

ERRATA of Diploma Thesis

Design, synthesis, and evaluation of heterocyclic compounds with potential antimicrobial activity III
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In the diploma thesis, the following corrections are made:

- 1) Correction of abbreviation MS-ASAP (Abbreviations)

MS-ASAP – Mass Spectrometry – Assisted Screening for Accelerated Process

Correction:

ASAP-MS – Atmospheric Solid Analysis Probe – Mass Spectrometry

- 2) Information on mode for Flash chromatography:

In section 9.1.1 Materials and Instrumentation, information on the mode for Flash chromatography was missing.

Equilibration time was set for 10 minutes using column F0040 – 37 g (20 bar). Hexane and EtOAc were used in a gradient inversely proportional, starting at 80% Hexane and 20% EtOAc and finishing at 100% EtOAc for 30-45 minutes. Channels 1 and 2 were set at 254 and 280 nm, respectively.

3) Correction of Scheme 1

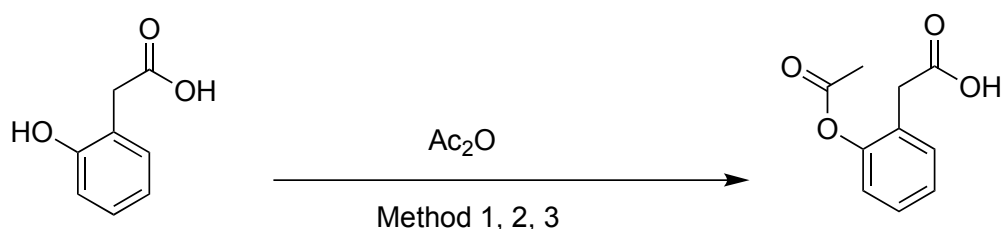
in section 9.2.1.3 Method 3, page 33, the scheme was incorrect. The acetylation reagent was acetic acid anhydride (Ac_2O), **not acetic acid**.

Previous scheme:



Conditons: Method 1 - $\text{CHCl}_3/\text{H}_2\text{O}$, NaOH, RT, 12 h
Method 2 - PhMe/THF, pyridine, RT, 12 h
Method 3 - without solvent, H_2SO_4 , RT, 1 h

Updated scheme:



Conditions: Method 1 - $\text{CHCl}_3/\text{H}_2\text{O}$, NaOH, RT, 12h
Method 2 - PhMe/THF, pyridine, RT, 12h
Method 3 - without solvent, H_2SO_4 , RT, 1h

4) Correction of incubation time in the antibacterial activity assay in section 9.5, page 48

Incorrectly stated:

Antibacterial activity was assessed as the Minimum Inhibitory Concentration (MIC) after 24 and **48 hours** of static incubation in a dark and humidified environment at $35^\circ\pm 2^\circ\text{C}$.

Correction:

Antibacterial activity was assessed as the Minimum Inhibitory Concentration (MIC) after 24 hours of static incubation in a dark and humidified environment at $35^\circ\pm 2^\circ\text{C}$.

5) Antifungal screening results

In section 9.5 Biological Activity Assay, page 50, the **results from the antifungal assay were missing**. Added data:

Code	MINIMUM INHIBITORY CONCENTRATION (µg/mL)							
	<i>Candida albicans</i>	<i>Candida krusei</i>	<i>Candida parapsilosis</i>	<i>Candida tropicalis</i>	<i>Aspergillus fumigatus</i>	<i>Aspergillus flavus</i>	<i>Lichtheimia corymbifera</i>	<i>Trichophyton interdigitale</i>
1	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
2	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
3	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
4	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
5	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
6	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
7	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
8	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
9	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
10	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500	≥ 500
AMPHOTERICIN B	1	1	0.5	1	4	4	1	1

*The IC₉₀ of amphotericin B is the lowest concentration giving rise to an inhibition of growth of 90% of that of the drug-free control. Results were read after 24 h (yeasts) or 48 h (moulds) cultivation without agitation at 35±2 °C in a humidified atmosphere. Measured on a microplate reader (Synergy™ HTX, BioTek Instruments, Inc., USA) at wavelength 530 nm.

6) Corrections to Table 1

In section 9.2.2.3 Method 6 on page 33, Table I was filled with **incorrect values in the last column** – the isolated yield in percent to theoretical yield.

Previous version:

Code	Acid		Amino compound			Product – Isolated yield	
	n (mmol)	m (mg)	R	n (mmol)	m (mg)	m (mg)	% to theoretical
1	4.5	685	2-NH ₂ -5-Cl-Pz	3.5	453	27	6
2	4.5	685	2-NH ₂ -5-Cl-Py	3.5	450	18	4
3	4.5	685	3-NH ₂ -6-Cl-Py	3.5	450	130	29
4	4.5	685	2-NH ₂ -6-Cl-Py	3.5	450	27	6
5	4.5	685	3-NH ₂ -5-Cl-Py	3.5	450	72	16
6	4.5	685	3-NH ₂ -2-Cl-Py	3.5	450	45	10
7	4.5	685	2-NH ₂ -Pz	3.5	333	17	5

Corrected version:

Code	Acid		Amino compound			Product – Isolated yield	
	n (mmol)	m (mg)	R	n (mmol)	m (mg)	m (mg)	% to theoretical
1	4.5	685	2-NH ₂ -5-Cl-Pz	3.5	453	27	3
2	4.5	685	2-NH ₂ -5-Cl-Py	3.5	450	18	2
3	4.5	685	3-NH ₂ -6-Cl-Py	3.5	450	130	14
4	4.5	685	2-NH ₂ -6-Cl-Py	3.5	450	27	3
5	4.5	685	3-NH ₂ -5-Cl-Py	3.5	450	72	8
6	4.5	685	3-NH ₂ -2-Cl-Py	3.5	450	45	5
7	4.5	685	2-NH ₂ -Pz	3.5	333	17	2

7) Weights of products 8-10

In section 9.3.2.1 Method 7 on page 34, the information on weights and yields were missing for compounds 8–10.

Added information:

Code	Starting material	Product – Isolated yield	
	m (mg)	m (mg)	% to theoretical
8	40	27	68
9	100	64	64
10	100	57	57