

# **Transition-Metal Catalyst Free C=N Coupling with Phenol / Phenoxide: Green Synthesis of Benzoxazole Scaffold by Anodic Oxidation Reaction**

Yachen Shih, Chengyi Ke, Chinghao Pan and Yungtzung Huang\*

Department of Applied Chemistry, National University of Kaohsiung

No. 700, Kaohsiung University Rd., Kaohsiung 81148, Taiwan, R.O.C.

*Corresponding Author, Phone: 886-7-591-9418; Fax: 886-7-591-9348; Email: ythuang@nuk.edu.tw*

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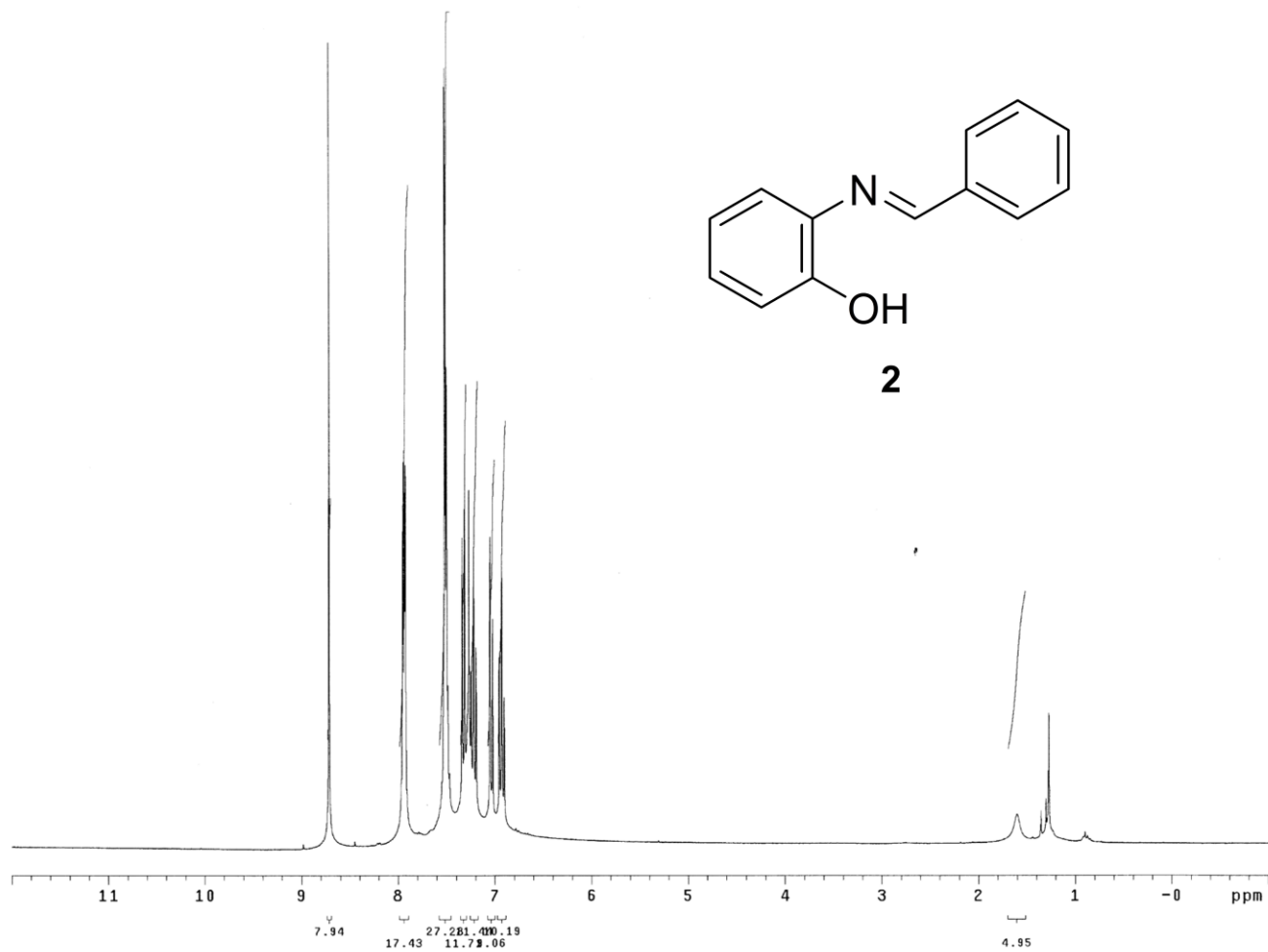
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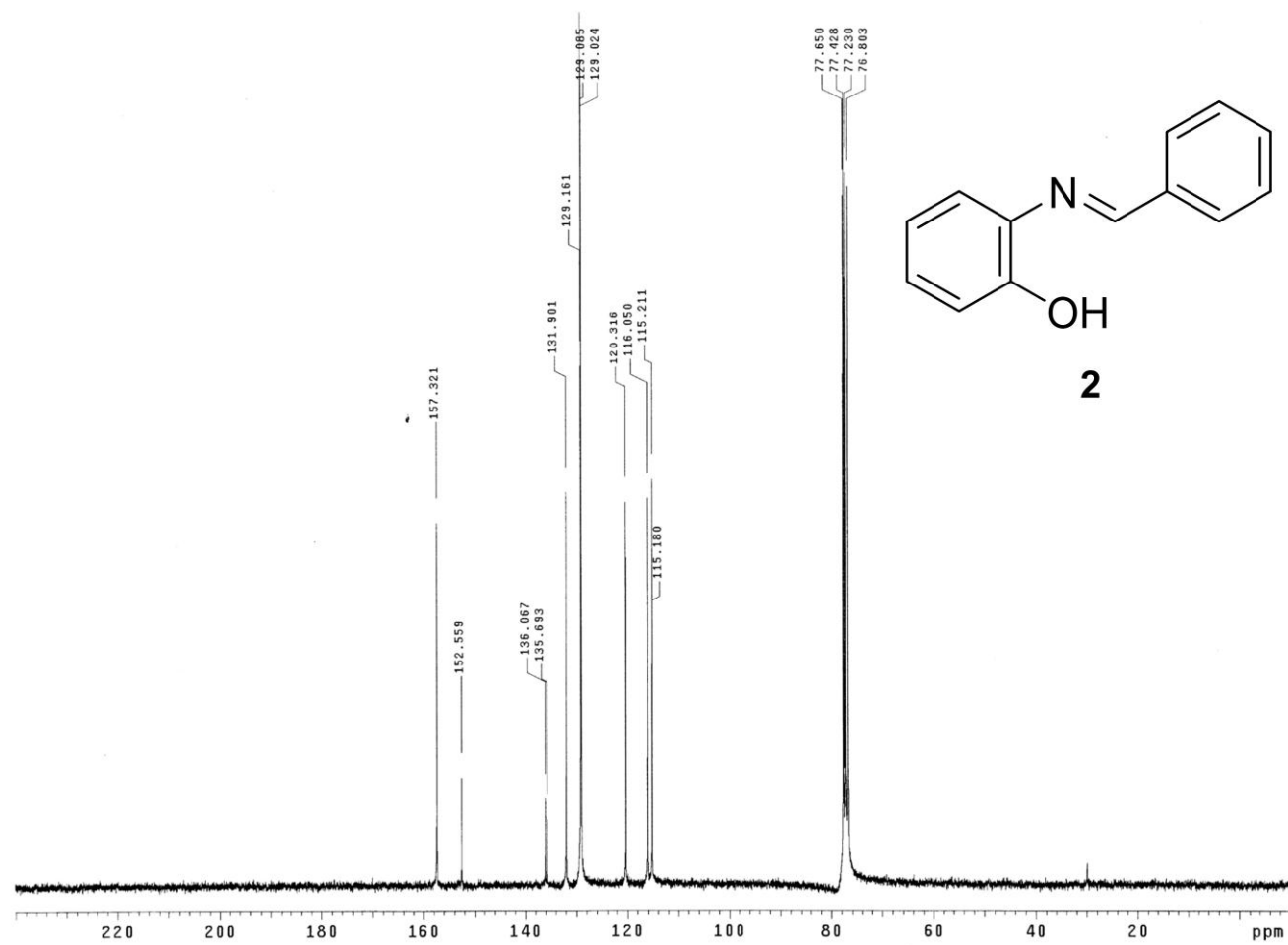
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## I. NMR spectra:

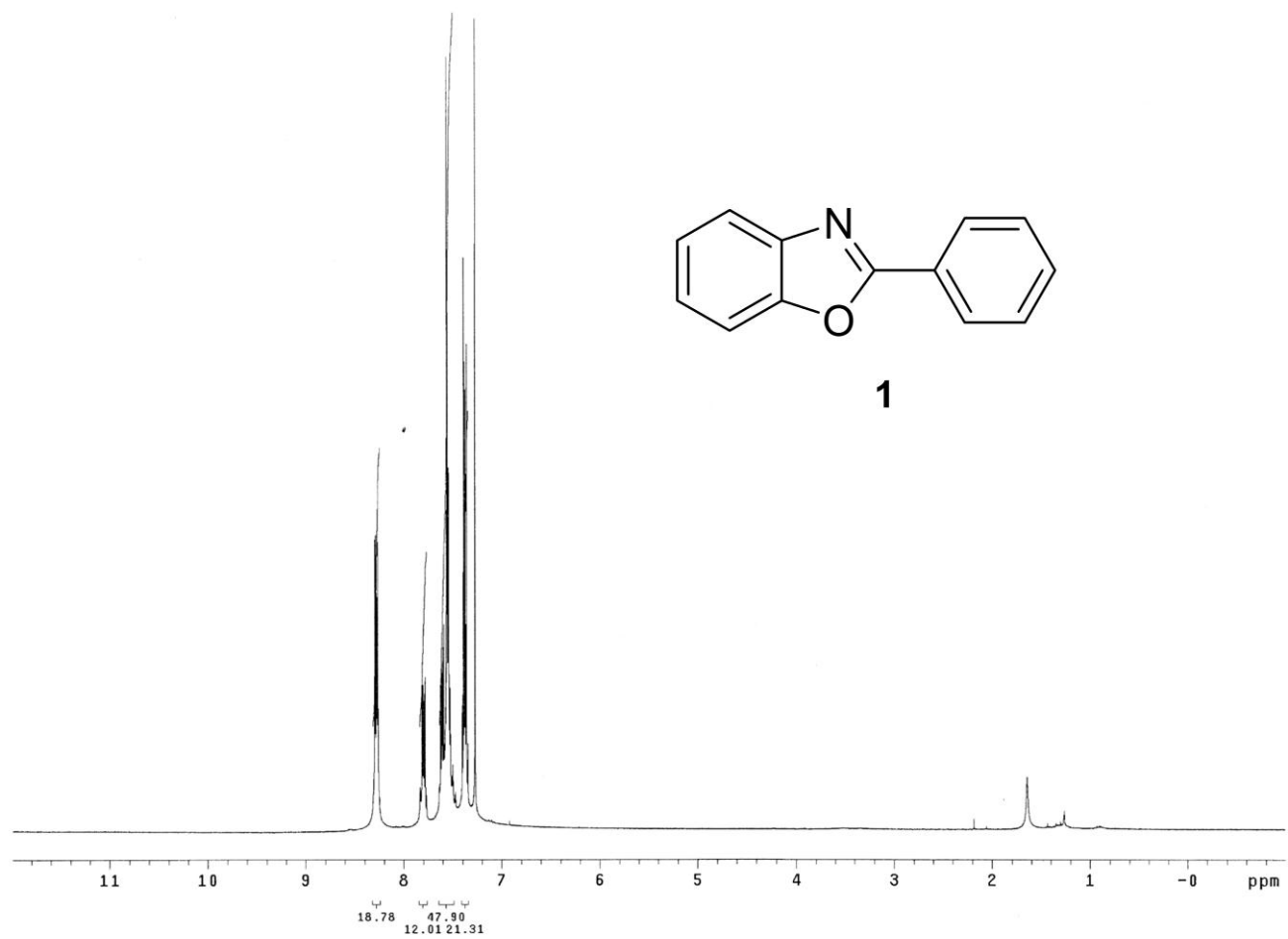
1.  $^1\text{H}$ -NMR spectrum of phenolic Schiff base (**2**):



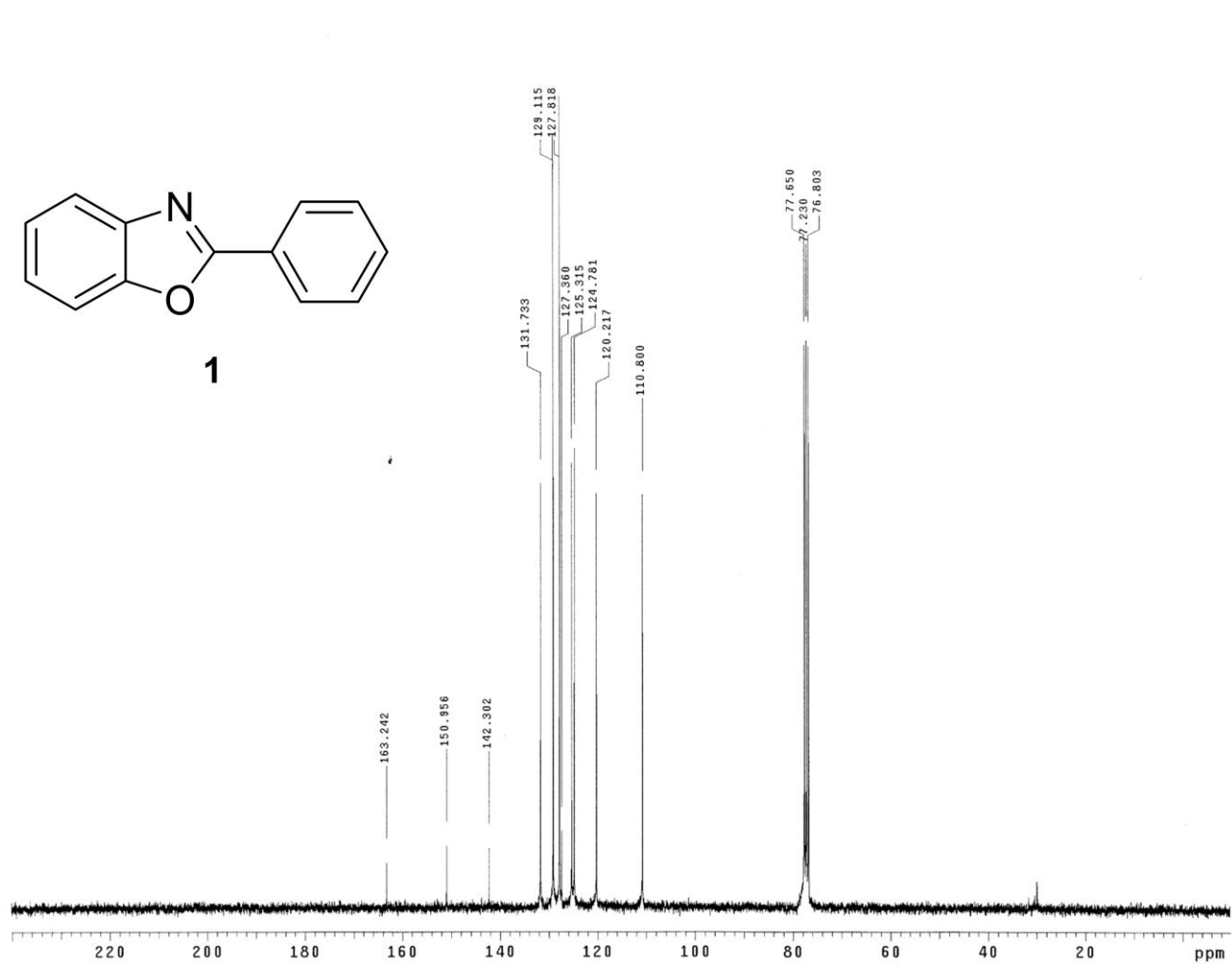
2.  $^{13}\text{C}$ -NMR spectrum of phenolic Schiff base (**2**):



3.  $^1\text{H-NMR}$  spectrum of benzoxazole (**1**):

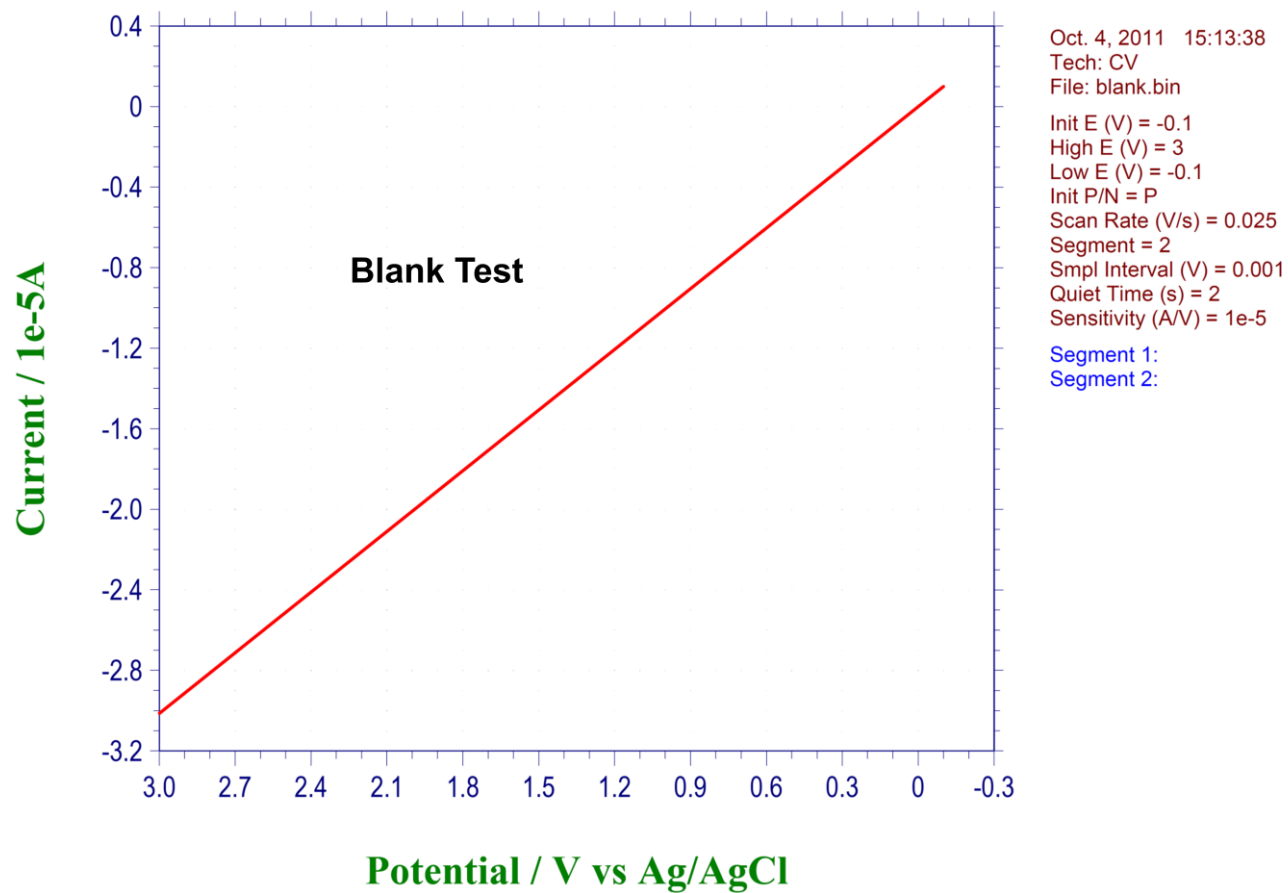


4.  $^{13}\text{C}$ -NMR spectrum of benzoxazole (**1**):

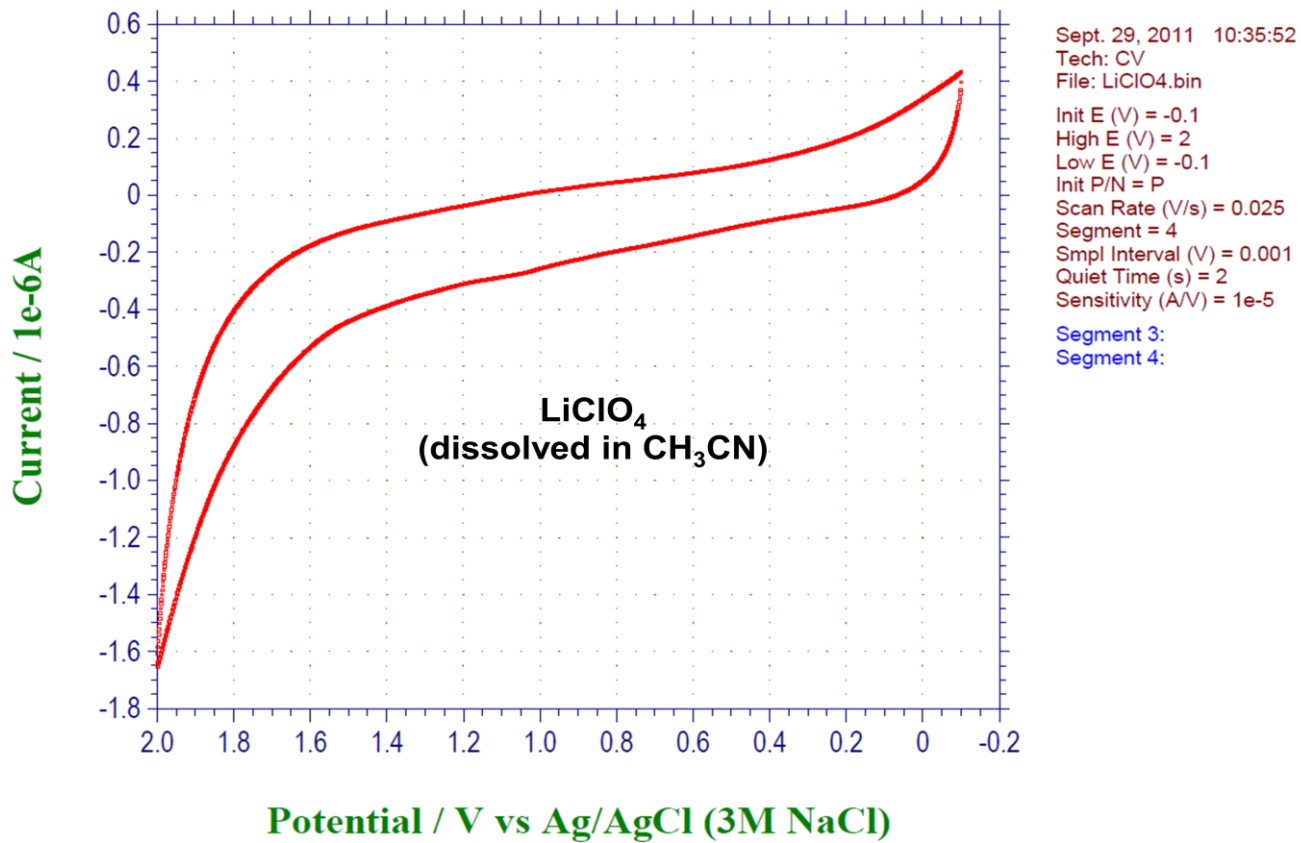


## II. CV spectra:

### 1. CV spectrum of blank test:

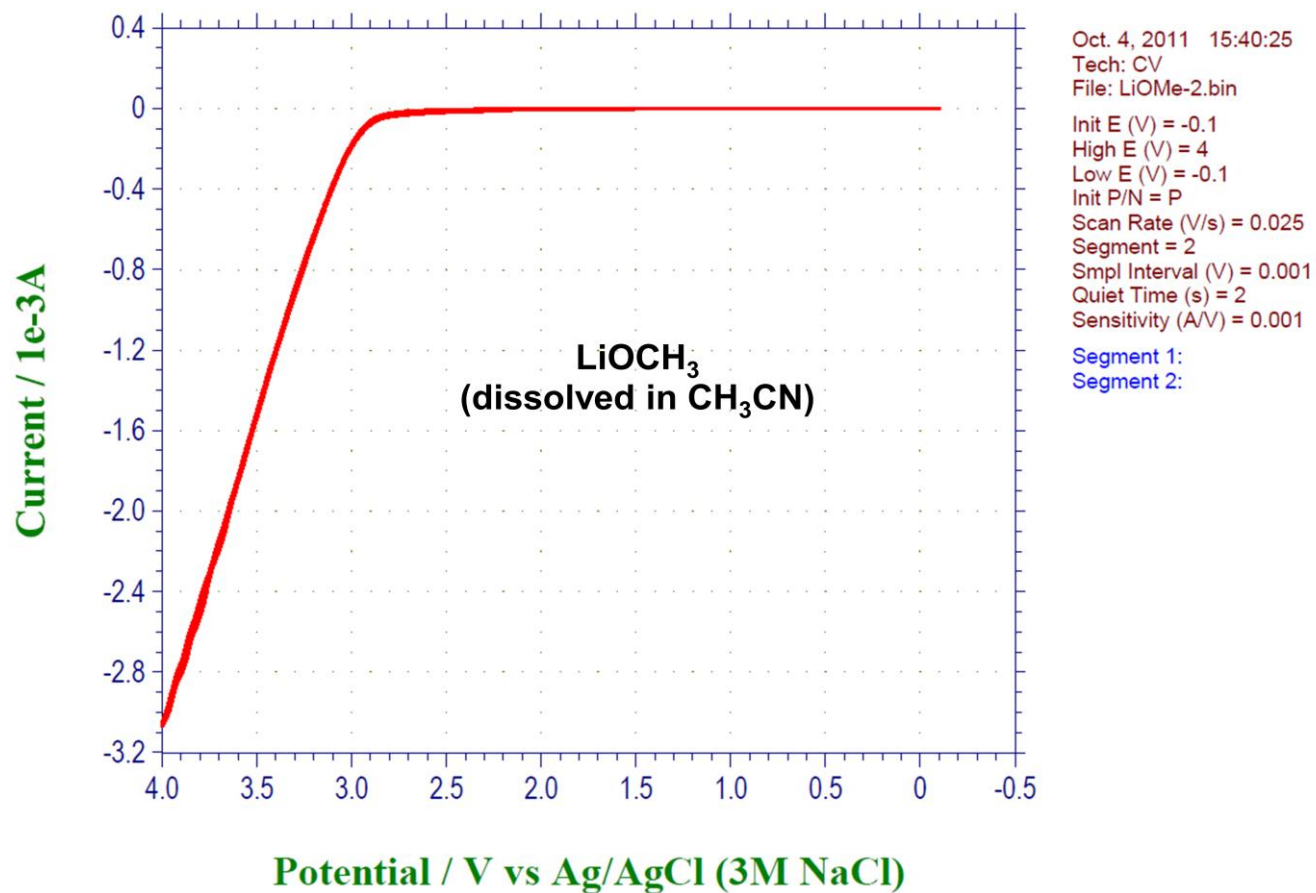


2. CV spectrum of  $\text{LiClO}_4$  in  $\text{CH}_3\text{CN}$ :

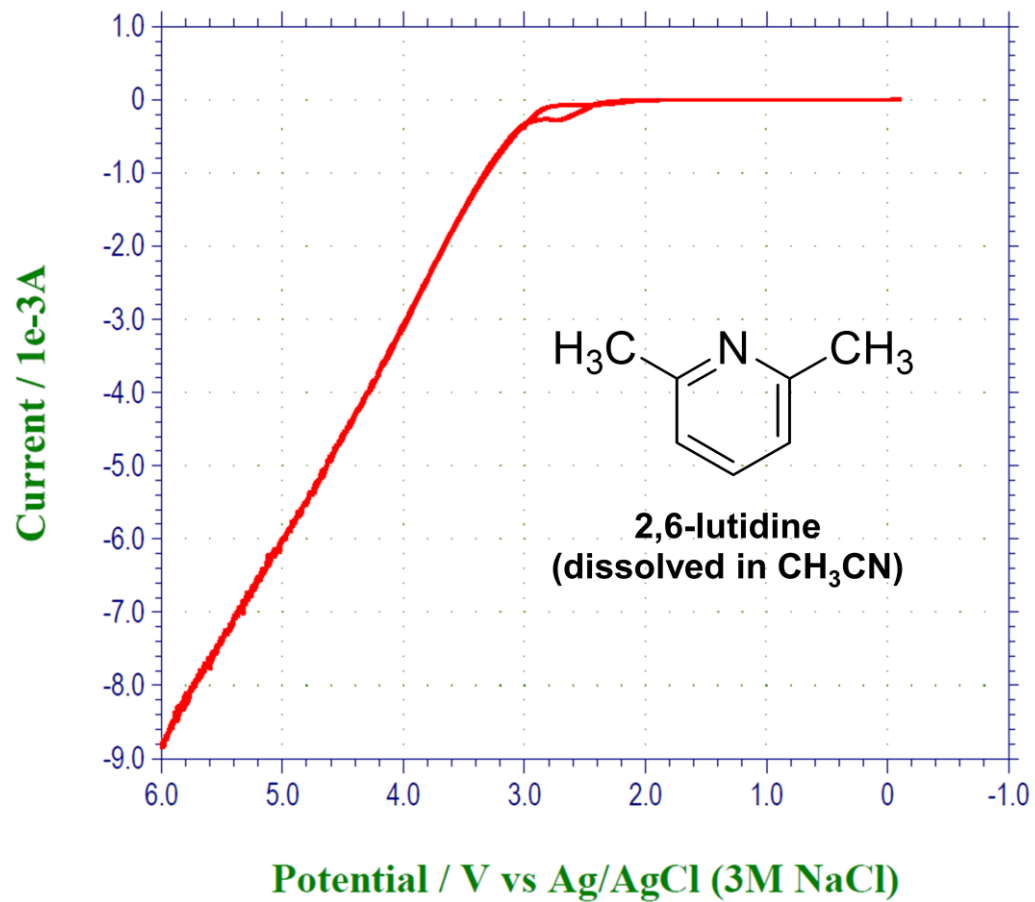




3. CV spectrum of LiOCH<sub>3</sub> in CH<sub>3</sub>CN:



4. CV spectrum of 2,6-lutidine in CH<sub>3</sub>CN:



Sept. 29, 2011 17:15:06

Tech: CV

File: 2,6-lutidine-1-2.bin

Init E (V) = -0.1

High E (V) = 6

Low E (V) = -0.1

Init P/N = P

Scan Rate (V/s) = 0.025

Segment = 2

Smpl Interval (V) = 0.001

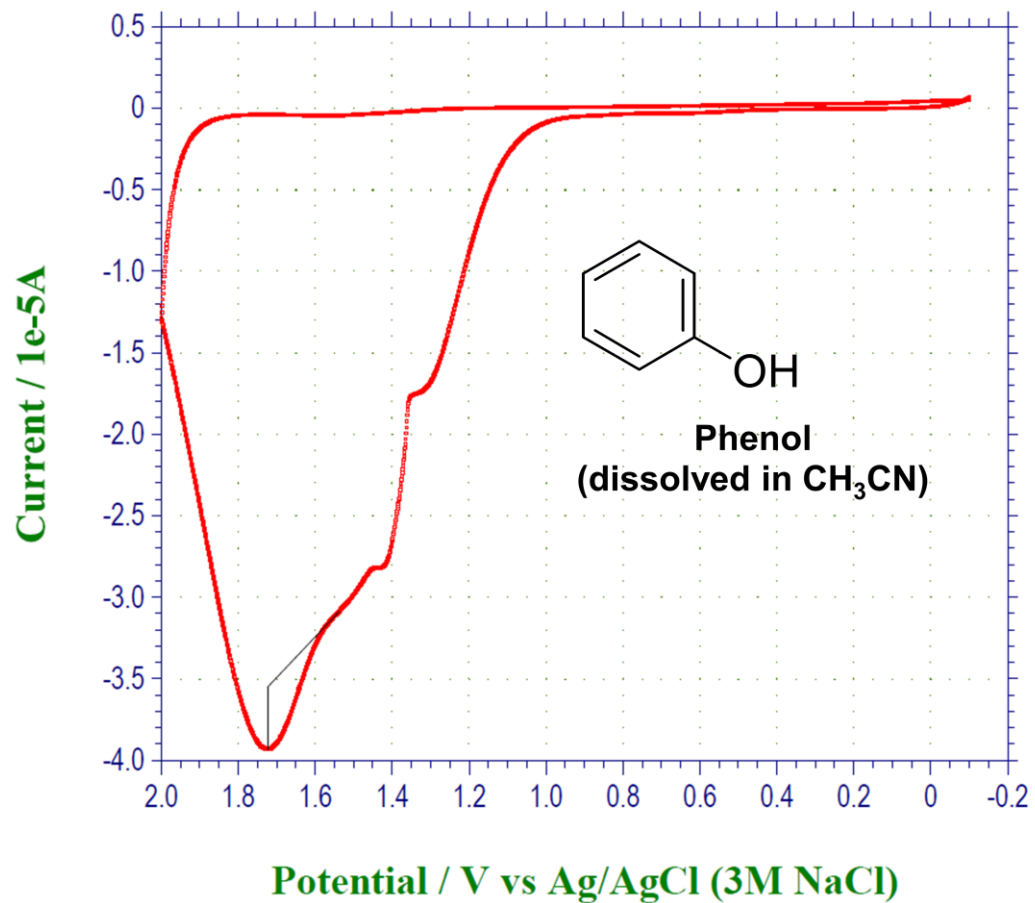
Quiet Time (s) = 2

Sensitivity (A/V) = 0.001

Segment 1:

Segment 2:

5. CV spectrum of phenol in CH<sub>3</sub>CN:



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Tech: CV

File: phenol-5-1.bin

Init E (V) = -0.1

High E (V) = 2

Low E (V) = -0.1

Init P/N = P

Scan Rate (V/s) = 0.025

Segment = 2

Smpl Interval (V) = 0.001

Quiet Time (s) = 2

Sensitivity (A/V) = 1e-5

Segment 1:

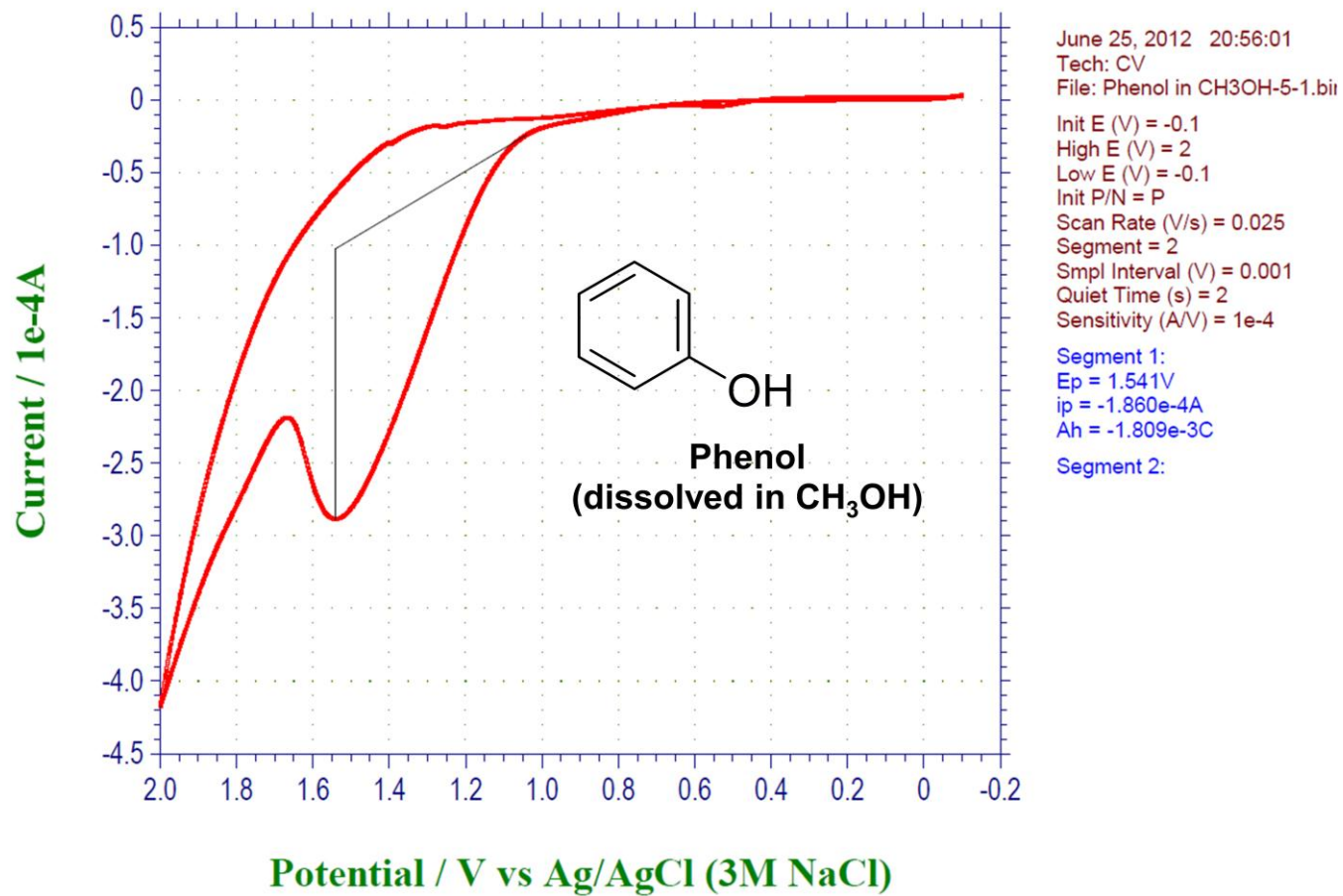
Ep = 1.724V

ip = -3.798e-6A

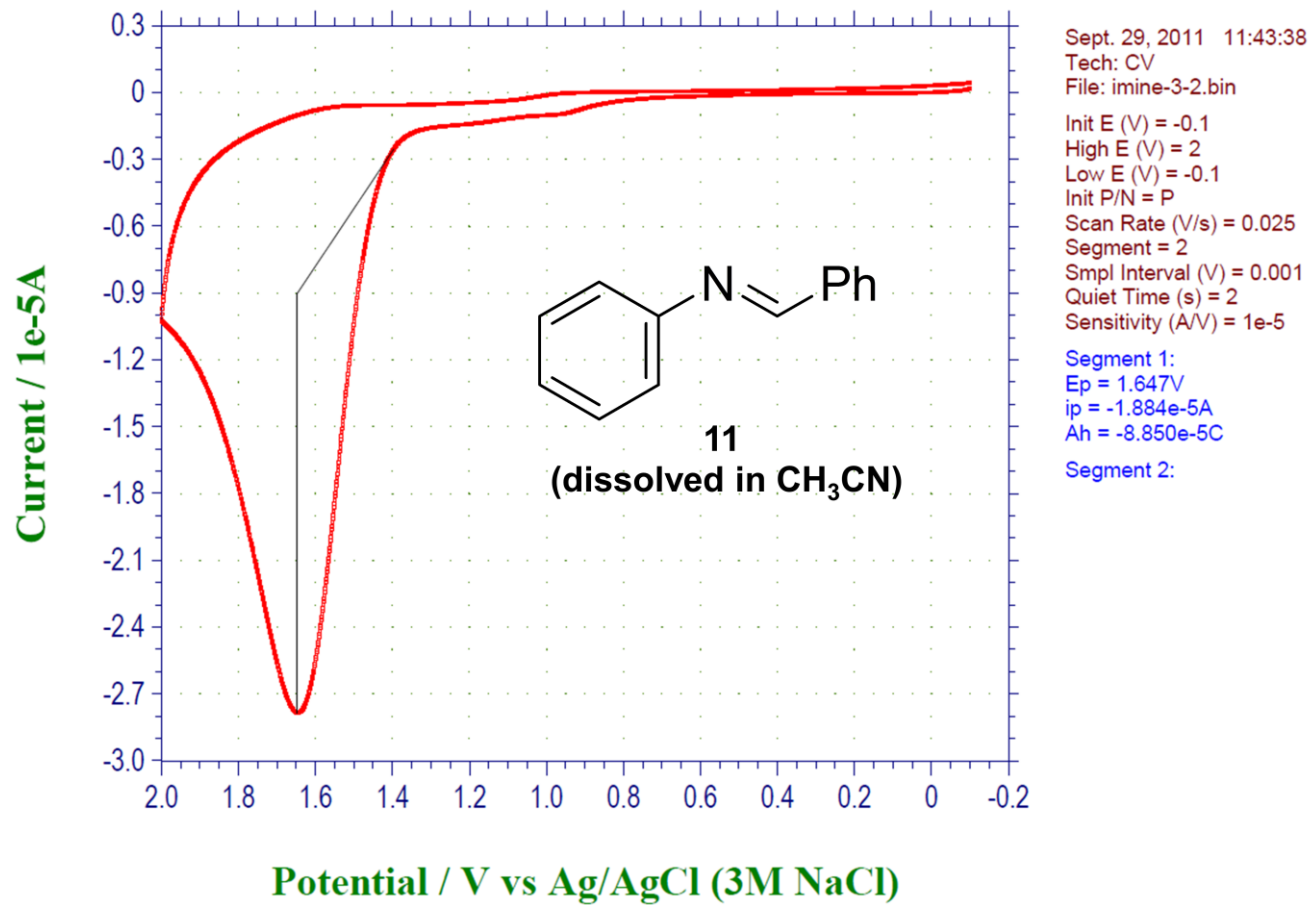
Ah = -1.380e-5C

Segment 2:

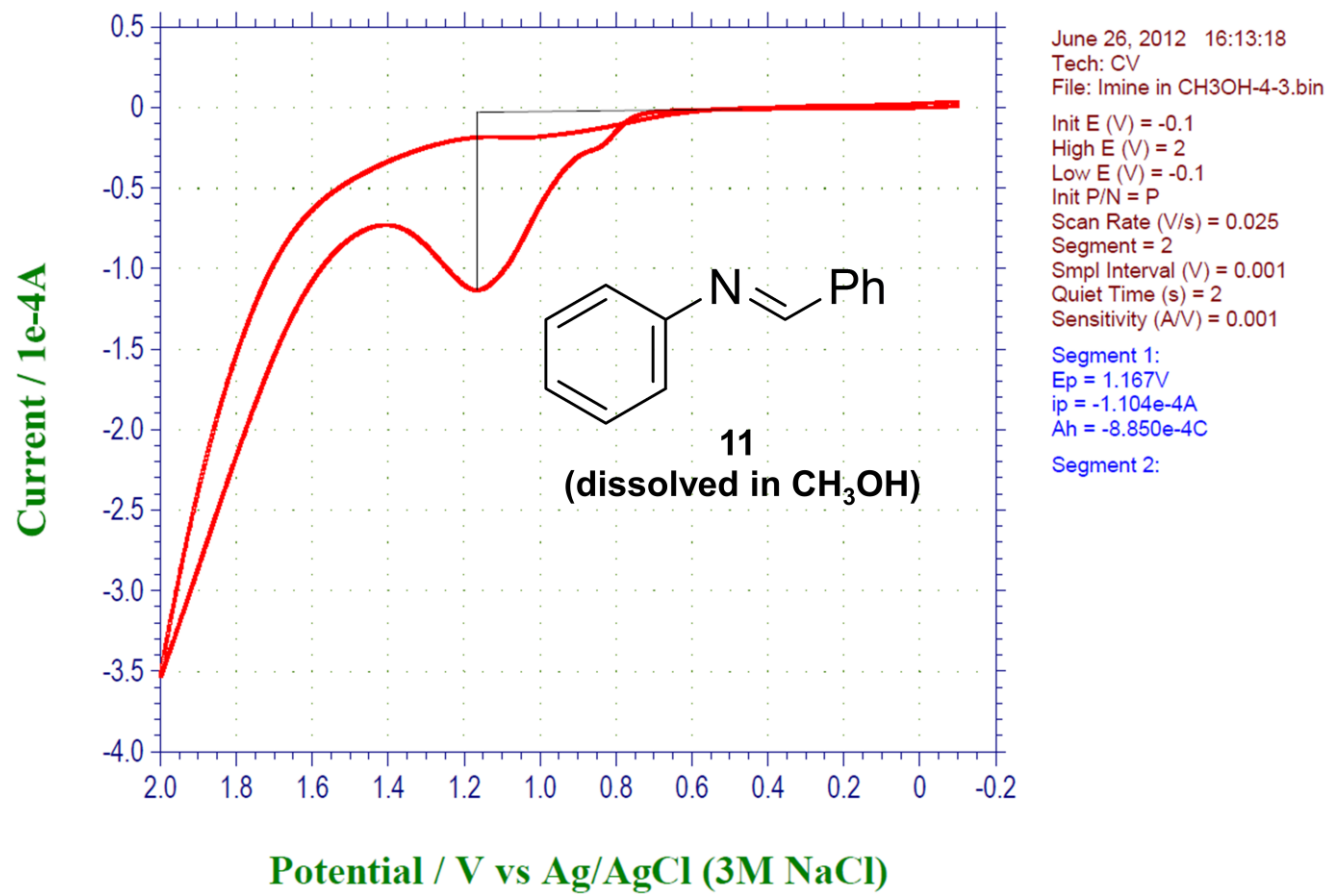
6. CV spectrum of phenol in CH<sub>3</sub>OH:



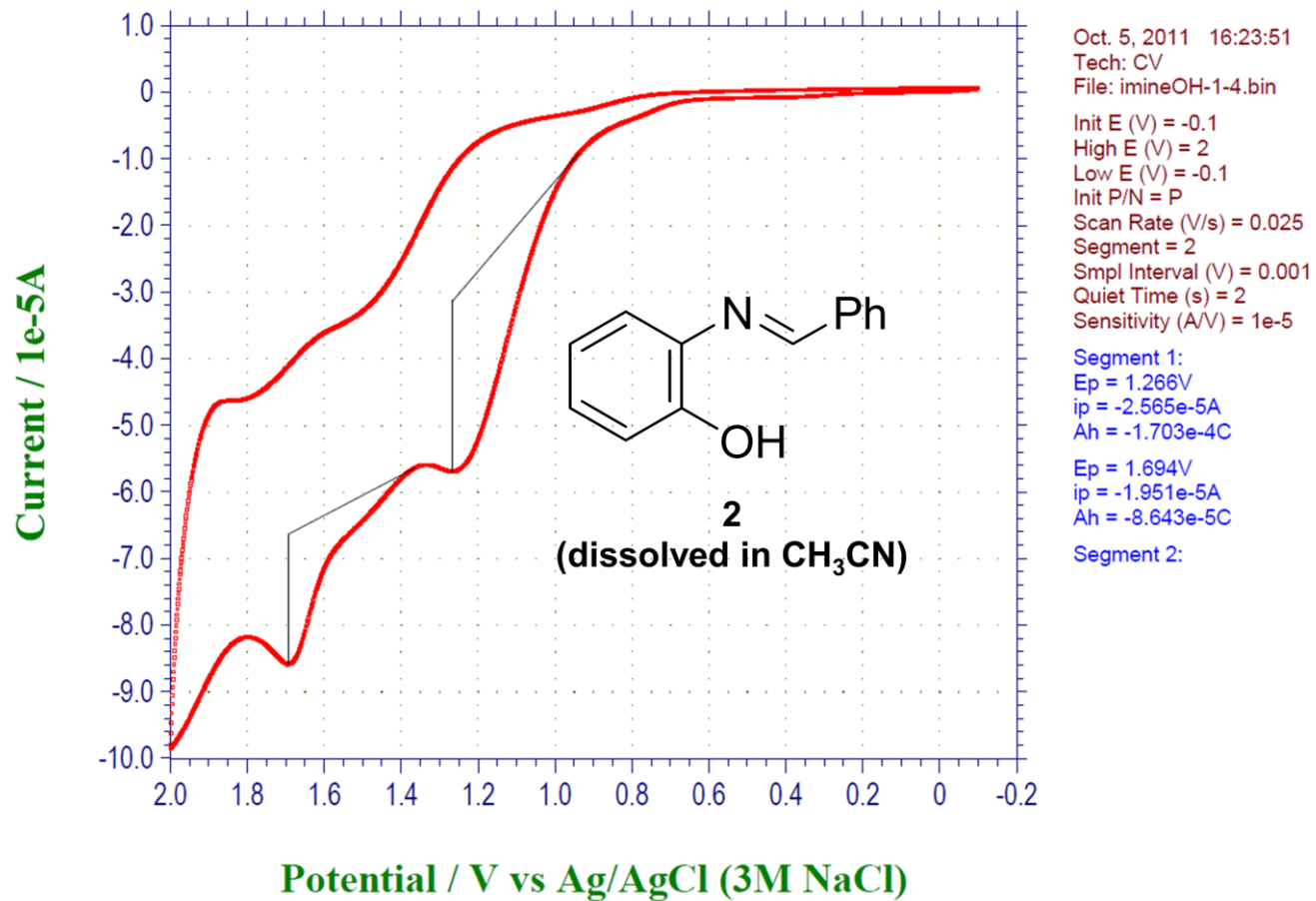
7. CV spectrum of imine (9) in CH<sub>3</sub>CN:



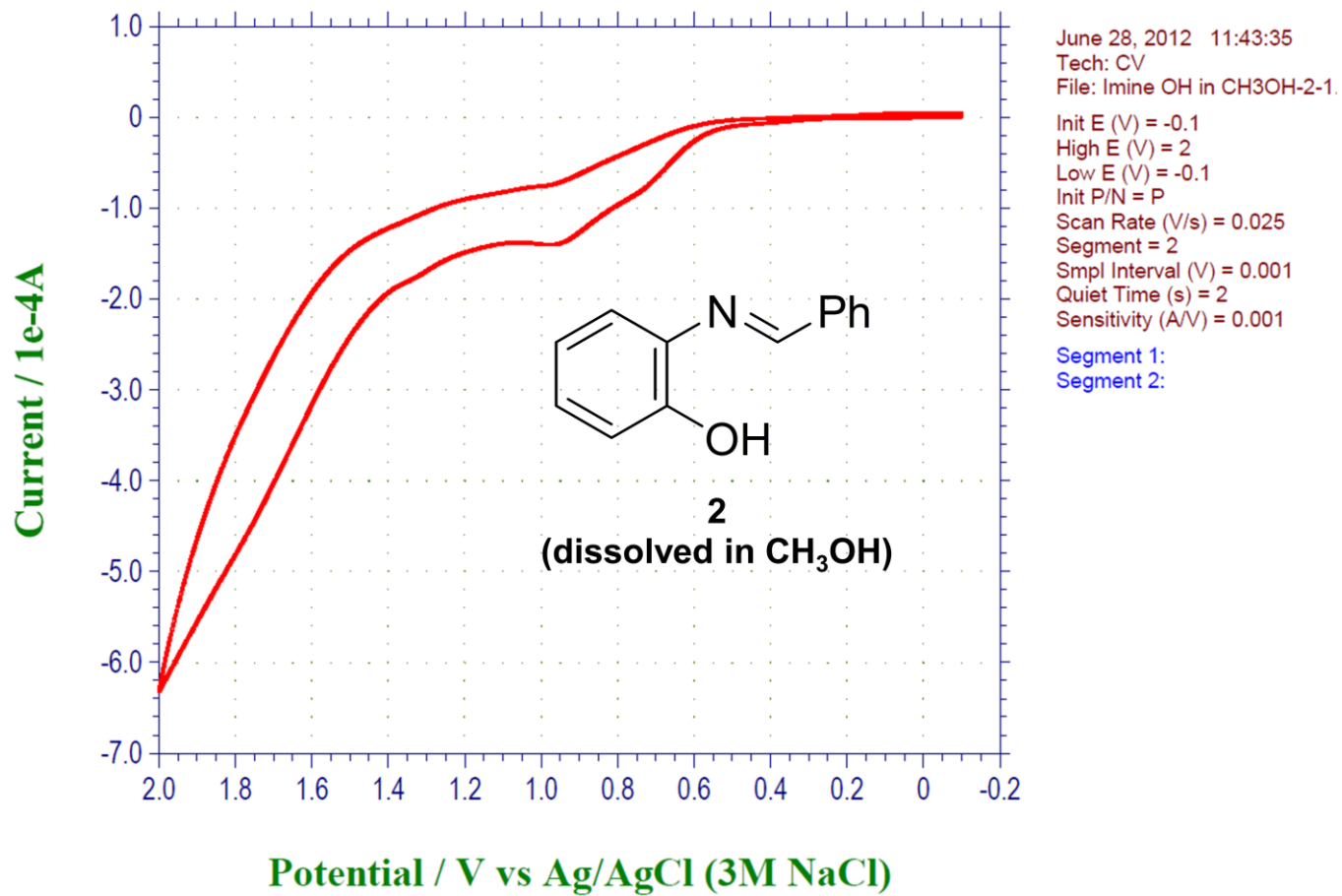
8. CV spectrum of imine (9) in CH<sub>3</sub>OH:



9. CV spectrum of phenolic Schiff base (**2**) in CH<sub>3</sub>CN:

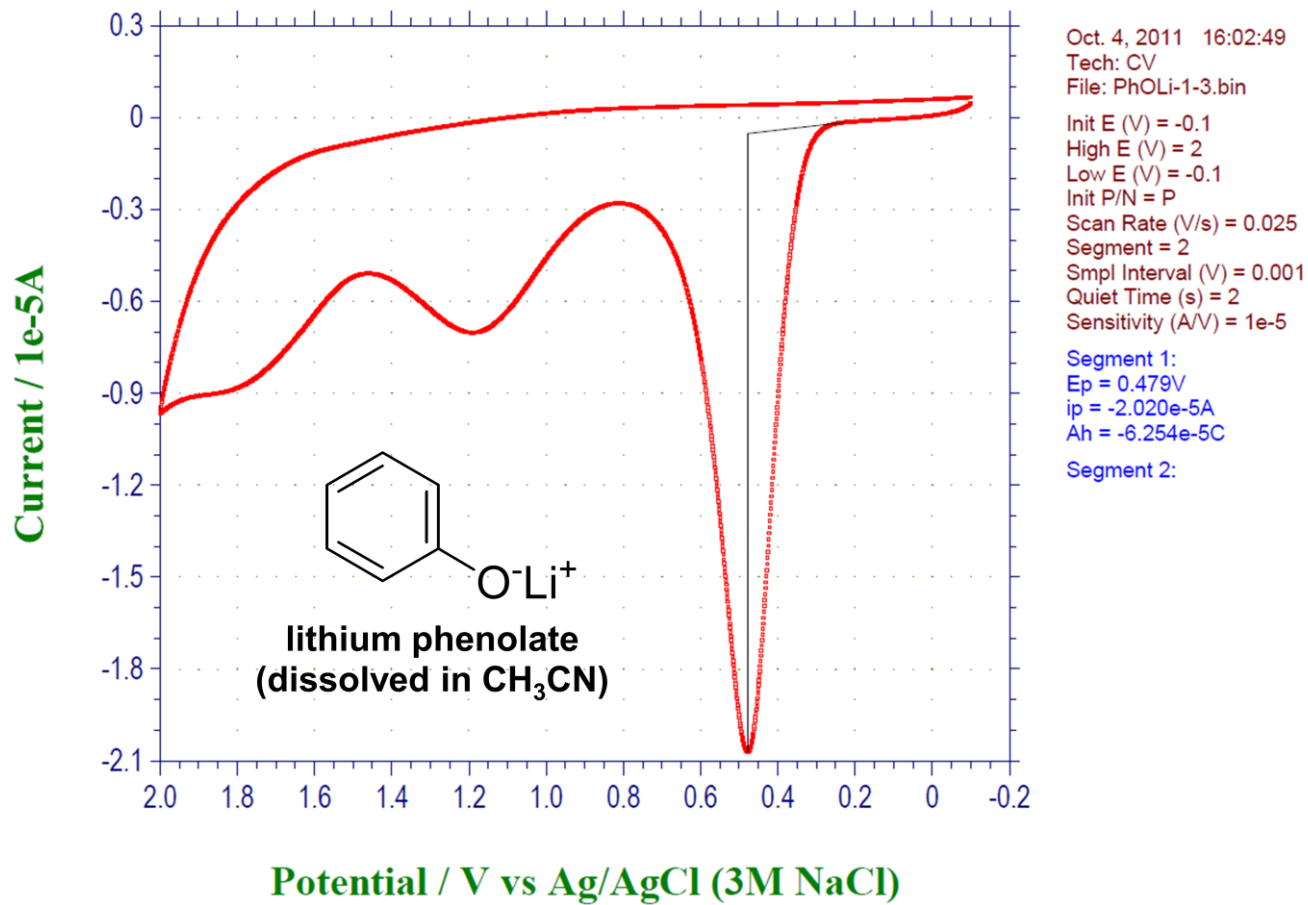


10. CV spectrum of phenolic Schiff base (**2**) in CH<sub>3</sub>OH:





11. CV spectrum of lithium phenolate in CH<sub>3</sub>CN:



12. CV spectrum of phenolate Schiff base (**7**) in CH<sub>3</sub>CN:

