

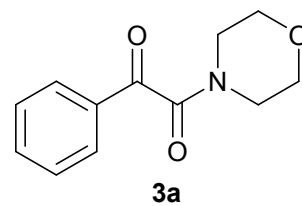
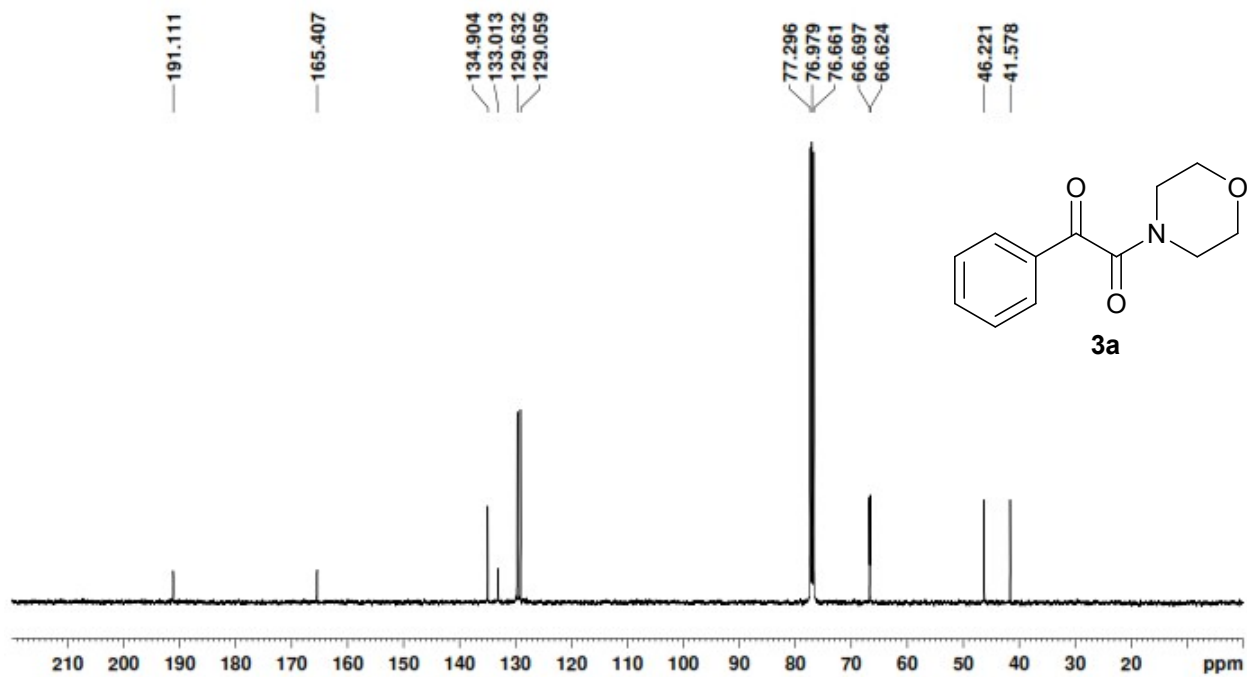
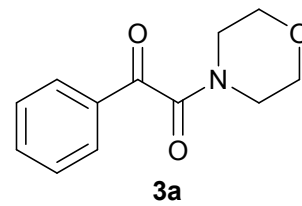
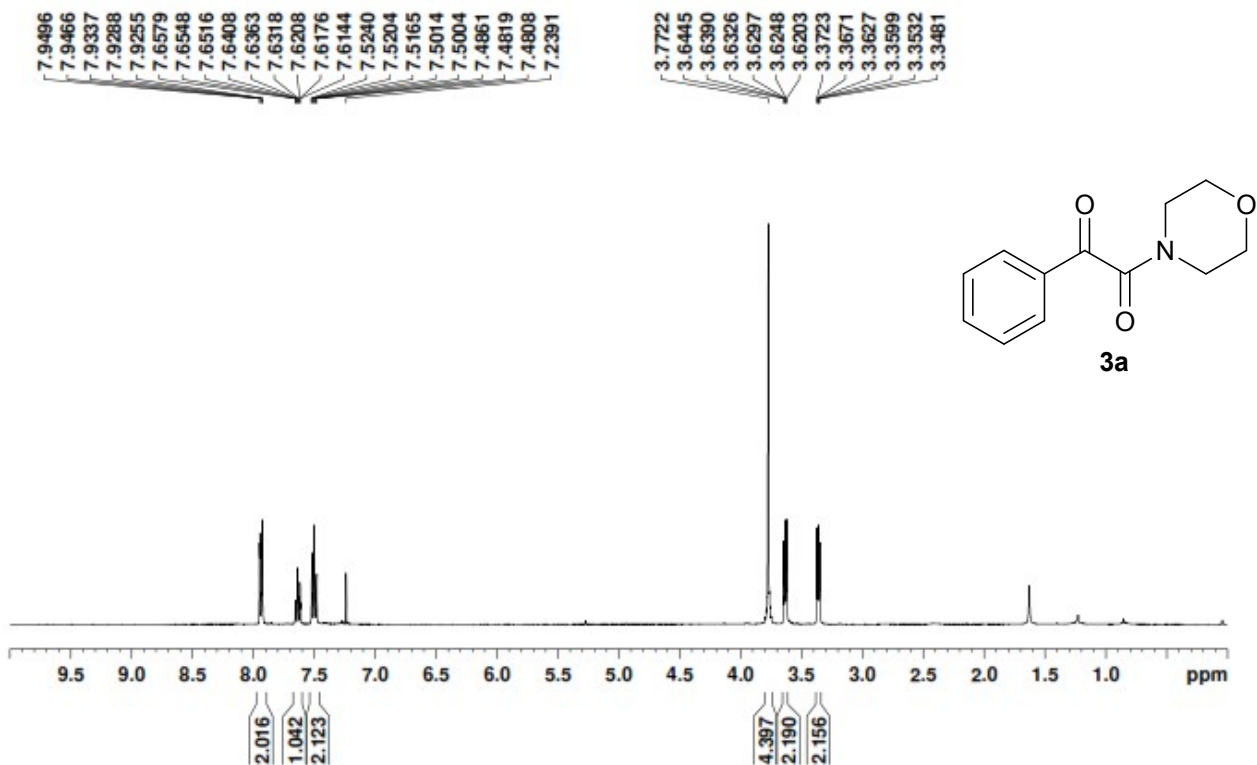
Supporting Information

One Pot Synthesis of α -Ketoamides from Ethylarenes and Amines: A Metal Free Difunctionalization Strategy

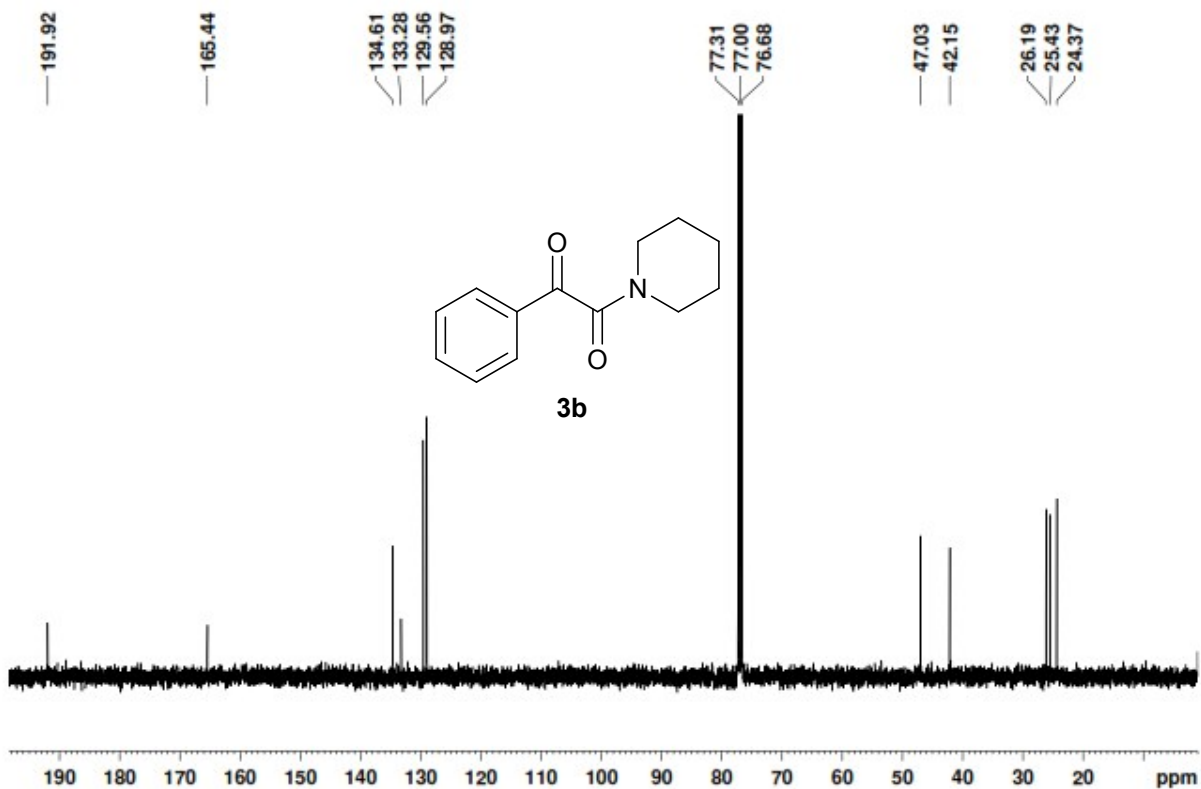
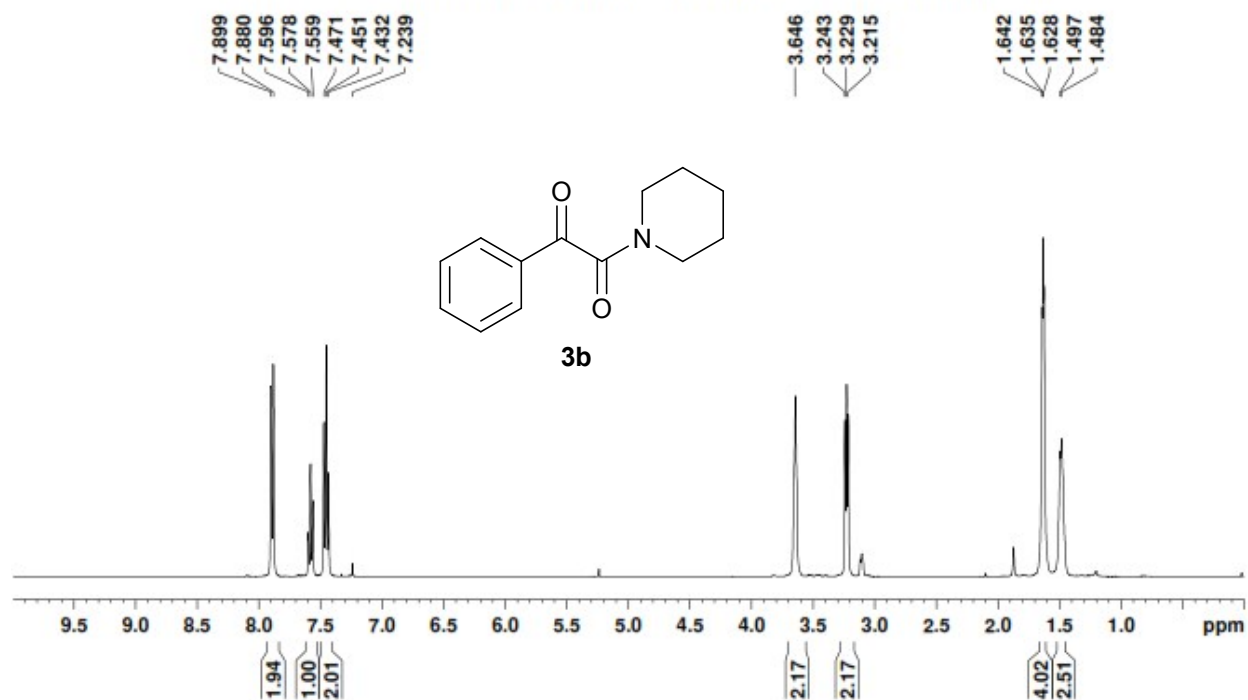
Mani Ramanathan, Chun-Kai Kuo and Shiuh-Tzung Liu*

Department of Chemistry, National Taiwan University, Taipei 106, Taiwan.

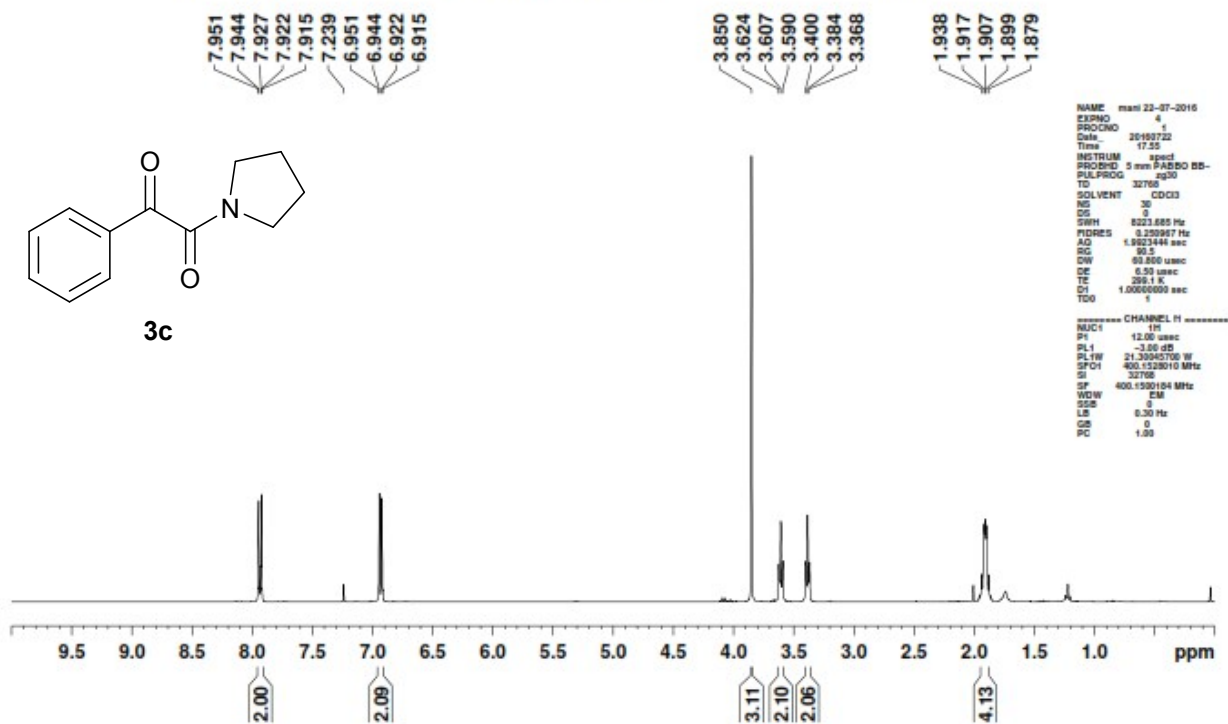
^1H and ^{13}C spectra for all the compounds (28 pages)



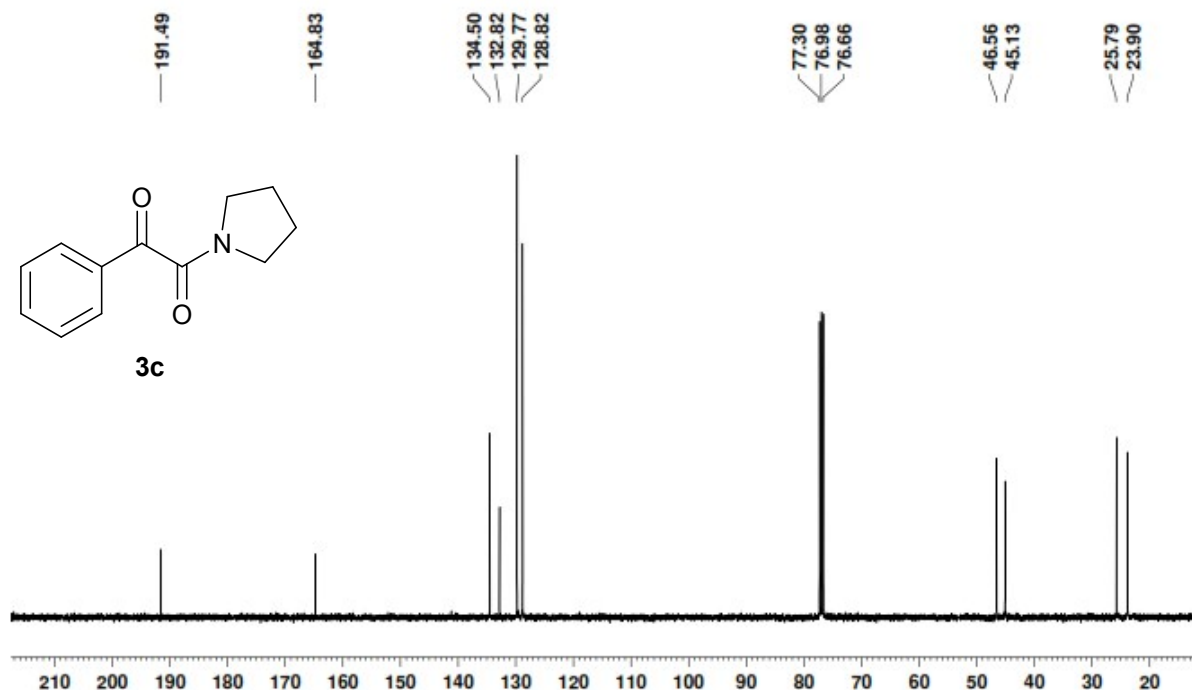
EtBz-I2-Py-TBHP, 80deg, 10h, NaI-Piperidine-TBHP, rt, 6h, purified

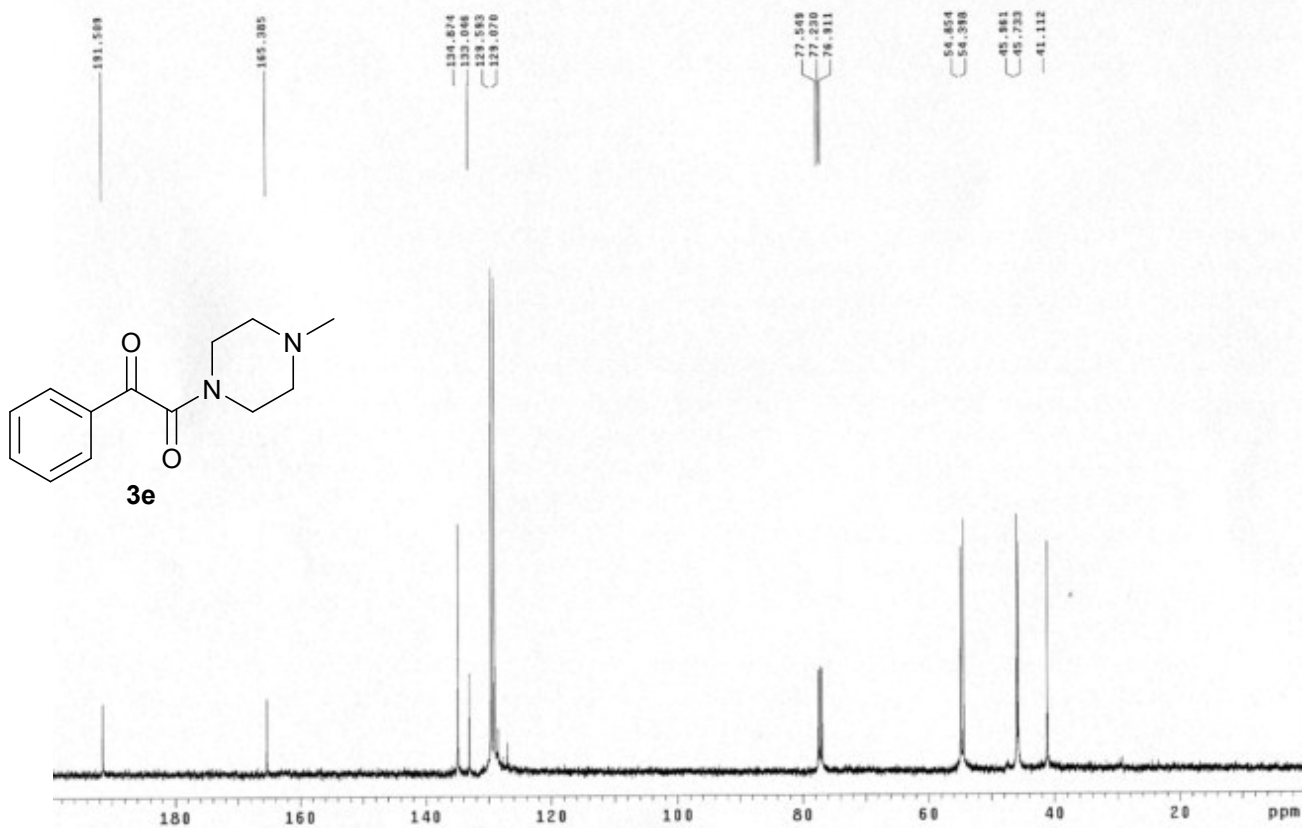
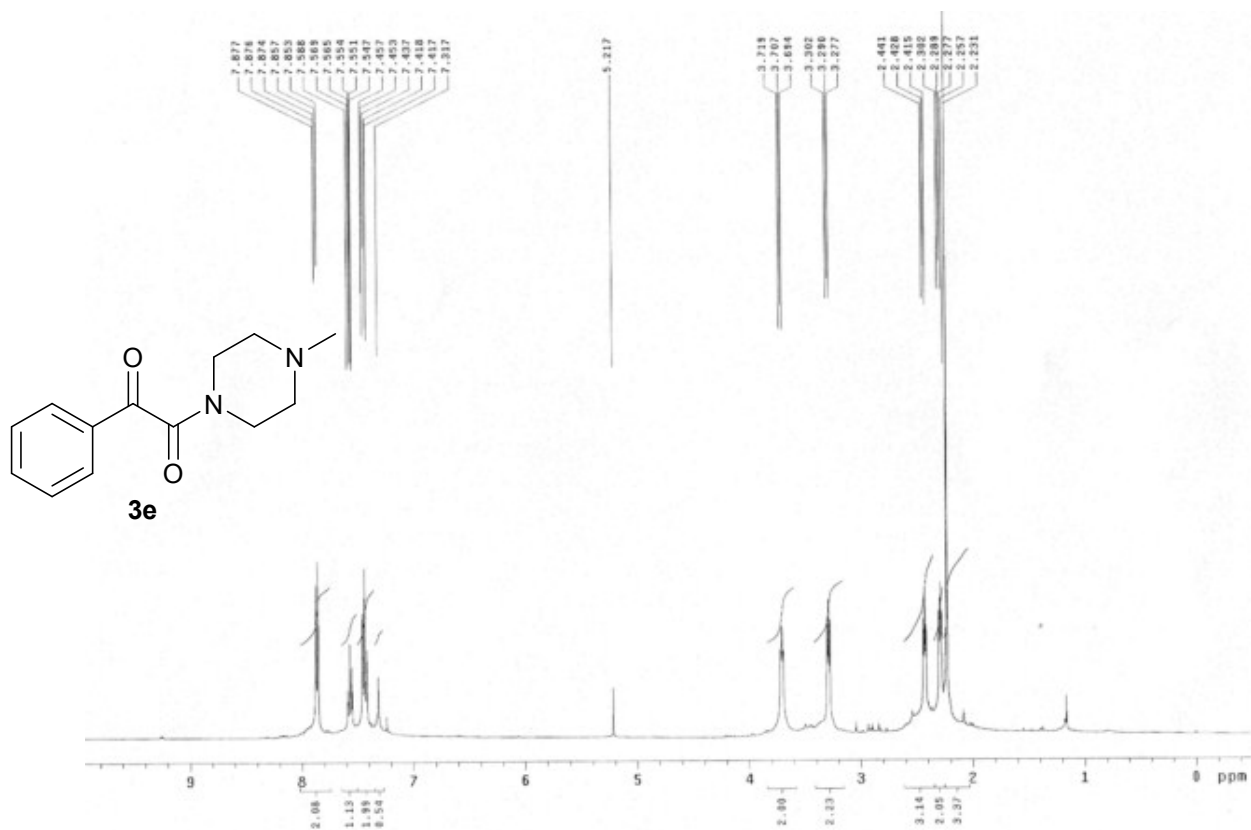


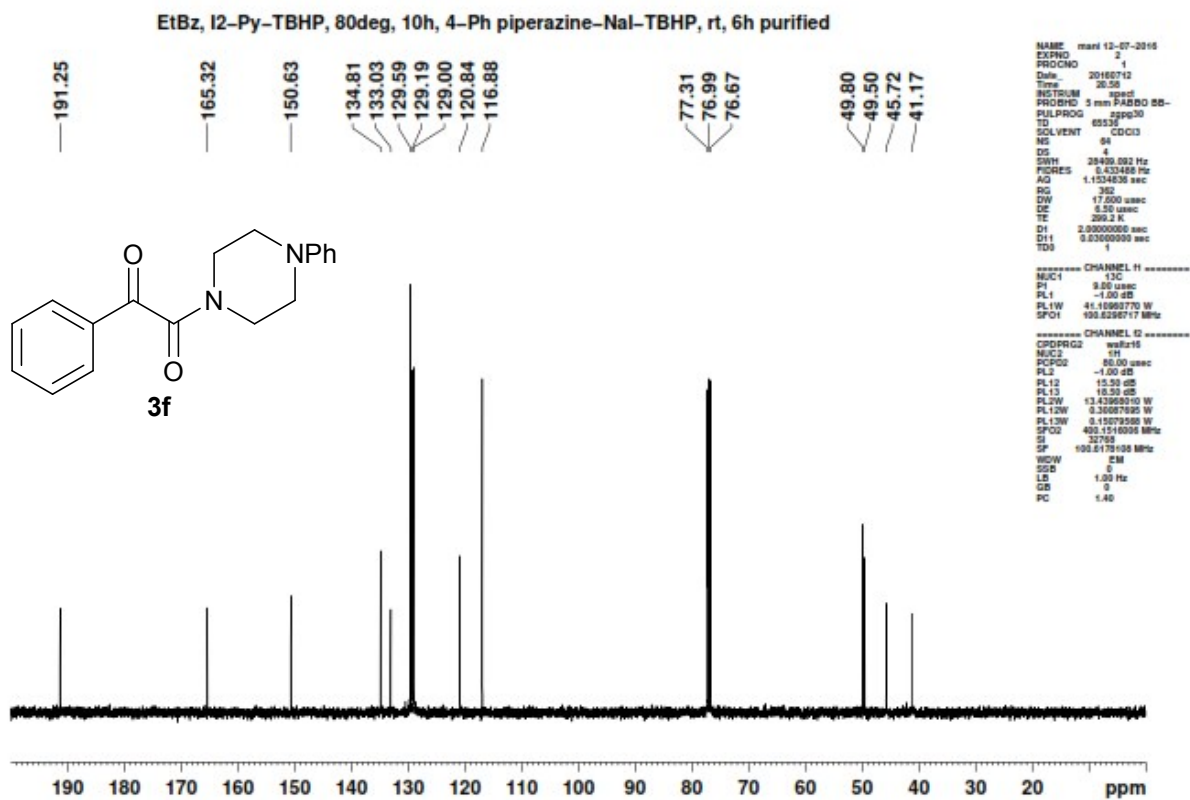
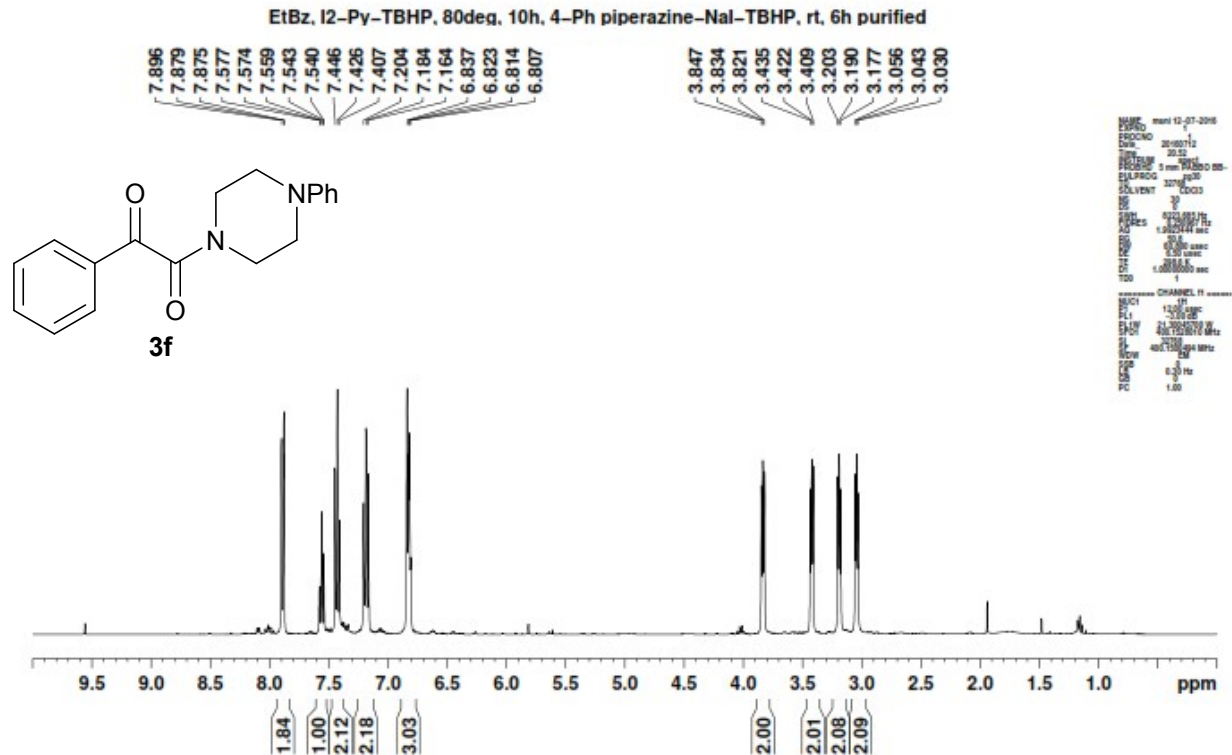
4-OMe EtBz, I2-Py-TBHP, 80deg, 10h, NaI-pyrrolidine-TBHP, rt, 6h, purified



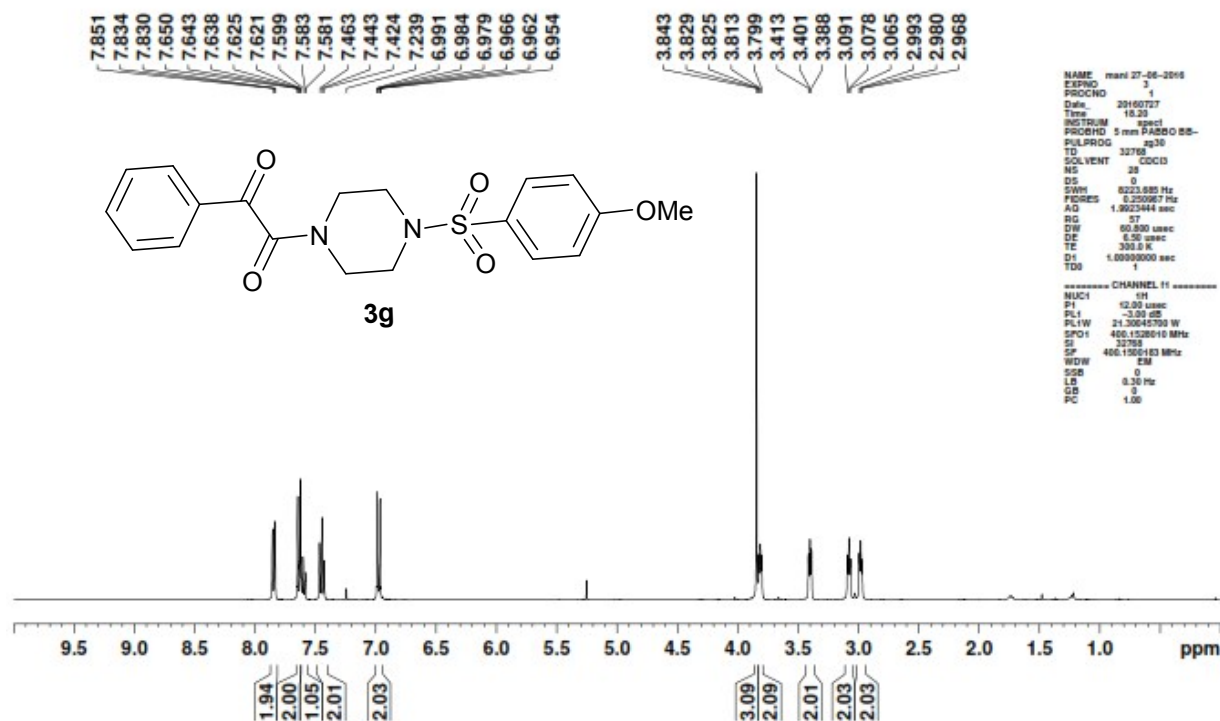
EtBz, I2-Py-TBHP, 80deg, 10h, Pyrrolidine-NaI-TBHP, rt, 6h purified



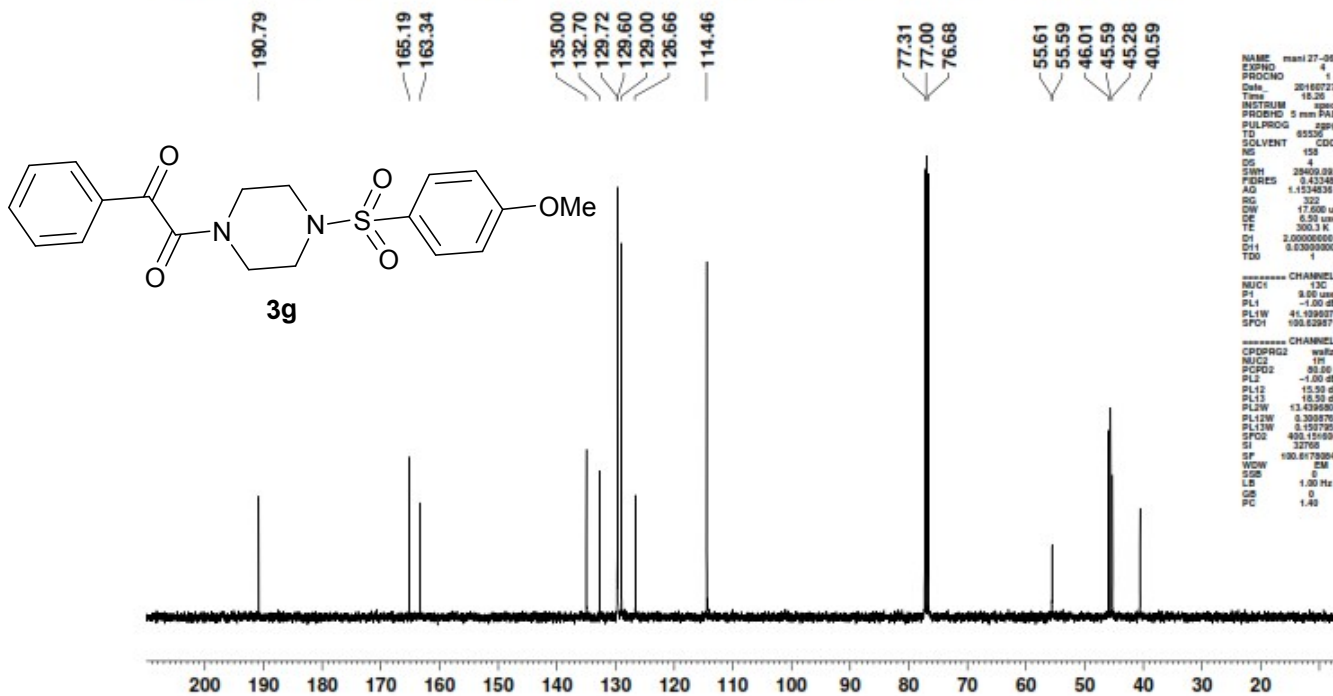




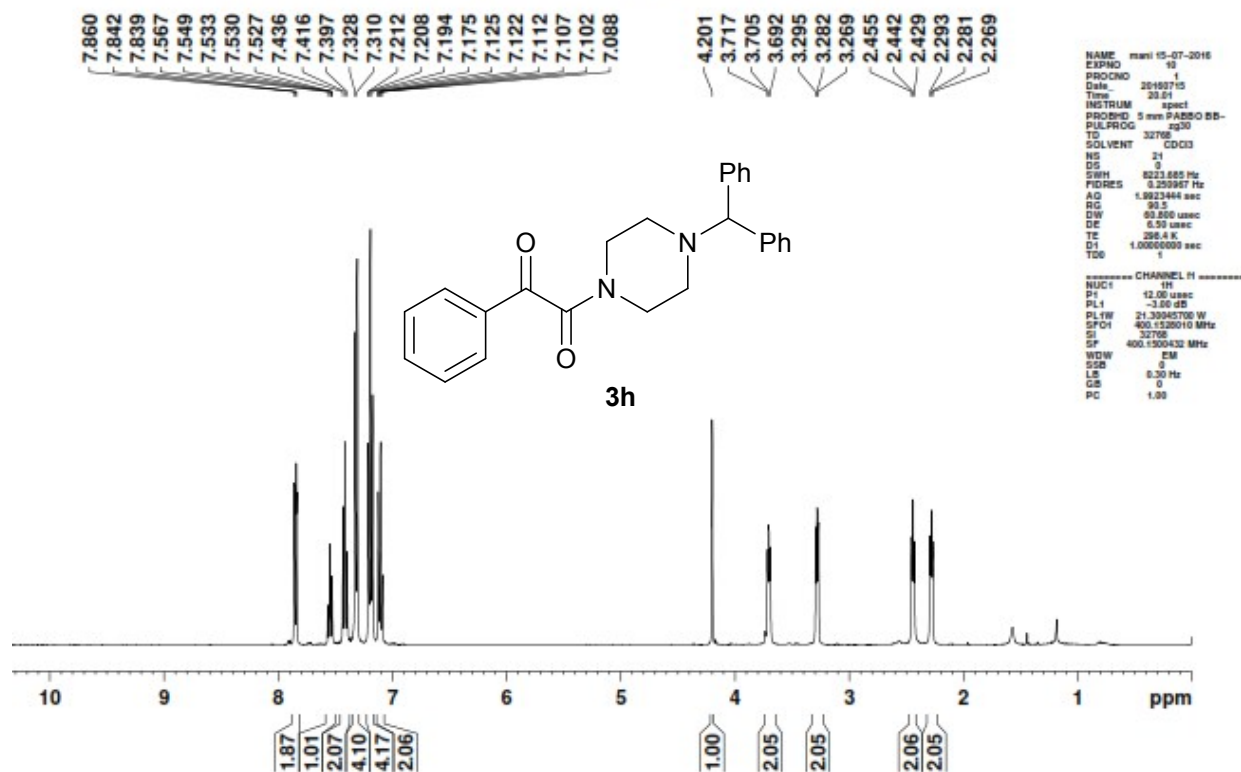
EtBz, I2-Py-TBHP, 80deg, 10h, NaI-N-(4-OMe phenylsulfonyl)piperazine-TBHP, rt 12h, purified



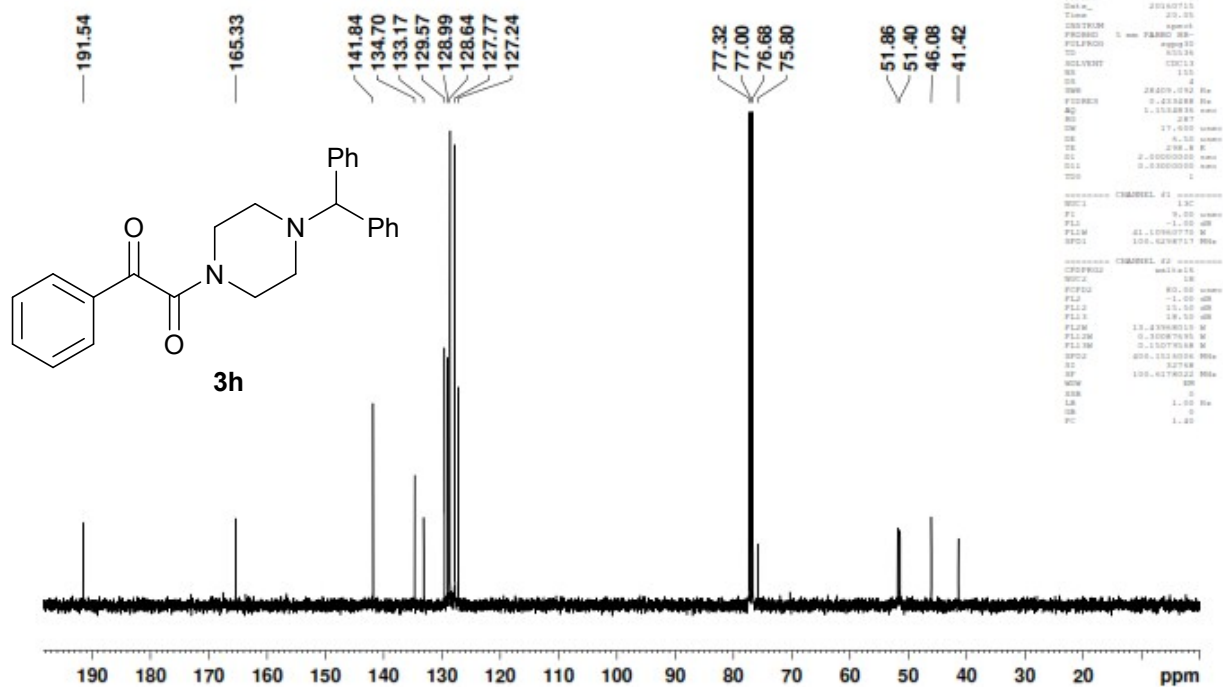
EtBz, I2-Py-TBHP, 80deg, 10h, NaI-N-(4-OMe phenylsulfonyl)piperazine-TBHP, rt 12h, purified



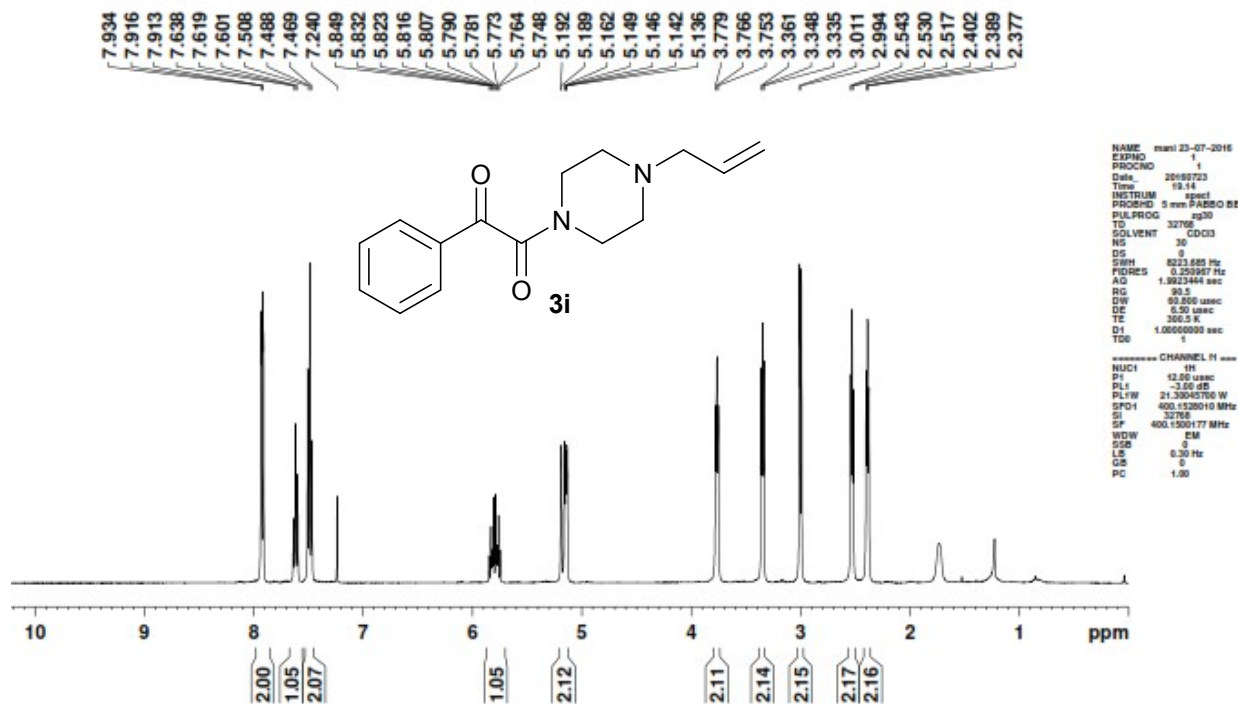
EtBz, I2-Py-TBHP, 80deg, 10h, 4-diphenylmethyl piperazine, TBHP, rt, 6h, purified



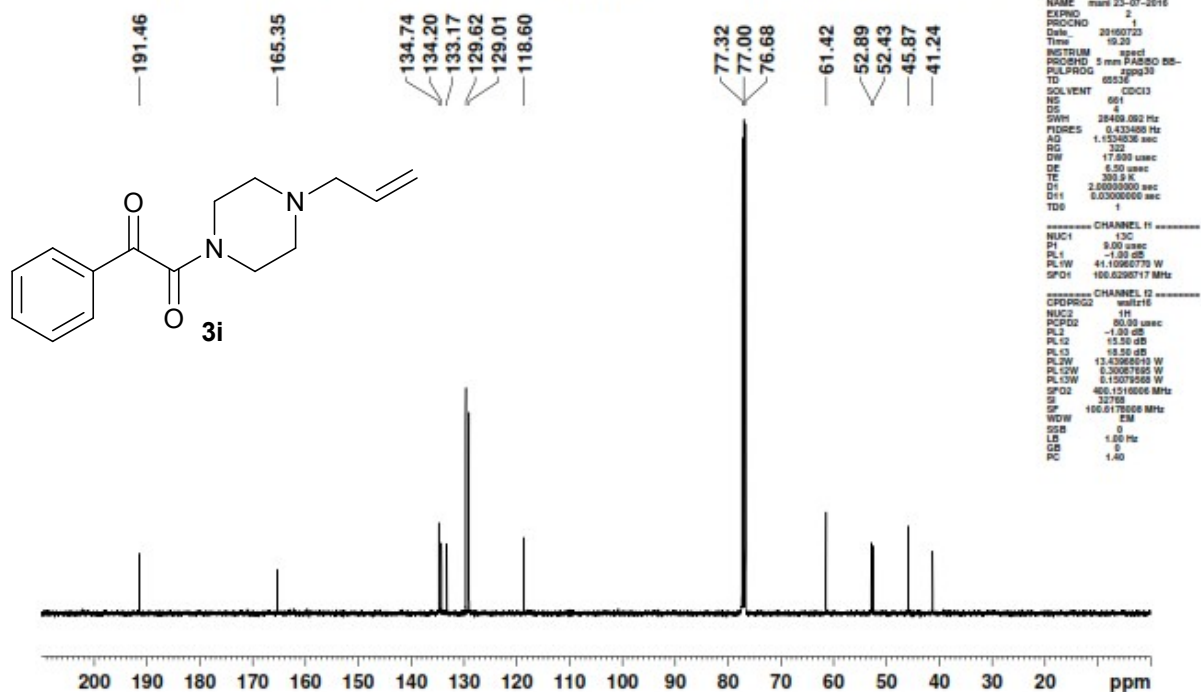
EtBz, I2-Py-TBHP, 80deg, 10h, 4-diphenylmethyl piperazine, TBHP, rt, 6h, purif



EtBz, I2-Py-TBHP, 80deg, 10h, NaI-N-allylpiperazine-TBHP, rt, 6h, purified



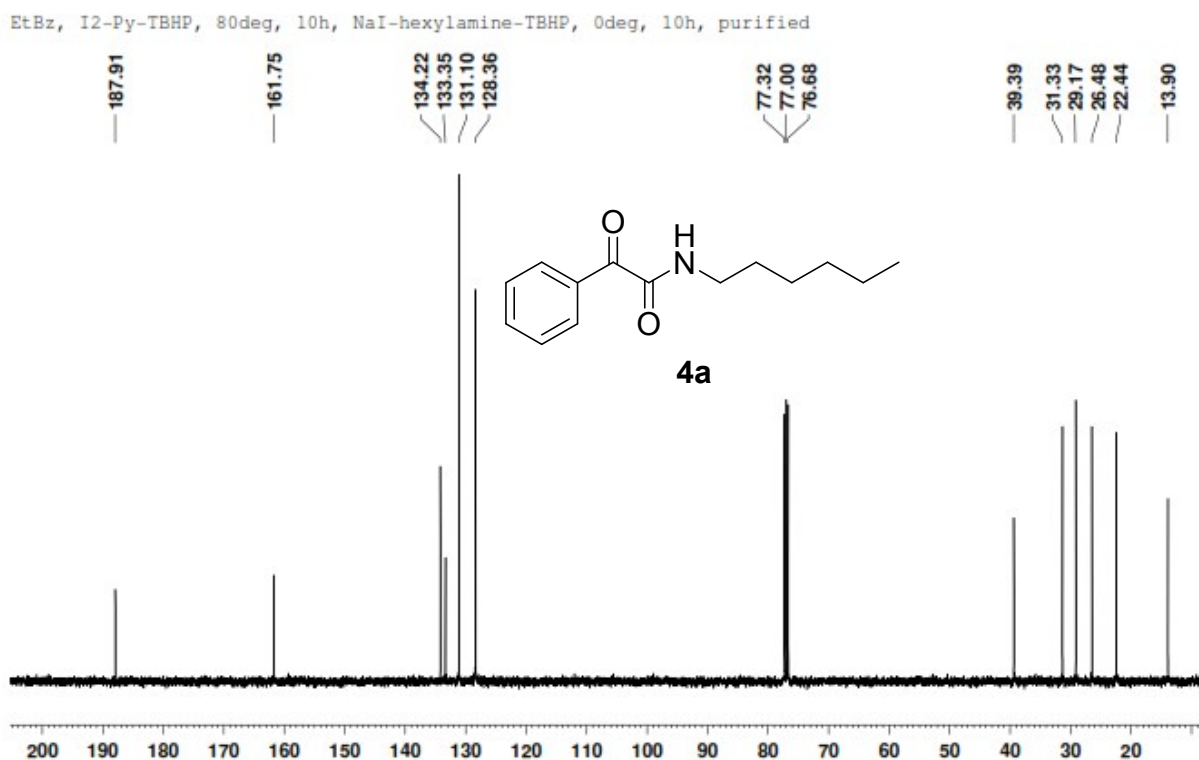
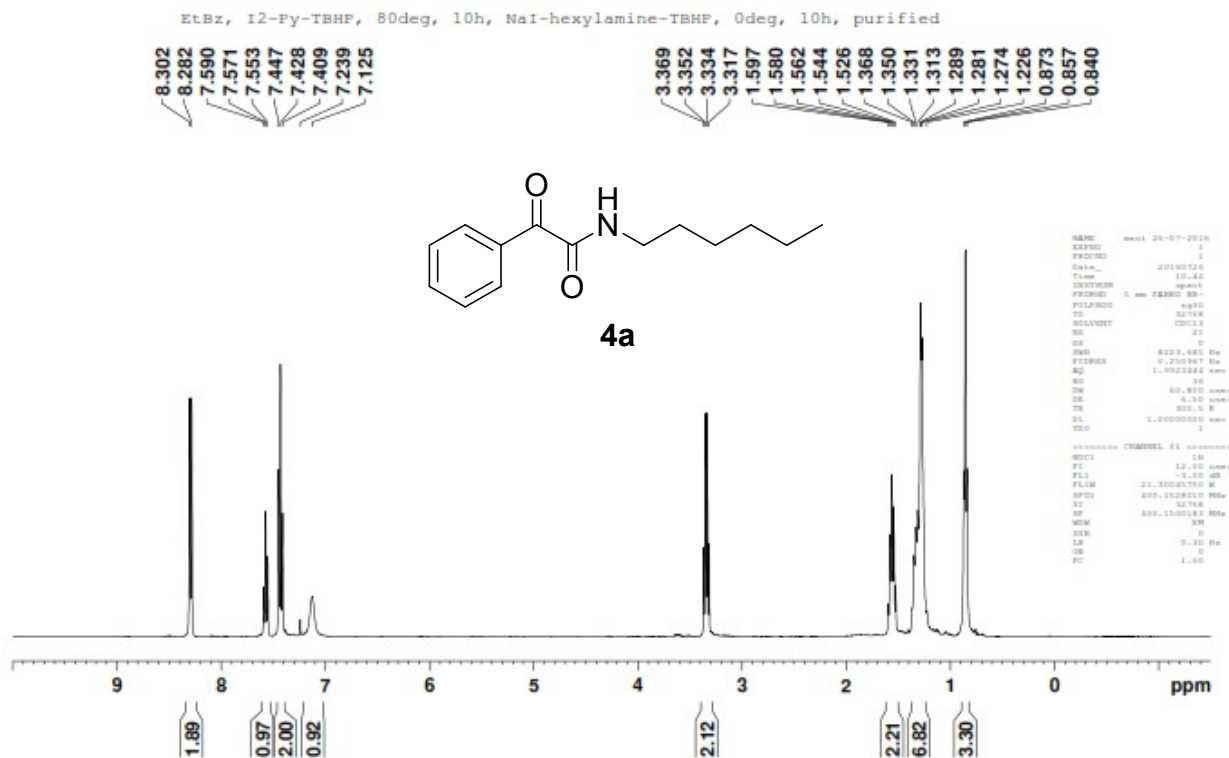
EtBz, I2-Py-TBHP, 80deg, 10h, NaI-N-allylpiperazine-TBHP, rt, 6h, purified

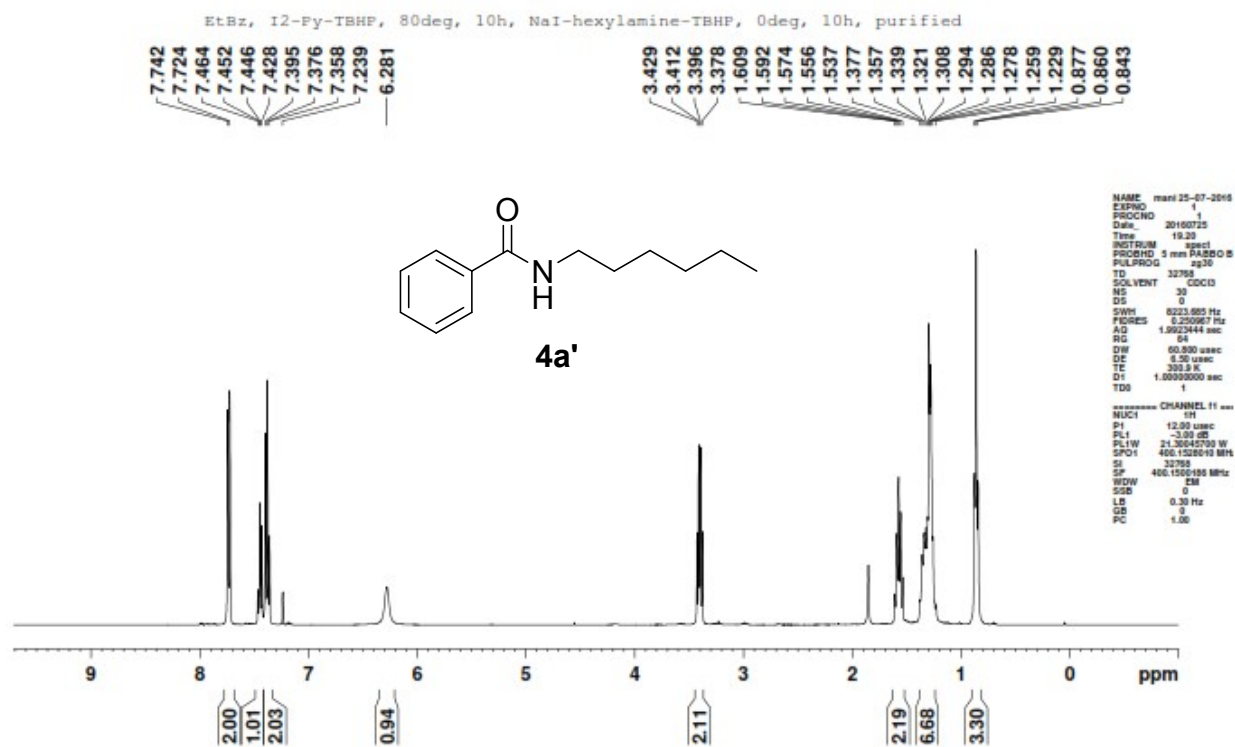


Chemical structure of **3j** is shown above the spectrum. The spectrum displays peaks from 1.0 to 8.0 ppm. Aromatic protons appear as a multiplet between 7.2 and 7.9 ppm. The piperidine ring protons show a complex pattern between 3.3 and 4.2 ppm. The ethyl ester group is visible as a quartet at ~4.1 ppm and a triplet at ~1.2 ppm. Integration values are provided below the baseline.

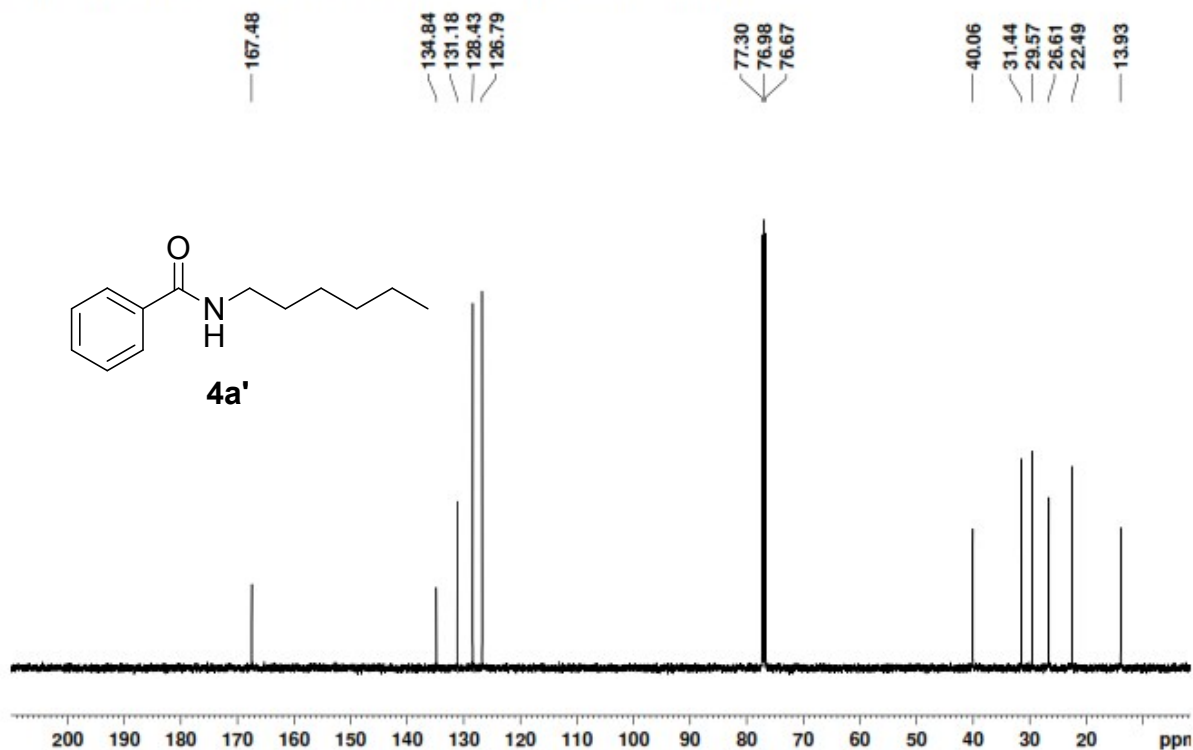
Chemical structure of **3j** (ethyl 1-(benzoylcarbamoyl)piperazine-4-carboxylate) is shown as an inset. The structure consists of a piperazine ring with a benzoylcarbamoyl group at position 1 and an ethyl ester group at position 4.

¹³C NMR spectrum (CDCl₃) of compound **3j** showing peaks at the following chemical shifts (ppm): 191.01, 165.51, 155.15, 134.91, 132.91, 129.60, 129.03, 77.29, 76.97, 76.66, 61.79, 45.64, 41.07, and 14.51.

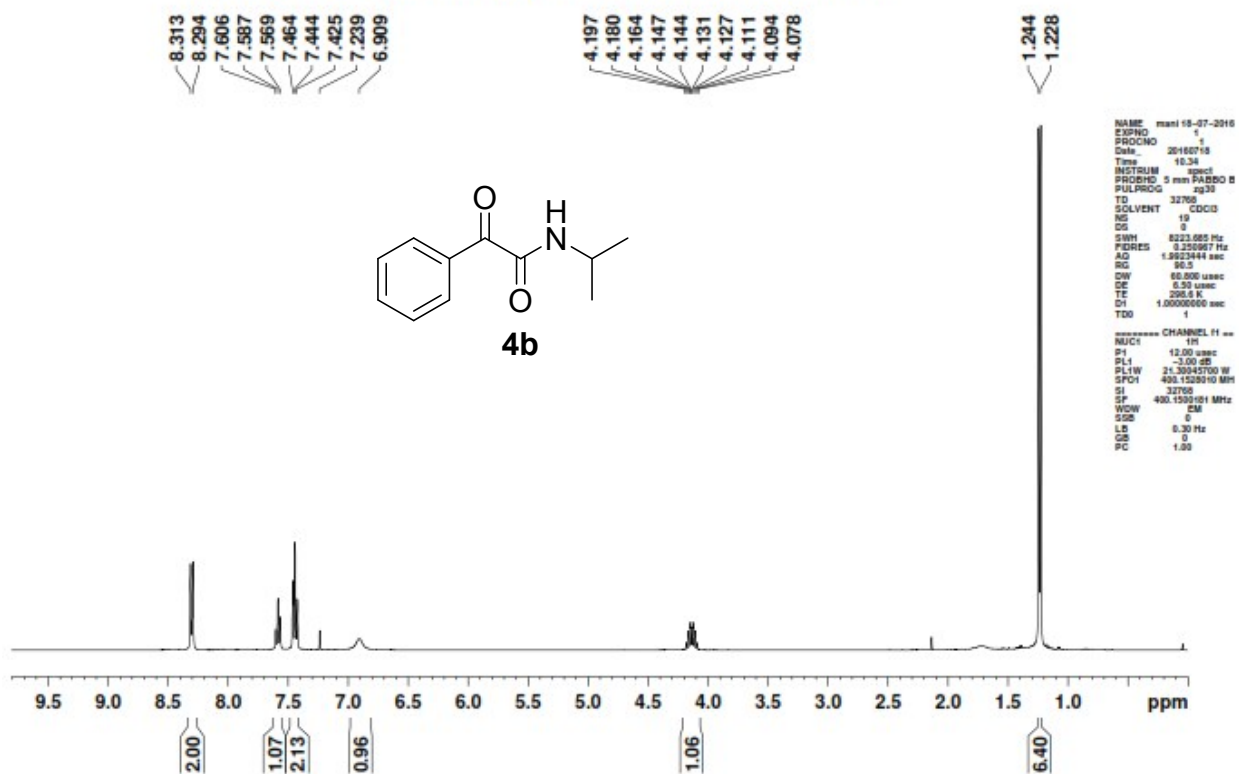




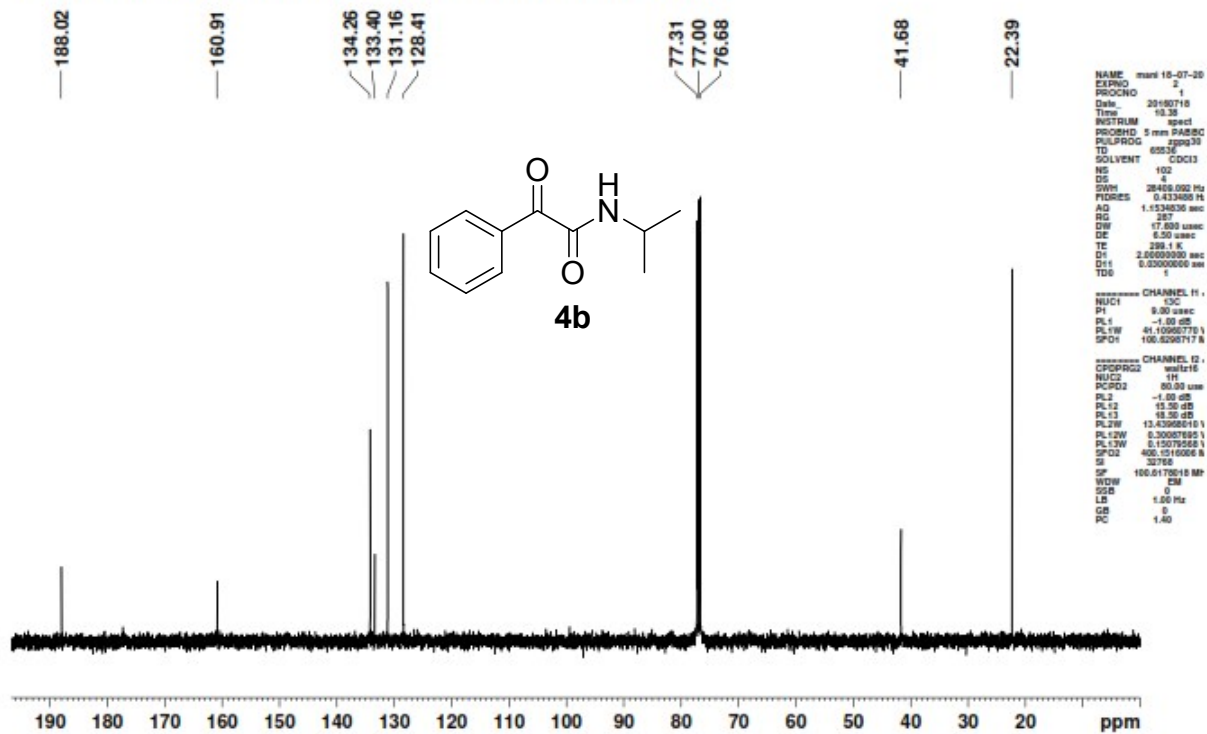
EtBz, I2-Py-TBHP, 80deg, 10h, NaI-hexylamine-TBHP, 0deg, 10h, purified



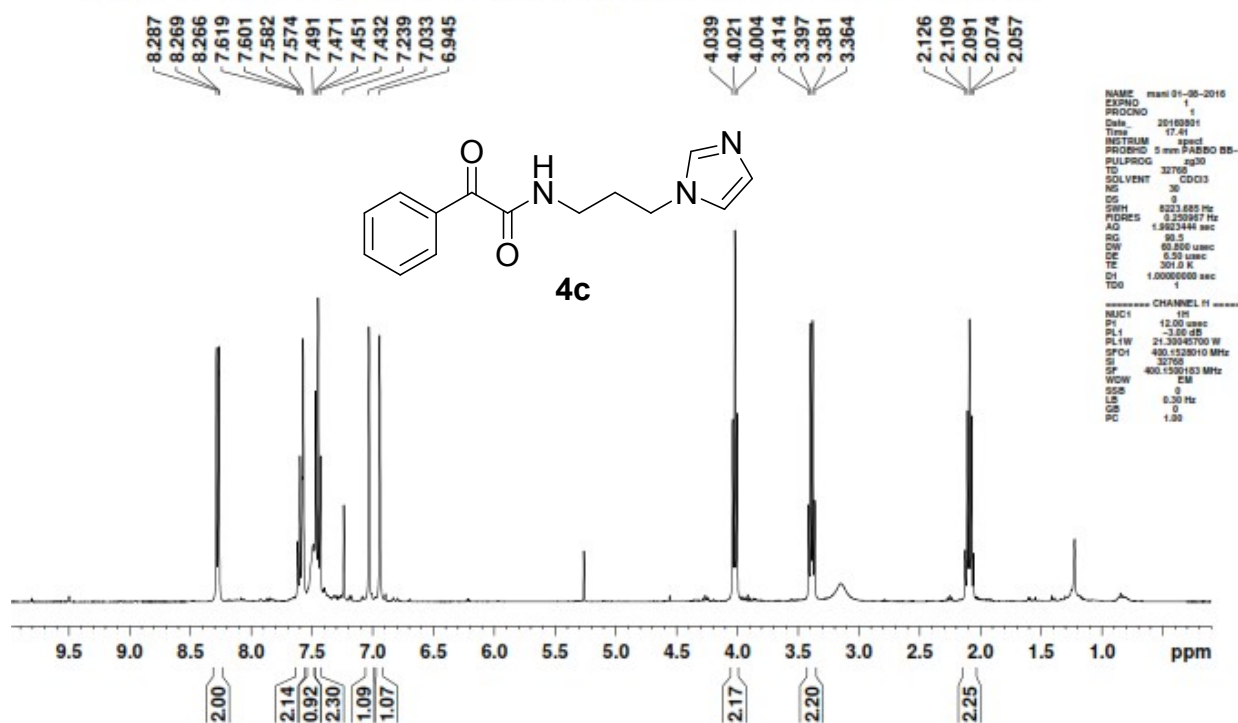
EtBz, I2-Py-TBHP, 80deg, 10h, isopropylamine, NaI, TBHP.0deg, 10h, purified



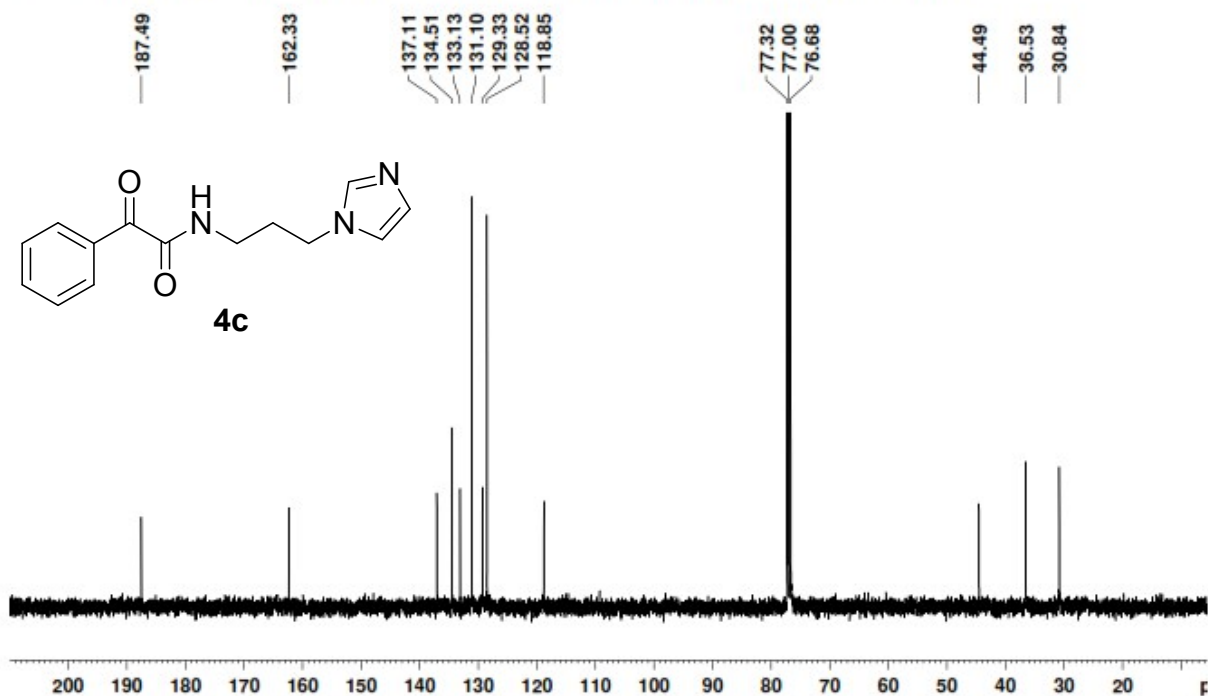
EtBz, I2-Py-TBHP, 80deg, 10h, isopropylamine, NaI, TBHP.0deg, 10h, purified



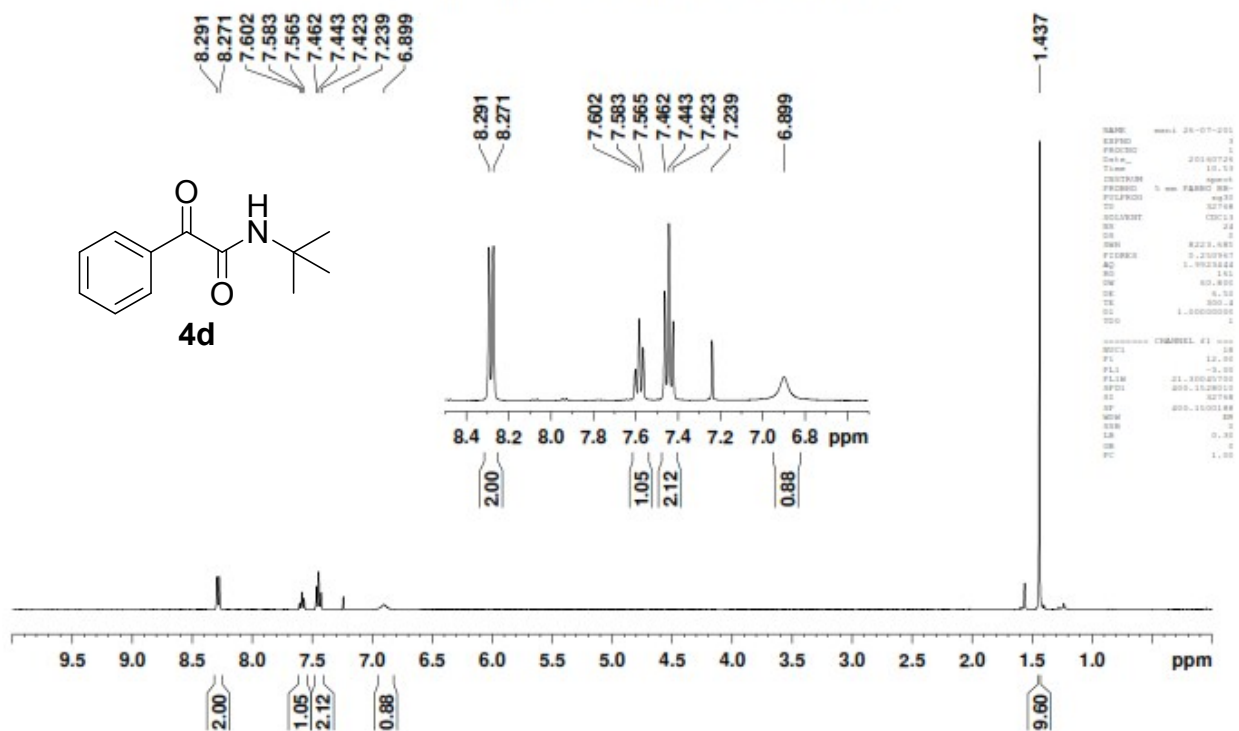
EtBz, I2-Py-TBHP, 80deg, 10h, NaI-3-(imidazolo)propylamine-TBHP, 0deg, 10h, purified



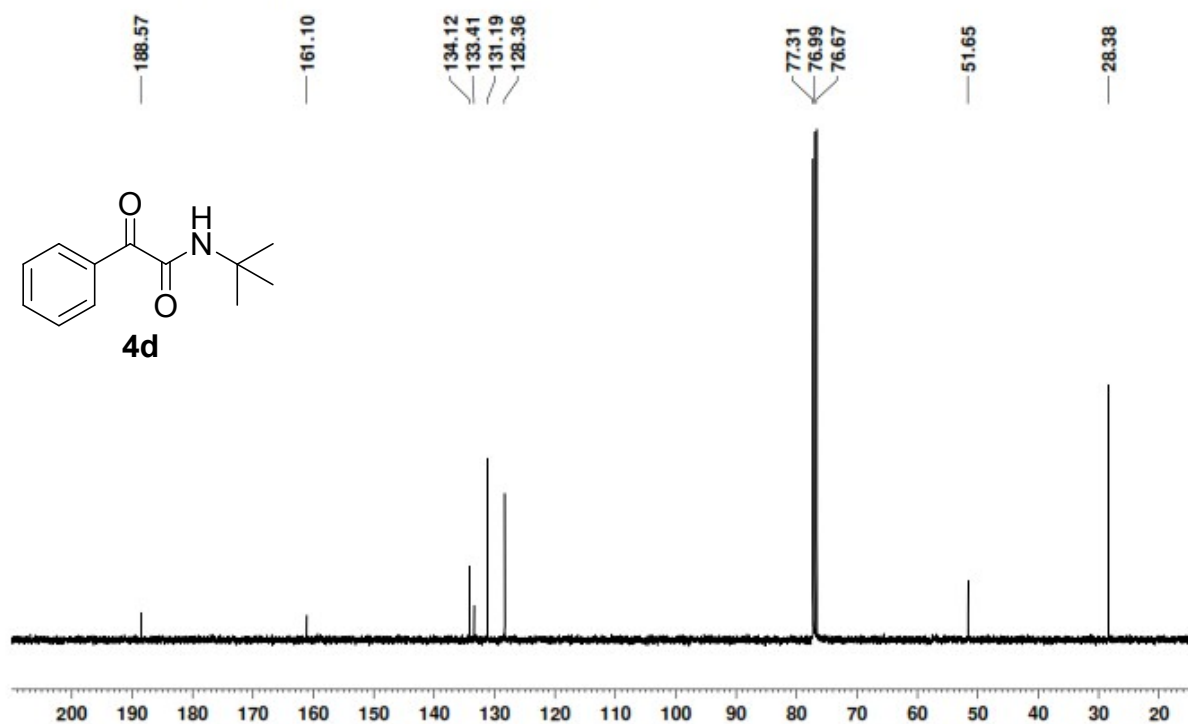
EtBz, I2-Py-TBHP, 80deg, 10h, NaI-3-(imidazolo)propylamine-TBHP, 0deg, 10h, purified

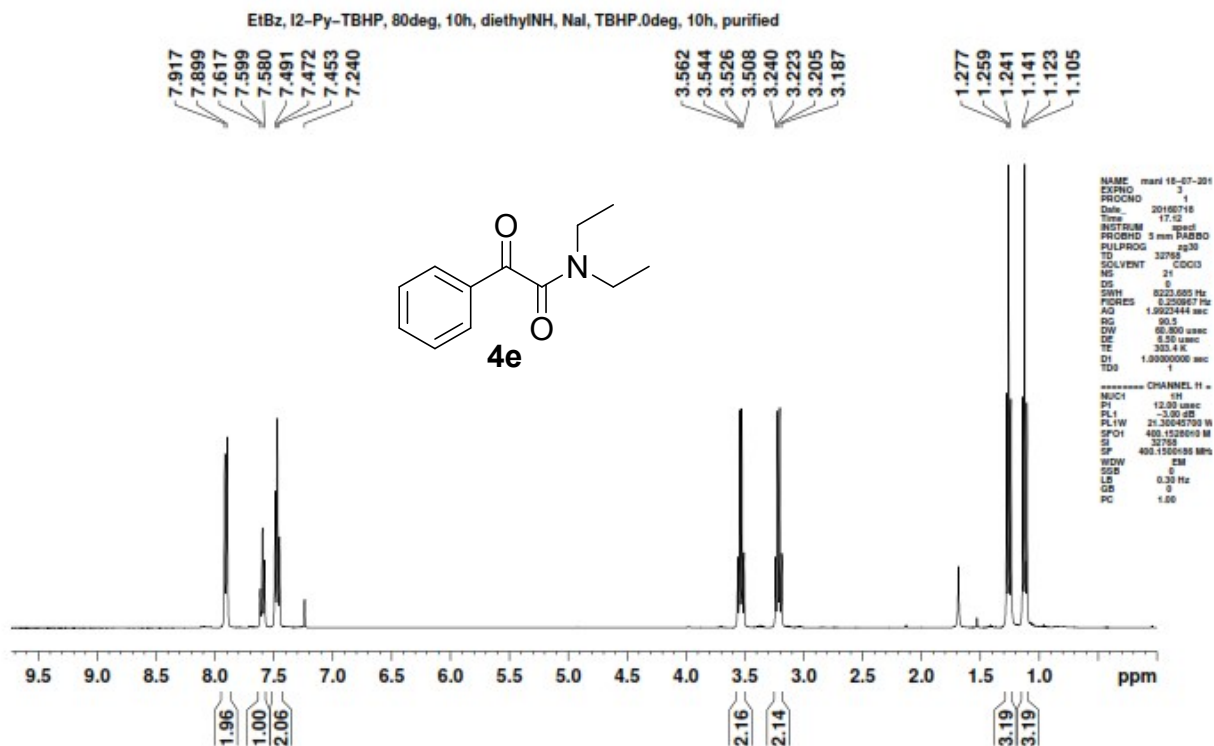


EtBz, 12-Py-TBHP, 80deg, 10h, NaI-tBuNH2-TBHP, 0deg, 10h, purified

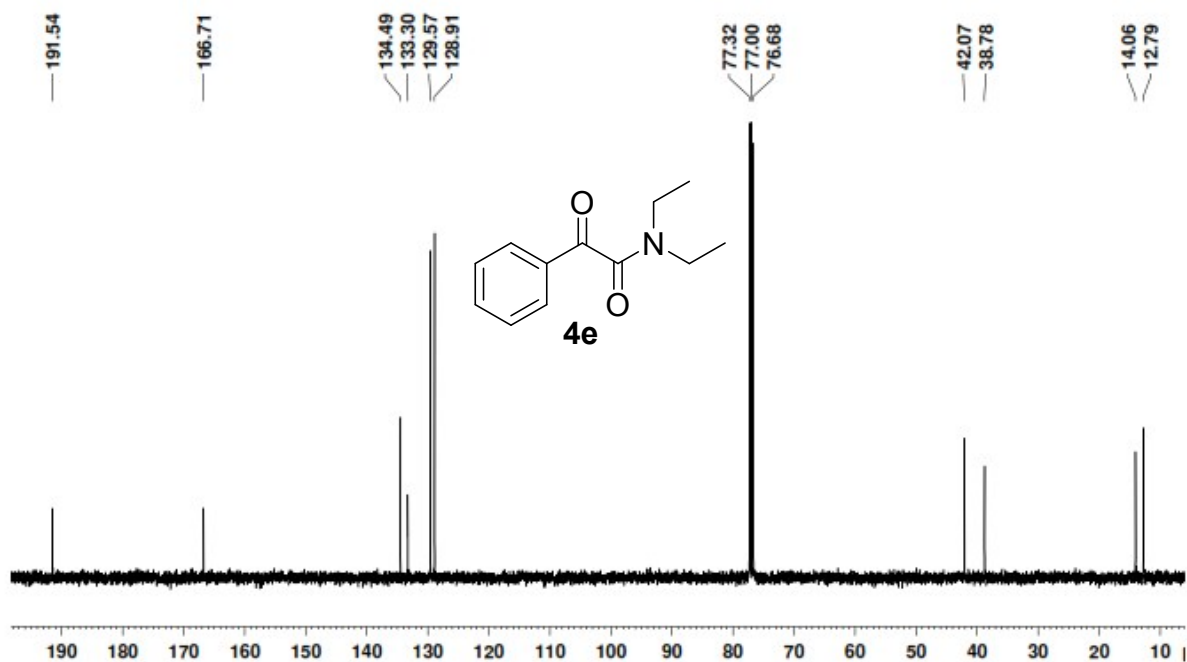


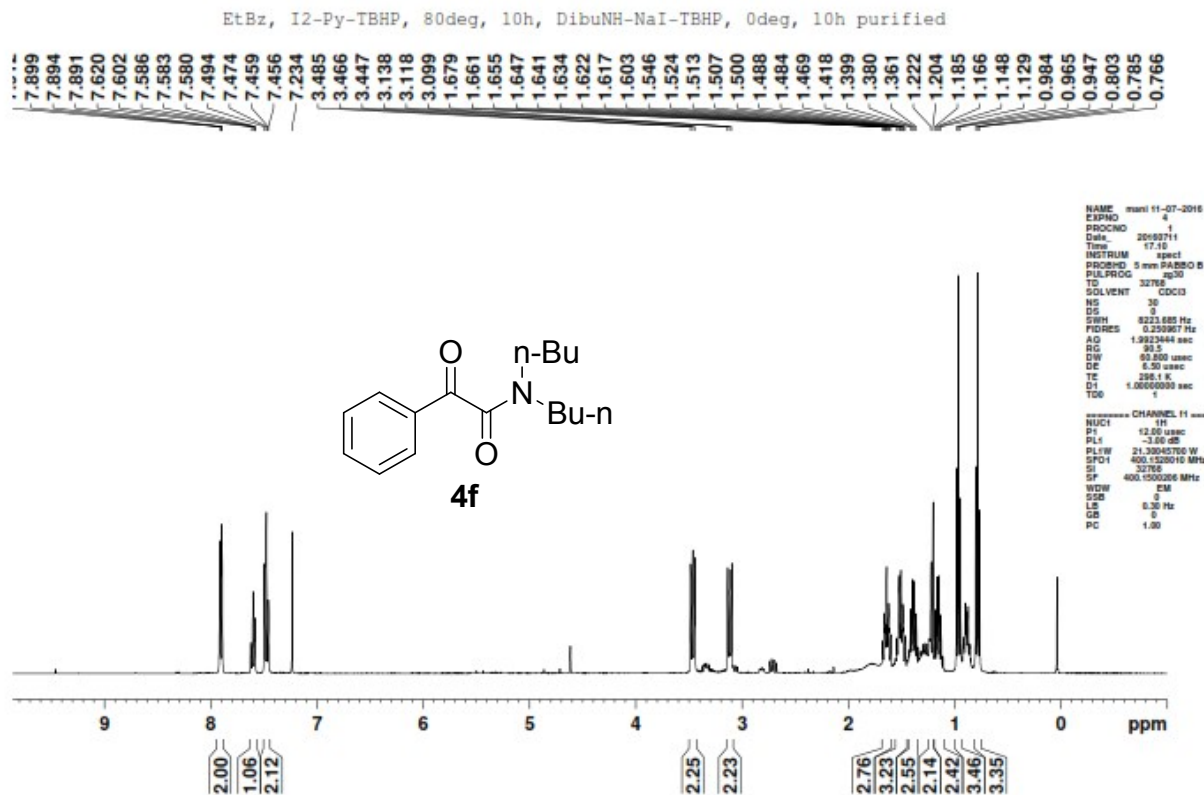
EtBz, 12-Py-TBHP, 80deg, 10h, NaI-tBuNH2-TBHP, 0deg, 10h, purified



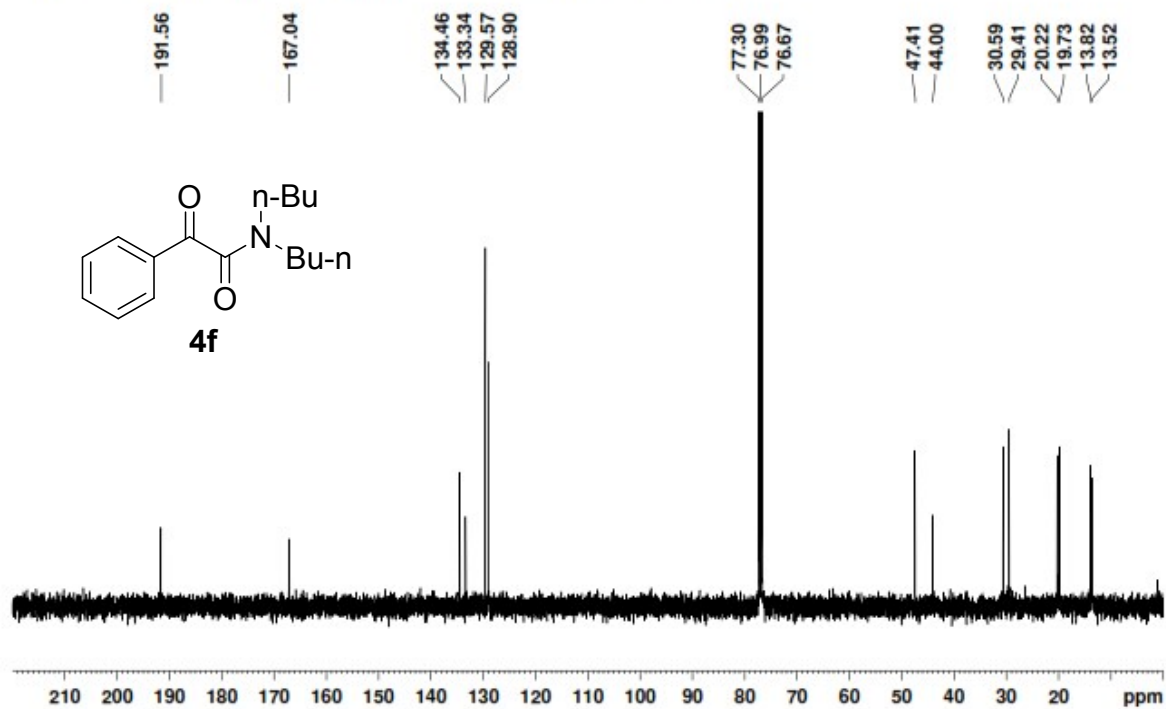


EtBz, I2-Py-TBHP, 80deg, 10h, diethylNH, NaI, TBHP.0deg, 10h, purified

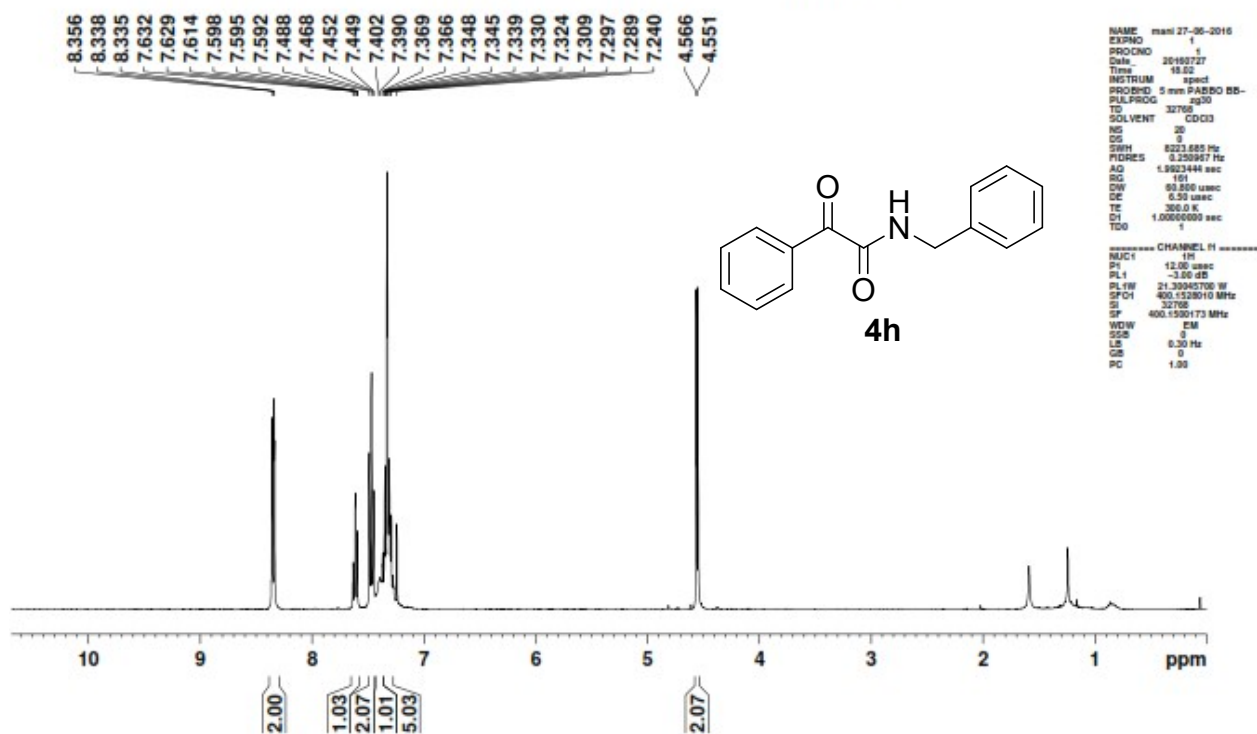




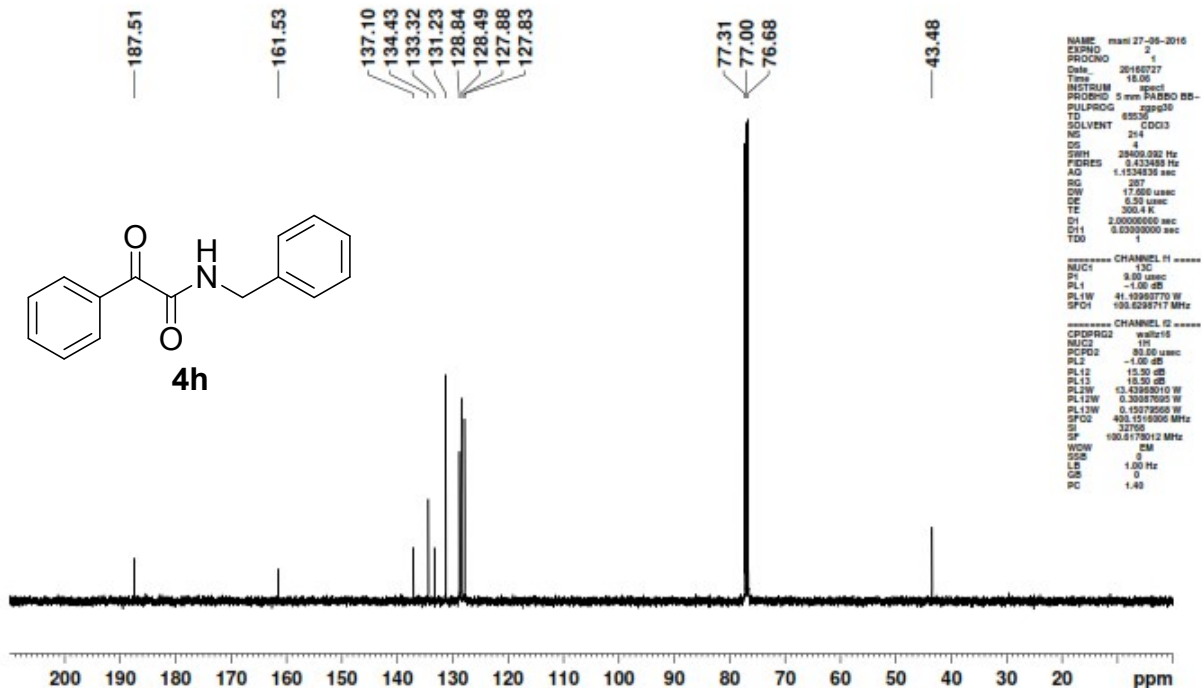
EtBz, I2-Py-TBHP, 80deg, 10h, DibuNH-NaI-TBHP, 0deg, 10h purified



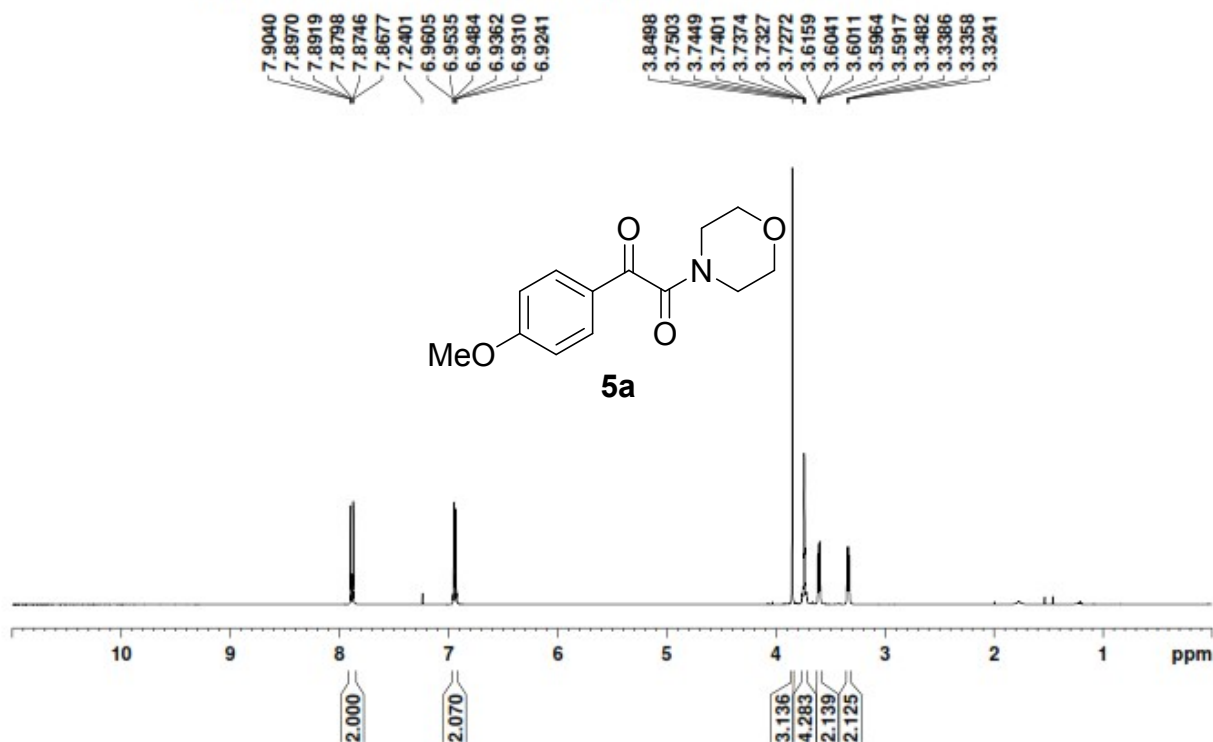
EtBz, I2-Py-TBHP, 80deg, 10h, NaI-benzylamine-TBHP, 0deg, 10h, purified



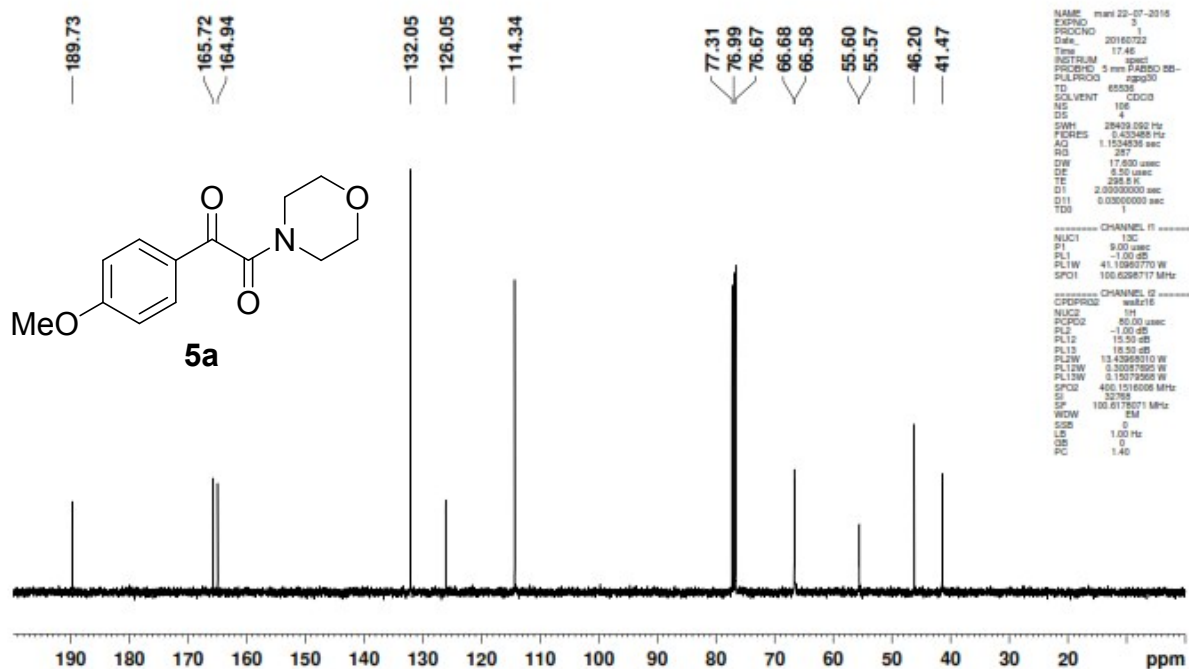
EtBz, I2-Py-TBHP, 80deg, 10h, NaI-benzylamine-TBHP, 0deg, 10h, purified



4-OMe EtBz, I2-Py-TBHP, 80deg, 10h, NaI-Morpholine-TBHP, rt, 6h, purified



4-OMe EtBz, I2-Py-TBHP, 80deg, 10h, NaI-Morpholine-TBHP, rt, 6h, purified

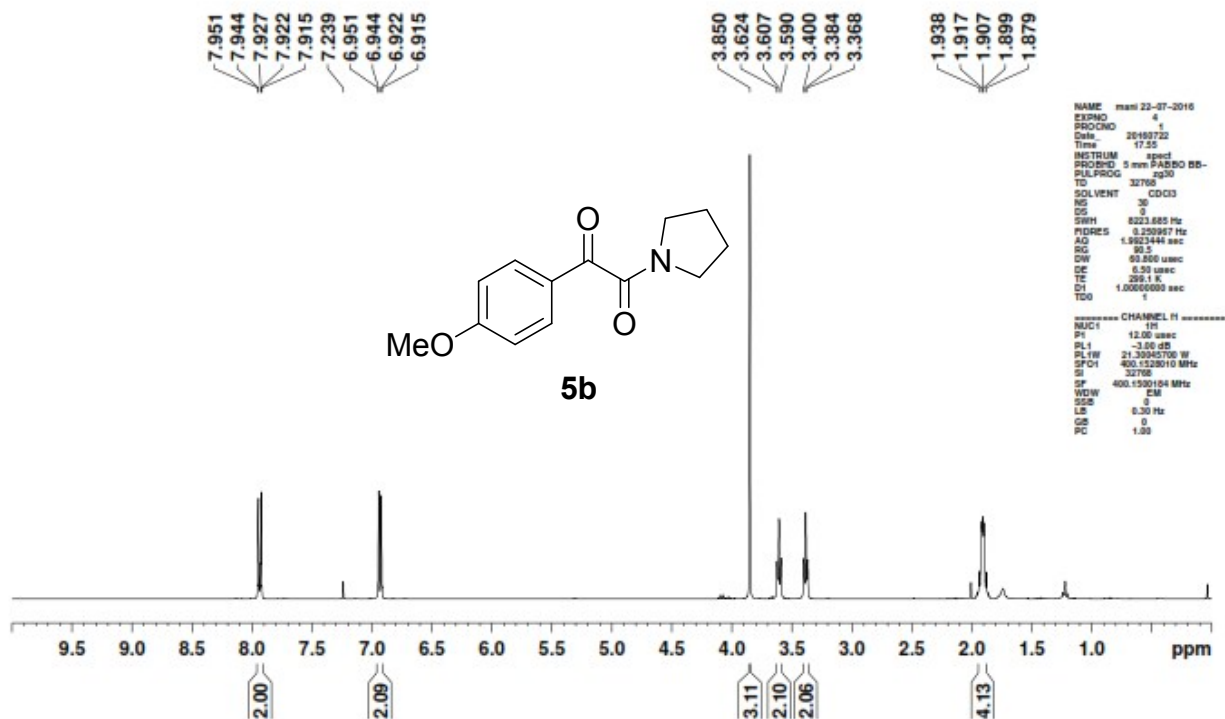


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SWH: 28432.000 Hz
F2RES: 0.433486 Hz
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TE: 298.2 K
D1: 2.00000000 sec
D11: 0.03000000 sec
TDS: 1

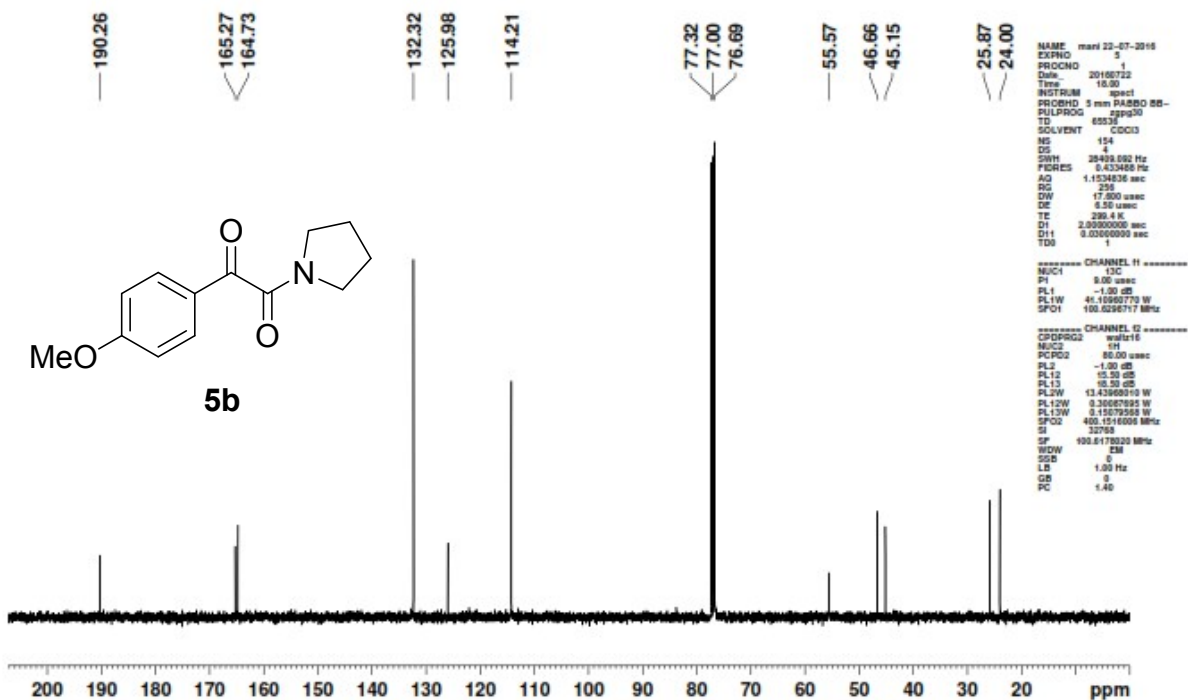
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PL1: 1.00 dB
PL1W: 41.10960770 W
SFO1: 100.626117 MHz

===== CHANNEL f2 =====
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NUC2: 1H
PCPD2: 85.00 usec
PL2: -1.00 dB
PL12: 15.50 dB
PL13: 18.50 dB
PLW: 13.43968010 W
PL1W: 0.30317655 W
PL13W: 0.15079268 W
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SF: 100.617621 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
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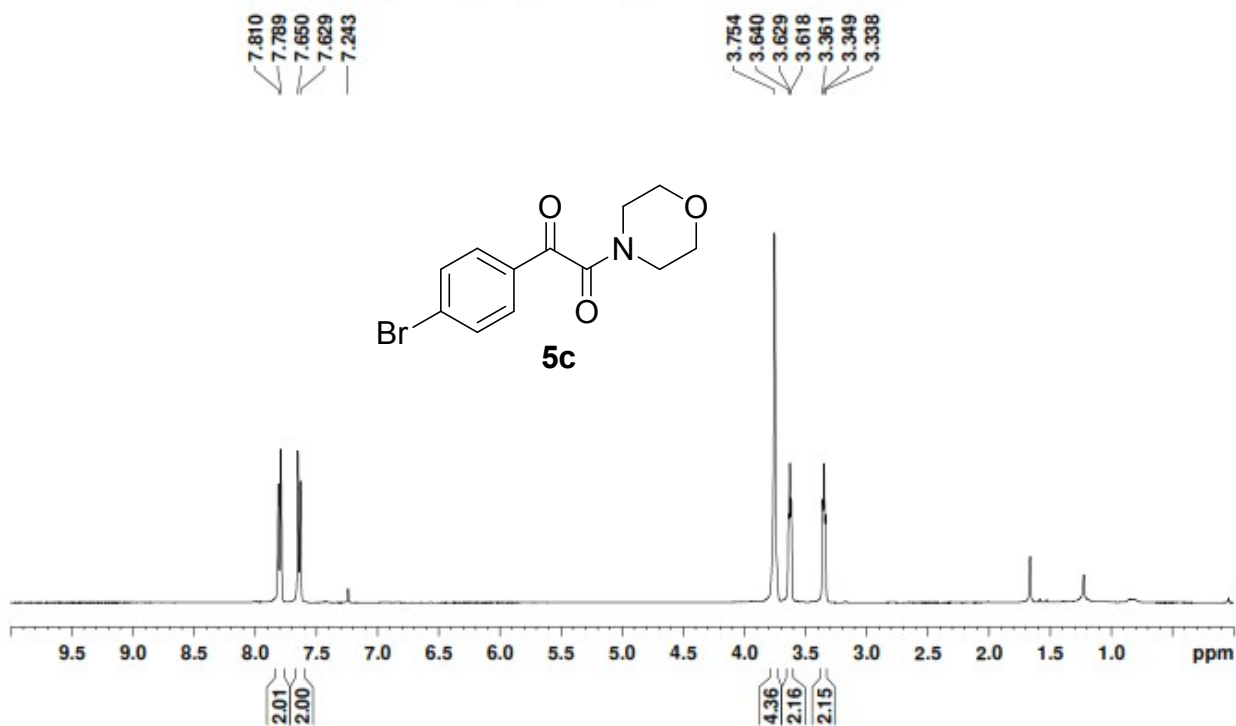
4-OMe EtBz, I2-Py-TBHP, 80deg, 10h, NaI-pyrrolidine-TBHP, rt, 6h, purified



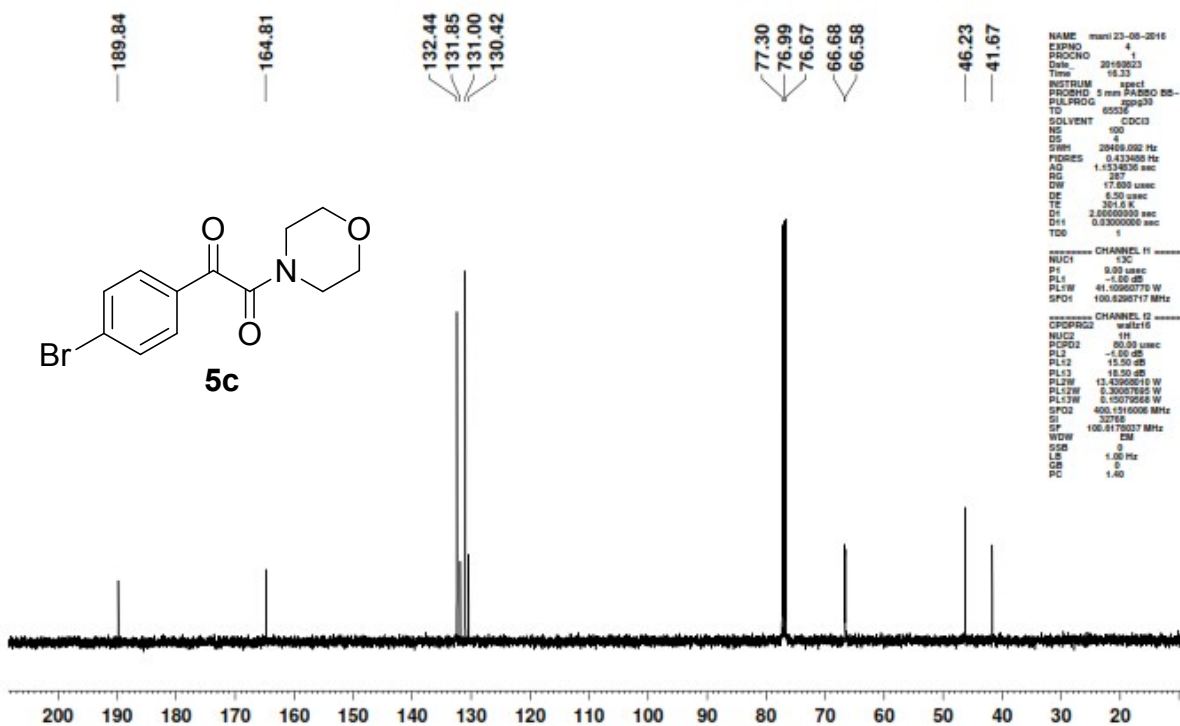
4-OMe EtBz, I2-Py-TBHP, 80deg, 10h, NaI-pyrrolidine-TBHP, rt, 6h, purified



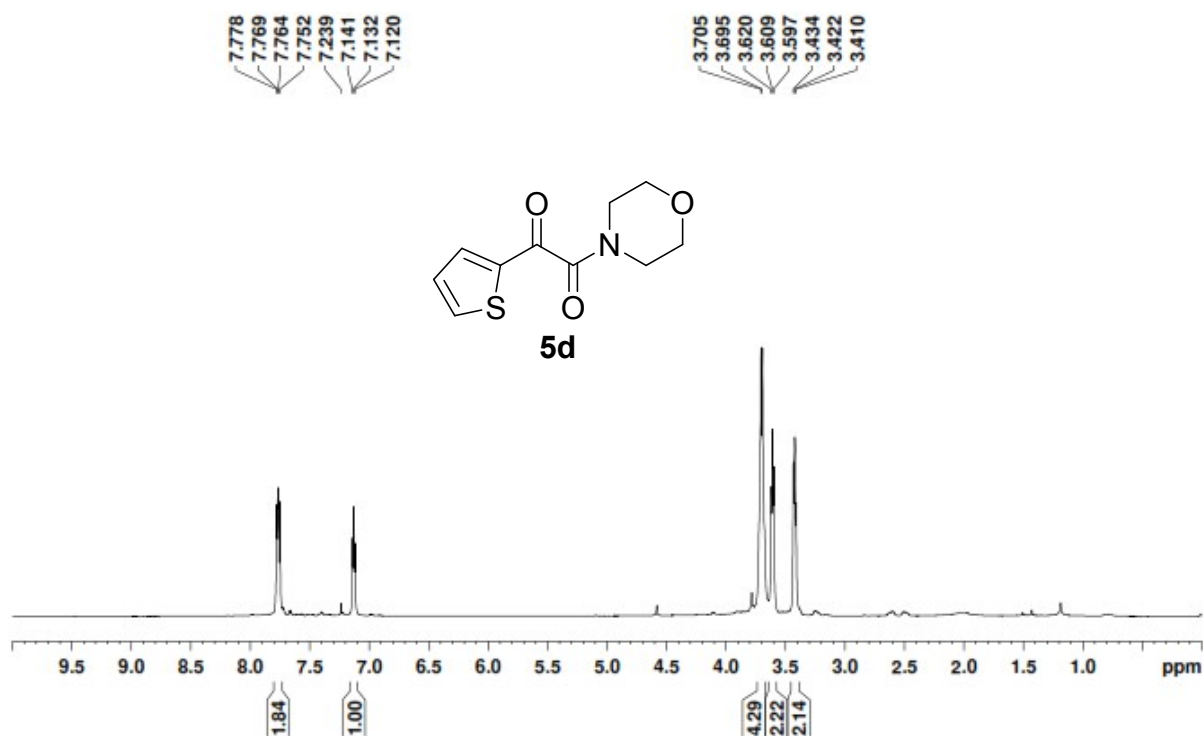
4-BrEtBz, 12-Py-TBHP, 80deg, 10h, NaI-morpholine-TBHP, rt, 6h, purified



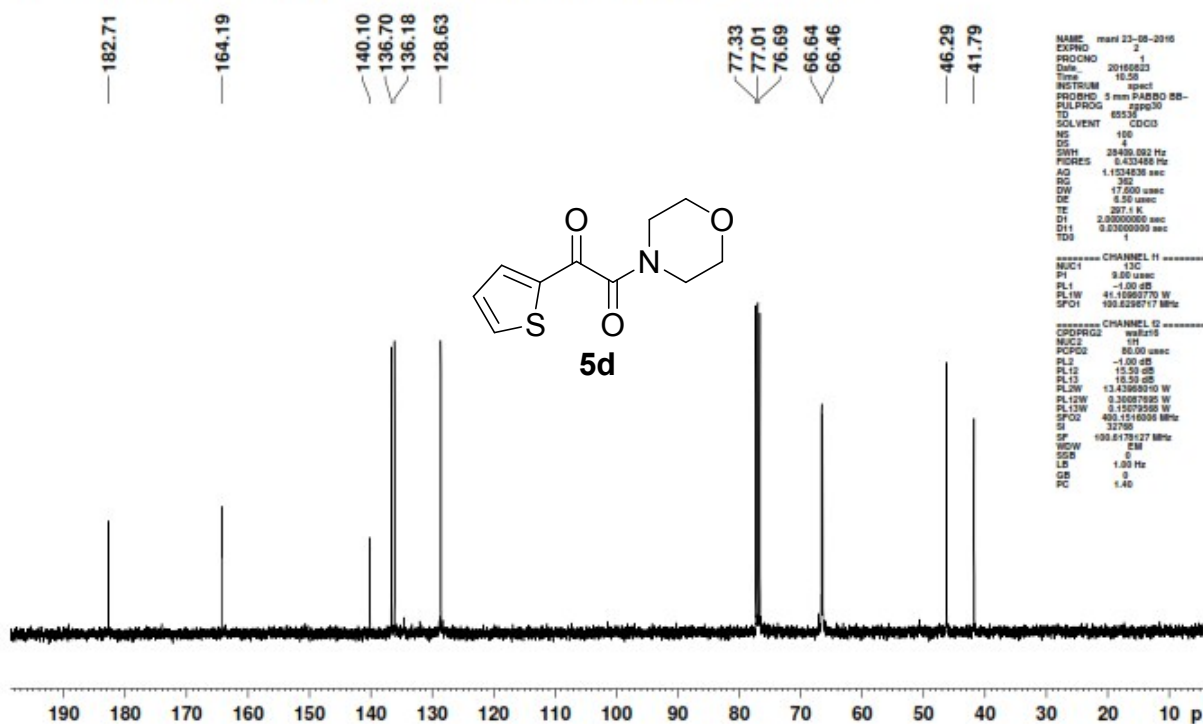
4-BrEtBz, 12-Py-TBHP, 80deg, 10h, NaI-morpholine-TBHP, rt, 6h, purified

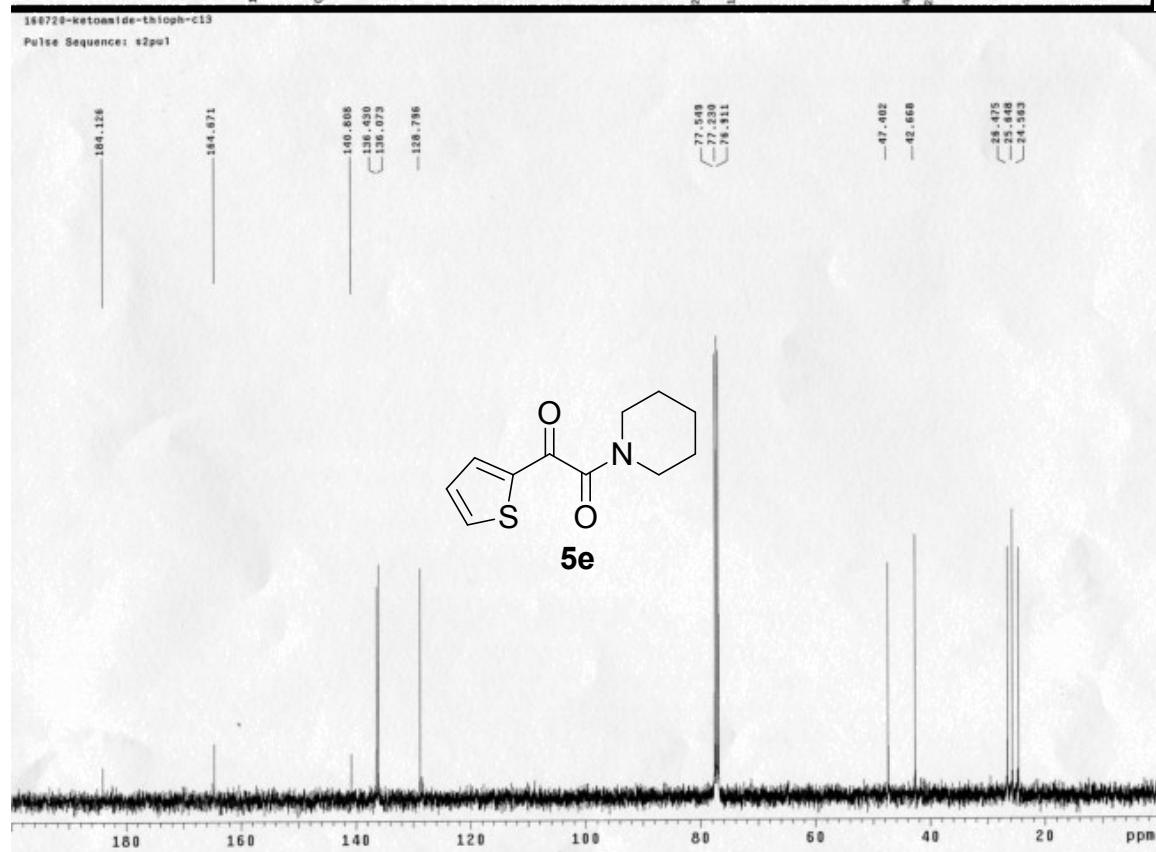
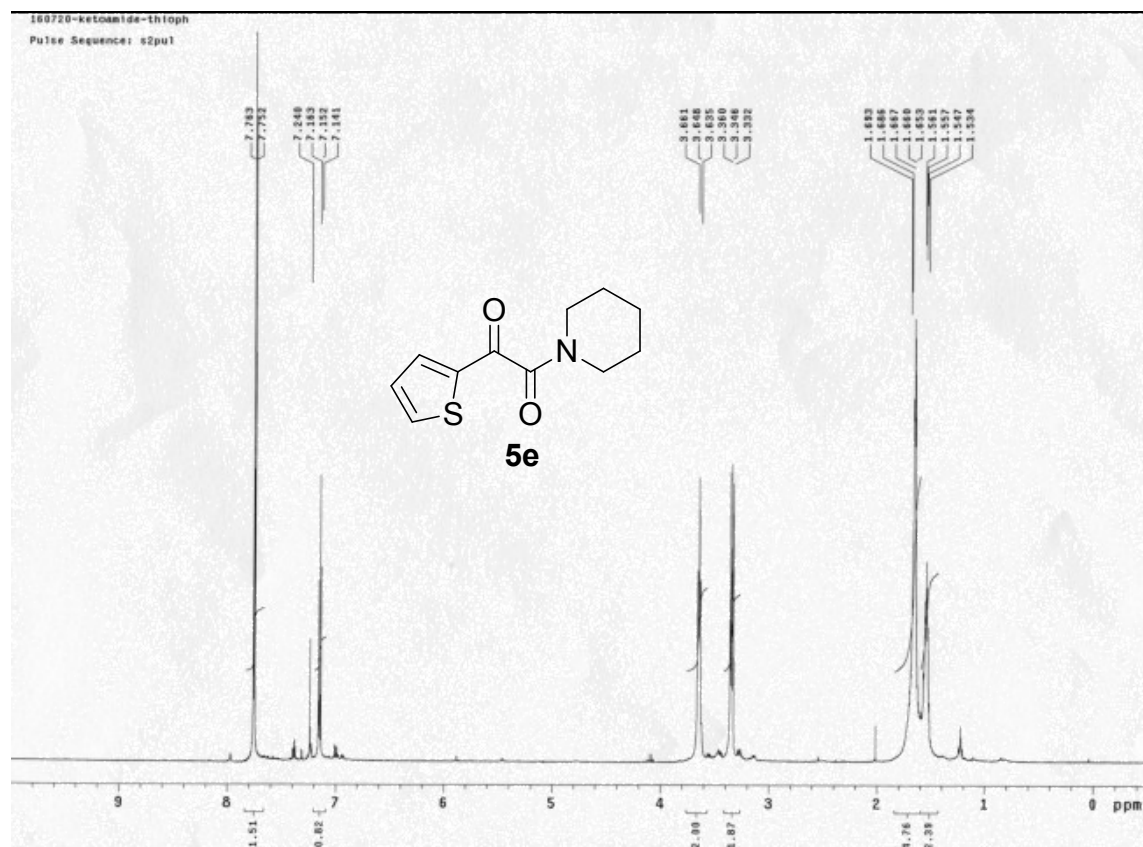


2-Et-thiobenz, I2-Py-TBHP, 80deg, 10h, NaI-morpholine-TBHP, rt, 6h, purified

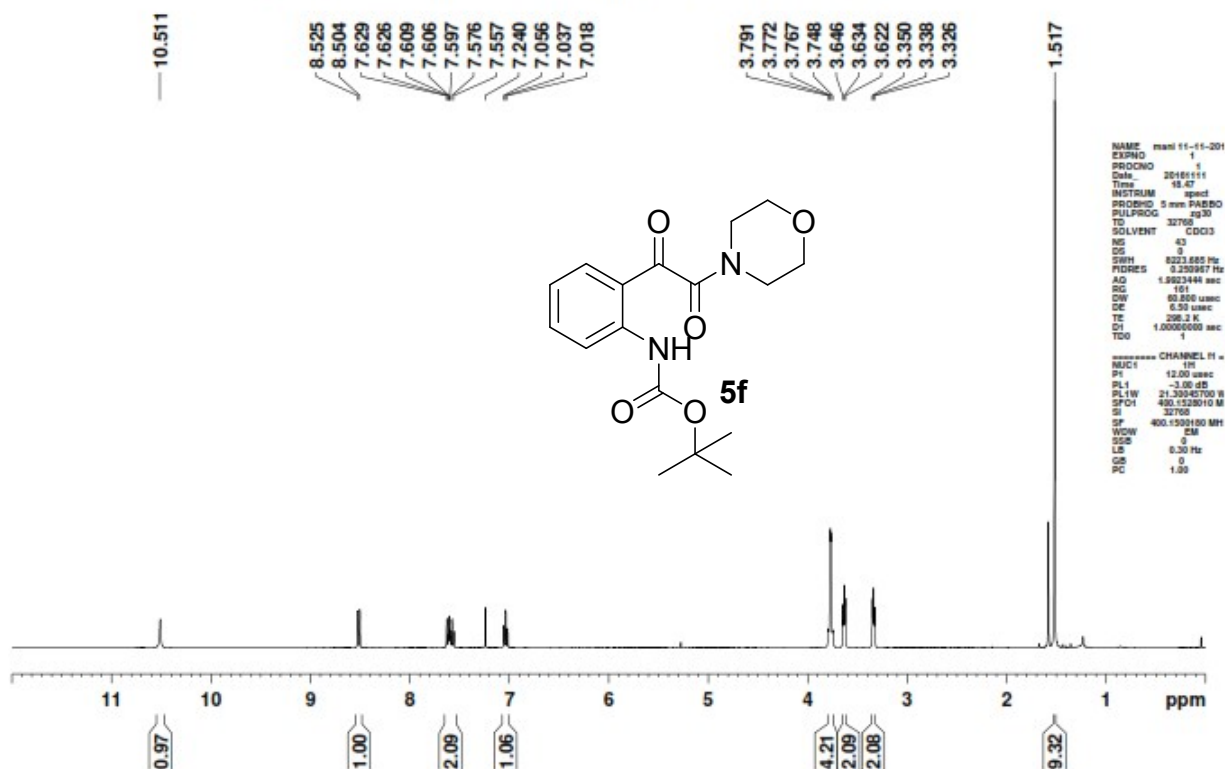


2-Et-thiobenz, I2-Py-TBHP, 80deg, 10h, NaI-morpholine-TBHP, rt, 6h, purified

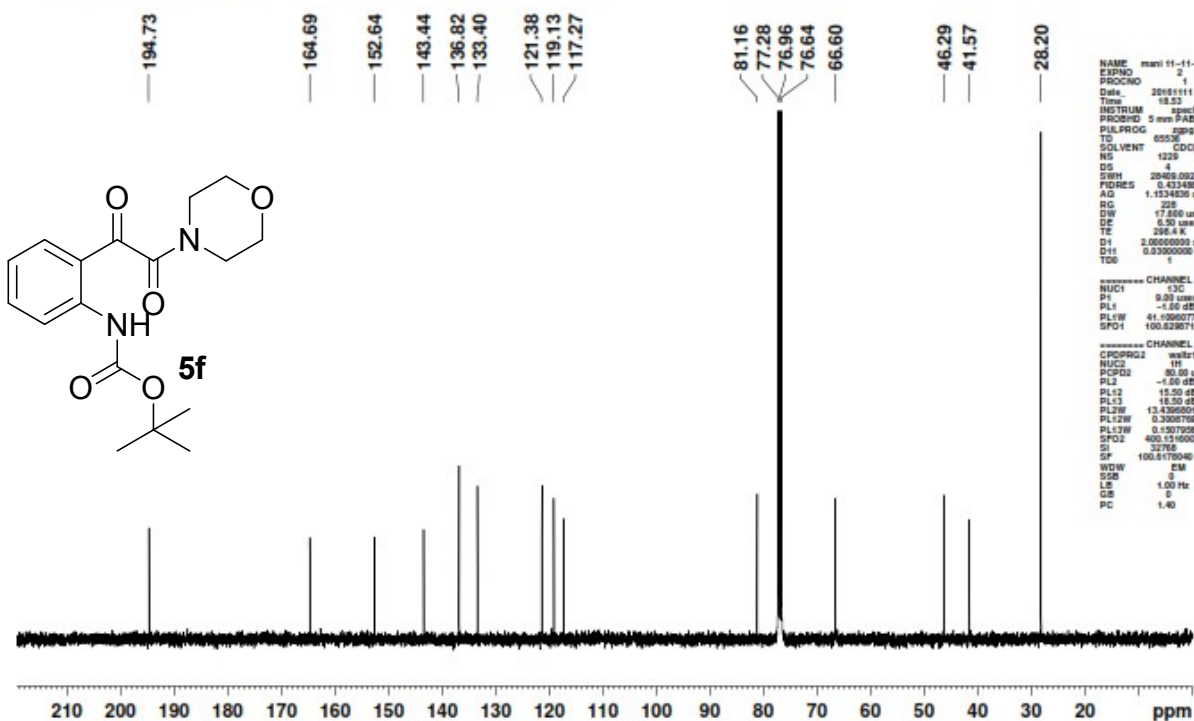




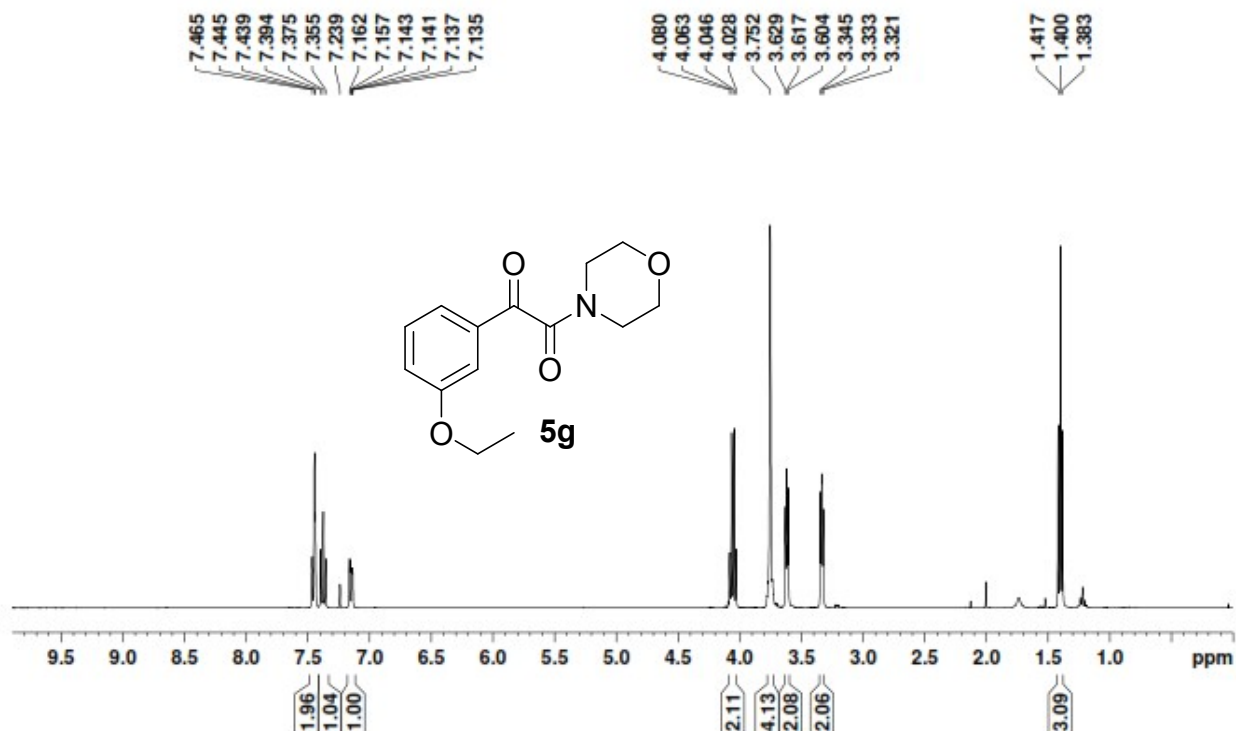
2-NH Boc ethyl benzene + Morpholine ketoamide purified



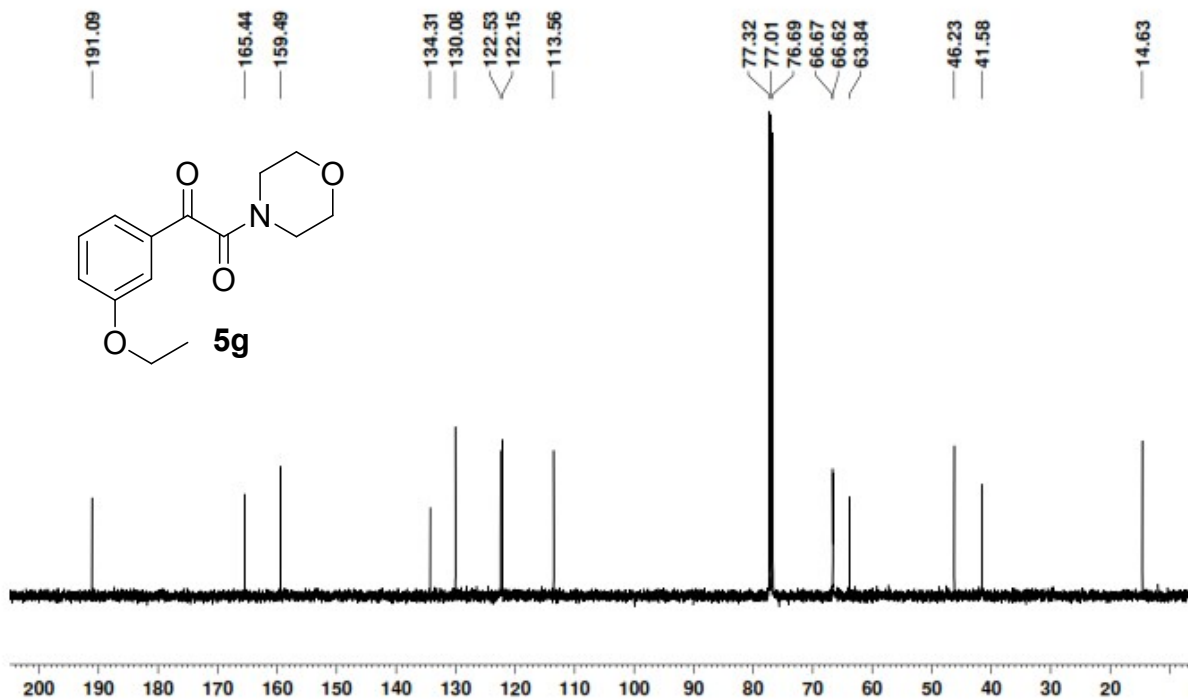
2-NH Boc ethyl benzene + Morpholine ketoamide purified



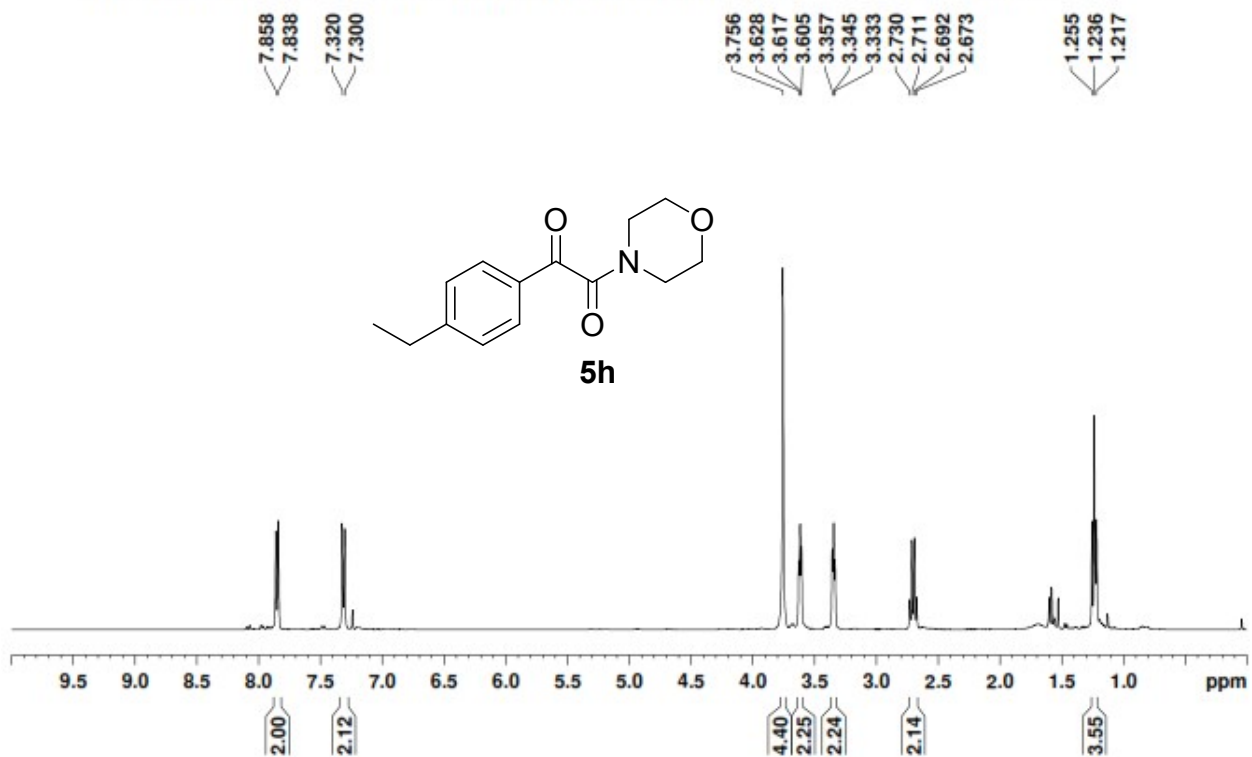
3-ethoxy-EtBz-I2-Py-TBHP, 80deg, 10h, NaI-Morpholine-TBHP,rt, 6h, purified



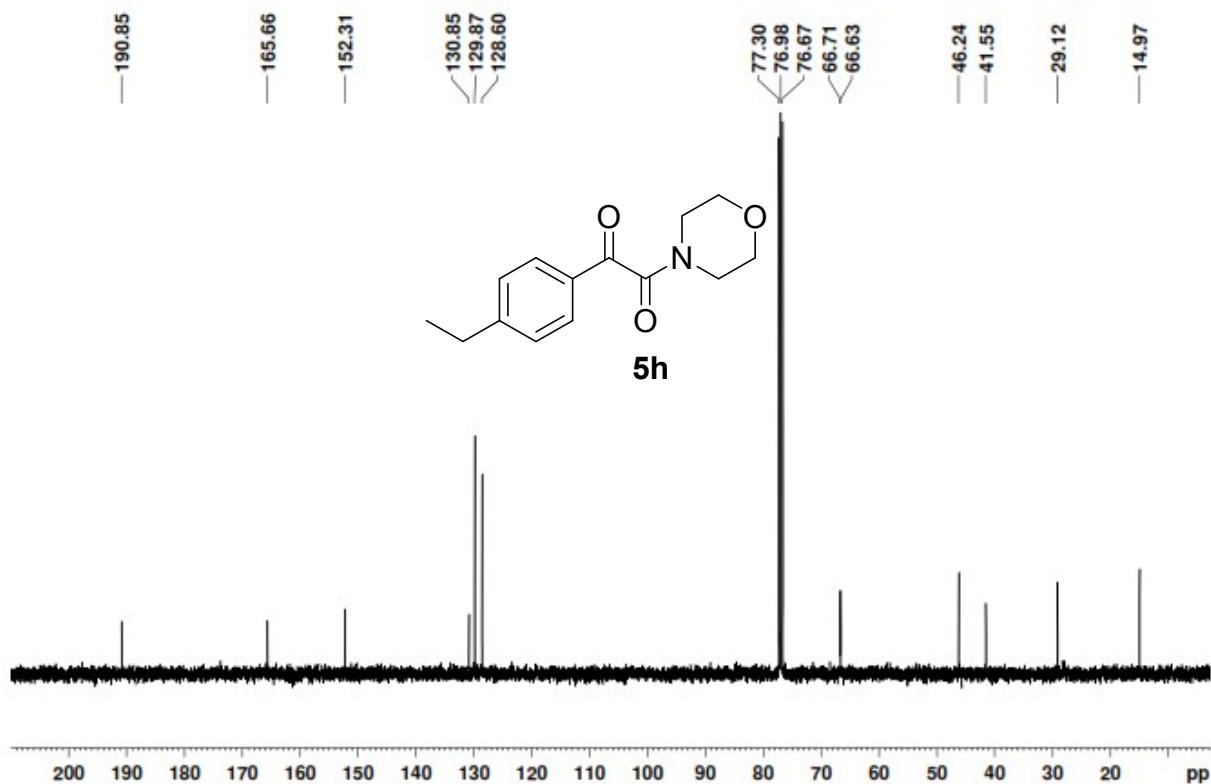
3-ethoxy-EtBz-I2-Py-TBHP, 80deg, 10h, NaI-Morpholine-TBHP,rt, 6h, purified



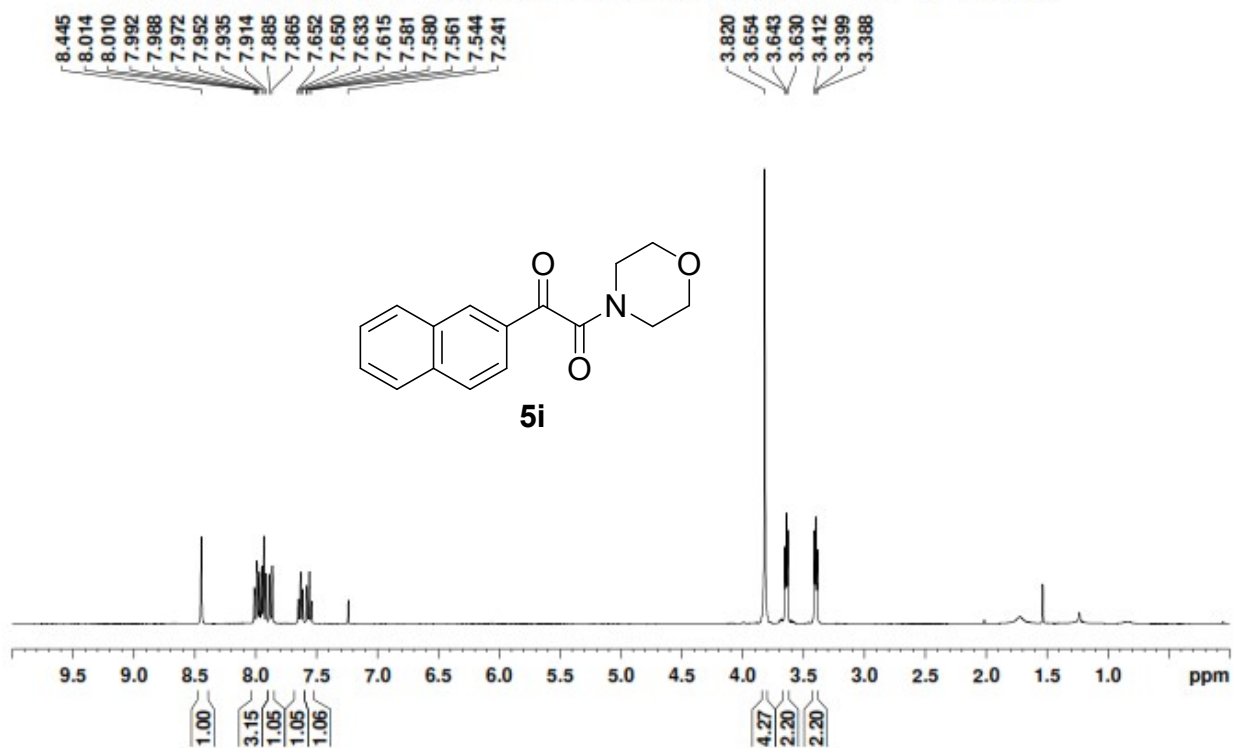
1,4-diethyl benzene, I2-Py-TBHP, 80deg, 12h, NaI-Morpholine-TBHP, rt, 12h, purified (30% EH)



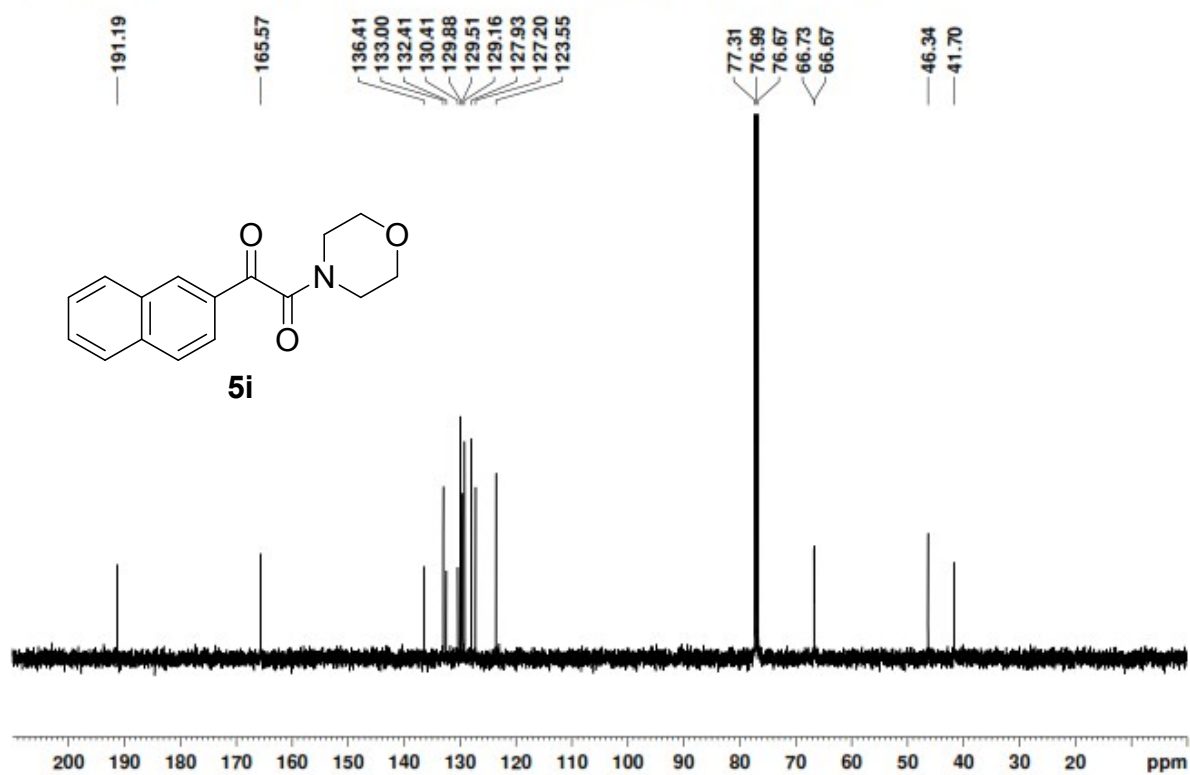
1,4-diethyl benzene, I2-Py-TBHP, 80deg, 12h, NaI-Morpholine-TBHP, rt, 12h, purified (30% EH)



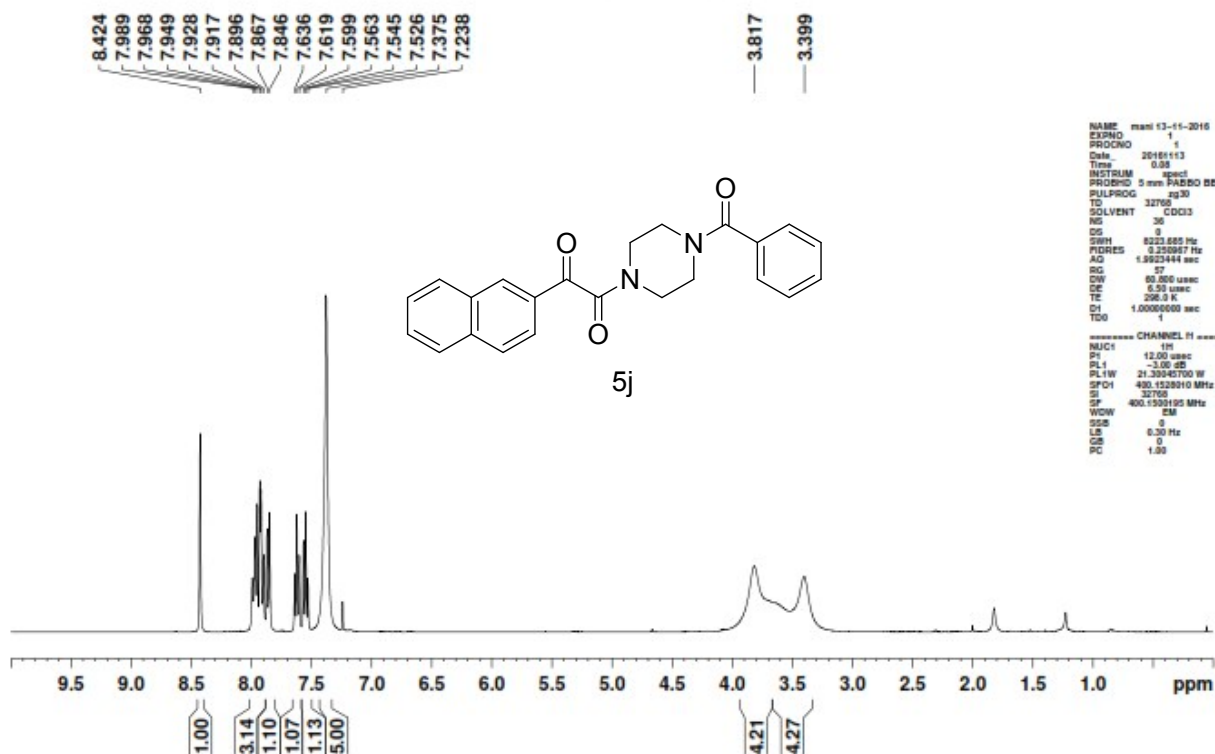
2-ethyl naphthalene, I2-Py-TBHP, 80deg, 10h, NaI-TBHP-Morpholine, rt, 6h, purified



2-ethyl naphthalene, I2-Py-TBHP, 80deg, 10h, NaI-TBHP-Morpholine, rt, 6h, purified



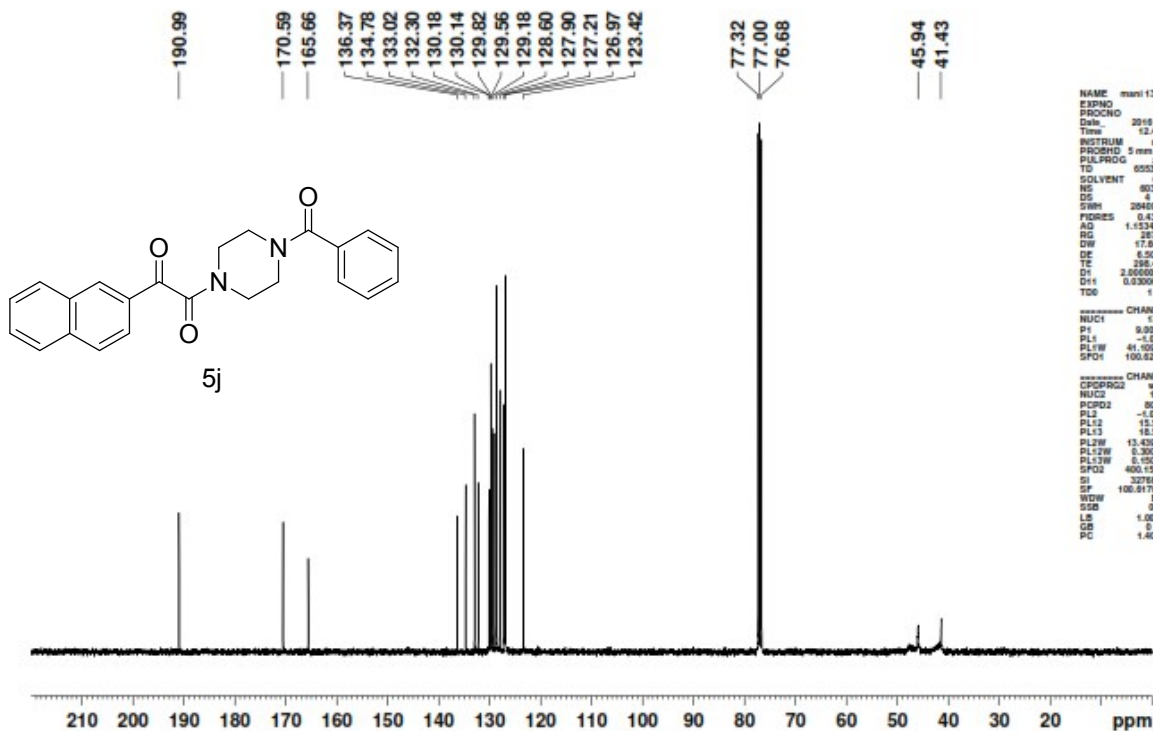
Anti HIV natural product, purified



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 DE: 6.50 usec
 TE: 306.0 K
 D1: 1.00000000 sec
 TDO: 1

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 NUC1: 1H
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 PL1: -3.00 dB
 PL1W: 21.30045700 W
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 SI: 32768
 SF: 400.1500105 MHz
 WDW: EM
 SSB: 0
 LB: 6.30 Hz
 GB: 0
 PC: 1.00

Anti HIV natural product, purified



NAME: mani 13-11-2016
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 NS: 603
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 SWH: 28469.000 Hz
 FIDRES: 0.433060 Hz
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 RG: 257
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 DE: 6.50 usec
 TE: 306.0 K
 D1: 2.00000000 sec
 D11: 0.03000000 sec
 TDO: 1

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 9.00 usec
 PL1: -1.00 dB
 PL1W: 41.00000770 W
 SFO1: 100.626017 MHz

===== CHANNEL f2 =====
 NUC2: 1H
 P2: 80.00 usec
 PL2: -1.00 dB
 PL2W: 15.50 dB
 PL3: 15.50 dB
 PL3W: 13.43000010 W
 PL4W: 0.30007895 W
 PL1W: 0.15072668 W
 SFO2: 400.1516006 MHz
 SI: 32768
 SF: 100.6175085 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40