DBU-Catalysis of *N*,*N'*-Carbonyldiimidazole-Mediated Amidations

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General Experimental Procedures

Common substrates and reagents were obtained from commercial suppliers and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were obtained on a Varian NMR 400 MHz spectrometer in $CDCl_3$. High resolution mass spectrometry was performed via infusion on a Thermo 7T LTQ FT Ultra mass spectrometer. Thin layer chromatography was performed with glass-backed TLC sheet of 250 µm thickness (Silica Gel 60 F_{254}). All flash chromatography was performed on a CombiFlash Companion with a RediSepRf column (40 g). HPLC data were collected on an Agilent 1100 Series with a diode array detector. LCMS data were collected on an Agilent 1100 LC/MSD using an Electrospray source. GC data were collected on an Agilent 6890 Gas Chromatograph using an RTX-5 Amine capillary column with flame ionization detection (FID).

General Procedure for Automated Reaction Monitoring

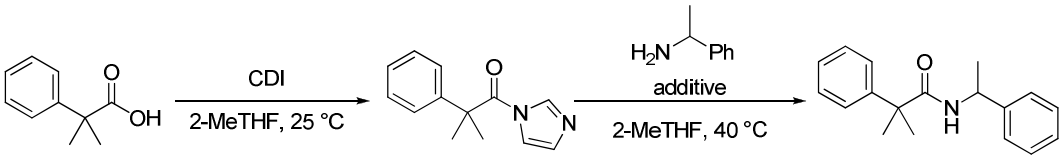
This procedure was used to form acyl imidazole **8** from 2-methyl-2-phenylpropanoic acid (**7**) and to perform the amidation screens (Figure 2, $t_{1/2}$ values from Table 1, Supporting Information S4).

To a one-neck 500 mL round-bottomed flask were charged **7** (9.8 g, 59.5 mmol) and 2-methyltetrahydrofuran (150 mL). The solid acid dissolved to give a colorless solution. *N,N'*-Carbonyldiimidazole (11.9 g, 71.4 mmol, 1.2 equiv) was then charged. The reaction mixture was stirred at 23 °C overnight. The mixture was concentrated *in vacuo*, and the resulting yellow oil was dissolved in 2-methyltetrahydrofuran (49 mL). The solution was then divided into seven equal portions (7 × 9ml) and transferred into seven 20 mL reaction vessels (RVs) for the ReactArray. The appropriate amine (1.2 equiv, 10.2 mmol) was then added to each RV. The appropriate additive (0.5 equiv, 4.25 mmol) was then charged. The RVs were placed into the RS10 block on the ReactArray and heated to the appropriate temperature (60 or 80 °C). Each RV was sampled at appropriate time intervals. At each sample point, 100 µL of the reaction mixture was dissolved in 900 µL of 2-methyltetrahydrofuran and assayed by GC or HPLC.

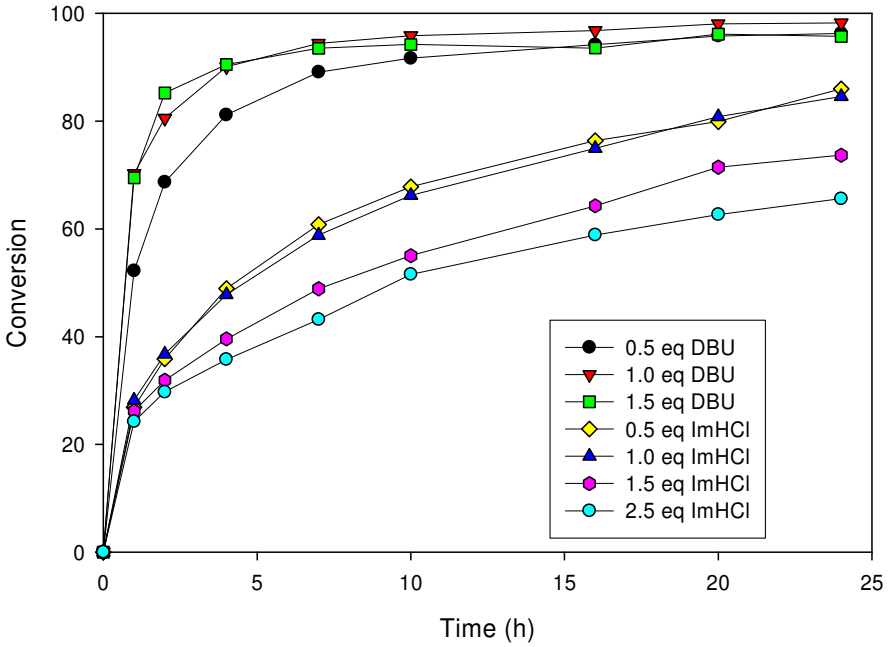
General Procedure for CO_2 Comparison Experiments (Figure 3)

To a one-neck round-bottomed flask were charged *o*-toluic acid (**19**, 2 g, 14.7 mmol) and 2-methyltetrahydrofuran (30 mL). The solid acid dissolved to give a colorless solution. *N*,*N'*-Carbonyldiimidazole (2.5 g, 15.4 mmol, 1.05 equiv) was then charged. The reaction was stirred at 23 °C overnight. The mixture was concentrated *in vacuo* and dissolved in 2-methyltetrahydrofuran (40 mL). The solution was equally divided and transferred into four identical 3-necked flasks equipped with stir bars. The flasks were then sparged with the appropriate head space gas (either N_2 or CO_2). The CO_2 experiments were left under a CO_2 balloon. When the sparge was complete, *sec*-phenethylamine (**11**, 0.49 g, 4.05 mmol, 1.1 equiv) was added to each flask. As necessary, DBU was also added to the reactions. The reactions were allowed to stir at ambient temperature and sampled periodically for LCMS analysis.

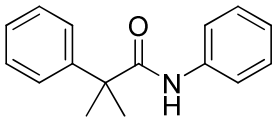
Variation of DBU and Imidazole•HCl Loading



7 **8** **18**



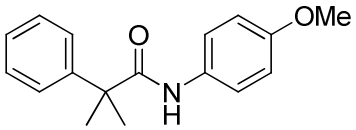
2-Methyl-*N*,2-diphenylpropanamide (12)



2-Methyl-2-phenylpropanoic acid (**7**, 1 g, 6.09 mmol), 2-methyltetrahydrofuran (6 mL) and *N,N'*-carbonyldiimidazole (1.2 equiv, 1.18 g, 7.31 mmol) were charged to a dry one-neck round-bottomed flask under N_2. The reaction was stirred at 23 °C for two hours. When acid consumption was confirmed by HPLC, the mixture was concentrated *in vacuo* to a yellow oil, which was dissolved in 2-methyltetrahydrofuran (5 mL). The solution was transferred to an RV for the AS2410. DBU (0.455 mL, 0.5 equiv, 3.03 mmol) and aniline (0.67 mL, 1.2 equiv, 7.31 mmol) were charged, and the reaction was stirred at 80 °C for 24 h. The reaction mixture was then cooled and diluted with 2-MeTHF (20 mL). The solution was washed with 1 N HCl (2 × 15 mL) and 0.1 N NaOH (2 × 15 mL). The organic layer was dried over $MgSO_4$, filtered and concentrated *in vacuo*. The crude material was then purified by flash chromatography (10 to 40% EtOAc in hexanes) to give 1.07 g (73%) of a pale yellow solid. Spectral data were in agreement with those previously published.[1]

[1] (a) Dunn, P. J.; Hoffman, W.; Kang, Y.; Mitchell, J. C.; Snowden, M. J. *Org. Process Res. Dev.* **2005**, *9*, 956-961. (b) Olsen, E. O. *Acta Chem. Scand.* **1975**, *B29*, 953-962.

***N*-(4-methoxyphenyl)-2-methyl-2-phenylpropanamide (13)**



2-Methyl-2-phenylpropanoic acid (**7**, 1 g, 6.09 mmol), 2-methyltetrahydrofuran (6 mL) and *N*,*N'*-carbonyldiimidazole (1.18 g , 1.2 equiv, 7.31 mmol) were charged to a dry one-neck round-bottomed flask under N_2. The reaction was stirred at 23 °C for two hours. When acid consumption was confirmed by HPLC, the mixture was concentrated *in vacuo* to a yellow oil. The oil was dissolved in 2-methyltetrahydrofuran (5mL) and transferred to an RV for the AS2410. DBU (0.455 mL, 0.5 equiv, 3.03 mmol) and *p*-anisidine (0.9 g, 1.20 equiv, 7.31 mmol) were added and the reaction was stirred at 80°C for 8 h. The reaction mixture was then cooled and diluted with 2-methyltetrahydrofuran (20 mL). The solution was washed with 1 N HCl (2 × 15 mL) and 0.1 N NaOH (2 × 15 mL). The organic layer was dried over $MgSO_4$, filtered and concentrated *in vacuo* to give 1.32 g (80%) of a pale yellow solid. HRMS (ES, N_2) found *m/z* 270.14901 (M^+), $C_{17}H_{20}N_1O_2$ requires 270.14886.

Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.55	621.6	1.0000
2	2.50	999.9	0.0410
3	3.33	1330.1	0.0881
4	3.70	1481.3	0.7460
5	6.83	2731.8	0.1725
6	6.85	2740.8	0.1876
7	7.21	2884.4	0.0160
8	7.23	2892.8	0.0529
9	7.25	2899.2	0.0443
10	7.32	2929.1	0.0480
11	7.34	2937.3	0.1682
12	7.36	2943.9	0.3505
13	7.38	2951.2	0.0511
14	7.47	2985.7	0.1868
15	7.49	2994.7	0.1731
16	8.97	3585.9	0.1107

Table of Integrals

No.	(ppm)	Value
1	[1.48 .. 1.64]	6
2	[3.66 .. 3.76]	3
3	[6.77 .. 6.90]	2
4	[7.18 .. 7.52]	7
5	[8.91 .. 9.03]	1

Table of Annotations

No.	(ppm)	Annotation
1	2.50	DMSO-d6
2	3.33	Water

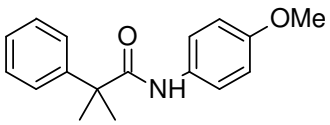


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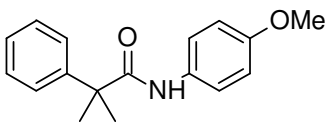
Table of Peaks

No.	(ppm)	(Hz)	Height
1	26.82	2697.9	0.3361
2	38.88	3910.8	0.1491
3	39.09	3931.9	0.4366
4	39.30	3952.8	0.8624
5	39.51	3973.9	1.0000
6	39.72	3994.8	0.8473
7	39.93	4015.7	0.4160
8	40.14	4036.8	0.1453
9	47.01	4728.3	0.1607
10	55.09	5541.0	0.1300
11	113.47	11412.9	0.3715
12	121.89	12259.7	0.4064
13	125.66	12638.4	0.3838
14	126.25	12698.0	0.1803
15	128.24	12898.5	0.3780
16	132.26	13302.8	0.1140
17	146.00	14684.3	0.1156
18	155.25	15615.0	0.1118
19	174.26	17526.6	0.1356

Table of Annotations

No.	(ppm)	Annotation
1	39.51	DMSO-d6



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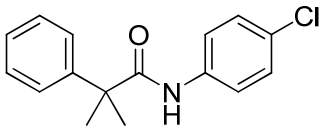
***N*-(4-Chlorophenyl)-2-methyl-2-phenylpropanamide (14)**



2-Methyl-2-phenylpropionic acid (**7**, 1 g, 6.09 mmol), 2-methyltetrahydrofuran (6 mL) and *N*,*N*′-carbonyldiimidazole (1.2 equiv, 1.18 g, 7.31 mmol) were charged to a dry one-neck round-bottomed flask under N_2. The reaction was stirred at 23 °C for two hours. When acid consumption was confirmed by HPLC, the mixture was concentrated *in vacuo* to a yellow oil. The oil was dissolved in 2-methyltetrahydrofuran (5 mL) and the solution was transferred to an RV for the AS2410. *p*-Chloroaniline (1.17 g, 1.5 equiv; 9.13 mmol) and DBU (0.46 mL, 0.5 equiv, 3.03 mmol) were then charged and the mixture was stirred at 80 °C for 24 h. The reaction mixture was then cooled and diluted with 2-methyltetrahydrofuran (20 mL). The solution was washed with 1 N HCl (2 × 15 mL) and 0.1 N NaOH (2 × 15 mL). The organic layer was dried over $MgSO_4$, filtered and concentrated *in vacuo* to give 1.21 g (73%) of a pale yellow solid. HRMS (ES, N_2) found *m/z* 274.09938 (M^+), $C_{16}H_{17}{}^{35}ClNO$ requires 274.09932.

Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.56	625.3	1.0000
2	2.50	999.9	0.0285
3	3.34	1334.6	0.0376
4	7.22	2886.7	0.0159
5	7.23	2890.2	0.0286
6	7.25	2900.4	0.0458
7	7.26	2903.7	0.0306
8	7.31	2922.1	0.1804
9	7.33	2931.0	0.2256
10	7.35	2939.2	0.3041
11	7.36	2943.0	0.4599
12	7.65	3057.8	0.2086
13	7.67	3066.6	0.1842
14	9.23	3693.3	0.1166

Table of Integrals

No.	(ppm)	Value
1	[1.48 .. 1.63]	6
2	[7.17 .. 7.75]	9
3	[9.17 .. 9.30]	1

Table of Annotations

No.	(ppm)	Annotation
1	2.50	DMSO-d6
2	3.34	Water

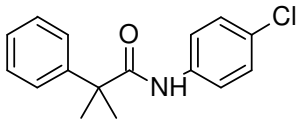


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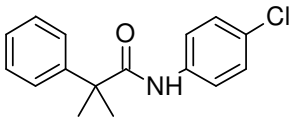
Table of Peaks

No.	(ppm)	(Hz)	Height
1	26.72	2687.2	0.5646
2	38.88	3910.8	0.1450
3	39.09	3931.9	0.4278
4	39.30	3953.0	0.8549
5	39.51	3973.9	1.0000
6	39.72	3994.8	0.8641
7	39.93	4015.9	0.4236
8	40.14	4036.8	0.1397
9	47.32	4759.6	0.2689
10	121.69	12239.0	0.6621
11	125.65	12637.8	0.6294
12	126.37	12710.7	0.2995
13	126.82	12755.8	0.1773
14	128.23	12897.1	0.6405
15	128.32	12906.0	0.6708
16	138.20	13899.7	0.2101
17	145.59	14643.0	0.1580
18	174.82	17583.2	0.2235

Table of Annotations

No.	(ppm)	Annotation
1	39.51	DMSO-d6



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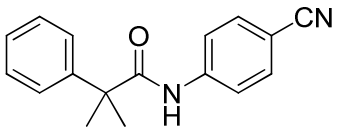
***N*-(4-Cyanophenyl)-2-methyl-2-phenylpropanamide (15)**



2-Methyl-2-phenylpropionic acid (**7,** 5 g, 30.45 mmol), 2-methyltetrahydrofuran (75 mL) and *N*,*N'*-carbonyldiimidazole (5.184 g ,1.05 equiv) were charged to a dry one-neck round-bottomed flask under N_2. The reaction was stirred at 23 °C overnight. When acid consumption was confirmed by LCMS, the mixture was concentrated *in vacuo* to a yellow oil and dissolved in 2-methyltetrahydrofuran (20 mL). The solution was transferred to a 3-neck flask equipped with a stir bar, thermocouple, and reflux condenser. *p*-Aminobenzonitrile (3.96 g, 1.1 equiv; 33.49 mmol) and DBU (4.58 mL, 1 equiv, 30.45 mmol) were added, and the mixture was stirred at 80 °C for 24 h.[2] The reaction mixture was then cooled to room temperature. The cooled reaction mixture was diluted with 2-methyltetrahydrofuran (80 mL) and 1N HCl (50 mL). The layers were then allowed to separate. The organic phase was washed four times with 1 N HCl (4 × 50 mL) to completely remove remaining p-aminobenzonitrile. The organic phase was dried over $MgSO_4$, filtered and concentrated *in vacuo* to a tan solid (6.94 g, 86%). HRMS (ES, N_2) found *m/z* 265.13358 (M^+), $C_{17}H_{17}N_2O$ requires 265.13358 .

[2] One equivalent of DBU was used to ensure reaction completion in 24 h.

Table of Integrals

No.	(ppm)	Value
1	[1.62 .. 1.71]	6
2	[6.88 .. 7.03]	1
3	[7.20 .. 7.61]	9

Table of Annotations

No.	(ppm)	Annotation
1	1.62	Water
2	7.27	CHLOROFORM-d

Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.62	647.0	0.0776
2	1.68	670.4	1.0000
3	6.98	2791.6	0.0521
4	7.27	2907.7	0.0412
5	7.33	2931.6	0.0172
6	7.34	2935.7	0.0332
7	7.35	2939.9	0.0550
8	7.36	2944.1	0.0498
9	7.37	2948.1	0.0343
10	7.43	2970.2	0.3307
11	7.44	2974.3	0.3002
12	7.48	2992.0	0.0906
13	7.50	3000.7	0.1981
14	7.53	3013.3	0.1898
15	7.56	3022.0	0.0859

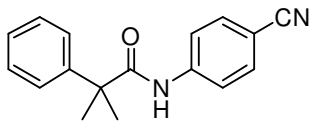


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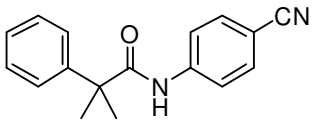
Table of Peaks

No.	(ppm)	(Hz)	Height
1	26.76	2691.6	0.6370
2	48.23	4851.0	0.3048
3	76.68	7712.5	0.6995
4	77.00	7744.6	0.7237
5	77.32	7776.6	0.7130
6	106.69	10731.1	0.2013
7	118.72	11941.1	0.1741
8	119.37	12006.1	1.0000
9	126.25	12698.2	0.9333
10	127.57	12831.1	0.4857
11	129.05	12980.2	0.9314
12	132.98	13374.7	0.9951
13	141.95	14277.4	0.2304
14	143.73	14456.2	0.2432
15	175.92	17694.0	0.2211

Table of Annotations

No.	(ppm)	Annotation
1	77.00	CHLOROFORM-d



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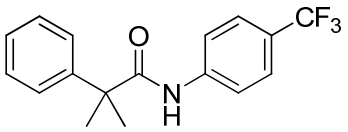
2-Methyl-2-phenyl-*N*-(4-(trifluoromethyl)phenyl)propanamide (16)



2-Methyl-2-phenylpropionic acid (**7**, 3 g, 18.27 mmol), 2-methyltetrahydrofuran (45 mL) and *N*,*N'*-carbonyldiimidazole (3.1 g, 1.05 equiv) were charged to a dry one-neck round-bottomed flask under N_2. The reaction was stirred at 23 °C. When acid consumption was confirmed by LCMS, the mixture was concentrated *in vacuo* to a yellow oil and dissolved in 2-methyltetrahydrofuran (12 mL). The solution was transferred to a 3-neck flask equipped with a stir bar, thermocouple, and reflux condenser. *p*-(Trifluoromethyl)aniline (3.24 g, 1.1 equiv; 20.1 mmol) and DBU (2.7 mL, 1 equiv, 18.3 mmol) were then charged and the mixture was heated to 80 °C for 48 h. The reaction mixture was then cooled to room temperature and concentrated *in vacuo*. The crude material was then purified by flash chromatography (15% EtOAc in *n*-heptane) to give 4.0 g (71%) of a pale yellow solid. HRMS (ES, N_2) found *m/z* 308.12551 (M^+), $C_{17}H_{17}O_1N_1F_3$ requires 308.12568.

Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.55	619.2	0.0963
2	1.69	674.7	1.0000
3	6.90	2761.2	0.0311
4	7.27	2907.7	0.1489
5	7.34	2933.8	0.0146
6	7.35	2940.5	0.0325
7	7.37	2946.3	0.0314
8	7.37	2948.3	0.0197
9	7.41	2963.9	0.0287
10	7.43	2972.1	0.1249
11	7.45	2978.4	0.2678
12	7.47	2988.5	0.0522
13	7.49	2997.5	0.1717
14	7.51	3004.1	0.1717
15	7.53	3013.1	0.0490

Table of Integrals

No.	(ppm)	Value
1	[1.53 .. 1.57]	0.6
2	[1.63 .. 1.74]	6
3	[6.81 .. 6.99]	1
4	[7.31 .. 7.57]	9

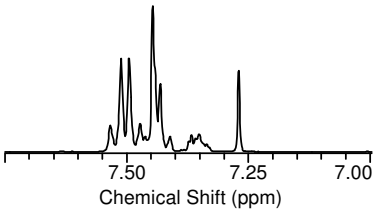
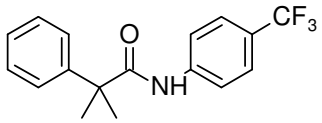


Table of Annotations

No.	(ppm)	Annotation
1	1.55	water
2	7.27	CHLOROFORM-d



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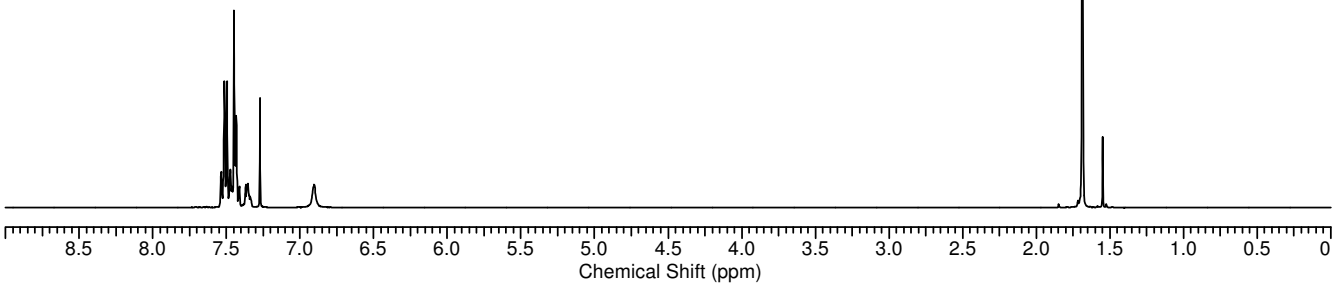
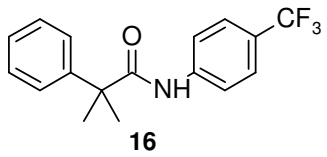


Table of Peaks

No.	(ppm)	(Hz)	Height
1	26.93	2708.1	0.3163
2	48.25	4852.7	0.1959
3	76.68	7712.3	0.9090
4	77.00	7744.6	0.9893
5	77.32	7776.8	0.8509
6	119.13	11982.2	1.0000
7	126.06	12678.9	0.0904
8	126.10	12682.8	0.3202
9	126.14	12686.6	0.3219
10	126.17	12690.4	0.0753
11	126.40	12713.5	0.8234
12	127.62	12836.2	0.3974
13	129.14	12988.9	0.4516
14	140.97	14179.0	0.0573
15	144.09	14492.0	0.1057
16	175.84	17685.4	0.1066

Table of Annotations

No.	(ppm)	Annotation
1	77.00	CHLOROFORM-d



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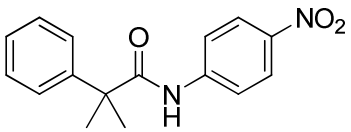
2-Methyl-*N*-(4-nitrophenyl)-2-phenylpropanamide (17)



2-Methyl-2-phenylpropionic acid (**7**, 3 g, 18.27 mmol), 2-methyltetrahydrofuran (45 mL) and *N*,*N'*-carbonyldiimidazole (3.11 g ,1.05 equiv) were charged to a dry one-neck round-bottomed flask under N_2. The reaction was stirred at 23 °C for three hours. When acid consumption was confirmed by LCMS, the mixture was concentrated *in vacuo* to a yellow oil and dissolved in 2-methyltetrahydrofuran (12 mL). The solution was transferred to a 3-neck round-bottomed flask equipped with a stir bar, thermocouple, and reflux condenser. *p*-Nitroaniline (2.78 g, 1.1 equiv; 20.1 mmol) and DBU (2.75 mL, 1 equiv, 18.27 mmol) were then charged and the mixture was stirred at 80 °C for 24 h.[2] The reaction mixture was then cooled to room temperature, and diluted with 2-methyltetrahydrofuran (45 mL) and 1 N HCl (30 mL). The layers were allowed to separate. The organic phase was washed with 1 N HCl (2 × 30 mL), followed by 1 N NaOH (1 × 15 mL). The organic phase was then washed with brine (15 mL), dried over $MgSO_4$ and concentrated *in vacuo* to a yellow solid (4.27 g, 82%). HRMS (ES, N_2) found *m/z* 285.12330 (M^+), $C_{16}H_{17}N_2O_3$ requires 285.12337.

Table of Integrals

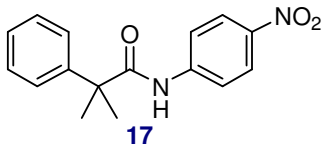
No.	(ppm)	Value
1	[1.65 .. 1.76]	6.000
2	[7.04 .. 7.14]	0.907
3	[7.32 .. 7.40]	0.952
4	[7.40 .. 7.48]	3.696
5	[7.50 .. 7.60]	1.900
6	[8.08 .. 8.20]	1.833

Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.69	674.9	1.0000
2	7.10	2837.5	0.0212
3	7.27	2906.2	0.0268
4	7.34	2932.7	0.0083
5	7.34	2936.0	0.0107
6	7.35	2937.3	0.0178
7	7.36	2941.3	0.0342
8	7.37	2946.3	0.0225
9	7.38	2949.8	0.0239
10	7.39	2954.0	0.0071
11	7.43	2971.9	0.2245
12	7.44	2975.9	0.2865
13	7.52	3007.3	0.0120
14	7.53	3010.4	0.1205
15	7.54	3012.4	0.0343
16	7.55	3017.5	0.0361
17	7.55	3019.5	0.1362
18	7.56	3022.5	0.0135
19	8.12	3245.9	0.0127
20	8.13	3248.8	0.1234
21	8.13	3251.0	0.0333
22	8.14	3256.0	0.0331
23	8.15	3258.1	0.1180
24	8.16	3261.1	0.0110

Table of Annotations

No.	(ppm)	Annotation
1	7.27	CHLOROFORM-d



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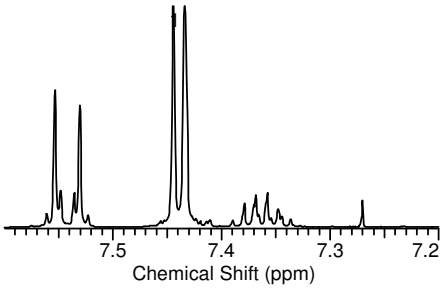
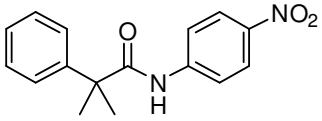


Table of Peaks

No.	(ppm)	(Hz)	Height
1	26.83	2696.8	0.9711
2	48.39	4864.5	0.1299
3	76.68	7708.7	0.5366
4	77.00	7740.6	0.5374
5	77.32	7772.6	0.5249
6	118.85	11947.4	0.9601
7	124.92	12557.5	1.0000
8	126.35	12701.6	0.8551
9	127.78	12845.0	0.4838
10	129.23	12990.7	0.7782
11	143.29	14404.6	0.0773
12	143.60	14435.4	0.1897
13	143.71	14446.7	0.1606
14	176.02	17694.6	0.1225

Table of Annotations

No.	(ppm)	Annotation
1	77.00	CHLOROFORM-d



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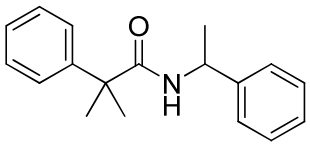
2-Methyl-2-phenyl-*N*-(1-phenylethyl)propanamide (18)



2-Methyl-2-phenylpropionic acid (**7**, 5 g, 30.45 mmoles), 2-methyltetrahydrofuran (75 mL) and *N*,*N'*-carbonyldiimidazole (5.2 g, 1.05 equiv) were charged to a dry one-neck round-bottomed flask under N_2. The reaction was stirred at 23 °C for 5 hours. When acid consumption was confirmed by LCMS, the mixture was concentrated *in vacuo* to a yellow oil and dissolved in 2-methyltetrahydrofuran (25 mL). The solution was transferred to a 3-neck flask equipped with a stir bar, thermocouple, and reflux condenser. *Sec*-Phenethylamine (**11**, 4.32 mL, 1.1 equiv; 33.49 mmol) and DBU (2.29 mL, 0.5 equiv, 15.22 mmol) were then added and the mixture was stirred at 60 °C for 24 h. The reaction mixture was then cooled and diluted with 2-MeTHF (80 mL) and 1 N HCl (50 mL). The layers were then allowed to separate. The organic phase was washed with 1 N HCl (2 × 50 mL). The organic phase was dried over $MgSO_4$, concentrated *in vacuo*, and dried under vacuum overnight to afford a white solid (7.6 g, 93% yield). HRMS (ES, N_2) found *m/z* 268.16959 (M^+), $C_{18}H_{22}N_1O_1$ requires 268.16959.

Table of Integrals

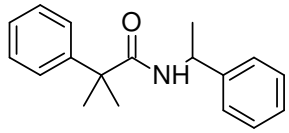
No.	(ppm)	Value
1	[1.24 .. 1.39]	3
2	[1.52 .. 1.60]	6
3	[4.98 .. 5.14]	1
4	[5.24 .. 5.46]	1
5	[7.07 .. 7.38]	9

Table of Annotations

No.	(ppm)	Annotation
1	1.61	water
2	7.27	chloroform-d

Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.32	526.6	0.5795
2	1.33	533.7	0.5873
3	1.55	618.4	0.9964
4	1.58	631.9	1.0000
5	5.03	2012.0	0.0146
6	5.05	2019.0	0.0525
7	5.07	2026.4	0.0772
8	5.08	2033.7	0.0591
9	5.10	2040.7	0.0170
10	5.33	2133.1	0.0353
11	5.35	2139.3	0.0334
12	7.11	2842.2	0.1539
13	7.13	2850.6	0.1716
14	7.18	2873.6	0.0283
15	7.20	2881.0	0.1033
16	7.22	2888.0	0.0965
17	7.25	2898.4	0.1927
18	7.25	2899.6	0.2053
19	7.26	2904.3	0.1901
20	7.27	2905.8	0.2410
21	7.28	2912.9	0.1330
22	7.34	2933.9	0.8544
23	7.35	2938.2	0.4783



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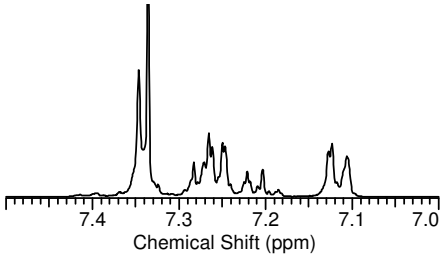
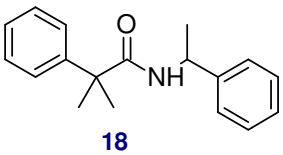


Table of Peaks

No.	(ppm)	(Hz)	Height
1	21.92	2205.1	0.2837
2	27.25	2741.1	0.3055
3	27.34	2749.5	0.2872
4	47.26	4753.2	0.2348
5	48.94	4922.2	0.2940
6	77.00	7744.6	0.9930
7	77.32	7776.6	1.0000
8	77.64	7808.4	0.9873
9	126.11	12684.0	0.8111
10	126.66	12739.6	0.8227
11	127.29	12802.5	0.4408
12	127.38	12811.4	0.4600
13	128.78	12952.3	0.8191
14	128.95	12969.4	0.8501
15	143.61	14444.3	0.1791
16	145.42	14626.3	0.1716
17	176.77	17779.2	0.1730

No.	(ppm)	Annotation
1	77.00	CHLOROFORM-d



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