Supporting Information

Chemoselective synthesis of *N*-aroylureas and imides *via* selective amidation of Boc and amide groups of *N*-R-*N*-Boc arylamides

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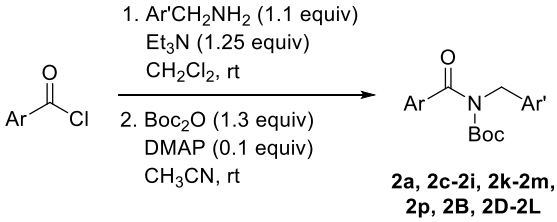
General Information

All reactions were conducted under an atmosphere of dry nitrogen with oven-dried glassware or vacuum line techniques. All anhydrous solvents were purchased from Sigma-Aldrich and directly used without further purification. Unless otherwise stated, reagents were commercially available and used as purchased without further purification. Chemicals were purchased from Sigma-Aldrich, TCI China, Acros, Alfa Aesar or J&K.

Progress of reactions was monitored by thin-layer chromatography using TLC plates and visualized by short-wave ultraviolet light. Flash chromatography was performed with Qingdao Haiyang flash silica gel (200–300 mesh). The NMR spectra were obtained using a Bruker AVANCE III 500 MHz spectrometer with TMS as the internal standard. The infrared spectra were obtained with KBr plates by using an FTIR650 FT-IR Spectrometer. High resolution mass spectrometry (HRMS) data were obtained on an Agilent Q-TOF 1290 LC/6224 MS system using electrospray ionization (ESI) in positive or negative mode. Melting points were determined on a Thermal Values analytical microscope and were uncorrected.

Synthesis of Starting material

General Procedure A



2a, 2c-2i, 2k-2m, 2p, 2B, 2D-2L

N-R-*N*-Boc arylamides **2a**, **2c-2i**, **2k-2m**, **2p**, **2b'**, **2d'-2l'** used in this study have been prepared according to the literature procedures.[1] Arylmethylamine (11 mmol, 1.1 equiv) and Et_3N (1.730 mL, 12.5 mmol, 1.25 equiv) was added dropwise to arylformyl chloride (10 mmol, 1.0 equiv) in CH_2Cl_2 (15 mL) successively under nitrogen atmosphere, and the reaction was left to stir at room temperature for 2 h. Reaction mixture was extracted with EtOAc (3 × 25 mL), and the combined organic extracts were washed successively with 1.0 M HCl (70 mL) and brine (70 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The resulting crude solid material was used in the subsequent step without further purification.

To a flask containing the crude material from the previous step was added DMAP (122.2 mg, 1 mmol, 0.1 equiv) in anhydrous CH_3CN (10 mL) under nitrogen atmosphere. Boc_2O (2.70 g, 13 mmol, 1.3 equiv) was added in one portion and the reaction was allowed to stir at room temperature for 16 h. The reaction

was quenched by addition of 20 mL saturated aqueous $NaHCO_3$ and extracted with EtOAc (3 × 25 mL). The combined organic extracts were dried over Na_2SO_4, filtered and concentrated. The crude material was loaded onto a silica gel column and purified by flash chromatography.

Compounds **1a**-**1n**, **1f'**, **1n'**, **2b**, **2j**, **2n**, **2o** and **2c'** were commercially available. The NMR data for other amides are given in the section below.

Synthesis of *N*-aroylureas

General Procedure B

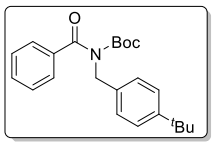
An oven-dried 10 mL vial equipped with a stir bar was charged with *N*-R-*N*-Boc benzamides **2** (0.1 mmol, 1.0 equiv) and KO^{t}Bu (33.7 mg, 0.3 mmol, 3.0 equiv) under a nitrogen atmosphere. A solution of benzamide (12.1 mg, 0.1 mmol, 1.0 equiv) in 1 mL of dry DME was added to the reaction by syringe at room temperature. The colorless mixture turned to white suspension. The vial was capped, removed from the glovebox, and stirred for 12 h at 100 °C in an oil bath. After cooling to room temperature, the reaction mixture was quenched with three drops of H_2O, passed through a short pad of silica gel and eluted with ethyl acetate (1 mL × 3). The combined organic solution was concentrated under reduced pressure. The crude material was loaded onto a silica gel column and purified by flash chromatography.

Synthesis of imides

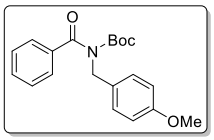
General Procedure C

An oven-dried 10 mL vial equipped with a stir bar was charged with *N*-Bn-*N*-Boc arylamides (0.1 mmol, 1.0 equiv) and LiOH (7.2 mg, 0.3 mmol, 3.0 equiv) under a nitrogen atmosphere. A solution of benzamide (12.1 mg, 0.1 mmol, 1.0 equiv) in 1 mL of dry DME was added to the reaction by syringe at room temperature. The mixture turned to colorless. The vial was capped, removed from the glovebox, and stirred for 12 h at 100 °C in an oil bath. After cooling to room temperature, the reaction mixture was quenched with three drops of H_2O, passed through a short pad of silica gel and eluted with ethyl acetate (1 mL × 3). The combined organic solution was concentrated under reduced pressure. The crude material was loaded onto a silica gel column and purified by flash chromatography.

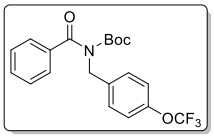
Characterization Data for Starting Materials



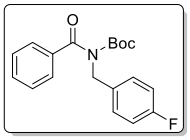
***tert*-Butyl benzoyl(4-(*tert*-butyl)benzyl)carbamate (2a).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 4-*tert*-butylbenzylamine (1.937 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.94 g, 80% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.54 – 7.49 (m, 2H), 7.49 – 7.43 (m, 1H), 7.41 – 7.37 (m, 2H), 7.37 – 7.33 (m, 4H), 4.96 (s, 2H), 1.31 (s, 9H), 1.13 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 173.2, 153.7, 150.3, 138.0, 134.9, 131.1, 128.2, 128.0, 127.6, 125.5, 83.2, 48.7, 34.6, 31.5, 27.5; IR (thin film): 2964, 1731, 1677, 1368, 1229, 1144, 853, 725, 697 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{23}H_{29}NNaO_3$ 390.2040; found 390.2036.



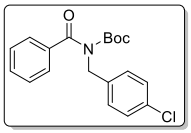
***tert*-Butyl benzoyl(4-methoxybenzyl)carbamate (2c).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 4-Methoxybenzylamine (1.437 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 8:1) to give the product (2.32 g, 68% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.50 – 7.47 (m, 2H), 7.47 – 7.43 (m, 1H), 7.42 – 7.33 (m, 4H), 6.90 – 6.82 (m, 2H), 4.92 (s, 2H), 3.79 (s, 3H), 1.12 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.2, 159.0, 153.6, 137.9, 131.1, 130.1, 129.9, 128.1, 127.5, 113.9, 83.1, 55.3, 48.4, 27.4. The NMR spectral data match the previously published data.[2]



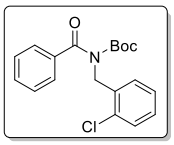
***tert*-Butyl benzoyl(4-(trifluoromethoxy)benzyl)carbamate (2d).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), [4-(trifluoromethoxy)phenyl]methanamine (1.679 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 8:1) to give the product (2.13 g, 54% yield) as a colorless liquid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.54 – 7.44 (m, 5H), 7.42 – 7.36 (m, 2H), 7.35 – 7.13 (m, 2H), 4.98 (s, 2H), 1.12 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 173.2, 153.4, 148.7 (q, $J^2_{C\text{-}F}$ = 1.3 Hz), 137.6, 136.7, 131.3, 129.9, 128.2, 127.6, 120.6 (q, $J^1_{C\text{-}F}$ = 257.0 Hz), 121.1, 83.2, 48.2, 27.4; IR (thin film): 2980, 2934, 1732, 1674, 1368, 1344, 1256, 1159, 851, 696 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{20}H_{20}F_3NNaO_4$ 418.1237; found 418.1220.



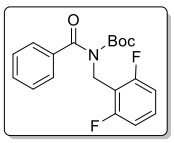
***tert*-Butyl benzoyl(4-fluorobenzyl)carbamate (2e).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 4-fluorobenzylamine (1.250 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.53 g, 77% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.51 – 7.48 (m, 2H), 7.47 – 7.41 (m, 3H), 7.40 – 7.36 (m, 2H), 7.05 – 6.98 (m, 2H), 4.95 (s, 2H), 1.12 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 173.2, 162.3 (d, $J^1_{C\text{-}F}$ = 245.5 Hz), 153.5, 137.8, 133.8 (d, $J^4_{C\text{-}F}$ = 3.2 Hz), 131.2, 130.3 (d, $J^3_{C\text{-}F}$ = 8.1 Hz), 128.2, 127.5, 115.4 (d, $J^2_{C\text{-}F}$ = 21.4 Hz), 83.4, 48.3, 27.4; IR (thin film): 2980, 2935, 1731, 1674, 1369, 1344, 1227, 1142, 852 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{19}H_{20}FNNaO_3$ 352.1319; found 352.1333.



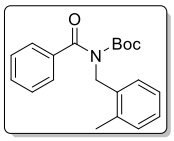
***tert*-Butyl benzoyl(4-chlorobenzyl)carbamate (2f).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 4-chlorobenzylamine (1.335 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.59 g, 75% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.52 – 7.48 (m, 2H), 7.48 – 7.44 (m, 1H), 7.41 – 7.36 (m, 4H), 7.34 – 7.27 (m, 2H), 4.94 (s, 2H), 1.12 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 173.1, 153.4, 137.7, 136.5, 133.4, 131.3, 129.9, 128.7, 128.2, 127.5, 83.5, 48.3, 27.4; IR (thin film): 2979, 1731, 1673, 1369, 1229, 1142, 792, 728, 697 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{19}H_{20}ClNNaO_3$ 368.1024; found 368.1021.



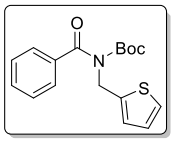
***tert*-Butyl benzoyl(2-chlorobenzyl)carbamate (2g).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 2-chlorobenzylamine (1.331 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.45 g, 71% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.57 – 7.67 (m, 2H), 7.52 – 7.47 (m, 1H), 7.44 – 7.40 (m, 2H), 7.39 – 7.35 (m, 1H), 7.35 – 7.32 (m, 1H), 7.27 – 7.23 (m, 1H), 7.22 – 7.19 (m, 1H), 5.12 (s, 2H), 1.14 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 173.2, 153.3, 137.4, 135.3, 133.1, 131.4, 129.6, 128.5, 128.2, 128.2, 127.7, 126.9, 83.5, 46.9, 27.5; IR (thin film): 2979, 2932, 1737, 1679, 1369, 1231, 1148, 750, 696 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{19}H_{20}ClNNaO_3$ 368.1024; found 368.1009.



***tert*-Butyl benzoyl(2,6-difluorobenzyl)carbamate (2h).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 2,6-difluorobenzylamine (1.315 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.26 g, 65% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.55 – 7.49 (m, 2H), 7.48 – 7.42 (m, 1H), 7.40 – 7.33 (m, 2H), 7.27 – 7.17 (m, 1H), 6.92 – 6.85 (m, 2H), 5.12 (s, 2H), 1.14 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.9, 161.7 (dd, $J^1_{C(Ar)-F}$ = 249.6, 8.1 Hz), 153.2, 137.6, 131.2, 129.2 (t, $J^3_{C(Ar)-F}$ = 10.5 Hz), 128.1, 127.7, 113.9 (t, $J^2_{C(Ar)-F}$ = 17.8 Hz), 111.5 (dd, $J^2_{C(Ar)-F}$ = 20.2, 5.7 Hz), 83.4, 37.8 (dd, J^3_{C-F} = 20.2, 5.7 Hz), 27.4; IR (thin film): 2980, 1730, 1691, 1626, 1594, 1471, 1333, 783, 697 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{19}H_{19}F_2NaNO_3$ 370.1225; found 370.1223.

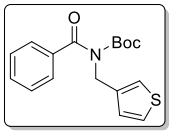


***tert*-Butyl benzoyl(2-methylbenzyl)carbamate (2i).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 2-methylbenzylamine (1.364 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.18 g, 67% yield) as a white solid. °C; ^1H NMR (500 MHz, $CDCl_3$): δ 7.62 – 7.57 (m, 2H), 7.51 – 7.47 (m, 1H), 7.44 – 7.39 (m, 2H), 7.38 – 7.28 (m, 1H), 7.23 – 7.15 (m, 3H), 5.04 (s, 2H), 2.44 (s, 3H), 1.15 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 173.1, 153.6, 137.7, 135.8, 135.6, 131.2, 130.3, 128.1, 127.6, 127.1, 126.7, 126.1, 83.2, 46.4, 27.4, 19.3; IR (thin film): 2978, 1731, 1674, 1339, 1232, 1148, 741, 724, 696 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{20}H_{23}NNaO_3$ 348.1570; found 348.1572.

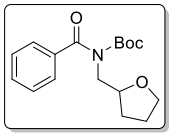


***tert*-Butyl benzoyl(thiophen-2-ylmethyl)carbamate (2k).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 2-thiophenemethylamine (1.127 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (1.99 g, 63% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.53 – 7.42 (m, 3H), 7.41 – 7.34 (m, 2H), 7.28 – 7.17 (m, 1H), 7.18 – 7.08 (m, 1H), 7.00 – 6.90 (m, 1H), 5.14 (s, 2H), 1.17 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 172.9, 153.1, 139.8, 137.7, 131.2, 128.2, 127.6, 127.6, 126.6, 125.7, 83.6, 43.6, 27.5; IR (thin film): 2979, 1731, 1673, 1368, 1328, 1248, 1139, 726, 697 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{17}H_{19}NNaO_3S$ 340.0978; found

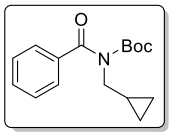
340.0973.



***tert*-Butyl benzoyl(thiophen-3-ylmethyl)carbamate (2l).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 3-thiophenemethylamine (1.24 g, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (1.90 g, 60% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.49 – 7.43 (m, 3H), 7.39 – 7.34 (m, 2H), 7.33 – 7.29 (m, 1H), 7.29 – 7.23 (m, 1H), 7.22 – 7.18 (m, 1H), 4.97 (s, 2H), 1.13 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 173.0, 153.4, 138.4, 137.9, 131.1, 128.2, 128.1, 127.5, 125.7, 123.7, 83.3, 44.0, 27.5; IR (thin film): 2978, 1731, 1673, 1368, 1335, 1240, 1137, 728, 696 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{17}H_{19}NNaO_3S$ 340.0978; found 340.0959.

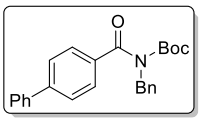


***tert*-Butyl benzoyl((tetrahydrofuran-2-yl)methyl)carbamate (2m).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), 2-tetrahydrofurfurylamine (1.147 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 15:1) to give the product (1.56 g, 51% yield) as a colorless liquid; ^1H NMR (500 MHz, $CDCl_3$): δ 7.59 – 7.52 (m, 2H), 7.46 – 7.44 (m, 1H), 7.40 – 7.29 (m, 2H), 4.31 (m, 1H), 4.05 – 3.95 (m, 1H), 3.76 – 3.66 (m, 3H), 2.10 – 1.75 (m, 3H), 1.70 – 1.60 (m, 1H), 1.08 (s, 9H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 173.5, 153.9, 138.1, 131.0, 128.1, 127.7, 82.9, 77.1, 67.7, 49.1, 29.1, 27.4, 25.6; IR (thin film): 2977, 2936, 1731, 1679, 1368, 1233, 1144, 726, 698 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{17}H_{23}NNaO_4$ 328.1519; found 328.1504.

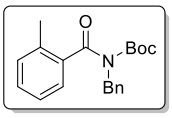


***tert*-Butyl benzoyl(cyclopropylmethyl)carbamate (2p).** The reaction was performed following General Procedure A with benzoyl chloride (1.160 mL, 10 mmol), cyclopropanemethylamine (0.943 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 30:1) to give the product (1.38 g, 50% yield) as a colorless liquid; ^1H NMR (500 MHz, $CDCl_3$): δ 7.55 – 7.49 (m, 2H), 7.48 – 7.42 (m, 1H), 7.41 – 7.33 (m, 2H), 3.68 (d, J = 7.2 Hz, 2H), 1.32 – 1.23 (m, 1H), 1.13 (s, 9H), 0.51 – 0.46 (m, 2H), 0.38 – 0.33 (m, 2H); $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 173.6, 153.9, 138.3, 130.9, 128.1, 127.4, 82.8, 50.2, 27.4, 10.7, 3.6; IR (thin film): 2979, 2935, 1729, 1678, 1358, 1241, 1140, 725, 697 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{16}H_{21}NO_3$ 298.1414;

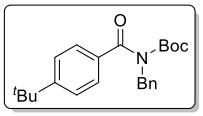
found 298.1418.



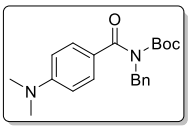
***tert*-Butyl ([1,1'-biphenyl]-4-carbonyl)(benzyl)carbamate (2b').** The reaction was performed following General Procedure A with 4-biphenylcarbonyl chloride (2.17 g, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.90 g, 75% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.64 – 7.58 (m, 6H), 7.48 – 7.41 (m, 4H), 7.41 – 7.36 (m, 1H), 7.36 – 7.32 (m, 2H), 7.30 – 7.32 (m, 1H), 5.01 (s, 2H), 1.16 (s, 9H). The NMR spectral data match the previously published data.[3]



***tert*-Butyl benzyl(2-methylbenzoyl)carbamate (2d').** The reaction was performed following General Procedure A with 2-toluoyl chloride (1.305 mL, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.05 g, 63% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.52 – 7.43 (m, 2H), 7.41 – 7.33 (m, 2H), 7.32 – 7.26 (m, 2H), 7.21 – 7.11 (m, 3H), 5.05 (s, 2H), 2.34 (s, 3H), 1.10 (s, 9H). The NMR spectral data match the previously published data.[1]

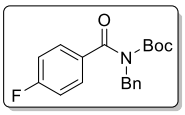


***tert*-Butyl benzyl(4-(*tert*-butyl)benzoyl)carbamate (2e').** The reaction was performed following General Procedure A with 4-*tert*-butylbenzoyl chloride (1.989 mL, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.61 g, 71% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.49 – 7.44 (m, 2H), 7.44 – 7.42 (m, 2H), 7.41 – 7.37 (m, 2H), 7.36 – 7.28 (m, 2H), 7.28 – 7.22 (m, 1H), 4.98 (s, 2H), 1.32 (s, 9H), 1.11 (s, 9H). The NMR spectral data match the previously published data.[3]

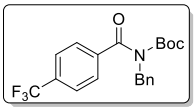


***tert*-Butyl benzyl(4-(dimethylamino)benzoyl)carbamate (2f').** The reaction was performed following General Procedure A with 4-dimethylaminobenzoylchloride (1.539 mL, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 8:1) to give the product (2.30 g, 65% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.56 – 7.49 (m, 2H), 7.44 – 7.39 (m, 2H), 7.35 – 7.27 (m, 2H), 7.26 – 7.21 (m, 1H), 6.65 – 6.58 (m, 2H), 4.94 (s, 2H), 3.01 (s, 6H), 1.22 (s, 9H). The NMR spectral data match the previously

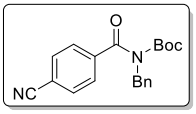
published data.[1]



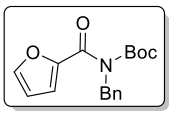
***tert*-Butyl benzyl(4-fluorobenzoyl)carbamate (2g').** The reaction was performed following General Procedure A with 4-fluorobenozyl chloride (1.117 mL, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 20:1) to give the product (2.47 g, 75% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.58 – 7.52 (m, 2H), 7.46 – 7.39 (m, 2H), 7.37 – 7.31 (m, 2H), 7.30 – 7.26 (m, 1H), 7.11 – 7.05 (m, 2H), 4.98 (s, 2H), 1.18 (s, 9H). The NMR spectral data match the previously published data.[3]



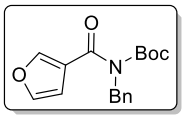
***tert*-Butyl benzyl(4-(trifluoromethyl)benzoyl)carbamate (2h').** The reaction was performed following General Procedure A with 4-(trifluoromethyl)benzoyl chloride (1.105 mL, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 24:1) to give the product (2.65 g, 70% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.54 – 7.49 (m, 2H), 7.49 – 7.43 (m, 1H), 7.41 – 7.37 (m, 2H), 7.37 – 7.33 (m, 4H), 4.96 (s, 2H), 1.31 (s, 9H), 1.13 (s, 9H). The NMR spectral data match the previously published data.[1]



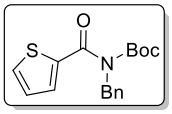
***tert*-Butyl benzyl(4-cyanobenzoyl)carbamate (2i').** The reaction was performed following General Procedure A with 4-cyanobenzoyl chloride (1.66 g, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (2.18 g, 65% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.72 – 7.65 (m, 2H), 7.61 – 7.54 (m, 2H), 7.43 – 7.37 (m, 2H), 7.37 – 7.31 (m, 2H), 7.31 – 7.25 (m, 1H), 4.99 (s, 2H), 1.17 (s, 9H). The NMR spectral data match the previously published data.[4]



***tert*-Butyl benzyl(furan-2-carbonyl)carbamate (2j').** The reaction was performed following General Procedure A with 2-furoyl chloride (0.986 mL, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 24:1) to give the product (1.67 g, 56% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.49 (m, 1H), 7.43 – 7.36 (m, 2H), 7.34 – 7.29 (m, 2H), 7.28 – 7.20 (m, 1H), 7.14 – 7.04 (m, 1H), 6.51 (m, 1H), 4.92 (s, 2H), 1.29 (s, 9H). The NMR spectral data match the previously published data.[3]

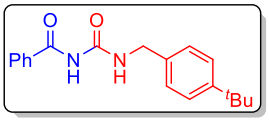


***tert*-Butyl benzyl(furan-3-carbonyl)carbamate (2k').** The reaction was performed following General Procedure A with 3-furoyl chloride (1.31 g, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 24:1) to give the product (1.66 g, 55% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.93 – 7.85 (m, 1H), 7.41 – 7.37 (m, 1H), 7.37 – 7.29 (m, 4H), 7.25 (s, 1H), 6.60 – 6.52 (m, 1H), 4.92 (s, 2H), 1.31 (s, 9H). The NMR spectral data match the previously published data.[1]

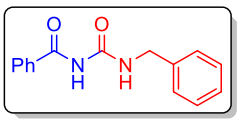


***tert*-Butyl benzyl(thiophene-2-carbonyl)carbamate (2l').** The reaction was performed following General Procedure A with 2-thiophenecarbonyl chloride (1.47 g, 10 mmol), benzylamine (1.202 mL, 11 mmol) and Boc_2O (2.70 g, 13 mmol, 1.3 equiv). The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (1.62 g, 51% yield) as a white solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.60 – 7.54 (m, 2H), 7.54 – 7.50 (m, 2H), 7.36 – 7.31 (m, 2H), 7.27 – 7.24 (m, 1H), 7.22 – 7.16 (m, 1H), 4.92 (s, 2H), 1.06 (s, 9H). The NMR spectral data match the previously published data.[3]

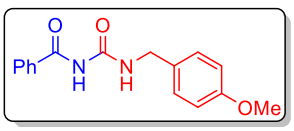
Characterization Data for *N*-aroylureas



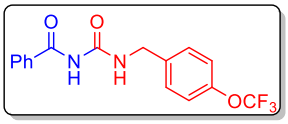
***N*-((4-(*tert*-butyl)benzyl)carbamoyl)benzamide (3aa).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol) and *tert*-butyl benzoyl(4-(*tert*-butyl)benzyl)carbamate **2a** (36.7 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (22.3 mg, 72% yield) as a white solid. mp: 128−130 °C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.77 (s, 1H), 9.04 (t, J = 5.9 Hz, 1H), 8.00 – 7.93 (m, 2H), 7.61 (t, J = 7.0 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.40 – 7.32 (m, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.41 (d, J = 5.9 Hz, 2H), 1.27 (s, 9H); ^{13}C NMR (126 MHz, DMSO-d$_6$) δ 168.3, 153.6, 149.4, 136.2, 132.8, 132.6, 128.5, 128.1, 127.1, 125.2, 42.4, 34.2, 31.2; IR (thin film): 3276, 2961, 1694, 1660, 1600, 1508, 1331, 1270, 850, 702 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{19}H_{22}N_2NaO_2$ 333.1573; found 333.1570.



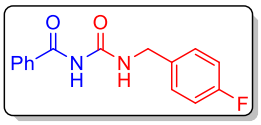
***N*-(benzylcarbamoyl)benzamide (3ab).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (13.2 mg, 52% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.75 (s, 1H), 9.05 (t, J = 6.0 Hz, 1H), 7.93 (dd, J = 8.0, 1.0 Hz, 2H), 7.60 – 7.57 (m, 1H), 7.49 – 7.45 (m, 2H), 7.32 – 7.30 (m, 4H), 7.24 – 7.21 (m, 1H), 4.42 (d, J = 6.0 Hz, 2H). The NMR spectral data match the previously published data.[5]



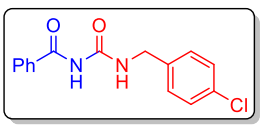
***N*-((4-methoxybenzyl)carbamoyl)benzamide (3ac).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(4-methoxybenzyl)carbamate **2c** (34.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (17.3 mg, 61% yield) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.38 (s, 1H), 9.00 (t, J = 6.0 Hz, 1H), 7.88 – 7.87 (m, 2H), 7.52 – 7.49 (m, 1H), 7.40 – 7.38 (m, 2H), 7.21 – 7.20 (m, 2H), 6.81 – 6.79 (m, 2H), 4.43 (d, J = 6.0 Hz, 2H), 3.73 (s, 3H). The NMR spectral data match the previously published data.[6]



***N*-((4-(trifluoromethoxy)benzyl)carbamoyl)benzamide (3ad).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(4-(trifluoromethoxy)benzyl)carbamate **2d** (39.5 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (18.6 mg, 55% yield) as a white solid. mp: 174−176 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.77 (s, 1H), 9.12 (t, J = 6.0 Hz, 1H), 7.95 – 7.93 (m, 2H), 7.61 – 7.58 (m, 1H), 7.49 – 7.42 (m, 4H), 7.31 (d, J = 8.0 Hz, 2H), 4.44 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 168.3, 153.8, 147.3, 139.0, 132.8, 132.6, 129.1, 128.5, 128.2, 121.1, 42.1, one resonance was not observed due to coincidental overlap; IR (thin film): 3296, 2944, 1697, 1666, 1508, 1307, 1274, 850, 699 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{16}H_{13}F_3N_2NaO_3$ 361.0770; found 361.0774.

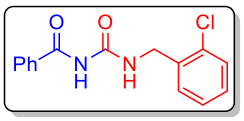


***N*-((4-fluorobenzyl)carbamoyl)benzamide (3ae).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(4-fluorobenzyl)carbamate **2e** (32.9 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (14.1 mg, 52% yield) as a white solid. mp: 115−117 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.75 (s, 1H), 9.05 (t, J = 6.0 Hz ,1H), 7.94 – 7.92 (m, 2H), 7.59 – 7.56 (m, 1H), 7.48 – 7.45 (m, 2H), 7.36 – 7.33 (m, 2H), 7.15 – 7.11 (m, 2H), 4.41 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 168.3, 161.3 (d, $J^1_{C(Ar)\text{-}F}$ = 242.3 Hz), 153.7, 135.6 (d, $J^4_{C(Ar)\text{-}F}$ = 3.0 Hz), 132.8, 132.6, 129.4 (d, $J^3_{C(Ar)\text{-}F}$ = 8.1 Hz), 128.5, 128.2, 115.1 (d, $J^2_{C(Ar)\text{-}F}$ = 21.3 Hz), 42.1; IR (thin film): 3297, 2943, 1691, 1666, 1542, 1274, 836, 703 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{15}H_{13}FN_2NaO_2$ 295.0853; found 295.0846.

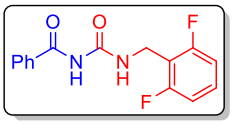


***N*-((4-chlorobenzyl)carbamoyl)benzamide (3af).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(4-chlorobenzyl)carbamate **2f** (34.5 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (15.8 mg, 55% yield) as a white solid. mp: 169−172 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ

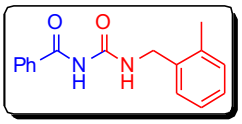
10.75 (s, 1H), 9.07 (t, J = 6.0 Hz, 1H), 7.92 (d, J = 8.0 Hz, 2H), 7.58 (t, J = 7.5 Hz, 1H), 7.46 (t, J = 7.5 Hz, 2H), 7.37 – 7.31 (m, 4H), 4.40 (d, J = 6.0 Hz, 2H); $^{13}C\{^1H\}$ NMR (125 MHz, DMSO-d_6): δ 168.3, 153.7, 138.5, 132.8, 132.6, 131.5, 129.2, 128.5, 128.4, 128.2, 42.1; IR (thin film): 3298, 2924, 1694, 1665, 1538, 1272, 797, 694 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{15}H_{13}ClN_2NaO_2$ 311.0558; found 311.0565.



***N*-((2-chlorobenzyl)carbamoyl)benzamide (3ag).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(2-chlorobenzyl)carbamate **2g** (34.5 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (17.6 mg, 61% yield) as a white solid. mp: 163−165 °C; ^1H NMR (500 MHz, DMSO-d_6): δ 10.81 (s, 1H), 9.12 (t, J = 6.0 Hz, 1H), 7.95 – 7.94 (m, 2H), 7.60 – 7.57 (m, 1H), 7.48 – 7.43 (m, 3H), 7.38 – 7.37 (m, 1H), 7.33 – 7.27 (m, 2H), 4.49 (d, J = 6.0 Hz, 2H); $^{13}C\{^1H\}$ NMR (125 MHz, DMSO-d_6): δ 168.5, 153.8, 136.2, 132.9, 132.6, 132.2, 129.3, 129.0, 128.96, 128.6, 128.3, 127.4, 40.9; IR (thin film): 3289, 2924, 1686, 1665, 1561, 1471, 1275, 756, 705 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{15}H_{13}ClN_2NaO_2$ 311.0558; found 311.0560.

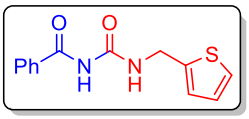


***N*-((2,6-difluorobenzyl)carbamoyl)benzamide (3ah).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(2,6-difluorobenzyl)carbamate **2h** (34.7 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (20.0 mg, 69% yield) as a white solid. mp: 183−185 °C; ^1H NMR (500 MHz, DMSO-d_6): δ 10.78 (s, 1H), 9.04 (t, J = 6.0 Hz, 1H), 7.91 – 9.89 (m, 2H), 7.59 – 7.56 (m, 1H), 7.47 – 7.44 (m, 2H), 7.41 – 7.36 (m, 1H), 7.11 – 7.08 (m, 2H), 4.51 (d, J = 6.0 Hz, 2H); $^{13}C\{^1H\}$ NMR (125 MHz, DMSO-d_6): δ 168.5, 161.3 (dd, J^1 = 247.4, 8.3 Hz), 153.3, 132.9, 132.4, 130.6 (t, J^4 = 10.5 Hz), 129.0, 128.6, 114.6 (t, J^3 = 19.3 Hz), 112.2 (dd, J^2 = 19.9, 5.6 Hz), 31.1; IR (thin film): 3315, 2969, 1698, 1668, 1537, 1471, 1267, 781, 708 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{15}H_{12}F_2N_2NaO_2$ 313.0759; found 313.0760.



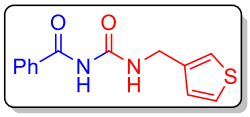
***N*-((2-methylbenzyl)carbamoyl)benzamide (3ai).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(2-methylbenzyl)carbamate **2i** (32.5 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (20.9 mg, 78% yield) as a white solid. mp: 128−130 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.78 (s, 1H), 8.94 (t, J = 6.0 Hz, 1H), 7.94 – 7.93 (m, 2H), 7.60 – 7.57 (m, 1H), 7.48 – 7.45 (m, 2H), 7.24 – 7.22 (m, 1H), 7.15 – 7.14 (m, 3H), 4.40 (d, J = 6.0 Hz, 2H), 2.28 (s, 3H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 168.4, 153.6, 136.8, 135.5, 132.8, 132.5, 130.1, 128.5, 128.2, 127.3, 127.1, 126.0, 40.9, 18.6; IR (thin film): 3311, 2922, 1683, 1554, 1269, 743, 709 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{16}H_{16}N_2NaO_2$ 291.1104; found 291.1109.

***N*-((furan-2-ylmethyl)carbamoyl)benzamide (3aj).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(furan-2-ylmethyl)carbamate **2i** (30.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (11.2 mg, 46% yield) as a white solid. mp: 133−135 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.99 (s, 1H), 9.16 (t, J = 5.7 Hz, 1H), 8.08 – 7.95 (m, 2H), 7.63 – 7.55 (m, 1H), 7.50 – 7.45 (m, 2H), 7.38 – 7.36 (m, 1H), 6.34 – 6.30 (m, 1H), 6.27 – 6.23 (m, 1H), 4.56 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 168.3, 154.4, 151.2, 142.5, 133.3, 132.4, 129.0, 127.9, 110.5, 107.6, 37.0; IR (thin film): 3308, 2925, 1689, 1666, 1600, 1504, 1270, 700 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{13}H_{12}N_2NaO_3$ 267.0740; found 267.0747.

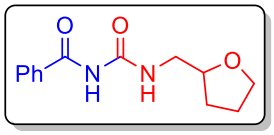


***N*-((thiophen-2-ylmethyl)carbamoyl)benzamide (3ak).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(thiophen-2-ylmethyl)carbamate **2k** (31.7 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (13.8 mg, 53% yield) as a white solid. mp: 153−155 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.77 (s, 1H), 9.06 (t, J = 6.0 Hz, 1H), 7.91 (dd, J = 8.5, 1.0 Hz, 2H), 7.59 – 7.56 (m, 1H), 7.47 – 7.44 (m, 2H), 7.37 – 7.36 (m, 1H), 7.00 – 6.99 (m, 1H), 6.94 – 6.92 (m, 1H), 4.58 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H}

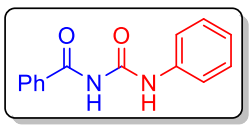
NMR (125 MHz, DMSO-d_6): δ 168.3, 153.5, 142.1, 132.8, 132.5, 128.5, 128.2, 126.8, 125.8, 125.3, 37.8; IR (thin film): 3226, 2920, 1702, 1690, 1541, 1268, 698 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{13}H_{12}N_2NaO_2S$ 283.0512; found 283.0520.



***N*-((thiophen-3-ylmethyl)carbamoyl)benzamide (3al).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(thiophen-3-ylmethyl)carbamate **2l** (31.7 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (11.4 mg, 44% yield) as a white solid. mp: 159−162 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.75 (s, 1H), 8.99 (t, J = 6.0 Hz, 1H), 7.94 – 7.92 (m, 2H), 7.60 – 7.57 (m, 1H), 7.49 – 7.45 (m, 3H), 7.36 (s, 1H), 7.09 – 7.07 (m, 1H), 4.42 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 168.3, 153.6, 140.0, 132.8, 132.6, 128.5, 128.2, 127.5, 126.6, 122.1, 38.3; IR (thin film): 3290, 2938, 1702, 1689, 1544, 1271, 702 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{13}H_{12}N_2NaO_2S$ 283.0512; found 283.0515.

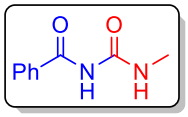


***N*-(((tetrahydrofuran-2-yl)methyl)carbamoyl)benzamide (3am).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl((tetrahydrofuran-2-yl)methyl)carbamate **2m** (30.5 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (20.6 mg, 83% yield) as a white solid. mp: 115−117 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.75 (s, 1H), 8.81 (t, J = 6.0 Hz, 1H), 7.97 – 7.96 (m, 2H), 7.64 – 7.61 (m, 1H), 7.53 – 7.50 (m, 2H), 3.97 – 3.93 (m, 1H), 3.82 – 3.77 (m, 1H), 3.68 – 3.63 (m, 1H), 3.43 – 3.39 (m, 1H), 3.26 – 3.24 (m, 1H), 1.97 – 1.90 (m, 1H), 1.87 – 1.79 (m, 2H), 1.58 – 1.51 (m, 1H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 168.4, 153.7, 132.8, 132.6, 128.5, 128.2, 77.0, 67.4, 43.1, 28.3, 25.4; IR (thin film): 3307, 2938, 1686, 1671, 1549, 1477, 1268, 719 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{13}H_{17}N_2O_3$ 271.1059; found 271.1028.

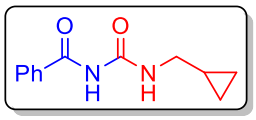


***N*-(phenylcarbamoyl)benzamide (3an).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(phenyl)carbamate **2n** (29.7 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (13.0 mg, 54%

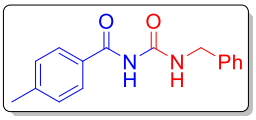
yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.02 (s, 1H), 10.82 (s, 1H), 8.01 – 7.99 (m, 2H), 7.65 – 7.62 (m, 1H), 7.58 – 7.49 (m, 4H), 7.36 – 7.32 (m, 2H), 7.11 – 7.07 (m, 1H). The NMR spectral data match the previously published data.[5]



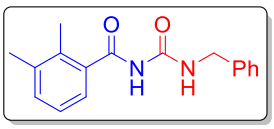
***N*-(methylcarbamoyl)benzamide (3ao).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(methyl)carbamate **2o** (23.5 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (9.6 mg, 54% yield) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.50 (s, 1H), 8.67 (s, 1H), 7.98 – 7.96 (m, 2H), 7.60 – 7.57 (m, 1H), 7.50 – 7.47 (m, 2H), 2.95 (d, J = 4.5 Hz, 3H). The NMR spectral data match the previously published data.[5]



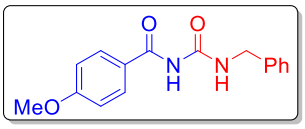
***N*-((cyclopropylmethyl)carbamoyl)benzamide (3ap).** The reaction was performed following General Procedure B with benzamide **1a** (12.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(cyclopropylmethyl)carbamate **2p** (27.5 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (16.4 mg, 75% yield) as a white solid. mp: 123−126 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.65 (s, 1H), 8.72 (t, J = 6.0 Hz, 1H), 7.92 – 7.91 (m, 2H), 7.58 – 7.56 (m, 1H), 7.48 – 7.45 (m, 2H), 3.07 (dd, J = 7.0, 6.0 Hz, 2H), 1.02 – 0.95 (m, 1H), 0.43 – 0.40 (m, 2H), 0.20 – 0.17 (m, 2H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 168.3, 153.5, 132.74, 132.72, 128.5, 128.1, 43.6, 11.0, 3.2; IR (thin film): 3321, 1694, 1667, 1273, 1026, 701 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{12}H_{14}N_2NaO_2$ 241.0947; found 241.0948.



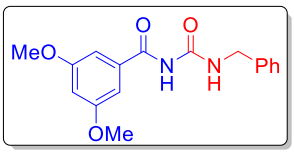
***N*-(benzylcarbamoyl)-4-methylbenzamide (3bb).** The reaction was performed following General Procedure B with 4-methylbenzamide **1b** (13.5 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (20.1 mg, 75% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.67 (s, 1H), 9.07 (t, J = 6.0 Hz, 1H), 7.86 – 7.84 (m, 2H), 7.33 – 7.26 (m, 6H), 7.24 – 7.21 (m, 1H), 4.42 (d, J = 6.0 Hz, 2H), 2.32 (s, 3H). The NMR spectral data match the previously published data.[6]



***N*-(benzylcarbamoyl)-2,3-dimethylbenzamide (3cb).** The reaction was performed following General Procedure B with 2,3-dimethylbenzamide **1c** (14.9 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (14.1 mg, 50% yield) as a white solid. mp: 164−167 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.85 (s, 1H), 8.67 (t, J = 6.0 Hz, 1H), 7.29 – 7.24 (m, 4H), 7.23 – 7.18 (m, 3H), 7.06 – 7.03 (m, 1H), 4.42 (d, J = 6.0 Hz, 2H), 2.25 (s, 3H), 2.22 (s, 3H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 171.5, 153.9, 138.5, 138.2, 135.1, 134.75, 132.8, 128.8, 127.9, 127.6, 125.7, 124.8, 43.9, 20.4, 16.5; IR (thin film): 3268, 2935, 1712, 1667, 1549, 1300, 745, 700 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{17}H_{18}N_2NaO_2$ 305.1260; found 305.1267.

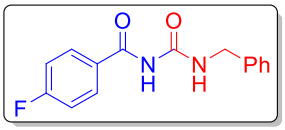


***N*-(benzylcarbamoyl)-4-methoxybenzamide (3db).** The reaction was performed following General Procedure B with 4-methoxybenzamide **1d** (15.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (25.0 mg, 88% yield) as a white solid. mp: 176−178 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.61 (s, 1H), 9.12 (t, J = 6.0 Hz, 1H), 7.99 – 7.97 (m, 2H), 7.35 – 7.30 (m, 4H), 7.26 – 7.24 (m, 1H), 7.03 – 7.01 (m, 2H), 4.43 (d, J = 6.0 Hz, 2H), 3.82 (s, 3H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 167.5, 162.9, 153.9, 139.3, 130.3, 128.4, 127.2, 126.9, 124.4, 113.8, 55.5, 42.7; IR (thin film): 3224, 2930, 1710, 1655, 1543, 1311, 844, 702 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{16}H_{16}N_2NaO_3$ 307.1053; found 307.1060.

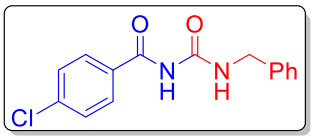


***N*-(benzylcarbamoyl)-3,5-dimethoxybenzamide (3eb).** The reaction was performed following General Procedure B with 3,5-dimethoxybenzamide **1e** (18.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (17.9 mg, 57% yield) as a white solid. mp: 131−132 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.80 (s, 1H), 9.09 (t, J = 6.0 Hz, 1H), 7.26 – 7.25 (m, 4H), 7.22 – 7.18 (m, 1H), 7.06 – 7.05 (m, 2H), 6.56 – 7.55 (m, 1H), 4.49 (d, J = 6.0 Hz, 2H), 3.71 (s, 6H); ^{13}C{^{1}H} NMR (125

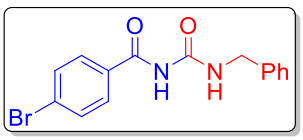
MHz, $CDCl_3$): δ 168.4, 161.1, 138.1, 134.5, 128.8, 127.7, 127.6, 105.8, 105.5, 55.7, 43.9, one resonance was not observed due to coincidental overlap; IR (thin film): 3283, 2936, 1691, 1663, 1530, 1308, 768, 699 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{17}H_{18}N_2NaO_4$ 337.1159; found 337.1154.



***N*-(benzylcarbamoyl)-4-fluorobenzamide (3fb).** The reaction was performed following General Procedure B with 4-fluorobenzamide **1f** (13.9 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (22.0 mg, 81% yield) as a white solid. mp: 163−164 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.79 (s, 1H), 9.02 (t, J = 6.0 Hz, 1H), 8.03 – 8.00 (m, 2H), 7.32 – 7.28 (m, 6H), 7.24 – 7.20 (m, 1H), 4.42 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 167.2, 164.8 (d, J^1 = 250.9 Hz) , 153.6, 139.2, 131.1 (d, J^3 = 9.4 Hz), 129.1 (d, J^4 = 2.8 Hz), 128.5, 127.3, 127.0, 115.6 (d, J^2 = 22.0 Hz), 42.8; IR (thin film): 3291, 2925, 1689, 1659, 1545, 1475, 1238, 765, 701 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{15}H_{13}FN_2NaO_2$ 295.0853; found 295.0823.

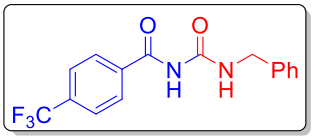


***N*-(benzylcarbamoyl)-4-chlorobenzamide (3gb).** The reaction was performed following General Procedure B with 4-chlorobenzamide **1g** (15.5 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (21.3 mg, 74% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.00 (s, 1H), 8.94 (t, J = 6.0 Hz, 1H), 8.05 – 8.04 (m, 2H), 7.96 – 7.94 (m, 2H), 7.33 – 7.29 (m, 4H), 7.25 – 7.21 (m, 1H), 4.42 (d, J = 6.0 Hz, 2H) . The NMR spectral data match the previously published data.[6]

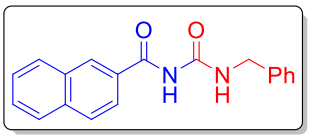


***N*-(benzylcarbamoyl)-4-bromobenzamide (3hb).** The reaction was performed following General Procedure B with 4-bromobenzamide **1h** (18.9 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (18.9 mg, 57% yield) as a white solid. mp: 198−201 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.84 (s, 1H), 8.99 (t, J = 6.0 Hz, 1H), 7.87 – 7.86 (m, 2H), 7.70 – 7.68 (m, 2H), 7.34 – 7.29 (m, 4H), 7.25 – 7.22 (m, 1H), 4.42 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 167.5, 153.6,

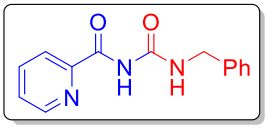
139.2, 131.8, 131.6, 130.3, 128.4, 127.3, 127.0, 126.7, 42.8; IR (thin film): 3286, 2933, 1692, 1661, 1547, 1270, 747, 698, 599 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{15}H_{13}BrN_2NaO_2$ 355.0053; found 355.0064.



***N*-(benzylcarbamoyl)-4-(trifluoromethyl)benzamide (3ib).** The reaction was performed following General Procedure B with 4-(trifluoromethyl)benzamide **1i** (18.9 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (18.0 mg, 56% yield) as a white solid. mp: 107−110 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.01 (s, 1H), 8.99 (t, J = 6.0 Hz, 1H), 8.12 – 8.11 (m, 2H), 7.87 – 7.85 (m, 2H), 7.33 – 7.32 (m, 4H), 7.27 – 7.22 (m, 1H), 4.44 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 167.4, 153.5, 139.2, 136.6, 132.3 (q, $J^2_{C(Ar)-F}$ = 32.0 Hz), 129.2, 128.5, 127.4, 127.1, 125.5 (q, $J^3_{C(Ar)-F}$ = 3.7 Hz), 123.8 (q, J^1_{C-F} =272.6 Hz), 42.9; IR (thin film): 3315, 2929, 1693, 1673, 1546, 1296, 724 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{16}H_{13}F_3N_2NaO_2$ 345.0821; found 345.0830.

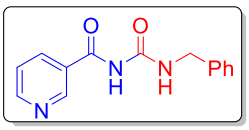


***N*-(benzylcarbamoyl)-2-naphthamide (3jb).** The reaction was performed following General Procedure B with 2-naphthamide **1j** (17.1 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (25.8 mg, 85% yield) as a white solid. mp: 162−164 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.89 (s, 1H), 9.10 (t, J = 6.0 Hz, 1H), 8.63 (s, 1H), 8.02 – 7.94 (m, 4H), 7.65 – 7.57 (m, 2H), 7.33 – 7.31 (m, 4H), 7.26 – 7.21 (m, 1H), 4.45 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 168.5, 153.8, 139.3, 134.8, 131.9, 129.9, 129.4, 128.6, 128.5, 128.2, 127.7, 127.3, 127.10, 127.07, 124.3, 42.8, one resonance was not observed due to coincidental overlap; IR (thin film): 3294, 2928, 1686, 1664, 1560, 1293, 775, 698 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{19}H_{16}N_2NaO_2$ 327.1104; found 327.1116.

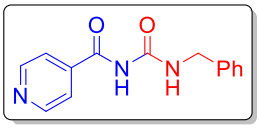


***N*-(benzylcarbamoyl)picolinamide (3kb).** The reaction was performed following General Procedure B with picolinamide **1k** (12.2 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by

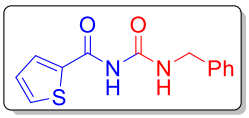
flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (12.8 mg, 50% yield) as a white solid. mp: 180−183 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.82 (s, 1H), 9.13 (t, J = 6.0 Hz, 1H), 8.64 – 8.62 (m, 2H), 7.81 –7.79 (m, 2H), 7.32 – 7.19 (m, 5H), 4.50 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 167.0, 154.9, 153.4, 150.6, 139.5, 137.7, 128.8, 128.4, 127.7, 127.2, 121.6, 43.9; IR (thin film): 3293, 3030, 2922, 1686, 1665, 1560, 1508, 1283, 760, 695 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{14}H_{13}N_3NaO_2$ 278.0900; found 278.0910.



***N*-(benzylcarbamoyl)nicotinamide (3lb).** The reaction was performed following General Procedure B with nicotinamide **1l** (12.2 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (14.8 mg, 58% yield) as a white solid. mp: 163−165 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.80 (s, 1H), 9.19 (s, 1H), 9.14 (t, J = 6.0 Hz, 1H), 8.72 – 8.70 (m, 1H), 8.28 – 8.26 (m, 1H), 7.27–7.26 (m, 4H), 7.25 – 7.19 (m, 2H), 4.49 (d, J = 6.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 168.4, 154.5, 136.8, 133.40, 133.35, 132.4, 129.03, 128.96, 128.95, 127.9, 43.3, one resonance was not observed due to coincidental overlap; IR (thin film): 3295, 3032, 2920, 1687, 1666, 1561, 1508, 1280, 860, 759, 707, 693 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{14}H_{13}N_3NaO_2$ 278.0900; found 278.0909.

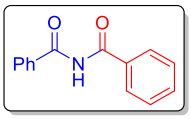


***N*-(benzylcarbamoyl)isonicotinamide (3mb).** The reaction was performed following General Procedure B with isonicotinamide **1m** (12.2 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (13.8 mg, 54% yield) as a white solid. mp: 154−156 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.03 (s, 1H), 8.74 (t, J = 6.0 Hz, 1H), 8.68 – 8.66 (m, 1H), 8.11 – 8.03 (m, 2H), 7.70 – 7.67 (m, 1H), 7.32 – 7.29 (m, 4H), 7.24 – 7.20(m, 1H), 4.41 (d, J = 6.0 Hz, 2H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 168.2, 154.4, 136.6, 133.3, 133.2, 133.21, 128.9, 128.8, 127.8, 43.2; IR (thin film): 3293, 3038, 2920, 1687, 1660, 1561, 1510, 1281, 860, 760, 710, 693 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{14}H_{13}N_3NaO_2$ 278.0900; found 278.0895.

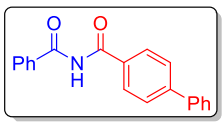


***N*-(benzylcarbamoyl)thiophene-2-carboxamide (3nb).** The reaction was performed following General Procedure B with thiophene-2-carboxamide **1n** (12.7 mg, 0.1 mmol), KO^{t}Bu (33.7 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C for 12 h. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 10:1) to give the product (19.5 mg, 75% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.85 (s, 1H), 8.89 (t, J = 6.0 Hz, 1H), 8.18 (dd, J = 4.0, 1.0 Hz, 1H), 7.94 (dd, J = 5.0, 1.0 Hz, 1H), 7.34 – 7.26 (m, 4H), 7.26 – 7.20 (m, 1H), 7.18 (dd, J = 5.0, 4.0 Hz, 1H), 4.41 (d, J = 6.0 Hz, 2H). The NMR spectral data match the previously published data.[6]

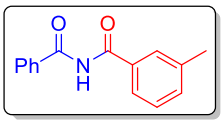
Characterization Data for Imides



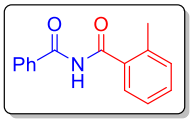
***N*-benzoylbenzamide (4ab).** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (16.7 mg, 74% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.32 (s, 1H), 7.90 – 7.89 (m, 4H), 7.62 – 7.60 (m, 2H), 7.51 – 7.49 (m, 4H). The NMR spectral data match the previously published data.[7]



***N*-benzoyl-[1,1'-biphenyl]-4-carboxamide (4ab').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl ([1,1'-biphenyl]-4-carbonyl)(benzyl)carbamate **2b'** (38.7 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (23.2 mg, 77% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.34 (s, 1H), 7.99 – 7.96 (m, 2H), 7.90 – 7.88 (m, 2H), 7.80 – 7.77 (m, 2H), 7.72 – 7.70 (m, 2H), 7.62 – 7.58 (m, 1H), 7.51 – 7.46 (m, 4H), 7.41 – 7.37 (m, 1H). The NMR spectral data match the previously published data.[8]

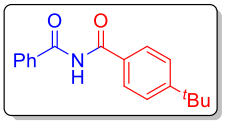


***N*-benzoyl-3-methylbenzamide (4ac').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzyl(3-methylbenzoyl)carbamate **2c'** (32.5 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (14.1 mg, 59% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.25 (s, 1H), 7.89 – 7.87 (m, 2H), 7.72 (s, 1H), 7.69 – 7.68 (m, 1H), 7.62 – 7.59 (m, 1H), 7.51 – 7.48 (m, 2H), 7.42 – 7.36 (m, 2H), 2.36 (s, 3H). The NMR spectral data match the previously published data.[9]

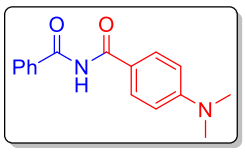


***N*-benzoyl-2-methylbenzamide (4ad').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzyl(2-methylbenzoyl)carbamate **2d'** (32.5 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (19.8 mg, 83% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.42 (s, 1H), 7.91 – 7.89 (m, 2H), 7.62 – 7.59 (m, 1H), 7.51 – 7.44 (m,

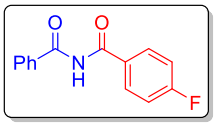
3H), 7.39 – 7.35 (m, 1H), 7.28 – 7.21 (m, 2H), 2.35 (s, 3H). The NMR spectral data match the previously published data.[7]



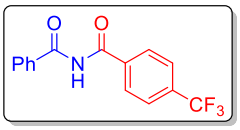
***N*-benzoyl-4-(*tert*-butyl)benzamide (4ae').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2mg, 0.3 mmol), and *tert*-butyl benzyl(4-(*tert*-butyl)benzoyl)carbamate **2e'** (36.7 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (18.0 mg, 64% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.22 (s, 1H), 7.88 – 7.87 (m, 2H), 7.84 – 7.82 (m, 2H), 7.61 – 7.59 (m, 1H), 7.52 – 7.48 (m, 4H), 1.29 (s, 9H). The NMR spectral data match the previously published data.[7]



***N*-benzoyl-4-(dimethylamino)benzamide (4af').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzyl(4-(dimethylamino)benzoyl)carbamate **2f'** (35.4 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 2:1) to give the product (17.2 mg, 64% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.26 (s, 1H), 8.19 – 8.13 (m, 4H), 7.94 – 7.91 (m, 1H), 7.84 – 7.81 (m, 2H), 7.06 – 7.04 (m, 2H), 3.33 (s, 6H). The NMR spectral data match the previously published data.[10]

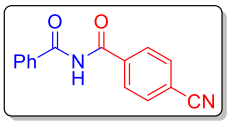


***N*-benzoyl-4-fluorobenzamide (4ag').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzyl(4-fluorobenzoyl)carbamate **2g'** (32.9 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (19.9 mg, 82% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.26 (s, 1H), 7.92 – 7.90 (m, 2H), 7.83 – 7.81 (m, 2H), 7.56 – 7.53 (m, 1H), 7.45 – 7.42 (m, 2H), 7.28 – 7.25 (m, 2H). The NMR spectral data match the previously published data.[7]

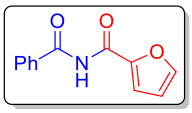


***N*-benzoyl-4-(trifluoromethyl)benzamide (4ah').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzyl(4-(trifluoromethyl)benzoyl)carbamate **2h'** (37.9 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The

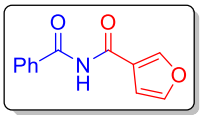
crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (17.0 mg, 58% yield) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.15 (s, 1H), 7.95– 7.93 (m, 2H), 7.88 – 7.87 (m, 2H), 7.74– 7.73 (m, 2H), 7.63 – 7.60 (m, 1H), 7.51 – 7.49 (m, 2H). The NMR spectral data match the previously published data.[7]



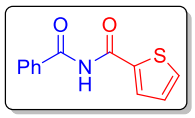
***N*-benzoyl-4-cyanobenzamide (4ai').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzyl(4-cyanobenzoyl)carbamate **2i'** (33.6 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (16.5 mg, 66% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.58 (s, 1H), 8.05 – 7.99 (m, 4H), 7.96 – 7.93 (m, 2H), 7.68 – 7.64 (m, 1H), 7.56 – 7.53 (m, 2H). The NMR spectral data match the previously published data.[11]



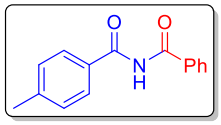
***N*-benzoylfuran-2-carboxamide (4aj').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzyl(furan-2-carbonyl)carbamate **2j'** (30.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (11.0 mg, 51% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.09 (s, 1H), 7.98– 7.97 (m, 1H), 7.84 – 7.82 (m, 2H), 7.62 – 7.59 (m, 1H), 7.56 (dd, J = 3.5, 1.0 Hz, 1H), 7.51 – 7.48 (m, 2H), 6.70 (dd, J = 3.5, 2.0 Hz, 1H). The NMR spectral data match the previously published data.[7]



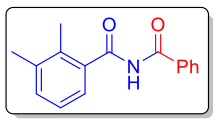
***N*-benzoylfuran-3-carboxamide (4ak').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzyl(furan-3-carbonyl)carbamate **2k'** (30.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (10.5 mg, 49% yield) as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.07 (s, 1H), 8.27 (s, 1H), 7.82 – 7.85 (m, 2H), 7.58 – 7.56 (m, 1H), 7.49 – 7.45 (m, 3H), 6.82 (d, J = 3.0 Hz, 1H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 166.9, 162.0, 148.1, 144.0, 133.4, 133.1, 128.8, 128.2, 121.8, 109.7; IR (thin film): 3276, 1717, 1669, 1481, 1157, 759, 707 cm^{-1}; HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{12}H_9NNaO_3$ 238.0475; found 238.0480.



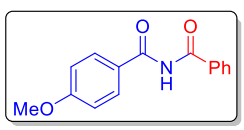
***N*-benzoylthiophene-2-carboxamide (4al').** The reaction was performed following General Procedure C with benzamide **1a** (12.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzyl(thiophene-2-carbonyl)carbamate **2l'** (31.7 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (14.3 mg, 62% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.27 (s, 1H), 8.13 (dd, J = 4.0, 1.0 Hz, 1H), 7.97 (dd, J = 5.0, 1.0 Hz, 1H), 7.85 – 7.84 (m, 2H), 7.63 – 7.60 (m, 1H), 7.52 – 7.50 (m, 2H), 7.22 (dd, J = 5.0, 4.0 Hz, 1H). The NMR spectral data match the previously published data.[7]



***N*-benzoyl-4-methylbenzamide (4bb).** The reaction was performed following General Procedure C with 4-methylbenzamide **1b** (13.5 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (20.3 mg, 85% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.21 (s, 1H), 7.89 – 7.87 (m, 4H), 7.61 – 7.58 (m, 1H), 7.50 – 7.47 (m, 2H), 7.30 – 7.29 (m, 2H), 2.33 (s, 3H). The NMR spectral data match the previously published data.[9]

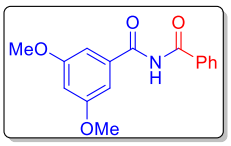


***N*-benzoyl-2,3-dimethylbenzamide (4cb).** The reaction was performed following General Procedure C with 2,3-dimethylbenzamide **1c** (14.9 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (15.2 mg, 60% yield) as a white solid. mp: 139−141 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.43 (s, 1H), 7.91 – 7.88 (m, 2H), 7.62 – 7.59 (m, 1H), 7.50 – 7.47 (m, 2H), 7.26 – 7.22 (m, 2H), 7.15 – 7.12 (m, 1H), 2.26 (s, 3H), 2.22 (s, 3H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 170.9, 166.6, 137.1, 137.0, 133.4, 133.2, 132.8, 131.1, 128.6, 128.4, 125.3, 124.7, 19.8, 16.1; IR (thin film): 3245, 2919, 1719, 1679, 1511, 1384, 1241, 1150, 704 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{16}H_{15}NNaO_2$ 276.0995; found 276.1005.

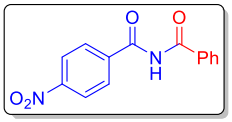


***N*-benzoyl-4-methoxybenzamide (4db).** The reaction was performed following General Procedure C with 4-methoxybenzamide **1d** (14.9 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (17.9 mg, 70% yield)

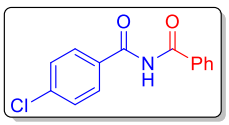
as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.14 (s, 1H), 7.90 – 7.85 (m, 4H), 7.60 – 7.58 (m, 1H), 7.50 – 7.47 (m, 2H), 7.03 – 7.01 (m, 2H), 3.81 (s, 3H). The NMR spectral data match the previously published data.[7]



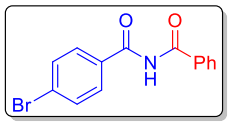
***N*-benzoyl-3,5-dimethoxybenzamide (4eb).** The reaction was performed following General Procedure C with 3,5-dimethoxybenzamide **1e** (18.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (20.0 mg, 70% yield) as a white solid. mp: 130−132 °C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.27 (s, 1H), 7.90 – 7.88 (m, 2H), 7.66 – 7.62 (m, 1H), 7.54 – 7.51 (m, 2H), 7.10 – 7.09 (m, 2H), 6.77 – 6.76 (m, 1H), 3.78 (s, 6H); ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 168.0, 166.9, 160.4, 135.7, 134.0, 132.6, 128.7, 128.4, 106.4, 104.6, 55.6; IR (thin film): 3256, 2939, 1713, 1674, 1597, 1499, 1206, 761, 695 cm^{-1}; HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{16}H_{15}NNaO_4$ 308.0893; found 308.0900.



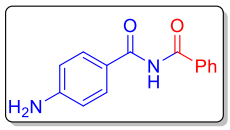
***N*-benzoyl-4-nitrobenzamide (4fb').** The reaction was performed following General Procedure C with 4-nitrobenzamide **1f'** (16.6 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (21.1 mg, 78% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.62 (s, 1H), 8.31 – 8.29 (m, 2H), 8.08 – 8.06 (m, 2H), 7.93 – 7.91 (m, 2H), 7.64 – 7.61(m, 1H), 7.53 – 7.50 (m, 2H). The NMR spectral data match the previously published data.[7]



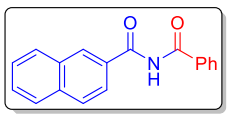
***N*-benzoyl-4-chlorobenzamide (4gb).** The reaction was performed following General Procedure C with 4-chlorobenzamide **1g** (15.5 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (20.8 mg, 80% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.37 (s, 1H), 7.90 – 7.87 (m, 4H), 7.62 – 7.59 (m, 1H), 7.57 – 7.55 (m, 2H), 7.51 – 7.48 (m, 2H). The NMR spectral data match the previously published data.[7]



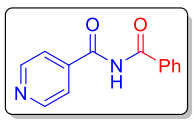
***N*-benzoyl-4-bromobenzamide (4hb).** The reaction was performed following General Procedure C with 4-bromobenzamide **1h** (19.9 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (19.6 mg, 65% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.37 (s, 1H), 7.89 – 7.88 (m, 2H), 7.83 – 7.81 (m, 2H), 7.72 – 7.70 (m, 2H), 7.63 – 7.60 (m, 1H), 7.51 – 7.48 (m, 2H). The NMR spectral data match the previously published data.[7]



4-Amino-*N*-benzoylbenzamide (4ib'). The reaction was performed following General Procedure C with 4-aminobenzamide **1i'** (13.7 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 1:1) to give the product (15.1 mg, 63% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.81 (s, 1H), 7.83 – 7.81 (m, 2H), 7.66 – 7.64 (m, 2H), 7.59 – 7.56 (m, 1H), 7.49 – 7.46 (m, 2H), 6.57 – 6.55 (m, 2H), 6.00 (s, 2H). The NMR spectral data match the previously published data.[12]

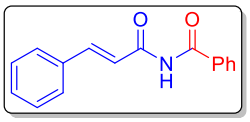


***N*-benzoyl-2-naphthamide (4jb).** The reaction was performed following General Procedure C with 2-naphthamide **1j** (17.1 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (22.6 mg, 82% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.45 (s, 1H), 8.58 (s, 1H), 8.07 – 8.06 (m, 1H), 8.01 – 7.97 (m, 2H), 7.94 – 7.70 (m, 3H), 7.65 – 7.57 (m, 3H), 7.52 – 7.50 (m, 2H). The NMR spectral data match the previously published data.[7]



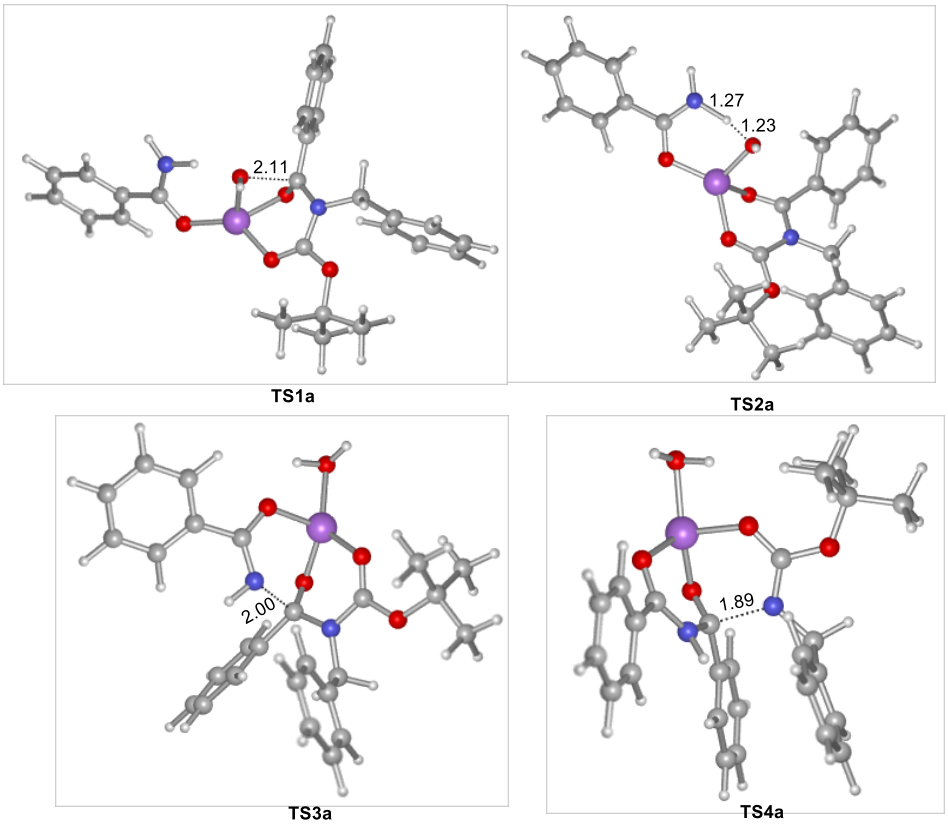
***N*-benzoylisonicotinamide (4mb).** The reaction was performed following General Procedure C with isonicotinamide **1m** (12.2 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (15.4 mg, 68% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.56 (s, 1H), 8.74 – 8.73 (m, 2H), 7.92 – 7.90 (m, 2H), 7.75 – 7.74(m, 2H), 7.64 –

7.61 (m, 1H), 7.52 – 7.49 (m, 2H). The NMR spectral data match the previously published data.[7]

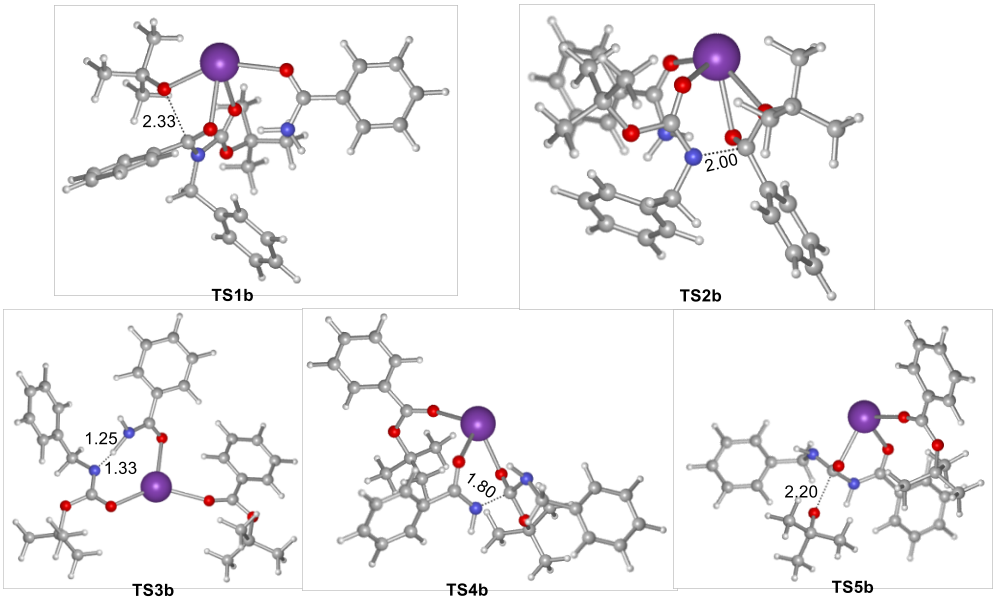


***N*-cinnamoylbenzamide (4nb').** The reaction was performed following General Procedure C with cinnamamide **1n'** (14.7 mg, 0.1 mmol), LiOH (7.2 mg, 0.3 mmol), and *tert*-butyl benzoyl(benzyl)carbamate **2b** (31.1 mg, 0.1 mmol) dissolved in DME (1 mL) at 100 °C. The crude material was purified by flash chromatography on silica gel (eluted with hexanes:EtOAc = 5:1) to give the product (13.0 mg, 52% yield) as a white solid. ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.12 (s, 1H), 7.93 – 7.91 (m, 2H), 7.71 – 7.60 (m, 4H), 7.52 – 7.50 (m, 2H), 7.45 – 7.41 (m, 3H), 7.32 – 7.29 (m, 1H). The NMR spectral data match the previously published data.[7]

Computational details



Supplementary Figure 1. Optimized 3D structures of the transition states shown in Figure 1. Bond lengths are shown in Å.



Supplementary Figure 2. Optimized 3D structures of the transition states shown in Figure 2. Bond lengths are shown in Å.

Computational methods

The B3LYP[12] density functional method was employed to carry out all the calculations. The 6-31G(d)[13] basis set was used for all atoms. Vibrational frequency analyses at the same level of the theory were performed on all the optimized geometries to characterize them as local minima (no imaginary frequency) or transition states (one imaginary frequency). In addition, intrinsic reaction coordinate (IRC) calculations were used to verify that the transition state connect with appropriate reactant and product.[14] The gas-phase Gibbs energies for all species were obtained at 298.15 K and 1 atm at their respective optimized structures. Solution phase single-point energies were calculated based on the optimized structures with the M06-2X[Error! Reference source not found.] method, SMD solvation model,[15] and 6-311++G(d,p) basis set. The Gibbs energy was determined by adding the single-point energy and the gas-phase thermal correction to the Gibbs energy obtained from the vibrational frequency analyses. All calculations were carried out with the Gaussian 09 suite of programs.[17] The 3D structures of the optimized intermediates or transition states were demonstrated using the software of CYLView.[19]

Cartesian Coordinates and Energies

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.718340	-0.136625	-0.034129
2	6	0	-0.220321	-0.022361	-0.018635
3	6	0	0.515173	-1.207918	0.109591
4	6	0	0.460485	1.196958	-0.143684
5	6	0	1.907128	-1.173802	0.137667
6	1	0	-0.028317	-2.144033	0.184587
7	6	0	1.854874	1.229660	-0.123076
8	1	0	-0.091870	2.120597	-0.294005
9	6	0	2.579945	0.045673	0.024005
10	1	0	2.469052	-2.097628	0.245087
11	1	0	2.374463	2.177980	-0.230328
12	1	0	3.666232	0.072497	0.042219
13	7	0	-2.420739	1.023584	0.207602
14	1	0	-3.417687	0.900293	0.328241
15	1	0	-1.996623	1.768531	0.741496
16	8	0	-2.287968	-1.194104	-0.272619

Zero-point correction= 0.128082 (Hartree/Particle)
Thermal correction to Energy= 0.135541
Thermal correction to Enthalpy= 0.136485
Thermal correction to Gibbs Free Energy= 0.095884
Sum of electronic and zero-point Energies= -400.822970
Sum of electronic and thermal Energies= -400.815511
Sum of electronic and thermal Enthalpies= -400.814567
Sum of electronic and thermal Free Energies= -400.855167
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-400.905998

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	1.405831	-0.492329	2.119963
2	6	0	1.507079	-0.440271	0.911467
3	6	0	2.839164	-0.326572	0.238985
4	7	0	0.361405	-0.487158	0.050143
5	6	0	3.899791	0.227625	0.970857
6	6	0	3.076975	-0.827273	-1.049437
7	6	0	-0.679385	-1.372158	0.375065
8	6	0	0.157353	0.591321	-0.931985
9	6	0	5.173101	0.302160	0.413316
10	1	0	3.705353	0.589121	1.975435
11	6	0	4.356324	-0.764759	-1.600271
12	1	0	2.265052	-1.285826	-1.605865
13	8	0	-0.575516	-2.276801	1.174482
14	8	0	-1.758719	-1.089667	-0.382108
15	1	0	1.150007	0.970761	-1.191619
16	1	0	-0.270900	0.165112	-1.842511
17	6	0	-0.709650	1.745148	-0.444915
18	6	0	5.403090	-0.193748	-0.873261
19	1	0	5.988274	0.741345	0.981563
20	1	0	4.537298	-1.165267	-2.593876
21	6	0	-3.007689	-1.865001	-0.246273
22	6	0	-1.345256	2.558696	-1.390909
23	6	0	-0.854039	2.048101	0.913682
24	1	0	6.398473	-0.140489	-1.306123
25	6	0	-3.558852	-1.707559	1.174225
26	6	0	-2.762339	-3.329671	-0.621793
27	6	0	-3.925249	-1.185302	-1.265605
28	6	0	-2.104242	3.658736	-0.991664
29	1	0	-1.248204	2.327448	-2.450055
30	6	0	-1.618474	3.146364	1.313996
31	1	0	-0.379402	1.422065	1.663682
32	1	0	-4.541776	-2.187409	1.240124
33	1	0	-2.894287	-2.166429	1.907931
34	1	0	-3.679337	-0.646586	1.418074
35	1	0	-2.096068	-3.814010	0.093281
36	1	0	-3.717266	-3.867032	-0.635617
37	1	0	-2.320834	-3.397966	-1.622343
38	1	0	-4.914357	-1.655024	-1.251455
39	1	0	-4.039444	-0.122146	-1.032316
40	1	0	-3.514866	-1.275142	-2.276969
41	6	0	-2.243588	3.956437	0.365453
42	1	0	-2.592418	4.277972	-1.739863
43	1	0	-1.724501	3.366367	2.373124
44	1	0	-2.838074	4.809989	0.680106

Zero-point correction= 0.364918 (Hartree/Particle)
Thermal correction to Energy= 0.386512
Thermal correction to Enthalpy= 0.387456
Thermal correction to Gibbs Free Energy= 0.312301
Sum of electronic and zero-point Energies= -1016.760523
Sum of electronic and thermal Energies= -1016.738929
Sum of electronic and thermal Enthalpies= -1016.737985
Sum of electronic and thermal Free Energies= -1016.813140
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1016.992929

4aa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.409386	2.322082	-0.326326
2	6	0	1.257970	1.126831	-0.178823
3	6	0	2.425293	0.185724	-0.042391
4	6	0	2.367403	-1.183266	-0.341683
5	6	0	3.641302	0.742279	0.378790
6	6	0	3.501736	-1.983701	-0.204329

7	1	0	1.453252	-1.630372	-0.724183
8	6	0	4.769925	-0.059351	0.525966
9	1	0	3.676479	1.807156	0.583589
10	6	0	4.701998	-1.425037	0.237235
11	1	0	3.449077	-3.040638	-0.450265
12	1	0	5.704628	0.380082	0.862981
13	1	0	5.583861	-2.050137	0.347966
14	6	0	-1.257964	1.126831	-0.178468
15	6	0	-2.425281	0.185694	-0.042222
16	6	0	-3.641433	0.742308	0.378469
17	6	0	-2.367266	-1.183374	-0.341142
18	6	0	-4.770077	-0.059317	0.525520
19	1	0	-3.676686	1.807231	0.583006
20	6	0	-3.501606	-1.983812	-0.203895
21	1	0	-1.453006	-1.630581	-0.723264
22	6	0	-4.702022	-1.425074	0.237170
23	1	0	-5.704892	0.380180	0.862141
24	1	0	-3.448834	-3.040815	-0.449520
25	1	0	-5.583892	-2.050180	0.347808
26	7	0	0.000011	0.504962	-0.102319
27	1	0	0.000076	-0.460205	0.194821
28	8	0	-1.409387	2.322059	-0.326177

Zero-point correction= 0.219118 (Hartree/Particle)
Thermal correction to Energy= 0.232951
Thermal correction to Enthalpy= 0.233895
Thermal correction to Gibbs Free Energy= 0.175829
Sum of electronic and zero-point Energies= -745.116563
Sum of electronic and thermal Energies= -745.102730
Sum of electronic and thermal Enthalpies= -745.101786
Sum of electronic and thermal Free Energies= -745.159852
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-745.246653

INT1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.177876	-0.257696	-0.164735
2	3	0	-3.371476	1.187568	0.292663
3	1	0	-4.872792	-0.795196	0.232895
4	6	0	-0.961512	0.087043	0.041659
5	6	0	0.535294	0.004212	0.021012
6	6	0	1.264189	1.188804	-0.149029
7	6	0	1.224815	-1.206577	0.178993
8	6	0	2.656568	1.160263	-0.186376
9	1	0	0.720637	2.121779	-0.252067
10	6	0	2.618445	-1.233138	0.151650
11	1	0	0.678442	-2.128826	0.358097
12	6	0	3.336727	-0.050722	-0.037697
13	1	0	3.212367	2.083051	-0.328612
14	1	0	3.143047	-2.175147	0.285547
15	1	0	4.422944	-0.072522	-0.061929
16	7	0	-1.679464	-1.000737	-0.244089
17	1	0	-1.216398	-1.825427	-0.597205
18	8	0	-1.509811	1.187589	0.329105
19	1	0	-2.763220	-0.903712	-0.242319

Zero-point correction= 0.142152 (Hartree/Particle)
Thermal correction to Energy= 0.152859
Thermal correction to Enthalpy= 0.153804
Thermal correction to Gibbs Free Energy= 0.105572
Sum of electronic and zero-point Energies= -484.240100
Sum of electronic and thermal Energies= -484.229392
Sum of electronic and thermal Enthalpies= -484.228448
Sum of electronic and thermal Free Energies= -484.276679
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-484.336324

INT2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.431691	0.545807	-1.913639
2	8	0	0.325487	0.644388	0.857450
3	6	0	-0.690084	0.907226	0.232570
4	6	0	-1.064011	2.338084	-0.045963
5	7	0	-1.543169	-0.101560	-0.269749
6	6	0	-2.004068	3.030143	0.725976
7	6	0	-0.345675	2.993168	-1.057969
8	6	0	-1.115481	-1.443352	-0.273424
9	6	0	-2.851754	0.238154	-0.862288
10	6	0	-2.233207	4.385007	0.480596
11	1	0	-2.550490	2.520663	1.514290
12	6	0	-0.594380	4.345013	-1.298166
13	1	0	0.389129	2.416956	-1.624634
14	8	0	0.042987	-1.803803	-0.147631
15	8	0	-2.157023	-2.259469	-0.451973
16	1	0	-2.739672	1.210143	-1.345778
17	1	0	-3.048835	-0.490114	-1.651295
18	6	0	-4.024484	0.277451	0.105349
19	6	0	-1.532769	5.041876	-0.532755
20	1	0	-2.958249	4.925119	1.083469
21	1	0	-0.044894	4.858364	-2.083143
22	6	0	-1.988621	-3.733472	-0.567080
23	6	0	-5.231351	0.832958	-0.340813
24	6	0	-3.957578	-0.228539	1.406591
25	1	0	-1.715343	6.096592	-0.722179
26	6	0	-1.422478	-4.288633	0.742073
27	6	0	-1.113689	-4.064473	-1.778596
28	6	0	-3.428820	-4.201166	-0.784427
29	6	0	-6.347956	0.876756	0.492125
30	1	0	-5.295530	1.238116	-1.348865
31	6	0	-5.074039	-0.179352	2.245691
32	1	0	-3.031660	-0.661336	1.772241
33	1	0	-1.419361	-5.383240	0.696678
34	1	0	-0.401879	-3.944014	0.914752
35	1	0	-2.049279	-3.986848	1.588073
36	1	0	-0.084364	-3.732996	-1.634393
37	1	0	-1.112078	-5.148954	-1.934186
38	1	0	-1.516983	-3.594595	-2.682295
39	1	0	-3.455863	-5.292554	-0.865580
40	1	0	-4.064882	-3.897918	0.052852
41	1	0	-3.842410	-3.776098	-1.704649
42	6	0	-6.272585	0.370096	1.791797
43	1	0	-7.274812	1.312928	0.129043
44	1	0	-5.002715	-0.573382	3.256071
45	1	0	-7.140180	0.407572	2.444859
46	3	0	1.533506	-0.479793	-0.376426
47	1	0	1.393396	0.076279	-2.760678
48	6	0	4.239422	-0.042757	-0.343561
49	6	0	5.635827	-0.079153	0.212272
50	6	0	5.812327	-0.506604	1.534632
51	6	0	6.758817	0.281654	-0.544880
52	6	0	7.086000	-0.547913	2.098016
53	1	0	4.936266	-0.800917	2.102912
54	6	0	8.035069	0.229501	0.015343
55	1	0	6.642645	0.573446	-1.585379
56	6	0	8.200292	-0.179048	1.340209
57	1	0	7.211439	-0.870888	3.128158
58	1	0	8.899964	0.501076	-0.584131
59	1	0	9.194419	-0.216364	1.778109
60	7	0	3.972996	0.777669	-1.366556
61	1	0	4.657390	1.468404	-1.638826

62	8	0	3.360687	-0.783017	0.161133
63	1	0	2.936564	0.804171	-1.714723

Zero-point correction= 0.508536 (Hartree/Particle)
Thermal correction to Energy= 0.542225
Thermal correction to Enthalpy= 0.543169
Thermal correction to Gibbs Free Energy= 0.438158
Sum of electronic and zero-point Energies= -1501.036682
Sum of electronic and thermal Energies= -1501.002994
Sum of electronic and thermal Enthalpies= -1501.002050
Sum of electronic and thermal Free Energies= -1501.107061
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1501.360375

INT3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.675365	0.879249	-2.089646
2	8	0	0.285408	0.939423	0.554286
3	6	0	-0.828608	1.097298	0.078243
4	6	0	-1.363127	2.492731	-0.082946
5	7	0	-1.607294	0.011898	-0.380102
6	6	0	-2.466621	2.991980	0.620515
7	6	0	-0.607553	3.342779	-0.906172
8	6	0	-1.034896	-1.278732	-0.460049
9	6	0	-2.998994	0.194342	-0.838569
10	6	0	-2.818598	4.336121	0.491352
11	1	0	-3.040201	2.343459	1.275430
12	6	0	-0.981715	4.678321	-1.044424
13	1	0	0.255529	2.941486	-1.431408
14	8	0	0.161376	-1.510342	-0.428483
15	8	0	-1.990088	-2.195085	-0.600213
16	1	0	-3.073320	1.210511	-1.230136
17	1	0	-3.156643	-0.483328	-1.679825
18	6	0	-4.076692	-0.035304	0.210617
19	6	0	-2.082768	5.177641	-0.344563
20	1	0	-3.667135	4.724106	1.047972
21	1	0	-0.403665	5.332414	-1.691156
22	6	0	-1.674513	-3.645986	-0.748103
23	6	0	-5.412222	0.169774	-0.162087
24	6	0	-3.796784	-0.434286	1.520463
25	1	0	-2.363188	6.222650	-0.445551
26	6	0	-0.978597	-4.147189	0.519144
27	6	0	-0.841389	-3.870414	-2.011794
28	6	0	-3.069115	-4.257673	-0.889339
29	6	0	-6.445016	-0.020189	0.754025
30	1	0	-5.645024	0.482729	-1.178222
31	6	0	-4.831254	-0.621919	2.441598
32	1	0	-2.769102	-0.600570	1.829397
33	1	0	-0.863836	-5.234901	0.458048
34	1	0	0.010125	-3.701549	0.639431
35	1	0	-1.584255	-3.920559	1.403072
36	1	0	0.159140	-3.445901	-1.916628
37	1	0	-0.745740	-4.947089	-2.189597
38	1	0	-1.337995	-3.428697	-2.882723
39	1	0	-2.987858	-5.345580	-0.979005
40	1	0	-3.684003	-4.024461	-0.014780
41	1	0	-3.575264	-3.874517	-1.781246
42	6	0	-6.157124	-0.417003	2.062434
43	1	0	-7.474566	0.144177	0.447519
44	1	0	-4.595059	-0.930178	3.456518
45	1	0	-6.960622	-0.563557	2.778842
46	3	0	1.640102	-0.171405	-0.414554
47	1	0	1.717804	0.321656	-2.882196
48	6	0	4.324173	0.170777	-0.367099
49	6	0	5.682378	-0.014071	0.275960

50	6	0	5.749338	-0.519586	1.581022
51	6	0	6.878460	0.286115	-0.390131
52	6	0	6.978425	-0.694090	2.215231
53	1	0	4.819191	-0.771335	2.079431
54	6	0	8.110943	0.100367	0.236855
55	1	0	6.848632	0.643312	-1.416471
56	6	0	8.164508	-0.384584	1.545039
57	1	0	7.012878	-1.076514	3.232663
58	1	0	9.029515	0.328751	-0.298338
59	1	0	9.124176	-0.526432	2.036013
60	7	0	4.145714	1.040729	-1.340872
61	1	0	4.970009	1.599026	-1.542265
62	8	0	3.375473	-0.555018	0.089527
63	1	0	2.695141	1.077601	-1.881412

Zero-point correction= 0.508635 (Hartree/Particle)
Thermal correction to Energy= 0.542385
Thermal correction to Enthalpy= 0.543329
Thermal correction to Gibbs Free Energy= 0.437847
Sum of electronic and zero-point Energies= -1501.036211
Sum of electronic and thermal Energies= -1501.002462
Sum of electronic and thermal Enthalpies= -1501.001518
Sum of electronic and thermal Free Energies= -1501.107000
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1501.363695

INT4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.122296	-2.121601	-3.410737
2	8	0	0.186705	0.643339	-2.444760
3	6	0	-0.457150	1.185934	-1.551970
4	6	0	-0.164360	2.619863	-1.222517
5	7	0	-1.521535	0.531702	-0.900823
6	6	0	0.072613	3.080337	0.080588
7	6	0	-0.009728	3.496543	-2.306138
8	6	0	-1.756019	-0.839486	-1.134948
9	6	0	-2.496654	1.255104	-0.052528
10	6	0	0.433643	4.410390	0.291588
11	1	0	0.003535	2.394795	0.917040
12	6	0	0.333345	4.829094	-2.087043
13	1	0	-0.156476	3.124075	-3.315054
14	8	0	-0.969033	-1.607245	-1.666890
15	8	0	-2.963541	-1.178606	-0.692862
16	1	0	-2.271690	2.316800	-0.153109
17	1	0	-3.492199	1.099793	-0.474748
18	6	0	-2.491012	0.845413	1.410782
19	6	0	0.555446	5.288473	-0.787379
20	1	0	0.627171	4.758379	1.302414
21	1	0	0.438084	5.504638	-2.931358
22	6	0	-3.409942	-2.597061	-0.615763
23	6	0	-3.642668	1.082583	2.172569
24	6	0	-1.370849	0.268810	2.022852
25	1	0	0.832473	6.325247	-0.616400
26	6	0	-2.457153	-3.381252	0.289207
27	6	0	-3.517265	-3.183130	-2.025011
28	6	0	-4.790227	-2.457955	0.029417
29	6	0	-3.677684	0.758971	3.528801
30	1	0	-4.520066	1.521979	1.701287
31	6	0	-1.413832	-0.060163	3.381508
32	1	0	-0.461737	0.073620	1.450887
33	1	0	-2.867145	-4.382982	0.458595
34	1	0	-1.467066	-3.482898	-0.158503
35	1	0	-2.356597	-2.882304	1.258346
36	1	0	-2.536890	-3.281526	-2.492854
37	1	0	-3.979984	-4.174670	-1.967344

38	1	0	-4.150561	-2.550498	-2.656288
39	1	0	-5.237625	-3.448056	0.163382
40	1	0	-4.712387	-1.973971	1.007608
41	1	0	-5.456170	-1.861439	-0.602798
42	6	0	-2.560301	0.183310	4.138235
43	1	0	-4.578750	0.949316	4.106208
44	1	0	-0.539275	-0.509863	3.844535
45	1	0	-2.586466	-0.075299	5.193535
46	3	0	0.861185	-1.171083	-2.156416
47	1	0	1.944136	-3.067971	-3.521590
48	6	0	2.508431	-0.760726	0.075101
49	6	0	3.915324	-0.921602	0.614163
50	6	0	4.548623	-2.169581	0.532153
51	6	0	4.616915	0.146266	1.191560
52	6	0	5.833925	-2.353773	1.040278
53	1	0	4.011450	-2.991118	0.069427
54	6	0	5.909405	-0.029823	1.686014
55	1	0	4.155648	1.129979	1.231108
56	6	0	6.520359	-1.283530	1.618635
57	1	0	6.303992	-3.332680	0.981409
58	1	0	6.442090	0.813755	2.118362
59	1	0	7.525969	-1.423560	2.007264
60	7	0	1.669323	0.106404	0.575986
61	1	0	2.106522	0.590563	1.362060
62	8	0	2.191669	-1.553171	-0.898076
63	1	0	2.618079	-2.057365	-2.554615

Zero-point correction= 0.510034 (Hartree/Particle)
Thermal correction to Energy= 0.543935
Thermal correction to Enthalpy= 0.544879
Thermal correction to Gibbs Free Energy= 0.440407
Sum of electronic and zero-point Energies= -1501.027340
Sum of electronic and thermal Energies= -1500.993439
Sum of electronic and thermal Enthalpies= -1500.992495
Sum of electronic and thermal Free Energies= -1501.096967
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1501.359387

INT5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.814770	-3.868904	-2.510080
2	8	0	0.600659	-0.376056	-2.430439
3	6	0	0.361893	0.304758	-1.363047
4	6	0	0.404753	1.847312	-1.563158
5	7	0	-1.020090	-0.089749	-0.692060
6	6	0	0.289574	2.782368	-0.523216
7	6	0	0.649754	2.310537	-2.858592
8	6	0	-1.219975	-1.416355	-0.475354
9	6	0	-2.183352	0.802634	-0.741112
10	6	0	0.418637	4.148848	-0.776367
11	1	0	0.058918	2.460553	0.489917
12	6	0	0.776478	3.677084	-3.114058
13	1	0	0.748063	1.572913	-3.647236
14	8	0	-0.368904	-2.304774	-0.635821
15	8	0	-2.472869	-1.676718	-0.034282
16	1	0	-1.961925	1.591169	-1.463117
17	1	0	-3.036810	0.246187	-1.139672
18	6	0	-2.592767	1.436703	0.582644
19	6	0	0.664878	4.601214	-2.074290
20	1	0	0.319700	4.858620	0.041000
21	1	0	0.968202	4.019340	-4.128030
22	6	0	-2.945868	-3.040306	0.250316
23	6	0	-3.538300	2.471168	0.567820
24	6	0	-2.083956	1.015033	1.814597
25	1	0	0.766924	5.665214	-2.271826

26	6	0	-2.134678	-3.653889	1.396701
27	6	0	-2.905467	-3.894771	-1.021220
28	6	0	-4.393404	-2.796380	0.687917
29	6	0	-3.967400	3.067053	1.752844
30	1	0	-3.939863	2.815048	-0.383674
31	6	0	-2.507686	1.613401	3.004319
32	1	0	-1.349181	0.216197	1.840487
33	1	0	-2.574090	-4.616248	1.683004
34	1	0	-1.095738	-3.812987	1.104961
35	1	0	-2.159133	-2.996115	2.272304
36	1	0	-1.879749	-4.070556	-1.348077
37	1	0	-3.385733	-4.861030	-0.829553
38	1	0	-3.452156	-3.398607	-1.830461
39	1	0	-4.870656	-3.744963	0.955861
40	1	0	-4.425341	-2.130878	1.556137
41	1	0	-4.969729	-2.334690	-0.120379
42	6	0	-3.452022	2.639572	2.979035
43	1	0	-4.700097	3.869432	1.719104
44	1	0	-2.098723	1.272954	3.952516
45	1	0	-3.782436	3.104368	3.904183
46	3	0	1.002573	-2.110287	-1.998520
47	1	0	1.382182	-4.540243	-1.958896
48	6	0	2.442526	-0.767497	-0.183905
49	6	0	3.492355	-0.462766	0.850457
50	6	0	4.206264	-1.531242	1.408533
51	6	0	3.800819	0.846893	1.245229
52	6	0	5.191282	-1.298305	2.365495
53	1	0	3.975930	-2.539609	1.080644
54	6	0	4.796465	1.080115	2.194100
55	1	0	3.291694	1.690300	0.785413
56	6	0	5.487924	0.008459	2.761461
57	1	0	5.731149	-2.134901	2.800894
58	1	0	5.037639	2.099514	2.482687
59	1	0	6.260735	0.190984	3.503360
60	7	0	1.385145	0.064608	-0.213205
61	1	0	1.388827	0.783879	0.496666
62	8	0	2.583996	-1.767467	-0.919572
63	1	0	2.574732	-3.567494	-1.977148

Zero-point correction= 0.510539 (Hartree/Particle)
Thermal correction to Energy= 0.543756
Thermal correction to Enthalpy= 0.544700
Thermal correction to Gibbs Free Energy= 0.442746
Sum of electronic and zero-point Energies= -1501.023052
Sum of electronic and thermal Energies= -1500.989836
Sum of electronic and thermal Enthalpies= -1500.988892
Sum of electronic and thermal Free Energies= -1501.090845
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1501.362811

INT6a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.657686	-2.884919	-2.696910
2	8	0	-0.481427	0.053802	-2.626661
3	6	0	0.406418	0.535539	-1.927292
4	6	0	0.579439	2.010278	-1.802357
5	7	0	-1.104169	0.017637	0.615478
6	6	0	1.792535	2.619583	-1.450287
7	6	0	-0.533871	2.811762	-2.097983
8	6	0	-2.270381	-0.517536	0.386387
9	6	0	-1.011052	0.985181	1.697545
10	6	0	1.887204	4.008617	-1.387097
11	1	0	2.677580	2.025174	-1.244055
12	6	0	-0.438412	4.197667	-2.025603
13	1	0	-1.464221	2.327801	-2.373522

14	8	0	-2.501091	-1.363765	-0.550051
15	8	0	-3.309722	-0.123101	1.209704
16	1	0	-1.559569	1.914958	1.470155
17	1	0	-1.472838	0.604087	2.624685
18	6	0	0.432178	1.344706	2.007142
19	6	0	0.772624	4.798944	-1.670980
20	1	0	2.832031	4.471490	-1.117945
21	1	0	-1.307825	4.810742	-2.245199
22	6	0	-4.663436	-0.641493	1.114303
23	6	0	0.809032	2.667787	2.266001
24	6	0	1.419775	0.350450	2.084288
25	1	0	0.847348	5.881729	-1.617806
26	6	0	-4.690305	-2.154687	1.371102
27	6	0	-5.297144	-0.266184	-0.232596
28	6	0	-5.386557	0.091255	2.252339
29	6	0	2.128136	2.994629	2.590817
30	1	0	0.059281	3.453745	2.204750
31	6	0	2.741638	0.670626	2.403235
32	1	0	1.132031	-0.679770	1.893835
33	1	0	-5.725544	-2.514402	1.406627
34	1	0	-4.153423	-2.693466	0.589450
35	1	0	-4.217792	-2.379805	2.333923
36	1	0	-4.769591	-0.741933	-1.060081
37	1	0	-6.349501	-0.573837	-0.255141
38	1	0	-5.257094	0.819723	-0.375135
39	1	0	-6.439670	-0.208500	2.295632
40	1	0	-4.918257	-0.139417	3.214913
41	1	0	-5.338771	1.174565	2.100355
42	6	0	3.102083	1.997550	2.657534
43	1	0	2.394916	4.030604	2.786687
44	1	0	3.488216	-0.117918	2.463112
45	1	0	4.129218	2.248773	2.910606
46	3	0	-1.311043	-1.583888	-1.983535
47	1	0	-3.085655	-2.612720	-1.856769
48	6	0	1.363747	-1.638705	-1.210074
49	6	0	2.537434	-2.245747	-0.517172
50	6	0	2.372287	-3.515847	0.055343
51	6	0	3.789240	-1.615520	-0.452846
52	6	0	3.436987	-4.134906	0.703661
53	1	0	1.402000	-3.996334	-0.010469
54	6	0	4.857531	-2.245197	0.184582
55	1	0	3.942343	-0.651087	-0.928013
56	6	0	4.680768	-3.500831	0.769436
57	1	0	3.299045	-5.112136	1.157303
58	1	0	5.827973	-1.758447	0.218729
59	1	0	5.512817	-3.987314	1.271020
60	7	0	1.362995	-0.250201	-1.277557
61	1	0	1.876554	0.212820	-0.534724
62	8	0	0.475590	-2.342569	-1.687506
63	1	0	-2.352960	-3.792597	-2.542939

Zero-point correction= 0.508826 (Hartree/Particle)
Thermal correction to Energy= 0.543184
Thermal correction to Enthalpy= 0.544128
Thermal correction to Gibbs Free Energy= 0.438364
Sum of electronic and zero-point Energies= -1501.032726
Sum of electronic and thermal Energies= -1500.998368
Sum of electronic and thermal Enthalpies= -1500.997424
Sum of electronic and thermal Free Energies= -1501.103188
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1501.364132

INT7a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.532102	3.593988	0.149241

2	7	0	0.090767	1.264562	-0.963047
3	6	0	1.164099	0.872502	-0.263780
4	6	0	-0.839739	0.353808	-1.619152
5	8	0	1.818829	1.653180	0.471787
6	8	0	1.489106	-0.418448	-0.436997
7	1	0	-1.309800	0.921841	-2.432227
8	1	0	-0.282341	-0.463962	-2.081651
9	6	0	-1.916635	-0.200294	-0.695409
10	6	0	2.643982	-1.047509	0.227456
11	6	0	-2.355676	-1.520614	-0.839785
12	6	0	-2.510132	0.612381	0.281915
13	6	0	2.463865	-1.008128	1.748361
14	6	0	3.943869	-0.377995	-0.229592
15	6	0	2.567403	-2.488196	-0.286225
16	6	0	-3.373285	-2.027232	-0.028706
17	1	0	-1.895779	-2.159773	-1.591100
18	6	0	-3.524222	0.103414	1.094436
19	1	0	-2.168954	1.638695	0.410046
20	1	0	3.255374	-1.596724	2.225856
21	1	0	2.511312	0.014210	2.126033
22	1	0	1.498970	-1.444754	2.027562
23	1	0	4.000736	0.653974	0.119668
24	1	0	4.801292	-0.932914	0.167714
25	1	0	4.011514	-0.386128	-1.322978
26	1	0	3.381777	-3.083041	0.140273
27	1	0	1.615162	-2.947776	-0.003049
28	1	0	2.653348	-2.514614	-1.377366
29	6	0	-3.960565	-1.214994	0.941928
30	1	0	-3.700579	-3.056732	-0.151200
31	1	0	-3.976217	0.741173	1.850080
32	1	0	-4.750314	-1.607043	1.577687
33	3	0	0.994548	3.281383	0.847215
34	1	0	-0.255022	2.238241	-0.703438
35	1	0	-1.033946	4.316622	-0.243158

Zero-point correction= 0.289111 (Hartree/Particle)
Thermal correction to Energy= 0.307673
Thermal correction to Enthalpy= 0.308617
Thermal correction to Gibbs Free Energy= 0.241600
Sum of electronic and zero-point Energies= -755.890060
Sum of electronic and thermal Energies= -755.871498
Sum of electronic and thermal Enthalpies= -755.870553
Sum of electronic and thermal Free Energies= -755.937571
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-756.085059

TS1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.043097	0.550179	-1.380812
2	8	0	0.122153	0.629392	1.053311
3	6	0	-0.461234	1.014650	0.031156
4	6	0	-0.517080	2.477806	-0.313111
5	7	0	-1.532855	0.182926	-0.533278
6	6	0	-0.355900	3.389890	0.735035
7	6	0	-0.701603	2.957253	-1.617723
8	6	0	-1.365116	-1.189010	-0.549666
9	6	0	-2.891520	0.735477	-0.701487
10	6	0	-0.392917	4.763598	0.487457
11	1	0	-0.194803	3.008808	1.738017
12	6	0	-0.738680	4.326547	-1.863811
13	1	0	-0.782689	2.249357	-2.435388
14	8	0	-0.314191	-1.775566	-0.296597
15	8	0	-2.496052	-1.804493	-0.924364
16	1	0	-2.778771	1.813234	-0.828220
17	1	0	-3.316864	0.347938	-1.630361

18	6	0	-3.842562	0.460026	0.454371
19	6	0	-0.587390	5.234874	-0.810345
20	1	0	-0.268399	5.463203	1.309719
21	1	0	-0.873280	4.688810	-2.879679
22	6	0	-2.620052	-3.278654	-0.946835
23	6	0	-5.217310	0.381851	0.200447
24	6	0	-3.390282	0.333148	1.773335
25	1	0	-0.614642	6.303819	-1.005314
26	6	0	-2.384849	-3.841323	0.457755
27	6	0	-1.666308	-3.871413	-1.988195
28	6	0	-4.078536	-3.468831	-1.371695
29	6	0	-6.126138	0.186346	1.240803
30	1	0	-5.579654	0.471453	-0.821846
31	6	0	-4.299286	0.130897	2.814221
32	1	0	-2.326361	0.381299	1.988084
33	1	0	-2.611793	-4.913349	0.460942
34	1	0	-1.349716	-3.702902	0.773449
35	1	0	-3.045643	-3.349715	1.179416
36	1	0	-0.624068	-3.741027	-1.693916
37	1	0	-1.869370	-4.942713	-2.097807
38	1	0	-1.823400	-3.396374	-2.962953
39	1	0	-4.320127	-4.535994	-1.411792
40	1	0	-4.752919	-2.982843	-0.659920
41	1	0	-4.252425	-3.038086	-2.363368
42	6	0	-5.668532	0.058953	2.553671
43	1	0	-7.189773	0.126099	1.024561
44	1	0	-3.932660	0.030501	3.832555
45	1	0	-6.373237	-0.098399	3.365899
46	3	0	1.271566	-0.686856	0.048329
47	1	0	0.715655	0.104764	-2.178223
48	6	0	4.011847	-0.367205	-0.169487
49	6	0	5.443707	-0.540550	0.243676
50	6	0	5.706717	-1.094468	1.503413
51	6	0	6.516338	-0.183639	-0.585678
52	6	0	7.019730	-1.265308	1.936654
53	1	0	4.867738	-1.382466	2.127961
54	6	0	7.830376	-0.364274	-0.155375
55	1	0	6.330039	0.203678	-1.583893
56	6	0	8.084189	-0.899253	1.109120
57	1	0	7.214077	-1.686616	2.919254
58	1	0	8.654903	-0.094621	-0.809726
59	1	0	9.108406	-1.037041	1.445451
60	7	0	3.726890	0.550323	-1.107729
61	1	0	4.422519	1.229319	-1.377902
62	8	0	3.124694	-1.076398	0.355746
63	1	0	2.711052	0.698448	-1.347448

Zero-point correction= 0.509168 (Hartree/Particle)
Thermal correction to Energy= 0.541894
Thermal correction to Enthalpy= 0.542838
Thermal correction to Gibbs Free Energy= 0.441024
Sum of electronic and zero-point Energies= -1501.030063
Sum of electronic and thermal Energies= -1500.997337
Sum of electronic and thermal Enthalpies= -1500.996393
Sum of electronic and thermal Free Energies= -1501.098207
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1501.352516

TS2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.604756	0.669623	-1.941485
2	8	0	0.303790	0.775909	0.752640
3	6	0	-0.744412	1.015754	0.174095
4	6	0	-1.152325	2.442323	-0.073460
5	7	0	-1.577388	-0.011344	-0.322912

6	6	0	-2.164758	3.085376	0.648724
7	6	0	-0.378585	3.154190	-1.003192
8	6	0	-1.108726	-1.342244	-0.355078
9	6	0	-2.926946	0.279832	-0.843293
10	6	0	-2.408833	4.442771	0.434774
11	1	0	-2.754533	2.536376	1.376971
12	6	0	-0.644559	4.506289	-1.218699
13	1	0	0.411676	2.630312	-1.539397
14	8	0	0.062390	-1.667368	-0.255663
15	8	0	-2.126437	-2.183080	-0.534941
16	1	0	-2.898212	1.294432	-1.244913
17	1	0	-3.107106	-0.391862	-1.684757
18	6	0	-4.060521	0.156115	0.163955
19	6	0	-1.653888	5.152333	-0.500889
20	1	0	-3.188346	4.943942	1.002051
21	1	0	-0.052447	5.058880	-1.943205
22	6	0	-1.919644	-3.653543	-0.660976
23	6	0	-5.363324	0.433884	-0.271834
24	6	0	-3.861078	-0.212812	1.497048
25	1	0	-1.849046	6.208587	-0.666477
26	6	0	-1.325022	-4.198631	0.639397
27	6	0	-1.048844	-3.952679	-1.883408
28	6	0	-3.349365	-4.156745	-0.866008
29	6	0	-6.442523	0.345820	0.605392
30	1	0	-5.533570	0.723693	-1.307072
31	6	0	-4.941976	-0.299071	2.379134
32	1	0	-2.860181	-0.436801	1.854029
33	1	0	-1.295281	-5.292562	0.589097
34	1	0	-0.310895	-3.830619	0.802319
35	1	0	-1.949835	-3.915921	1.493321
36	1	0	-0.025810	-3.599466	-1.745935
37	1	0	-1.023547	-5.035413	-2.048328
38	1	0	-1.471989	-3.485426	-2.779410
39	1	0	-3.348444	-5.247874	-0.954094
40	1	0	-3.983737	-3.875421	-0.019972
41	1	0	-3.783555	-3.737084	-1.779204
42	6	0	-6.234761	-0.021098	1.937550
43	1	0	-7.445651	0.565822	0.249908
44	1	0	-4.768078	-0.586143	3.412739
45	1	0	-7.074506	-0.088712	2.623618
46	3	0	1.581637	-0.368130	-0.333759
47	1	0	1.564789	0.159148	-2.765037
48	6	0	4.263130	-0.013269	-0.332625
49	6	0	5.654498	-0.111455	0.242880
50	6	0	5.802197	-0.531721	1.571174
51	6	0	6.801734	0.188079	-0.504248
52	6	0	7.067212	-0.624014	2.148793
53	1	0	4.908304	-0.781665	2.132885
54	6	0	8.069608	0.084086	0.068228
55	1	0	6.707569	0.477111	-1.547889
56	6	0	8.205087	-0.315800	1.399100
57	1	0	7.167395	-0.940501	3.184050
58	1	0	8.951360	0.309585	-0.526293
59	1	0	9.192497	-0.393324	1.847241
60	7	0	4.018189	0.800185	-1.351425
61	1	0	4.777291	1.407338	-1.635949
62	8	0	3.356043	-0.726004	0.193500
63	1	0	2.808750	0.830829	-1.750262

Zero-point correction=	0.505173 (Hartree/Particle)
Thermal correction to Energy=	0.538515
Thermal correction to Enthalpy=	0.539459
Thermal correction to Gibbs Free Energy=	0.434769
Sum of electronic and zero-point Energies=	-1501.038464
Sum of electronic and thermal Energies=	-1501.005123
Sum of electronic and thermal Enthalpies=	-1501.004179
Sum of electronic and thermal Free Energies=	-1501.108868

M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1501.361095

TS3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.444397	-4.085024	-2.236226
2	8	0	0.499981	-0.622094	-2.365377
3	6	0	0.190809	0.238538	-1.511961
4	6	0	0.733245	1.651395	-1.716656
5	7	0	-1.174254	0.147708	-0.937264
6	6	0	0.750471	2.663440	-0.742731
7	6	0	1.299467	1.917200	-2.969565
8	6	0	-1.701505	-1.099260	-0.694033
9	6	0	-2.047388	1.318217	-0.761470
10	6	0	1.317120	3.906854	-1.020656
11	1	0	0.312892	2.492132	0.236297
12	6	0	1.863060	3.162925	-3.248132
13	1	0	1.299062	1.126831	-3.711456
14	8	0	-1.094701	-2.167869	-0.783584
15	8	0	-2.992175	-1.014823	-0.326591
16	1	0	-1.594904	2.144794	-1.310304
17	1	0	-3.003337	1.109339	-1.248990
18	6	0	-2.306992	1.738104	0.679409
19	6	0	1.875715	4.162321	-2.275334
20	1	0	1.321120	4.676652	-0.253408
21	1	0	2.296416	3.349126	-4.227327
22	6	0	-3.775416	-2.196238	0.086525
23	6	0	-3.288139	2.707786	0.926280
24	6	0	-1.597150	1.207425	1.762045
25	1	0	2.317642	5.131808	-2.489638
26	6	0	-3.143167	-2.832860	1.327966
27	6	0	-3.908730	-3.178378	-1.081374
28	6	0	-5.133045	-1.576361	0.429542
29	6	0	-3.552883	3.142195	2.224331
30	1	0	-3.851982	3.124967	0.093774
31	6	0	-1.863154	1.641448	3.064142
32	1	0	-0.833060	0.455049	1.584555
33	1	0	-3.801719	-3.622112	1.707691
34	1	0	-2.169180	-3.268609	1.100320
35	1	0	-3.019955	-2.082446	2.116008
36	1	0	-2.947351	-3.624673	-1.338398
37	1	0	-4.606733	-3.977303	-0.806584
38	1	0	-4.308667	-2.667923	-1.964272
39	1	0	-5.823145	-2.354033	0.773025
40	1	0	-5.026305	-0.828500	1.221191
41	1	0	-5.569714	-1.090219	-0.449001
42	6	0	-2.839628	2.608731	3.300783
43	1	0	-4.318266	3.894762	2.396047
44	1	0	-1.302799	1.218536	3.894168
45	1	0	-3.045654	2.944242	4.313691
46	3	0	0.589006	-2.359329	-1.660791
47	1	0	1.041458	-4.863677	-1.822091
48	6	0	2.179354	-1.126021	0.171768
49	6	0	3.433644	-0.931091	0.989918
50	6	0	4.035266	-2.051171	1.579278
51	6	0	4.028871	0.326447	1.162270
52	6	0	5.190756	-1.915110	2.346186
53	1	0	3.580435	-3.024369	1.426069
54	6	0	5.194292	0.461811	1.916978
55	1	0	3.599842	1.201300	0.679992
56	6	0	5.774164	-0.657252	2.517299
57	1	0	5.640072	-2.790640	2.807998
58	1	0	5.652781	1.440722	2.030455
59	1	0	6.679309	-0.550904	3.109575
60	7	0	1.273801	-0.157525	0.120175

61	1	0	1.563021	0.676082	0.622769
62	8	0	2.028027	-2.242898	-0.410114
63	1	0	2.116435	-3.779139	-1.591869

Zero-point correction= 0.509761 (Hartree/Particle)
Thermal correction to Energy= 0.542577
Thermal correction to Enthalpy= 0.543521
Thermal correction to Gibbs Free Energy= 0.442887
Sum of electronic and zero-point Energies= -1501.017385
Sum of electronic and thermal Energies= -1500.984568
Sum of electronic and thermal Enthalpies= -1500.983624
Sum of electronic and thermal Free Energies= -1501.084258
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1501.352099

TS4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.319302	-3.066813	-2.895950
2	8	0	-0.455692	0.148267	-2.660147
3	6	0	0.130273	0.585705	-1.635966
4	6	0	0.632122	2.029222	-1.718235
5	7	0	-1.108860	0.710288	-0.211007
6	6	0	1.759048	2.530060	-1.057072
7	6	0	-0.085154	2.885737	-2.565289
8	6	0	-2.036537	-0.240584	-0.122746
9	6	0	-1.102003	1.840069	0.708331
10	6	0	2.157156	3.858193	-1.233260
11	1	0	2.350884	1.903700	-0.397532
12	6	0	0.304979	4.211591	-2.735478
13	1	0	-0.943132	2.483792	-3.092722
14	8	0	-2.084415	-1.269671	-0.842696
15	8	0	-2.962491	-0.033283	0.863389
16	1	0	-0.878769	2.748596	0.140639
17	1	0	-2.102987	1.974676	1.130680
18	6	0	-0.097144	1.721959	1.850029
19	6	0	1.430531	4.704220	-2.069186
20	1	0	3.038920	4.225789	-0.715057
21	1	0	-0.264573	4.860432	-3.395861
22	6	0	-4.126397	-0.895717	1.067945
23	6	0	0.482666	2.878012	2.390458
24	6	0	0.246145	0.483209	2.406689
25	1	0	1.740578	5.736907	-2.205789
26	6	0	-3.690742	-2.308450	1.477490
27	6	0	-5.024242	-0.890862	-0.175098
28	6	0	-4.842091	-0.209990	2.237942
29	6	0	1.373090	2.801856	3.461801
30	1	0	0.237195	3.846977	1.960900
31	6	0	1.143356	0.401929	3.474701
32	1	0	-0.194940	-0.422657	2.001110
33	1	0	-4.569066	-2.900433	1.759419
34	1	0	-3.168083	-2.815484	0.665811
35	1	0	-3.022161	-2.259391	2.343990
36	1	0	-4.519546	-1.335682	-1.033796
37	1	0	-5.942143	-1.454991	0.025672
38	1	0	-5.305668	0.135607	-0.433928
39	1	0	-5.749814	-0.762177	2.504213
40	1	0	-4.189719	-0.168048	3.116094
41	1	0	-5.124413	0.813368	1.970307
42	6	0	1.709068	1.560987	4.007841
43	1	0	1.811851	3.711384	3.864773
44	1	0	1.397693	-0.569647	3.891152
45	1	0	2.407143	1.498635	4.838557
46	3	0	-1.070035	-1.577709	-2.463512
47	1	0	-2.717147	-2.839282	-2.033944
48	6	0	1.318737	-1.625348	-1.207771

49	6	0	2.472184	-2.232657	-0.460113
50	6	0	2.420995	-3.604017	-0.175222
51	6	0	3.596994	-1.492878	-0.067518
52	6	0	3.462549	-4.219702	0.514299
53	1	0	1.556240	-4.171063	-0.503009
54	6	0	4.643806	-2.112641	0.614449
55	1	0	3.676644	-0.440919	-0.326648
56	6	0	4.575571	-3.474657	0.912488
57	1	0	3.409107	-5.281381	0.739323
58	1	0	5.516111	-1.533384	0.904024
59	1	0	5.390837	-3.956103	1.445815
60	7	0	1.113477	-0.300113	-0.984871
61	1	0	1.544439	0.070161	-0.148447
62	8	0	0.629294	-2.338690	-1.956485
63	1	0	-1.796602	-3.867449	-2.727995

Zero-point correction= 0.509134 (Hartree/Particle)
Thermal correction to Energy= 0.542356
Thermal correction to Enthalpy= 0.543300
Thermal correction to Gibbs Free Energy= 0.439608
Sum of electronic and zero-point Energies= -1501.020739
Sum of electronic and thermal Energies= -1500.987516
Sum of electronic and thermal Enthalpies= -1500.986572
Sum of electronic and thermal Free Energies= -1501.090264
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1501.355762

Li^+_1a2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.910268	-0.206138	0.196709
2	6	0	-5.373981	-0.011307	0.359118
3	6	0	-5.823810	1.226111	0.843726
4	6	0	-6.308366	-1.009698	0.038300
5	6	0	-7.185111	1.452726	1.026775
6	1	0	-5.096122	1.995239	1.078550
7	6	0	-7.669855	-0.775737	0.214008
8	1	0	-5.987431	-1.956247	-0.388402
9	6	0	-8.109026	0.452576	0.714324
10	1	0	-7.526607	2.409084	1.411189
11	1	0	-8.387933	-1.547181	-0.046904
12	1	0	-9.171211	0.631758	0.853237
13	7	0	-3.430255	-1.465495	0.141244
14	1	0	-4.010531	-2.264964	0.345171
15	8	0	-3.135216	0.774227	0.112988
16	1	0	-2.429707	-1.604195	0.048265
17	8	0	-0.327362	-0.644605	-0.070232
18	6	0	0.805375	-0.841830	-0.529403
19	6	0	1.173256	-2.209084	-0.982190
20	7	0	1.752834	0.185019	-0.660265
21	6	0	0.788997	-3.301782	-0.189435
22	6	0	1.775611	-2.429940	-2.231989
23	6	0	1.338776	1.530798	-0.721075
24	6	0	3.214623	-0.142897	-0.478043
25	6	0	1.038590	-4.600148	-0.626770
26	1	0	0.319350	-3.124473	0.773143
27	6	0	1.995954	-3.731866	-2.676256
28	1	0	2.040767	-1.588618	-2.866407
29	8	0	0.158007	1.876900	-0.779053
30	8	0	2.363312	2.355223	-0.753677
31	1	0	3.442247	-1.002051	-1.103884
32	1	0	3.766714	0.708067	-0.868649
33	6	0	3.573032	-0.433497	0.964774
34	6	0	1.638619	-4.816214	-1.870374
35	1	0	0.762506	-5.443507	-0.001119
36	1	0	2.444101	-3.900262	-3.650660

37	6	0	2.218517	3.851151	-0.938650
38	6	0	3.549929	0.578382	1.936288
39	6	0	3.951705	-1.727591	1.342360
40	1	0	1.823699	-5.829616	-2.214048
41	6	0	1.442653	4.436268	0.240119
42	6	0	1.562029	4.123413	-2.290812
43	6	0	3.677426	4.303487	-0.925217
44	6	0	3.889118	0.296655	3.258634
45	1	0	3.280822	1.592790	1.654788
46	6	0	4.299248	-2.008471	2.665344
47	1	0	3.984717	-2.518799	0.597649
48	1	0	1.473753	5.528716	0.172689
49	1	0	0.396876	4.124923	0.236770
50	1	0	1.902463	4.148473	1.191335
51	1	0	0.522665	3.791399	-2.315022
52	1	0	1.580871	5.201603	-2.480276
53	1	0	2.116935	3.632679	-3.097017
54	1	0	3.722998	5.388487	-1.059468
55	1	0	4.158646	4.055504	0.025833
56	1	0	4.241428	3.834371	-1.737122
57	6	0	4.264486	-0.998191	3.626121
58	1	0	3.872405	1.089538	4.000983
59	1	0	4.599149	-3.015108	2.942042
60	1	0	4.535548	-1.214747	4.655326
61	3	0	-1.337417	0.967819	-0.134459

Zero-point correction= 0.497994 (Hartree/Particle)
Thermal correction to Energy= 0.529988
Thermal correction to Enthalpy= 0.530932
Thermal correction to Gibbs Free Energy= 0.428487
Sum of electronic and zero-point Energies= -1425.059462
Sum of electronic and thermal Energies= -1425.027468
Sum of electronic and thermal Enthalpies= -1425.026524
Sum of electronic and thermal Free Energies= -1425.128969
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1425.380697

OH_anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.109707
2	1	0	0.000000	0.000000	-0.877653

Zero-point correction= 0.007784 (Hartree/Particle)
Thermal correction to Energy= 0.010145
Thermal correction to Enthalpy= 0.011089
Thermal correction to Gibbs Free Energy= -0.008512
Sum of electronic and zero-point Energies= -75.712989
Sum of electronic and thermal Energies= -75.710629
Sum of electronic and thermal Enthalpies= -75.709685
Sum of electronic and thermal Free Energies= -75.729285
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-75.849228

LiOH_1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.177876	-0.257696	-0.164735
2	3	0	-3.371476	1.187568	0.292663
3	1	0	-4.872792	-0.795196	0.232895
4	6	0	-0.961512	0.087043	0.041659
5	6	0	0.535294	0.004212	0.021012
6	6	0	1.264189	1.188804	-0.149029
7	6	0	1.224815	-1.206577	0.178993
8	6	0	2.656568	1.160263	-0.186376

9	1	0	0.720637	2.121779	-0.252067
10	6	0	2.618445	-1.233138	0.151650
11	1	0	0.678442	-2.128826	0.358097
12	6	0	3.336727	-0.050722	-0.037697
13	1	0	3.212367	2.083051	-0.328612
14	1	0	3.143047	-2.175147	0.285547
15	1	0	4.422944	-0.072522	-0.061929
16	7	0	-1.679464	-1.000737	-0.244089
17	1	0	-1.216398	-1.825427	-0.597205
18	8	0	-1.509811	1.187589	0.329105
19	1	0	-2.763220	-0.903712	-0.242319

Zero-point correction= 0.142152 (Hartree/Particle)
Thermal correction to Energy= 0.152859
Thermal correction to Enthalpy= 0.153804
Thermal correction to Gibbs Free Energy= 0.105572
Sum of electronic and zero-point Energies= -484.240100
Sum of electronic and thermal Energies= -484.229392
Sum of electronic and thermal Enthalpies= -484.228448
Sum of electronic and thermal Free Energies= -484.276679
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-484.336324

LiOH_2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.203437	-3.927637	-0.509294
2	8	0	0.988715	-1.858736	1.629615
3	6	0	1.105973	-1.045741	0.721211
4	6	0	2.471272	-0.608419	0.276896
5	7	0	-0.024697	-0.543304	0.035401
6	6	0	2.996271	0.662985	0.537537
7	6	0	3.253683	-1.602891	-0.334035
8	6	0	-1.279898	-1.158449	0.211805
9	6	0	0.098939	0.551355	-0.947056
10	6	0	4.314656	0.947788	0.179070
11	1	0	2.389563	1.421615	1.023589
12	6	0	4.563381	-1.293097	-0.701930
13	1	0	2.800907	-2.586124	-0.512944
14	8	0	-1.445759	-2.274931	0.683313
15	8	0	-2.250843	-0.364511	-0.233221
16	1	0	1.096313	0.471605	-1.383469
17	1	0	-0.616228	0.354541	-1.748033
18	6	0	-0.115445	1.953412	-0.397950
19	6	0	5.095826	-0.027119	-0.444627
20	1	0	4.728844	1.930147	0.389285
21	1	0	5.174856	-2.051260	-1.184340
22	6	0	-3.675572	-0.798955	-0.265801
23	6	0	0.075619	3.037927	-1.265083
24	6	0	-0.490758	2.206774	0.924156
25	1	0	6.121187	0.199529	-0.725866
26	6	0	-4.167748	-1.040628	1.163034
27	6	0	-3.821720	-2.030527	-1.162358
28	6	0	-4.363464	0.419025	-0.884563
29	6	0	-0.105193	4.346296	-0.820768
30	1	0	0.372224	2.855457	-2.296217
31	6	0	-0.668209	3.518592	1.372830
32	1	0	-0.645200	1.380147	1.611059
33	1	0	-5.245171	-1.237566	1.143209
34	1	0	-3.666626	-1.894822	1.620799
35	1	0	-3.997010	-0.153149	1.781572
36	1	0	-3.326445	-2.903068	-0.733868
37	1	0	-4.885887	-2.259163	-1.286063
38	1	0	-3.400621	-1.835383	-2.154406
39	1	0	-5.441975	0.242516	-0.947941
40	1	0	-4.191231	1.311980	-0.276018

41	1	0	-3.984784	0.609692	-1.893739
42	6	0	-0.477859	4.591628	0.503376
43	1	0	0.049097	5.174888	-1.506810
44	1	0	-0.956768	3.697364	2.405252
45	1	0	-0.615998	5.611089	0.852820
46	3	0	0.160284	-3.440483	0.740774
47	1	0	1.110070	-4.588675	-1.205747

Zero-point correction= 0.379456 (Hartree/Particle)
Thermal correction to Energy= 0.404662
Thermal correction to Enthalpy= 0.405606
Thermal correction to Gibbs Free Energy= 0.322734
Sum of electronic and zero-point Energies= -1100.165738
Sum of electronic and thermal Energies= -1100.140532
Sum of electronic and thermal Enthalpies= -1100.139588
Sum of electronic and thermal Free Energies= -1100.222460
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1100.415180

INT1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.399750	0.106745	0.028202
2	6	0	-1.060981	0.342009	-0.026298
3	6	0	-2.514461	-0.055036	-0.010145
4	6	0	-3.457089	0.903916	0.383023
5	6	0	-2.959347	-1.328558	-0.391649
6	6	0	-4.813532	0.588530	0.423351
7	1	0	-3.103128	1.893042	0.654075
8	6	0	-4.318301	-1.641785	-0.363022
9	1	0	-2.249570	-2.072180	-0.744563
10	6	0	-5.247806	-0.686251	0.051583
11	1	0	-5.534120	1.337565	0.741227
12	1	0	-4.650951	-2.629469	-0.670950
13	1	0	-6.306264	-0.931594	0.077589
14	7	0	-0.141183	-0.624133	0.076291
15	1	0	-0.445615	-1.568194	0.267289
16	8	0	-0.762582	1.554842	-0.131277
17	1	0	0.927957	-0.404519	0.066948
18	6	0	3.406314	-0.847739	0.089187
19	6	0	3.304215	-1.817279	-1.114122
20	1	0	4.095472	-2.579259	-1.115538
21	1	0	2.336037	-2.333822	-1.103464
22	1	0	3.367725	-1.251638	-2.052012
23	6	0	3.302610	-1.657249	1.405425
24	1	0	2.339228	-2.180769	1.454856
25	1	0	4.099389	-2.406328	1.509488
26	1	0	3.354192	-0.975653	2.263284
27	6	0	4.786262	-0.148647	0.046367
28	1	0	4.879036	0.433154	-0.880606
29	1	0	4.879254	0.542606	0.894526
30	1	0	5.626457	-0.854776	0.089235
31	19	0	1.668870	2.376137	-0.217001

Zero-point correction= 0.252294 (Hartree/Particle)
Thermal correction to Energy= 0.269531
Thermal correction to Enthalpy= 0.270475
Thermal correction to Gibbs Free Energy= 0.203666
Sum of electronic and zero-point Energies= -1233.735397
Sum of electronic and thermal Energies= -1233.718161
Sum of electronic and thermal Enthalpies= -1233.717217
Sum of electronic and thermal Free Energies= -1233.784026
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1233.925844

INT2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.129594	1.798424	1.790136
2	8	0	-0.507348	0.569945	-1.746677
3	6	0	0.670428	0.712582	-1.422398
4	6	0	1.420608	1.913503	-1.918335
5	7	0	1.332422	-0.187030	-0.575542
6	6	0	1.416403	2.199442	-3.289856
7	6	0	1.979479	2.818003	-1.000201
8	6	0	0.589324	-0.988044	0.317754
9	6	0	2.808129	-0.219511	-0.472744
10	6	0	2.014604	3.369264	-3.754227
11	1	0	0.948515	1.505931	-3.983026
12	6	0	2.549235	3.999671	-1.477986
13	1	0	1.908554	2.590096	0.073368
14	8	0	-0.620931	-0.923498	0.462122
15	8	0	1.403865	-1.818799	0.964460
16	1	0	3.177850	0.655943	-1.005280
17	1	0	3.074117	-0.090075	0.576766
18	6	0	3.441818	-1.465186	-1.064697
19	6	0	2.580649	4.270625	-2.847960
20	1	0	2.030566	3.583027	-4.819532
21	1	0	2.968791	4.712056	-0.772071
22	6	0	0.899306	-2.823459	1.930131
23	6	0	4.572646	-2.019346	-0.453737
24	6	0	2.968787	-2.040611	-2.249858
25	1	0	3.037986	5.187472	-3.211380
26	6	0	0.044868	-3.847953	1.178614
27	6	0	0.140010	-2.144902	3.072967
28	6	0	2.196348	-3.455641	2.439987
29	6	0	5.219201	-3.122044	-1.014261
30	1	0	4.946947	-1.584779	0.470357
31	6	0	3.608287	-3.147941	-2.808726
32	1	0	2.088922	-1.627348	-2.736493
33	1	0	-0.246144	-4.652659	1.862897
34	1	0	-0.861971	-3.387951	0.780049
35	1	0	0.614714	-4.289554	0.354144
36	1	0	-0.831953	-1.774535	2.744664
37	1	0	-0.014469	-2.870662	3.879680
38	1	0	0.720893	-1.306492	3.468657
39	1	0	1.964706	-4.270772	3.133437
40	1	0	2.783580	-3.856959	1.608616
41	1	0	2.804720	-2.714155	2.967662
42	6	0	4.737208	-3.692157	-2.193833
43	1	0	6.095567	-3.539161	-0.524843
44	1	0	3.224867	-3.584200	-3.727633
45	1	0	5.236246	-4.553692	-2.629369
46	6	0	1.708864	2.225612	2.964016
47	6	0	2.978653	1.390925	3.288771
48	1	0	2.714505	0.327588	3.355878
49	1	0	3.709731	1.503399	2.477895
50	1	0	3.465647	1.684928	4.229574
51	6	0	2.125372	3.719594	2.872523
52	1	0	2.858394	3.855359	2.066915
53	1	0	1.247223	4.333832	2.631860
54	1	0	2.568936	4.105406	3.801600
55	6	0	0.721696	2.081017	4.158512
56	1	0	-0.165514	2.710466	3.989654
57	1	0	0.386812	1.038415	4.240267
58	1	0	1.153405	2.375775	5.125578
59	19	0	-1.267414	1.681793	1.105465
60	6	0	-4.090257	0.100211	-0.498263
61	6	0	-5.543507	-0.274832	-0.564792
62	6	0	-6.338521	-0.017438	0.559698
63	6	0	-6.131751	-0.844756	-1.702881
64	6	0	-7.691474	-0.348643	0.557400

65	1	0	-5.875608	0.443237	1.426118
66	6	0	-7.488725	-1.166746	-1.708480
67	1	0	-5.543448	-1.004941	-2.602512
68	6	0	-8.269174	-0.925770	-0.576253
69	1	0	-8.297421	-0.153833	1.438056
70	1	0	-7.937443	-1.597803	-2.599225
71	1	0	-9.325801	-1.179574	-0.580307
72	7	0	-3.251460	-0.543018	-1.341144
73	1	0	-3.553076	-1.366855	-1.837988
74	8	0	-3.698422	0.969863	0.294350
75	1	0	-2.250352	-0.350961	-1.301510

Zero-point correction= 0.618786 (Hartree/Particle)
Thermal correction to Energy= 0.660053
Thermal correction to Enthalpy= 0.660997
Thermal correction to Gibbs Free Energy= 0.536477
Sum of electronic and zero-point Energies= -2250.508602
Sum of electronic and thermal Energies= -2250.467334
Sum of electronic and thermal Enthalpies= -2250.466390
Sum of electronic and thermal Free Energies= -2250.590910
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.930873

INT3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.409351	-1.336964	-0.902948
2	8	0	-0.842760	0.169637	-1.493097
3	6	0	-1.852537	0.058027	-0.680562
4	6	0	-2.996002	1.068931	-0.984822
5	7	0	-1.409941	0.150664	0.809672
6	6	0	-2.956811	1.678349	-2.244841
7	6	0	-4.072549	1.381888	-0.141105
8	6	0	-0.571649	-0.820810	1.290391
9	6	0	-1.404659	1.461330	1.499324
10	6	0	-3.958758	2.558524	-2.655902
11	1	0	-2.115018	1.445092	-2.886989
12	6	0	-5.070957	2.272585	-0.541087
13	1	0	-4.140707	0.938061	0.846727
14	8	0	-0.220998	-1.844289	0.702065
15	8	0	-0.177455	-0.541641	2.564479
16	1	0	-2.228345	2.039835	1.087978
17	1	0	-1.626188	1.292663	2.555241
18	6	0	-0.140793	2.303531	1.378950
19	6	0	-5.021852	2.862406	-1.805038
20	1	0	-3.903441	3.013588	-3.642091
21	1	0	-5.887760	2.503164	0.138629
22	6	0	0.749019	-1.418339	3.293530
23	6	0	0.594738	2.645223	2.520272
24	6	0	0.260677	2.830931	0.142369
25	1	0	-5.799672	3.554006	-2.118545
26	6	0	2.100775	-1.484829	2.573698
27	6	0	0.128103	-2.805082	3.501360
28	6	0	0.897120	-0.700412	4.639375
29	6	0	1.710752	3.481117	2.436079
30	1	0	0.284487	2.255170	3.485915
31	6	0	1.375951	3.667233	0.054080
32	1	0	-0.290160	2.561838	-0.753683
33	1	0	2.826609	-2.013272	3.202638
34	1	0	2.016226	-2.006791	1.619917
35	1	0	2.480515	-0.474460	2.389021
36	1	0	0.019393	-3.333849	2.554012
37	1	0	0.766317	-3.397187	4.167493
38	1	0	-0.857784	-2.712995	3.970944
39	1	0	1.553863	-1.274266	5.301820
40	1	0	1.330558	0.294845	4.501496

41	1	0	-0.076786	-0.590777	5.127891
42	6	0	2.106793	3.994623	1.200483
43	1	0	2.266943	3.733105	3.335586
44	1	0	1.664400	4.076555	-0.911548
45	1	0	2.969718	4.652159	1.131563
46	6	0	-3.523067	-2.071981	-0.342942
47	6	0	-3.688764	-1.947979	1.180372
48	1	0	-2.787280	-2.284288	1.699097
49	1	0	-3.906517	-0.928144	1.499036
50	1	0	-4.523040	-2.582717	1.502805
51	6	0	-4.833458	-1.729349	-1.076236
52	1	0	-5.192108	-0.727150	-0.838605
53	1	0	-4.675497	-1.783047	-2.158860
54	1	0	-5.619306	-2.445582	-0.805359
55	6	0	-3.157239	-3.536796	-0.660226
56	1	0	-3.050352	-3.678033	-1.743627
57	1	0	-2.218358	-3.806587	-0.163771
58	1	0	-3.937523	-4.223634	-0.312595
59	19	0	-0.163367	-2.299030	-1.912700
60	6	0	2.777326	-0.534167	-1.671372
61	6	0	4.260531	-0.304408	-1.551519
62	6	0	5.105186	-1.409895	-1.717410
63	6	0	4.827322	0.953803	-1.302624
64	6	0	6.487060	-1.267247	-1.615183
65	1	0	4.653709	-2.373512	-1.928072
66	6	0	6.211191	1.098241	-1.206988
67	1	0	4.198142	1.834435	-1.206911
68	6	0	7.043757	-0.012193	-1.358039
69	1	0	7.131138	-2.133838	-1.738885
70	1	0	6.639017	2.079626	-1.020717
71	1	0	8.121921	0.101583	-1.281683
72	7	0	1.958634	0.414692	-1.183763
73	1	0	2.312628	1.191486	-0.645936
74	8	0	2.352092	-1.575576	-2.206744
75	1	0	0.927912	0.318141	-1.236368

Zero-point correction= 0.621947 (Hartree/Particle)
Thermal correction to Energy= 0.661051
Thermal correction to Enthalpy= 0.661995
Thermal correction to Gibbs Free Energy= 0.547565
Sum of electronic and zero-point Energies= -2250.505112
Sum of electronic and thermal Energies= -2250.466009
Sum of electronic and thermal Enthalpies= -2250.465065
Sum of electronic and thermal Free Energies= -2250.579495
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.944486

INT4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-5.063583	-1.855757	0.499717
2	8	0	-2.959671	-1.356782	-0.185535
3	6	0	-4.077881	-1.007310	0.178590
4	6	0	-4.495202	0.417576	0.313786
5	7	0	2.075894	-1.116239	0.469858
6	6	0	-3.571358	1.424033	-0.007281
7	6	0	-5.781683	0.768650	0.754191
8	6	0	2.506958	-2.007406	-0.418923
9	6	0	2.767381	-0.976949	1.752199
10	6	0	-3.933619	2.764260	0.112746
11	1	0	-2.573781	1.170400	-0.349730
12	6	0	-6.136342	2.110024	0.872436
13	1	0	-6.493664	-0.010220	1.001288
14	8	0	1.916288	-2.256358	-1.501206
15	8	0	3.677608	-2.679770	-0.094508
16	1	0	2.009463	-0.870031	2.541865

17	1	0	3.355223	-1.871614	1.993773
18	6	0	3.679001	0.243392	1.820815
19	6	0	-5.213481	3.109466	0.552117
20	1	0	-3.210789	3.535256	-0.138658
21	1	0	-7.132573	2.376431	1.214578
22	6	0	4.180508	-3.790899	-0.890485
23	6	0	4.764859	0.375170	0.940140
24	6	0	3.435173	1.279761	2.729996
25	1	0	-5.492823	4.155717	0.645633
26	6	0	4.593434	-3.312120	-2.288698
27	6	0	3.146355	-4.923375	-0.956515
28	6	0	5.412680	-4.246211	-0.099094
29	6	0	5.576493	1.509153	0.969206
30	1	0	4.963405	-0.423373	0.230976
31	6	0	4.245844	2.418792	2.764745
32	1	0	2.594362	1.196405	3.416070
33	1	0	5.056717	-4.134758	-2.847136
34	1	0	3.724756	-2.946632	-2.837229
35	1	0	5.327403	-2.501739	-2.208134
36	1	0	2.262107	-4.601229	-1.508295
37	1	0	3.579619	-5.799885	-1.453125
38	1	0	2.846615	-5.219482	0.055745
39	1	0	5.901360	-5.088838	-0.601206
40	1	0	6.136198	-3.428792	-0.010983
41	1	0	5.128452	-4.560863	0.910799
42	6	0	5.318867	2.539138	1.880403
43	1	0	6.414952	1.590669	0.281316
44	1	0	4.037603	3.209812	3.481661
45	1	0	5.952677	3.422159	1.903066
46	6	0	-4.907253	-3.325620	0.465376
47	6	0	-6.289759	-3.812681	0.906794
48	1	0	-6.528286	-3.442584	1.908934
49	1	0	-7.062611	-3.462725	0.215007
50	1	0	-6.312567	-4.907090	0.926921
51	6	0	-4.603399	-3.788050	-0.963105
52	1	0	-5.356736	-3.401344	-1.657788
53	1	0	-3.617811	-3.455569	-1.292571
54	1	0	-4.633530	-4.882417	-1.004881
55	6	0	-3.834549	-3.759616	1.468861
56	1	0	-2.844691	-3.406360	1.175547
57	1	0	-4.065902	-3.372383	2.466897
58	1	0	-3.811093	-4.853406	1.526276
59	19	0	-0.378673	-1.199577	-0.879986
60	6	0	0.595427	2.153173	-0.840037
61	6	0	0.497896	3.648482	-0.969406
62	6	0	-0.460917	4.170151	-1.848482
63	6	0	1.300227	4.529646	-0.230865
64	6	0	-0.600632	5.547662	-2.004910
65	1	0	-1.083757	3.476180	-2.403459
66	6	0	1.153438	5.908855	-0.381426
67	1	0	2.020450	4.146873	0.487558
68	6	0	0.207758	6.420397	-1.271920
69	1	0	-1.338421	5.941757	-2.698843
70	1	0	1.774287	6.583505	0.201796
71	1	0	0.097802	7.495094	-1.390678
72	7	0	1.754110	1.637882	-0.405997
73	1	0	2.551367	2.223708	-0.205696
74	8	0	-0.382278	1.437466	-1.142484
75	1	0	1.844732	0.622158	-0.179967

Zero-point correction=	0.619987 (Hartree/Particle)
Thermal correction to Energy=	0.661047
Thermal correction to Enthalpy=	0.661991
Thermal correction to Gibbs Free Energy=	0.535526
Sum of electronic and zero-point Energies=	-2250.551905
Sum of electronic and thermal Energies=	-2250.510845
Sum of electronic and thermal Enthalpies=	-2250.509901

Sum of electronic and thermal Free Energies= -2250.636366
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.963451

INT5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	5.383926	-1.464770	0.991871
2	8	0	3.172258	-1.135444	0.611268
3	6	0	4.348754	-0.891203	0.362054
4	6	0	4.790742	0.075680	-0.681880
5	7	0	-2.990653	-0.437544	-0.578744
6	6	0	3.835565	0.920518	-1.268457
7	6	0	6.130853	0.142858	-1.097191
8	6	0	-2.762462	-1.758392	-0.698750
9	6	0	-4.221238	0.267624	-0.916489
10	6	0	4.221423	1.814068	-2.266258
11	1	0	2.797882	0.909259	-0.947528
12	6	0	6.506768	1.036087	-2.097087
13	1	0	6.866447	-0.508346	-0.638964
14	8	0	-1.674843	-2.291649	-0.435062
15	8	0	-3.852116	-2.441394	-1.135933
16	1	0	-3.946978	1.159507	-1.492184
17	1	0	-4.815042	-0.375259	-1.570188
18	6	0	-5.037008	0.686865	0.296499
19	6	0	5.552540	1.871841	-2.684308
20	1	0	3.471532	2.460434	-2.712928
21	1	0	7.543515	1.080233	-2.419379
22	6	0	-3.795524	-3.875585	-1.447346
23	6	0	-5.523274	-0.272297	1.195773
24	6	0	-5.322488	2.035405	0.532738
25	1	0	5.848339	2.567653	-3.465273
26	6	0	-3.494061	-4.682507	-0.179567
27	6	0	-2.775284	-4.137796	-2.560933
28	6	0	-5.216284	-4.163356	-1.942592
29	6	0	-6.276053	0.110665	2.304373
30	1	0	-5.307668	-1.322784	1.018480
31	6	0	-6.078487	2.423238	1.642331
32	1	0	-4.950776	2.789487	-0.158247
33	1	0	-3.569550	-5.754046	-0.397498
34	1	0	-2.491838	-4.465084	0.191687
35	1	0	-4.221469	-4.443997	0.604380
36	1	0	-1.760891	-3.922213	-2.222058
37	1	0	-2.829410	-5.187694	-2.870572
38	1	0	-2.996935	-3.514391	-3.434266
39	1	0	-5.315224	-5.220570	-2.210625
40	1	0	-5.951027	-3.933210	-1.164191
41	1	0	-5.448902	-3.558850	-2.825297
42	6	0	-6.556313	1.461392	2.531653
43	1	0	-6.647741	-0.644744	2.992271
44	1	0	-6.289251	3.476163	1.811389
45	1	0	-7.142804	1.759567	3.396747
46	6	0	5.218212	-2.473677	2.058402
47	6	0	6.666962	-2.803207	2.427433
48	1	0	7.205786	-3.204603	1.563036
49	1	0	7.190491	-1.907373	2.775969
50	1	0	6.688824	-3.551080	3.226840
51	6	0	4.483132	-1.855681	3.252008
52	1	0	4.992743	-0.944418	3.582493
53	1	0	3.449978	-1.609447	3.002153
54	1	0	4.482191	-2.566029	4.086183
55	6	0	4.507203	-3.712307	1.503746
56	1	0	3.471311	-3.493883	1.239647
57	1	0	5.028115	-4.085486	0.615410
58	1	0	4.514994	-4.505458	2.259565
59	19	0	0.555310	-0.930843	0.058603

60	6	0	-0.159430	1.993069	-0.178047
61	6	0	-0.126710	3.508046	-0.058894
62	6	0	1.045400	4.194457	-0.402536
63	6	0	-1.238340	4.251757	0.361360
64	6	0	1.116786	5.582884	-0.300807
65	1	0	1.896101	3.616420	-0.747995
66	6	0	-1.176558	5.643100	0.449136
67	1	0	-2.167832	3.740503	0.600450
68	6	0	0.004407	6.313228	0.124829
69	1	0	2.039165	6.098351	-0.558332
70	1	0	-2.052010	6.204363	0.767013
71	1	0	0.055633	7.396809	0.197272
72	7	0	-0.985242	1.274401	0.580007
73	1	0	-1.476393	1.864691	1.249620
74	8	0	0.636169	1.464418	-1.015923
75	1	0	-2.219502	0.133628	-0.164330

Zero-point correction= 0.620541 (Hartree/Particle)
Thermal correction to Energy= 0.661576
Thermal correction to Enthalpy= 0.662520
Thermal correction to Gibbs Free Energy= 0.535383
Sum of electronic and zero-point Energies= -2250.553745
Sum of electronic and thermal Energies= -2250.512710
Sum of electronic and thermal Enthalpies= -2250.511766
Sum of electronic and thermal Free Energies= -2250.638903
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.964822

INT6b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.109928	-1.346399	1.143774
2	8	0	-2.936357	-1.527230	-0.791608
3	6	0	-3.974788	-1.296504	-0.178978
4	6	0	-5.251348	-0.927936	-0.862512
5	7	0	2.670404	0.053631	-1.379402
6	6	0	-5.279759	-0.918370	-2.263945
7	6	0	-6.408656	-0.592117	-0.144782
8	6	0	1.975833	-0.191037	-0.091371
9	6	0	3.822032	0.965109	-1.363760
10	6	0	-6.447660	-0.577332	-2.940811
11	1	0	-4.380293	-1.185226	-2.808683
12	6	0	-7.575192	-0.248291	-0.824861
13	1	0	-6.385425	-0.600276	0.938696
14	8	0	1.060682	-1.092090	-0.158466
15	8	0	2.996923	-0.288498	0.918151
16	1	0	3.793599	1.533710	-2.305279
17	1	0	3.752529	1.709700	-0.557534
18	6	0	5.172466	0.272807	-1.288205
19	6	0	-7.597145	-0.240502	-2.221511
20	1	0	-6.463313	-0.573535	-4.027119
21	1	0	-8.468357	0.013934	-0.264824
22	6	0	3.180290	-1.490109	1.701795
23	6	0	6.246109	0.885575	-0.631969
24	6	0	5.395998	-0.949399	-1.933884
25	1	0	-8.508681	0.027369	-2.748936
26	6	0	3.417810	-2.725097	0.819073
27	6	0	1.989946	-1.708821	2.651020
28	6	0	4.445596	-1.178275	2.513499
29	6	0	7.513172	0.298163	-0.621385
30	1	0	6.086572	1.831626	-0.117937
31	6	0	6.659559	-1.541562	-1.924939
32	1	0	4.558066	-1.434833	-2.425187
33	1	0	3.629211	-3.599084	1.448668
34	1	0	2.537777	-2.926172	0.206521
35	1	0	4.275411	-2.559242	0.160222

36	1	0	1.086071	-1.907781	2.074236
37	1	0	2.188070	-2.551770	3.325458
38	1	0	1.828435	-0.814093	3.265686
39	1	0	4.696437	-2.017882	3.172423
40	1	0	5.291094	-0.990858	1.844499
41	1	0	4.294282	-0.286234	3.132134
42	6	0	7.725255	-0.919553	-1.269729
43	1	0	8.332150	0.788959	-0.100666
44	1	0	6.813139	-2.493048	-2.429242
45	1	0	8.709214	-1.381866	-1.260507
46	6	0	-3.001581	-1.677706	2.080931
47	6	0	-3.705542	-1.588232	3.437480
48	1	0	-4.073464	-0.572766	3.617380
49	1	0	-4.554101	-2.278643	3.482462
50	1	0	-3.004781	-1.847882	4.237209
51	6	0	-2.510660	-3.101772	1.812809
52	1	0	-3.340163	-3.814878	1.874261
53	1	0	-2.041910	-3.183027	0.831013
54	1	0	-1.767630	-3.374467	2.569798
55	6	0	-1.885250	-0.634839	1.979483
56	1	0	-1.235874	-0.777327	1.113858
57	1	0	-2.307148	0.376084	1.958413
58	1	0	-1.249813	-0.713413	2.868462
59	19	0	-0.648615	-0.998480	-1.953230
60	6	0	0.382692	1.848359	-0.316154
61	6	0	-0.231362	3.070731	0.318286
62	6	0	-0.851631	4.006025	-0.521039
63	6	0	-0.228620	3.298353	1.702007
64	6	0	-1.435099	5.155749	0.007211
65	1	0	-0.863507	3.810033	-1.588132
66	6	0	-0.821177	4.444385	2.232569
67	1	0	0.213880	2.568572	2.374857
68	6	0	-1.420783	5.379008	1.386228
69	1	0	-1.902858	5.878646	-0.656251
70	1	0	-0.818272	4.604513	3.307560
71	1	0	-1.878647	6.273842	1.799675
72	7	0	1.348942	1.215782	0.349469
73	1	0	1.682417	1.582048	1.230284
74	8	0	-0.023122	1.480040	-1.449324
75	1	0	1.955539	0.463053	-1.978147

Zero-point correction= 0.620606 (Hartree/Particle)
Thermal correction to Energy= 0.660731
Thermal correction to Enthalpy= 0.661676
Thermal correction to Gibbs Free Energy= 0.537804
Sum of electronic and zero-point Energies= -2250.501427
Sum of electronic and thermal Energies= -2250.461301
Sum of electronic and thermal Enthalpies= -2250.460357
Sum of electronic and thermal Free Energies= -2250.584228
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.930379

INT7b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.798139	0.631838	0.855059
2	8	0	-3.638374	-1.135487	0.024523
3	6	0	-4.693445	-0.588513	0.334400
4	6	0	-6.023824	-1.245056	0.163582
5	7	0	3.164640	-1.881780	-0.723340
6	6	0	-6.063440	-2.552536	-0.340506
7	6	0	-7.222032	-0.592517	0.489659
8	6	0	1.947059	-1.277266	-0.555037
9	6	0	4.322573	-1.352476	-1.435225
10	6	0	-7.282818	-3.200658	-0.517509
11	1	0	-5.130620	-3.048575	-0.586828

12	6	0	-8.440878	-1.243421	0.310369
13	1	0	-7.190534	0.418370	0.879176
14	8	0	1.026345	-1.949330	-0.027176
15	8	0	3.489166	1.189830	1.305590
16	1	0	4.352535	-1.744944	-2.462908
17	1	0	4.173625	-0.272696	-1.505088
18	6	0	5.622298	-1.686598	-0.729555
19	6	0	-8.473749	-2.546153	-0.192693
20	1	0	-7.306378	-4.214326	-0.907592
21	1	0	-9.366335	-0.733886	0.563249
22	6	0	2.792280	1.204167	2.558908
23	6	0	6.503072	-2.631214	-1.267115
24	6	0	5.952798	-1.058873	0.481181
25	1	0	-9.425963	-3.051022	-0.331056
26	6	0	2.492285	-0.234823	3.012869
27	6	0	1.487916	2.008472	2.423222
28	6	0	3.745603	1.892299	3.541124
29	6	0	7.695737	-2.950847	-0.612738
30	1	0	6.255884	-3.118038	-2.208864
31	6	0	7.143409	-1.377080	1.133410
32	1	0	5.275534	-0.316003	0.898206
33	1	0	1.994354	-0.246541	3.990978
34	1	0	1.842216	-0.745500	2.292942
35	1	0	3.422615	-0.807396	3.095319
36	1	0	0.823086	1.537429	1.689694
37	1	0	0.956505	2.066097	3.381677
38	1	0	1.700559	3.027063	2.081715
39	1	0	3.301878	1.959560	4.541031
40	1	0	4.683605	1.331329	3.615346
41	1	0	3.981648	2.904025	3.194155
42	6	0	8.017454	-2.324033	0.590735
43	1	0	8.370502	-3.686008	-1.044353
44	1	0	7.394466	-0.879670	2.067133
45	1	0	8.945332	-2.567779	1.102200
46	6	0	-3.635308	1.520928	1.124852
47	6	0	-4.313103	2.764820	1.704316
48	1	0	-4.991876	3.214089	0.972269
49	1	0	-4.886270	2.513200	2.602486
50	1	0	-3.555450	3.507543	1.973238
51	6	0	-2.720235	0.869477	2.163944
52	1	0	-3.280659	0.629048	3.074014
53	1	0	-2.262273	-0.044329	1.782237
54	1	0	-1.918930	1.566739	2.429685
55	6	0	-2.917229	1.858683	-0.183209
56	1	0	-2.358412	1.017023	-0.594681
57	1	0	-3.637598	2.204830	-0.932418
58	1	0	-2.203638	2.669644	-0.006029
59	19	0	-1.334051	-1.999089	-0.882536
60	6	0	0.841889	0.566387	-1.527845
61	6	0	0.882397	2.056903	-1.786350
62	6	0	-0.119445	2.616663	-2.592928
63	6	0	1.878295	2.897738	-1.267385
64	6	0	-0.133423	3.982365	-2.872431
65	1	0	-0.877211	1.954482	-2.997930
66	6	0	1.859705	4.265946	-1.541247
67	1	0	2.658633	2.487194	-0.637649
68	6	0	0.857288	4.813557	-2.344718
69	1	0	-0.914207	4.398191	-3.505142
70	1	0	2.635789	4.905348	-1.127735
71	1	0	0.850315	5.879234	-2.560881
72	7	0	1.908939	0.055245	-0.897908
73	1	0	2.903169	0.813800	0.607229
74	8	0	-0.155052	-0.069663	-1.972693
75	1	0	3.205686	-2.834636	-0.386826

Zero-point correction= 0.620655 (Hartree/Particle)
Thermal correction to Energy= 0.661765

Thermal correction to Enthalpy= 0.662709
Thermal correction to Gibbs Free Energy= 0.537358
Sum of electronic and zero-point Energies= -2250.548314
Sum of electronic and thermal Energies= -2250.507204
Sum of electronic and thermal Enthalpies= -2250.506260
Sum of electronic and thermal Free Energies= -2250.631611
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.970043

INT8b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.918891	0.167085	0.234208
2	8	0	-1.065965	-0.991633	-0.361438
3	6	0	-1.624277	0.073024	-0.105352
4	6	0	-0.953918	1.400494	-0.141992
5	6	0	0.450182	1.467355	-0.175617
6	6	0	-1.714828	2.583268	-0.159242
7	6	0	1.069547	2.716590	-0.231492
8	1	0	1.092121	0.581395	-0.127034
9	6	0	-1.082757	3.820877	-0.224417
10	1	0	-2.796770	2.523202	-0.128115
11	8	0	2.753903	-0.810984	-0.155332
12	6	0	0.313024	3.888881	-0.261119
13	1	0	2.154529	2.762231	-0.249094
14	1	0	-1.676368	4.730807	-0.245520
15	6	0	3.979697	-0.496135	0.381661
16	1	0	0.807877	4.855712	-0.309030
17	6	0	3.813206	0.131106	1.791382
18	6	0	4.731598	0.511982	-0.527772
19	6	0	4.855880	-1.771581	0.518362
20	1	0	4.770763	0.382633	2.269486
21	1	0	3.213134	1.047134	1.724766
22	1	0	3.276109	-0.570236	2.442778
23	1	0	4.137048	1.427722	-0.639072
24	1	0	5.721967	0.791853	-0.141063
25	1	0	4.861103	0.079064	-1.528070
26	1	0	5.850941	-1.577357	0.943639
27	1	0	4.345716	-2.499371	1.163966
28	1	0	4.992433	-2.231683	-0.469984
29	6	0	-3.816980	-1.000681	0.320874
30	6	0	-5.149107	-0.362208	0.723481
31	1	0	-5.050704	0.167307	1.676264
32	1	0	-5.481440	0.352546	-0.036265
33	1	0	-5.918111	-1.133970	0.832809
34	6	0	-3.935874	-1.677722	-1.048549
35	1	0	-4.228949	-0.947815	-1.810840
36	1	0	-2.994214	-2.140666	-1.347943
37	1	0	-4.709213	-2.452754	-1.006210
38	6	0	-3.325833	-1.957867	1.411770
39	1	0	-2.371652	-2.413453	1.142522
40	1	0	-3.205283	-1.424241	2.360376
41	1	0	-4.065563	-2.752487	1.560139
42	19	0	1.129725	-2.233559	-1.023678

Zero-point correction= 0.352855 (Hartree/Particle)
Thermal correction to Energy= 0.375958
Thermal correction to Enthalpy= 0.376902
Thermal correction to Gibbs Free Energy= 0.296402
Sum of electronic and zero-point Energies= -1410.737328
Sum of electronic and thermal Energies= -1410.714225
Sum of electronic and thermal Enthalpies= -1410.713281
Sum of electronic and thermal Free Energies= -1410.793782
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1410.990227

3aa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.983504	2.249985	0.096512
2	6	0	0.640938	2.548990	-0.118465
3	6	0	2.485584	1.201629	0.983156
4	8	0	0.271991	3.658719	-0.439852
5	1	0	3.501164	1.501562	1.267556
6	1	0	1.903567	1.162422	1.914661
7	6	0	2.537979	-0.190572	0.365387
8	6	0	2.419178	-1.318692	1.189173
9	6	0	2.745239	-0.374498	-1.007470
10	6	0	2.517971	-2.604543	0.654999
11	1	0	2.253794	-1.188501	2.257019
12	6	0	2.837205	-1.660362	-1.543550
13	1	0	2.824470	0.496531	-1.651513
14	6	0	2.726928	-2.778222	-0.714767
15	1	0	2.426065	-3.468803	1.307407
16	1	0	2.994788	-1.787664	-2.611167
17	1	0	2.797889	-3.778173	-1.133708
18	6	0	-1.596073	1.441651	0.033693
19	6	0	-2.247882	0.082062	0.050510
20	6	0	-3.604965	0.038799	-0.300838
21	6	0	-1.599396	-1.108385	0.410888
22	6	0	-4.294433	-1.170349	-0.314348
23	1	0	-4.096620	0.970688	-0.558946
24	6	0	-2.293810	-2.318495	0.404363
25	1	0	-0.559816	-1.112571	0.727617
26	6	0	-3.639479	-2.353619	0.036787
27	1	0	-5.343411	-1.191046	-0.596867
28	1	0	-1.781516	-3.232668	0.691343
29	1	0	-4.177086	-3.298042	0.029242
30	7	0	-0.196257	1.424592	0.031070
31	1	0	0.253979	0.521968	-0.049291
32	8	0	-2.253939	2.463221	0.026910
33	1	0	2.537681	3.094376	0.039996

Zero-point correction= 0.265265 (Hartree/Particle)
Thermal correction to Energy= 0.281558
Thermal correction to Enthalpy= 0.282502
Thermal correction to Gibbs Free Energy= 0.218213
Sum of electronic and zero-point Energies= -839.741889
Sum of electronic and thermal Energies= -839.725595
Sum of electronic and thermal Enthalpies= -839.724651
Sum of electronic and thermal Free Energies= -839.788940
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-839.915187

TS1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.279036	-2.071346	0.348711
2	8	0	-0.563089	-0.815589	-1.362981
3	6	0	-1.549774	-0.239294	-0.886321
4	6	0	-2.828084	-0.184897	-1.665611
5	7	0	-1.369748	0.724025	0.174648
6	6	0	-2.753585	-0.499338	-3.029310
7	6	0	-4.069069	0.183955	-1.124815
8	6	0	-0.466338	0.455579	1.197422
9	6	0	-1.856741	2.112671	0.008058
10	6	0	-3.891907	-0.450081	-3.834457
11	1	0	-1.793594	-0.787166	-3.444184
12	6	0	-5.202798	0.241577	-1.929267
13	1	0	-4.147355	0.394257	-0.064493
14	8	0	0.216223	-0.550467	1.306043

15	8	0	-0.459291	1.479246	2.076387
16	1	0	-2.637945	2.084887	-0.751298
17	1	0	-2.318086	2.447535	0.938783
18	6	0	-0.778137	3.092411	-0.427546
19	6	0	-5.119490	-0.075834	-3.289154
20	1	0	-3.816488	-0.700416	-4.889457
21	1	0	-6.158142	0.520013	-1.492395
22	6	0	0.482476	1.520929	3.210706
23	6	0	-0.664234	4.339353	0.196290
24	6	0	0.080374	2.792781	-1.494835
25	1	0	-6.007358	-0.033707	-3.914513
26	6	0	1.924195	1.533845	2.691566
27	6	0	0.213640	0.359326	4.172482
28	6	0	0.136742	2.858169	3.872019
29	6	0	0.285635	5.269751	-0.231285
30	1	0	-1.324053	4.582451	1.025999
31	6	0	1.032847	3.719187	-1.921461
32	1	0	0.001376	1.830928	-1.994359
33	1	0	2.612670	1.680613	3.531356
34	1	0	2.175725	0.595385	2.194597
35	1	0	2.065525	2.360332	1.986708
36	1	0	0.467847	-0.599084	3.718618
37	1	0	0.814506	0.492149	5.079529
38	1	0	-0.842119	0.342016	4.462823
39	1	0	0.779325	3.021983	4.743388
40	1	0	0.284195	3.684354	3.169505
41	1	0	-0.906224	2.865993	4.205243
42	6	0	1.139564	4.961147	-1.290710
43	1	0	0.360130	6.233028	0.266743
44	1	0	1.685014	3.475577	-2.756803
45	1	0	1.879965	5.682992	-1.624942
46	6	0	-3.172875	-2.422671	1.344238
47	6	0	-3.422447	-1.268411	2.351473
48	1	0	-2.472986	-0.953374	2.800420
49	1	0	-3.860124	-0.397726	1.850639
50	1	0	-4.103400	-1.562518	3.161700
51	6	0	-4.529880	-2.879269	0.747044
52	1	0	-4.988135	-2.067797	0.172914
53	1	0	-4.360486	-3.714565	0.056571
54	1	0	-5.245977	-3.204196	1.515569
55	6	0	-2.589031	-3.616953	2.156948
56	1	0	-2.408655	-4.469442	1.486637
57	1	0	-1.635973	-3.325152	2.621612
58	1	0	-3.256669	-3.961861	2.958858
59	19	0	0.039817	-2.959403	0.095535
60	6	0	3.104276	-1.475690	-0.928519
61	6	0	4.595952	-1.296292	-0.917052
62	6	0	5.360195	-2.220706	-0.193004
63	6	0	5.245902	-0.265097	-1.610119
64	6	0	6.747002	-2.101969	-0.140307
65	1	0	4.845598	-3.025854	0.320830
66	6	0	6.635154	-0.151687	-1.564560
67	1	0	4.675126	0.432196	-2.217470
68	6	0	7.387463	-1.065737	-0.824491
69	1	0	7.330028	-2.819183	0.431041
70	1	0	7.129985	0.645000	-2.113260
71	1	0	8.469792	-0.975394	-0.787554
72	7	0	2.354557	-0.394339	-1.250704
73	1	0	2.754186	0.531810	-1.228930
74	8	0	2.598338	-2.576454	-0.665995
75	1	0	1.335270	-0.468858	-1.193056

Zero-point correction= 0.619157 (Hartree/Particle)
Thermal correction to Energy= 0.658931
Thermal correction to Enthalpy= 0.659875
Thermal correction to Gibbs Free Energy= 0.542402
Sum of electronic and zero-point Energies= -2250.498774

Sum of electronic and thermal Energies= -2250.459000
Sum of electronic and thermal Enthalpies= -2250.458056
Sum of electronic and thermal Free Energies= -2250.575529
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.925645

TS2b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.419407	0.149478	-1.657410
2	8	0	0.689853	-1.098776	-1.148223
3	6	0	1.813827	-0.726371	-0.730038
4	6	0	2.713205	-1.785847	-0.097441
5	7	0	1.411551	0.453706	0.838024
6	6	0	2.506368	-3.097525	-0.548067
7	6	0	3.717359	-1.560157	0.851876
8	6	0	0.956985	1.689870	0.619573
9	6	0	1.175515	-0.169469	2.146816
10	6	0	3.296913	-4.149236	-0.082955
11	1	0	1.712620	-3.275509	-1.265290
12	6	0	4.503675	-2.611176	1.326222
13	1	0	3.868499	-0.561447	1.242011
14	8	0	0.918162	2.278451	-0.483323
15	8	0	0.518626	2.341315	1.763950
16	1	0	1.954259	-0.917015	2.308124
17	1	0	1.286404	0.580388	2.936345
18	6	0	-0.168702	-0.873279	2.319085
19	6	0	4.301683	-3.910023	0.855481
20	1	0	3.123657	-5.156902	-0.452402
21	1	0	5.271189	-2.413302	2.070141
22	6	0	0.126567	3.746617	1.758843
23	6	0	-1.325198	-0.166910	2.683507
24	6	0	-0.265412	-2.263152	2.161819
25	1	0	4.915809	-4.727688	1.223724
26	6	0	-1.130853	3.963359	0.905806
27	6	0	1.289582	4.637506	1.302171
28	6	0	-0.187227	4.013905	3.236631
29	6	0	-2.538688	-0.827091	2.883282
30	1	0	-1.262986	0.908086	2.816221
31	6	0	-1.476126	-2.930687	2.363013
32	1	0	0.618800	-2.829058	1.881227
33	1	0	-1.503620	4.985739	1.041857
34	1	0	-0.914053	3.803552	-0.150895
35	1	0	-1.921650	3.269705	1.212948
36	1	0	1.524204	4.461216	0.251845
37	1	0	1.026144	5.693266	1.437806
38	1	0	2.181882	4.430517	1.903892
39	1	0	-0.478671	5.060074	3.381251
40	1	0	-1.008980	3.377701	3.582756
41	1	0	0.689870	3.808539	3.859034
42	6	0	-2.620254	-2.214386	2.726170
43	1	0	-3.420451	-0.260667	3.173281
44	1	0	-1.523071	-4.010671	2.244547
45	1	0	-3.560719	-2.731724	2.900194
46	6	0	3.761477	0.705063	-1.816308
47	6	0	4.198235	1.591488	-0.644294
48	1	0	3.424584	2.330855	-0.428750
49	1	0	4.400279	1.020150	0.261190
50	1	0	5.122660	2.114204	-0.918447
51	6	0	4.790434	-0.388306	-2.140958
52	1	0	5.021436	-1.015935	-1.279483
53	1	0	4.419588	-1.031735	-2.946240
54	1	0	5.723645	0.078521	-2.477882
55	6	0	3.574271	1.598767	-3.056203
56	1	0	3.226320	1.004878	-3.909784
57	1	0	2.846738	2.389530	-2.842394

58	1	0	4.520388	2.073993	-3.336869
59	19	0	0.012620	1.035982	-2.570826
60	6	0	-2.916325	-0.564858	-1.496469
61	6	0	-4.402168	-0.624655	-1.273373
62	6	0	-5.185059	0.416175	-1.789657
63	6	0	-5.029978	-1.679558	-0.595863
64	6	0	-6.566767	0.416406	-1.612602
65	1	0	-4.688446	1.216062	-2.328675
66	6	0	-6.414250	-1.683454	-0.425788
67	1	0	-4.445617	-2.515422	-0.222648
68	6	0	-7.184719	-0.633333	-0.928599
69	1	0	-7.163257	1.233104	-2.010411
70	1	0	-6.891523	-2.510446	0.093058
71	1	0	-8.263141	-0.636503	-0.793706
72	7	0	-2.140750	-1.321756	-0.696518
73	1	0	-2.499935	-1.695758	0.171614
74	8	0	-2.450409	0.154223	-2.400381
75	1	0	-1.119578	-1.273235	-0.781013

Zero-point correction= 0.620798 (Hartree/Particle)
Thermal correction to Energy= 0.659898
Thermal correction to Enthalpy= 0.660842
Thermal correction to Gibbs Free Energy= 0.546187
Sum of electronic and zero-point Energies= -2250.499230
Sum of electronic and thermal Energies= -2250.460131
Sum of electronic and thermal Enthalpies= -2250.459187
Sum of electronic and thermal Free Energies= -2250.573842
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.929742

TS3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	5.359874	-1.494073	0.426088
2	8	0	3.139032	-1.124584	0.154232
3	6	0	4.308019	-0.784951	-0.002710
4	6	0	4.717859	0.468187	-0.697635
5	7	0	-2.541157	-0.735688	-0.669603
6	6	0	3.723677	1.376275	-1.094207
7	6	0	6.066707	0.750269	-0.968298
8	6	0	-2.514509	-1.998259	-0.236057
9	6	0	-3.634590	-0.213096	-1.486989
10	6	0	4.079560	2.548560	-1.758561
11	1	0	2.677378	1.187264	-0.877779
12	6	0	6.413996	1.923084	-1.634162
13	1	0	6.832459	0.048571	-0.658353
14	8	0	-1.576805	-2.480500	0.438070
15	8	0	-3.602118	-2.759092	-0.597441
16	1	0	-3.196757	0.440945	-2.252459
17	1	0	-4.141651	-1.030106	-2.010538
18	6	0	-4.652456	0.596079	-0.693233
19	6	0	5.421525	2.823224	-2.031348
20	1	0	3.301347	3.243382	-2.060885
21	1	0	7.458718	2.134920	-1.844297
22	6	0	-3.660987	-4.198111	-0.350240
23	6	0	-5.409469	-0.002541	0.324962
24	6	0	-4.847211	1.957566	-0.954405
25	1	0	5.695061	3.737366	-2.551797
26	6	0	-3.675342	-4.486408	1.156156
27	6	0	-2.505651	-4.914317	-1.062006
28	6	0	-4.999872	-4.594222	-0.982907
29	6	0	-6.335158	0.740346	1.056704
30	1	0	-5.267675	-1.058792	0.535272
31	6	0	-5.774968	2.706277	-0.223948
32	1	0	-4.265454	2.437173	-1.739175
33	1	0	-3.825284	-5.558776	1.329347

34	1	0	-2.736877	-4.175170	1.616137
35	1	0	-4.499606	-3.947132	1.636679
36	1	0	-1.547332	-4.633662	-0.622429
37	1	0	-2.631123	-6.000126	-0.976982
38	1	0	-2.499156	-4.655665	-2.127185
39	1	0	-5.174151	-5.669224	-0.863510
40	1	0	-5.825404	-4.054748	-0.507024
41	1	0	-5.007368	-4.357785	-2.052142
42	6	0	-6.521590	2.099076	0.785837
43	1	0	-6.916035	0.258285	1.839530
44	1	0	-5.912646	3.761899	-0.445935
45	1	0	-7.244045	2.677062	1.356541
46	6	0	5.228503	-2.785689	1.134767
47	6	0	6.687924	-3.165023	1.398483
48	1	0	7.239560	-3.262504	0.457941
49	1	0	7.180887	-2.404124	2.011908
50	1	0	6.735960	-4.121769	1.928708
51	6	0	4.475835	-2.584657	2.453674
52	1	0	4.950256	-1.795618	3.046840
53	1	0	3.431798	-2.317584	2.283422
54	1	0	4.508020	-3.512365	3.035469
55	6	0	4.557827	-3.816744	0.221988
56	1	0	3.517485	-3.556648	0.020223
57	1	0	5.095081	-3.891546	-0.729542
58	1	0	4.583179	-4.800031	0.704337
59	19	0	0.488081	-0.978233	-0.056603
60	6	0	-0.464599	2.004088	0.096614
61	6	0	-0.425784	3.457382	0.507006
62	6	0	0.809842	4.117696	0.533647
63	6	0	-1.585247	4.173972	0.835143
64	6	0	0.890325	5.457644	0.907604
65	1	0	1.701463	3.562290	0.261056
66	6	0	-1.507510	5.520316	1.193739
67	1	0	-2.557167	3.689901	0.779253
68	6	0	-0.269328	6.163380	1.238352
69	1	0	1.856902	5.954392	0.938106
70	1	0	-2.415249	6.067770	1.434110
71	1	0	-0.208707	7.210533	1.523614
72	7	0	-1.419938	1.210874	0.600988
73	1	0	-2.055407	1.661932	1.250676
74	8	0	0.422160	1.574425	-0.685764
75	1	0	-1.905469	0.224002	-0.002648

Zero-point correction= 0.615522 (Hartree/Particle)
Thermal correction to Energy= 0.656206
Thermal correction to Enthalpy= 0.657150
Thermal correction to Gibbs Free Energy= 0.531586
Sum of electronic and zero-point Energies= -2250.547853
Sum of electronic and thermal Energies= -2250.507170
Sum of electronic and thermal Enthalpies= -2250.506226
Sum of electronic and thermal Free Energies= -2250.631790
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.957096

TS4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.148091	-1.172736	1.285261
2	8	0	-2.865426	-1.712382	-0.508470
3	6	0	-3.937947	-1.378903	-0.012874
4	6	0	-5.172511	-1.164048	-0.825779
5	7	0	2.644614	-0.085856	-1.409864
6	6	0	-5.122840	-1.438106	-2.199708
7	6	0	-6.366272	-0.697649	-0.255931
8	6	0	2.120251	-0.237714	-0.057099
9	6	0	3.836399	0.749218	-1.591958

10	6	0	-6.249393	-1.247842	-2.995318
11	1	0	-4.196536	-1.805714	-2.628523
12	6	0	-7.491113	-0.504922	-1.055351
13	1	0	-6.403777	-0.486857	0.806470
14	8	0	1.210194	-1.103166	0.104353
15	8	0	3.196118	-0.138159	0.833709
16	1	0	3.781485	1.147300	-2.615651
17	1	0	3.837188	1.621404	-0.921760
18	6	0	5.152883	0.003803	-1.450820
19	6	0	-7.435150	-0.779232	-2.423868
20	1	0	-6.204646	-1.463995	-4.059065
21	1	0	-8.412588	-0.140210	-0.610422
22	6	0	3.294362	-0.967017	2.020191
23	6	0	6.302308	0.684364	-1.032279
24	6	0	5.266015	-1.348992	-1.792430
25	1	0	-8.314377	-0.628622	-3.044405
26	6	0	3.416450	-2.450467	1.640653
27	6	0	2.113703	-0.724233	2.972610
28	6	0	4.599590	-0.480894	2.663707
29	6	0	7.536157	0.034964	-0.958562
30	1	0	6.228691	1.734157	-0.754245
31	6	0	6.496423	-2.003459	-1.716695
32	1	0	4.371592	-1.881815	-2.100259
33	1	0	3.610037	-3.054473	2.536097
34	1	0	2.499897	-2.798862	1.162531
35	1	0	4.250048	-2.588102	0.944083
36	1	0	1.179216	-1.031727	2.501914
37	1	0	2.257109	-1.290309	3.901481
38	1	0	2.046432	0.339047	3.234025
39	1	0	4.806887	-1.041814	3.582441
40	1	0	5.438223	-0.614135	1.973501
41	1	0	4.530705	0.583271	2.915398
42	6	0	7.638188	-1.314466	-1.301027
43	1	0	8.415583	0.581790	-0.626463
44	1	0	6.564188	-3.056236	-1.981926
45	1	0	8.596151	-1.824950	-1.240304
46	6	0	-3.096464	-1.319026	2.327326
47	6	0	-3.865208	-0.956686	3.600443
48	1	0	-4.220993	0.077829	3.557474
49	1	0	-4.728406	-1.616668	3.733724
50	1	0	-3.211235	-1.060896	4.471968
51	6	0	-2.620683	-2.772881	2.370683
52	1	0	-3.466679	-3.451114	2.527190
53	1	0	-2.105952	-3.051676	1.449727
54	1	0	-1.922875	-2.899302	3.205402
55	6	0	-1.955383	-0.327623	2.084126
56	1	0	-1.279758	-0.636931	1.285553
57	1	0	-2.350761	0.667977	1.856050
58	1	0	-1.357335	-0.248243	2.998612
59	19	0	-0.563943	-1.225818	-1.672335
60	6	0	0.370876	1.847162	-0.488346
61	6	0	-0.338176	3.103225	-0.035915
62	6	0	-1.005809	3.875600	-0.995881
63	6	0	-0.374467	3.512419	1.304559
64	6	0	-1.671928	5.043882	-0.629911
65	1	0	-0.987986	3.538835	-2.027233
66	6	0	-1.050676	4.675400	1.674743
67	1	0	0.108667	2.908332	2.068178
68	6	0	-1.696324	5.447902	0.707355
69	1	0	-2.174777	5.640028	-1.387366
70	1	0	-1.076491	4.975816	2.719188
71	1	0	-2.219225	6.356523	0.994689
72	7	0	1.378094	1.376122	0.228915
73	1	0	1.679715	1.901136	1.041187
74	8	0	-0.024121	1.294743	-1.560758
75	1	0	1.879584	0.328820	-1.940894

Zero-point correction= 0.620071 (Hartree/Particle)
Thermal correction to Energy= 0.659742
Thermal correction to Enthalpy= 0.660686
Thermal correction to Gibbs Free Energy= 0.539355
Sum of electronic and zero-point Energies= -2250.501053
Sum of electronic and thermal Energies= -2250.461382
Sum of electronic and thermal Enthalpies= -2250.460438
Sum of electronic and thermal Free Energies= -2250.581770
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.926226

TS5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.562131	0.381954	0.811399
2	8	0	-3.285444	-0.928023	-0.534494
3	6	0	-4.342472	-0.675737	0.037770
4	6	0	-5.547546	-1.552670	-0.073016
5	7	0	2.452668	-1.319107	-0.829002
6	6	0	-5.472432	-2.694036	-0.883233
7	6	0	-6.739265	-1.266371	0.609216
8	6	0	1.674705	-0.459935	-0.063055
9	6	0	3.746564	-0.925503	-1.426258
10	6	0	-6.571520	-3.538985	-1.011411
11	1	0	-4.546227	-2.905199	-1.407146
12	6	0	-7.837359	-2.114221	0.479931
13	1	0	-6.796311	-0.384048	1.235870
14	8	0	0.670304	-0.902949	0.521741
15	8	0	3.191321	0.253436	1.355953
16	1	0	3.638848	-0.881869	-2.517607
17	1	0	3.993453	0.075277	-1.070730
18	6	0	4.853832	-1.889986	-1.058466
19	6	0	-7.756006	-3.250115	-0.328961
20	1	0	-6.506357	-4.421765	-1.641316
21	1	0	-8.757714	-1.889040	1.011286
22	6	0	2.962117	0.251837	2.732279
23	6	0	5.370861	-2.790119	-1.996567
24	6	0	5.366440	-1.888407	0.248020
25	1	0	-8.614126	-3.909435	-0.427471
26	6	0	2.746835	-1.192819	3.245682
27	6	0	1.717405	1.101188	3.096992
28	6	0	4.198769	0.861099	3.433701
29	6	0	6.388085	-3.679981	-1.641398
30	1	0	4.981941	-2.790059	-3.013446
31	6	0	6.381081	-2.777372	0.600574
32	1	0	4.943348	-1.177619	0.956905
33	1	0	2.585026	-1.228303	4.331937
34	1	0	1.876228	-1.637943	2.752549
35	1	0	3.623878	-1.809383	3.013683
36	1	0	0.833294	0.700228	2.591087
37	1	0	1.524564	1.115809	4.178663
38	1	0	1.861839	2.139891	2.769077
39	1	0	4.077854	0.914204	4.524833
40	1	0	5.091608	0.262648	3.216043
41	1	0	4.377448	1.875385	3.056078
42	6	0	6.894062	-3.674957	-0.341144
43	1	0	6.784638	-4.372749	-2.379634
44	1	0	6.777678	-2.767652	1.612947
45	1	0	7.686775	-4.365096	-0.062788
46	6	0	-3.543892	1.427183	1.117898
47	6	0	-4.340771	2.379980	2.012783
48	1	0	-5.208416	2.781105	1.478807
49	1	0	-4.692823	1.864647	2.912228
50	1	0	-3.706213	3.216746	2.320936
51	6	0	-2.375795	0.809434	1.887986
52	1	0	-2.744791	0.224866	2.737736

53	1	0	-1.742527	0.175059	1.266494
54	1	0	-1.743403	1.611557	2.282786
55	6	0	-3.109844	2.128819	-0.170756
56	1	0	-2.479262	1.497451	-0.797836
57	1	0	-3.986282	2.450282	-0.744604
58	1	0	-2.529339	3.021392	0.086660
59	19	0	-0.902581	-1.418219	-1.434244
60	6	0	0.854129	1.574663	-1.188800
61	6	0	0.957135	3.072551	-1.257113
62	6	0	0.164424	3.734433	-2.205178
63	6	0	1.793041	3.827802	-0.420557
64	6	0	0.209314	5.121786	-2.322791
65	1	0	-0.479576	3.137581	-2.842041
66	6	0	1.833859	5.216719	-0.537086
67	1	0	2.408821	3.347359	0.333801
68	6	0	1.045467	5.867122	-1.488468
69	1	0	-0.406468	5.622058	-3.065685
70	1	0	2.482441	5.791020	0.118734
71	1	0	1.082022	6.949702	-1.577907
72	7	0	1.774298	0.936189	-0.445726
73	1	0	2.452582	1.349123	0.220043
74	8	0	-0.037711	0.978223	-1.832041
75	1	0	2.477767	-2.238184	-0.399159

Zero-point correction= 0.618699 (Hartree/Particle)
Thermal correction to Energy= 0.658888
Thermal correction to Enthalpy= 0.659832
Thermal correction to Gibbs Free Energy= 0.536269
Sum of electronic and zero-point Energies= -2250.492603
Sum of electronic and thermal Energies= -2250.452414
Sum of electronic and thermal Enthalpies= -2250.451470
Sum of electronic and thermal Free Energies= -2250.575033
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2250.907865

K^+_1a2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.665090	-0.789454	-1.081781
2	6	0	-4.105444	-0.914694	-0.710899
3	6	0	-5.016464	-0.029742	-1.304866
4	6	0	-4.575803	-1.887874	0.184366
5	6	0	-6.371335	-0.100187	-0.991590
6	1	0	-4.645178	0.707298	-2.008922
7	6	0	-5.933547	-1.962723	0.489415
8	1	0	-3.894810	-2.615570	0.617136
9	6	0	-6.831840	-1.065628	-0.092847
10	1	0	-7.069632	0.593631	-1.450512
11	1	0	-6.292006	-2.726673	1.173072
12	1	0	-7.889600	-1.124767	0.146998
13	7	0	-1.749016	-1.339329	-0.249455
14	1	0	-1.973782	-1.624691	0.693074
15	8	0	-2.313688	-0.206738	-2.124164
16	1	0	-0.768592	-1.232563	-0.484935
17	8	0	1.189616	-0.832528	-1.481632
18	6	0	2.089792	-0.543204	-0.693802
19	6	0	3.370529	-1.287717	-0.683045
20	7	0	1.943661	0.523538	0.234757
21	6	0	3.374893	-2.615307	-1.145406
22	6	0	4.581711	-0.676257	-0.313402
23	6	0	1.299262	1.695759	-0.182791
24	6	0	2.174505	0.230259	1.685909
25	6	0	4.568564	-3.327043	-1.212058
26	1	0	2.437440	-3.074537	-1.442219
27	6	0	5.775658	-1.387364	-0.399604
28	1	0	4.588364	0.359732	0.012068

29	8	0	1.024961	1.927110	-1.355048
30	8	0	1.098790	2.520854	0.839952
31	1	0	3.087035	-0.361792	1.753125
32	1	0	2.351322	1.182380	2.181962
33	6	0	1.016655	-0.524166	2.312986
34	6	0	5.769020	-2.713854	-0.840278
35	1	0	4.566771	-4.356707	-1.556518
36	1	0	6.711050	-0.908099	-0.127436
37	6	0	0.599649	3.922541	0.656553
38	6	0	-0.071299	0.156610	2.876170
39	6	0	1.015657	-1.926474	2.320348
40	1	0	6.700912	-3.268648	-0.898478
41	6	0	-0.817999	3.890888	0.084593
42	6	0	1.582154	4.701546	-0.218795
43	6	0	0.602546	4.454057	2.090131
44	6	0	-1.141744	-0.549248	3.427525
45	1	0	-0.074253	1.242060	2.888728
46	6	0	-0.054841	-2.635461	2.869034
47	1	0	1.863185	-2.469074	1.907522
48	1	0	-1.233949	4.903752	0.101837
49	1	0	-0.826835	3.533023	-0.946130
50	1	0	-1.466088	3.250002	0.691414
51	1	0	1.601425	4.322257	-1.241941
52	1	0	1.280212	5.753704	-0.245828
53	1	0	2.592820	4.653463	0.199869
54	1	0	0.267644	5.495750	2.096364
55	1	0	-0.074130	3.875400	2.727108
56	1	0	1.607965	4.415425	2.520478
57	6	0	-1.138025	-1.947226	3.422471
58	1	0	-1.972280	-0.009143	3.873435
59	1	0	-0.034929	-3.721582	2.879822
60	1	0	-1.962974	-2.496351	3.868045
61	19	0	-0.180001	0.586055	-3.271007

Zero-point correction= 0.495601 (Hartree/Particle)
Thermal correction to Energy= 0.528654
Thermal correction to Enthalpy= 0.529598
Thermal correction to Gibbs Free Energy= 0.424938
Sum of electronic and zero-point Energies= -2017.416728
Sum of electronic and thermal Energies= -2017.383675
Sum of electronic and thermal Enthalpies= -2017.382731
Sum of electronic and thermal Free Energies= -2017.487391
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-2017.769996

O^{t}Bu_anion

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000422	-0.002049	1.483797
2	6	0	0.000088	-0.000220	0.159522
3	6	0	-1.140961	-0.915601	-0.437425
4	1	0	-2.108285	-0.559600	-0.055183
5	1	0	-1.197333	-0.956303	-1.541619
6	1	0	-0.999755	-1.938835	-0.061005
7	6	0	1.363912	-0.529076	-0.437557
8	1	0	1.429995	-0.550669	-1.541754
9	1	0	2.179007	0.101762	-0.055160
10	1	0	1.537531	-1.547374	-0.061317
11	6	0	-0.223323	1.446477	-0.435238
12	1	0	-0.233950	1.515860	-1.539352
13	1	0	-1.178731	1.835876	-0.055455
14	1	0	0.569846	2.106199	-0.055348

Zero-point correction= 0.120309 (Hartree/Particle)
Thermal correction to Energy= 0.126797
Thermal correction to Enthalpy= 0.127742

Thermal correction to Gibbs Free Energy= 0.091523
Sum of electronic and zero-point Energies= -232.918967
Sum of electronic and thermal Energies= -232.912478
Sum of electronic and thermal Enthalpies= -232.911534
Sum of electronic and thermal Free Energies= -232.947753
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-233.069240

KO^{t}Bu_1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.399750	0.106745	0.028202
2	6	0	-1.060981	0.342009	-0.026298
3	6	0	-2.514461	-0.055036	-0.010145
4	6	0	-3.457089	0.903916	0.383023
5	6	0	-2.959347	-1.328558	-0.391649
6	6	0	-4.813532	0.588530	0.423351
7	1	0	-3.103128	1.893042	0.654075
8	6	0	-4.318301	-1.641785	-0.363022
9	1	0	-2.249570	-2.072180	-0.744563
10	6	0	-5.247806	-0.686251	0.051583
11	1	0	-5.534120	1.337565	0.741227
12	1	0	-4.650951	-2.629469	-0.670950
13	1	0	-6.306264	-0.931594	0.077589
14	7	0	-0.141183	-0.624133	0.076291
15	1	0	-0.445615	-1.568194	0.267289
16	8	0	-0.762582	1.554842	-0.131277
17	1	0	0.927957	-0.404519	0.066948
18	6	0	3.406314	-0.847739	0.089187
19	6	0	3.304215	-1.817279	-1.114122
20	1	0	4.095472	-2.579259	-1.115538
21	1	0	2.336037	-2.333822	-1.103464
22	1	0	3.367725	-1.251638	-2.052012
23	6	0	3.302610	-1.657249	1.405425
24	1	0	2.339228	-2.180769	1.454856
25	1	0	4.099389	-2.406328	1.509488
26	1	0	3.354192	-0.975653	2.263284
27	6	0	4.786262	-0.148647	0.046367
28	1	0	4.879036	0.433154	-0.880606
29	1	0	4.879254	0.542606	0.894526
30	1	0	5.626457	-0.854776	0.089235
31	19	0	1.668870	2.376137	-0.217001

Zero-point correction= 0.252294 (Hartree/Particle)
Thermal correction to Energy= 0.269531
Thermal correction to Enthalpy= 0.270475
Thermal correction to Gibbs Free Energy= 0.203666
Sum of electronic and zero-point Energies= -1233.735397
Sum of electronic and thermal Energies= -1233.718161
Sum of electronic and thermal Enthalpies= -1233.717217
Sum of electronic and thermal Free Energies= -1233.784026
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1233.925844

KO^{t}Bu_2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.132037	-0.132476	0.162645
2	8	0	-0.721769	0.487672	-2.323316
3	6	0	-0.276803	0.838165	-1.239292
4	6	0	-0.459199	2.259386	-0.773899
5	7	0	0.423160	-0.042793	-0.391368
6	6	0	0.493534	3.244255	-1.059503
7	6	0	-1.671254	2.589980	-0.148837
8	6	0	0.431627	-1.430497	-0.645854

9	6	0	1.083486	0.461697	0.828898
10	6	0	0.238567	4.570960	-0.709077
11	1	0	1.427463	2.980404	-1.548202
12	6	0	-1.908642	3.921780	0.196638
13	1	0	-2.391969	1.786500	0.053517
14	8	0	-0.314000	-2.007952	-1.417241
15	8	0	1.378040	-2.014507	0.097804
16	1	0	0.527014	1.345117	1.144921
17	1	0	0.951427	-0.287784	1.610702
18	6	0	2.556580	0.806925	0.679921
19	6	0	-0.961062	4.910365	-0.080030
20	1	0	0.977037	5.337200	-0.929495
21	1	0	-2.843864	4.186476	0.683888
22	6	0	1.591299	-3.481803	0.092299
23	6	0	3.234853	1.300849	1.802726
24	6	0	3.259467	0.665238	-0.519600
25	1	0	-1.156431	5.944618	0.192066
26	6	0	2.024776	-3.932930	-1.305048
27	6	0	0.329226	-4.197381	0.581152
28	6	0	2.734676	-3.642092	1.096700
29	6	0	4.583164	1.644830	1.728450
30	1	0	2.699962	1.418924	2.743188
31	6	0	4.611510	1.011107	-0.597170
32	1	0	2.754018	0.280029	-1.400272
33	1	0	2.295017	-4.994257	-1.275324
34	1	0	1.223895	-3.796566	-2.033415
35	1	0	2.904020	-3.367858	-1.632359
36	1	0	-0.489457	-4.101240	-0.133699
37	1	0	0.549176	-5.261853	0.719145
38	1	0	0.005752	-3.790074	1.544813
39	1	0	3.017665	-4.696962	1.172969
40	1	0	3.609996	-3.066979	0.779795
41	1	0	2.432308	-3.292579	2.088977
42	6	0	5.278139	1.501231	0.524815
43	1	0	5.091383	2.027245	2.609755
44	1	0	5.141544	0.894714	-1.539005
45	1	0	6.329173	1.770246	0.464137
46	6	0	-3.626573	-0.457244	1.403858
47	6	0	-4.262477	-1.876721	1.389823
48	1	0	-4.668794	-2.188198	2.362846
49	1	0	-5.082461	-1.905365	0.658407
50	1	0	-3.508376	-2.617593	1.087292
51	6	0	-4.718502	0.553879	1.845746
52	1	0	-5.523339	0.570977	1.100073
53	1	0	-5.158961	0.318855	2.825461
54	1	0	-4.292296	1.563648	1.897708
55	6	0	-2.490173	-0.450035	2.463895
56	1	0	-1.711044	-1.166848	2.169842
57	1	0	-2.031792	0.545930	2.508053
58	1	0	-2.833311	-0.712988	3.474854
59	19	0	-2.807688	-1.103039	-2.008413

Zero-point correction= 0.489502 (Hartree/Particle)
Thermal correction to Energy= 0.521293
Thermal correction to Enthalpy= 0.522237
Thermal correction to Gibbs Free Energy= 0.421307
Sum of electronic and zero-point Energies= -1849.659369
Sum of electronic and thermal Energies= -1849.627577
Sum of electronic and thermal Enthalpies= -1849.626633
Sum of electronic and thermal Free Energies= -1849.727563
M06-2X /6-311++G (d, p)/SMD// B3LYP /6-31G(d) energy=-1850.004292

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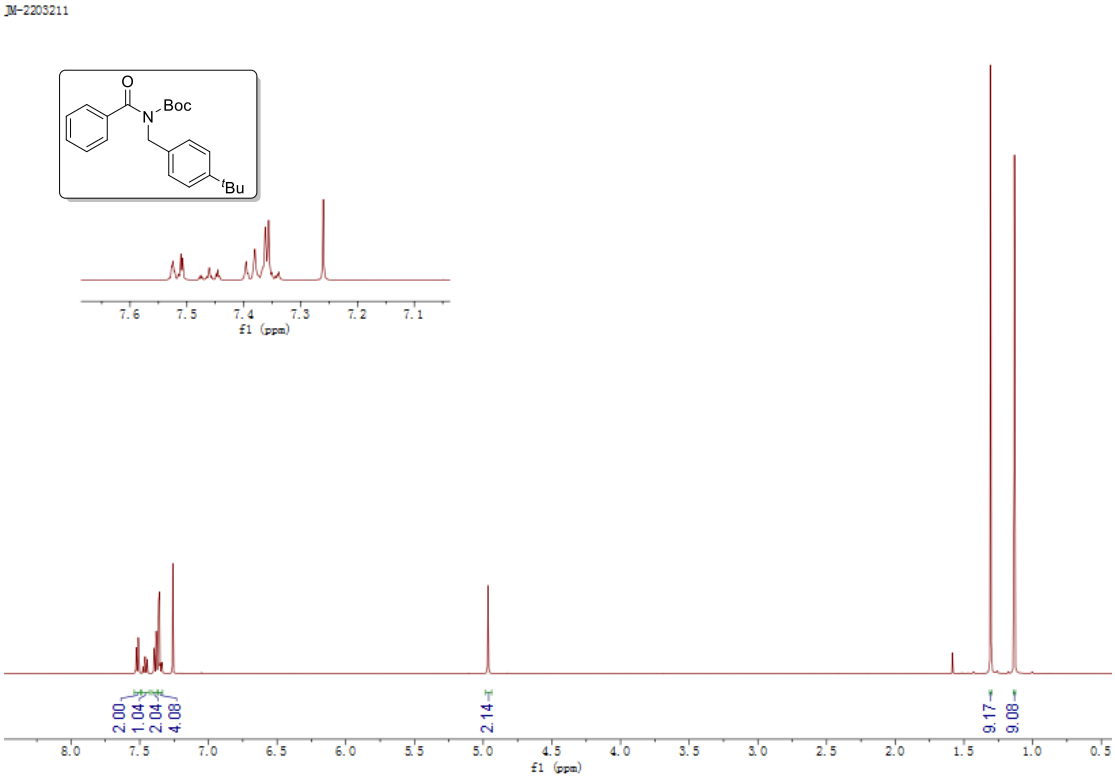
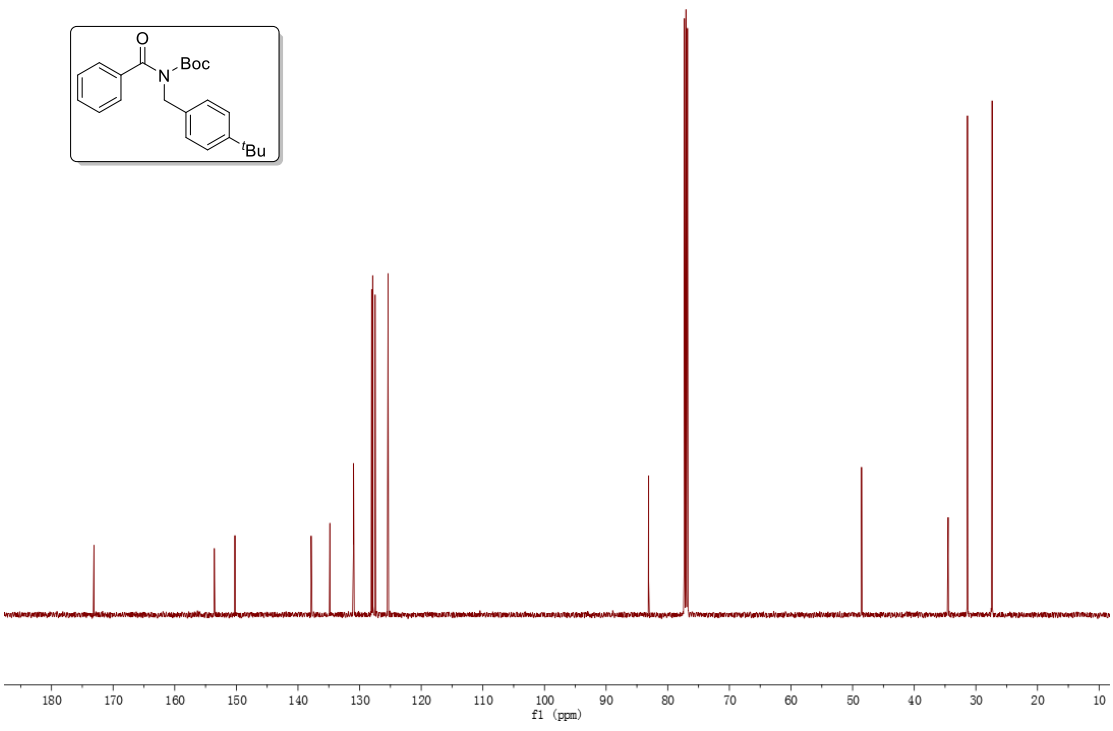
NMR Spectra

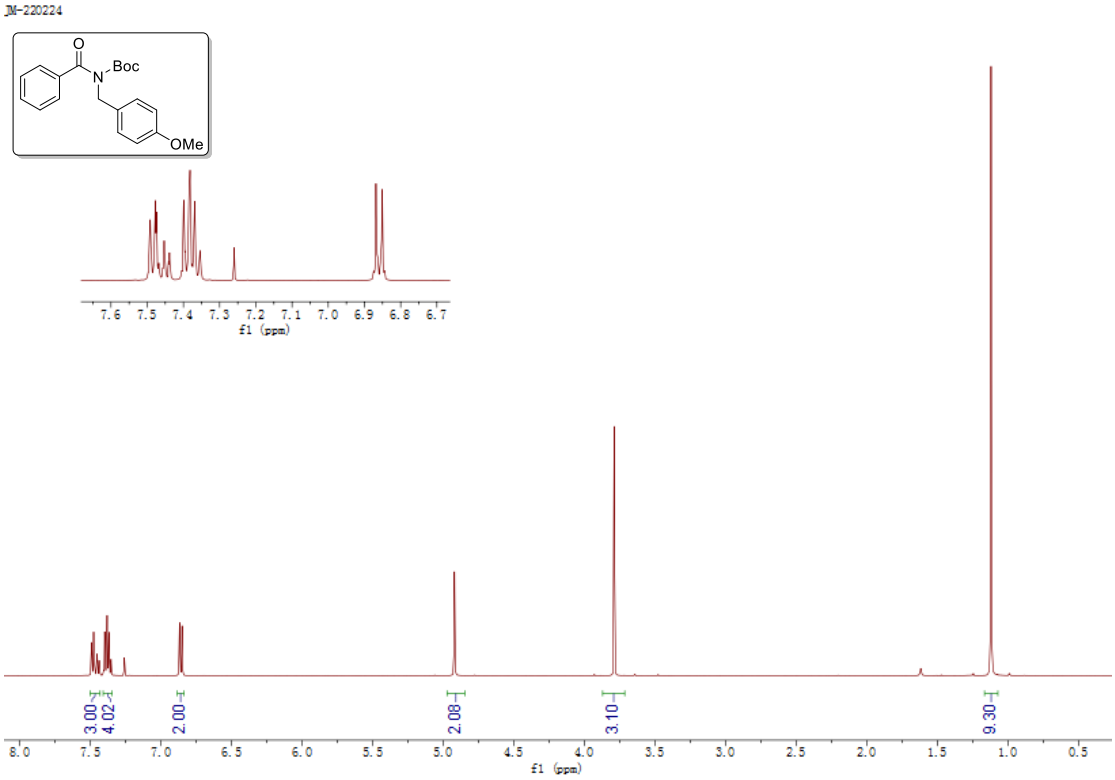
Supplementary Figure 3. ^{1}H NMR Spectrum of 2a (500 MHz, $CDCl_3$)



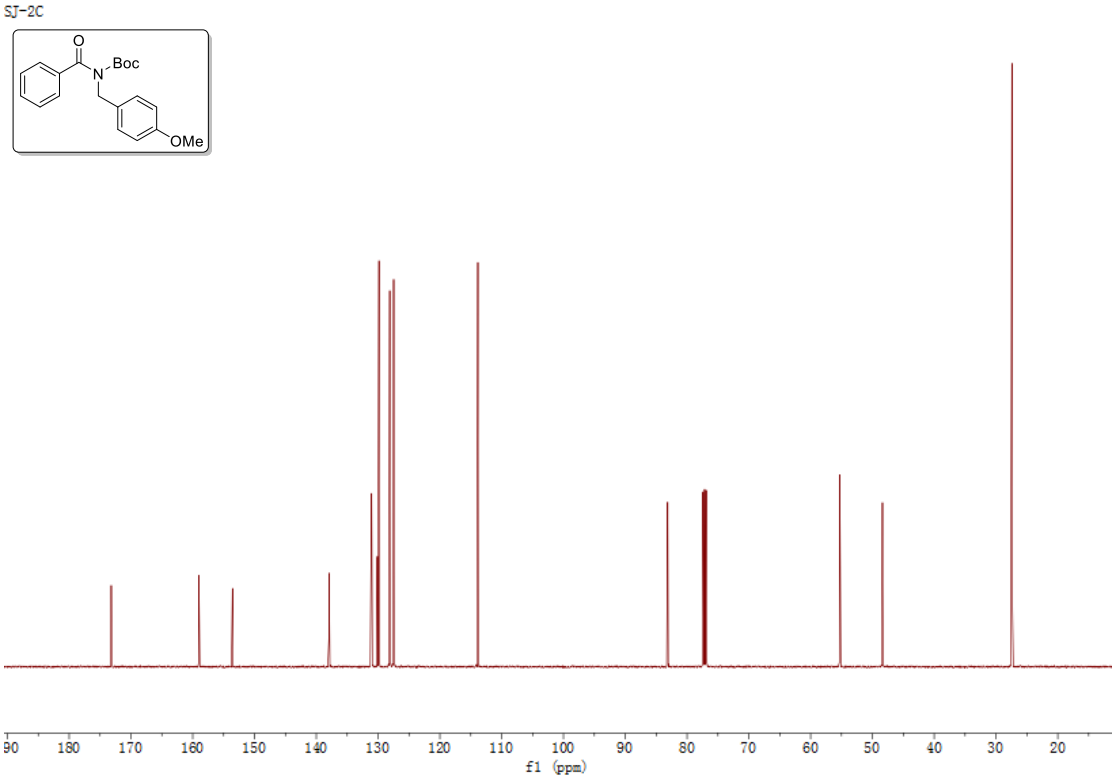
Supplementary Figure 4. ^{13}C NMR Spectrum of 2a (125 MHz, $CDCl_3$)



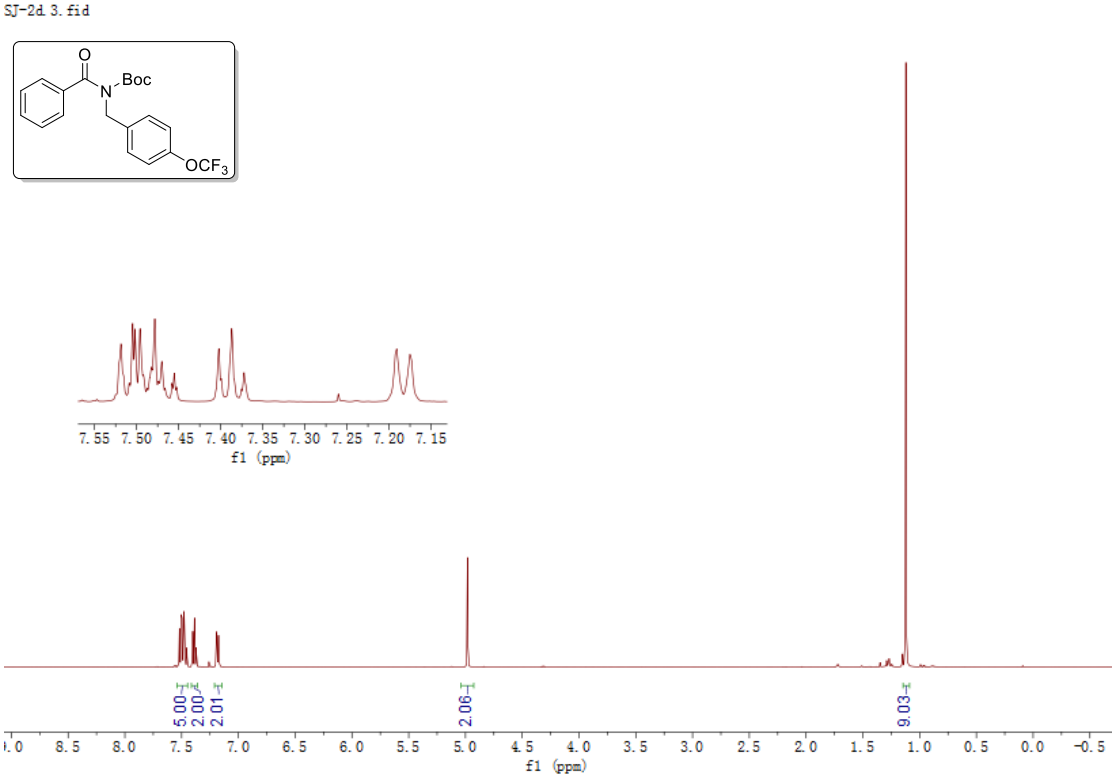
Supplementary Figure 5. ^{1}H NMR Spectrum of 2c (500 MHz, $CDCl_3$)



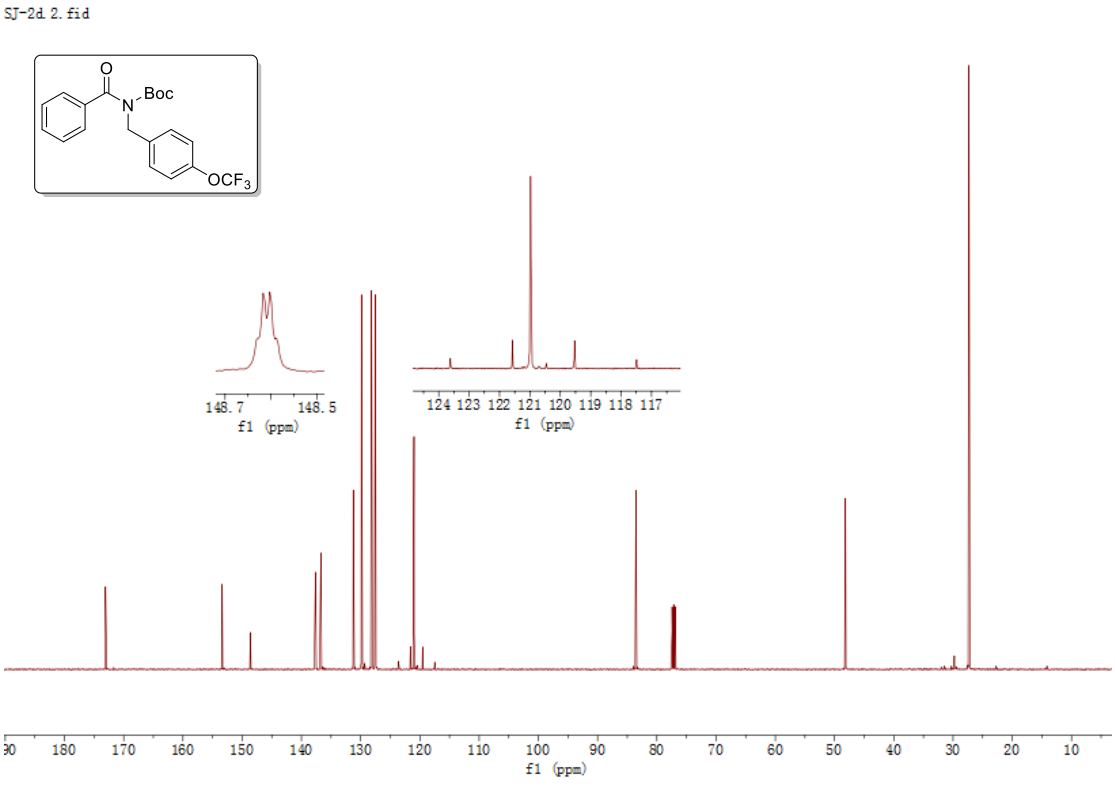
Supplementary Figure 6. ^{13}C NMR Spectrum of 2c (125 MHz, $CDCl_3$)



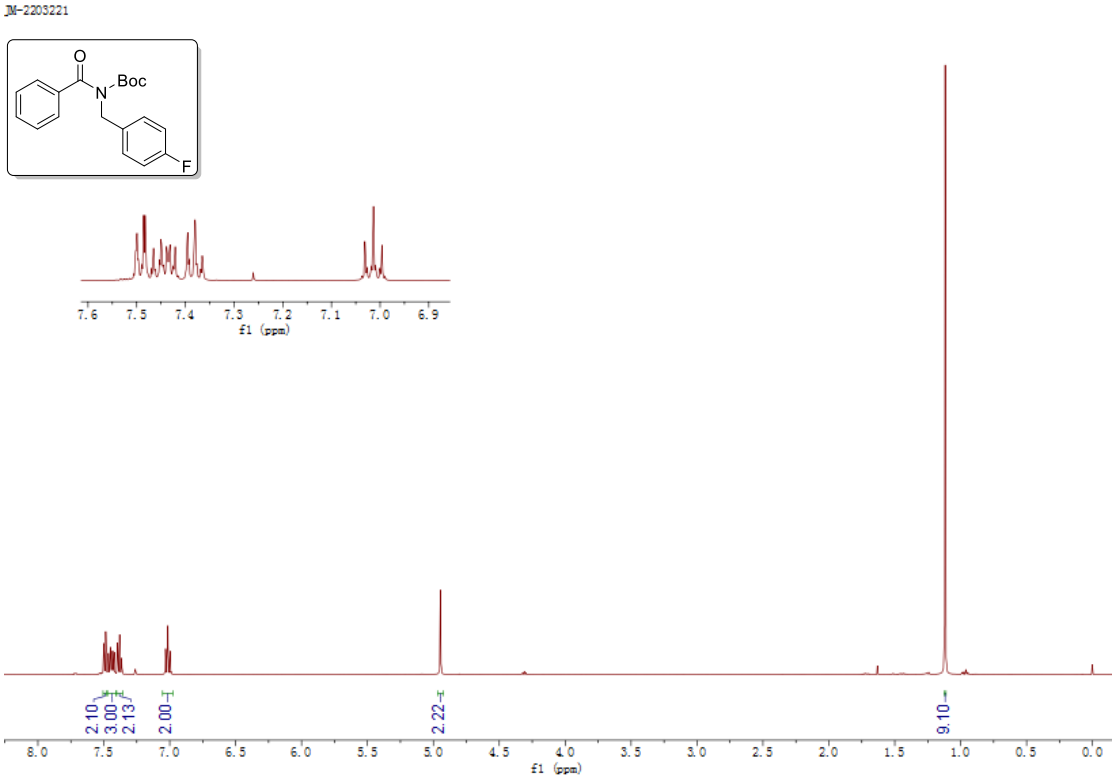
Supplementary Figure 7. ^{1}H NMR Spectrum of 2d (500 MHz, $CDCl_3$)



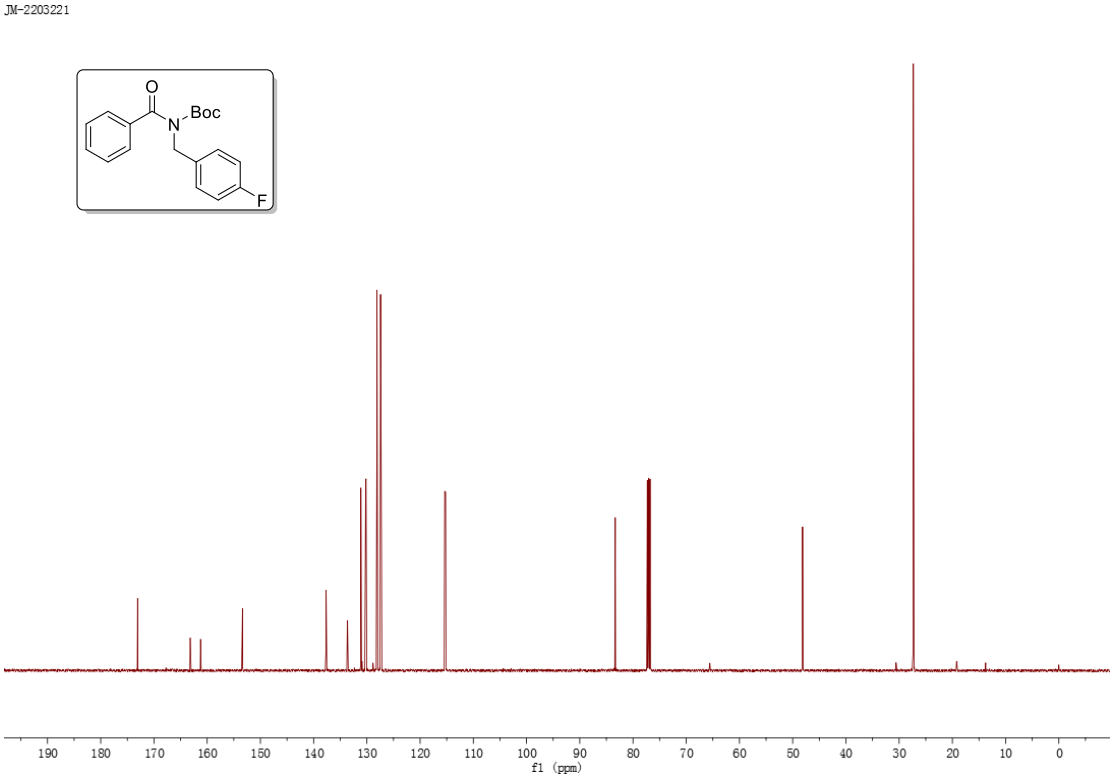
Supplementary Figure 8. ^{13}C NMR Spectrum of 2d (125 MHz, $CDCl_3$)



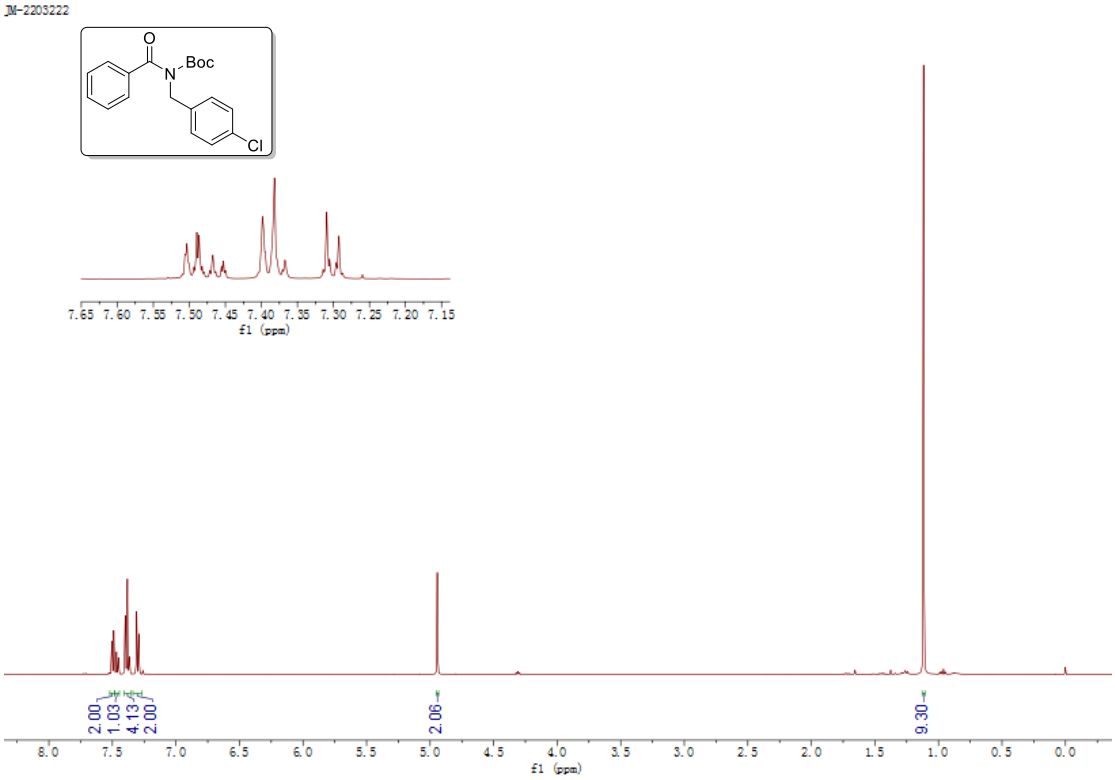
Supplementary Figure 9. ^{1}H NMR Spectrum of 2e (500 MHz, $CDCl_3$)



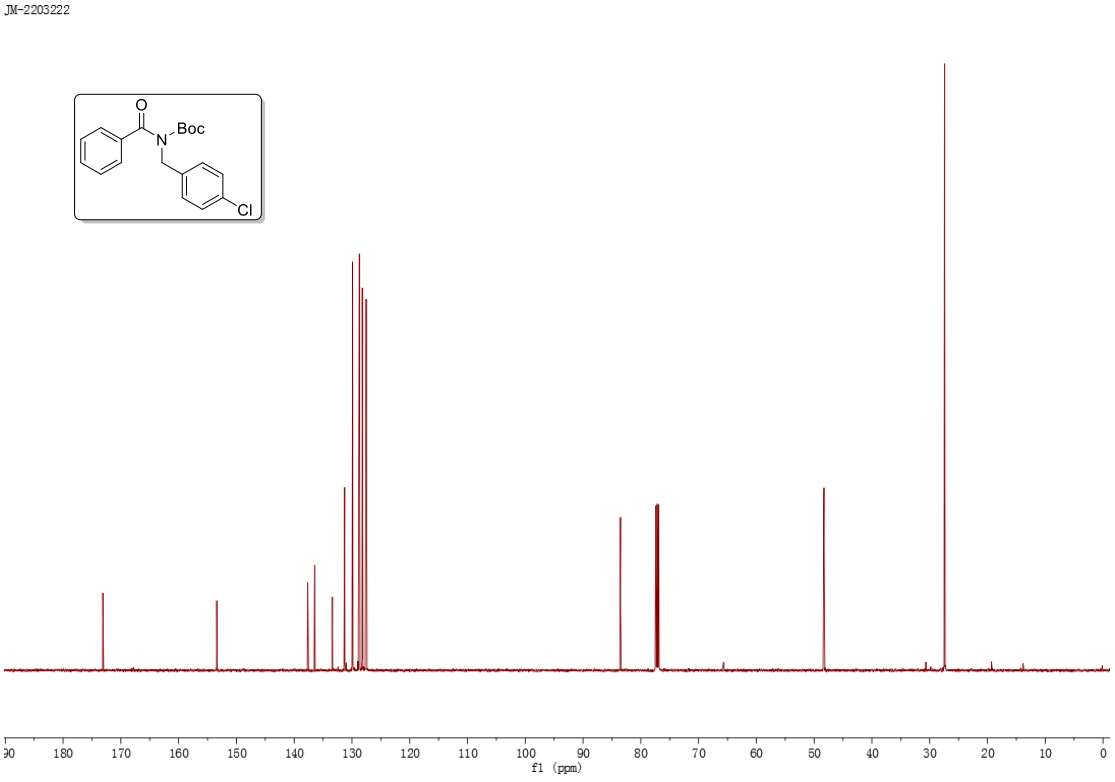
Supplementary Figure 10. ^{13}C NMR Spectrum of 2e (125 MHz, $CDCl_3$)



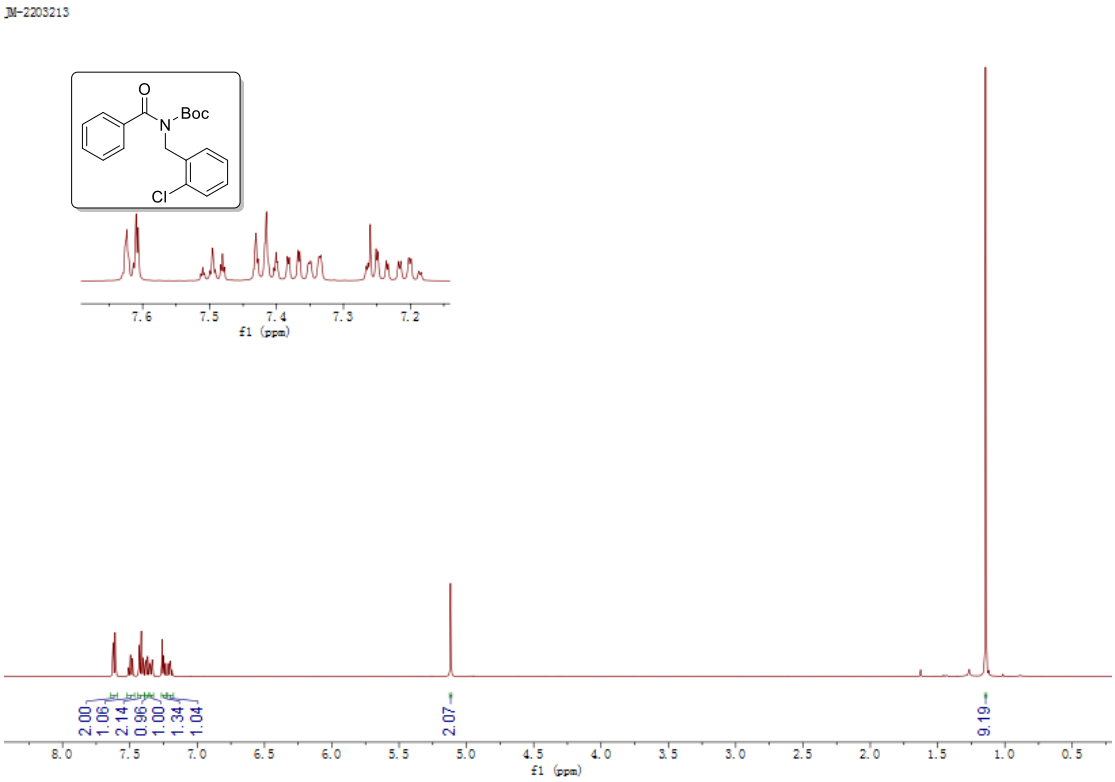
Supplementary Figure 11. ^{1}H NMR Spectrum of 2f (500 MHz, $CDCl_3$)



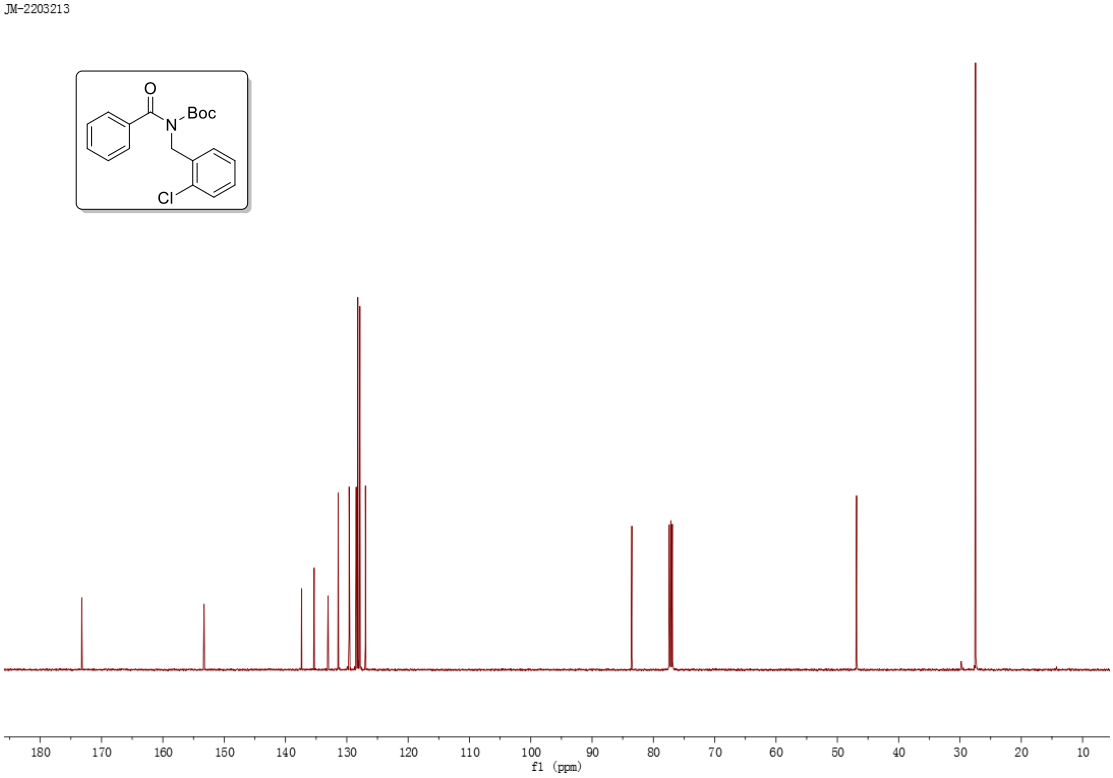
Supplementary Figure 12. ^{13}C NMR Spectrum of 2f (125 MHz, $CDCl_3$)



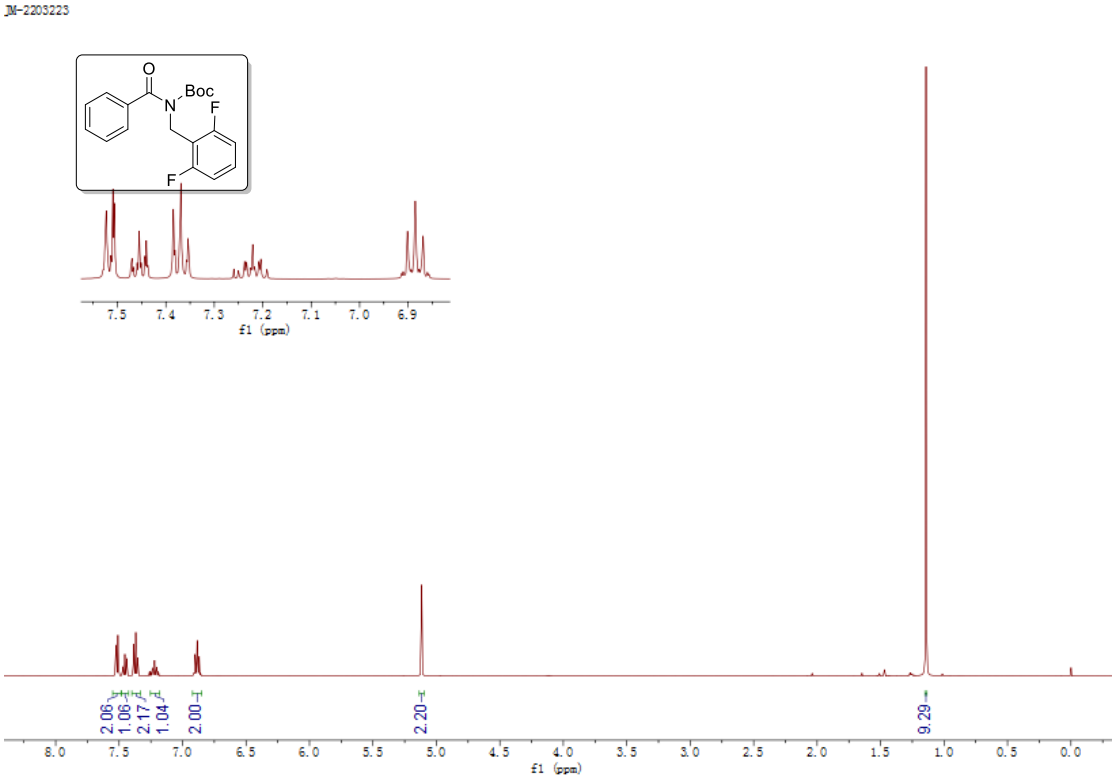
Supplementary Figure 13. ^{1}H NMR Spectrum of 2g (500 MHz, $CDCl_3$)



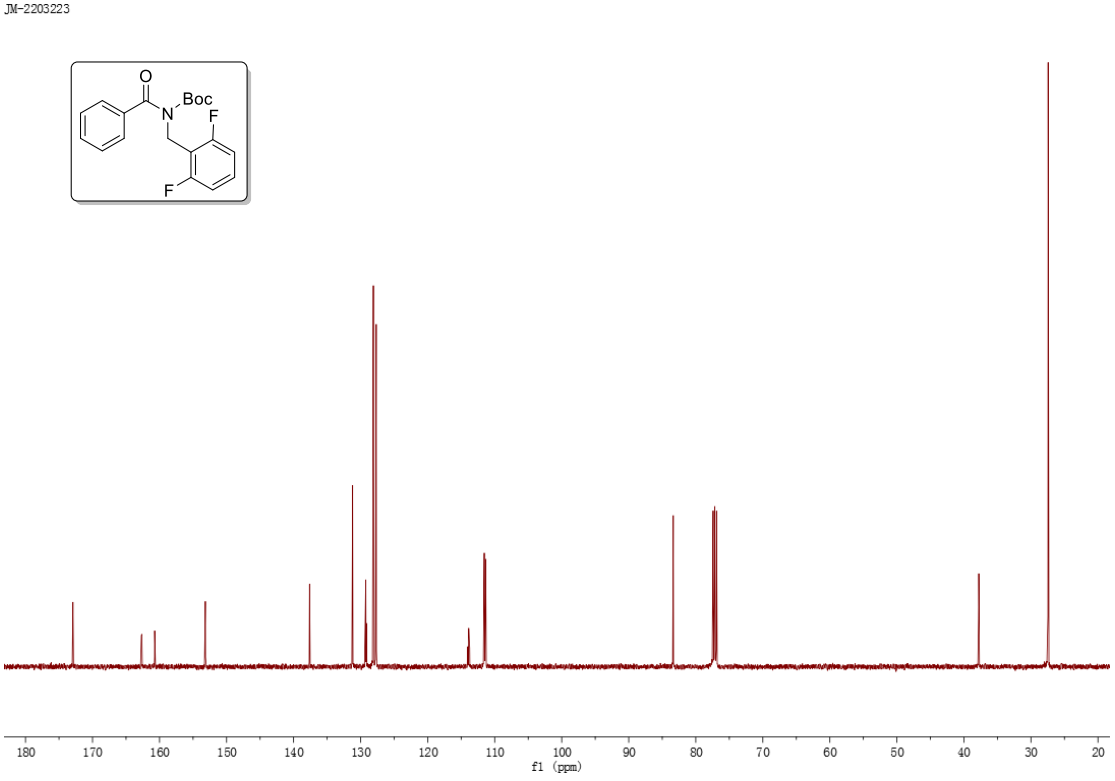
Supplementary Figure 14. ^{13}C NMR Spectrum of 2g (125 MHz, $CDCl_3$)



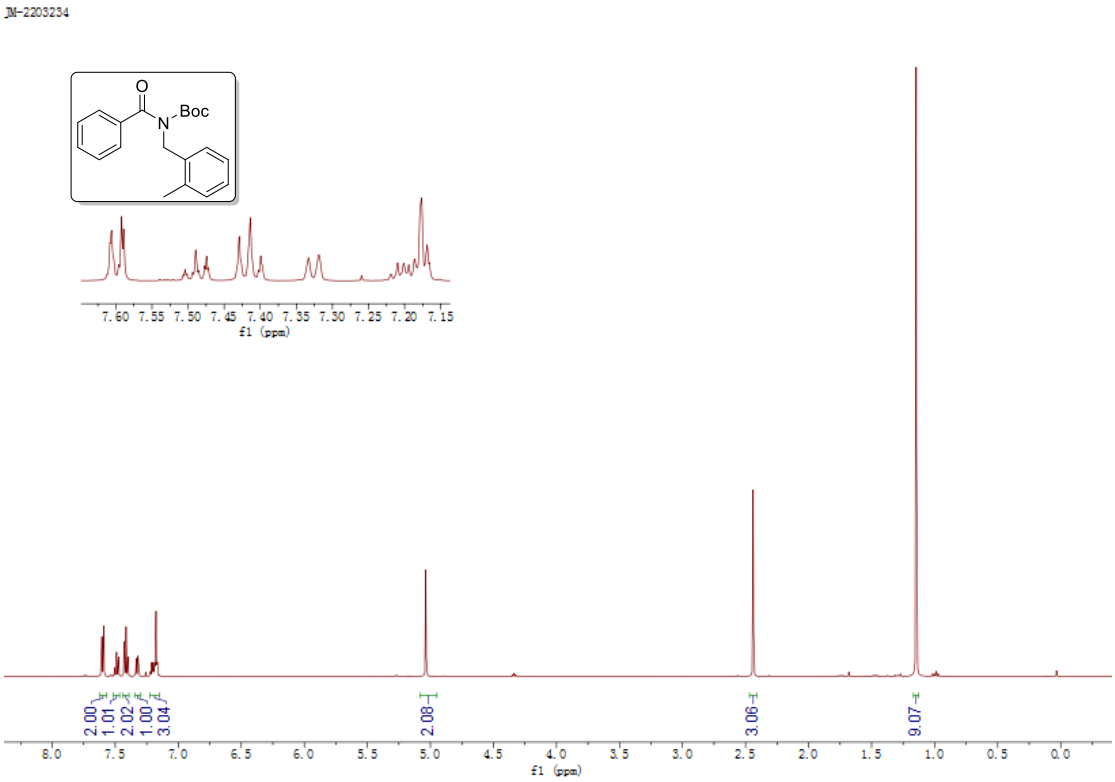
Supplementary Figure 15. ^{1}H NMR Spectrum of 2h (500 MHz, $CDCl_3$)



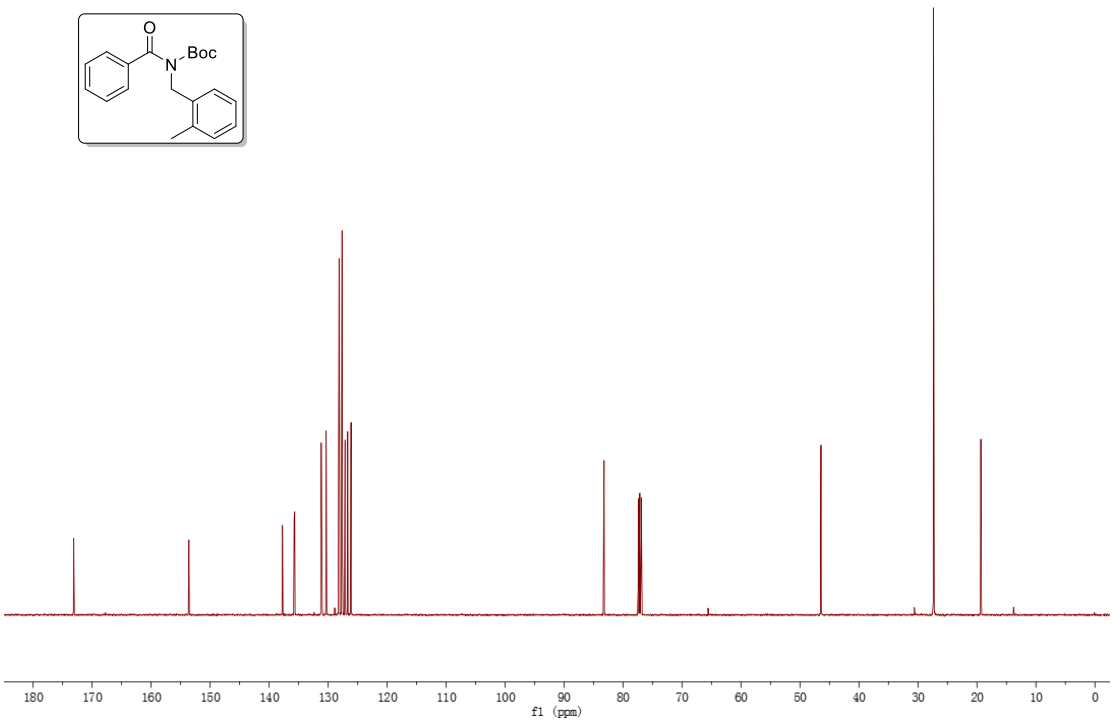
Supplementary Figure 16. ^{13}C NMR Spectrum of 2h (125 MHz, $CDCl_3$)



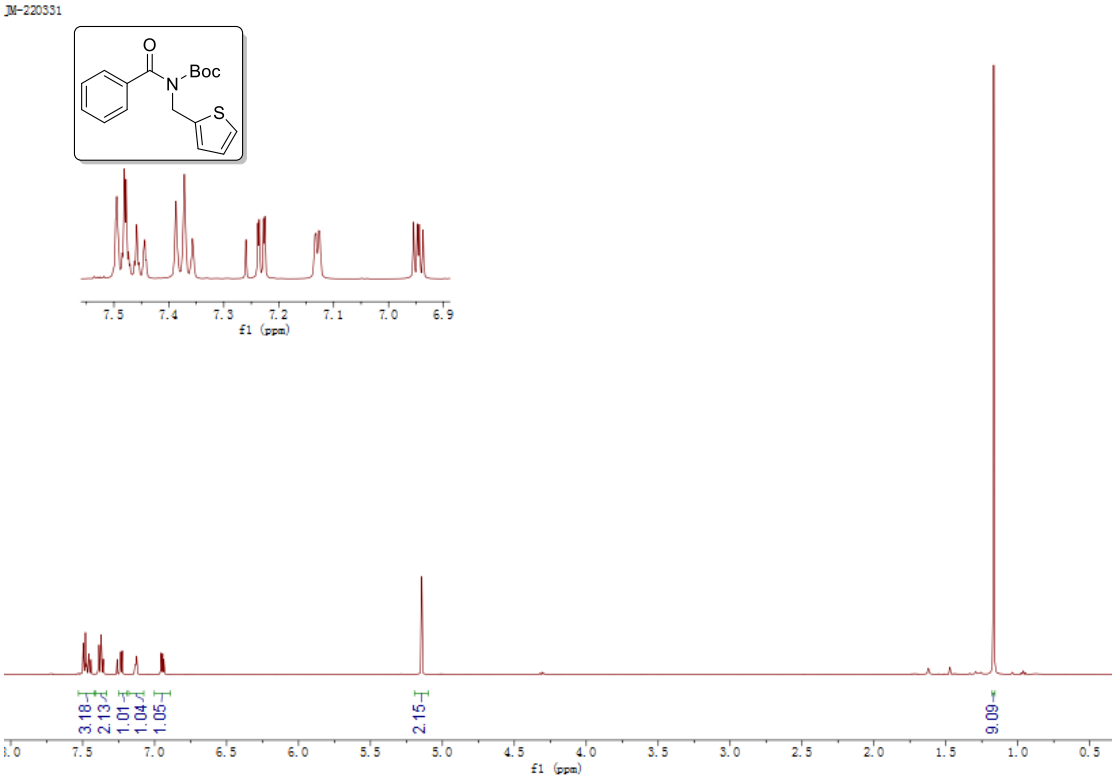
Supplementary Figure 17. ^{1}H NMR Spectrum of 2i (500 MHz, $CDCl_3$)



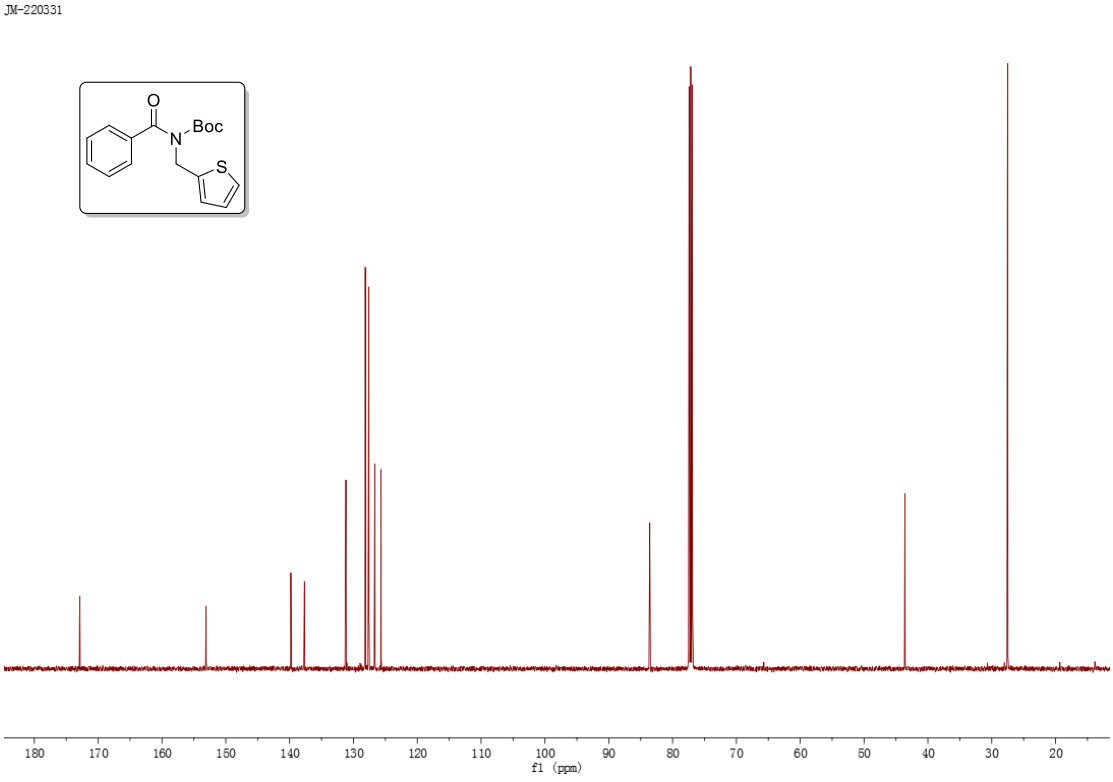
Supplementary Figure 18. ^{13}C NMR Spectrum of 2i (125 MHz, $CDCl_3$)



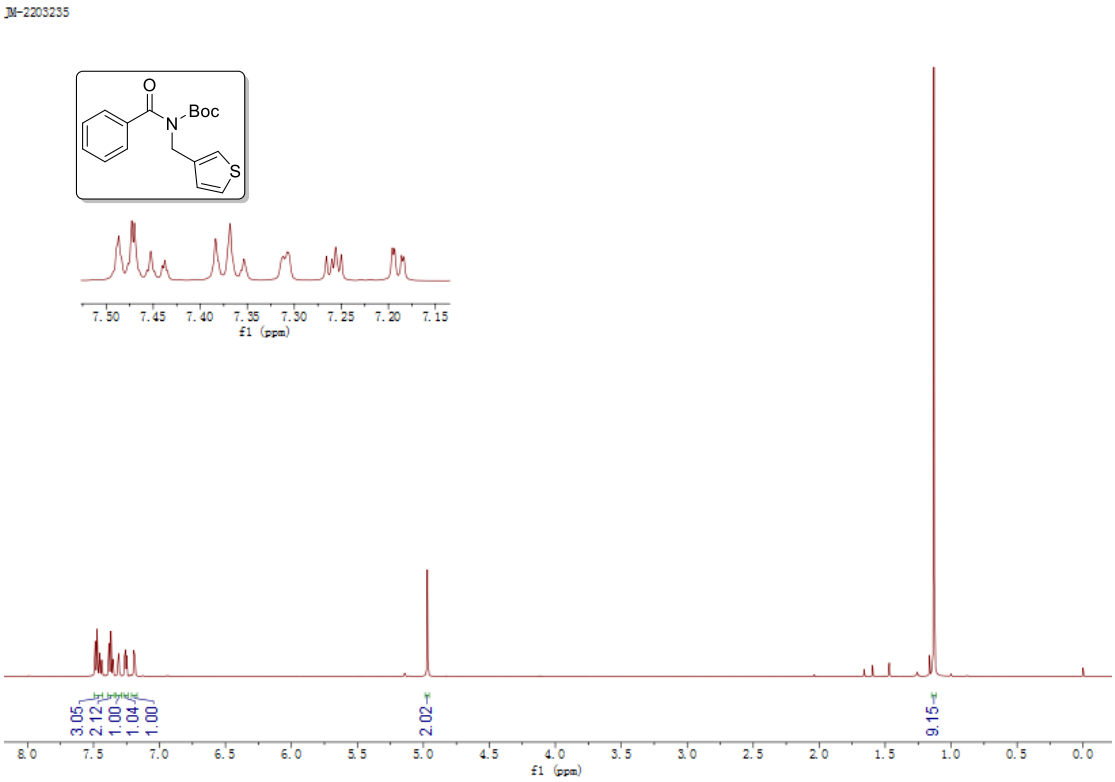
Supplementary Figure 19. ^{13}H NMR Spectrum of 2k (500 MHz, $CDCl_3$)



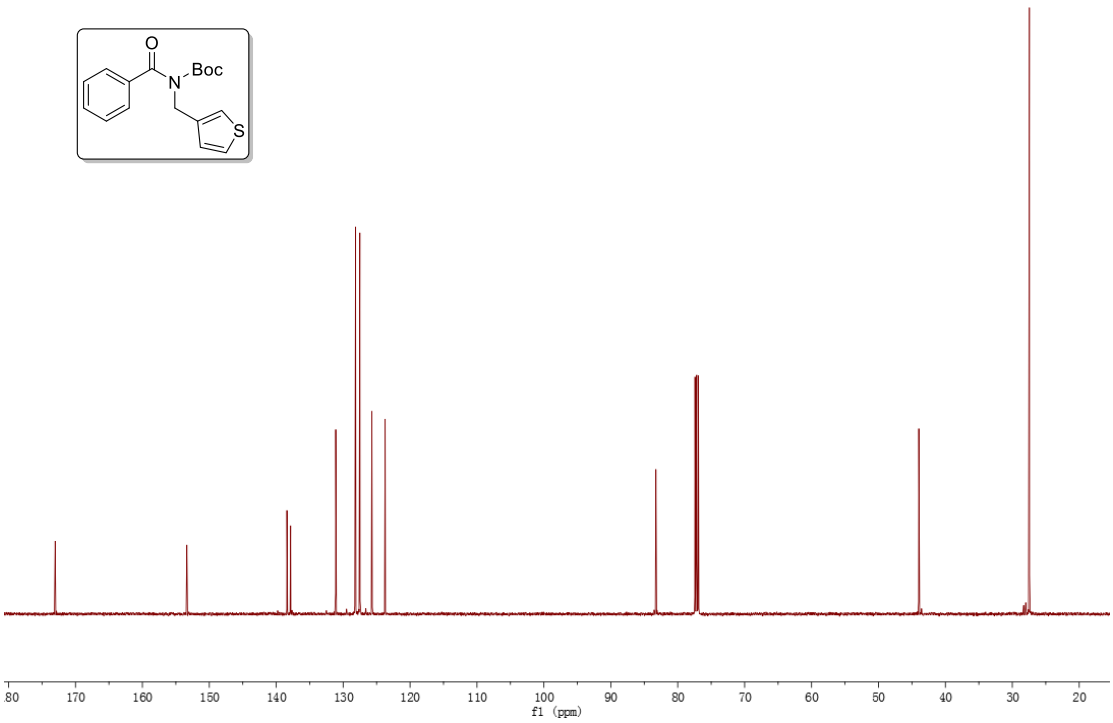
Supplementary Figure 20. ^{13}C NMR Spectrum of 2k (125 MHz, $CDCl_3$)



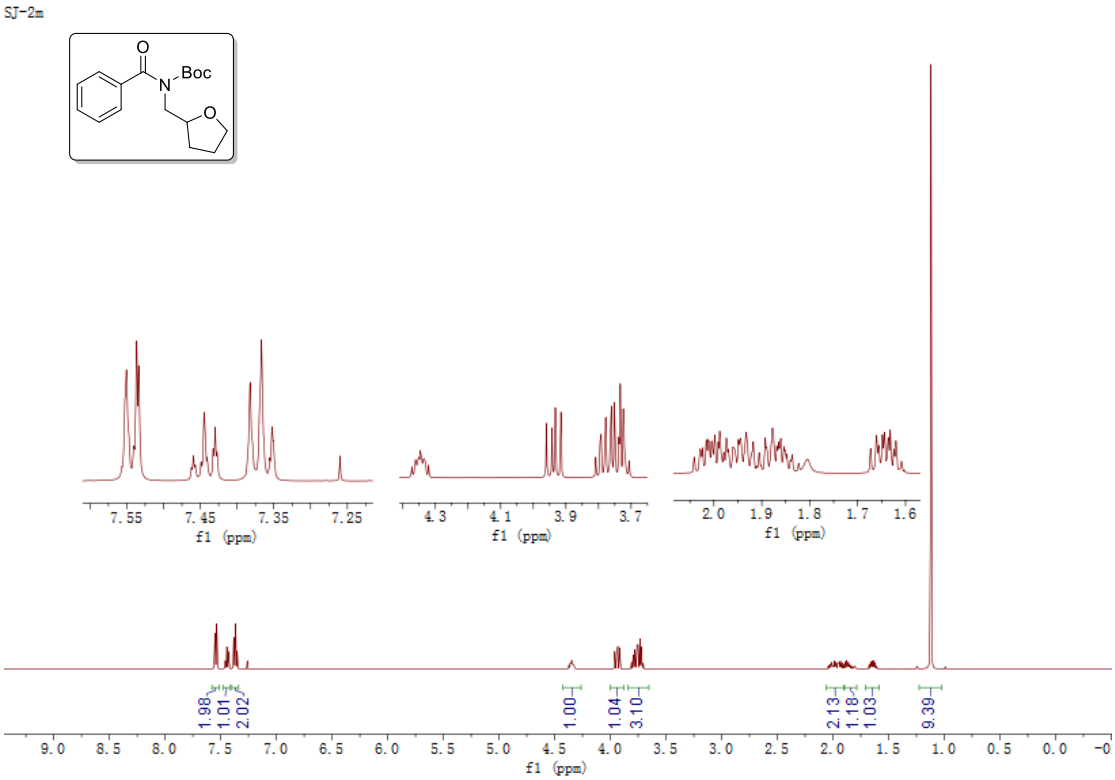
Supplementary Figure 21. ^{1}H NMR Spectrum of 2l (500 MHz, $CDCl_3$)



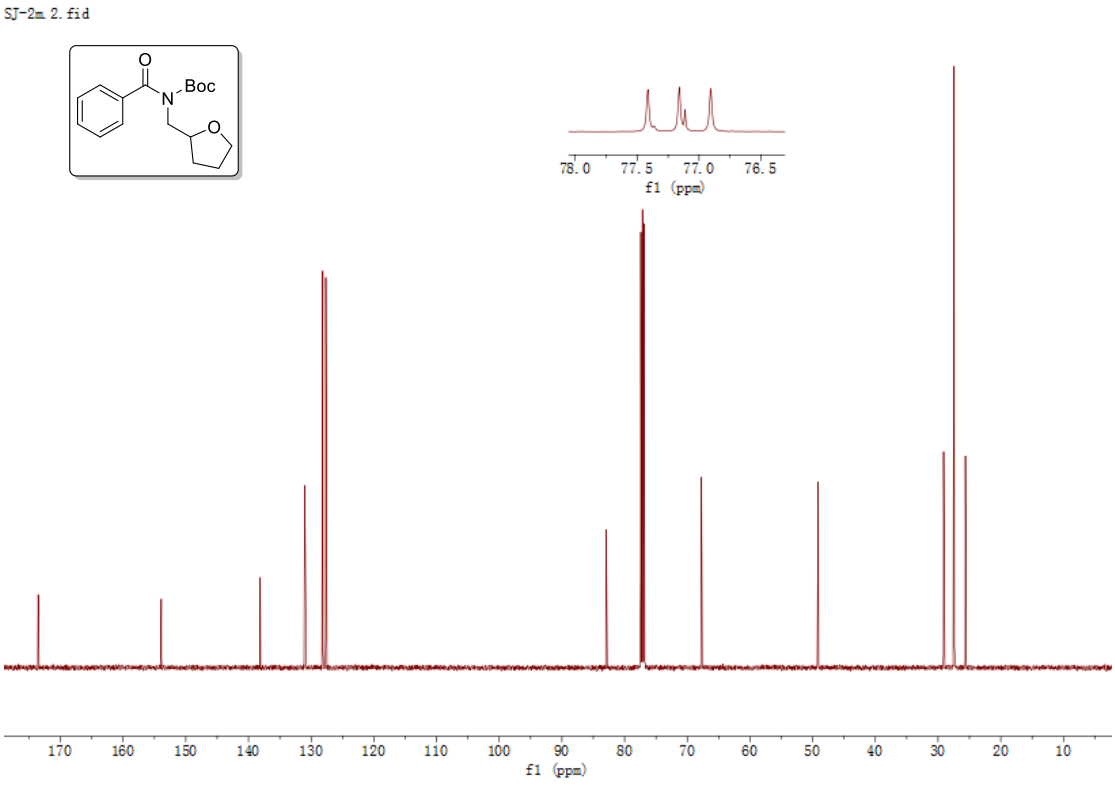
Supplementary Figure 22. ^{13}C NMR Spectrum of 2l (125 MHz, $CDCl_3$)



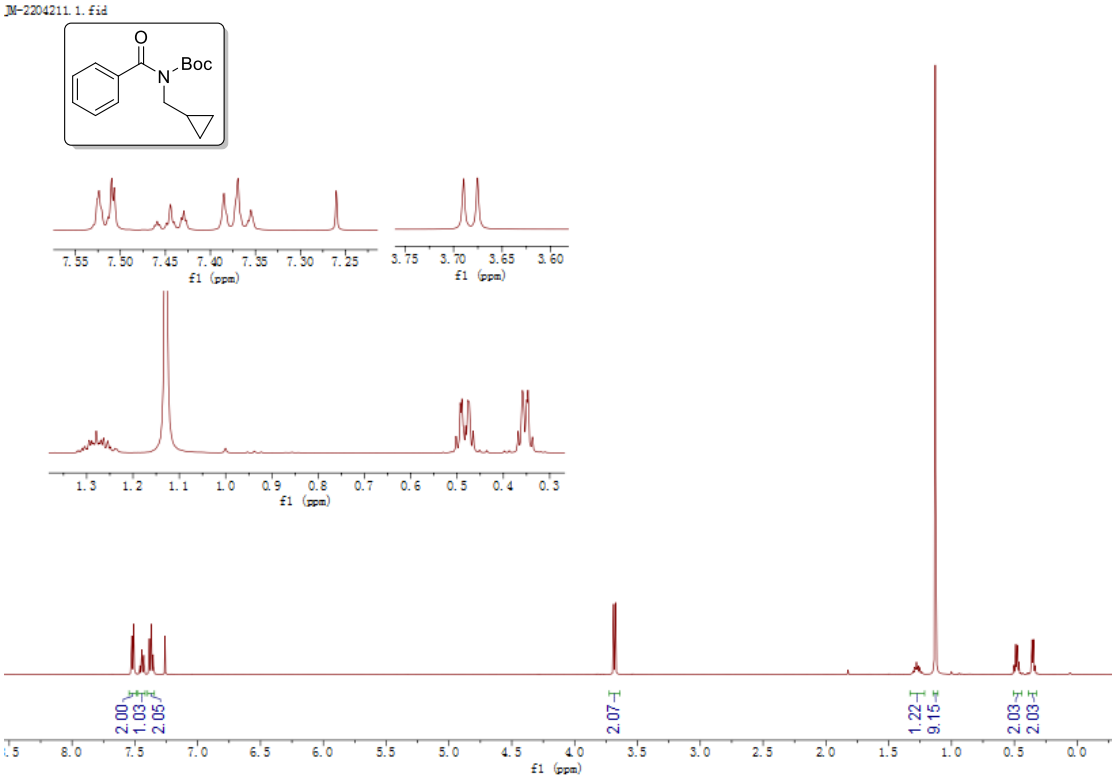
Supplementary Figure 23. ^{1}H NMR Spectrum of 2m (500 MHz, $CDCl_3$)



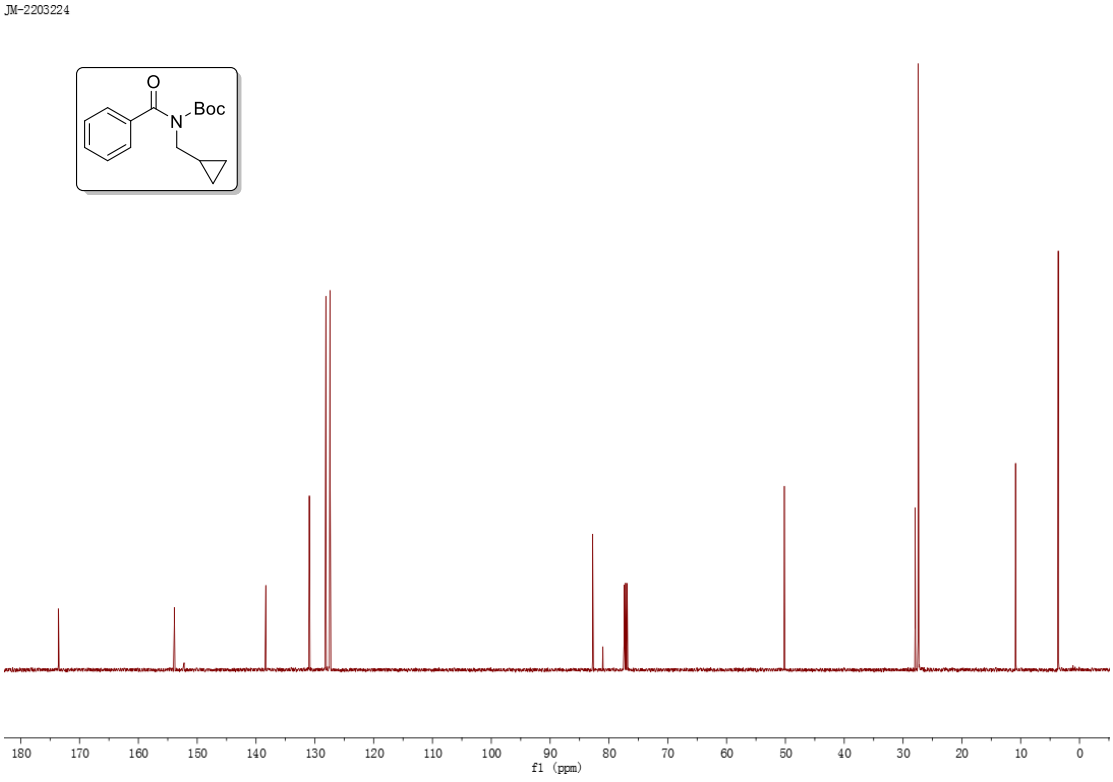
Supplementary Figure 24. ^{13}C NMR Spectrum of 2m (125 MHz, $CDCl_3$)



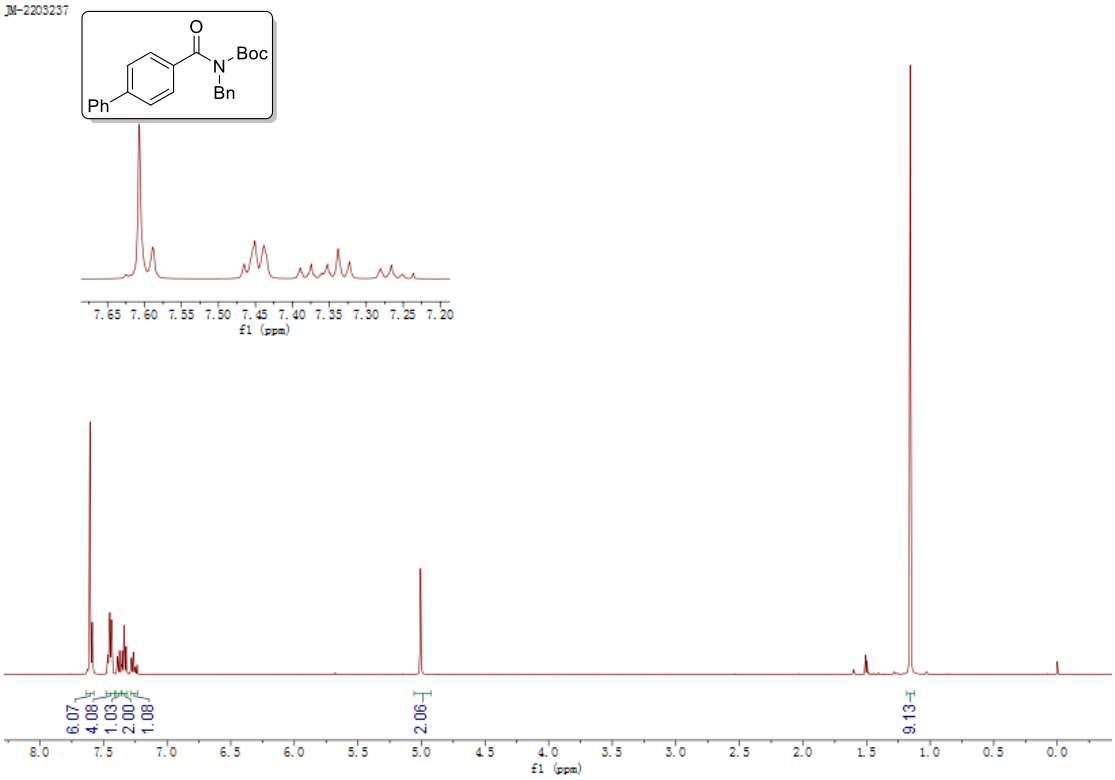
Supplementary Figure 25. ^{1}H NMR Spectrum of 2p (500 MHz, $CDCl_3$)



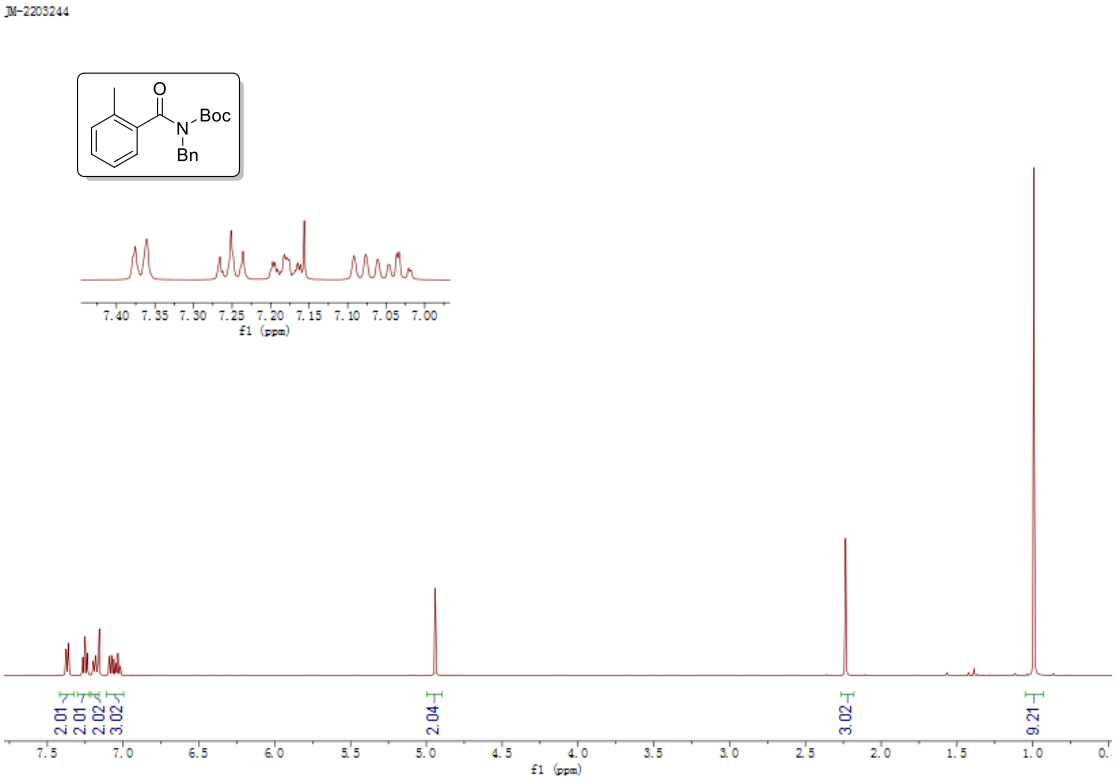
Supplementary Figure 26. ^{13}C NMR Spectrum of 2p (125 MHz, $CDCl_3$)



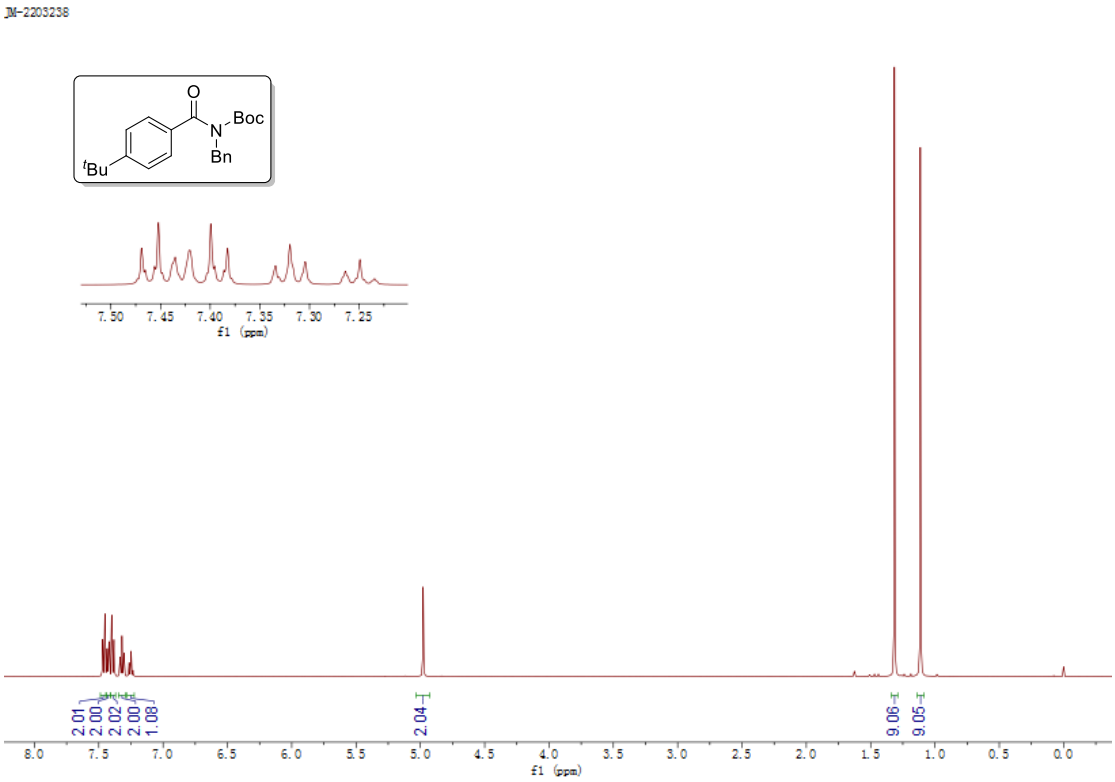
Supplementary Figure 27. ^{1}H NMR Spectrum of 2b' (500 MHz, $CDCl_3$)



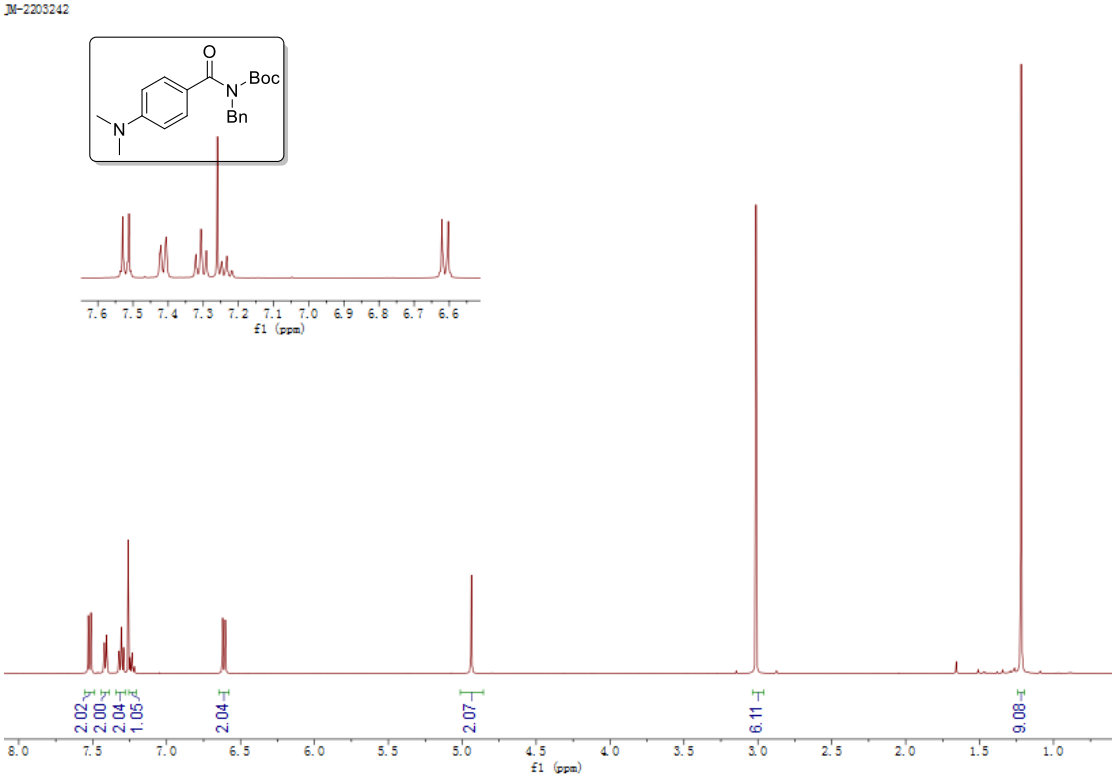
Supplementary Figure 28. ^{1}H NMR Spectrum of 2d' (500 MHz, $CDCl_3$)



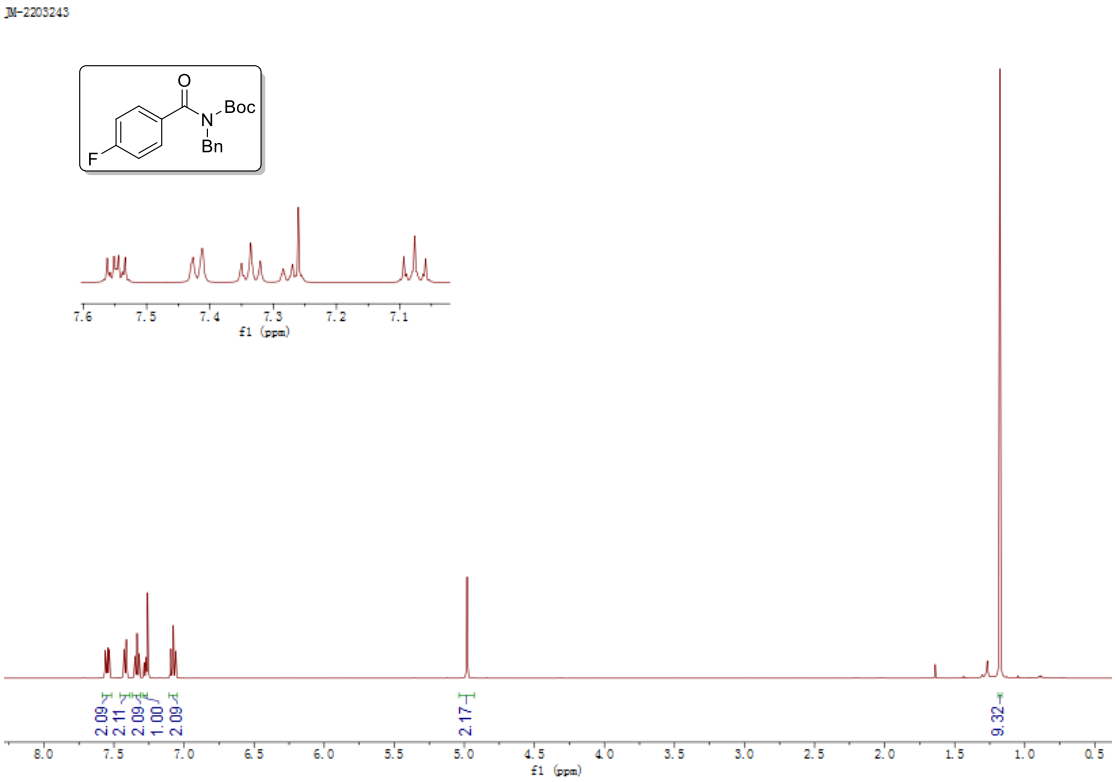
Supplementary Figure 29. ^{1}H NMR Spectrum of 2e' (500 MHz, $CDCl_3$)



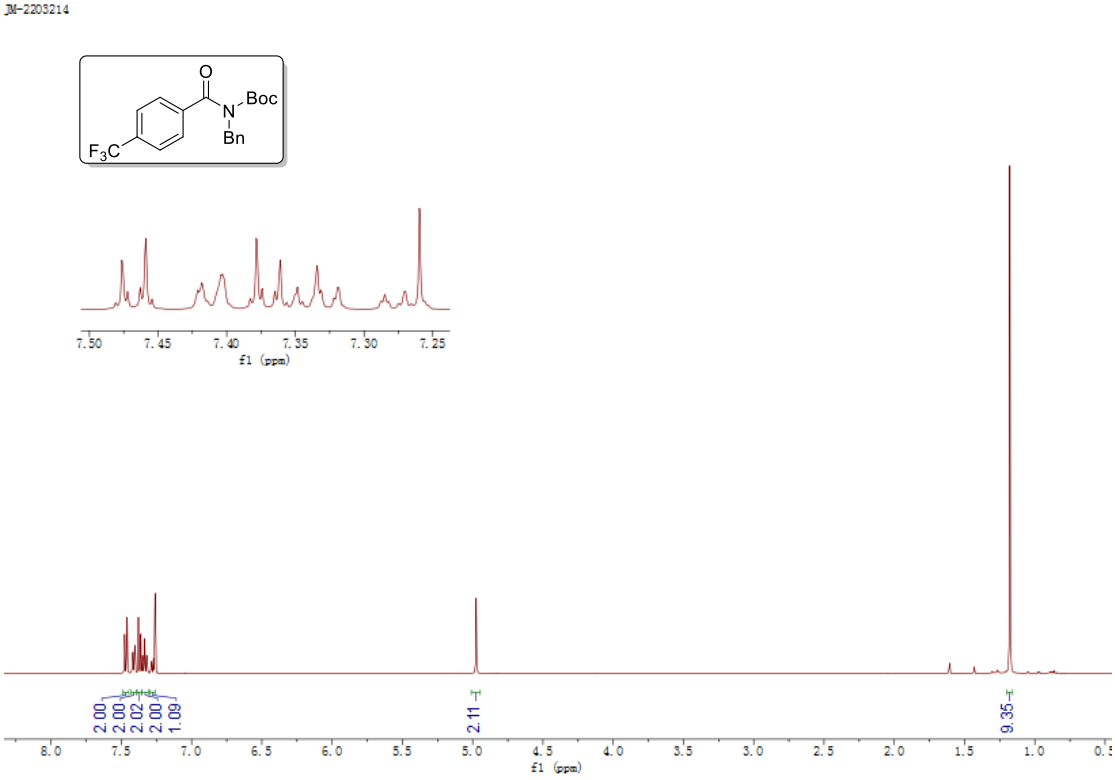
Supplementary Figure 30. ^{1}H NMR Spectrum of 2f' (500 MHz, $CDCl_3$)



Supplementary Figure 31. ^{1}H NMR Spectrum of 2g' (500 MHz, $CDCl_3$)

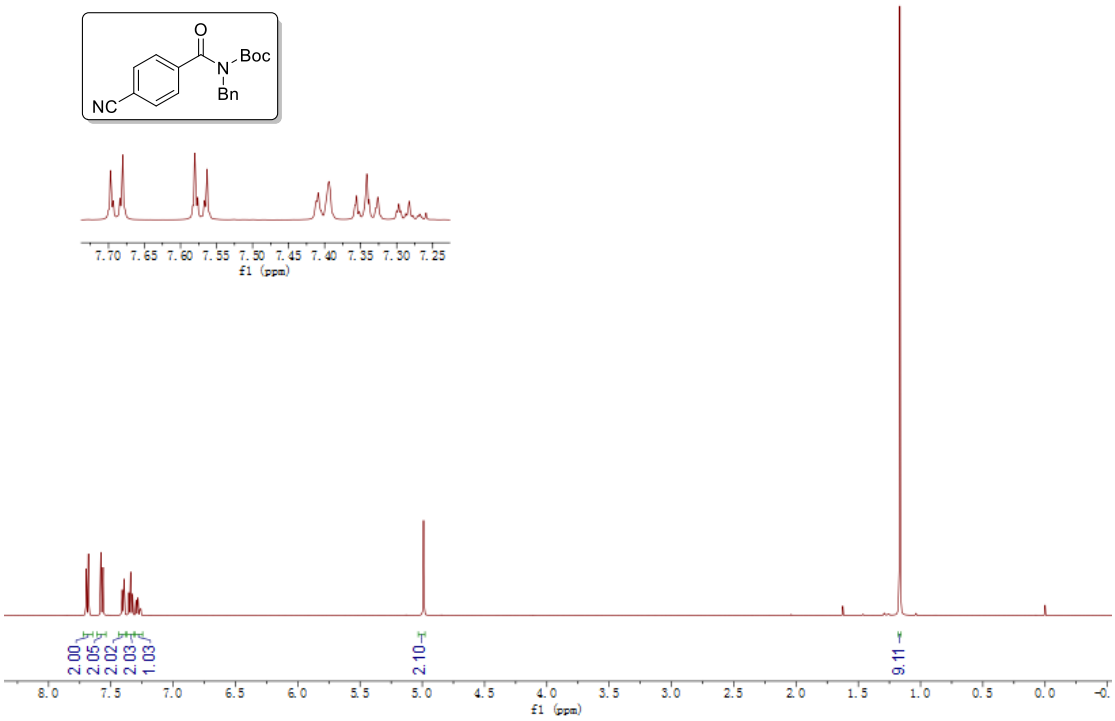


Supplementary Figure 32. ^{1}H NMR Spectrum of 2h' (500 MHz, $CDCl_3$)



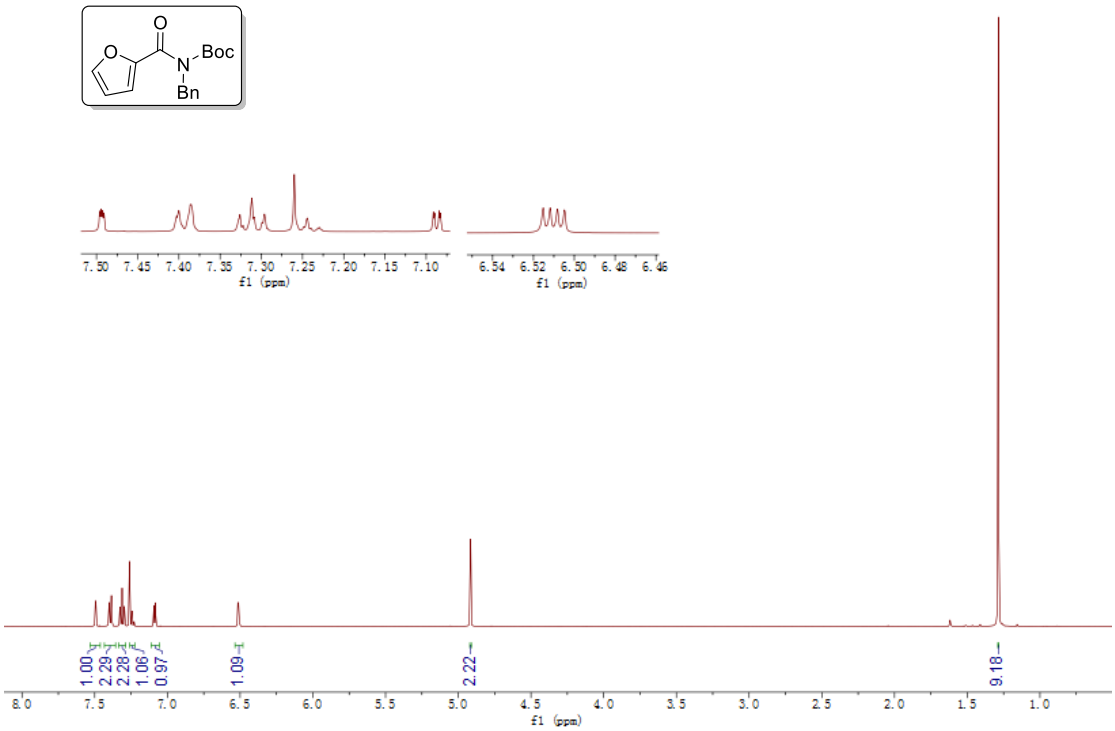
Supplementary Figure 33. ^{1}H NMR Spectrum of 2i' (500 MHz, $CDCl_3$)

JM-2203225

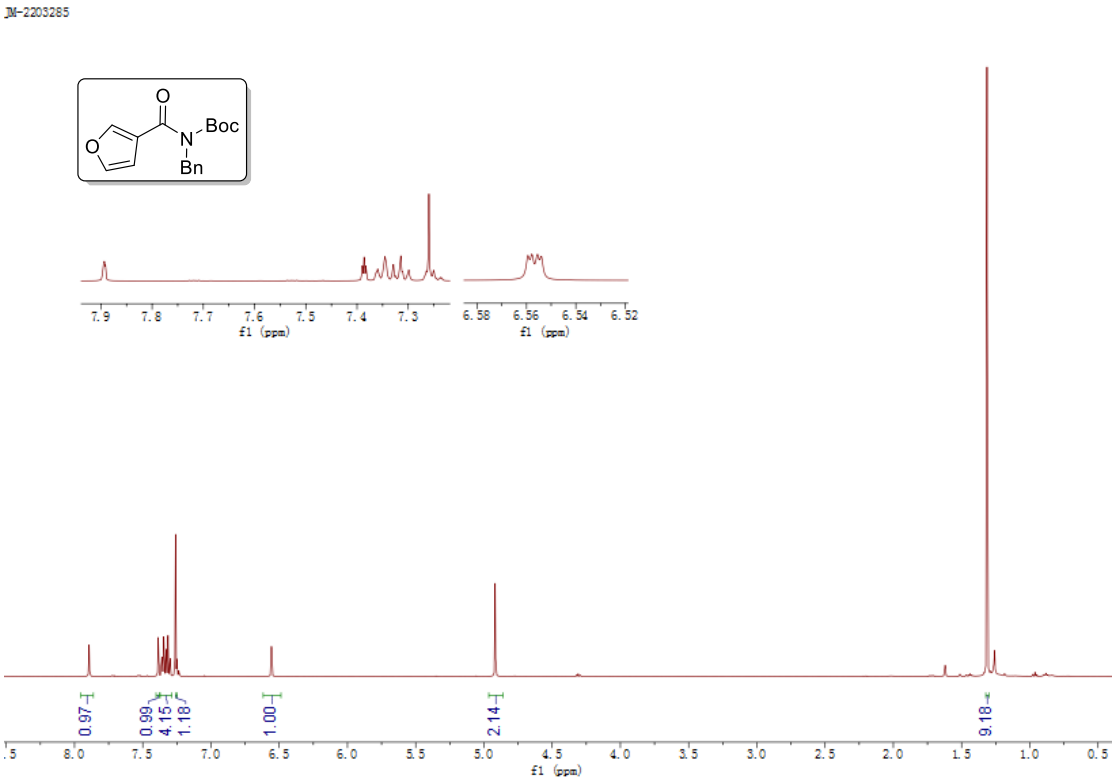


Supplementary Figure 34. ^{1}H NMR Spectrum of 2j' (500 MHz, $CDCl_3$)

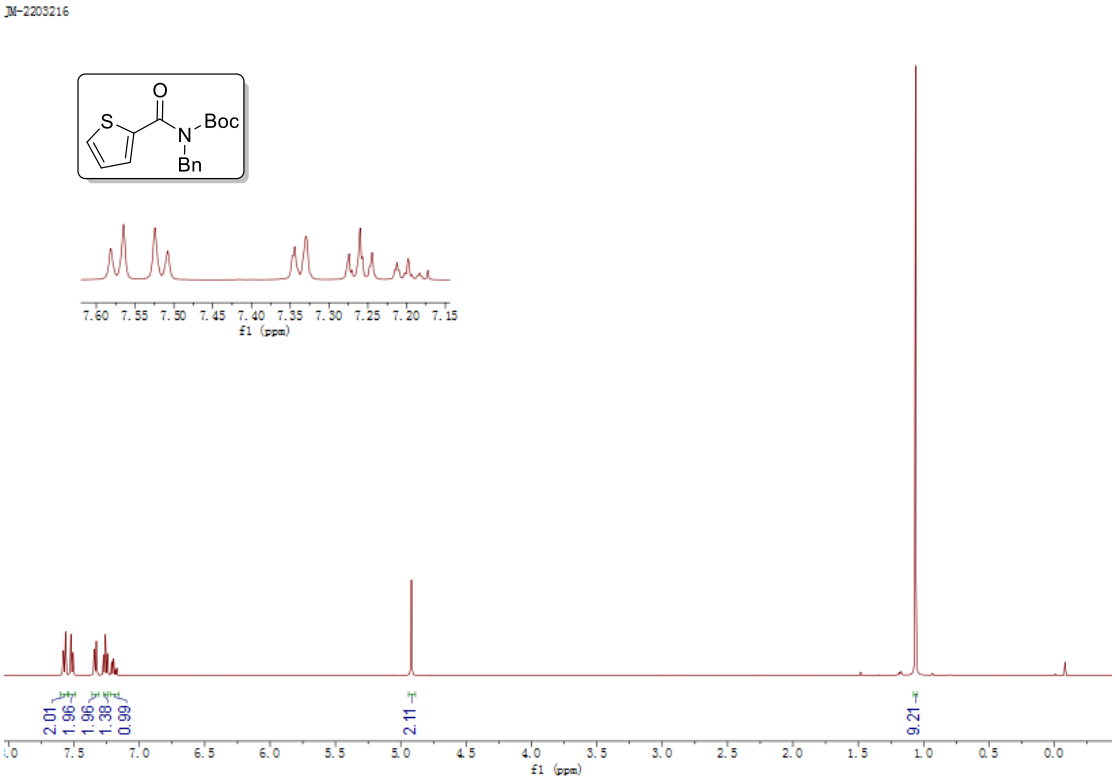
JM-2203215



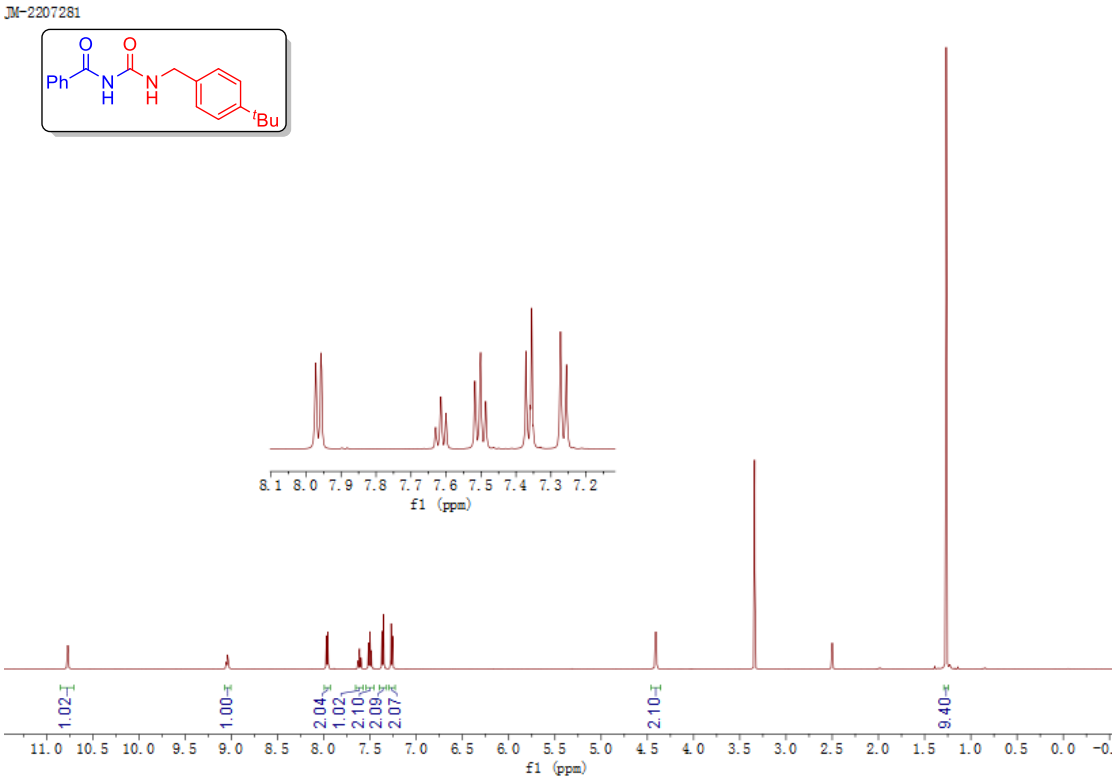
Supplementary Figure 35. ^{1}H NMR Spectrum of 2k' (500 MHz, $CDCl_3$)



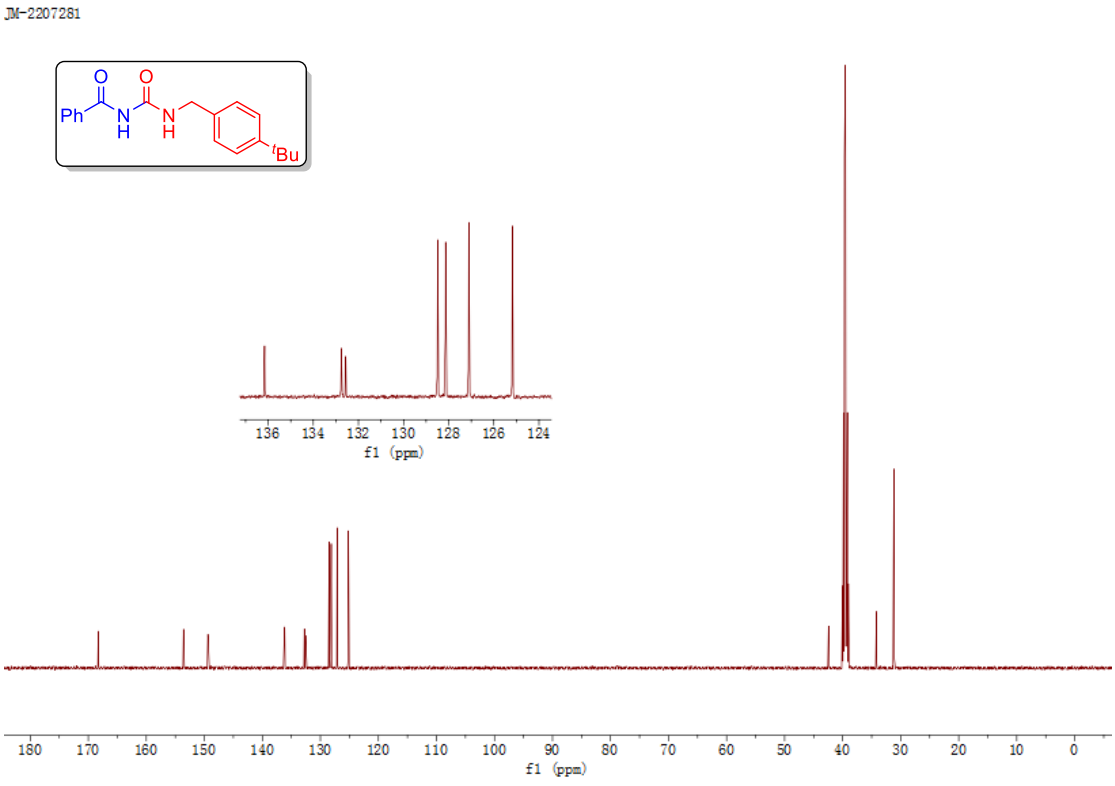
Supplementary Figure 36. ^{1}H NMR Spectrum of 2l' (500 MHz, $CDCl_3$)



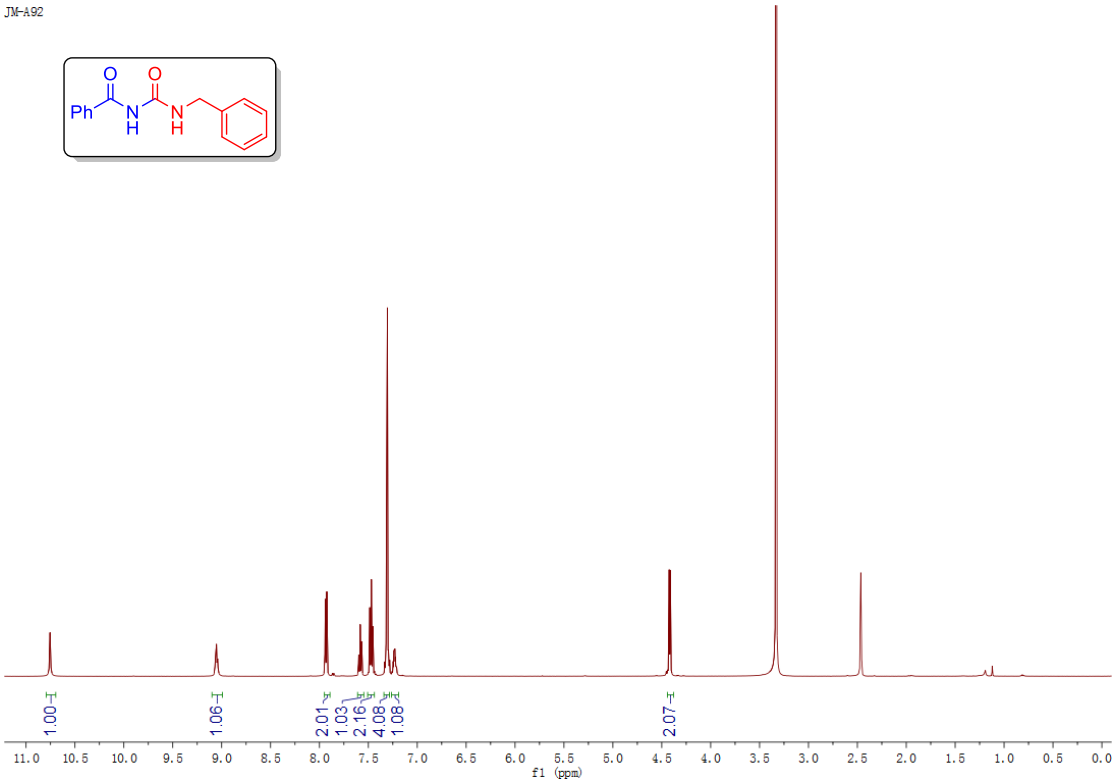
Supplementary Figure 37. ^{1}H NMR Spectrum of 3aa (500 MHz, DMSO-d$_6$)



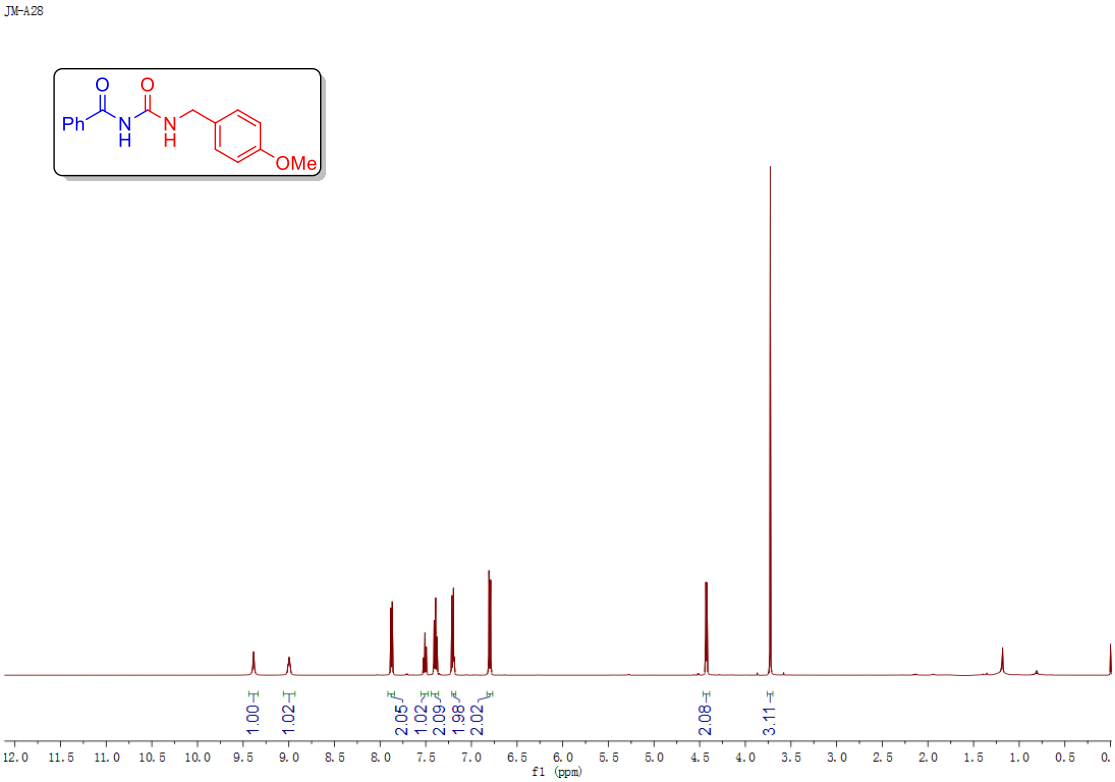
Supplementary Figure 38. ^{13}C NMR Spectrum of 3aa (125 MHz, DMSO-d$_6$)



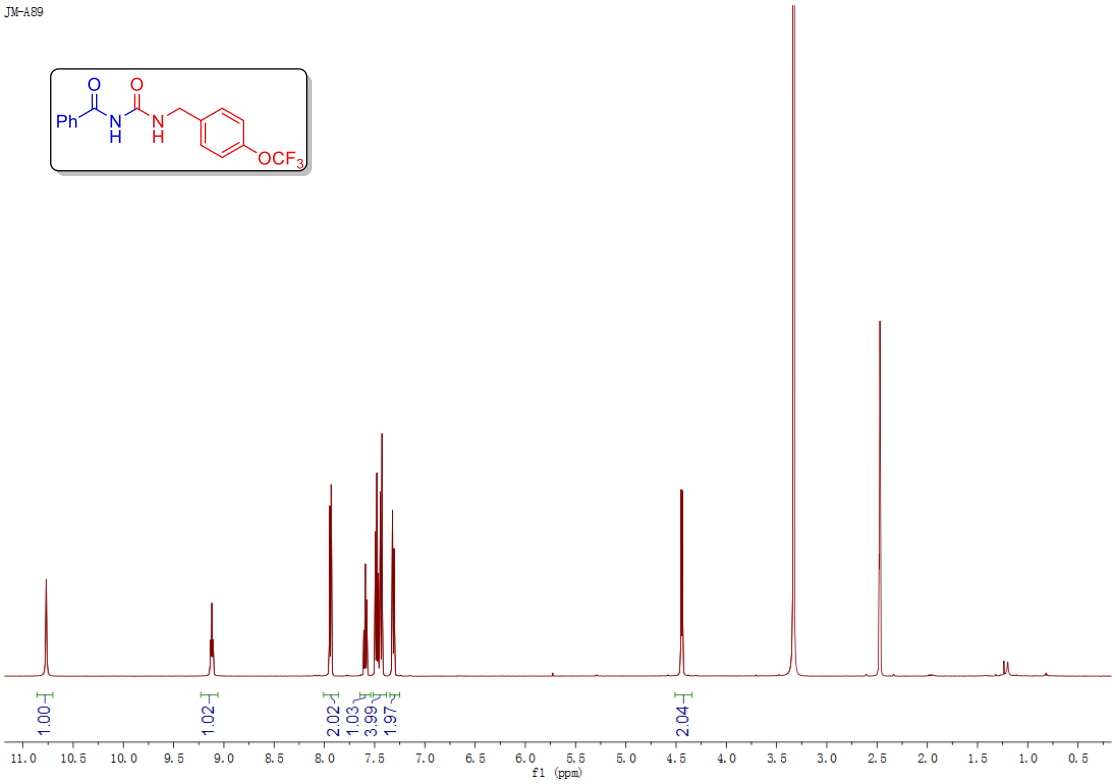
Supplementary Figure 39. ^{1}H NMR Spectrum of 3ab (500 MHz, DMSO-d_6)



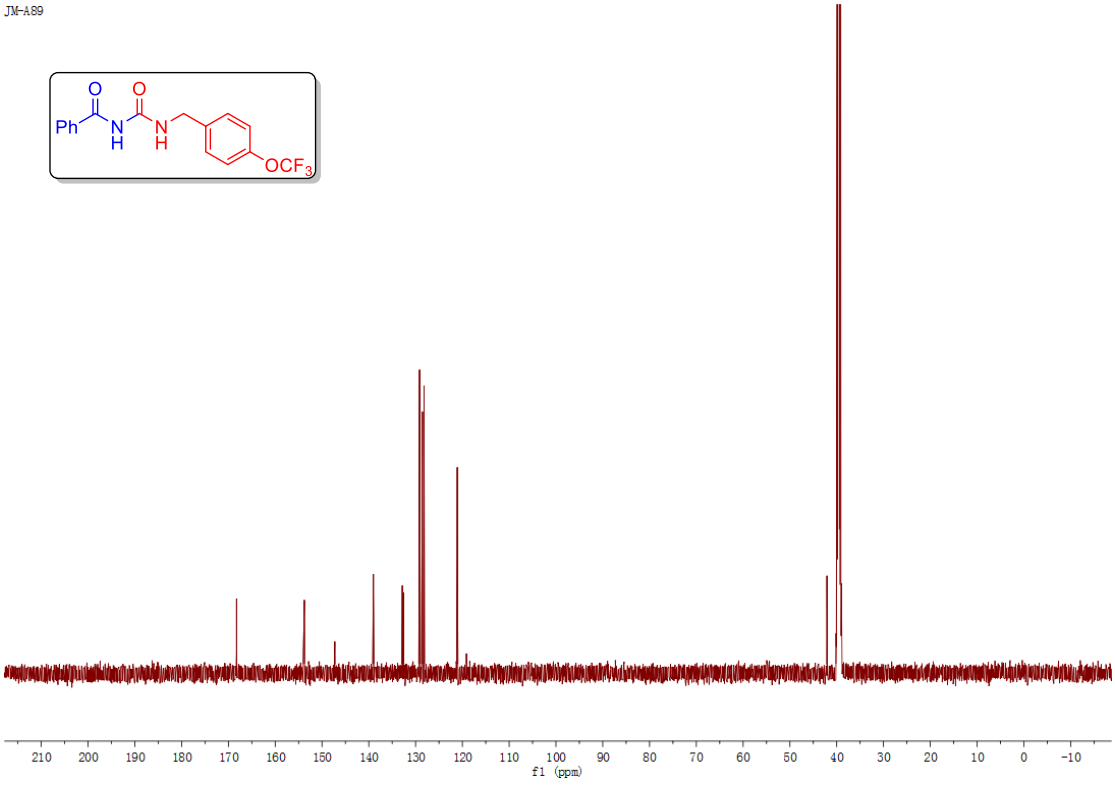
Supplementary Figure 40. ^{1}H NMR Spectrum of 3ac (500 MHz, $CDCl_3$)



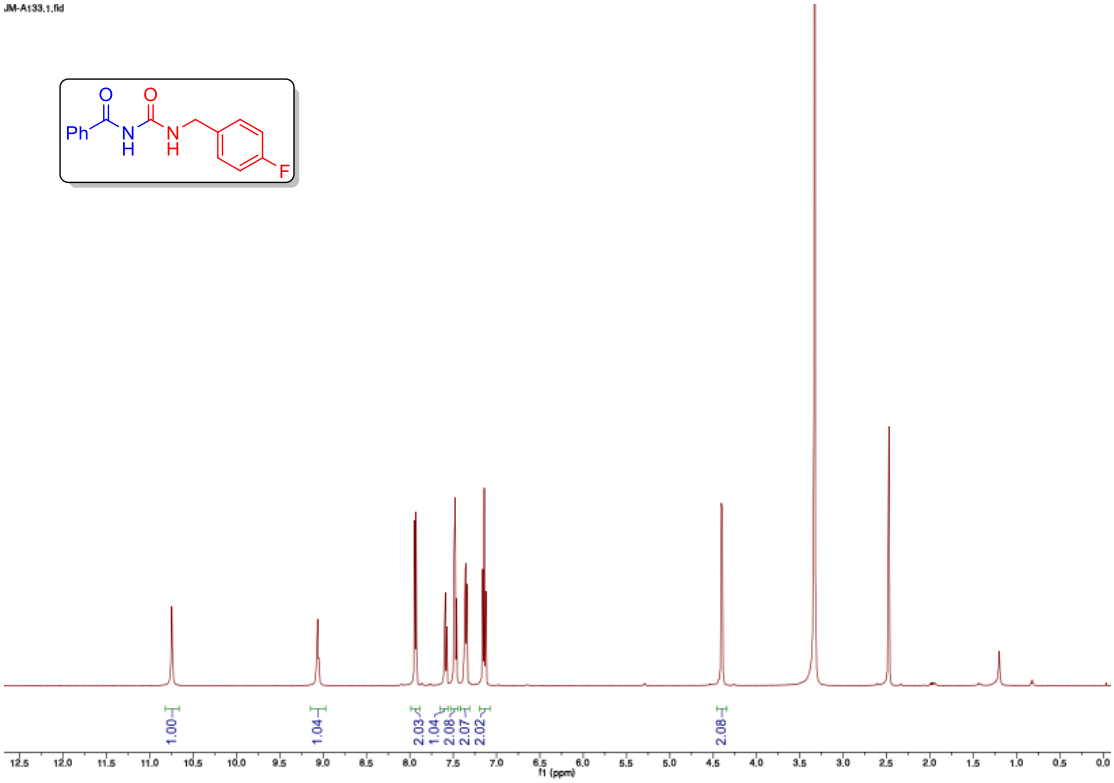
Supplementary Figure 41. ^{1}H NMR Spectrum of 3ad (500 MHz, DMSO-d_6)



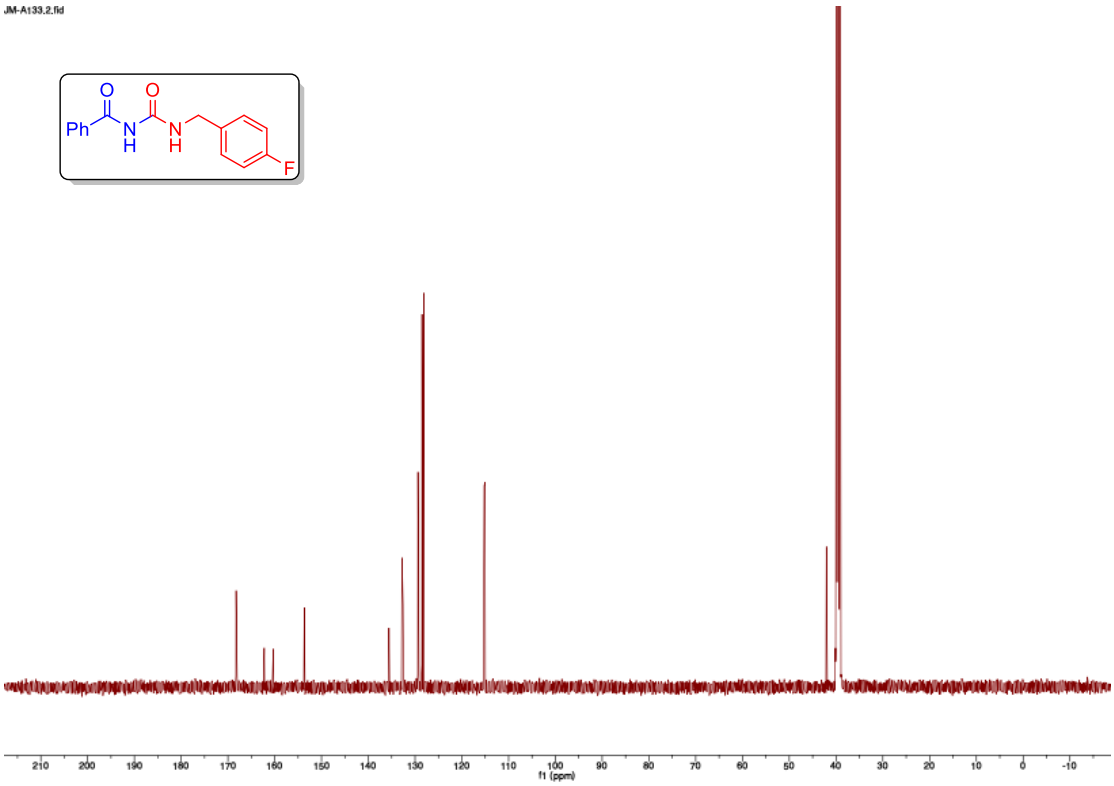
Supplementary Figure 42. ^{13}C NMR Spectrum of 3ad (125 MHz, DMSO-d_6)



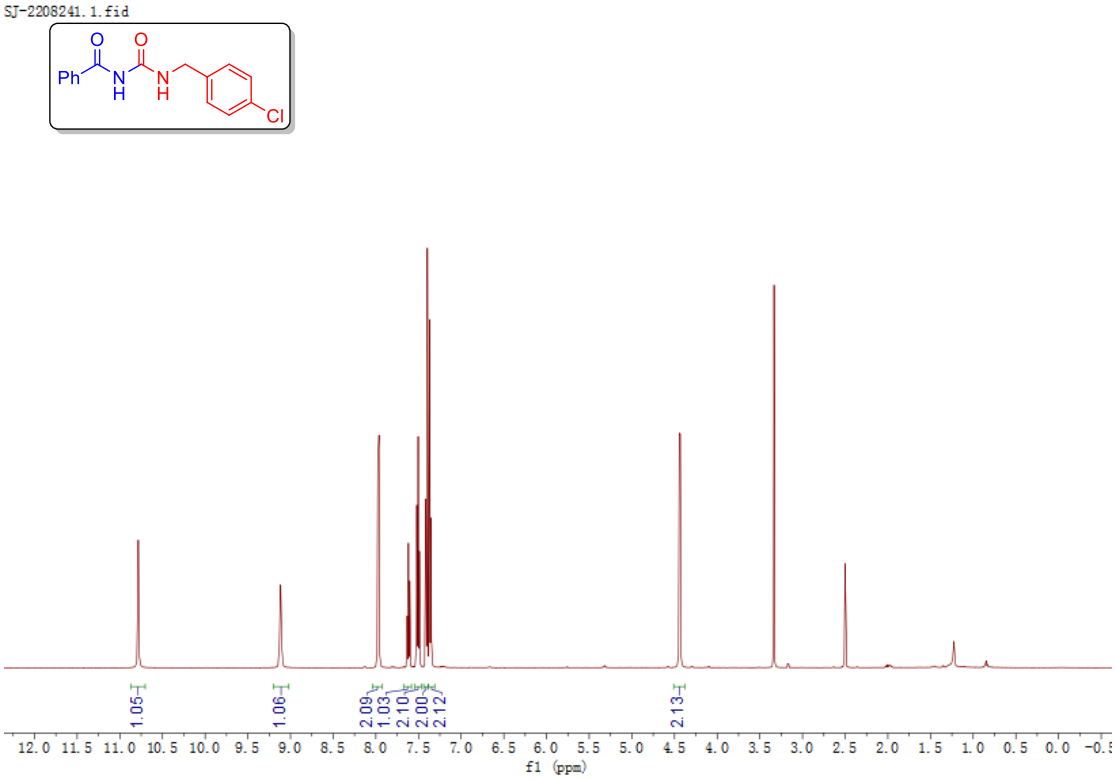
Supplementary Figure 43. ^{1}H NMR Spectrum of 3ae (500MHz, DMSO-d_6)



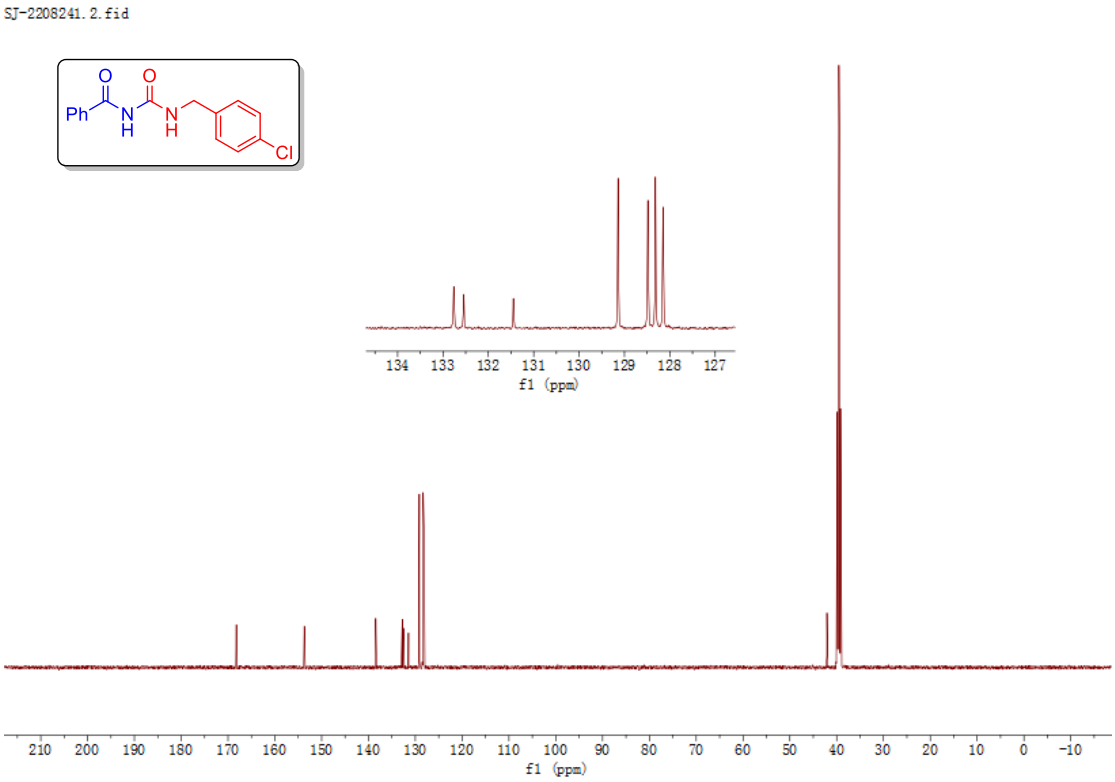
Supplementary Figure 44. ^{13}C NMR Spectrum of 3ae (125 MHz, DMSO-d_6)



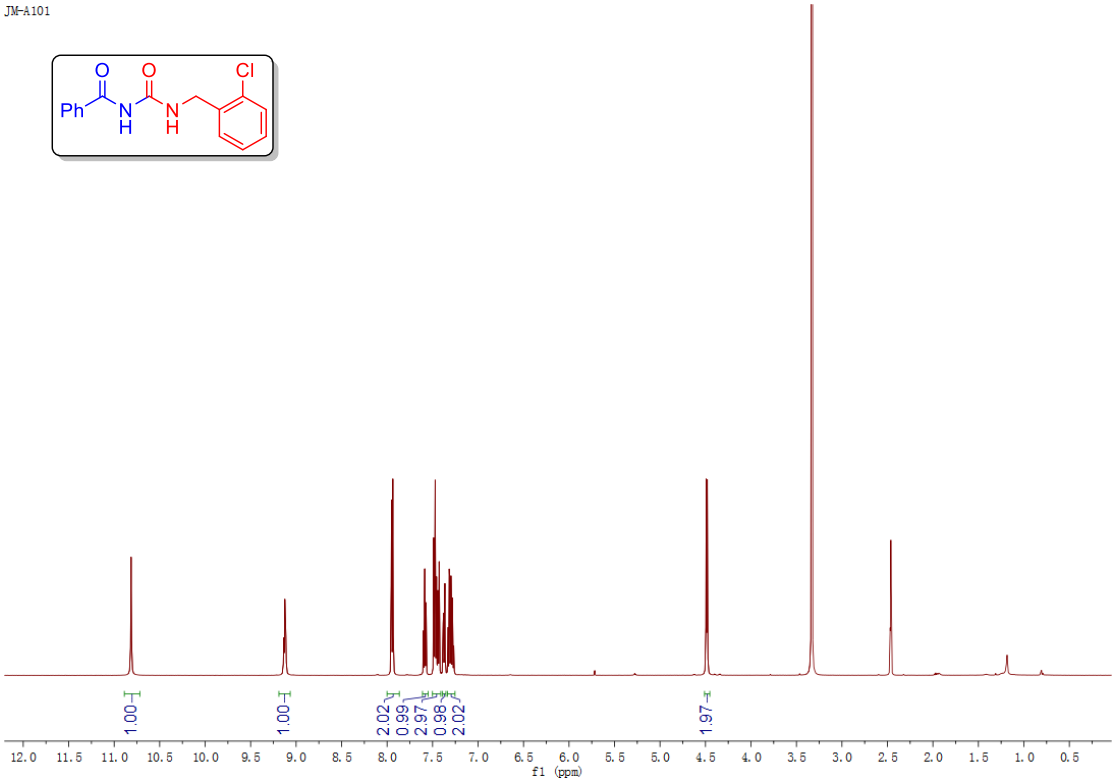
Supplementary Figure 45. ^{1}H NMR Spectrum of 3af (500MHz, DMSO-d_6)



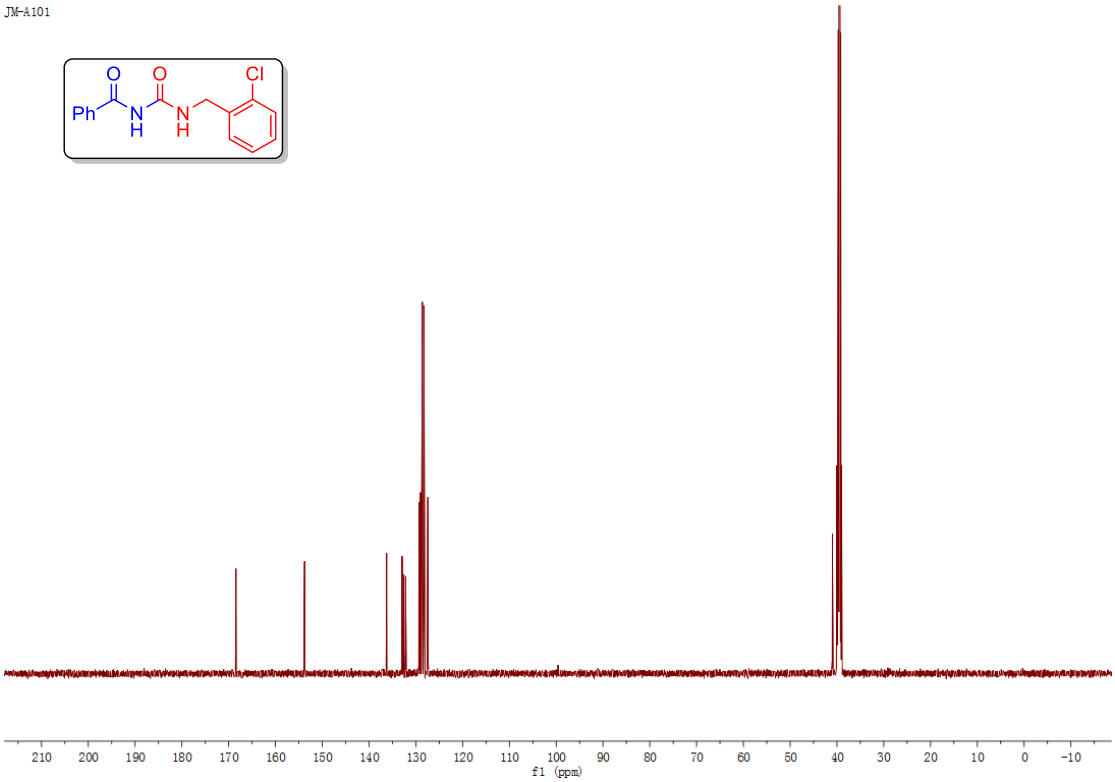
Supplementary Figure 46. ^{13}C NMR Spectrum of 3af (125 MHz, DMSO-d_6)



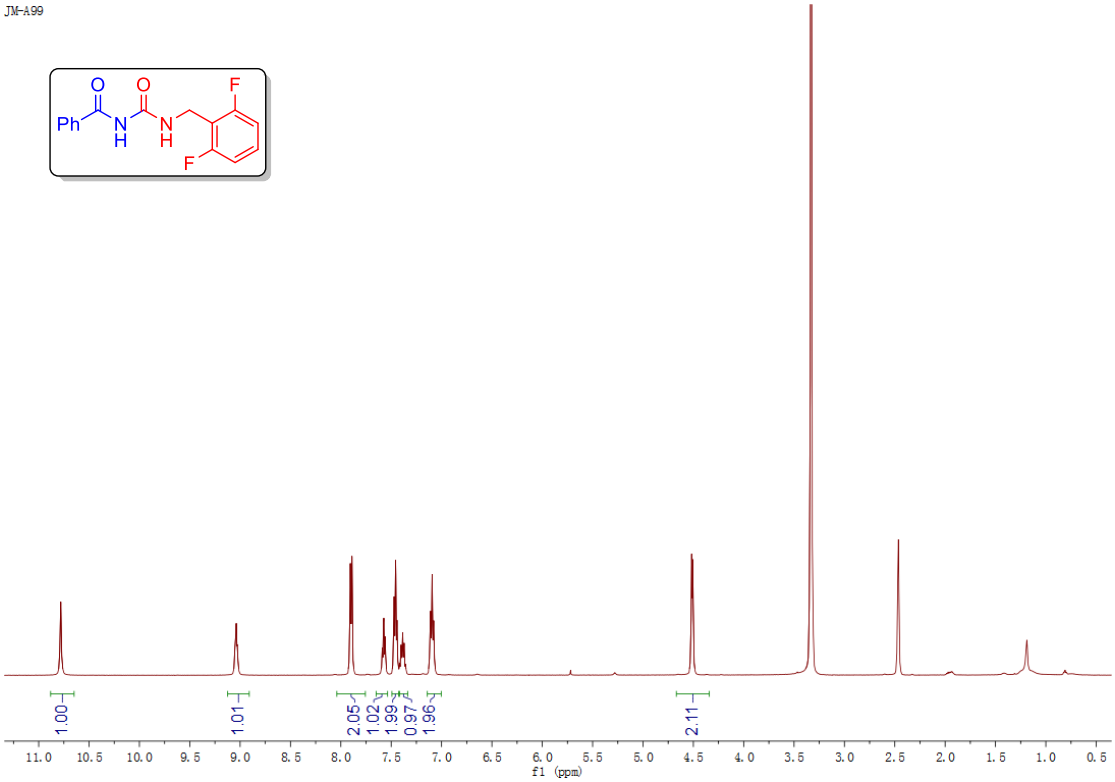
Supplementary Figure 47. ^{1}H NMR Spectrum of 3ag (500MHz, DMSO-d_6)



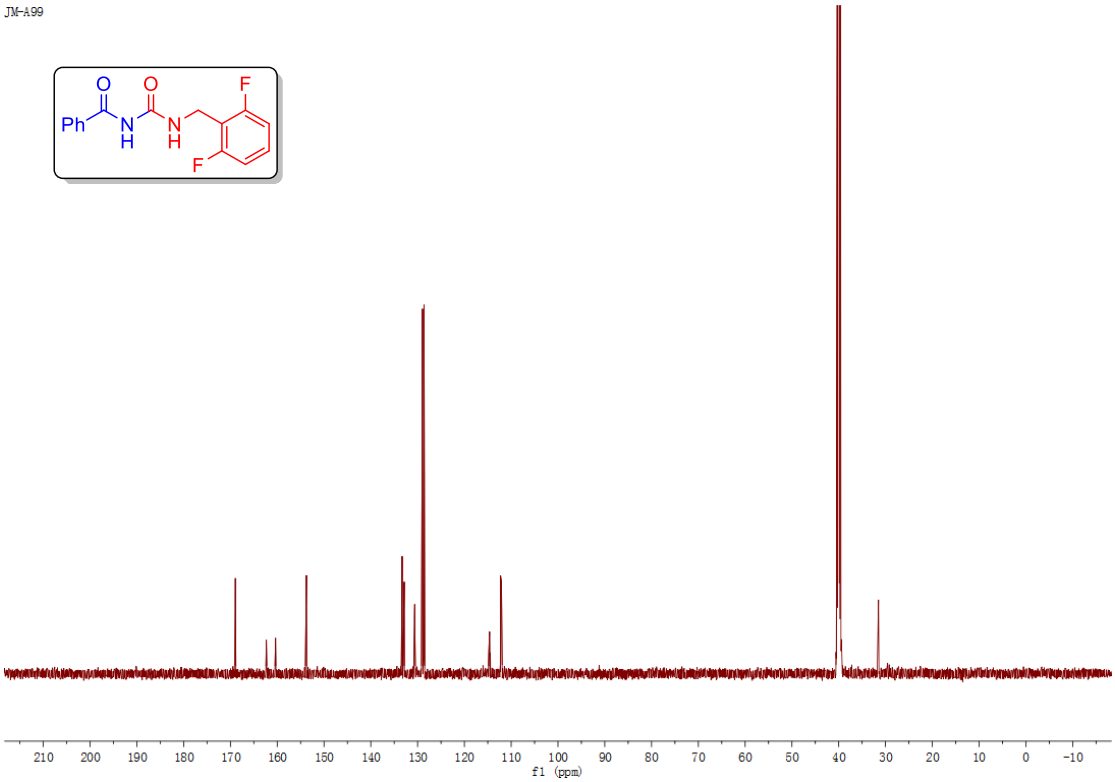
Supplementary Figure 48. ^{13}C NMR Spectrum of 3ag (125 MHz, DMSO-d_6)



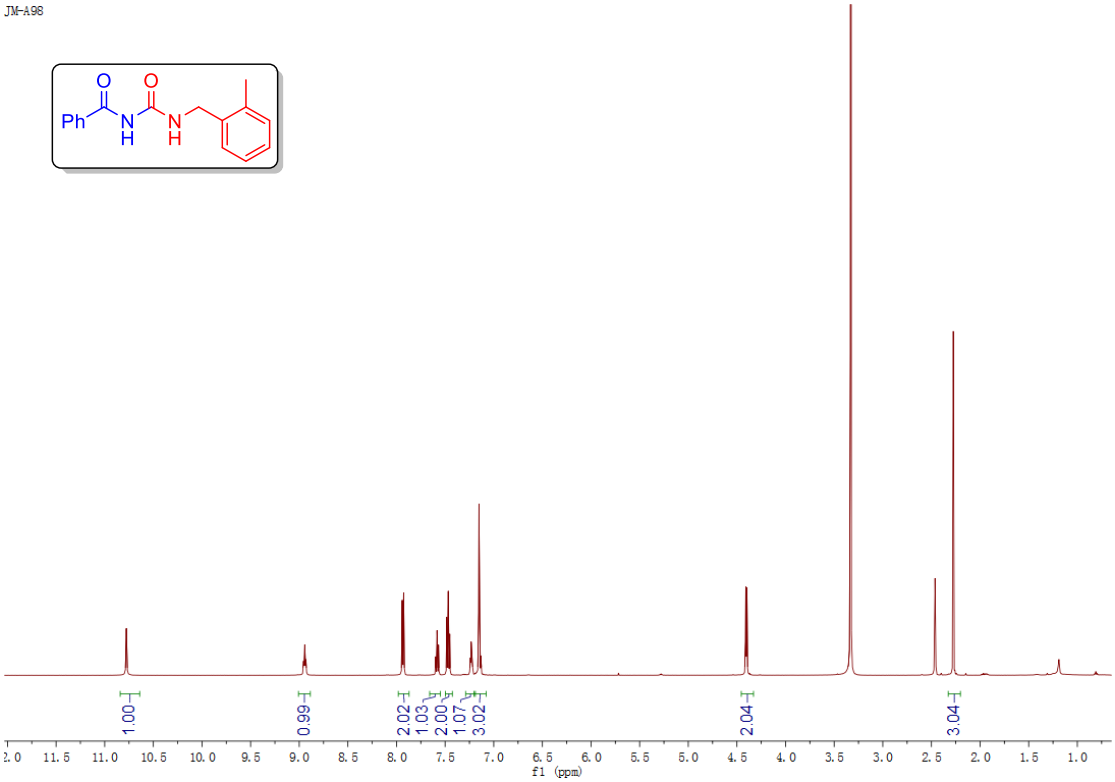
Supplementary Figure 49. ^{1}H NMR Spectrum of 3ah (500MHz, DMSO-d_6)



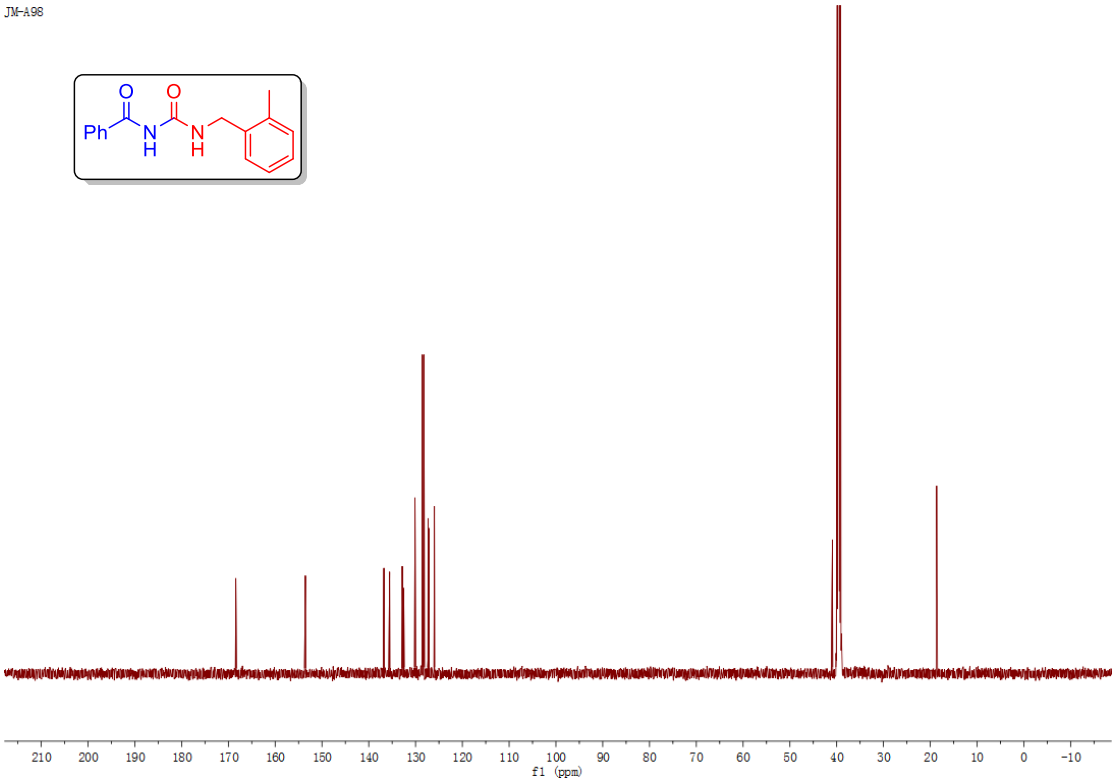
Supplementary Figure 50. ^{13}C NMR Spectrum of 3ah (125 MHz, DMSO-d_6)



Supplementary Figure 51. ^{1}H NMR Spectrum of 3ai (500MHz, DMSO-d_6)



Supplementary Figure 52. ^{13}C NMR Spectrum of 3ai (125 MHz, DMSO-d_6)



Supplementary Figure 53. ^{1}H NMR Spectrum of 3aj (500MHz, $CDCl_3$)

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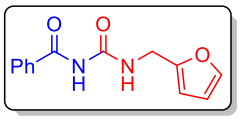
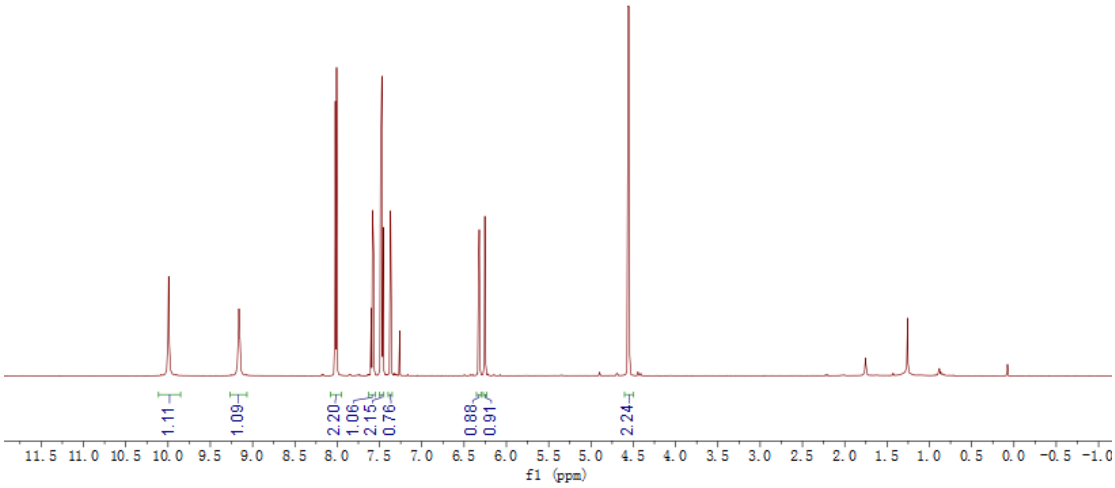
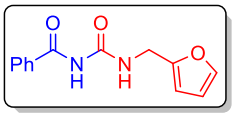
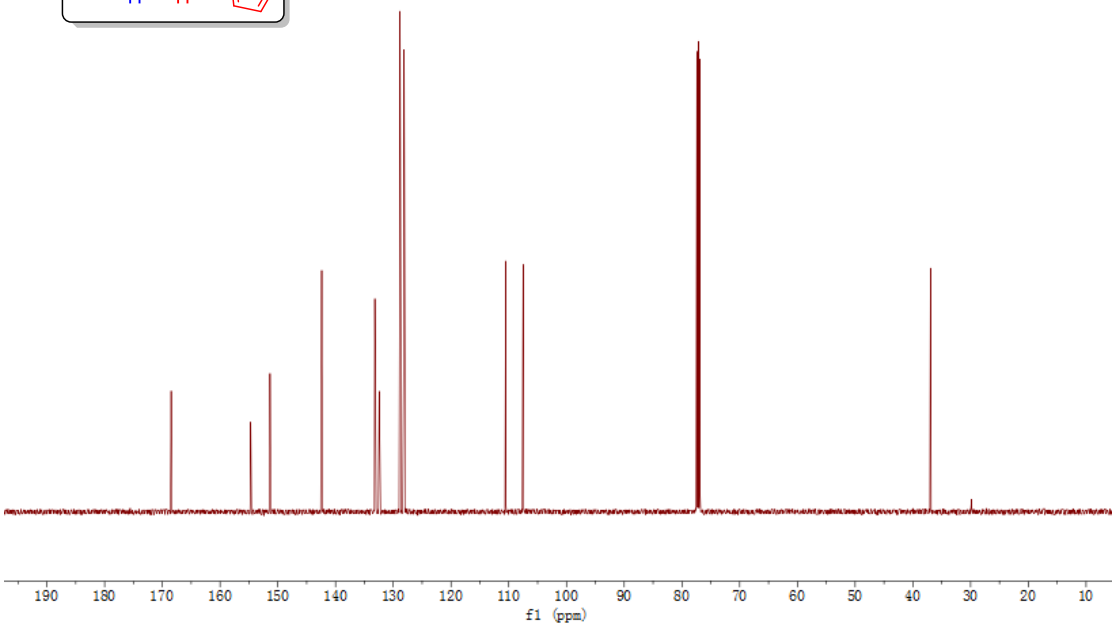




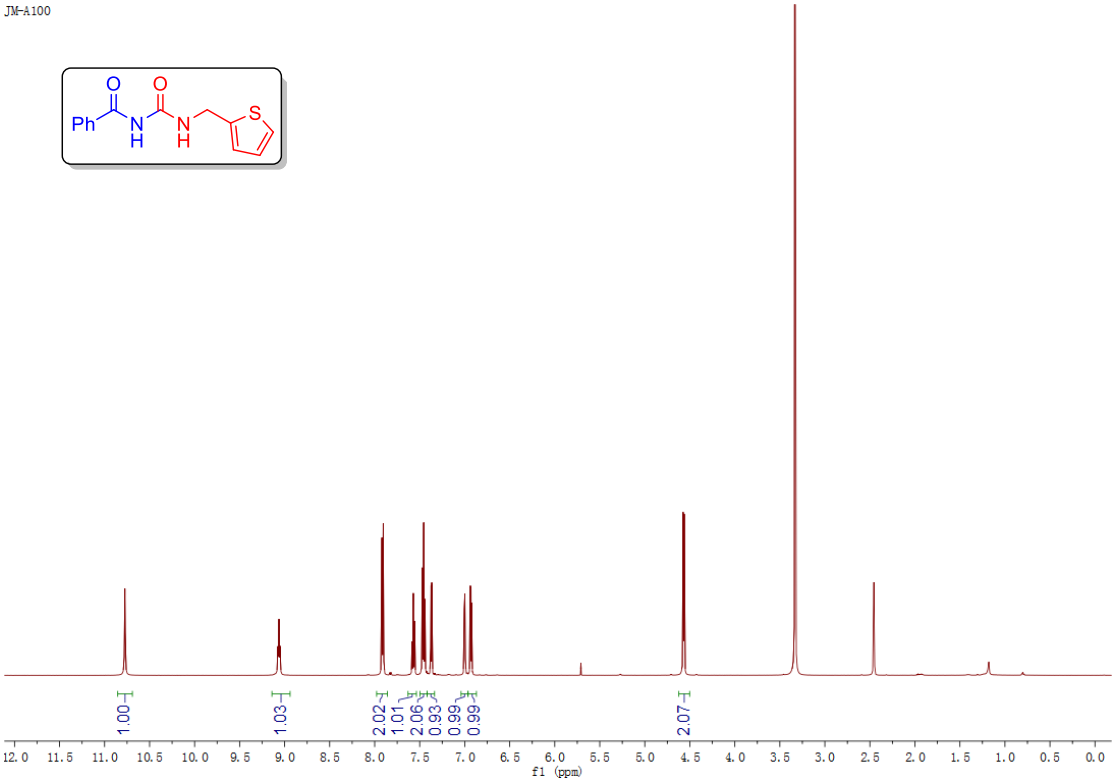
Supplementary Figure 54. ^{13}C NMR Spectrum of 3aj (125 MHz, $CDCl_3$)

SJ-2208242.2.fid

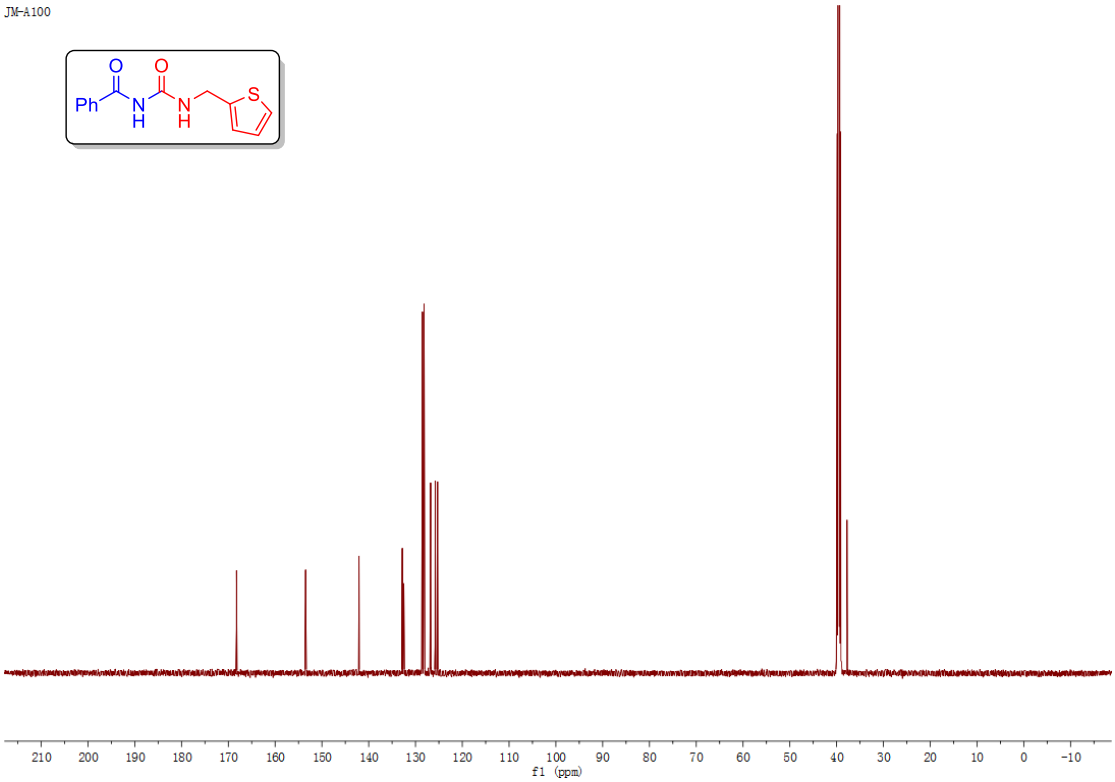




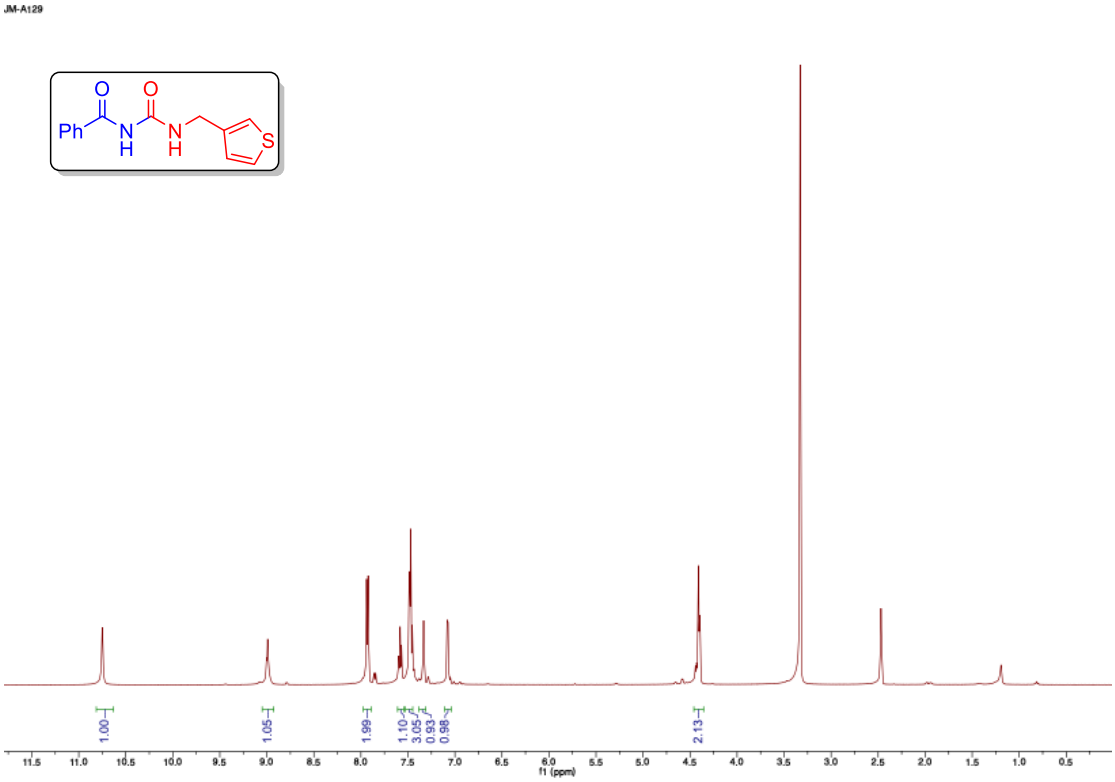
Supplementary Figure 55. ^{1}H NMR Spectrum of 3ak (500MHz, DMSO-d_6)



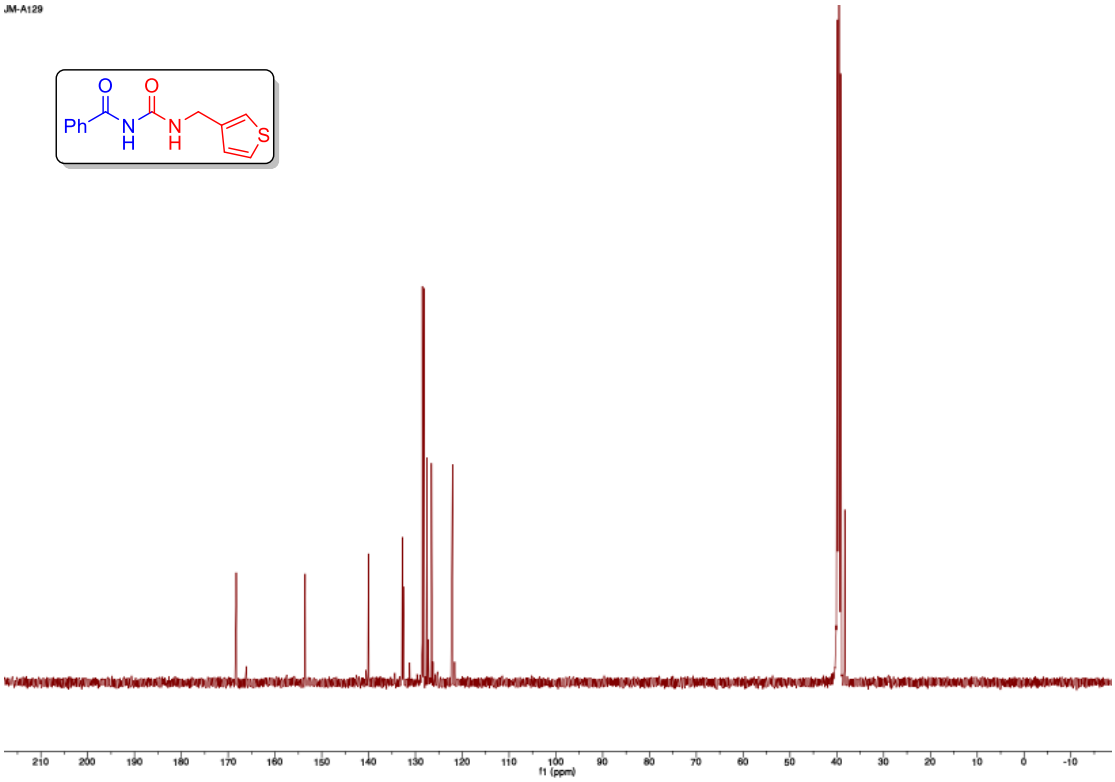
Supplementary Figure 56. ^{13}C NMR Spectrum of 3ak (125 MHz, DMSO-d_6)



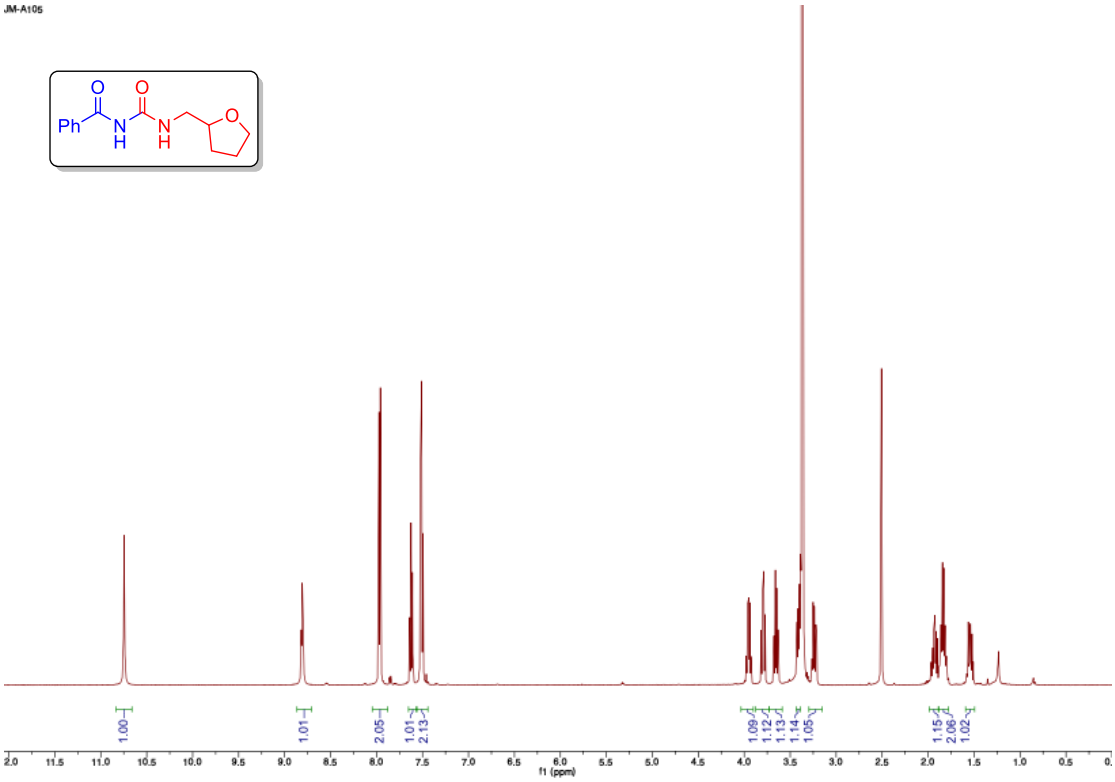
Supplementary Figure 57. ^{1}H NMR Spectrum of 3al (500MHz, DMSO-d_6)



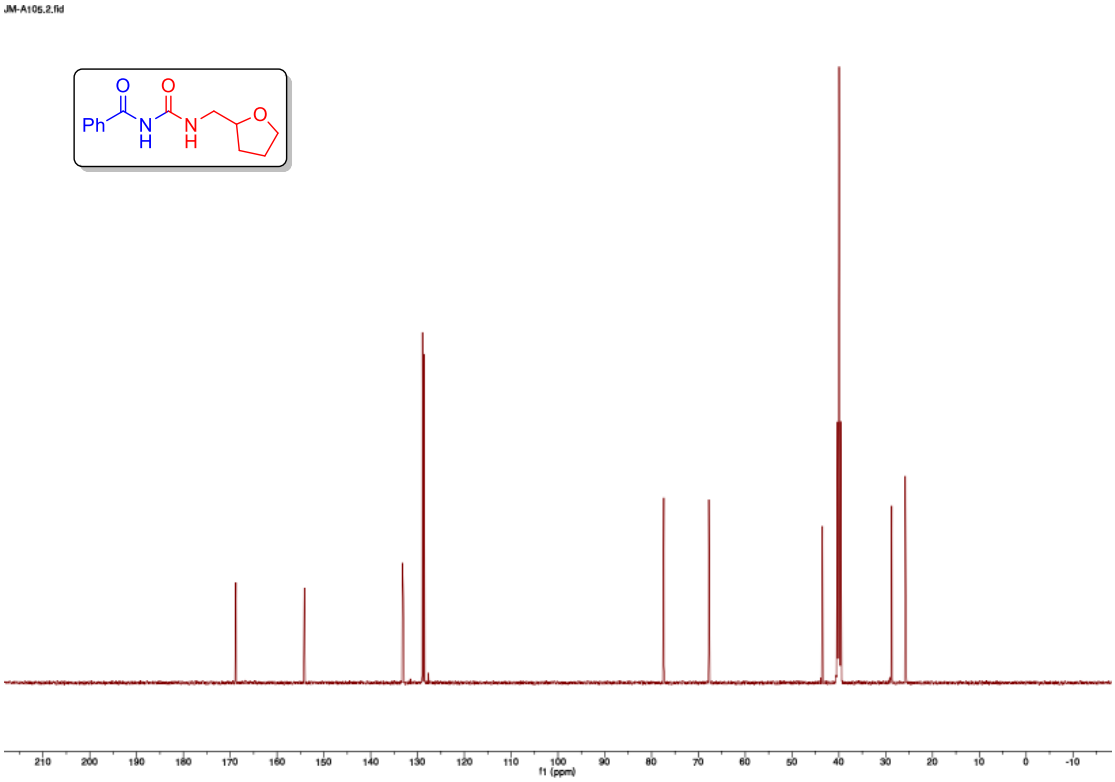
Supplementary Figure 58. ^{13}C NMR Spectrum of 3al (125 MHz, DMSO-d_6)



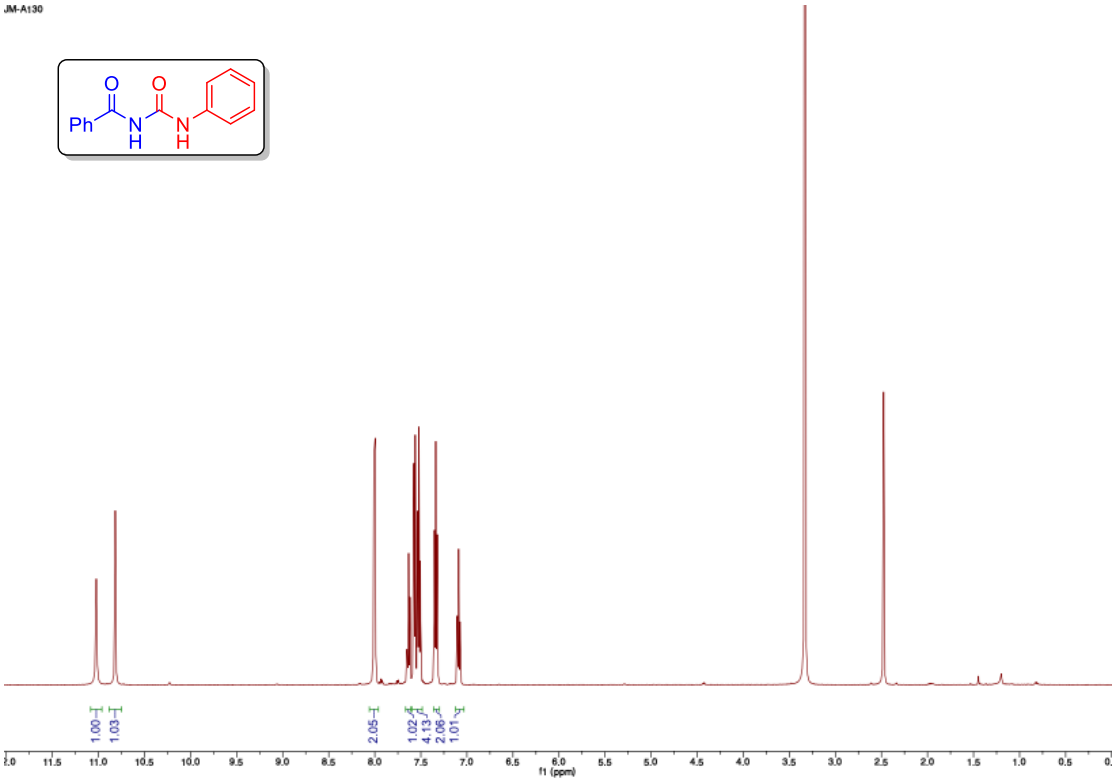
Supplementary Figure 59. ^{1}H NMR Spectrum of 3am (500MHz, DMSO-d_6)



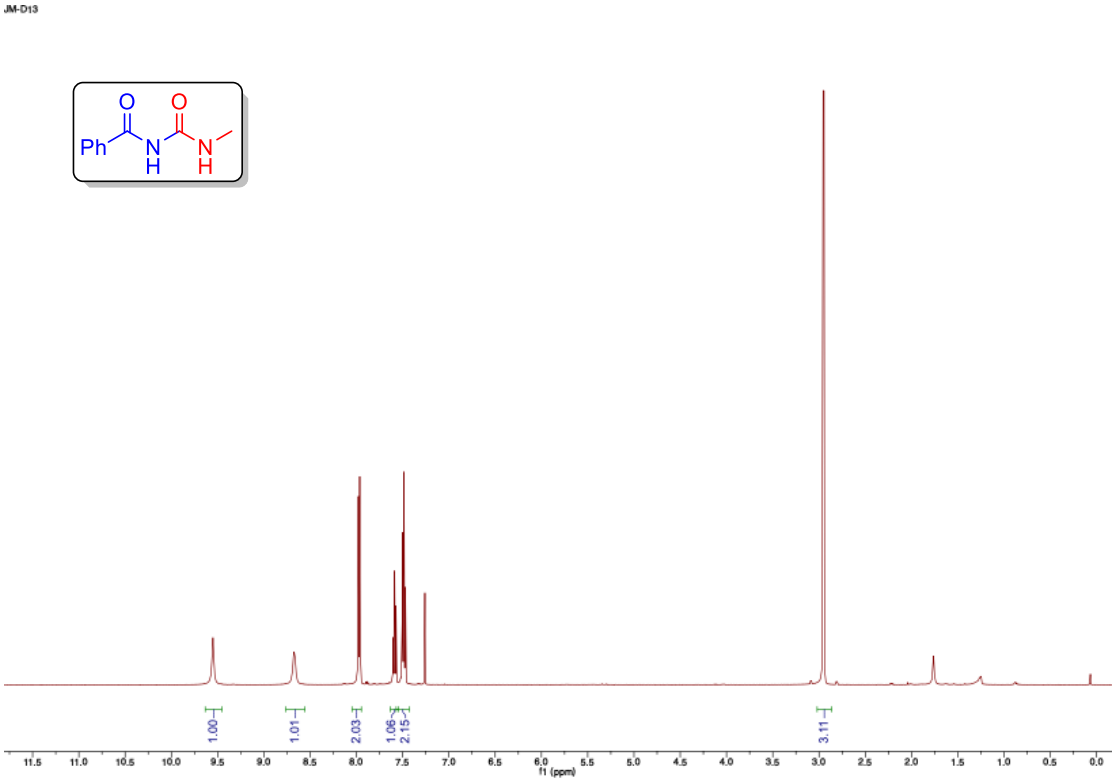
Supplementary Figure 60. ^{13}C NMR Spectrum of 3am (125 MHz, DMSO-d_6)



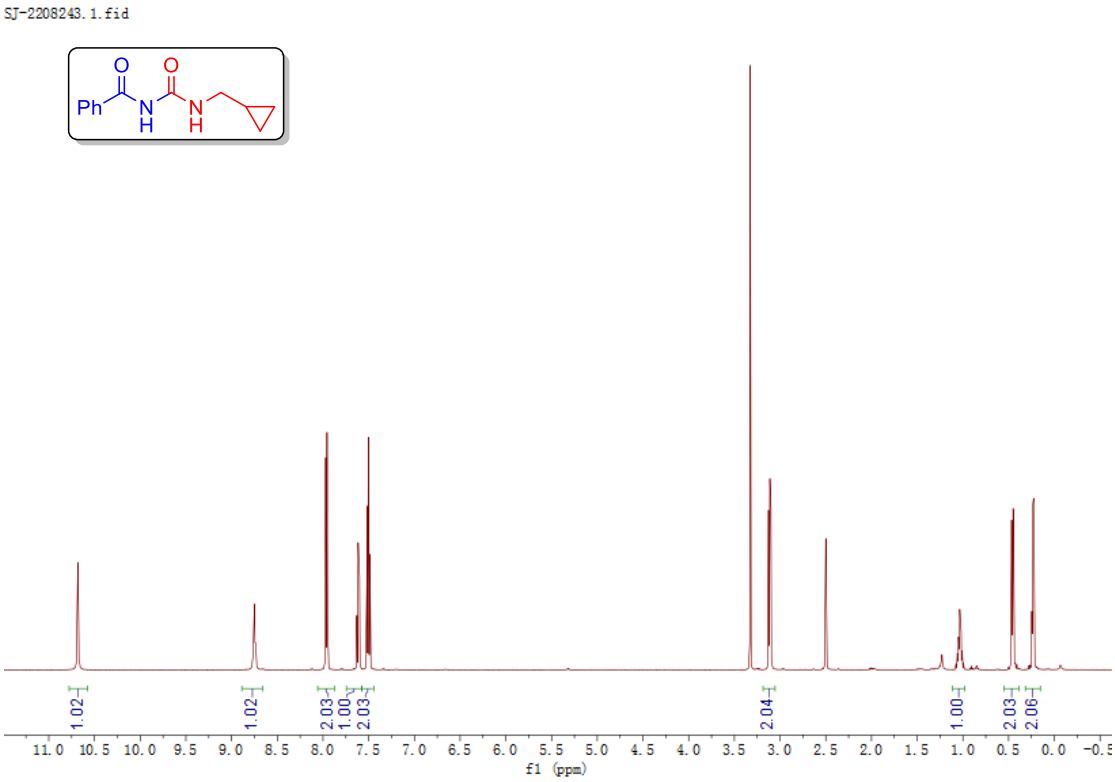
Supplementary Figure 61. ^{1}H NMR Spectrum of 3an (500MHz, DMSO-d_6)



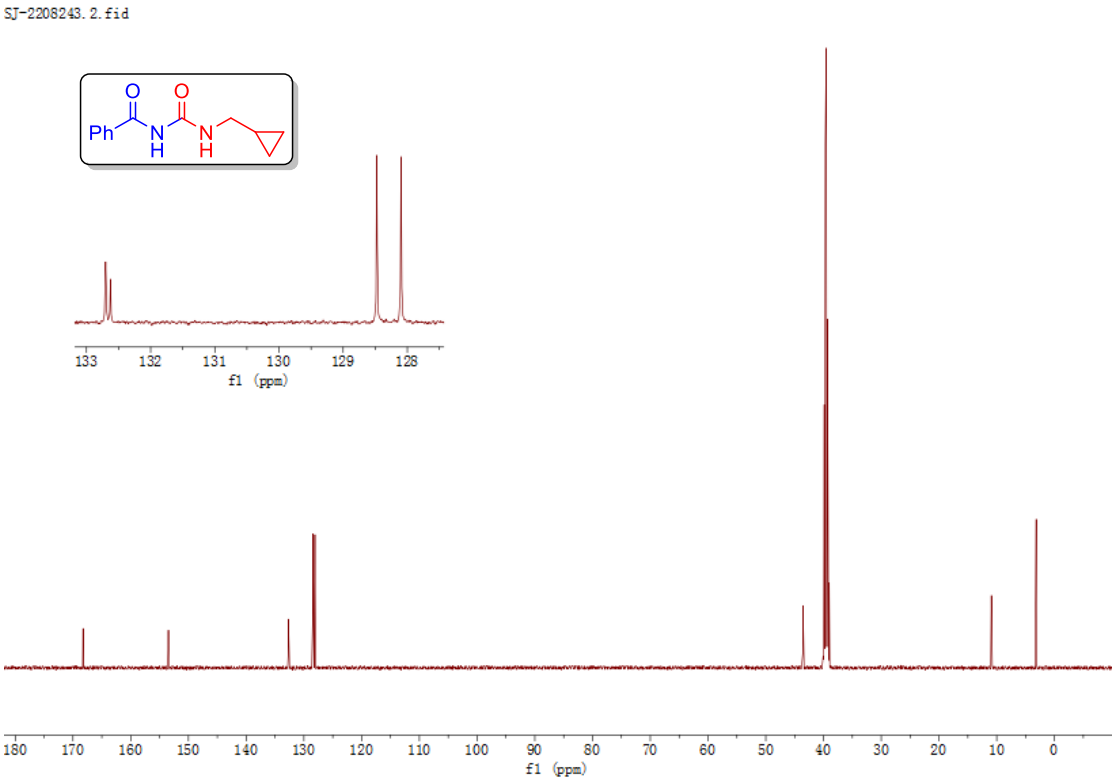
Supplementary Figure 62. ^{1}H NMR Spectrum of 3ao (500MHz, $CDCl_3$)



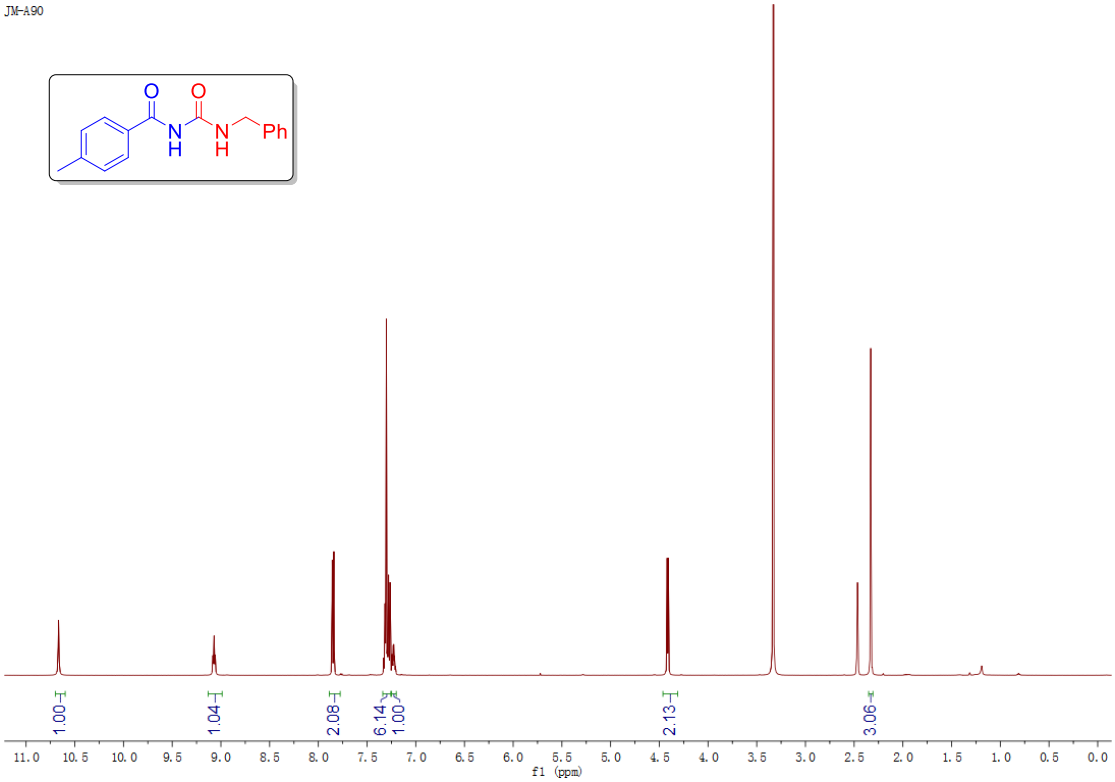
Supplementary Figure 63. ^{1}H NMR Spectrum of 3ap (500MHz, DMSO-d_6)



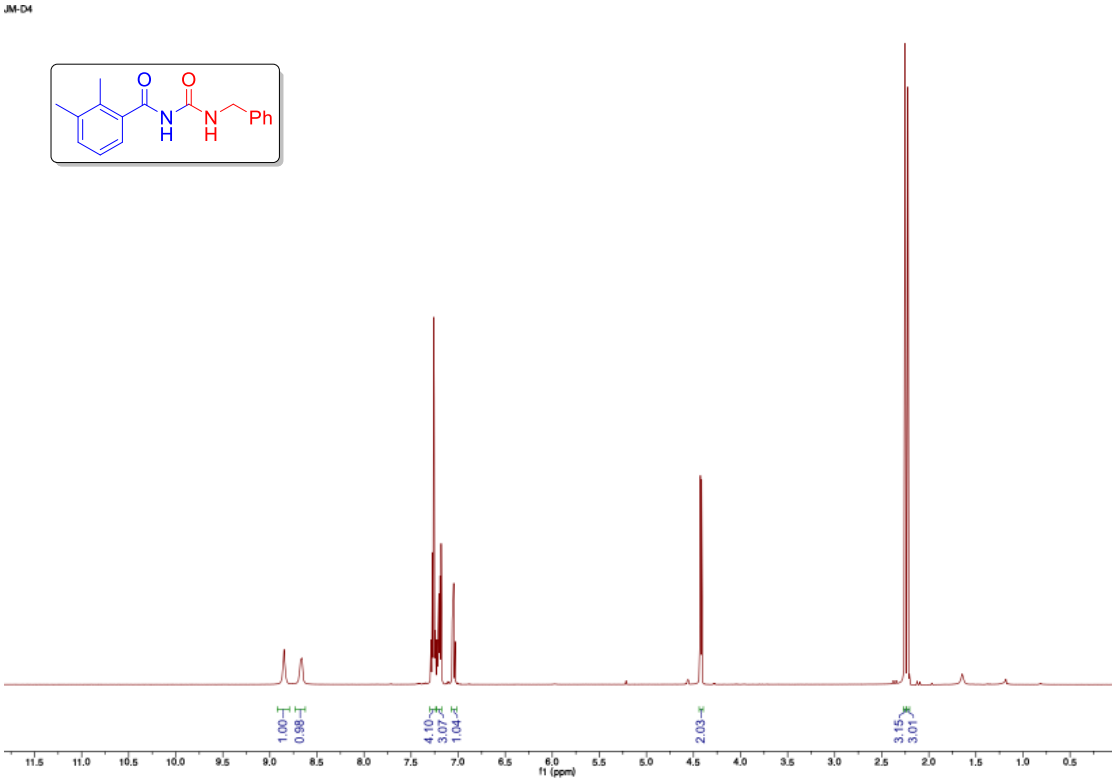
Supplementary Figure 64. ^{13}C NMR Spectrum of 3ap (125 MHz, DMSO-d_6)



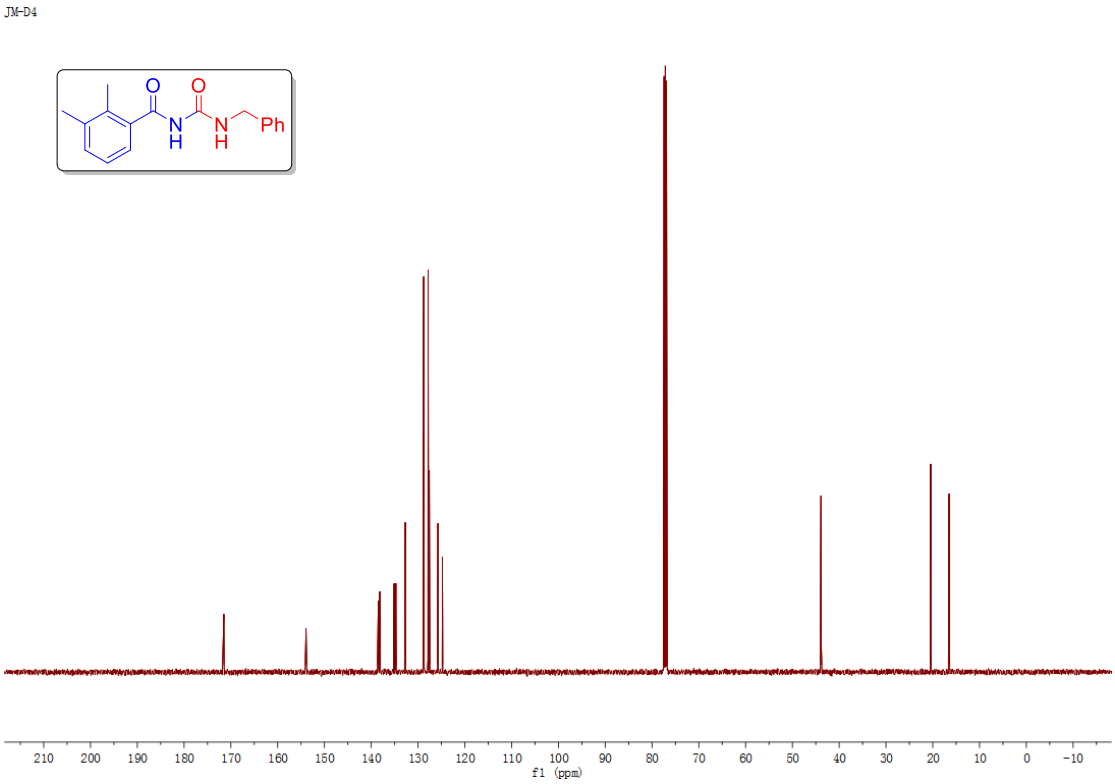
Supplementary Figure 65. ^{1}H NMR Spectrum of 3bb (500MHz, DMSO-d_6)



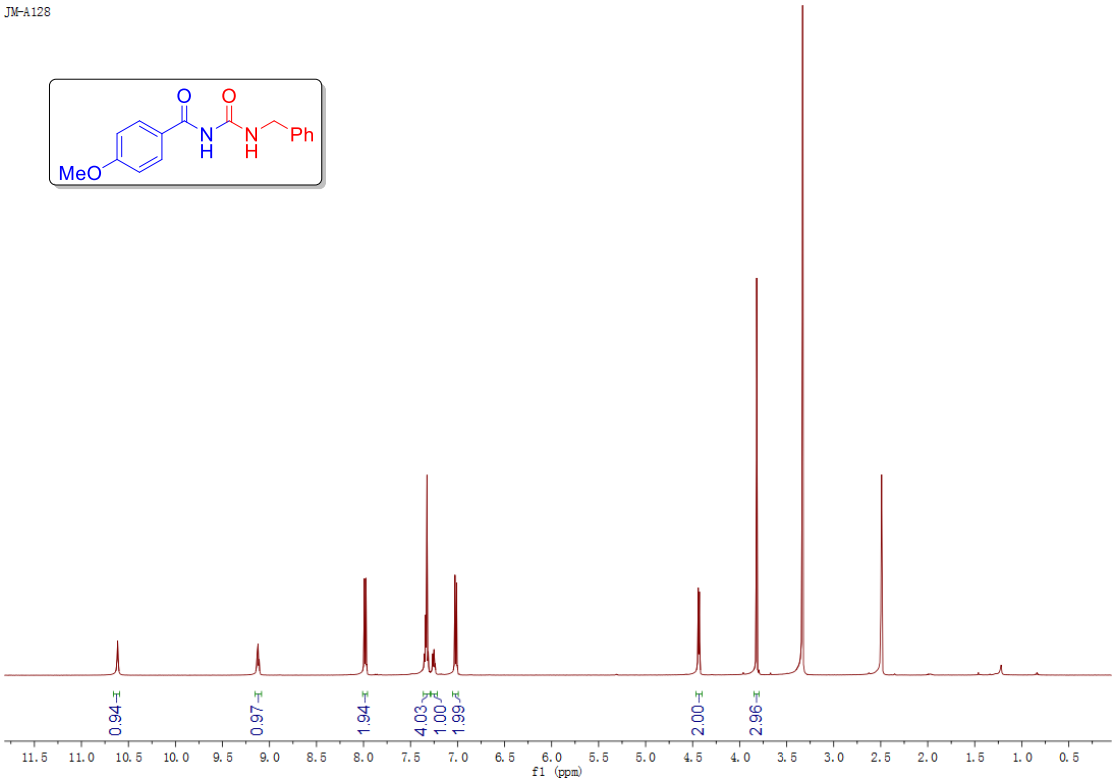
Supplementary Figure 66. ^{1}H NMR Spectrum of 3cb (500MHz, $CDCl_3$)



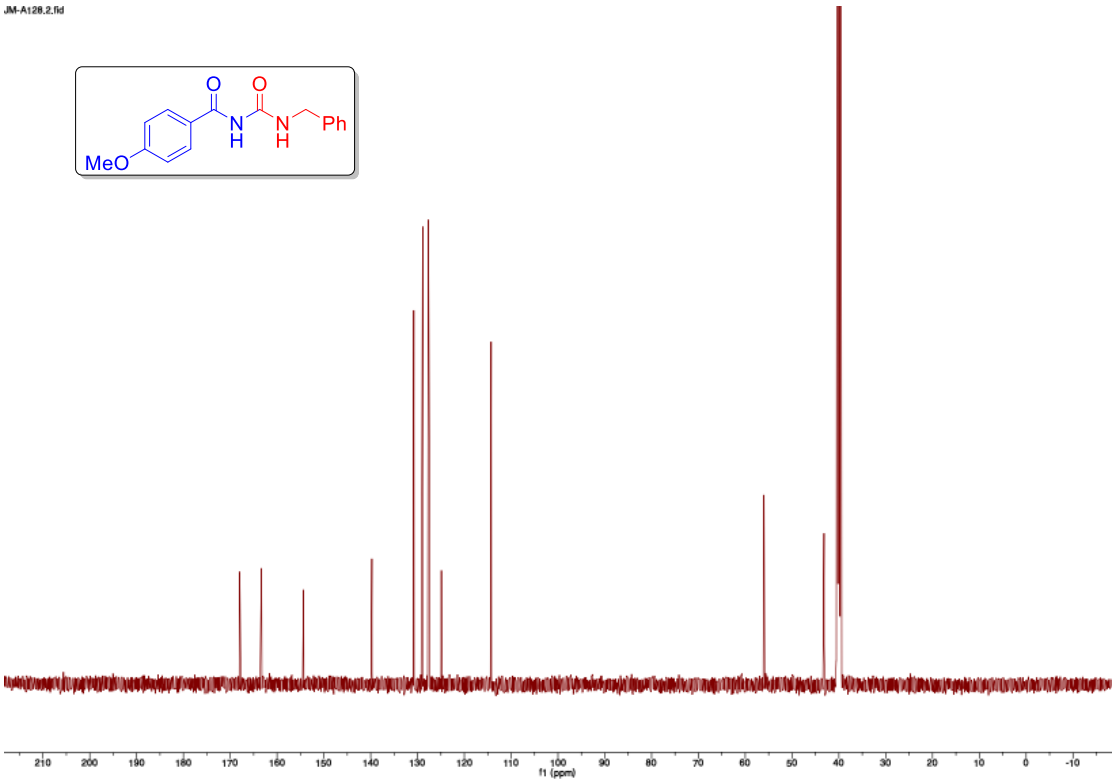
Supplementary Figure 67. ^{13}C NMR Spectrum of 3cb (125 MHz, $CDCl_3$)



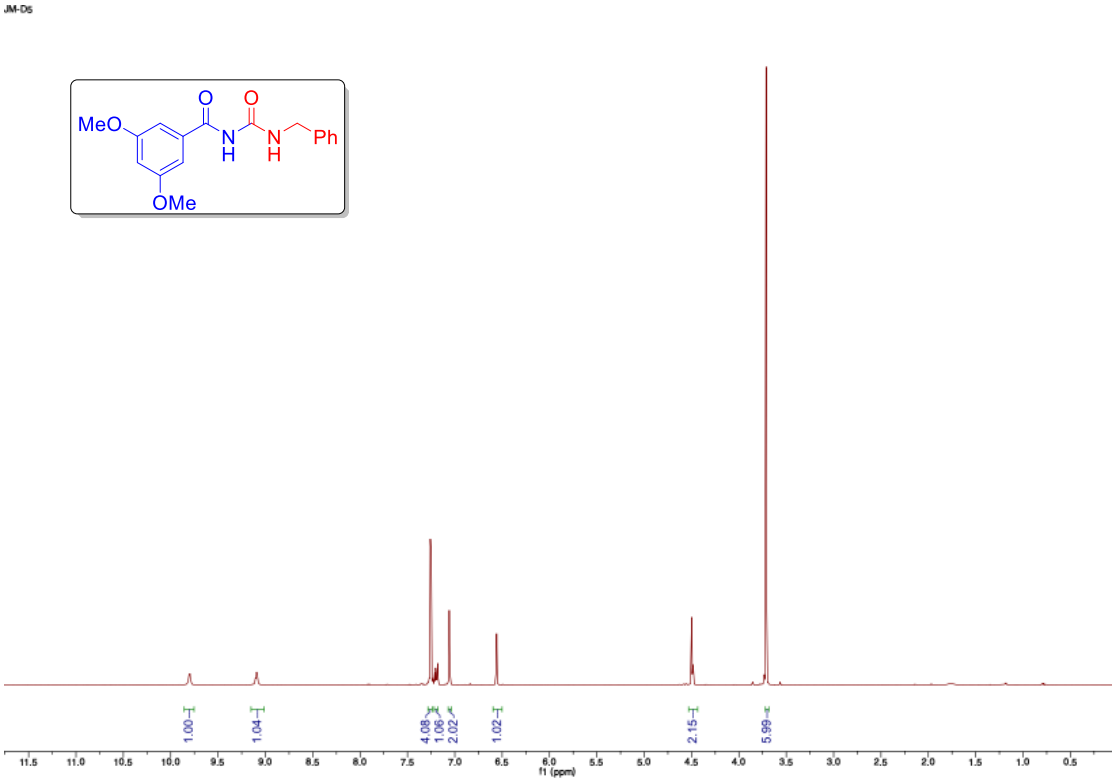
Supplementary Figure 68. ^{1}H NMR Spectrum of 3db (500MHz, DMSO-d_6)



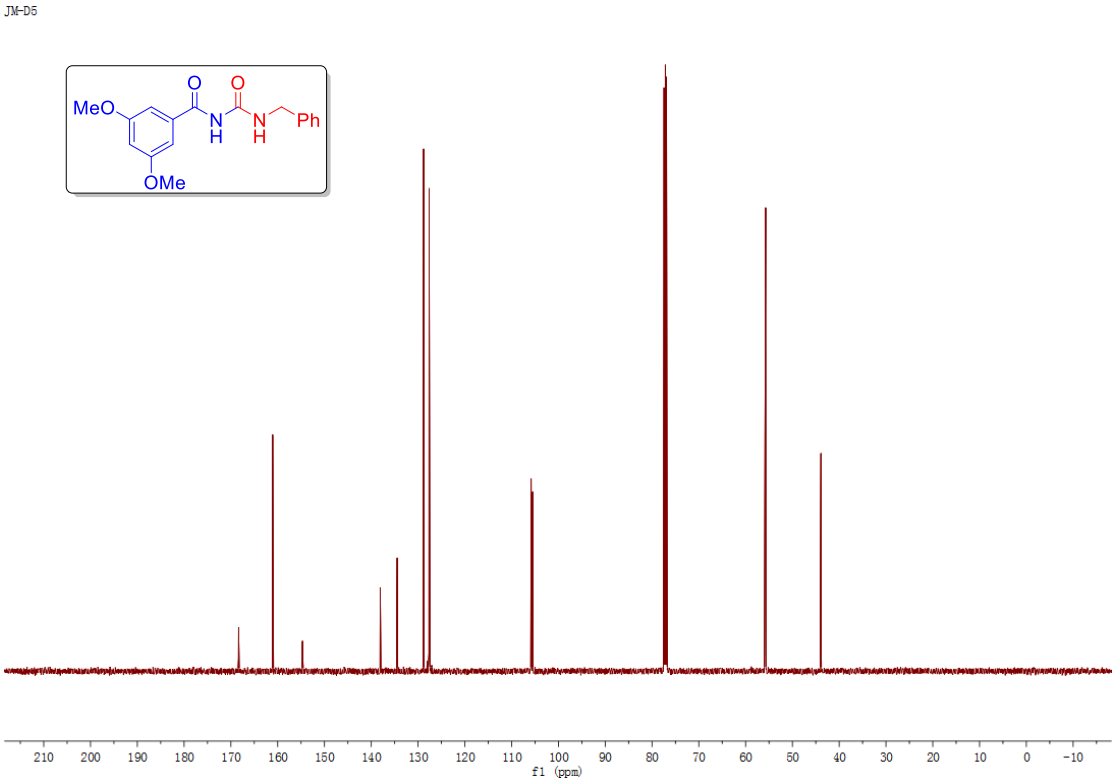
Supplementary Figure 69. ^{13}C NMR Spectrum of 3db (125 MHz, DMSO-*d*$_6$)



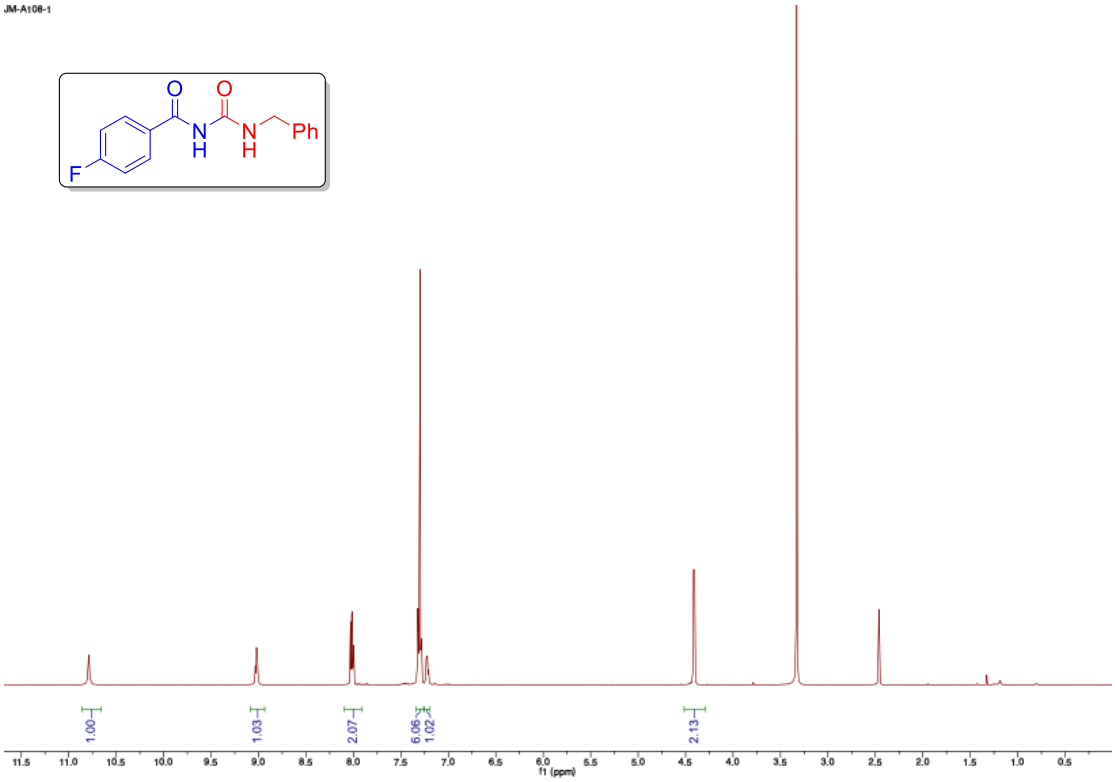
Supplementary Figure 70. ^{1}H NMR Spectrum of 3eb (500MHz, CDCl$_3$)



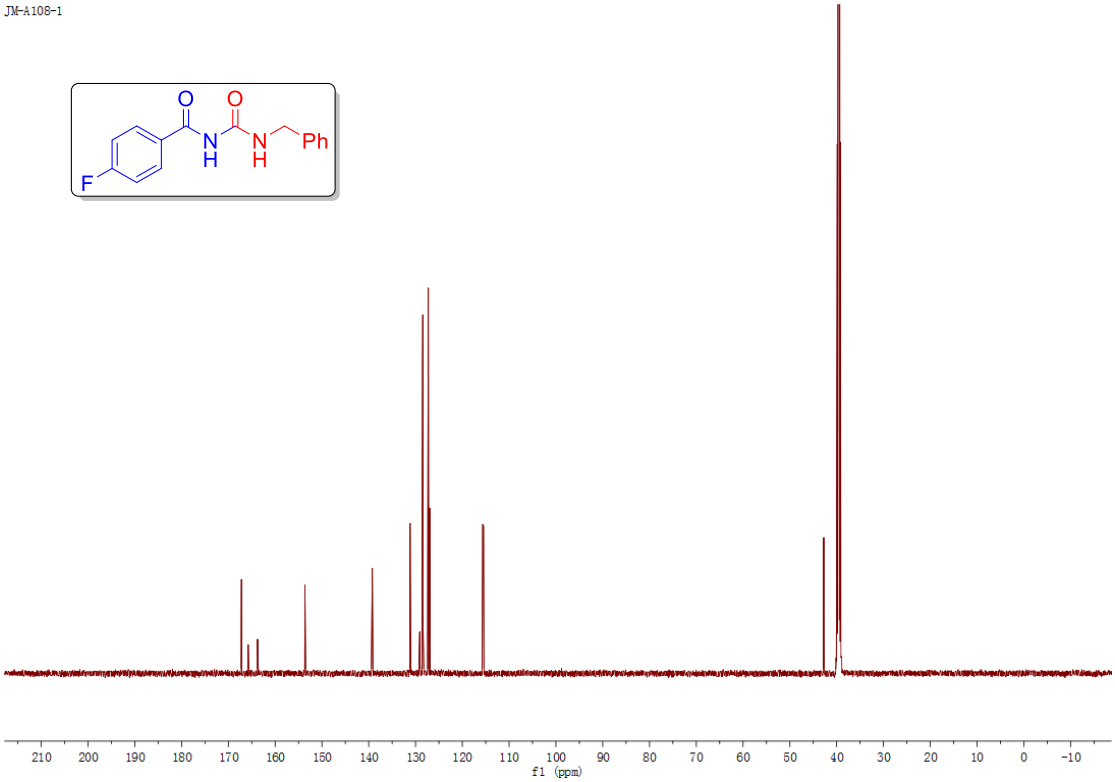
Supplementary Figure 71. ^{13}C NMR Spectrum of 3eb (125 MHz, $CDCl_3$)



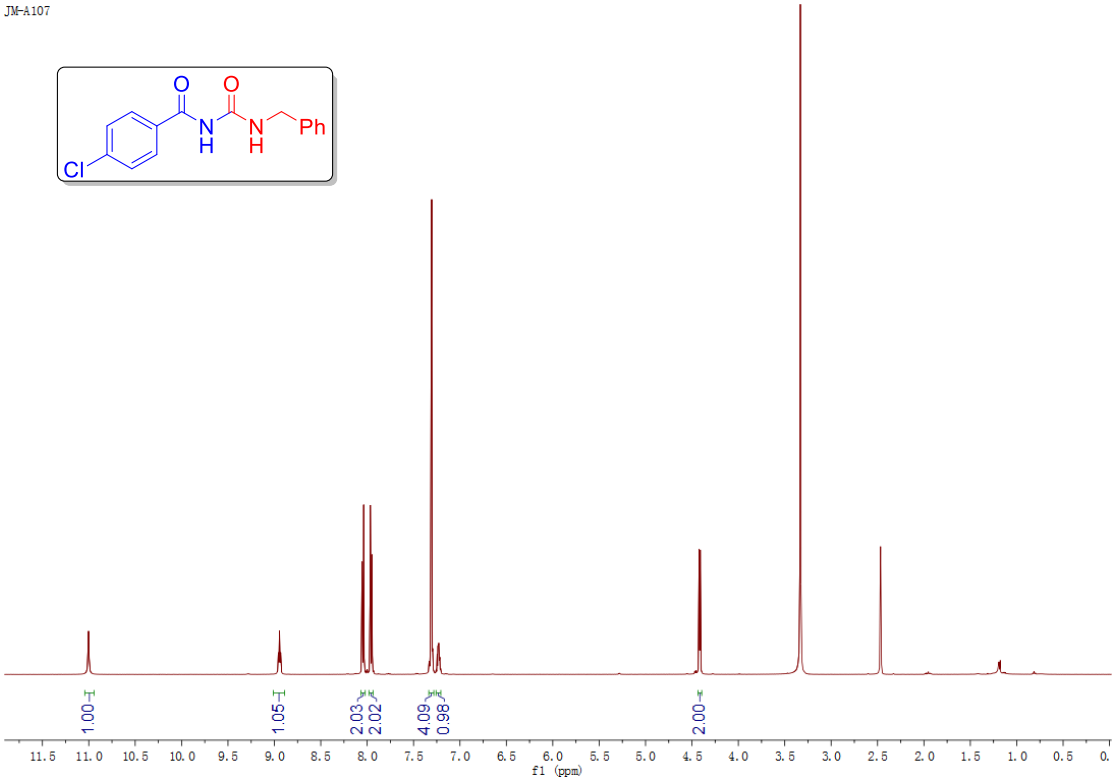
Supplementary Figure 72. ^{1}H NMR Spectrum of 3fb (500MHz, DMSO-d_6)



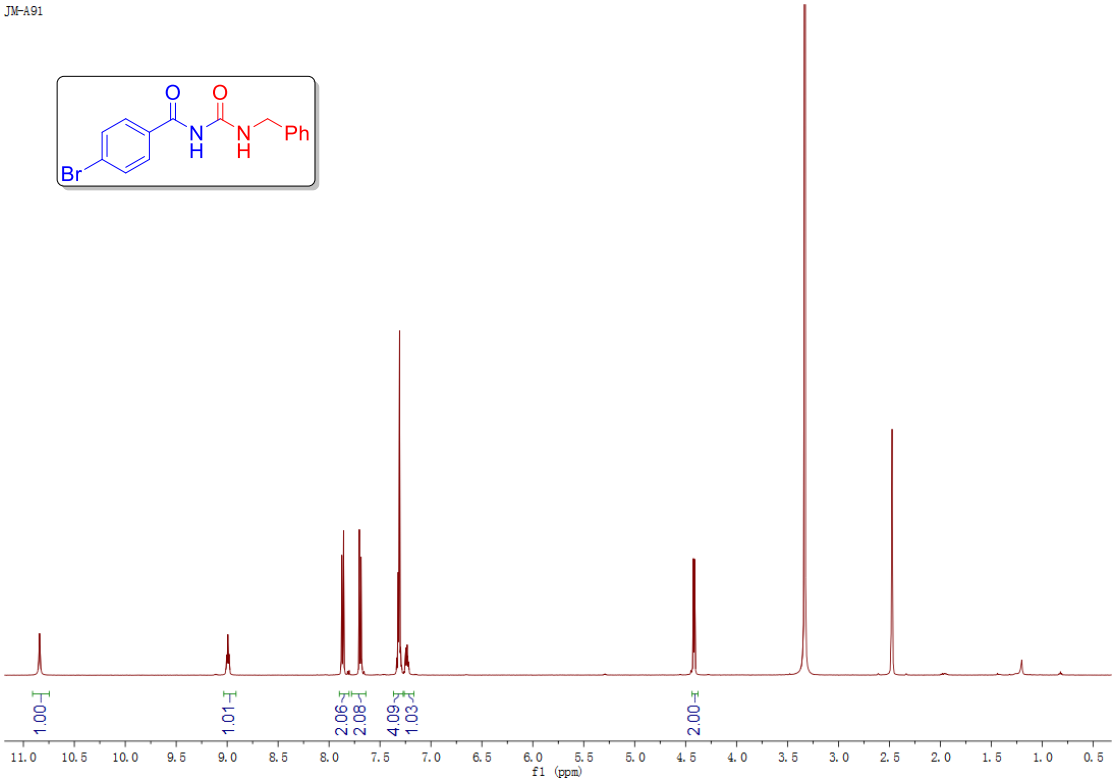
Supplementary Figure 73. ^{13}C NMR Spectrum of 3fb (125 MHz, DMSO-d_6)



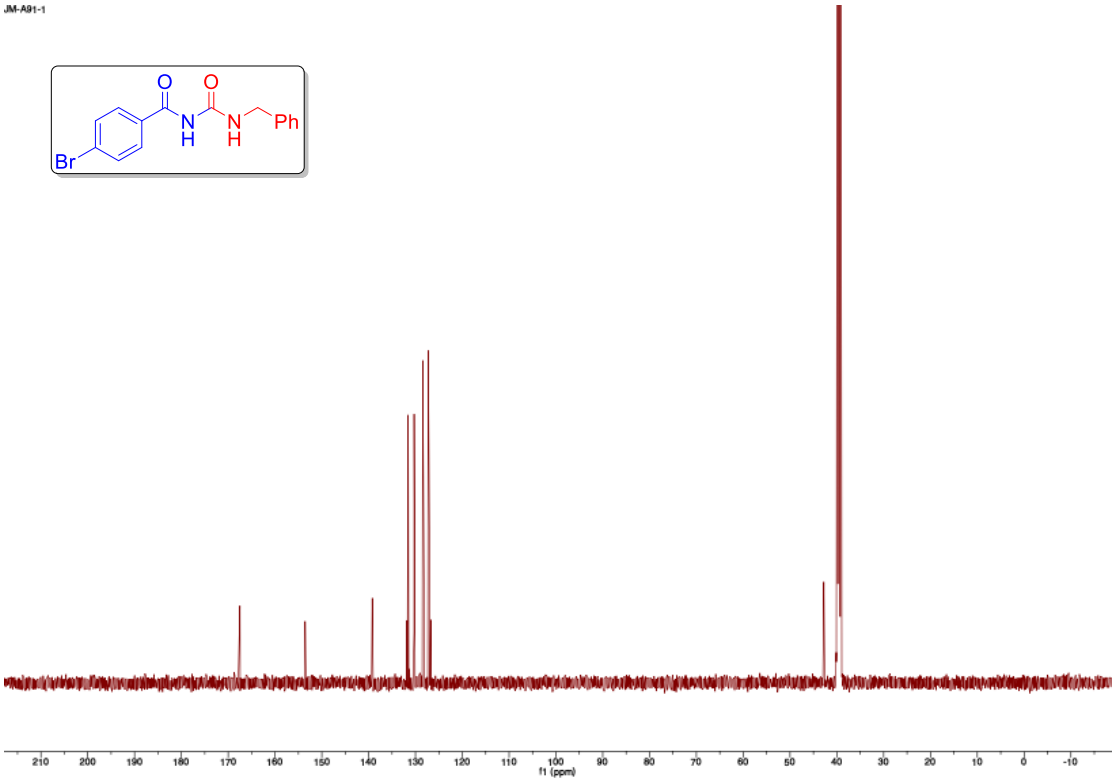
Supplementary Figure 74. ^{1}H NMR Spectrum of 3gb (500MHz, DMSO-d_6)



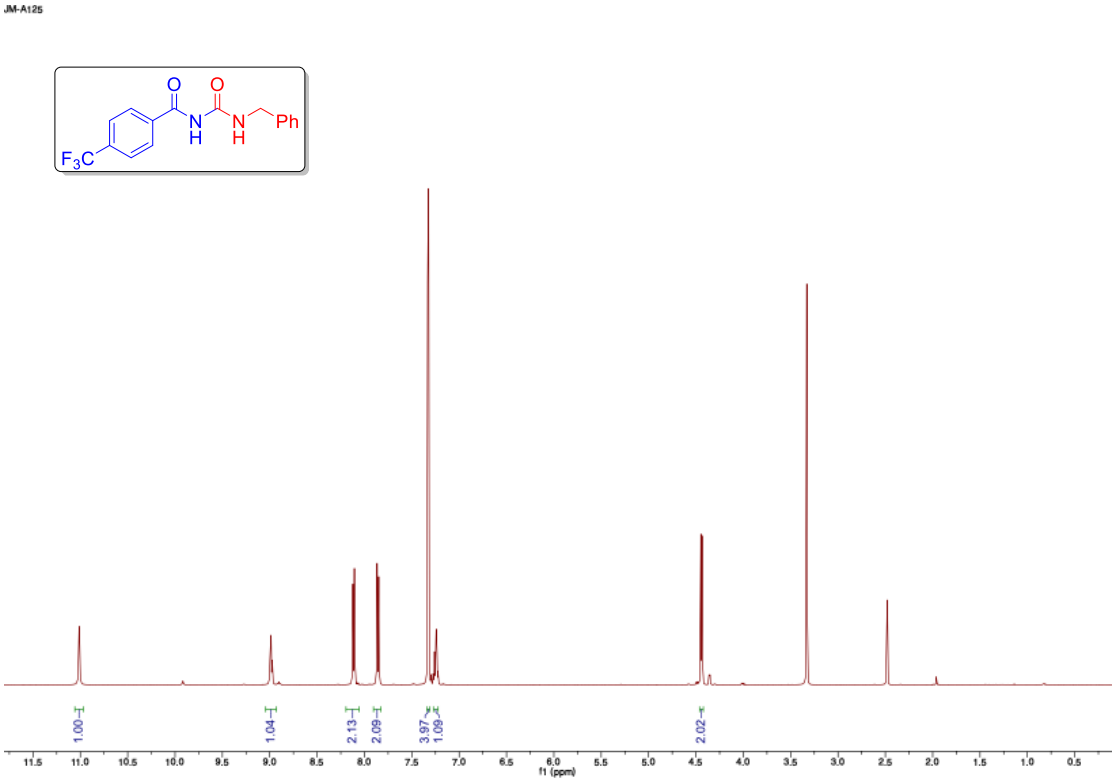
Supplementary Figure 75. ^{1}H NMR Spectrum of 3hb (500MHz, DMSO-d_6)



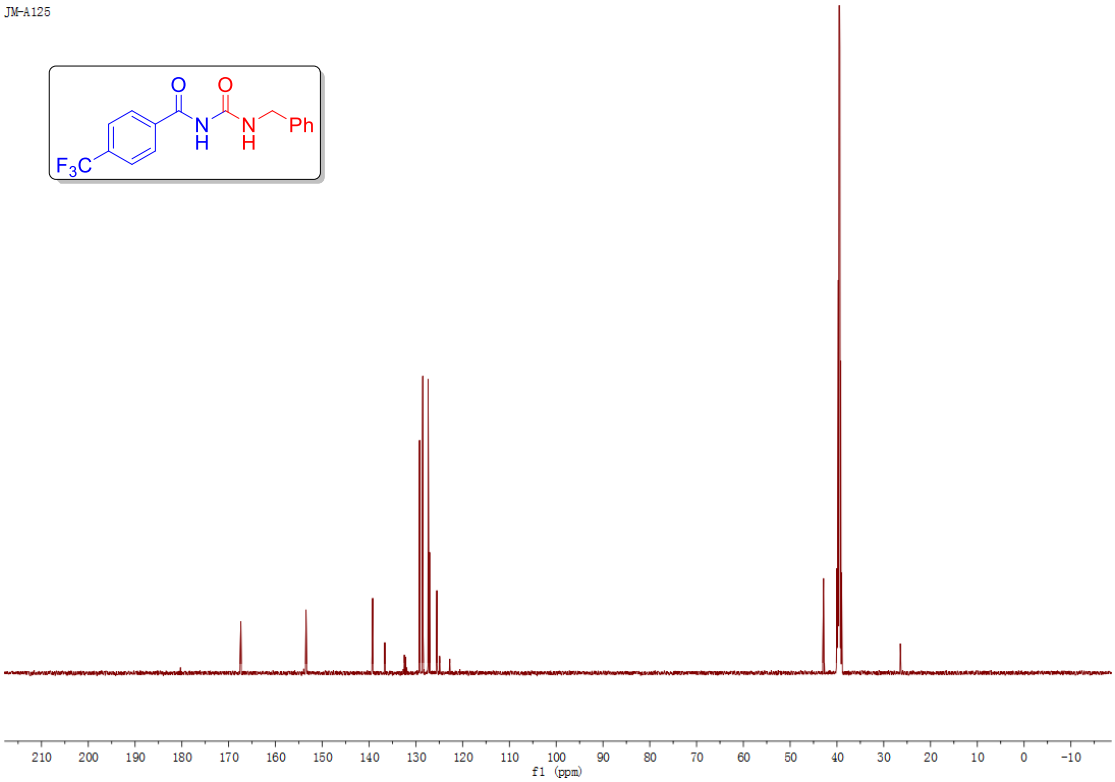
Supplementary Figure 76. ^{13}C NMR Spectrum of 3hb (125 MHz, DMSO-d_6)



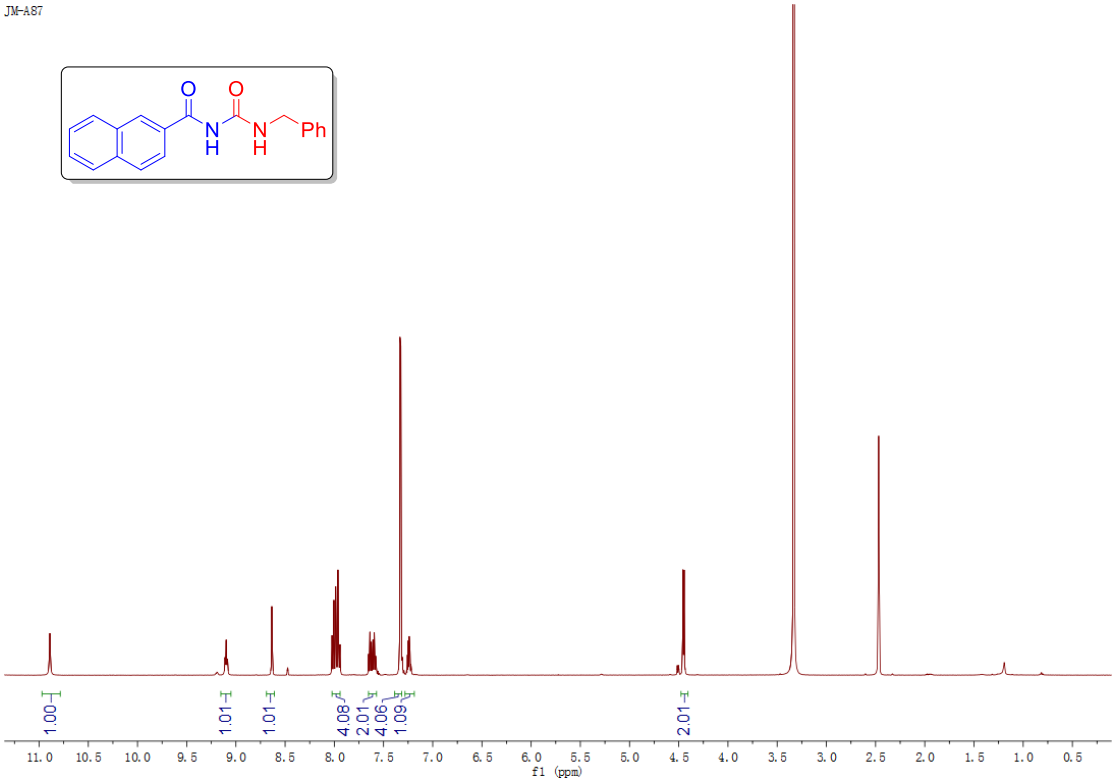
Supplementary Figure 77. ^{1}H NMR Spectrum of 3ib (500MHz, DMSO-d_6)



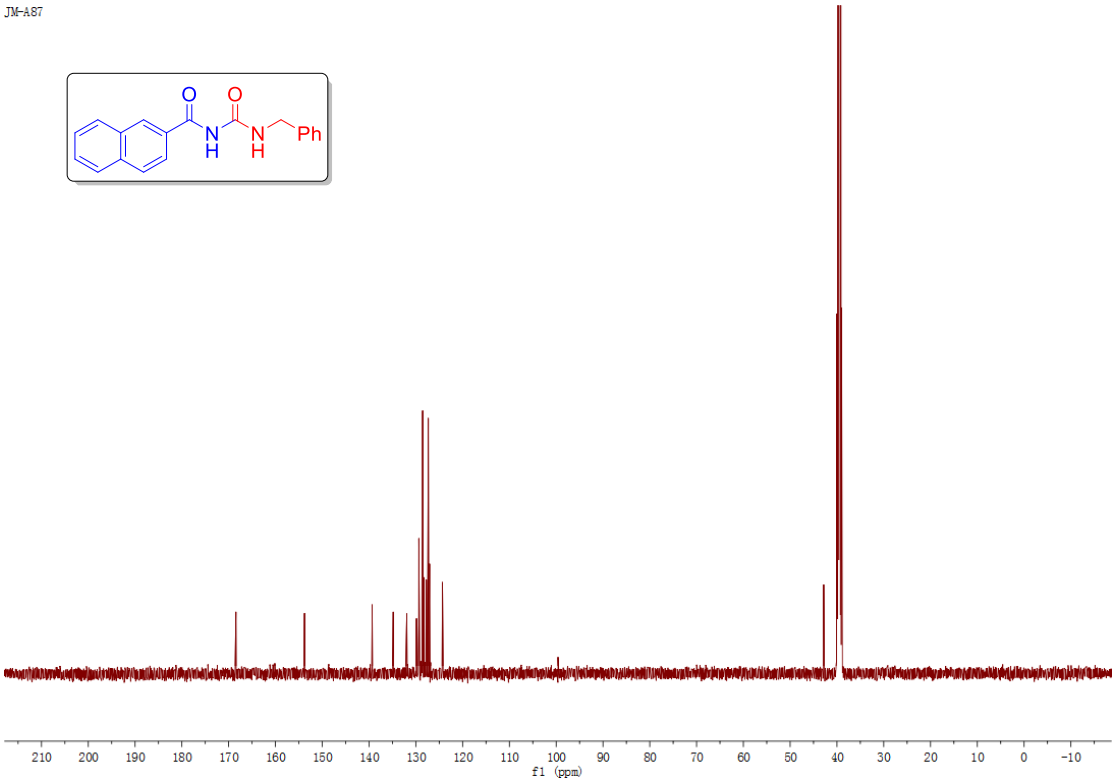
Supplementary Figure 78. ^{13}C NMR Spectrum of 3ib (125 MHz, DMSO-d_6)



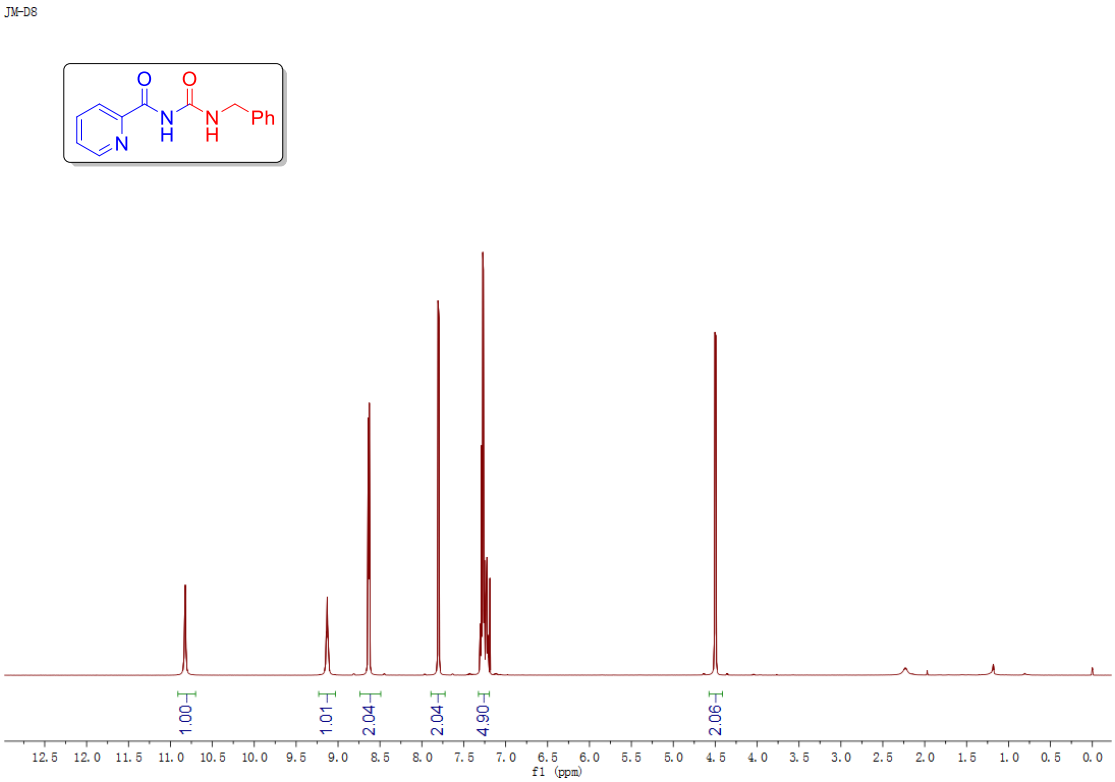
Supplementary Figure 79. ^{1}H NMR Spectrum of 3jb (500MHz, DMSO-d_6)



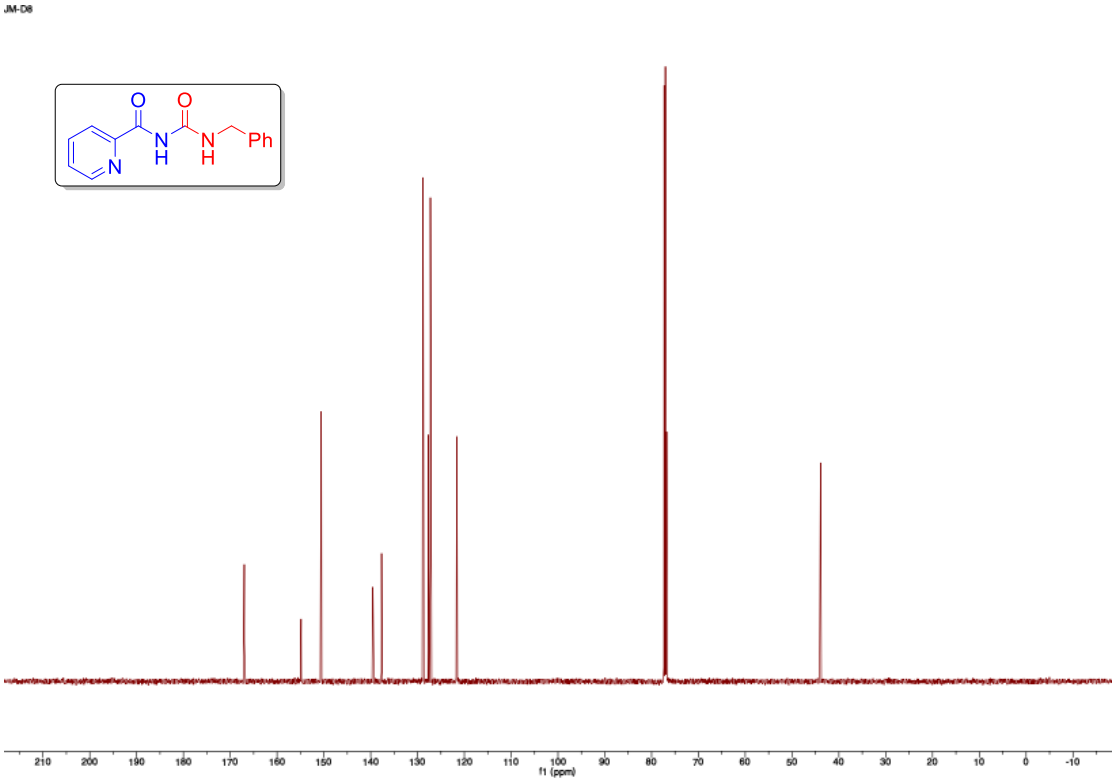
Supplementary Figure 80. ^{13}C NMR Spectrum of 3jb (125 MHz, DMSO-d_6)



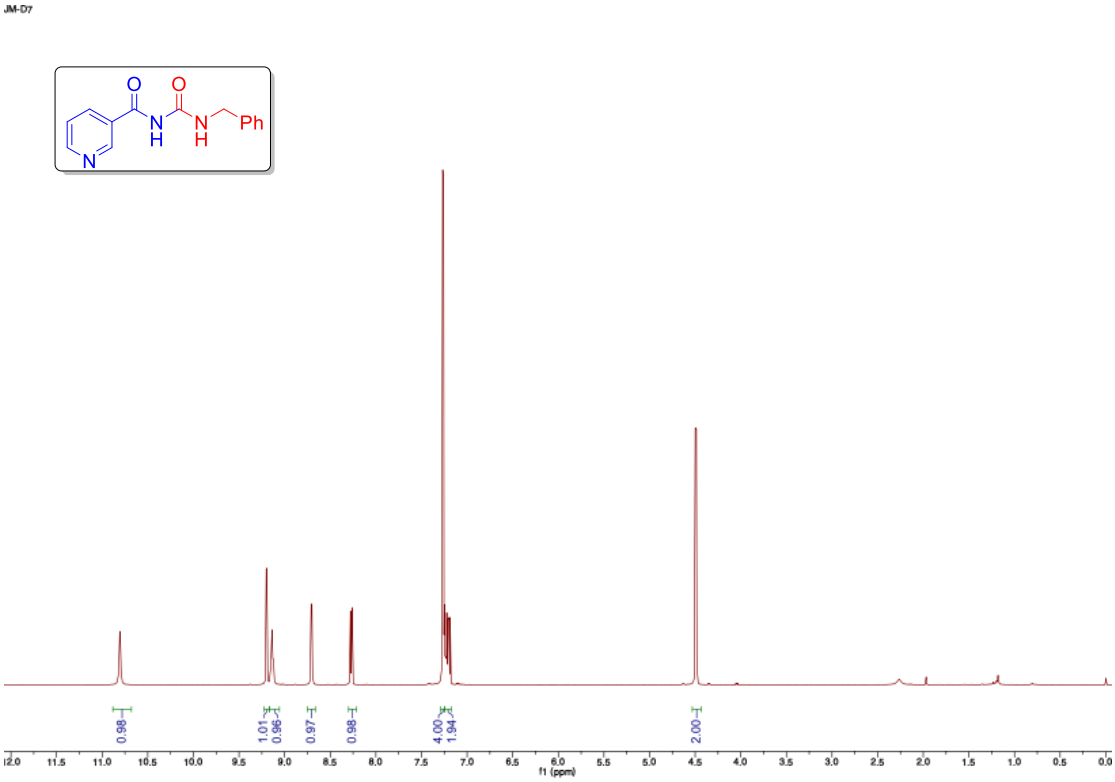
Supplementary Figure 81. ^{1}H NMR Spectrum of 3kb (500MHz, $CDCl_3$)



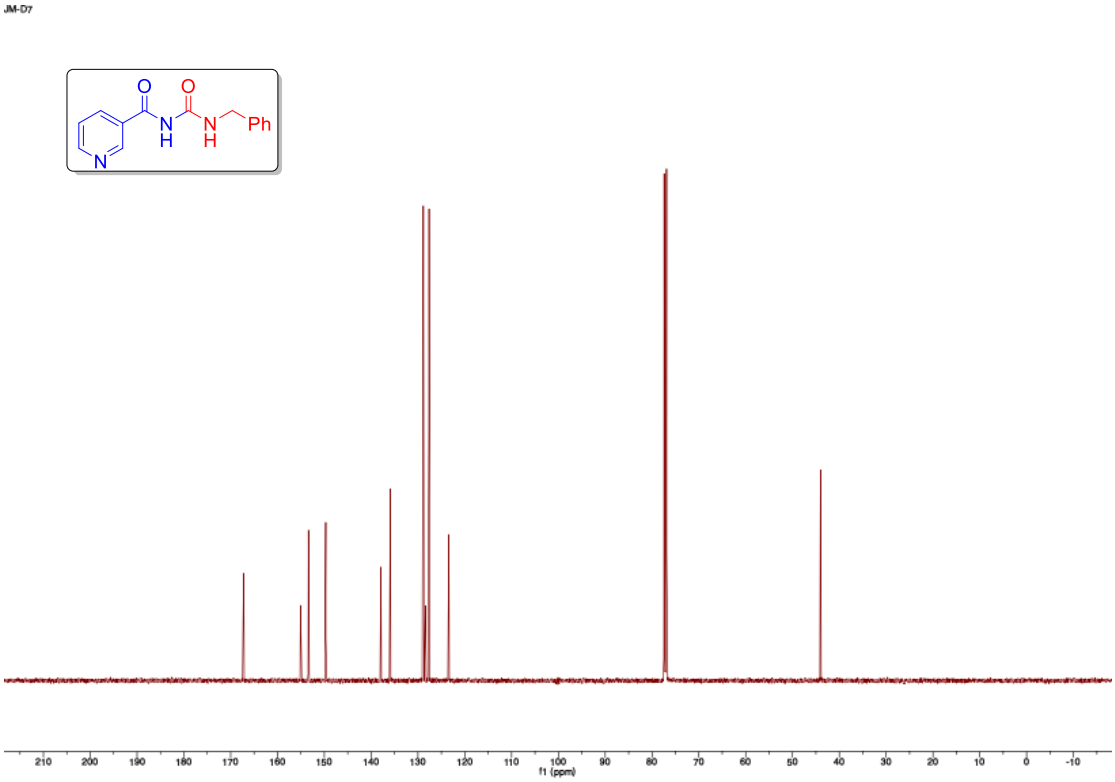
Supplementary Figure 82. ^{13}C NMR Spectrum of 3kb (125 MHz, $CDCl_3$)



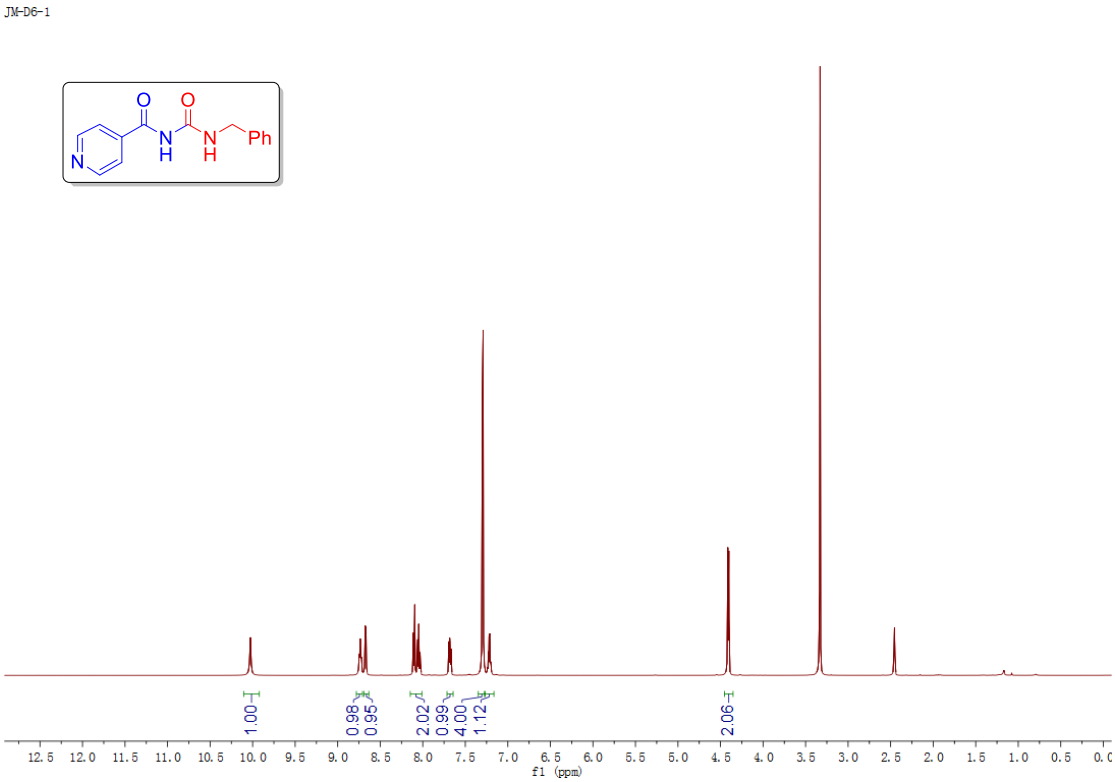
Supplementary Figure 83. ^{1}H NMR Spectrum of 3lb (500MHz, $CDCl_3$)



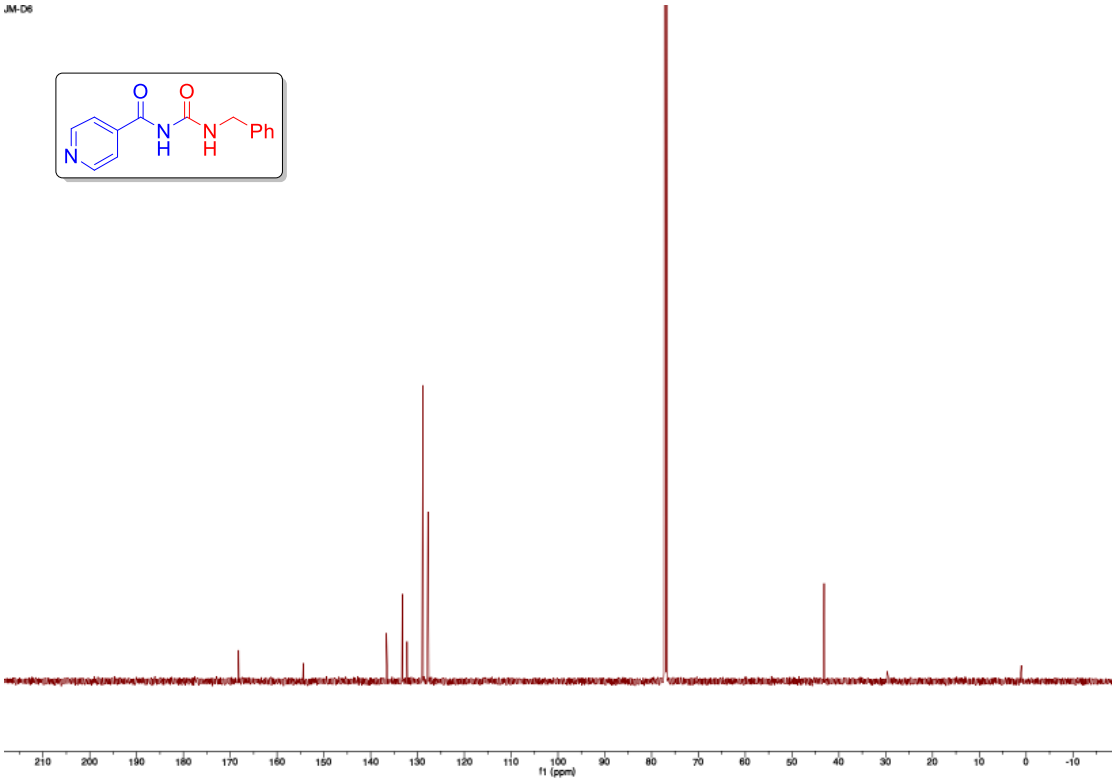
Supplementary Figure 84. ^{13}C NMR Spectrum of 3lb (125 MHz, $CDCl_3$)



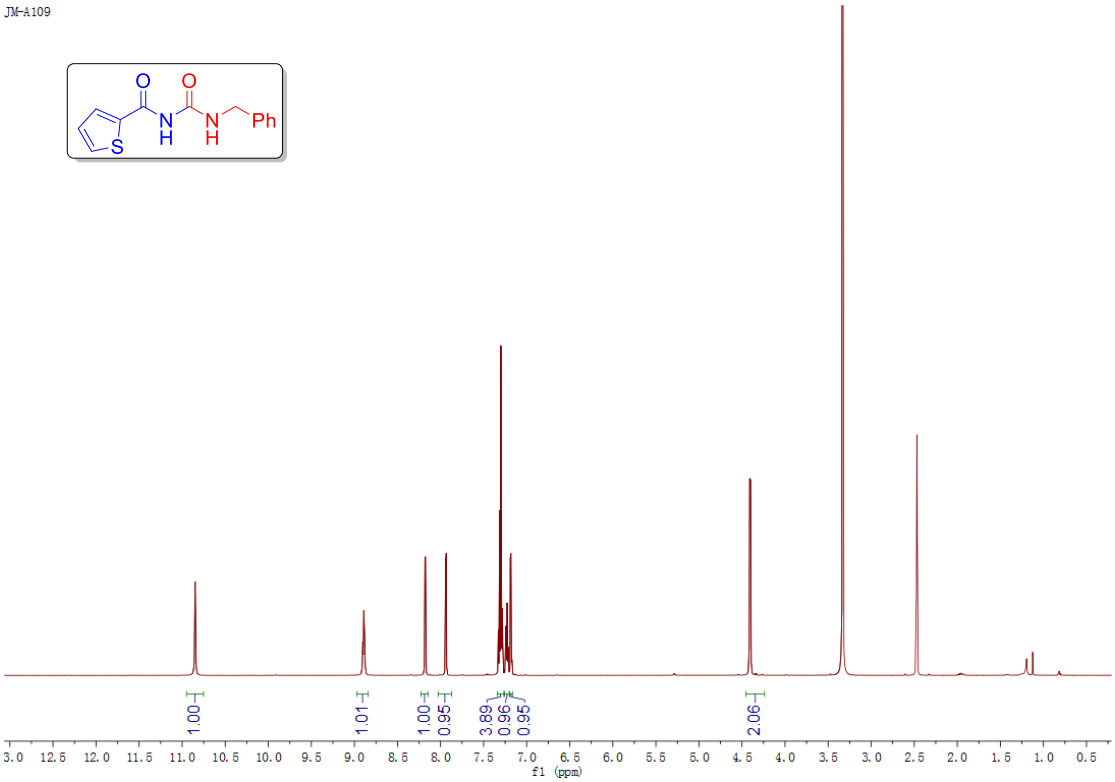
Supplementary Figure 85. ^{1}H NMR Spectrum of 3mb (500MHz, DMSO-d_6)



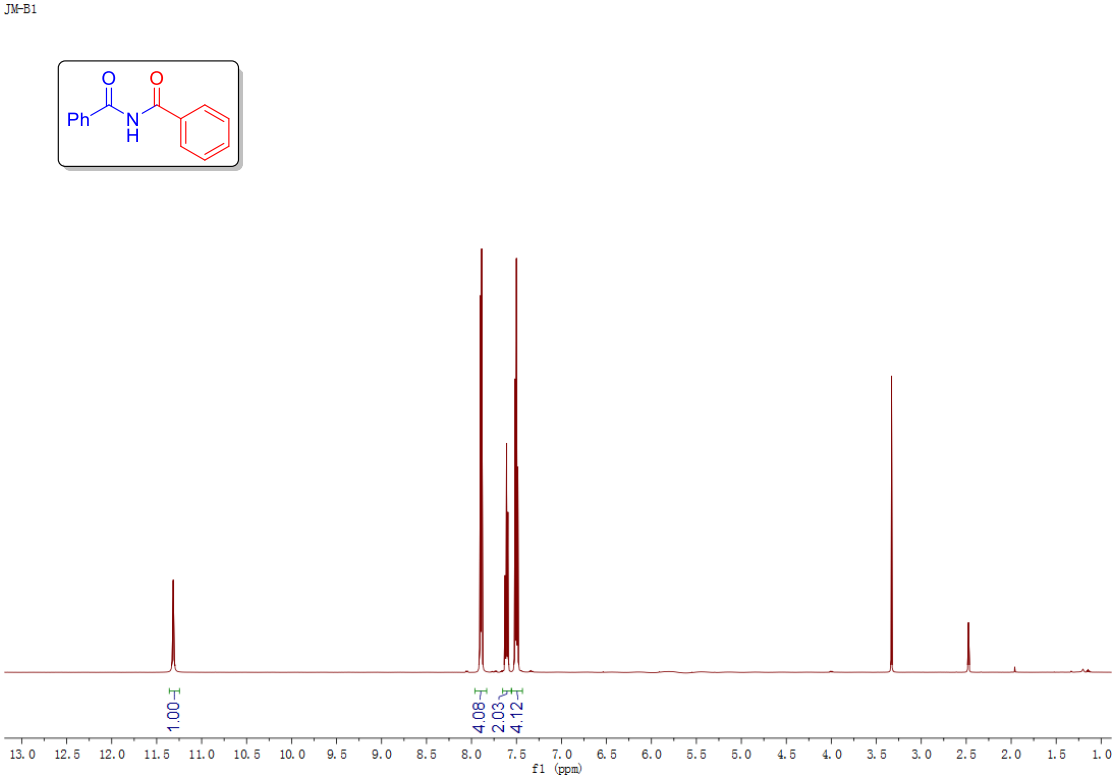
Supplementary Figure 86. ^{13}C NMR Spectrum of 3mb (125 MHz, $CDCl_3$)



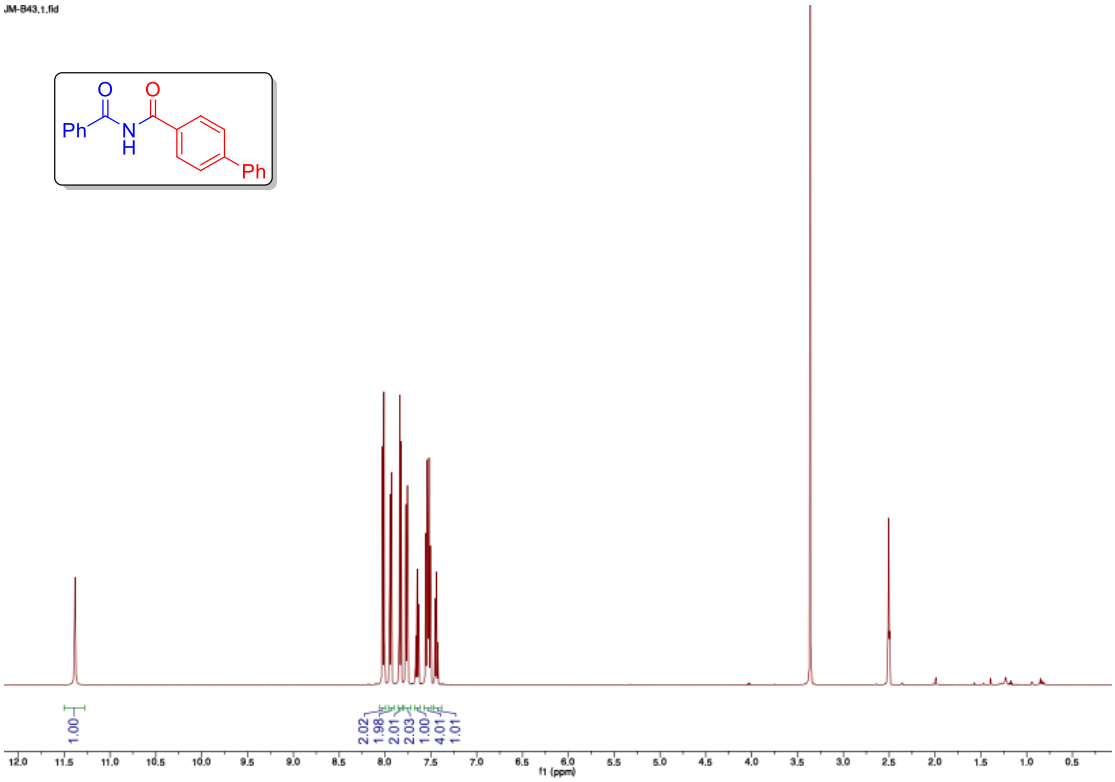
Supplementary Figure 87. ^{1}H NMR Spectrum of 3nb (500MHz, DMSO-d_6)



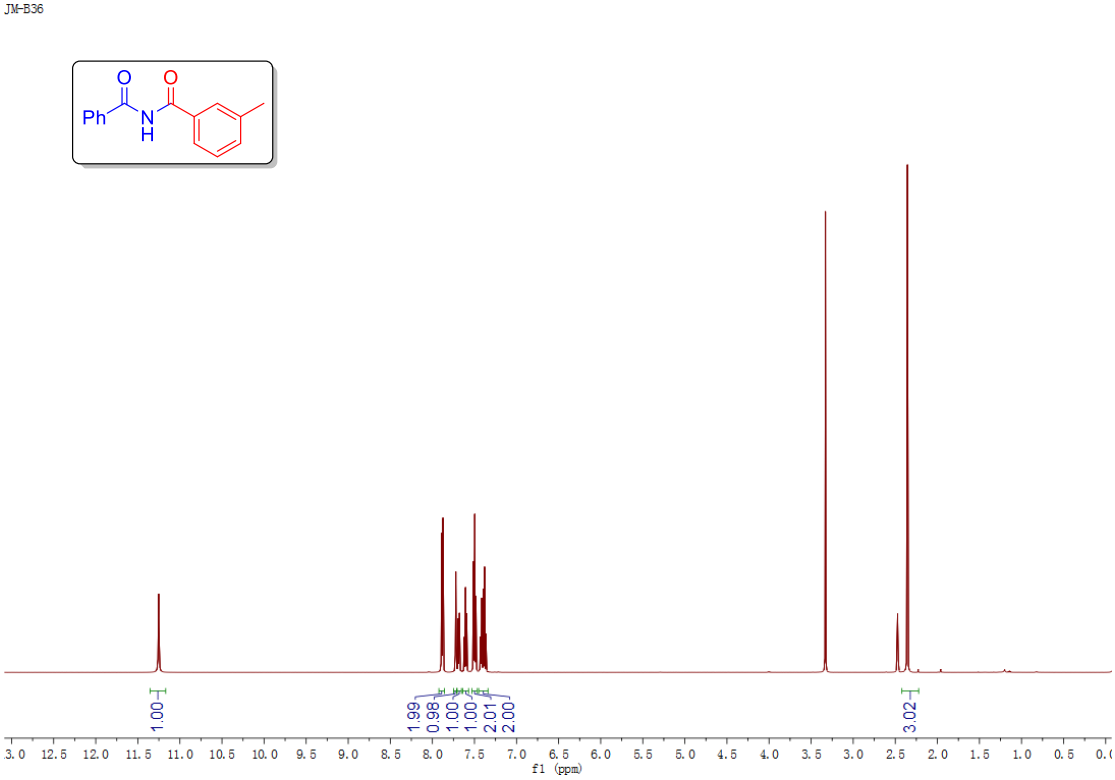
Supplementary Figure 88. ^{1}H NMR Spectrum of 4ab (500MHz, DMSO-d_6)



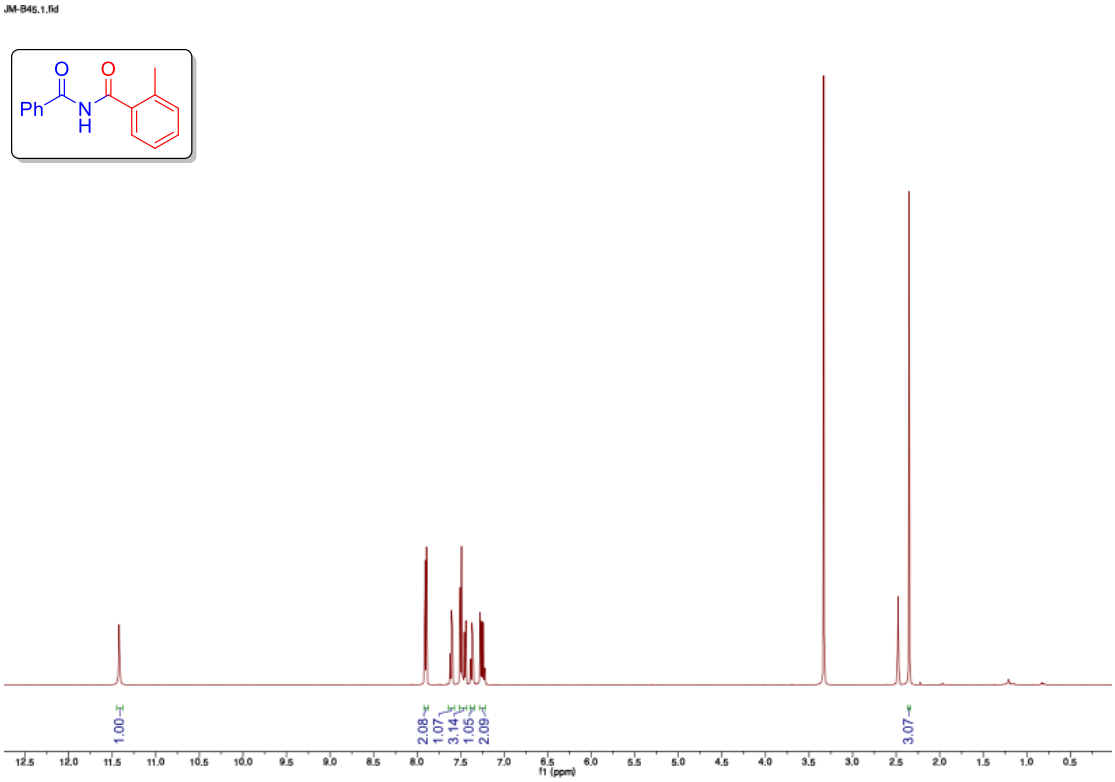
Supplementary Figure 89. ^{1}H NMR Spectrum of 4ab' (500MHz, DMSO-d_6)



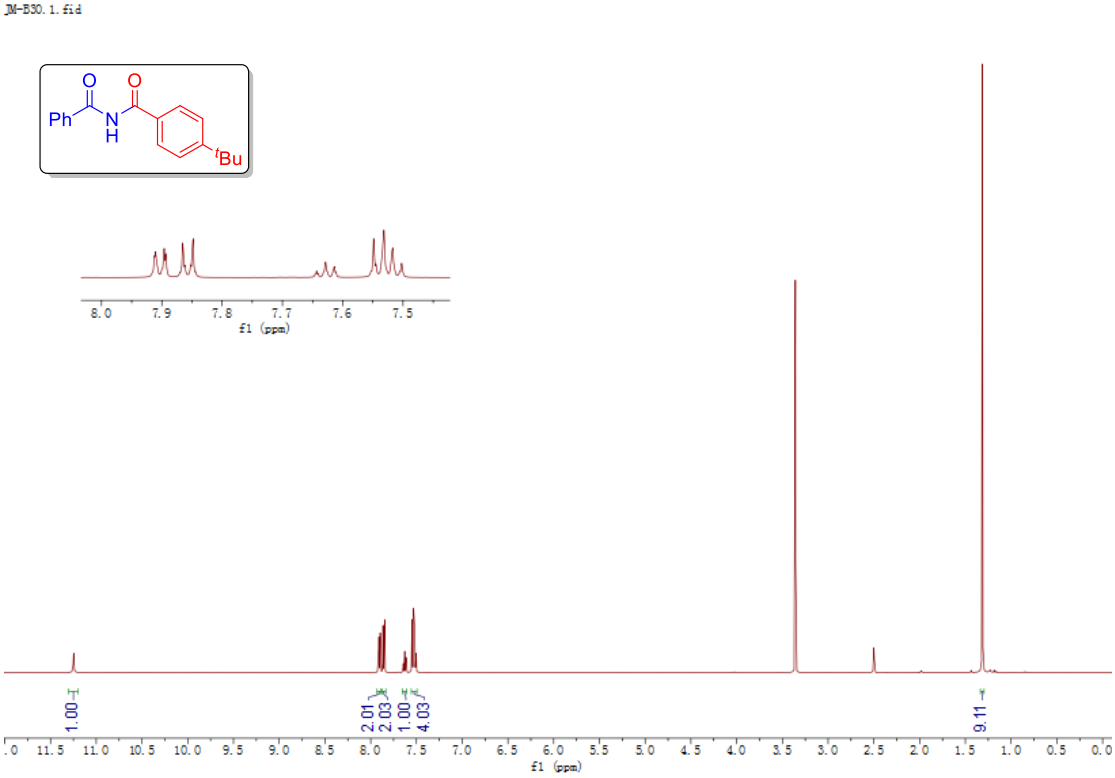
Supplementary Figure 90. ^{1}H NMR Spectrum of 4ac' (500MHz, DMSO-d_6)



Supplementary Figure 91. ^{1}H NMR Spectrum of 4ad' (500MHz, DMSO-d_6)

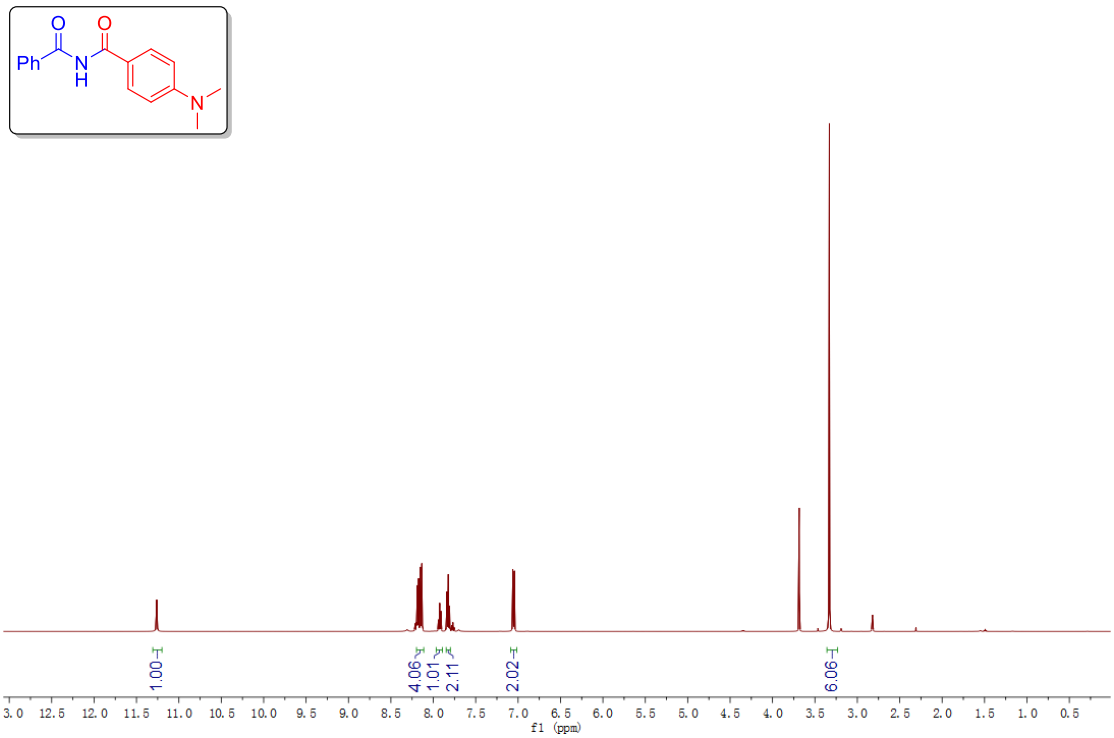


Supplementary Figure 92. ^{1}H NMR Spectrum of 4ae' (500MHz, DMSO-d_6)



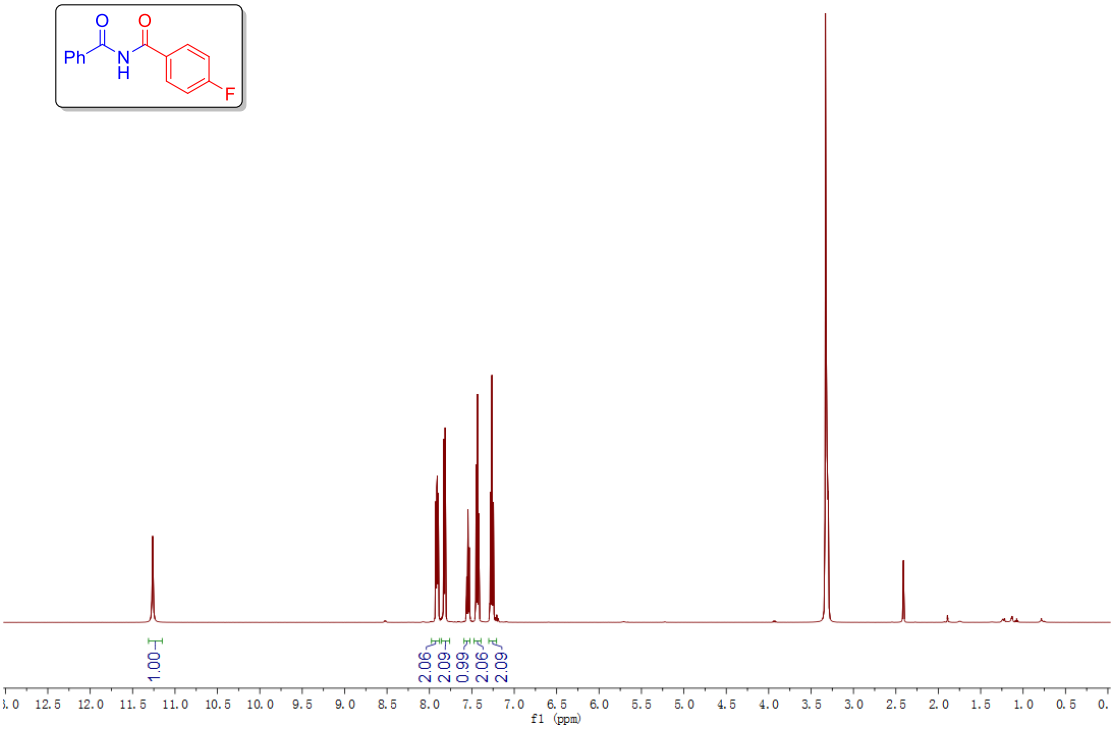
Supplementary Figure 93. ^{1}H NMR Spectrum of 4af' (500MHz, DMSO-d_6)

JM-B31

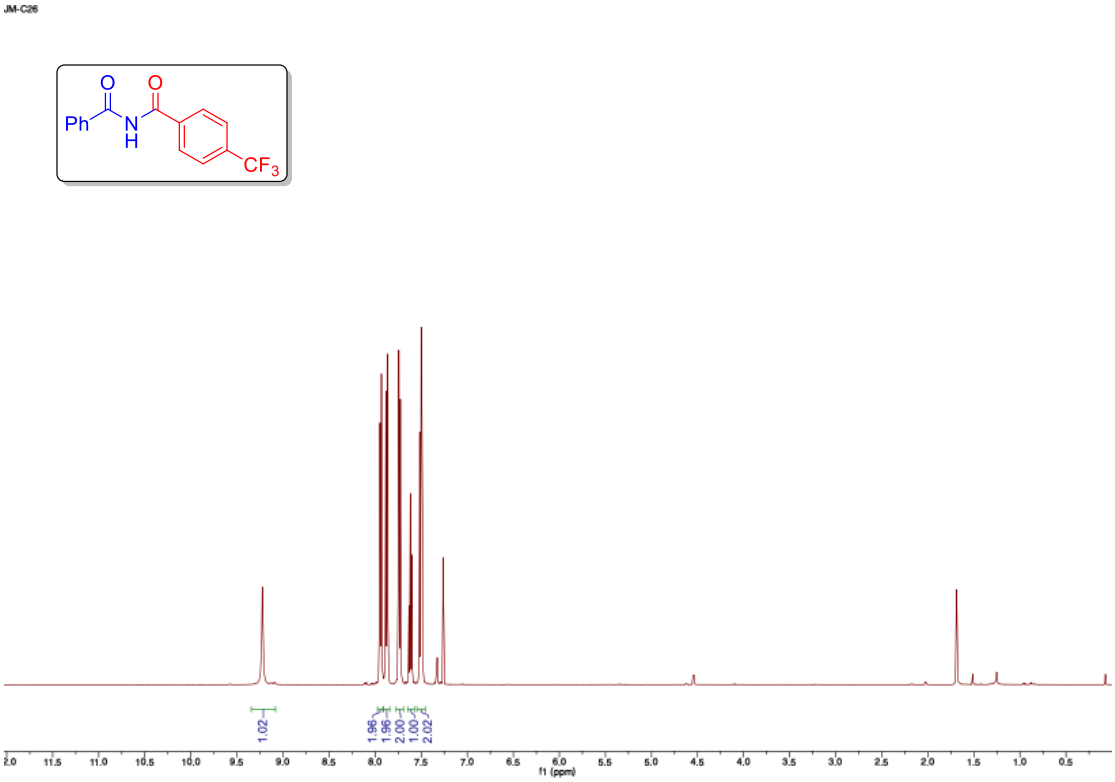


Supplementary Figure 94. ^{1}H NMR Spectrum of 4ag' (500MHz, DMSO-d_6)

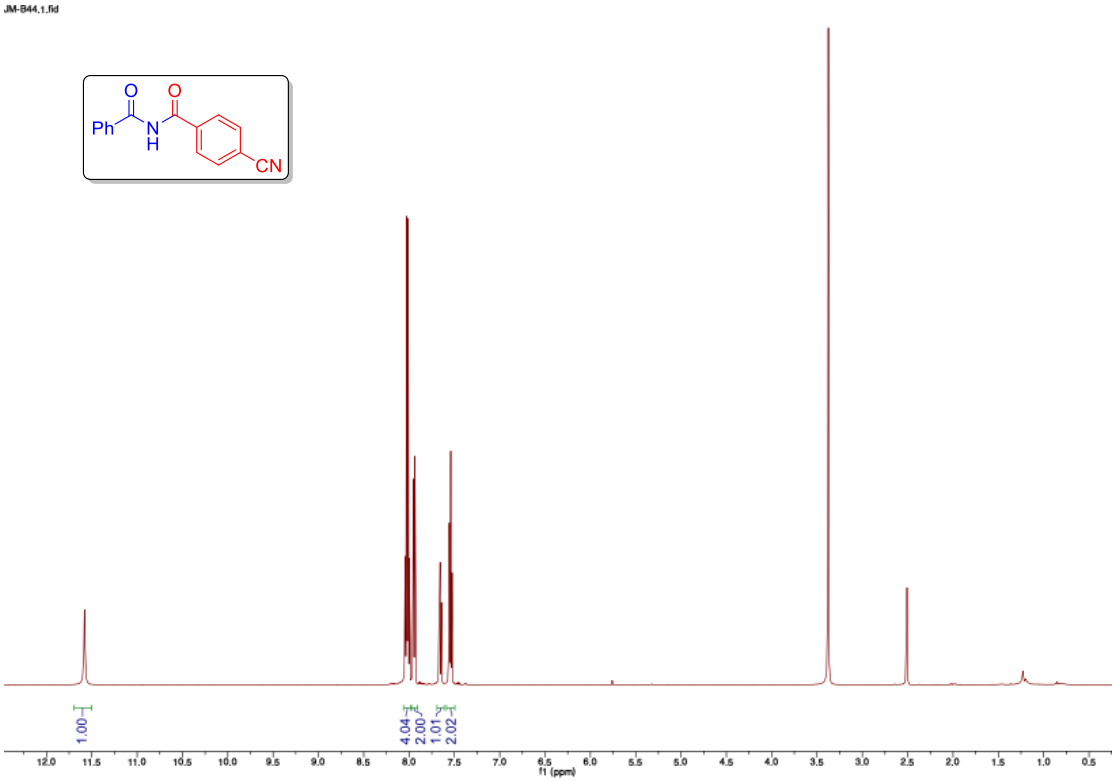
JM-B13



Supplementary Figure 95. ^{1}H NMR Spectrum of 4ah' (500MHz, $CDCl_3$)

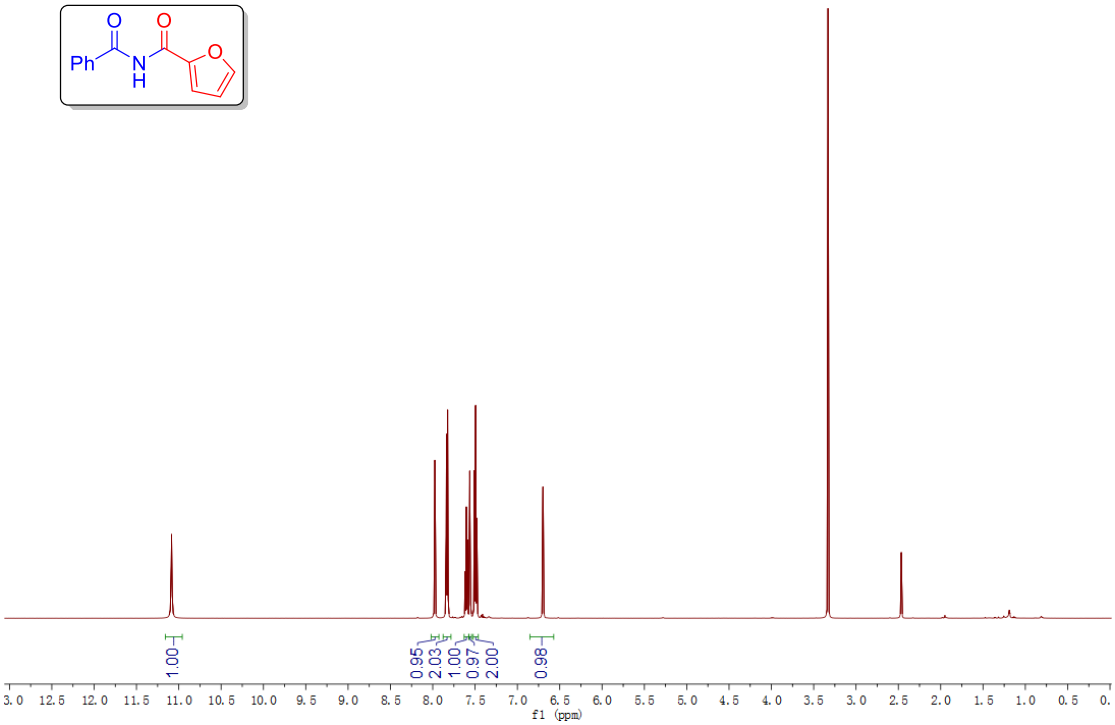


Supplementary Figure 96. ^{1}H NMR Spectrum of 4ai' (500MHz, DMSO-d_6)



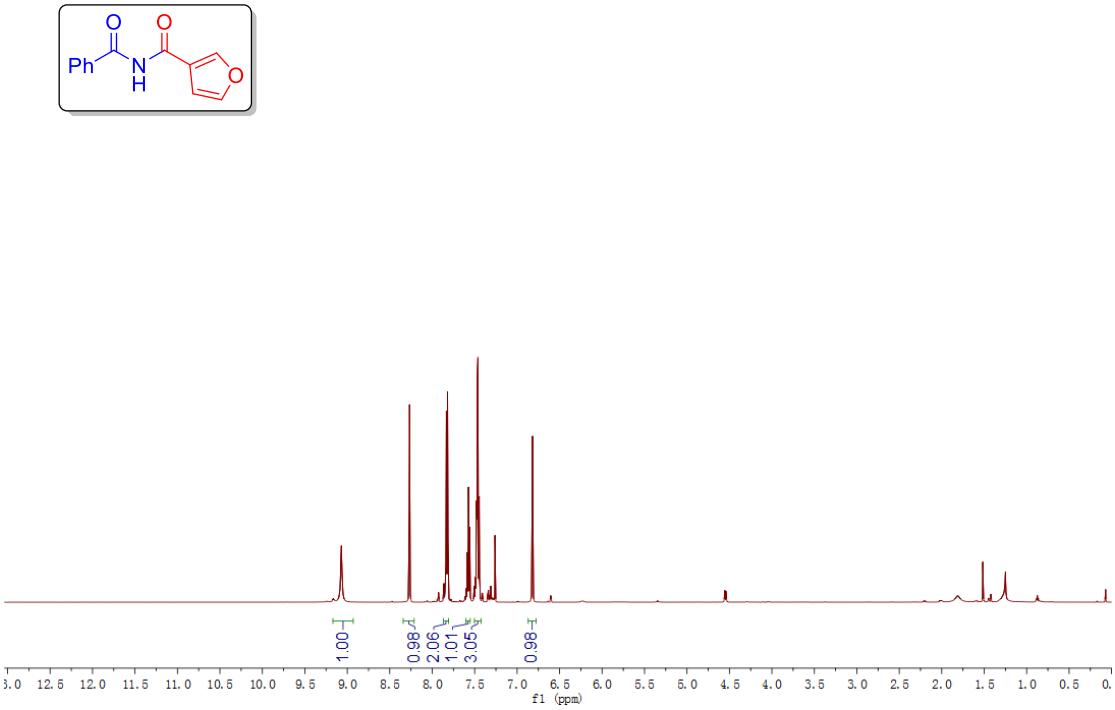
Supplementary Figure 97. ^{1}H NMR Spectrum of 4aj' (500MHz, DMSO-d_6)

JM-B34

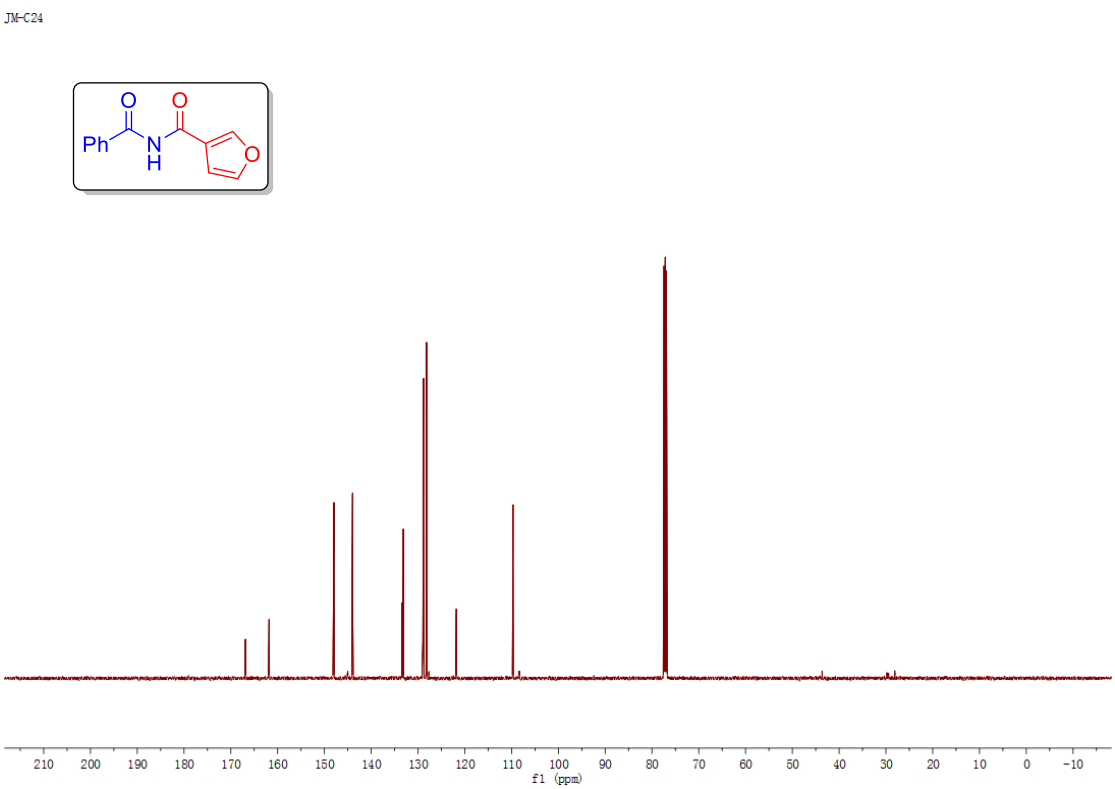


Supplementary Figure 98. ^{1}H NMR Spectrum of 4ak' (500MHz, $CDCl_3$)

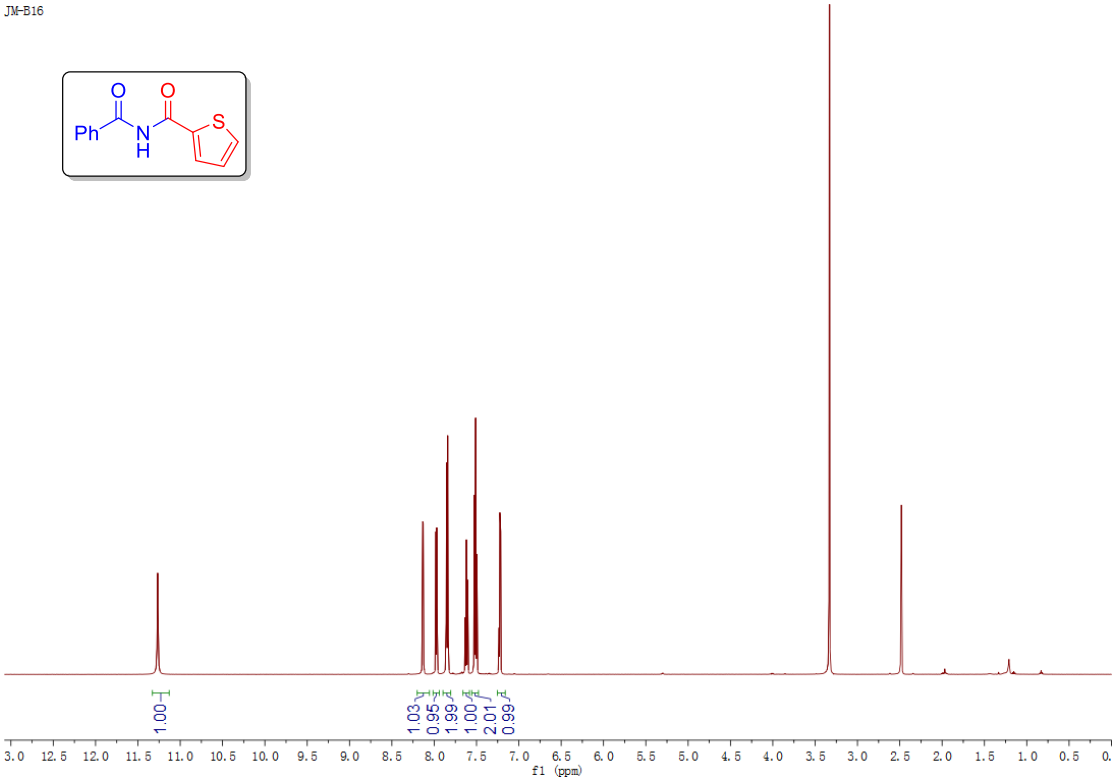
JM-C24



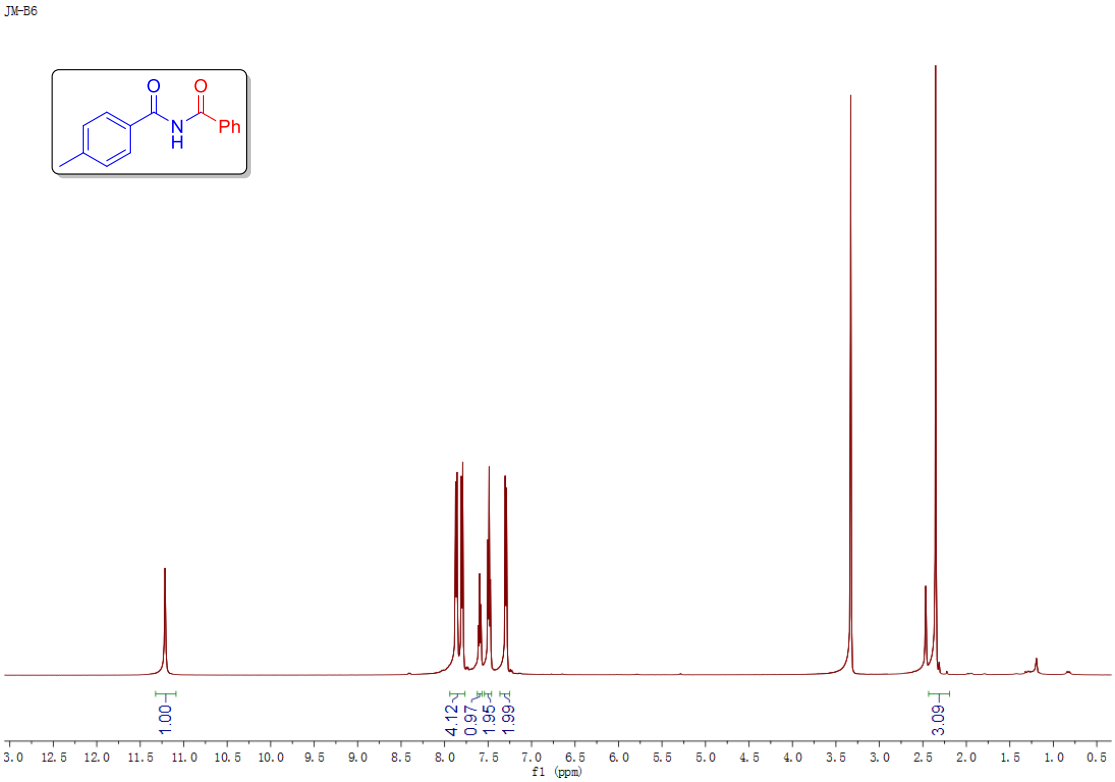
Supplementary Figure 99. ^{13}C NMR Spectrum of 4ak' (125MHz, $CDCl_3$)



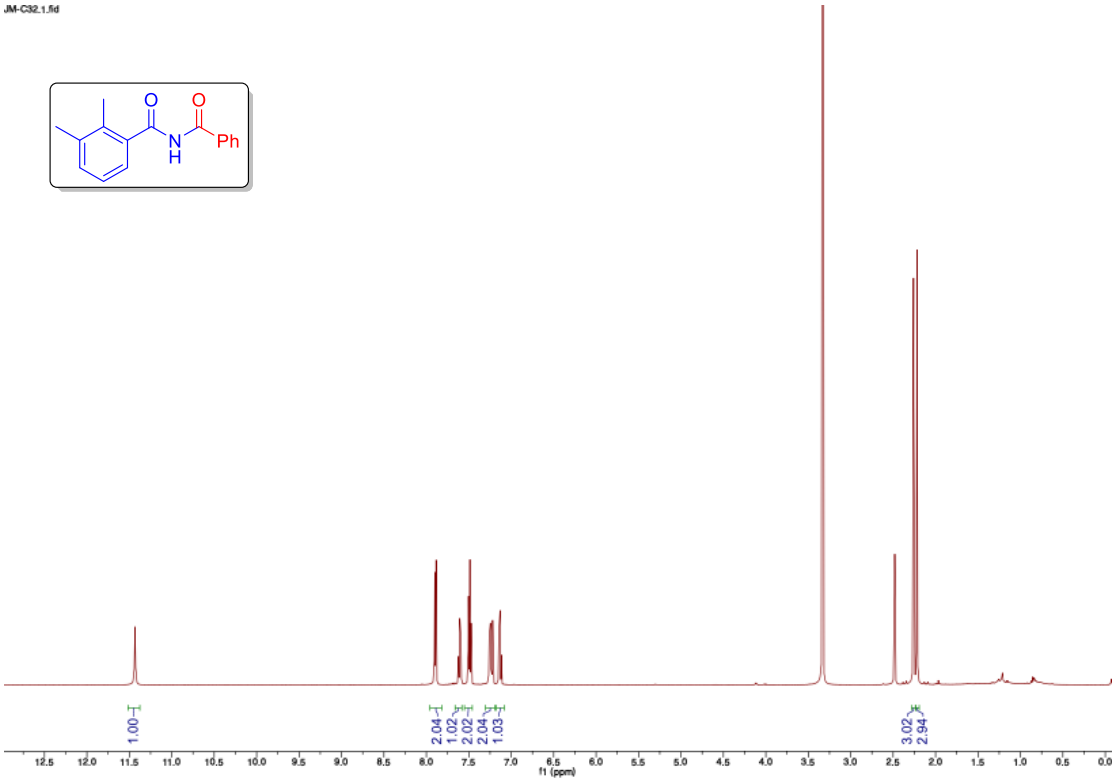
Supplementary Figure 100. ^{1}H NMR Spectrum of 4al' (500MHz, DMSO-d_6)



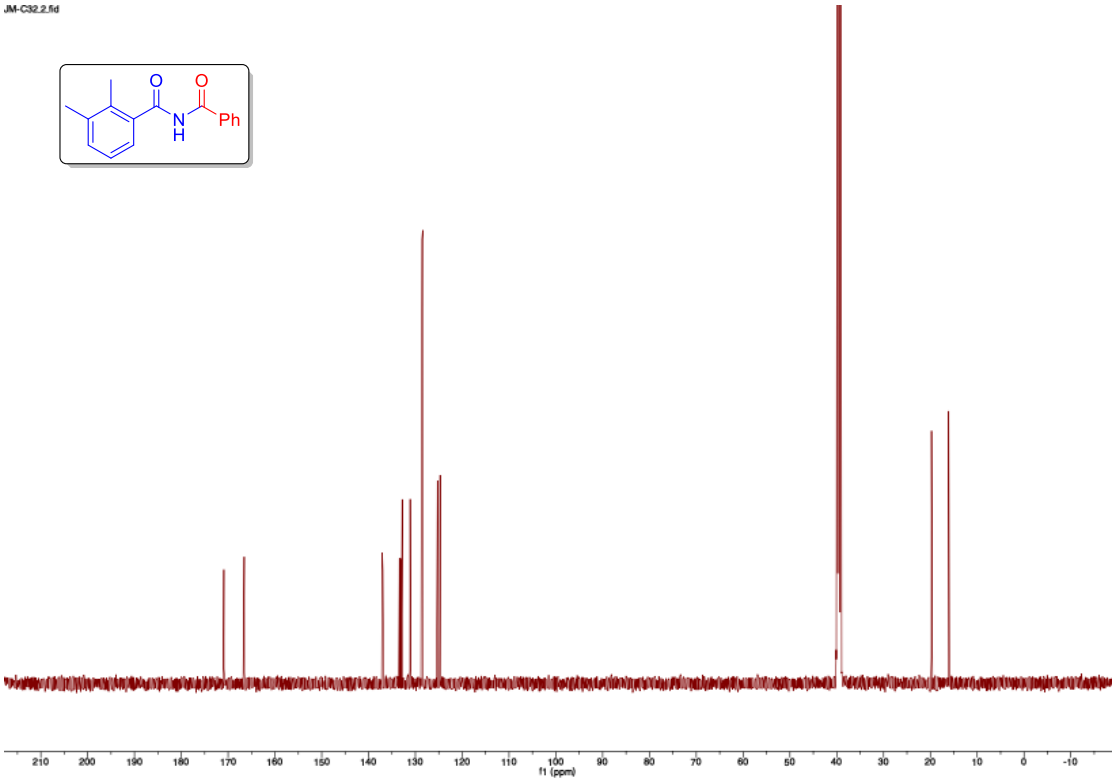
Supplementary Figure 101. ^{1}H NMR Spectrum of 4bb (500MHz, DMSO-d_6)



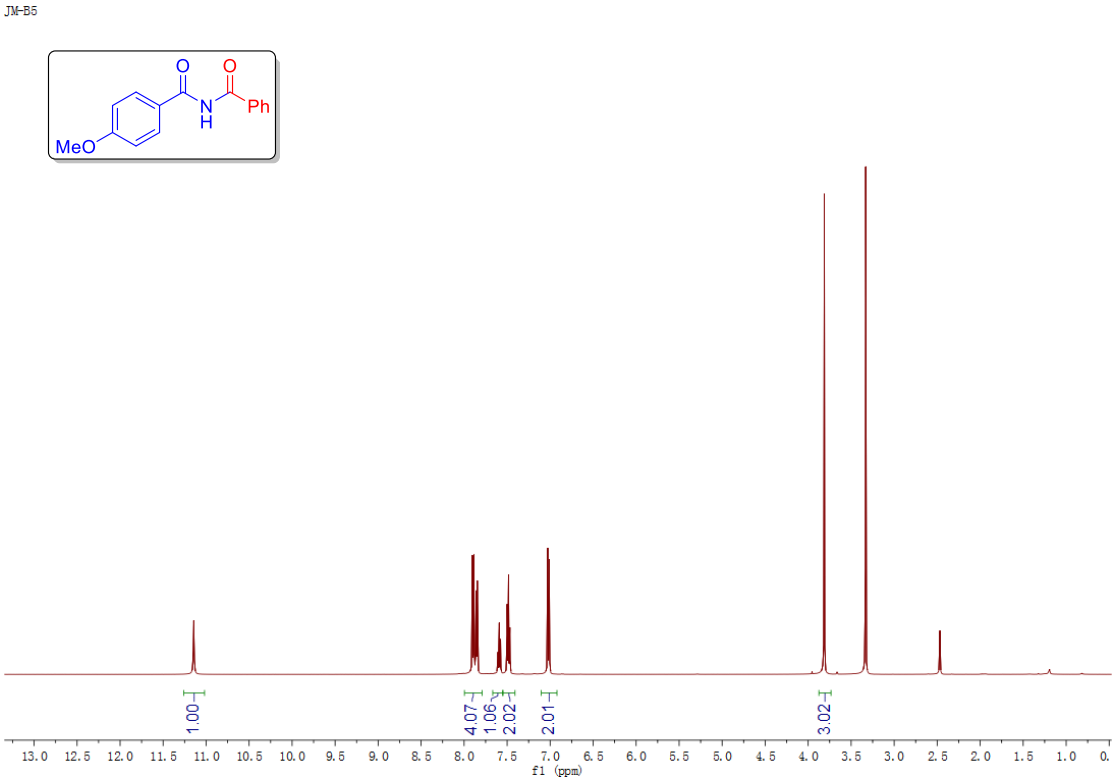
Supplementary Figure 102. ^{1}H NMR Spectrum of 4cb (500MHz, DMSO-d_6)



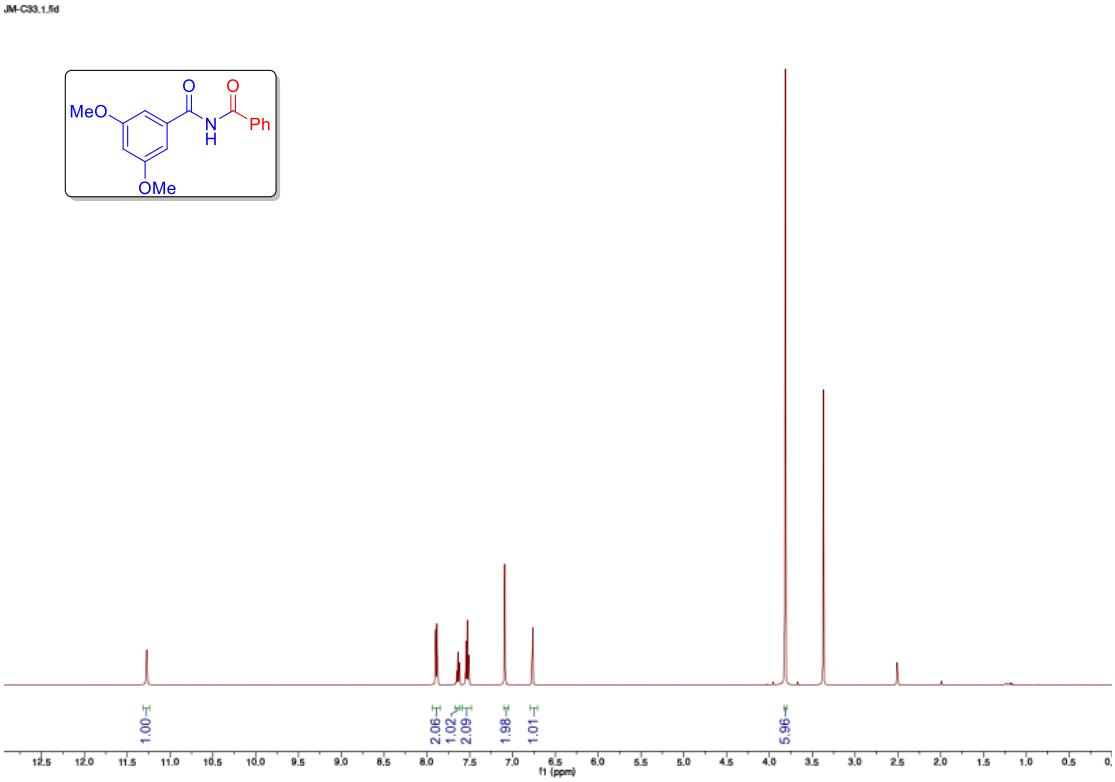
Supplementary Figure 103. ^{13}C NMR Spectrum of 4cb (125MHz, DMSO-d_6)



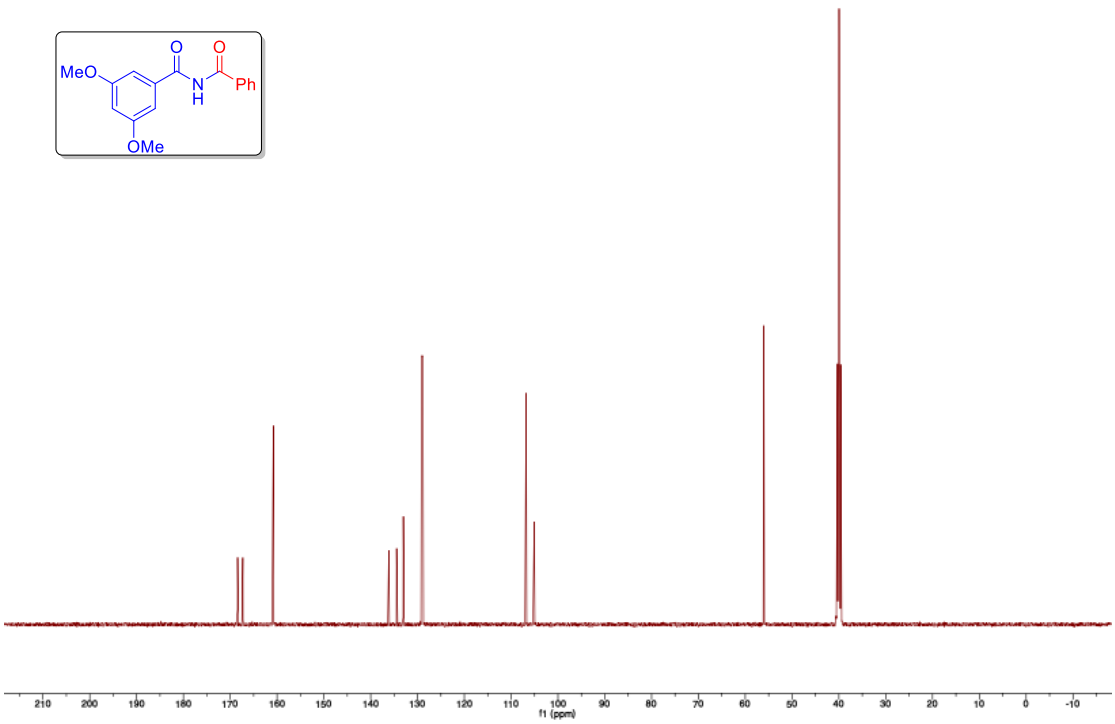
Supplementary Figure 104. ^{1}H NMR Spectrum of 4db (500MHz, DMSO-d_6)



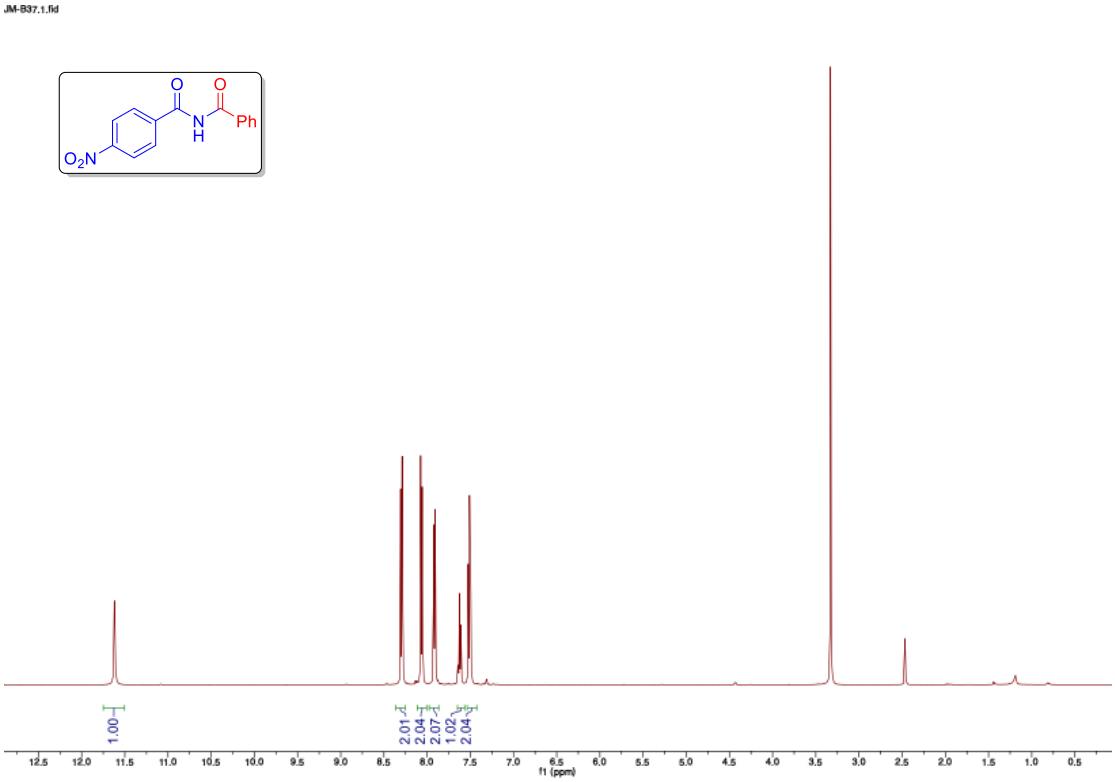
Supplementary Figure 105. ^{1}H NMR Spectrum of 4eb (500MHz, DMSO-d_6)



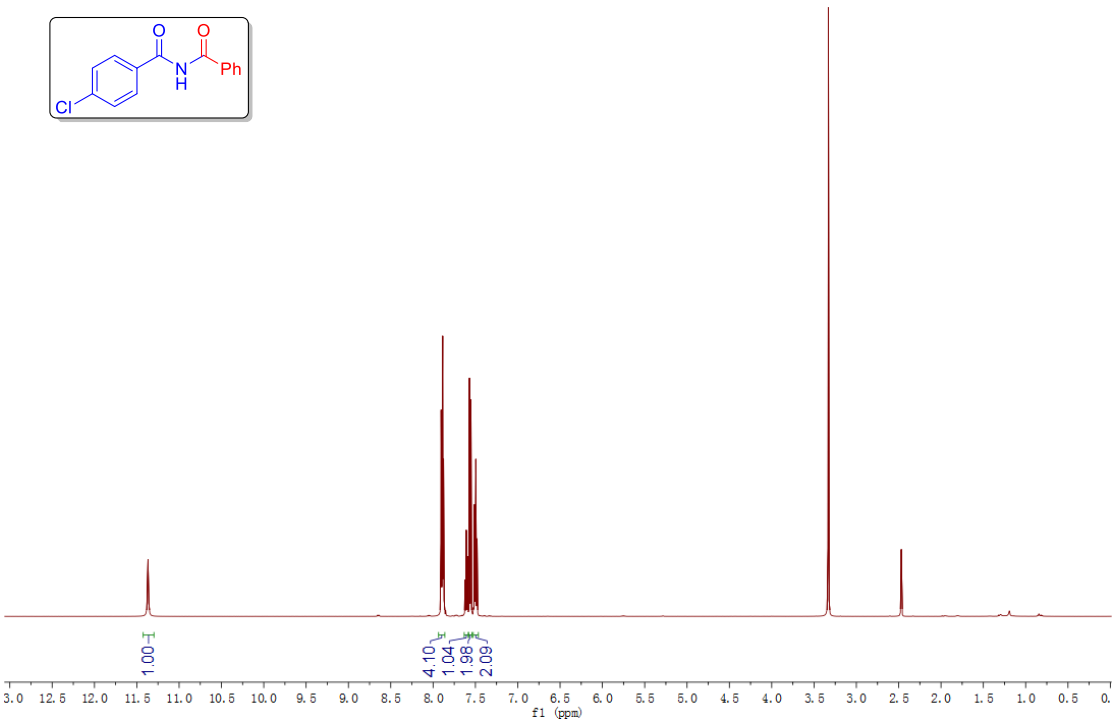
Supplementary Figure 106. ^{13}C NMR Spectrum of 4eb (125MHz, DMSO-d_6)



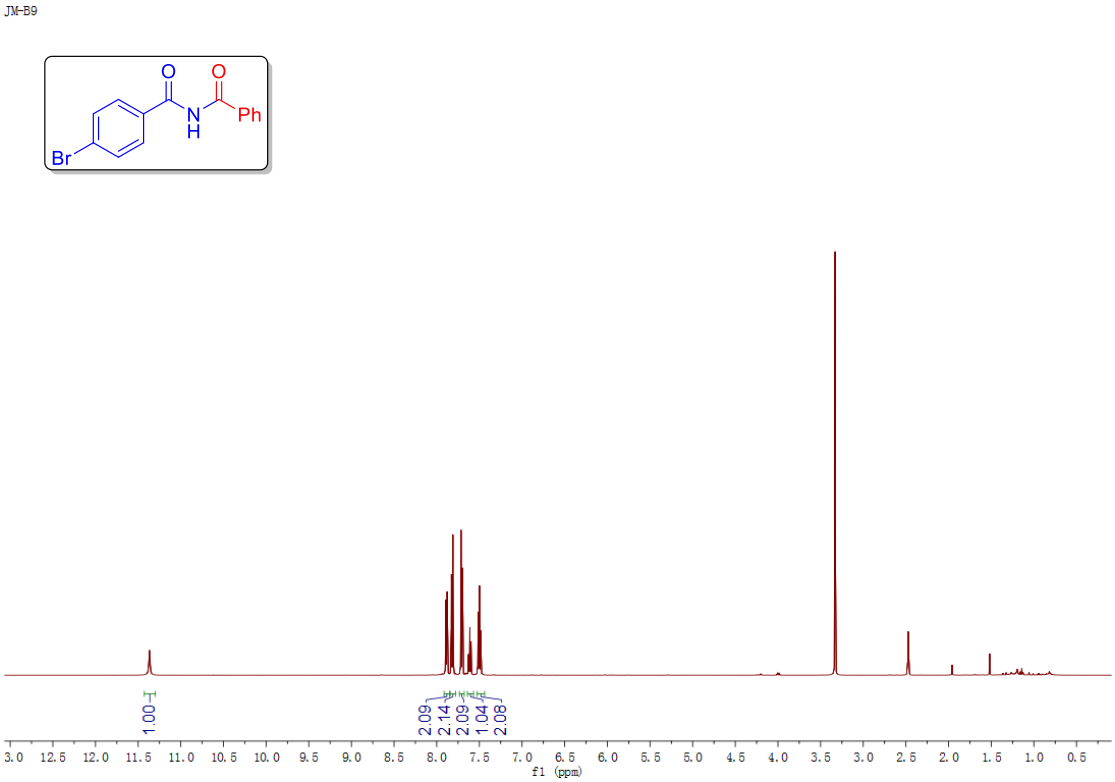
Supplementary Figure 107. ^{1}H NMR Spectrum of 4fb' (500MHz, DMSO-d_6)



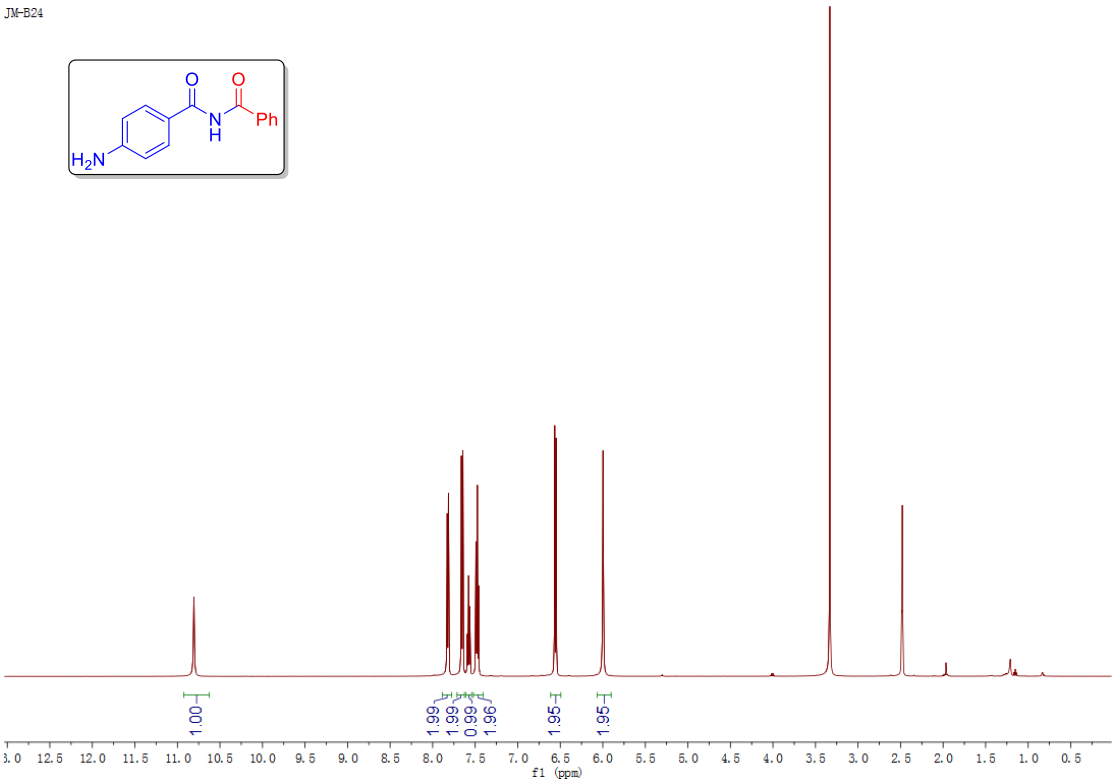
Supplementary Figure 108. ^{1}H NMR Spectrum of 4gb (500MHz, DMSO-d_6)



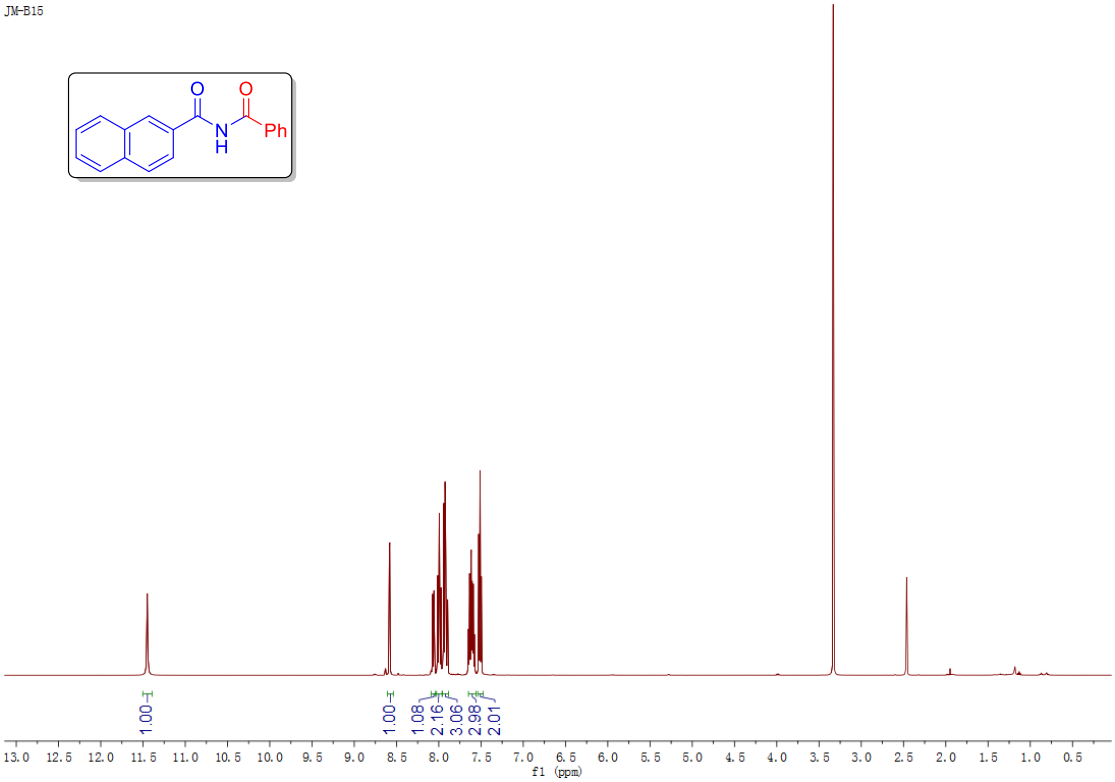
Supplementary Figure 109. ^{1}H NMR Spectrum of 4hb (500MHz, DMSO-d_6)



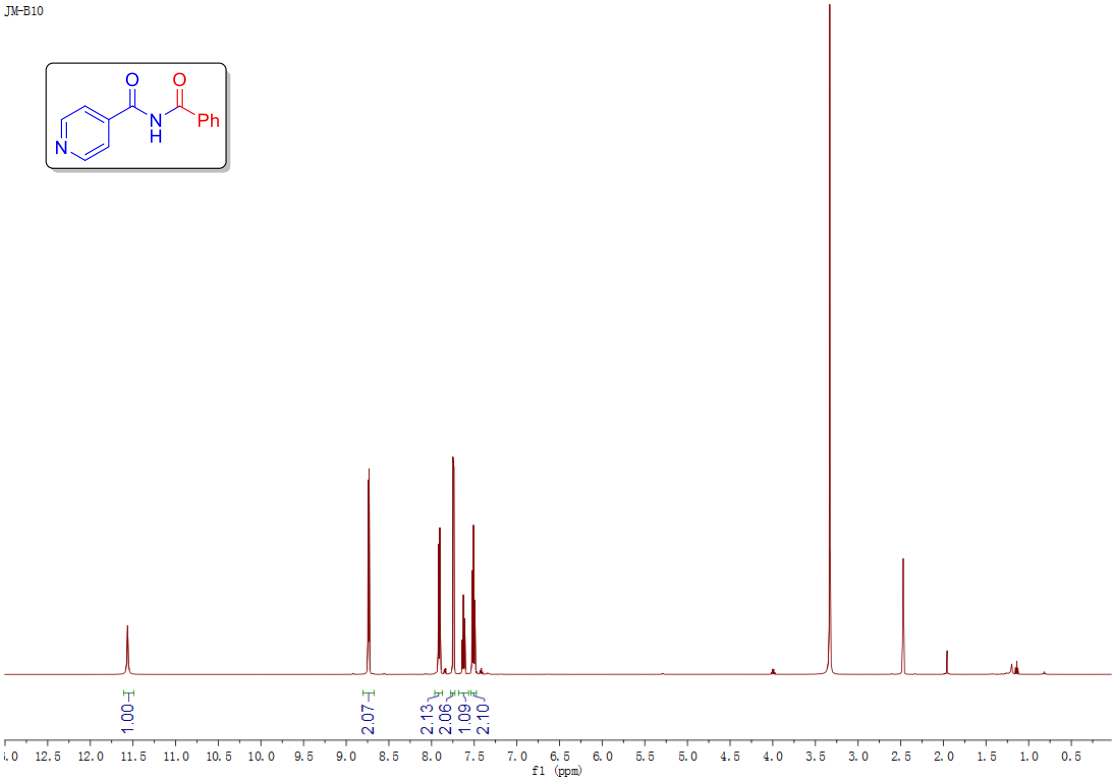
Supplementary Figure 110. ^{1}H NMR Spectrum of 4ib' (500MHz, DMSO-d_6)



Supplementary Figure 111. ^{1}H NMR Spectrum of 4jb (500MHz, DMSO-d_6)



Supplementary Figure 112. ^{1}H NMR Spectrum of 4mb (500MHz, DMSO-d_6)



Supplementary Figure 113. ^{1}H NMR Spectrum of 4nb' (500MHz, DMSO-d_6)