A Highly Efficient Copper Catalyzed Methodology for the Synthesis of 2-Hydroxy-benzamides in Neat Water

Shah Jaimin Balkrishna and Sangit Kumar*

Department of Chemistry, Indian Institute of Science Education and Research (IISER) Bhopal, MP, India 462 023

sangitkumar@iiserbhopal.ac.in

Content

$^1$H NMR, $^{13}$C NMR, Mass spectra for 2-Hydroxy-benzamides

S2-S67
Figure S1: 1H NMR (400 MHz) spectrum of crude 1 (after work up of reaction mixture) in CDCl₃.
Figure S2 $^{13}$C NMR (400 MHz) spectrum of 1 in CDCl$_3$ (Crude Reaction Mixture)
Figure S3 | 1H NMR (400 MHz) spectrum of 1 in CDCl₃
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Figure S24: 1H NMR (400 MHz) spectrum of 8 in CDCl₃

**Figure Legend:**

- **Chemical Structure:**
  - 1. **Parameter**
    - 1. Data File Name
    - 2. Title
    - 3. Origin
    - 4. Comment
    - 5. Data Set
    - 6. Phase Correction
    - 7. Acquisition Date
    - 8. Acquisition Time
    - 9. Temperature
    - 10. Spectrum Width
    - 11. Sample Size Frequency 400.13 (MHz)
    - 12. Spectrum Width
    - 13. Total Number of Scans
    - 14. Processing
    - 15. Acquisition
    - 16. Instrument
    - 17. Manufacturer
    - 18. Software
    - 19. Date Created
    - 20. Date Modified

- **Spectral Details:**
  - **Chemical Shift (δ ppm):**
    - 0.5 - 3.0
    - 3.1 - 5.0
    - 5.1 - 7.0
    - 7.1 - 10.0

- **Resonance Assignments:**
  - H1: 6.55 ppm
  - H2: 7.89 ppm
  - CH3: 2.07 ppm

- **Additional Observations:**
  - Clear resonances at specific chemical shifts indicating the presence of hydrogen nuclei in the molecule.

- **Note:**
  - The NMR spectrum provides a clear visualization of the molecular structure and its chemical environment.

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**Chemical Structure: 8**

- Benzene ring
- Oxide group
- Side chain with hydrogens
Figure S25: $^1$C NMR (100 MHz) spectrum of 8 in CDCl₃
Figure S26 HRMS (ESI) spectrum of $8 \ m/z \ 280.0919$ (calcd for $\text{C}_{15}\text{H}_{15}\text{NO}_3 + \text{Na}: 280.0944$).
Figure S27 $^1$H NMR (400 MHz) spectrum of 9 in CDCl$_3$
Figure S28 $^{13}$C NMR (100 MHz) spectrum of 9 in CDCl$_3$
Figure S29 HRMS (ESI) spectrum of $9 \text{ m/z } 344.1260$ (calcd for $\text{C}_{20}\text{H}_{19}\text{NO}_{3} + \text{Na}$: 344.1257).
Figure S30 $^1$H NMR (400 MHz) spectrum 10 in CDCl$_3$
Figure S31 $^{13}$C NMR (100 MHz) spectrum of 10 in CDCl$_3$
Figure S32 ESMS (ESI negative mode) spectrum of $10 \text{m/z} 180.0708$ (calcd for $\text{C}_9\text{H}_{11}\text{NO}_3 - \text{H}^+\colon 180.0655$).
Figure S33 $^1$H NMR (400 MHz) spectrum of 11 in CDCl$_3$
Figure S34 $^{13}$C NMR (100 MHz) spectrum of 11 in CDCl$_3$
Figure S35 HRMS (ESI) spectrum of **11 m/z 284.0437** (calcd for C$_{14}$H$_{12}$ClNO$_2$+ Na: 284.0449).
Figure S36: $^1$H NMR (400 MHz) spectrum of compound 12 in CDCl$_3$
Figure S37 $^{13}$C NMR (100 MHz) spectrum of 12 in CDCl$_3$
Figure S38 ESMS (ESI) spectrum of 12 m/z 300.0977 (calcd for $\text{C}_{17}\text{H}_{15}\text{NO}_2 + \text{Na}$: 300.0995).
Figure S40 $^{13}$C NMR (100 MHz) spectrum of 13 in CDCl$_3$
Figure S41 ESMS (ESI) spectrum of 13 \( m/z \) 251.0781 (calcd for \( \text{C}_{13}\text{H}_{12}\text{N}_{2}\text{O}_{2} + \text{Na} \): 251.0791).
Figure S42 $^1$H NMR (400 MHz) spectrum of 14 in CDCl$_3$
Figure S43 $^{13}$C NMR (100 MHz) spectrum of 14 in CDCl$_3$
Figure S44 ESMS (ESI in negative mode) spectrum of $^{14}\text{m/z}$ 232.0434 (calcd for $\text{C}_{12}\text{H}_{11}\text{NO}_2\text{S} - \text{H}^+$: 232.0427).
Figure S45 $^1$H NMR (400 MHz) spectrum 15 in CDCl$_3$
Figure S46. $^{13}$C NMR (100 MHz) spectrum of 15 in CDCl₃.
Figure S47 HRMS (ESI in negative mode) spectrum of 15 m/z 232.0426 (calcd for C_{12}H_{11}NO_{2}S – H^+: 232.0427).
Figure S48: 1H NMR (400 MHz) spectrum of compound 16 in CDCl$_3$. 

- Chemical shifts and splitting patterns are indicated in the spectrum. 
- The spectrum shows the presence of aromatic and amine functionalities.
Figure S49 $^1$H NMR (400 MHz) spectrum 17 in CDCl$_3$
Figure S50 $^{13}$C NMR (100 MHz) spectrum of 17 in CDCl$_3$
Figure S51 HRMS (ESI) spectrum of 17 m/z 389.1906 (calcd for C_{24}H_{24}N_{2}O_{3} + H'^{+}: 389.1860).
Figure S52 $^1$H NMR (400 MHz) spectrum 18 in CDCl$_3$
Figure S53 $^{13}$C NMR (100 MHz) spectrum of 18 in CDCl$_3$
Figure S54 HRMS (ESI) spectrum of $\textbf{18}$ m/z 507.2137 (calcd for $\text{C}_{28}\text{H}_{32}\text{N}_{2}\text{O}_{7}$ - H⁺: 507.2126).
Figure S55: 1H NMR (400 MHz) spectrum 19 in DMSO-d$_6$. 

[Diagram of 1H NMR spectrum with assigned peak labels and chemical structure]
Figure S56 $^{13}$C NMR (100 MHz) spectrum of 19 in DMSO-d$_6$
Figure S57 HRMS (ESI) spectrum of 19 m/z 323.1027 (calcd for C_{16}H_{16}N_{2}O_{4} + Na: 323.1002).
Figure S58 $^1$H NMR (400 MHz) spectrum 20 in DMSO-$d_6$
Figure S59 $^{13}$C NMR (100 MHz) spectrum of 20 in DMSO-d$_6$
Figure S60ESMS (ESI) spectrum of $20 \text{ m/z } 337.1192$ (calcd for $\text{C}_{17}\text{H}_{18}\text{N}_{2}\text{O}_{4} + \text{Na}$: 337.1159).
Figure S61 $^1$H NMR (400 MHz) spectrum 21 in DMSO-d$_6$
Figure S62 $^{13}$C NMR (100 MHz) spectrum 21 in DMSO-d$_6$
Figure S63 HRMS (ESI) spectrum of 21 m/z 445.1356 (calcd for C$_{20}$H$_{22}$N$_{4}$O$_{8}^{80}$Se - H$^+$: 445.1354).
Figure S64 $^1$H NMR (400 MHz) spectrum 22 in CDCl$_3$
Figure S65: $^1$C NMR (100 MHz) spectrum of 22 in CDCl$_3$. 

![NMR Spectrum Diagram](image)
Figure S66 ESMS (ESI) spectrum of $22 \, m/z \, 377.1471$ (calcd for $C_{20}H_{22}N_{2}O_{4} + Na: 377.1472$).