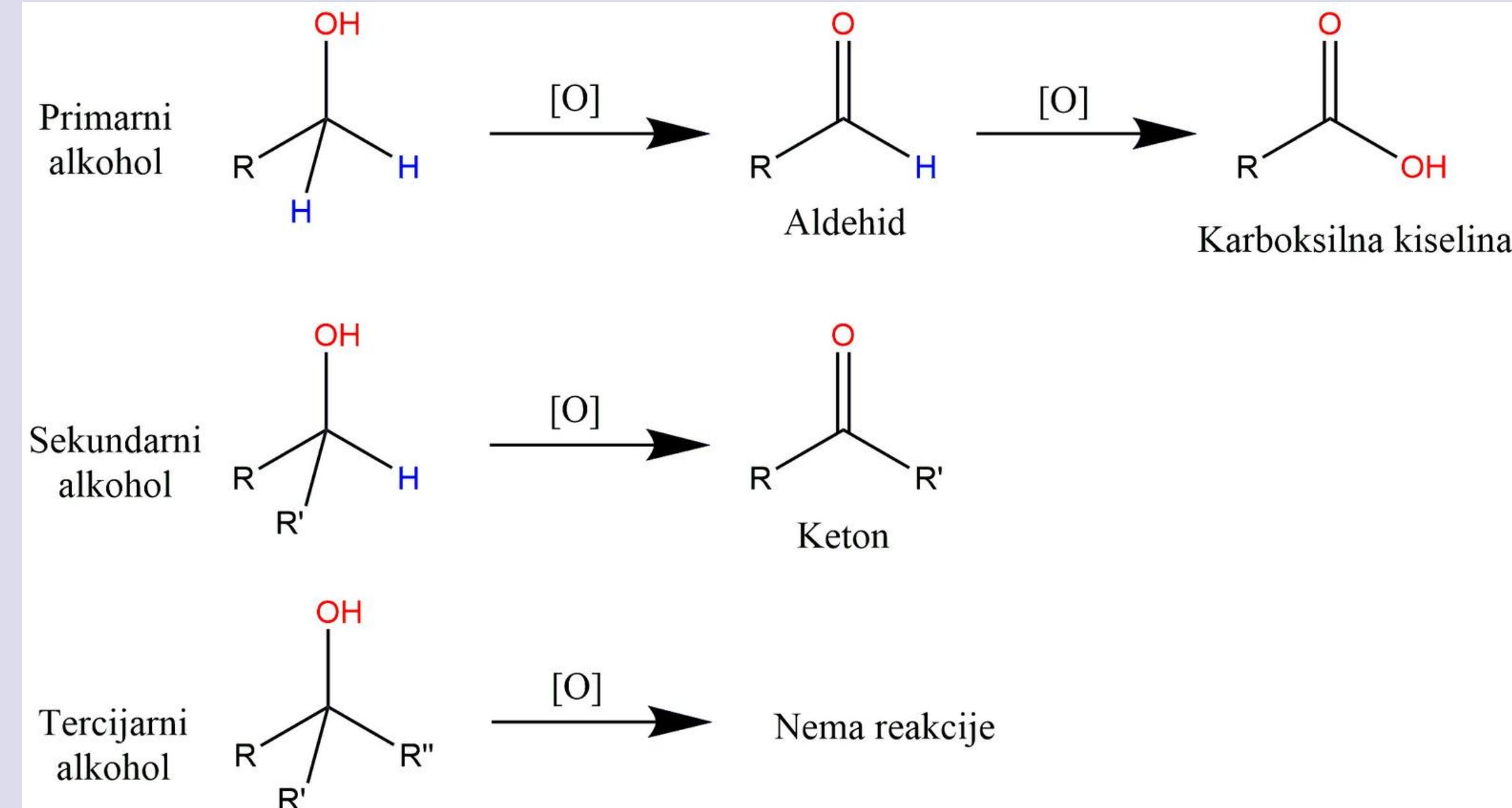


1. Oksidacija alkohola
2. Parametri katalitičkih reakcija
3. Benzilni alkohol
4. Derivati benzilnog alkohola
5. Zaključak

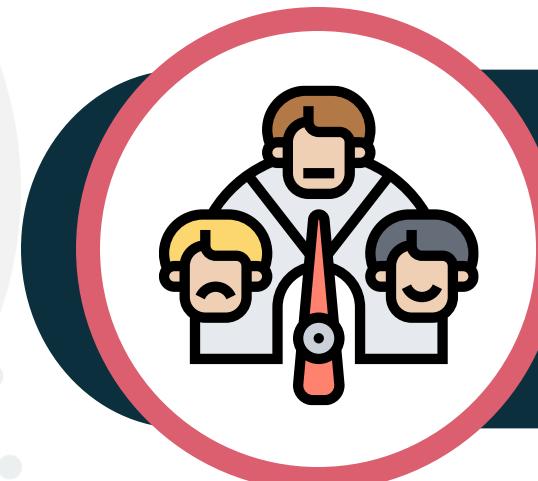




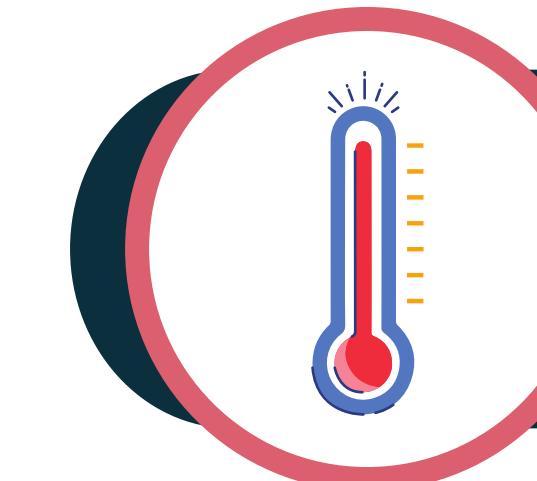
## OKSIDACIJA ALKOHOLA



## PARAMETRI KATALIZE



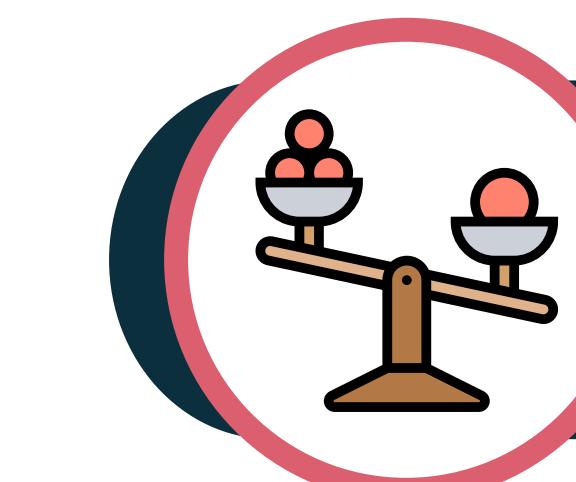
AKTIVNA POVRŠINA KATALIZATORA



TEMPERATURA



TLAK



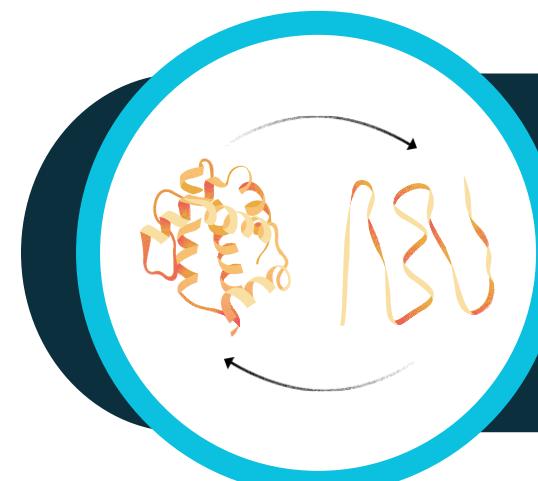
KONCENTRACIJA REAKTANTA /  
KATALIZATORA



VRSTA OKSIDANSA



VRIJEME REAKCIJE



INHIBITORI / PROMOTORI



HOMOGENI / HETEROGENI  
KATALIZATORI

...



# Vodikov peroksid



Djelovanje pri pH  
vrijednosti sedam

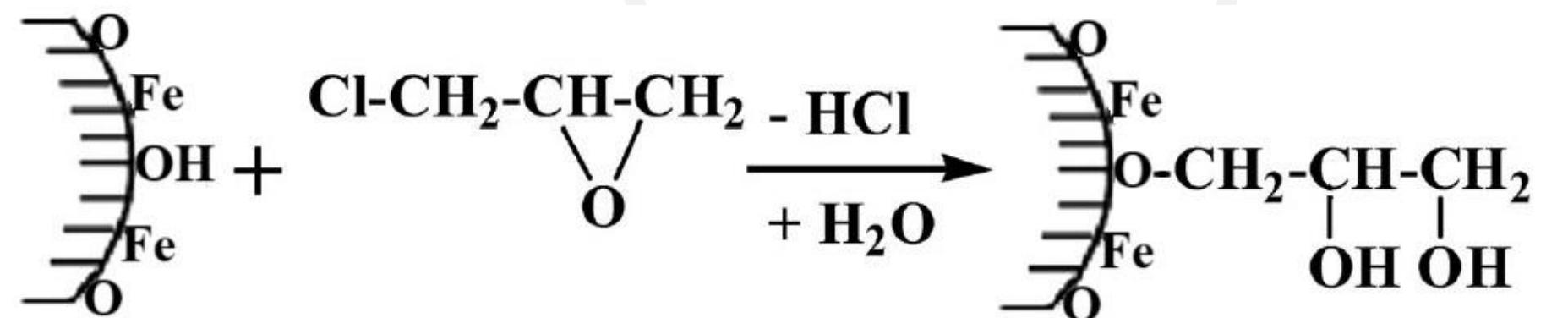


Razgradnja na vodu i kisik



- Visoka selektivnost
- Manje štetnih nusprodukata
- Primjena u različitim industrijama

# Fe<sub>3</sub>O<sub>4</sub>-ECH-D



••—

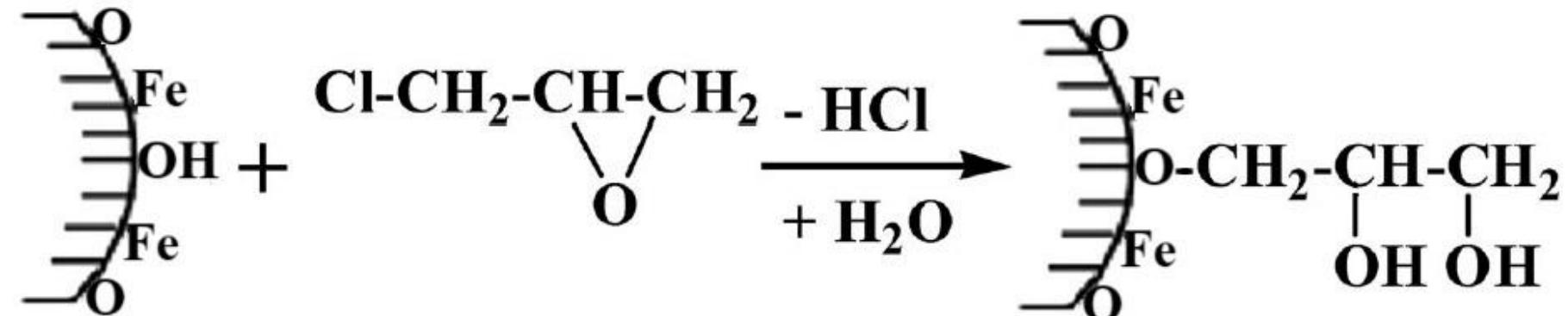
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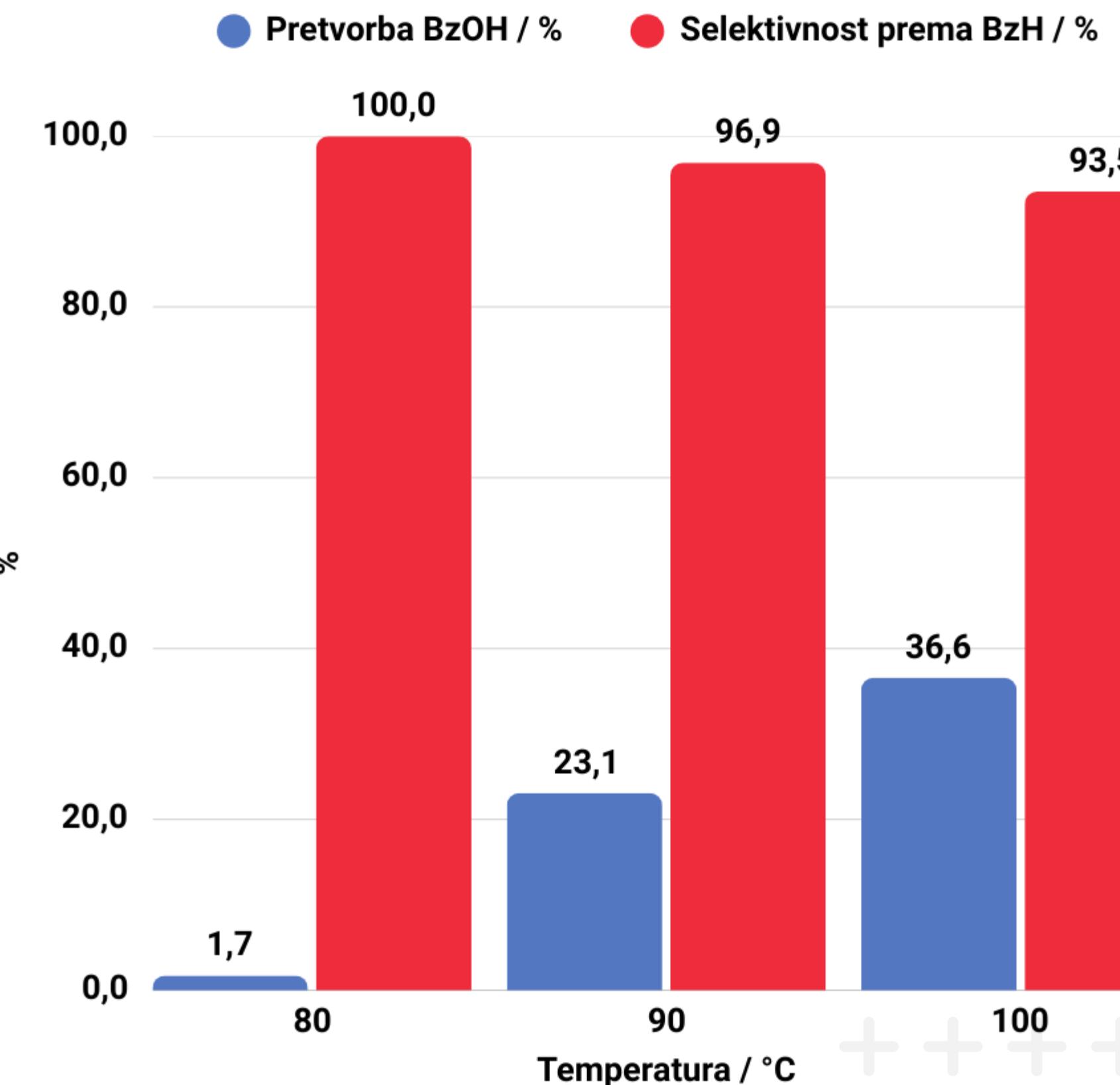
## TEMPERATURA

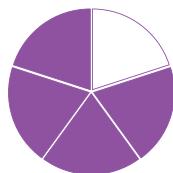
# $\text{Fe}_3\text{O}_4$ -ECH-D



Uvjeti reakcije:

BzOH (40 mmol), katalizator (0,2 g),  
 $\text{H}_2\text{O}_2$  (80 mmol),  $\text{H}_2\text{O}$  (8 mL), 1,5 h



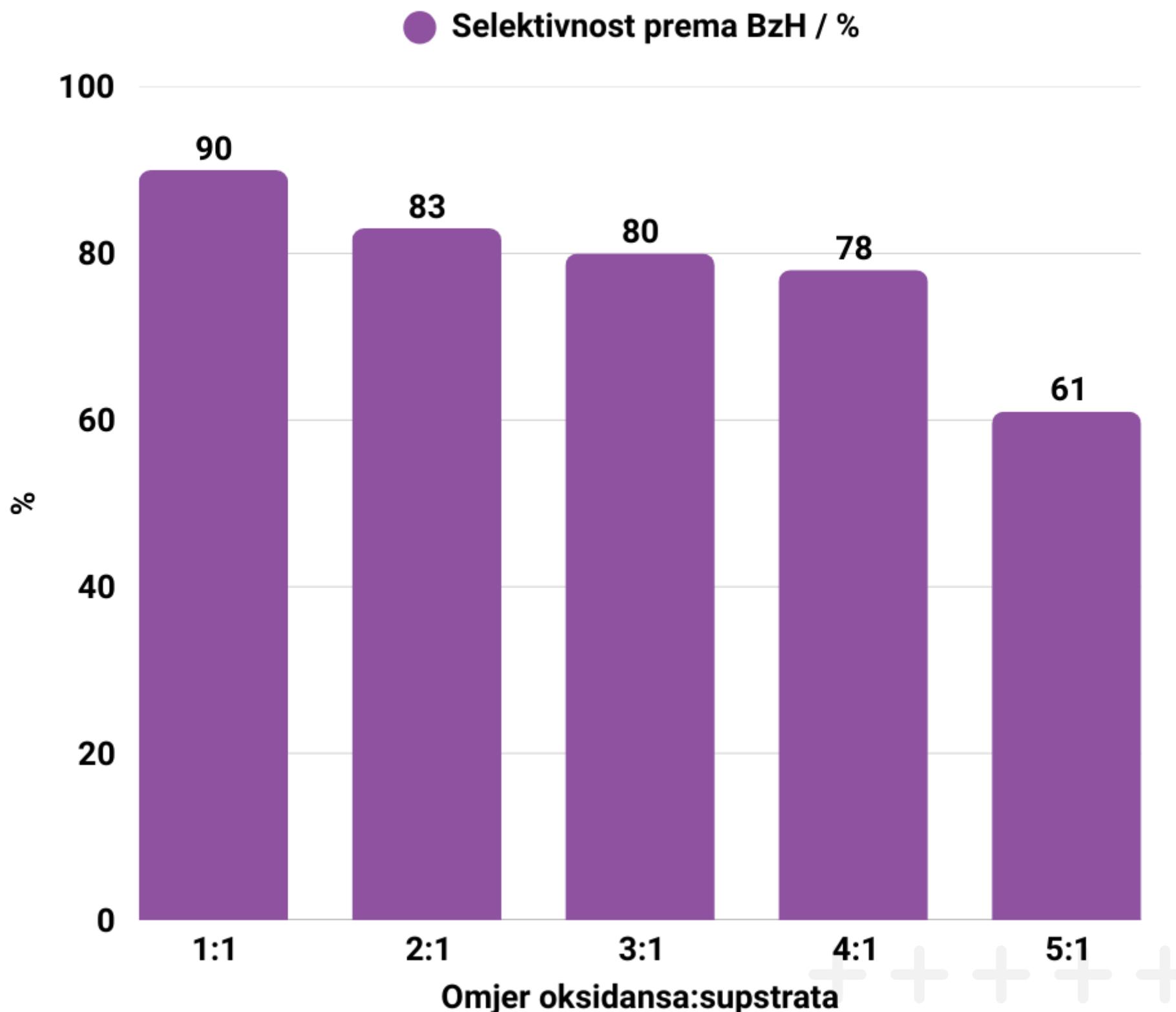


## OMJER OKSIDANSA I SUPSTRATA

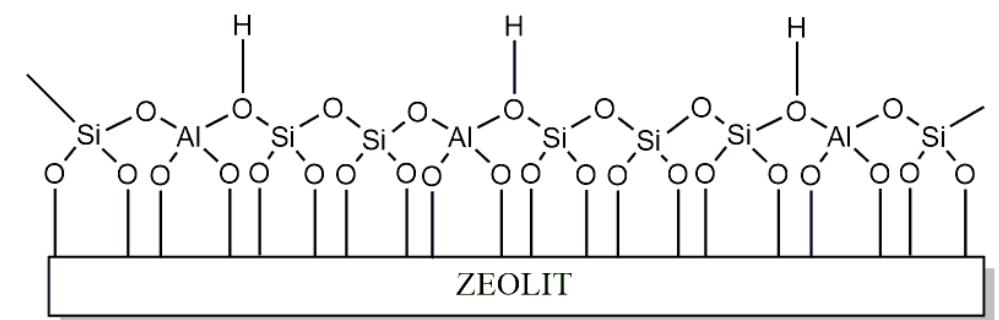


Pretvorba BzOH 95 - 100 %

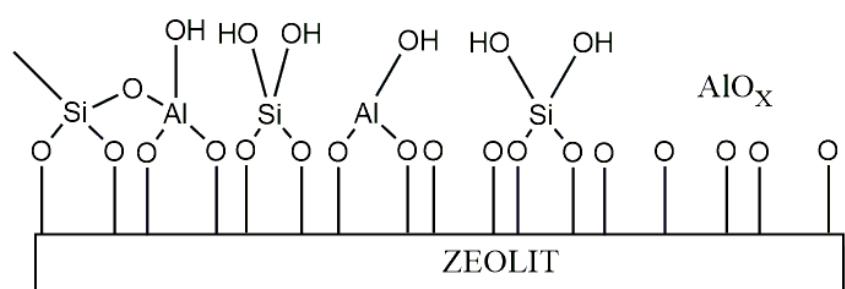
Uvjeti reakcije:  
BzOH (1 mmol), katalizator (0,0015 mmol),  
 $\text{H}_2\text{O}_2$  (30 %),  $\text{H}_2\text{O}$  (3 mL), 90 °C, 6 h

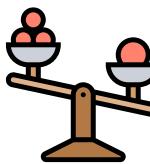


# 25ZSM(AT-0,5)



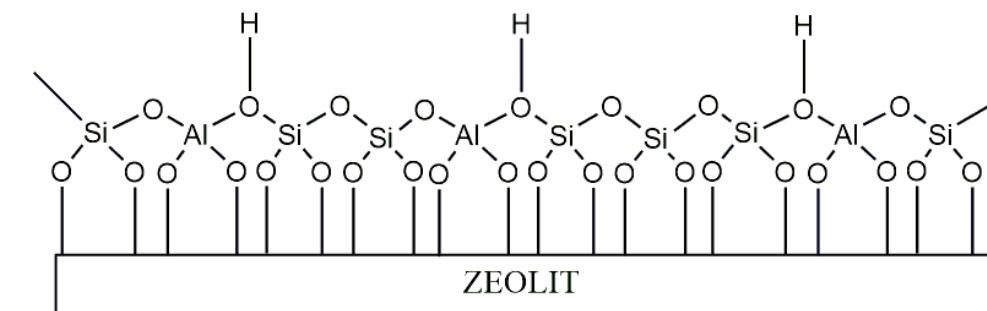
Lužnati tretman



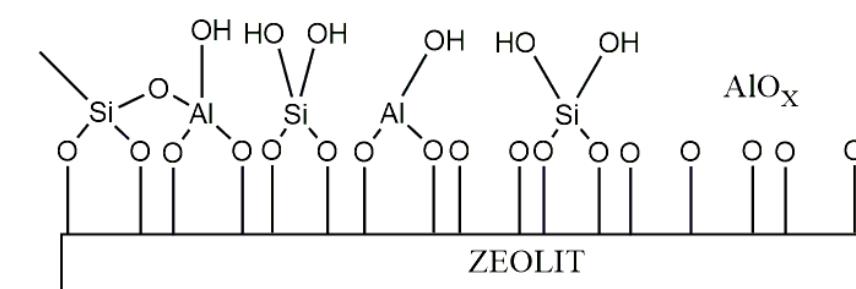


## KOLIČINA KATALIZATORA

# 25ZSM(AT-0,5)

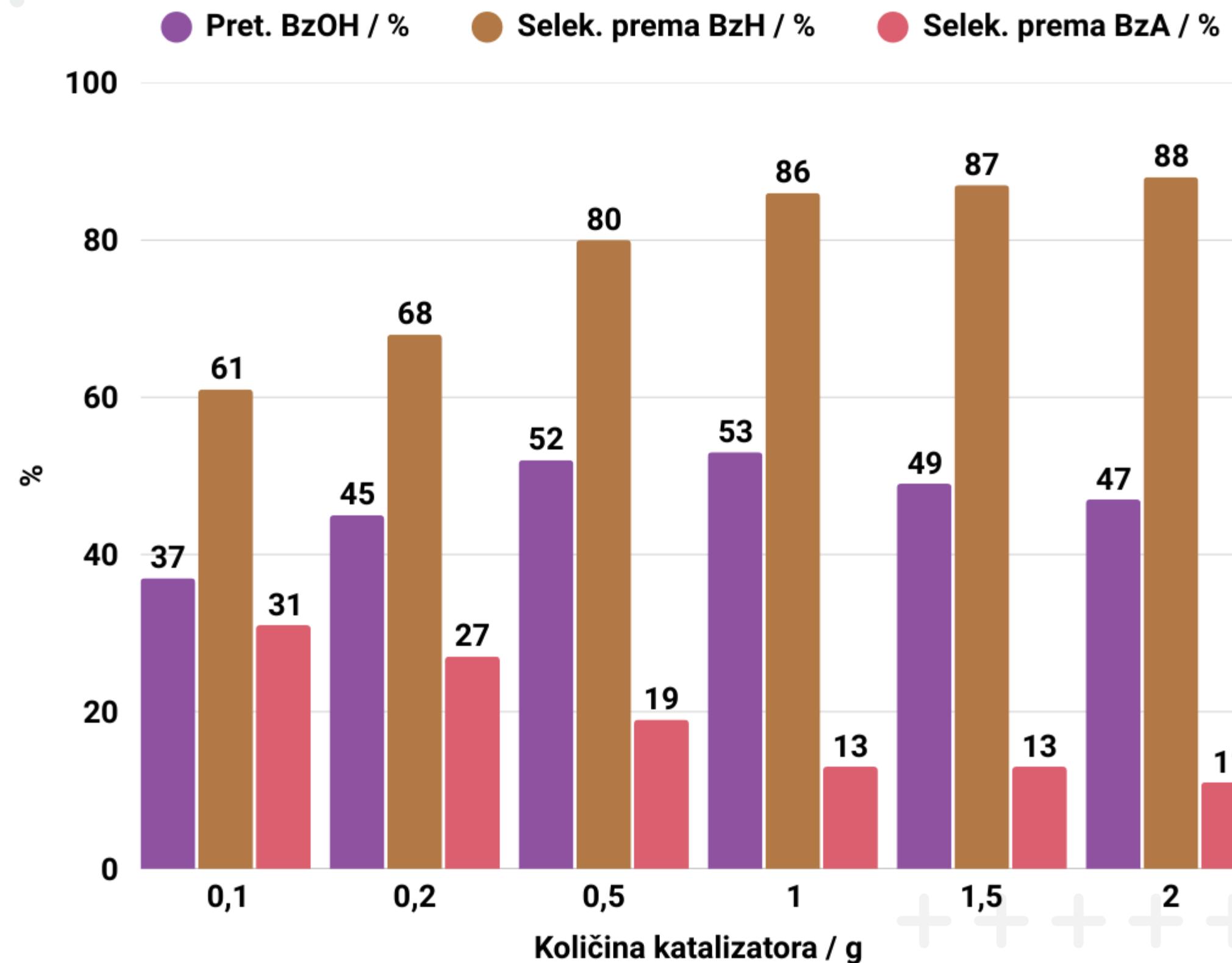


Lužnati tretman

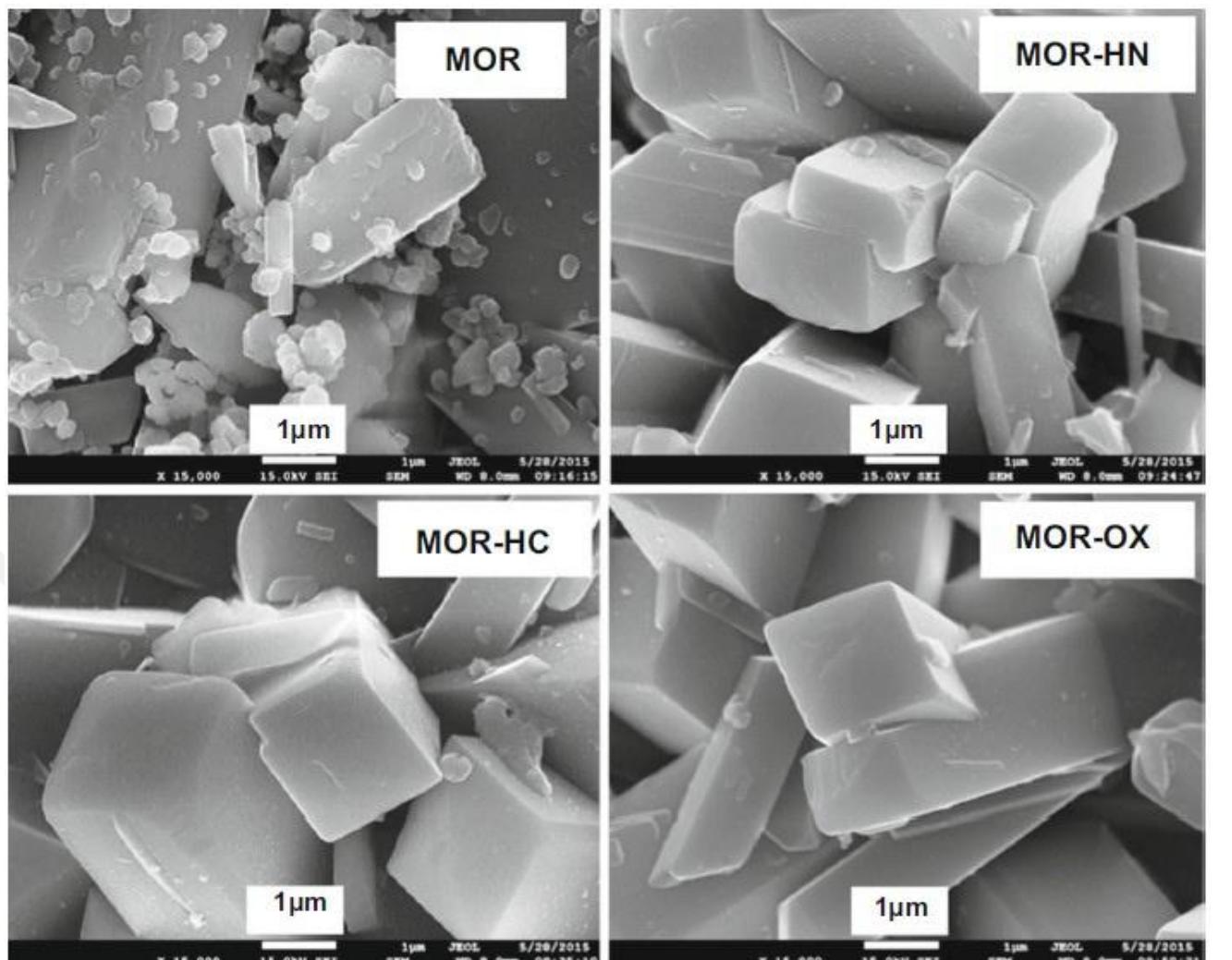


Uvjeti reakcije:

katalizator (0,1 – 2 g),  $\text{H}_2\text{O}_2/\text{BzOH}$  (1:3),  
deionizirana  $\text{H}_2\text{O}$  (26 mL), reflux, 4 h



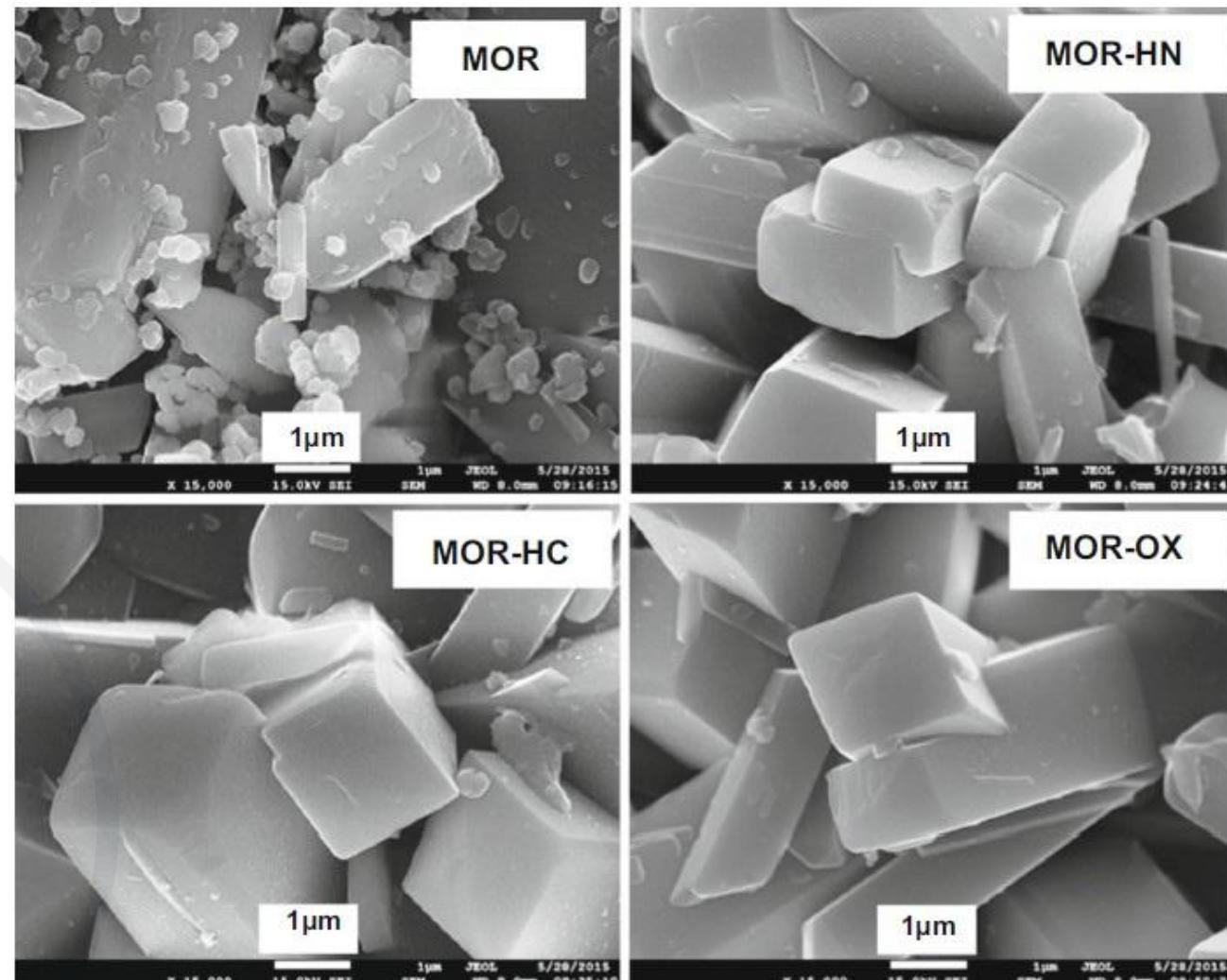
# MOR + promjene



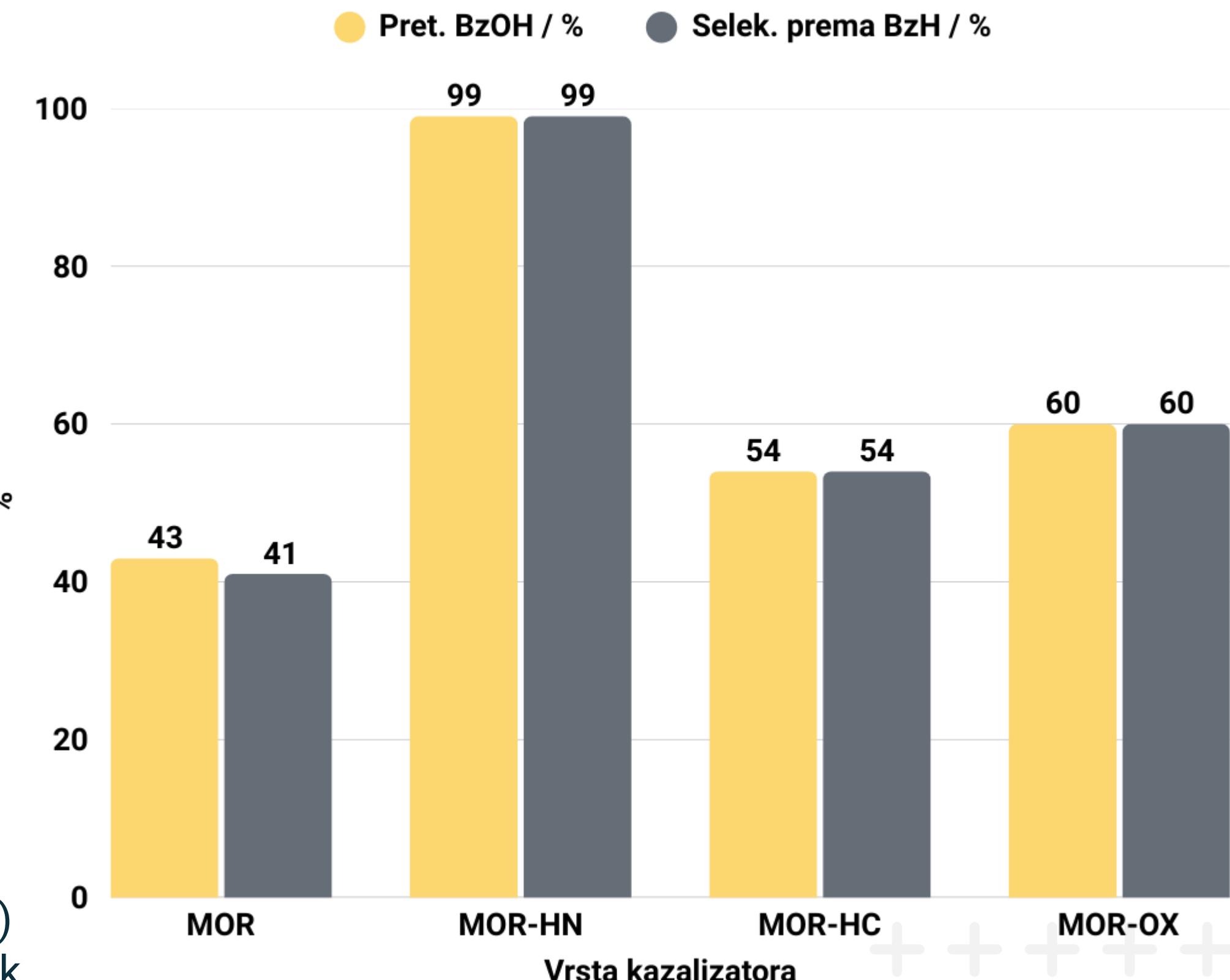


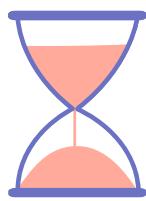
## PROMJENA KATALIZATORA

# MOR + promjene



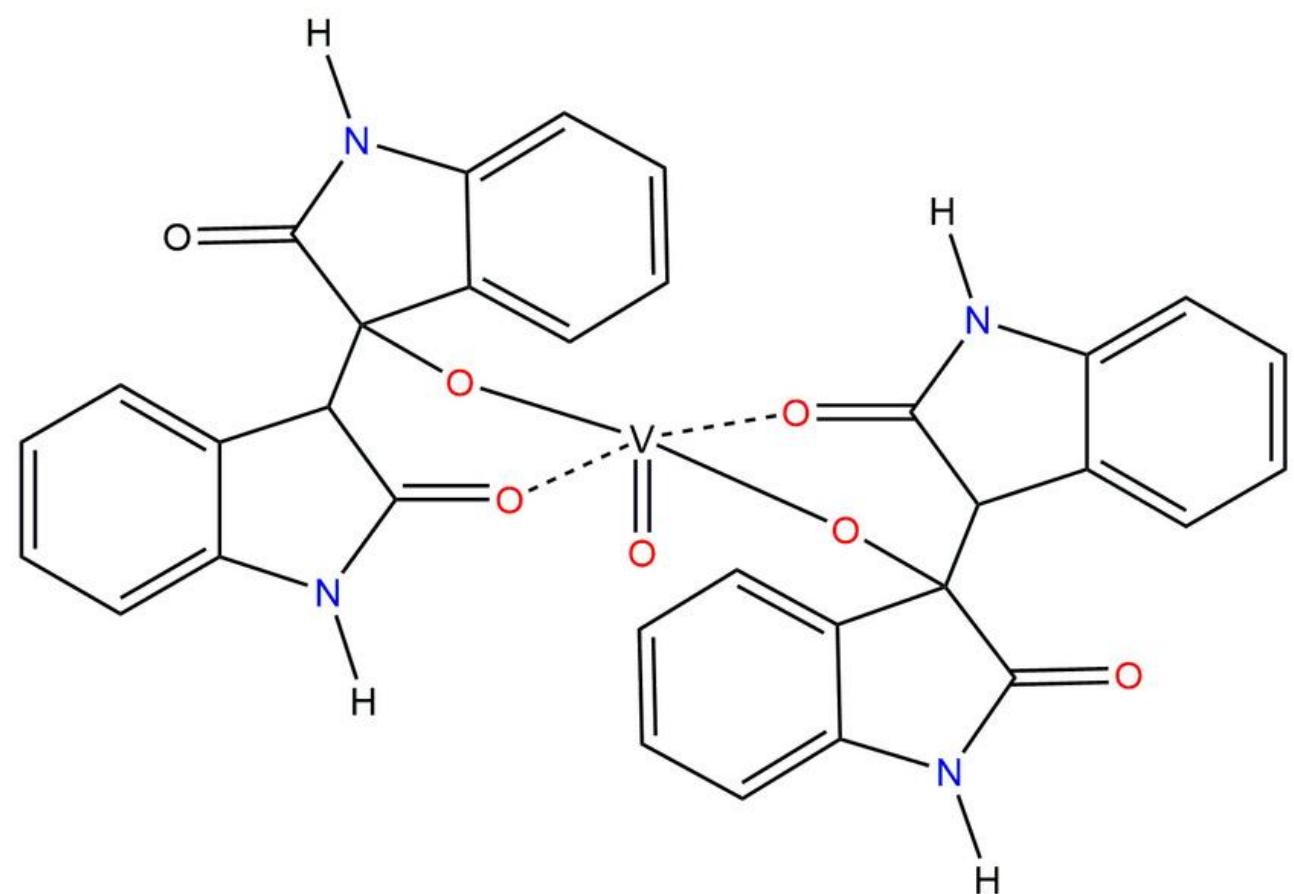
Uvjeti reakcije:  
katalizator (0,5 g), BzOH (14 mL), H<sub>2</sub>O<sub>2</sub>(30 %, 13 mL)  
deionizirana H<sub>2</sub>O (26 mL), 90 °C, 4 h, atmosferski tlak





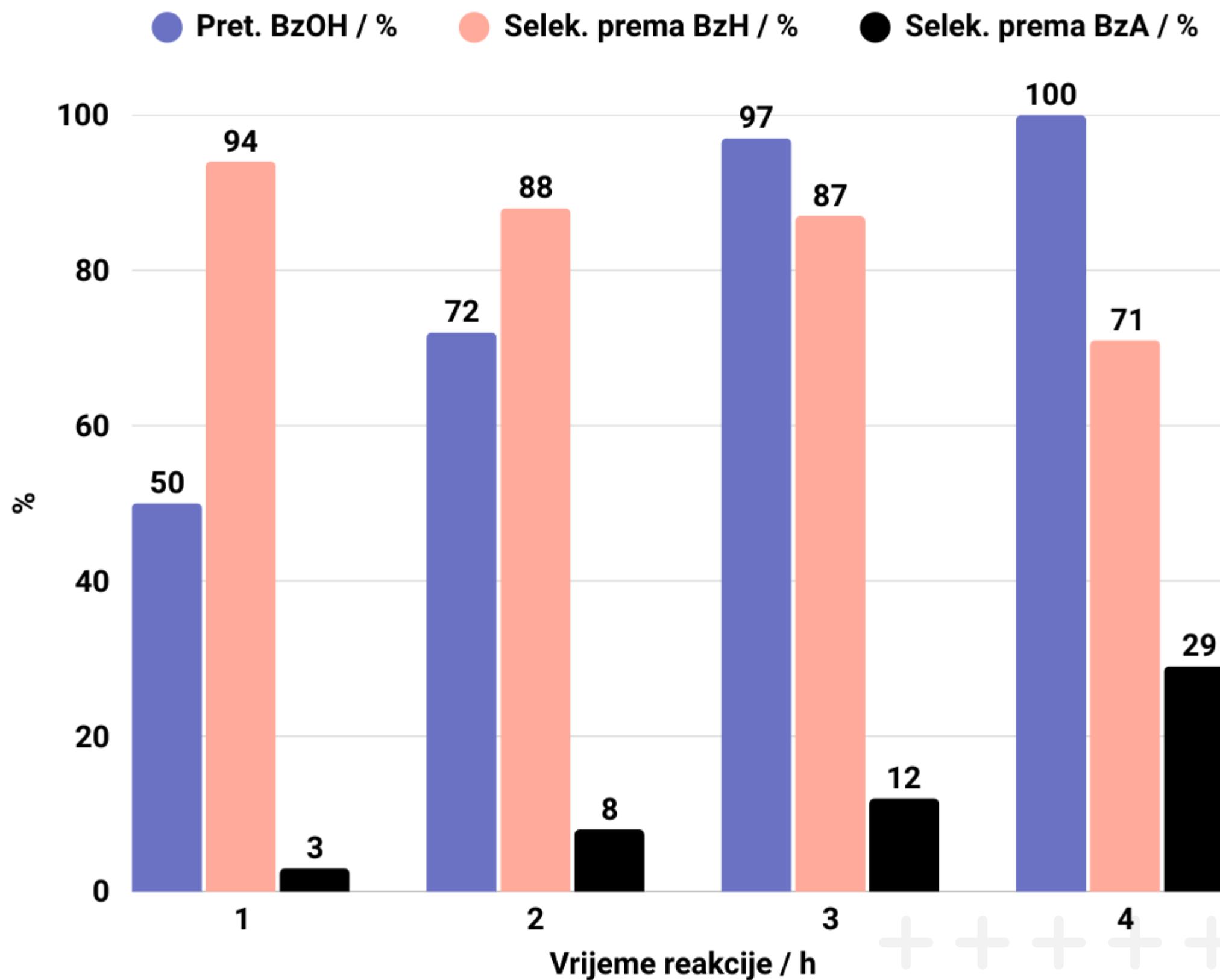
VRIJEME

# [VOH<sub>2</sub>ID]

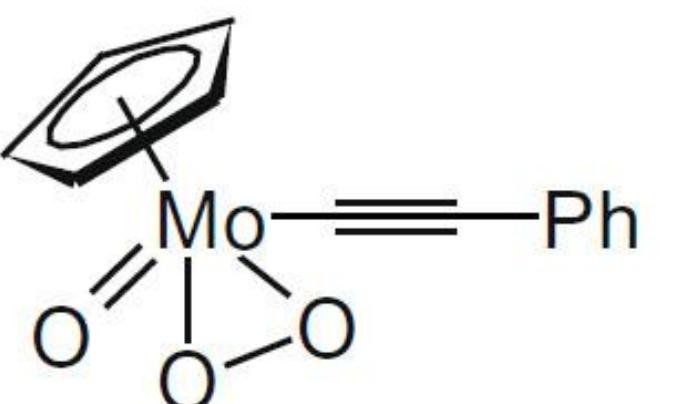


Uvjeti reakcije:

BzOH (1 mmol), [VOH<sub>2</sub>ID] (0,02 mmol),  
H<sub>2</sub>O<sub>2</sub> (3 mmol), CH<sub>3</sub>CN (10 mL), 85 °C



# [CpMo(CO)<sub>3</sub>(CC≡Ph)]

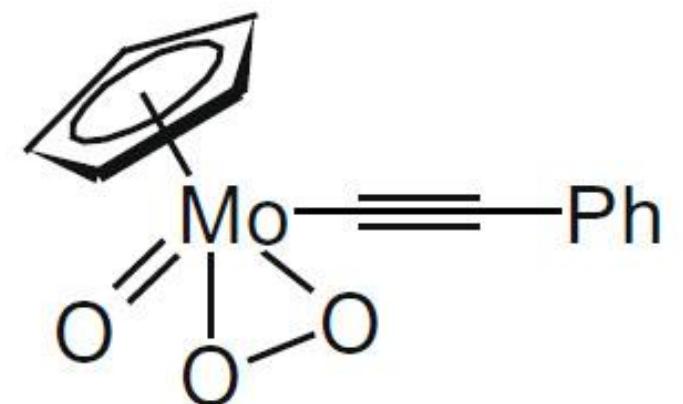


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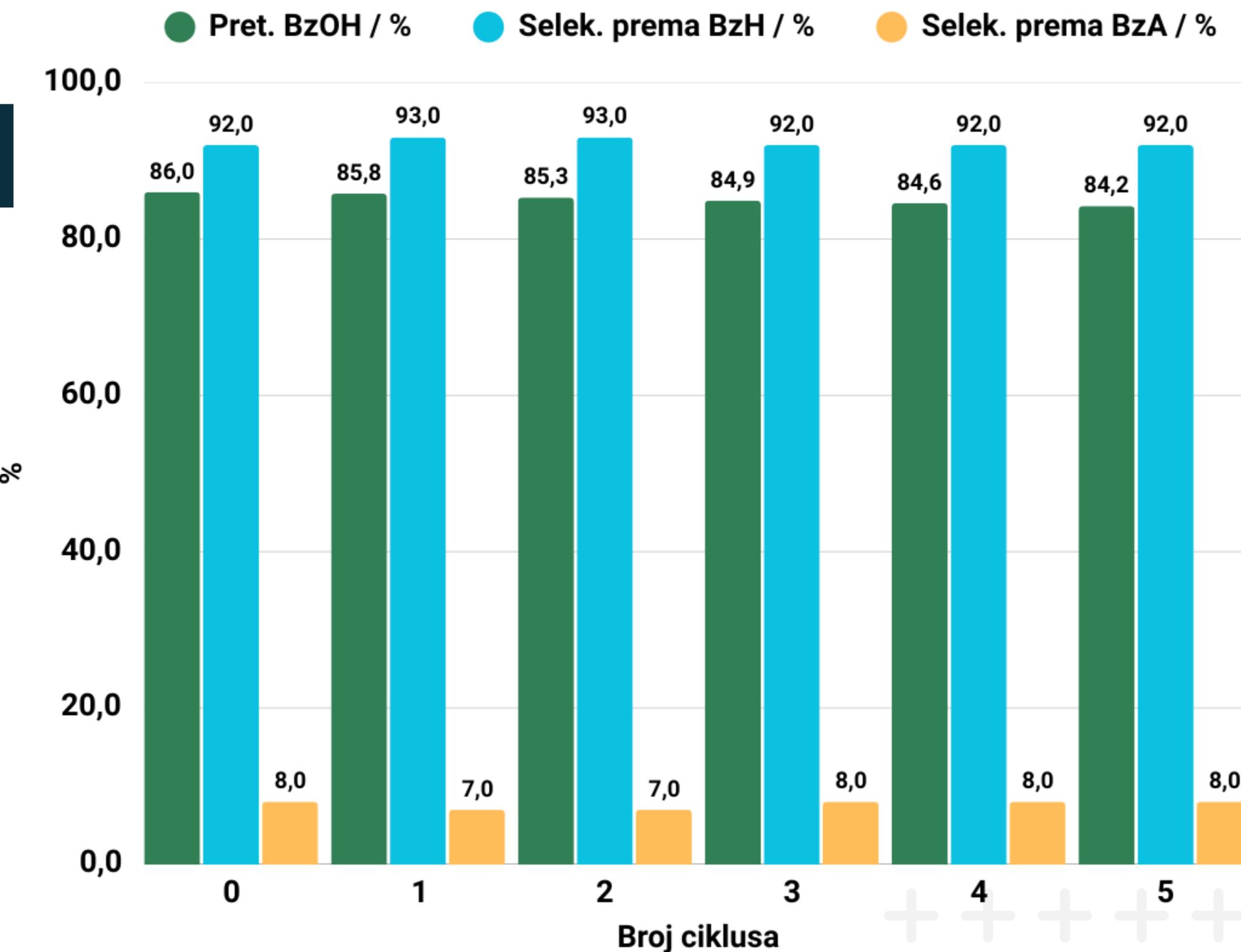


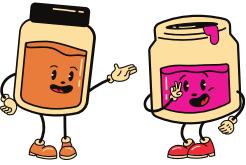
## RECIKLIRANJE KATALIZATORA

# [CpMo(CO)<sub>3</sub>(CC≡Ph)]

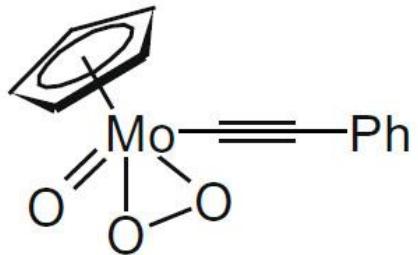


Uvjeti reakcije:  
BzOH (0,05 mol), [CpMo(CO)<sub>3</sub>(CC≡Ph)] (0,1 mmol),  
 $\text{H}_2\text{O}_2$  (0,1 mol), 8 h, 80 °C



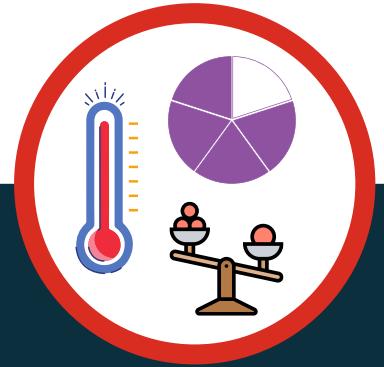


# DERIVATI BENZILNOG ALKOHOLA



Uvjeti reakcije:  
BzOH (0.05 mol),  
[CpMo(CO)<sub>3</sub>(CC≡Ph)]  
(0,1 mmol),  
H<sub>2</sub>O<sub>2</sub> (0,1 mol),  
8 h, 80 °C

Supstrat	Pret. alkohola / %	Selek. prema aldehidu / %	Selek. prema kiselini / %
<chem>Cc1ccccc1CO</chem>	86	92	8
<chem>Cc1ccccc1CO</chem>	90	87	13
<chem>COc1ccccc1CO</chem>	90	90	10
<chem>COc1ccccc1CO</chem>	83	85	15
<chem>[N+](=O)[O-]c1ccccc1CO</chem>	60	88	12
<chem>Clc1ccccc1CO</chem>	65	91	9
<chem>Clc1cc(Cl)c(cc1)CO</chem>	78	90	10



Viša temperatura = veća pretvorba BzOH, minimalno smanjenje selektivnosti

Veći omjer oksidansa i supstrata = manja selektivnost

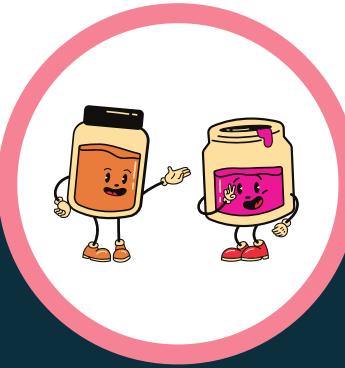
Veća količina katalizatora = prvotno veća pretvorba BzOH, a zatim smanjenje pretvorbe; veća selektivnost prema BzH



Promjene katalizatora = ovisno o promjeni pozitivan / negativan učinak

Duže vrijeme reakcije = veća pretvorba BzOH, ali manja selektivnost prema BzH

Mogućnost recikliranja homogenog katalizatora tijekom pet ciklusa



Elektron-donirajuće skupine = povećanje pretvorbe BzOH i selektivnosti prema BzH

Elektron-odvlačeće skupine = smanjenje pretvorbe BzOH i minimalan utjecaj na selektivnost prema BzH



HVALA  
NA PAŽNJI!

