Electronic Supplementary Material (ESI) for Green Chemistry.

Electronic Supplementary Information:

Hydrogen Bond Mediated Conversion of Benzenenitriles and Arylacetonitriles to Amides: An "On / In-Water" Reaction Strategy

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NMR Spectroscopy characterization

Benzamide (9). To a 25 mL round bottom flask (RB), was added benzonitrile (103 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 3 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9** was obtained as a white solid (113 mg, 94%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.98 (s, 1H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.66 (m, 3H), 7.37 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 168.0, 134.3, 131.2, 128.2, 127.5.

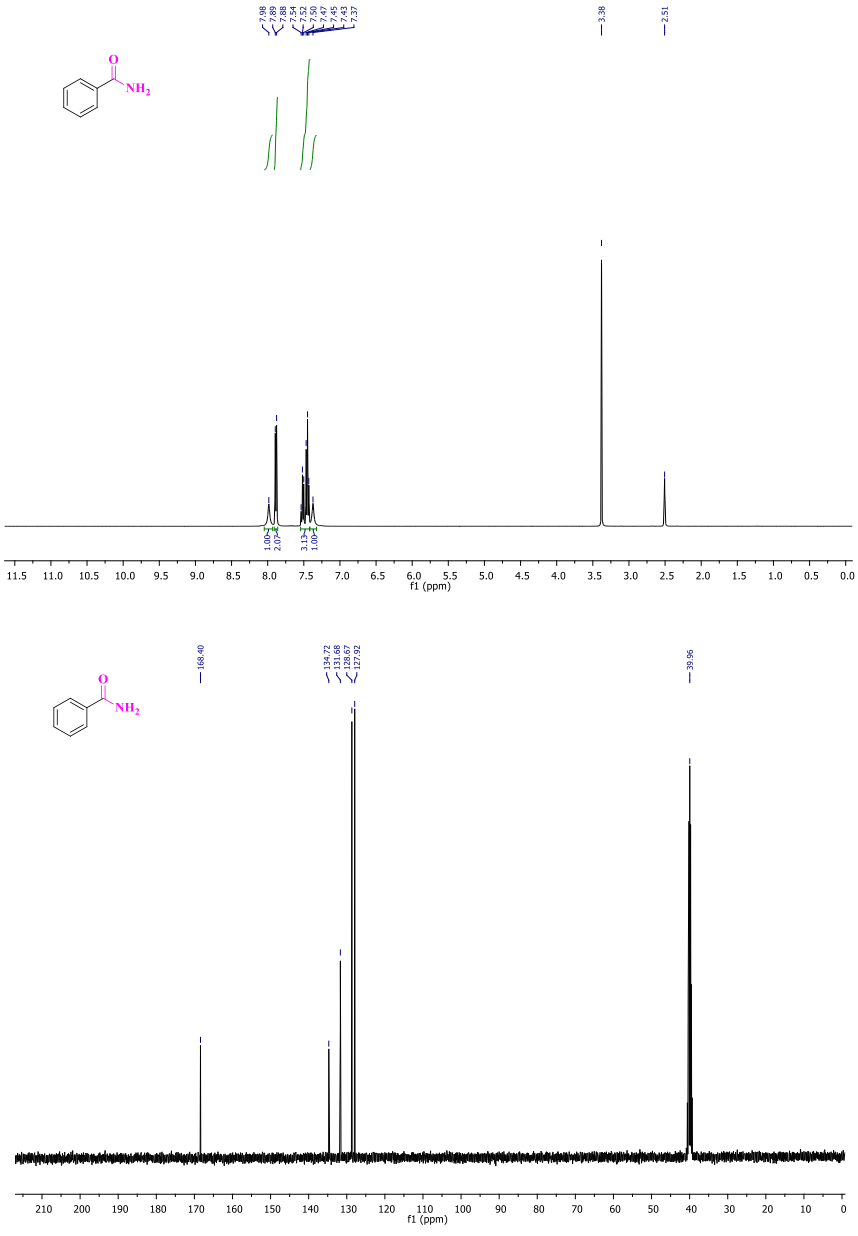


Figure S1. ^{1}H and ^{13}C spectra of benzamide (**9**) in DMSO-d6.

2-methylbenzamide (9a). To a 25 mL round bottom flask (RB), was added 2-methylbenzonitrile (118 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9a** was obtained as a white solid (121 mg, 90%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.92 (s, 1H), 7.70 (m, 2H), 7.33 (d, *J* = 4.0 Hz, 2H), 7.31 (s, 1H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 168.0, 137.4, 134.3, 131.8, 128.0, 128.0, 124.6, 21.0.

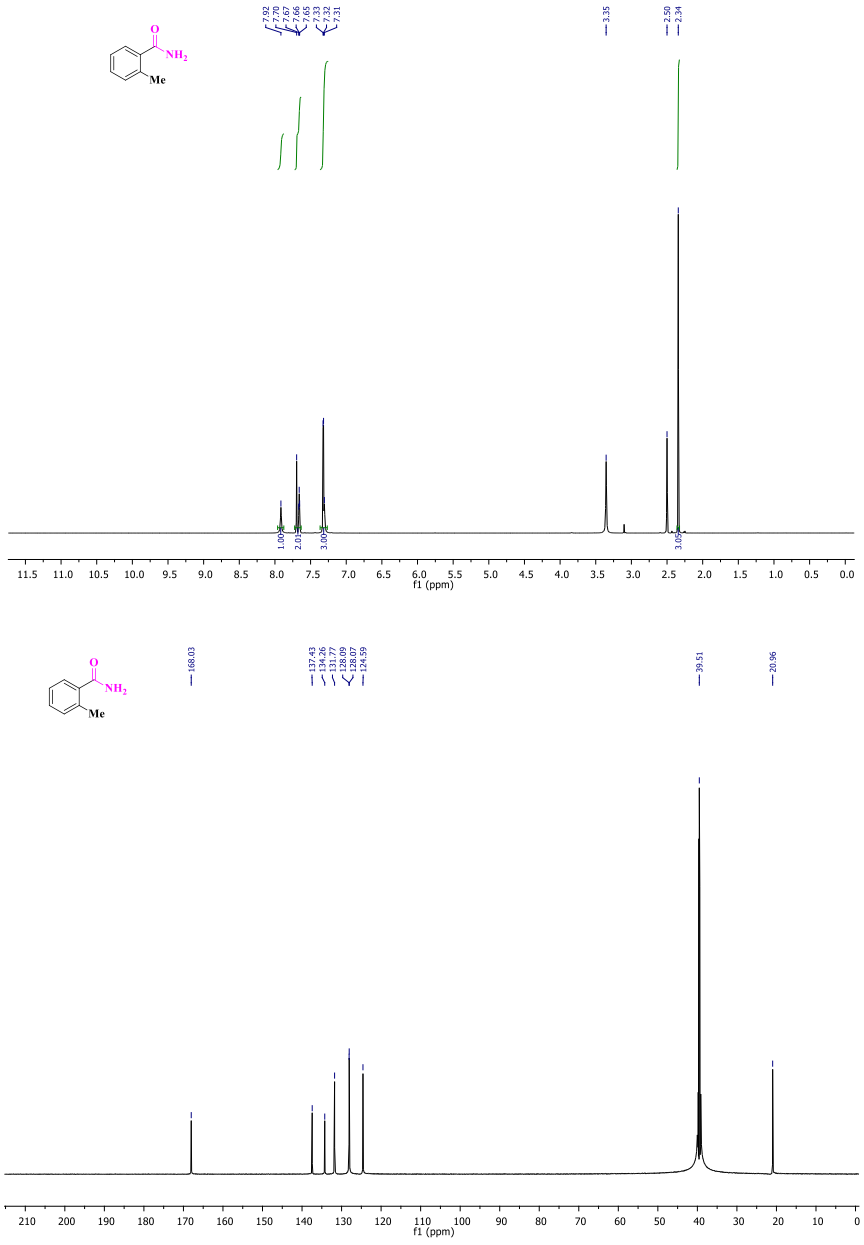


Figure S2. ^{1}H and ^{13}C spectra of 2-methylbenzamide (**9a**) in DMSO-d6.

3-methylbenzamide (9b). To a 25 mL round bottom flask (RB), was added 3-methylbenzonitrile (120 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9b** was obtained as a white solid (109 mg, 81%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.90 (s, 1H), 7.69 (s, 1H), 7.66 (m, 2H), 7.33 (d, *J* = 4.0 Hz, 2H), 7.29 (s, 1H), 3.34 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 168.0, 137.4, 134.2, 131.7, 128.1, 128.1, 124.6, 21.0.

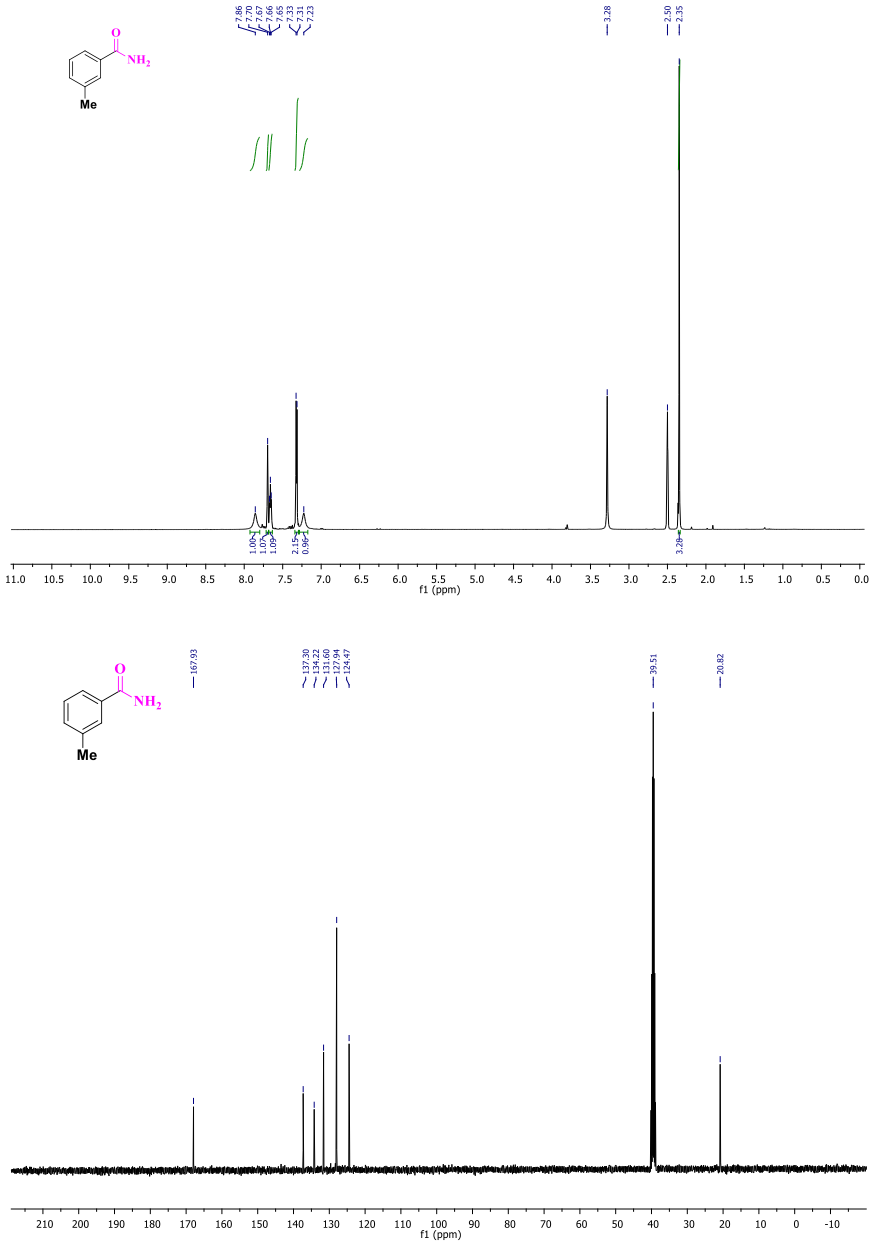


Figure S3. ^{1}H and ^{13}C spectra of 3-methylbenzamide (**9b**) in DMSO-d6.

4-methylbenzamide (9c). To a 25 mL round bottom flask (RB), was added 4-methylbenzonitrile (119 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9c** was obtained as a white solid (108 mg, 80%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.87 (s, 1H), 7.46 (m, 4H), 7.09 (dd, *J* = 4.0 Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 167.9, 134.3, 131.2, 128.2, 127.5.

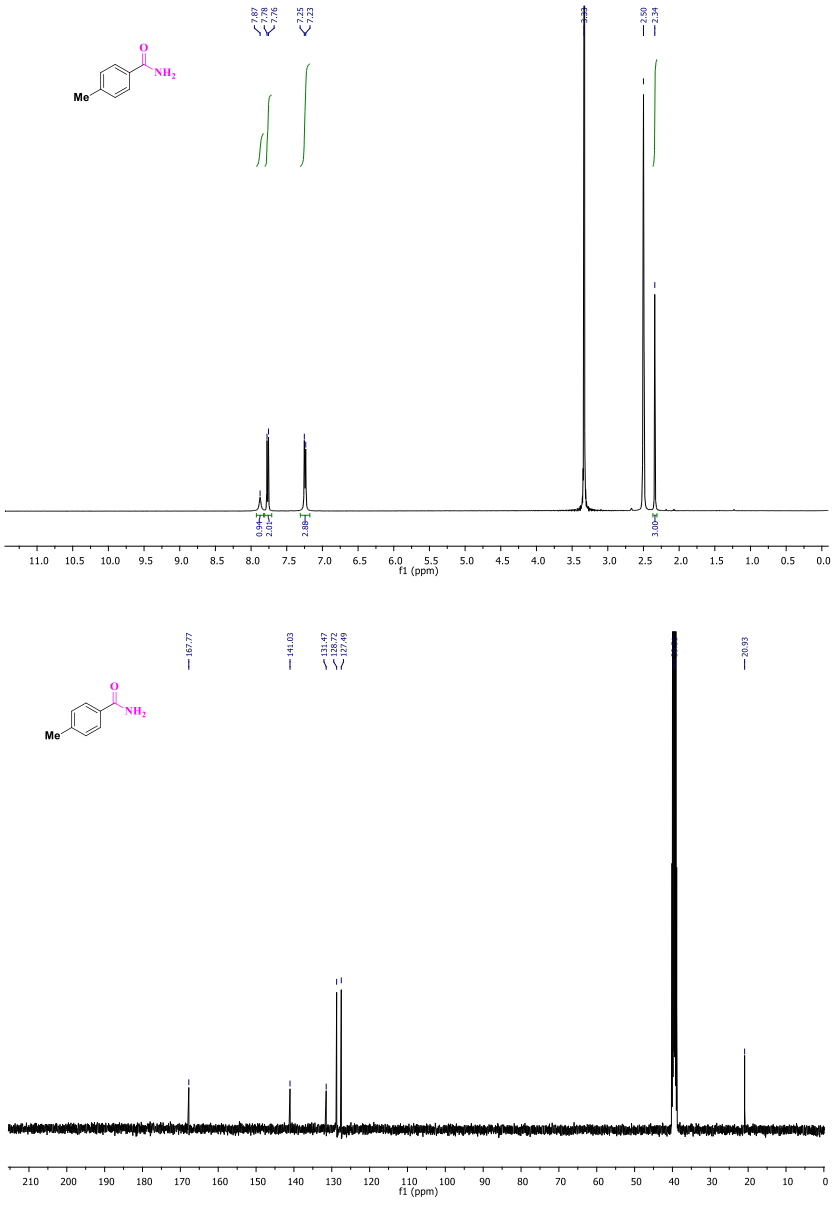


Figure S4. ^{1}H and ^{13}C spectra of 4-methylbenzamide (**9c**) in DMSO-d6.

3-methoxybenzamide (9d). To a 25 mL round bottom flask (RB), was added 3-methoxybenzonitrile (123 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 6 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9d** was obtained as a white solid (119 mg, 79%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.96 (s, 1H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 167.7, 159.1, 135.7, 129.3, 119.7, 117.0, 112.7, 55.2.

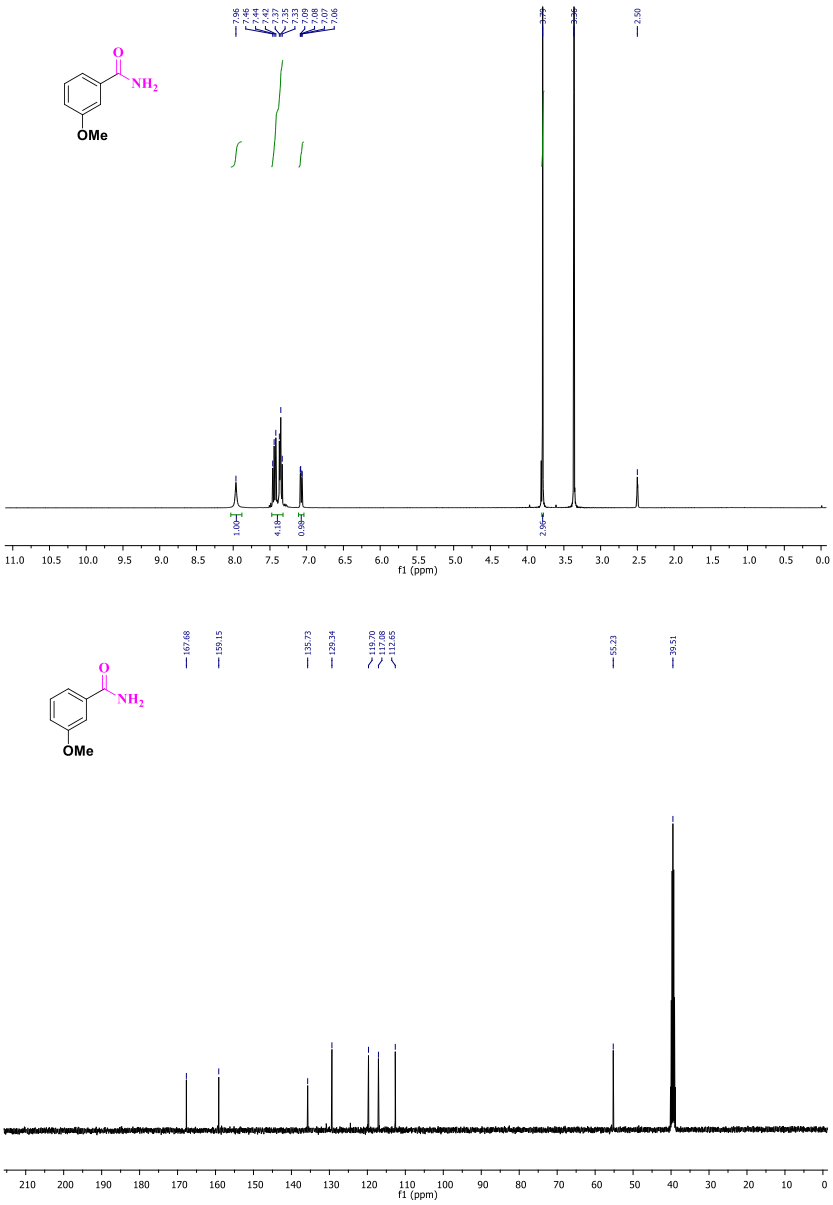


Figure S5. ^{1}H and ^{13}C spectra of 3-methoxybenzamide (**9d**) in DMSO-d6.

4-methoxybenzamide (9e). To a 25 mL round bottom flask (RB), was added 4-methoxybenzonitrile (133 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 3 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9e** was obtained as a light yellow solid (127 mg, 84%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.85 (m, 4H), 7.16 (s, 1H), 6.98 (d, *J* = 8.0 Hz, 1H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 167.4, 161.6, 129.3, 126.5, 113.4, 55.3.

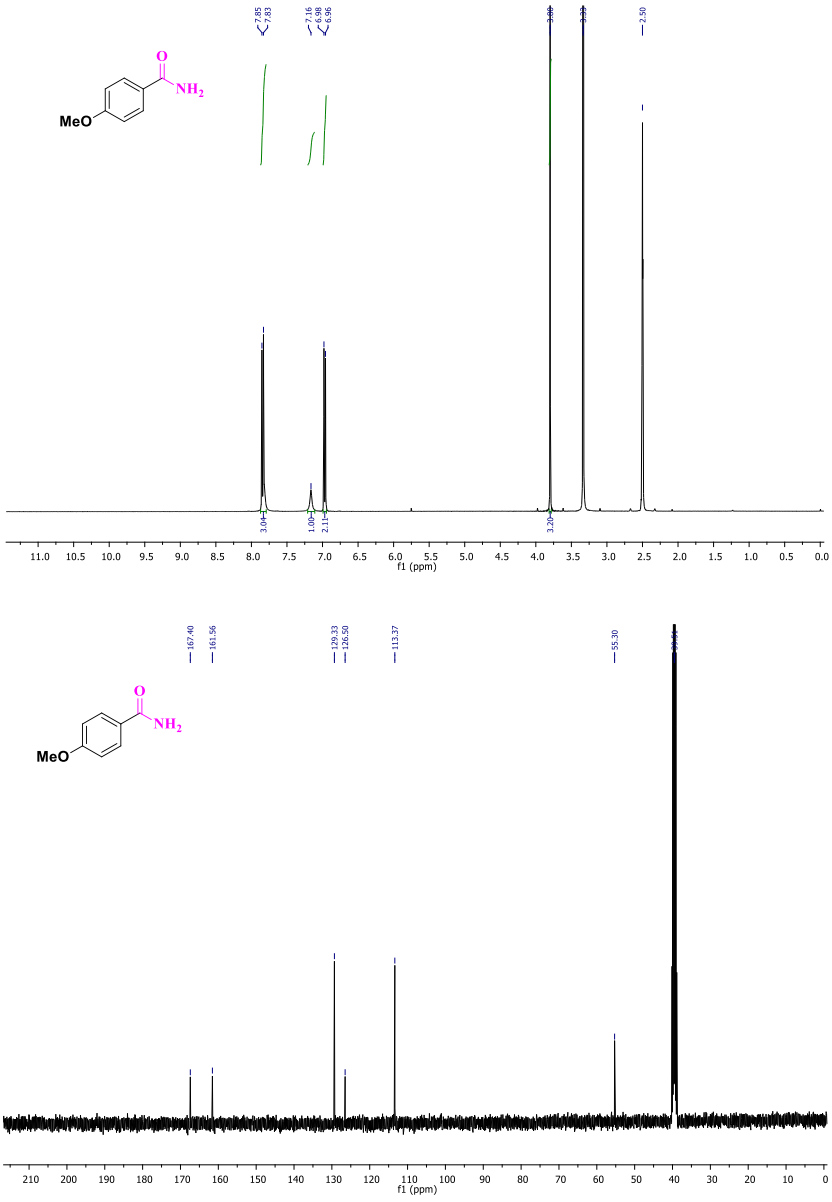


Figure S6. ^{1}H and ^{13}C spectra of 4-methoxybenzamide (**9e**) in DMSO-d6.

2-fluorobenzamide (9f). To a 25 mL round bottom flask (RB), was added 2-fluorobenzonitrile (138 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 4 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9f** was obtained as a white solid (107 mg, 77%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.68-7.64 (m, 2H), 7.54-7.49 (m, 2H), 7.28-7.23 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d6) δ 165.1, 159.2 (d, $J_{C\text{-}F}$ = 247.0 Hz), 132.4 (d, $J_{C\text{-}F}$ = 9.0 Hz), 130.1 (d, $J_{C\text{-}F}$ = 3.0 Hz), 124.3 (d, $J_{C\text{-}F}$ = 4.0 Hz), 123.8 (d, $J_{C\text{-}F}$ = 14.0 Hz), 116.1 (d, $J_{C\text{-}F}$ = 22.0 Hz).

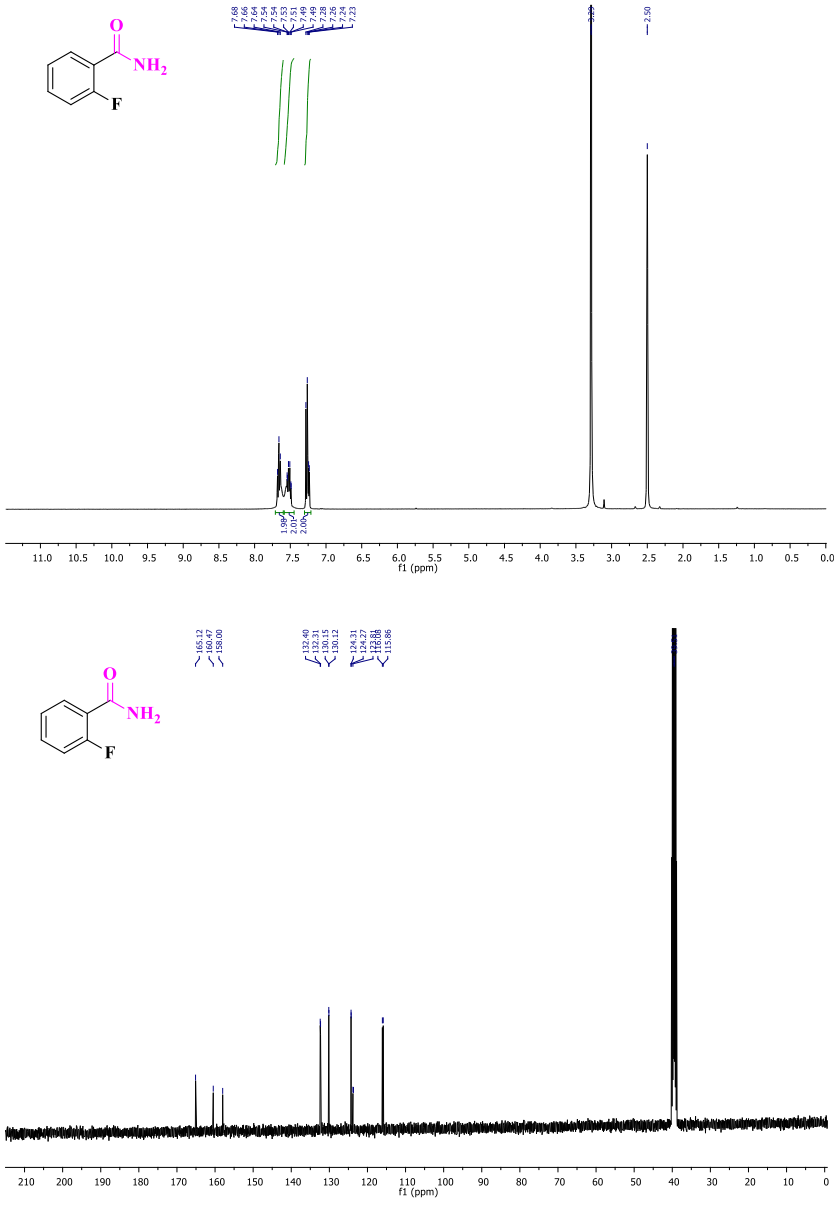


Figure S7. ^{1}H and ^{13}C spectra of 2-fluorobenzamide (**9f**) in DMSO-d6.

3-fluorobenzamide (9g). To a 25 mL round bottom flask (RB), was added 3-fluorobenzonitrile (106 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 5 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9g** was obtained as a white solid (117 mg, 84%). ^{1}H NMR (400 Hz, DMSO-d6) δ 7.73 (s, 1H), 7.78 (t, J = 8.0 Hz, 2H), 7.54-7.49 (m, 1H), 7.26 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 165.8, 159.7 (d, $J_{C\text{-}F}$ = 247.0 Hz), 133.0 (d, $J_{C\text{-}F}$ = 8.0 Hz),130.7 (d, $J_{C\text{-}F}$ = 3.0 Hz), 124.9 (d, $J_{C\text{-}F}$ = 4.0 Hz), 124.6 (d, $J_{C\text{-}F}$ = 14.0 Hz), 116.7 (d, $J_{C\text{-}F}$ = 22.0 Hz).

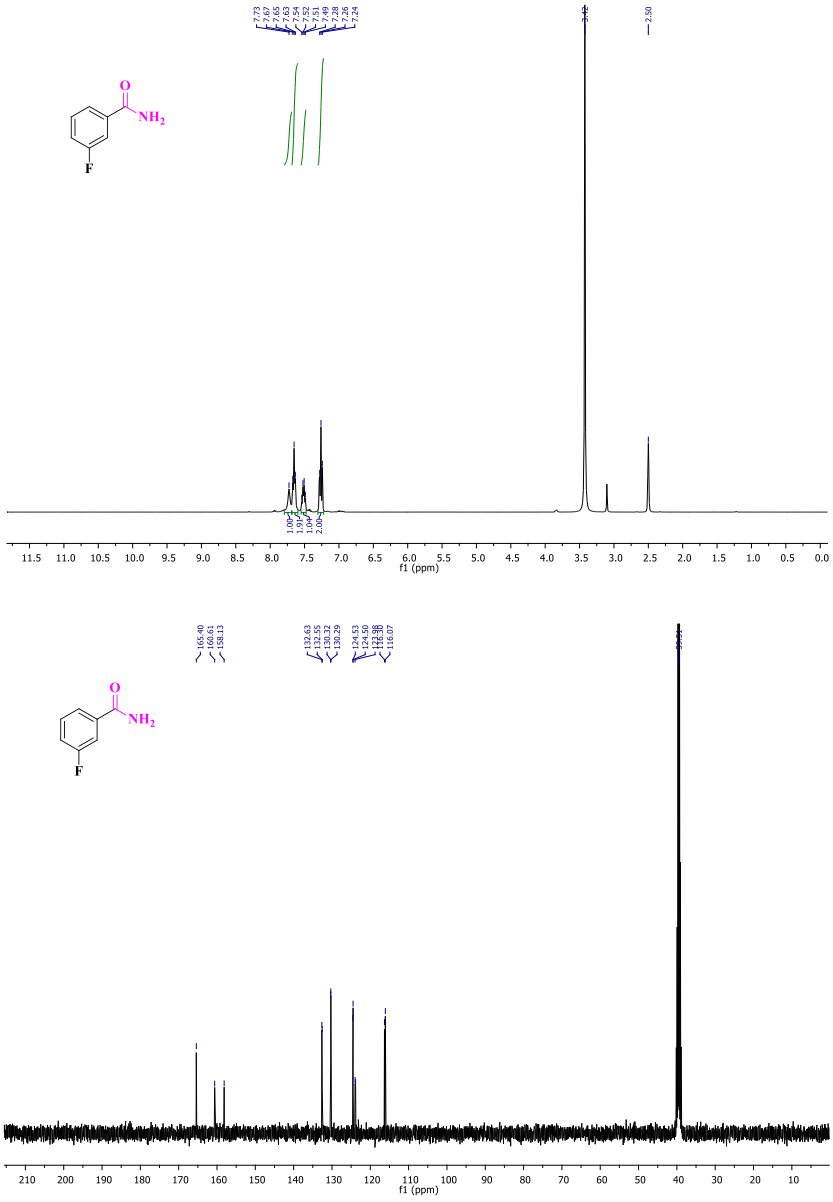


Figure S8. ^{1}H and ^{13}C spectra of 3-fluorobenzamide (**9g**) in DMSO-d6.

4-fluorobenzamide (9h). To a 25 mL round bottom flask (RB), was added 4-fluorobenzonitrile (109 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 4 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9h** was obtained as a white solid (127 mg, 91%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.99 (s, 1H), 7.96-7.92 (m, 2H), 7.39 (s, 1H), 7.29-7.25 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d6) δ 166.8, 163.9 (d, $J_{C\text{-}F}$ = 247.0 Hz), 130.8 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.2 (d, $J_{C\text{-}F}$ = 9.0 Hz), 115.2 (d, $J_{C\text{-}F}$ = 22.0 Hz).

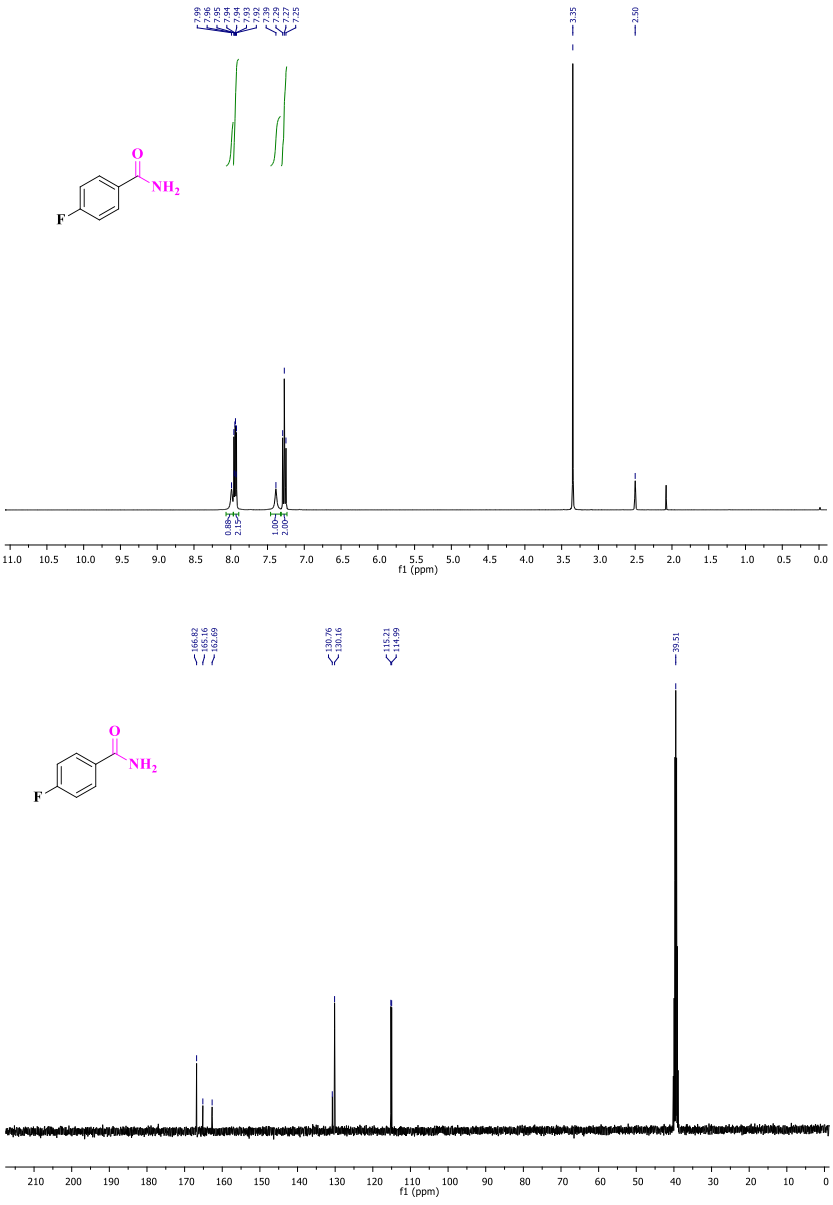


Figure S9. ^{1}H and ^{13}C spectra of 4-fluorobenzamide (**9h**) in DMSO-d6.

2-chlorobenzamide (9i). To a 25 mL round bottom flask (RB), was added 2-chlorobenzonitrile (138 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 6 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9i** was obtained as a white solid (137 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77-7.75 (m, 1H), 7.43-7.31 (m, 3H), 6.45-6.41 (d, *J* = 6.0 Hz 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 133.9, 131.8, 130.8, 130.6, 130.4, 127.2.

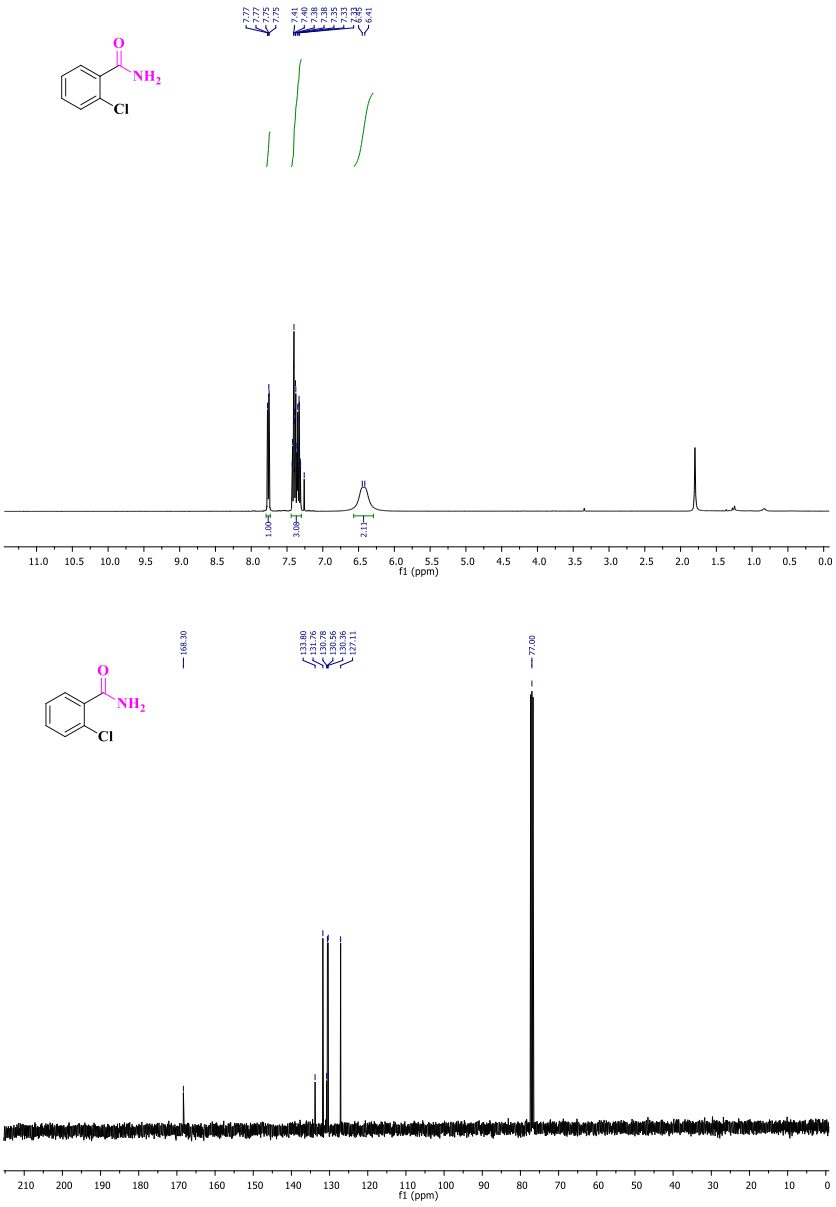


Figure S10. ^{1}H and ^{13}C spectra of 2-chlorobenzamide (**9i**) in $CDCl_3$.

3-chlorobenzamide (9j). To a 25 mL round bottom flask (RB), was added 3-chlorobenzonitrile (138 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 6 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9j** was obtained as a white solid (115 mg, 74%). ^{1}H NMR (400 MHz, DMSO-d6) δ 8.09 (s, 1H), 7.91 (t, *J* = 4.0 Hz, 1H), 7.84 (s, 1H), 7.60-7.57(m, 1H), 7.51-7.47 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d6) δ 166.4, 136.3, 133.1, 131.0,130.2, 127.3, 126.2.

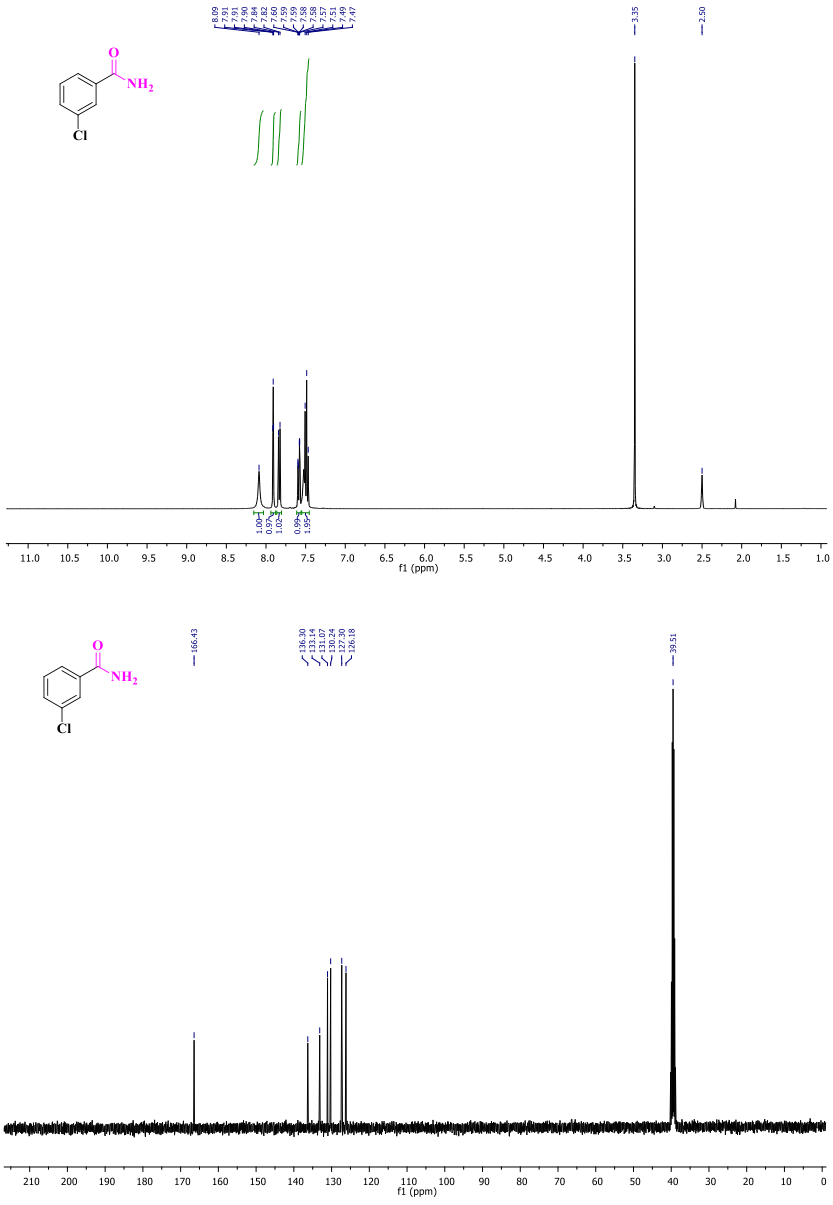


Figure S11. ^{1}H and ^{13}C spectra of 3-chlorobenzamide (**9j**) in DMSO-d6.

4-chlorobenzamide (9k). To a 25 mL round bottom flask (RB), was added 4-chlorobenzonitrile (138 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9k** was obtained as a white solid (139 mg, 89%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.90 (s, 1H), 7.89-7.88 (d, *J* = 4.0 Hz, 2H), 7.69 (s, 1H), 7.67 (d, *J* = 2.0 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d6) δ 168.0, 134.3, 131.3, 128.3, 127.5.

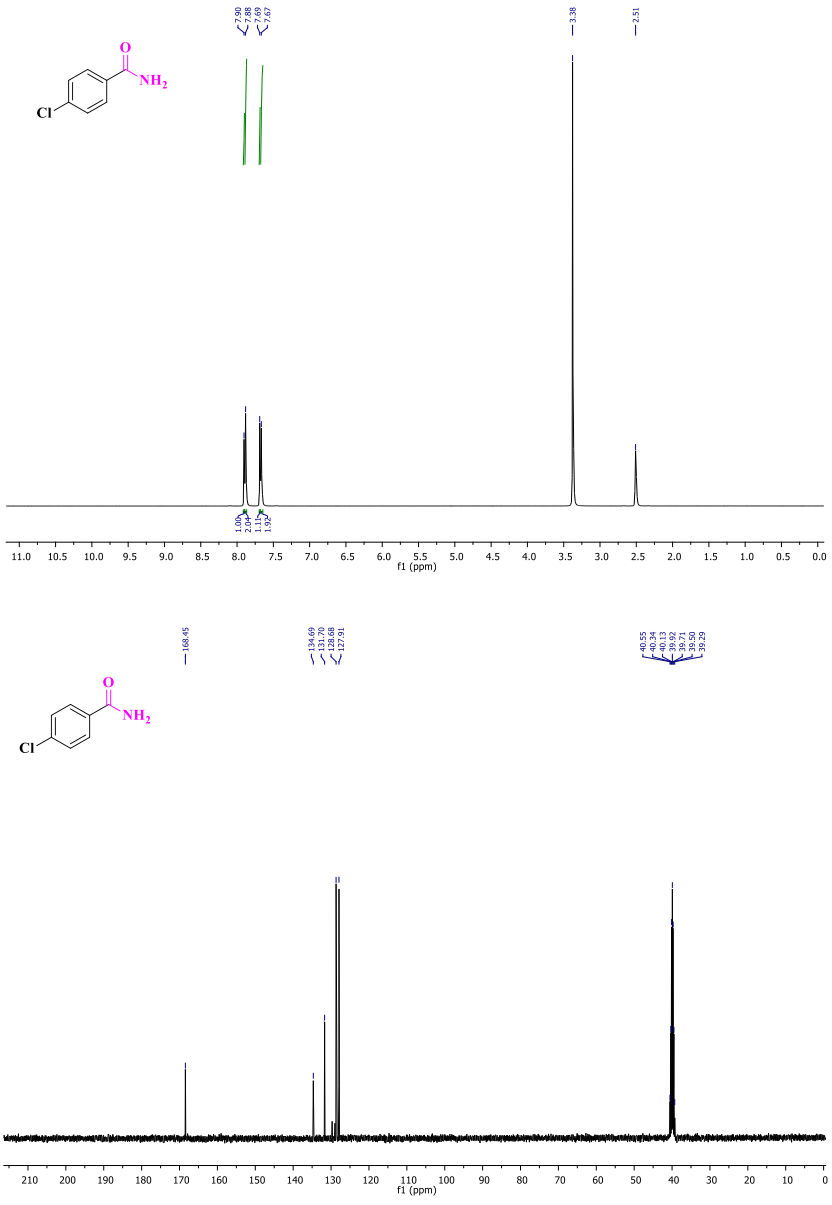


Figure S12. ^{1}H and ^{13}C spectra of 4-chlorobenzamide (**9k**) in DMSO-d6.

2-bromobenzamide (9l). To a 25 mL round bottom flask (RB), was added 2-bromobenzonitrile (182 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9l** was obtained as a white solid (174 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 (s, 1H), 7.82 (d, *J* = 4.0 Hz, 2H), 7.67 (d, *J* = 4.0 Hz 2H) 7.45 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 138.8, 132.2, 130.0, 128.0, 127.0, 118.0.

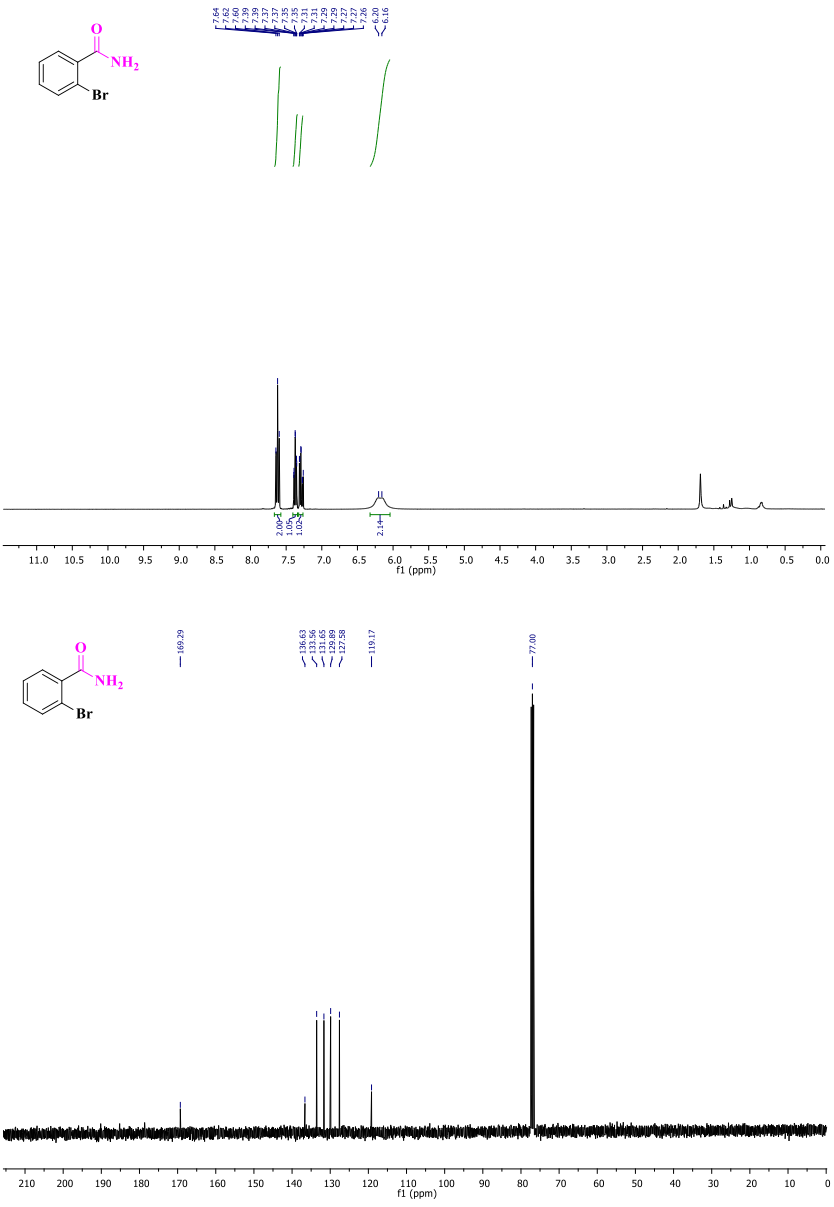


Figure S13. ^{1}H and ^{13}C spectra of 2-bromobenzamide (**9l**) in $CDCl_3$.

3-bromobenzamide (9m). To a 25 mL round bottom flask (RB), was added 3-bromobenzonitrile (182 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 4 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9m** was obtained as a white solid (158 mg, 79%). ^{1}H NMR (400 MHz, DMSO-d6) δ 8.85 (s, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.55 (s, 1H), 7.42-7.49 (m, 2H), 7.35-7.31 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 166.3, 136.5, 134.0, 130.5,130.2, 126.5, 121.6.

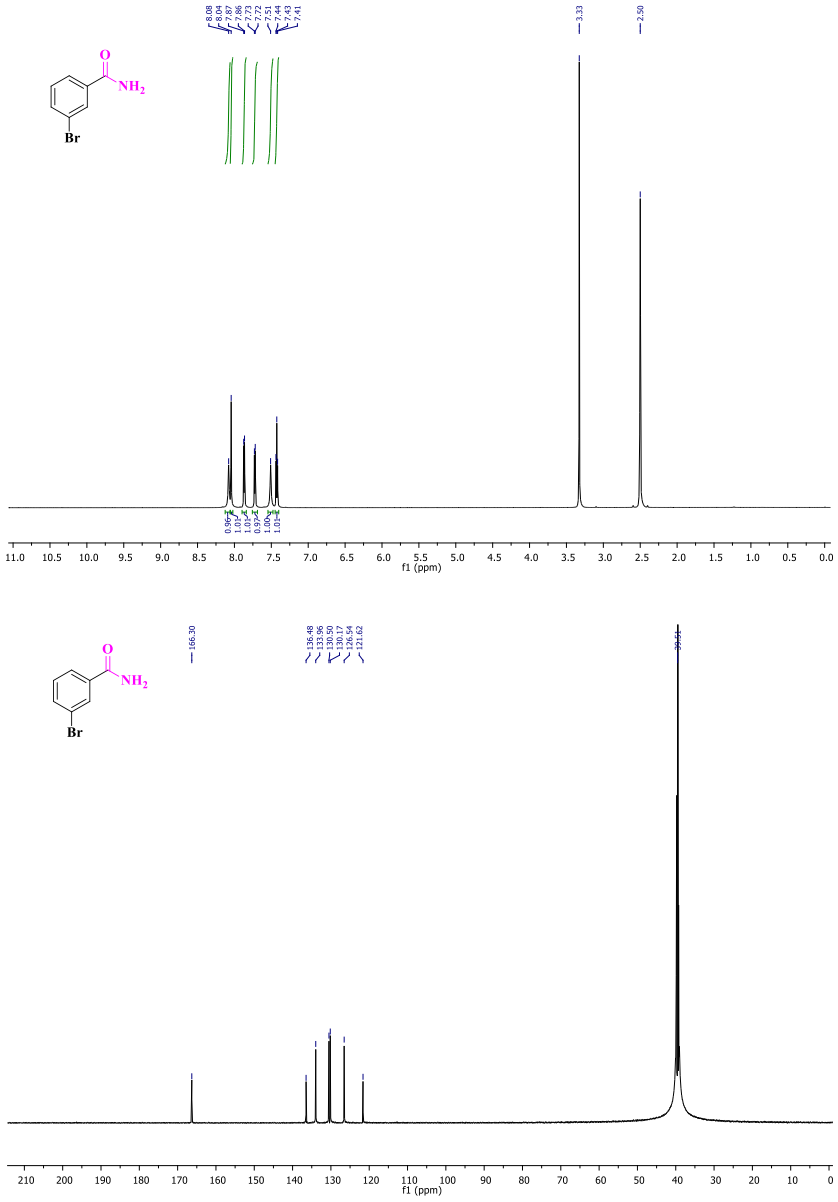


Figure S14. ^{1}H and ^{13}C spectra of 3-bromobenzamide (**9m**) in DMSO-d6.

4-bromobenzamide (9n). To a 25 mL round bottom flask (RB), was added 4-bromobenzonitrile (182 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 4 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9n** was obtained as a white solid (180 mg, 90%). ^{1}H NMR (400 MHz, DMSO-d6) δ 8.04 (s, 1H), 7.82 (d, *J* = 4.0 Hz, 2H), 7.67 (d, *J* = 4.0 Hz 2H) 7.45 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 166.9, 133.4, 131.2, 129.6, 125.0.

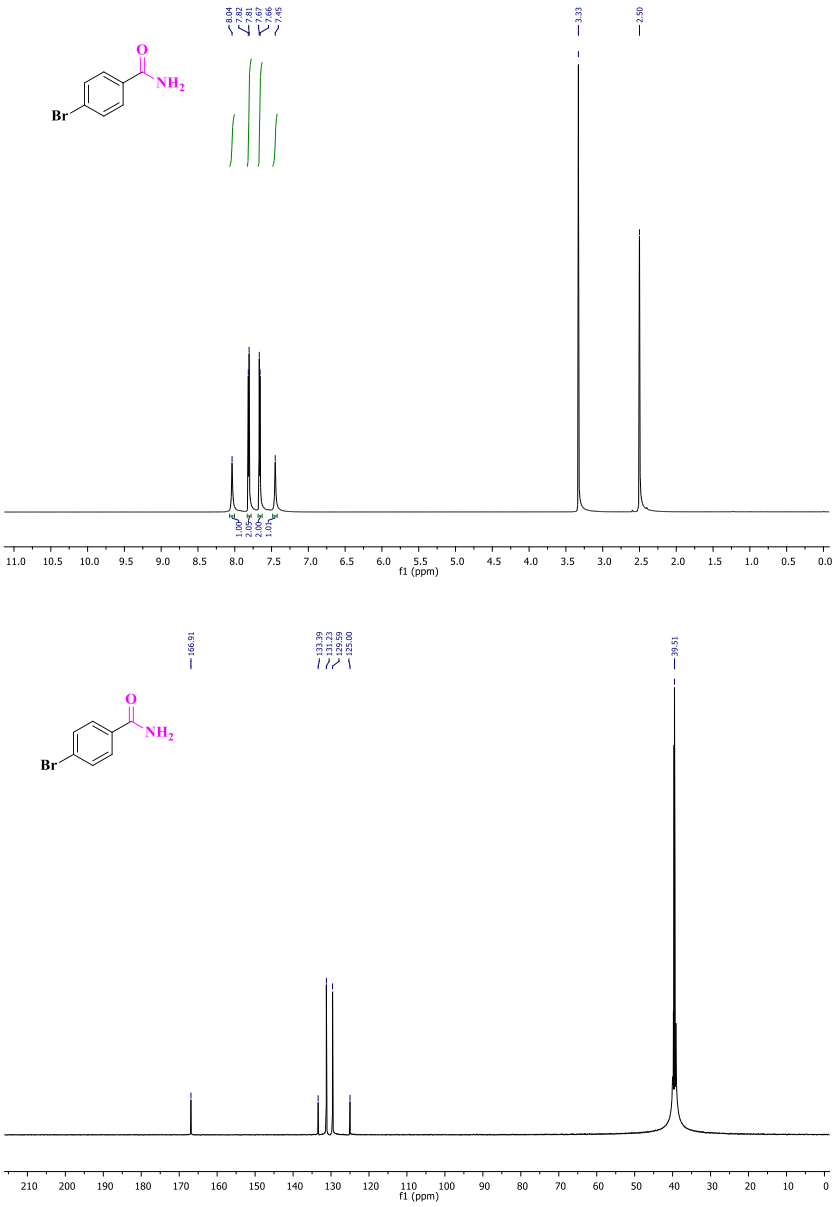


Figure S15. ^{1}H and ^{13}C spectra of 4-bromobenzamide (**9n**) in DMSO-d6.

4-nitrobenzamide (9o). To a 25 mL round bottom flask (RB), was added 4-nitrobenzonitrile (148 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9o** was obtained as a white solid (153 mg, 92%). ^{1}H NMR (400 MHz, DMSO-d6) δ 8.31-8.29 (m, 3H), 8.10-8.08 (d, *J* = 4.0 Hz, 2H), 7.72 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 166.2, 149.0, 140.0, 128.9, 123.5.

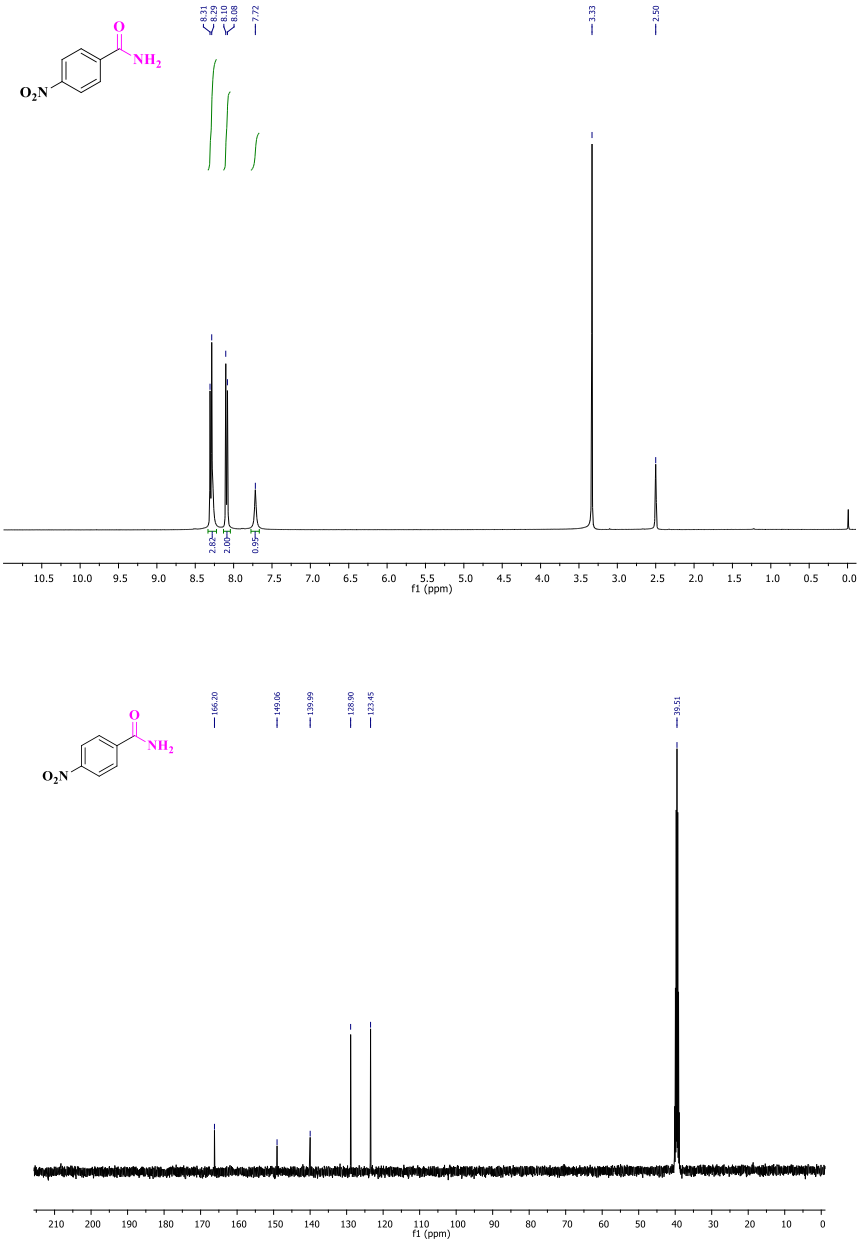


Figure S16. ^{1}H and ^{13}C spectra of 4-nitrobenzamide (**9o**) in DMSO-d6.

3,4-dimethoxybenzamide (9p). To a 25 mL round bottom flask (RB), was added 3,4-dimethoxybenzonitrile (163 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 3 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9p** was obtained as a white solid (161 mg, 89%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.87 (s, 1H), 7.50-7.49 (d, *J* = 4.0 Hz, 1H), 7.46 (s, 1H), 7.22 (s, 1H), 6.99-6.98 (d, *J* = 4.0 Hz, 2H), 3.79 (s, 3H), 7.78 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 167.5, 151.3, 148.2, 126.6, 120.8, 110.9, 110.8, 55.6, 55.5.

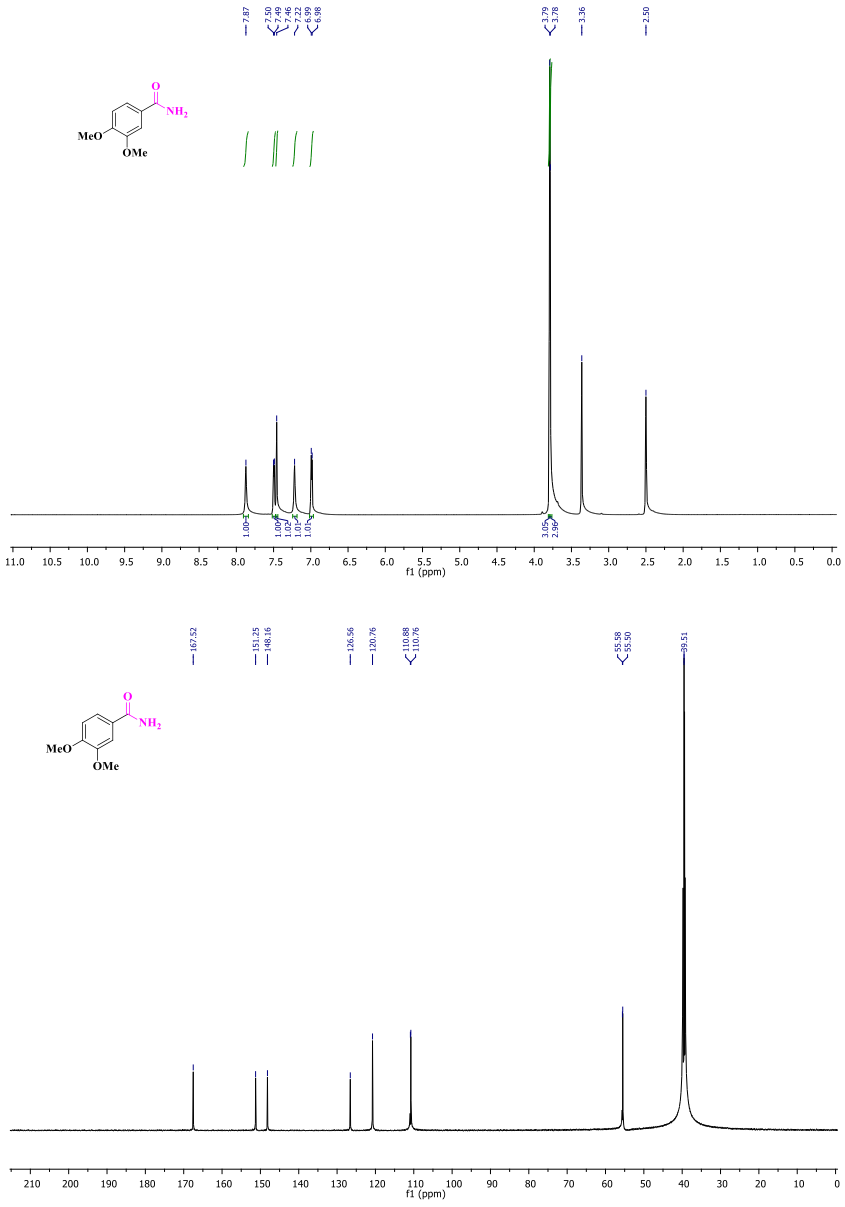


Figure S17. ^{1}H and ^{13}C spectra of 3,4-dimethoxybenzamide (**9p**) in DMSO-d6.

5-bromo-2-fluorobenzamide (9q). To a 25 mL round bottom flask (RB), was added 5-bromo-2-fluorobenzonitrile (200 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9q** was obtained as a light yellow solid (177 mg, 81%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.84 (s, 1H), 7.77-7.76 (m, 2H), 7.71-7.69 (m, 1H), 7.30-7.27 (t, J = 8.0, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 163.9, 158.4 (d, $J_{C\text{-}F}$ = 142.0 Hz), 135.0 (d, $J_{C\text{-}F}$ = 5.0 Hz), 132.4 (d, $J_{C\text{-}F}$ = 2.0 Hz), 126.2 (d, $J_{C\text{-}F}$ = 9.0 Hz), 118.8 (d, $J_{C\text{-}F}$ = 14.0 Hz), 116.1 (d, $J_{C\text{-}F}$ = 2.0 Hz).

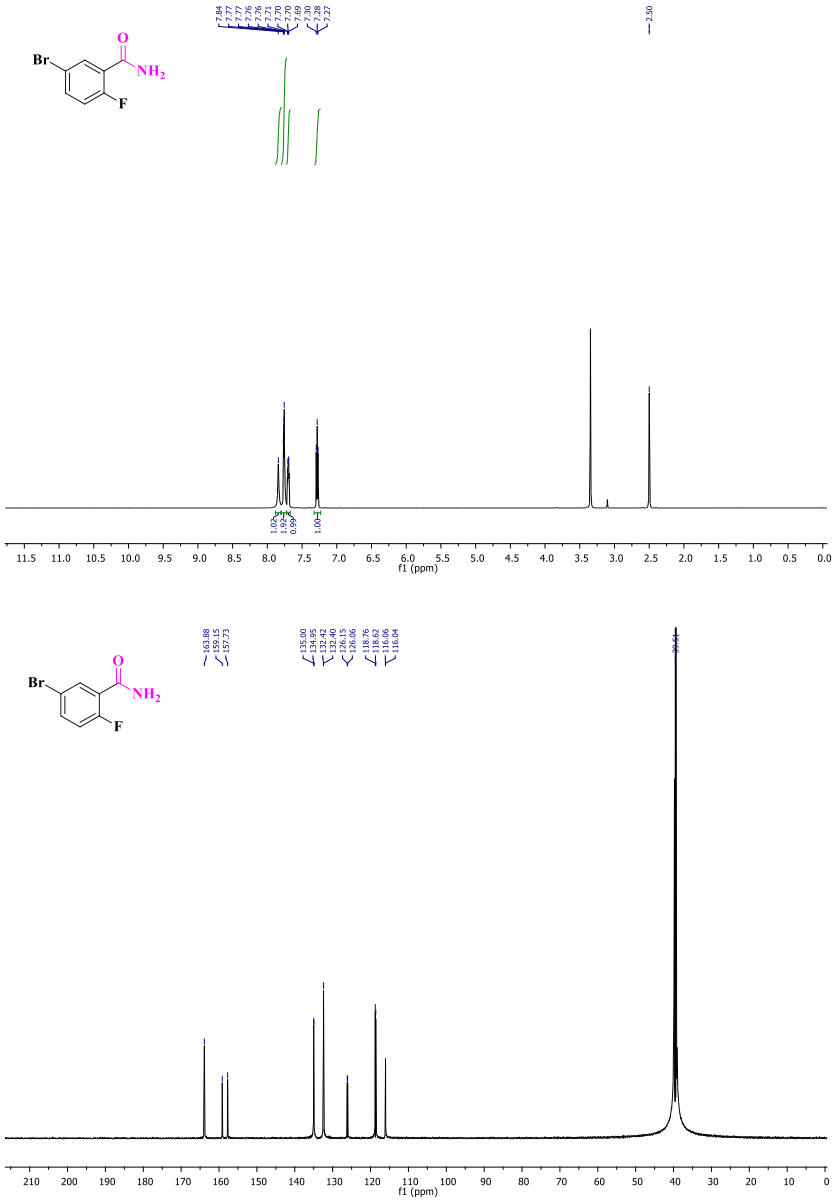


Figure S18. ^{1}H and ^{13}C spectra of 5-bromo-2-fluorobenzamide (**9q**) in DMSO-d6.

Nicotinamide (9r). To a 25 mL round bottom flask (RB), was added nicotinonitrile (104 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9r** was obtained as a white solid (98 mg, 80%). ^{1}H NMR (400 MHz, DMSO-d6) δ 9.02 (s, 1H), 8.70-8.69 (d, *J* = 4.0 Hz, 1H), 8.21-8.19 (d, *J* = 8.0 Hz, 2H), 7.62 (s, 1H), 7.51-7.48 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 166.6, 152.0, 148.8, 135.3, 129.7, 123.6.

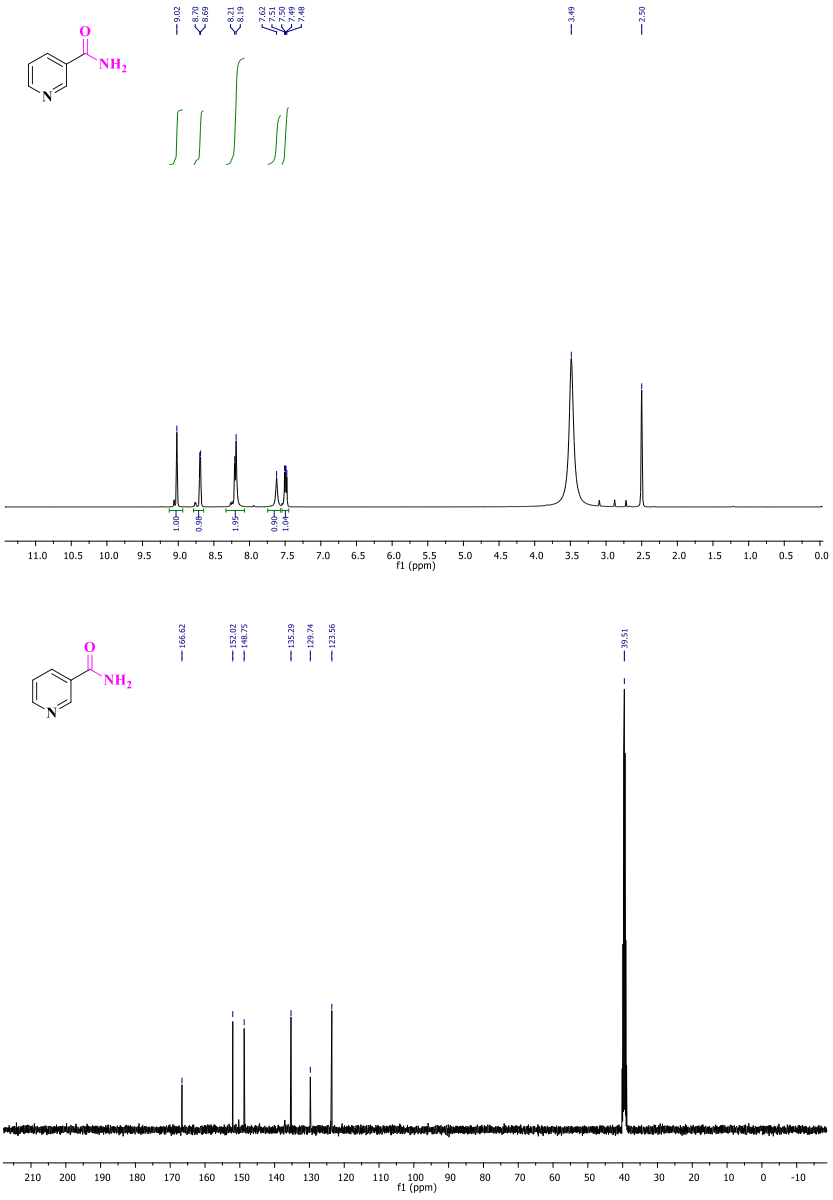


Figure S19. ^{1}H and ^{13}C spectra of Nicotinamide (**9r**) in DMSO-d6.

Isonicotinamide (9s). To a 25 mL round bottom flask (RB), was added isonicotinonitrile (104 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9s** was obtained as a white solid (105 mg, 86%). ^{1}H NMR (400 MHz, DMSO-d6) δ 8.72-8.71 (d, *J* = 4.0 Hz, 2H), 8.23 (s, 1H), 7.77-7.76 (d, *J* = 4.0 Hz, 2H), 7.71 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 166.3, 150.2, 141.3, 121.4.

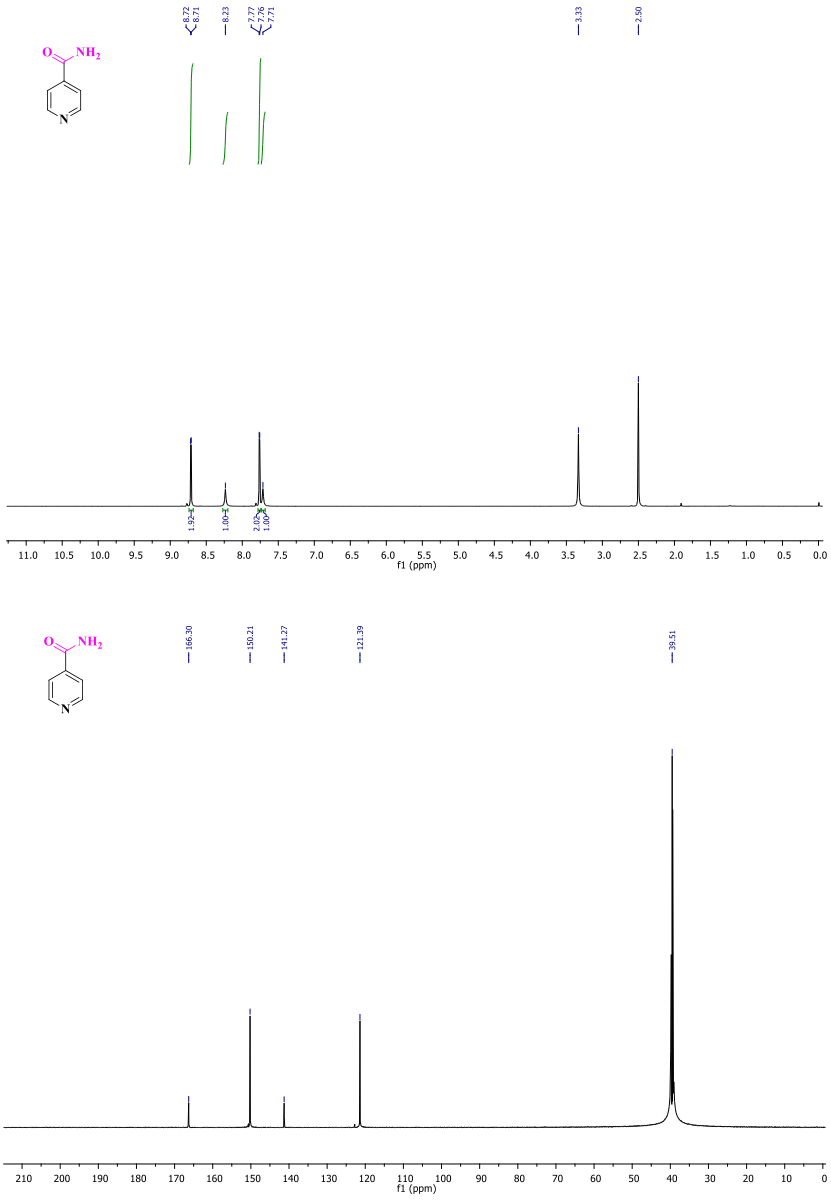


Figure S20. ^{1}H and ^{13}C spectra of Isonicotinamide (**9s**) in DMSO-d6.

2-chloro-6-(trifluoromethyl)nicotinamide (9t). To a 25 mL round bottom flask (RB), was added 2-chloro-6-(trifluoromethyl)nicotinonitrile (137 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 5 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9t** was obtained as a white solid (175 mg, 78%). ^{1}H NMR (400 MHz, DMSO-d6) δ 8.21-8.20 (d, *J* = 4.0 Hz, 1H), 8.17 (s, 1H), 8.03-8.02 (d, *J* = 4.0 Hz, 1H), 7.97 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 165.8, 147.0, 146.2 (d, $J_{C\text{-}F}$ = 2.0 Hz), 140.0, 136.9, 121.3, 120.3 (d, $J_{C\text{-}F}$ = 1.0 Hz).

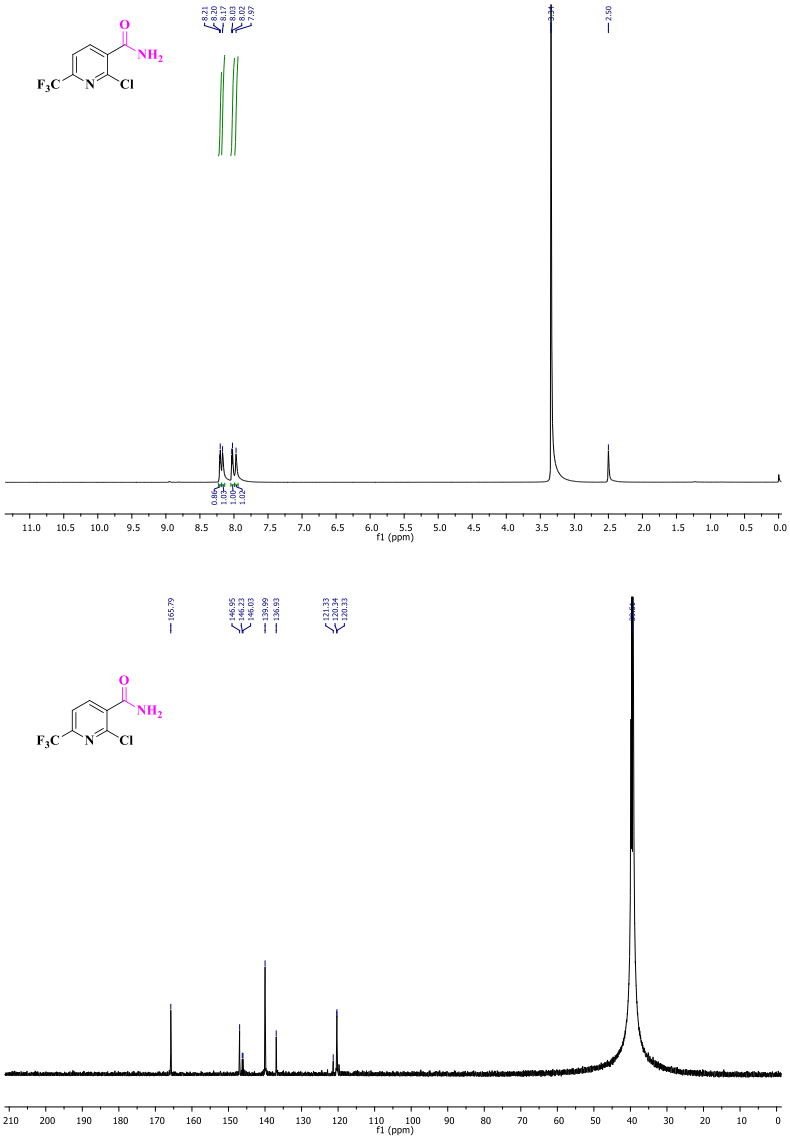


Figure S21. ^{1}H and ^{13}C spectra of 2-chloro-6-(trifluoromethyl)nicotinamide (**9t**) in DMSO-d6.

furan-2-carboxamide (9u). To a 25 mL round bottom flask (RB), was added furan-2-carbonitrile (87 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 3 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9u** was obtained as a white solid (99 mg, 89%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.79 (s, 1H), 7.76 (s, 1H), 7.36 (s, 1H), 7.10-7.09 (d, *J* = 4.0 Hz, 2H), 6.60-6.58 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 159.5, 148.1, 145.0, 113.6, 111.8.

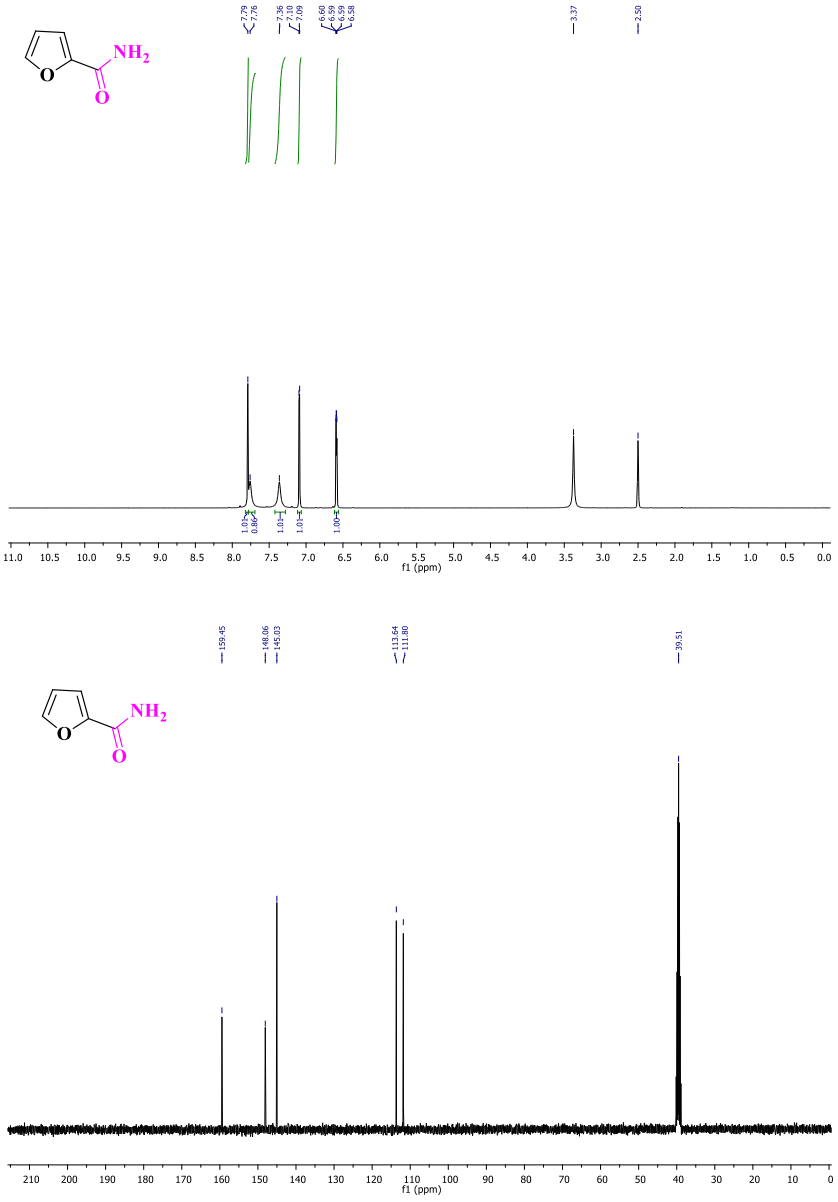


Figure S22. ^{1}H and ^{13}C spectra of furan-2-carboxamide (**9u**) in DMSO-d6.

furan-3-carboxamide (9v). To a 25 mL round bottom flask (RB), was added furan-3-carbonitrile (87 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 3 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9v** was obtained as a white solid (96 mg, 86%). ^{1}H NMR (400 MHz, DMSO-d6) δ 8.15 (s, 1H), 7.70-7.69 (t, *J* = 4.0 Hz, 1H), 7.64 (s, 1H), 7.18 (s, 1H), 6.80-6.80 (d, *J* = 2.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 163.4, 145.3, 143.9, 122.9, 109.3.

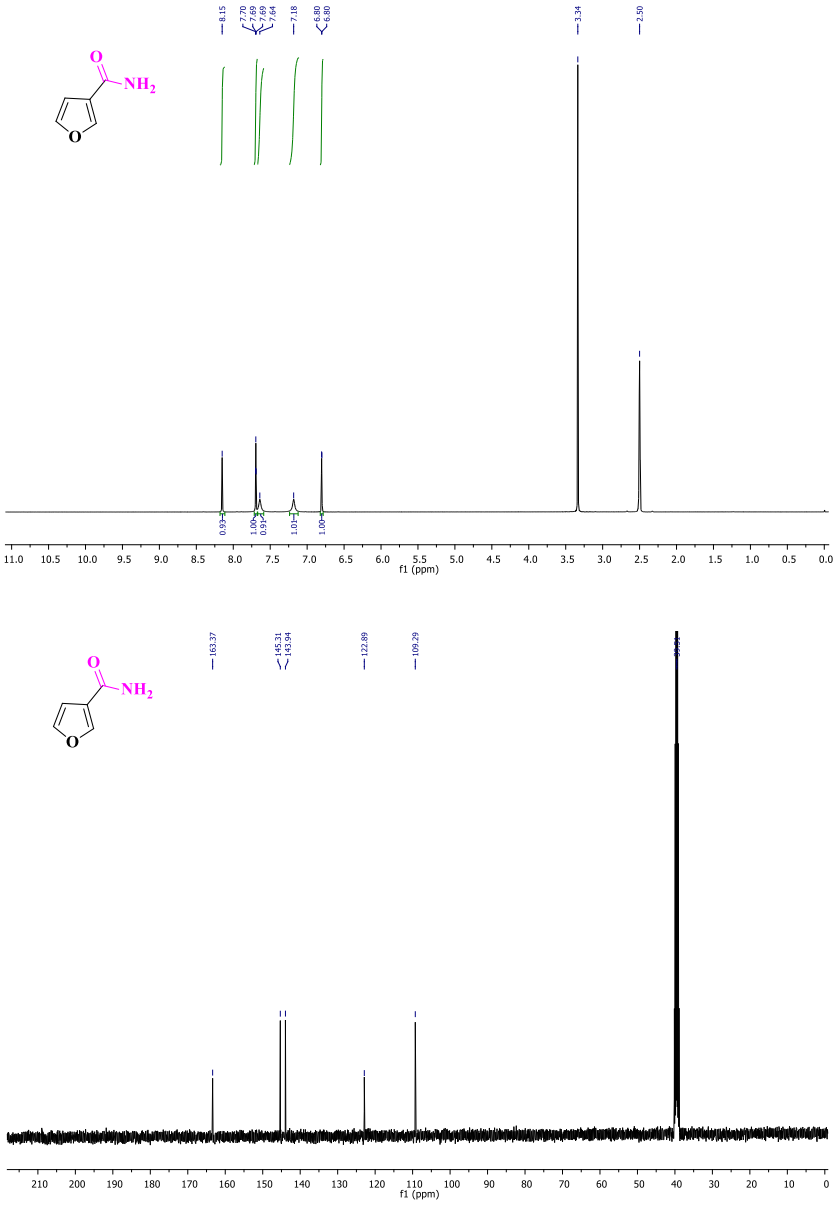


Figure S23. ^{1}H and ^{13}C spectra of furan-3-carboxamide (**9v**) in DMSO-d6.

thiophene-2-carboxamide (9w). To a 25 mL round bottom flask (RB), was added thiophene-2-carbonitrile (93 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 4 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9w** was obtained as a white solid (118 mg, 93%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.96 (s, 1H), 7.75-7.72 (m, 2H), 7.37 (s, 1H), 6.60-6.58 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 162.9, 140.3, 131.0, 128.7, 127.9.

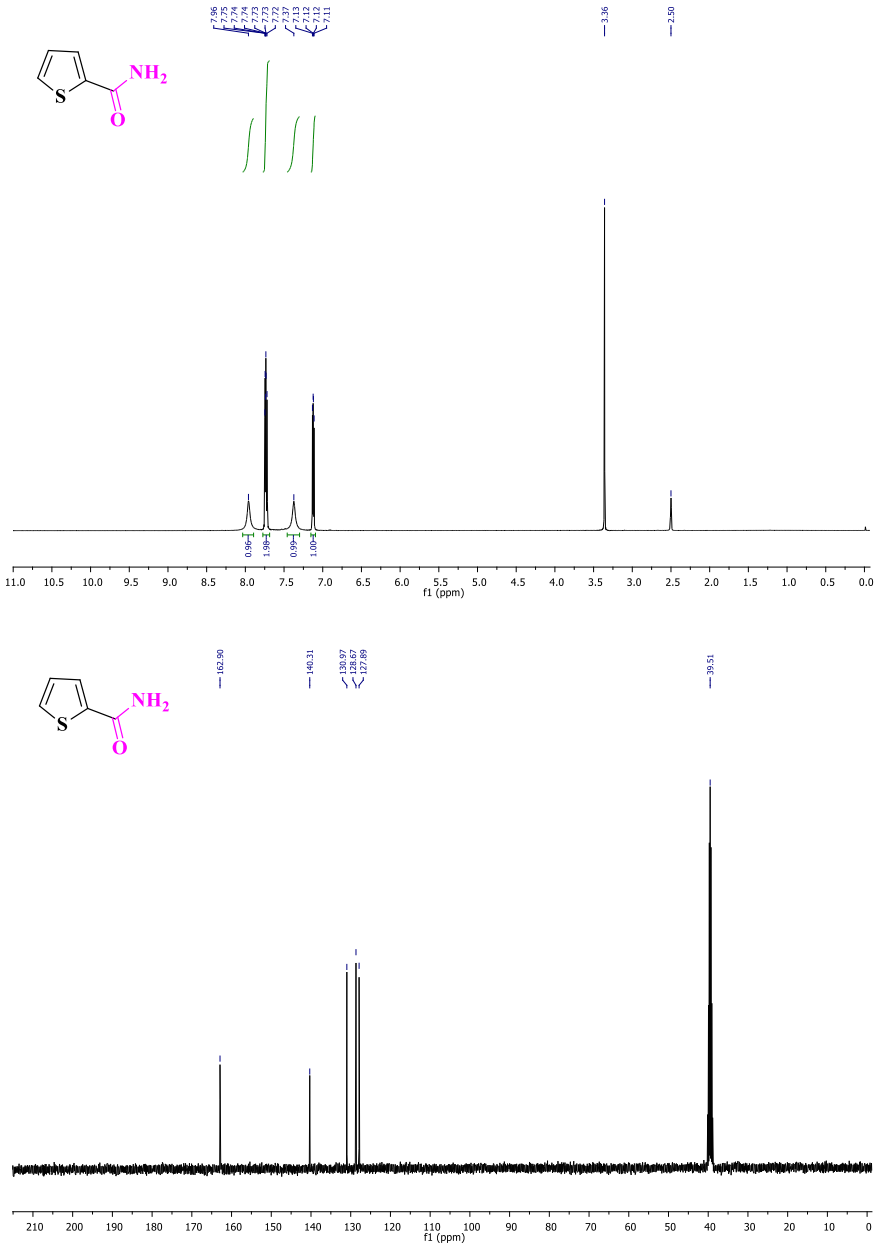


Figure S24. ^{1}H and ^{13}C spectra of thiophene-2-carboxamide (**9w**) in DMSO-d6.

thiophene-3-carboxamide (9x). To a 25 mL round bottom flask (RB), was added thiophene-3-carbonitrile (91 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 4 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9x** was obtained as a white solid (107 mg, 84%). ^{1}H NMR (400 MHz, DMSO-d6) δ 8.13-8.12 (d, *J* = 4.0 Hz, 1H), 7.77 (s, 1H), 7.56-7.54 (dd, *J* = 4.0, 4.0, 1H), 7.49-7.47 (d, *J* = 8.0 Hz, 1H), 7.22 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 163.7, 138.0, 129.0, 127.2, 126.5.

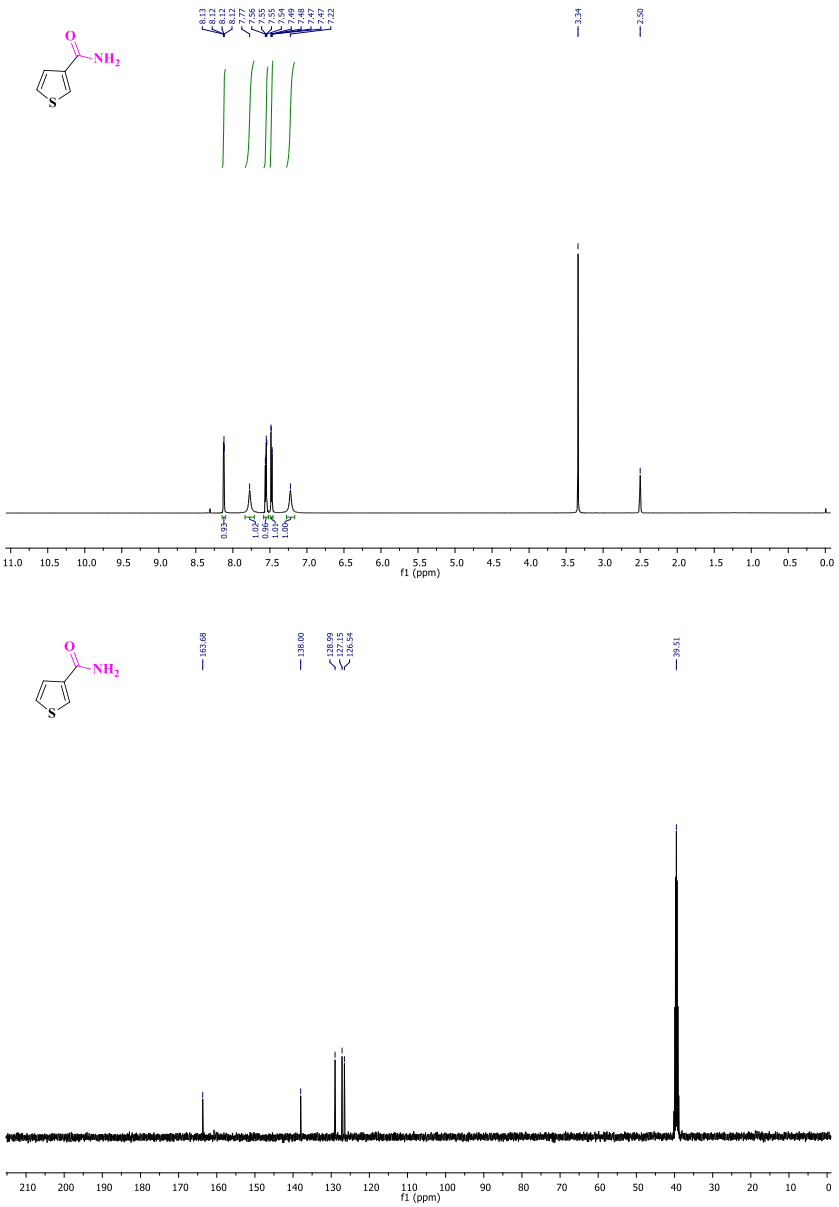


Figure S25. ^{1}H and ^{13}C spectra of thiophene-3-carboxamide (**9x**) in DMSO-d6.

4-(2-amino-2-oxoethyl)benzamide (9y). To a 25 mL round bottom flask (RB), was added 4-(cyanomethyl)benzonitrile (142 mg, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9y** was obtained as a light pink solid (141 mg, 79%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.93 (s, 1H), 7.81-7.79 (d, *J* = 8.0 Hz, 2H), 7.52 (s, 1H), 7.33-7.31 (d, *J* = 16.0 Hz, 1H), 6.94 (s, 3H), 3.42-3.36 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 171.8, 167.8, 139.9, 132.4, 128.9, 127.4.

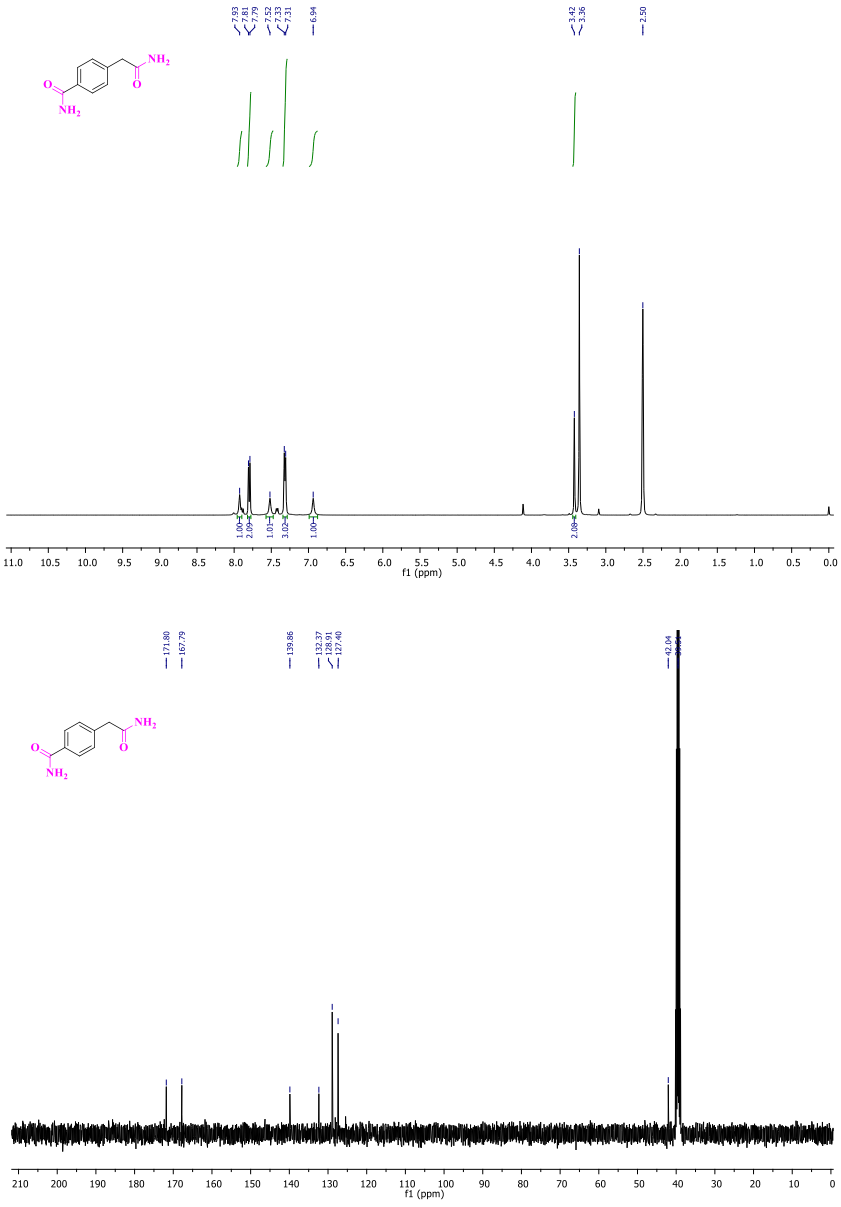


Figure S26. ^{1}H and ^{13}C spectra of 4-(2-amino-2-oxoethyl)benzamide (**9y**) in DMSO-d6.

(E)-3-(4-methoxyphenyl)acrylamide (9z). To a 25 mL round bottom flask (RB), was added (E)-3-(4-methoxyphenyl)acrylonitrile (145 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9z** was obtained as a white solid (143 mg, 81%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.51-7.49 (d, *J* = 8.0 Hz, 2H), 7.43 (s, 1H), 7.38-7.34 (d, *J* = 16.0 Hz, 1H), 6.98-6.96 (d, *J* = 8.0 Hz, 3H), 6.47-6.43 (d, *J* = 16.0 Hz, 1H), 3.8 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 166.9, 160.3, 138.8, 129.1, 127.4, 119.8, 114.4, 55.2.

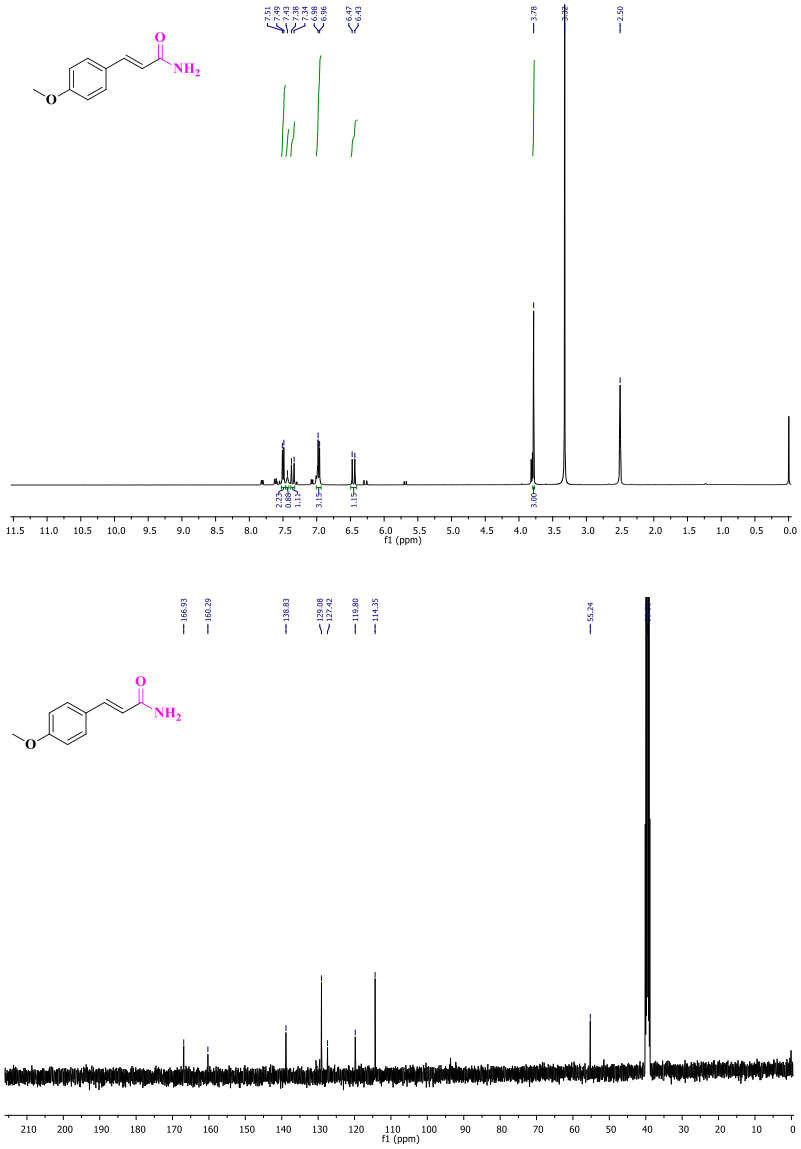


Figure S27. ^{1}H and ^{13}C spectra of (E)-3-(4-methoxyphenyl)acrylamide (**9z**) in DMSO-d6.

2-phenylacetamide (9aa). To a 25 mL round bottom flask (RB), was added 2-phenylacenitrile (115 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 5 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9aa** was obtained as a white solid (116 mg, 86%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.50 (s, 1H), 7.31-7.21 (m, 5H), 6.89 (s, 1H), 3.36 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ 172.5, 136.6, 129.2, 128.3, 126.4.

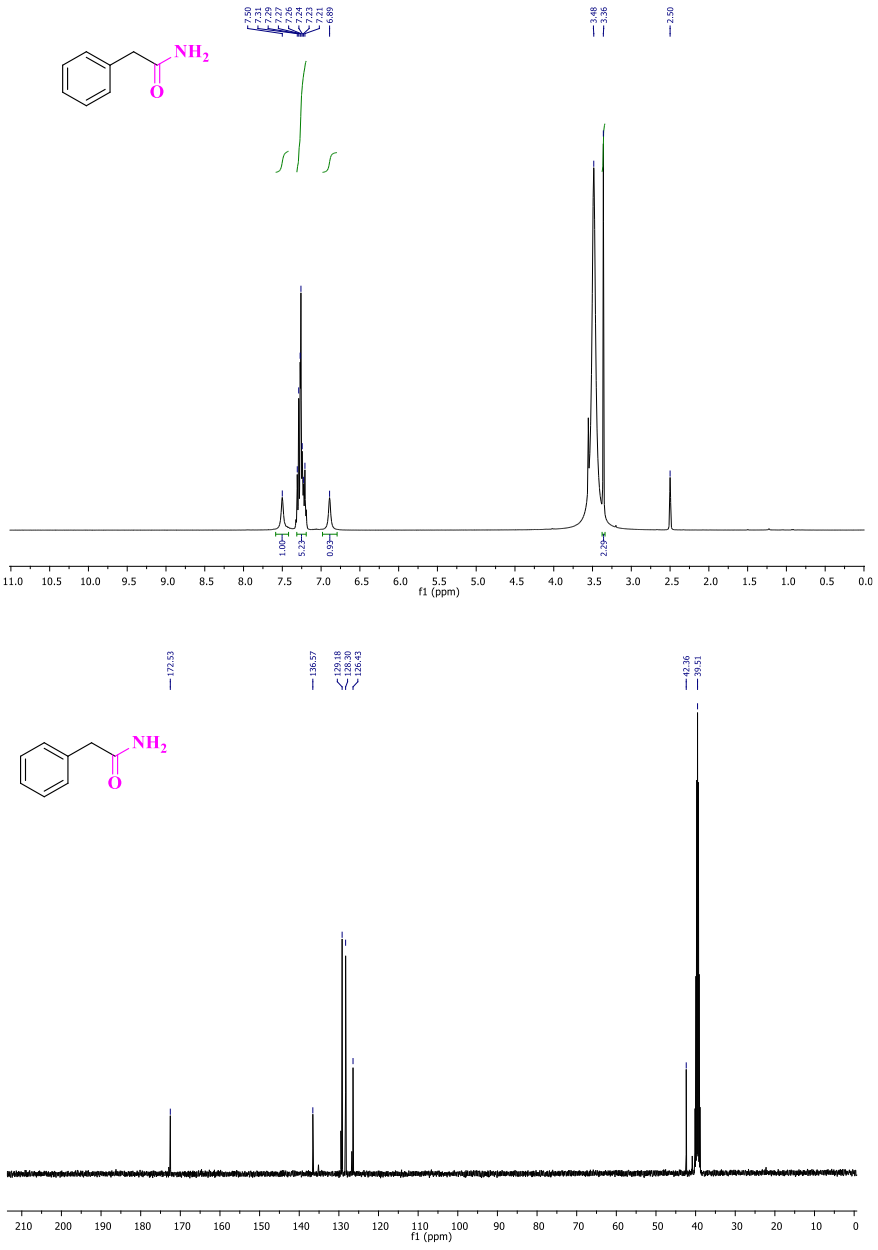


Figure S28. ^{1}H and ^{13}C spectra of 2-phenylacetamide (**9aa**) in DMSO-d6.

2-(m-tolyl)acetamide (9ab). To a 25 mL round bottom flask (RB), was added 2-(m-tolyl)acetonitrile (132 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 6 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9ab** was obtained as a white solid (128 mg, 86%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.45 (s, 1H), 7.19-7.15 (t, *J* = 8.0 Hz, 1H), 7.07-7.01 (m, 3H), 6.84 (s, 1H), 3.09 (s, 2H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 172.2, 137.1, 136.4, 129.7, 128.0, 126.9, 126.1, 42.2, 21.0.

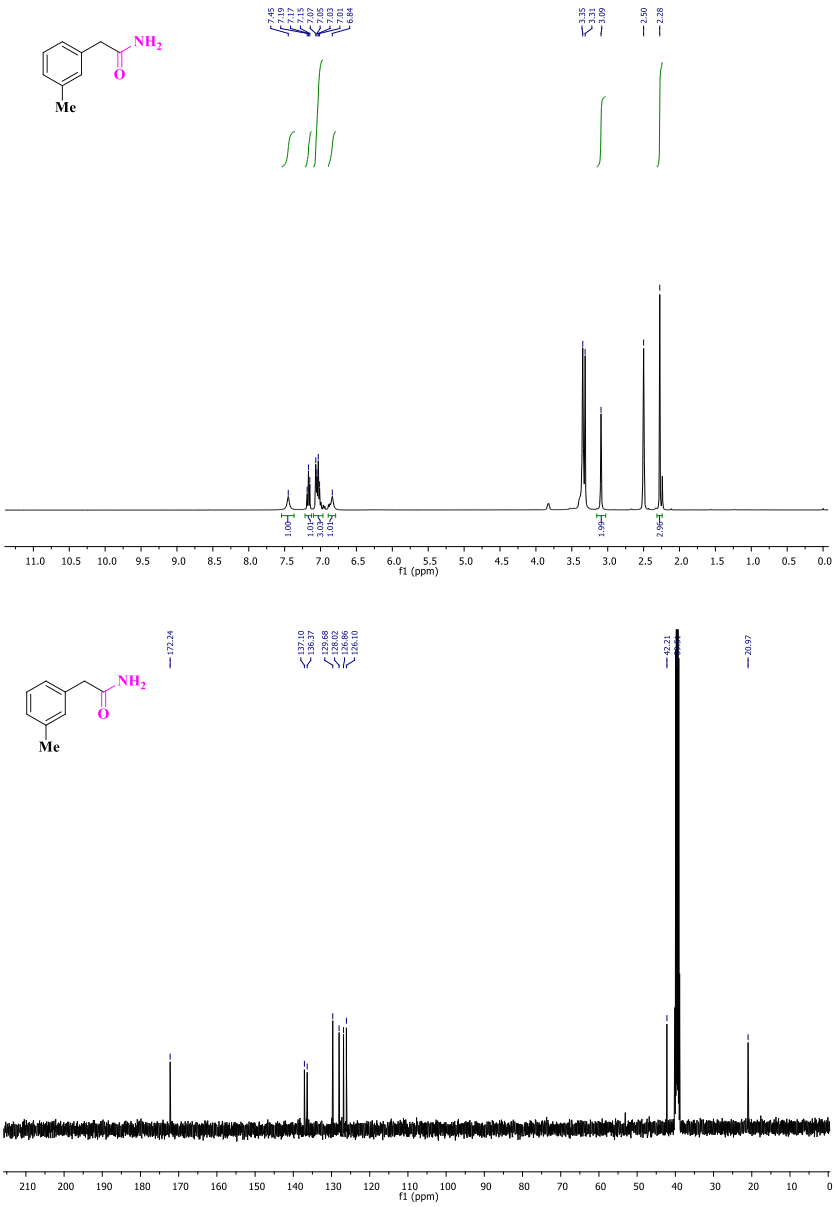


Figure S29. ^{1}H and ^{13}C spectra of 2-(m-tolyl)acetamide (**9ab**) in DMSO-d6.

2-(p-tolyl)acetamide (9ac). To a 25 mL round bottom flask (RB), was added 2-(p-tolyl)acetonitrile (132 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9ac** was obtained as a white solid (121 mg, 81%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.39 (s, 1H), 7.14-7.08 (m, 4H), 6.82 (s, 1H), 3.30 (s, 2H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6) δ 172.4, 135.2, 133.4, 128.9, 128.7, 41.8, 20.6.

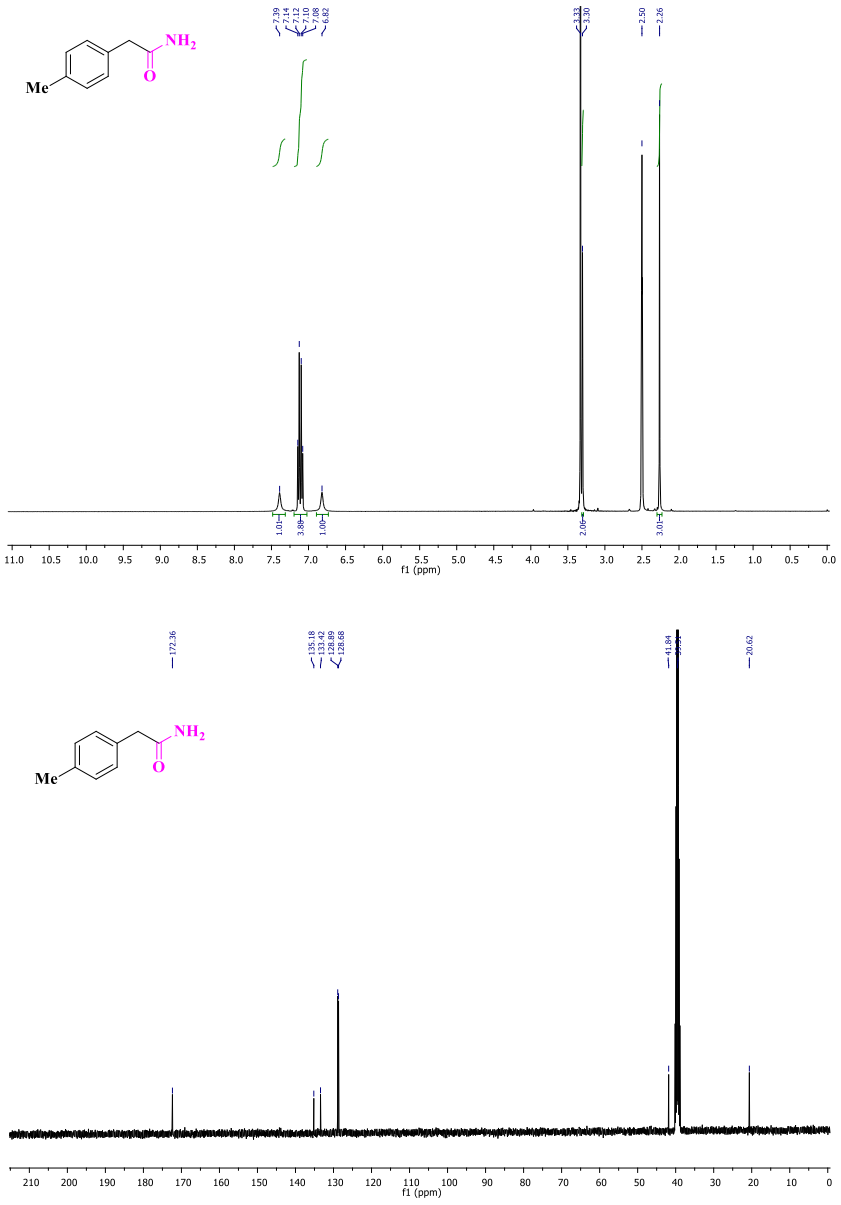


Figure S30. ^{1}H and ^{13}C spectra of 2-(p-tolyl)acetamide (**9ac**) in DMSO-d6.

2-(4-methoxyphenyl)acetamide (9ad). To a 25 mL round bottom flask (RB), was added 2-(4-methoxyphenyl)acetonitrile (145 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 2 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9ad** was obtained as a white solid (134 mg, 81%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.37 (s, 1H), 7.17-7.15 (d, *J* = 8.0 Hz, 2H), 6.86-6.84 (d, *J* = 8.0 Hz, 2H), 6.80 (s, 1H), 3.72 (s, 3H), 3.28 (s, 2H); ^{13}C NMR (176 MHz, $CDCl_3$) δ 173.7, 156.0, 130.5, 126.8, 114.5, 55.3, 42.4.

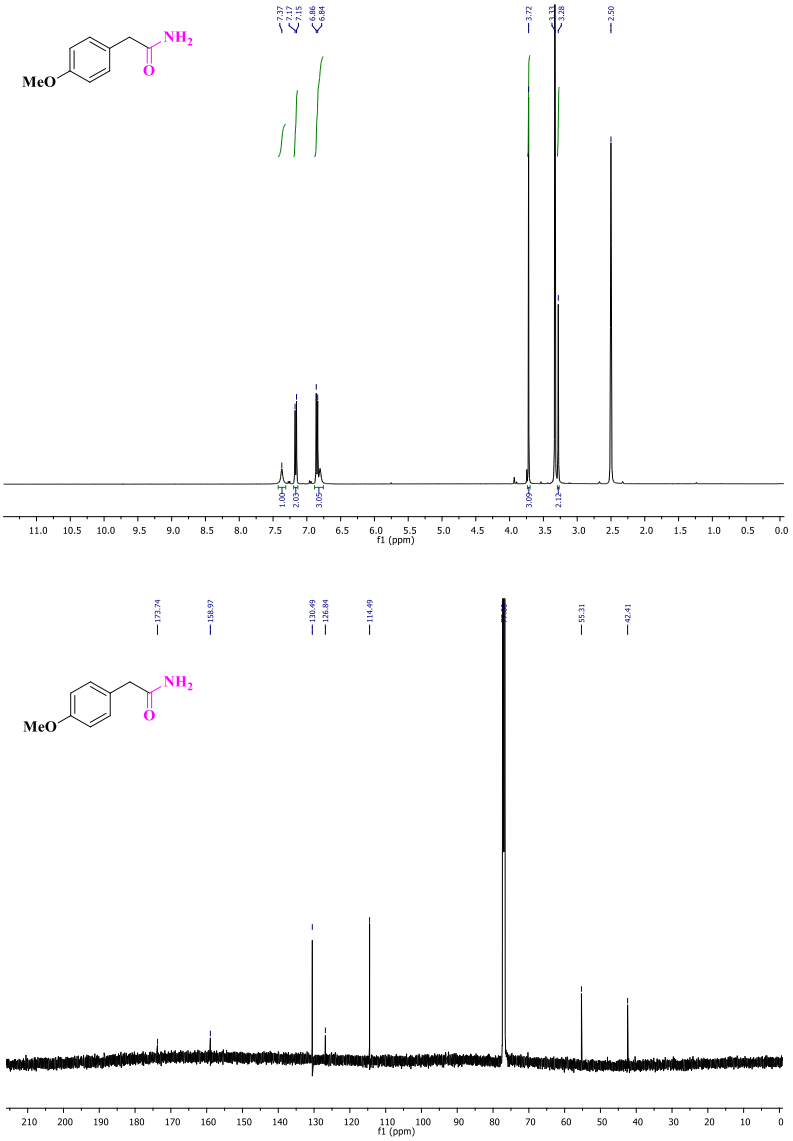


Figure S31. ^{1}H and ^{13}C spectra of 2-(4-methoxyphenyl)acetamide (**9ad**) in DMSO-d6 and $CDCl_3$ respectively.

2-(3-fluorophenyl)acetamide (9ae). To a 25 mL round bottom flask (RB), was added 2-(3-flurophenyl)acetonitrile (116 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 5 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9ae** was obtained as a white solid (132 mg, 86%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.47 (s, 1H), 7.32-7.26 (m, 2H), 7.15-7.12 (m, 2H), 6.95 (s, 1H), 3.44 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d6) δ 171.1, 160.6 (d, $J_{C\text{-}F}$ = 139.0 Hz), 131.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 128.5 (d, $J_{C\text{-}F}$ = 5.0 Hz), 124.1 (d, $J_{C\text{-}F}$ = 3.0 Hz), 123.5 (d, $J_{C\text{-}F}$ = 9.0 Hz), 115.0 (d, $J_{C\text{-}F}$ = 12.0 Hz), 35.1.

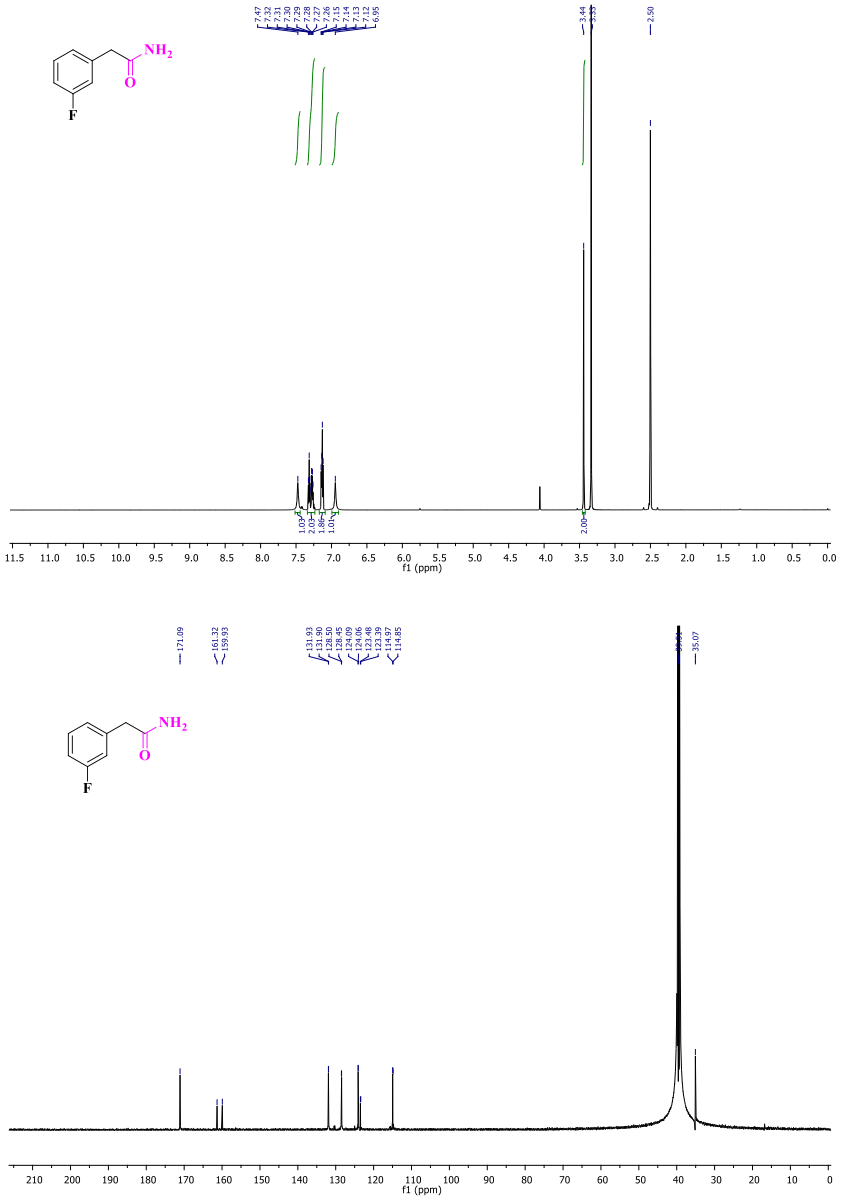


Figure S32. ^{1}H and ^{13}C spectra of 2-(3-fluorophenyl)acetamide (**9ae**) in DMSO-d6.

2-(4-fluorophenyl)acetamide (9af). To a 25 mL round bottom flask (RB), was added 2-(4-fluorophenyl)acetonitrile (120 µL, 1 mmol) and water (3 mL). This was followed by the addition of ChOH (13.15 µL, 5 mol%). The reaction mixture was stirred at 80 °C for 4 hours in air, and the progress of the reaction was continuously monitored through TLC. After the completion of the reaction, the product was extracted in ethyl acetate/water (4:1, 3x 50 mL). The resultant solution was concentrated under vacuum. The catalyst was removed in the workup process, and **9af** was obtained as a yellow solid (135 mg, 88%). ^{1}H NMR (400 MHz, DMSO-d6) δ 7.46 (s, 1H), 7.30-7.26 (m, 2H), 7.13-7.09 (t, *J* = 8.0, 2H), 6.28 (s, 1H), 3.36 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d6) δ 172.4, 161.0 (d, $J_{C\text{-}F}$ = 240.0 Hz), 132.7 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.9 (d, $J_{C\text{-}F}$ = 8.0 Hz), 114.9 (d, $J_{C\text{-}F}$ = 21.0 Hz), 41.2.

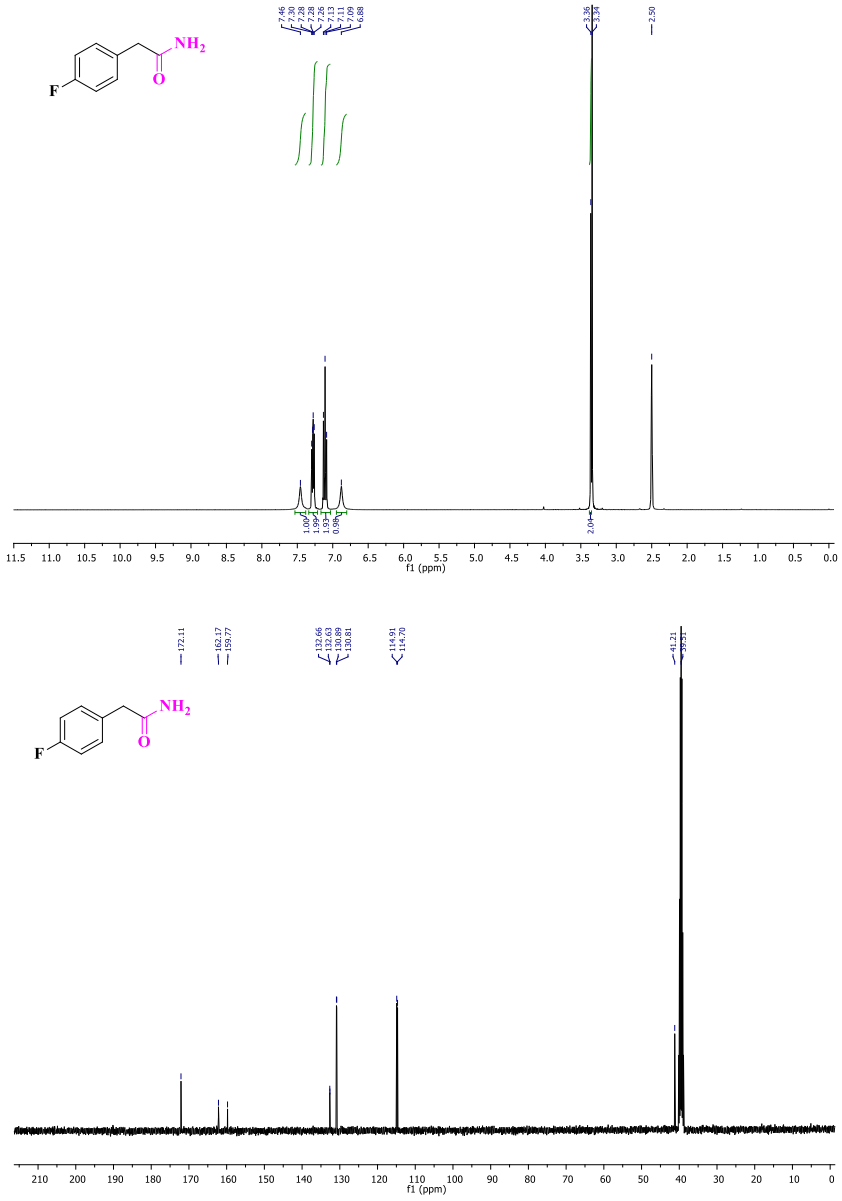


Figure S33. ^{1}H and ^{13}C spectra of 2-(4-fluorophenyl)acetamide (**9af**) in DMSO-d6.

^{19}F NMR Spectra:

2-fluorobenzamide (9f). ^{19}F NMR (376 MHz, DMSO-d6) δ -113.78.

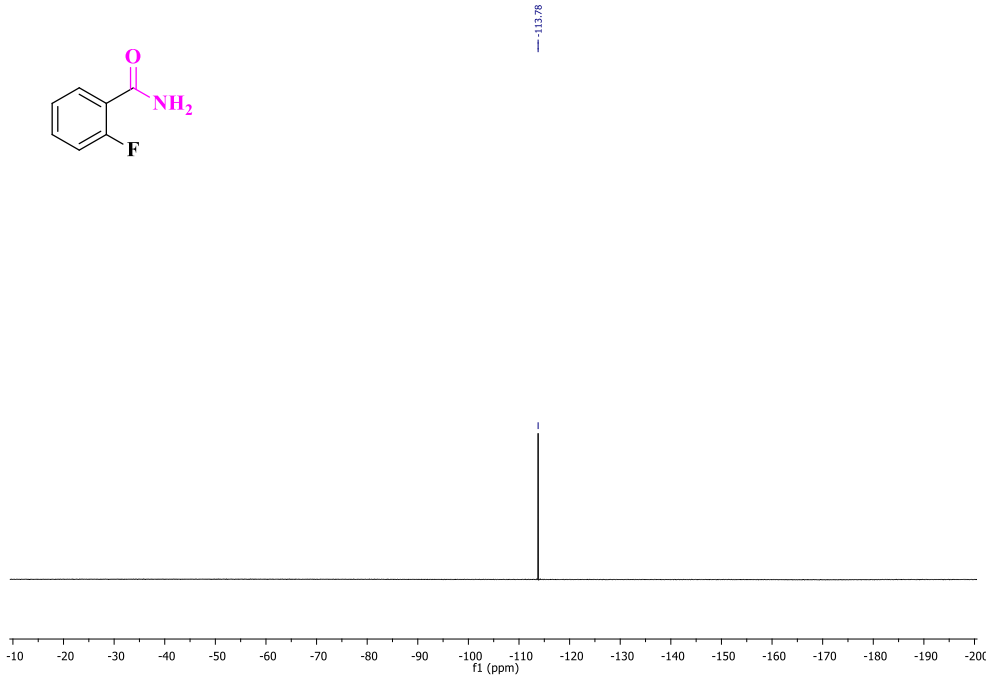


Figure S34. ^{19}F spectra of 2-fluorobenzamide **(9f)**.in DMSO-d6.

3-fluorobenzamide (9g). ^{19}F NMR (376 MHz, DMSO-d6) δ -113.78.

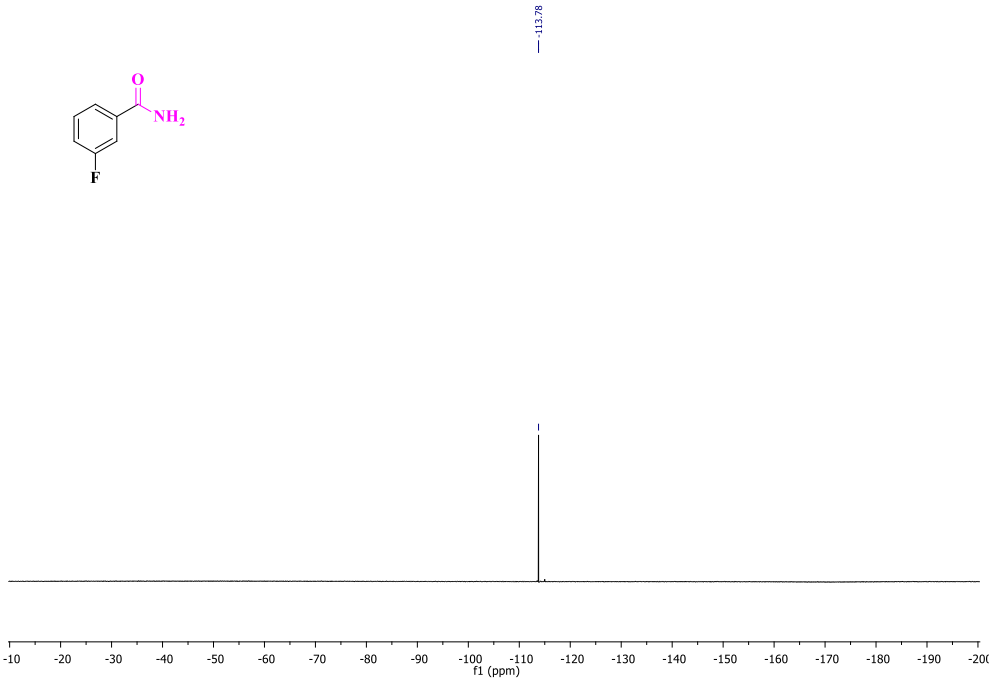


Figure S35. ^{19}F spectra of 3-fluorobenzamide **(9g)**.in DMSO-d6.

4-fluorobenzamide (9h). ^{19}F NMR (376 MHz, DMSO-d6) δ -109.62.

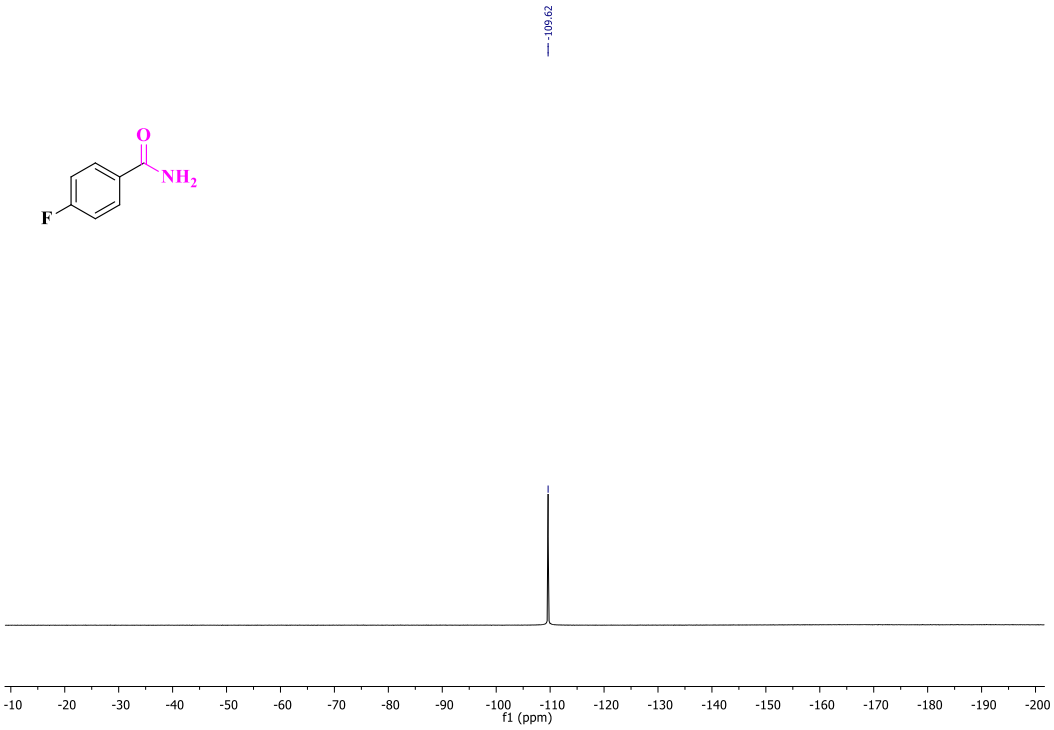


Figure S36. ^{19}F spectra of 4-fluorobenzamide **(9h)**.in DMSO-d6.

5-bromo-2-fluorobenzamide (9q). ^{19}F NMR (376 MHz, DMSO-d6) δ -115.72.

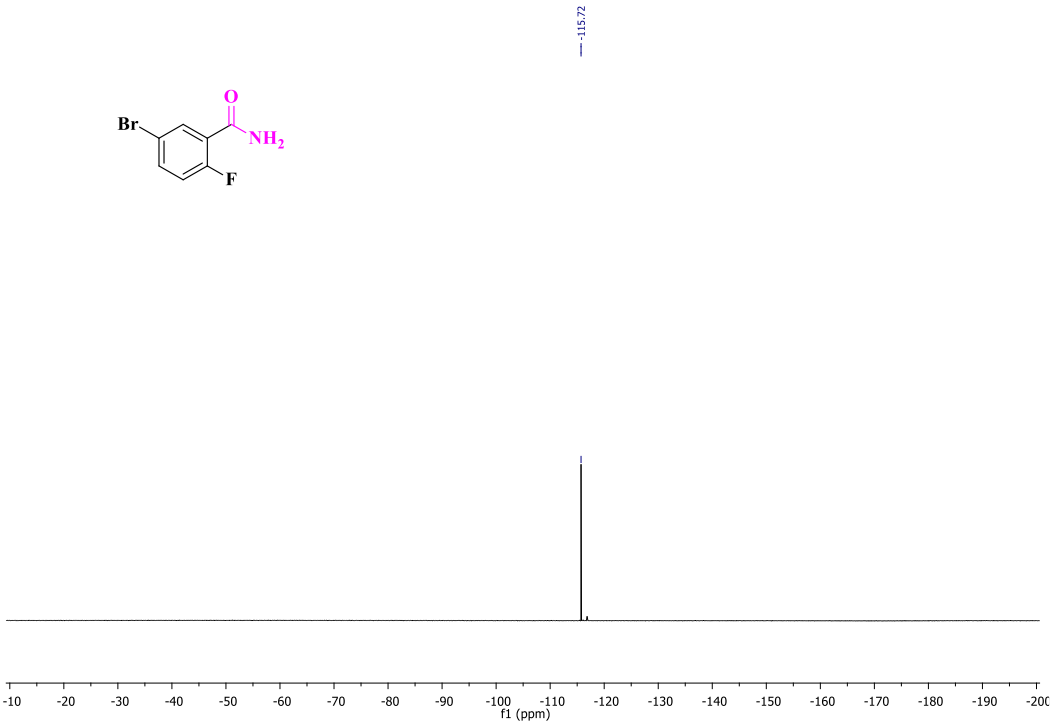


Figure S37. ^{19}F spectra of 5-bromo-2-fluorobenzamide **(9q)**.in DMSO-d6.

2-chloro-6-(trifluoromethyl)nicotinamide (9t). ^{19}F NMR (376 MHz, DMSO-d6) δ -67.25.

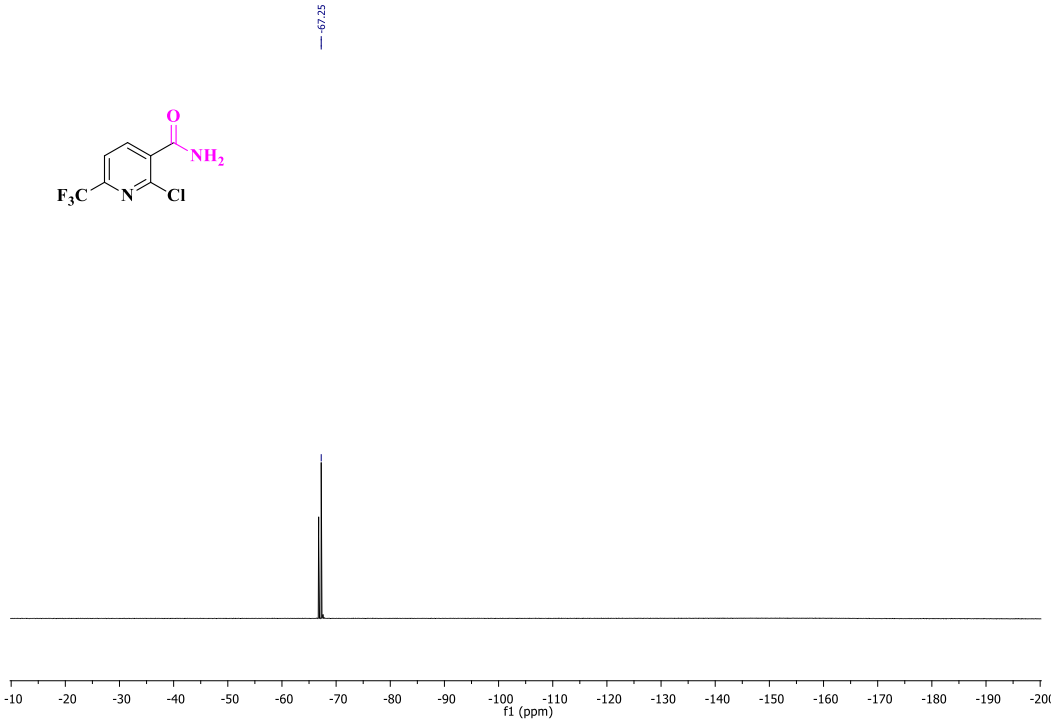


Figure S38. ^{19}F spectra of 2-chloro-6-(trifluoromethyl)nicotinamide **(9t)**.in DMSO-d6.

2-(3-fluorophenyl)acetamide (9ae). ^{19}F NMR (376 MHz, DMSO-d6) δ -117.48.

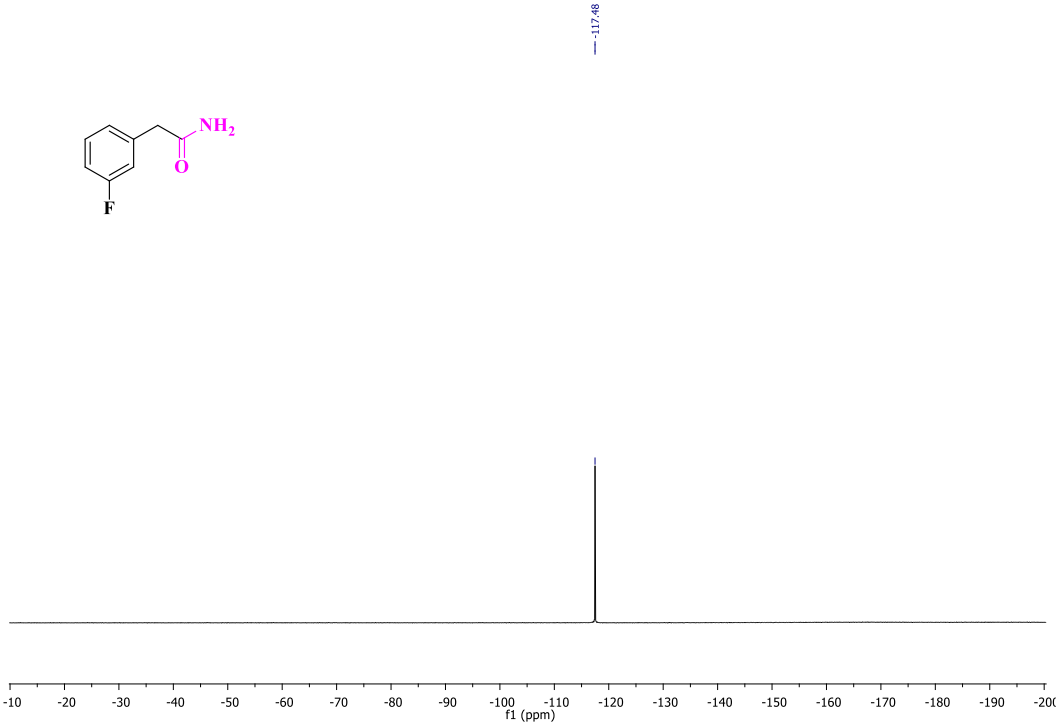


Figure S39. ^{19}F spectra of 2-(3-fluorophenyl)acetamide **(9ae)**.in DMSO-d6.

2-(4-fluorophenyl)acetamide (9af). ^{19}F NMR (376 MHz, DMSO-d6) δ -117.07.

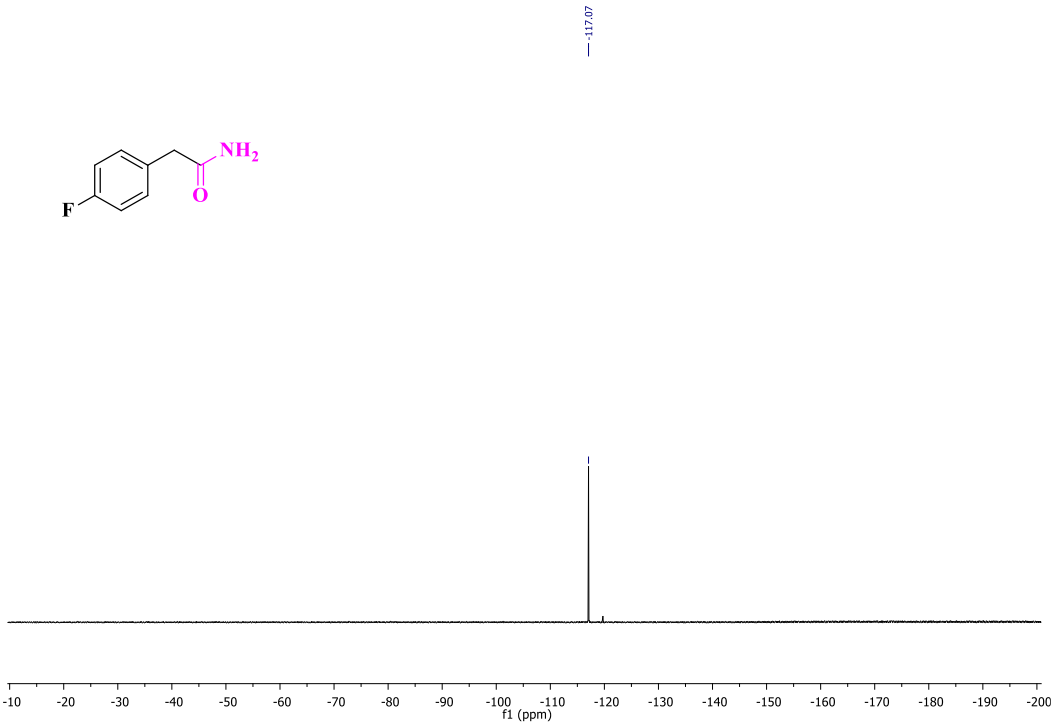


Figure S40. ^{19}F spectra of 2-(4-fluorophenyl)acetamide **(9af)**.in DMSO-d6.

Kinetic Results:

For our experimental monitoring, p-fluorobenzonitrile (**8h**) was taken as the model substrate with p-fluoroanisole in DMSO-d6 as the calibrant. The reaction was scaled down to 0.25 mmol of the reactant in order to carry out the reaction in the NMR tube itself. This brings down the catalyst load to ~3.29 µL, which is very negligible and hence, the reaction did not proceed at all. After careful consideration, the catalyst load was increased to 10 µL for all further experiments. The general reaction scheme used for our experimental monitoring has been shown below in **Figure S41**.

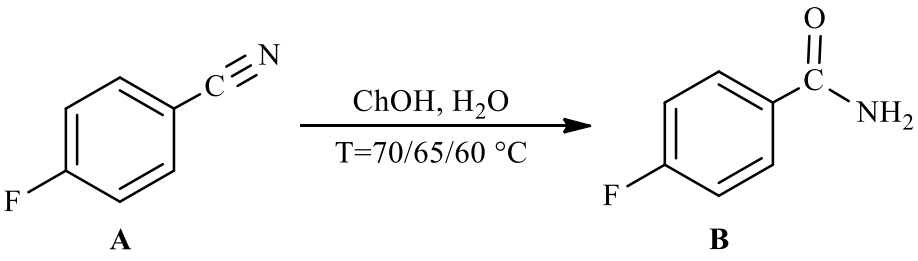
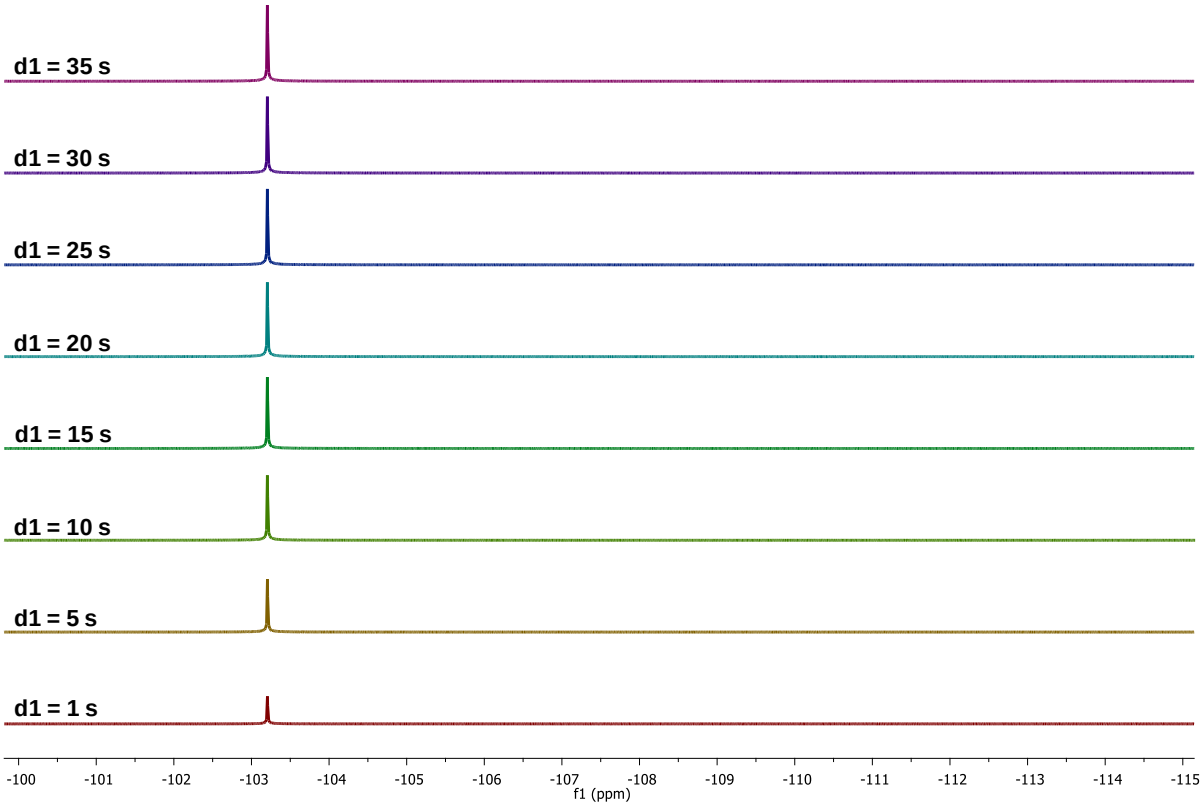


Figure S41. Reaction scheme for the experimental monitoring.

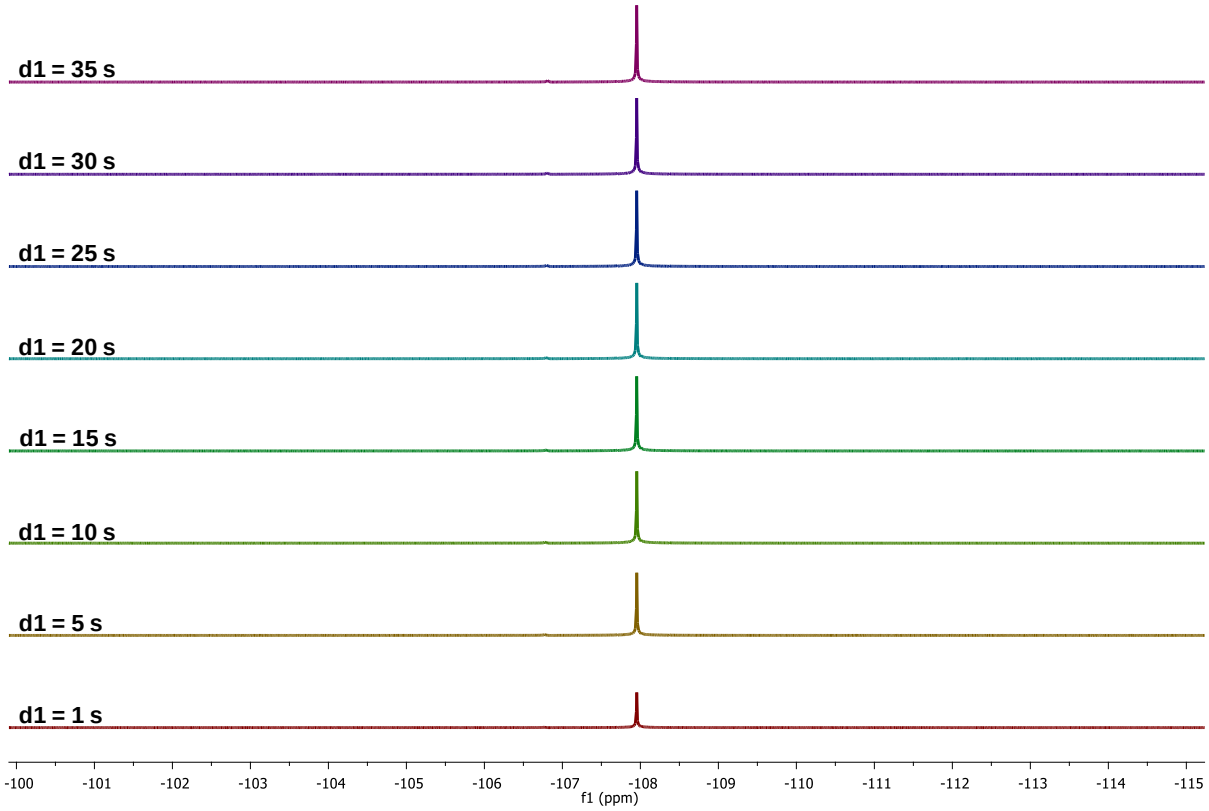
A simple derivation for the time-dependence of the concentration of the product would lead us to equation 1. Now, a plot of product concentration with respect to time would help us find out the rate constant, k.

$$[B] = 0.25(1 - e^{-kt}) \qquad \text{----------1}$$

The progress of the reaction was appreciable at all the three planned temperatures, 70 °C, 65 °C and 60 °C. Some preliminary experiments were performed to estimate the relaxation delay (d1) of the reactant and the product separately. The d1 values were varied from 1 s to 35 s and it was observed that both the reactant and the product relaxed almost completely within around 25 s. The corresponding stacked NMR spectra have been shown in **Figure S42 (a)** reactant and **(b)** product for reference. Moreover, it is recommended to use d1 = 30 s to ensure reliable quantification.[1] Hence, d1 was set at 30 s for all kinetic measurements.



(a)



(b)

Figure S42. Corresponding ^{19}F NMR stacked plots for the relaxation experiments **(a)** reactant and **(b)** product.

A few of the selected ^{19}F NMR spectra for the data at 70 °C have been shown below in **Figure S43** to represent the general nature of the spectra obtained.

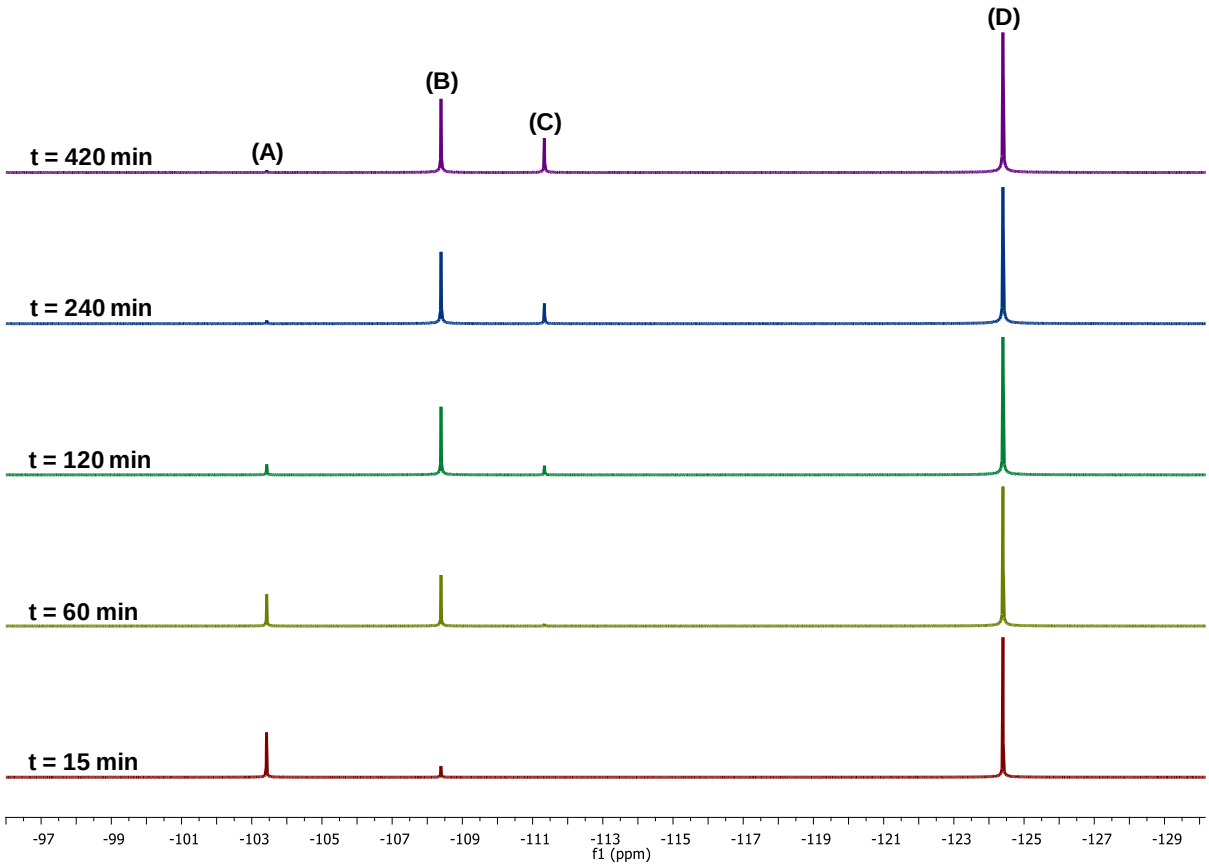


Figure S43. A representative ^{19}F NMR stacked plot for the data at 70 °C. p-fluorobenzonitrile (**A**), p-fluorobenzamide (**B**), p-fluorobenzamide with catalyst (**C**) and p-fluoroanisole (**D**).

The reaction was monitored separately at 70 °C, 65 °C and 60 °C at regular intervals continuously for 7 hours each and the results were analysed by plotting the respective time-dependent concentrations of the product. The peak (**C**) has been attributed to the interaction of the product with the regenerated catalyst, verified from additional NMR measurements. Hence, the sum of the integration value for peak (**B**) and peak (**C**) was taken as the product. The best fitting obtained further validates our claims. Keeping in mind the guidelines laid down by the University of Oxford for Quantitative NMR Spectroscopy, the measurements were performed and the concentration of product was calculated using the formula shown below.[1]

$$[B] = \frac{I_B}{I_{cal}} \times \frac{N_{cal}}{N_B} \times C_{cal} \qquad \text{----------2}$$

where, I_B is the integration value for the product

I_{cal} is the integration value for the calibrant

N_{cal} is the number of nuclei for the calibrant

N_B is the number of nuclei for the product

C_{cal} is the concentration of the calibrant taken

In our case, the number of nuclei is the same in both the product and the calibrant. Moreover, the integration value for the calibrant is being normalized to 1 for simplicity. Hence, the equation now reduces to –

$$[B] = I_B \times C_{cal} \qquad \text{----------3}$$

Different types of exponential fitting were tried and the best fit was obtained with ExpDec1 for all the measurements. The general fitting equation is –

$$y = y_0 + A_1 e^{-\frac{x}{t_1}} \qquad \text{----------4}$$

Comparing this equation with equation 1, we know that k from equation 1 should be the reciprocal of t_1 from equation 4. Let us assume that the rate constants are k_1, k_2 and k_3 at 70 °C, 65 °C and 60 °C respectively.

At 70 °C, t_1 = 83.41975 min

$$k_1 = \frac{1}{t_1}$$

$$\Rightarrow k_1 = \frac{1}{83.41975}\ min^{-1} = 0.012\ min^{-1} \qquad \text{----------5}$$

At 65 °C, t_1 = 114.07359 min

$$k_2 = \frac{1}{t_1}$$

$$\Rightarrow k_2 = \frac{1}{114.07359}\ min^{-1} = 0.009\ min^{-1} \qquad \text{----------6}$$

At 60 °C, t_1 = 169.02648 min

$$k_3 = \frac{1}{t_1}$$

$$\Rightarrow k_3 = \frac{1}{169.02648}\ min^{-1} = 0.006\ min^{-1} \qquad \text{----------7}$$

Based on the obtained values of rate constants, an Arrhenius plot was made and the activation energy barrier was determined using the slope of the fitted curve.

$$Slope\ of\ the\ curve\ \left(-\frac{E_a}{R}\right) = -7930.14648\ K$$

$$\Rightarrow -\frac{E_a}{R} = -7930.14648\ K$$

$$\Rightarrow E_a = 7930.14648 \times 8.31446\ J\ mol^{-1}$$

$$\Rightarrow E_a = 65.93488\ kJ\ mol^{-1} = \sim 65.9\ kJ\ mol^{-1} \quad \text{----------8}$$

Computational Method:

The geometry optimizations and frequency calculations were performed using density functional theory (DFT) with the B3LYP functional and 6-31+G(d,p) basis set. Solvent effects were incorporated by using PCM solvation model. The structures of reactants, intermediates, transition states and products were optimized in gas phase and single point energy calculations were performed for the optimized geometries in the solution phase taking H_2O as the solvent, without symmetry constraints. The Gibbs free energy corrections were added to the single-point electronic energies calculated to obtain the free energies. The QTAIM was performed at the same level of theory and all the calculations were performed with Gaussian-16 software package.[2] Optimized Cartesian coordinates, electronic energies, Gibbs energies of all reactants, transition states and products are provided below.

Molecule	E (au)	G (au)	E+G (au)
ChOH	-404.752702	0.172380	-404.580322

C	-1.144263000	-1.438415000	-0.328977000
H	-1.603694000	-1.946637000	-1.201439000
H	-0.677212000	-2.248214000	0.265338000
C	-0.068708000	-0.542084000	-0.956855000
H	0.506168000	-1.079260000	-1.717297000
H	-0.572554000	0.328085000	-1.383184000
O	-2.070269000	-0.746302000	0.433779000
H	-2.039336000	0.316695000	0.176049000
N	0.988776000	0.035753000	0.016766000

C	0.445047000	0.319444000	1.403947000
H	1.273687000	0.718230000	1.994492000
H	-0.371515000	1.040570000	1.289329000
H	0.071787000	-0.606679000	1.835843000
C	2.131872000	-0.923059000	0.130790000
H	1.753576000	-1.879205000	0.495258000
H	2.591534000	-1.056030000	-0.850000000
H	2.866728000	-0.525474000	0.832930000
C	1.456942000	1.345020000	-0.561581000
H	1.833812000	1.168062000	-1.570910000
H	0.582668000	2.003581000	-0.578923000
H	2.252406000	1.746972000	0.070301000
O	-1.668123000	1.617325000	-0.150779000
H	-2.407690000	2.235411000	-0.163099000

Molecule	**E (au)**	**G (au)**	**E+G (au)**
Reactant (8)	-324.5213113	0.069445	-324.451866

C	0.000000000	0.000000000	0.610632000
C	0.000000000	1.218590000	-0.091086000
C	0.000000000	-1.218590000	-0.091086000
C	0.000000000	1.211917000	-1.485242000
C	0.000000000	-1.211917000	-1.485242000
C	0.000000000	0.000000000	-2.182796000
H	0.000000000	2.154066000	0.458215000
H	0.000000000	-2.154066000	0.458215000
H	0.000000000	2.152764000	-2.026833000
H	0.000000000	-2.152764000	-2.026833000
H	0.000000000	0.000000000	-3.268668000
C	0.000000000	0.000000000	2.046696000
N	0.000000000	0.000000000	3.210664000

Molecule	E (au)	G (au)	E+G (au)
INT-1	-729.263787	0.261207	-729.002580

C	-2.453281000	1.697356000	0.447705000
C	-2.249864000	0.445050000	-0.425513000
O	-1.894026000	2.820526000	-0.201400000
N	-3.231275000	-0.701463000	-0.175318000
C	-3.175451000	-1.113037000	1.278387000
C	-4.624342000	-0.322979000	-0.567487000
C	-2.768942000	-1.876158000	-1.012435000
O	-0.392868000	-1.755827000	0.638875000
H	-3.515793000	1.925007000	0.589765000
H	-2.006725000	1.543698000	1.437851000
H	-2.372783000	0.729027000	-1.473999000
H	-1.262286000	0.004993000	-0.257753000
H	-0.924002000	2.806671000	-0.078491000
H	-3.835665000	-1.973433000	1.409972000
H	-2.114510000	-1.380488000	1.460355000
H	-3.524958000	-0.282326000	1.892953000
H	-4.977516000	0.500380000	0.052286000
H	-4.630162000	-0.024347000	-1.617318000
H	-5.273236000	-1.188633000	-0.425588000
H	-2.755522000	-1.562659000	-2.058543000
H	-1.761184000	-2.139513000	-0.628580000
H	-3.483977000	-2.690980000	-0.875117000
C	1.764259000	1.573275000	0.114298000
N	0.915051000	2.366245000	0.175697000
H	-0.029046000	-2.482710000	1.161971000
C	2.805586000	0.592133000	0.025698000
C	2.463093000	-0.771587000	0.088845000

C	4.141526000	1.007668000	-0.132929000
C	3.490335000	-1.712942000	-0.012787000
C	5.146328000	0.048450000	-0.229428000
C	4.820096000	-1.312155000	-0.170146000
H	1.412876000	-1.083952000	0.227189000
H	4.378641000	2.065956000	-0.179013000
H	3.242254000	-2.769494000	0.032435000
H	6.179560000	0.359204000	-0.351029000
H	5.606691000	-2.057911000	-0.247045000

Molecule	E (au)	G (au)	E+G (au)
TS-1	-729.2620597	0.263784	-728.998275

C	-2.450523000	1.744583000	0.259873000
C	-2.645569000	0.477031000	-0.602700000
O	-1.603802000	2.549933000	-0.456853000
N	-3.445352000	-0.703607000	0.005020000
C	-2.869309000	-1.080683000	1.345446000
C	-4.889997000	-0.336783000	0.151723000
C	-3.315007000	-1.877074000	-0.921470000
O	0.235705000	-0.698229000	0.335519000
H	-3.422648000	2.238142000	0.451012000
H	-2.037096000	1.454427000	1.247213000
H	-3.153917000	0.736842000	-1.534841000
H	-1.659069000	0.068272000	-0.818175000
H	-0.492431000	2.065034000	-0.358225000
H	-3.307287000	-2.031552000	1.657589000
H	-1.784750000	-1.149803000	1.236830000
H	-3.113741000	-0.303232000	2.067015000
H	-4.967970000	0.541727000	0.790863000
H	-5.298091000	-0.107952000	-0.833790000

H	-5.431785000	-1.174528000	0.596080000
H	-3.673472000	-1.586532000	-1.909796000
H	-2.261800000	-2.153305000	-0.978044000
H	-3.907189000	-2.710928000	-0.537093000
C	1.119319000	0.449512000	-0.009590000
N	0.689584000	1.575326000	-0.275951000
H	0.782013000	-1.376258000	0.759780000
C	2.565267000	0.038696000	0.001335000
C	3.528192000	1.032180000	0.249710000
C	3.009884000	-1.268149000	-0.263219000
C	4.887175000	0.724987000	0.254909000
C	4.375240000	-1.575096000	-0.270275000
C	5.318844000	-0.582054000	-0.003826000
H	3.176244000	2.043498000	0.424869000
H	2.295472000	-2.050129000	-0.507350000
H	5.614645000	1.506536000	0.457430000
H	4.697948000	-2.589109000	-0.491504000
H	6.378981000	-0.819718000	-0.004181000

Molecule	**E (au)**	**G (au)**	**E+G (au)**
INT-2	-729.2721803	0.265480	-729.006700

C	2.519151000	1.685068000	-0.440883000
C	2.757042000	0.502833000	0.542159000
O	1.669399000	2.500711000	0.203792000
N	3.642823000	-0.712197000	0.087613000
C	3.027845000	-1.352168000	-1.122587000
C	5.029038000	-0.243966000	-0.230461000
C	3.697609000	-1.715469000	1.198261000
O	-0.373570000	-0.418009000	-0.522539000
H	3.509128000	2.148553000	-0.691300000

H	2.136380000	1.267394000	-1.409110000
H	3.231081000	0.883486000	1.450212000
H	1.788574000	0.063882000	0.783489000
H	0.067500000	1.950899000	0.260553000
H	3.583876000	-2.260153000	-1.369459000
H	1.985851000	-1.579364000	-0.896649000
H	3.061307000	-0.646034000	-1.950106000
H	4.977535000	0.489649000	-1.033226000
H	5.452111000	0.225563000	0.658557000
H	5.640504000	-1.098500000	-0.530848000
H	4.121195000	-1.238624000	2.082882000
H	2.683109000	-2.050441000	1.416360000
H	4.317241000	-2.565037000	0.897718000
C	-1.297204000	0.540005000	-0.036537000
N	-0.957232000	1.683977000	0.349442000
H	-0.857704000	-1.058727000	-1.062777000
C	-2.715928000	0.063209000	-0.004635000
C	-3.744609000	1.020347000	0.002684000
C	-3.062119000	-1.297463000	0.032476000
C	-5.080322000	0.625569000	0.031231000
C	-4.403286000	-1.693243000	0.066817000
C	-5.416429000	-0.733516000	0.060841000
H	-3.464184000	2.068032000	-0.009019000
H	-2.289554000	-2.061086000	0.076091000
H	-5.863566000	1.378457000	0.030294000
H	-4.652303000	-2.750068000	0.106598000
H	-6.458574000	-1.039204000	0.084126000

Molecule	**E (au)**	**G (au)**	**E+G (au)**
TS-2	-729.2332117	0.261055	-728.972157

C	1.465310000	-1.373003000	-0.680455000
C	2.647396000	-0.360790000	-0.799239000
O	0.692951000	-1.208860000	-1.771015000
N	3.444530000	-0.019416000	0.493415000
C	2.575012000	0.779905000	1.426503000
C	3.887570000	-1.282414000	1.169205000
C	4.645669000	0.800732000	0.129680000
O	-1.525223000	2.728700000	-0.251594000
H	1.900174000	-2.396530000	-0.577000000
H	0.942433000	-1.182885000	0.299080000
H	3.386192000	-0.726047000	-1.517690000
H	2.245727000	0.592571000	-1.144347000
H	0.036240000	0.344510000	-1.564646000
H	3.151308000	1.031350000	2.319390000
H	2.249845000	1.683894000	0.911741000
H	1.700079000	0.187577000	1.687194000
H	3.007043000	-1.853574000	1.458913000
H	4.485149000	-1.864603000	0.466777000
H	4.482179000	-1.029128000	2.049826000
H	5.290221000	0.213172000	-0.524910000
H	4.311043000	1.696492000	-0.394506000
H	5.187590000	1.078596000	1.037236000
C	-1.413779000	1.447334000	-0.525499000
N	-0.308234000	1.279491000	-1.202510000
H	-0.434197000	2.597468000	-0.945884000
C	-2.415999000	0.450180000	-0.099991000
C	-2.249190000	-0.908827000	-0.420162000
C	-3.542557000	0.870827000	0.623744000
C	-3.212020000	-1.832369000	-0.008818000
C	-4.498612000	-0.060634000	1.030646000
C	-4.334189000	-1.413340000	0.714380000
H	-1.372320000	-1.229846000	-0.986646000
H	-3.652857000	1.925549000	0.853018000
H	-3.087218000	-2.882180000	-0.259145000

H	-5.371336000	0.267092000	1.588540000
H	-5.080857000	-2.138344000	1.027630000

Molecule	E (au)	G (au)	E+G (au)
INT-3	-729.3096743	0.266031	-729.043643

C	-1.575617000	0.143761000	1.735541000
C	-2.285653000	0.609422000	0.422063000
O	-0.873085000	1.183424000	2.226406000
N	-2.725923000	-0.491262000	-0.579927000
C	-1.510354000	-1.102208000	-1.226895000
C	-3.507888000	-1.552181000	0.136465000
C	-3.581588000	0.124636000	-1.646844000
O	1.985729000	2.365494000	-1.467655000
H	-2.365471000	-0.231271000	2.429089000
H	-0.957714000	-0.762058000	1.487173000
H	-3.188783000	1.179460000	0.656989000
H	-1.595847000	1.244150000	-0.136582000
H	0.161113000	1.877519000	1.194668000
H	-1.832357000	-1.892758000	-1.907702000
H	-0.978872000	-0.324177000	-1.774944000
H	-0.858838000	-1.503013000	-0.452390000
H	-2.864285000	-2.022138000	0.878348000
H	-4.358925000	-1.084831000	0.633145000
H	-3.854400000	-2.292241000	-0.588059000
H	-4.482346000	0.532374000	-1.186875000
H	-3.018990000	0.926439000	-2.126163000
H	-3.849511000	-0.636351000	-2.383932000
C	1.573876000	1.791678000	-0.446990000
N	0.711551000	2.364925000	0.422584000
H	0.466111000	3.320165000	0.197196000

C	2.035955000	0.383522000	-0.135379000
C	1.792761000	-0.254185000	1.092507000
C	2.768888000	-0.289523000	-1.125457000
C	2.273309000	-1.549330000	1.313140000
C	3.241029000	-1.583806000	-0.903553000
C	2.994698000	-2.217966000	0.319499000
H	1.223224000	0.251453000	1.869692000
H	2.966678000	0.232743000	-2.055980000
H	2.090360000	-2.031001000	2.269999000
H	3.810661000	-2.092810000	-1.676579000
H	3.371154000	-3.221563000	0.499725000

Molecule	**E (au)**	**G (au)**	**E+G (au)**
Water	-76.4422838	0.003620	-76.438664

O	0.000000000	0.000000000	0.116517000
H	0.000000000	0.769487000	-0.466066000
H	0.000000000	-0.769487000	-0.466066000

Molecule	**E (au)**	**G (au)**	**E+G (au)**
INT-4	-805.7719155	0.287391	-805.484525

C	2.410183000	1.100279000	1.308096000
C	2.331818000	-0.438618000	1.258630000
O	1.840994000	1.727147000	0.227326000
N	3.007981000	-1.108702000	0.047663000
C	2.243863000	-0.828412000	-1.230889000
C	4.430122000	-0.645741000	-0.110243000

C	2.986288000	-2.589083000	0.286670000
O	-0.716351000	-0.952582000	0.128283000
H	1.905628000	1.338947000	2.271392000
H	3.467876000	1.398650000	1.461001000
H	2.819236000	-0.873335000	2.139656000
H	1.289353000	-0.761687000	1.206407000
H	0.265277000	1.459312000	0.090068000
H	2.727625000	-1.390428000	-2.033389000
H	1.210620000	-1.144252000	-1.080367000
H	2.273673000	0.242155000	-1.414477000
H	4.440907000	0.403284000	-0.414858000
H	4.949935000	-0.782896000	0.840081000
H	4.902412000	-1.256428000	-0.882652000
H	3.577046000	-2.818902000	1.174909000
H	1.952084000	-2.902620000	0.433642000
H	3.409575000	-3.096294000	-0.582622000
C	-1.370461000	0.107764000	0.052388000
N	-0.792040000	1.320464000	0.015330000
H	-1.366415000	2.137864000	-0.121811000
C	-2.879424000	0.044059000	-0.008674000
C	-3.468949000	-1.154221000	-0.436222000
C	-3.708953000	1.113052000	0.362763000
C	-4.856467000	-1.274691000	-0.515307000
C	-5.098775000	0.990077000	0.295001000
C	-5.676095000	-0.201849000	-0.150604000
H	-2.818041000	-1.981339000	-0.698599000
H	-3.280628000	2.038467000	0.737154000
H	-5.299627000	-2.205630000	-0.857696000
H	-5.728859000	1.822096000	0.596180000
H	-6.756873000	-0.296051000	-0.206677000
O	3.814226000	2.279288000	-1.307818000
H	2.981530000	2.203035000	-0.720634000
H	3.996238000	3.217194000	-1.429625000

Molecule	E (au)	G (au)	E+G (au)
Product (9)	-805.7671874	0.292205	-805.474982

C	2.213544000	-2.019074000	-0.834330000
C	2.719587000	-0.573040000	-0.830026000
O	1.156606000	-2.275887000	0.054936000
N	3.189587000	-0.029045000	0.527459000
C	2.008477000	0.297181000	1.419589000
C	4.076148000	-1.012070000	1.228427000
C	3.952582000	1.245993000	0.267642000
O	-0.407575000	-0.403253000	-0.883619000
H	1.925632000	-2.208386000	-1.881078000
H	3.020477000	-2.723354000	-0.599187000
H	3.583567000	-0.491562000	-1.497778000
H	1.934546000	0.107191000	-1.164551000
H	0.757023000	2.343938000	-0.902608000
H	2.401097000	0.749181000	2.333078000
H	1.342388000	0.988565000	0.898816000
H	1.481019000	-0.629926000	1.631163000
H	3.492890000	-1.893793000	1.490592000
H	4.901488000	-1.285282000	0.568290000
H	4.467429000	-0.543201000	2.132876000
H	4.850088000	1.003532000	-0.304827000
H	3.303913000	1.925094000	-0.295232000
H	4.232908000	1.681271000	1.228894000
C	-1.113412000	0.548321000	-0.407481000
N	-0.620582000	1.757573000	-0.203505000
H	-1.329021000	2.410093000	0.122305000
C	-2.563297000	0.222513000	-0.084855000
C	-3.157887000	-0.885657000	-0.706947000

C	-3.331435000	0.973223000	0.818705000
C	-4.488440000	-1.222109000	-0.451391000
C	-4.659051000	0.631539000	1.087641000
C	-5.244807000	-0.464784000	0.448249000
H	-2.553826000	-1.472242000	-1.390770000
H	-2.889097000	1.819734000	1.336861000
H	-4.934811000	-2.077725000	-0.951202000
H	-5.233945000	1.218871000	1.798665000
H	-6.278648000	-0.728771000	0.653477000
O	1.652168000	2.664738000	-1.277080000
H	0.401140000	-1.684796000	-0.223693000
H	1.459060000	3.054856000	-2.137009000

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