

## LAMPIRAN

### Lampiran A: Perhitungan Sintesis Senyawa 5(4-bromobutil)-2,3-dimetil-1,4-benzokuinon

#### A.1 Sintesis 2,3-dimetil-1,4-benzokuinon DBQ

##### A.1.1 Perhitungan massa DMHQ

$$\text{BM DMHQ} = 138,16 \text{ g/mol}$$

$$\text{Mol DMHQ} = 9 \text{ mmol} \times \frac{1 \text{ mol}}{1000 \text{ mmol}} = 0,009 \text{ mol}$$

$$\text{Massa DMHQ} = \text{mol} \times \text{BM} = 0,009 \text{ mol} \times 138,16 \text{ g/mol} = 1,240 \text{ g}$$

##### A.1.2 Perhitungan massa KBrO<sub>3</sub>

$$\text{BM KBrO}_3 = 167 \text{ g/mol}$$

$$\text{Mol KBrO}_3 = 3 \text{ mmol} \times \frac{1 \text{ mol}}{1000 \text{ mmol}} = 0,003 \text{ mol}$$

$$\text{Massa KBrO}_3 = \text{mol} \times \text{BM} = 0,003 \text{ mol} \times 167 \text{ g/mol} = 0,501 \text{ g}$$

#### A.2 Sintesis bromo alkil benzokuinon

##### A.2.1 Perhitungan massa DMBQ

$$\text{BM DMBQ} = 136,15 \text{ g/mol}$$

$$\text{Mol DMBQ} = 2 \text{ mmol} \times \frac{1 \text{ mol}}{1000 \text{ mmol}} = 0,002 \text{ mol}$$

$$\text{Massa DMBQ} = \text{mol} \times \text{BM} = 0,002 \text{ mol} \times 136,15 \text{ g/mol} = 0,272 \text{ g}$$

##### A.2.2 Perhitungan massa HOOC(CH<sub>2</sub>)<sub>4</sub>Br

$$\text{BM HOOC(CH}_2)_4\text{Br} = 181,02 \text{ g/mol}$$

$$\text{Mol HOOC(CH}_2)_4\text{Br} = 2,1 \text{ mmol} \times \frac{1 \text{ mol}}{1000 \text{ mmol}} = 0,0021 \text{ mol}$$

$$\text{Massa HOOC(CH}_2)_4\text{Br} = 0,0021 \text{ mol} \times 181,02 \text{ g/mol} = 0,380 \text{ g}$$

##### A.2.3 Perhitungan massa AgNO<sub>3</sub>

$$\text{BM AgNO}_3 = 170 \text{ g/mol}$$

$$\text{Mol AgNO}_3 = 1 \text{ mmol} \times \frac{1 \text{ mol}}{1000 \text{ mmol}} = 0,001 \text{ mol}$$

$$\text{Massa AgNO}_3 = 0,001 \text{ mol} \times 170 \text{ g/mol} = 0,170 \text{ g}$$

#### A.2.4 Perhitungan massa $(\text{NH}_4)_2\text{S}_2\text{O}_8$

$$\text{BM } (\text{NH}_4)_2\text{S}_2\text{O}_8 = 228,20 \text{ g/mol}$$

$$\text{Mol } (\text{NH}_4)_2\text{S}_2\text{O}_8 = 2 \text{ mmol} \times \frac{1 \text{ mol}}{1000 \text{ mmol}} = 0,002 \text{ mol}$$

$$\text{Massa } (\text{NH}_4)_2\text{S}_2\text{O}_8 = 0,002 \text{ mol} \times 228,20 \text{ g/mol} = 0,456 \text{ g}$$

### A.3 Penentuan koefisien partisi

#### A.3.1 Perhitungan massa $\text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O}$ 0.1 M

$$\text{BM } \text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O} = 138 \text{ g/mol}$$

$$\text{Mol } \text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O} = 0.1 \text{ mol/L} \times 0.1 \text{ L} = 0.01 \text{ mol}$$

$$\text{Massa } \text{NaH}_2\text{PO}_4 \cdot \text{H}_2\text{O} = \text{mol} \times \text{BM} = 0.01 \text{ mol} \times 138 \text{ g/mol} = 1.38 \text{ g}$$

#### A.3.2 Perhitungan massa $\text{Na}_2\text{HPO}_4 \cdot 7\text{H}_2\text{O}$ 0.1 M

$$\text{BM } \text{Na}_2\text{HPO}_4 \cdot \text{H}_2\text{O} = 268 \text{ g/mol}$$

$$\text{Mol } \text{Na}_2\text{HPO}_4 \cdot 7\text{H}_2\text{O} = 0,1 \text{ mol/L} \times 0.1 \text{ L} = 0.01 \text{ mol}$$

$$\text{Massa } \text{Na}_2\text{HPO}_4 \cdot 7\text{H}_2\text{O} = \text{mol} \times \text{BM} = 0.01 \text{ mol} \times 268 \text{ g/mol} = 2.68 \text{ g}$$

### A.4 Perhitungan massa uji kelarutan oktanol-air

#### A.4.1 Perhitungan massa (5-(4-bromobutil)-2,3-dimetil-1,4-benzokuinon) dalam 3 mL 1-oktanol

$$\text{BM } \text{C}_{12}\text{H}_{15}\text{O}_2\text{Br} = 270,9 \text{ g/mol}$$

$$M = \frac{\text{massa}}{\text{BM}} \times \frac{1000}{\text{mL}}$$

$$10 \text{ mM} = \frac{\text{massa}}{270,9 \text{ g/mol}} \times \frac{1000}{3 \text{ mL}}$$

$$0,01 \text{ M} = \frac{\text{massa}}{270,9 \text{ g/mol}} \times \frac{1000}{3 \text{ mL}}$$

$$\text{Massa} = 8,127 \text{ mg}$$

#### A.4.2 Perhitungan massa Timokuinon dalam 3 mL 1-oktanol

$$\text{BM } \text{C}_{10}\text{H}_{12}\text{O}_2 = 164,2 \text{ g/mol}$$

$$M = \frac{\text{massa}}{\text{BM}} \times \frac{1000}{\text{mL}}$$

$$10 \text{ mM} = \frac{\text{massa}}{164,2 \text{ g/mol}} \times \frac{1000}{3 \text{ mL}}$$

$$0,01 \text{ M} = \frac{\text{massa}}{164,2 \text{ g/mol}} \times \frac{1000}{3 \text{ mL}}$$

$$\text{Massa} = 4,926 \text{ mg}$$

## **A.5 Perhitungan *yield* produk**

### **A.5.1 Perhitungan *yield* (%) produk DBQ 1**

$$\text{Massa produk} = 0,29 \text{ g}$$

$$\begin{aligned} \text{Yield} &= \frac{\text{mol produk}}{\text{mol reaktan}} \times 100\% \\ &= \frac{0,29 \text{ g} / 136,15 \text{ g/mol}}{9 \text{ mmol}} \times 100\% \\ &= \frac{2,13 \text{ mmol}}{9 \text{ mmol}} \times 100\% \\ &= 23,667 \% \end{aligned}$$

### **A.5.2 Perhitungan *yield* (%) produk DBQ 2**

$$\text{Massa produk} = 1,29 \text{ g}$$

$$\begin{aligned} \text{Yield} &= \frac{\text{mol produk}}{\text{mol reaktan}} \times 100\% \\ &= \frac{1,29 \text{ g} / 136,15 \text{ g/mol}}{18 \text{ mmol}} \times 100\% \\ &= \frac{9,475 \text{ mmol}}{18 \text{ mmol}} \times 100\% \\ &= 52,638 \% \end{aligned}$$

### **A.5.3 Perhitungan *yield* (%) produk C4-1**

$$\text{Massa produk} = 0,04 \text{ g}$$

$$\begin{aligned} \text{Yield} &= \frac{\text{mol produk}}{\text{mol reaktan}} \times 100\% \\ &= \frac{0,04 \text{ g} / 270,9 \text{ g/mol}}{2 \text{ mmol}} \times 100\% \\ &= \frac{0,148 \text{ mmol}}{4,1 \text{ mmol}} \times 100\% \\ &= 3,601 \% \end{aligned}$$

### **A.5.4 Perhitungan *yield* (%) produk C4-2**

$$\text{Massa produk} = 0,13 \text{ g}$$

$$\begin{aligned} \text{Yield} &= \frac{\text{mol produk}}{\text{mol reaktan}} \times 100\% \\ &= \frac{0,13 \text{ g} / 270,9 \text{ g/mol}}{8,2 \text{ mmol}} \times 100\% \\ &= \frac{0,450 \text{ mmol}}{8,2 \text{ mmol}} \times 100\% \\ &= 5,582 \% \end{aligned}$$

## A.6 Perhitungan nilai koefisien partisi (log P)

### A.6.1 Koefisien partisi (log $P_{7,4}$ ) timokuinon dalam oktanol-air (3:7)

oktanol:air (3:7),  $\lambda_{maks} = 254 \text{ nm}$

$$\text{Log}P = \log \frac{A_o/V_o}{A_a/V_a} = \log \frac{63970392V/3 \text{ mL}}{920323 V/7 \text{ mL}} = 2,21$$

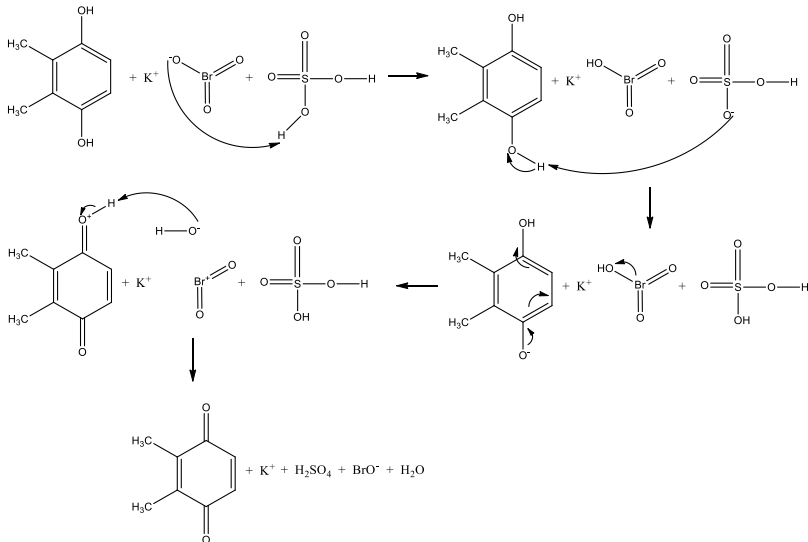
### A.6.2 Koefisien partisi (log $P_{7,4}$ ) C4 2 dalam oktanol-air (3:7)

oktanol:air (3:7),  $\lambda_{maks} = 259 \text{ nm}$

$$\text{Log} P = \log \frac{A_o/V_o}{A_a/V_a} = \log \frac{36350375V/3 \text{ mL}}{87531V/7 \text{ mL}} = 2.99$$

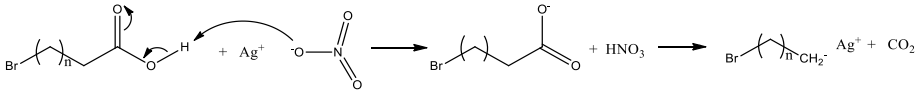
## Lampiran B : Mekanisme Reaksi

### B.1 Sintesis 2,3-dimetil-1,4-benzokuinon (DBQ)



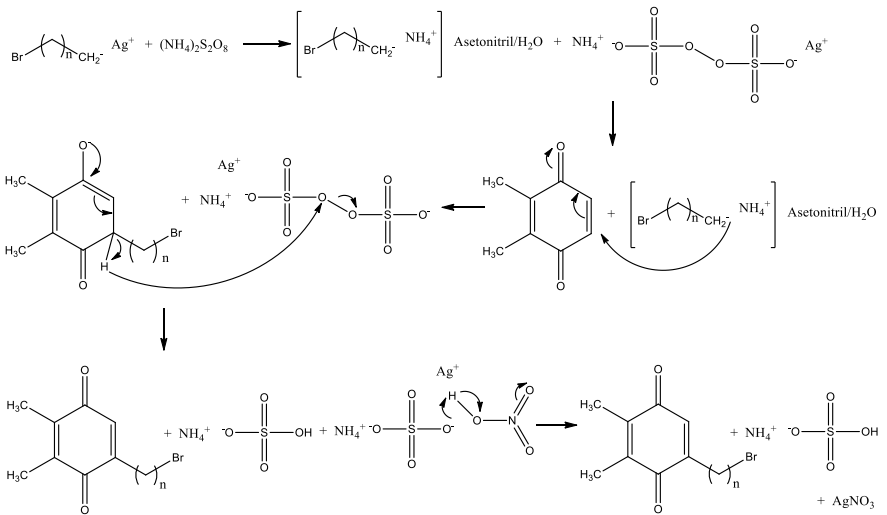
## B.2 Sintesis bromoalkil benzokuinon

### B.2.1 Reaksi dekarboksilasi bromopentanoat



Keterangan :  $n = 3$

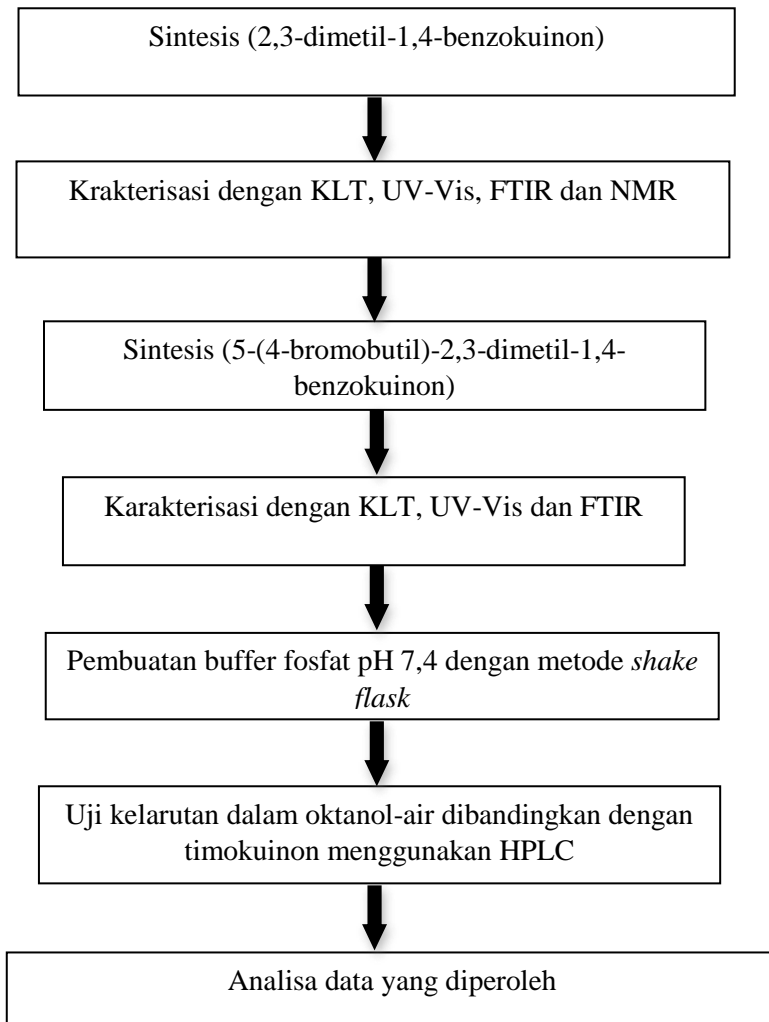
### B.2.2 Reaksi alkilasi



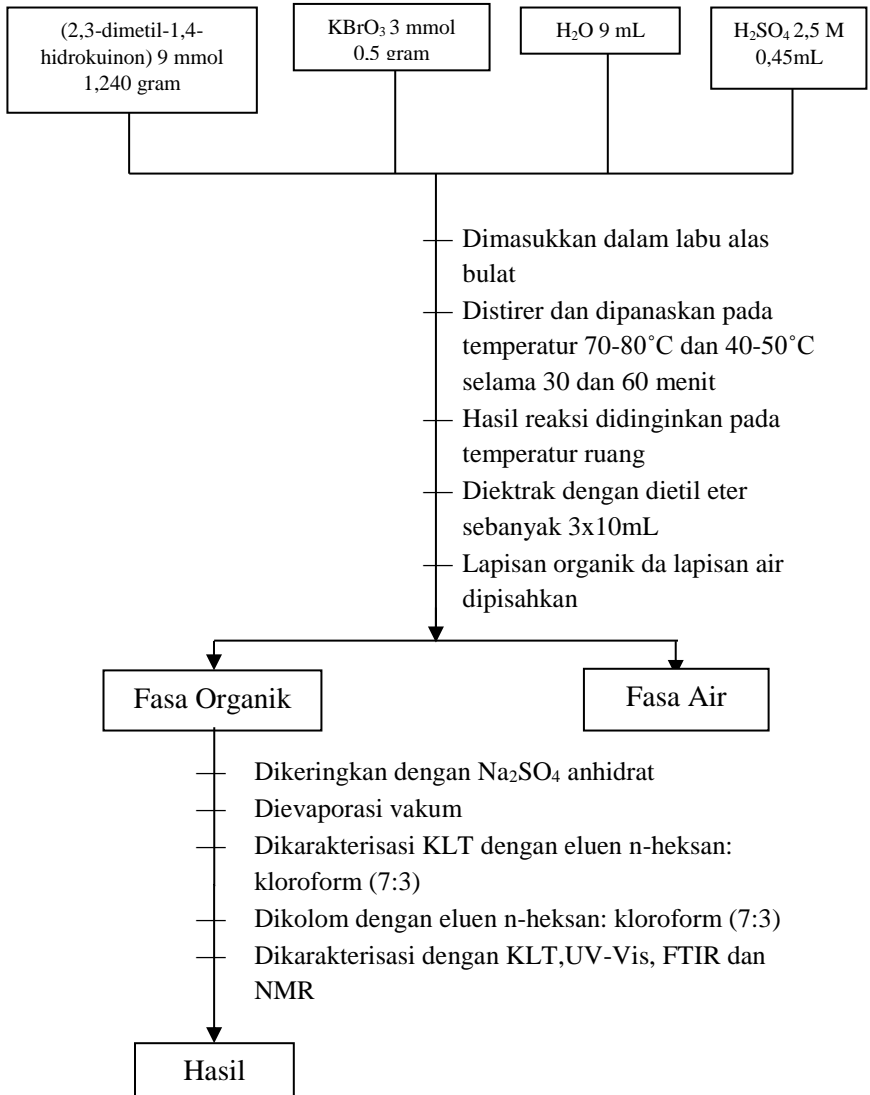
Keterangan:  $n = 4$

## Lampiran C : Skema Kerja

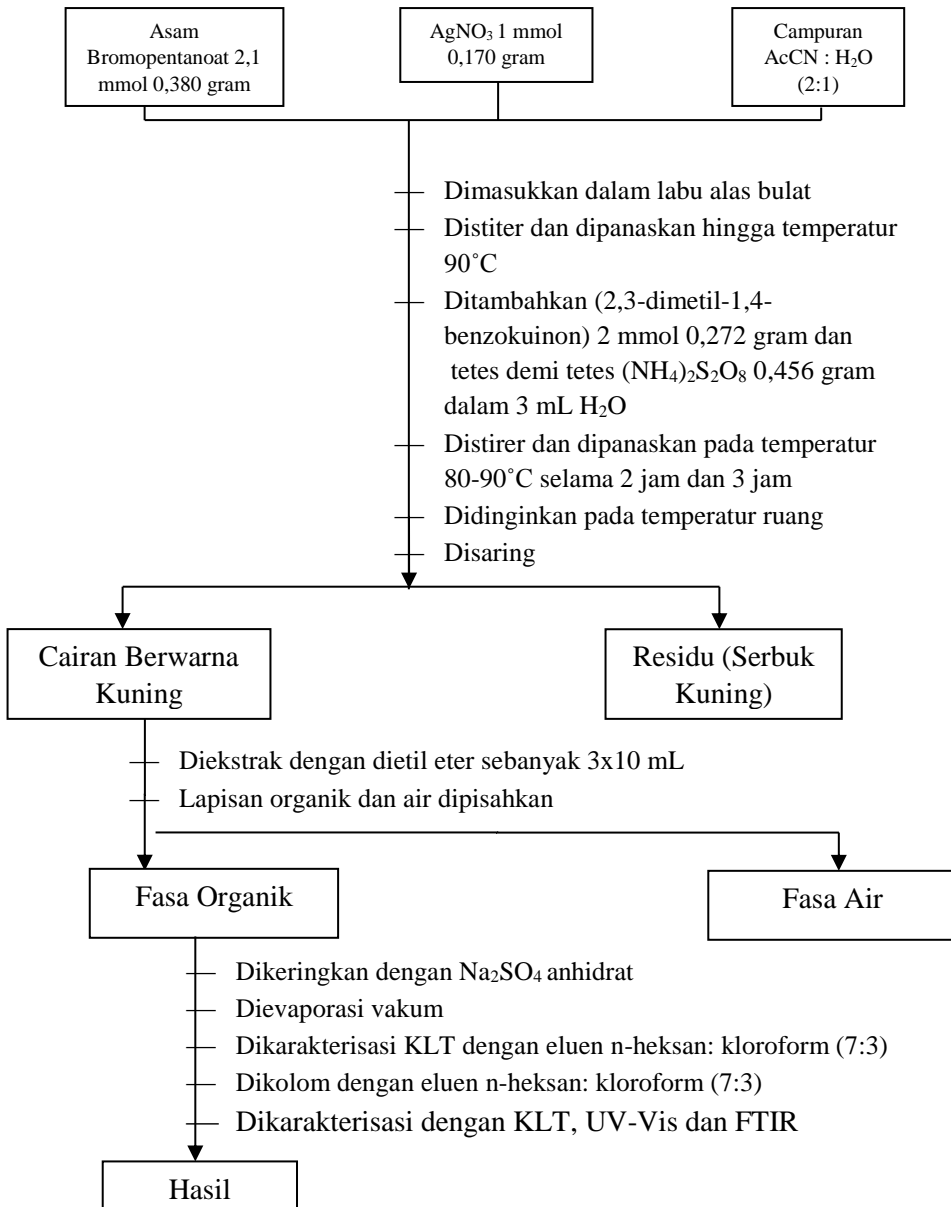
### C.1 Diagram alir penelitian



## C.2 Diagram alir sintesis 2,3-dimetil-1,4-benzokuinon (DBQ)



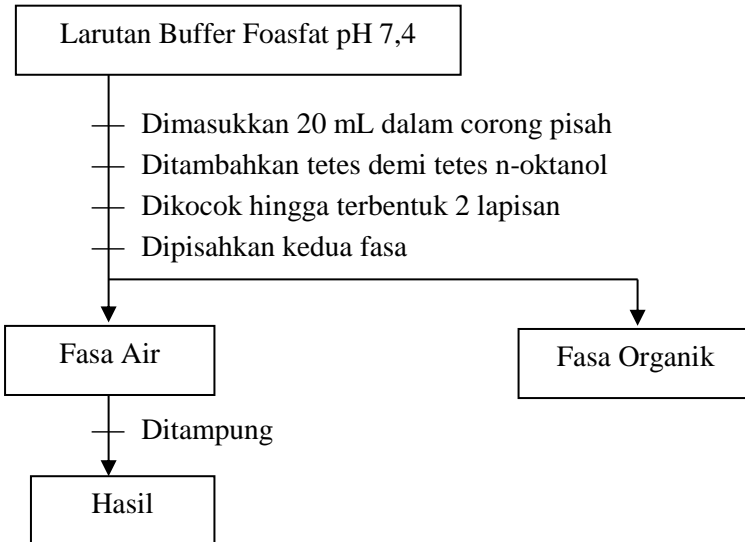
### C.3 Diagram alir sintesis 5-(4-bromobutil)-2,3-dimetil-1,4-benzokuinon (C4)



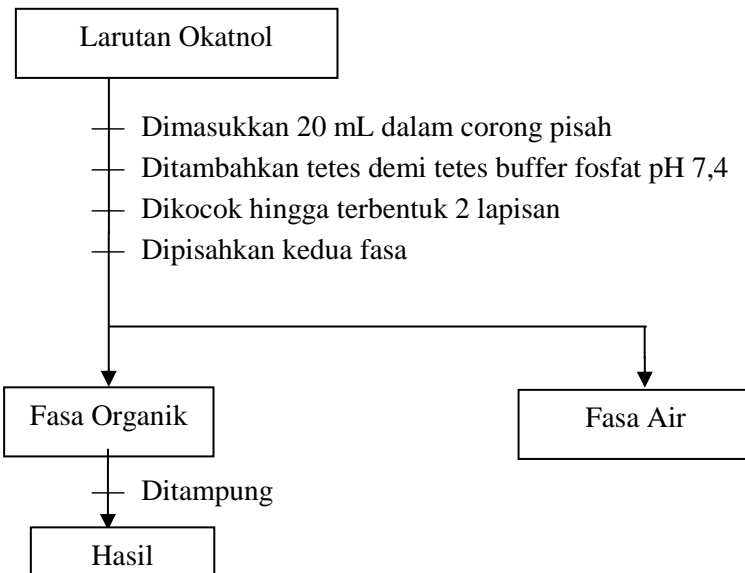


#### C.4 Diagram alir uji kelarutan dalamoktanol-air

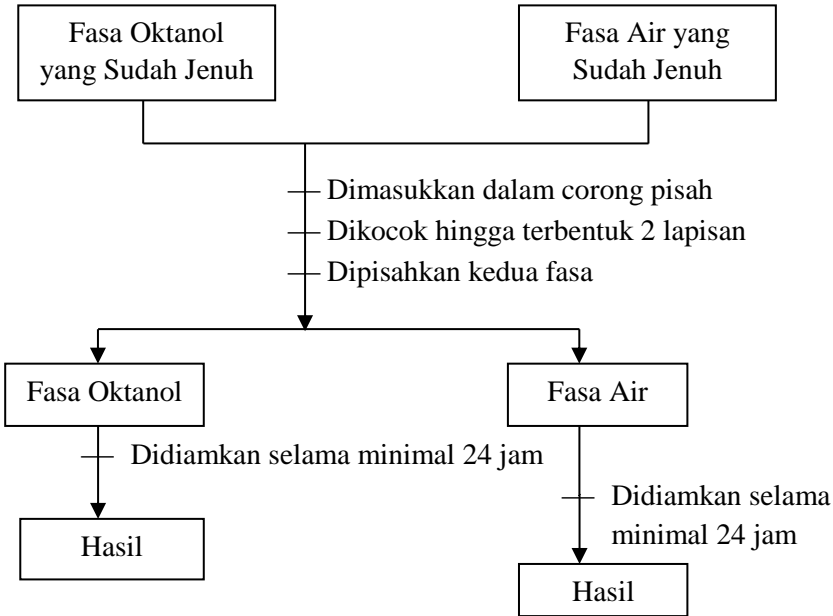
##### Penjenuhan fasa air dengan n-okatanol



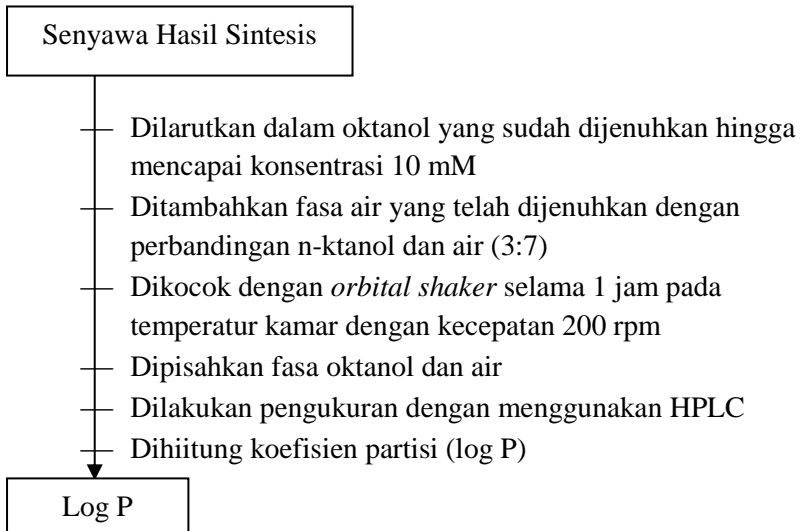
##### Penjenuhan fasa n-oktanol dengan fasa air



## Preparasi n-oktanol dan air untuk pengukuran kelarutan



## Pengukuran kelarutan menggunakan HPLC

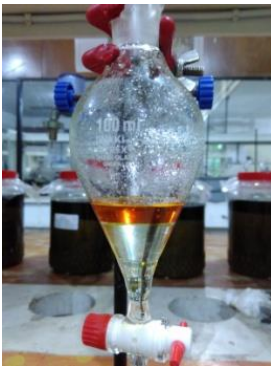


## Lampiran D : Dokumentasi Penelitian

### D.1 Rangkaian alat reaksi



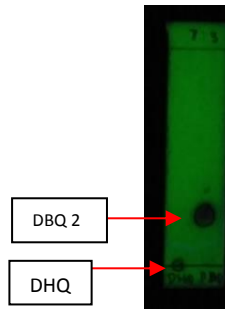
### D.2 Ekstraksi dengan dietil eter



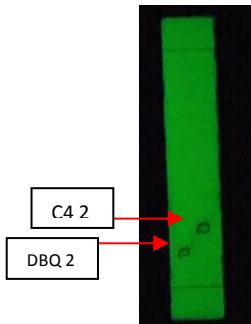
### D.3 Rangkaian alat kromatografi kolom



### D.4 Hasil KLT DHQ dengan DBQ 2



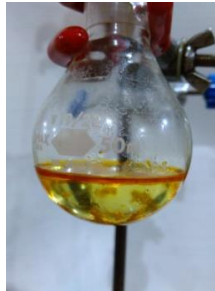
### D.5 Hasil KLT DBQ 2 dengan C4-2



### D.6 Hasil reaksi DBQ



### D.7 Hasil reaksi C4-2



### D.8 Produk DBQ



### D.9 Produk C4-2

