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−Electronic Supplementary Information−

Mukaiyama aldol reaction of *in situ* generated nitrosocarbonyl compounds: selective C–N bond formation and N–O bond cleavage in one-pot for α-amination of ketones

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General Procedures

All non-aqueous reactions were carried out under an atmosphere of nitrogen in flame-dried glassware and were stirred using a magnetic stir plate. All reactions were carried out using anhydrous solvent unless otherwise noted. Anhydrous pyridine, CH_3CN, and CH_2Cl_2 were dried over calciumhydride. Dry THF was prepared by distilling over sodium ketyl. The CuCl is purchased from Sigma-Aldrich Company.

All reactions were monitored by thin layer chromatography (TLC) on WhatmanPartisil® K6F TLC plates (silica gel 60 Å, 0.25 mm thickness) and visualized using a UV lamp (366 or 254 nm) or by use of one of the following visualization reagents: PMA: 10 g phosphomolybdic acid/ 100 mL ethanol; $KMnO_4$: 0.75 g potassium permanganate, 5 g K_2CO_3, / 100 mL water. Products were isolated by column chromatography (Merck silica gel 100-200μm). Yields refer to chromatographically and spectroscopically homogenous materials unless noted otherwise. ^{13}C and ^{1}H NMR spectra were recorded on a Bruker 400 or Bruker 500 MHz spectrometers. Chemical shift values (δ) are reported in ppm and calibrated to the residual solvent peak $CDCl_3$ δ = 7.2600 ppm for ^{1}H, δ = 77.16 for ^{13}C; or calibrated to tetramethylsilane (δ = 0.00). All NMR spectra were recorded at ambient temperature (290 K) unless otherwise noted. ^{1}H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constant, integration). The following abbreviations are used to indicate multiplicities: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sext, sextet; sept, septet; m, multiplet; dd, doublet of doublet; dt, doublet of triplet; dq, doublet of quartet; td, triplet of doublet; tt, triplet of triplet; dq, doublet of quartet; br, broad; app, apparent.

Infrared spectra were recorded on a Thermo Nicolet iS10 FT spectrometer. Mass spectra were recorded by electron spry ionization (ESI) method on a Q-TOF Micro with lock spray source. The crystal data were collected and integrated using a BrukerAxs kappa apex2 CCD diffractometer, with graphite monochromated Mo-Kα radiation.

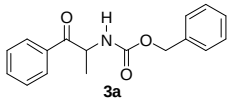
The silyl enol ethers were synthesized following literature procedures published previously and were purified by silica gel column chromatography or distillation (*Angew. Chem. Int. Ed.* **2008**, *47*, 3795; *Angew. Chem. Int. Ed.* **2012**, *51*, 1942). *N*-Boc-hydroxylamine, *N*-Cbz-hydroxylamine, *N*-Fmoc-hydroxylamine, and *N*-Troc-hydroxylamine were synthesized following literature procedures (*J. Org. Chem.* **2007**, *72*, 5587; *J. Am. Chem. Soc.***2011**, *133*, 10430). The

chiral menthol substituted hydroxamic acid was prepared according to protocol developed by Kibayashi et *al*. (*J. Org. Chem.* **1998**, *63*, 8397).

General procedure for *N*-selective nitrosocarbonyl Mukaiyama aldol reaction:

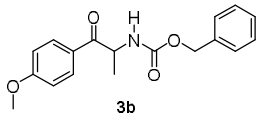
CuCl (20 mol%) was taken in a 16x100 mm oven dried test tube equipped with a magnetic stir. The test tube was capped with a septum and kept under vacuum for 10 min and then purged with nitrogen. Dry CH_3CN (1.5 mL) and pyridine (10 mol%) were added. After 1h stirring at room temperature, silyl enol ether (0.15, mmol, 1.0 equiv.) and 1 mL dry CH_3CN were added to the mixture. The nitrogen gas was replaced using oxygen balloon and then a solution of hydroxamic acid (1.3 equiv.) in CH_3CN (1.5 mL) was added slowly *via* syringe pump for a period of 12h. After the addition, the reaction mixture was allowed to stir for additional 7h at room temperature. The reaction mixture was transfer to a pear shape flask after dilution with CH_2Cl_2 and the solvent was evaporated to dryness. The crude reaction mixture was loaded directly onto silica gel column and purified to provide pure nitrosocarbonyl aldol product **3**.

Reaction can also be performed under open air instead of using oxygen balloon, however, slightly diminished yield was observed.



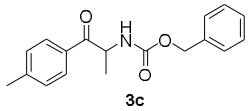
3a

3a: Compound **3a** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (42 mg, 98%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.97 (d, *J* = 7.48 Hz, 2H), 7.62-7.58 (m, 1H), 7.51-7.47 (m, 2H), 7.37-7.29 (m, 5H), 5.88 (d, *J* = 5.72 Hz, 1H), 5.39-5.31 (m, 1H), 5.13 (s, 2H), 1.44 (d, *J* = 7.08 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 199.0, 155.8, 136.6, 134.1, 134.0, 129.0, 128.8, 128.7, 128.3, 128.2, 67.0, 51.8, 20.1; HRMS (TOF MS ES$^+$) $C_{17}H_{17}NO_3Na^+$ m/z (%) = 306.12 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3344, 2979, 2361, 1735, 1687, 1595, 1505, 1450, 1347, 1221, 1058.



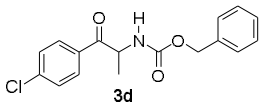
3b

3b: Compound **3b** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (43 mg, 91.0%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.96 (d, *J* = 8.80 Hz, 2H), 7.36-7.30 (m, 5H), 6.95 (d, *J* = 8.8 Hz, 2H), 5.91 (d , *J* = 6.96 Hz, 1H), 5.33-5.25 (m, 1H), 5.12 (s, 2H), 3.87 (s, 3H), 1.43 (d, *J* = 7.04 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.4, 164.3, 155.8, 136.6, 131.2, 128.6, 128.2 (2×C), 126.9, 114.2, 66.9, 55.7, 51.3, 20.4; HRMS (TOF MS ES$^+$) $C_{18}H_{19}NO_4Na^+$ m/z (%) = 336.12 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3608, 3347, 2965, 2937, 1796, 1721, 1677, 1600, 1511, 1454, 1262, 1232, 1166, 1027.



3c

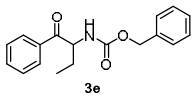
3c: Compound **3c** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (40 mg, 90%) as waxy solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.87 (d, *J* = 8.0Hz,2H), 7.36-7.30 (m, 5H), 7.29-7.27 (m, 2H), 5.88 (d, *J* = 6.36 Hz, 1H), 5.35-5.28 (m, 1H), 5.13 (s, 2H), 2.42 (s, 3H), 1.43 (d, *J* = 7.04 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.6, 155.8, 145.0, 136.6, 131.6, 129.7, 129.0, 128.7, 128.2 (2×C), 66.9, 51.7, 21.8, 20.3; HRMS (TOF MS ES$^+$) $C_{18}H_{19}NO_3H^+$ m/z (%) = 298.14 ([M+H]$^+$, 100%).



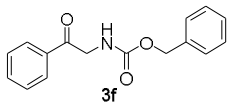
3d

3d: Compound **3d** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (46 mg, 96%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.91 (d, *J* = 8.48 Hz, 2H), 7.47 (d, *J* = 8.60 Hz, 2H), 7.36-7.25 (m, 5H), 5.79 (d, *J* = 6.83 Hz, 1H), 5.33-5.25 (m, 1H), 5.12 (s , 2H), 1.42 (d, *J* = 7.12 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.9, 155.7, 140.6, 136.5, 132.5, 130.2, 129.4, 128.7, 128.3, 128.2, 67.1, 51.7,

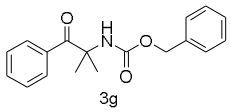
19.9; HRMS (TOF MS ES$^+$) $C_{17}H_{16}ClNO_3H^+$ m/z (%) = 318.76 ([M+H]$^+$, 100%); IR(cm^{-1}): 3342, 2979, 2361, 2333, 1735, 1688, 1590, 1503, 1450, 1401, 1346, 1220, 1091, 1059.



3e: Compound **3e** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (46 mg, 96%) as waxy solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.97 (d, *J* = 7.52 Hz, 2H), 7.62-7.58 (m, 1H), 7.50-7.47 (m, 2H), 7.37-7.30(m, 5H), 5.83 (d, *J* = 7.36 Hz, 1H), 5.37-5.31 (m, 1H), 5.13 (s, 2H), 2.05-1.97 (m, 1H), 1.71-1.61 (m, 1H), 0.88 (t, *J* = 7.44 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.9, 156.1, 136.6, 134.7, 133.9, 129.0, 128.7 (2×C), 128.3, 128.2, 67.0, 56.7, 26.7, 9.1; HRMS (TOF MS ES$^+$) $C_{18}H_{19}NO_3H^+$ m/z (%) = 298.14 ([M+H]$^+$, 100%).

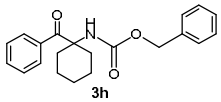


3f: Compound **3f** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (37 mg, 92%) as waxy solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.96 (d, *J* = 7.52 Hz, 2H), 7.61 (t, *J* = 7.44 Hz,1H), 7.51-7.47 (m, 2H), 7.40-7.30 (m, 5H), 5.83 (s, 1H), 5.16 (s, 2H), 4.72 (d, *J* =4.4, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 194.1, 156.4, 136.5, 134.5, 134.2, 129.0, 128.7, 128.3, 128.2, 128.0, 67.2, 48.0; HRMS (TOF MS ES$^+$) $C_{16}H_{15}NO_3Na^+$ m/z (%) = 292.09 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3304, 2361, 1731, 1693, 1607, 1534, 1470, 1390, 1328, 1214, 1010.

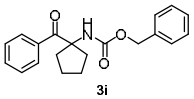


3g: Compound **3g** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (40 mg, 90%) as white solid. ^{1}H NMR (400 MHz,

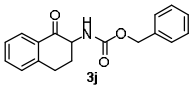
$CDCl_3$): δ = 7.94 (d, *J* = 7.6 Hz, 2H), 7.48 (t, *J* = 7.32 Hz,1H), 7.39-7.35 (m, 2H), 7.27-7.25 (m, 3H), 7.17 (s, 2H), 5.64 (s, 1H), 4.95 (s, 2H), 1.67 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 201.7, 154.8, 136.5, 135.7, 132.1, 128.7, 128.6, 128.3, 128.2, 128.1, 66.6, 61.1, 26.1; HRMS (TOF MS ES^+) $C_{18}H_{19}NO_3H^+$ m/z (%) = 298.14 ($[M+Na]^+$, 100%); IR(cm^{-1}): 3349, 2929, 2858, 1710, 1517, 1452, 1380, 1272, 1167, 1082.



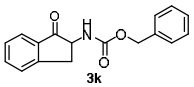
3h: Compound **3h** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (38 mg, 74 %) as white solid. ^1H NMR (400 MHz, $CDCl_3$): δ = 7.88 (d, *J* = 6.56 Hz, 2H), 7.44-7.43 (m, 1H), 7.32-7.26 (m, 5H), 7.11 (s, 2H), 5.34-5.25 (m,1H), 4.91 (s, 2H), 2.19-2.16 (m, 2H), 1.98-1.92 (m, 2H), 1.68-1.61 (m, 3H), 1.50-1.47 (m, 2H), 1.33-1.30 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 202.8, 154.7, 136.9, 136.4, 131.6, 128.8, 128.6, 128.3, 128.1, 66.8, 63.7, 32.8, 25.2, 21.6; HRMS (TOF MS ES^+) $C_{21}H_{23}NO_3H^+$ m/z (%) = 338.17 ($[M+H]^+$, 100%); IR(cm^{-1}): 3339, 3060, 3034, 2957, 2874, 1788, 1694, 1589, 1519, 1450, 1267, 1112, 1016.



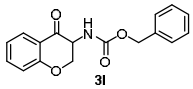
3i: Compound **3i** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (34 mg, 70%) as white solid. ^1H NMR (500 MHz, $CDCl_3$): δ = 7.87-7.77 (m, 2H), 7.47-7.46 (m, 1H), 7.36 (t, *J* = 5.28, 2H), 7.25-7.24 (m, 3H), 7.08-7.03 (m, 2H), 5.41 (s, 1H), 4.87 (s, 2H), 2.52 (s, 2H), 1.98-1.96 (m, 2H), 1.80 (s, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 201.4, 155.0, 136.4, 131.8, 128.5, 128.1, 127.9, 70.09, 66.6, 37.9, 24.8; HRMS (TOF MS ES^+) $C_{20}H_{21}NO_3H^+$ m/z (%) = 324.15 ($[M+H]^+$, 100%); IR(cm^{-1}): 3338, 3060, 2957, 2874, 1788, 1694, 1519, 1499, 1321, 1267, 1113, 1017.



3j: Compound **3j** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (38 mg, 86%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.01 (dd, J^1 = 7.84 Hz, J^2 = 1.92 Hz, 1H), 7.51 (td, J^1 = 7.52 Hz, J^2 = 1.32 Hz, 1H), 7.38-7.30 (m, 6H), 7.27-7.25 (m, 1H), 5.97 (brs , 1H), 5.15 (s , 2H), 4.50-4.44 (m, 1H), 3.24-3.20 (m, 1H), 3.02 (dq, J^1 = 4.00 Hz, J^2 = 2.45 Hz, 1H), 2.79 (d, J = 11.0 Hz, 1H), 1.94 (qd, J^1 = 17.40 Hz, J^2 = 4.40 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 195.5, 156.3, 143.9, 136.5, 134.2, 131.5, 129.0, 128.7, 128.3 (2×C), 127.8, 126.9, 67.0, 58.1, 31.1, 28.5; HRMS (TOF MS ES$^+$) $C_{18}H_{17}NO_3Na^+$ m/z (%) = 318.12 ([M+Na]$^+$, 100%);IR(cm^{-1}): 3376, 2970, 2364, 1730, 1690, 1533, 1364, 1171.

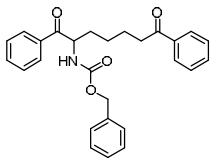


3k: Compound **3k** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→15% EtOAc : hexane) to provide pure compound (39 mg, 91%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.78 (d, J = 7.56 Hz, 1H), 7.63 (t, J = 7.36 Hz, 1H), 7.46-7.36 (m, 7H), 5.47 (brs, 1H), 5.14 (s , 2H), 4.40 (brs, 1H), 3.73 (dd, J^1 = 16.08 Hz, J^2 = 7.6 Hz, 1H), 3.07-3.01 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 202.8, 156.6, 151.3, 136.3, 135.9, 134.7, 128.7, 128.4, 128.3, 128.1, 126.8, 124.5, 67.3, 57.5, 35.0; HRMS (TOF MS ES$^+$) $C_{17}H_{15}NO_3Na^+$ m/z (%) = 304.08 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3321, 2930, 2361, 1730, 1609, 1536, 1457, 1262, 1058.



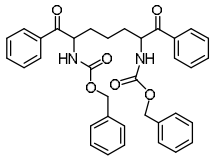
3l: Compound **3l** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (39 mg, 86%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.87 (dd, J^1 = 1.58 Hz, J^2 = 7.92 Hz, 1H), 7.53-7.49 (m, 1H), 7.38-7.32 (m, 5H), 7.06-7.02 (m,1H), 6.99 (d, J = 8.4 Hz , 1H), 5.72 (s, 1H), 5.15 (s, 2H), 4.95-4.91 (m, 1H), 4.75-

4.70 (m, 1H), 4.06 (dd, J^1 = 13.32 Hz, J^2 = 10.62 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.1, 161.9, 156.2, 136.8, 136.1, 128.8, 128.5, 128.4, 127.6, 121.9, 119.6, 118.1, 69.7, 67.5, 54.3; HRMS (TOF MS ES$^+$) $C_{17}H_{15}NO_4Na^+$ m/z (%) = 320.09 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3304, 2361, 1693, 1607, 1470, 1390, 1328, 1214, 1147, 1010.



3m

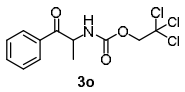
3m: Compound **3m** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→25% EtOAc : hexane) to provide pure compound (64 mg, 99%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.97 (d, J = 7.48 Hz, 2H), 7.91-7.89 (m, 2H), 7.60 (t, J = 7.40 Hz, 1H), 7.56-7.41 (m, 5H), 7.36-7.30 (m, 5H), 5.81 (d, J = 7.96 Hz, 1H), 5.38 (td, J^1 = 7.72 Hz, J^2 = 4.38 Hz, 1H), 5.12 (s, 2H), 2.91-2.89 (m, 2H), 2.03-1.94 (m, 1H), 1.80-1.59 (m, 3H), 1.51-1.45 (m, 1H), 1.42-1.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 199.9, 198.9, 156.1, 137.0, 136.5, 134.5, 134.0, 133.1, 129.0, 128.7 (2×C), 128.6, 128.2 (2×C), 128.1, 67.0, 55.6, 38.3, 33.6, 24.8, 23.9; HRMS (TOF MS ES$^+$) $C_{27}H_{27}NO_4H^+$ m/z (%) = 430.20 ([M+H]$^+$, 100%); IR(cm^{-1}): 3348, 3062, 2941, 2863, 1718, 1685, 1590, 1510, 1451, 1354, 1324, 1224, 1058.



3n

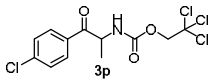
3n: Compound **3n** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→25% EtOAc : hexane) to provide pure compound (82 mg, 95%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.91-7.89 (m, 4H), 7.60-7.56 (m, 2H), 7.46 (dd, J^1 = 12.84 Hz, J^2 = 7.44 Hz, 4H), 7.36-7.30 (m, 10H), 5.82 (d, J = 7.68 Hz, 1H), 5.73 (d, J = 7.68 Hz, 1H), 5.30-5.28 (m, 2H), 5.14-5.00 (m, 4H), 1.83-1.26 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.6, 197.5, 155.2, 155.1, 135.4, 135.3, 133.4 (2×C), 132.8, 127.9, 127.6, 127.5 (2×C), 127.1, 127.0, 66.0, 54.1,

54.0, 32.0, 31.7, 19.7, 19.6; HRMS (TOF MS ES$^+$) $C_{35}H_{34}N_2O_6Na^+$ m/z (%) = 601.23 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3338, 3059, 2949, 2846, 1691, 1518, 1449, 1352, 1229, 1057.



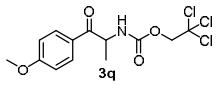
3o

3o: Compound **3o** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10 % EtOAc : hexane) to provide pure compound (43 mg, 87%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.99-7.97 (m, 2H), 7.62 (tt, J^1 = 6.72 Hz, J^2 = 1.24 Hz, 1H), 7.53-7.49 (m, 2H), 6.12 (d, J = 6.8 HZ ,1H), 5.38-5.31 (m, 1H), 4.79-4.71 (m, 2H), 1.48 (d, J = 7.08 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.4, 154.0, 134.2, 133.9, 129.1, 128.9, 95.6, 74.8, 52.1, 20.0; HRMS (TOF MS ES$^+$) $C_{12}H_{12}NO_3Cl_3Na^+$ m/z (%) = 345.97 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3420, 2985, 1740, 1690, 1599, 1506, 1450, 1220, 1112, 1046.



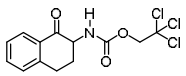
3p

3p: Compound **3p** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (46 mg, 85%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.94-7.90 (m, 2H), 7.50-7.47 (m, 2H), 6.08 (d, J = 7.20 Hz, 1H), 5.33-5.26 (m , 1H), 4.78-4.70 (m, 2H), 1.46 (d, J = 7.12 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.3, 154.0, 140.8, 132.2, 130.2, 129.5, 95.5, 74.8, 52.0, 19.9.



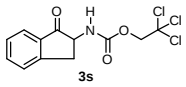
3q

3q: Compound **3q** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (47 mg, 89%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.96 (d, J = 8.92 Hz, 2H), 6.97 (d, J = 8.94 Hz, 2H), 6.16 (d, J = 7.12 Hz, 1H), 5.29 (quint, J = 7.12 Hz, 1H), 4.78-4.70 (m, 2H), 3.88 (s, 3H), 1.47 (d, J = 7.08 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 196.8, 164.4, 154.0, 131.3, 126.6, 114.3, 95.6, 74.7, 55.7, 51.7, 20.4.



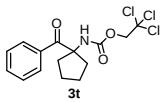
3r

3r: Compound **3r** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (49 mg, 96%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.03 (dd, J^1 = 7.84 Hz, J^2 = 0.76 Hz, 1H), 7.53 (td, J^1 = 7.52 Hz, J^2 = 1.36 Hz, 1H), 7.34 (t, J = 7.6 1H), 7.27 (d, J = 7.8 Hz, 1H), 6.21 (d, J = 2.1 Hz, 1H), 4.76 (q, J = 11.88 Hz, 2H), 4.49 (dt, J^1 = 13.6 Hz, J^2 = 4.92 Hz, 1H), 3.26-3.21 (m, 1H), 3.08-3.02 (m, 1H), 2.84-2.79 (m, 1H), 2.01-1.97 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 195.0, 154.5, 143.8, 134.4, 131.4, 129.0, 127.9, 127.1, 95.6, 74.8, 58.1, 30.7, 28.4.



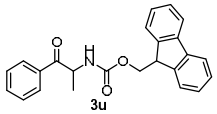
3s

3s: Compound **3s** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (40 mg, 82%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.79 (d, J = 7.68 Hz, 1H), 7.65 (td, J^1 = 7.56 Hz, J^2 = 1.12 Hz, 1H), 7.47 (d, J = 7.72 Hz, 1H), 7.44-7.40 (m, 1H), 5.74 (d, J = 4.08 Hz, 1H), 4.79-4.72 (m, 2H), 4.46-4.41 (m, 1H), 3.76 (dd, J^1 = 16.64 Hz, J^2 = 8.08 Hz, 1H), 3.07 (dd, J^1 = 16.72 Hz, J^2 = 5.44 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 202.2, 154.8, 151.2, 136.0, 134.6, 128.3, 126.9, 124.6, 95.4, 74.9, 57.5, 34.8.



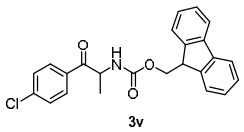
3t

3t: Compound **3t** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (40 mg, 76%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.85 (d, J = 7.4 Hz, 2H), 7.45 (t, J = 7.32 Hz, 1H), 7.38-7.34 (m, 2H), 5.59 (s, 1H), 4.50 (s, 2H), 2.60-2.53 (m, 2H), 2.04-1.98 (m, 2H), 1.85-1.82 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 201.0, 153.2, 136.2, 131.9, 128.6, 128.2, 95.5, 74.2, 71.1, 37.8, 24.8.



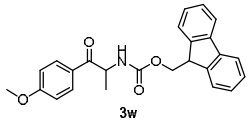
3u

3u: Compound **3u** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (55 mg, 99%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.90 (d, *J* = 7.56 Hz, 2H), 7.68 (d, *J* =7.52 Hz, 2H), 7.52 (t, *J* = 7.30 Hz, 3H), 7.43-7.39 (m, 2H), 7.31 (t, *J* = 7.36 Hz, 2H), 7.23 (t, *J* = 7.36 Hz, 2H), 5.84 (d, *J* = 6.36 Hz, 1H), 5.31-5.24 (m, 1H), 4.33-4.31 (m, 2H), 4.15 (t, *J* = 6.96 Hz, 1H), 1.37 (d, *J* = 7.05 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 199.1, 155.8, 144.1, 144.0, 141.4, 134.0, 129.0, 128.8, 127.8, 127.2, 125.3, 124.8, 120.2, 120.1, 67.1, 51.7, 47.3, 20.1; HRMS (TOF MS ES$^+$) $C_{24}H_{21}NO_3Na^+$ m/z (%) = 394.14 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3417, 3340, 3064, 2954, 2932, 1717, 1684, 1595, 1504, 1450, 1378, 1347, 1321, 1225, 1102.



3v

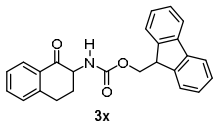
3v: Compound **3v** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (50 mg, 82%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.93 (d, *J* = 8.52 Hz, 2H), 7.76 (d, *J* = 7.52 Hz, 2H), 7.61 (d, *J* = 7.12 Hz, 2H), 7.48 (d, *J* = 8.52 Hz, 2H), 7.40 (t, *J* = 7.44 Hz, 2H), 7.31 (t, *J* = 7.44 Hz, 2H) 5.84 (d, *J* = 7.36 Hz, 1H), 5.34-5.27 (m, 1H), 4.41-4.40 (m, 2H), 4.25-4.21 (m, 1H), 1.44 (d, *J* = 7.08 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 198.0, 155.8, 144.0, 143.9, 141.4, 140.6, 132.4, 130.2, 129.4, 127.9, 127.2, 125.2, 120.1, 67.2, 51.7, 47.3, 20.0.



3w

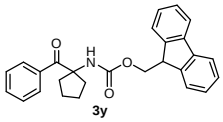
3w: Compound **3w** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (56 mg, 93%) as waxy solid. ^{1}H NMR (400 MHz,

$CDCl_3$): δ = 7.98 (d, *J* = 8.84 Hz, 2H), 7.76 (d, *J* = 7.48 Hz, 2H), 7.62 (d, *J* = 7.36 Hz, 2H),7.42-7.38 (m, 2H), 7.31 (t, *J* = 7.44 Hz, 2H), 6.97 (d, *J* = 8.88 Hz, 2H), 5.95 (d, *J* = 7.36 Hz, 1H), 5.35-5.27 (m, 1H), 4.40-4.38 (m, 2H), 4.24 (t, *J* = 7.16 Hz, 1H), 3.88 (s, 3H), 1.45 (d, *J* = 7.04 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 197.5, 164.3, 155.8, 144.1, 144.0, 141.4, 131.2, 127.8, 127.2, 126.9, 125.3, 120.1, 114.3, 67.1, 55.7, 51.4, 47.3, 20.5.



3x

3x: Compound **3x** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (57 mg, 98 %) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.03 (d, *J* = 7.28 Hz, 1H), 7.76 (d, *J* = 7.24 Hz, 2H), 7.64 (d, *J* = 6.76 Hz, 2H), 7.53-7.50 (m, 1H), 7.43-7.39 (m, 2H), 7.35-7.31 (m , 3H), 7.27-7.25 (m, 1H), 6.03 (brs, 1H), 4.51-4.41 (m, 3H), 4.28-4.24 (m, 1H), 3.29-3.22 (m, 1H), 3.05-3.01 (m, 1H), 2.81-2.79 (m, 1H), 2.01-1.95 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 195.6, 156.3, 144.1, 144.0, 143.9, 141.5, 134.2, 131.5, 129.0, 127.9, 127.8, 127.2, 127.0, 125.3, 120.1, 67.2, 58.1, 47.4, 31.1, 28.5.



3y

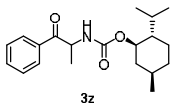
3y: Compound **3y** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (46 mg, 75%) as waxy solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.87 (d, *J* = 6.76 Hz, 1H), 7.73 (d, *J* = 7.28 Hz, 2H), 7.41-7.23 (m, 10H), 5.30 (s, 1H), 4.21 (d, *J* = 6.56 Hz, 2H), 3.95-3.92 (m, 1H), 2.50-2.33 (m, 2H), 1.96-1.93 (m, 2H), 1.85-1.78 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 201.3, 155.0, 143.9, 141.4, 131.8, 130.1, 128.5, 128.1, 127.8, 127.1, 125.0, 120.0, 70.9, 66.6, 47.3, 37.8, 24.8.

Gram scale synthesis of compound 3a:

CuCl (0.075 mmol, 74 mg, 20 mol%) was taken in a 250 ml oven dried round bottom flask equipped with a magnetic stir. The flask was capped with a septum and kept under vacuum

for 10 min and then purged with nitrogen. Under nitrogen atmosphere dry CH_3CN (40 mL) and pyridine (0.03mmol, 30 µL, 10 mol%) were added via syringe and stirred for 1h at room temperature. After that, substrate silyl enol ether **1a** (4 mmol, 1.06g, 1equiv.) and 30 ml CH_3CN were added via syringe. The flask was carefully purged with oxygen and a balloon with oxygen was placed. Then solution of hydroxamic acid **2a** (4.81 mmol, 0.87 g, 1.3 equiv.) in CH_3CN (30 mL) was added slowly via syringe pump during a period of 12 h. After the addition, the reaction was further stirrer for 7 h. The solvent was evaporated to dryness and the crude reaction mixture was loaded directly onto silica gel column and purified to provide pure nitrosocarbonyl aldol product **3a** (1.11 g, 97% yield).

Diastereoselective nitrosocarbonyl Mukaiyama aldol reaction:



3z

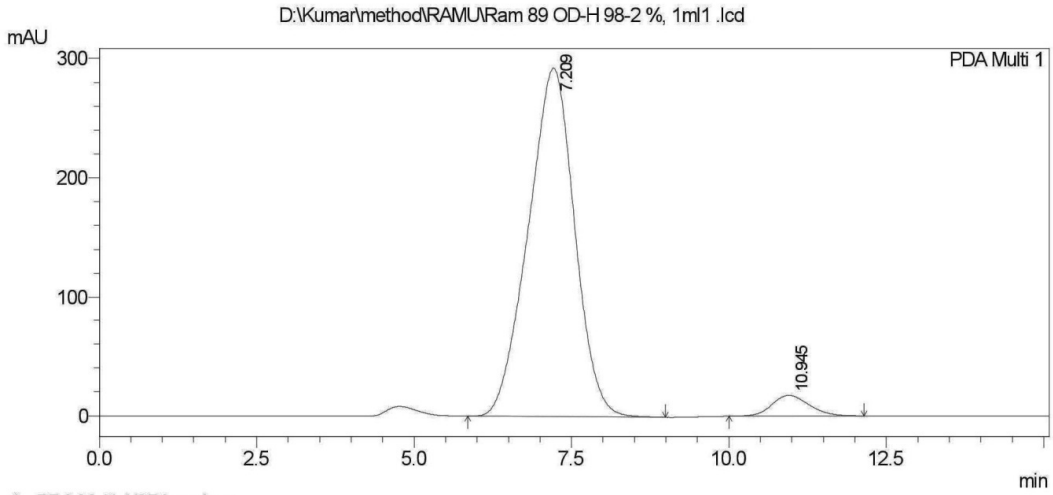
3z: Compound **3z** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol described above and purified by silica gel column chromatography (1→10% EtOAc : hexane) to provide pure compound (41 mg, 81%, d.r. = 19:1) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.98-7.97 (m, 2H), 7.62-7.58 (m, 1H), 7.51-7.47 (m, 2H), 5.67 (d, *J* = 6.56 Hz,1H), 5.34-5.30 (m, 1H), 4.56-4.55 (m, 1H), 2.07 (d, *J* = 11.72 Hz, 1H) 1.92-1.89 (m, 1H), 1.69-1.62 (m, 2H), 1.49-1.47 (m, 1H), 1.46 (d, *J* = 7.08 Hz, 3H), 1.35-1.29 (m, 1H), 1.07-1.00 (m, 2H), 0.91-0.86 (m, 7H), 0.76 (d, *J* = 6.86, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 199.4, 156.0, 134.4, 134.0, 129.1, 128.9, 75.1, 51.8, 47.7, 41.7, 34.6, 31.7, 26.4, 23.8, 22.3, 21.0, 20.2, 16.7; HRMS (TOF MS ES$^+$) $C_{20}H_{29}NO_3H^+$ m/z (%) = 332.22 ([M+H]$^+$, 100%); IR(cm^{-1}): 3333, 2952, 2866, 1687, 1590, 1502, 1452, 1375, 1296, 1224, 1089, 1051.

==== Shimadzu LCsolution Analysis Report ====

D:\Kumar\method\RAMU\Ram 89 OD-H 98-2 %, 1ml1 .lcd

Acquired by	: Admin
Sample Name	: Ram 89 OD-H 98-2 %, 1ml 1
Sample ID	: Ram 89 OD-H 98-2 %, 1ml 1
Vail #	:
Injection Volume	: 20 uL
Data File Name	: Ram 89 OD-H 98-2 %, 1ml1 .lcd
Method File Name	: OD-H+ 2IPA+1ml.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 4/9/2015 11:49:38 PM
Data Processed	: 4/10/2015 12:14:23 AM

<Chromatogram>



1 PDA Multi 1/254nm 4nm

PeakTable

PDA Ch1 254nm 4nm

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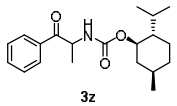
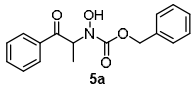


3z

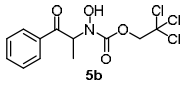
General procedure for *N*-selective nitrosocarbonyl Mukaiyama aldol reaction of TMS- and TBS-substituted silyl enol ethers:

CuCl (20 mol%) was taken in a 16x100 mm oven dried test tube equipped with a magnetic stir. The test tube was capped with a septum and kept under vacuum for 10 min and then purged with nitrogen. Dry CH_3CN (1.5 mL) and pyridine (10 mol%) were added. After 1 h stirring at room temperature, silyl enol ether **4** (0.19 mmol, 1.0 equiv.) and 1 mL dry CH_3CN were added to the mixture. The nitrogen gas was replaced using oxygen balloon and then a solution of hydroxamic acid (1.3 equiv.) in CH_3CN (1.5 mL) was added slowly *via* syringe pump for a period of 12 h. After the addition, the reaction mixture was allowed to stir for additional 7 h at room temperature. The reaction mixture was transfer to a pear shape flask after dilution with CH_2Cl_2 and the solvent was evaporated to dryness. The crude reaction mixture was loaded directly onto silica gel column and purified to provide pure nitrosocarbonyl aldol product **5**.



5a

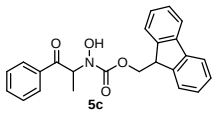
5a: Compound **5a** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→25% EtOAc : hexane) to provide pure compound (43 mg, 76%) as yellow waxy solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.80-7.78 (m, 2H), 7.51-7.47 (m, 1H), 7.37-7.34 (m, 2H), 7.26-7.15 (m, 5H), 6.64 (brs, 1H), 5.59 (q, *J* = 7.26 Hz, 1H), 5.10 (s, 2H), 1.48 (d, *J* = 7.28 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.8, 157.3, 135.9, 134.4, 134.0, 129.0, 128.7 (2×C), 128.4, 128.2, 68.3, 59.5, 14.5; HRMS (TOF MS ES$^+$) $C_{17}H_{17}NO_4Na^+$ m/z (%) = 322.10 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3346, 2940, 1699, 1597, 1449, 1415, 1293, 1228, 1122.



5b

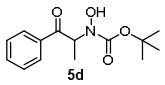
5b: Compound **5b** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→25% EtOAc : hexane) to provide pure compound (43 mg, 66%) as yellow waxy solid. ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.92 (d, *J* = 7.36 Hz, 2H), 7.64-7.60 (m, 1H), 7.51-7.47 (m, 2H), 5.76-5.74 (m, 1H), 4.80 (s, 2H), 1.64 (d, *J* = 7.08 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ =

200.5, 155.3, 134.3, 134.1, 129.1, 128.8, 95.1, 75.5, 59.8, 14.8; HRMS (TOF MS ES^+) $C_{12}H_{12}NO_4Cl_3Na^+$ m/z (%) = 361.97 ($[M+Na]^+$, 100%); IR(cm^{-1}): 3353, 2945, 1722, 1696, 1597, 1449, 1228, 1129, 1051.



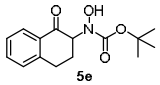
5c

5c: Compound **5c** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→15% EtOAc : hexane) to provide pure compound (62 mg, 84 %) as yellow waxy solid. ^{1}H NMR (400 MHz, $CDCl_3$); δ = 7.74 (d, *J* = 7.6 Hz, 2H), 7.61 (dd, J^1 = 12.32 Hz, J^2 = 7.56 Hz, 2H), 7.52-7.46 (m, 3H), 7.38-7.34 (m, 2H), 7.30-7.23 (m, 2H), 7.19-7.13 (m, 2H), 5.46 (s, 1H), 4.40 (d, *J* = 6.8 Hz, 2H), 4.16 (t, *J* = 6.76 Hz, 1H), 1.44 (d, *J* = 7.28 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.7, 157.2, 143.7, 143.6, 141.4 (2×C), 134.3, 134.0, 128.9, 128.8, 127.9, 127.3, 127.2, 125.2, 125.1, 120.1, 120.0, 68.2, 59.5, 47.2, 14.5; HRMS (TOF MS ES^+) $C_{24}H_{21}NO_4Na^+$ m/z (%) = 410.13 ($[M+Na]^+$, 100%); IR(cm^{-1}): 3363, 3062, 2955, 1801, 1704, 1609, 1597, 1476, 1450, 1411, 1285, 1227, 1127, 1080.



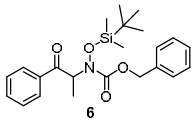
5d

5d: Compound **5d** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→20% EtOAc : hexane) to provide pure compound (30 mg, 59%) as yellow waxy solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.92-7.90 (m, 2 H), 7.59 (tt, J^1 = 7.40 Hz, J^2 = 1.2 Hz, 1H), 7.49-7.45 (m, 2 H), 5.54 (q, *J* = 7.27 Hz, 1H), 1.55 (d, *J* = 7.24 Hz, 3H), 1.45 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 200.8, 156.8, 134.8, 133.8, 128.9, 128.7, 82.5, 59.8, 28.3, 14.4; HRMS (TOF MS ES^+) $C_{14}H_{19}NO_4Na^+$m/z (%) = 288.12 ($[M+Na]^+$, 100%); IR(cm^{-1}): 3342, 2975, 2930, 1696, 1692, 1590, 1449, 1369, 1226, 1166, 1128. 1009.



5e

5e: Compound **5e** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→15% EtOAc : hexane) to provide pure compound (33 mg, 62 %) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.97 (dd, J^1 = 7.86 Hz, J^2 = 1.18 Hz, 1H), 7.43 (td, J^1 = 7.52 Hz, J^2 = 1.44 Hz, 1H), 7.25 (t, J = 7.6 Hz, 1H), 7.19 (d, J = 6.72 Hz, 1H), 6.05 (brs, 1H), 4.78 (d, J = 11.32 Hz, 1H), 3.15-3.10 (m, 1H), 3.04-2.98 (m, 1H), 2.49 (qd, J^1 =13.04 Hz, J^2 = 4.68 Hz, 1H), 2.37-2.31 (m, 1H), 1.45 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 194.7, 158.1, 144.1, 134.3, 132.0, 129.0, 127.9, 127.0, 82.6, 66.0, 29.1, 28.3, 27.7; HRMS (TOF MS ES$^+$) $C_{15}H_{19}NO_4Na^+$ m/z (%) = 300.12 ([M+Na]$^+$, 100%); IR(cm^{-1}): 3323, 2977, 1699, 1600, 1455, 1367, 1311, 1228, 1159.



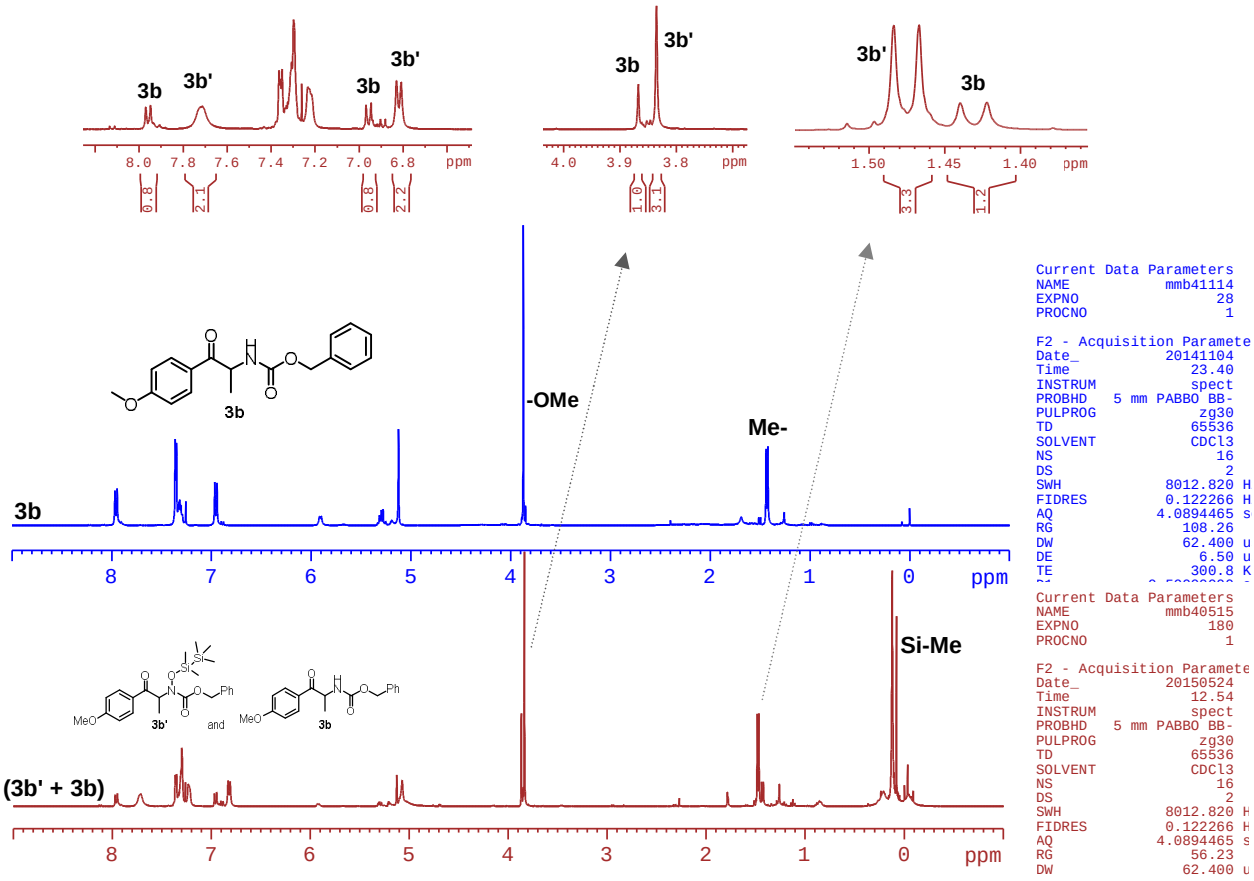
6

6: Compound **6** was prepared following general *N*-selective nitrosocarbonyl Mukaiyama aldol protocol described above and purified by silica gel column chromatography (1→5% EtOAc : hexane) to provide pure compound (72 mg, 91%) as oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.94-7.92 (m, 2H), 7.54-7.51 (m, 1H), 7.41-7.37 (m, 2H), 7.34-7.31 (m, 5H), 5.46 (q, J = 6.84 Hz, 1H), 5.20-5.13 (m, 2H), 1.49 (d, J = 6.84 Hz, 3H) 0.82 (s, 9H), -0.02 (s, 3H), -0.18 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 196.8, 158.7, 135.8, 135.6, 133.1, 128.8, 128.7, 128.6 (2×C), 68.5, 61.9, 25.9, 18.4, 13.0, -4.6, -4.7.

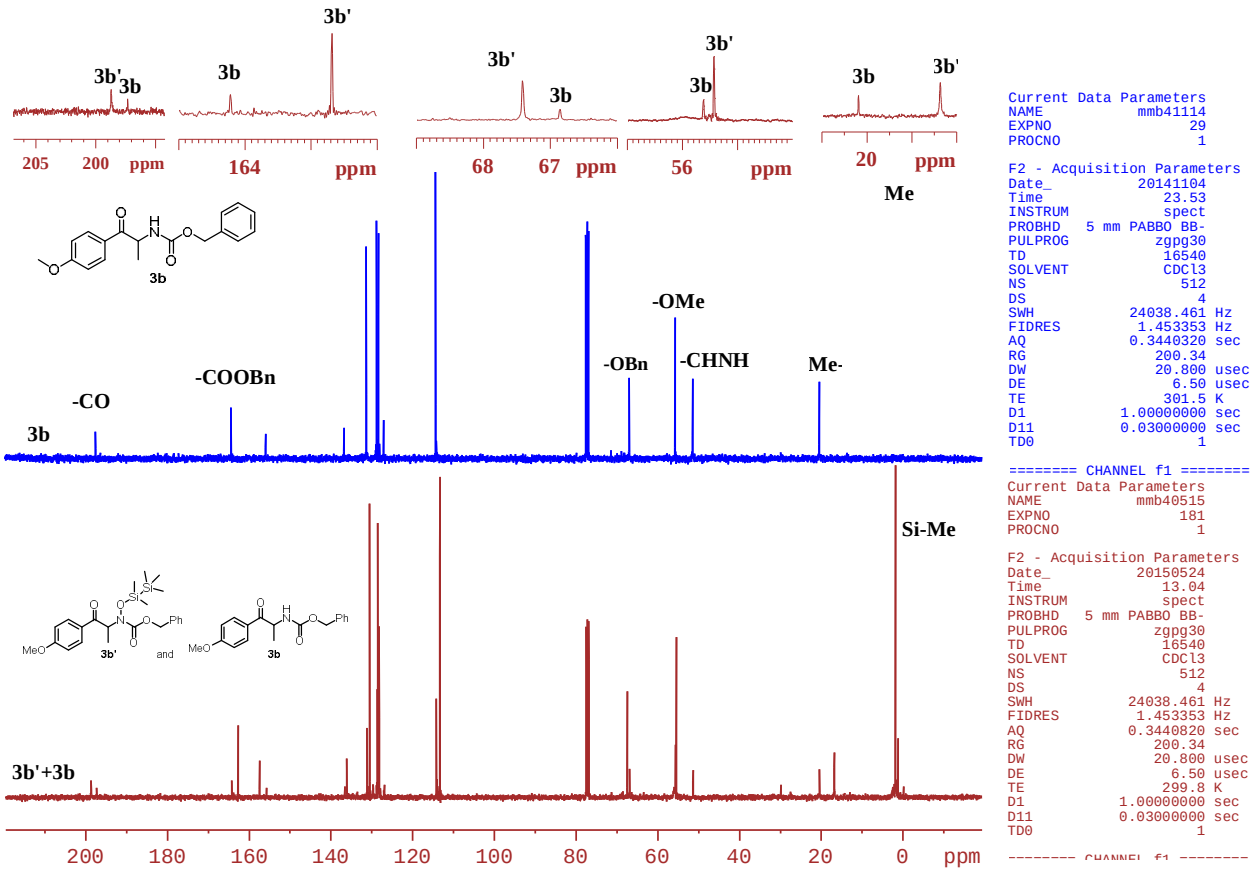
Identification of the intermediate 3b′:

CuCl (20 mol%) was taken in a 16x100 mm oven dried test tube equipped with a magnetic stir. The test tube was capped with a septum and kept under vacuum for 10 min and then purged with nitrogen. Dry THF (1.5 mL) and 2-ethyl-2-oxazoline (10 mol%) were added. After 1h stirring at 25 ^{o}C, silyl enol ether **1b** (0.15 mmol, 1.0 equiv.) and 1 mL dry THF were added to the mixture. The nitrogen gas was replaced using oxygen balloon and then a solution of hydroxamic acid **2a** (1.3 equiv.) in THF (1.5 ml) was added slowly *via* syringe pump for a period of 4 h.

After the addition, the reaction mixture was allowed to stir for additional thirty minutes at 25 ^{o}C. The reaction mixture was immediately transferred to a pear-shape flask after dilution with CH_2Cl_2 and the solvent was evaporated to dryness quickly. The crude reaction mixture was loaded directly onto celite column and purified rapidly with hexane and CH_2Cl_2. The ^{1}H and ^{13}C-NMR spectra confirmed the presence of 3:1 mixture of compounds **3b′** and **3b**.



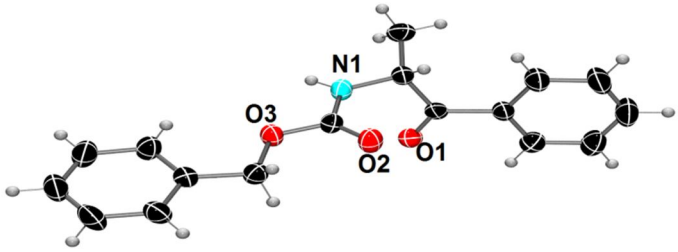
^{1}H NMR of (**3b′** + **3b**) was recorded after quick column through celite.



^{13}C NMR of (**3b′** + **3b**) was recorded after quick column through celite.

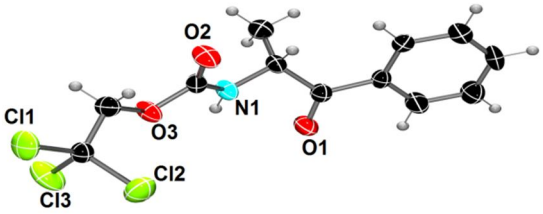
Crystallographic Experimental Section:

Crystal structure of compound **3a**:



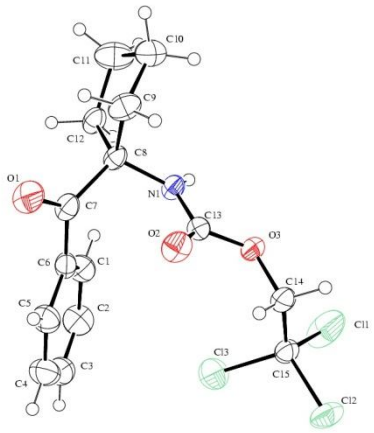
Crystal data	*Data collection*	*Refinement*
$C_{17}H_{17}NO_3$	Bruker kappa apex2 CCD Diffractometer	Refinement on F^2
M_r = 283.31	ω and φ scan	Least-squares matrix: full
Triclinic, *P*1	Absorption correction: multi-scan	$R[F^2 > 2\sigma(F^2)]$ = 0.066
a = 6.0589 (4) Å	*SADABS* (Bruker, 2012)	$wR(F^2)$ = 0.199
b = 8.0710 (5) Å	T_{min} = 0.922, T_{max} = 0.971	*S* = 1.10
c = 15.6647 (10) Å	9021 measured reflections	2516 reflections
α = 100.410 (4)°	2516 independent reflections	196 parameters
β = 96.485 (4)°	2008 reflections with $I > 2\sigma(I)$	0 restraints
γ = 93.141 (4)°	R_{int} = 0.179	Hydrogen site location: mixed
V = 746.38 (8) Å^3	θ_{max} = 25.0°, θ_{min} = 1.3°	H atoms treated by a mixture of independent and
Z = 2	*h* = −7→7	constrained refinement
F(000) = 300	*k* = −9→9	$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.3494P]$
D_x = 1.261 Mg m^{-3}	*l* = −17→18	where $P = (F_o^2 + 2F_c^2)/3$
Mo $K\alpha$ radiation, λ = 0.71073 Å		$(\Delta/\sigma)_{max} < 0.001$
Cell parameters from 2516 reflections		$\Delta\rho_{max}$ = 0.26 e Å^{-3}
θ = 1.3–27.5°		$\Delta\rho_{min}$ = −0.33 e Å^{-3}
μ = 0.09 mm^{-1}		Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
T = 296 K		Extinction coefficient: 0.049 (10)
Block, colourless		
0.30 × 0.25 × 0.10 mm		

Crystal structure of compound **3o**:



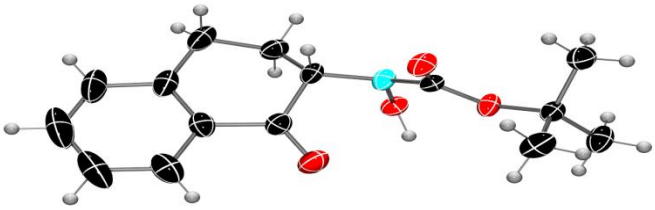
Empirical formula	C12 H12 Cl3 N O3	
Formula weight	324.58	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6581(5) Å	α= 101.560(3)°.
	b = 11.8588(8) Å	β= 104.761(2)°.
	c = 14.7395(10) Å	γ = 90.004(3)°.
Volume	1431.65(16) $Å^3$	
Z	4	
Density (calculated)	1.506 Mg/m^3	
Absorption coefficient	0.642 mm^{-1}	
F(000)	664	
Crystal size	0.300 x 0.300 x 0.250 mm^3	
Theta range for data collection	2.436 to 24.997°.	
Index ranges	-10<=h<=10, -14<=k<=14, -17<=l<=17	
Reflections collected	34468	
Independent reflections	34468 [R(int) = ?]	
Completeness to theta = 24.997°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8599 and 0.8291	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	34468 / 2 / 354	
Goodness-of-fit on F^2	0.965	
Final R indices [I>2sigma(I)]	R1 = 0.0615, wR2 = 0.1122	
R indices (all data)	R1 = 0.1316, wR2 = 0.1409	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.456 and -0.455 $e.Å^{-3}$	

Crystal structure of compound **3t**:

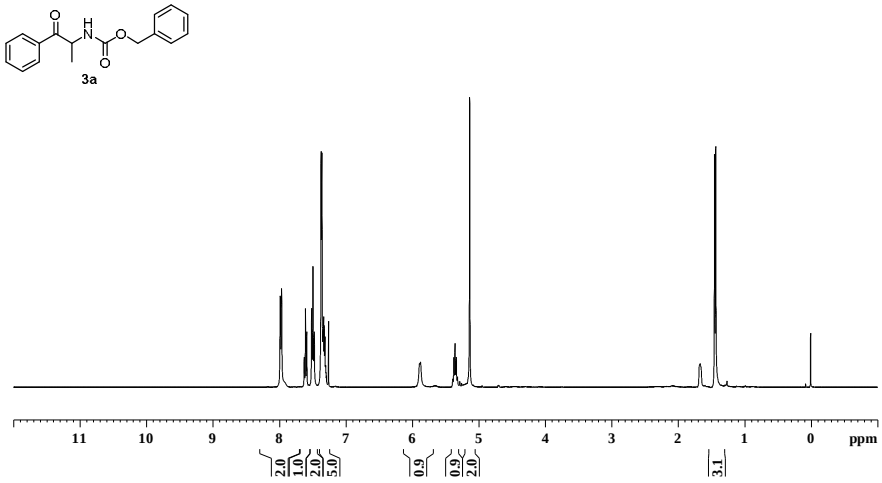


Crystal data	*Data collection*	*Refinement*
$C_{15}H_{16}Cl_3NO_3$	Bruker kappa apex2 CCD Diffractometer	Refinement on F_2
M_r = 364.64	ω and φ scan	Least-squares matrix: full
Triclinic, *P*1	Absorption correction: multi-scan	$R[F_2 > 2\sigma(F_2)]$ = 0.037
a = 6.0347 (2) Å	*SADABS* (Bruker, 2012)	$wR(F_2)$ = 0.090
b = 11.3911 (4) Å	T_{min} = 0.801, T_{max} = 0.882	*S* = 1.04
c = 13.0283 (4) Å	11909 measured reflections	2871 reflections
α = 67.611 (2)°	2871 independent reflections	203 parameters
β = 89.839 (2)°	2550 reflections with $I > 2\sigma(I)$	0 restraints
γ = 85.877 (2)°	R_{int} = 0.016	Hydrogen site location: mixed
V = 825.64 (5) Å$_3$	θ_{max} = 25.0°, θ_{min} = 1.7°	H atoms treated by a mixture of independent and
Z = 2	*h* = −7→7	constrained refinement
F(000) = 376	*k* = −13→13	$w = 1/[\sigma_2(F_o$
D_x = 1.467 Mg m$_{-3}$	*l* = −15→15	$_2) + (0.0317P)_2 + 0.5977P]$
Mo $K\alpha$ radiation, λ = 0.71073 Å		where $P = (F_o$
Cell parameters from 2871 reflections		$_2 + 2F_c$
θ = 1.7–27.2°		$_2)/3$
μ = 0.56 mm$_{-1}$		$(\Delta/\sigma)_{max} < 0.001$
T = 296 K		$\Delta\rho_{max}$ = 0.52 e Å$_{-3}$
Block, colourless		$\Delta\rho_{min}$ = −0.44 e Å$_{-3}$
0.25 × 0.22 × 0.10 mm		

Crystal structure of compound **5e**:



Crystal data	*Data collection*	*Refinement*
$C_{15}H_{19}NO_4$ M_r = 277.31 Orthorhombic, *Pca*2$_1$ *a* = 11.5083 (8) Å *b* = 13.3657 (9) Å *c* = 9.5834 (6) Å *V* = 1474.08 (17) Å^3 *Z* = 4 *F*(000) = 592 D_x = 1.250 Mg m^{-3} Mo *Kα* radiation, *λ* = 0.71073 Å Cell parameters from 2467 reflections *θ* = 1.5–25.5° *μ* = 0.09 mm^{-1} *T* = 296 K Block, pale-yellow 0.40 × 0.10 × 0.10 mm	Bruker kappa apex2 CCD Diffractometer *ω* and *φ* scan Absorption correction: multi-scan *SADABS* (Bruker, 2012) T_{min} = 0.880, T_{max} = 0.965 9969 measured reflections 2467 independent reflections 1741 reflections with $I > 2\sigma(I)$ R_{int} = 0.043 θ_{max} = 25.0°, θ_{min} = 1.5° *h* = −13→13 *k* = −15→15 *l* = −11→10	Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)]$ = 0.045 $wR(F^2)$ = 0.114 *S* = 1.01 2467 reflections 188 parameters 1 restraint Hydrogen site location: mixed H atoms treated by a mixture of independent and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.0972P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} < 0.001$ $\Delta\rho_{max}$ = 0.12 e Å^{-3} $\Delta\rho_{min}$ = −0.15 e Å^{-3} Absolute structure: Flack x determined using 610 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons and Flack (2004), Acta Cryst. A60, s61). Absolute structure parameter: 0.6 (10)

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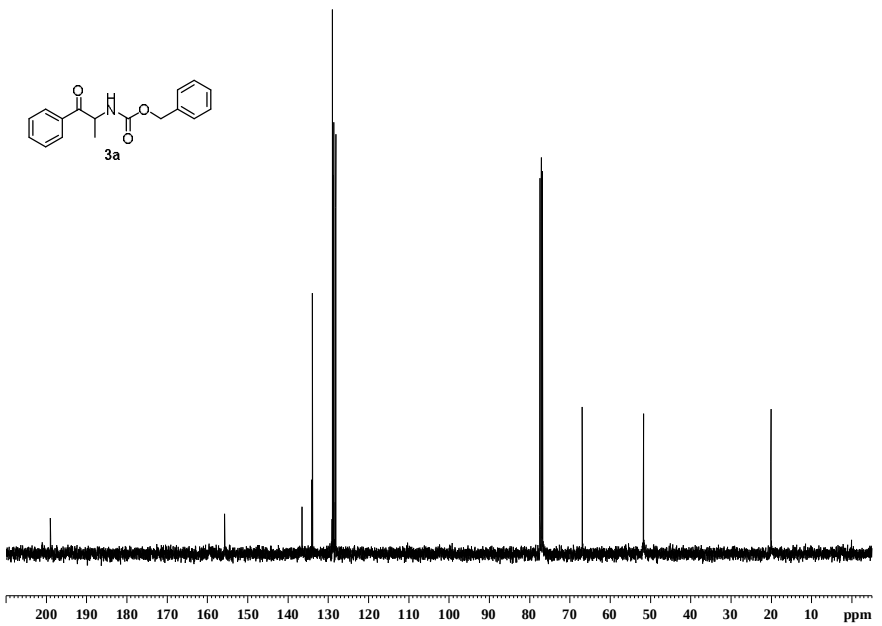


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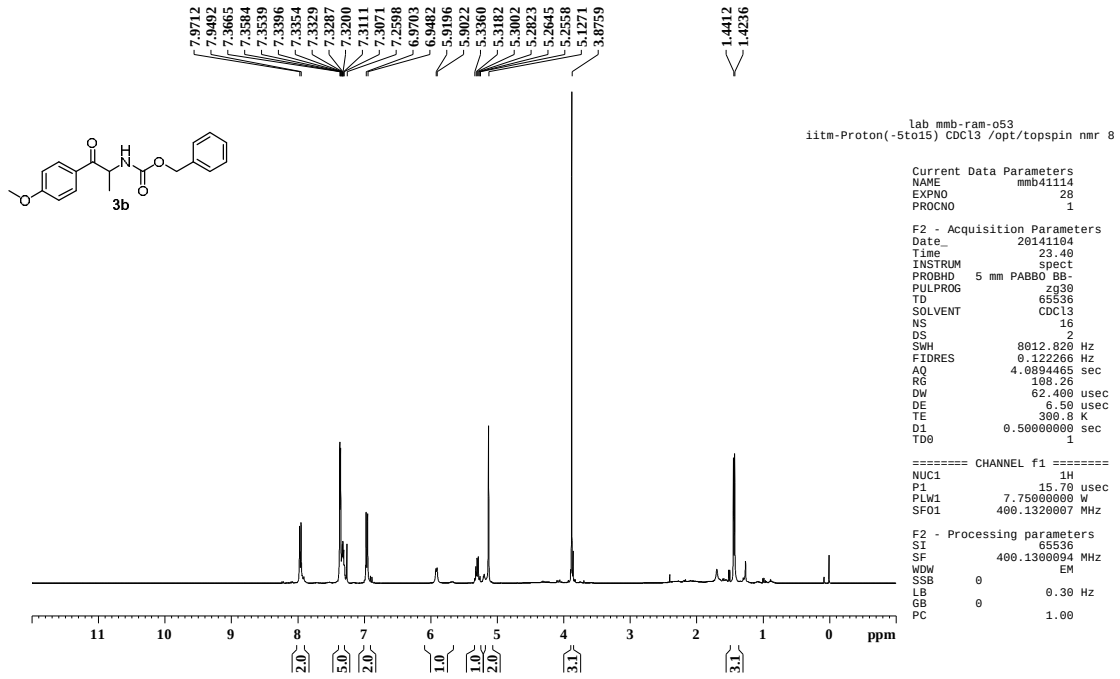
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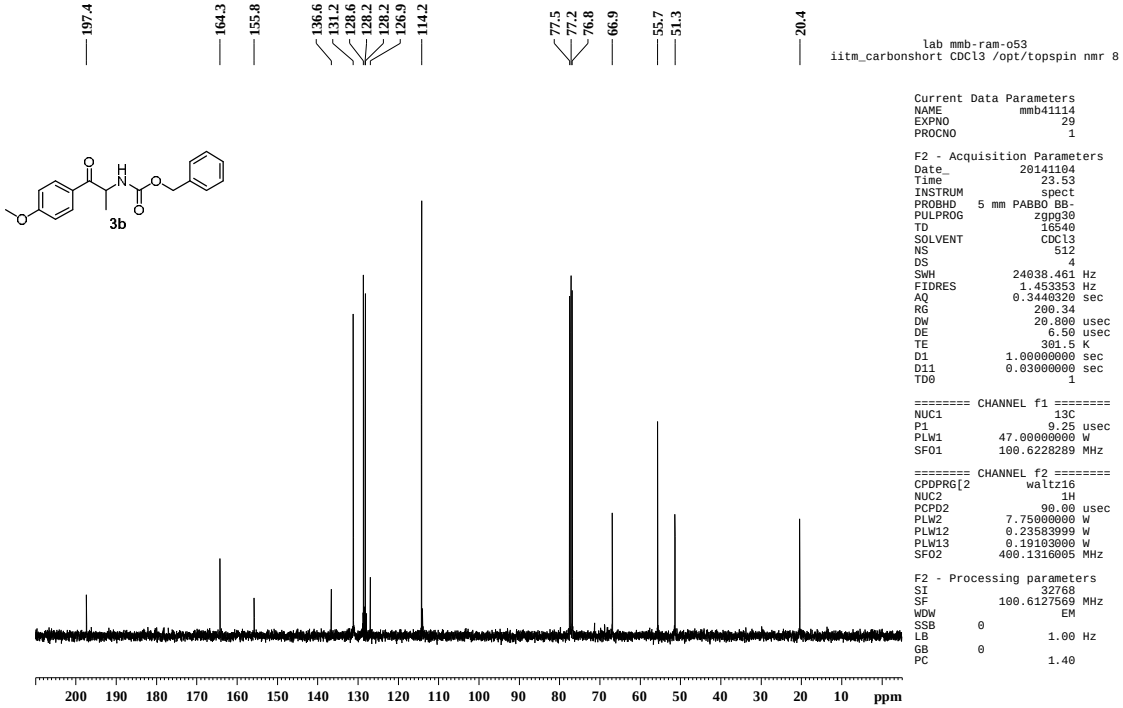
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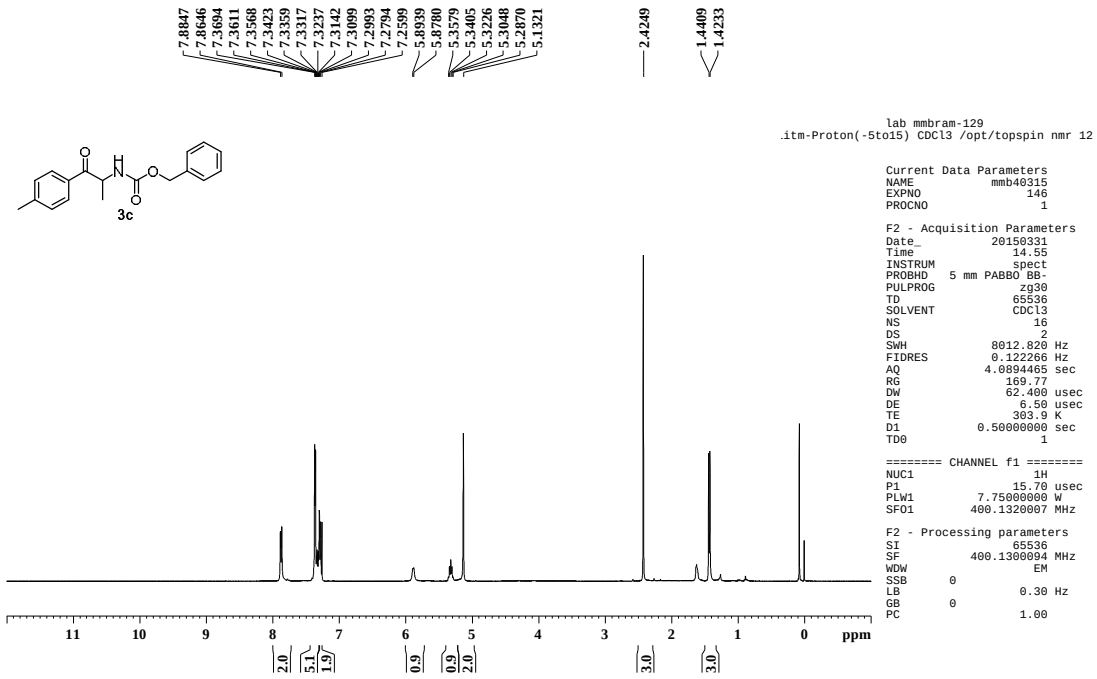
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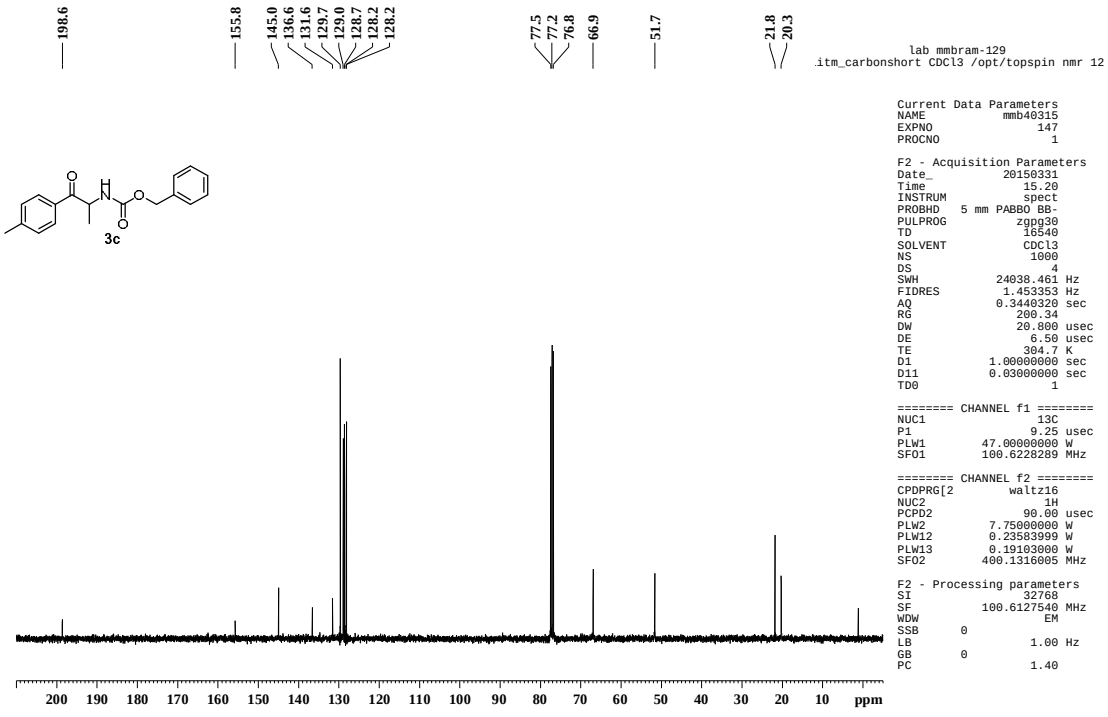
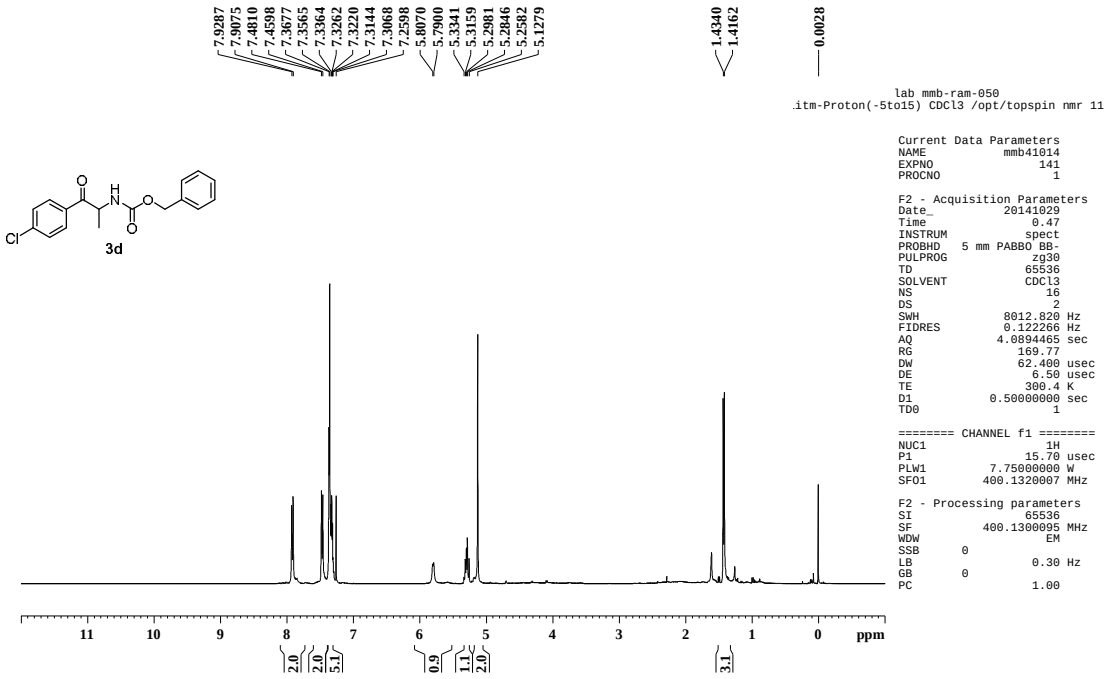
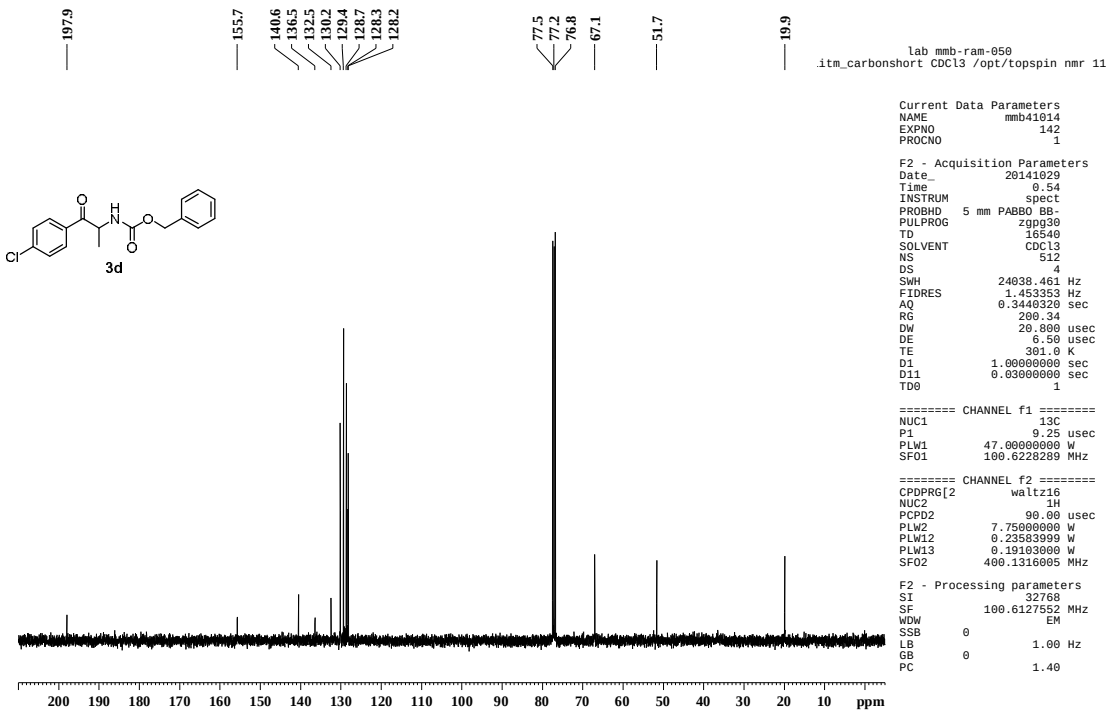
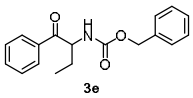
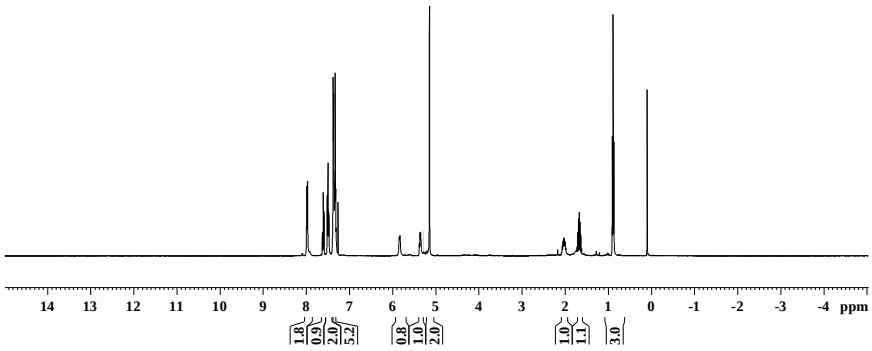
7.3423
7.3359
7.3317
7.3237
7.3142
7.3099
7.2993
7.2794
7.2599
5.8939
5.8780
5.3579
5.3405
5.3226
5.3048
5.2870
5.1321
2.4249
1.4409
1.4233
3c
lab mmbram-129
.itm-Proton(-5to15) CDCl3 /opt/topspin nmr 12
Current Data Parameters
NAME mmb40315
EXPNO 146
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150331
Time 14.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.77
DW 62.400 usec
DE 6.50 usec
TE 303.9 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.0 5.1 1.9 0.9 0.9 2.0 3.0 3.0


198.6
155.8
145.0
136.6
131.6
129.7
129.0
128.7
128.2
128.2
77.5
77.2
76.8
66.9
51.7
21.8
20.3
3c
lab mmbram-129
.itm_carbonshort CDCl3 /opt/topspin nmr 12
Current Data Parameters
NAME mmb40315
EXPNO 147
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150331
Time 15.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 1000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 304.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

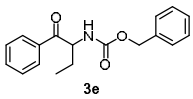

7.9287
7.9075
7.4810
7.4598
7.3677
7.3565
7.3364
7.3262
7.3220
7.3144
7.3068
7.2598
5.8070
5.7900
5.3341
5.3159
5.2981
5.2846
5.2582
5.1279
1.4340
1.4162
0.0028
lab mmb-ram-050
.itm-Proton(-5to15) CDCl3 /opt/topspin nmr 11
3d
Current Data Parameters
NAME mmb41014
EXPNO 141
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141029
Time 0.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.77
DW 62.400 usec
DE 6.50 usec
TE 300.4 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.0 2.0 5.1 0.9 1.1 2.0 3.1

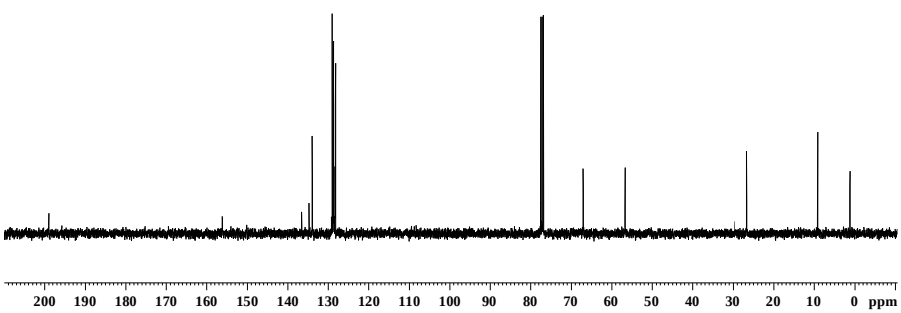

197.9
155.7
140.6
136.5
132.5
130.2
129.4
128.7
128.3
128.2
77.5
77.2
76.8
67.1
51.7
19.9
lab mmb-ram-050
.itm_carbonshort CDCl3 /opt/topspin nmr 11
3d
Current Data Parameters
NAME mmb41014
EXPNO 142
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141029
Time 0.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 301.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127552 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



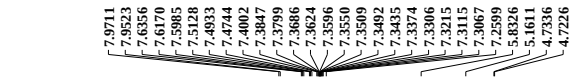


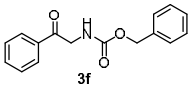

```
lab mmb-ram-126
oton(-5to15) CDCl3 /opt/topspin

Current Data Parameters
NAME            mmb40315
EXPNO                130
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150329
Time               23.40
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                95.73
DW              62.400 usec
DE               6.50 usec
TE              302.8 K
D1           0.50000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.70 usec
PLW1          7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                65536
SF          400.1300093 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```

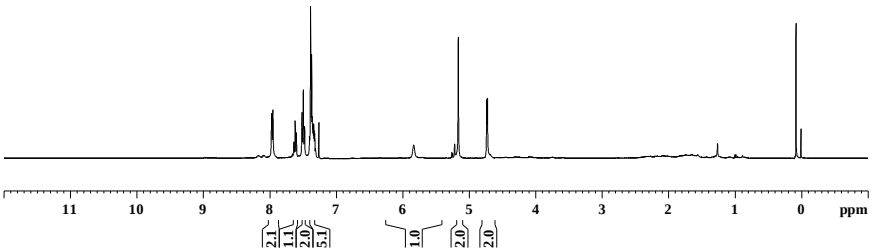




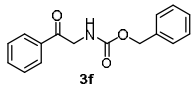

```
lab mmb-ram-126 re
n_carbonshort CDCl3 /opt/topspin nmr

Current Data Parameters
NAME            mmb4051
EXPNO               23
PROCNO               1

F2 - Acquisition Parame
Date_           2015052
Time               23.3
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg3
TD                 1654
SOLVENT           CDCl3
NS                   25
DS                    4
SWH            24038.46
FIDRES          1.45335
AQ             0.344032
RG                200.3
DW                20.80
DE                 6.5
TE                299.4
D1           1.0000000
D11          0.0300000
TD0                   1

======== CHANNEL f1 ===
NUC1                13
P1                 9.2
PLW1         47.0000000
SFO1        100.6228285

======== CHANNEL f2 ===
CPDPRG[2         waltz1
NUC2                1H
PCPD2            90.00
PLW2          7.7500000
PLW12         0.2358399
PLW13         0.1910300
SFO2        400.1316005

F2 - Processing paramet
SI                32768
SF           100.6127566
WDW                  EM
SSB       0
```

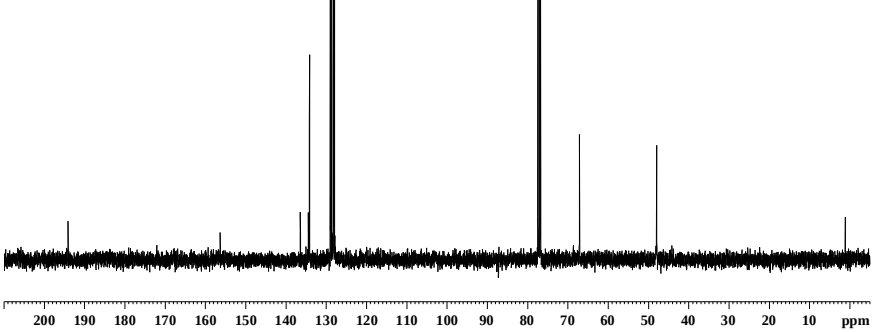




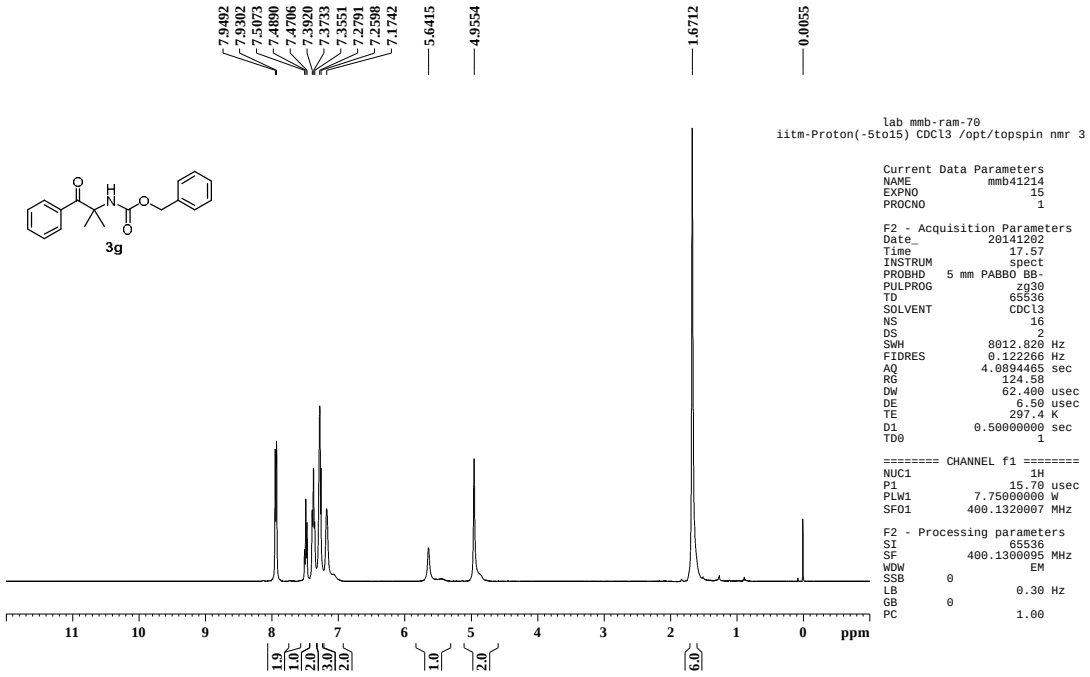


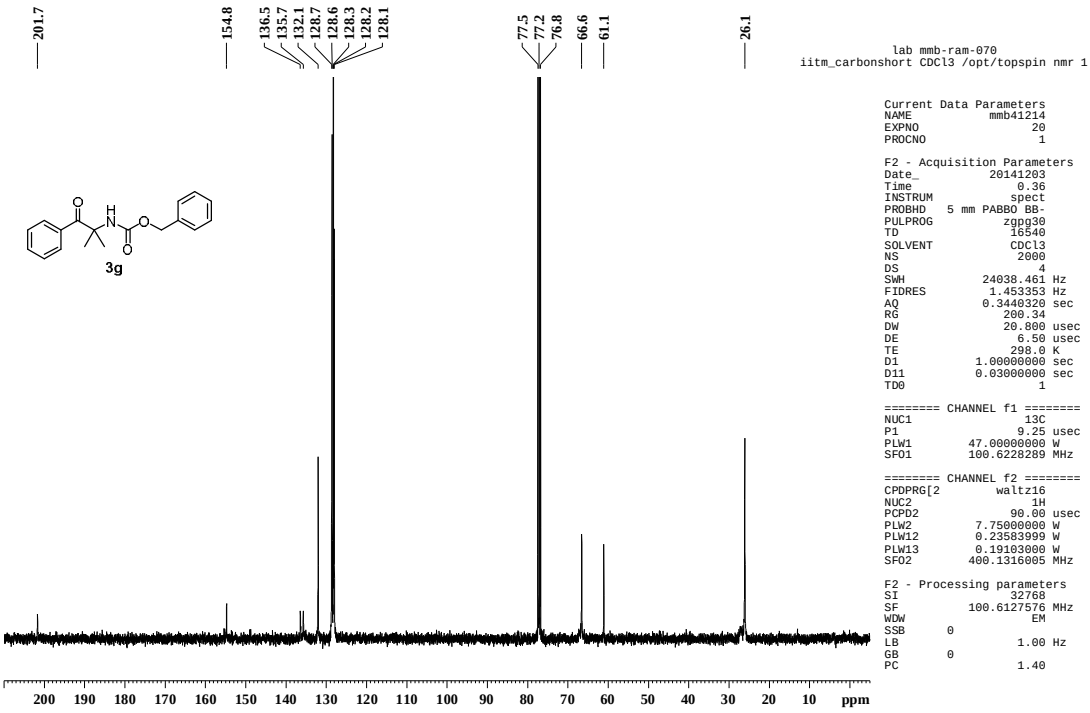

```
lab mmbram-067
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 3

Current Data Parameters
NAME            mmb41114
EXPNO                145
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141129
Time                11.41
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 138.85
DW                 62.400 usec
DE                  6.50 usec
TE                 298.5 K
D1            0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.70 usec
PLW1          7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300094 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

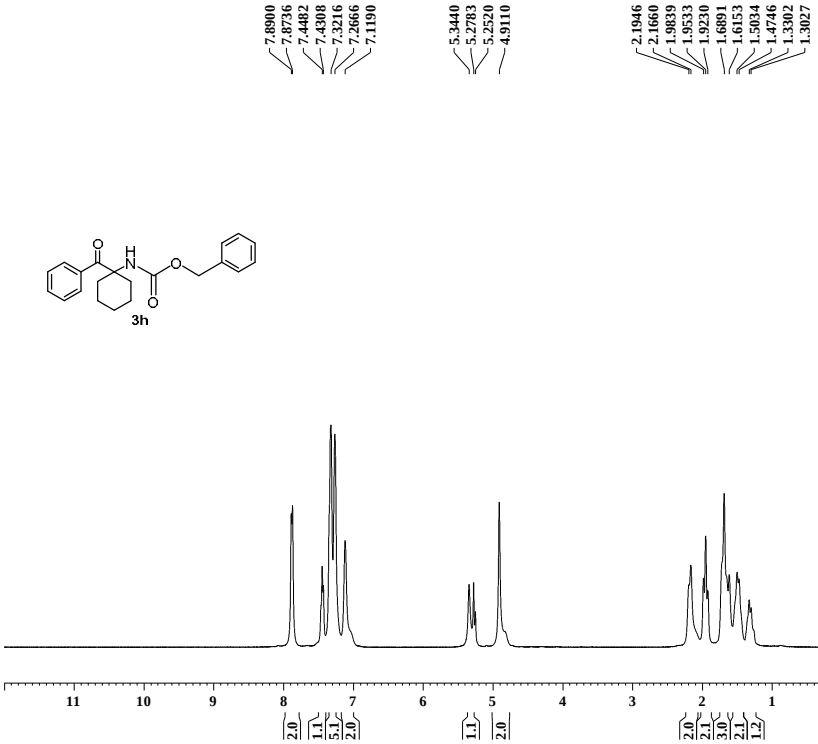




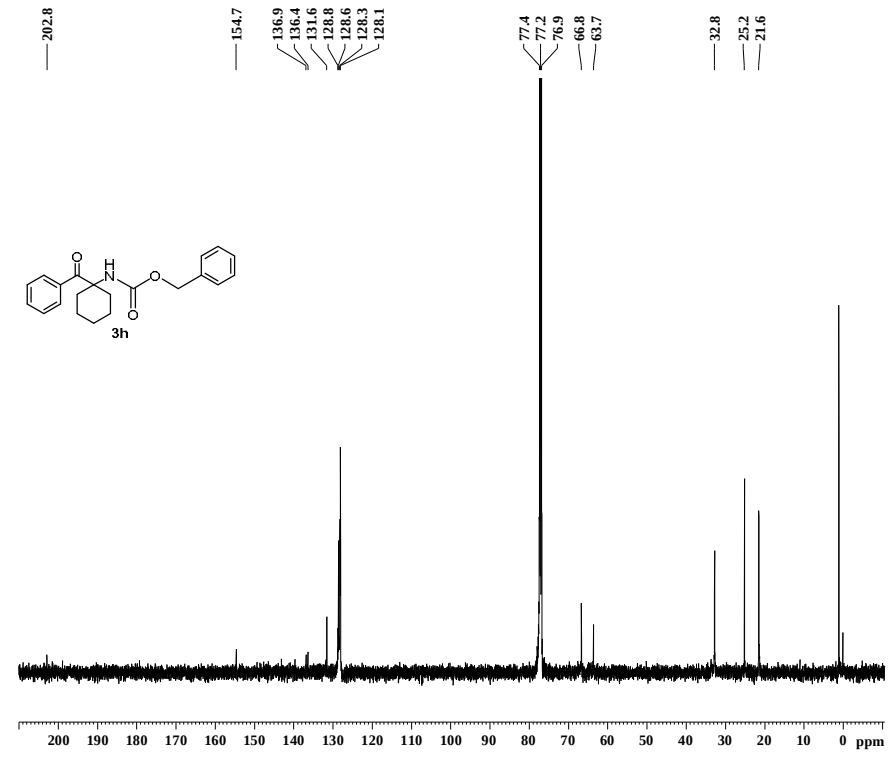

```
lab mmbram-067
iitm_carbonshort CDCl3 /opt/topspin nmr 3

Current Data Parameters
NAME            mmb41114
EXPNO                146
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141129
Time                11.48
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES          1.453353 Hz
AQ              0.3440320 sec
RG                 200.34
DW                 20.800 usec
DE                  6.50 usec
TE                 299.2 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.25 usec
PLW1         47.00000000 W
SFO1        100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2          7.75000000 W
PLW12         0.23583999 W
PLW13         0.19103000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127573 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


7.9492
7.9302
7.5073
7.4890
7.4706
7.3920
7.3733
7.3551
7.2791
7.2598
7.1742
5.6415
4.9554
1.6712
0.0055
3g
lab mmb-ram-70
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 3
Current Data Parameters
NAME mmb41214
EXPNO 15
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141202
Time 17.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 124.58
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.9 1.0 1.0 2.0 3.0 2.0 1.0 2.0 6.0

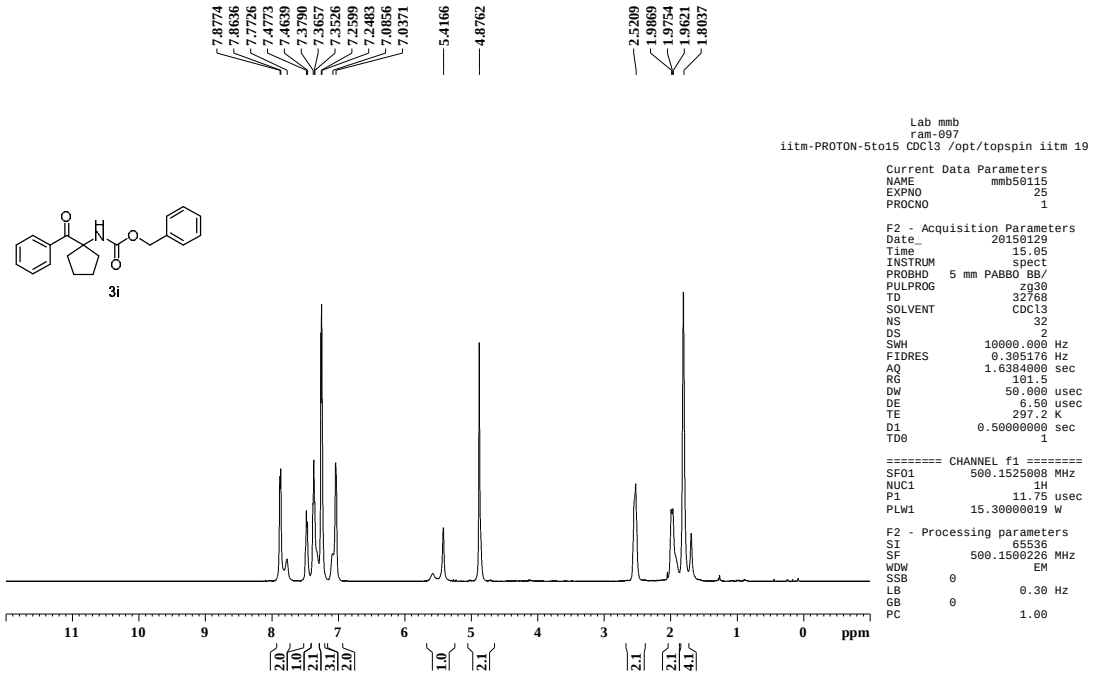

201.7
154.8
136.5
135.7
132.1
128.7
128.6
128.3
128.2
128.1
77.5
77.2
76.8
66.6
61.1
26.1
3g
lab mmb-ram-070
iitm_carbonshort CDCl3 /opt/topspin nmr 1
Current Data Parameters
NAME mmb41214
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141203
Time 0.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127576 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



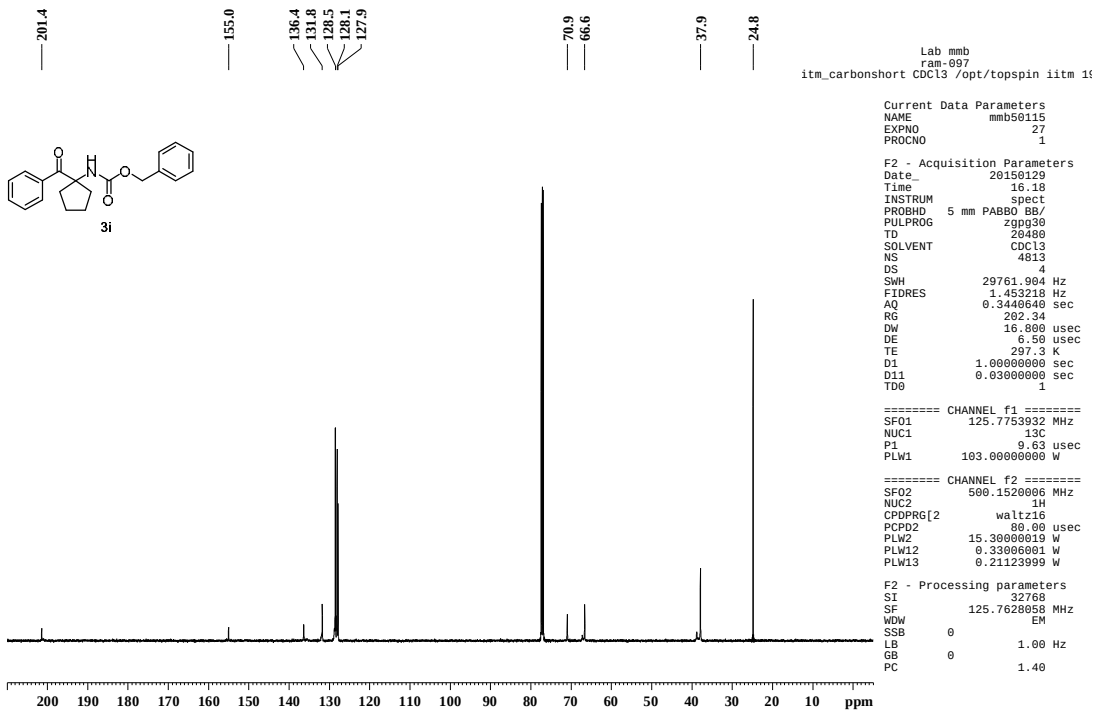

```
lab mmb-ram-095
roton(-5to15) CDCl3 /opt/topspin

Current Data Parameters
NAME            mmb40115
EXPNO                158
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150116
Time                5.31
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                153.13
DW                62.400 usec
DE                 6.50 usec
TE                301.2 K
D1            0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.70 usec
PLW1          7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300114 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



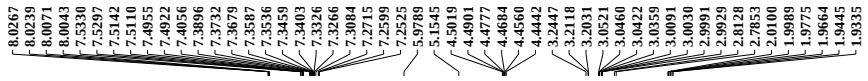

```
Lab mmb
ram-095
onshort CDCl3 /opt/topspir

Current Data Parameters
NAME            mmb50415
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150403
Time               19.52
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 20480
SOLVENT            CDCl3
NS                  8000
DS                     4
SWH            29761.904 Hz
FIDRES          1.453218 Hz
AQ              0.3440640 sec
RG                202.34
DW                16.800 usec
DE                 6.50 usec
TE                298.1 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7753932 MHz
NUC1                  13C
P1                  9.63 usec
PLW1        103.00000000 W

======== CHANNEL f2 ========
SFO2         500.1520006 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         15.30000019 W
PLW12         0.33006001 W
PLW13         0.21123999 W

F2 - Processing parameters
SI                 32768
SF          125.7628029 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

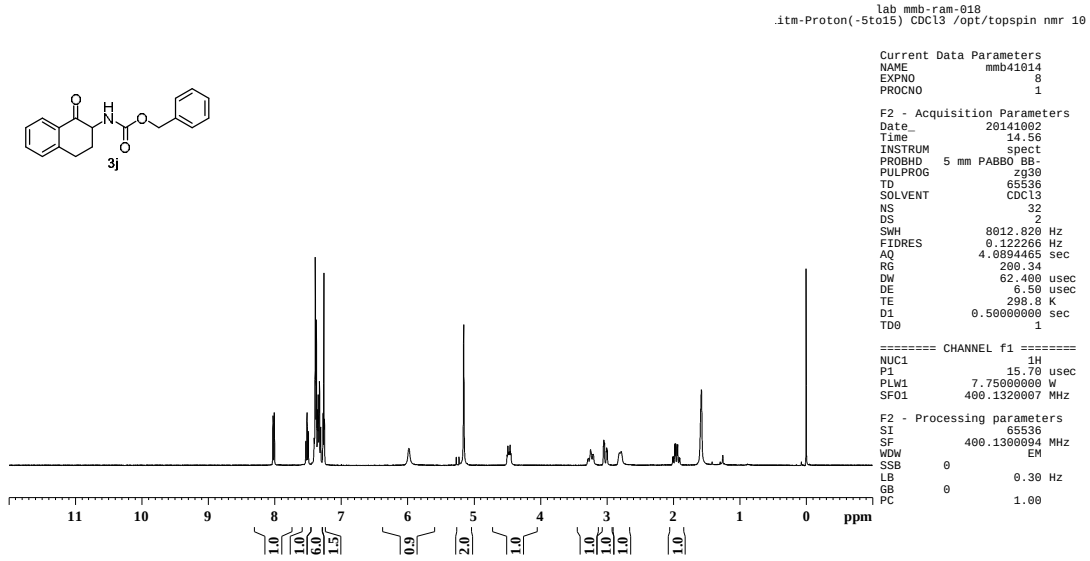


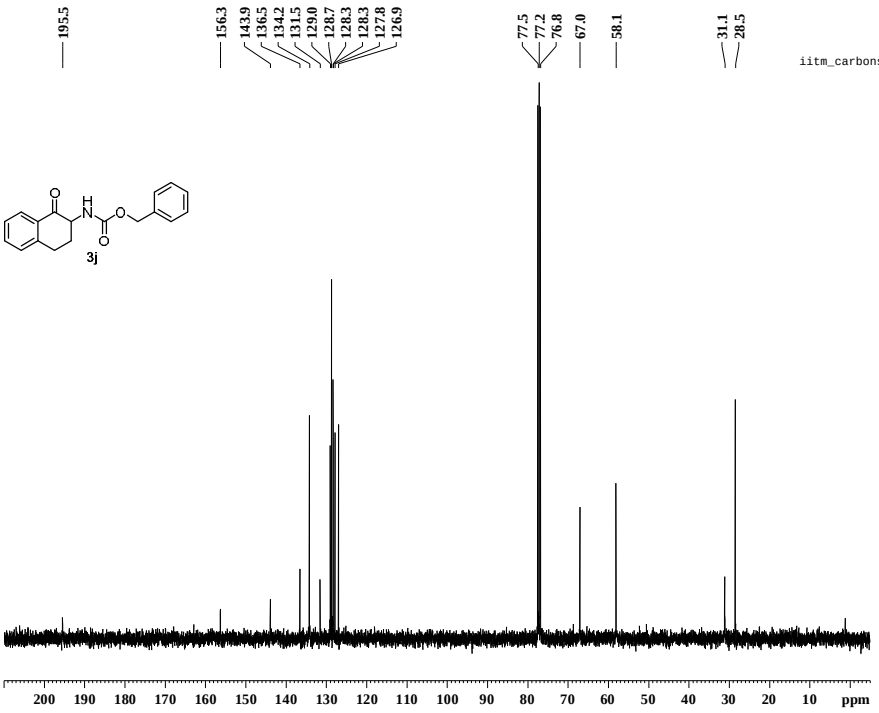

```
Lab mmb
ram-097
iitm-PROTON-5to15 CDCl3 /opt/topspin iitm 19

Current Data Parameters
NAME            mmb50115
EXPNO                 25
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150129
Time              15.05
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ            1.6384000 sec
RG                101.5
DW               50.000 usec
DE                6.50 usec
TE                297.2 K
D1           0.50000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         500.1525008 MHz
NUC1                 1H
P1                11.75 usec
PLW1        15.30000019 W

F2 - Processing parameters
SI                65536
SF           500.1500226 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```

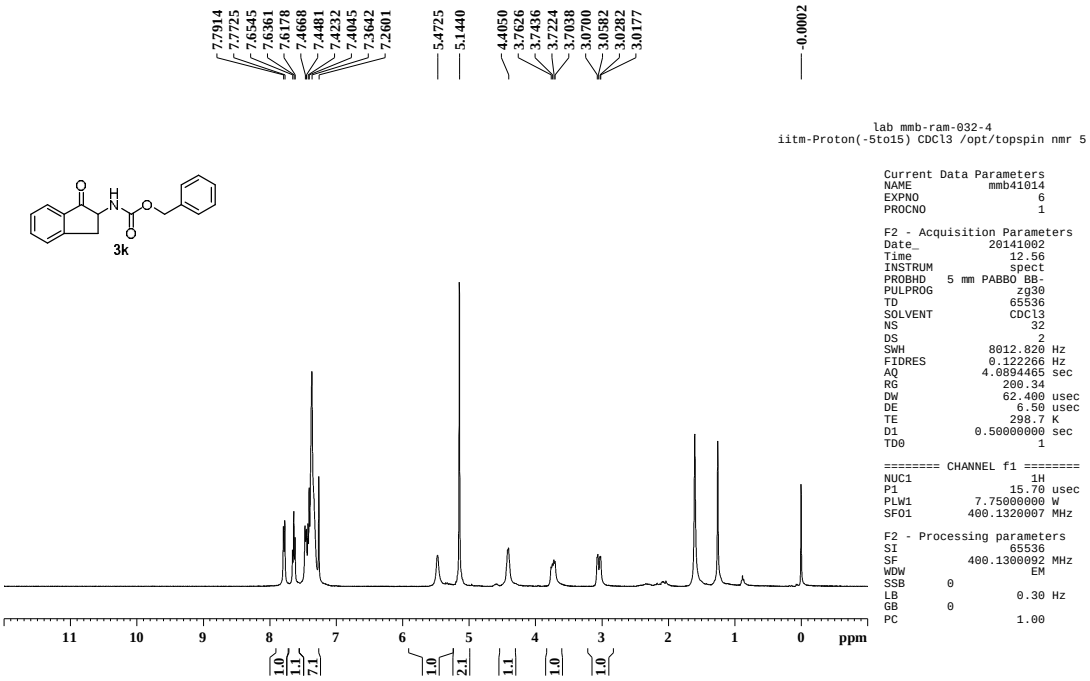



```
Lab mmb
ram-097
itm_carbonshort CDCl3 /opt/topspin iitm 19

Current Data Parameters
NAME            mmb50115
EXPNO                 27
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150129
Time              16.18
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                20480
SOLVENT           CDCl3
NS                 4813
DS                    4
SWH           29761.904 Hz
FIDRES         1.453218 Hz
AQ            0.3440640 sec
RG                202.34
DW               16.800 usec
DE                6.50 usec
TE                297.3 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7753932 MHz
NUC1                 13C
P1                9.63 usec
PLW1       103.00000000 W

======== CHANNEL f2 ========
SFO2         500.1520006 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.30000019 W
PLW12        0.33006001 W
PLW13        0.21123999 W

F2 - Processing parameters
SI                32768
SF           125.7628058 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

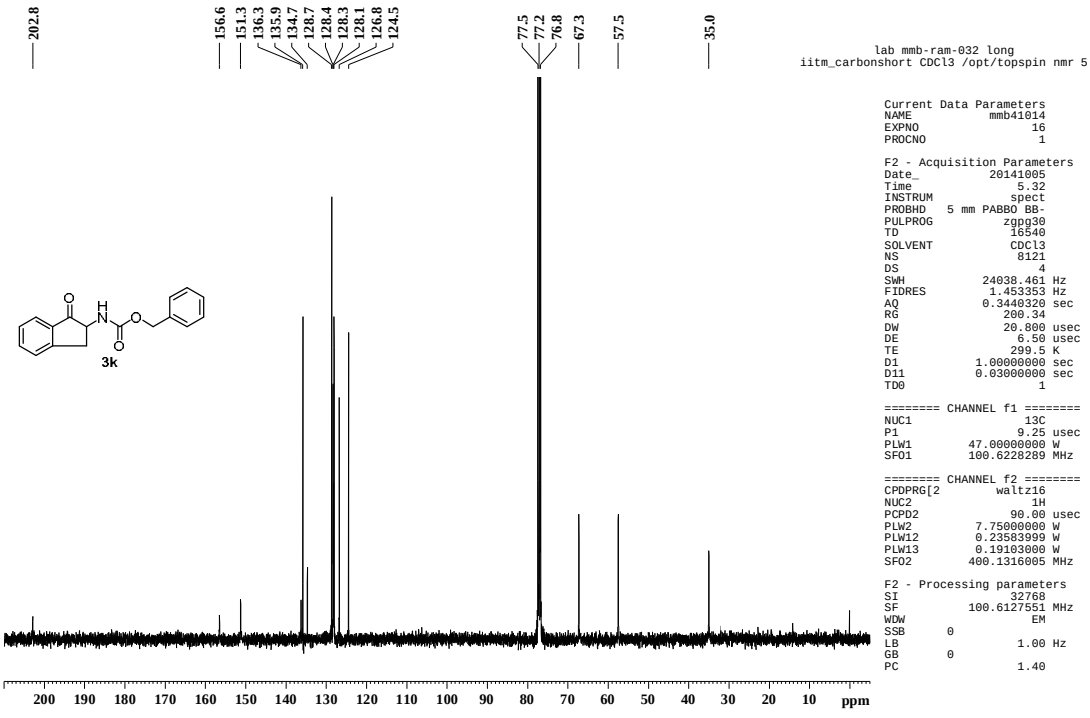

8.0267
8.0239
8.0071
8.0043
7.5330
7.5297
7.5142
7.5110
7.4955
7.4922
7.4056
7.3896
7.3732
7.3679
7.3587
7.3536
7.3459
7.3403
7.3326
7.3266
7.3084
7.2715
7.2599
7.2525
5.9789
5.1545
4.5019
4.4901
4.4777
4.4684
4.4560
4.4442
3.2447
3.2118
3.2031
3.0521
3.0460
3.0422
3.0359
3.0091
3.0030
2.9991
2.9929
2.8128
2.7853
2.0100
1.9989
1.9775
1.9664
1.9445
1.9335


lab mmb-ram-018
.itm-Proton(-5to15) CDCl3 /opt/topspin nmr 10
3j
Current Data Parameters
NAME mmb41014
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141002
Time 14.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.0 1.0 6.0 1.5 0.9 2.0 1.0 1.0 1.0 1.0 1.0

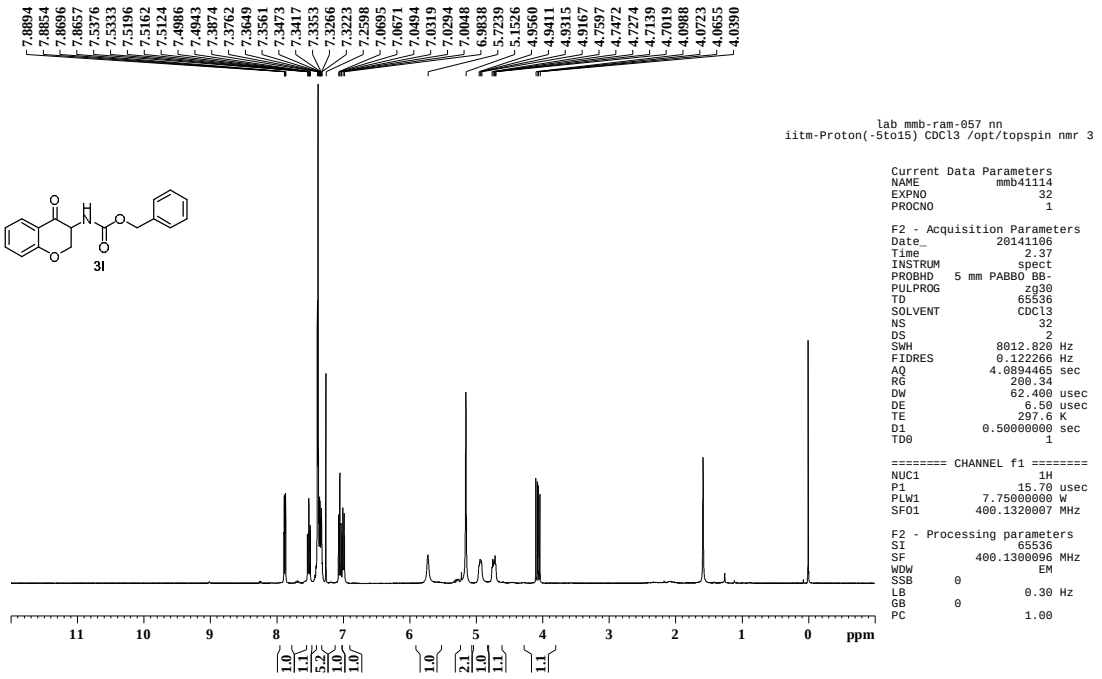

195.5
156.3
143.9
136.5
134.2
131.5
129.0
128.7
128.3
128.3
127.8
126.9
77.5
77.2
76.8
67.0
58.1
31.1
28.5
lab mmb-ran-019
iitm_carbonshort CDCl3 /opt/topspin nmr 7
3j
Current Data Parameters
NAME mmb40315
EXPNO 17
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150303
Time 14.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127560 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



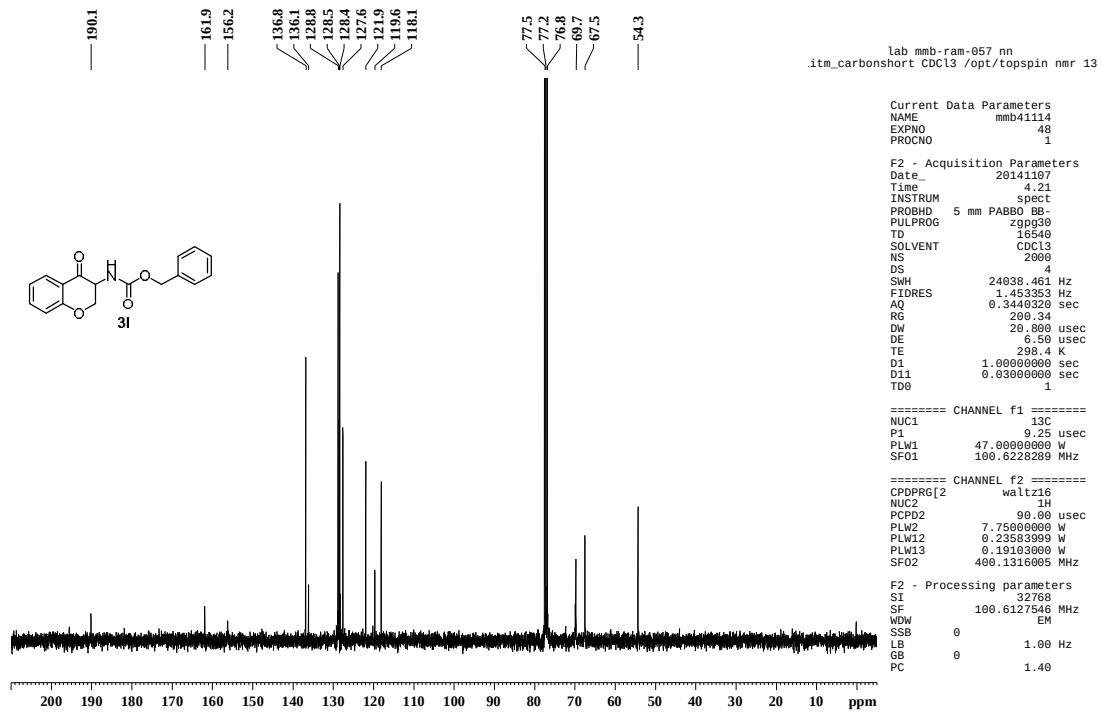

```
lab mmb-ram-032-4
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 5

Current Data Parameters
NAME              mmb41014
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_            20141002
Time                12.56
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                200.34
DW                62.400 usec
DE                 6.50 usec
TE                298.7 K
D1             0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.70 usec
PLW1         7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF            400.1300092 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



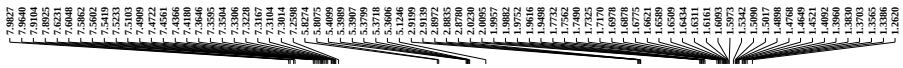

```
lab mmb-ram-032 long
iitm_carbonshort CDCl3 /opt/topspin nmr 5

Current Data Parameters
NAME              mmb41014
EXPNO                   16
PROCNO                   1

F2 - Acquisition Parameters
Date_            20141005
Time                 5.32
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 16540
SOLVENT            CDCl3
NS                  8121
DS                     4
SWH            24038.461 Hz
FIDRES          1.453353 Hz
AQ              0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                299.5 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PLW1         47.00000000 W
SFO1        100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2          7.75000000 W
PLW12         0.23583999 W
PLW13         0.19103000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127551 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

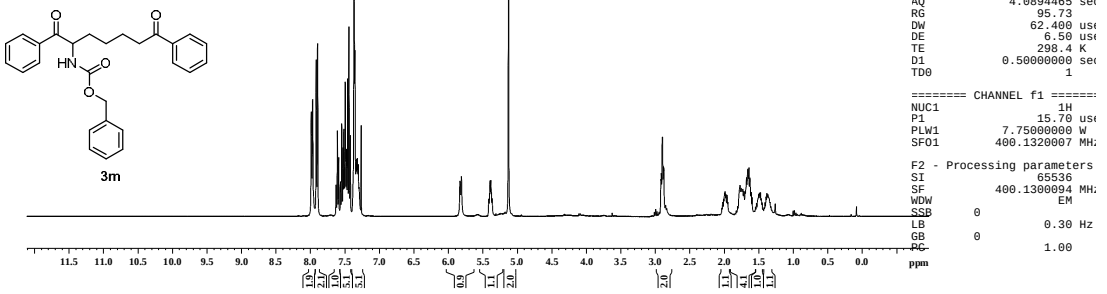



```
lab mmb-ram-057 nn
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 3

Current Data Parameters
NAME            mmb41114
EXPNO                 32
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141106
Time                2.37
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                200.34
DW                62.400 usec
DE                 6.50 usec
TE                297.6 K
D1            0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.70 usec
PLW1          7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300096 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```

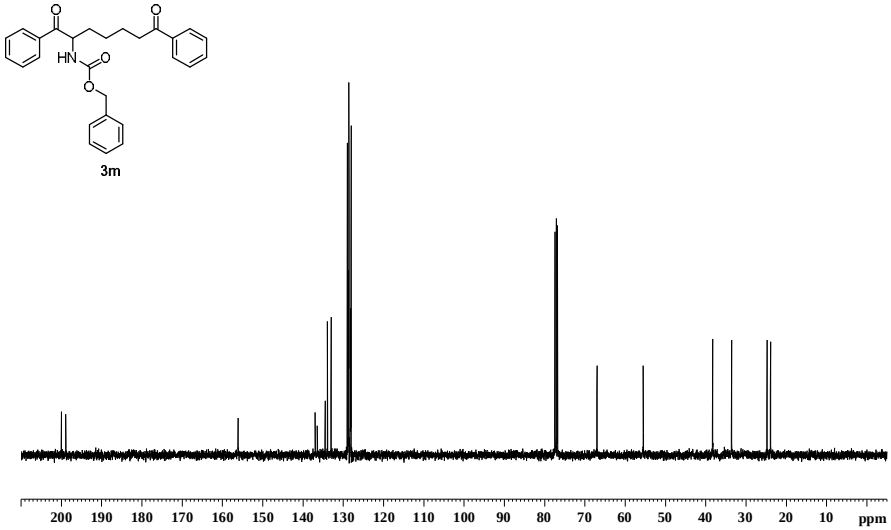



```
lab mmb-ram-057 nn
itm_carbonshort CDCl3 /opt/topspin nmr 13

Current Data Parameters
NAME            mmb41114
EXPNO                 48
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141107
Time                4.21
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 16540
SOLVENT            CDCl3
NS                  2000
DS                     4
SWH            24038.461 Hz
FIDRES          1.453353 Hz
AQ              0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                298.4 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.25 usec
PLW1         47.00000000 W
SFO1        100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2          7.75000000 W
PLW12         0.23583999 W
PLW13         0.19103000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127546 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

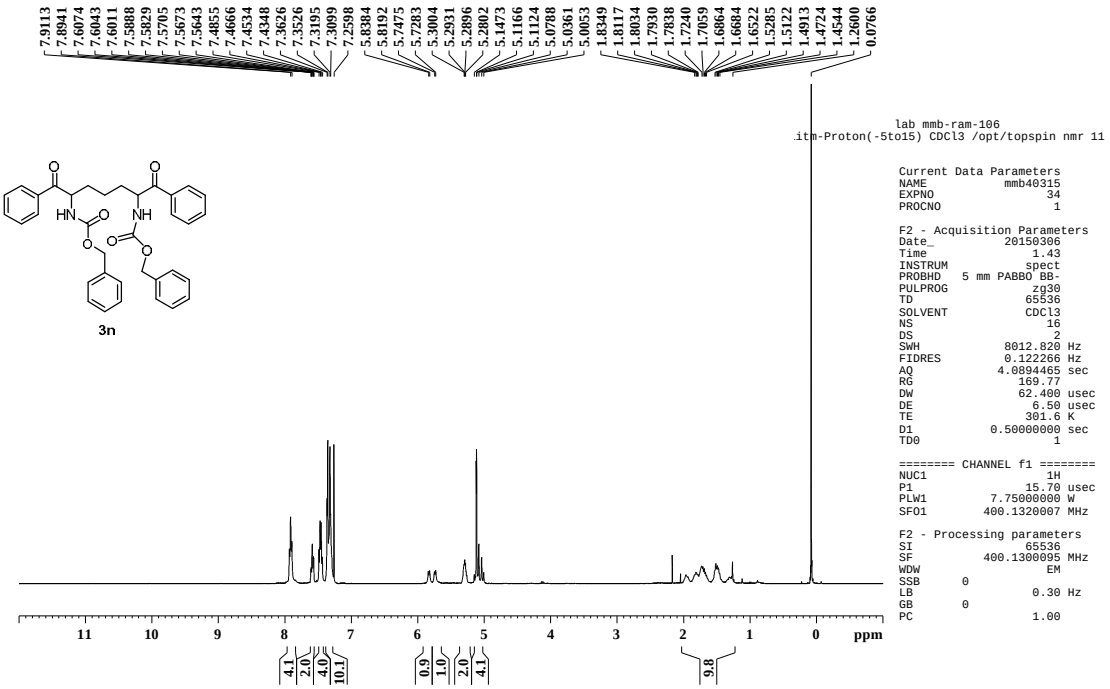


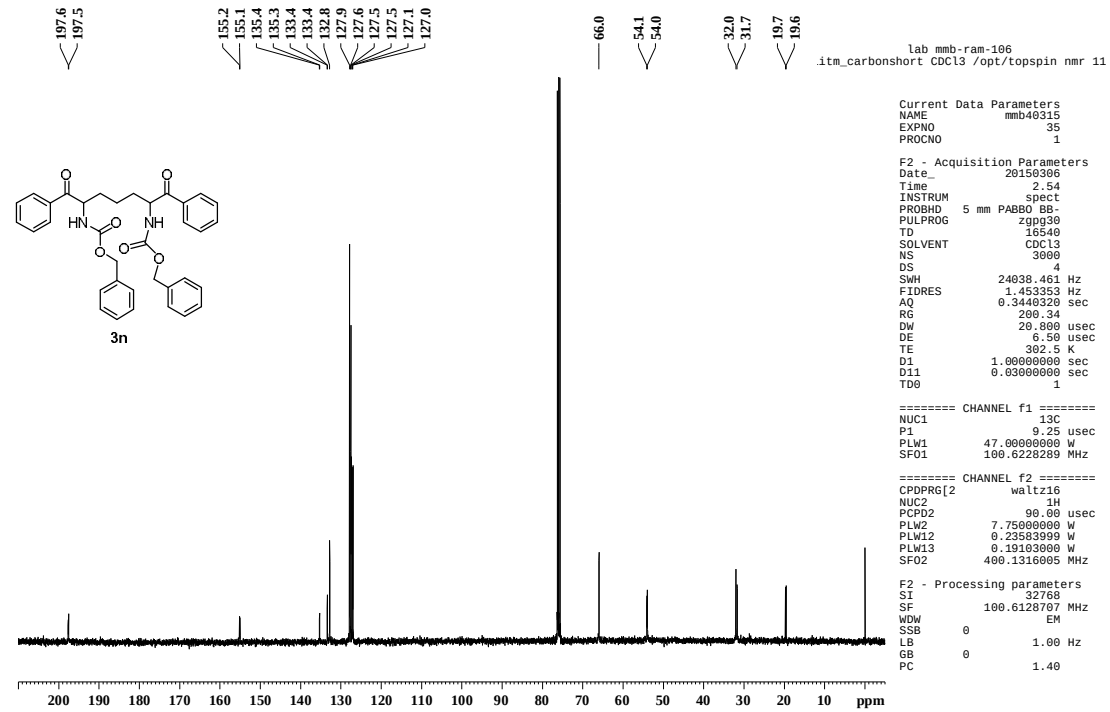


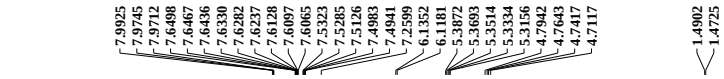

```
lab mmb-ram-107
oton(-5to15) CDCl3 /opt/topspin

Current Data Parameters
NAME            mmb40215
EXPNO                 42
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150204
Time              19.55
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES        0.122256 Hz
AQ            4.0894465 sec
RG                95.73
DW               62.400 usec
DE                6.50 usec
TE                298.4 K
D1           0.50000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.70 usec
PLW1         7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                65536
SF          400.1300094 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC                1.00
```

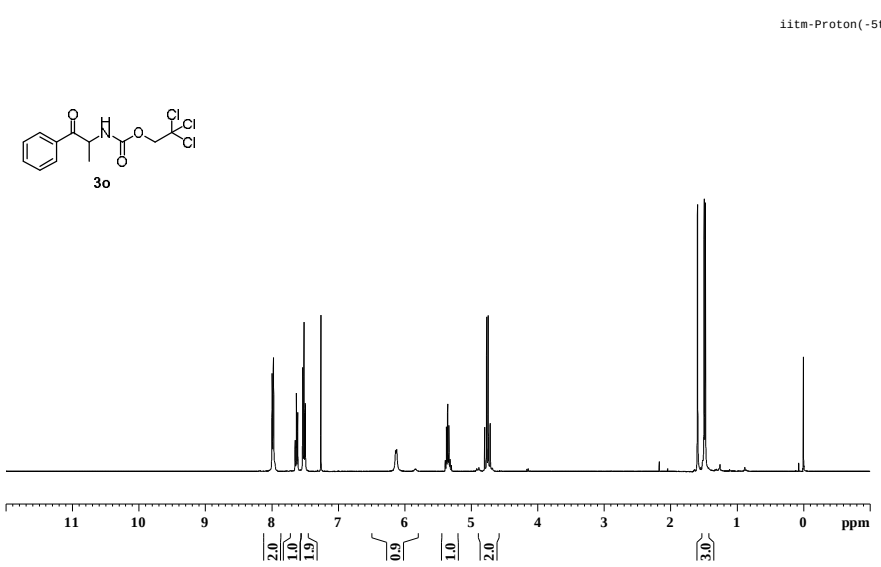


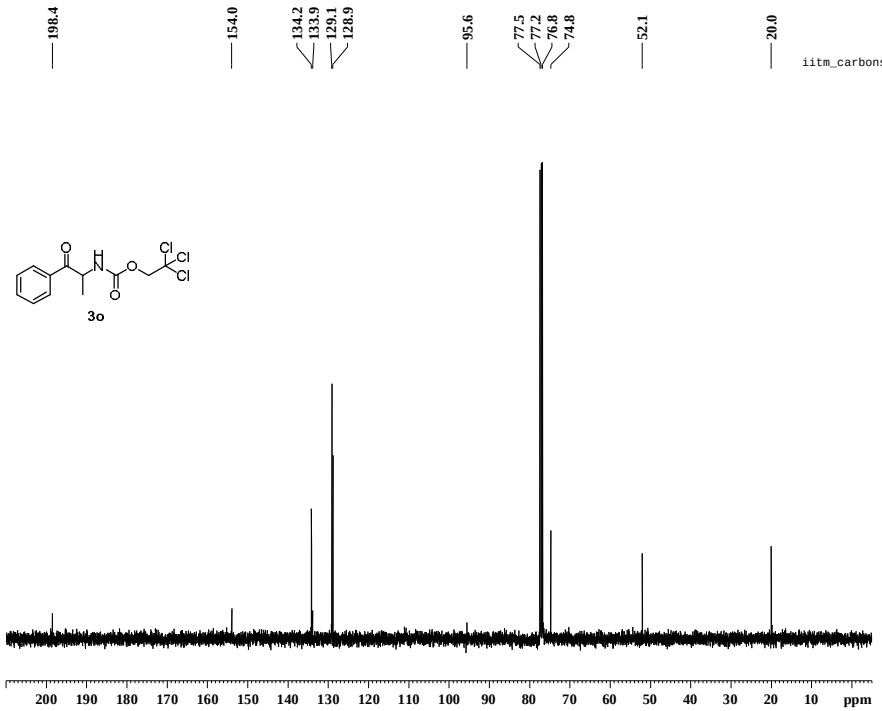

```
lab mmb-ram-107
iitm_carbonshort CDCl3 /opt/topspin nmr 3

Current Data Parameters
NAME            mmb40215
EXPNO                 43
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150204
Time              20.02
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               16540
SOLVENT          CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ            0.3440320 sec
RG                200.34
DW               20.800 usec
DE                6.50 usec
TE                299.3 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                9.25 usec
PLW1        47.00000000 W
SFO1       100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2         7.75000000 W
PLW12        0.23583999 W
PLW13        0.19103000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127595 MHz
WDW                  EM
SSB       0
LB              1.00 Hz
GB        0
PC                1.40
```

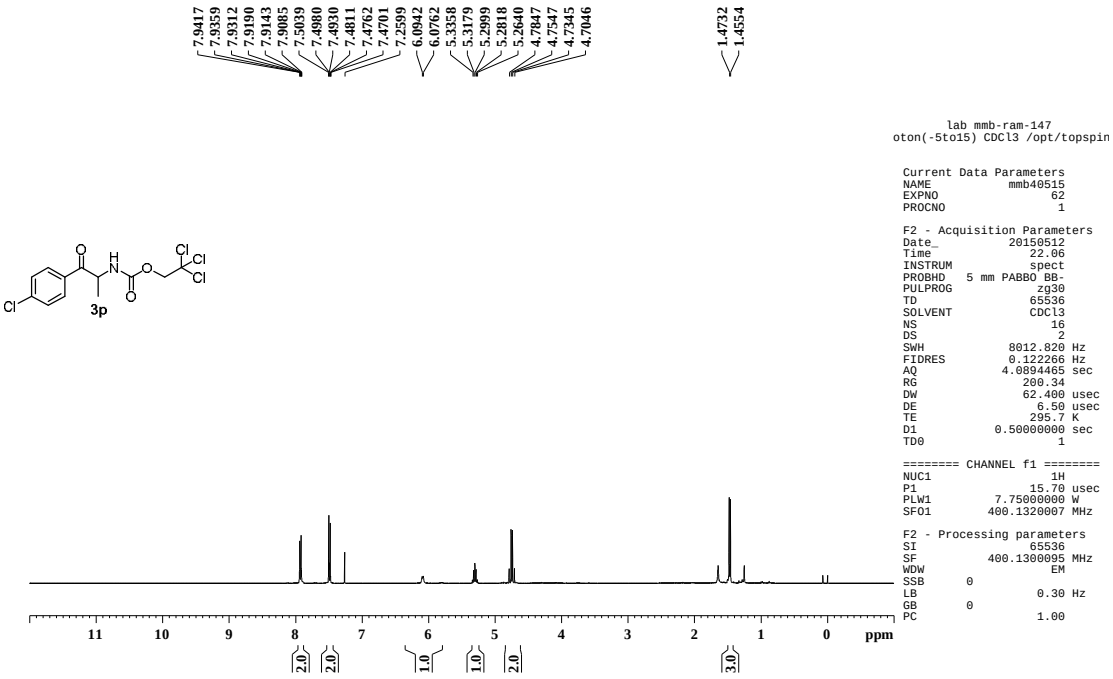

7.9113
7.8941
7.6074
7.6043
7.6011
7.5888
7.5829
7.5705
7.5673
7.5643
7.4855
7.4666
7.4534
7.4348
7.3626
7.3526
7.3195
7.3099
7.2598
5.8384
5.8192
5.7475
5.7283
5.3004
5.2931
5.2896
5.2802
5.1473
5.1166
5.1124
5.0788
5.0361
5.0053
1.8349
1.8117
1.8034
1.7930
1.7838
1.7240
1.7059
1.6864
1.6684
1.6522
1.5285
1.5122
1.4913
1.4724
1.4544
1.2600
0.0766
lab mmb-ram-106
.itm-Proton(-5to15) CDCl3 /opt/topspin nmr 11
3n
Current Data Parameters
NAME mmb40315
EXPNO 34
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150306
Time 1.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 169.77
DW 62.400 usec
DE 6.50 usec
TE 301.6 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
4.1 2.0 4.0 10.1 0.9 1.0 2.0 4.1 9.8


197.6
197.5
155.2
155.1
135.4
135.3
133.4
133.4
132.8
127.9
127.6
127.5
127.5
127.1
127.0
66.0
54.1
54.0
32.0
31.7
19.7
19.6
lab mmb-ram-106
.itm_carbonshort CDCl3 /opt/topspin nmr 11
3n
Current Data Parameters
NAME mmb40315
EXPNO 35
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150306
Time 2.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 3000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 302.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128707 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

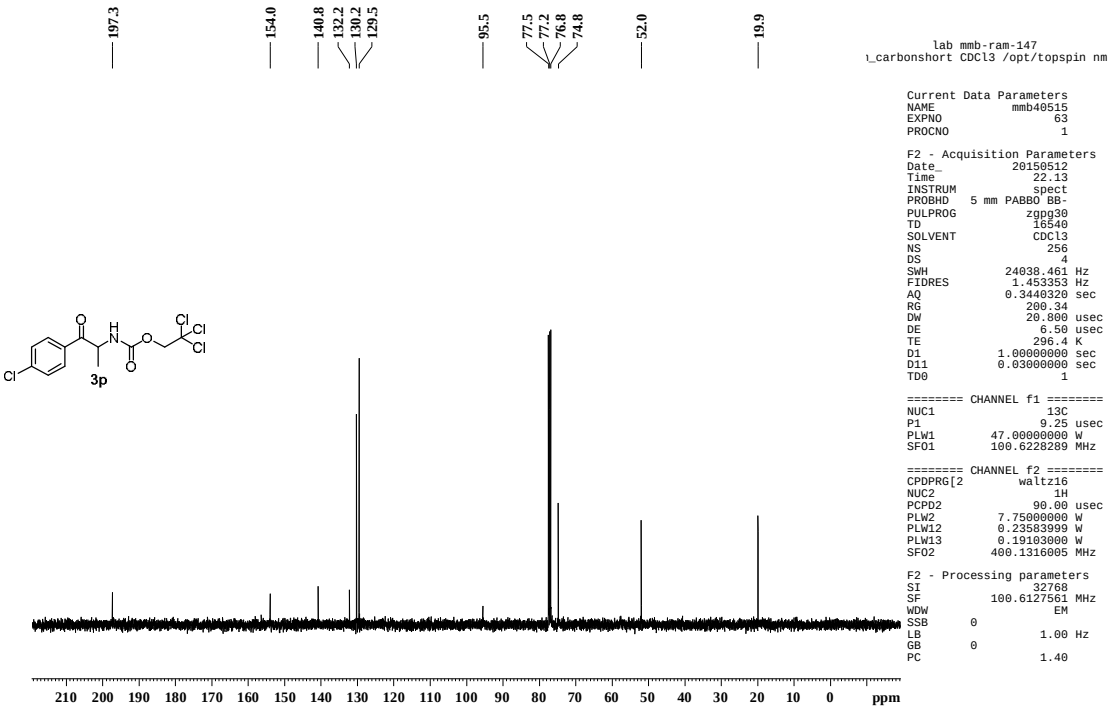

7.9925
7.9745
7.9712
7.6498
7.6467
7.6436
7.6330
7.6282
7.6237
7.6128
7.6097
7.6065
7.5323
7.5285
7.5126
7.4983
7.4941
7.2599
6.1352
6.1181
5.3872
5.3693
5.3514
5.3334
5.3156
4.7942
4.7643
4.7417
4.7117
1.4902
1.4725


lab mmb-ram-061
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 3
Current Data Parameters
NAME mmb41114
EXPNO 84
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141112
Time 20.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
3o
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.0 1.0 1.9 0.9 1.0 2.0 3.0

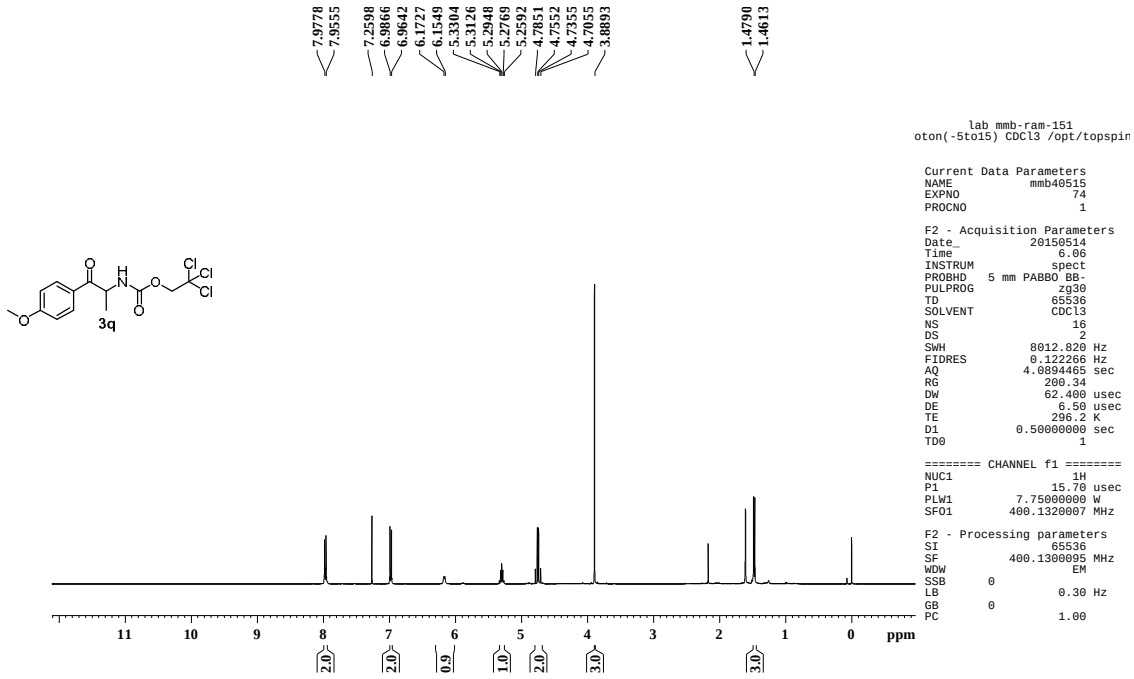

198.4
154.0
134.2
133.9
129.1
128.9
95.6
77.5
77.2
76.8
74.8
52.1
20.0
lab mmb-ram-061
iitm_carbonshort CDCl3 /opt/topspin nmr 3
Current Data Parameters
NAME mmb41114
EXPNO 85
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141112
Time 21.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 301.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
3o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

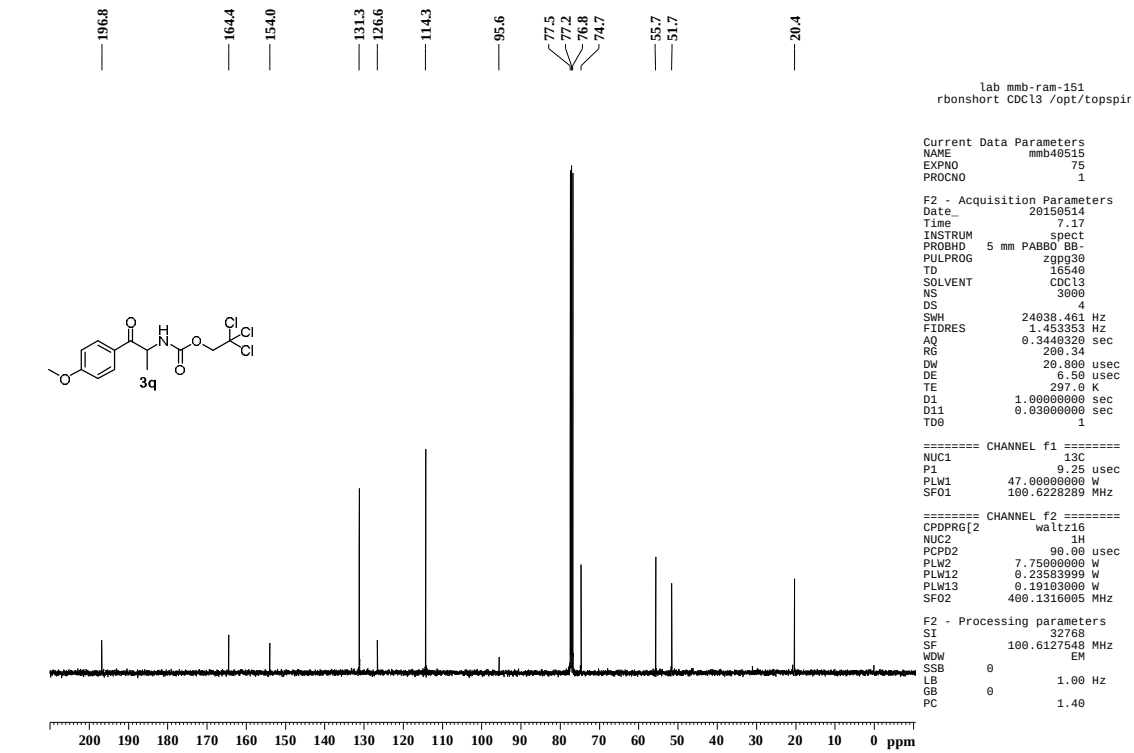


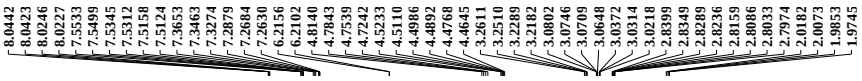

```
lab mmb-ram-147
oton(-5to15) CDCl3 /opt/topspin

Current Data Parameters
NAME            mmb40515
EXPNO                 62
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150512
Time              22.06
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                200.34
DW                62.400 usec
DE                 6.50 usec
TE                295.7 K
D1           0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.70 usec
PLW1         7.75000000 W
SFO1       400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300095 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```

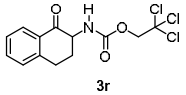



```
lab mmb-ram-147
1_carbonshort CDCl3 /opt/topspin nm

Current Data Parameters
NAME            mmb40515
EXPNO                 63
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150512
Time              22.13
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                16540
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ             0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                296.4 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PLW1        47.00000000 W
SFO1       100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2         7.75000000 W
PLW12        0.23583999 W
PLW13        0.19103000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127561 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

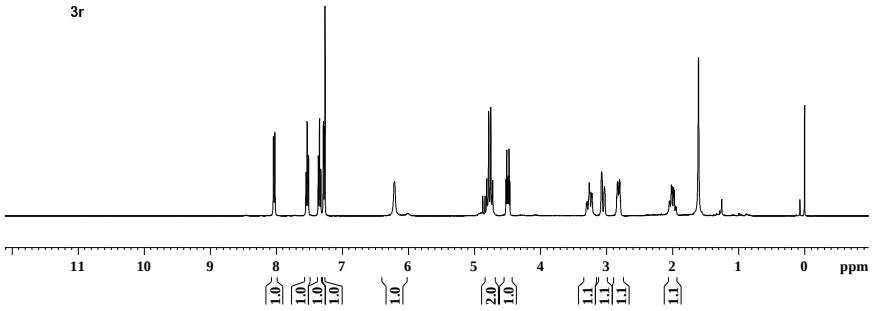

7.9778
7.9555
7.2598
6.9866
6.9642
6.1727
6.1549
5.3304
5.3126
5.2948
5.2769
5.2592
4.7851
4.7552
4.7355
4.7055
3.8893
1.4790
1.4613
3q
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.0 2.0 0.9 1.0 2.0 3.0 3.0
lab mmb-ram-151
oton(-5to15) CDCl3 /opt/topspin
Current Data Parameters
NAME mmb40515
EXPNO 74
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150514
Time 6.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


196.8
164.4
154.0
131.3
126.6
114.3
95.6
77.5
77.2
76.8
74.7
55.7
51.7
20.4
3q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
lab mmb-ram-151
rbonshort CDCl3 /opt/topspin
Current Data Parameters
NAME mmb40515
EXPNO 75
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150514
Time 7.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 3000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127548 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

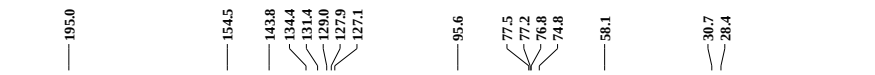


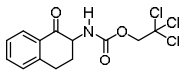


3r



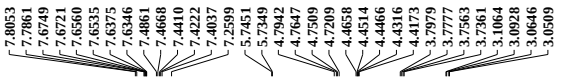

```
lab mmb-ram-141-alp+troc
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 2

Current Data Parameters
NAME            mmb40515
EXPNO                 19
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150508
Time               7.06
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ           4.0894465 sec
RG                200.34
DW              62.400 usec
DE               6.50 usec
TE               298.0 K
D1           0.50000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                9.00 usec
PLW1         8.50000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                65536
SF         400.1300088 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```

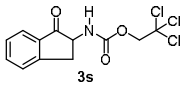


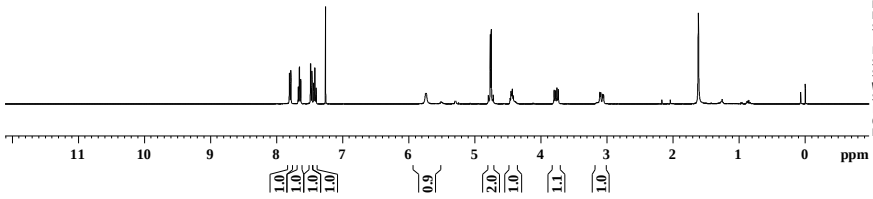


3r

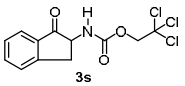

```
lab mmb-ram-141 long
rbonshort CDCl3 /opt/topspir

Current Data Parameters
NAME            mmb40515
EXPNO                 38
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150508
Time              23.59
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD               16540
SOLVENT           CDCl3
NS                 1500
DS                    4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ            0.3440320 sec
RG                200.34
DW              20.800 usec
DE               6.50 usec
TE               299.6 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                9.25 usec
PLW1        47.00000000 W
SFO1       100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2         7.75000000 W
PLW12        0.23583999 W
PLW13        0.19103000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127547 MHz
WDW                  EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```

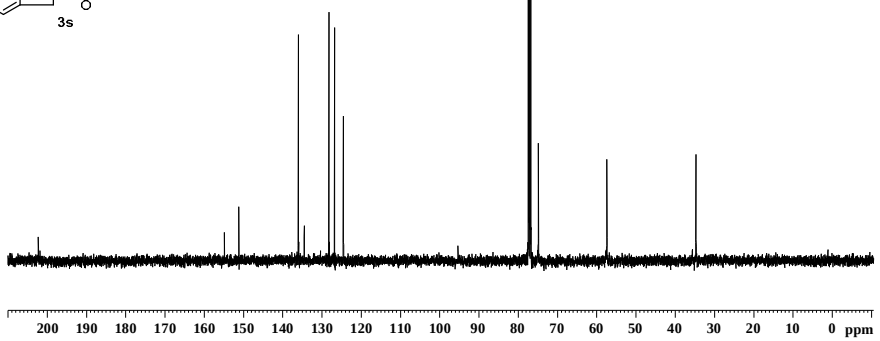




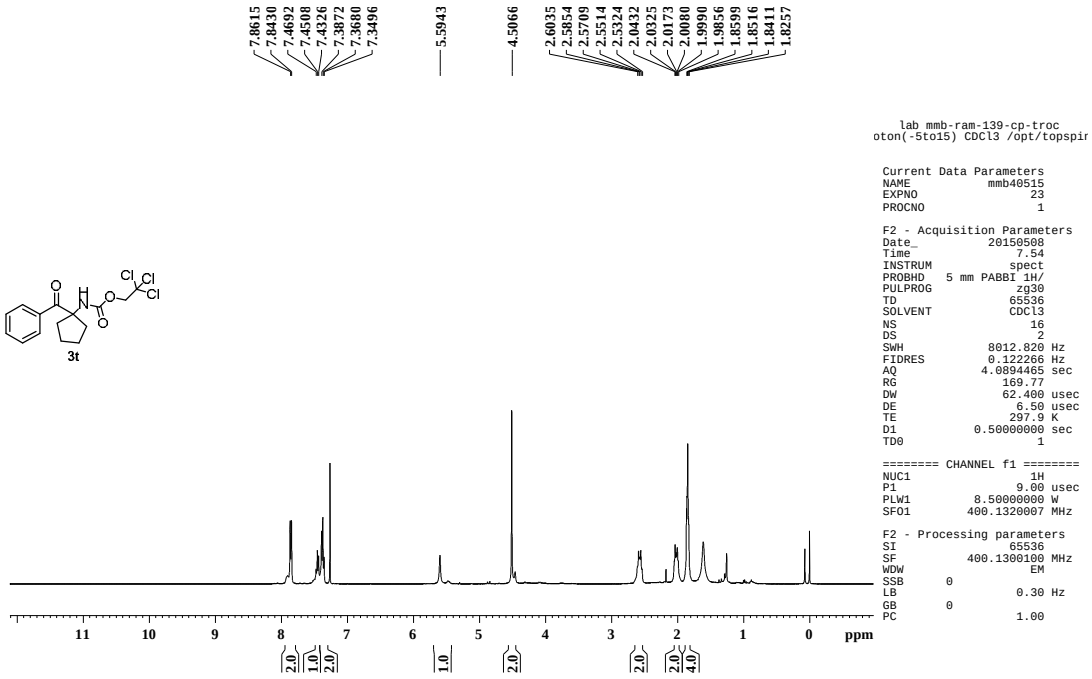



```
lab mmb-ram-149-ind+troc
oton(-5to15) CDCl3 /opt/topspin

Current Data Parameters
NAME                  mmb40515
EXPNO                       72
PROCNO                       1

F2 - Acquisition Parameters
Date_               20150514
Time                    4.49
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                     200.34
DW                     62.400 usec
DE                      6.50 usec
TE                     296.3 K
D1                  0.50000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.70 usec
PLW1                7.75000000 W
SFO1               400.1320007 MHz

F2 - Processing parameters
SI                         65536
SF                 400.1300095 MHz
WDW                           EM
SSB                0
LB                      0.30 Hz
GB                 0
PC                      1.00
```

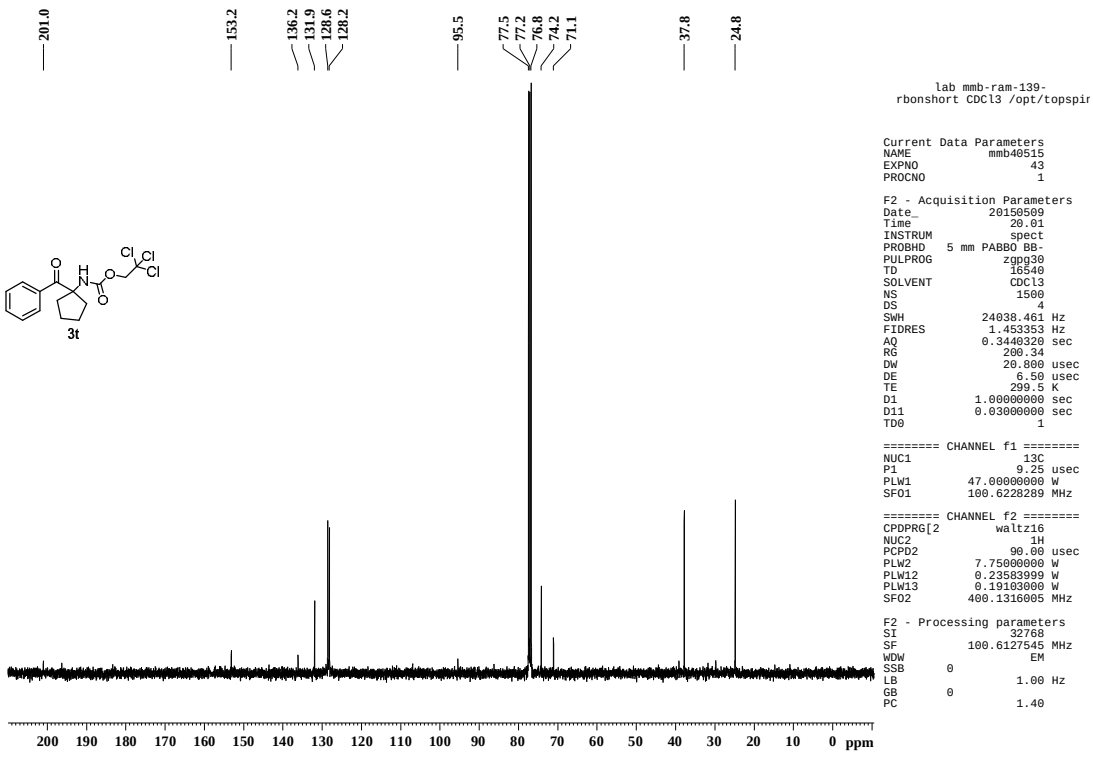




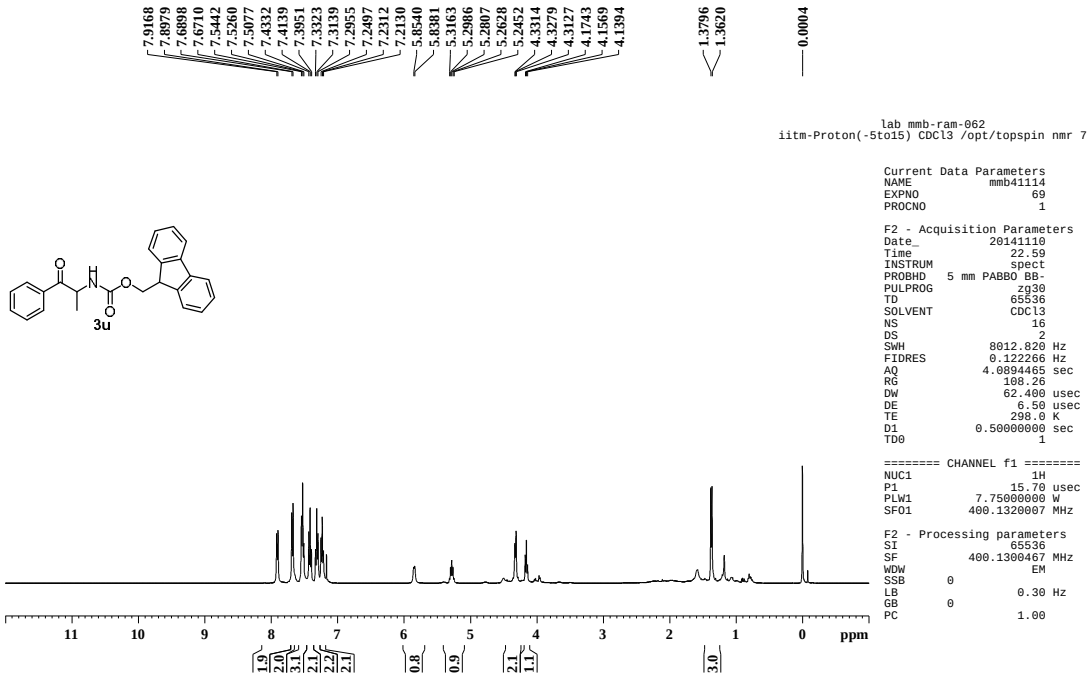

```
lab mmb-ram-149-ind+troc
rbonshort CDCl3 /opt/topspin

Current Data Parameters
NAME                  mmb40515
EXPNO                       73
PROCNO                       1

F2 - Acquisition Parameters
Date_               20150514
Time                    6.01
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     16540
SOLVENT                CDCl3
NS                      3000
DS                         4
SWH                24038.461 Hz
FIDRES              1.453353 Hz
AQ                  0.3440320 sec
RG                     200.34
DW                     20.800 usec
DE                      6.50 usec
TE                     297.0 K
D1                  1.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.25 usec
PLW1               47.00000000 W
SFO1              100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                       1H
PCPD2                  90.00 usec
PLW2                7.75000000 W
PLW12               0.23583999 W
PLW13               0.19103000 W
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                 100.6127549 MHz
WDW                           EM
SSB                0
LB                      1.00 Hz
GB                 0
PC                      1.40
```



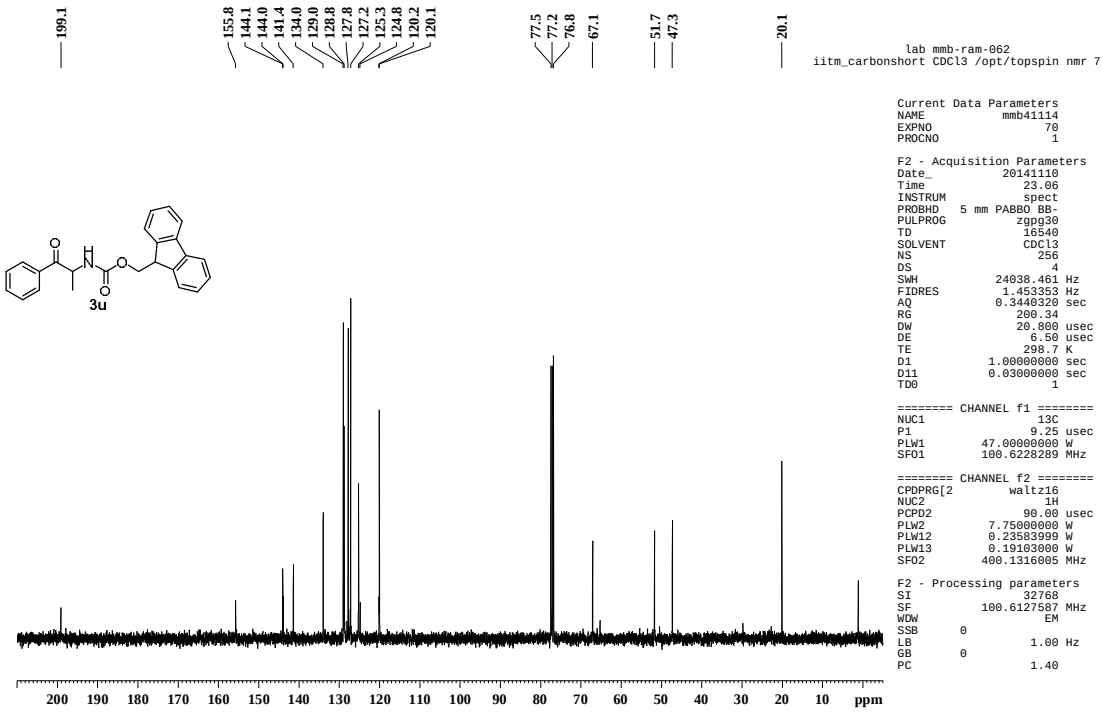

```
lab mmb-ram-139-cp-troc
oton(-5to15) CDCl3 /opt/topspir

Current Data Parameters
NAME            mmb40515
EXPNO                 23
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150508
Time               7.54
INSTRUM           spect
PROBHD   5 mm PABBI 1H/
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ            4.0894465 sec
RG               169.77
DW               62.400 usec
DE                6.50 usec
TE               297.9 K
D1            0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  9.00 usec
PLW1          8.50000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300100 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



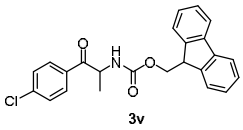

```
lab mmb-ram-139-
rbonshort CDCl3 /opt/topspir

Current Data Parameters
NAME            mmb40515
EXPNO                 43
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150509
Time              20.01
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               16540
SOLVENT           CDCl3
NS                 1500
DS                    4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ            0.3440320 sec
RG               200.34
DW               20.800 usec
DE                6.50 usec
TE               299.5 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.25 usec
PLW1         47.00000000 W
SFO1        100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2          7.75000000 W
PLW12         0.23583999 W
PLW13         0.19103000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127545 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



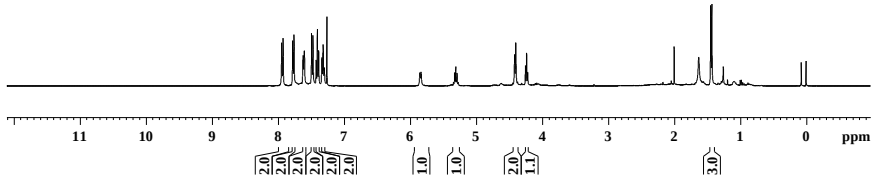

```
lab mmb-ram-062
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 7

Current Data Parameters
NAME            mmb41114
EXPNO                 69
PROCNO                 1

F2 - Acquisition Parameters
Date_          20141110
Time              22.59
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                108.26
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1           0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.70 usec
PLW1         7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300467 MHz
WDW                   EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```




```
lab mmb-ram-062
iitm_carbonshort CDCl3 /opt/topspin nmr 7

Current Data Parameters
NAME            mmb41114
EXPNO                 70
PROCNO                 1

F2 - Acquisition Parameters
Date_          20141110
Time              23.06
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               16540
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ             0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                298.7 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PLW1        47.00000000 W
SFO1       100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2         7.75000000 W
PLW12        0.23583999 W
PLW13        0.19103000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127587 MHz
WDW                   EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```



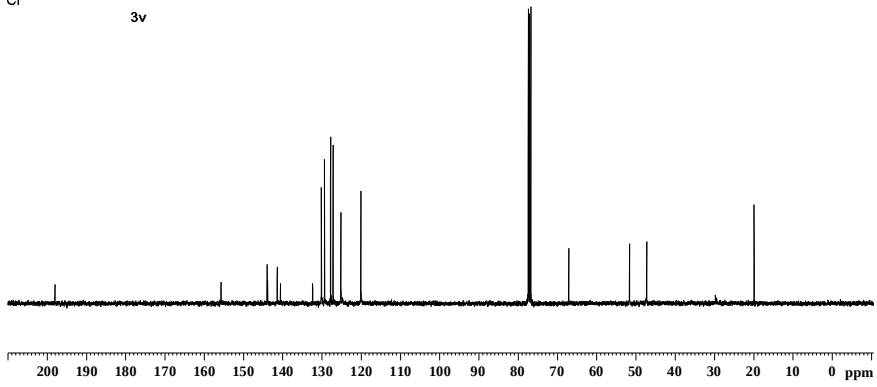
3v

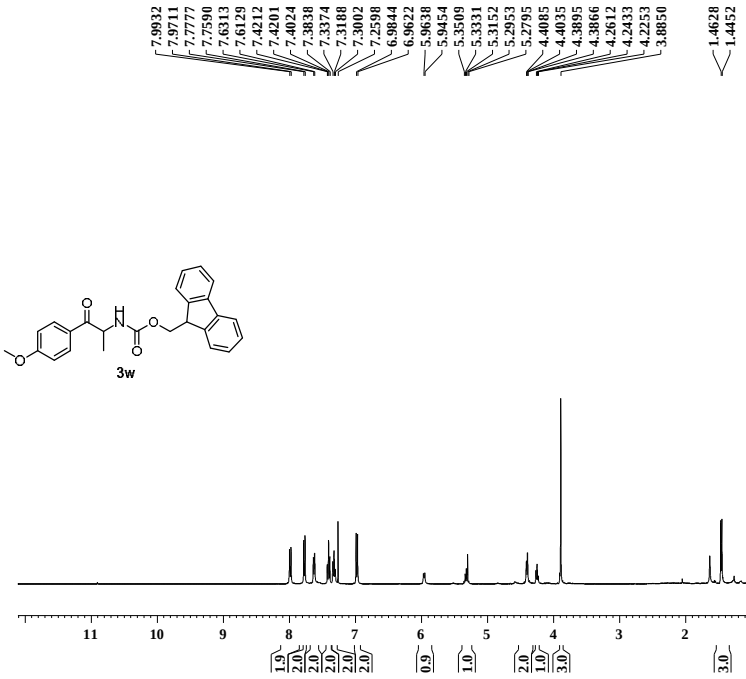



```
lab mmb-ram-148-pclp-Fmoc
oton(-5to15) CDCl3 /opt/topspin

Current Data Parameters
NAME            mmb40515
EXPNO                 53
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150511
Time              20.36
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ            4.0894465 sec
RG               169.77
DW               62.400 usec
DE                6.50 usec
TE               295.9 K
D1            0.50000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               15.70 usec
PLW1         7.75000000 W
SFO1       400.1320007 MHz

F2 - Processing parameters
SI                65536
SF         400.1300095 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```

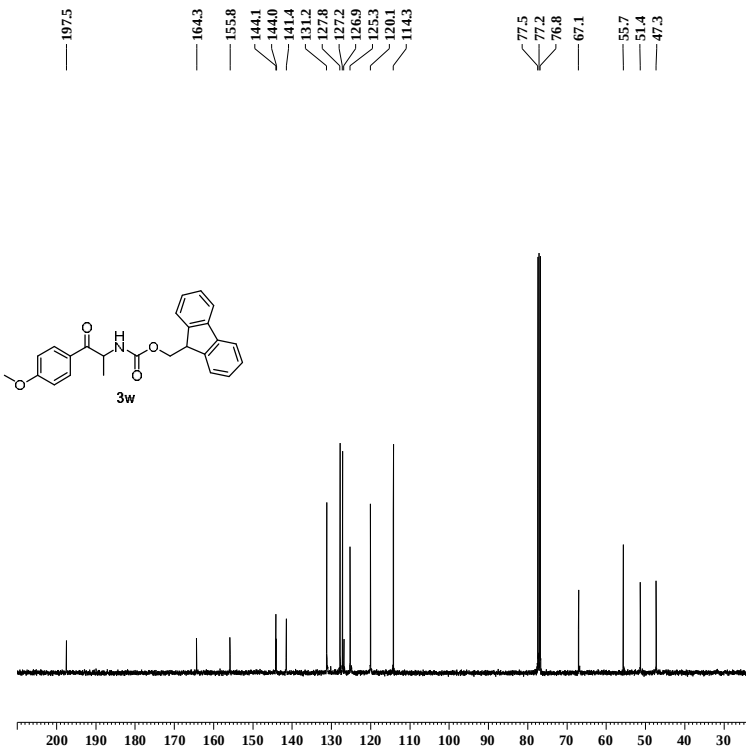

```
lab mmb-ram-148-pclp-Fmoc
rbonshort CDCl3 /opt/topspin

Current Data Parameters
NAME            mmb40515
EXPNO                 54
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150511
Time              21.20
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               16540
SOLVENT          CDCl3
NS                1800
DS                   4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ            0.3440320 sec
RG               200.34
DW               20.800 usec
DE                6.50 usec
TE               296.8 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1               9.25 usec
PLW1        47.00000000 W
SFO1       100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            90.00 usec
PLW2         7.75000000 W
PLW12        0.23583999 W
PLW13        0.19103000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6127565 MHz
WDW                  EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

3v

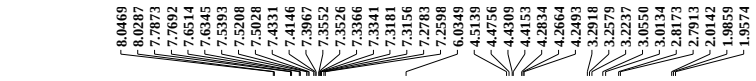


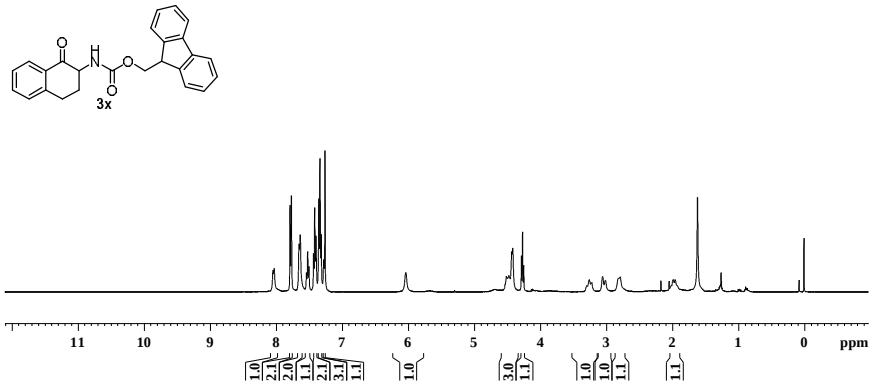



```
lab mmb-ram-152
ɔton(-5to15) CDCl3 /opt/topspin

Current Data Parameters
NAME            mmb40515
EXPNO                 76
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150514
Time               0.49
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                153.13
DW                62.400 usec
DE                 6.50 usec
TE                296.4 K
D1            0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.70 usec
PLW1          7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300095 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

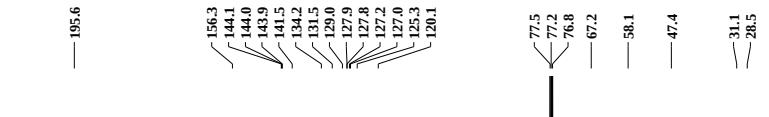


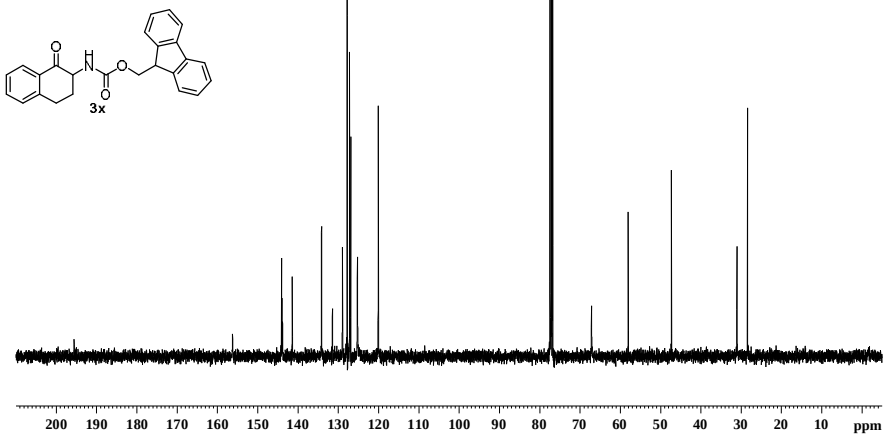

```
lab mmb-ram-152
·bonshort CDCl3 /opt/topspin

Current Data Parameters
NAME            mmb40515
EXPNO                 77
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150514
Time               2.00
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               16540
SOLVENT           CDCl3
NS                 3000
DS                    4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ             0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE                296.9 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PLW1         47.00000000 W
SFO1        100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2          7.75000000 W
PLW12         0.23583999 W
PLW13         0.19103000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127563 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



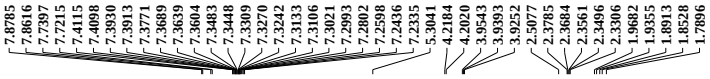


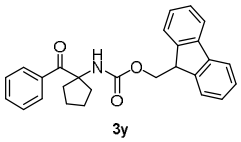

```
lab mmb-ram-142-alp+Fmoc
-Proton(-5to15) CDCl3 /opt/topspin n

Current Data Parameters
NAME                  mmb40515
EXPNO                       21
PROCNO                       1

F2 - Acquisition Parameters
Date_              20150508
Time                    7.24
INSTRUM                spect
PROBHD   5 mm PABBI 1H/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                8012.820 Hz
FIDRES             0.122266 Hz
AQ                 4.0894465 sec
RG                    138.85
DW                    62.400 usec
DE                     6.50 usec
TE                    298.0 K
D1                 0.50000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     9.00 usec
PLW1              8.50000000 W
SFO1             400.1320007 MHz

F2 - Processing parameters
SI                        65536
SF                400.1300100 MHz
WDW                         EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```



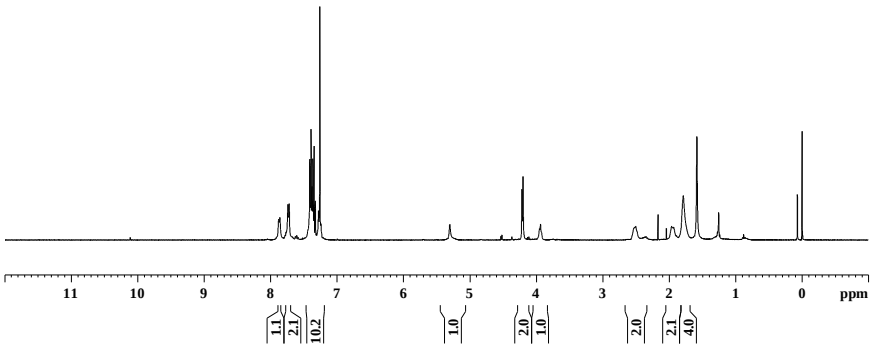



```
lab mmb-ram-142
rbonshort CDCl3 /opt/topspin

Current Data Parameters
NAME                  mmb40515
EXPNO                       44
PROCNO                       1

F2 - Acquisition Parameters
Date_              20150509
Time                   20.41
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     16540
SOLVENT                CDCl3
NS                      1500
DS                         4
SWH               24038.461 Hz
FIDRES             1.453353 Hz
AQ                 0.3440320 sec
RG                    200.34
DW                    20.800 usec
DE                     6.50 usec
TE                    299.5 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     9.25 usec
PLW1              47.00000000 W
SFO1             100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                      1H
PCPD2                  90.00 usec
PLW2               7.75000000 W
PLW12              0.23583999 W
PLW13              0.19103000 W
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127558 MHz
WDW                         EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

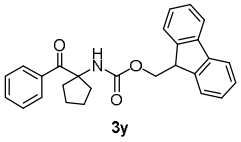




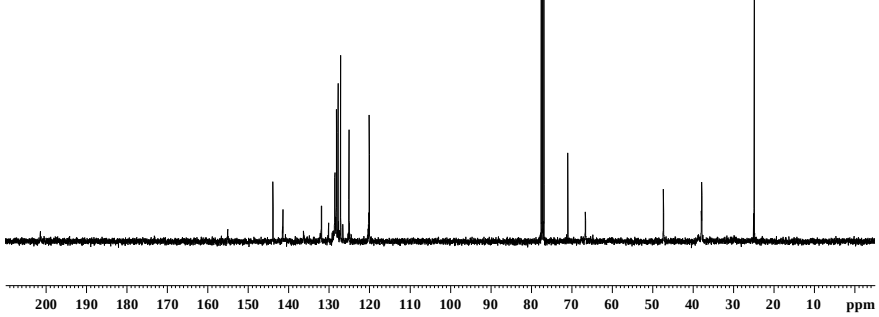
3y



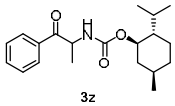

```
lab mmb-ram-140 re
›ton(-5to15) CDCl3 /opt/topspin

Current Data Parameters
NAME                  mmb40515
EXPNO                      255
PROCNO                       1

F2 - Acquisition Parameters
Date_               20150530
Time                    0.25
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                     200.34
DW                     62.400 usec
DE                      6.50 usec
TE                     298.7 K
D1                  0.50000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.70 usec
PLW1                7.75000000 W
SFO1               400.1320007 MHz

F2 - Processing parameters
SI                         65536
SF                 400.1300096 MHz
WDW                           EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

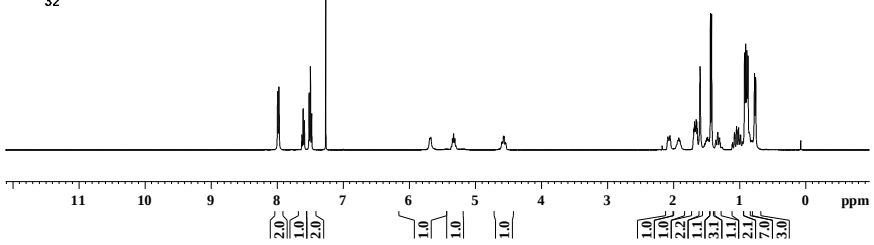


3y

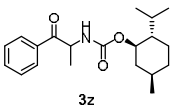


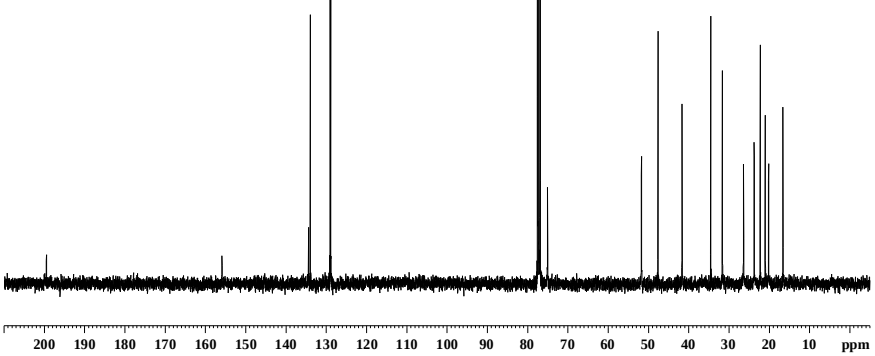

```
lab mmbram-140
_carbonshort CDCl3 /opt/topspin nm

Current Data Parameters
NAME                  mmb40515
EXPNO                      246
PROCNO                       1

F2 - Acquisition Parameters
Date_               20150529
Time                    3.34
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                     16540
SOLVENT                CDCl3
NS                      1500
DS                         4
SWH                24038.461 Hz
FIDRES              1.453353 Hz
AQ                  0.3440320 sec
RG                     200.34
DW                     20.800 usec
DE                      6.50 usec
TE                     299.6 K
D1                  1.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       9.25 usec
PLW1               47.00000000 W
SFO1              100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                       1H
PCPD2                   90.00 usec
PLW2                7.75000000 W
PLW12               0.23583999 W
PLW13               0.19103000 W
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                 100.6127570 MHz
WDW                           EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```



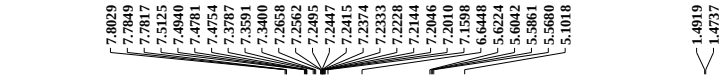


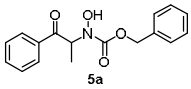

```
lab mmb-ram-089 repte
oton(-5to15) CDCl3 /opt/topspin

Current Data Parameters
NAME            mmb40115
EXPNO                147
PROCNO                 1

F2 - Acquisition Parameters
Date_            20150115
Time                8.25
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 200.34
DW                62.400 usec
DE                 6.50 usec
TE                 301.7 K
D1             0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.70 usec
PLW1          7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300095 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



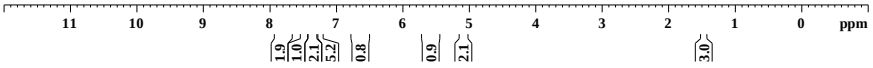



```
lab mmb-ram-089
iitm_carbonshort CDCl3 /opt/topspin nmr 8

Current Data Parameters
NAME            mmb40115
EXPNO                154
PROCNO                 1

F2 - Acquisition Parameters
Date_            20150115
Time               18.41
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                 16540
SOLVENT            CDCl3
NS                  3500
DS                     4
SWH            24038.461 Hz
FIDRES          1.453353 Hz
AQ              0.3440320 sec
RG                 200.34
DW                20.800 usec
DE                 6.50 usec
TE                 302.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.25 usec
PLW1         47.00000000 W
SFO1        100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2          7.75000000 W
PLW12         0.23583999 W
PLW13         0.19103000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127431 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

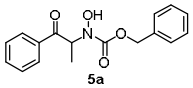




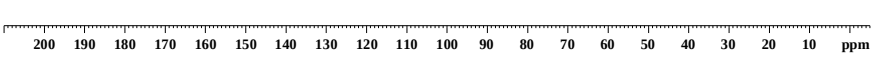
5a



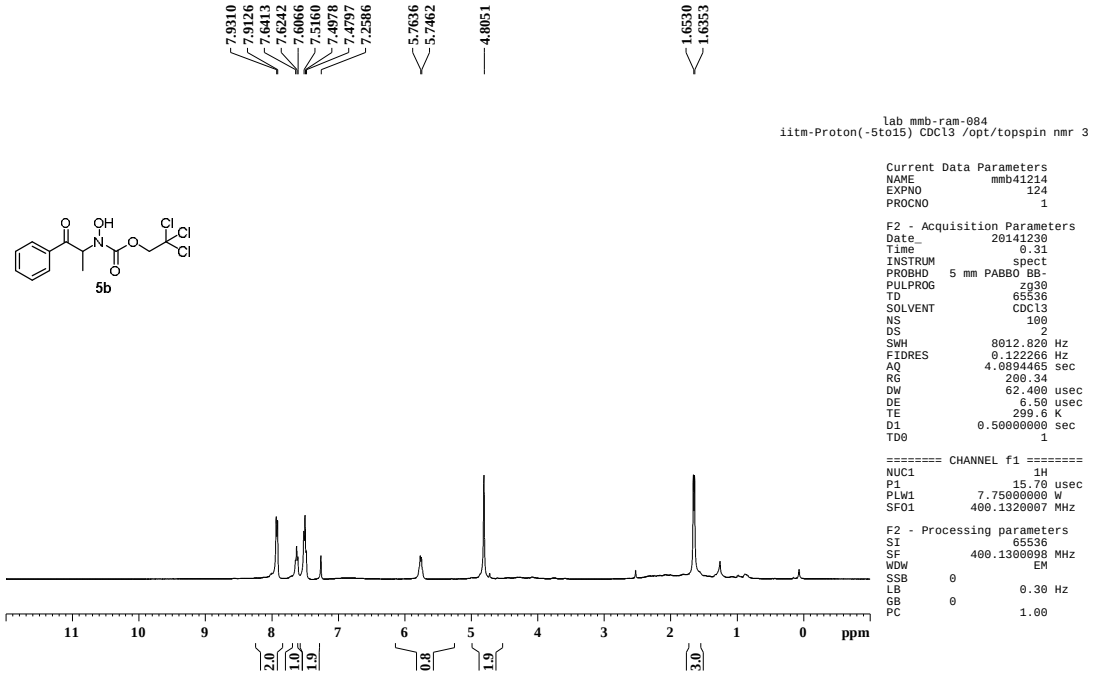

```
lab mmb-ram-083
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 4

Current Data Parameters
NAME            mmb41214
EXPNO                 89
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141219
Time               15.44
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                108.26
DW                62.400 usec
DE                 6.50 usec
TE         0 K
D1          0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.70 usec
PLW1          7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF          400.1300494 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

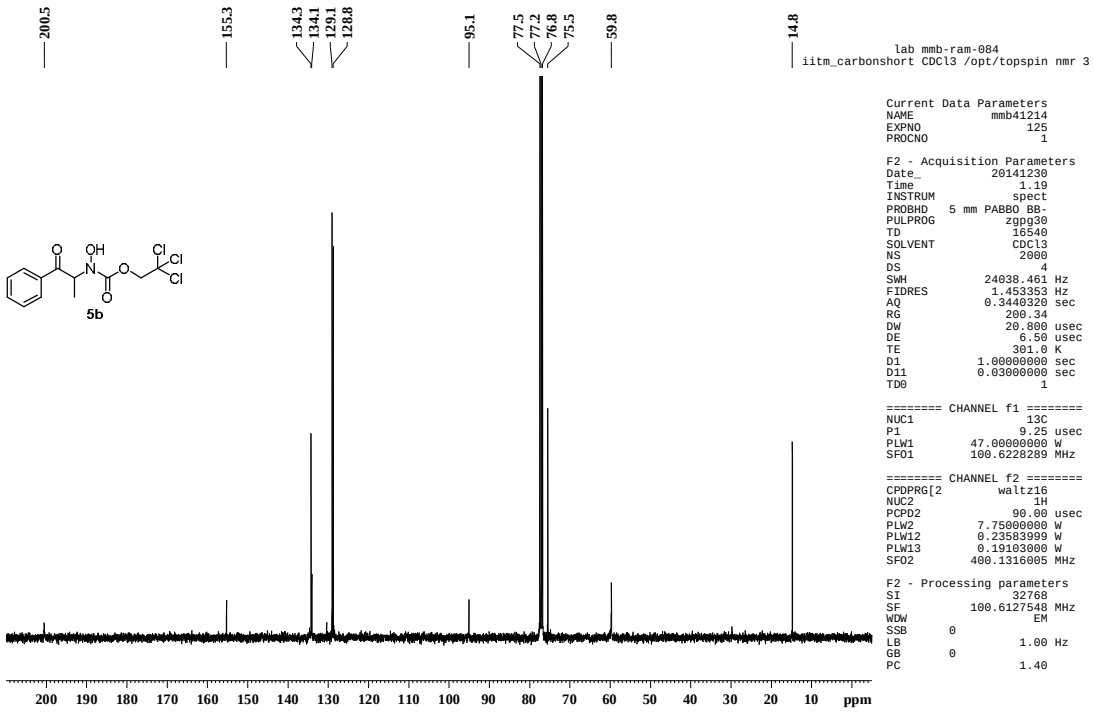


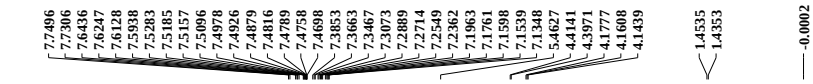
5a

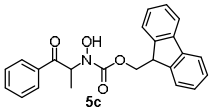


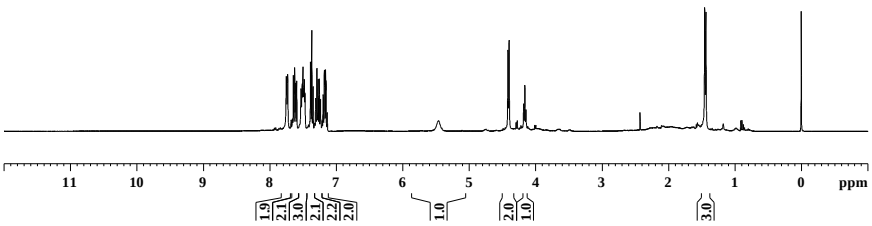

```
lab mmb-ram-083
iitm_carbonshort CDCl3 /opt/topspin nmr 4

Current Data Parameters
NAME            mmb41214
EXPNO                 90
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141219
Time               15.51
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                16540
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         1.453353 Hz
AQ             0.3440320 sec
RG                200.34
DW                20.800 usec
DE                 6.50 usec
TE         0 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PLW1         47.00000000 W
SFO1        100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2          7.75000000 W
PLW12         0.23583999 W
PLW13         0.19103000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127578 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


7.9310
7.9126
7.6413
7.6242
7.6066
7.5160
7.4978
7.4797
7.2586
5.7636
5.7462
4.8051
1.6530
1.6353
lab mmb-ram-084
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 3
Current Data Parameters
NAME mmb41214
EXPNO 124
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141230
Time 0.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 100
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 200.34
DW 62.400 usec
DE 6.50 usec
TE 299.6 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
5b
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.0 1.0 1.9 0.8 1.9 3.0

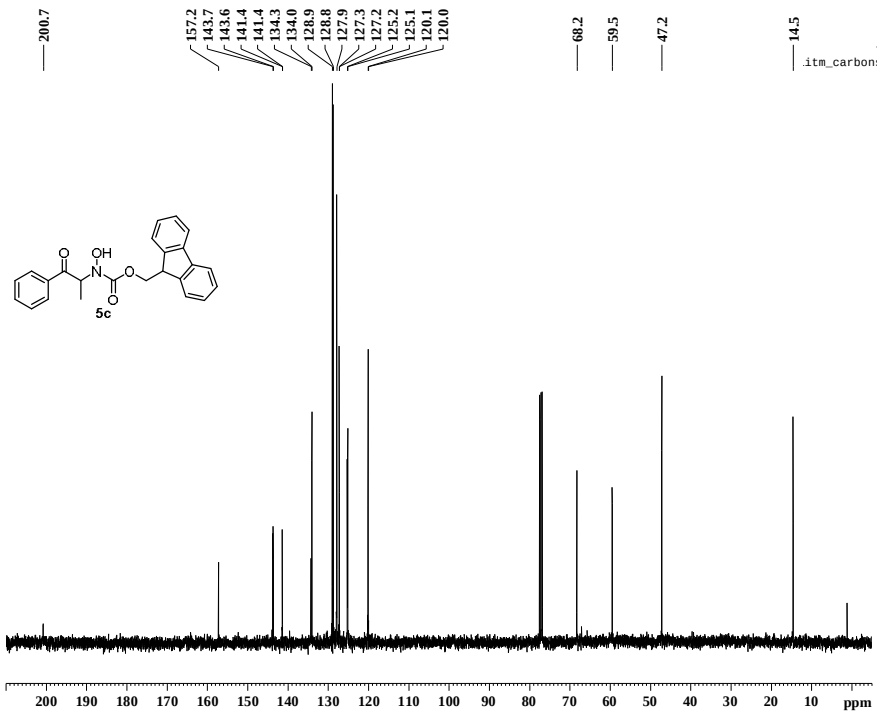

200.5
155.3
134.3
134.1
129.1
128.8
95.1
77.5
77.2
76.8
75.5
59.8
14.8
lab mmb-ram-084
iitm_carbonshort CDCl3 /opt/topspin nmr 3
Current Data Parameters
NAME mmb41214
EXPNO 125
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141230
Time 1.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 301.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127548 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
5b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



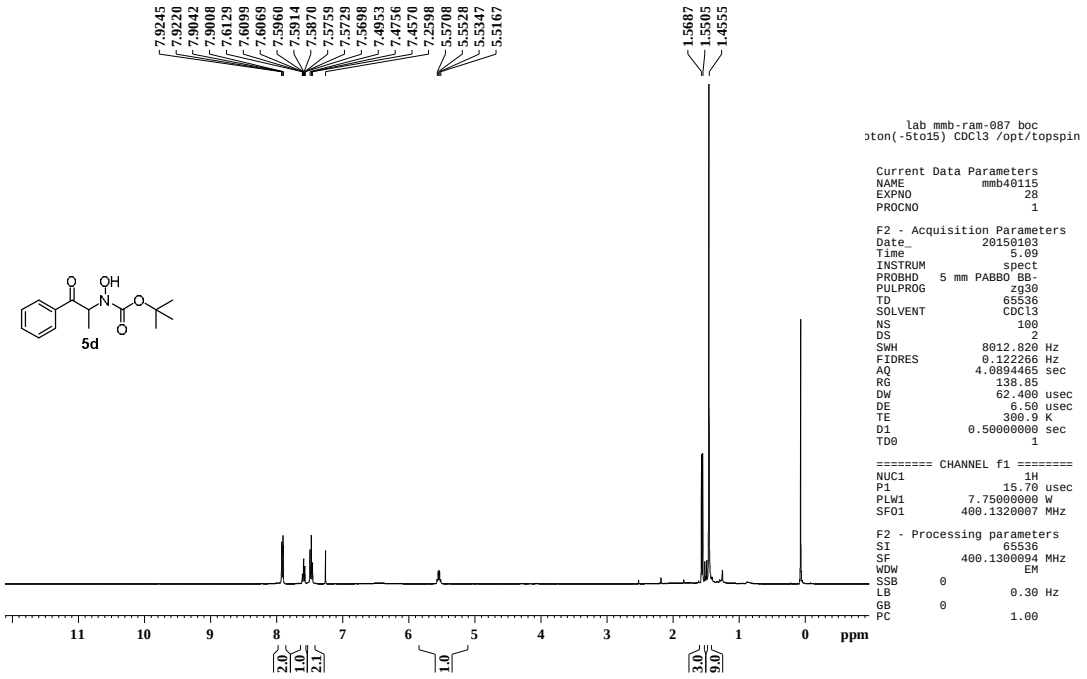


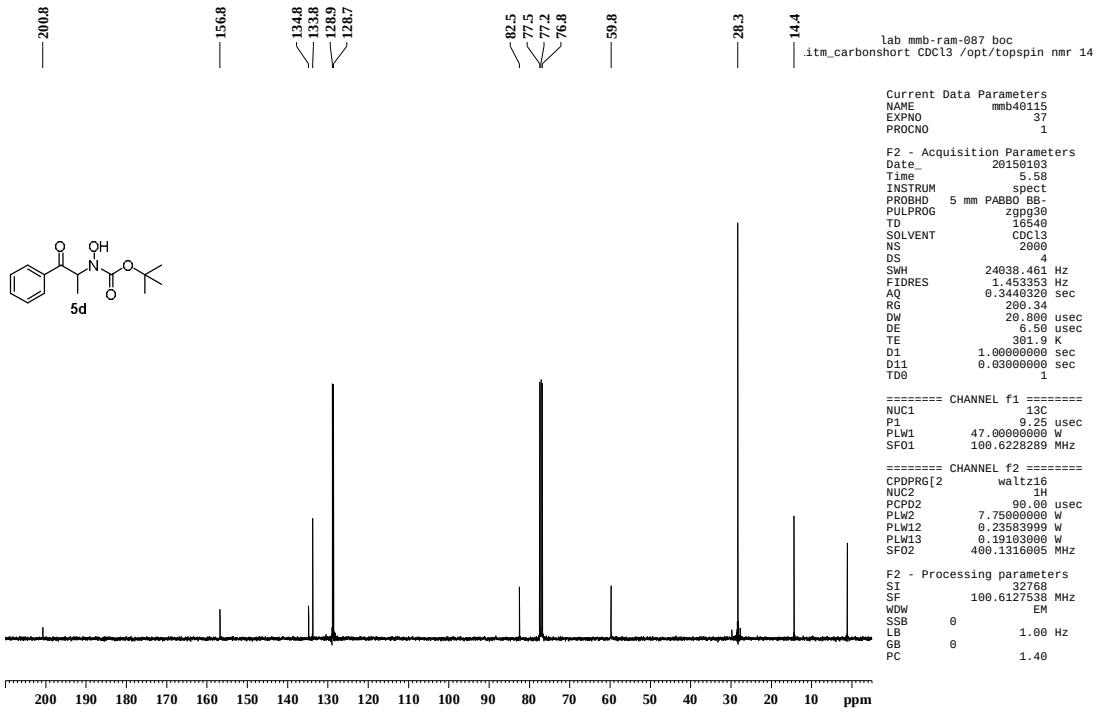


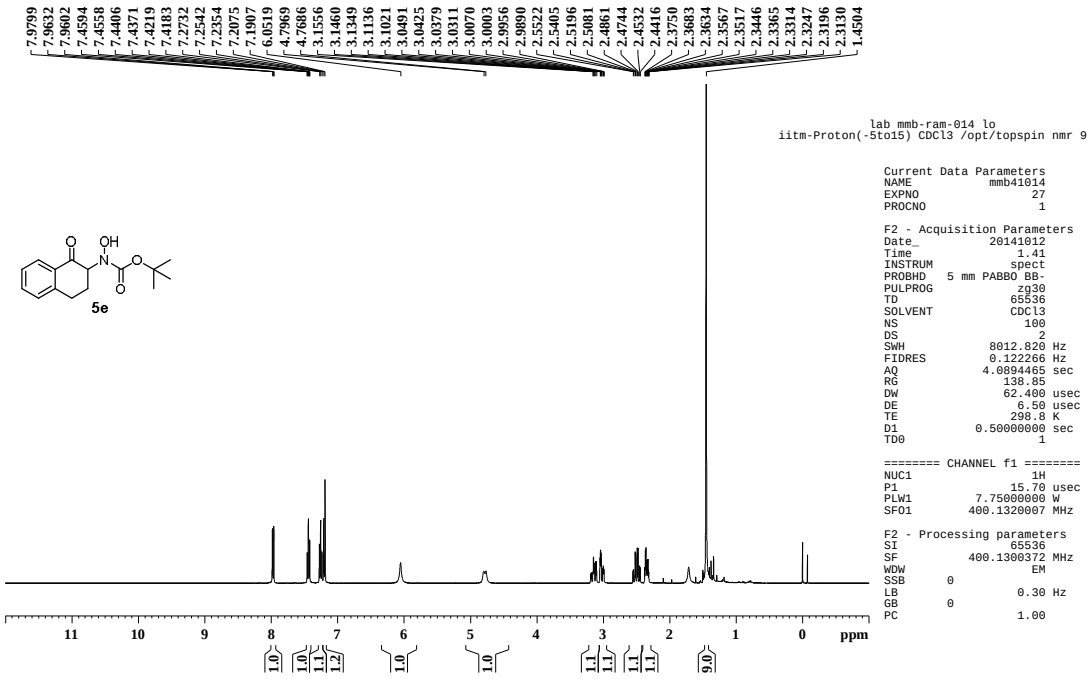

```
lab mmb-ram-086 fmoc
.itm-Proton(-5to15) CDCl3 /opt/topspin nmr 10

Current Data Parameters
NAME            mmb40315
EXPNO                 32
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150306
Time                1.31
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                  79.8
DW                 62.400 usec
DE                  6.50 usec
TE                 301.6 K
D1              0.50000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.70 usec
PLW1         7.75000000 W
SFO1        400.1320007 MHz

F2 - Processing parameters
SI                 65536
SF            400.1300495 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

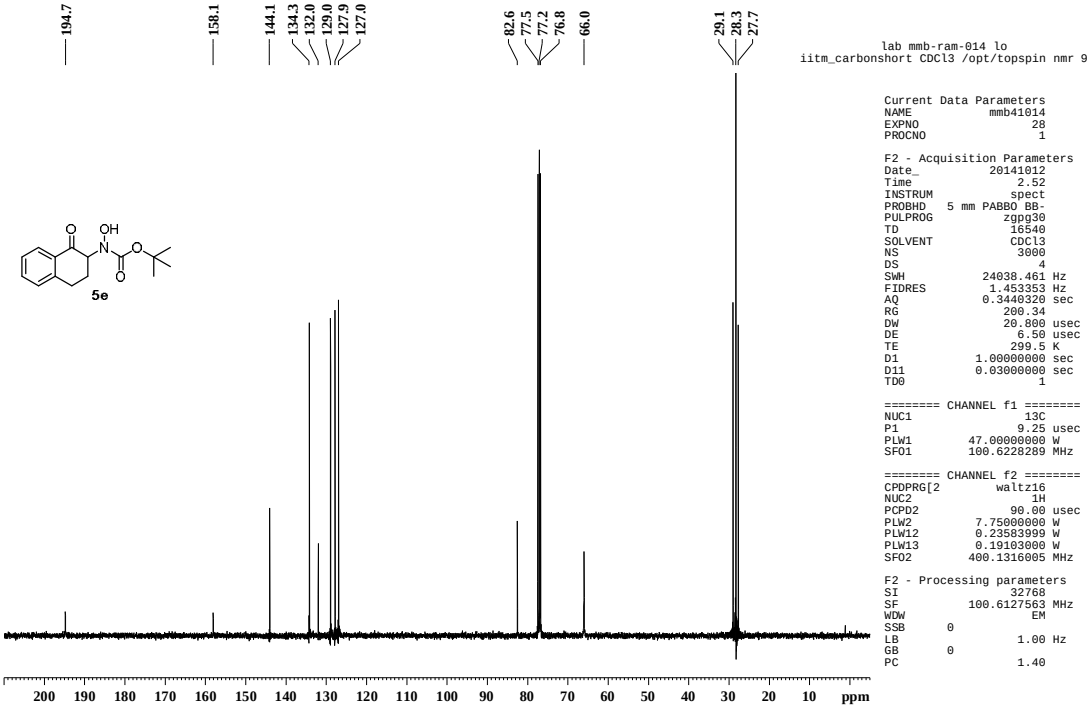


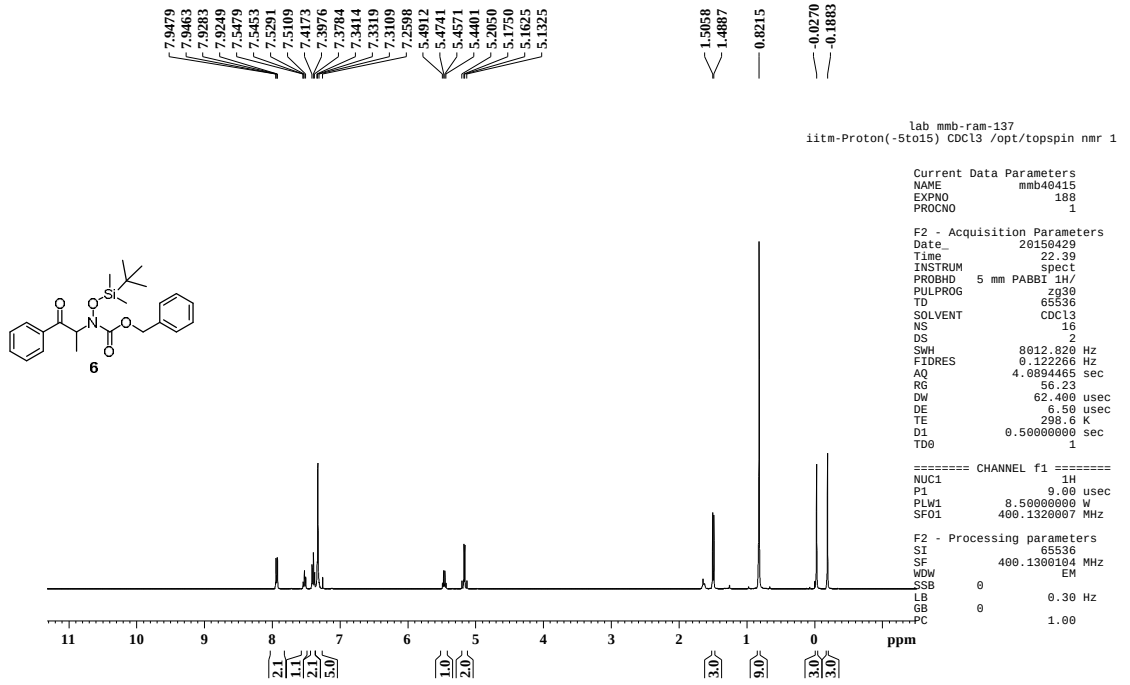

```
lab mmb-ram-086 fmoc
.itm_carbonshort CDCl3 /opt/topspin nmr 10

Current Data Parameters
NAME            mmb40315
EXPNO                 33
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150306
Time                1.36
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 16540
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES          1.453353 Hz
AQ              0.3440320 sec
RG                  200.34
DW                 20.800 usec
DE                  6.50 usec
TE                 302.2 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.25 usec
PLW1        47.00000000 W
SFO1       100.6228289 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2         7.75000000 W
PLW12        0.23583999 W
PLW13        0.19103000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127597 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

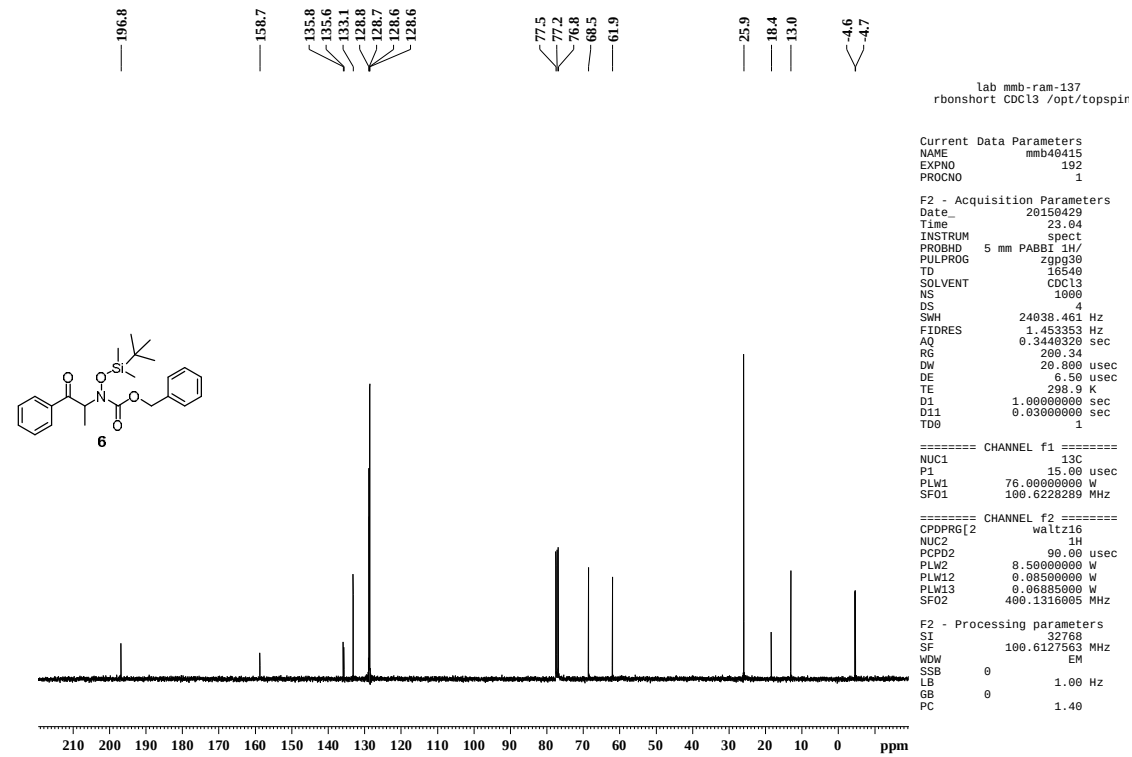

7.9245
7.9220
7.9042
7.9008
7.6129
7.6099
7.6069
7.5960
7.5914
7.5870
7.5759
7.5729
7.5698
7.4953
7.4756
7.4570
7.2598
5.5708
5.5528
5.5347
5.5167
1.5687
1.5505
1.4555
5d
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.0 1.0 2.1 1.0 3.0 9.0
lab mmb-ram-087 boc
ɔton(-5to15) CDCl3 /opt/topspin
Current Data Parameters
NAME mmb40115
EXPNO 28
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150103
Time 5.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 100
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 6.50 usec
TE 300.9 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


200.8
156.8
134.8
133.8
128.9
128.7
82.5
77.5
77.2
76.8
59.8
28.3
14.4
5d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
lab mmb-ram-087 boc
.itm_carbonshort CDCl3 /opt/topspin nmr 14
Current Data Parameters
NAME mmb40115
EXPNO 37
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150103
Time 5.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 2000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 301.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127538 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


7.9799
7.9632
7.9602
7.4594
7.4558
7.4406
7.4371
7.4219
7.4183
7.2732
7.2542
7.2354
7.2075
7.1907
6.0519
4.7969
4.7686
3.1556
3.1460
3.1349
3.1136
3.1021
3.0491
3.0425
3.0379
3.0311
3.0070
3.0003
2.9956
2.9890
2.5522
2.5405
2.5196
2.5081
2.4861
2.4744
2.4532
2.4416
2.3750
2.3683
2.3634
2.3567
2.3517
2.3446
2.3365
2.3314
2.3247
2.3196
2.3130
1.4504
lab mmb-ram-014 lo
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 9
Current Data Parameters
NAME mmb41014
EXPNO 27
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141012
Time 1.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 100
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 138.85
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.70 usec
PLW1 7.75000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300372 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OH
N
O
O
O
5e
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.0
1.0
1.1
1.2
1.0
1.0
1.1
1.1
1.1
1.1
9.0


194.7
158.1
144.1
134.3
132.0
129.0
127.9
127.0
82.6
77.5
77.2
76.8
66.0
29.1
28.3
27.7
lab mmb-ram-014 lo
iitm_carbonshort CDCl3 /opt/topspin nmr 9
Current Data Parameters
NAME mmb41014
EXPNO 28
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141012
Time 2.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 3000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.25 usec
PLW1 47.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 7.75000000 W
PLW12 0.23583999 W
PLW13 0.19103000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127563 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OH
N
O
O
O
5e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.9479
7.9463
7.9283
7.9249
7.5479
7.5453
7.5291
7.5109
7.4173
7.3976
7.3784
7.3414
7.3319
7.3109
7.2598
5.4912
5.4741
5.4571
5.4401
5.2050
5.1750
5.1625
5.1325
1.5058
1.4887
0.8215
-0.0270
-0.1883
lab mmb-ram-137
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 1
Current Data Parameters
NAME mmb40415
EXPNO 188
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150429
Time 22.39
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 56.23
DW 62.400 usec
DE 6.50 usec
TE 298.6 K
D1 0.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.00 usec
PLW1 8.50000000 W
SFO1 400.1320007 MHz
F2 - Processing parameters
SI 65536
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
6
11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.1 1.1 2.1 5.0 1.0 2.0 3.0 9.0 3.0 3.0


196.8
158.7
135.8
135.6
133.1
128.8
128.7
128.6
128.6
77.5
77.2
76.8
68.5
61.9
25.9
18.4
13.0
-4.6
-4.7
lab mmb-ram-137
rbonshort CDCl3 /opt/topspin
Current Data Parameters
NAME mmb40415
EXPNO 192
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150429
Time 23.04
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 16540
SOLVENT CDCl3
NS 1000
DS 4
SWH 24038.461 Hz
FIDRES 1.453353 Hz
AQ 0.3440320 sec
RG 200.34
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 15.00 usec
PLW1 76.00000000 W
SFO1 100.6228289 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 8.50000000 W
PLW12 0.08500000 W
PLW13 0.06885000 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127563 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm