



## APPENDICES

**Appendix 1. Quantities of Reagents Used and Yields of Products**

**Table 1. Quantities of reagents used and yields of TsIm**

<b>Experiments</b>	<b>I</b>	<b>II</b>	<b>III</b>
Imidazole	6.808 g	6.808 g	6.808 g
Tosyl chloride	19.064 g	19.064 g	19.064 g
Dichloromethane	80 mL	80 mL	80 mL
Hexylamine	1 mL	1 mL	1 mL
Sodium carbonate	9.24 g	9.24 g	9.24 g
Water	100 mL	100 mL	100 mL
Actual mass of tosyl imidazole	19.2652 g	18.7735 g	19.6486 g
Theoretical mass of tosyl imidazole	22.226 g	22.226 g	22.226 g
Yield (%)	86.68	84.47	88.40

**Table 2. Quantities of reagents used and yields of CD-OTs**

<b>Experiments</b>	<b>I</b>	<b>II</b>	<b>III</b>
$\beta$ -CD	11.35 g	11.35 g	11.35 g
Tosyl imidazole	3.334 g	3.334 g	3.334 g
Water	100 mL	100 mL	100 mL
Sodium hydroxide	4 g	4 g	4 g
Actual mass of CD-OTs	4.8477 g	4.621 g	4.8006 g
Theoretical mass of CD-OTs	12.8919 g	12.8919 g	12.8919 g
Yield (%)	37.60	35.84	37.24

**Table 3. Quantities of reagents used and yields of CD-N<sub>3</sub>**

<b>Experiments</b>	<b>I</b>	<b>II</b>	<b>III</b>
CD-OTs	12.8919 g	12.8919 g	12.8919 g
Sodium azide	5.2008 g	5.2008 g	5.2008 g
Water	250 mL	250 mL	250 mL
Actual mass of CD-N <sub>3</sub>	10.6036 g	11.1637 g	10.8946 g
Theoretical mass of CD-N <sub>3</sub>	11.6002 g	11.6002 g	11.6002 g
Yield (%)	91.41	96.24	93.92

Table 4. Quantities of reagents used and yields of CD-NH<sub>2</sub>

<b>Experiments</b>	<b>I</b>	<b>II</b>	<b>III</b>
CD-N <sub>3</sub>	11.60 g	11.60 g	11.60 g
Triphenylphosphine	2.886 g	2.886 g	2.886 g
DMF	20 mL	20 mL	20 mL
Water	2 mL	2 mL	2 mL
Actual mass of CD-NH <sub>2</sub>	10.4303 g	10.6221 g	10.4705 g
Theoretical mass of CD-NH <sub>2</sub>	11.34 g	11.34 g	11.34 g
Yield (%)	91.98	93.67	92.33

Table 5. Quantities of reagents used and yields of CD-NH<sub>3</sub>Cl

<b>Experiments</b>	<b>I</b>	<b>II</b>	<b>III</b>
CD-NH <sub>2</sub>	9.072 g	9.072 g	9.072 g
HCl	25 mL	25 mL	25 mL
Water	20 mL	20 mL	20 mL
Actual mass of CD-NH <sub>3</sub> Cl	9.0475 g	8.5862 g	8.7961 g
Theoretical mass of CD-NH <sub>3</sub> Cl	9.3637 g	9.3637 g	9.3637 g
Yield (%)	96.62	91.70	93.94

Table 6. Quantities of reagents used and yields of CD-PrAmOTs

<b>Experiments</b>	<b>I</b>	<b>II</b>	<b>III</b>
CD-OTs	3.867 g	3.867 g	3.867 g
<i>n</i> -propylamine	0.5325 g	0.5325 g	0.5325 g
DMF	7.5 mL	7.5 mL	7.5 mL
Actual mass of CD-PrAmOTs	3.3397 g	3.5395 g	3.3879 g
Theoretical mass of CD-PrAmOTs	4.0443 g	4.0443 g	4.0443 g
Yield (%)	82.58%	87.52%	83.77%

Table 7. Quantities of reagents used and yields of CD-PrAmCl

<b>Experiments</b>	<b>I</b>	<b>II</b>	<b>III</b>
CD-PrAmCl	3.3397 g	3.5395 g	3.3879 g
HCl	10 mL	10.5 mL	10 mL
Water	10 mL	10 mL	10 mL
Actual mass of CD-PrAmCl	2.2768 g	2.4256 g	2.1695 g
Theoretical mass of CD-PrAmCl	3.0036 g	3.1833 g	3.0469 g
Yield (%)	75.80%	76.20%	71.20%

## Appendix 2. Preparation TsIm and $\beta$ -CD Solution

### TsIm Stock Solution

Mass	: 0.1111g
Mr	: 222.26 g/mol
Mol	: $5 \times 10^{-4}$ mol
Total Volume	: 100 mL
Concentration	: $5 \times 10^{-3}$ M

### TsIm Dilute Solution

Solution I (diluted from stock solution)	
Concentration Solution I	: $5 \times 10^{-3}$ M
Volume stock solution	: 10 mL
Volume final solution	: 100 mL
Solution II (diluted from solution I)	
Concentration Solution II	: $5 \times 10^{-4}$ M
Volume stock solution	: 10 mL
Volume final solution	: 100 mL

### $\beta$ -CD Stock Solution

Mass	: 1.3333 gram
Mr	: 1333 g/mol
Mol	: $1 \times 10^{-3}$ mol
Total Volume	: 100 mL
Concentration	: $10 \times 10^{-3}$ M

### $\beta$ -CD Dilute Solution

Solution I (diluted from stock solution)	
Concentration Solution I	: $8 \times 10^{-3}$ M
Volume stock solution	: 20 mL
Volume final solution	: 25 mL
Solution II (diluted from stock solution)	
Concentration Solution II	: $6 \times 10^{-3}$ M
Volume stock solution	: 15 mL
Volume final solution	: 25 mL
Solution III (diluted from stock solution)	
Concentration Solution III	: $4 \times 10^{-3}$ M
Volume stock solution	: 10 mL
Volume final solution	: 25 mL
Solution IV (diluted from stock solution)	
Concentration Solution IV	: $2 \times 10^{-3}$ M
Volume stock solution	: 5 mL
Volume final solution	: 25 mL

### Appendix 25. Melting Point Test Result

Table 1. Melting Point of TsIm

Experiment	Melting Point (°C)	Mean (°C)
1	75-76	75.5
2	75-77	76
3	76-77	76.5
<b>Mean ± Standard Deviation</b>	<b>76 ± 0.5</b>	

Table 2. Melting Point of CD-OTs

Experiment	Melting Point (°C)
1	164
2	164
3	163
<b>Mean ± Standard Deviation</b>	<b>164 ± 0.58</b>

Table 3. Melting Point of CD-N<sub>3</sub>

Experiment	Melting Point (°C)
1	178
2	178
3	179
<b>Mean ± Standard Deviation</b>	<b>178 ± 0.58</b>

Table 4. Melting Point of CD-NH<sub>3</sub>Cl

Experiment	Melting Point (°C)
1	190
2	192
3	188
<b>Mean ± Standard Deviation</b>	<b>190 ± 2.00</b>

Table 5. Melting Point of CD-PrAmCl

Experiment	Melting Point (°C)
1	178
2	179
3	178
<b>Mean ± Standard Deviation</b>	<b>178 ± 0.58</b>