Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

$CuCl_2$ mediated (aza)oxindole synthesis by oxidative coupling of C_{sp}^2−H and C_{sp}^3−H centers: Substrate scope and DFT study

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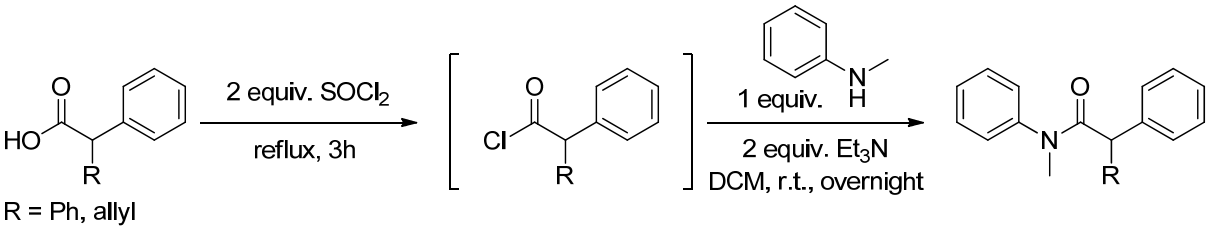
CONTENTS:

1. General Information:

Toluene, THF, and CH_2Cl_2 were dried by filtration on Al_2O_3 drying columns (Solvtek® system). Triethylamine was dried over CaH_2 and distilled under nitrogen. DMF (Acros) was dried over activated 4Å molecular sieves. NaO*t*Bu and KO*t*Bu were sublimed and stored in a glove box. All reactions were carried out under nitrogen in glassware dried by heating under vacuum. Weighing of $CuCl_2$, NaO*t*Bu, KO*t*Bu was performed in the glove box. Proton (^{1}H) and carbon (^{13}C{H}) NMR spectra were recorded on Bruker AMX-400 or AMX-500 FT spectrometers using an internal deuterium lock. Chemical shifts are quoted in parts per million (ppm) downfield of tetramethylsilane. Coupling constants *J* are quoted in Hz. Infrared spectra were recorded on a Perkin–Elmer Spectrum One spectrophotometer using a diamond ATR Golden Gate sampler. Electron impact (EI) mass spectra were obtained using Varian CH–4 or SM–1 instruments operating at 40–70eV. Electrospray ionization (ESI) HRMS measurements were obtained on a VG analytical 7070E instrument. Analytical thin layer chromatography (TLC) was performed on Merck precoated plastic-backed TLC plates (silica gel 60 F_{254}) and visualized by UV lamp (254 nm), potassium permanganate. Flash chromatography (FC) was performed using silica gel 60 (23-400 mesh). Technical grade solvents were employed. Melting points were determined on a Büchi 510 apparatus.

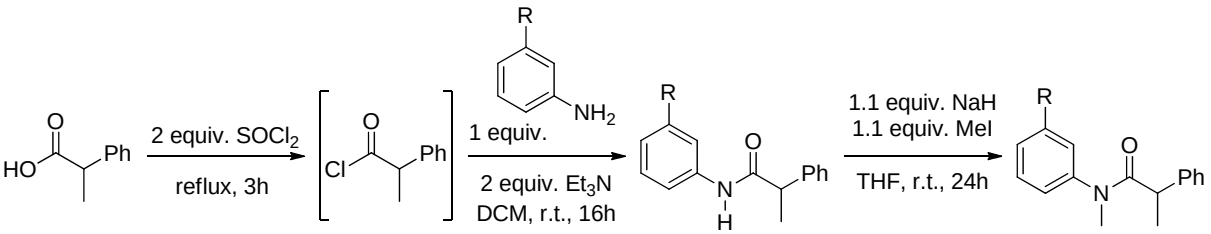
2. Synthesis and analytical data of the substrates:

*General procedure **A** for preparing substrates **1a**, **1b**:*



The carboxylic acid (1.0 equiv.) was refluxed with $SOCl_2$ (2.0 equiv.) for 3h. After evaporating the excess $SOCl_2$ the reaction mixture was diluted with CH_2Cl_2 (0.8M with respect to (w.r.t.) the carboxylic acid). The acid chloride solution was added to the solution of *N*-methyl aniline (1.0 equiv.) and triethyl amine (2.0 equiv.) in CH_2Cl_2 (0.8M w.r.t. the *N*-methyl aniline) at 0 ^oC. The mixture was stirred for overnight (12-18h) at room temperature (r.t.). The reaction mixture was extracted with water and EtOAc (3 times). The combined organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated. The product was purified by flash chromatography. The eluant used for the flash chromatography was described under the discussion for each molecule. The yields of the products are based on two steps.

*General procedure **B** for preparing substrates **1c-e**:*

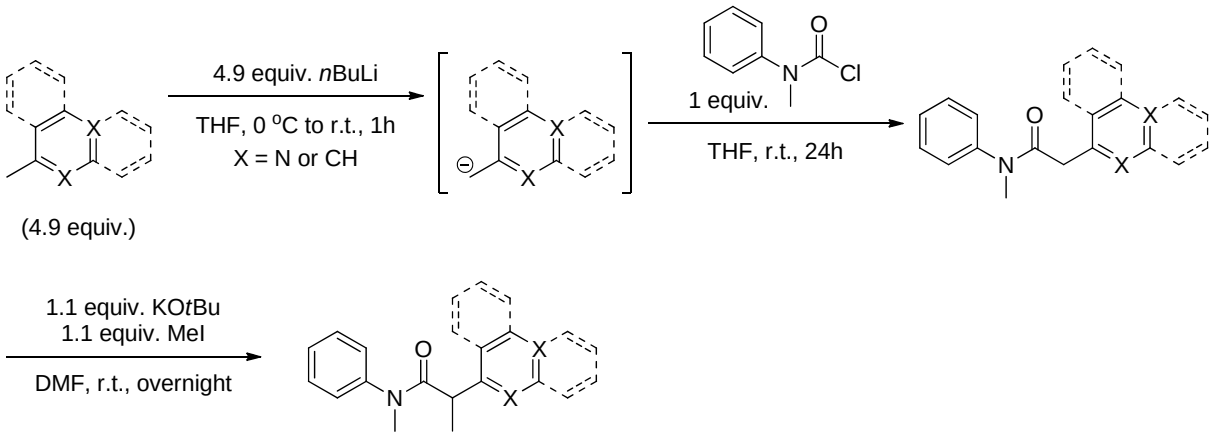


The 2-phenylpropionic acid (1.0 equiv.) was heated under reflux with $SOCl_2$ (2.0 equiv.) for 3h. After evaporating the excess $SOCl_2$, the reaction mixture was diluted with CH_2Cl_2 (0.8M w.r.t. the carboxylic acid). The acid chloride solution was added to the solution of *m*-substituted aniline (1.0 equiv.) and triethyl amine (2.0 equiv.) in CH_2Cl_2 (0.8M w.r.t. the substituted aniline) at 0 ^oC. The mixture was stirred for overnight at r.t. The N-H amide was passed through a small pad of silica. The solvent was evaporated and the crude amide was used for the next step.

The solution of amide (1.0 equiv.) in THF (0.3M w.r.t. the amide) was added to a suspension of NaH (1.1 equiv.) in THF (0.3M w.r.t. the NaH) at 0 ^{o}C and the mixture was stirred for 1h at r.t., followed by the addition of MeI (1.1 equiv.) at 0 ^{o}C. Stirring was continued for 24h at r.t.. The reaction mixture was quenched with brine and extracted with EtOAc (3 times). The combined organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated. The product was purified by flash chromatography.

The eluant used for the flash chromatography for both the steps was same and described under the discussion for each molecule. The yields of the products are based on three steps.

General procedure ***C*** *for preparing substrates* ***1f*** and ***1h-1i****:*



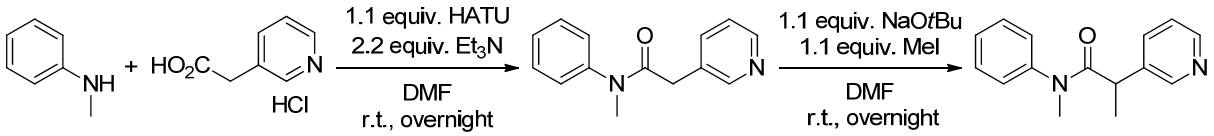
Methylpyridine (or methylquinoline) (4.9 equiv.) in dry THF (1.4M w.r.t. the methylpyridine or methylquinoline) was treated dropwise with *n*BuLi (1.6 M in THF, 4.9 equiv.) at 0 °C. After addition, the mixture was warmed to r.t. and stirred for 1h. The resulting mixture was cooled to 0 ^{o}C and the solution of *N*-methyl-*N*-phenyl carbamoyl chloride (1.0 equiv.) in THF (0.3M w.r.t. the carbamoyl chloride) was added dropwise. This mixture was stirred for overnight at r.t.. The reaction was quenched with H_2O (~1 mL) and the solvent was evaporated. The crude mixture was extracted with water and CH_2Cl_2 (three times). The combined organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated. The amide was purified by chromatography.

The solution of the amide (1.0 equiv.) in DMF (0.2M w.r.t. the amide) was added to a solution of KO*t*Bu (1.1 equiv.) in DMF (0.2M w.r.t. the KO*t*Bu) at 0 ^{o}C and the mixture was stirred for 1h at r.t., followed by the addition of MeI (1.1 equiv.) at 0 ^{o}C. Stirring was continued for

24h at r.t.. The reaction mixture was quenched with brine and extracted with EtOAc (3 times). The combined organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated. The product was purified by flash chromatography.

The eluant used for the flash chromatography for both the steps was same and described under the discussion for each molecule. The yields of the products are based on three steps.

*General procedure **D** for preparing substrates **1g**:*

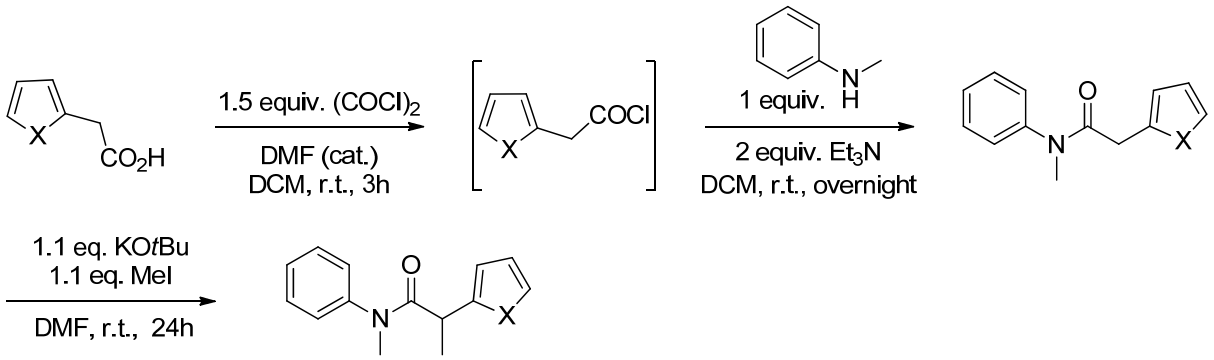


To the solution of 3-pyridyl acetic acid-hydrochloride (1.1 equiv.), and HATU (1.1 equiv.) in DMF (0.3M w.r.t. the acid), 2.2 equiv. Et_3N was added and the resulting mixture was stirred at r.t. for 1h. The solution of *N*-methyl aniline (1.0 equiv.) in DMF (0.5M w.r.t. the *N*-methyl aniline) was added to the reaction mixture and stirred at r.t. for overnight. The crude mixture was extracted with brine and EtOAc (three times). The combined organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated. The amide was purified by chromatography.

The solution of the amide (1.0 equiv.) in DMF (0.2M w.r.t. the amide) was added to a solution of NaO*t*Bu (1.1 equiv.) in DMF (0.2M w.r.t. the NaO*t*Bu) at 0 ^{o}C and the mixture was stirred for 1h at r.t., followed by the addition of MeI (1.1 equiv.) at 0 ^{o}C. Stirring was continued for 24h at r.t.. The reaction mixture was quenched with brine and extracted with EtOAc (3 times). The combined organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated. The product was purified by flash chromatography.

The eluant used for the flash chromatography for both the steps was same and described under the discussion for each molecule. The yields of the products are based on two steps.

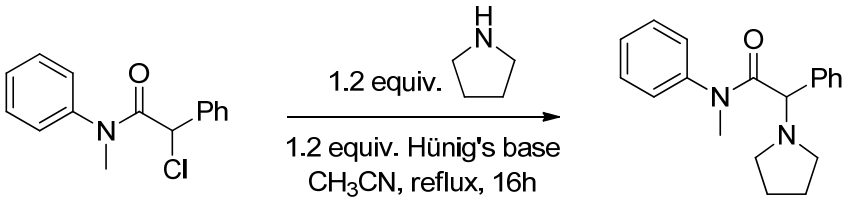
*General procedure **E** for preparing substrates **1o-p**:*



To a solution of the carboxylic acid (1.0 equiv.) in DCM (0.5M w.r.t. to the acid) was added oxalyl chloride (1.5 equiv.) at r.t. followed by addition of a drop of DMF as catalyst. The mixture was stirred at r.t. until gas evolution seized. After removing all volatiles under vacuum, the reaction mixture was diluted with CH_2Cl_2 (0.8M w.r.t. the carboxylic acid). The acid chloride solution was added to the solution of *N*-methyl aniline (1.0 equiv.) and triethyl amine (2.0 equiv.) in CH_2Cl_2 (0.8M w.r.t. the *N*-methyl aniline) at 0 ^oC. The mixture was stirred for overnight (12-18 hours) at r.t.. The N-H amide was passed through a small pad of silica. The solvent was evaporated and the crude amide was used for the next step.

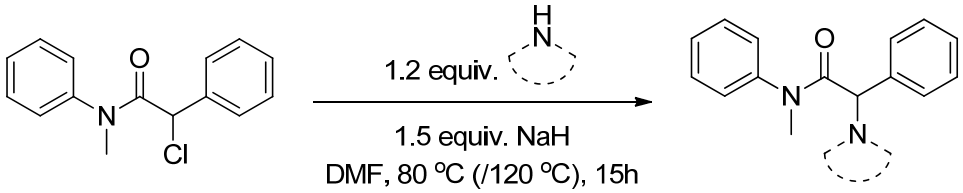
The solution of the amide (1.0 equiv.) in DMF (0.2M w.r.t. the amide) was added to a solution of KO*t*Bu (1.1 equiv.) in DMF (0.2M w.r.t. the KO*t*Bu) at 0 ^oC and the mixture was stirred for 1h at r.t., followed by the addition of MeI (1.1 equiv.) at 0 ^oC. Stirring was continued for 24h at r.t.. The reaction mixture was quenched with brine and extracted with EtOAc (3 times). The combined organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated. The product was purified by flash chromatography. The eluant used for the flash chromatography for both the steps was same and described under the discussion for each molecule. The yields of the products are based on three steps.

*General procedure **F** for preparing substrates **1k**:*



To a solution of the pyrrolidine (1.2 equiv.) and diisopropylethylamine (1.2 equiv.) in acetonitrile (0.2M w.r.t. the amine) was added the solution of 2-chloro-*N*-methyl-*N*,2-diphenylacetamide (1 equiv.) in acetonitrile (0.2M w.r.t. the amide). The solution was then heated under reflux for 16h, and then allowed to cool to room temperature. The solvent was evaporated and the crude amide was purified by flash column chromatography. The eluant used for the flash chromatography was described under each molecule discussion.

*General procedure **G** for preparing substrates **1l-n*** and ***1q**:*



To a vigorously stirred solution of lactam (1.2 equiv.) in dry DMF (0.30M w.r.t. the lactam), NaH (1.5 equiv.) was added in small portions, and the mixture was heated for 1h at 60 °C under nitrogen atmosphere. A solution of α-chloroacetanilide (1.0 equiv.) in the DMF (0.25M w.r.t. the amide) was added dropwise and the resulting mixture was heated at 80 °C for 15h. After cooling to r.t., the crude mixture was extracted with brine and EtOAc (five times). The combined organic phase was dried over anhydrous Na_2SO_4 and the solvent was evaporated. The product was purified by flash chromatography.

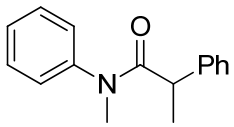
For synthesizing the substrate **1q**, a solution of potassium phthalimide and α-chloroacetanilide in DMF was heated at 120 °C for 15h. The reaction mixture was poured into ice-water. The resulting solid was filtered, washed with water. The product was purified by flash chromatography.

The eluant used for the flash chromatography was described under each molecule discussion.

2-phenylpropanoic acid, *N*-methyl aniline, 3-methyl aniline, 3-methoxy aniline, 3-trifluoromethyl aniline, 2-picoline, 4-picoline, 2-methylquinoline, 4-methylquinoline, 1-methylisoquinoline, *N*-methyl-*N*-phenylcarbamoyl chloride, 3-pyridylacetic acid hydrochloride, pyrrolidine, piperidine, hexamethyleneimine, 2-Pyrrolidone, 2-Pyperidinone, potassium phthalimide were bought and used as received.

2-phenylpent-4-enoic acid,[1] 2-(furan-2-yl)acetic acid,[2] 2-(thiophene-2-yl)acetic acid,[2] 3,3-dimethylpyrrolidin-2-one,[3] 3,3-dimethylpiperidin-2-one,[3] and substrate **1j**[4] were prepared according to the literature procedures.

_N_-methyl-_N_,2-diphenylpropanamide (1a)[4]:



The reaction was carried out according to the general procedure **A**. Purified by chromatography (pentane/Et_2O = 2:1), 84% yield, oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.37-7.32 (m, 3H), 7.22-7.16 (m, 3H), 7.03 (d, J = 6.8 Hz, 2H), 7.00 (brs, 2H), 3.65 (q, J = 6.9 Hz, 1H), 3.25 (s, 3H), 1.40 (d, J = 6.9 Hz, 3H).

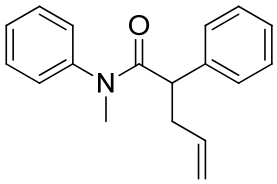
^{13}C NMR (125 MHz, $CDCl_3$): δ 174.1, 143.9, 142.1, 129.6, 128.4, 127.9, 127.6, 126.7, 43.2, 37.8, 20.4.

IR (neat, cm^{-1}): 3060, 3025, 2974, 2931, 1653, 1594, 1493, 1453, 1377, 1121, 1029, 773.1, 696.

HRMS (ESI): calcd. for $C_{16}H_{18}NO$ ($[M+H]^+$): 240.1382, found: 240.1382.

Anal. calcd. for $C_{16}H_{17}NO$: C, 80.30; H, 7.16; N, 5.85, found: C, 80.15; H, 7.54; N, 5.85.

_N_-methyl-_N_,2-diphenylpent-4-enamide (1b):



The reaction was carried out according to the general procedure **A**. Purified by chromatography (pentane/Et_2O = 2:1), 87% yield, oil.

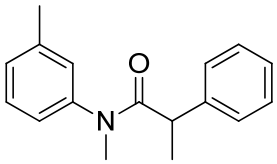
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39-7.36 (m, 3H), 7.24-7.19 (m, 3H), 7.06-7.04 (m, 2H), 6.99 (brs, 2H), 5.72-5.62 (m, 1H), 5.04-4.95 (m, 2H), 3.54 (dd, J = 8.7, 6.4 Hz, 1H) 3.25 (s, 3H), 2.89-2.82 (m, 1H), 2.40-2.33 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 172.7, 143.7, 139.9, 136.2, 129.6, 129.3, 128.4, 128.2, 128.0, 126.9, 116.6, 49.1, 39.4, 37.8.

IR (neat, cm^{-1}): 3063, 3029, 2920, 1653, 1594, 1493, 1377, 1268, 1118, 914, 772, 696, 554.

HRMS (ESI): calcd. for $C_{18}H_{20}NO$ ($[M+H]^+$): 266.1539, found: 266.1541.

_N_-methyl-2-phenyl-_N_-(_m_-tolyl)propanamide (1c):



The reaction was carried out according to the general procedure **B**. Purified by chromatography (pentane/Et_2O = 2:1), 78% yield, oil.

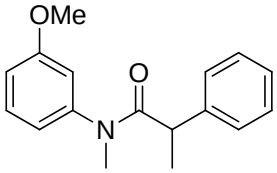
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.28-7.14 (m, 5H), 7.05 (d, J = 6.3 Hz, 2H), 6.83 (d, J = 6.2 Hz, 1H), 6.73 (brs, 1H), 3.64 (q, J = 6.7 Hz, 1H), 3.25 (s, 3H), 2.31 (s, 3H), 1.41 (d, J = 6.8 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 174.1, 143.7, 142.3, 139.6, 129.3, 128.7, 128.6, 128.4, 127.6, 126.6, 124.7, 43.3, 37.7, 21.3, 20.5.

IR (neat, cm^{-1}): 3027, 2970, 2929, 1656, 1603, 1586, 1490, 1453, 1377, 1281, 1120, 1032, 701, 502.

HRMS (ESI): calcd. for $C_{17}H_{20}NO$ ($[M+H]^+$): 254.1539, found: 254.1535.

_N_-(3-methoxyphenyl)-_N_-methyl-2-phenylpropanamide (1d):



The reaction was carried out according to the general procedure **B**. Purified by chromatography (cyclohexane/EtOAc = 3:2), 84% yield, oil.

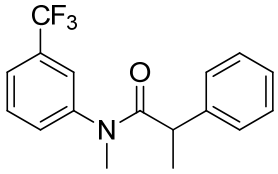
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.29-7.17 (m, 4H), 7.07 (d, J = 7.2 Hz, 2H), 6.89 (dd, J = 8.3, 2.0 Hz, 1H), 6.65 (d, J = 5.6 Hz, 1H), 6.45 (brs, 1H), 3.69 (brs, 4H; three methoxy protons and one benzylic proton overlapped), 3.25 (s, 3H), 1.41 (d, J = 6.9 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 174.0, 160.4, 144.9, 142.3, 130.3, 128.4, 127.6, 126.6, 119.9, 114.0, 113.3, 55.3, 43.2, 37.7, 20.5.

IR (neat, cm^{-1}): 2932, 1656, 1597, 1488, 1379, 1283, 1227, 1118, 1042, 700.

HRMS (ESI): calcd. for $C_{17}H_{20}NO_2$ ($[M+H]^+$): 270.1488, found: 270.1488.

_N_-methyl-2-phenyl-_N_-(3-(trifluoromethyl)phenyl)propanamide (1e):



The reaction was carried out according to the general procedure **B**. Purified by chromatography (cyclohexane/EtOAc = 3:2), 92% yield, oil.

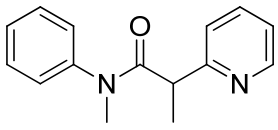
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.58 (d, J = 7.4 Hz, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.19-7.14 (m, 5H), 6.94 (brs, 2H), 3.53 (brs, 1H), 3.26 (s, 3H), 1.40 (d, J = 6.7 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 173.7, 144.3, 141.6, 132.1 (q, $^2J_{C,F}$ = 32.8 Hz), 131.4, 130.2, 128.7, 127.4, 126.9, 125.2, 124.7, 43.9, 37.8, 20.6.

IR (neat, cm^{-1}): 2977, 2934, 1661, 1492, 1447, 1376, 1332, 1249, 1167, 1124, 1069, 700, 524.

HRMS (ESI): calcd. for $C_{17}H_{17}F_3NO$ ($[M+H]^+$): 308.1256, found: 308.1252.

_N_-methyl-_N_-phenyl-2-(pyridin-2-yl)propanamide (1f):



The reaction was carried out according to the general procedure **C**. Purified by chromatography (EtOAc), 90% yield, oil.

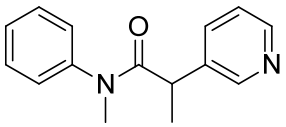
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (d, J = 4.3 Hz, 1H), 7.55 (td, J = 7.6, 1.5 Hz, 1H), 7.35-7.29 (m, 3H), 7.17 (d, J = 7.9 Hz, 1H), 7.09 (dd, J = 7.0, 5.3 Hz, 1H), 7.02 (d, J = 6.3 Hz, 2H), 3.93 (q, J = 7.0 Hz, 1H), 3.30 (s, 3H), 1.44 (d, J = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 173.4, 161.5, 149.2, 143.8, 136.6, 129.7, 127.9, 127.8, 121.9, 121.7, 45.9, 37.9, 18.9.

IR (neat, cm^{-1}): 3069, 2978, 2933, 1653, 1590, 1567, 1494, 1470, 1432, 1378, 1266, 1121, 1071, 1031, 750, 698, 554.

HRMS (ESI): calcd. for $C_{15}H_{17}N_2O$ ($[M+H]^+$): 241.1335, found: 241.1339.

_N_-methyl-_N_-phenyl-2-(pyridin-3-yl)propanamide (1g):



The reaction was carried out according to the general procedure **D**. Purified by chromatography (EtOAc), 48% yield, oil.

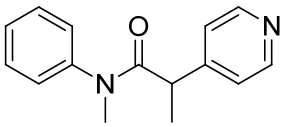
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.45 (d, J = 3.6 Hz, 1H), 8.04 (d, J = 1.5 Hz, 1H), 7.70 (d, J = 7.9 Hz, 1H), 7.44-7.38 (m, 3H), 7.24 (dd, J = 7.9, 4.8 Hz, 1H), 7.03 (brd, J = 3.4 Hz, 2H), 3.69 (q, J = 6.9 Hz, 1H), 3.26 (s, 3H), 1.42 (d, J = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 173.2, 148.8, 147.8, 143.6, 137.8, 135.6, 130.0, 128.4, 127.8, 123.8, 40.5, 37.9, 20.2.

IR (neat, cm^{-1}): 3059, 2978, 2934, 1655, 1594, 1495, 1424, 1382, 1123, 1027, 776, 702, 557.

HRMS (ESI): calcd. for $C_{15}H_{17}N_2O$ ($[M+H]^+$): 241.1335, found: 241.1329.

_N_-methyl-_N_-phenyl-2-(pyridin-4-yl)propanamide (1h):



The reaction was carried out according to the general procedure **C**. Purified by chromatography (EtOAc), 99% yield, oil.

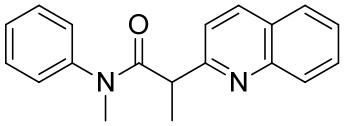
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (d, *J* = 4.9 Hz, 2H), 7.34-7.30 (m, 3H), 6.92-6.91 (m, 4H), 3.57 (q, *J* = 6.9 Hz, 1H), 3.19 (s, 3H), 1.32 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 172.5, 150.6, 149.8, 143.3, 129.8, 128.2, 127.6, 122.8, 42.5, 37.7, 19.7.

IR (neat, cm^{-1}): 3070, 2981, 2934, 1653, 1594, 1494, 1414, 1380, 1261, 1121, 1069, 1030, 829, 773, 728, 699, 555.

HRMS (ESI): calcd. for $C_{15}H_{17}N_2O$ ($[M+H]^+$): 241.1335, found: 241.1338.

_N_-methyl-_N_-phenyl-2-(quinolin-2-yl)propanamide (1i):



The reaction was carried out according to the general procedure **C**. Purified by chromatography (cyclohexane/EtOAc = 1:1), 90% yield, oil.

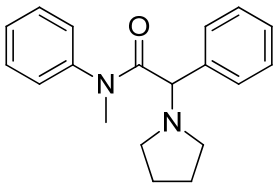
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.51-7.46 (m, 2H), 7.28 (brs, 3H), 7.01-7.00 (m, 2H), 4.13 (q, *J* = 6.9 Hz, 1H), 3.30 (s, 3H), 1.54 (d, *J* = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 173.2, 161.4, 147.6, 143.5, 136.5, 129.6, 129.24, 129.16, 127.9, 127.8, 127.4, 127.0, 126.1, 119.8, 46.8, 37.9, 18.8.

IR (neat, cm^{-1}): 3051, 2978, 2931, 1651, 1594, 1494, 1379, 1117, 1068, 1030, 756, 698.

HRMS (ESI): calcd. for $C_{19}H_{19}N_2O$ ($[M+H]^+$): 291.1491, found: 291.1493.

_N_-methyl-_N_,2-diphenyl-2-(pyrrolidin-1-yl)acetamide (1k):



The reaction was carried out according to the general procedure **F**. Purified by chromatography (pentane/Et_2O/Et_3N = 1:1:0.04), 78% yield, solid, m.p. = 94-96 ^oC.

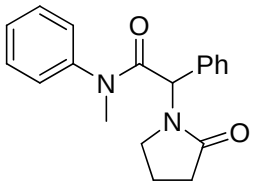
^1H NMR (400 MHz, $CDCl_3$): δ 7.29 (brs, 3H), 7.17-7.10 (m, 5H), 6.90 (brs, 2H), 3.78 (s, 1H), 3.16 (s, 3H), 2.46-2.44 (m, 2H), 2.25-2.23 (m, 2H), 1.67-1.65 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 171.2, 143.6, 137.7, 129.7, 129.1, 128.5, 128.2, 128.1, 127.9, 70.4, 52.5, 38.1, 23.2.

IR (neat, cm^{-1}): 3028, 2964, 2785, 1660, 1594, 1493, 1380, 1254, 1114, 723, 697, 558.

HRMS (ESI): calcd. for $C_{19}H_{23}N_2O$ ($[M+H]^+$): 295.1804, found: 295.1803.

_N_-methyl-2-(2-oxopyrrolidin-1-yl)-_N_,2-diphenylacetamide (1l):



The reaction was carried out according to the general procedure **G**. Purified by chromatography (cyclohexane/EtOAc/Et_3N = 3:1:0.08), 85% yield, solid, m.p. = 137-139 ^oC.

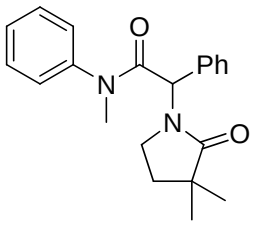
^1H NMR (400 MHz, $CDCl_3$): δ 7.28-7.22 (m, 6H), 7.04-7.02 (m, 2H), 6.98 (brs, 2H), 5.82 (s, 1H), 3.95-3.89 (m, 1H), 3.28 (s, 3H), 2.87-2.82 (m, 1H), 2.49-2.41 (m, 1H), 2.37-2.29 (m, 1H), 2.09-1.99 (m, 1H), 1.86-1.75 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 175.2, 170.2, 142.6, 134.4, 129.5, 129.2, 128.7, 128.3, 128.1, 127.9, 56.9, 45.6, 37.7, 31.2, 18.4.

IR (neat, cm^{-1}): 2970, 2956, 2890, 1681, 1660, 1494, 1416, 1283, 1120, 699, 512.

HRMS (ESI): calcd. for $C_{19}H_{21}N_2O_2$ ($[M+H]^+$): 309.1597, found: 309.1595.

2-(3,3-dimethyl-2-oxopyrrolidin-1-yl)-*N*-methyl-*N*,2-diphenylacetamide (1m):



The reaction was carried out according to the general procedure **G**. Purified by chromatography (pentane/EtOAc = 1:1), 82% yield, solid, m.p. = 128-130 ^{o}C.

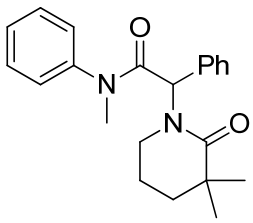
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.26-7.19 (m, 6H), 7.00-6.98 (m, 2H), 6.94 (brs, 2H), 5.74 (s, 1H), 3.81-3.76 (m, 1H), 3.23 (s, 3H), 2.69-2.65 (m, 1H), 1.85-1.80 (m, 1H), 1.64-1.58 (m, 1H), 1.18 (s, 3H), 1.05 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 179.8, 170.1, 142.6, 134.3, 129.5, 129.1, 128.6, 128.3, 128.0, 127.8, 57.1, 42.2, 40.8, 37.6, 34.5, 24.4, 24.1.

IR (neat, cm^{-1}): 2968, 2940, 2907, 2869, 1677, 1655, 1595, 1586, 1493, 1412, 1377, 1278, 1254, 1215, 1143, 1116, 830, 775, 700, 649, 559.

HRMS (ESI): calcd. for $C_{21}H_{25}N_2O_2$ ($[M+H]^+$): 337.1910, found: 337.1916.

2-(3,3-dimethyl-2-oxopiperidin-1-yl)-*N*-methyl-*N*,2-diphenylacetamide (1n):



The reaction was carried out according to the general procedure **G**. Purified by chromatography (pentane/EtOAc = 1:1), 69% yield, solid, m.p. = 96-98 ^{o}C.

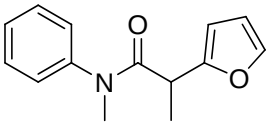
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.25-7.14 (m, 6H), 6.97-6.95 (m, 4H), 6.15 (s, 1H), 3.58-3.53 (m, 1H), 3.24 (s, 3H), 2.58-2.53 (m, 1H), 1.82-1.75 (m, 1H), 1.70-1.65 (m, 1H), 1.61-1.49 (m, 2H), 1.25 (s, 3H), 1.17 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 176.8, 170.4, 142.7, 134.8, 129.9, 129.3, 128.4, 128.1, 127.73, 127.69, 59.5, 46.5, 38.8, 37.6, 36.2, 28.1, 27.7, 19.9.

IR (neat, cm^{-1}): 2960, 2930, 2860, 1654, 1625, 1596, 1496, 1476, 1453, 1428, 1388, 1201, 1121, 770, 697, 558.

HRMS (ESI): calcd. for $C_{22}H_{27}N_2O_2$ ($[M+H]^+$): 351.2067, found: 351.2067.

2-(furan-2-yl)-*N*-methyl-*N*-phenylpropanamide (1o):



The reaction was carried out according to the general procedure **E**. Purified by chromatography (cyclohexane/EtOAc = 3:2), 80% yield, oil.

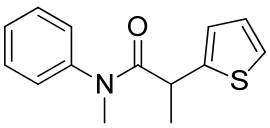
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44-7.34 (m, 3H), 7.28 (brs, 1H), 7.21-7.19 (m, 2H), 6.27 (dd, *J* = 2.9, 1.94 Hz, 1H), 6.04 (d, *J* = 3.1 Hz, 1H), 3.79 (q, *J* = 6.9 Hz, 1H), 3.30 (s, 3H), 1.4 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 172.4, 154.9, 143.9, 141.4, 129.9, 128.1, 127.6, 110.4, 105.9, 37.9, 36.9, 16.9.

IR (neat, cm^{-1}): 2934, 1660, 1594, 1496, 1382, 1121, 1072, 1009, 780, 700.

HRMS (ESI): calcd. for $C_{14}H_{16}NO_2$ ($[M+H]^+$): 230.1175, found: 230.1174.

***N*-methyl-*N*-phenyl-2-(thiophen-2-yl)propanamide (1p):**



The reaction was carried out according to the general procedure **E**. Purified by chromatography (cyclohexane/EtOAc = 3:2), 82% yield, oil.

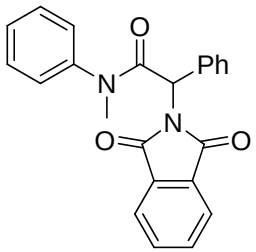
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45-7.36 (m, 3H), 7.16-7.14 (m, 3H), 6.87 (dd, *J* = 5.0, 3.5 Hz, 1H), 6.68 (d, *J* = 3.3 Hz, 1H), 3.97 (q, *J* = 6.9 Hz, 1H), 3.28 (s, 3H), 1.46 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): 173.5, 144.7, 143.9, 129.9, 128.2, 127.6, 126.4, 124.4, 124.3, 38.4, 37.8, 21.5.

IR (neat, cm^{-1}): 2973, 2931, 1654, 1594, 1494, 1381, 1308, 1258, 1118, 1029, 850, 773, 696, 554.

HRMS (ESI): calcd. for $C_{14}H_{16}NOS$ ($[M+H]^+$): 246.0947, found: 246.0948.

2-(1,3-dioxoisoindolin-2-yl)-*N*-methyl-*N*,2-diphenylacetamide (1q):



The reaction was carried out according to the general procedure **G** (the reaction mixture was heated at 120 ^{o}C). Purified by chromatography (EtOAc), 58% yield, solid, m.p. = 175-177 ^{o}C.

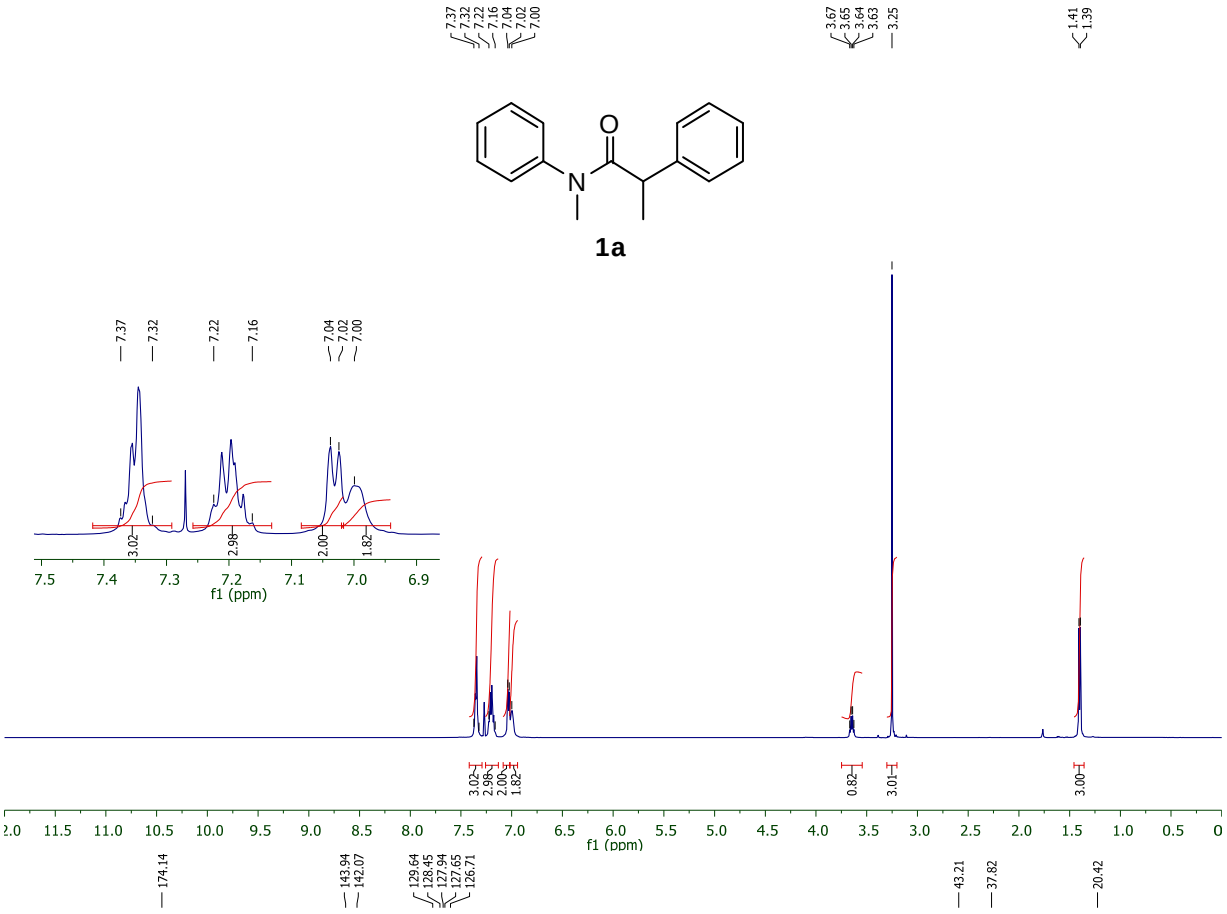
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79-7.66 (m, 4H), 7.30-7.19 (m, 8H), 7.00 (brs, 2H), 6.06 (s, 1H), 3.35 (s, 3H).

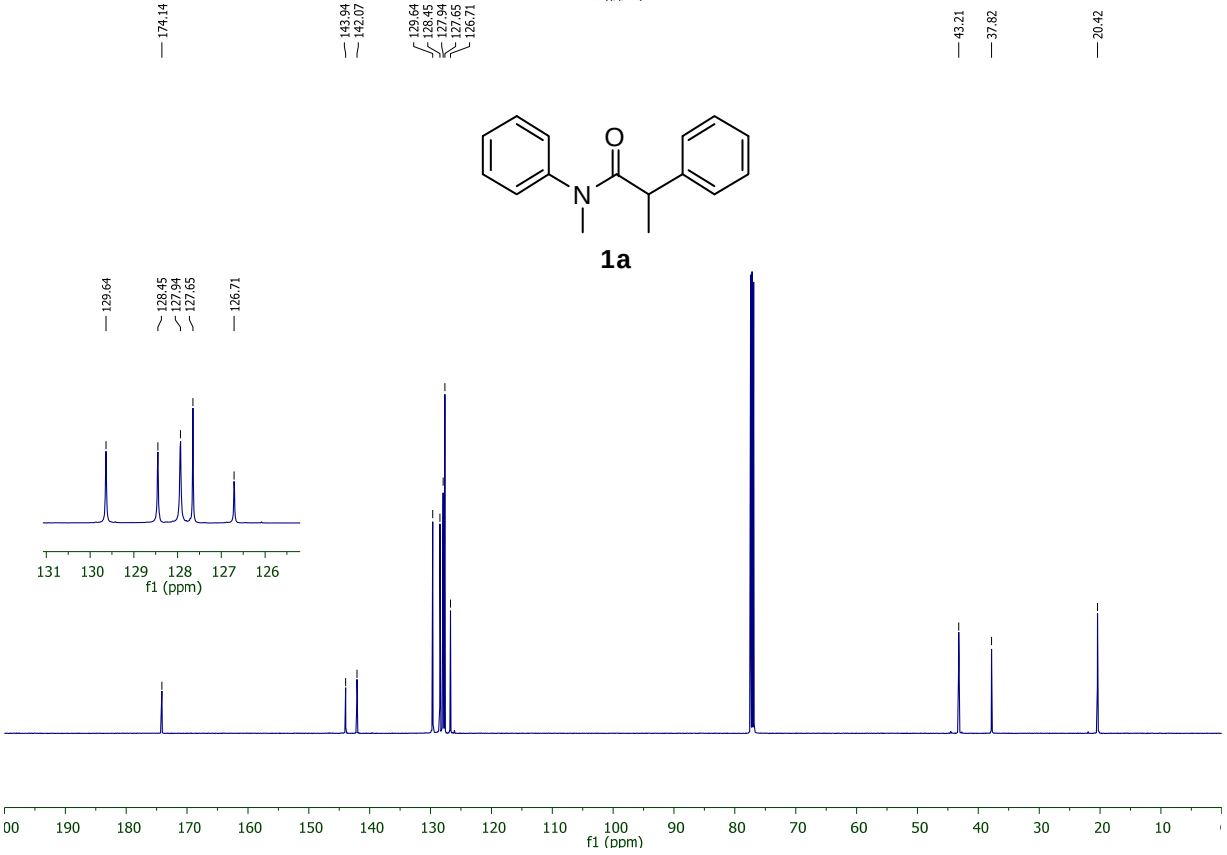
^{13}C NMR (75 MHz, $CDCl_3$): δ 167.7, 167.5, 142.6, 134.0, 133.9, 131.9, 130.2, 129.6, 128.3, 128.2, 128.0, 127.4, 123.4, 56.6, 38.5.

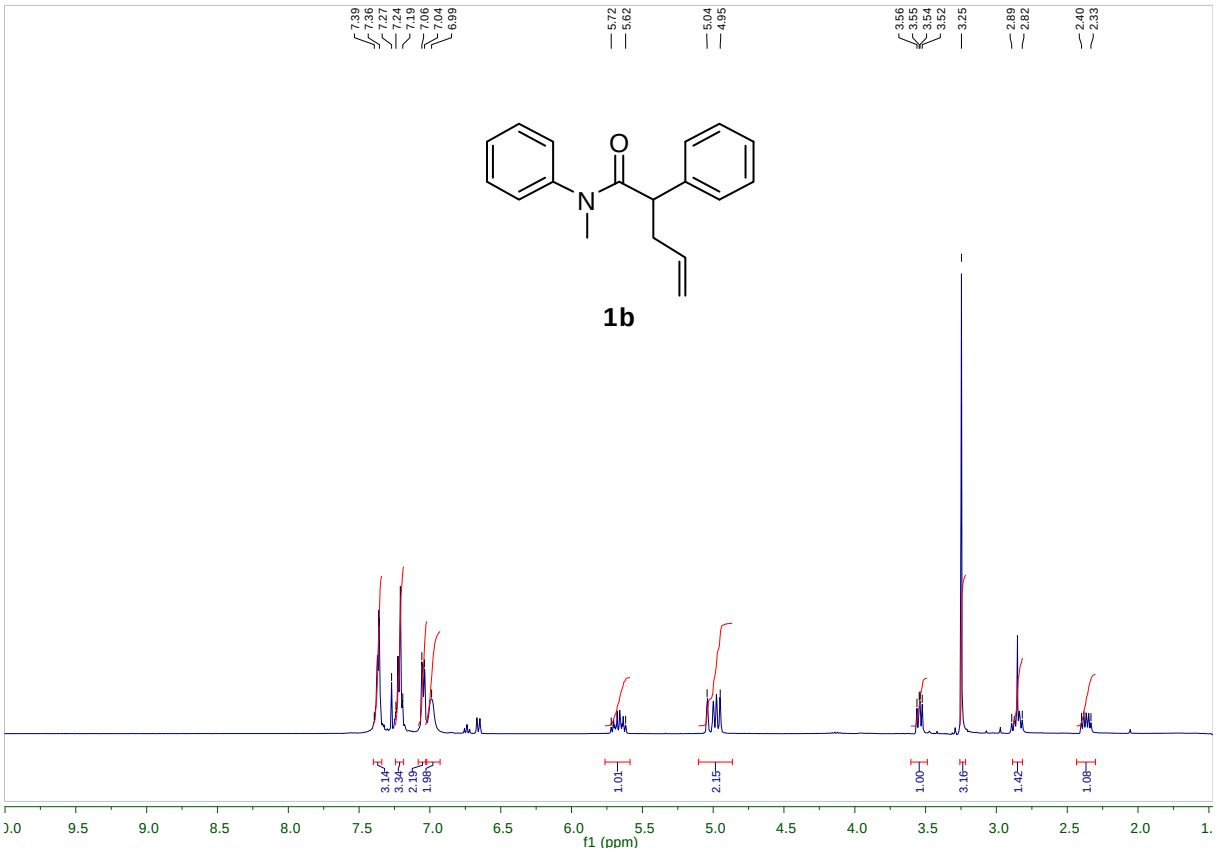
IR (neat, cm^{-1}): 3071, 3033, 2945, 1712, 1668, 1658, 1593, 1494, 1382, 1341, 1113, 1075, 1046, 897, 695, 640, 559, 505.

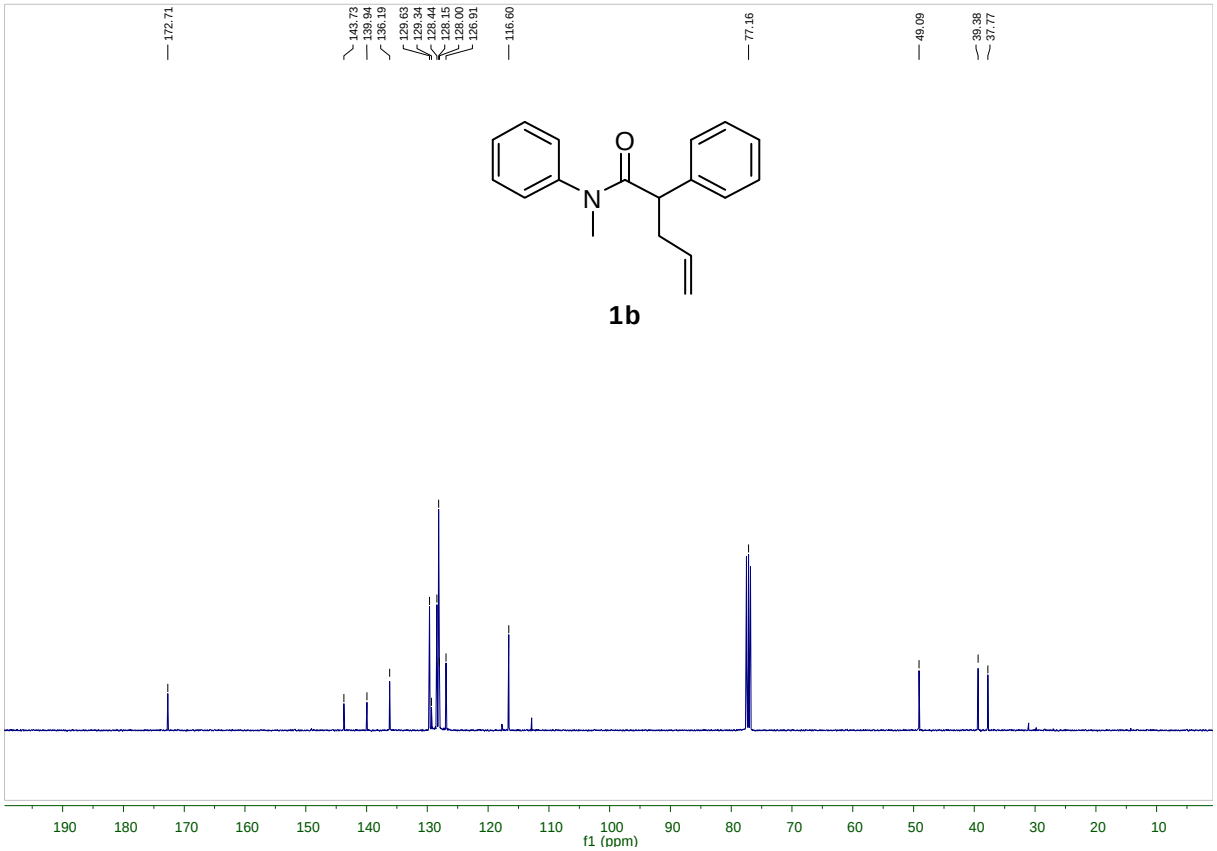
HRMS (ESI): calcd. for $C_{23}H_{19}N_2O_3$ ($[M+H]^+$): 371.1390, found: 371.1398.

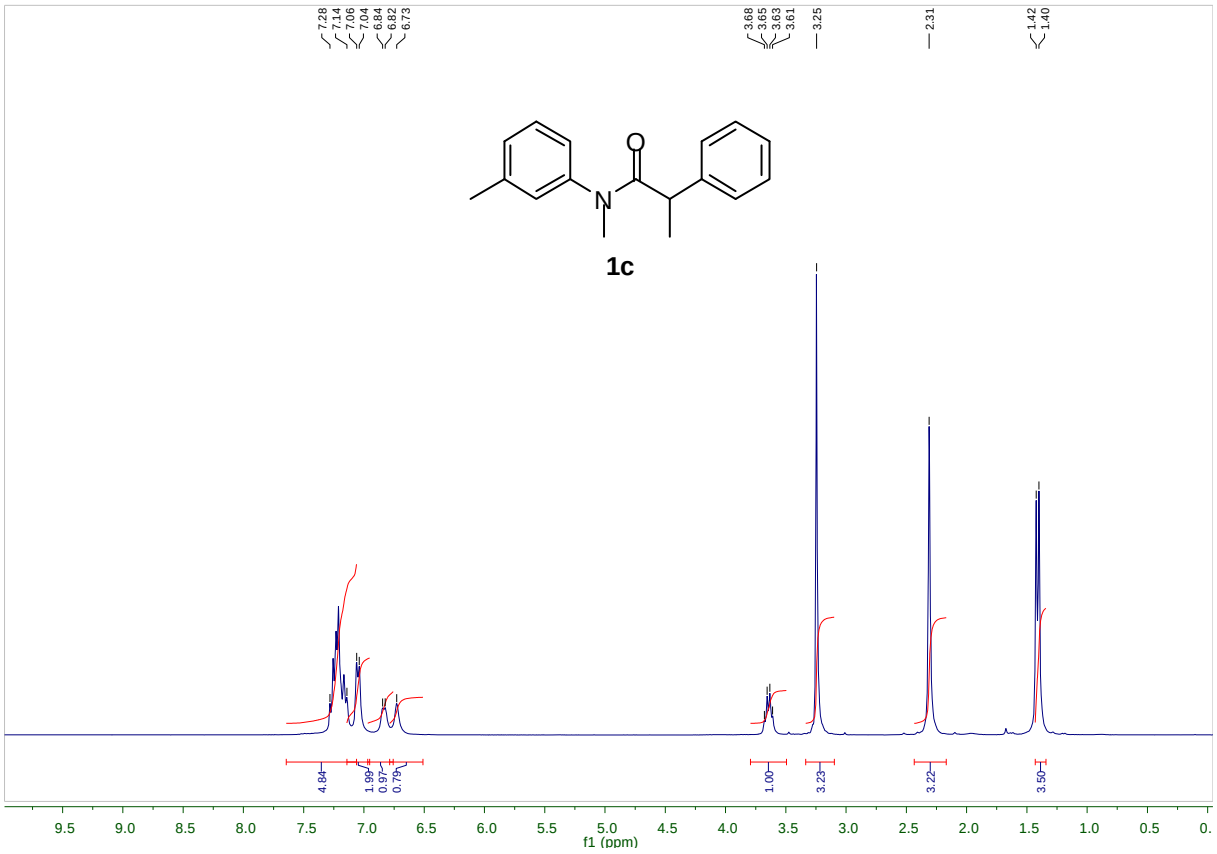
3. Spectra of the substrates and the products:

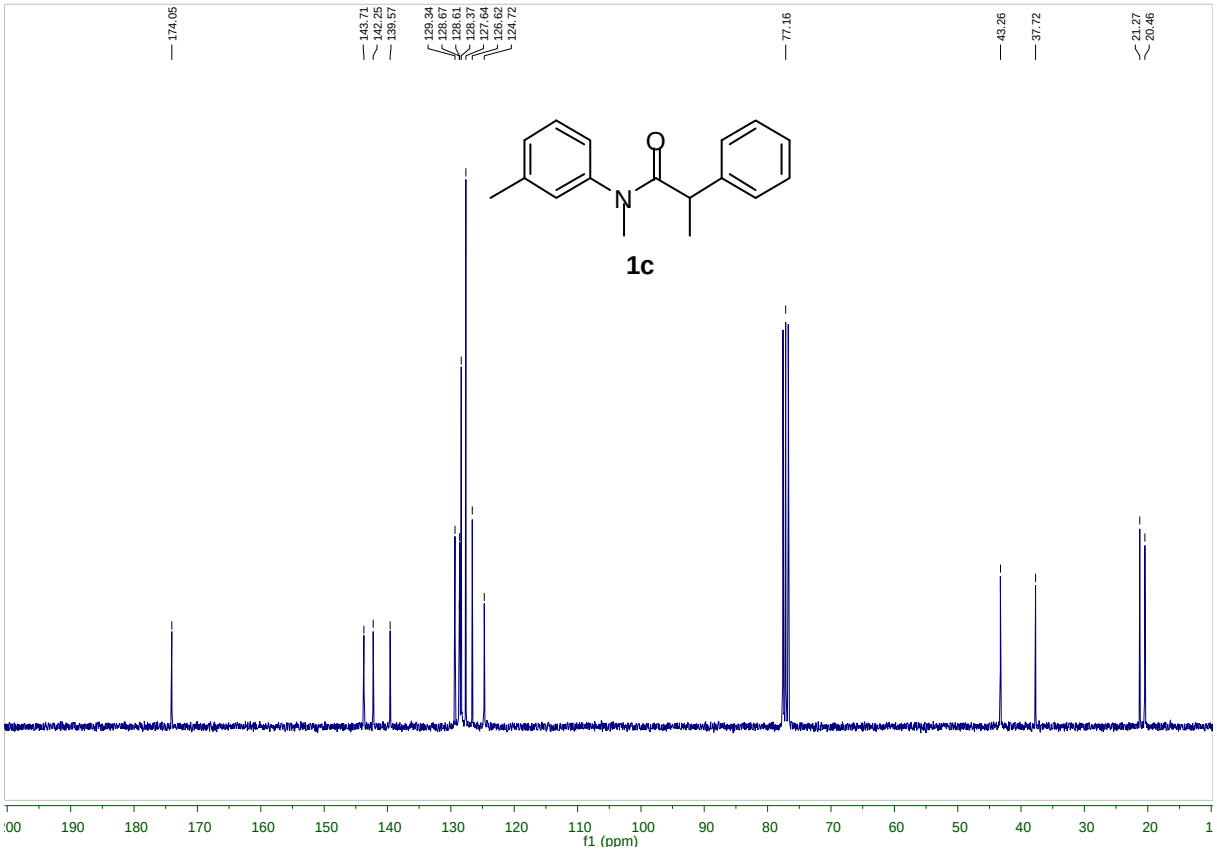


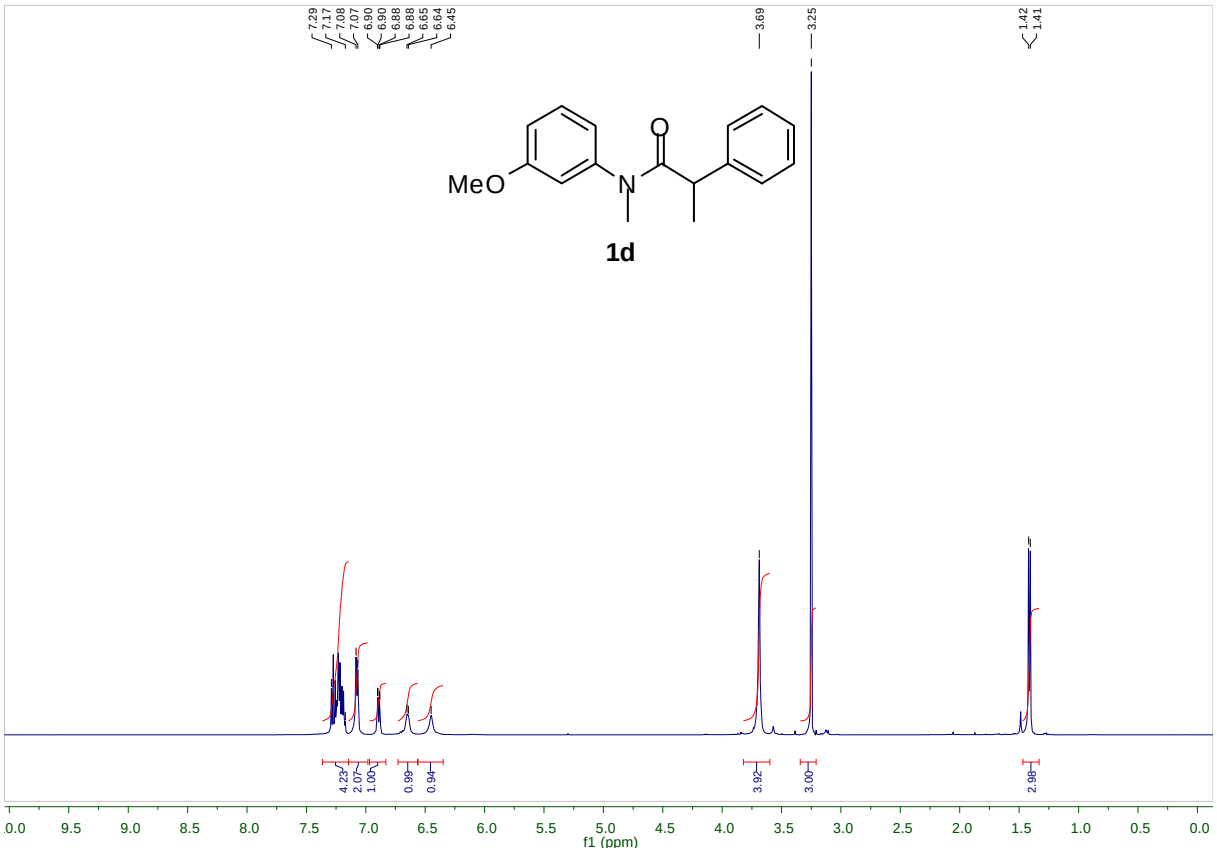


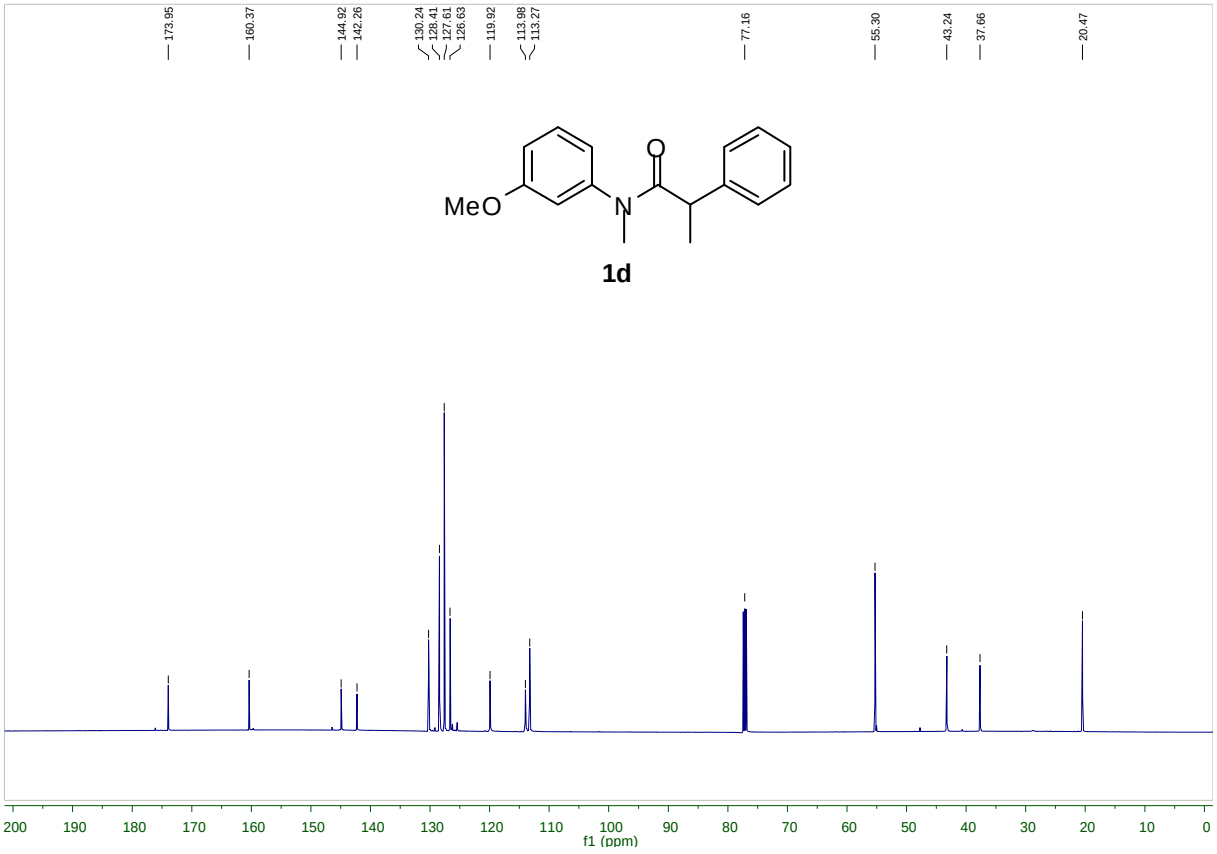


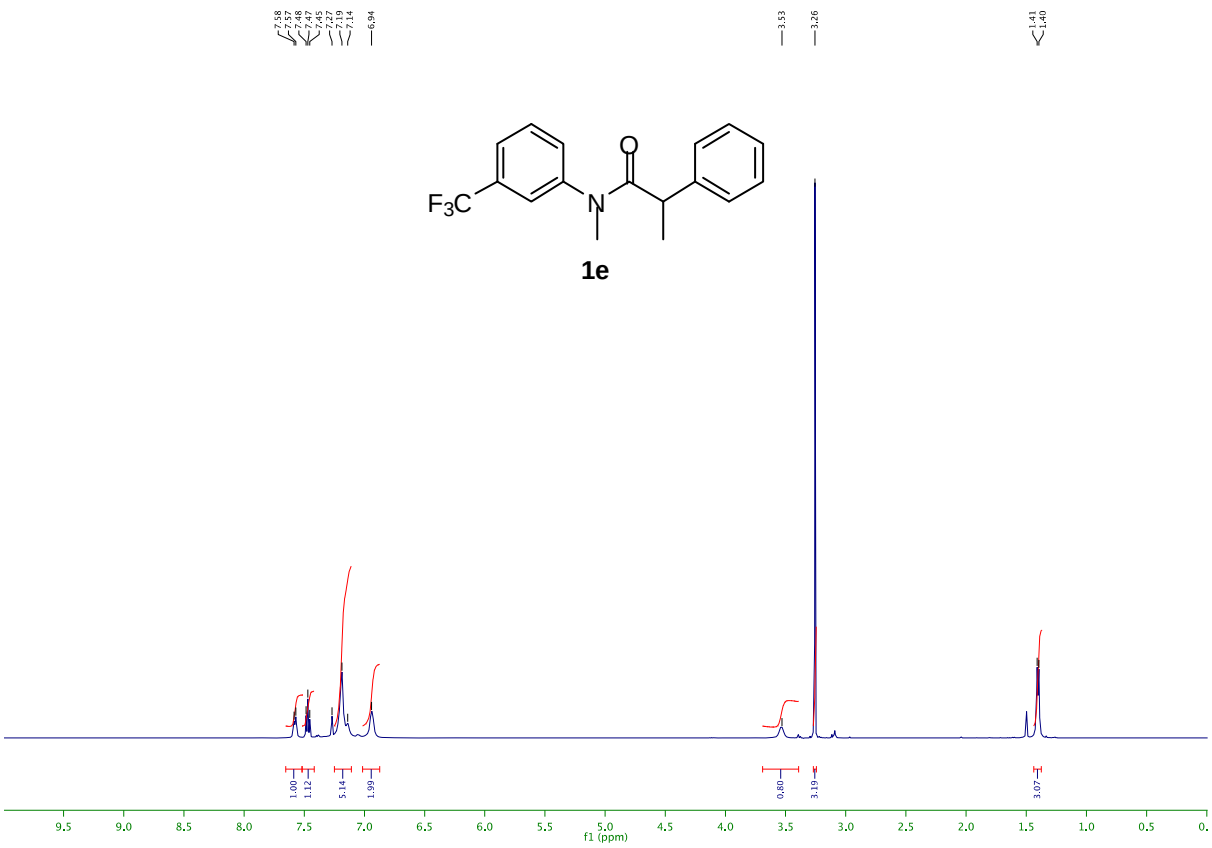


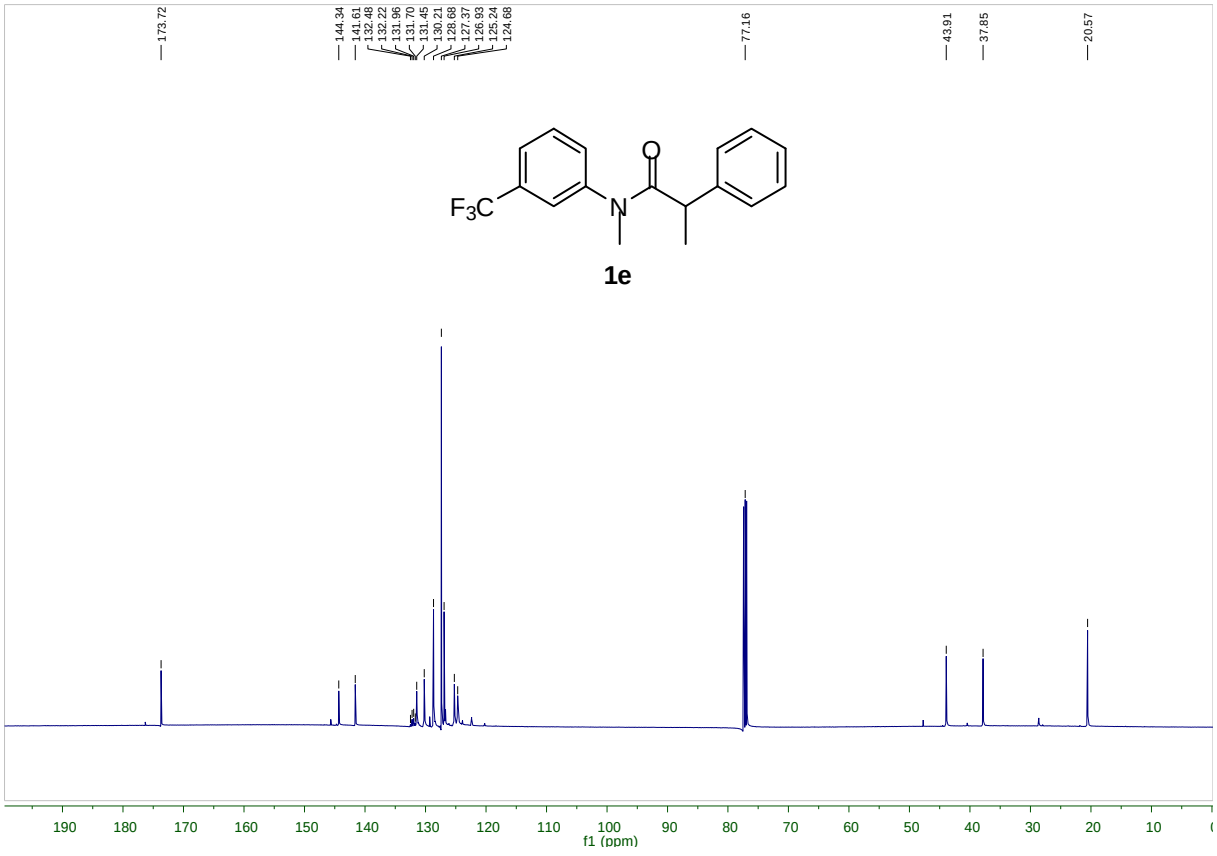


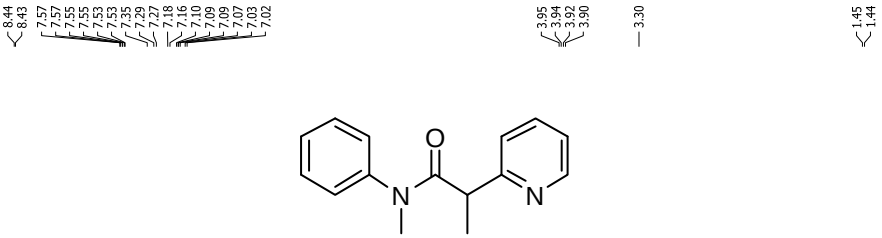












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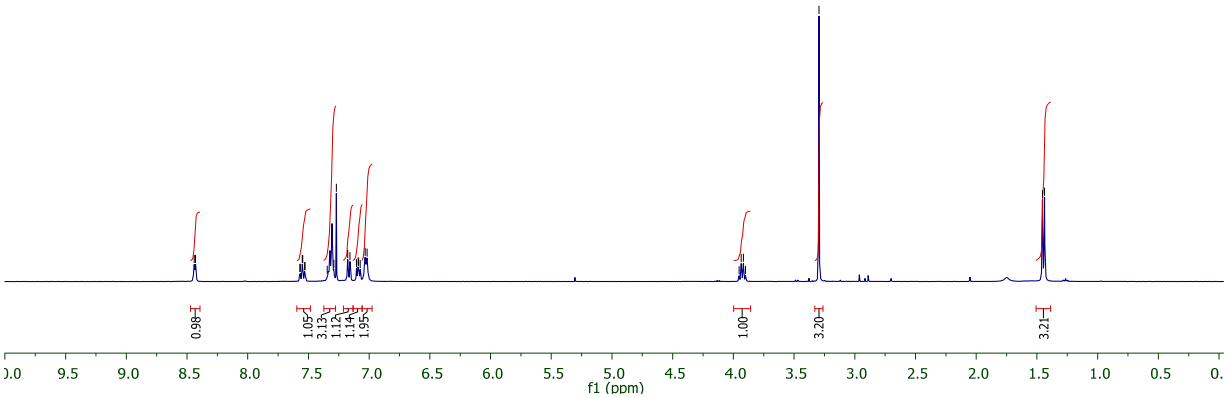

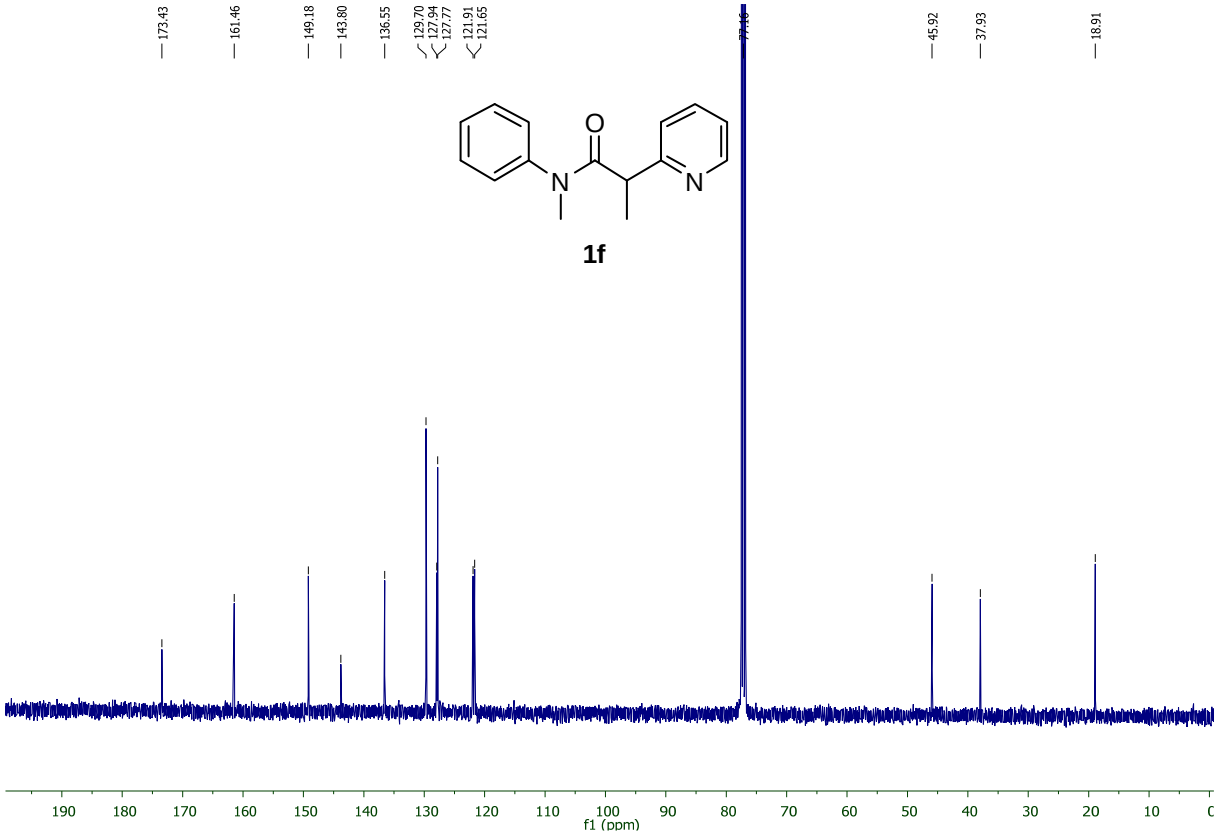

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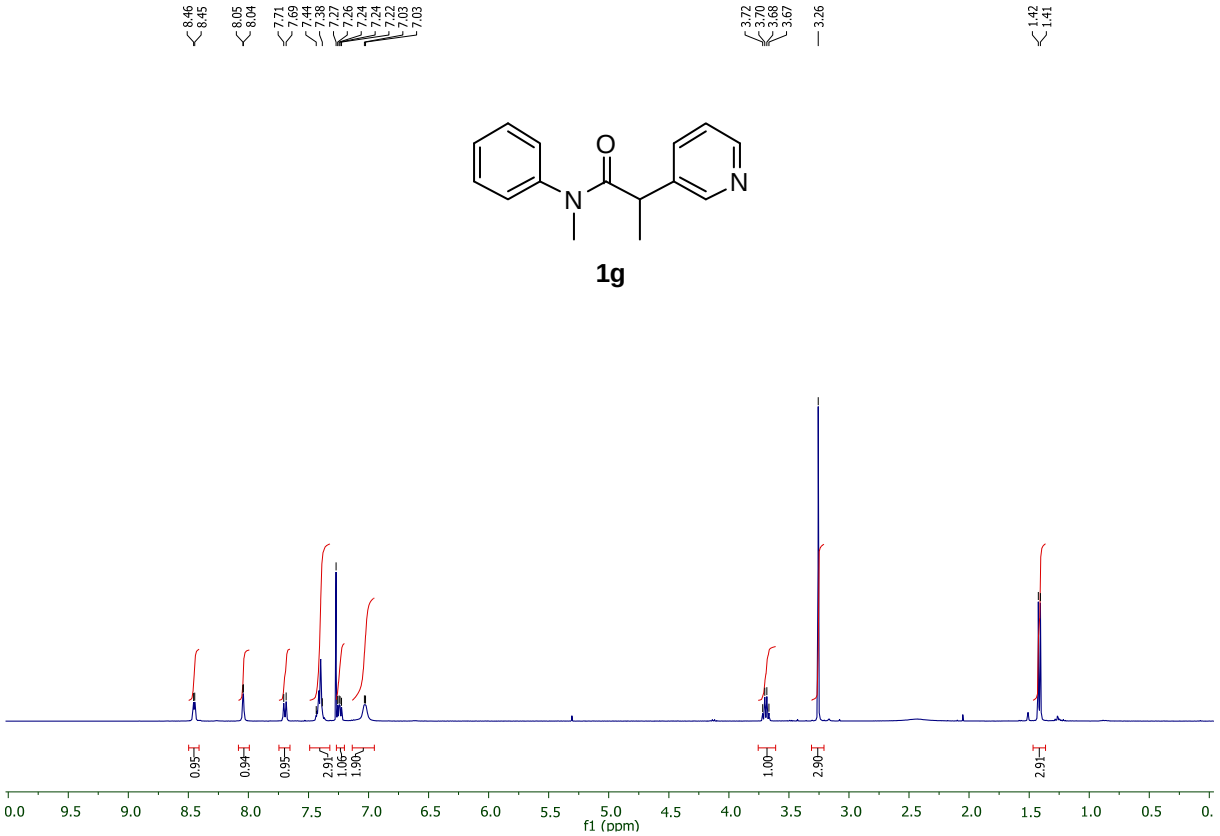

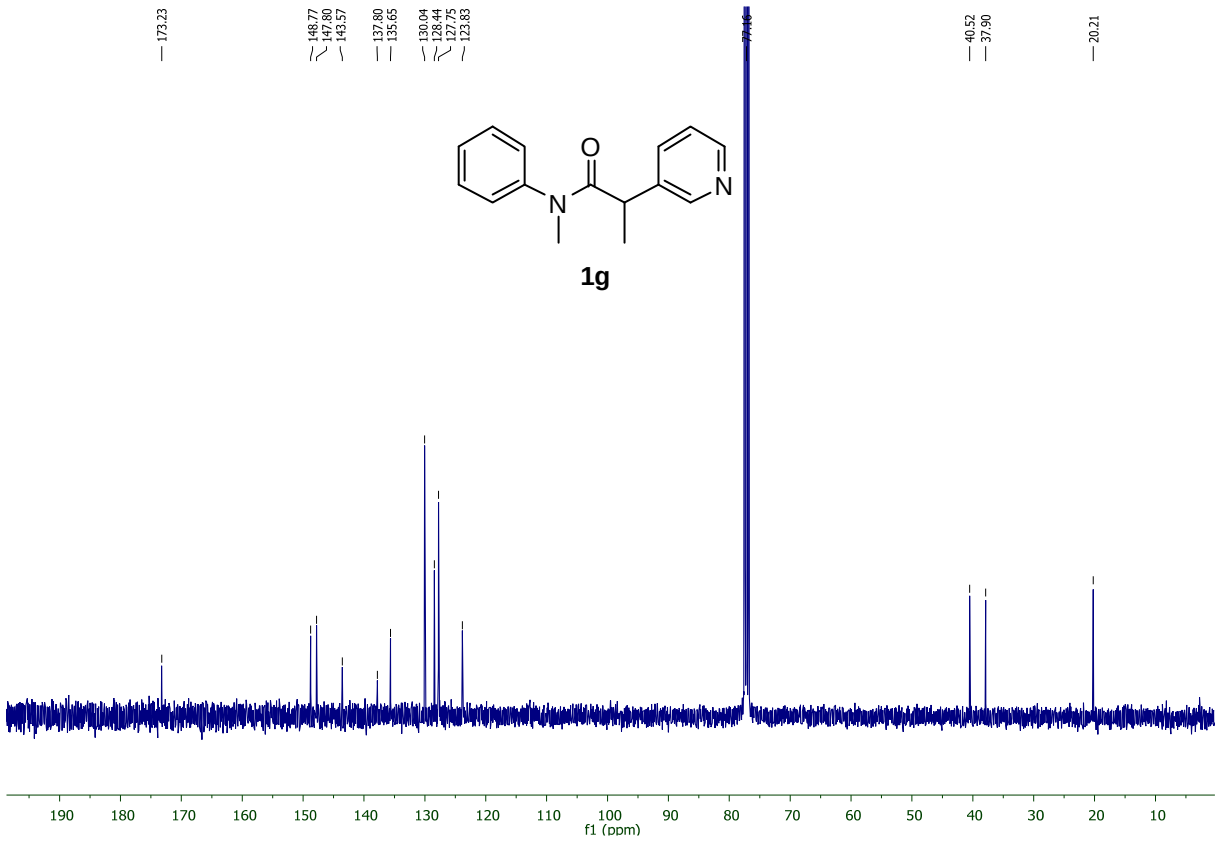

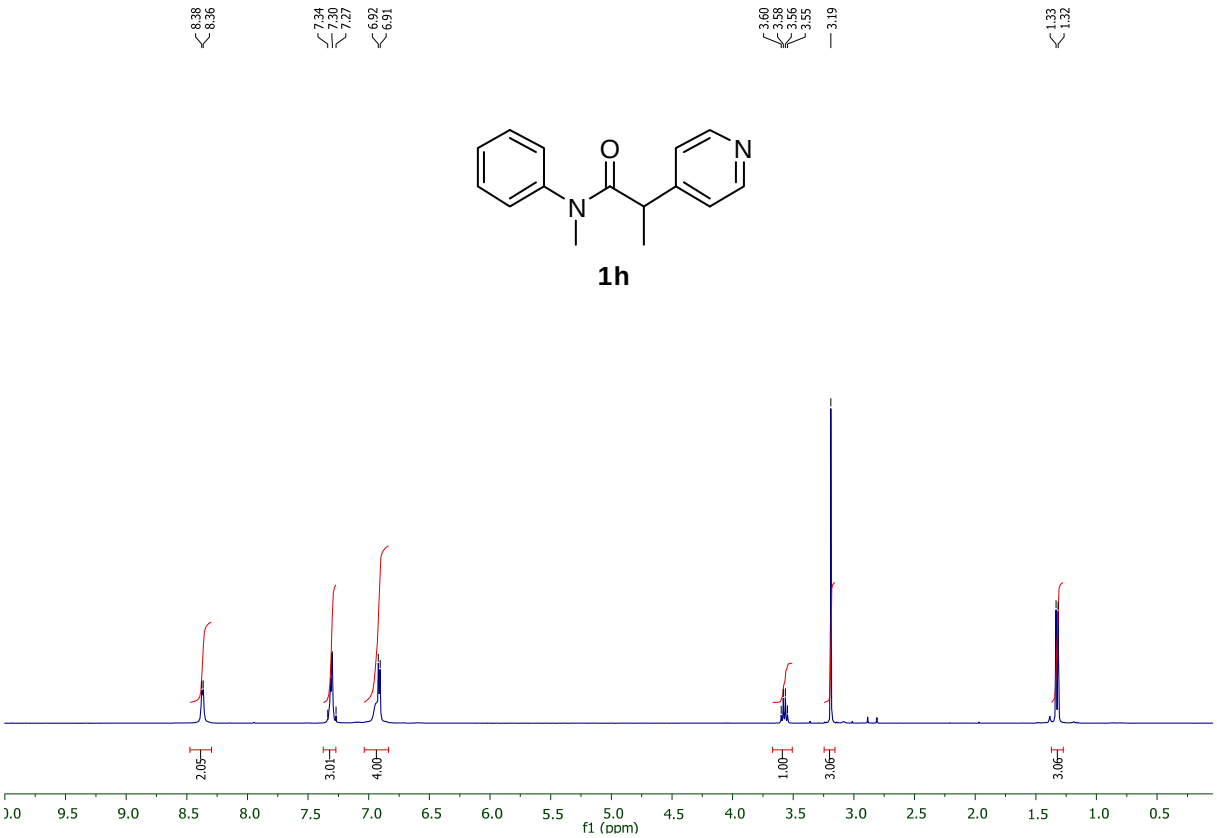

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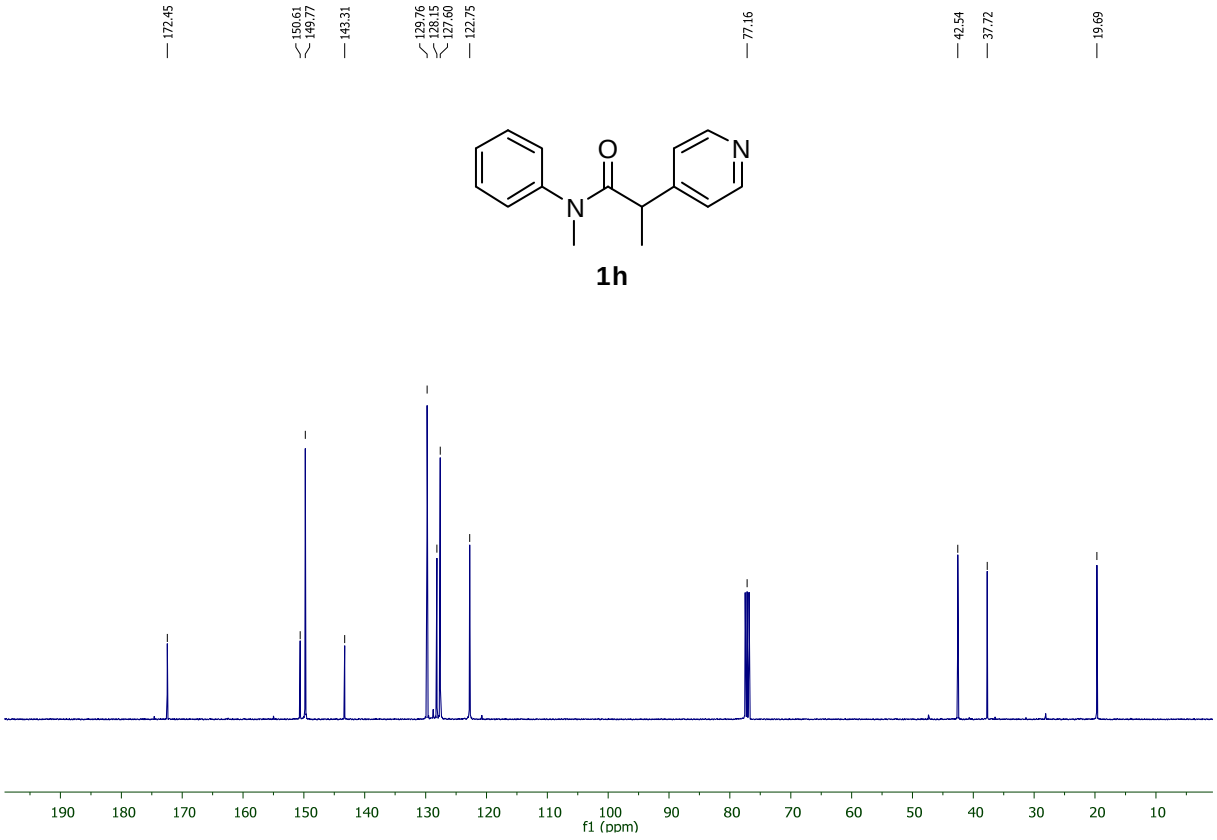
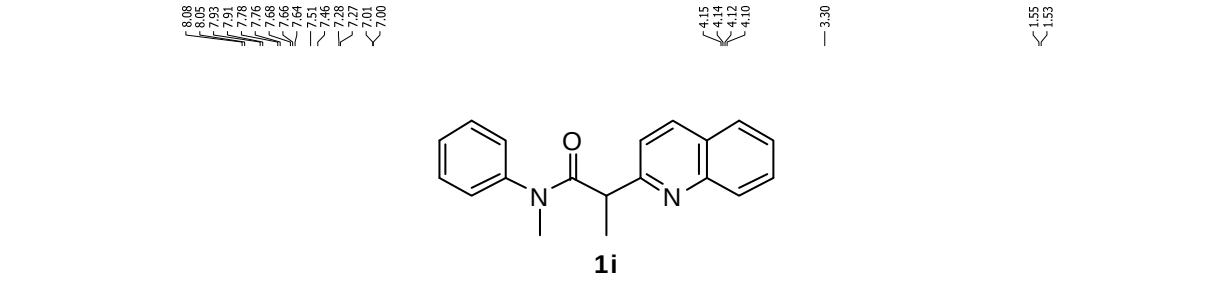


1h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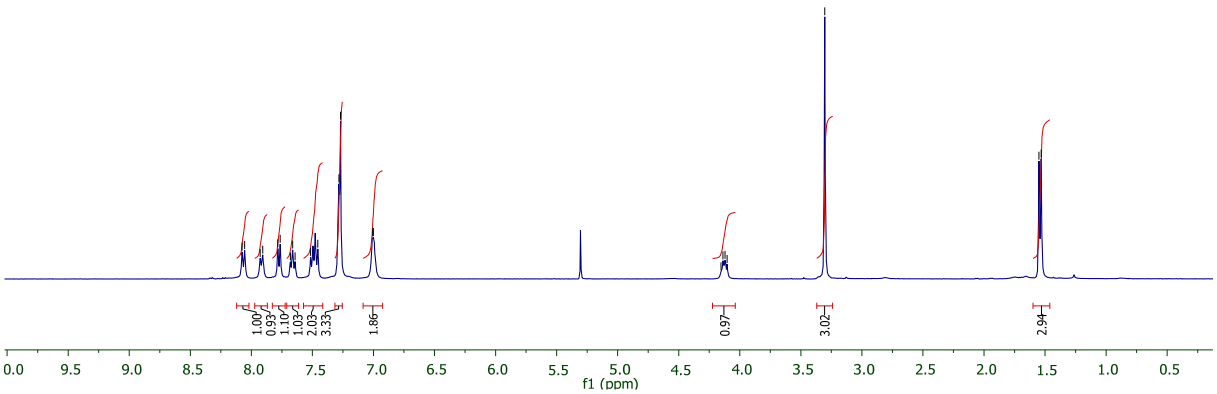
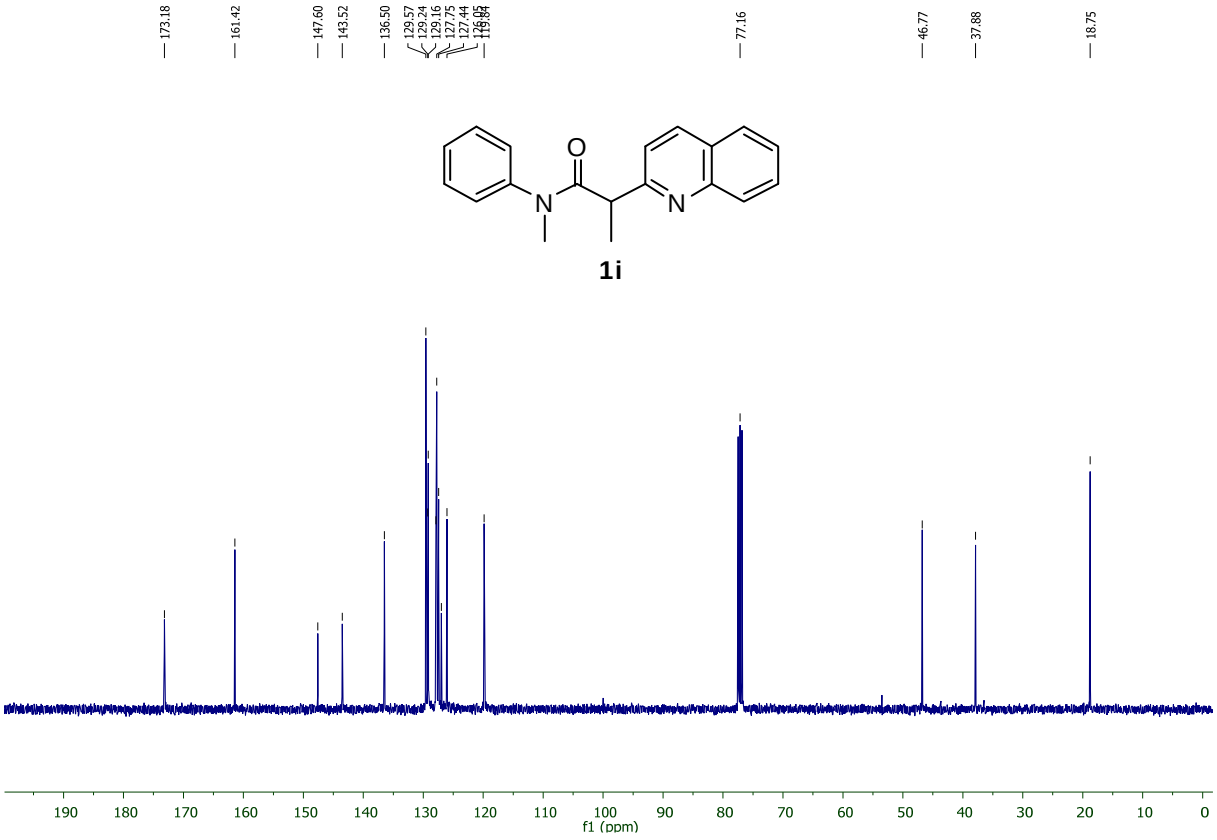
7.91
7.78
7.76
7.68
7.66
7.64
7.51
7.46
7.28
7.27
7.01
7.00
4.15
4.14
4.12
4.10
3.30
1.55
1.53
O
N
N

1i


1.00
0.93
1.10
1.03
2.03
3.33
1.86
0.97
3.02
2.94
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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77.16
46.77
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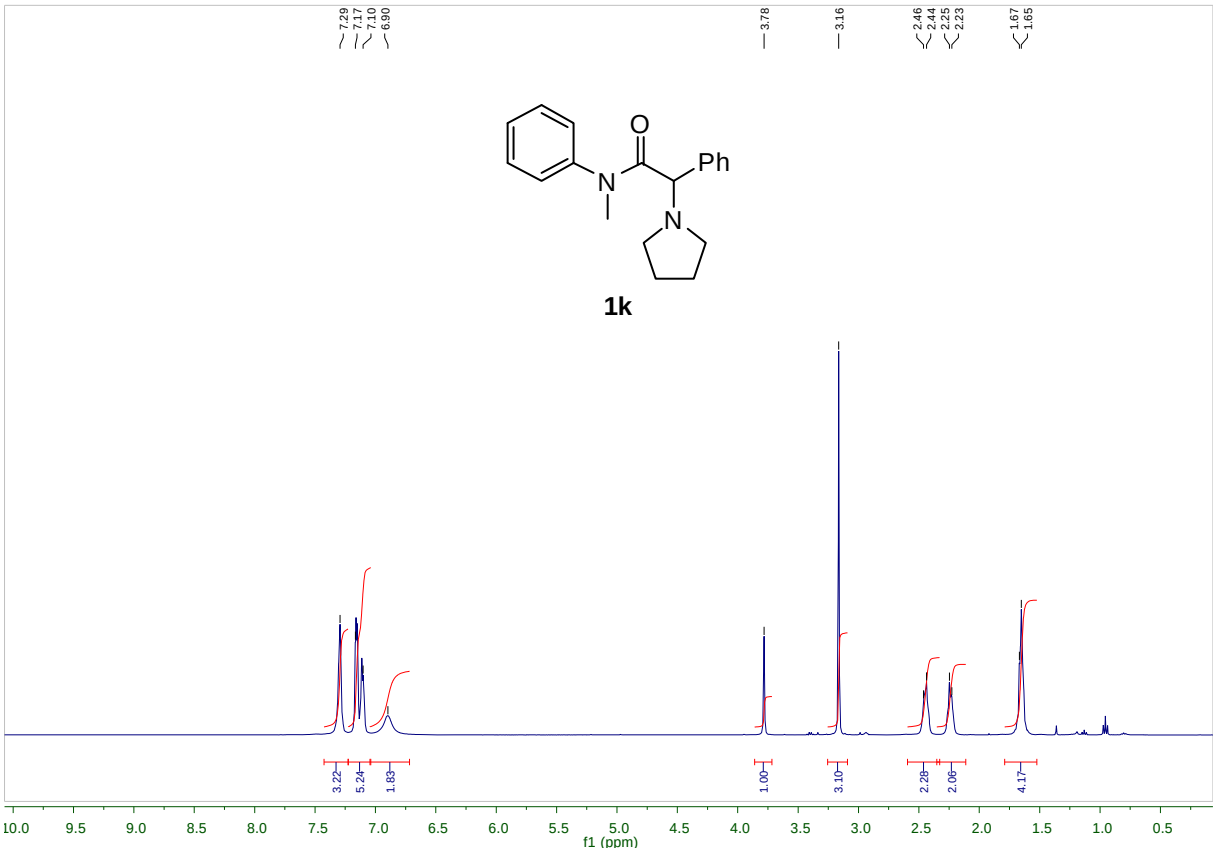
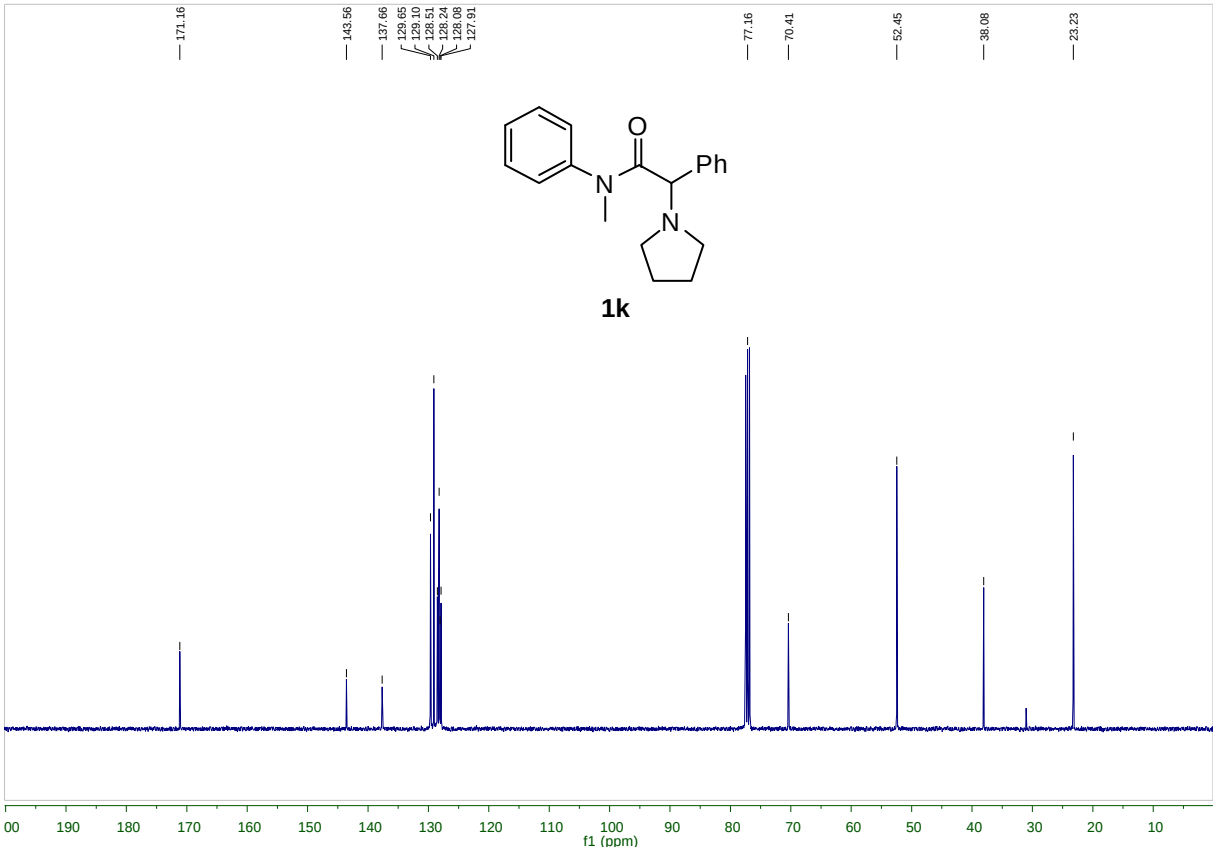
18.75
O
N
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

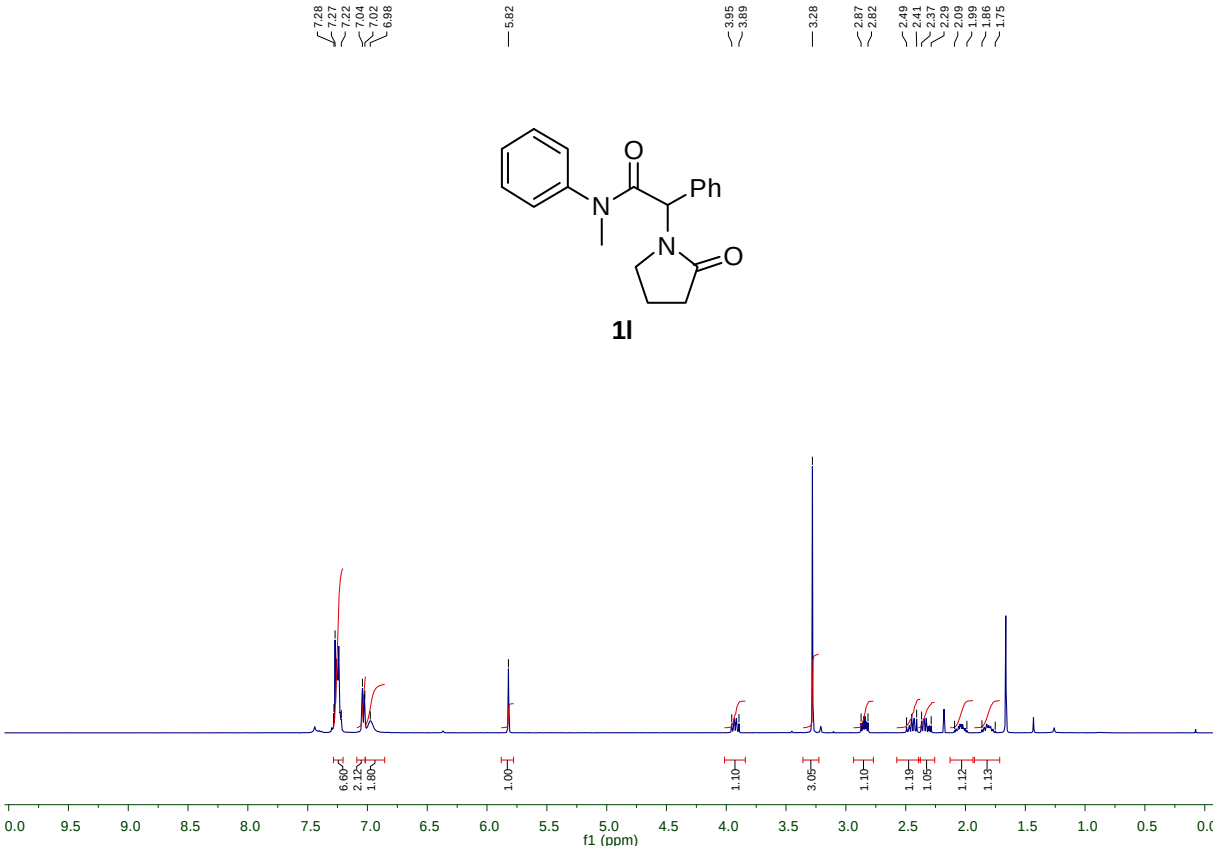
1i



1k



1k



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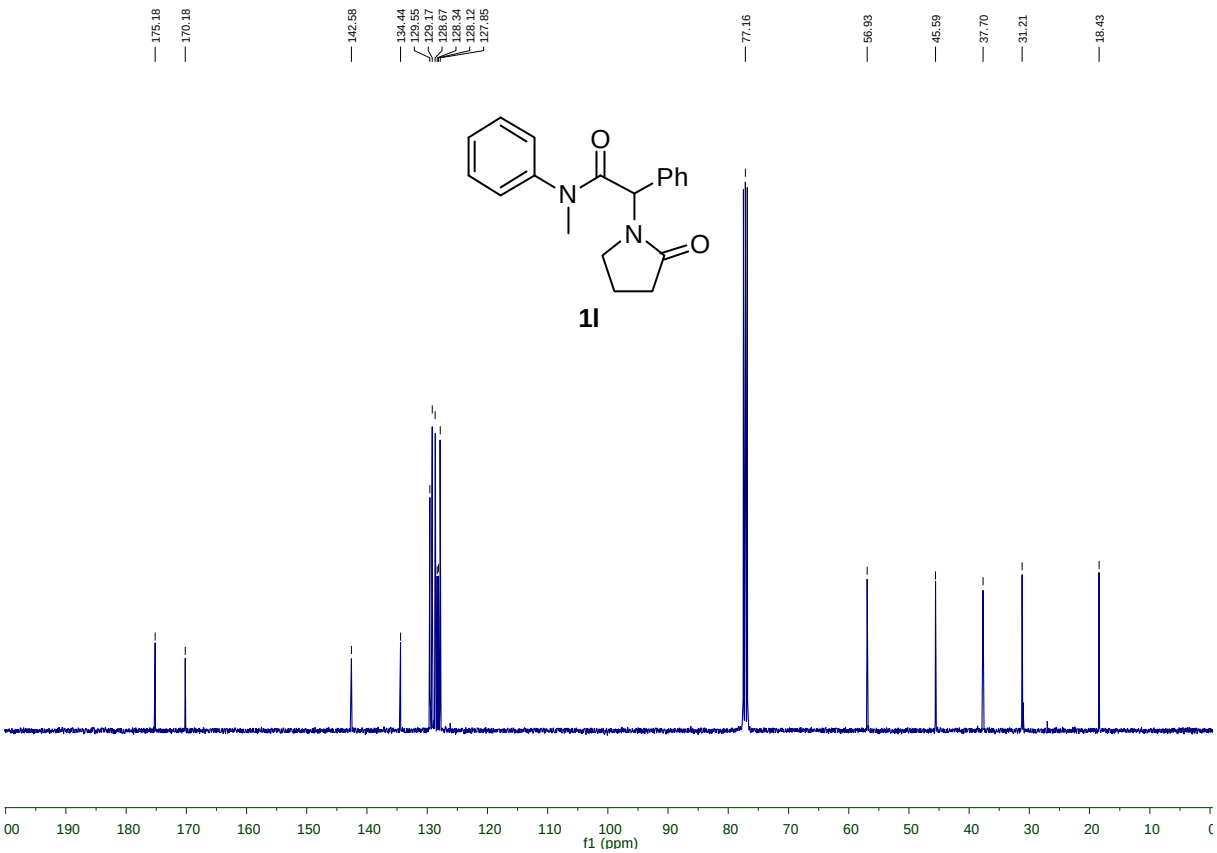

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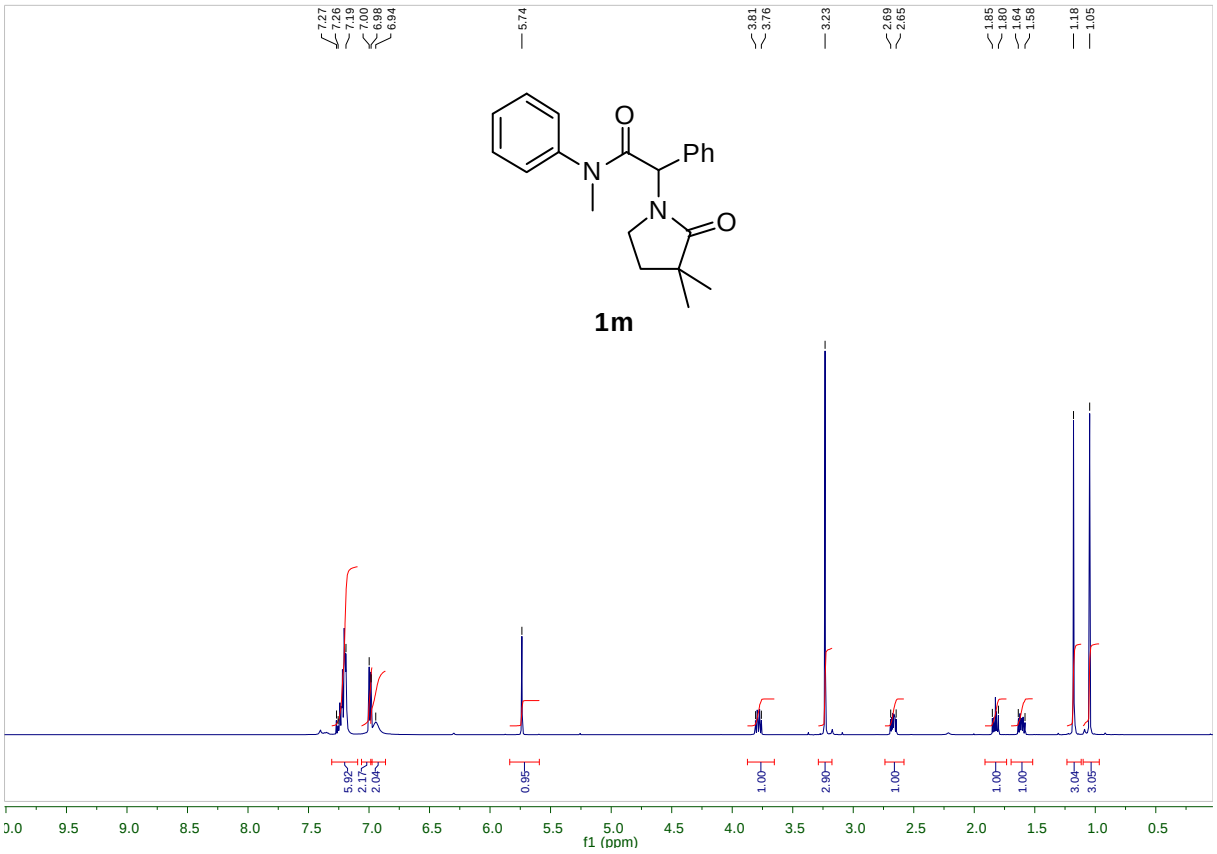

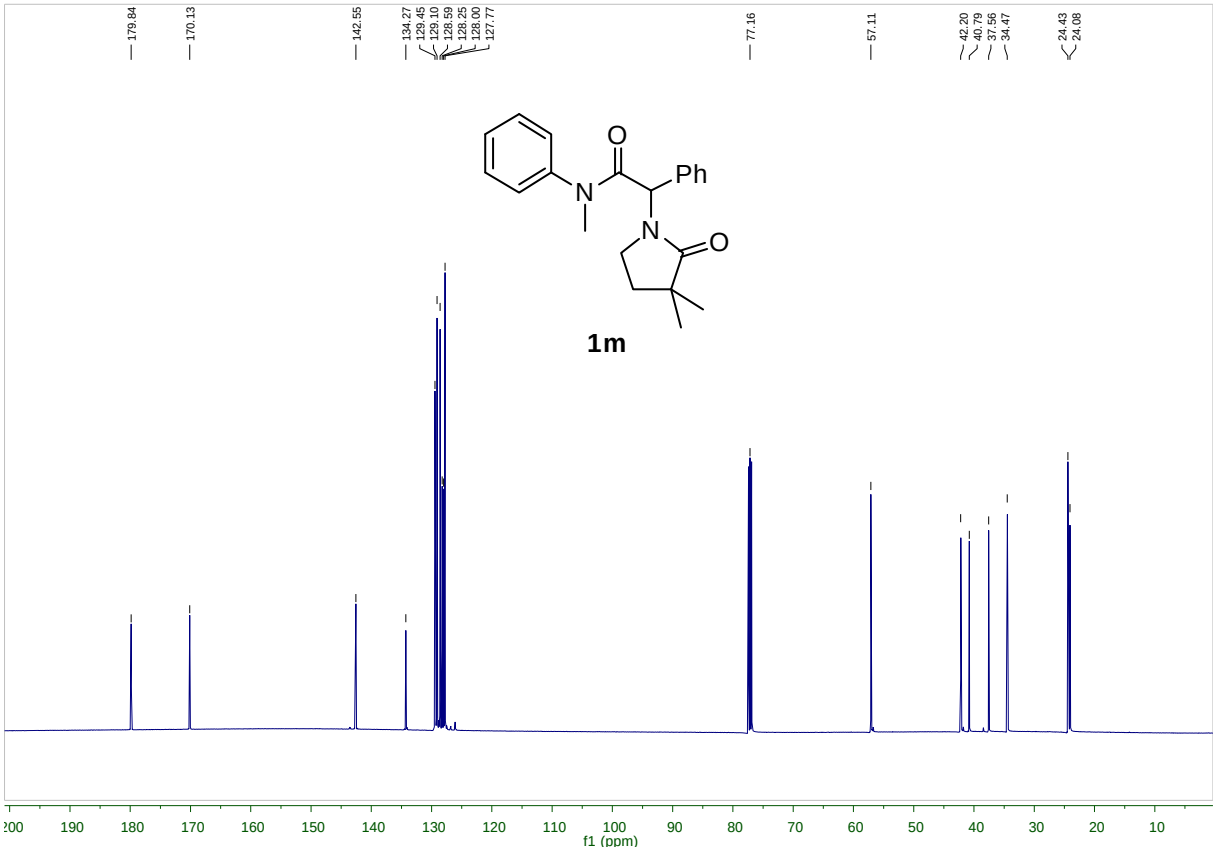

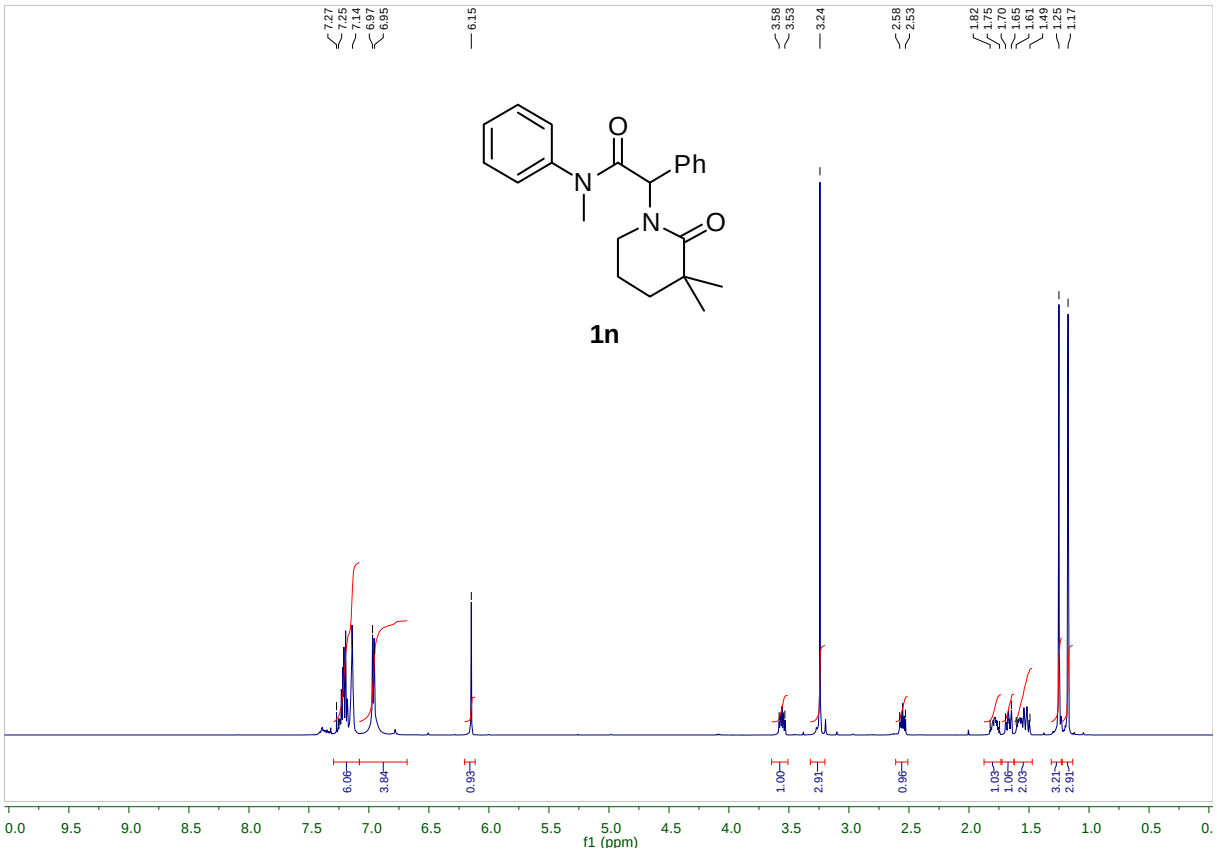

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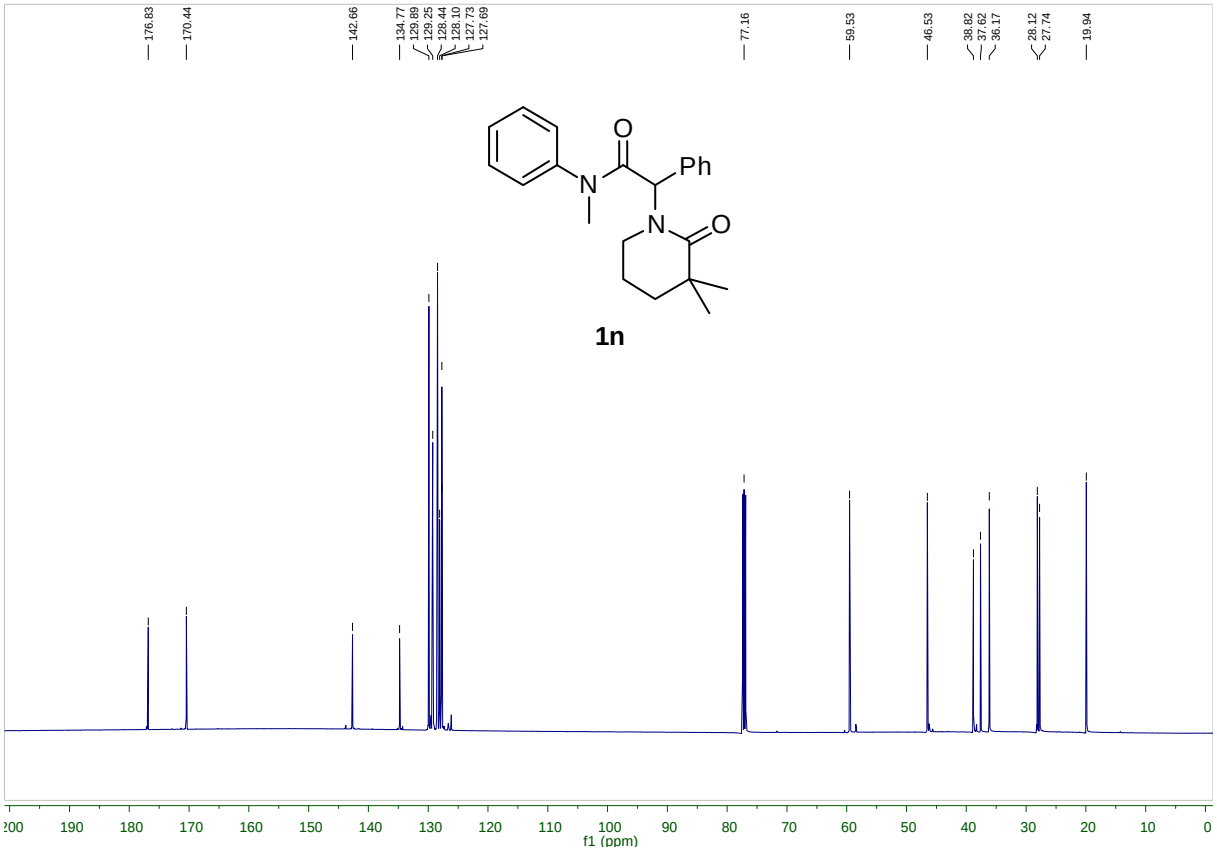

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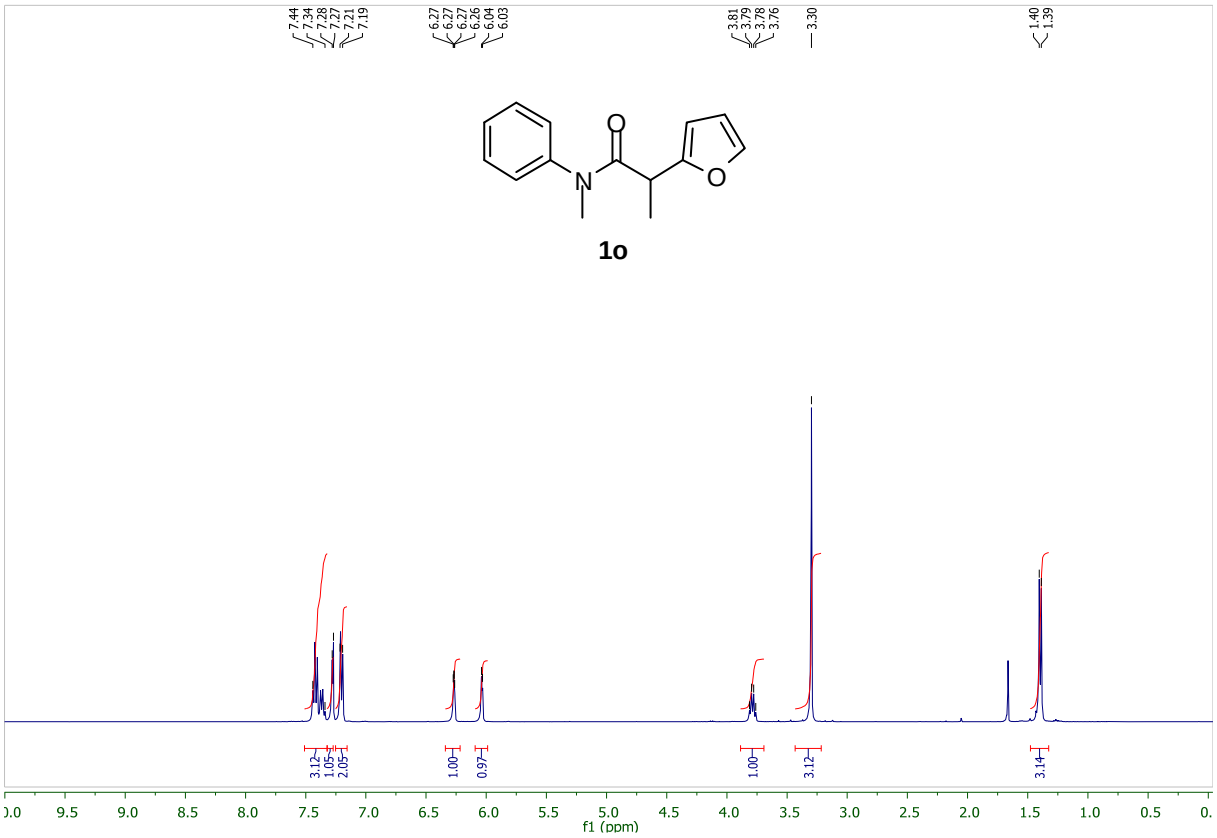

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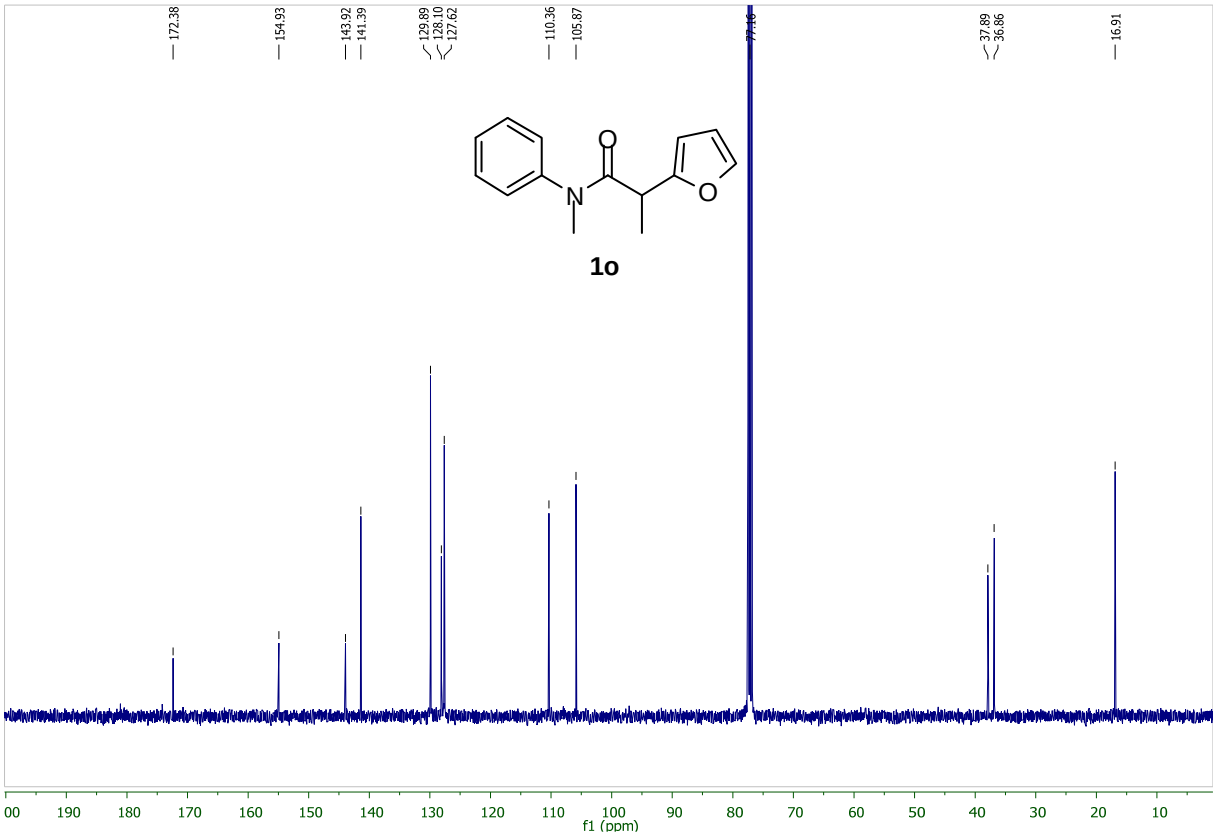

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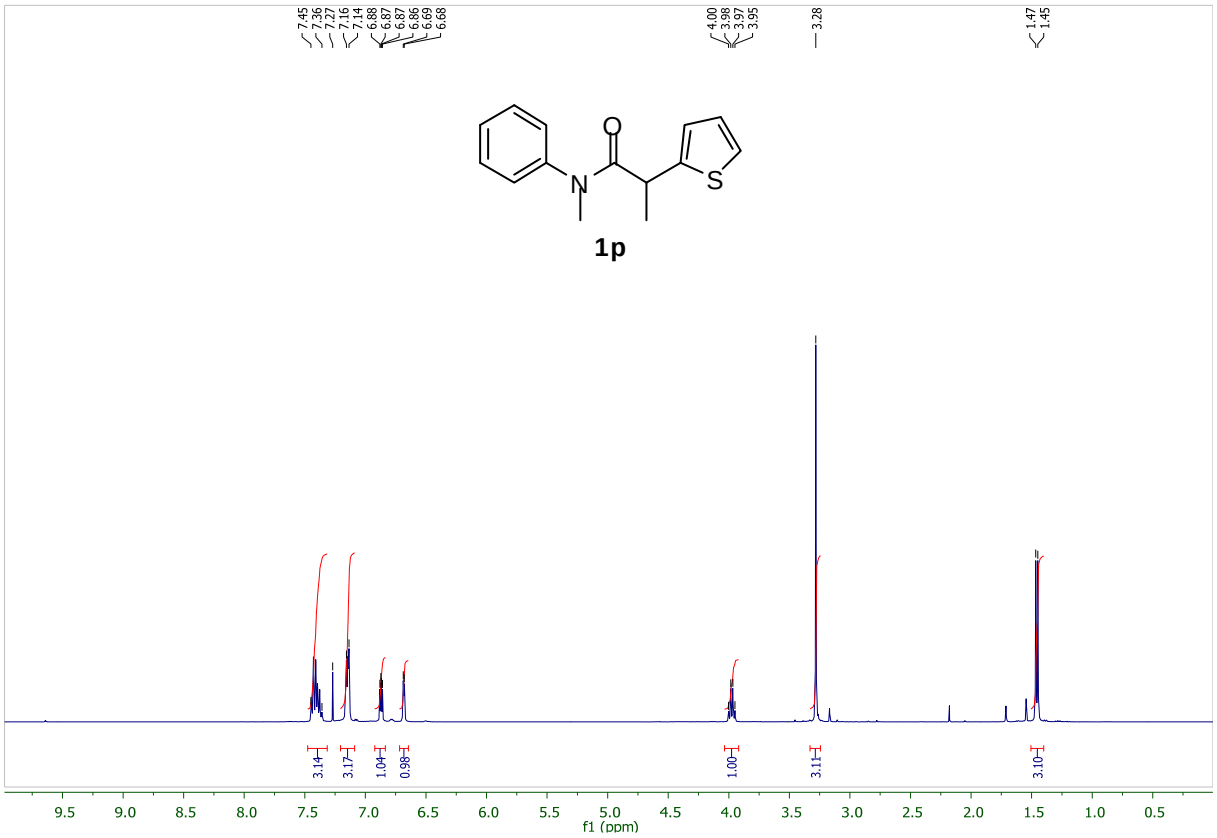

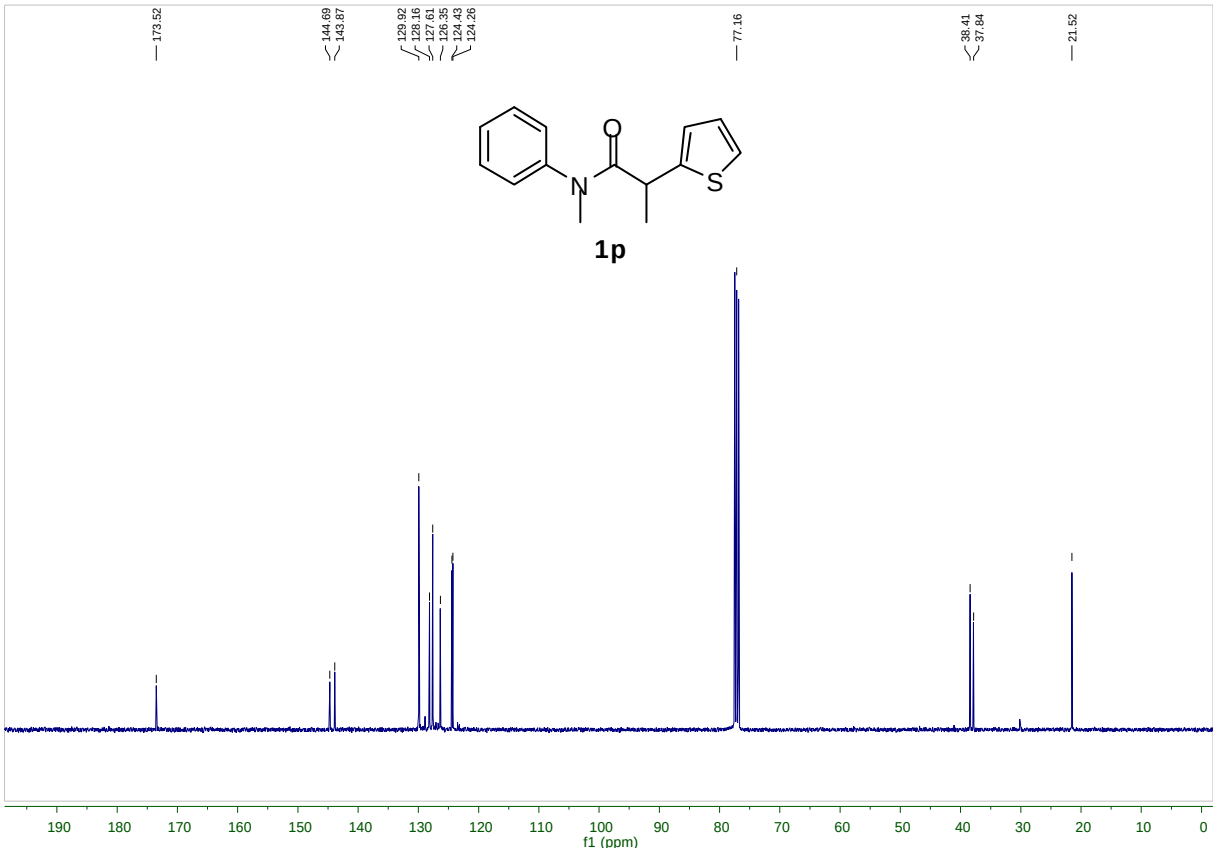

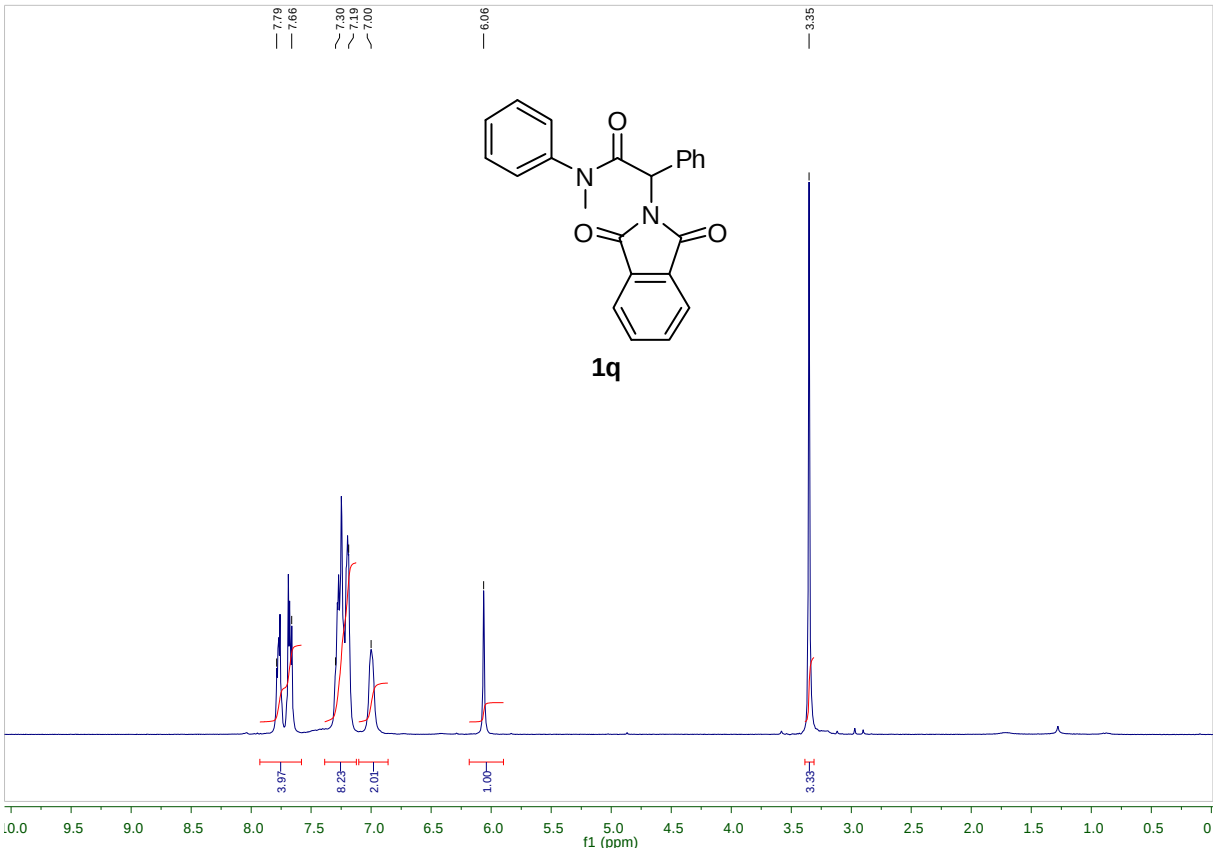

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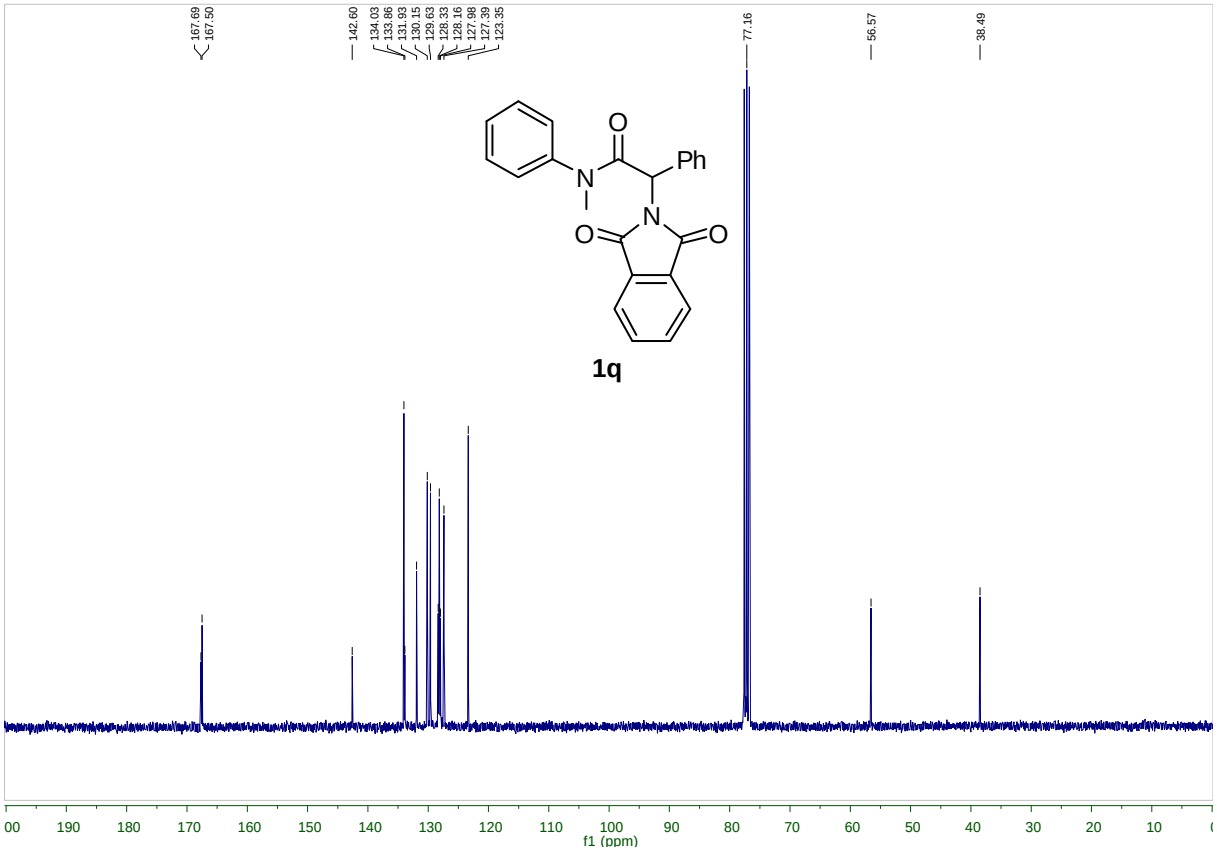

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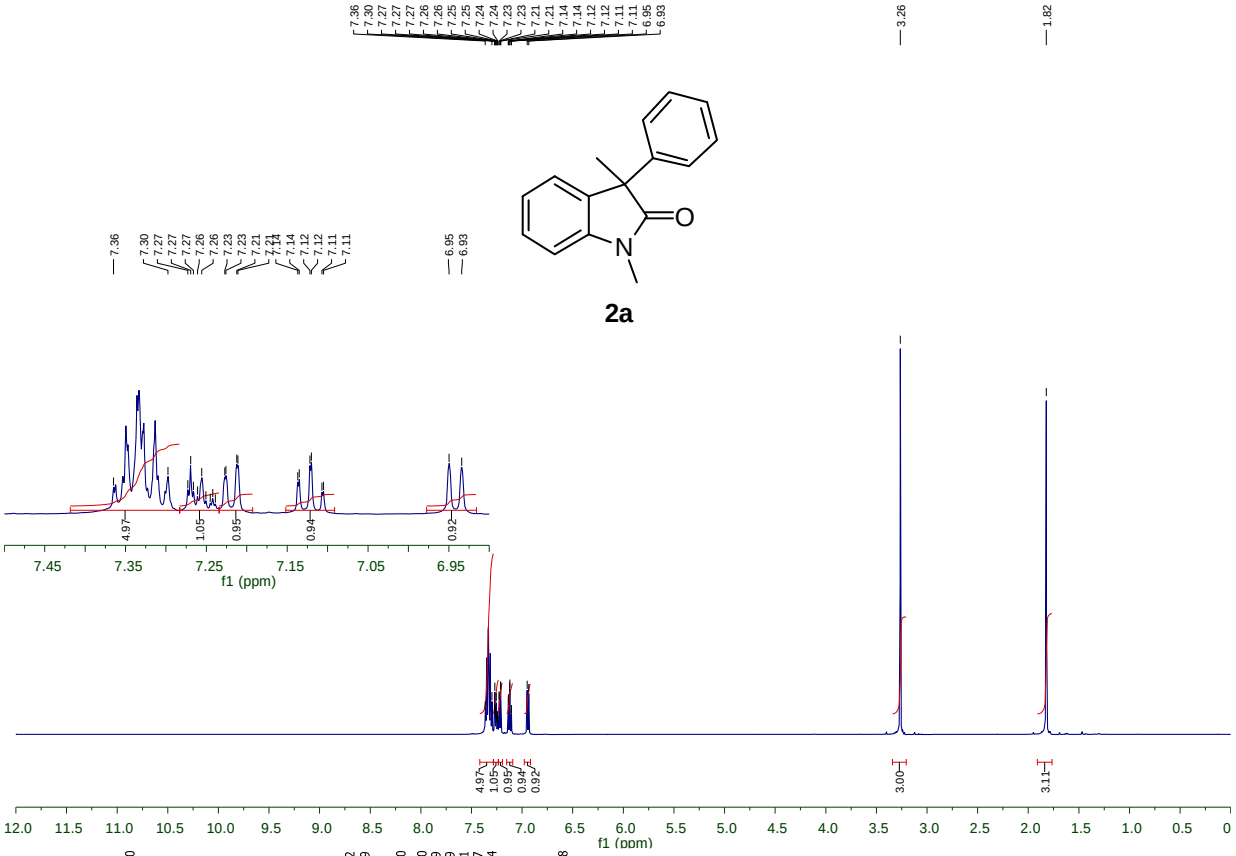
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7.27
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7.25
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7.24
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7.23
7.21
7.21
7.14
7.14
7.12
7.12
7.11
7.11
6.95
6.93
3.26
1.82
O
N
4.97
1.05
0.95
0.94
0.92
3.00
3.11
7.45
7.35
7.25
7.15
7.05
6.95
f1 (ppm)
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11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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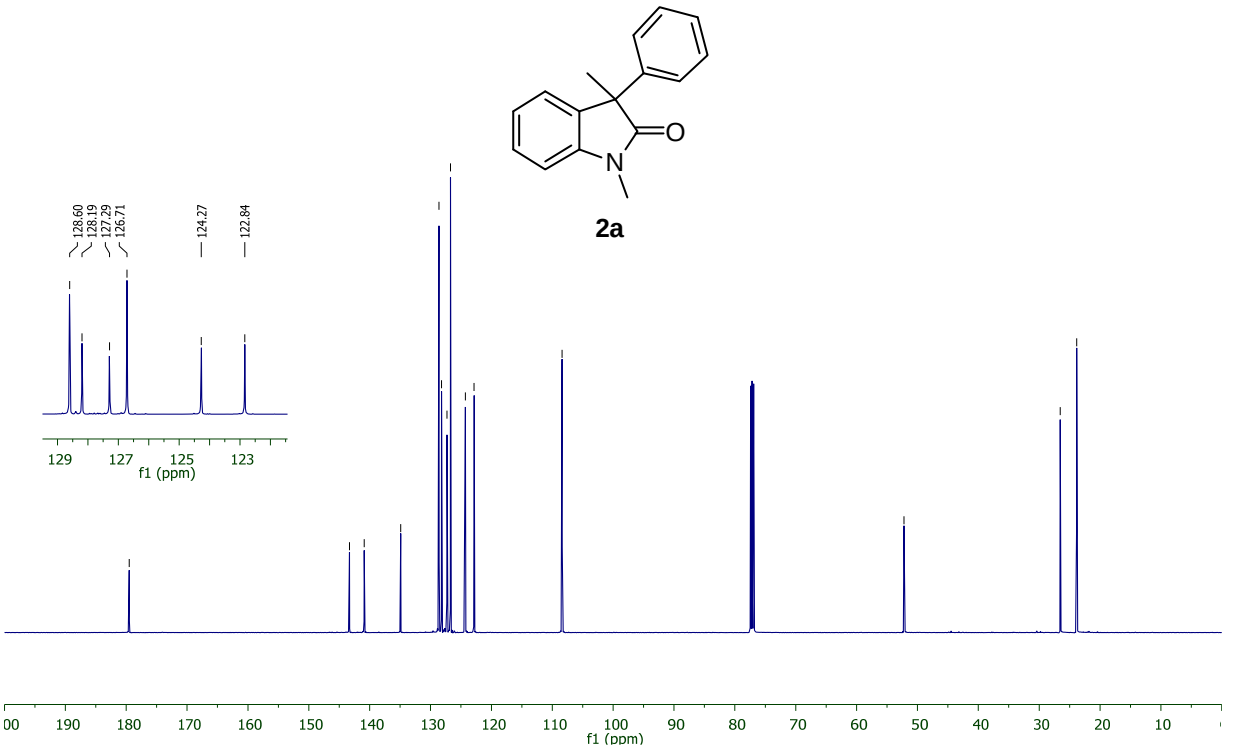
0

2a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126.71
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122.84
108.38
52.21
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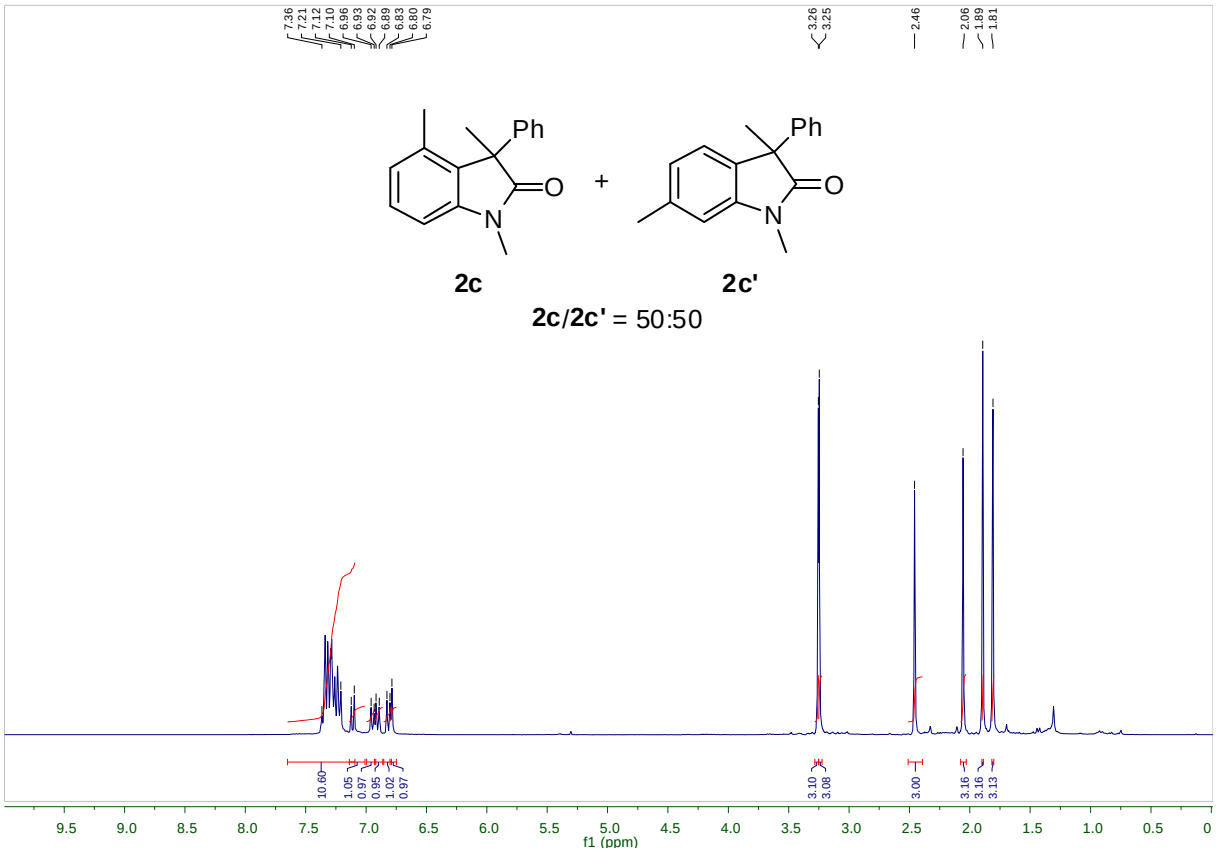
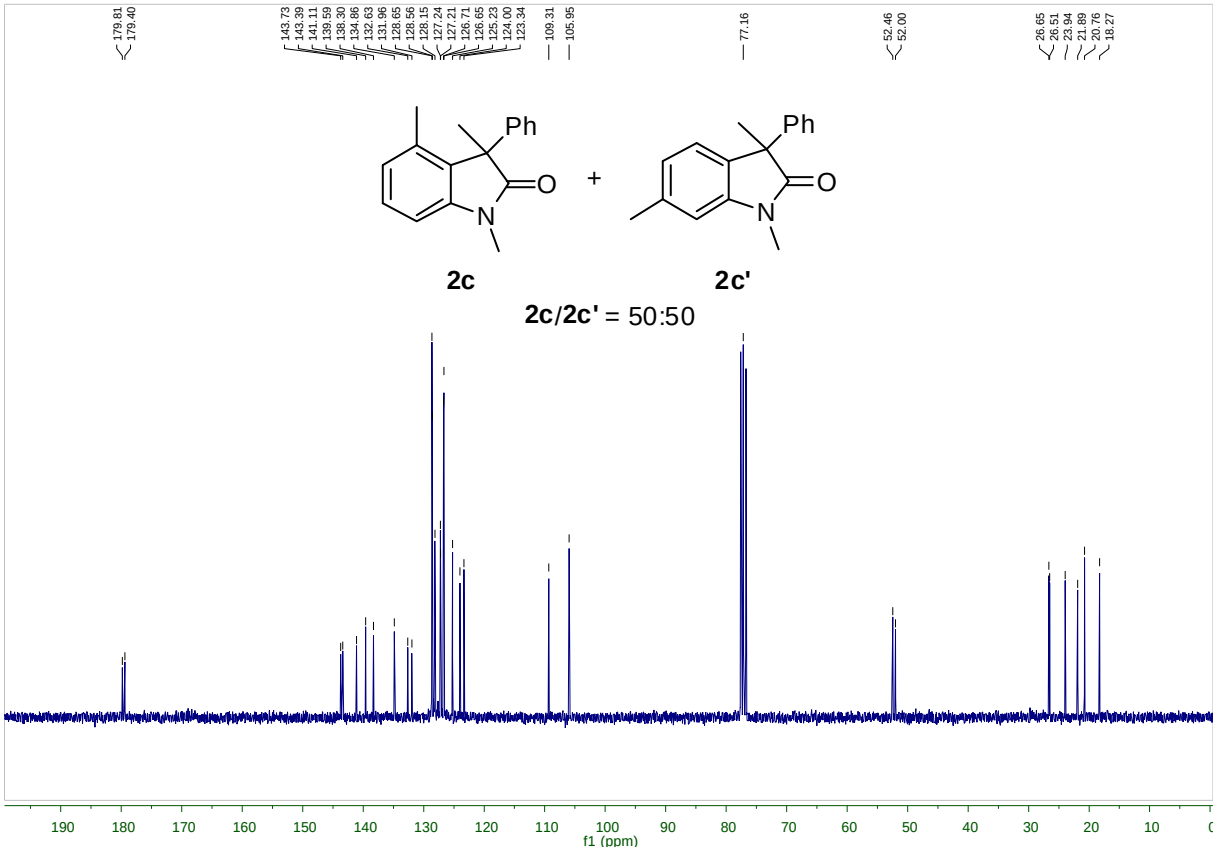
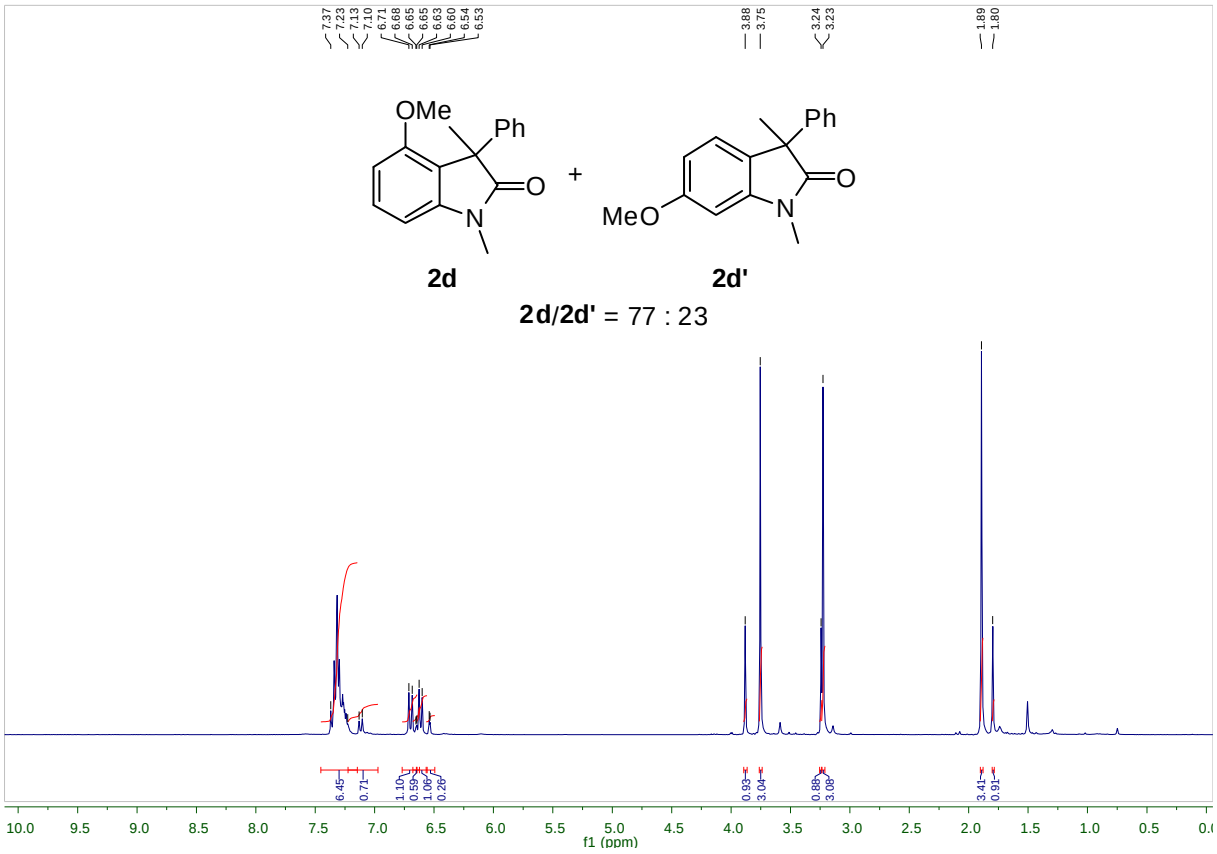
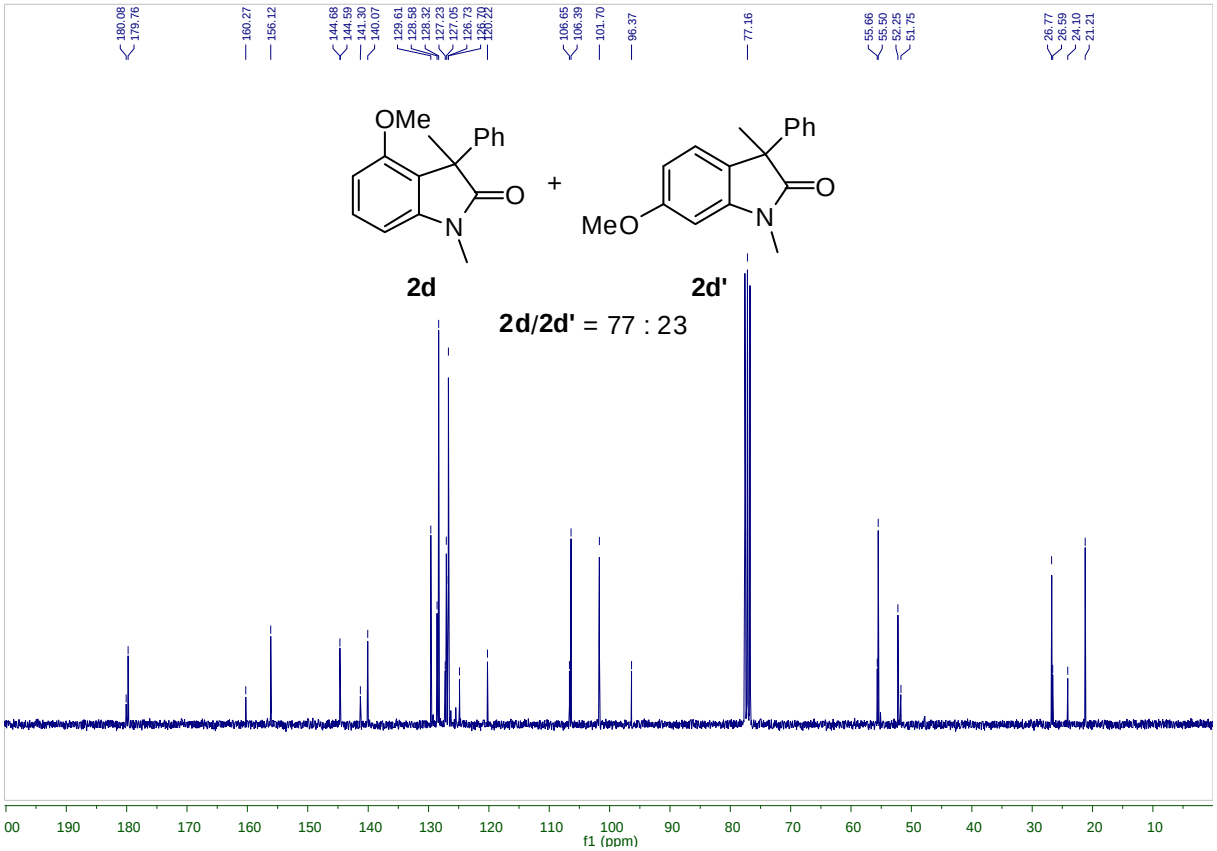
23.84
O
N
129
127
125
123
f1 (ppm)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

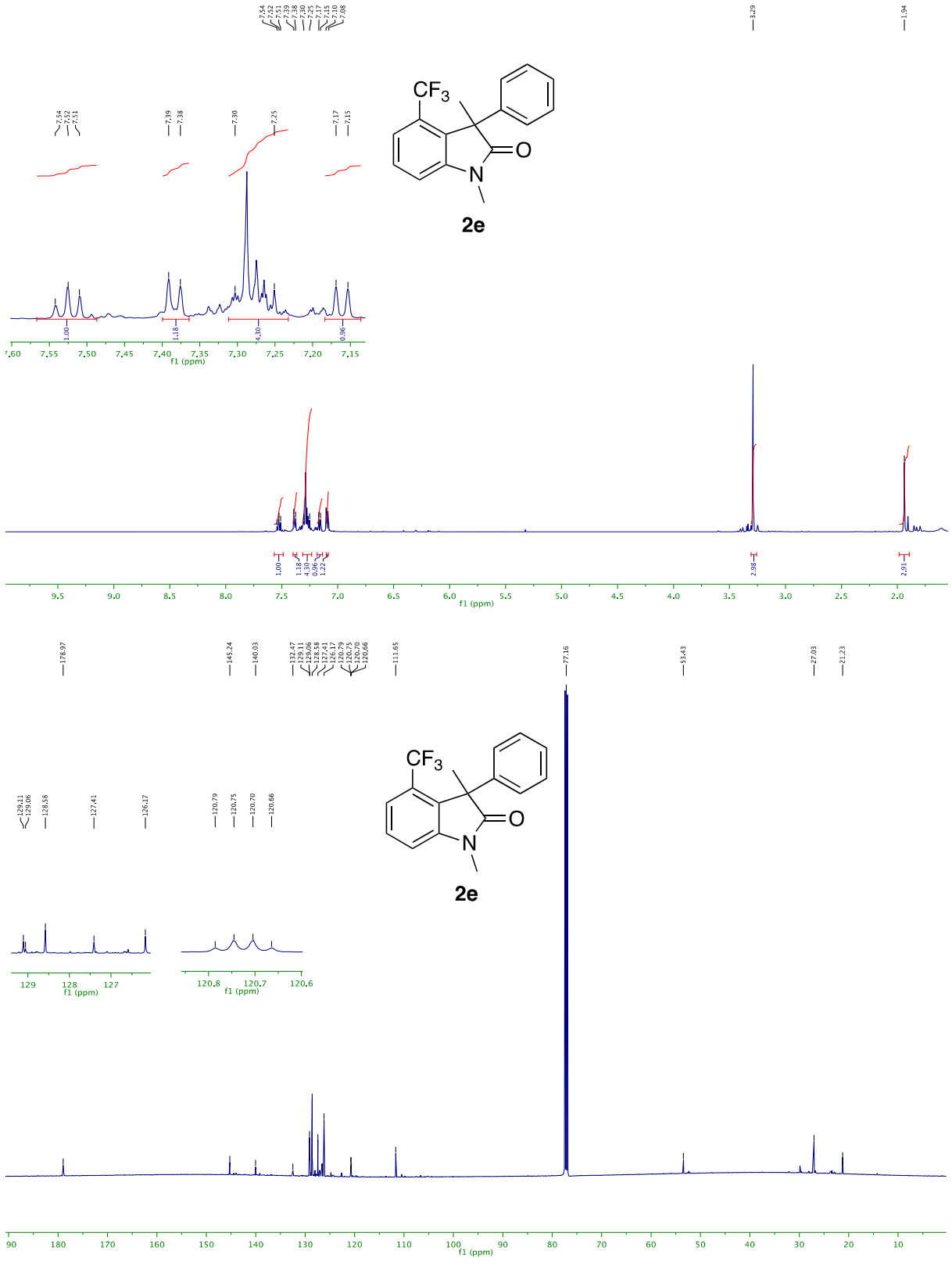
2a



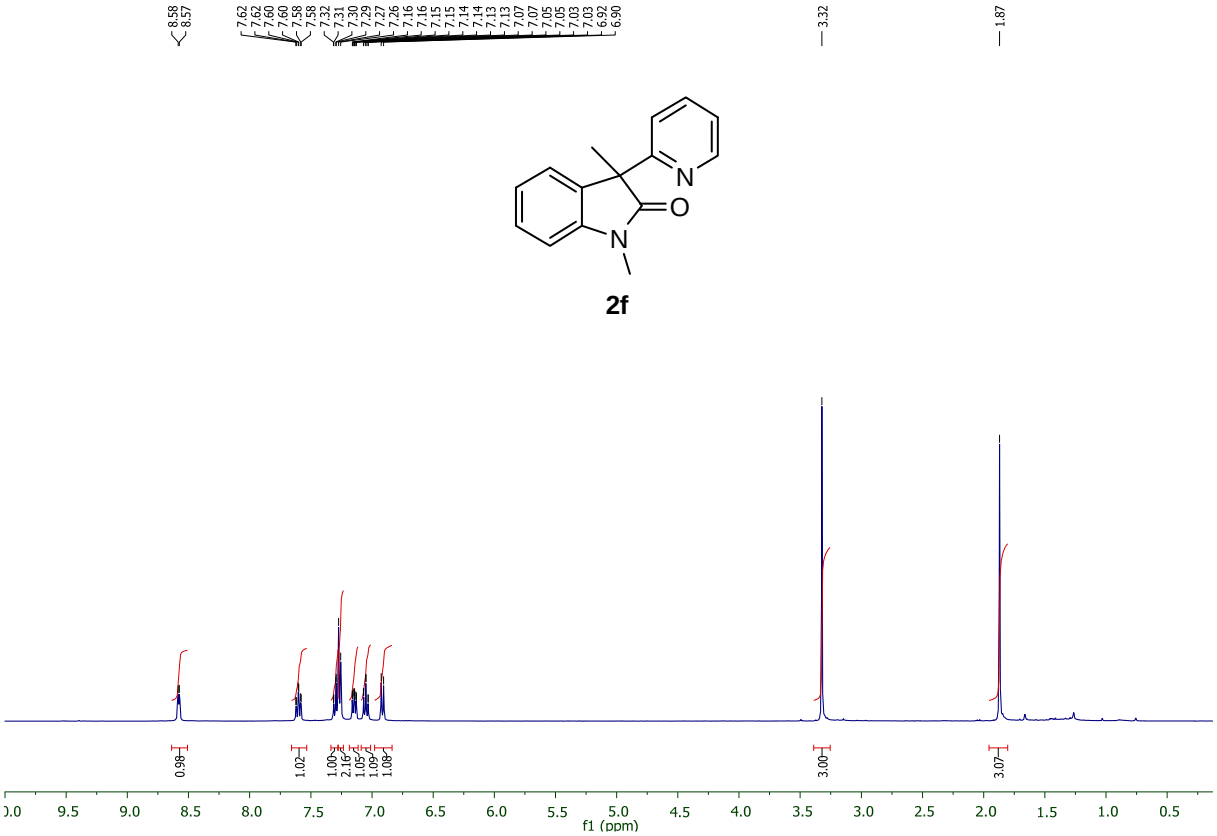




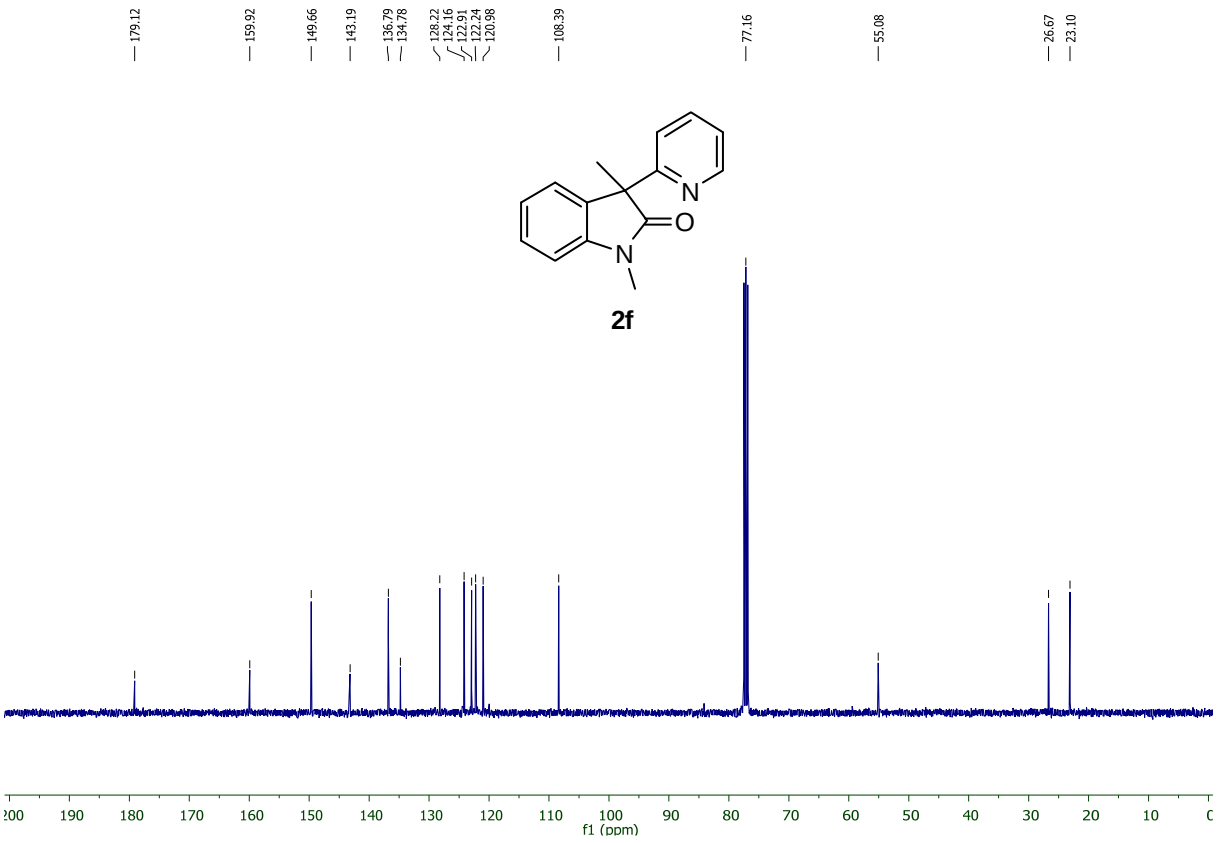




[**2e** was obtained together with an inseparable, unidentified impurity. In ^{13}C NMR, the peak of C(3)-methyl group (δ = 21.2 ppm) appeared as quartet presumably due to the coupling (through space- or long range-) with CF_3 group.]



2f



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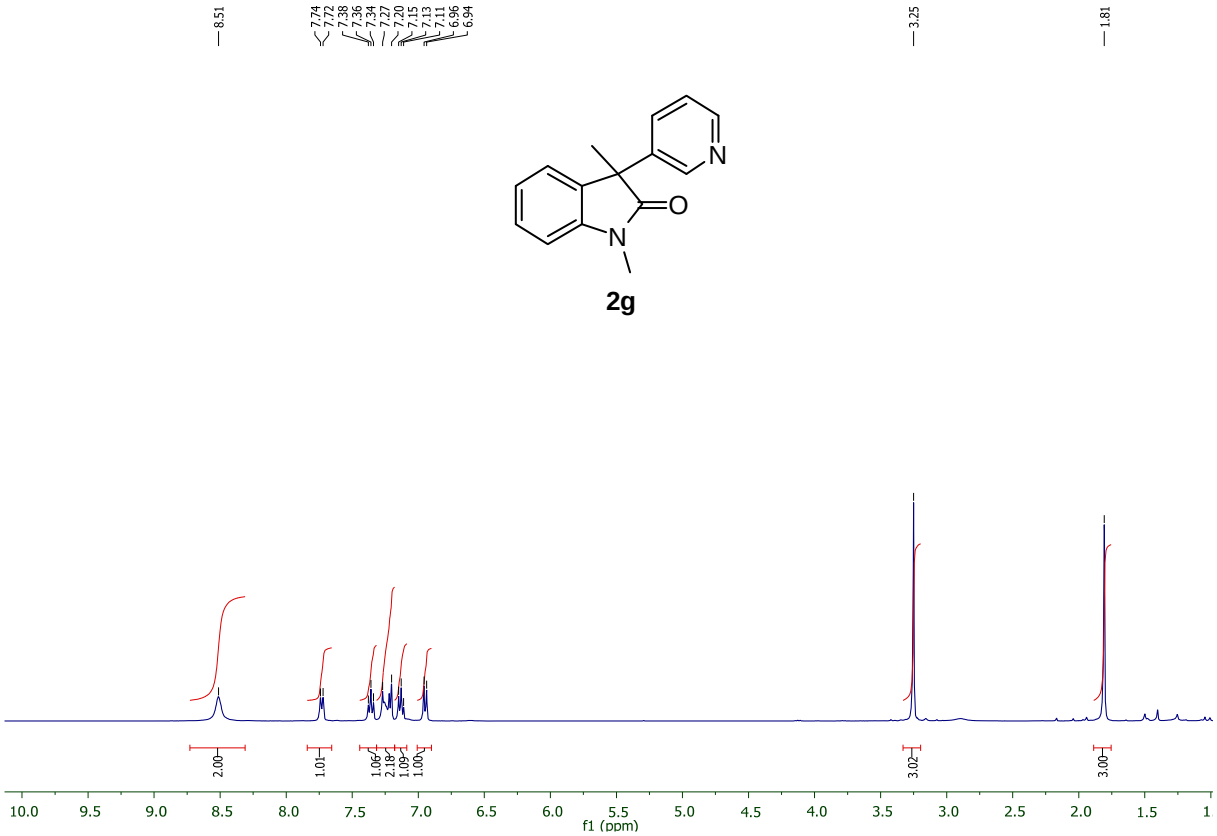
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N
O
N
2.00
1.01
1.06
2.18
1.09
1.00
3.02
3.00
10.0
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
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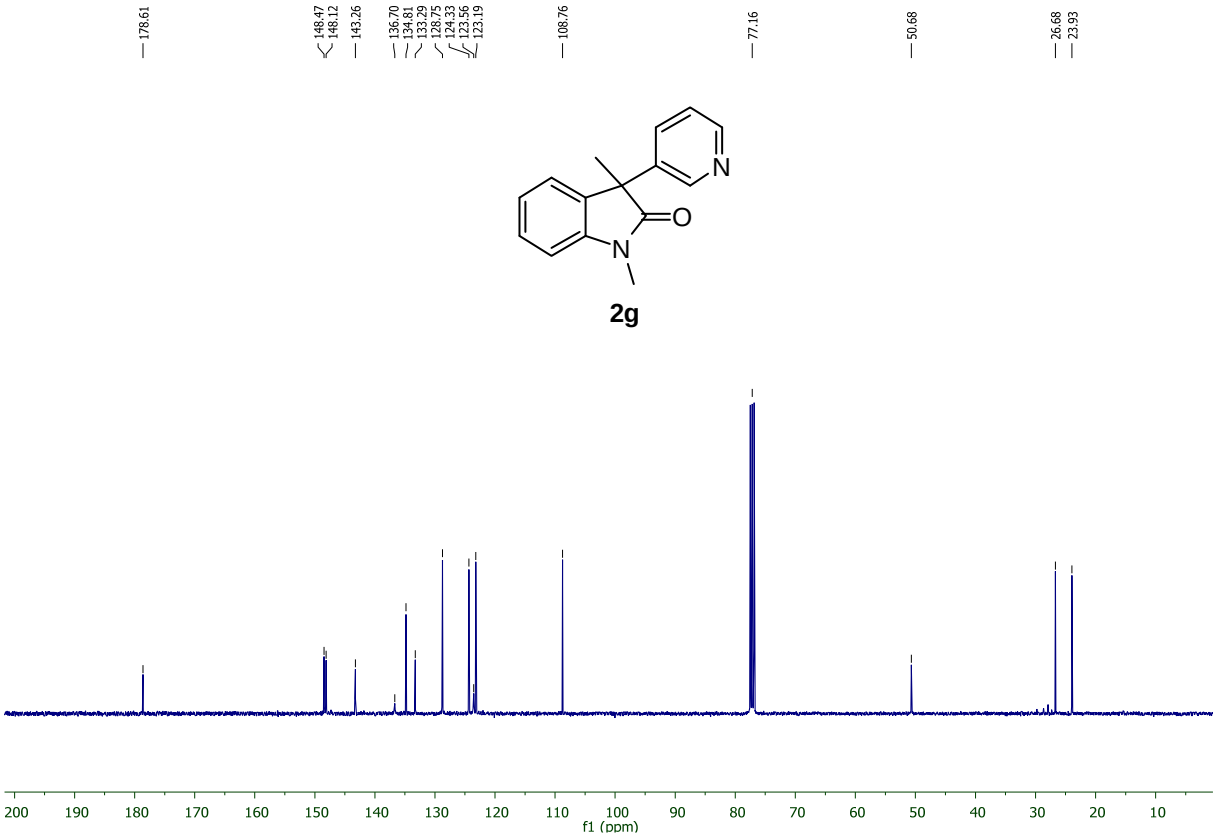
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1
f1 (ppm)

2g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136.70
134.81
133.29
128.75
124.33
123.56
123.19
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50.68
26.68
23.93
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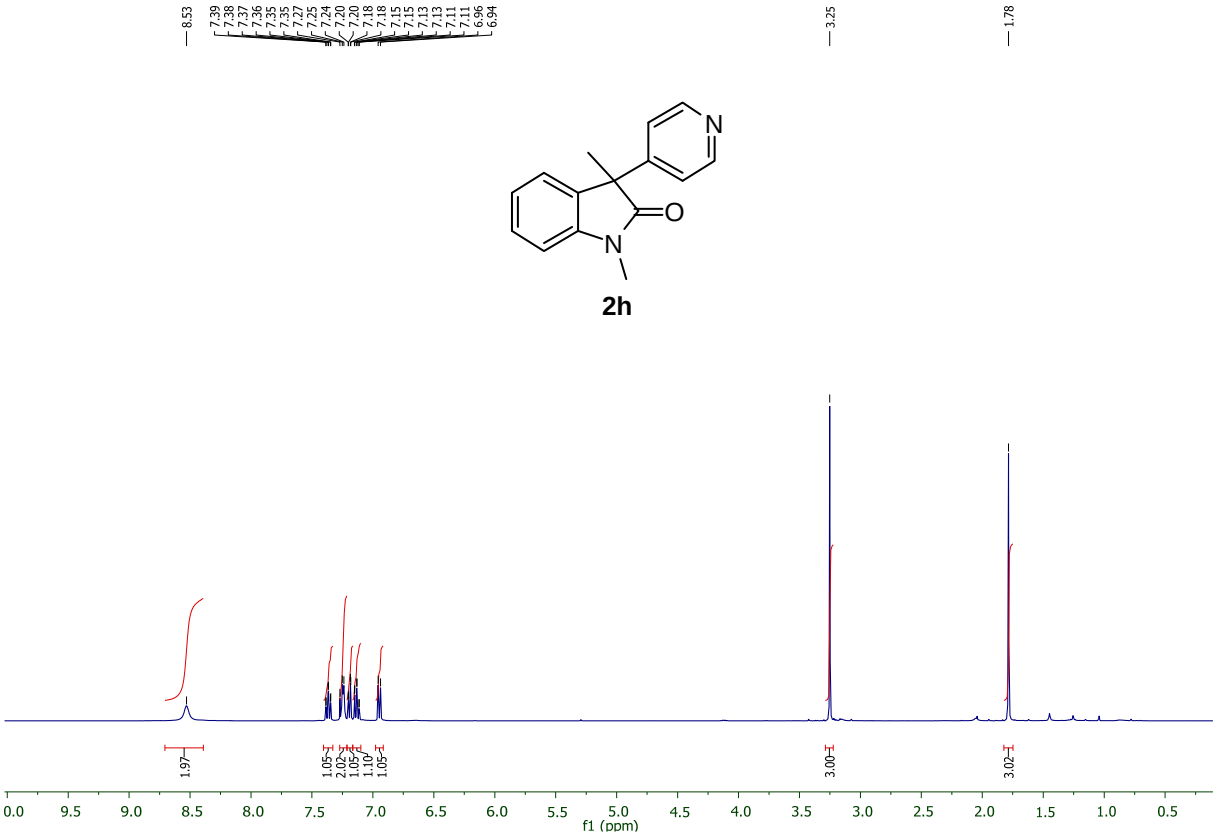
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

2g



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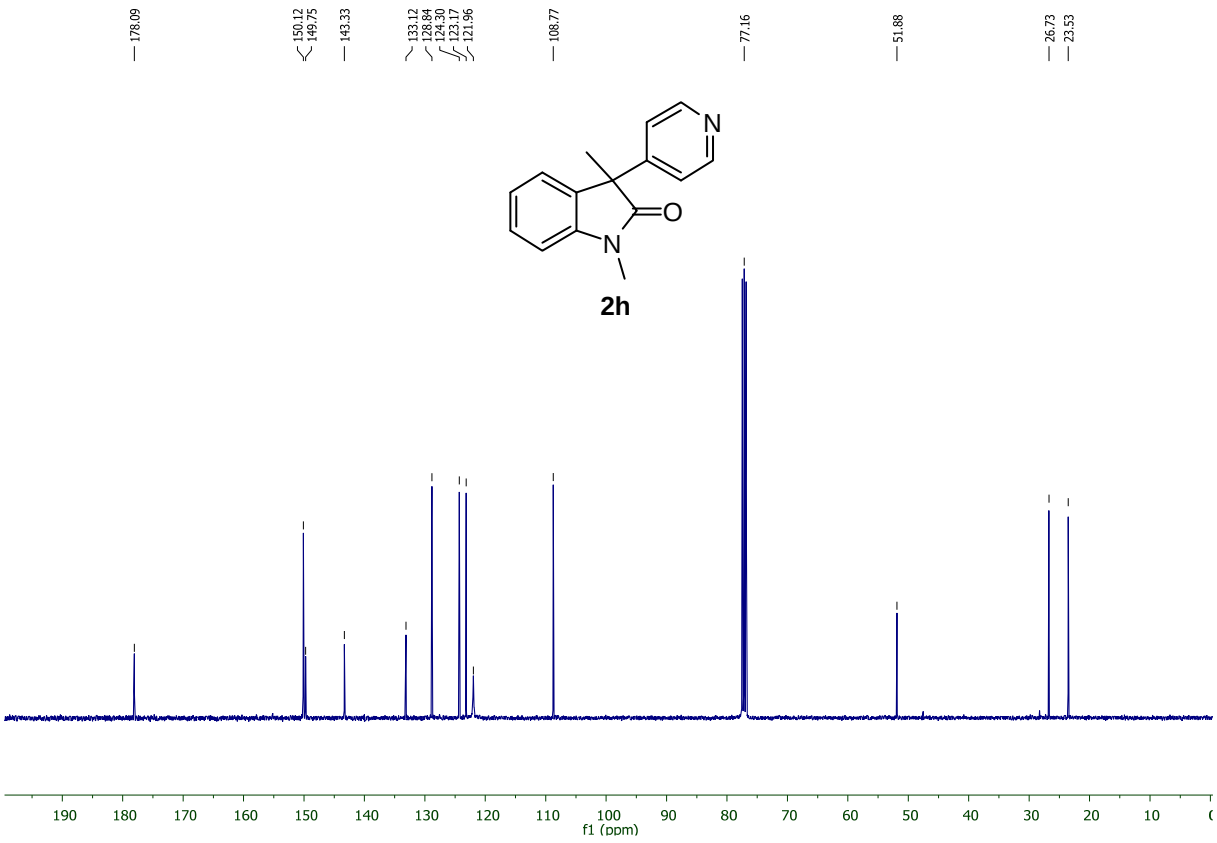

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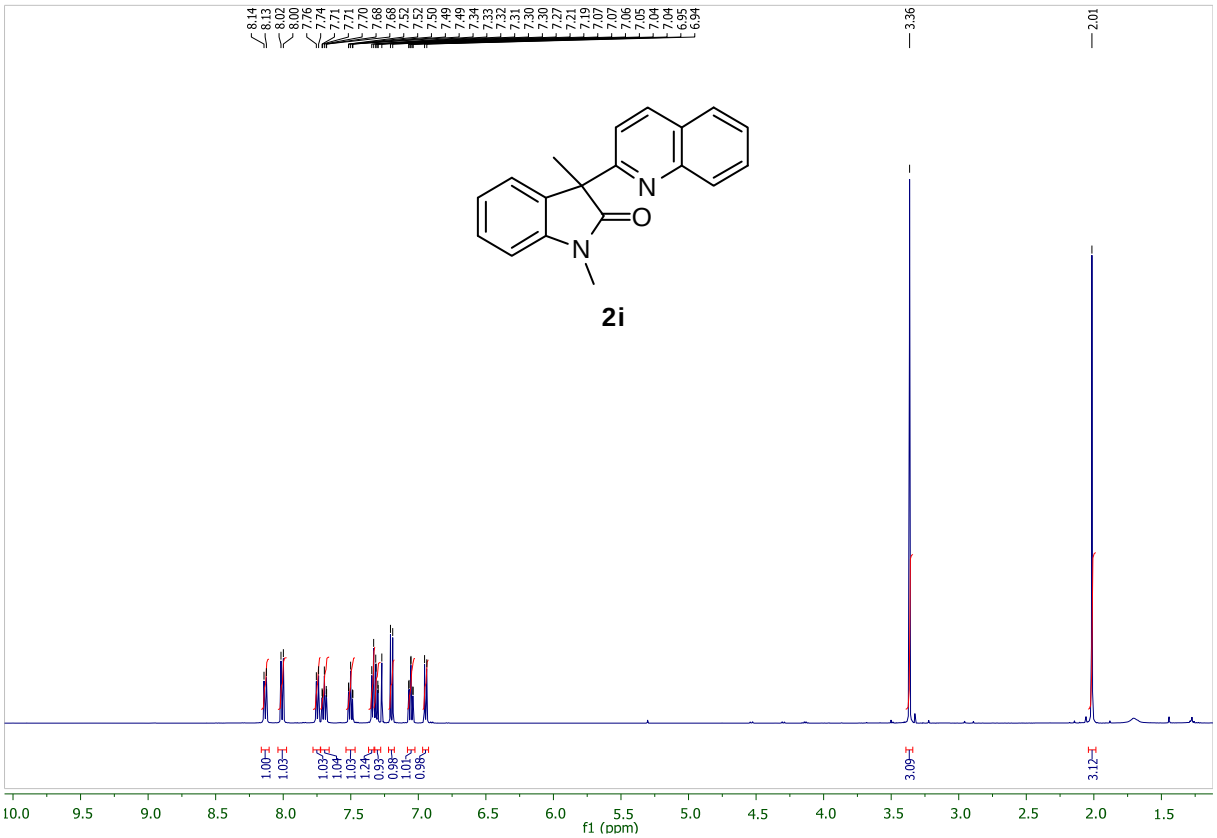
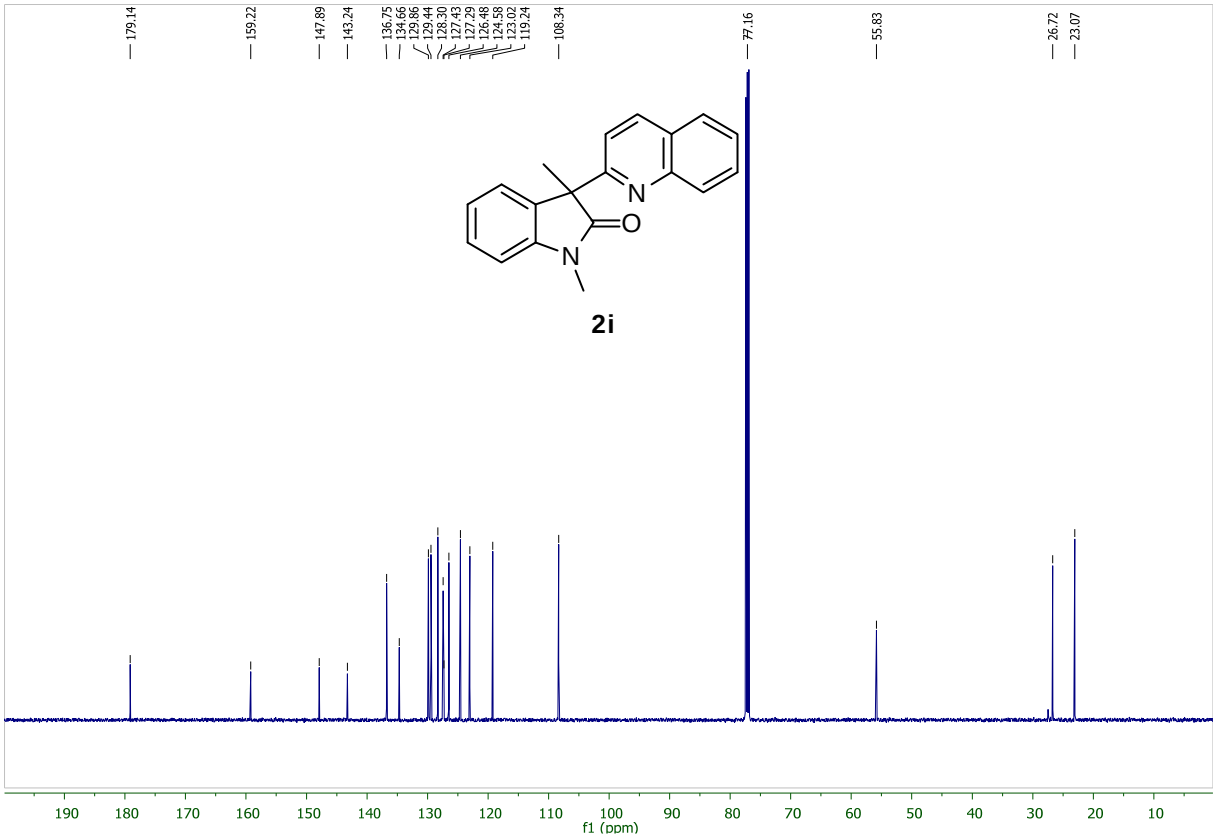
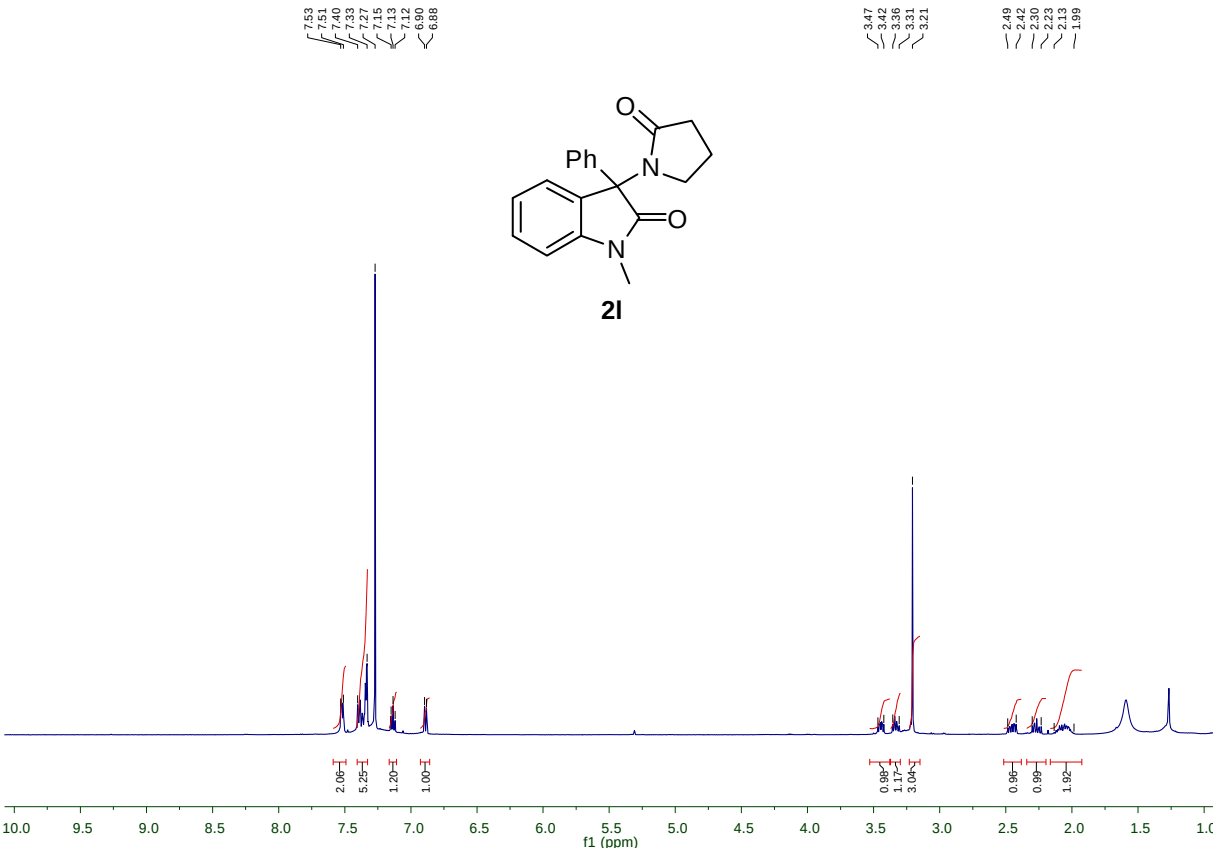
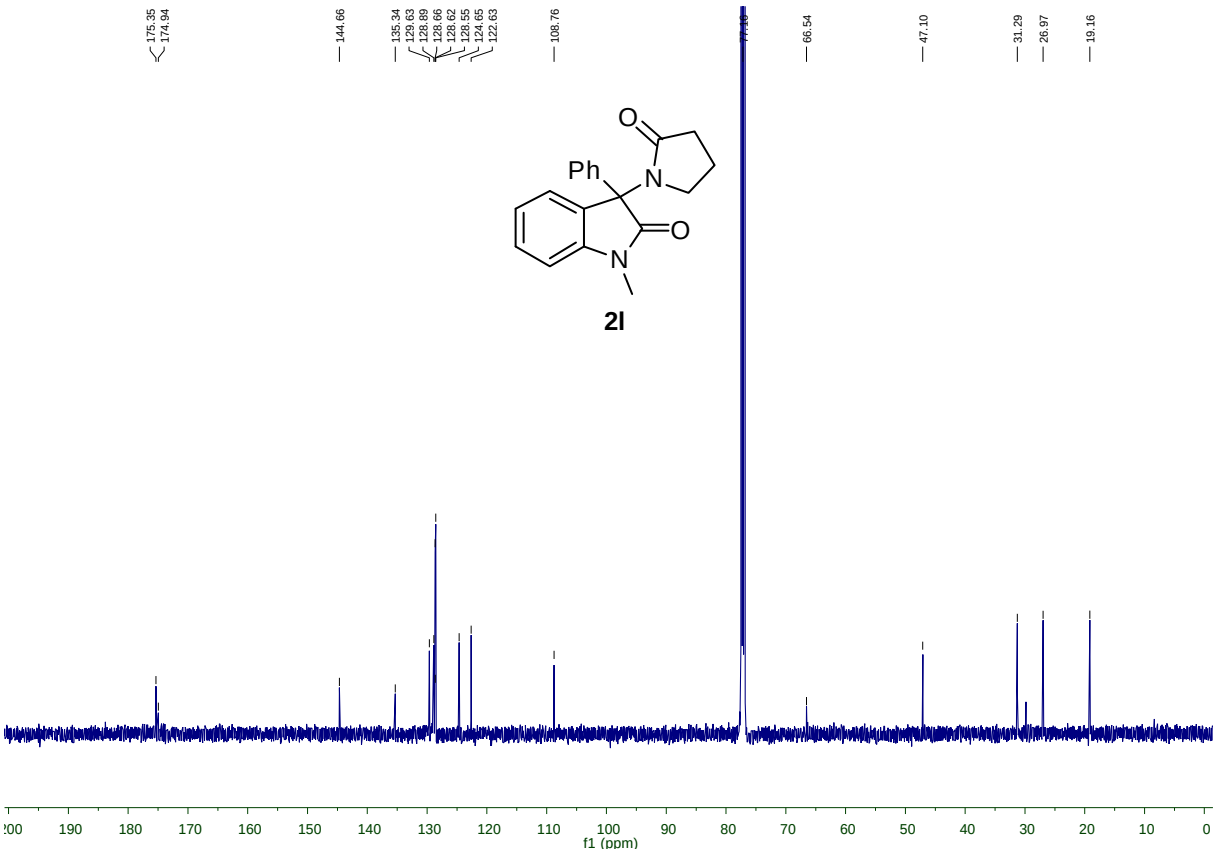


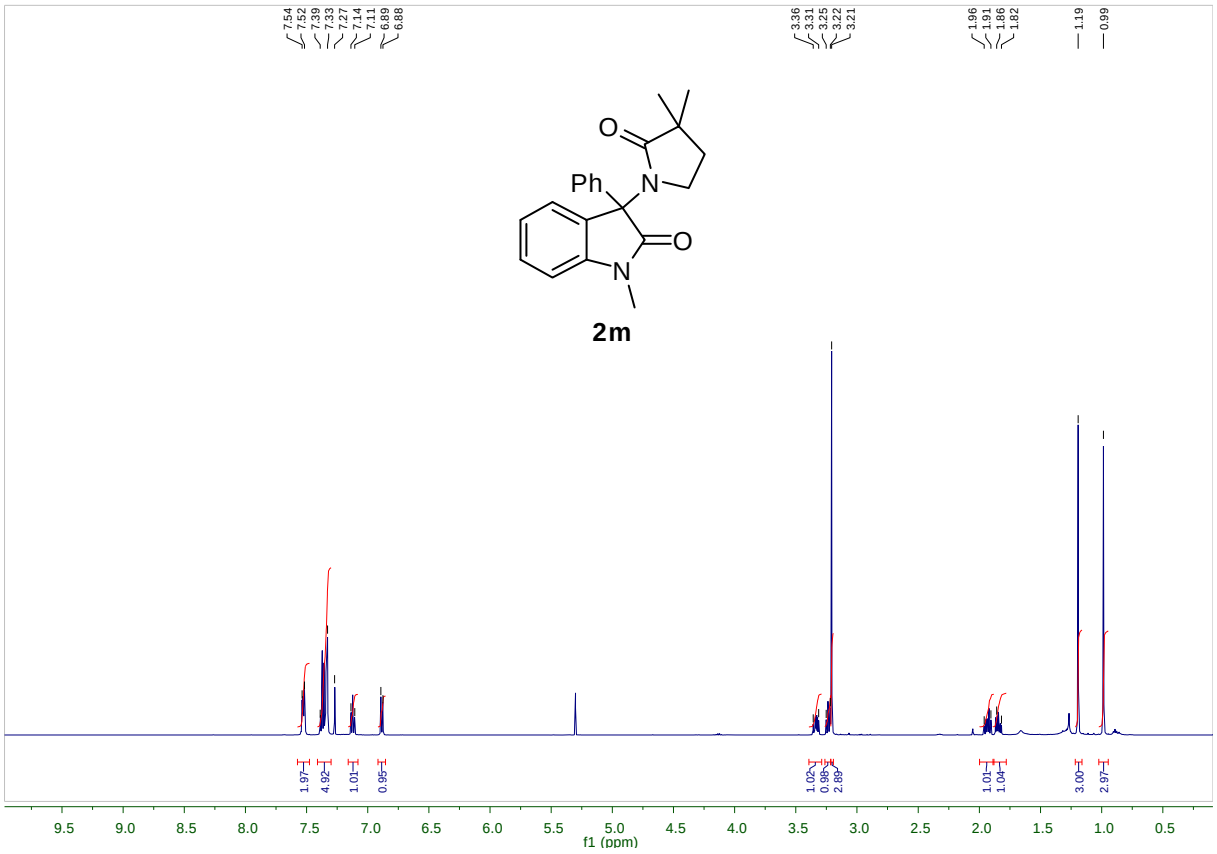


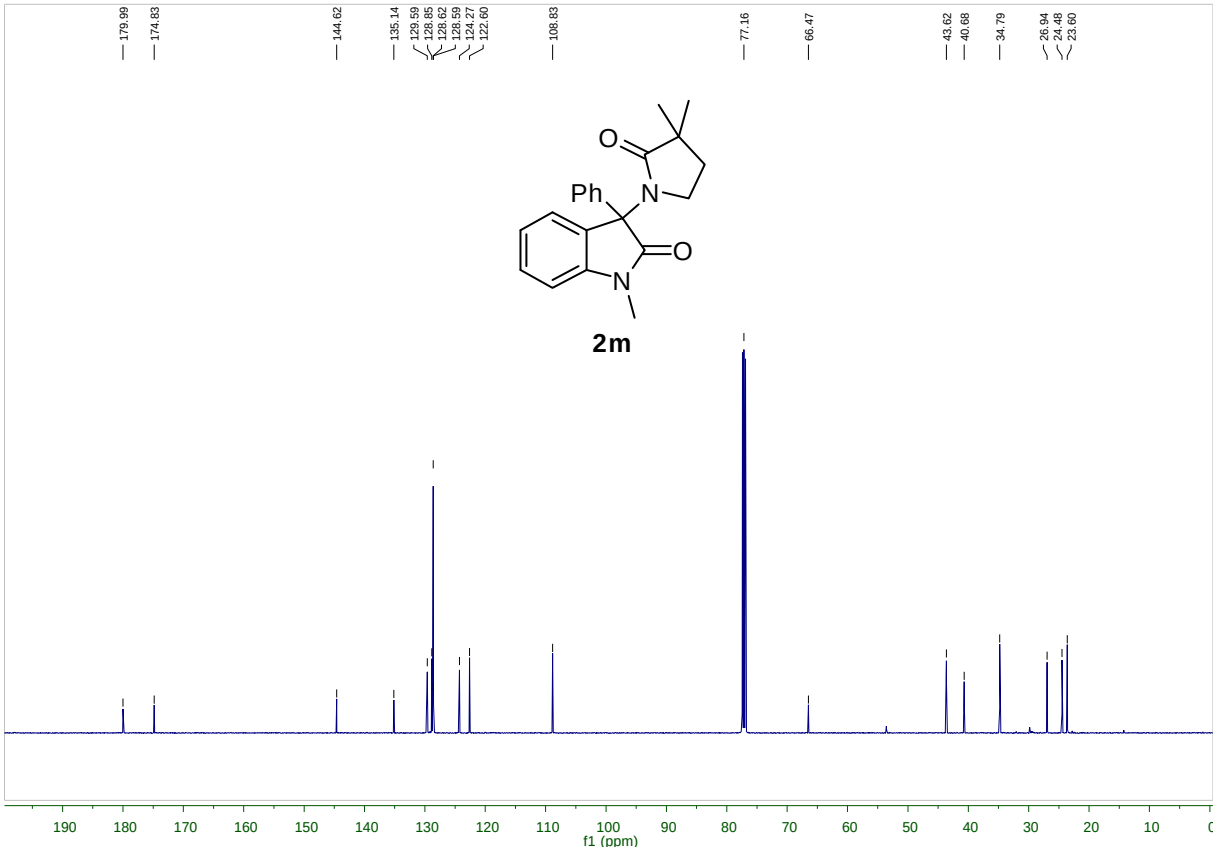


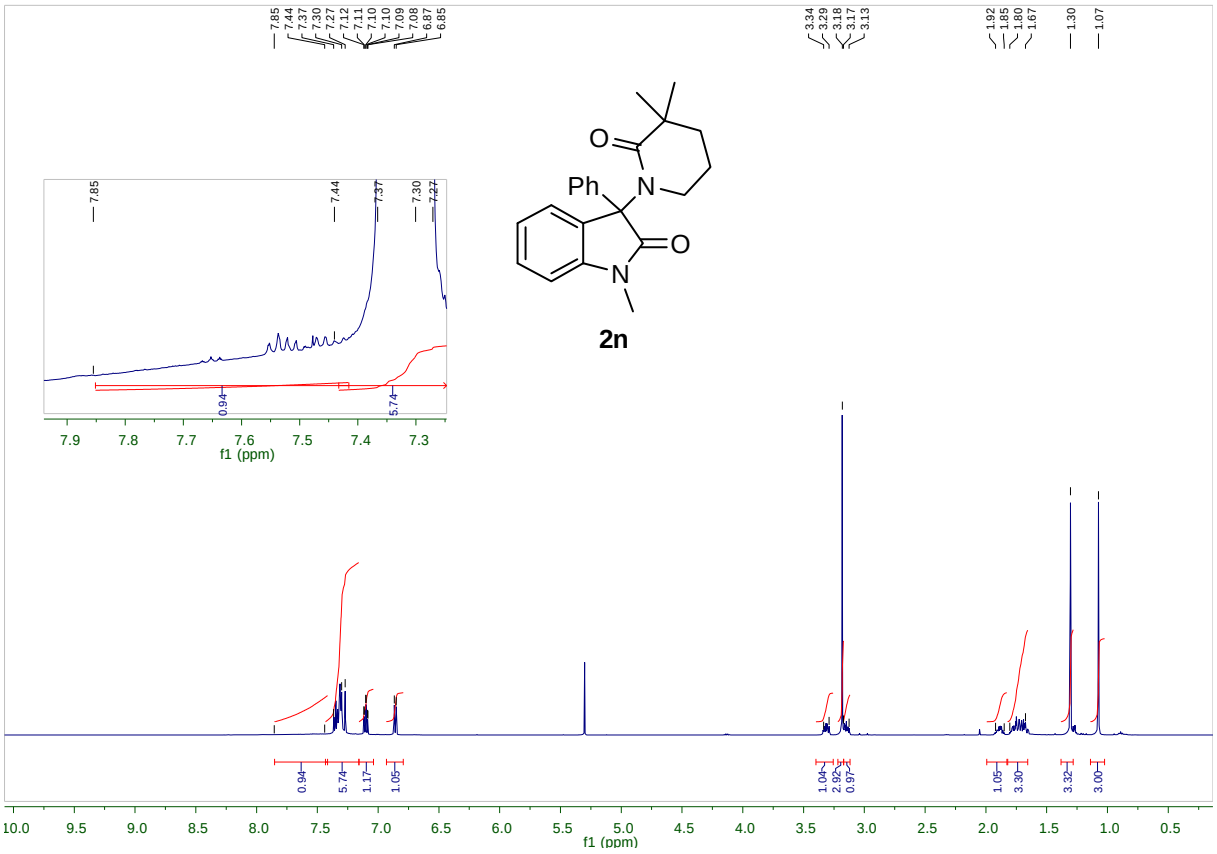
2l

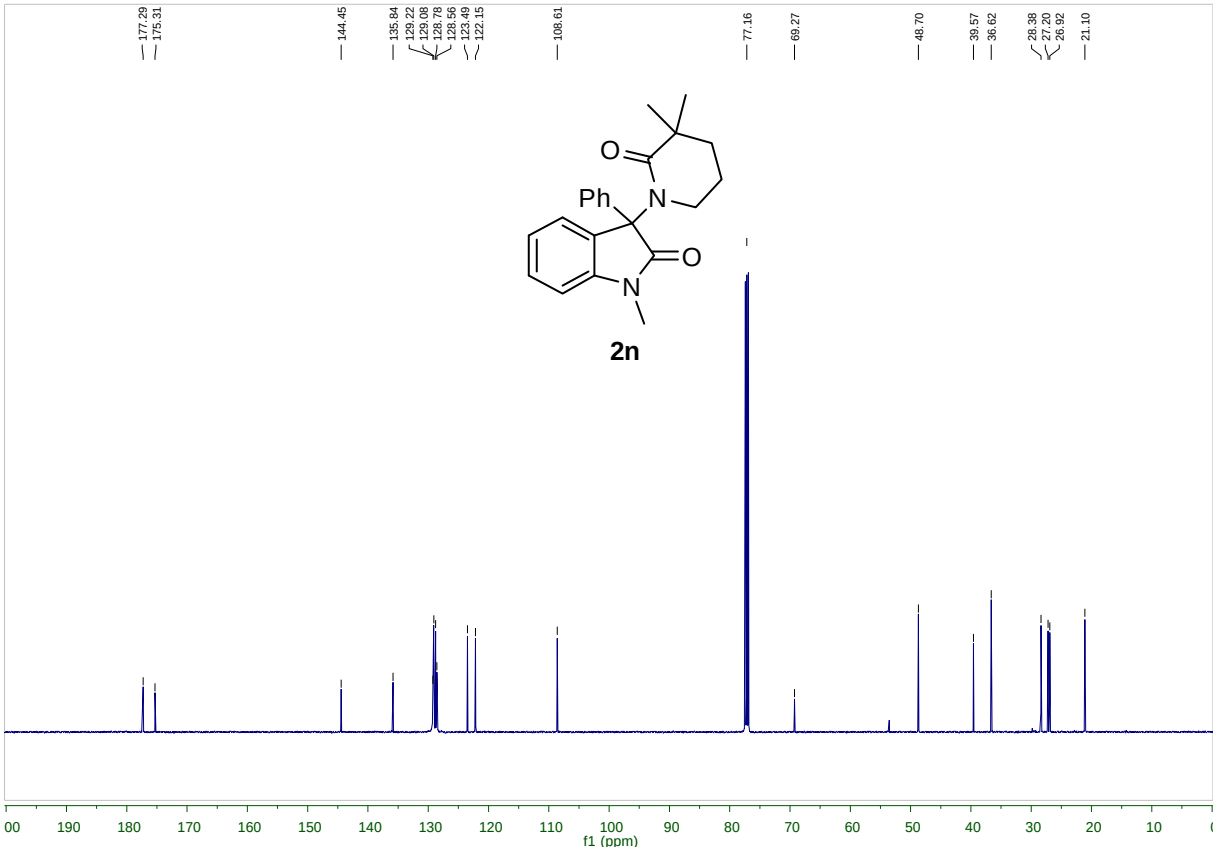


2l









4. Computational details:

Full reference 42**:** Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.

Computational method: UB3LYP with LANDL2 basis set on Cu, Cl and 6-31G(d,p) on other atoms. Solvation model: PCM single points in DMF or toluene at the same level of theory.

4.1 Reaction profiles

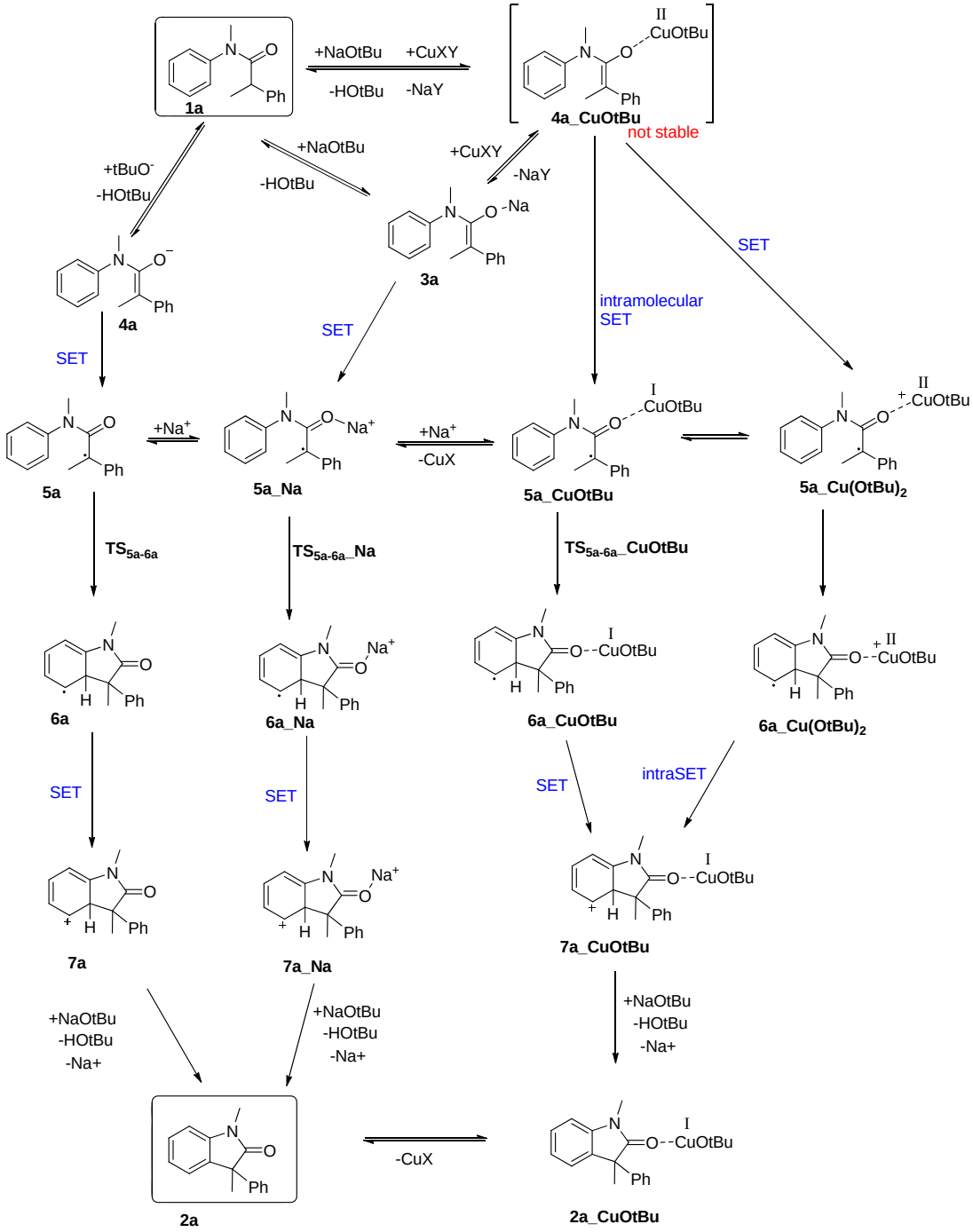


Figure 1. Different pathways for the cyclization. The first SET to amide enolate can be intermolecular (to form radical intermediate **5a**) or intramolecular (when copper (II) is coordinated to amide oxygen). The corresponding copper (II) intermediate **4a_CuOtBu** for the latter was not possible to locate by computations, since it spontaneously forms complex **5a_CuOtBu**.

Table 1. Free energies ΔG_{298} of stationary points for the copper (II) mediated oxindole formation.

Intermediate	ΔG_{298}, kJ/mol		Intermediate	ΔG_{298}, kJ/mol	
	gas phase	DMF		gas phase	DMF
1a	0.0	0.0	Catalytic cycle with Na^+		
3a	8.7	15.5	**5a_Na**	552.1	61.6
4a	534.2	57.6	**TS_{5a-6a}_Na**	633.2	**155.7**
5a	98.8	57.1	**6a_Na**	579.9	89.4
TS_{5a-6a}	**179.2**	**132.6**	**7a_Na**	**669.8**	-163.4
6a	124.4	48.4	Catalytic cycle with Cu(O*t*Bu)		
7a	110.7	99.3	**5a_CuOtBu**	39.2	3.4
2a	-27.8	-119.3	**TS_{5a-6a}_CuOtBu**	124.9	84.7
Catalytic cycle with $Cu(OtBu)_2$			**6a_CuOtBu**	70.2	1.1
5a_$Cu(OtBu)_2$	695.0	11.1	**7a_CuOtBu**	**733.4**	**118.8**
6a_$Cu(OtBu)_2$	731.6	5.5	**2a_CuOtBu**	-83.7	-161.4

Table 2. Free energies of intermediates and transition state **TS_{5-6}** for copper (II) mediated (aza)-oxindole formation (ΔG_{298} in toluene, kJ/mol).

Intermediate	ΔG_{298} (in toluene), kJ/mol				
	2a	**2r**	**2t‘‘**	**2t‘**	**2s**
1	0.0	0.0	0.0	0.0	0.0
5	81.3	71.6	80.6	81.0	73.6
TS_{5-6}	**159.6**	141.4	160.0	152.9	151.3
6	92.9	72.6	94.7	77.9	84.2
7	137.3	**145.6**	**196.5**	**165.5**	**155.1**

Table 3. Free energies of intermediates and transition state **TS_{5-6}** for copper (II) mediated (aza)-oxindole formation (ΔG_{298} in DMF. kJ/mol).

Intermediate	ΔG_{298} (in DMF), kJ/mol				
	2a	**2r**	**2t‘‘**	**2t‘**	**2s**
1	0.0	0.0	0.0	0.0	0.0
5	57.1	48.1	56.7	56.0	49.4
TS_{5-6}	**132.6**	**112.7**	134.8	121.7	**121.5**
6	48.4	28.1	48.2	38.6	39.8
7	99.3	107.3	**153.1**	**125.8**	112.6

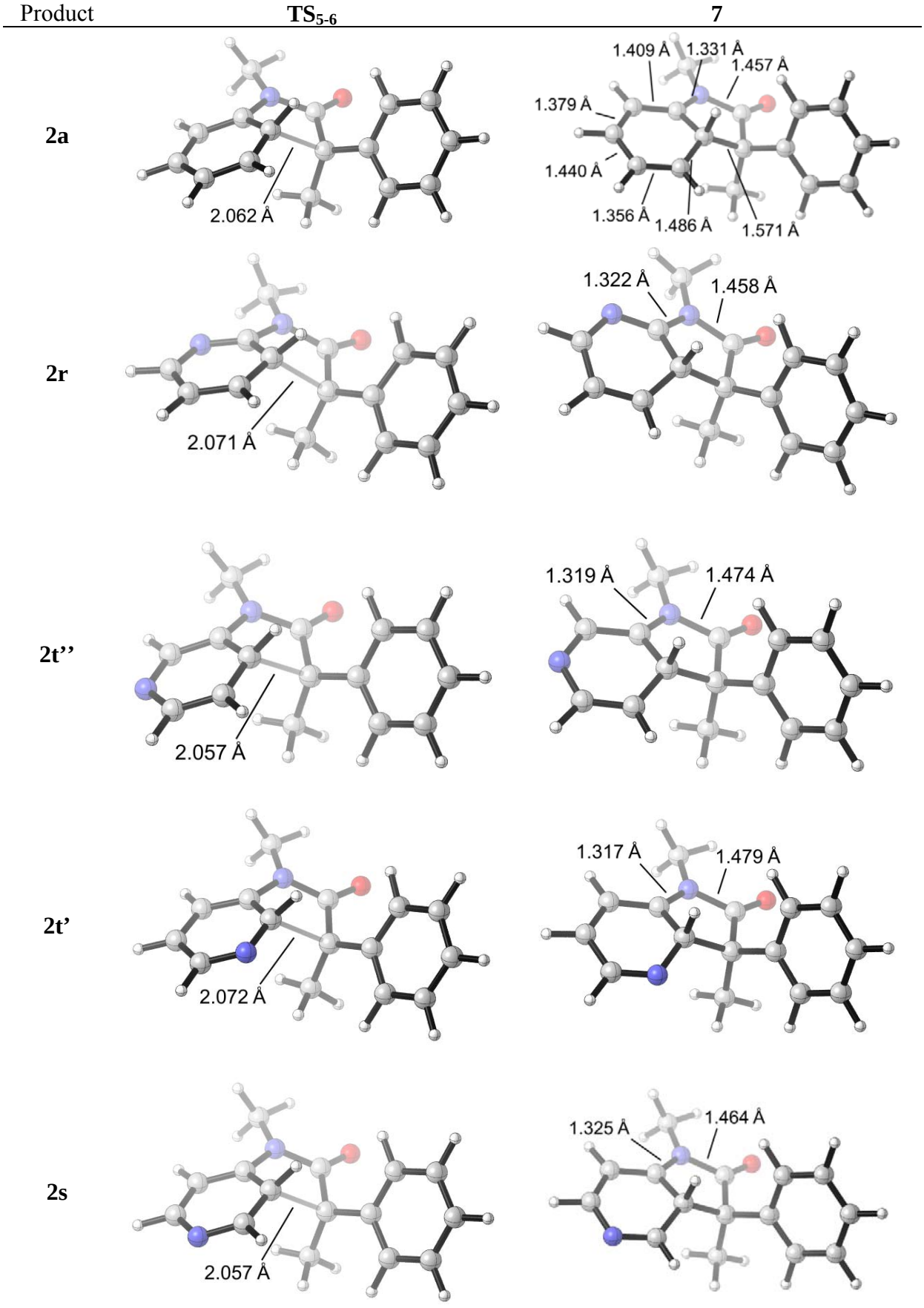


Figure 4. Structures of **TS$_{5-6}$** and **7** for the copper (II) mediated (aza)-oxindole formation.

4.2. Tables with energies

Table 4. **Oxindole synthesis.** Calculated energies of conformers at B3LYP level. Solvent effects in DMF are included by PCM single point calculations at the same level.

	E_{tot}	H_{298}	G_{298}	E_{tot}	G_{298}
	Gas phase	Gas phase	Gas phase	DMF	DMF
Inorganic species					
NaOtBu	-395.392189	-395.258993	-395.301618	-395.441771	-395.351200
$CuCl_2$	-1116.584892	-1116.577283	-1116.610178	-1116.594757	-1116.620043
$CuCl_2^-$	-1116.745895	-1116.738410	-1116.770471	-1116.829671	-1116.854246
CuCl	-656.375872	-656.371373	-656.398378	-656.399026	-656.421532
CuCl(O*t*Bu)	-889.463290	-889.327383	-889.373768	-889.478989	-889.389467
$CuCl(OtBu)^-$	-889.576971	-889.440861	-889.488468	-889.663206	-889.574702
$Cu(OtBu)_2$	-662.321409	-662.056254	-662.112837	-662.333887	-662.125315
$Cu(OtBu)_2^-$	-662.407942	-662.142868	-662.203958	-662.495827	-662.291843
Cu(O*t*Bu)	-429.216636	-429.082948	-429.125089	-429.235226	-429.143679
Cu	-196.116808	-196.114447	-196.133317	-196.117415	-196.133924
HOtBu	-233.689173	-233.545673	-233.582358	-233.702972	-233.596157
$tBuO^-$	-233.052141	-232.924927	-232.961198	-233.174695	-233.083752
NaCl	-622.560317	-622.555842	-622.581906	-622.621443	-622.643033
Na^+	-162.081230	-162.078869	-162.095659	-162.238306	-162.252735
Cl^-	-460.252233	-460.249873	-460.267256	-460.378847	-460.393869
Catalytic cycle					
1a	-749.957463	-749.647027	-749.710819	-749.980025	-749.733382
1	-749.952540	-749.641985	-749.704696	-749.977309	-749.729465
12	-749.946634	-749.635828	-749.697418	-749.970817	-749.721602
2	-749.957463	-749.647027	-749.710819	-749.980025	-749.733382
22	-749.948976	-749.638388	-749.701099	-749.971760	-749.723883
3a	-911.661625	-911.361835	-911.426760	-911.716378	-911.482538
e.1	-911.658233	-911.358804	-911.424866	-911.713446	-911.480079
z.1	-911.660600	-911.360909	-911.426760	-911.716378	-911.482538
z.1.2	-911.659738	-911.360166	-911.425960	-911.713595	-911.479817
z.2	-911.661625	-911.361835	-911.426270	-911.715197	-911.479842
4a	-749.366060	-749.070509	-749.130954	-749.448121	-749.213733
e.1	-749.362202	-749.066854	-749.127545	-749.444532	-749.209875
e.2	-749.359910	-749.064536	-749.126329	-749.443428	-749.209847
z.1	-749.365150	-749.069910	-749.130855	-749.448028	-749.213733
z.2	-749.366060	-749.070509	-749.130954	-749.448121	-749.213015
5a	-749.312717	-749.015592	-749.078567	-749.331149	-749.097125
e.1	-749.308010	-749.010849	-749.073804	-749.327556	-749.093350
e.2	-749.310747	-749.013885	-749.077307	-749.330565	-749.097125
z.1	-749.307650	-749.010454	-749.073010	-749.327859	-749.093219
z.2	-749.312717	-749.015592	-749.078567	-749.331149	-749.096998
TS_{5a-6a}	-749.283595	-748.988226	-749.047943	-749.304016	-749.068365
e.2	-749.280956	-748.985849	-749.046688	-749.302456	-749.068188
z.2	-749.283595	-748.988226	-749.047943	-749.304016	-749.068365

	E_{tot}	H_{298}	G_{298}	E_{tot}	G_{298}
	Gas phase	Gas phase	Gas phase	DMF	DMF
6a	-749.306105	-749.009158	-749.068821	-749.337698	-749.100414
e.2	-749.303770	-749.006886	-749.066854	-749.335782	-749.098866
z.2	-749.306105	-749.009158	-749.068821	-749.337698	-749.100414
7a	-749.095918	-748.796906	-748.855849	-749.204294	-748.964225
e.2	-749.094018	-748.795129	-748.854533	-749.203014	-748.963528
z.2	-749.095918	-748.796906	-748.855849	-749.204294	-748.964225
2a	-748.761739	-748.474263	-748.532182	-748.779342	-748.549785
e.2	-748.759524	-748.472147	-748.530509	-748.778684	-748.549669
z.2	-748.761739	-748.474263	-748.532182	-748.779342	-748.549785
Catalytic cycle with Na^+					
5a_Na	-911.479265	-911.178670	-911.246330	-911.595781	-911.362845
z.1	-911.477669	-911.176983	-911.243791	-911.582328	-911.348451
z.2	-911.479265	-911.178670	-911.246330	-911.595781	-911.362845
$TS_{5a\text{-}6a}$_Na					
z.2	-911.450910	-911.151870	-911.215456	-911.562444	-911.326990
6a_Na					
z.2	-911.473397	-911.172769	-911.235746	-911.589894	-911.352243
7a_Na					
z.2	-911.464172	-911.163741	-911.228064	-911.5824711	-911.346363
Catalytic cycle with Cu(OtBu)					
5a_CuOtBu	-1178.571280	-1178.138158	-1178.226360	-1178.606178	-1178.261258
z.1	-1178.566441	-1178.133459	-1178.222483	-1178.604107	-1178.260149
z.2	-1178.571280	-1178.138158	-1178.226360	-1178.606178	-1178.261258
$TS_{5a\text{-}6a}$_CuOtBu					
z.2	-1178.540081	-1178.108646	-1178.193725	-1178.57664	-1178.230284
6a_CuOtBu					
z.2	-1178.562561	-1178.129516	-1178.214553	-1178.610124	-1178.262115
7a_CuOtBu					
z.2	-1178.339183	-1177.904424	-1177.988499	-1178.465878	-1178.115194
2a_CuOtBu					
z.2	-1178.019485	-1177.595964	-1177.67855	-1178.050429	-1177.709494
Catalytic cycle with $Cu(OtBu)_2$					
5a_$Cu(OtBu)_2$					
z.2	-1178.349283	-1177.915645	-1178.003148	-1178.437915	-1178.091780
6a_$Cu(OtBu)_2$					
z.2	-1178.339180	-1177.905705	-1177.989195	-1178.443888	-1178.093903

	E_{tot}	H_{298}	G_{298}	E_{tot}	G_{298}
	Gas phase	Gas phase	Gas phase	DMF	DMF
Complexes of reactant with copper(II) salts					
1a_$CuCl_2$	-1866.569976	-1866.249716	-1866.330290	-1866.605748	-1866.366143
12	-1866.561948	-1866.241683	-1866.321520	-1866.600734	-1866.360307
1	-1866.566395	-1866.246270	-1866.327279	-1866.605260	-1866.366143
2	-1866.569976	-1866.249716	-1866.330290	-1866.605748	-1866.366063
22	-1866.562098	-1866.241879	-1866.322103	-1866.600760	-1866.360765
1a_CuCl(O*t*Bu)	-1639.433447	-1638.984177	-1639.078096	-1639.468915	-1639.112034
1_1	-1639.430525	-1638.980522	-1639.074521	-1639.466925	-1639.110921
1_2	-1639.430757	-1638.980816	-1639.073876	-1639.468915	-1639.112034
2_1	-1639.433447	-1638.984177	-1639.078096	-1639.467283	-1639.111932
2_2	-1639.431692	-1638.981688	-1639.074816	-1639.465805	-1639.108929
1a_Cu(O*t*Bu)$_2$	-1412.282935	-1411.703145	-1411.810164	-1412.314372	-1411.841599
1_1	-1412.279277	-1411.699515	-1411.804434	-1412.312765	-1411.837922
1_2	-1412.279451	-1411.699649	-1411.804323	-1412.313180	-1411.838052
2_1	-1412.282935	-1411.703144	-1411.810164	-1412.314369	-1411.841599
2_2	-1412.282935	-1411.703145	-1411.810158	-1412.314372	-1411.841595

Table 5. **Azaoxindole synthesis.** Calculated energies of conformers at B3LYP level. Solvent effects in DMF and toluene are included by PCM single point calculations at the same level.

	E_{tot}	H_{298}	G_{298}	E_{tot}	E_{tot}	G_{298}	G_{298}
	Gas phase	Gas phase	Gas phase	DMF	toluene	DMF	toluene
Inorganic species							
NaOtBu	-395.392189	-395.258993	-395.301618	-395.441771	-395.417837	-395.351200	-395.327265
Cu(O*t*Bu)$_2$	-662.321409	-662.056254	-662.112837	-662.333887	-662.326894	-662.125315	-662.118322
Cu(O*t*Bu)	-429.216636	-429.082948	-429.125089	-429.235226	-429.224709	-429.143679	-429.133162
HOtBu	-233.689173	-233.545673	-233.582358	-233.702972	-233.695082	-233.596157	-233.588267
tBuO$^-$	-233.052141	-232.924927	-232.961198	-233.174695	-233.118149	-233.083752	-233.027206
Cu(O*t*Bu)$_2^-$	-662.407942	-662.142868	-662.203958	-662.495827	-662.454871	-662.291843	-662.250887
Na$^+$	-162.081230	-162.078869	-162.095659	-162.238306	-162.174653	-162.252735	-162.189082
2a formation							
1a	-749.957463	-749.647027	-749.710819	-749.980025	-749.967478	-749.733382	-749.720834
2	-749.957463	-749.647027	-749.710819	-749.980025	-749.967478	-749.733382	-749.720834
5a							
z.2	-749.312717	-749.015592	-749.078567	-749.331149	-749.320911	-749.096998	-749.086761
TS$_{5a\text{-}6a}$							
z.2	-749.283595	-748.988226	-749.047943	-749.304016	-749.292582	-749.068365	-749.056930
6a							
z.2	-749.306105	-749.009158	-749.068821	-749.337698	-749.319627	-749.100414	-749.082343
7a							
z.2	-749.095918	-748.796906	-748.855849	-749.204294	-749.152479	-748.964225	-748.912409
2r formation							
1r	-765.996740	-765.697890	-765.760185	-766.022369	-766.007990	-765.785815	-765.771435
2_1	-765.996740	-765.697890	-765.760185	-766.022369	-766.007990	-765.785815	-765.771435
2_2	-765.994770	-765.695996	-765.759156	-766.021319	-766.006176	-765.785705	-765.770562
5r							
z.2	-765.354412	-765.069045	-765.131438	-765.375959	-765.364047	-765.152984	-765.141072

	E_{tot}	H_{298}	G_{298}	E_{tot}	E_{tot}	G_{298}	G_{298}
	Gas phase	Gas phase	Gas phase	DMF	toluene	DMF	toluene
TS_{5r-6r}							
z.2	-765.327169	-765.043623	-765.103481	-765.352076	-765.338178	-765.128388	-765.114489
6r							
z.2	-765.351174	-765.065997	-765.125833	-765.385922	-765.366026	-765.160581	-765.140685
7r							
z.2	-765.129044	-764.842037	-764.901670	-765.240979	-765.187228	-765.013606	-764.959854
2s formation							
1s	-765.991085	-765.692218	-765.754671	-766.019035	-766.003344	-765.782621	-765.766930
2_1	-765.991085	-765.692218	-765.754671	-766.019035	-766.003344	-765.782621	-765.766930
5s							
z.2	-765.347785	-765.062361	-765.124996	-765.372061	-765.358581	-765.149272	-765.135792
TS_{5s-6s}							
z.2	-765.317711	-765.034343	-765.093972	-765.345548	-765.329951	-765.121809	-765.106212
6s							
z.2	-765.341055	-765.056204	-765.115977	-765.378034	-765.356823	-765.152957	-765.131745
7s							
z.2	-765.119388	-764.832711	-764.891838	-765.235924	-765.179262	-765.008374	-764.951712
2t‘/2t‘‘ formation							
1t	-765.990771	-765.692270	-765.756103	-766.018116	-766.002902	-765.783489	-765.768234
2_1	-765.990771	-765.692270	-765.756103	-766.018116	-766.002902	-765.783447	-765.768234
2_2	-765.990350	-765.691841	-765.755734	-766.018104	-766.002548	-765.783489	-765.767932
2t‘‘ formation							
5t‘‘							
z.2	-765.346335	-765.061098	-765.123929	-765.369792	-765.356817	-765.147386	-765.134411
$TS_{5t''-6t''}$							
z.2	-765.317356	-765.033797	-765.093368	-765.341623	-765.328186	-765.117635	-765.104197

	E_{tot}	H_{298}	G_{298}	E_{tot}	E_{tot}	G_{298}	G_{298}
	Gas phase	Gas phase	Gas phase	DMF	toluene	DMF	toluene
6t‘‘							
z.2	-765.338640	-765.053491	-765.113031	-765.376200	-765.354678	-765.150591	-765.129069
7t‘‘							
z.2	-765.104570	-764.818405	-764.877488	-765.220921	-765.164337	-764.993839	-764.937255
2t‘ formation							
5t‘							
z.2	-765.346055	-765.060813	-765.123662	-765.370024	-765.356675	-765.147631	-765.134281
$TS_{5t'-6t'}$							
z.2	-765.318960	-765.035355	-765.094810	-765.346765	-765.331056	-765.122615	-765.106906
6t‘							
z.2	-765.347511	-765.061838	-765.120999	-765.380786	-765.361961	-765.154274	-765.135449
7t‘							
z.2	-765.117634	-764.830785	-764.889815	-765.232038	-765.176891	-765.004219	-764.949073

4.3 Coordinates of important stationary points (the best conformers)

Cu(O*t*Bu)$_2^-$
29 atoms
PCM Energy = -662.454870851
Cu -0.000065 0.596783 -0.000010
O 1.783131 0.688942 0.467678
O -1.783315 0.689290 -0.467572
C 2.780407 -0.153494 0.010595
C 2.520537 -1.619423 0.443949
C 2.906050 -0.105098 -1.533751
C 4.117128 0.320829 0.634722
H 2.420935 -1.664051 1.534377
H 1.575396 -1.962791 0.008704
H 3.320533 -2.309226 0.136687
H 3.086080 0.927723 -1.853274
H 3.719789 -0.737178 -1.919325
H 1.963116 -0.433311 -1.985650
H 4.973792 -0.298742 0.334051
H 4.312745 1.356407 0.334827
H 4.036292 0.299729 1.727139
C -2.780363 -0.153492 -0.010588
C -2.520275 -1.619268 -0.444325
C -2.905851 -0.105495 1.533784
C -4.117257 0.320715 -0.634441
H -2.420730 -1.663602 -1.534769
H -1.575057 -1.962610 -0.009223
H -3.320147 -2.309271 -0.137189
H -3.086096 0.927206 1.853574
H -3.719397 -0.737861 1.919296
H -1.962788 -0.433591 1.985499
H -4.973766 -0.299076 -0.333786
H -4.313020 1.356197 -0.334306
H -4.036562 0.299854 -1.726874

Cu(O*t*Bu)
15 atoms
PCM Energy = -429.224709350
Cu 1.696387 0.000002 -0.038341
O 0.051343 0.000025 -0.786097
C -1.117601 -0.000002 0.005012
C -1.191664 -1.262820 0.882773
C -1.191587 1.262670 0.882991
C -2.284570 0.000125 -1.008243
H -1.102149 -2.157473 0.259014
H -0.363762 -1.266031 1.604223
H -2.130730 -1.321403 1.445245
H -1.102018 2.157425 0.259385
H -2.130649 1.321213 1.445473
H -0.363685 1.265706 1.604442
H -3.254491 0.000112 -0.498660
H -2.222947 0.885936 -1.646758
H -2.223007 -0.885578 -1.646913

Cu(O*t*Bu)$_2$
29 atoms
PCM Energy = -662.326894178
Cu -0.000001 0.001022 -0.000020
O -1.639993 0.000704 -0.664628
O 1.639980 0.000694 0.664613
C -2.891259 -0.000269 0.000509
C -2.997100 -1.266114 0.872516
C -2.997219 1.262678 0.876659
C -3.981693 0.001430 -1.083410
H -2.871794 -2.160839 0.255261
H -2.218888 -1.266242 1.643865
H -3.972313 -1.320807 1.368100
H -2.872129 2.159443 0.262321
H -3.972370 1.315631 1.372554
H -2.218917 1.260397 1.647919
H -4.984625 0.000753 -0.643352
H -3.880631 0.888119 -1.716265
H -3.880645 -0.883262 -1.719053
C 2.891260 -0.000269 -0.000496
C 2.997132 -1.266122 -0.872486
C 2.997221 1.262669 -0.876659
C 3.981672 0.001456 1.083445
H 2.871825 -2.160841 -0.255223
H 2.218936 -1.266268 -1.643851
H 3.972356 -1.320809 -1.368050
H 2.872111 2.159440 -0.262334
H 3.972381 1.315628 -1.372537
H 2.218934 1.260371 -1.647933
H 4.984612 0.000787 0.643408
H 3.880584 0.888150 1.716289
H 3.880622 -0.883231 1.719095

HO*t*Bu
15 atoms
PCM Energy = -233.695081532
O -0.013341 0.000052 1.451842
C 0.005297 0.000003 0.014267
C -0.690127 -1.265596 -0.509565
C -0.691341 1.264890 -0.509671
C 1.489928 0.000690 -0.357864
H -0.209959 -2.158441 -0.098717
H -1.746412 -1.279643 -0.213696
H -0.652668 -1.321857 -1.602615
H -0.212061 2.158233 -0.098869
H -0.653906 1.321113 -1.602723
H -1.747652 1.277923 -0.213843
H 1.621303 0.000653 -1.444080
H 1.982229 0.886524 0.053701
H 1.983077 -0.884597 0.053864
H -0.939763 -0.000243 1.729243

NaO*t*Bu
15 atoms
PCM Energy = -395.417836595
O 0.759025 -0.003251 -0.000458
C -0.619761 -0.000166 -0.000064
C -1.145654 0.541451 1.351219
C -1.145478 0.901099 -1.143340
C -1.150802 -1.439179 -0.207477
H -0.772522 -0.085781 2.168928
H -0.771830 1.559464 1.510326
H -2.241594 0.564326 1.406886
H -0.775424 0.528290 -2.105276
H -2.241408 0.941912 -1.187906
H -0.768209 1.921566 -1.010112
H -2.246970 -1.494446 -0.212903
H -0.781220 -1.833866 -1.160866
H -0.777203 -2.088253 0.592779
Na 2.697668 -0.000585 -0.000020

***t*BuO$^-$**
14 atoms
PCM Energy = -233.118149095

O -0.001624 -0.000350 1.483502
C -0.000218 -0.000092 0.159447
C 0.502873 1.374350 -0.436257
C 0.939638 -1.122006 -0.436379
C -1.441094 -0.252029 -0.438148
H -0.146187 2.175408 -0.057869
H 1.513854 1.568936 -0.053933
H 0.529679 1.440779 -1.539121
H 0.601154 -2.095981 -0.058244
H 0.987321 -1.174851 -1.539209
H 1.956669 -0.962070 -0.054012
H -1.510351 -0.264122 -1.541041
H -1.810946 -1.213790 -0.058283
H -2.115398 0.527156 -0.058279

1a
35 atoms
PCM Energy = -749.967477884
C 2.234325 -2.236096 -0.667247
C 1.526228 -1.061281 -0.924523
C 1.890849 0.128614 -0.285302
C 2.977843 0.138448 0.596811
C 3.685001 -1.037048 0.848549
C 3.313771 -2.226288 0.217610
H 1.942329 -3.158286 -1.160722
H 0.684641 -1.059117 -1.609374
H 3.254839 1.068265 1.084673
H 4.523566 -1.024355 1.538433
H 3.864295 -3.141283 0.414717
N 1.197760 1.351252 -0.576351
C -0.002969 1.729246 -0.009450
O -0.564028 2.773784 -0.331315
C -0.623535 0.798224 1.043285
C -1.179707 1.647379 2.203163
H 0.146826 0.132263 1.439795
H -0.376747 2.201329 2.700660
H -1.906903 2.370843 1.830079
H -1.665068 1.002747 2.941273
C -1.711860 -0.074569 0.419636
C -2.712464 0.475347 -0.395161
C -1.749143 -1.448123 0.693302
C -3.722248 -0.331949 -0.919042
H -2.684766 1.536274 -0.621990
C -2.761450 -2.255538 0.172175
H -0.977954 -1.888618 1.320345
C -3.752267 -1.699138 -0.637144
H -4.488395 0.109495 -1.550379
H -2.773556 -3.318261 0.397879
H -4.540571 -2.325008 -1.045469
C 1.800675 2.211935 -1.596504
H 2.823560 2.480143 -1.312650
H 1.832545 1.699127 -2.564448
H 1.190966 3.110426 -1.678785

3a
35 atoms
PCM Energy = -911.715196796
O 0.010323 1.024073 1.517617
C -0.100523 1.110623 0.241084
C 0.880673 0.848316 -0.710472
C 2.194046 0.312378 -0.322069
C 2.710092 0.339773 1.008068
C 3.021027 -0.317882 -1.292167
C 3.936773 -0.250086 1.329810
H 2.156076 0.885630 1.762246
C 4.240572 -0.898449 -0.959255
H 2.698935 -0.348948 -2.326559
C 4.710680 -0.882348 0.357565
H 4.298286 -0.183857 2.353493
H 4.833303 -1.368447 -1.740043
H 5.664392 -1.334395 0.612224
C 0.591655 1.008723 -2.188134
H 0.528670 0.051250 -2.728287
H -0.359325 1.520895 -2.332428
H 1.375997 1.593586 -2.685435
N -1.471699 1.380559 -0.236170
C -1.998285 2.652707 0.252829
H -2.269684 2.625534 1.317141
H -1.228109 3.413933 0.114498
H -2.873296 2.945959 -0.334926
C -1.822981 -1.017223 -0.563166
C -2.311225 0.261688 -0.183252
C -2.638081 -2.148175 -0.507944
C -3.658264 0.337624 0.229222
C -3.964382 -2.056885 -0.081516
H -2.235628 -3.105087 -0.832530
C -4.460935 -0.801791 0.272452
H -4.080596 1.287405 0.532147
H -4.598126 -2.936820 -0.042781
H -5.492377 -0.701990 0.600226
Na 0.422124 -1.100253 1.357957
H -0.827610 -1.092319 -0.992585

4a
34 atoms
PCM Energy = -749.448120666
C -2.797901 -2.011546 0.899062
C -1.875763 -1.024201 0.579986
C -2.288217 0.205140 0.002662
C -3.679531 0.367957 -0.224268
C -4.589207 -0.637453 0.100513
C -4.167851 -1.840343 0.665110
H -2.436974 -2.935290 1.347162
H -0.821029 -1.174533 0.775945
H -4.050587 1.284292 -0.668287
H -5.646917 -0.469225 -0.095472
H -4.880535 -2.621175 0.916352
N -1.387383 1.202949 -0.321884
O 0.411935 2.033101 0.869389
C -1.897419 2.545696 -0.544126
H -2.389467 2.637862 -1.524281
H -2.621438 2.851673 0.225414
H -1.052401 3.230772 -0.494613
C 0.064094 1.153543 0.048162
C 0.848336 0.183103 -0.605793
C 0.295976 -0.616638 -1.766097
H 0.137806 -1.686068 -1.544426
H -0.663510 -0.216854 -2.096943
H 0.976305 -0.582590 -2.630875
C 2.230136 -0.066273 -0.221425
C 2.930917 0.682055 0.770993
C 2.978711 -1.113248 -0.832803
C 4.250004 0.400492 1.104695
H 2.397015 1.488623 1.255856
C 4.302304 -1.383202 -0.492099
H 2.506592 -1.737701 -1.583791
C 4.963049 -0.631804 0.481274
H 4.737322 1.005585 1.868997
H 4.821374 -2.199031 -0.994768
H 5.996834 -0.841461 0.746733

5a
34 atoms
PCM Energy = -749.320911264
C 2.192732 -2.076257 -1.083940
C 1.510505 -0.869310 -0.937711
C 2.076159 0.175629 -0.191092
C 3.351123 0.001562 0.367691
C 4.035918 -1.200732 0.198301
C 3.457905 -2.248646 -0.519881
H 1.739577 -2.876759 -1.661318
H 0.543157 -0.729383 -1.407068
H 3.800370 0.804850 0.942548
H 5.021695 -1.320095 0.638365
H 3.991159 -3.185784 -0.646128
N 1.398471 1.417493 -0.041165
O -0.555060 2.600597 0.023682
C 2.143043 2.644238 -0.340260
H 2.776151 2.947365 0.501918
H 2.774366 2.492461 -1.219424
H 1.417329 3.432076 -0.536440
C 0.032199 1.533317 0.214089
C -0.671431 0.358131 0.799664
C -0.046301 -0.346381 1.976432
H 0.145120 -1.408000 1.774747
H 0.903553 0.109775 2.256828
H -0.709771 -0.296797 2.849161
C -1.981901 -0.011049 0.337879
C -2.625270 0.640515 -0.753241
C -2.675103 -1.099804 0.936371
C -3.869452 0.224172 -1.203831
H -2.141022 1.489600 -1.217626
C -3.920852 -1.506535 0.477305
H -2.224854 -1.631761 1.766664
C -4.530051 -0.850300 -0.596559
H -4.334646 0.744802 -2.036132
H -4.421581 -2.341854 0.958752
H -5.504775 -1.169021 -0.953460

TS_{5a-6a}
34 atoms
PCM Energy = -749.292582200
C 1.144081 -2.141199 -0.664874
C 0.911075 -0.731894 -0.738942
C 2.024741 0.130584 -0.436273
C 3.284694 -0.368011 -0.152187
C 3.481805 -1.760719 -0.129192
C 2.400854 -2.632308 -0.342814
H 0.335764 -2.822100 -0.914155
H 0.207237 -0.387842 -1.494617
H 4.101247 0.304049 0.092615
H 4.468243 -2.159103 0.085076
H 2.565061 -3.705528 -0.304257
N 1.610363 1.455800 -0.240873
O -0.178545 2.657258 0.562788
C 2.499798 2.602746 -0.313093
H 3.233525 2.596802 0.502774
H 3.031532 2.606330 -1.268187
H 1.884921 3.498554 -0.225927
C 0.337481 1.578284 0.316606
C -0.283520 0.223620 0.643460
C 0.183637 -0.299156 1.991009
H 0.035819 -1.379436 2.073373
H 1.249005 -0.105739 2.139303
H -0.366199 0.188331 2.805165
C -1.690124 0.020464 0.263573
C -2.266219 0.744010 -0.804427
C -2.489955 -0.955716 0.893809
C -3.571805 0.500865 -1.218129
H -1.691527 1.523410 -1.293472
C -3.796987 -1.196327 0.477232
H -2.089425 -1.531100 1.720779
C -4.346839 -0.472307 -0.582027
H -3.989732 1.079103 -2.037318
H -4.389307 -1.952462 0.984908
H -5.366643 -0.659543 -0.904626

6a
34 atoms
PCM Energy = -749.319627000
C 1.083222 -2.151217 -0.096547
C 0.788035 -0.706592 -0.359849
C 2.031008 0.141418 -0.365171
C 3.292717 -0.366709 -0.512545
C 3.461007 -1.776094 -0.508045
C 2.357905 -2.631066 -0.242544
H 0.250386 -2.821290 0.095732
H 0.338022 -0.626834 -1.370415
H 4.157711 0.287152 -0.571191
H 4.453185 -2.196726 -0.630052
H 2.540143 -3.698040 -0.141929
N 1.638318 1.455770 -0.151819
O -0.206371 2.587162 0.661636
C 2.513065 2.609765 -0.238121
H 3.332811 2.532820 0.485492
H 2.935833 2.694468 -1.243788
H 1.912539 3.491587 -0.013328
C 0.344882 1.544710 0.363388
C -0.186945 0.102155 0.573167
C 0.074133 -0.223165 2.060074
H -0.137103 -1.272526 2.278545
H 1.124854 -0.049073 2.309740
H -0.545445 0.408334 2.701503
C -1.646751 -0.044492 0.162081
C -2.112933 0.591572 -0.999994
C -2.545882 -0.847073 0.875626
C -3.426223 0.429249 -1.434577
H -1.445656 1.236664 -1.564220
C -3.863052 -1.014043 0.441449
H -2.228871 -1.348679 1.783082
C -4.309266 -0.378085 -0.715082
H -3.761639 0.939430 -2.332919
H -4.539285 -1.642252 1.014270
H -5.334287 -0.504728 -1.050743

7a
34 atoms
PCM Energy = -749.152478572
C 1.104595 -2.159510 0.022994
C 0.809932 -0.726756 -0.241504
C 2.010180 0.155695 -0.351048
C 3.290886 -0.373147 -0.604115
C 3.438589 -1.739573 -0.487926
C 2.364686 -2.632852 -0.139054
H 0.269904 -2.820544 0.236357
H 0.390443 -0.742541 -1.267886
H 4.143162 0.269022 -0.792822
H 4.428232 -2.165201 -0.630843
H 2.583562 -3.688309 -0.021556
N 1.669124 1.425649 -0.146555
O -0.194951 2.586789 0.619418
C 2.521012 2.607172 -0.303502
H 3.333195 2.589164 0.427729

H 2.928468 2.642868 -1.315650
H 1.891707 3.479150 -0.126411
C 0.314966 1.530954 0.379933
C -0.209153 0.100589 0.620901
C 0.012984 -0.181573 2.125985
H -0.245479 -1.215276 2.365697
H 1.058061 -0.023640 2.408702
H -0.608184 0.485052 2.727191
C -1.653982 -0.059958 0.153778
C -2.006032 0.357942 -1.140039
C -2.640518 -0.630127 0.965070
C -3.306487 0.207141 -1.612169
H -1.266686 0.827802 -1.786927
C -3.946112 -0.784493 0.490832
H -2.413011 -0.953077 1.974260
C -4.282561 -0.369243 -0.795202
H -3.559567 0.543927 -2.612263
H -4.698365 -1.227802 1.135277
H -5.297621 -0.488016 -1.159908

2a
33 atoms
PCM Energy = -748.779342414
C 1.317218 -1.895336 0.797817
C 1.008199 -0.588074 0.449958
C 1.926767 0.160431 -0.304720
C 3.132751 -0.375736 -0.743978
C 3.419093 -1.703088 -0.399636
C 2.528870 -2.456175 0.365408
H 0.627817 -2.483259 1.397127
H 3.834392 0.211606 -1.326973
H 4.353908 -2.145940 -0.730356
H 2.773583 -3.479967 0.630094
N 1.444998 1.464102 -0.484871
O -0.357318 2.709195 0.248921
C 2.142585 2.529899 -1.173376
H 3.114983 2.727745 -0.708202
H 2.299461 2.276135 -2.227276
H 1.519799 3.422335 -1.103094
C 0.239989 1.649702 0.170801
C -0.184543 0.287068 0.793376
C -0.328805 0.469520 2.324235
H -0.643504 -0.470261 2.786316
H 0.623765 0.772756 2.769037
H -1.072850 1.236449 2.549198
C -1.523368 -0.153825 0.169610
C -1.664955 -1.356132 -0.533668
C -2.650889 0.671967 0.311772
C -2.901430 -1.734775 -1.062249
H -0.807792 -2.003321 -0.677379
C -3.882698 0.294954 -0.219356
H -2.551233 1.628323 0.811981
C -4.016251 -0.914291 -0.904466
H -2.986466 -2.674092 -1.601470
H -4.739905 0.951562 -0.100233
H -4.977599 -1.209007 -1.315197

Azaoxindole synthesis

1r
34 atoms
PCM Energy = -766.021318852
C 3.318837 -1.550908 -0.985400
C 1.990150 0.186458 -0.293219
C 3.393623 -0.917557 1.315976
C 3.824712 -1.765650 0.295913
H 3.645549 -2.171023 -1.818038
H 3.782036 -1.019553 2.325014
H 4.544484 -2.555814 0.480147
N 1.058333 1.194021 -0.657032
C -0.076357 1.543229 0.060254
O -0.658511 2.594865 -0.183477
C -0.675390 0.538975 1.059331
C -1.131132 1.280106 2.329843
H 0.065902 -0.210164 1.339004
H -0.279006 1.735377 2.847329
H -1.831179 2.077606 2.073248
H -1.621316 0.585822 3.017740
C -1.830197 -0.211236 0.391816
C -2.901821 0.466744 -0.207003
C -1.846361 -1.611455 0.406414
C -3.961473 -0.242912 -0.771121
H -2.888077 1.550884 -0.242862
C -2.907448 -2.322328 -0.156528
H -1.021338 -2.151647 0.864500
C -3.970164 -1.639043 -0.747026
H -4.782756 0.297655 -1.233299
H -2.900578 -3.408474 -0.134852
H -4.797119 -2.188966 -1.186959
C 1.376171 2.014148 -1.835338
H 1.955794 2.900144 -1.552215
H 1.947875 1.402669 -2.531640
H 0.446262 2.345573 -2.294410
N 2.420278 -0.606258 -1.280868
C 2.478516 0.088039 1.020044
H 2.161275 0.796979 1.776672

5r
33 atoms
PCM Energy = -765.375958526
C 2.233466 -2.109018 -1.000685
C 1.512306 -0.929653 -0.854599
C 2.114066 0.143646 -0.172455
C 4.057143 -1.046992 0.112571
C 3.536261 -2.181990 -0.504858
H 1.789680 -2.953143 -1.520389
H 0.516145 -0.831859 -1.268236
H 5.076362 -1.045443 0.494674
H 4.135517 -3.079979 -0.608814
N 1.431855 1.366529 0.024259
O -0.507267 2.546878 -0.076882
C 2.171762 2.619015 -0.177059
H 3.216016 2.440346 0.070944
H 2.084845 2.963115 -1.213729
H 1.752897 3.388202 0.471186
C 0.049081 1.478645 0.183699
C -0.688039 0.332182 0.779135
C -0.080819 -0.383233 1.959546
H 0.069177 -1.453734 1.769961
H 0.884779 0.043832 2.232031
H -0.738169 -0.302017 2.834515
C -2.008263 -0.008579 0.319899
C -2.632361 0.641541 -0.783242
C -2.731493 -1.067544 0.936235
C -3.887232 0.251506 -1.227953
H -2.123849 1.467554 -1.262464
C -3.987695 -1.447635 0.483280
H -2.297255 -1.596224 1.776967
C -4.577481 -0.793367 -0.602593
H -4.337150 0.769742 -2.069997
H -4.511961 -2.259849 0.978854
H -5.560446 -1.091129 -0.954946
N 3.370624 0.086960 0.287022

TS_{5r-6r}
33 atoms
PCM Energy = -765.352076408
C 1.177743 -2.165697 -0.623043
C 0.897373 -0.770861 -0.736900
C 2.013252 0.095574 -0.439064
C 3.480152 -1.619240 -0.158610
C 2.466533 -2.574719 -0.301235
H 0.400946 -2.891894 -0.841892
H 0.186937 -0.452787 -1.496083
H 4.511293 -1.919159 0.006218
H 2.710119 -3.629974 -0.224715
N 1.622861 1.420931 -0.239823
O -0.159597 2.644017 0.550801
C 2.566792 2.530665 -0.257529
H 3.034121 2.608929 -1.242181
H 2.005264 3.438101 -0.037926
H 3.350974 2.378906 0.489398
C 0.346397 1.561620 0.306291
C -0.291715 0.216679 0.640775
C 0.172444 -0.305234 1.989625
H 0.014113 -1.383541 2.078382
H 1.239178 -0.118782 2.138982
H -0.373029 0.191299 2.801111
C -1.698313 0.023281 0.258454
C -2.263915 0.745250 -0.816311
C -2.508730 -0.940624 0.893954
C -3.570480 0.511795 -1.231843
H -1.680505 1.515891 -1.308992
C -3.816971 -1.171236 0.475562
H -2.116234 -1.513352 1.726606
C -4.356292 -0.449450 -0.590577
H -3.980811 1.088124 -2.056064
H -4.418423 -1.917362 0.987092
H -5.376943 -0.629057 -0.914664
N 3.246303 -0.284402 -0.184317

6r
33 atoms
PCM Energy = -765.385922160
C 1.151995 -2.163775 -0.021356
C 0.776412 -0.747612 -0.336992
C 2.014858 0.112064 -0.379989
C 3.451546 -1.620112 -0.586511
C 2.450145 -2.556416 -0.233012
H 0.377799 -2.873815 0.252089
H 0.320885 -0.715575 -1.345905
H 4.464981 -1.941179 -0.803708
H 2.732958 -3.599296 -0.118827
N 1.643428 1.420679 -0.138017
O -0.186557 2.554764 0.704561
C 2.552326 2.553009 -0.214799
H 3.398461 2.404739 0.461506
H 2.936715 2.657580 -1.232312

H 1.989591 3.441906 0.069921
C 0.352519 1.514155 0.386002
C -0.194492 0.074503 0.585154
C 0.043670 -0.250899 2.076068
H -0.186219 -1.295732 2.296756
H 1.092492 -0.089037 2.341759
H -0.576281 0.391847 2.705524
C -1.652934 -0.052531 0.158062
C -2.096298 0.589193 -1.009586
C -2.570621 -0.841490 0.862555
C -3.406996 0.445835 -1.458369
H -1.413673 1.223893 -1.567555
C -3.885215 -0.989533 0.413953
H -2.271077 -1.347192 1.773646
C -4.309320 -0.347891 -0.747709
H -3.725108 0.960158 -2.360538
H -4.576830 -1.607212 0.979682
H -5.332375 -0.459648 -1.094270
N 3.241509 -0.263613 -0.569852

7r
33 atoms
PCM Energy = -765.240979380
C 1.189477 -2.161535 0.047677
C 0.794506 -0.761122 -0.281733
C 1.986520 0.133253 -0.391630
C 3.448594 -1.562659 -0.560854
C 2.484630 -2.532091 -0.089365
H 0.410342 -2.878810 0.288991
H 0.336891 -0.819368 -1.286396
H 4.445950 -1.906259 -0.831455
H 2.810901 -3.553082 0.072818
N 1.676505 1.391054 -0.125947
O -0.180411 2.549816 0.652349
C 2.558576 2.558037 -0.225507
H 2.978185 2.787143 0.756871
H 3.358730 2.335504 -0.929259
H 1.955288 3.401933 -0.560926
C 0.318363 1.494363 0.395086
C -0.216767 0.062447 0.608542
C 0.010096 -0.247545 2.107679
H -0.263169 -1.280526 2.333662
H 1.057927 -0.107455 2.389708
H -0.599960 0.418020 2.721256
C -1.664486 -0.076487 0.146591
C -2.016993 0.362904 -1.140116
C -2.654747 -0.642032 0.956847
C -3.321995 0.237053 -1.606515
H -1.274411 0.829887 -1.785391
C -3.964996 -0.771084 0.488132
H -2.427077 -0.980590 1.960864
C -4.301996 -0.334952 -0.790818
H -3.575720 0.589992 -2.600804
H -4.720265 -1.211043 1.131266
H -5.320672 -0.434108 -1.151202
N 3.234587 -0.268349 -0.690178

1s
34 atoms
PCM Energy = -766.003344452
C 2.167905 -2.325137 -0.300835
C 1.409790 -1.174822 -0.515241
C 1.989776 0.071452 -0.248436
C 3.987800 -1.125098 0.355634
H 1.730171 -3.301432 -0.500524
H 0.396067 -1.245677 -0.891450
H 5.020330 -1.129480 0.699948
N 1.293564 1.288413 -0.472173
C 0.044527 1.624424 0.034679
O -0.459830 2.702108 -0.265262
C -0.660809 0.679920 1.017900
C -1.154401 1.513767 2.220679
H 0.048659 -0.063432 1.388437
H -0.314706 1.986432 2.740668
H -1.832763 2.299435 1.883593
H -1.681138 0.868204 2.928705
C -1.821348 -0.067028 0.360452
C -2.738861 0.585224 -0.475961
C -2.016255 -1.427083 0.638525
C -3.818559 -0.110463 -1.020640
H -2.596245 1.637323 -0.699300
C -3.098547 -2.121952 0.096469
H -1.315553 -1.946138 1.288190
C -4.003652 -1.464833 -0.737322
H -4.518050 0.409446 -1.669159
H -3.231755 -3.175525 0.325271
H -4.845533 -2.003211 -1.162678
C 1.971525 2.334155 -1.254236
H 2.751867 1.874009 -1.860320
H 1.237892 2.821345 -1.896178
H 2.413968 3.099831 -0.607371
C 3.320408 0.087007 0.190645
H 3.822460 1.022969 0.410895
N 3.437461 -2.323864 0.124957

5s
33 atoms
PCM Energy = -765.358580549
C 2.300311 -2.039812 -1.072131
C 1.560907 -0.869622 -0.909380
C 2.111533 0.179522 -0.159173
C 4.052299 -1.218167 0.124049
H 1.882489 -2.861402 -1.651081
H 0.583260 -0.773130 -1.367071
H 5.050389 -1.378643 0.527695
N 1.418444 1.396015 0.047668
O -0.529721 2.555333 -0.027782
C 2.092248 2.666006 -0.259036
H 3.162417 2.489967 -0.354592
H 1.708834 3.084041 -1.194680
H 1.906219 3.393920 0.533404
C 0.032350 1.486838 0.218081
C -0.688323 0.321427 0.791601
C -0.068282 -0.419562 1.948867
H 0.107058 -1.479025 1.723130
H 0.887077 0.018166 2.239051
H -0.729030 -0.381752 2.823917
C -2.006282 -0.022985 0.328067
C -2.645591 0.650301 -0.752226
C -2.711215 -1.109515 0.917144
C -3.898037 0.256727 -1.200496
H -2.151000 1.495755 -1.211464
C -3.964885 -1.493145 0.460650
H -2.264366 -1.657999 1.738211
C -4.570305 -0.814996 -0.601725
H -4.359855 0.792811 -2.024670
H -4.474533 -2.327216 0.934502
H -5.551241 -1.115786 -0.957030
C 3.398592 -0.012417 0.364977
H 3.875661 0.754779 0.965514
N 3.529052 -2.233264 -0.575982

TS_{5s-6s}
33 atoms
PCM Energy = -765.329951143
C 1.198249 -2.152969 -0.622122
C 0.914802 -0.751268 -0.718759
C 2.024062 0.120529 -0.439037
C 3.414864 -1.799519 -0.153048
H 0.403816 -2.870049 -0.821177
H 0.198735 -0.445655 -1.479548
H 4.387758 -2.244510 0.041521
N 1.617726 1.442450 -0.253459
O -0.160403 2.647693 0.567898
C 2.521333 2.581714 -0.295828
H 3.064534 2.594052 -1.243989
H 1.914918 3.482458 -0.203259
H 3.243050 2.553410 0.529786
C 0.342675 1.567564 0.310530
C -0.284520 0.216415 0.644128
C 0.172197 -0.284823 2.003941
H -0.004681 -1.357620 2.116113
H 1.242656 -0.115320 2.146755
H -0.362952 0.239098 2.805019
C -1.690778 0.019377 0.257980
C -2.250522 0.731300 -0.825969
C -2.505204 -0.936082 0.900352
C -3.556532 0.497376 -1.243698
H -1.663359 1.494192 -1.326587
C -3.812594 -1.167359 0.479938
H -2.116940 -1.502831 1.738979
C -4.346779 -0.454793 -0.595014
H -3.962284 1.065877 -2.075559
H -4.417120 -1.907450 0.996434
H -5.366729 -0.635363 -0.920672
C 3.278086 -0.398646 -0.177070
H 4.124695 0.239995 0.051876
N 2.393860 -2.657409 -0.326085

6s
33 atoms
PCM Energy = -765.356823161
C 1.156196 -2.146717 -0.024138
C 0.794599 -0.720438 -0.339327
C 2.027719 0.135686 -0.374810
C 3.375506 -1.817428 -0.550821
H 0.368116 -2.830449 0.289461
H 0.337901 -0.698629 -1.349189
H 4.333840 -2.294040 -0.734117
N 1.644221 1.444923 -0.150090
O -0.192031 2.574376 0.685047
C 2.523798 2.596980 -0.232559
H 3.350865 2.505787 0.480375
H 2.933988 2.691969 -1.242273
H 1.929818 3.478455 0.009880
C 0.350688 1.532985 0.374460
C -0.185733 0.090581 0.581100
C 0.059273 -0.224951 2.073886
H -0.169625 -1.267860 2.304356
H 1.109517 -0.060688 2.332601
H -0.557836 0.421833 2.702039
C -1.643704 -0.048509 0.157159
C -2.090447 0.576459 -1.018189
C -2.558115 -0.829869 0.874143
C -3.401620 0.424232 -1.462640
H -1.409741 1.204175 -1.586375
C -3.873104 -0.986814 0.429848
H -2.255760 -1.323474 1.790863
C -4.300743 -0.361800 -0.739554
H -3.722480 0.925112 -2.371367
H -4.562002 -1.598947 1.004752
H -5.324001 -0.481014 -1.082967
C 3.269667 -0.400085 -0.565969
H 4.159667 0.213995 -0.659418
N 2.354365 -2.645367 -0.201986

7s
33 atoms
PCM Energy = -765.179262016
C 1.166435 -2.157102 0.048114
C 0.813903 -0.733769 -0.235213
C 2.005869 0.149991 -0.368886
C 3.370956 -1.777741 -0.480736
H 0.362297 -2.847296 0.303541
H 0.379462 -0.800276 -1.253522
H 4.335789 -2.259804 -0.615518
N 1.676112 1.415995 -0.157606
O -0.178668 2.577402 0.637709
C 2.532141 2.596561 -0.310175
H 3.330035 2.583747 0.436574
H 2.957371 2.620901 -1.315048
H 1.900410 3.470524 -0.152460
C 0.320558 1.521341 0.385999
C -0.207065 0.090449 0.625332
C 0.009824 -0.192116 2.131908
H -0.264070 -1.221296 2.374189
H 1.056037 -0.045672 2.417224
H -0.604123 0.483572 2.730273
C -1.651117 -0.063213 0.152286
C -1.990216 0.337030 -1.150544
C -2.648505 -0.605555 0.969039
C -3.290063 0.194606 -1.627003
H -1.241893 0.786629 -1.801903
C -3.953425 -0.751197 0.490151
H -2.430759 -0.914388 1.984726
C -4.277542 -0.354629 -0.804912
H -3.533591 0.516413 -2.634316
H -4.714551 -1.173785 1.137958
H -5.291943 -0.467433 -1.173165
C 3.269903 -0.413003 -0.636317
H 4.144535 0.189825 -0.850468
N 2.354516 -2.643253 -0.102969

1t
34 atoms
PCM Energy = -766.002547595
C 1.900352 0.116448 -0.264822
C 3.675524 -1.106118 0.792769
C 3.188540 -2.252561 0.162365
H 4.544416 -1.161980 1.440749
H 3.677988 -3.212602 0.314061
N 1.220084 1.338574 -0.561997
C 0.015297 1.727706 -0.002475
O -0.531462 2.775181 -0.333738
C -0.620217 0.807325 1.050122
C -1.182462 1.666726 2.199370
H 0.142251 0.139613 1.459702
H -0.382102 2.220981 2.700728
H -1.903761 2.390357 1.815588
H -1.676863 1.028238 2.936632
C -1.706096 -0.063737 0.418945
C -2.705784 0.491872 -0.393077
C -1.739740 -1.439733 0.679719
C -3.712209 -0.312977 -0.926686

H -2.680326 1.554654 -0.611358
C -2.747932 -2.244895 0.147256
H -0.968937 -1.886128 1.302990
C -3.738392 -1.683024 -0.658378
H -4.477804 0.132250 -1.555933
H -2.755088 -3.310102 0.359827
H -4.522921 -2.307393 -1.075960
C 1.834826 2.193336 -1.581720
H 2.855548 2.462597 -1.290967
H 1.872575 1.676091 -2.546758
H 1.227260 3.092384 -1.671934
C 3.019264 0.102335 0.572981
H 3.354189 1.022439 1.042998
C 1.503238 -1.089568 -0.856982
H 0.638200 -1.102248 -1.516300
N 2.123031 -2.255633 -0.648073

5t'
33 atoms
PCM Energy = -765.356674532
C 1.594437 -0.785971 -1.018346
C 2.109312 0.181180 -0.139724
C 3.350484 -2.207427 -0.650310
H 0.659936 -0.595099 -1.541256
H 3.815902 -3.165446 -0.872400
N 1.434903 1.412630 0.084288
O -0.520535 2.564902 -0.027964
C 2.119046 2.652061 -0.305328
H 3.189025 2.545226 -0.123386
H 1.959083 2.879776 -1.365874
H 1.723460 3.480598 0.281511
C 0.048712 1.504629 0.237813
C -0.667511 0.333875 0.809524
C -0.046383 -0.405298 1.967688
H 0.161354 -1.457300 1.732396
H 0.890999 0.056408 2.278186
H -0.721196 -0.397322 2.832616
C -1.980285 -0.021377 0.340003
C -2.625977 0.653990 -0.735329
C -2.675139 -1.119519 0.919643
C -3.874519 0.251959 -1.186865
H -2.139160 1.507578 -1.187542
C -3.924850 -1.511651 0.459804
H -2.222565 -1.672057 1.734813
C -4.536894 -0.830667 -0.596903
H -4.340991 0.789968 -2.007206
H -4.425863 -2.355231 0.926034
H -5.514762 -1.138133 -0.955036
C 3.330353 -0.096390 0.486611
H 3.763888 0.621132 1.176932
N 2.185867 -1.958912 -1.260870
C 3.964062 -1.306319 0.221488
H 4.910691 -1.553792 0.691381

TS$_{5t'-6t'}$
33 atoms
PCM Energy = -765.331055996
C 0.931508 -0.742634 -0.750861
C 2.038177 0.127018 -0.438205
C 2.257443 -2.585025 -0.351229
H 0.218688 -0.403433 -1.501571
H 2.328722 -3.668983 -0.268924
N 1.629225 1.443789 -0.218404
O -0.152628 2.639849 0.606156
C 2.521649 2.590267 -0.281493
H 3.036271 2.613416 -1.245588
H 1.910752 3.485252 -0.164447
H 3.268276 2.563062 0.521826
C 0.354961 1.561818 0.343390
C -0.274027 0.206563 0.642183
C 0.196963 -0.374751 1.963831
H 0.080328 -1.461977 1.977472
H 1.253517 -0.156350 2.138419
H -0.377893 0.047125 2.796819
C -1.680494 0.017359 0.256881
C -2.269000 0.798228 -0.762489
C -2.468113 -0.996709 0.839694
C -3.579197 0.575969 -1.172345
H -1.701493 1.603804 -1.215566
C -3.779306 -1.216687 0.426617
H -2.052224 -1.622097 1.620960
C -4.343633 -0.433393 -0.581543
H -4.008437 1.197354 -1.953040
H -4.362314 -2.004877 0.894286
H -5.366838 -0.605200 -0.902001
C 3.291287 -0.402262 -0.189557
H 4.139667 0.235695 0.037620
N 1.059550 -2.101899 -0.665845
C 3.412167 -1.802186 -0.178356
H 4.370270 -2.276265 0.005137

6t'
33 atoms
PCM Energy = -765.361960827
C 0.829006 -0.736633 -0.243048
C 2.057885 0.114312 -0.399612
C 2.250768 -2.543002 0.189460
H 0.411839 -0.887280 -1.258085
H 2.393334 -3.569519 0.531709
N 1.677200 1.435533 -0.357323
O -0.131881 2.685734 0.320422
C 2.555855 2.567170 -0.596713
H 3.385172 2.571623 0.119177
H 2.960960 2.525900 -1.612027
H 1.962537 3.472844 -0.471807
C 0.375657 1.594763 0.137591
C -0.183129 0.197751 0.498854
C -0.037812 0.053618 2.036709
H -0.336966 -0.953615 2.332462
H 0.997887 0.211271 2.357208
H -0.675697 0.783827 2.539887
C -1.640007 -0.035626 0.089765
C -2.583109 1.001265 0.043932
C -2.067587 -1.344311 -0.187638
C -3.911625 0.736216 -0.293471
H -2.272477 2.015362 0.262941
C -3.396971 -1.604327 -0.520929
H -1.357989 -2.163582 -0.124219
C -4.325107 -0.564525 -0.579286
H -4.624804 1.555005 -0.331933
H -3.705554 -2.624204 -0.733292
H -5.360030 -0.766764 -0.840234
C 3.302922 -0.444829 -0.524858
H 4.189835 0.152553 -0.710853
N 1.042522 -2.061088 0.311904
C 3.391155 -1.838047 -0.303929
H 4.341542 -2.353163 -0.387349

7t‘
33 atoms
PCM Energy = -765.176891485
C 0.809670 -0.737263 -0.280905
C 2.006986 0.154757 -0.383962
C 2.234584 -2.568004 -0.124940
H 0.367806 -0.756297 -1.294461
H 2.408637 -3.624250 0.074119
N 1.691051 1.406280 -0.122722
O -0.152546 2.549410 0.730974
C 2.542412 2.595667 -0.236908
H 3.323401 2.575103 0.527261
H 2.988195 2.640270 -1.231901
H 1.900877 3.462013 -0.076088
C 0.326424 1.495236 0.441466
C -0.201116 0.062560 0.620173
C 0.028269 -0.304002 2.105802
H -0.200516 -1.359448 2.261502
H 1.069051 -0.138594 2.401608
H -0.610609 0.307595 2.745068
C -1.648188 -0.062216 0.151901
C -2.010394 0.463695 -1.098370
C -2.622473 -0.710682 0.916804
C -3.313175 0.345040 -1.573439
H -1.277624 0.990313 -1.708230
C -3.929955 -0.832231 0.439452
H -2.380881 -1.127540 1.887216
C -4.278901 -0.307116 -0.802500
H -3.575776 0.764090 -2.539386
H -4.673532 -1.339260 1.045730
H -5.295650 -0.401817 -1.169549
C 3.281715 -0.399841 -0.693338
H 4.138663 0.220061 -0.932931
N 1.039295 -2.120028 0.035199
C 3.374711 -1.754786 -0.562575
H 4.322500 -2.256175 -0.737047

5t‘‘
33 atoms
PCM Energy = -765.356816753
C 2.259721 -1.995219 -1.201535
C 1.558962 -0.803885 -1.027658
C 2.081685 0.165150 -0.163315
C 3.470085 -2.167590 -0.530407
H 1.881655 -2.769919 -1.861084
H 0.625662 -0.623087 -1.550606
H 4.044676 -3.083284 -0.652459
N 1.428823 1.408669 0.063953
O -0.517473 2.579480 -0.028753
C 2.122673 2.637019 -0.344759
H 3.195221 2.510043 -0.196193
H 1.932965 2.869513 -1.399429
H 1.760653 3.471700 0.255150
C 0.047661 1.516733 0.235175
C -0.671450 0.352980 0.820095
C -0.052750 -0.367471 1.990906
H 0.157031 -1.422717 1.772531
H 0.884017 0.099440 2.295656
H -0.729217 -0.347008 2.854343
C -1.979071 -0.012278 0.345580
C -2.618336 0.649125 -0.742429
C -2.674300 -1.107194 0.931121
C -3.860411 0.235785 -1.201737
H -2.132480 1.502262 -1.197050
C -3.917602 -1.510543 0.463347
H -2.227323 -1.646730 1.758139
C -4.522655 -0.844475 -0.606958
H -4.322638 0.763694 -2.031027
H -4.419767 -2.350526 0.934870
H -5.495729 -1.160401 -0.970700
C 3.304630 -0.116202 0.466491
H 3.736563 0.613686 1.149495
N 3.993384 -1.244973 0.288174

TS$_{5t''-6t''}$
33 atoms
PCM Energy = -765.328185589
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C 0.904080 -0.745281 -0.741801
C 2.015852 0.113137 -0.439812
C 2.453668 -2.566812 -0.327434
H 0.399819 -2.868171 -0.887827
H 0.194441 -0.413456 -1.497117
H 2.673269 -3.631032 -0.264406
N 1.619380 1.439445 -0.235269
O -0.164278 2.642530 0.581878
C 2.519043 2.580464 -0.303268
H 3.049110 2.582886 -1.258948
H 1.911306 3.480747 -0.211906
H 3.252442 2.563359 0.511950
C 0.348049 1.565887 0.322604
C -0.281680 0.210385 0.640930
C 0.181210 -0.318317 1.987620
H 0.017863 -1.395585 2.073946
H 1.248928 -0.138277 2.135356
H -0.362468 0.180485 2.798731
C -1.689806 0.017024 0.257832
C -2.260934 0.755608 -0.802036
C -2.493934 -0.959919 0.880474
C -3.568838 0.526087 -1.215701
H -1.681348 1.535502 -1.284364
C -3.803347 -1.186948 0.464030
H -2.095683 -1.546466 1.700514
C -4.348862 -0.447958 -0.587026
H -3.984445 1.114962 -2.028218
H -4.400389 -1.943767 0.964668
H -5.370393 -0.624871 -0.909773
C 3.265431 -0.419877 -0.158348
H 4.110720 0.230176 0.058491
N 3.504857 -1.745074 -0.124398

6t‘‘
33 atoms
PCM Energy = -765.354677989
C 1.119610 -2.150733 -0.127933
C 0.781339 -0.717169 -0.371512
C 2.019947 0.124881 -0.376284
C 2.417020 -2.563048 -0.258635
H 0.322142 -2.868354 0.039887
H 0.324649 -0.638964 -1.378315
H 2.657407 -3.620418 -0.165689
N 1.646197 1.437242 -0.155961
O -0.187512 2.572414 0.679419
C 2.531204 2.586538 -0.232446
H 3.346537 2.498796 0.494172
H 2.957163 2.672474 -1.236101
H 1.935775 3.471112 -0.005270
C 0.351828 1.529229 0.370269
C -0.188748 0.087645 0.571782
C 0.077003 -0.252324 2.054474
H -0.141536 -1.302023 2.263609
H 1.129517 -0.087505 2.302784

H -0.536222 0.377365 2.703534
C -1.650677 -0.046502 0.163058
C -2.112949 0.595335 -0.997238
C -2.554272 -0.842555 0.877832
C -3.428556 0.445359 -1.429040
H -1.441562 1.235175 -1.562910
C -3.873815 -0.996913 0.446278
H -2.239675 -1.348795 1.783475
C -4.316764 -0.355140 -0.708246
H -3.761489 0.959435 -2.325958
H -4.554286 -1.619960 1.019504
H -5.343502 -0.472352 -1.041802
C 3.277316 -0.416923 -0.508422
H 4.159078 0.215520 -0.590108
N 3.495117 -1.753942 -0.498292

7t‘‘
33 atoms
PCM Energy = -765.164336860
C 1.160412 -2.158659 0.021707
C 0.807591 -0.741963 -0.250958
C 1.990930 0.148774 -0.374523
C 2.447977 -2.556829 -0.132808
H 0.367765 -2.869246 0.233525
H 0.375388 -0.772529 -1.273203
H 2.748082 -3.589769 0.005085
N 1.676002 1.408471 -0.143352
O -0.185874 2.569629 0.647625
C 2.530720 2.593124 -0.285367
H 3.325234 2.575492 0.464683
H 2.959562 2.625085 -1.288201
H 1.895279 3.463624 -0.122834
C 0.308886 1.512337 0.397870
C -0.214972 0.080343 0.621011
C 0.008797 -0.221408 2.122970
H -0.258797 -1.255869 2.347613
H 1.055402 -0.076387 2.406571
H -0.606754 0.442951 2.732370
C -1.659565 -0.068743 0.151719
C -2.003595 0.346542 -1.145135
C -2.653797 -0.621005 0.965966
C -3.305148 0.210001 -1.618146
H -1.257442 0.802350 -1.794748
C -3.960665 -0.760625 0.490567
H -2.431857 -0.941798 1.976994
C -4.289682 -0.348470 -0.798320
H -3.552461 0.542738 -2.620951
H -4.719391 -1.190656 1.136263
H -5.305492 -0.456776 -1.164024
C 3.282545 -0.417176 -0.638313
H 4.134993 0.207027 -0.896048
N 3.474695 -1.700002 -0.498581

5. References:

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