



Transition Metal Salen Complexes: Synthesis and Biological activity

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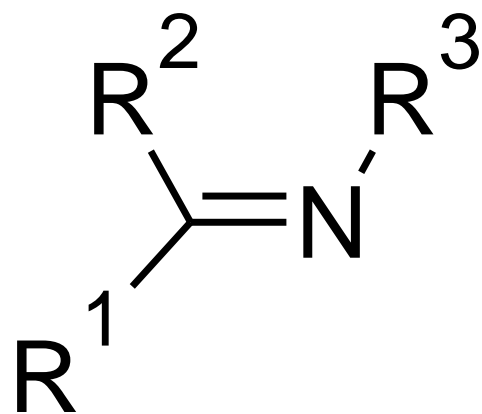
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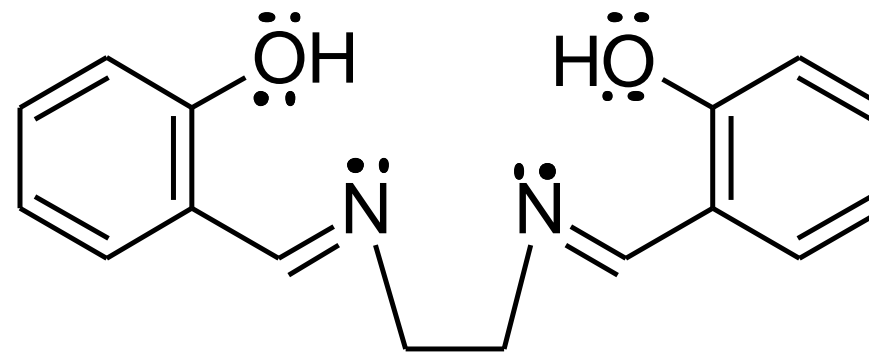
Supervisor: **Prof. E. Elizbarashvili**

November 18th, 2020

Introduction

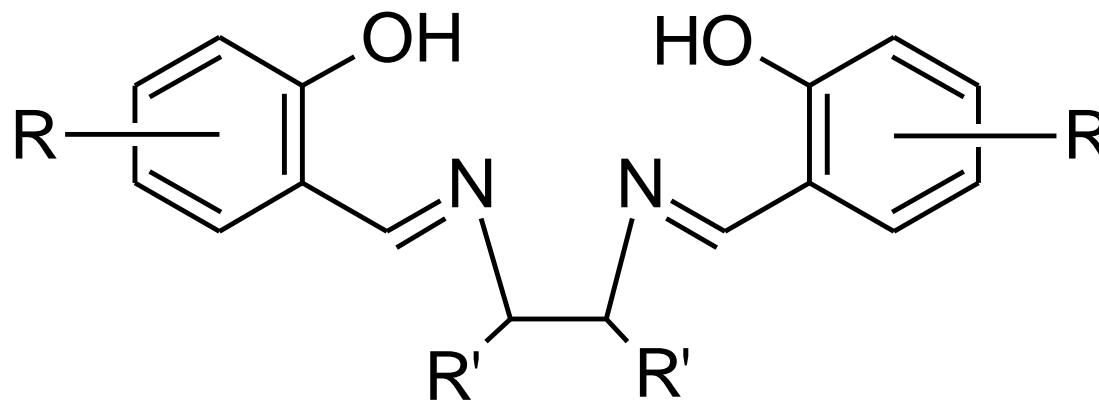


General structure of Schiff Bases



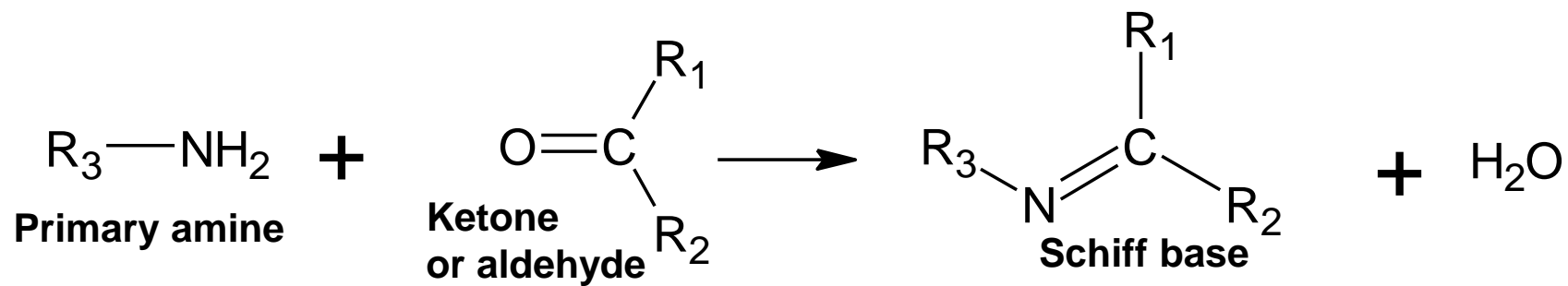
N,N'-ethylenebis (salicylimine)

Salen

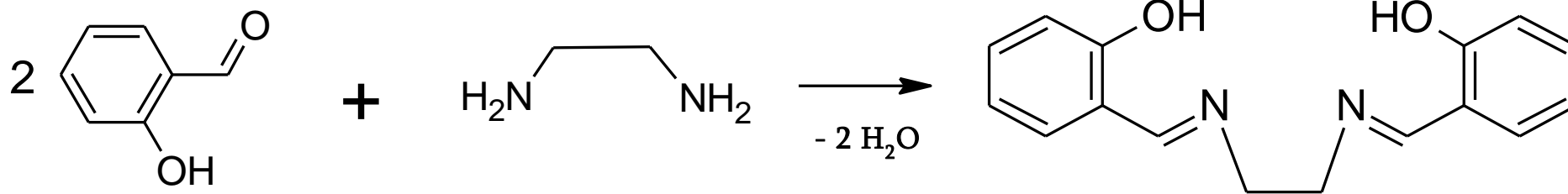


General structure of Salen-type ligands

Introduction

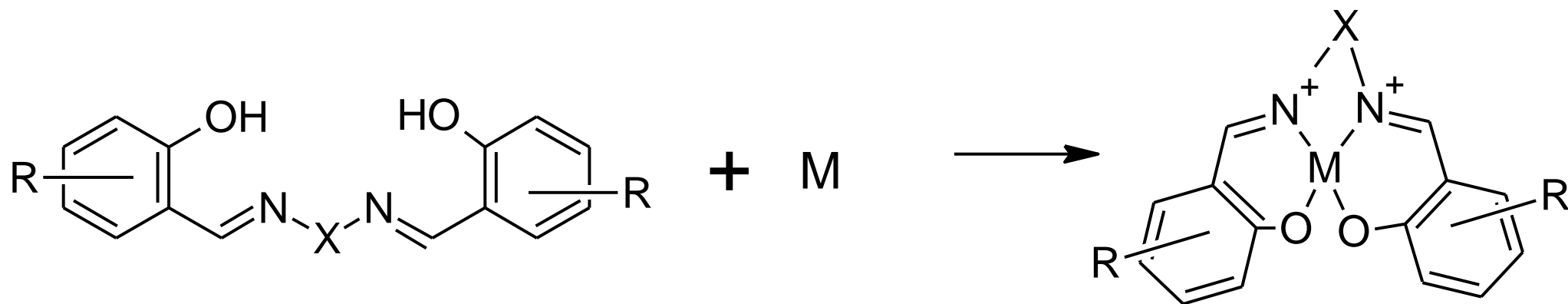


Synthesis of Schiff bases



Synthesis of Salen ligand

Introduction



R= OH, NH₂

X= none, -CH₂-CH₂-, -[CH₂]₄-, -[CH₂]₆-,

M= Fe²⁺, Fe³⁺, Mn²⁺, Co²⁺, Ni²⁺, Zn²⁺, Cu²⁺, Cd²⁺

Synthesis of Metal Salen complexes

Introduction

Advantages:

- ✓ Ease and flexibility of synthesis process
- ✓ High thermal stability

Fields of use :

- Catalysis
- Medicine and Biochemistry
- Thermoplastic Polyurethane (TPU) synthesis



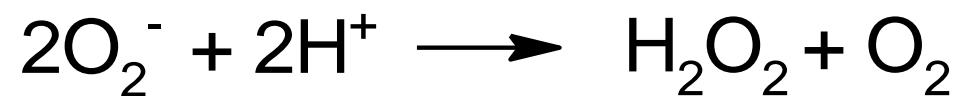
Thermoplastic Polyurethane (TPU)

Introduction

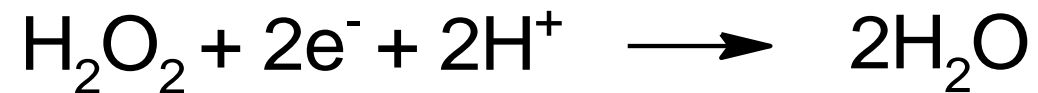
Biological activity of Salen complexes

Free radical elimination mechanism of enzymes

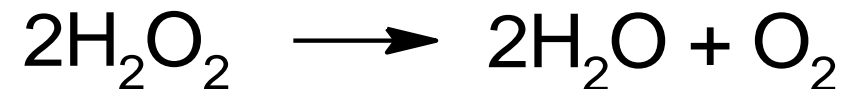
Superoxide-dismutase



Peroxidase



Catalase

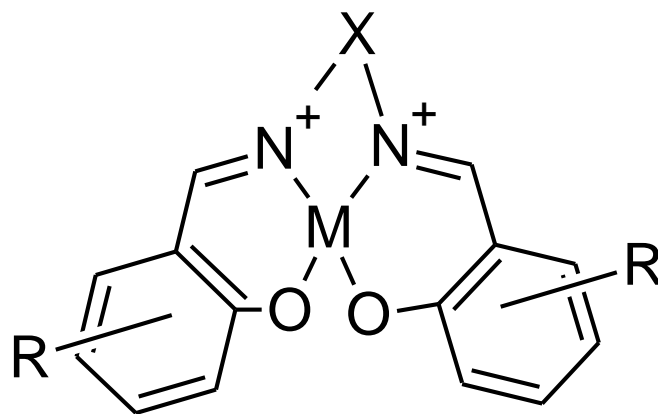


Introduction

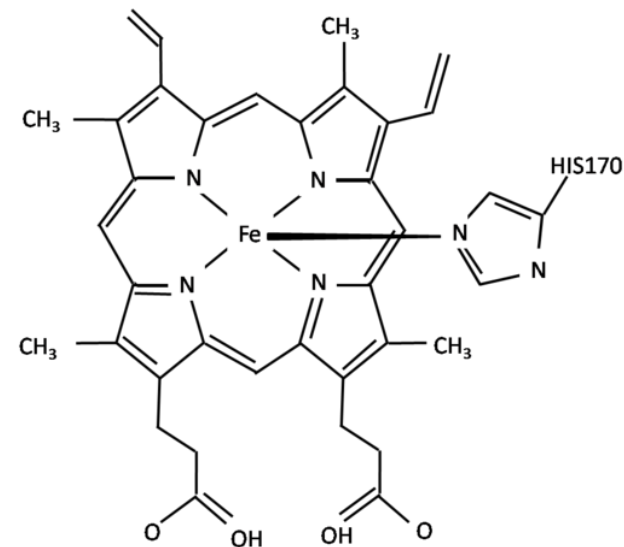
Biological activity of Salen complexes

„Enzyme Mimics“

- Antibacterial
- Antifungal
- Anti-inflammatory
- Antitumor



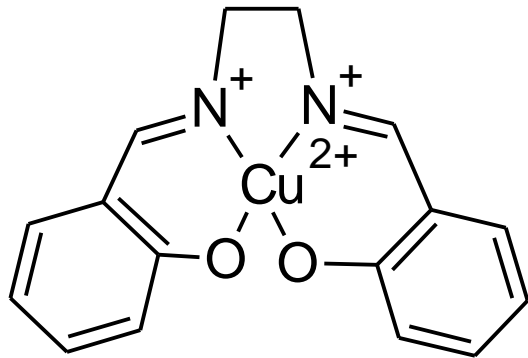
Metal Salen complex



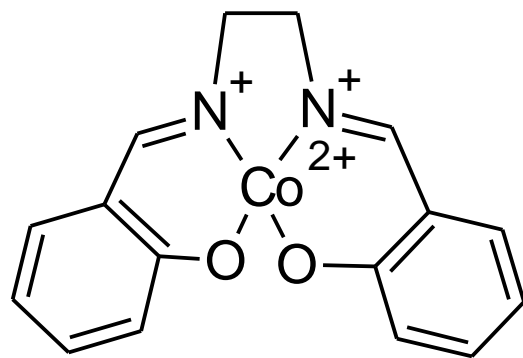
Active site of Peroxidase enzyme

Junior Project

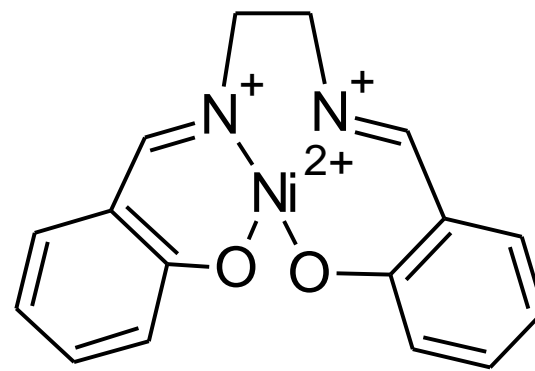
Synthesized Compounds



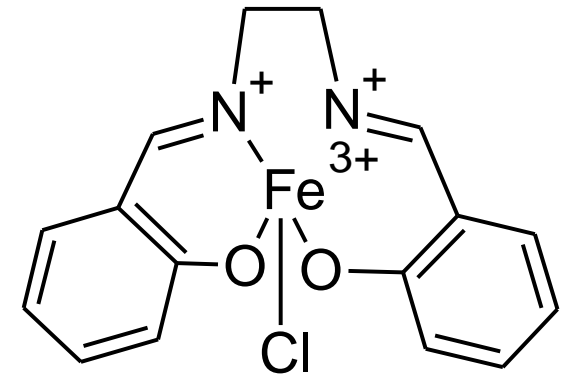
Copper(II) Salen



Cobalt(II) Salen



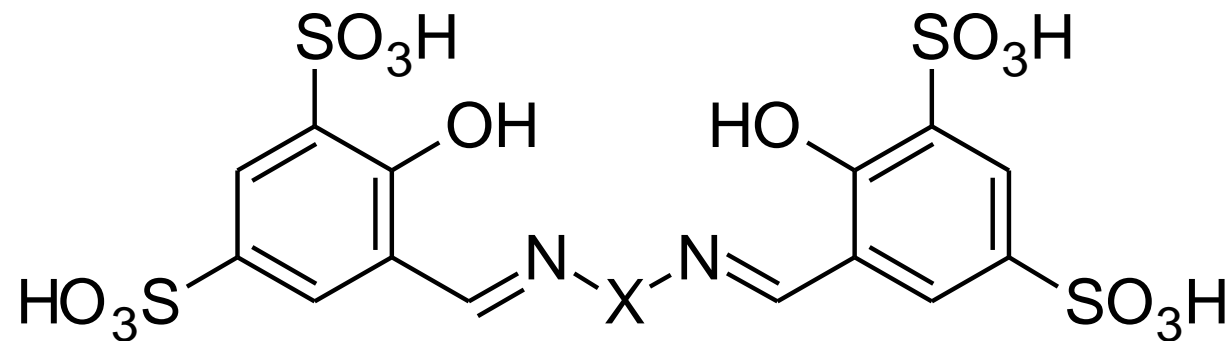
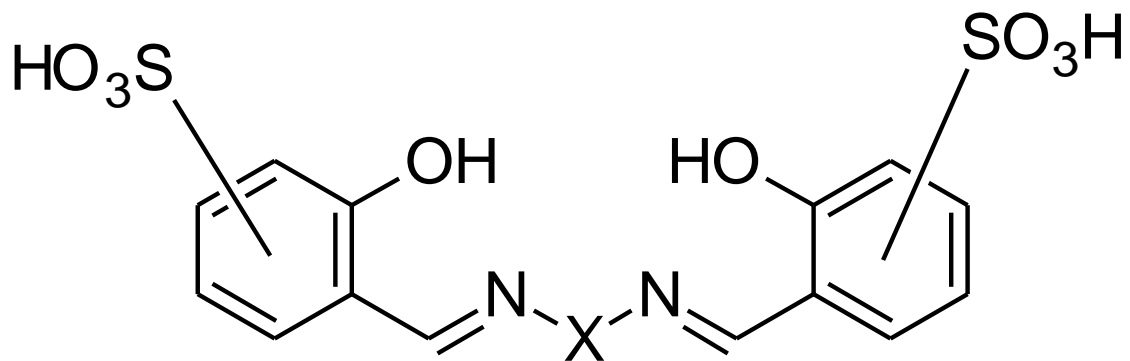
Nickel(II) Salen



Iron(III) Salen

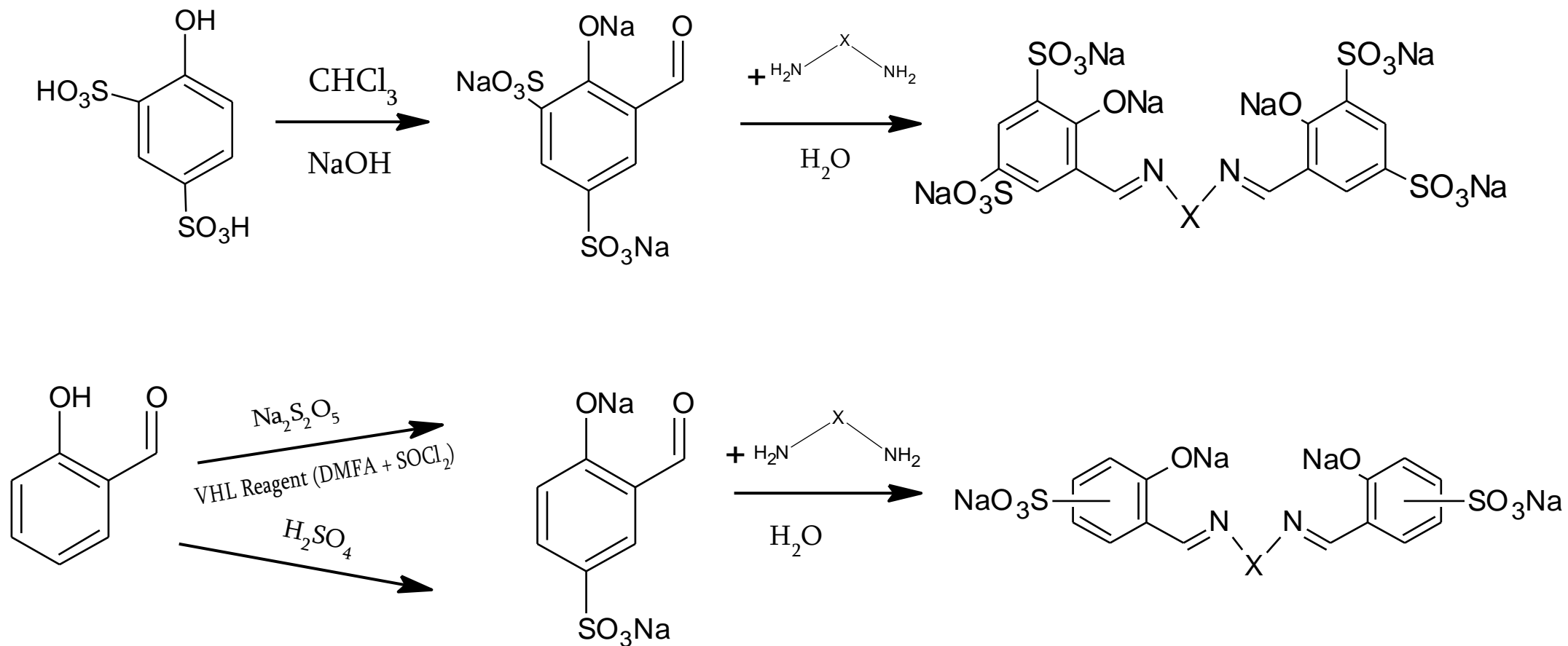
Senior project objective:

Synthesis of water soluble Salen-type ligands



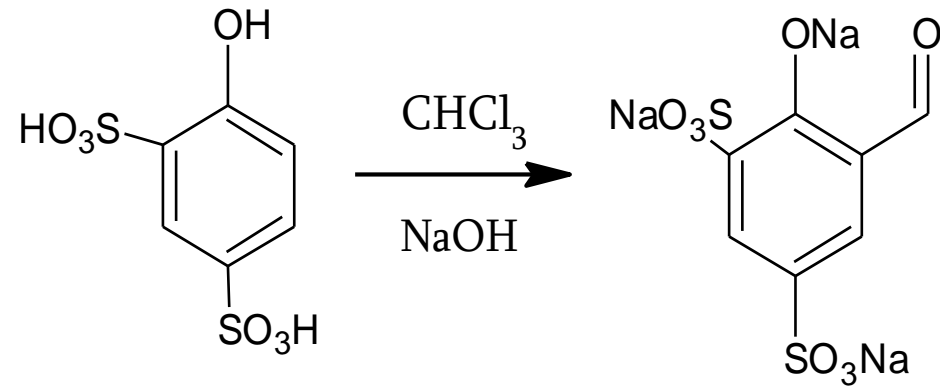
X= none, -CH₂-CH₂-, -[CH₂]₄-, -[CH₂]₆-,

Scheme of synthesis



Synthesis of ligand precursor

Carbonylation (Reimer-Tiemann reaction):

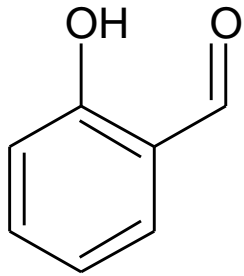


4-Hydroxybenzene-1,3-
disulfonic acid

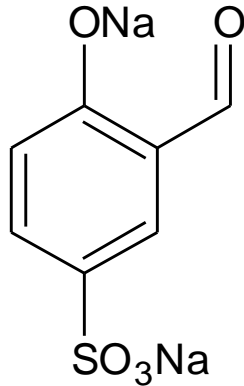
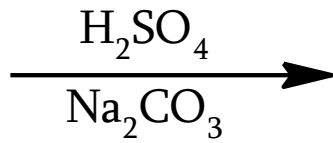
5-formyl-4-hydroxybenzene-
1,3-disulfonic acid sodium salt

Synthesis of ligand precursor

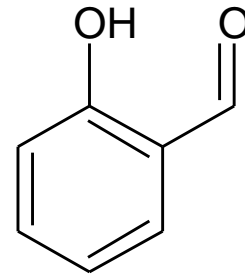
Sulfonation:



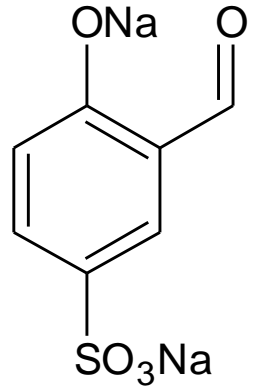
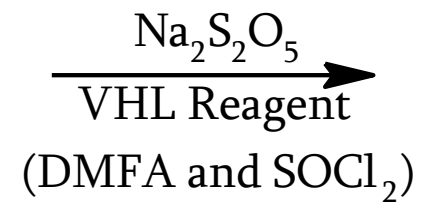
Salicylaldehyde



3-formyl- 4-
hydroxybenzenesulfonic acid
sodium salt



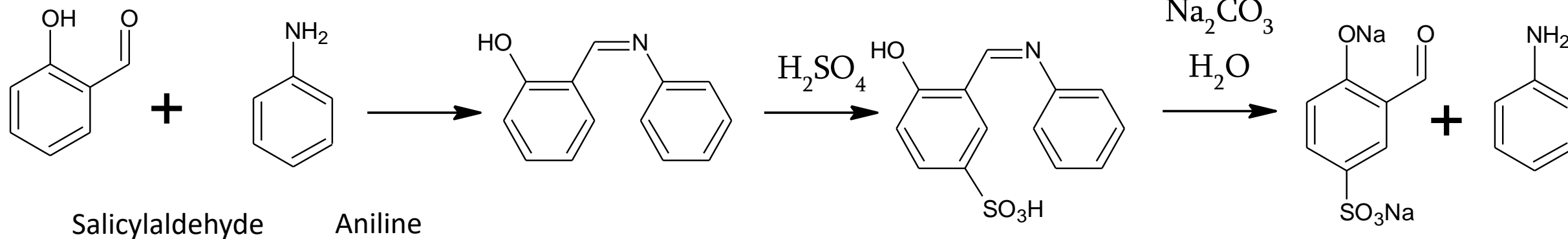
Salicylaldehyde



3-formyl- 4-
hydroxybenzenesulfonic acid
sodium salt

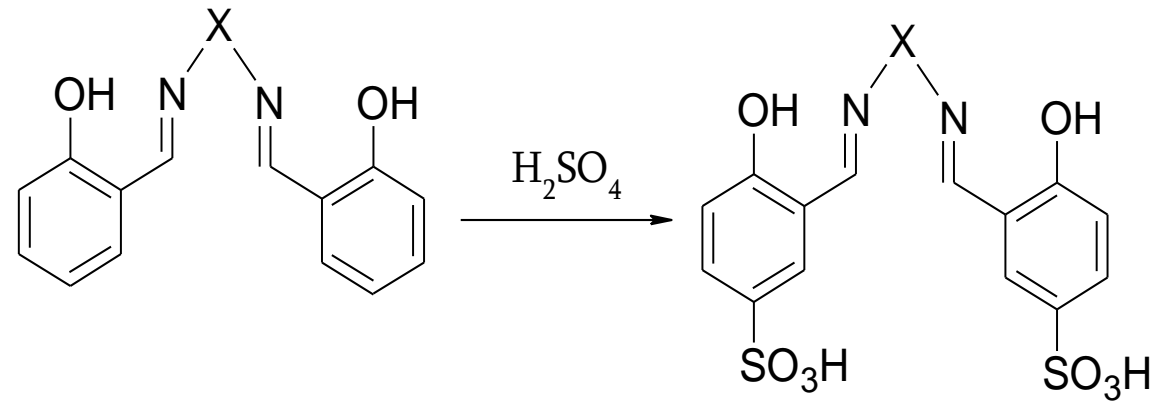
Synthesis of ligand precursor

Protection of carbonyl group and further sulfonation:



Synthesis of ligand

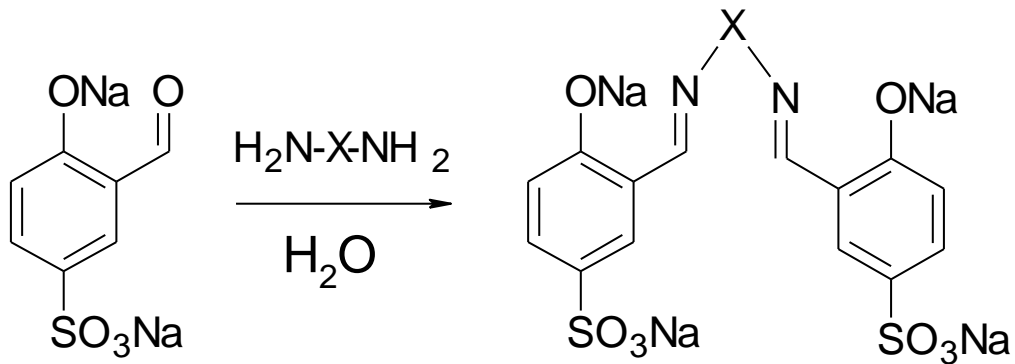
Direct sulfonation of salen ligand:



X= none, -(CH₂)₂-

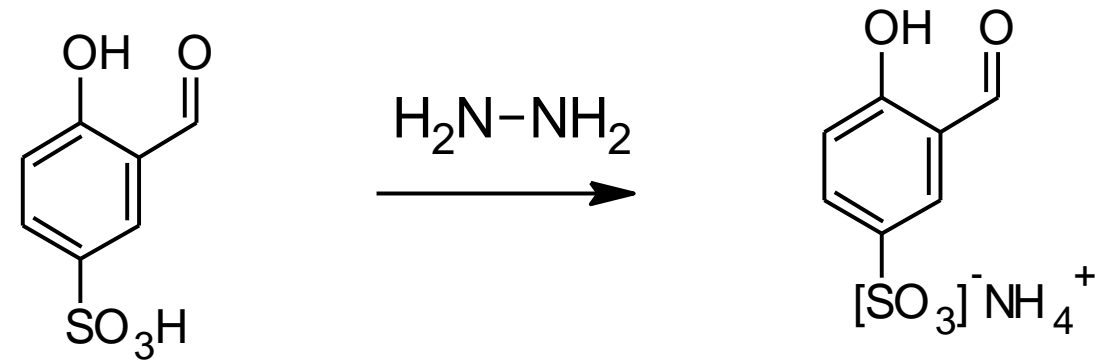
Synthesis of ligand

Precursor condensation with diamines:



X= none, $-(\text{CH}_2)_2-$

Precursor condensation with diamines (Alternative reaction):



Conclusions

- Transition metal (Ni, Co, Cu, Fe) Salen complexes were successfully synthesized with high Yield.
- Biological activity results weren't valid because of organic solvent's toxic effect.
- From water soluble groups sulfonate group has the lowest toxicity, is natural to human body and is easily metabolized.
- 4-hydroxybenzenesulfonic acid carbonylation with Reimer-Tiemman reaction has very low yield. This may be explained by sulfonic acid group effect on carbonyl group.
- It is shown, that favourable compound of sulfonation of salicylaldehyde with concentrated sulfonic acid is 2-hydroxyl-5-benzenesulfonic acid. This may be explained with oxidation of carbonyl group to carboxyl.
- Results have shown, that the most efficient way of synthesizing sulfonated salicylaldehyde is using protection for carbonyl group right before sulfonation. After sulfonation protecting group is removed by basic hydrolysis. Yield: 88%
- Sulfonated salicylaldehyde condensation reaction products aren't water soluble, that can be explained with sulfonic acid group to be reacting with basic reagents.

**THANK YOU
FOR
YOUR ATTENTION!**