Supplementary Information

Tunable synthesis of α,β-multifunctionalized azaheterocycles via the cascade reaction of saturated cyclic amines with diverse nucleophiles promoted by oxoammonium salt

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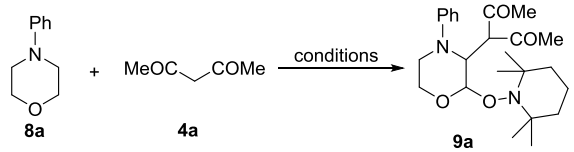
Contents

I. General Experimental Information

TEMPO salts were synthesized with a previously described procedure.[1] *N*-Aryl cyclic amines (**1**) were prepared based on a literature procedure.[2] Melting points were recorded with a micro melting point apparatus and uncorrected. The ^{1}H NMR spectra were recorded at 400 MHz or 600 MHz, and the ^{13}C NMR spectra were recorded at 100 MHz or 150 MHz. The ^{19}F NMR spectra were recorded at 376 MHz. Chemical shifts were expressed in parts per million (δ), and were reported as s (singlet), d (doublet), t (triplet), q (quadruplet), dd (doublet of doublet), td (doublet of triplet), m (multiplet), brs (broad singlet) etc. The coupling constants *J* were given in Hz. High-resolution mass spectra (HRMS) were performed on a microTOF mass spectrometer. All the reactions were monitored by thin-layer chromatography (TLC) using silica gel plates (silica gel 60 F254 0.25 mm), and components were visualized by observation under UV light (254 and 365 nm).

II. Experimental Procedures and Spectroscopic Data

1. Optimization studies for the formation of 9a[a]



entry	oxoammonium salt (equiv)	additive (equiv)	solvent	yield (%)[b] **9a**
1	$T^+BF_4^-$ (2)	$CaCl_2$ (0.5)	EtOAc	39
2	$T^+BF_4^-$ (2)	$CaCl_2$ (0.5)	THF	41
3	$T^+BF_4^-$ (2)	$CaCl_2$ (0.5)	1,4-dioxane	29
4	$T^+BF_4^-$ (2)	$CaCl_2$ (0.5)	DCM	38
5	$T^+BF_4^-$ (2)	$CaCl_2$ (0.5)	acetone	39
6	$T^+BF_4^-$ (2)	$CaCl_2$ (0.5)	CH_3CN	32
7	$T^+BF_4^-$ (2)	$CaCl_2$ (0.5)	DMF	24
8	$T^+ClO_4^-$ (2)	$CaCl_2$ (0.5)	THF	38
9	T^+OTf^- (2)	$CaCl_2$ (0.5)	THF	34
10	$T^+PF_6^-$ (2)	$CaCl_2$ (0.5)	THF	25
11	$T^+BF_4^-$ (2)	$FeCl_2$ (0.5)	THF	49
12	$T^+BF_4^-$ (2)	NaCl (1)	THF	48
13	$T^+BF_4^-$ (2)	CaF_2 (0.5)	THF	50
14	$T^+BF_4^-$ (2)	KF (1)	THF	54
15	$T^+BF_4^-$ (2)	CsF (1)	THF	65
16	$T^+BF_4^-$ (2)	K_2CO_3 (0.5)	THF	53
17	$T^+BF_4^-$ (2)	Na_2CO_3 (0.5)	THF	76
18	$T^+BF_4^-$ (2)	Na_2CO_3 (1)	THF	73
19	$T^+BF_4^-$ (2)	Na_2CO_3 (0.25)	THF	75
20	$T^+BF_4^-$ (3)	Na_2CO_3 (0.5)	THF	65
21[c]	$T^+BF_4^-$ (2)	Na_2CO_3 (0.5)	THF	67
22[d]	$T^+BF_4^-$ (2)	Na_2CO_3 (0.5)	THF	70
23[e]	**$T^+BF_4^-$ (2)**	**Na_2CO_3 (0.5)**	**THF**	**80**

[a] Reaction conditions: **8a** (0.2 mmol), **4a** (0.4 mmol), solvent (1 mL), rt, air, 1 h. [b] isolated yield. [c] under O_2. [d] under N_2. [e] 0.5 h.

2. A typical procedure for the synthesis of 3a and the spectroscopic data of 3a-3q

To a reaction tube equipped with a stir bar were added 1-(phenyl)piperidine (**1a**, 32 mg, 0.2 mmol), THF (1 mL), dimethyl malonate (**2a**, 46 μL, 0.4 mmol), $T^+BF_4^-$ (97 mg, 0.4 mmol), and $CaCl_2$ (11 mg, 0.1 mmol). The resulting mixture was then stirred at room temperature under air for 0.5 h. Upon completion, the mixture was diluted with ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (3:1) as the eluent to afford **3a** as yellow liquid in 37 mg (60%). **3b-3q** were obtained in an analogous manner.

Dimethyl 2-(3-oxo-1-phenylpiperidin-2-yl)malonate (**3a**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (37 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27 (t, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 6.87 (t, *J* = 7.6 Hz, 1H), 4.94 (d, *J* = 7.2 Hz, 1H), 4.00 (d, *J* = 7.6 Hz, 1H), 3.73 (s, 3H), 3.63 (s, 3H), 3.60-3.54 (m, 1H), 3.47-3.40 (m, 1H), 2.68-2.62 (m, 1H), 2.56-2.48 (m, 1H), 2.27-2.22 (m, 1H), 2.17-2.12 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 207.8, 167.7, 167.5, 148.1, 129.5, 120.0, 115.9, 66.5, 52.8, 52.7, 44.5, 37.1, 22.6. HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{16}H_{19}NO_5Na$ 328.1155; Found 328.1152.

Dimethyl 2-(1-(4-fluorophenyl)-3-oxopiperidin-2-yl)malonate (**3b**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (47 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.93-6.84 (m, 4H), 4.69 (d, *J* = 7.6 Hz, 1H), 3.86 (d, *J* = 7.2 Hz, 1H), 3.66 (s, 3H), 3.56 (s, 3H), 3.37-3.33 (m, 2H), 2.62-2.57 (m, 1H), 2.48-2.40 (m, 1H), 2.14-2.06 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 207.5, 167.55, 167.46, 157.6 (d, $^{1}J_{C\text{-}F}$ = 238.4 Hz), 144.8 (d, $^{4}J_{C\text{-}F}$ = 2.1 Hz), 119.1 (d, $^{3}J_{C\text{-}F}$ = 7.7 Hz), 115.9 (d, $^{2}J_{C\text{-}F}$ = 21.9 Hz), 67.3, 52.8, 52.74, 52.71, 46.6, 37.4, 23.0. ^{19}F{^{1}H} NMR ($CDCl_3$, 376 MHz): δ -123.1. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{19}FNO_5$ 324.1242; Found 324.1238.

Dimethyl 2-(1-(4-chlorophenyl)-3-oxopiperidin-2-yl)malonate (**3c**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (43 mg, 63%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24-7.20 (m, 2H), 6.90-6.86 (m, 2H), 4.88 (d, *J* = 7.6 Hz, 1H), 3.97 (d, *J* = 7.2 Hz, 1H), 3.73 (s, 3H), 3.64 (s, 3H), 3.56-3.50 (m, 1H), 3.45-3.38 (m, 1H), 2.69-2.62 (m, 1H), 2.55-2.48 (m, 1H), 2.27-2.21 (m, 1H), 2.17-2.12 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 207.4, 167.5, 167.3, 146.7, 129.3, 124.8, 116.9, 66.4, 52.9, 52.8, 52.7, 44.6, 37.0, 22.5. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{19}ClNO_5$ 340.0946; Found 340.0942.

Dimethyl 2-(1-(4-iodophenyl)-3-oxopiperidin-2-yl)malonate (**3d**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (52 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55-7.51 (m, 2H), 6.62 (dd, J_1 = 12.0 Hz, J_2 = 3.2 Hz, 2H), 4.90 (d, J = 7.2 Hz, 1H), 3.97 (d, J = 7.6 Hz, 1H), 3.73 (s, 3H), 3.64 (s, 3H), 3.57-3.51 (m, 1H), 3.43-3.37 (m, 1H), 2.68-2.61 (m, 1H), 2.55-2.47 (m, 1H), 2.27-2.22 (m, 1H), 2.17-2.12 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 207.3, 167.5, 167.3, 147.7, 138.1, 117.4, 81.4, 66.0, 52.91, 52.87, 52.7, 44.0, 36.8, 22.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{19}INO_5$ 432.0302; Found 432.0306.

Dimethyl 2-(1-(4-(*tert*-butyl)phenyl)-3-oxopiperidin-2-yl)malonate (**3e**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (30 mg, 42%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 8.8 Hz, 2H), 4.88 (d, J = 7.2 Hz, 1H), 3.99 (d, J = 7.2 Hz, 1H), 3.73 (s, 3H), 3.64 (s, 3H), 3.54-3.49 (m, 1H), 3.46-3.43 (m, 1H), 2.68-2.62 (m, 1H), 2.55-2.49 (m, 1H), 2.24-2.14 (m, 2H), 1.29 (s, 9H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 207.9, 167.8, 167.6, 145.7, 143.0, 126.3, 116.0, 66.7, 52.9, 52.74, 52.72, 45.0, 37.3, 34.0, 31.4, 22.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{28}NO_5$ 362.1962; Found 362.1954.

Dimethyl 2-(3-oxo-1-(*p*-tolyl)piperidin-2-yl)malonate (**3f**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (27 mg, 42%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.08 (d, J = 8.4 Hz, 2H), 6.87 (d, J = 8.4 Hz, 2H), 4.83 (d, J = 7.2 Hz, 1H), 3.97 (d, J = 7.6 Hz, 1H), 3.73 (s, 3H), 3.64 (s, 3H), 3.50-3.38 (m, 2H), 2.68-2.62 (m, 1H), 2.54-2.47 (m, 1H), 2.31 (s, 3H), 2.27-2.11 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 208.0, 167.7, 167.6, 146.0, 130.03, 129.99, 117.1, 67.0, 52.8, 52.74, 52.71, 45.8, 37.4, 22.8, 20.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{22}NO_5$ 320.1492; Found 320.1496.

Dimethyl 2-(3-oxo-1-(*m*-tolyl)piperidin-2-yl)malonate (**3g**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (28 mg, 44%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.16 (t, J = 7.6 Hz, 1H), 7.14-6.75 (m, 2H), 6.70 (d, J = 7.2 Hz, 1H), 4.92 (d, J = 7.6 Hz,

1H), 4.00 (d, *J* = 7.6 Hz, 1H), 3.73 (s, 3H), 3.64 (s, 3H), 3.59-3.53 (m, 1H), 3.45-3.39 (m, 1H), 2.67-2.62 (m, 1H), 2.55-2.48 (m, 1H), 2.32 (s, 3H), 2.31-2.11 (m, 2H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 208.0, 167.7, 167.5, 148.2, 139.3, 129.3, 120.9, 116.8, 113.1, 66.5, 52.82, 52.77, 52.74, 44.6, 37.1, 22.7, 21.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{22}NO_5$ 320.1492; Found 320.1494.

Dimethyl 2-(3-oxo-1-(*o*-tolyl)piperidin-2-yl)malonate (**3h**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (26 mg, 40%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21-7.13 (m, 3H), 7.08-7.04 (m, 1H), 4.54 (d, *J* = 6.4 Hz, 1H), 3.69-3.65 (m, 7H), 3.19-3.15 (m, 1H), 3.05-2.99 (m, 1H), 2.81-2.75 (m, 1H), 2.56-2.47 (m, 1H), 2.19-2.14 (m, 4H), 2.00-1.95 (m, 1H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 207.4, 167.9, 167.8, 147.6, 135.4, 131.5, 126.8, 125.3, 122.4, 68.3, 52.8, 52.6, 52.5, 51.7, 38.7, 23.3, 17.3. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{22}NO_5$ 320.1492; Found 320.1497.

Dimethyl 2-(1-(naphthalen-2-yl)-3-oxopiperidin-2-yl)malonate (**3i**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (40 mg, 56%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76-7.68 (m, 3H), 7.43-7.39 (m, 1H), 7.32-7.20 (m, 2H), 7.19 (s, 1H), 5.08 (d, *J* = 7.6 Hz, 1H), 4.08 (d, *J* = 7.6 Hz, 1H), 3.75-3.67 (m, 4H), 3.59-3.55 (m, 4H), 2.71-2.65 (m, 1H), 2.60-2.54 (m, 1H), 2.31-2.29 (m, 1H), 2.20-1.18 (m, 1H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 207.8, 167.6, 167.4, 145.8, 134.5, 129.3, 128.5, 127.5, 126.7, 126.6, 123.7, 118.4, 110.9, 66.6, 52.85, 52.80, 52.77, 44.9, 37.1, 22.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{22}NO_5$ 356.1492; Found 356.1498.

Dimethyl 2-(1-([1,1'-biphenyl]-4-yl)-3-oxopiperidin-2-yl)malonate (**3j**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (48 mg, 63%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56-7.52 (m, 4H), 7.41 (t, *J* = 8.0 Hz, 2H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.03-7.00 (m, 2H), 5.00 (d, *J* = 7.2 Hz, 1H), 4.05 (d, *J* = 7.6 Hz, 1H), 3.74 (s, 3H), 3.65-3.60 (m, 4H), 3.50-3.44 (m,

1H), 2.69-2.64 (m, 1H), 2.58-2.51 (m, 1H), 2.31-2.25 (m, 1H), 2.20-1.15 (m, 1H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 207.7, 167.7, 167.5, 147.3, 140.6, 132.5, 128.8, 128.1, 126.6, 126.5, 115.7, 66.3, 52.88, 52.86, 52.83, 44.3, 37.0, 22.6. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{24}NO_5$ 382.1649; Found 382.1644.

Diethyl-2-(1-([1,1'-biphenyl]-4-yl)-3-oxopiperidin-2-yl)malonate (**3k**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (49 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (t, *J* = 8.4 Hz, 4H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.29-7.24 (m, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 5.01 (d, *J* = 7.6 Hz, 1H), 4.25-4.01 (m, 5H), 3.64-3.60 (m, 1H), 3.51-3.45 (m, 1H), 2.68-2.50 (m, 2H), 2.29-2.14 (m, 2H), 1.26 (t, *J* = 7.2 Hz, 3H), 1.17 (t, *J* = 7.2 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 207.8, 167.3, 167.1, 147.5, 140.7, 132.3, 128.8, 128.0, 126.6, 126.5, 115.6, 66.3, 61.9, 53.3, 44.1, 37.1, 22.8, 14.0, 13.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{28}NO_5$ 410.1962; Found 410.1955.

Di-*tert*-butyl-2-(3-oxo-1-(*p*-tolyl)piperidin-2-yl)malonate (**3l**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (44 mg, 54%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.06 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 4.78 (d, *J* = 8.0 Hz, 1H), 3.80 (d, *J* = 8.0 Hz, 1H), 3.55-3.50 (m, 1H), 3.45-3.42 (m, 1H), 2.66-2.61 (m, 1H), 2.51-2.45 (m, 1H), 2.26-2.20 (m, 4H), 2.12-2.11 (m, 1H), 1.45 (s, 9H), 1.35 (s, 9H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 208.4, 166.6, 166.3, 146.4, 129.8, 129.1, 116.4, 82.1, 66.8, 55.3, 44.9, 37.4, 27.9, 27.7, 23.5, 20.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{34}NO_5$ 404.2431; Found 404.2436.

1,2-Diphenylpiperidin-3-one (**3m**)

Eluent: petroleum ether/ethyl acetate (10:1). Yellow liquid (21 mg, 42%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.31 (m, 4H), 7.29-7.20 (m, 3H), 6.79-6.76 (m, 3H), 5.33 (s, 1H), 3.73-3.66 (m, 2H), 2.60-2.54 (m, 1H), 2.48-2.44 (m, 1H), 2.14-2.06 (m, 2H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ

206.3, 148.5, 136.9, 129.4, 128.9, 127.7, 126.2, 118.1, 113.0, 69.2, 44.3, 36.9, 21.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{18}NO$ 252.1383; Found 252.1393.

2-(4-Methoxyphenyl)-1-phenylpiperidin-3-one (**3n**)

Eluent: petroleum ether/ethyl acetate (10:1). Yellow liquid (34 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25-7.20 (m, 4H), 6.85 (dd, J_1 = 8.8 Hz, J_2 = 3.2 Hz, 2H), 6.79-6.75 (m, 3H), 5.26 (s, 1H), 3.78 (s, 3H), 3.71-3.63 (m, 2H), 2.61-2.54 (m, 1H), 2.45-2.37 (m, 1H), 2.13-2.06 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 206.6, 159.2, 148.6, 129.4, 128.6, 127.4, 118.0, 114.4, 113.1, 68.7, 55.3, 44.2, 36.8, 21.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{20}NO_2$ 282.1489; Found 282.1491.

2-Allyl-1-(4-chlorophenyl)piperidin-3-one (**3o**)

Eluent: petroleum ether/ethyl acetate (5:1). Yellow liquid (21 mg, 43%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21-7.17 (m, 2H), 6.78-6.75 (m, 2H), 5.75-5.65 (m, 1H), 5.07-5.02 (m, 2H), 4.20 (t, *J* = 7.2 Hz, 1H), 3.53-3.37 (m, 2H), 2.56-2.45 (m, 4H), 2.16-2.08 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 208.4, 147.5, 133.4, 129.2, 123.7, 118.1, 116.3, 67.1, 42.9, 36.9, 34.0, 22.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{17}ClNO$ 250.0993; Found 250.0997.

1-(4-((((3a*R*,5*R*,6*R*,6a*R*)-5-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl)oxy)methyl)phenyl)-2-(4-methoxyphenyl)piperidin-3-one (3p)

Eluent: petroleum ether/ethyl acetate (2:1). Yellow liquid (50 mg, 45%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.23 (d, *J* = 7.6 Hz, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 6.73 (d, *J* = 8.4 Hz, 2H), 5.75 (d, *J* = 3.2 Hz, 1H), 5.28 (s, 1H), 4.69-4.57 (m, 3H), 4.37 (d, *J* = 11.6 Hz, 1H), 4.13-3.97 (m, 3H), 3.78 (s, 3H), 3.73-3.64 (m, 2H), 3.53-3.49 (m, 1H), 2.61-2.55 (m, 1H), 2.46-2.42 (m, 1H), 2.14-2.10 (m, 2H), 1.62 (s, 3H), 1.42 (s, 3H), 1.34 (s, 6H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 206.23, 206.20, 159.3, 148.51, 148.49, 129.67, 129.66, 128.45, 128.41, 127.35, 127.33,

126.22, 126.19, 114.4, 113.9, 112.82, 112.80, 108.5, 105.0, 82.7, 78.1, 76.54, 76.49, 75.5, 72.23, 72.21, 68.7, 67.1, 55.3, 44.3, 36.7, 26.9, 26.8, 26.4, 25.2, 21.02, 21.01. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{31}H_{40}NO_8$ 554.2748; Found 554.2740.

1-(4-((((1*S*,2*R*,5*S*)-2-Isopropyl-5-methylcyclohexyl)oxy)methyl)phenyl)-2-(4-methoxyphenyl)piperidin-3-one (3q)

Eluent: petroleum ether/ethyl acetate (5:1). Yellow liquid (37 mg, 41%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.20 (t, J = 8.4 Hz, 4H), 6.84 (dd, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 2H), 6.72 (d, J = 8.8 Hz, 2H), 5.25 (s, 1H), 4.53 (d, J = 10.8 Hz, 1H), 4.28 (d, J = 10.8 Hz, 1H), 3.77 (s, 3H), 3.70-3.63 (m, 2H), 3.16-3.10 (m, 1H), 2.59-2.53 (m, 1H), 2.46-2.37 (m, 1H), 2.27-2.24 (m, 1H), 2.18-2.05 (m, 3H), 1.66-1.59 (m, 3H), 1.36-1.21 (m, 3H), 0.94-0.86 (m, 7H), 0.68 (d, J = 6.8 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 206.5, 159.2, 148.1, 129.5, 128.61, 128.57, 127.4, 114.3, 113.05, 113.02, 78.34, 78.29, 70.22, 70.19, 68.7, 55.3, 48.3, 44.4, 40.4, 36.8, 34.6, 31.6, 25.49, 25.47, 23.31, 23.29, 22.4, 21.3, 21.0, 16.07, 16.06. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{29}H_{40}NO_3$ 450.3003; Found 450.2996.

3. A typical procedure for the synthesis of 5a and the spectroscopic data of 5a-5d

To a reaction tube equipped with a stir bar were added 1-(4-iodophenyl)piperidine (**1d**, 57 mg, 0.2 mmol), THF (1 mL), pentane-2,4-dione (**4a**, 41 μL, 0.4 mmol), $T^+BF_4^-$ (97 mg, 0.4 mmol), and $CaCl_2$ (11 mg, 0.1 mmol). The resulting mixture was then stirred at room temperature under air for 0.5 h. Upon completion, the mixture was diluted with ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (3:1) as the eluent to afford **5a** as yellow solid in 56 mg (73%). **5b-5d** were obtained in an analogous manner.

7-Acetyl-1-(4-iodophenyl)-1,2,3,4,7,7a-hexahydro-6*H*-cyclopenta[*b*]pyridin-6-one (**5a**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow solid (56 mg, 73%), mp 127-128 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (s, 1H), 7.39 (dd, J_1 = 12.0 Hz, J_2 = 3.2 Hz, 2H), 6.29 (dd, J_1 = 12.0 Hz, J_2 = 3.2 Hz, 2H), 3.55-3.41 (m, 2H), 3.15 (d, J = 18.4 Hz, 1H), 2.56-2.51 (m, 4H), 2.31-1.87 (m, 4H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 200.3, 193.7, 176.5, 144.9, 142.3, 138.0, 114.7, 78.5, 66.8, 50.1, 46.7, 42.1, 29.9, 23.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{17}INO_2$ 382.0298; Found 382.0288.

7-Acetyl-1-(2-bromophenyl)-1,2,3,4,7,7a-hexahydro-6*H*-cyclopenta[*b*]pyridin-6-one (**5b**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (37 mg, 56%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (s, 1H), 7.58 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.23-7.18 (m, 1H), 7.10 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.04-7.00 (m, 1H), 3.68-3.62 (m, 1H), 3.42-3.37 (m, 1H), 2.74 (d, J = 18.4 Hz, 1H), 2.54 (d, J = 18.4 Hz, 1H), 2.40 (s, 3H), 2.26-2.11 (m, 4H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 202.2, 194.5, 172.8, 143.6, 141.2, 134.2, 130.1, 128.3, 127.5, 125.5, 69.1, 52.4, 47.3, 39.4, 29.8, 23.6. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{17}BrNO_2$ 334.0437; Found 334.0432.

Ethyl-6-oxo-1-phenyl-2,3,4,6,7,7a-hexahydro-1*H*-cyclopenta[*b*]pyridine-7-carboxylate (**5c**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (25 mg, 44%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (s, 1H), 7.17 (t, J = 7.6 Hz, 2H), 6.73 (t, J = 7.6 Hz, 1H), 6.54 (d, J = 8.4 Hz, 2H), 4.31 (q, J = 7.2 Hz, 2H), 3.57-3.48 (m, 2H), 3.22 (d, J = 18.4 Hz, 1H), 2.51 (d, J = 18.0 Hz, 1H), 2.31-1.87 (m, 4H), 1.35 (t, J = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 198.9, 177.9, 161.2, 145.3, 135.5, 129.5, 117.4, 112.5, 66.9, 61.3, 50.0, 46.4, 42.0, 23.4, 14.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{20}NO_3$ 286.1438; Found 286.1430.

Ethyl 1-(4-bromophenyl)-6-oxo-2,3,4,6,7,7a-hexahydro-1*H*-cyclopenta[*b*]pyridine-7-carboxylate (**5d**)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (55 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.26 (s, 1H), 7.26-7.22 (m, 2H), 6.43-6.39 (m, 2H), 4.32 (q, *J* = 7.2 Hz, 2H), 3.56-3.42 (m, 2H), 3.14 (d, *J* = 18.4 Hz, 1H), 2.52 (d, *J* = 18.4 Hz, 1H), 2.30-1.88 (m, 4H), 1.35 (t, *J* = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 198.5, 177.1, 161.1, 144.3, 135.9, 132.1, 114.0, 109.4, 66.9, 61.4, 50.2, 46.3, 42.0, 23.4, 14.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{19}BrNO_3$ 364.0543; Found 364.0539.

4. A typical procedure for the synthesis of 5a and the spectroscopic data of 7a-7b

To a reaction tube equipped with a stir bar were added 1-(phenyl)piperidine (**1a**, 32 mg, 0.2 mmol), THF/H_2O (19/1, 1 mL), malononitrile (**6a**, 25 μL, 0.4 mmol), $T^+BF_4^-$ (97 mg, 0.4 mmol), and $CaCl_2$ (11 mg, 0.1 mmol). The resulting mixture was then stirred at room temperature under air for 1 h. Upon completion, the mixture was diluted with ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with dichloromethane/methanol (20:1) as the eluent to afford **7a** as yellow solid in 27 mg (53%, 5:1 dr). **7b** was obtained in an analogous manner.

7a-Hydroxy-2-oxo-4-phenyloctahydro-1*H*-pyrrolo[3,2-*b*]pyridine-3-carbonitrile (**7a**)

Eluent: dichloromethane/methanol (20:1). Yellow solid (27 mg, 53%, 5:1 dr), mp 94-95 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 (t, *J* = 8.4 Hz, 2H), 7.04-6.97 (m, 3H), 5.29 (s, 1H), 4.48 (d, *J* = 5.2 Hz, 1H), 4.24 (br s, 1H), 3.40 (d, *J* = 5.2 Hz, 1H), 3.22-3.19 (m, 2H), 2.01-1.70 (m, 4H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 167.2, 148.7, 129.7, 129.6, 122.2, 118.7, 116.3, 115.1, 86.2, 66.8, 47.0, 37.3, 33.5, 20.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{16}N_3O_2$ 258.1237; Found 258.1237.

7a-Hydroxy-2-oxo-4-(*p*-tolyl)octahydro-1*H*-pyrrolo[3,2-*b*]pyridine-3-carbonitrile (**7b**)

Eluent: dichloromethane/methanol (20:1). Yellow solid (22 mg, 40%, 9:1 dr), mp 148-149 ℃. ^{1}H NMR (400 MHz, acetone-d_6): δ 7.95 (br s, 1H), 7.09 (d, *J* = 8.4 Hz, 2H), 6.99 (d, *J* = 8.4 Hz, 2H), 5.46 (s, 1H), 4.56 (d, *J* = 7.2 Hz, 1H), 3.74 (d, *J* = 7.2 Hz, 1H), 3.30 (t, *J* = 6.0 Hz, 2H), 2.24 (s, 3H), 2.09-1.99 (m, 2H), 1.87-1.83 (m, 1H), 1.71-1.68 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 165.0, 147.4, 129.7, 117.8, 116.7, 114.4, 84.8, 67.4, 45.1, 36.1, 33.8, 20.3, 19.6. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{18}N_3O_2$ 272.1394; Found 272.1385.

5. A typical procedure for the synthesis of 9a and the spectroscopic data of 9a-9q

To a reaction tube equipped with a stir bar were added 4-phenylmorpholine (**8a**, 33 mg, 0.2 mmol), THF (1 mL), pentane-2,4-dione (**4a**, 41 μL, 0.4 mmol), $T^+BF_4^-$ (97 mg, 0.4 mmol), and Na_2CO_3 (11 mg, 0.1 mmol). The resulting mixture was then stirred at room temperature under air for 0.5 h. Upon completion, the mixture was diluted with ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (3:1) as the eluent to afford **9a** as white solid in 67 mg (80%, >20:1 dr). **9b-9q** were obtained in an analogous manner.

3-(4-Phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholin-3-yl)pentane-2,4-dione (9a)

Eluent: petroleum ether/ethyl acetate (3:1). White solid (67 mg, 80%, >20:1 dr), mp 119-120 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24-7.20 (m, 2H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.78 (t, *J* = 7.2 Hz, 1H), 4.94 (d, *J* = 10.8 Hz, 1H), 4.69 (d, *J* = 11.2 Hz, 1H), 4.59 (s, 1H), 4.27-4.22 (m, 1H), 3.60-3.53 (m, 2H), 3.35-3.32 (m, 1H), 2.21(s, 3H), 1.92 (s, 3H), 1.45-1.42 (m, 5H), 1.28-1.14 (m, 8H), 0.95-0.94 (m, 5H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 201.9, 201.3, 150.0, 129.2, 119.1, 116.4, 101.7, 69.3, 60.5, 59.3, 58.2, 57.7, 41.8, 40.8, 40.1, 33.84, 33.77, 31.3, 27.3, 20.6, 19.9, 17.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{37}N_2O_4$ 417.2748; Found 417.2776.

3-(4-(4-(Tert-butyl)phenyl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholin-3-yl)pentane-2,4-dione (9b)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow syrup (68 mg, 72%, >20:1 dr). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24 (dd, J_1 = 6.8 Hz, J_2 = 2.0 Hz, 2H), 6.89 (d, J = 8.8 Hz, 2H), 4.88 (d, J = 10.8 Hz, 1H), 4.69 (d, J = 10.8 Hz, 1H), 4.57 (s, 1H), 4.28-4.27 (m, 1H), 3.58-3.51 (m, 2H), 3.30-3.27 (m, 1H), 2.21 (s, 3H), 1.94 (s, 3H), 1.44-0.88 (m, 27H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 202.1, 201.5, 147.9, 142.2, 125.9, 116.5, 101.8, 69.4, 60.5, 59.3, 59.0, 57.6, 41.8, 40.8, 40.1, 33.9, 33.8, 31.4, 31.2, 27.2, 20.6, 19.8, 17.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{45}N_2O_4$ 473.3374; Found 473.3387.

3-(4-(4-Fluorophenyl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholin-3-yl)pentane-2,4-dione (9c)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow solid (71 mg, 82%, >20:1 dr), mp 124-125 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.94-6.90 (m, 4H), 4.80 (d, J = 10.8 Hz, 1H), 4.68 (d, J = 11.2 Hz, 1H), 4.59 (s, 1H), 4.28-4.22 (m, 1H), 3.62-3.53 (m, 2H), 3.26-3.23 (m, 1H), 2.22 (s, 3H), 1.95 (s, 3H), 1.46-1.43 (m, 5H), 1.26-1.15 (m, 7H), 0.98-0.93 (m, 6H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 201.8, 201.3, 156.6 (d, $^{1}J_{C\text{-}F}$ = 236.3 Hz), 146.7 (d, $^{4}J_{C\text{-}F}$ = 2.1 Hz), 118.0 (d, $^{3}J_{C\text{-}F}$ = 7.7 Hz), 115.6 (d, $^{2}J_{C\text{-}F}$ = 21.9 Hz), 101.7, 69.1, 60.5, 59.3, 59.1, 57.5, 42.4, 40.8, 40.1, 33.8, 33.7, 31.3, 27.6, 20.6, 19.9, 17.0. ^{19}F{^{1}H} NMR (376 MHz, $CDCl_3$): δ -125.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{36}FN_2O_4$ 435.2654; Found 435.2672.

3-(4-(4-Bromophenyl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholin-3-yl)pentane-2,4-dione (9d)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow syrup (75 mg, 76%, >20:1 dr). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33-7.29 (m, 2H), 6.86-6.82 (m, 2H), 4.86 (d, J = 11.2 Hz, 1H), 4.66 (d, J = 10.8

Hz, 1H), 4.60 (s, 1H), 4.25-4.18 (m, 1H), 3.59-3.52 (m, 2H), 3.32-3.28 (m, 1H), 2.22 (s, 3H), 1.95 (s, 3H), 1.46-0.96 (m, 18H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 201.6, 201.1, 149.1, 132.0, 117.8, 111.0, 101.6, 69.1, 60.5, 59.3, 58.0, 57.6, 42.1, 40.8, 40.1, 33.81, 33.76, 31.2, 27.6, 20.6, 19.9, 16.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{36}BrN_2O_4$ 495.1853; Found 495.1852.

3-(2-((2,2,6,6-Tetramethylpiperidin-1-yl)oxy)-4-(4-(trifluoromethyl)phenyl)morpholin-3-yl)pentane-2,4-dione (9e)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow solid (77 mg, 80%, >20:1 dr), mp 154-155 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47 (d, *J* = 8.8 Hz, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 5.00 (d, *J* = 11.2 Hz, 1H), 4.69 (d, *J* = 10.8 Hz, 1H), 4.63 (s, 1H), 4.26-4.20 (m, 1H), 3.62-3.56 (m, 2H), 3.45-3.41 (m, 1H), 2.24 (s, 3H), 1.98 (s, 3H), 1.45-0.91 (m, 18H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 201.4, 200.9, 152.4, 126.6 (q, $^{4}J_{C\text{-}F}$ = 3.3 Hz), 124.7 (q, $^{1}J_{C\text{-}F}$ = 269.1 Hz), 120.4 (q, $^{2}J_{C\text{-}F}$ = 32.7 Hz), 115.0, 101.6, 68.9, 60.6, 59.4, 57.7, 41.8, 40.8, 40.1, 33.8, 31.2, 27.7, 20.5, 19.7, 16.9. $^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$): δ -61.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{36}F_3N_2O_4$ 485.2622; Found 485.2612.

3-(4-([1,1'-Biphenyl]-4-yl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholin-3-yl)pentane-2,4-dione (9f)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow syrup (66 mg, 67%, >20:1 dr). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56-7.47 (m, 4H), 7.39 (t, *J* = 8.0 Hz, 2H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.04-7.01 (m, 2H), 4.98 (d, *J* = 10.8 Hz, 1H), 4.70 (d, *J* = 11.2 Hz, 1H), 4.62 (s, 1H), 4.30-4.24 (m, 1H), 3.64-3.38 (m, 3H), 2.23 (s, 3H), 1.97 (s, 3H), 1.59-0.86 (m, 18H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 201.9, 201.4, 149.4, 140.8, 131.8, 128.8, 128.7, 127.8, 126.4, 116.5, 101.7, 69.4, 60.6, 59.4, 58.1, 57.8, 42.0, 40.8, 40.2, 33.8, 31.3, 27.4, 20.6, 19.9, 17.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{41}N_2O_4$ 493.3061; Found 493.3067.

3-(4-(3-Nitrophenyl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholin-3-yl)pentane-2,4-dione (9g)

Eluent: petroleum ether/ethyl acetate (2:1). Orange solid (55 mg, 60%, >20:1 dr), mp 126-127 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (t, J = 2.4 Hz, 1H), 7.62 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.38 (t, J = 8.0 Hz, 1H), 7.30-7.27 (m, 1H), 4.97 (d, J = 11.2 Hz, 1H), 4.71 (d, J = 11.2 Hz, 1H), 4.65 (s, 1H), 4.27-4.24 (m, 1H), 3.63-3.60 (m, 2H), 3.49-3.45 (m, 1H), 2.26 (s, 3H), 2.04 (s, 3H), 1.44-0.85 (m, 18H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 201.1, 200.7, 150.9, 149.3, 129.9, 121.7, 113.6, 109.6, 101.6, 68.7, 60.6, 59.4, 58.2, 57.4, 42.0, 40.7, 40.1, 33.8, 31.2, 28.0, 20.5, 19.6, 16.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{36}N_3O_6$ 462.2599; Found 462.2602.

3-(2-((2,2,6,6-Tetramethylpiperidin-1-yl)oxy)-4-(*m*-tolyl)morpholin-3-yl)pentane-2,4-dione (9h)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow syrup (65 mg, 75%, >20:1 dr). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.10 (t, J = 8.0 Hz, 1H), 6.80 (s, 1H), 6.75 (dd, J_1 = 8.0 Hz, J_2 = 2.4 Hz, 1H), 6.61 (d, J = 7.2 Hz, 1H), 4.92 (d, J = 10.8 Hz, 1H), 4.68 (d, J = 11.2 Hz, 1H), 4.59 (s, 1H), 4.25-4.19 (m, 1H), 3.59-3.50 (m, 2H), 3.34-3.31 (m, 1H), 2.33-2.29 (m, 3H), 2.21 (s, 3H), 1.92 (s, 3H), 1.68-0.96 (m, 18H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 202.0, 201.4, 150.1, 138.9, 129.0, 120.0, 117.2, 113.6, 101.7, 69.6, 60.5, 59.3, 57.8, 57.7, 42.2, 40.8, 40.2, 33.8, 33.7, 31.3, 27.1, 21.8, 20.6, 19.9, 17.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{39}N_2O_4$ 431.2904; Found 431.2916.

Ethyl 3-oxo-2-(4-phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholin-3-yl)butanoate (9i)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow syrup (71 mg, 80%, >20:1 dr). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21-7.17 (m, 2H), 6.90 (d, J = 8.0 Hz, 2H), 6.73 (t, J = 7.2 Hz, 1H), 4.85 (d, J = 10.8 Hz, 1H), 4.76 (s, 1H), 4.44 (d, J = 11.2 Hz, 1H), 4.34-4.27 (m, 1H), 3.91-3.87 (m, 1H),

3.68-3.59 (m, 3H), 3.35-3.32 (m, 1H), 2.21 (s, 3H), 1.45-0.87 (m, 21H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 200.5, 167.1, 150.4, 128.9, 118.6, 115.9, 102.0, 61.6, 59.9, 58.26, 58.23, 41.3, 40.8, 40.2, 34.0, 33.8, 29.9, 20.6, 19.7, 17.0, 13.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{39}N_2O_5$ 447.2853; Found 447.2846.

Dimethyl 2-(4-phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholin-3-yl)malonate (9j)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow liquid (64 mg, 71%, >20:1 dr). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21 (t, *J* = 8.0 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 6.77-6.73 (m, 1H), 4.93 (s, 1H), 4.84 (d, *J* = 10.8 Hz, 1H), 4.33-4.27 (m, 2H), 3.71 (s, 3H), 3.66-3.60 (m, 2H), 3.31-3.26 (m, 4H), 1.47-0.93 (m, 18H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 167.9, 167.3, 150.1, 129.0, 118.8, 116.0, 101.7, 60.5, 59.4, 58.8, 58.3, 52.6, 52.1, 51.4, 41.1, 40.8, 40.2, 34.0, 33.8, 20.6, 19.8, 17.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{37}N_2O_6$ 449.2646; Found 449.2634.

2-(4-(4-Chlorophenyl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholin-3-yl)-1-phenylbutane-1,3-dione (9k)

Eluent: petroleum ether/ethyl acetate (3:1). Yellow syrup (60 mg, 59%, >20:1 dr). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 7.6 Hz, 2H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 2H), 7.05 (d, *J* = 8.8 Hz, 2H), 6.72 (d, *J* = 8.8 Hz, 2H), 5.53 (d, *J* = 10.8 Hz, 1H), 4.99 (d, *J* = 10.4 Hz, 1H), 4.86 (s, 1H), 4.32-4.27 (m, 1H), 3.59-3.55 (m, 1H), 3.40-3.33 (m, 1H), 3.14-3.11 (m, 1H), 2.23 (s, 3H), 1.51-0.76 (m, 18H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 200.8, 193.8, 149.4, 137.1, 133.8, 129.1, 128.7, 128.6, 123.7, 117.3, 102.2, 61.6, 60.7, 60.5, 59.4, 57.7, 41.8, 40.8, 40.2, 33.8, 30.4, 27.0, 20.6, 19.5, 17.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{29}H_{38}ClN_2O_4$ 513.2515; Found 513.2516.

3-(Nitromethyl)-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)-4-(*p*-tolyl)morpholine (9l)

Eluent: petroleum ether/ethyl acetate (5:1). Yellow liquid (34 mg, 44%, >20:1 dr). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.11 (d, *J* = 8.4 Hz, 2H), 6.84 (d, *J* = 8.4 Hz, 2H), 5.07 (s, 1H), 4.72-4.70 (m, 2H),

4.47-4.42 (m, 1H), 4.31-4.28 (m, 1H), 3.76-3.71 (m, 1H), 3.21-3.16 (m, 2H), 2.28 (s, 3H), 1.50-1.14 (m, 18H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 146.2, 130.2, 115.9, 101.1, 72.7, 60.6, 59.5, 59.0, 57.6, 42.2, 40.6, 40.0, 33.8, 33.6, 20.8, 20.4, 20.2, 17.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{34}N_3O_4$ 392.2544; Found 392.2539.

3-(4-Methoxyphenyl)-4-phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholine (9m)

Eluent: petroleum ether/ethyl acetate (5:1). Yellow liquid (42 mg, 50%, >20:1 dr). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29 (d, *J* = 8.8 Hz, 2H), 7.23-7.17 (m, 2H), 6.80-6.75 (m, 5H), 5.29 (d, *J* = 2.4 Hz, 1H), 4.81 (d, *J* = 2.0 Hz, 1H), 4.20-4.16 (m, 1H), 3.96-3.93 (m, 1H), 3.75 (s, 3H), 3.43-3.40 (m, 2H), 1.51-1.44 (m, 5H), 1.32-1.27 (m, 4H), 1.11 (br s, 6H), 0.99 (br s, 3H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 158.7, 150.4, 131.2, 129.1, 128.8, 118.9, 115.9, 113.7, 105.2, 62.7, 61.6, 60.6, 59.4, 55.3, 44.4, 40.5, 40.1, 34.2, 33.8, 20.8, 20.1, 17.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{37}N_2O_3$ 425.2799; Found 425.2790.

3-Allyl-4-phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholine (9n)

Eluent: petroleum ether/ethyl acetate (5:1). Yellow solid (39 mg, 54%, >20:1 dr), mp 73-74 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28-7.23 (m, 2H), 6.85 (d, *J* = 8.0 Hz, 2H), 6.81-6.78 (m, 1H), 5.76-5.66 (m, 1H), 5.10-5.01 (m, 2H), 4.98 (s, 1H), 4.28-4.22 (m, 1H), 4.05-4.01 (m, 1H), 3.74-3.70 (m, 1H), 3.31-3.17 (m, 2H), 2.52-2.44 (m, 1H), 2.24-2.18 (m, 1H), 1.50-1.13 (m, 18H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$): δ 150.0, 135.0, 129.3, 118.6, 117.9, 115.1, 102.0, 60.4, 59.3, 59.2, 58.5, 41.3, 40.6, 40.1, 34.3, 33.9, 31.8, 20.8, 20.2, 17.1. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{35}N_2O_2$ 359.2693; Found 359.2689.

3-(2-((4-Methoxy-2,2,6,6-tetramethylpiperidin-1-yl)oxy)-4-phenylmorpholin-3-yl)pentane-2,4-dione (**9o**)

Eluent: petroleum ether/ethyl acetate (2:1). Yellow liquid (75 mg, 84%). ^{1}H NMR (400 MHz,

$CDCl_3$): δ 7.22 (t, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 6.78 (t, *J* = 7.2 Hz, 1H), 4.93 (d, *J* = 11.2 Hz, 1H), 4.68 (d, *J* = 10.8 Hz, 1H), 4.59 (s, 1H), 4.28-4.21 (m, 1H), 4.61-3.54 (m, 2H), 3.40-3.29 (m, 5H), 2.21 (s, 3H), 1.93 (s, 3H), 1.87-1.84 (m, 2H), 1.38-1.19 (m, 8H), 1.01 (s, 3H), 1.98 (s, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$): δ 201.9, 201.3, 150.0, 129.2, 119.2, 116.3, 101.8, 71.4, 69.2, 60.9, 59.6, 58.3, 57.8, 55.8, 45.5, 44.8, 41.7, 34.0, 33.9, 31.2, 27.4, 21.6, 20.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{39}N_2O_5$ 447.2853; Found 447.2852.

3-(4-Phenyl-2-((2,2,6,6-tetramethyl-4-oxopiperidin-1-yl)oxy)morpholin-3-yl)pentane-2,4-dione (**9p**)

Eluent: petroleum ether/ethyl acetate (2:1). Yellow solid (60 mg, 70%), mp 133-134 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 7.22 (t, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 7.6 Hz, 2H), 6.79 (t, *J* = 7.2 Hz, 1H), 4.96 (d, *J* = 10.8 Hz, 1H), 4.71 (s, 1H), 4.69 (d, *J* = 10.8 Hz, 1H), 4.26-4.23 (m, 1H), 3.64-3.56 (m, 2H), 3.40-3.36 (m, 1H), 2.61-2.53 (m, 2H), 2.24 (s, 3H), 2.19-2.12 (m, 2H), 1.97 (s, 3H), 1.40 (s, 3H), 1.29 (s, 3H), 1.01 (s, 3H), 0.95 (s, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$): δ 207.5, 201.9, 201.1, 149.9, 129.3, 119.5, 116.3, 102.2, 69.1, 63.6, 62.5, 58.2, 57.9, 54.1, 53.6, 41.7, 33.7, 33.5, 31.1, 27.6, 22.4, 21.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{35}N_2O_5$ 431.2540; Found 431.2521.

3-(2-((4-Hydroxy-2,2,6,6-tetramethylpiperidin-1-yl)oxy)-4-phenylmorpholin-3-yl)pentane-2,4-dione (**9q**)

Eluent: petroleum ether/ethyl acetate (1:1). Yellow liquid (67 mg, 77%). ^1H NMR (400 MHz, $CDCl_3$): δ 7.22 (t, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 6.78 (t, *J* = 7.2 Hz, 1H), 4.93 (d, *J* = 11.2 Hz, 1H), 4.68 (d, *J* = 10.8 Hz, 1H), 4.59 (s, 1H), 4.28-4.22 (m, 1H), 4.14-4.09 (m, 1H), 3.61-3.54 (m, 2H), 3.36-3.33 (m, 1H), 2.22 (s, 3H), 2.03 (s, 1H), 1.94 (s, 3H), 1.88-1.78 (m, 2H), 1.45-1.39 (m, 2H), 1.27 (s, 3H), 1.18 (s, 3H), 1.00 (s, 3H), 0.97 (s, 3H). $^{13}C\{^1H\}$ NMR (150 MHz,

$CDCl_3$): δ 202.0, 201.3, 149.9, 129.2, 119.3, 116.3, 101.8, 69.2, 62.8, 61.0, 59.7, 58.4, 57.7, 49.1, 48.4, 41.7, 33.9, 33.8, 31.2, 27.4, 21.5, 20.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{37}N_2O_5$ 433.2697; Found 433.2695.

6. Control Experiments

6.1. To a reaction tube equipped with a stir bar were added 1-(phenyl)piperidine (**1a**, 32 mg, 0.2 mmol), THF (1 mL), dimethyl malonate (**2a**, 46 μL, 0.4 mmol), $T^+BF_4^-$ (97 mg, 0.4 mmol), $CaCl_2$ (11 mg, 0.1 mmol), and BHT (44 mg, 0.4 mmol). The resulting mixture was then stirred at room temperature under air for 0.5 h. Upon completion, the mixture was diluted with ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (3:1) as the eluent to afford **3a** as yellow liquid in 34 mg (56%).

6.2. To a reaction tube equipped with a stir bar were added 4-phenylmorpholine (**8a**, 33 mg, 0.2 mmol), THF (1 mL), pentane-2,4-dione (**4a**, 41 μL, 0.4 mmol), $T^+BF_4^-$ (97 mg, 0.4 mmol), Na_2CO_3 (11 mg, 0.1 mmol), and BHT (44 mg, 0.4 mmol) The resulting mixture was then stirred at room temperature under air for 0.5 h. Upon completion, the mixture was diluted with ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (3:1) as the eluent to afford **9a** as white solid in 61 mg (73%).

6.3. To a reaction tube equipped with a stir bar were added 1-(phenyl)piperidine (**1a**, 32 mg, 0.2 mmol), THF (1 mL), dimethyl malonate (**2a**, 46 μL, 0.4 mmol), $T^+BF_4^-$ (97 mg, 0.4 mmol), and $CaCl_2$ (11 mg, 0.1 mmol). The resulting mixture was then stirred at room temperature under air for

5 min. Subsequent HRMS analysis of the mixture showed that 5-oxo-1-phenyl-2,3,4,5-tetrahydropyridin-1-ium (**i**, Calc'd, 174.0913, Found, 174.0913) was formed (Fig. S1).

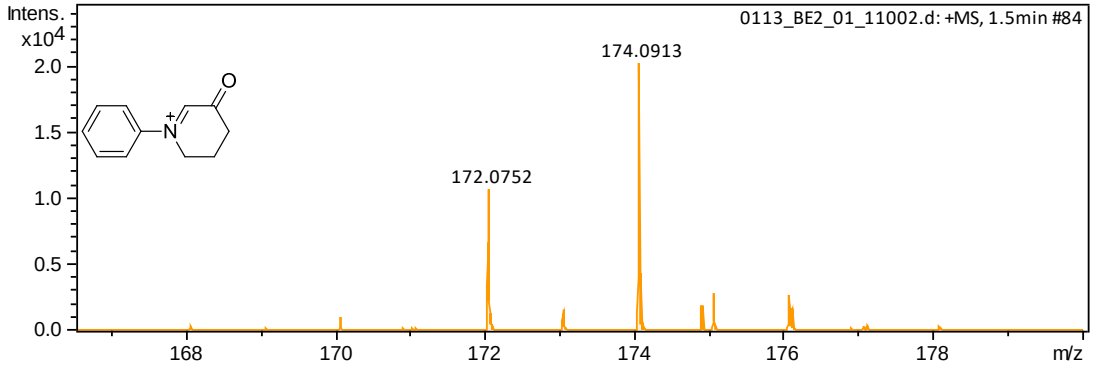


Fig. S1 Copy of HRMS Spectrum of the Reaction Mixture for the Formation of 3a

6.4. To a reaction tube equipped with a stir bar were added 4-phenylmorpholine (**8a**, 33 mg, 0.2 mmol), THF (1 mL), pentane-2,4-dione (**4a**, 41 μL, 0.4 mmol), $T^+BF_4^-$ (97 mg, 0.4 mmol), and Na_2CO_3 (11 mg, 0.1 mmol). The resulting mixture was then stirred at room temperature under air for 5 min. Subsequent HRMS analysis of the mixture showed that 6-oxo-4-phenyl-3,6-dihydro-2*H*-1,4-oxazin-4-ium was not formed, but 4-phenyl-6-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)-3,6-dihydro-2*H*-1,4-oxazin-4-ium (**ii**, Calc'd, 317.2224, Found, 317.2217) was formed (Fig. S2).

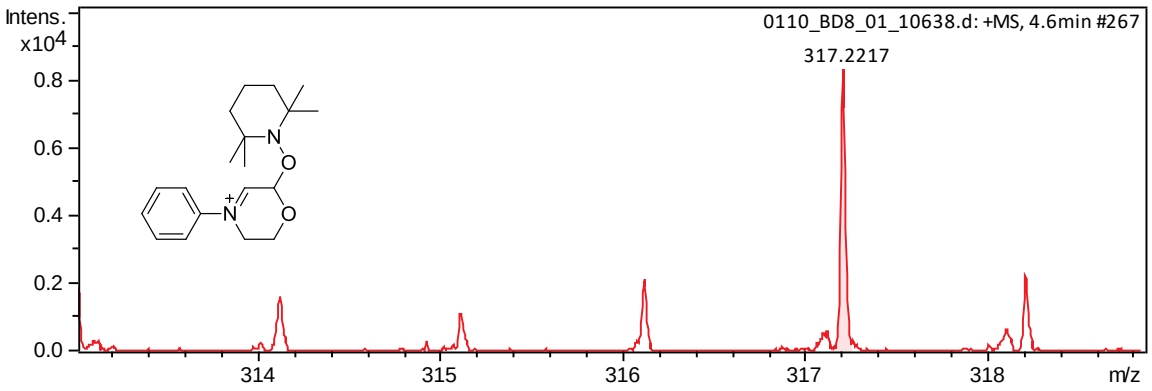
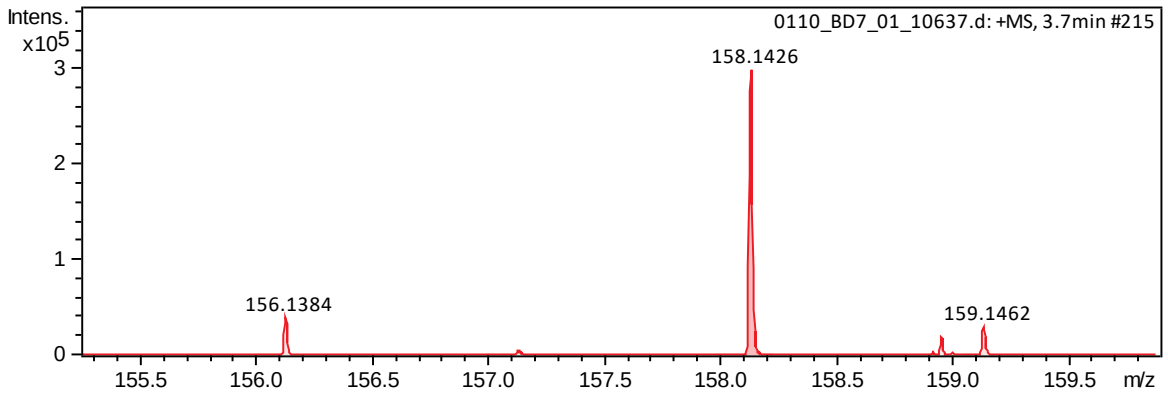


Fig. S2 Copy of HRMS Spectrum of the Reaction Mixture for the Formation of 9a

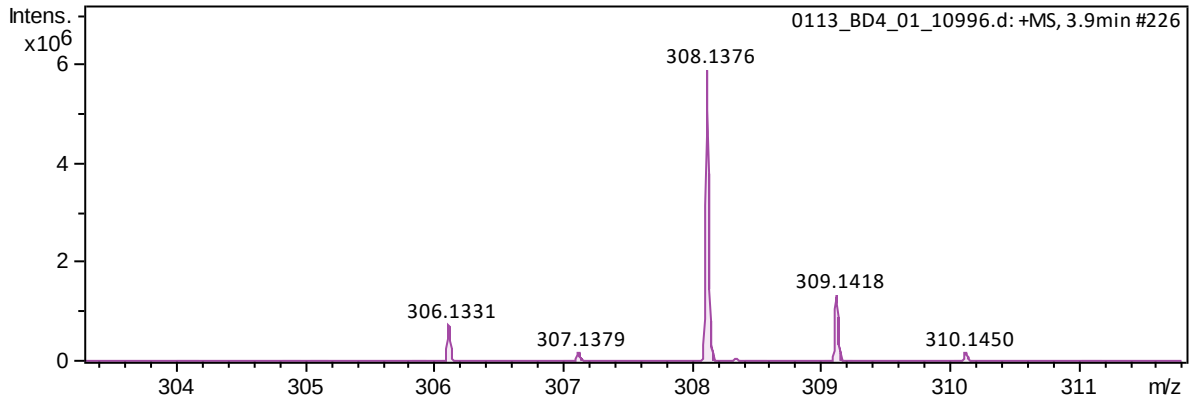
6.5. To a reaction tube equipped with a stir bar were added 1-(phenyl)piperidine (**1a**, 32 mg, 0.2

mmol), THF (1 mL), dimethyl malonate (**2a**, 46 μL, 0.4 mmol), TEMP$^{18}O^{+}BF_4^{-}$ (98 mg, 0.4 mmol, 88%) (Fig. S3), and $CaCl_2$ (11 mg, 0.1 mmol). The resulting mixture was then stirred at room temperature under air for 0.5 h. Subsequent HRMS analysis of the mixture showed that [^{18}O]-**3a** and [^{16}O]-**3a** were formed in a ratio of 7.9:1 (Fig. S4). Meanwhile, the mixture was diluted with ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (3:1) as the eluent to afford [^{18}O]-**3a** in 33 mg (54%).



m/z	Res.	S/N	I	I%	FWHM
156.1384	10866	298.9	38763	9.9	0.0144
158.1426	10576	2263.5	295842	75.8	0.0150

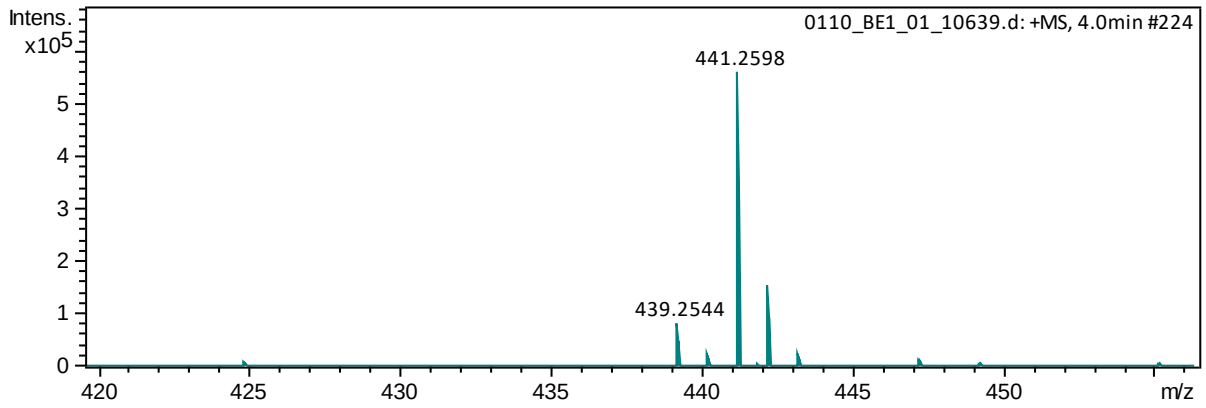
Fig. S3 Copy of HRMS Spectrum of the Mixture of TEMPO^{+}/TEMP$^{18}O^{+}$



m/z	Res.	S/N	I	I%	FWHM
306.1331	11747	5686.4	5686.4	12.6	0.0261
308.1376	11585	44718.9	44718.9	100	0.0266

Fig. S4 Copy of HRMS Spectrum of the Mixture of [^{16}O]-3a/[^{18}O]-3a

6.6. To a reaction tube equipped with a stir bar were added 4-phenylmorpholine (**8a**, 33 mg, 0.2 mmol), THF (1 mL), pentane-2,4-dione (**4a**, 41 μL, 0.4 mmol), TEMP$^{18}O^{+}BF_4^{-}$ (98 mg, 0.4 mmol, 88%) (Fig. S2), and Na_2CO_3 (11 mg, 0.1 mmol). The resulting mixture was then stirred at room temperature under air for 0.5 h. Subsequent HRMS analysis of the mixture showed that [^{18}O]-**9a** and [^{16}O]-**9a** were formed in a ratio of 7:1 (Fig. S5). Meanwhile, the mixture was diluted with ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (3:1) as the eluent to afford [^{18}O]-**9a** in 59 mg (71%).

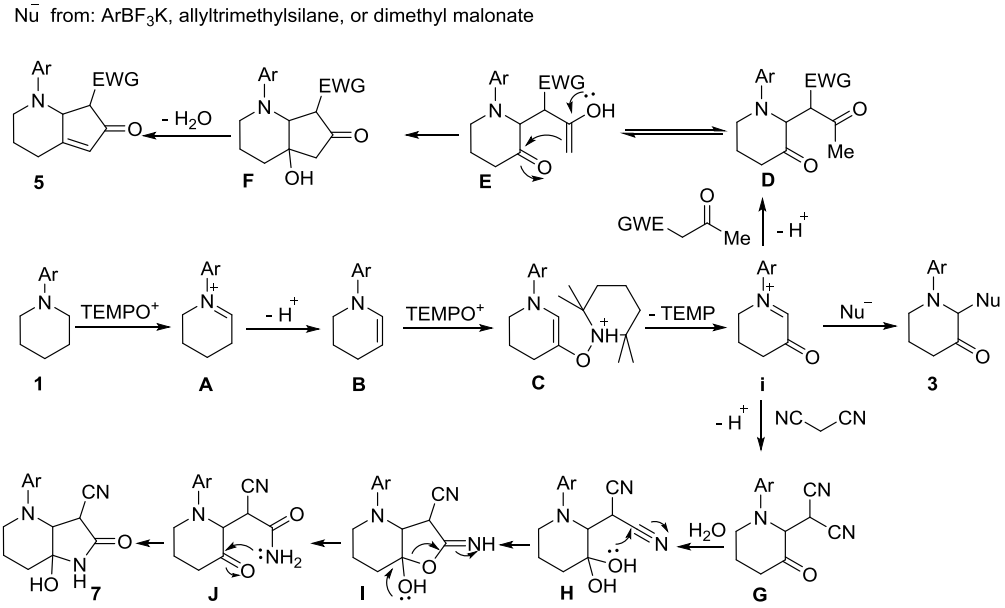


m/z	Res.	S/N	I	I%	FWHM
439.2544	11511	568.3	81864	0.9	0.0382
441.2598	12057	3867.8	556272	6.3	0.0366

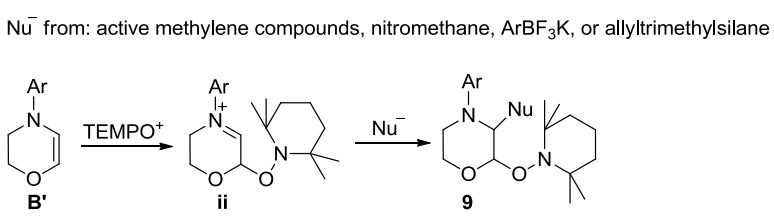
Fig. S5 Copy of HRMS Spectrum of the Mixture of [^{16}O]-9a/[^{18}O]-9a

7. Possible mechanisms.

7.1 Possible mechanisms for the synthesis of 3, 5 and 7[3].



7.2 Possible mechanism for the synthesis of 9.



8. Synthetic and pharmaceutical application.

8.1. To a reaction tube equipped with a stir bar were added 2-(4-methoxyphenyl)-1-phenylpiperidin-3-one (**3n**, 28 mg, 0.1 mmol), EtOAc (2 mL), and ^{t}BuONO (26 μL, 0.2 mmol, 90%). The resulting mixture was then stirred at rt for 12 h. Then the mixture was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (5:1) as the eluent to afford **10** as yellow liquid in 21 mg (64%).

***N*-(5-(4-Methoxyphenyl)-4,5-dioxopentyl)-*N*-phenylnitrous amide (10)**

Eluent: petroleum ether/ethyl acetate (5:1). Yellow liquid (21 mg, 64%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (dd, J_1 = 6.8 Hz, J_2 = 2.0 Hz, 2H), 7.61 (dd, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 2H), 7.51-7.47 (m, 2H), 7.39-7.35 (m, 1H), 6.97 (dd, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 2H), 4.16-4.12 (m, 2H), 3.89 (s, 3H), 2.88 (t, J = 6.8 Hz, 2H), 1.99-1.96 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 202.1, 190.1, 165.0, 141.4, 132.9, 129.7, 127.5, 124.7, 119.4, 114.3, 55.6, 42.6, 35.6, 20.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}N_2O_4$ 327.1339; Found 327.1341.

8.2. To a reaction tube equipped with a stir bar were added 3-(4-methoxyphenyl)-4-phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)morpholine (**9m**, 64 mg, 0.15 mmol), THF (2 mL), H_2O (3 mL), AcOH (2 mL), and Zn (96 mg, 1.5 mmol). The resulting mixture was then stirred at rt for 1 h. Next, Zn (96 mg, 1.5 mmol) was added to the mixture and the resulting mixture stirred at 70 ^{o}C for another 2 h. Then, the mixture was diluted with ethyl acetate and aqueous NaOH (4M). The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (2:1) as the eluent to afford **11** as yellow liquid in 24 mg (56%).

3-(4-Methoxyphenyl)-4-phenylmorpholin-2-ol (11)

Eluent: petroleum ether/ethyl acetate (2:1). Yellow liquid (24 mg, 56%, mixture of diastereomers). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25-7.15 (m, 4H), 6.90-6.87 (m, 3H), 6.76-6.74 (m, 2H), 5.20-5.14 (m, 1H), 4.35-4.34 (m, 1H), 4.20-3.88 (m, 2H), 3.72 (s, 3H), 3.42-3.07 (m, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 158.9, 150.5, 130.7, 129.8, 129.0, 121.5, 120.1, 119.4, 113.8, 113.5, 95.3, 65.8, 61.7, 55.1, 47.6. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{20}NO_3$ 286.1438; Found 286.1438.

8.3. To a reaction tube equipped with a stir bar were added 1,2-diphenylpiperidin-3-one (**3m**, 50 mg, 0.2 mmol), MeOH (2 mL), and $NaBH_4$ (11 mg, 0.3 mmol). The resulting mixture was then stirred at 0 ^{o}C for 20 min. Then the mixture was quenched by aqueous NH_4Cl and diluted by ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (2:1) as the eluent to afford **12** as yellow liquid in 46 mg (90%).

1,2-Diphenylpiperidin-3-ol (12)

Eluent: petroleum ether/ethyl acetate (2:1). Yellow liquid (46 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.25 (m, 2H), 7.21-7.17 (m, 2H), 7.14-7.08 (m, 3H), 6.93-6.91 (m, 2H), 6.84-6.81 (m, 1H), 4.34 (d, *J* = 2.8 Hz, 1H), 4.01-3.97 (m, 1H), 3.53-3.47 (m, 1H), 3.00-2.93 (m, 1H), 2.23-2.14 (m, 1H), 2.06-2.00 (m, 2H), 2.00-1.66 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 152.0, 140.3, 128.7, 128.35, 128.29, 126.9, 122.1, 121.9, 70.2, 67.3, 55.4, 30.3, 21.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{20}NO$ 254.1539; Found 254.1537.

8.4. To a reaction tube equipped with a stir bar were added 1,2-diphenylpiperidin-2-ol (**12**, 25 mg, 0.1 mmol), DMF (0.5 mL), and NaH (12 mg, 0.3 mmol, 60% susp.) at 0 ^{o}C. The resulting mixture was then warmed to room temperature and stirred for additional 1 h. To the mixture was added

3,5-bis(trifluoromethyl)benzyl bromide (92 mg, 0.3 mmol). After completion of the addition, the reaction mixture was heated to 70 ^{o}C and stirred for additional 0.5 h. The resulting solution was cooled to room temperature, quenched by H_2O and diluted by ethyl acetate. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (2:1) as the eluent to afford **13** as yellow liquid in 42 mg (88%).

3-((3,5-Bis(trifluoromethyl)benzyl)oxy)-1,2-diphenylpiperidine (13)

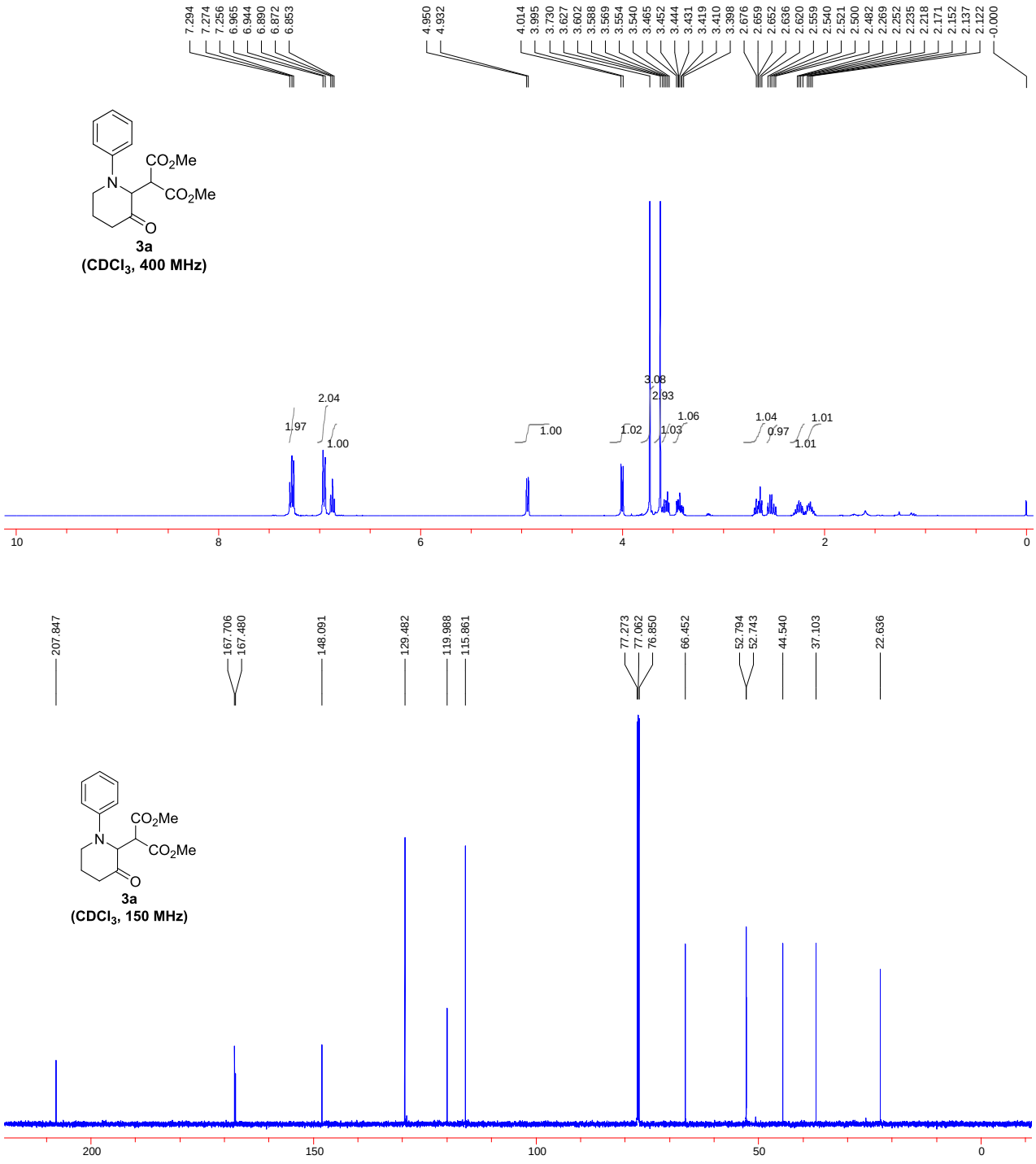
Eluent: petroleum ether/ethyl acetate (2:1). Yellow liquid (42 mg, 88%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (s, 1H), 7.57 (s, 2H), 7.42 (d, *J* = 7.2 Hz, 2H), 7.24-7.12 (m, 5H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.79-6.76 (m, 1H), 4.75-4.72 (m, 1H), 4.58 (d, *J* = 14.4 Hz, 1H), 4.36 (d, *J* = 14.4 Hz, 1H), 3.91-3.88 (m, 1H), 3.48-3.43 (m, 1H), 3.25-3.20 (m, 1H), 2.11-2.03 (m, 2H), 1.87-1.76 (m, 2H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 151.4, 141.1, 139.9, 131.4 (q, $^{2}J_{C\text{-}F}$ = 32.7 Hz), 128.9, 128.6, 128.0, 127.4, 126.9, 123.3 (q, $^{1}J_{C\text{-}F}$ = 271.2 Hz), 121.3 (q, $^{4}J_{C\text{-}F}$ = 3.3 Hz), 120.1, 118.8, 78.7, 70.7, 64.1, 50.0, 26.5, 21.8. ^{19}F{^{1}H} NMR ($CDCl_3$, 376 MHz):δ - 62.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{24}F_6NO$ 480.1757; Found 480.1752.

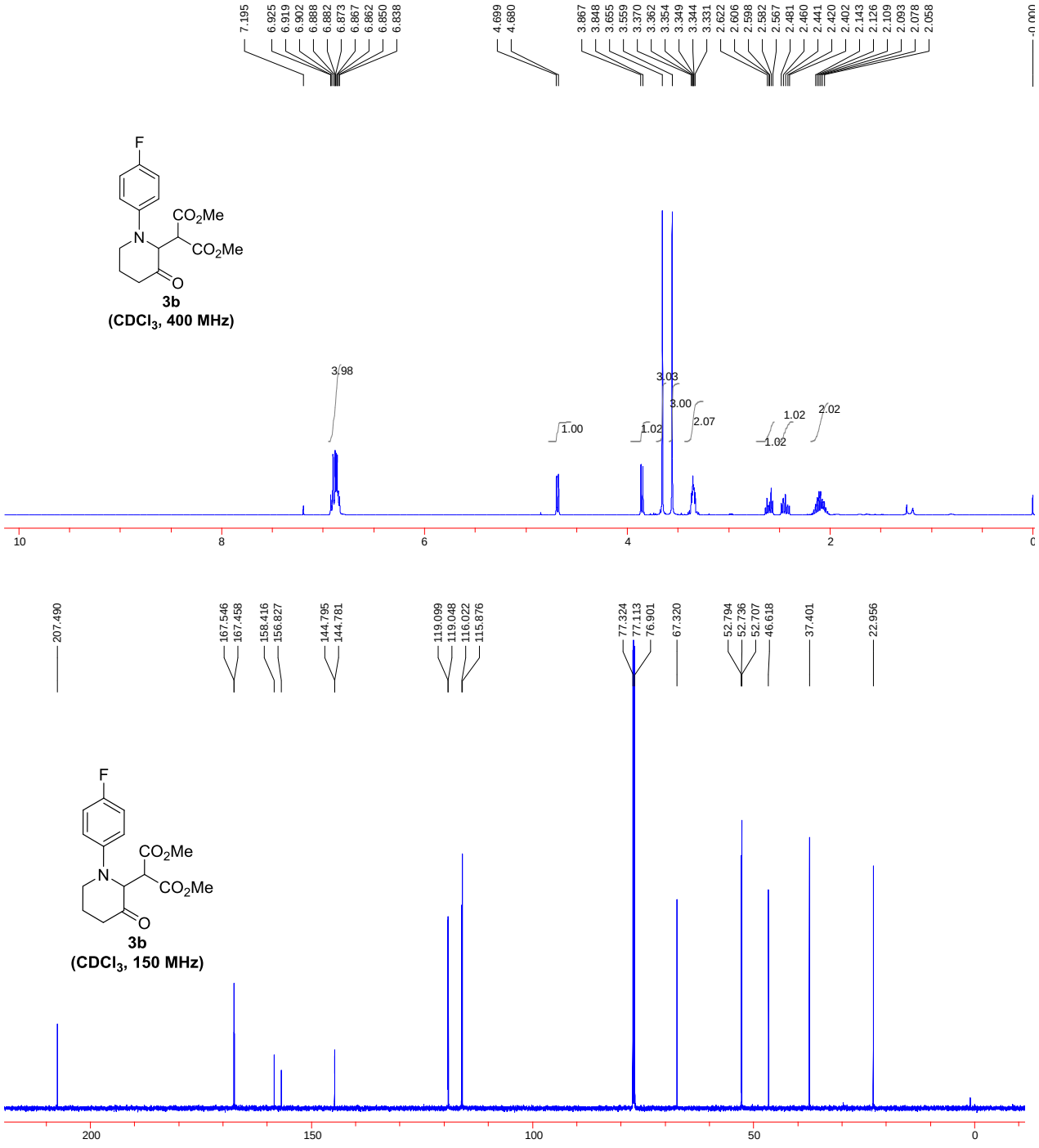
8.5. To a reaction tube equipped with a stir bar were added 1-(phenyl)piperidine (**1a**, 32 mg, 0.2 mmol), THF (1 mL), ethyl 3-oxo-4-(4-oxoquinazolin-3(4*H*)-yl)butanoate (**14**, 82 mg, 0.3 mmol), $T^+BF_4^-$ (97 mg, 0.4 mmol), and $CaCl_2$ (11 mg, 0.1 mmol). The resulting mixture was then stirred at room temperature under air for 0.5 h. Upon completion, the mixture was diluted with ethyl acetate and aqueous NaCl. The organic layer was dried over anhydrous Na_2SO_4 and filtered. Then, the solvent was evaporated under vacuum and the crude product was purified by column chromatography on silica-gel with petroleum ether/ethyl acetate (1:1) as the eluent to afford **15** as white solid in 45 mg (51%).

Ethyl 3-oxo-2-(3-oxo-1-phenylpiperidin-2-ylidene)-4-(4-oxoquinazolin-3(4*H*)-yl)butanoate (15)

Eluent: petroleum ether/ethyl acetate (1:1). White solid (45 mg, 51%), mp 124-125 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 8.04 (s, 1H), 7.80-7.72 (m, 2H), 7.54-7.50 (m, 1H), 7.18-7.14 (m, 2H), 6.83 (t, *J* = 7.6 Hz, 1H), 6.49 (d, *J* = 8.0 Hz, 2H), 5.65 (d, *J* = 17.6 Hz, 1H), 5.48 (d, *J* = 17.6 Hz, 1H), 4.41-4.33 (m, 2H), 3.78-3.74 (m, 1H), 3.52-3.48 (m, 1H), 2.34-2.20 (m, 2H), 2.08-2.04 (m, 2H), 1.39 (t, *J* = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 193.4, 187.9, 162.6, 160.9, 148.1, 146.1, 142.3, 134.8, 129.3, 127.7, 126.8, 121.8, 120.6, 115.1, 110.8, 109.3, 61.1, 51.4, 46.5, 41.2, 22.1, 14.3. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{24}N_3O_5$ 446.1710; Found 446.1707.

III. Copies of the NMR Spectra of 3a-3q

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6.882
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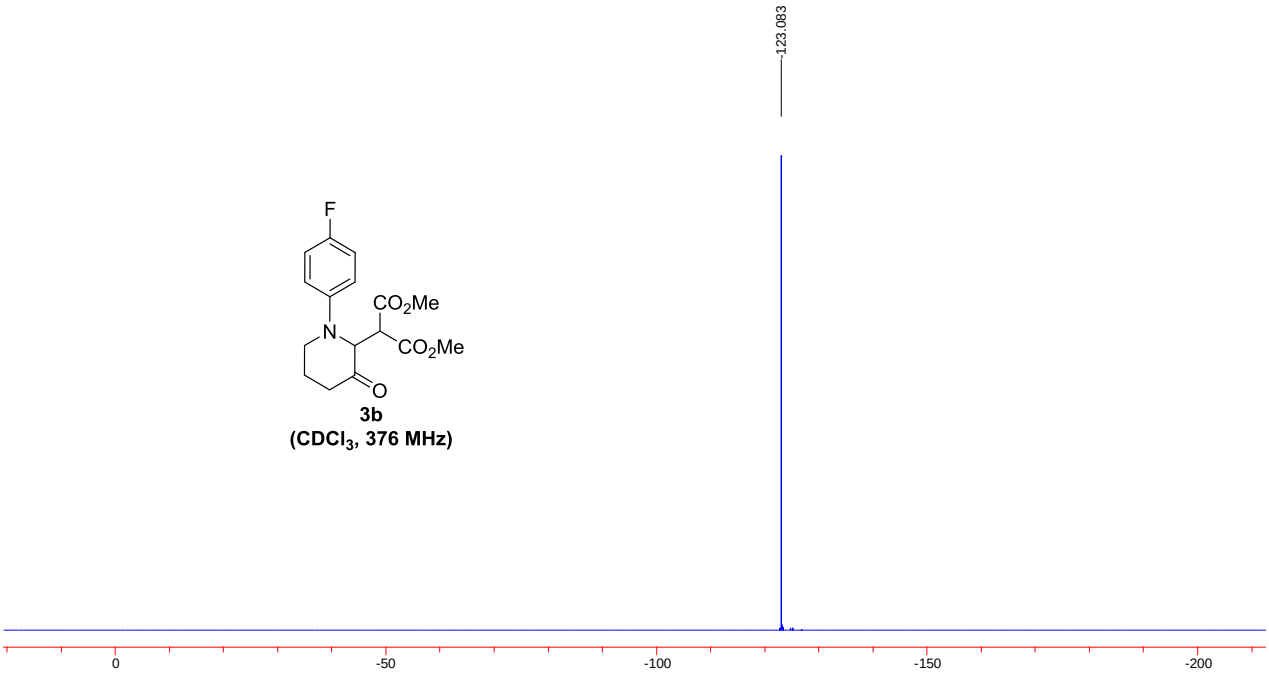
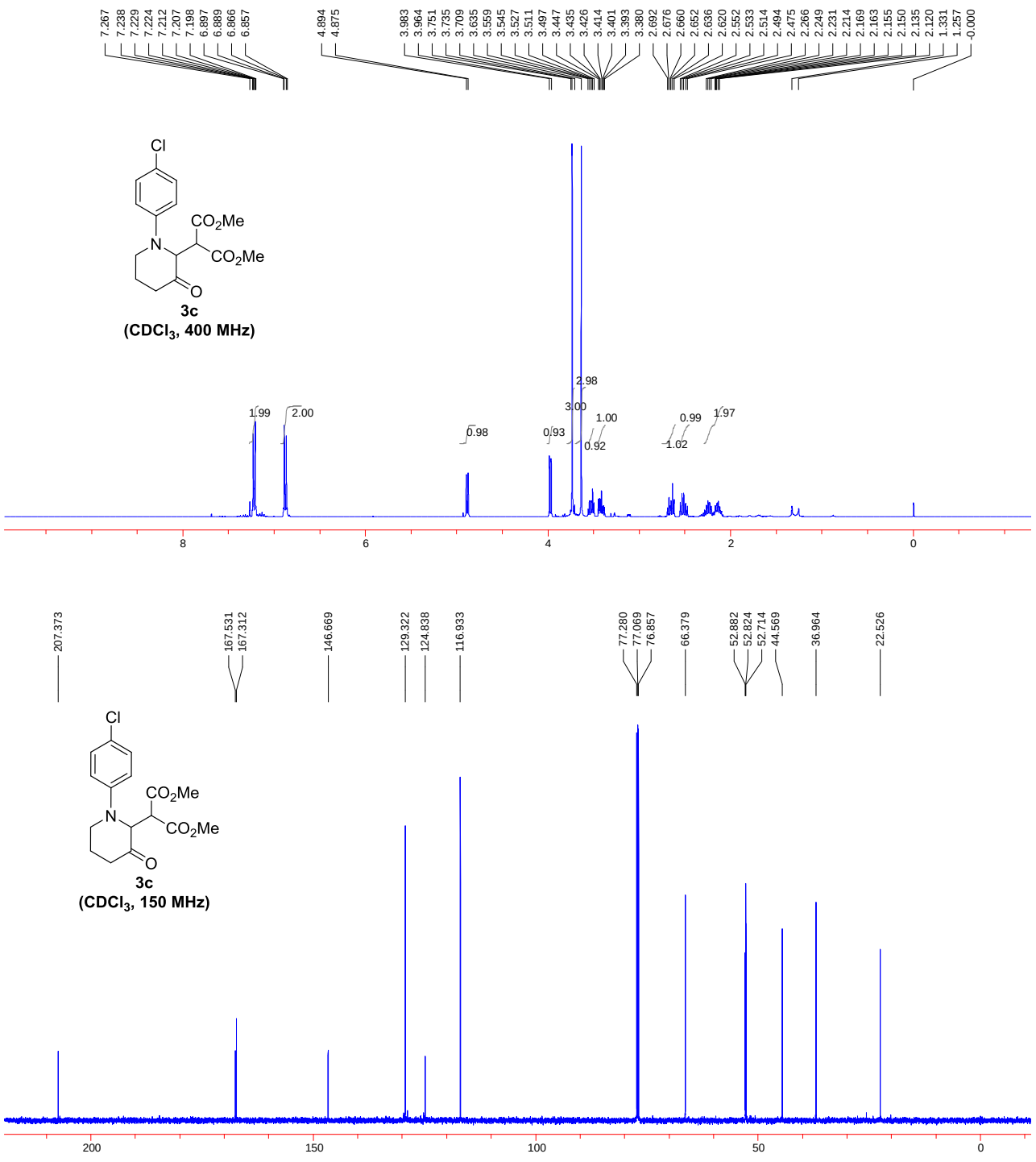
6.867
6.862
6.850
6.838
4.699
4.680
3.867
3.848
3.655
3.559
3.370
3.362
3.354
3.349
3.344
3.331
2.622
2.606
2.598
2.582
2.567
2.481
2.460
2.441
2.420
2.402
2.143
2.126
2.109
2.093
2.078
2.058
F
CO2Me
CO2Me
N
O
3b
(CDCl3, 400 MHz)
3.98
1.00
3.03
3.00
1.02
2.07
1.02
1.02
2.02
10
8
6
4
2
0
207.490
167.546
167.458
158.416
156.827
144.795
144.781
119.099
119.048
116.022
115.876
77.324
77.113
76.901
67.320
52.794
52.736
52.707
46.618
37.401
22.956
F
CO2Me
CO2Me
N
O
3b
(CDCl3, 150 MHz)
200
150
100
50
0



3b
($CDCl_3$, 376 MHz)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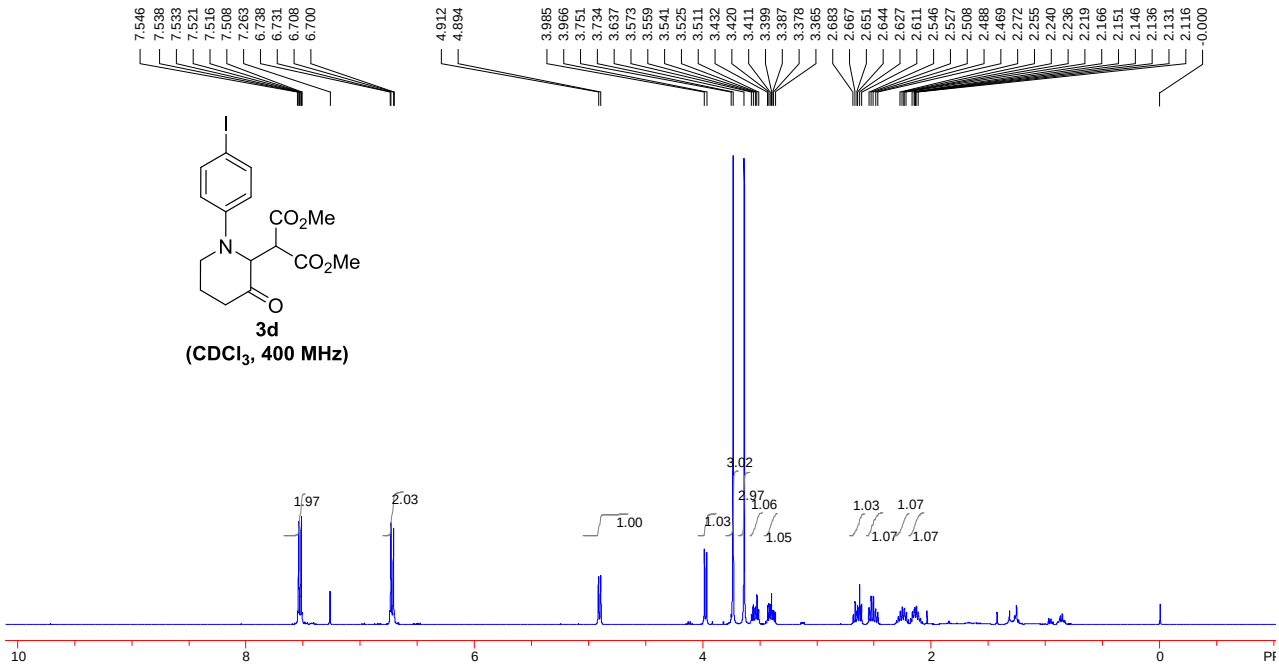
7.238
7.229
7.224
7.212
7.207
7.198
6.897
6.889
6.866
6.857
4.894
4.875
3.983
3.964
3.751
3.735
3.709
3.635
3.559
3.545
3.527
3.511
3.497
3.447
3.435
3.426
3.414
3.401
3.393
3.380
2.692
2.676
2.660
2.652
2.636
2.620
2.552
2.533
2.514
2.494
2.475
2.266
2.249
2.231
2.214
2.169
2.163
2.155
2.150
2.135
2.120
1.331
1.257
-0.000
Cl
CO2Me
N
CO2Me
O
3c
(CDCl3, 400 MHz)
1.99
2.00
0.98
0.93
2.98
3.00
1.00
0.92
0.99
1.02
1.97
8
6
4
2
0
207.373
167.531
167.312
146.669
129.322
124.838
116.933
77.280
77.069
76.857
66.379
52.882
52.824
52.714
44.569
36.964
22.526
Cl
CO2Me
N
CO2Me
O
3c
(CDCl3, 150 MHz)
200
150
100
50
0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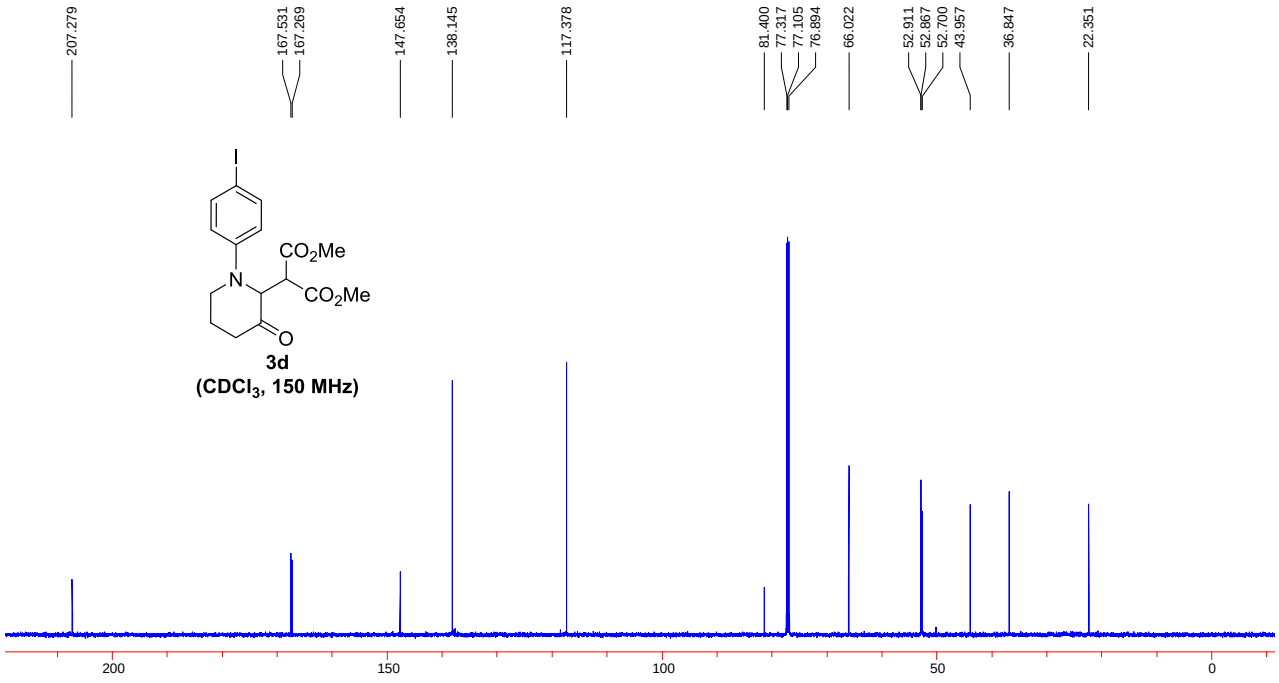
7.516
7.508
7.263
6.738
6.731
6.708
6.700
4.912
4.894
3.985
3.966
3.751
3.734
3.637
3.573
3.559
3.541
3.525
3.511
3.432
3.420
3.411
3.399
3.387
3.378
3.365
2.683
2.667
2.651
2.644
2.627
2.611
2.546
2.527
2.508
2.488
2.469
2.272
2.255
2.240
2.236
2.219
2.166
2.151
2.146
2.136
2.131
2.116
-0.000
I
CO2Me
N
CO2Me
O
3d
(CDCl3, 400 MHz)
1.97
2.03
1.00
1.03
3.02
2.97
1.06
1.05
1.03
1.07
1.07
1.07
10
8
6
4
2
0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167.269
147.654
138.145
117.378
81.400
77.317
77.105
76.894
66.022
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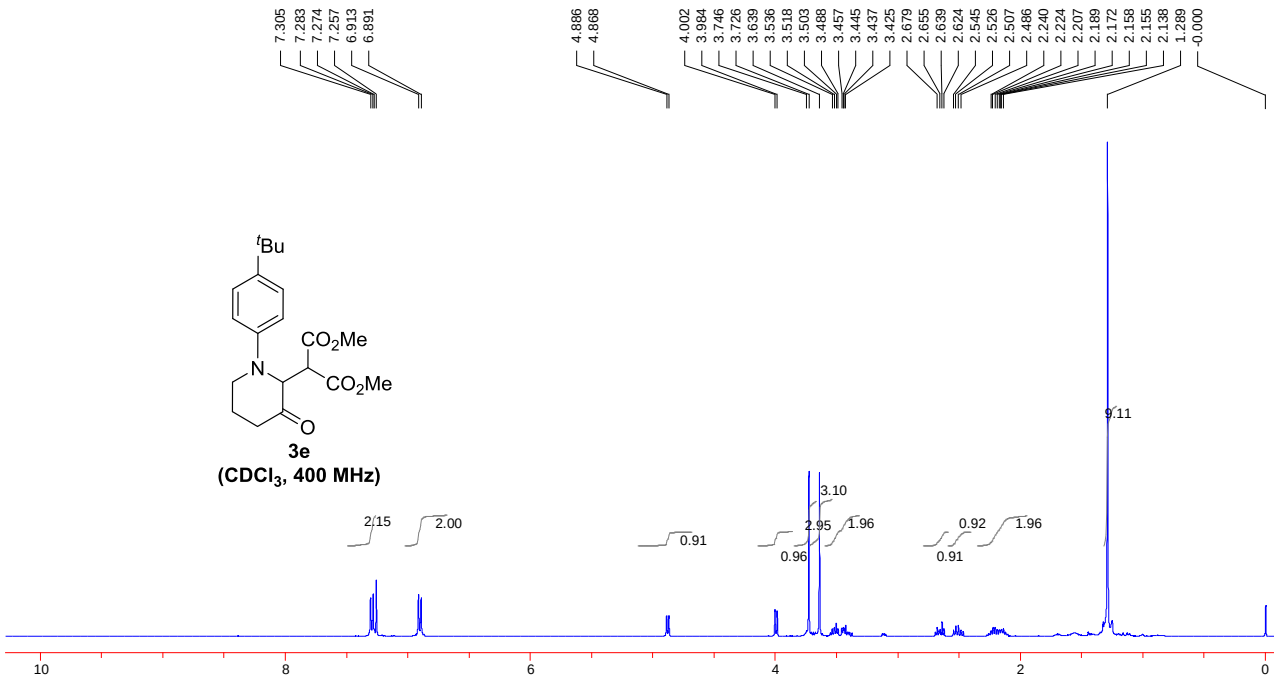
52.867
52.700
43.957
36.847
22.351
I
CO2Me
N
CO2Me
O
3d
(CDCl3, 150 MHz)
200
150
100
50
0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7.274
7.257
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6.891
4.886
4.868
4.002
3.984
3.746
3.726
3.639
3.536
3.518
3.503
3.488
3.457
3.445
3.437
3.425
2.679
2.655
2.639
2.624
2.545
2.526
2.507
2.486
2.240
2.224
2.207
2.189
2.172
2.158
2.155
2.138
1.289
-0.000
tBu
CO2Me
CO2Me
N
O
3e
(CDCl3, 400 MHz)
9.11
3.10
2.15
2.00
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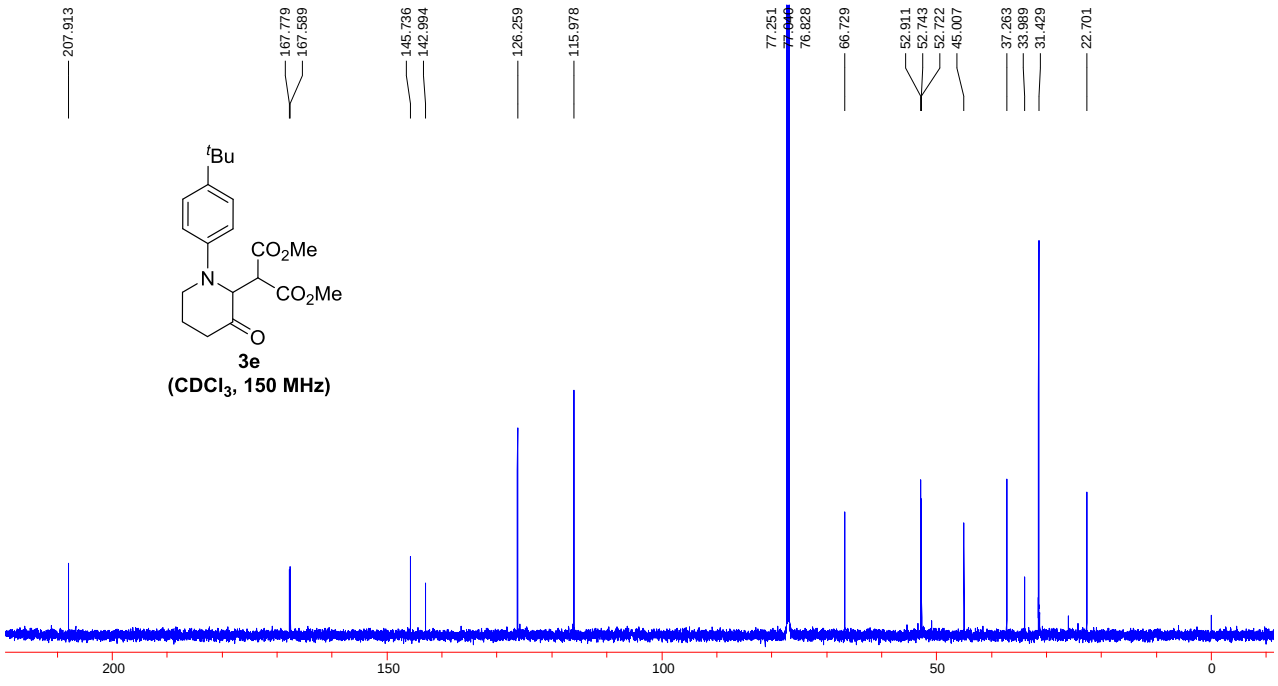
2.95
1.96
0.96
0.92
1.96
0.91
10
8
6
4
2
0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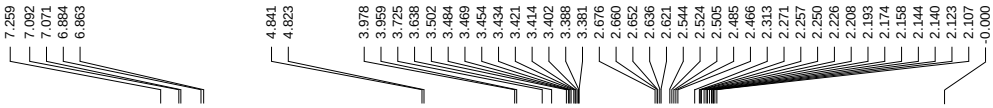
167.589
145.736
142.994
126.259
115.978
77.251
77.040
76.828
66.729
52.911
52.743
52.722
45.007
37.263
33.989
31.429
22.701
tBu
CO2Me
CO2Me
N
O
3e
(CDCl3, 150 MHz)
200
150
100
50
0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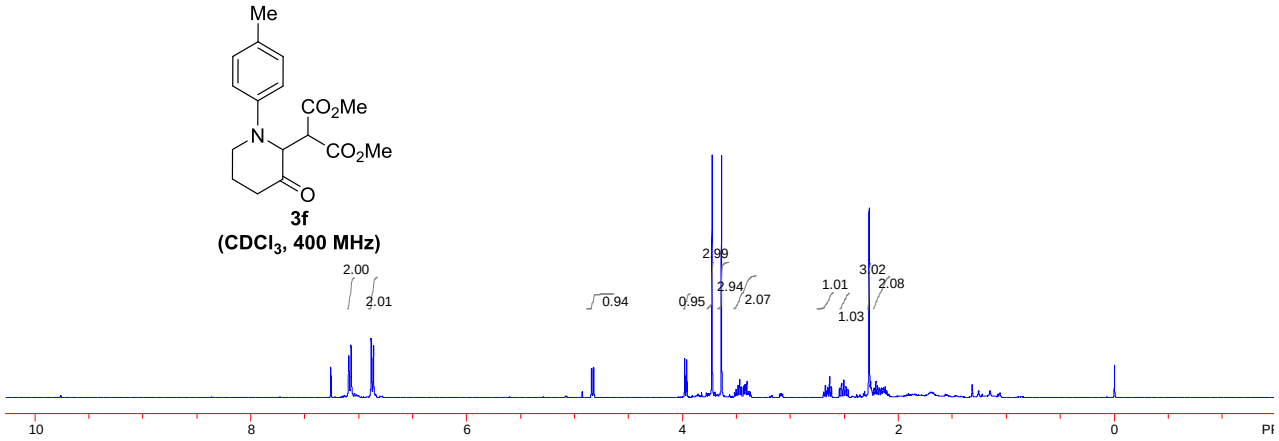
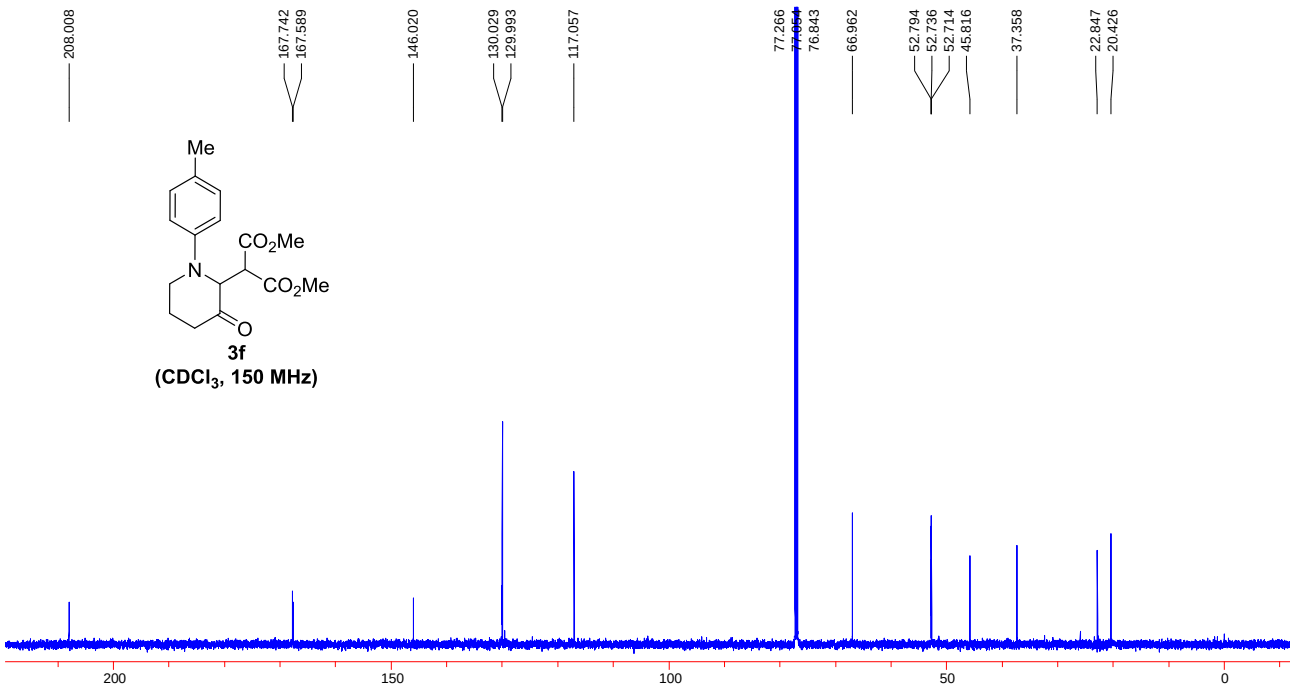
7.092
7.071
6.884
6.863
4.841
4.823
3.978
3.959
3.725
3.638
3.502
3.484
3.469
3.454
3.434
3.421
3.414
3.402
3.388
3.381
2.676
2.660
2.652
2.636
2.621
2.544
2.524
2.505
2.485
2.466
2.313
2.271
2.257
2.250
2.226
2.208
2.193
2.174
2.158
2.144
2.140
2.123
2.107
-0.000


Me
CO2Me
CO2Me
N
O
3f
(CDCl3, 400 MHz)
2.00
2.01
0.94
2.99
0.95
2.94
2.07
1.01
1.03
3.02
2.08
10
8
6
4
2
0
Pf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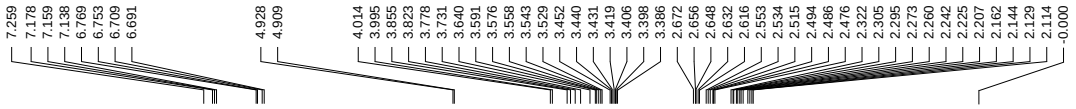
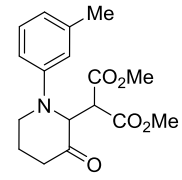
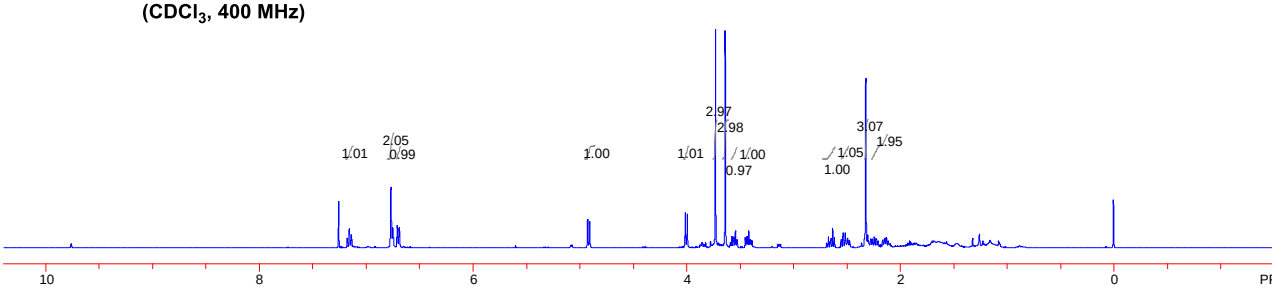
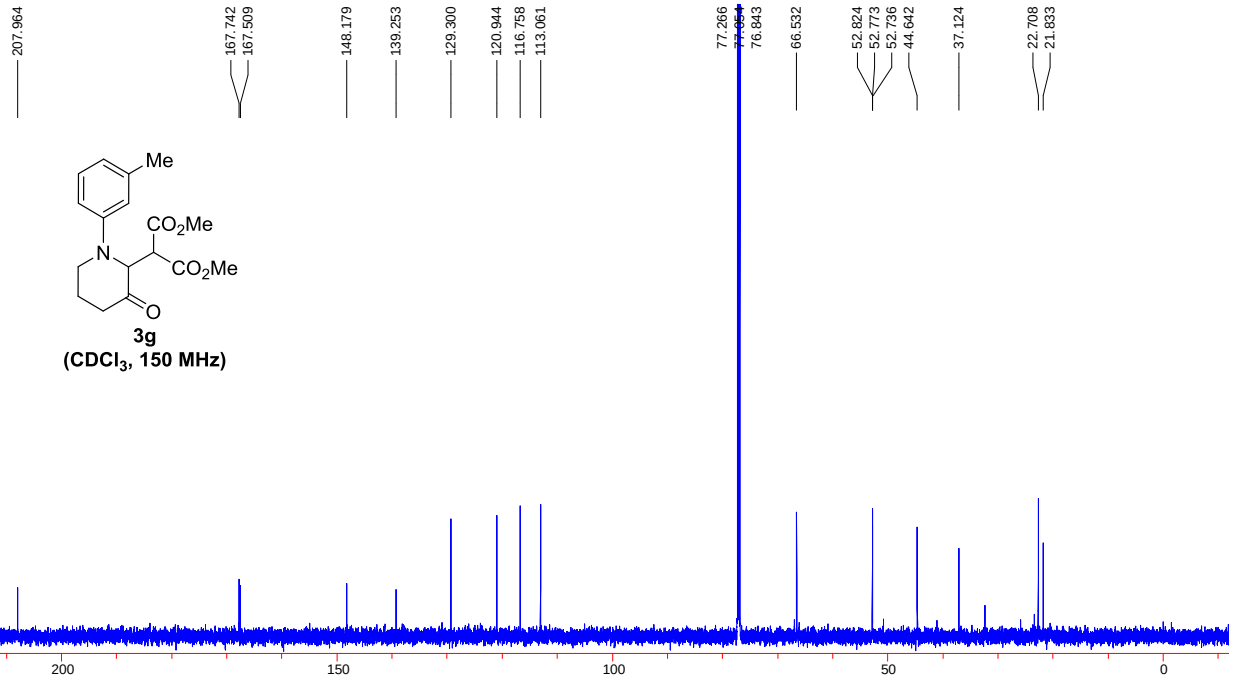
167.589
146.020
130.029
129.993
117.057
77.266
77.054
76.843
66.962
52.794
52.736
52.714
45.816
37.358
22.847
20.426
Me
CO2Me
CO2Me
N
O
3f
(CDCl3, 150 MHz)
200
150
100
50
0



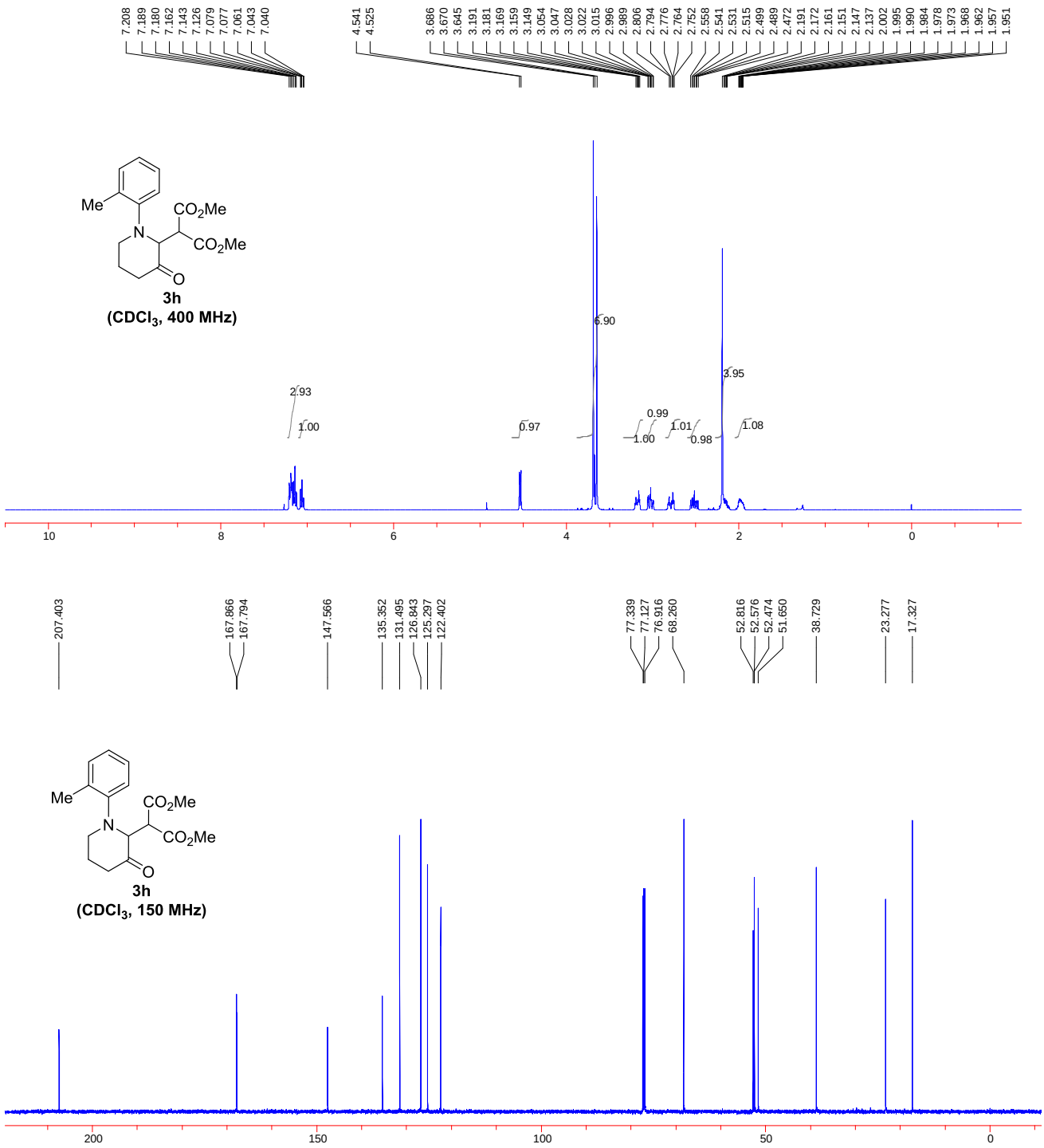


3g
($CDCl_3$, 400 MHz)





3g
($CDCl_3$, 150 MHz)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7.126
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7.077
7.061
7.043
7.040
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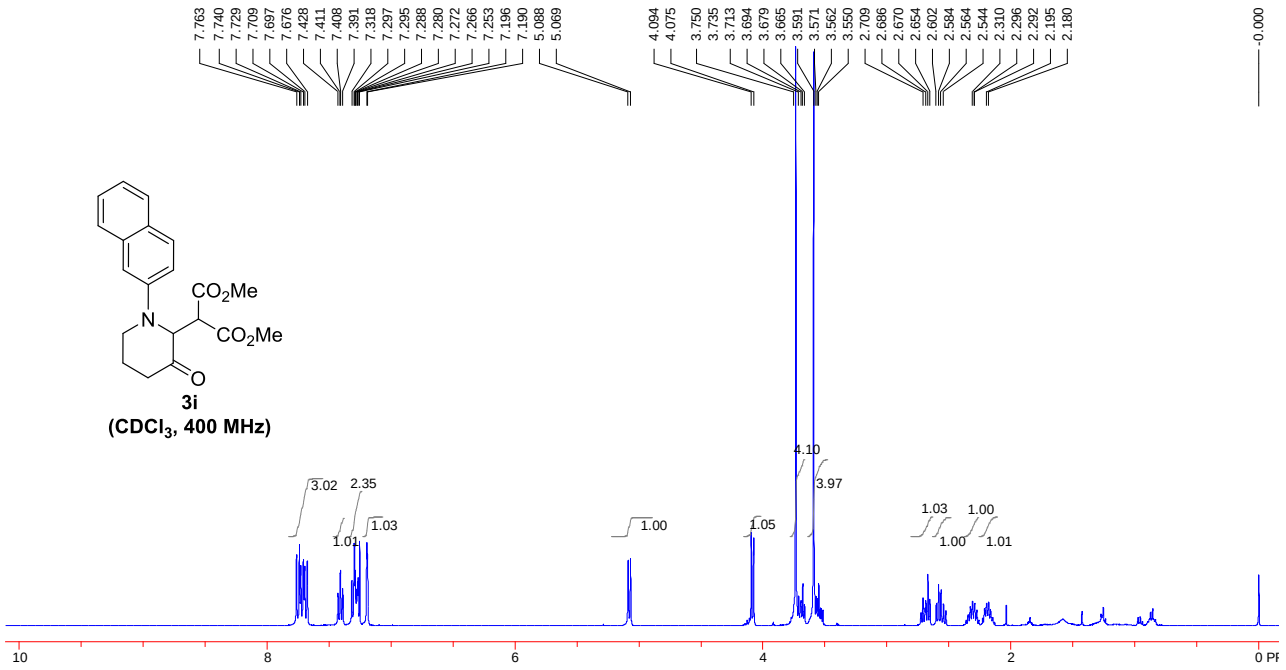
4.525
3.686
3.670
3.645
3.191
3.181
3.169
3.159
3.149
3.054
3.047
3.028
3.022
3.015
2.996
2.989
2.806
2.794
2.776
2.764
2.752
2.558
2.541
2.531
2.515
2.499
2.489
2.472
2.191
2.172
2.161
2.151
2.147
2.137
2.002
1.995
1.990
1.984
1.978
1.973
1.968
1.962
1.957
1.951
Me
CO2Me
CO2Me
N
O
3h
(CDCl3, 400 MHz)
6.90
3.95
2.93
1.00
0.97
0.99
1.00
1.01
0.98
1.08
10
8
6
4
2
0
207.403
167.866
167.794
147.566
135.352
131.495
126.843
125.297
122.402
77.339
77.127
76.916
68.260
52.816
52.576
52.474
51.650
38.729
23.277
17.327
Me
CO2Me
CO2Me
N
O
3h
(CDCl3, 150 MHz)
200
150
100
50
0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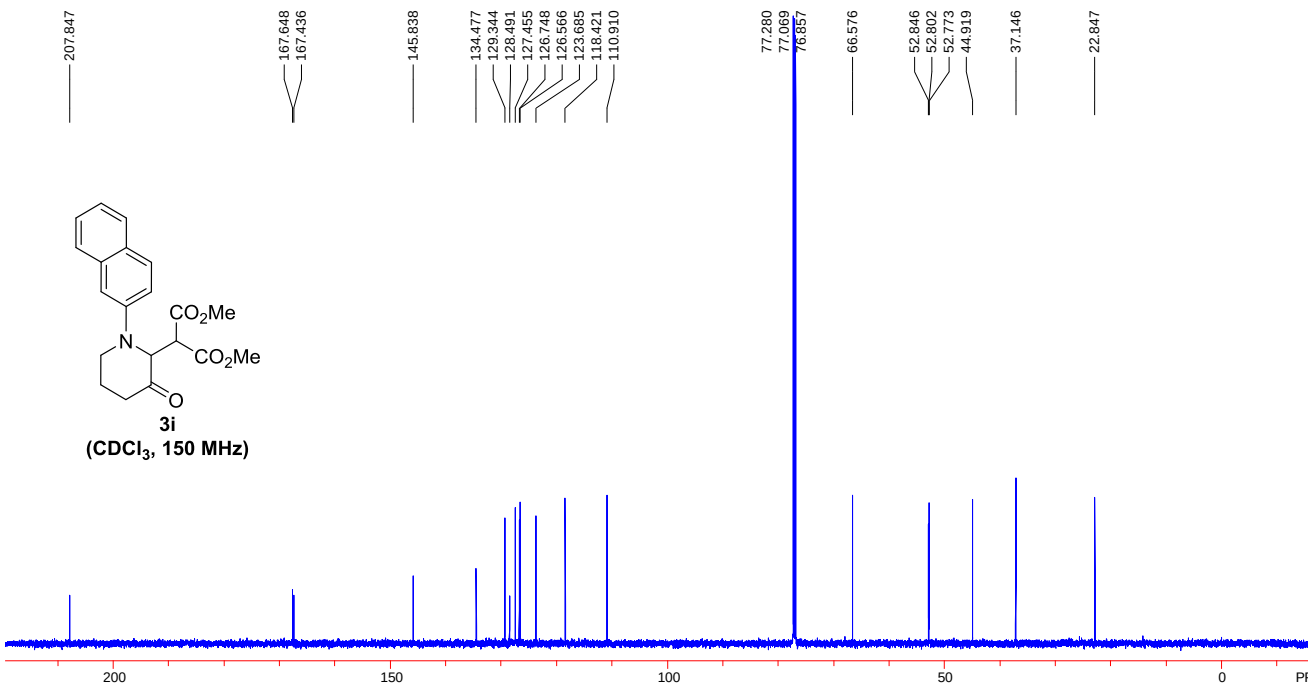
4.094 4.075 3.750 3.735 3.713 3.694 3.679 3.665 3.591 3.571 3.562 3.550 2.709 2.686 2.670 2.654 2.602 2.584 2.564 2.544 2.310 2.296 2.292 2.195 2.180
-0.000
CO2Me
CO2Me
N
O
3i
(CDCl3, 400 MHz)
3.02 2.35 1.03 1.01 1.00 1.05 4.10 3.97 1.03 1.00 1.00 1.01
10 8 6 4 2 0 PI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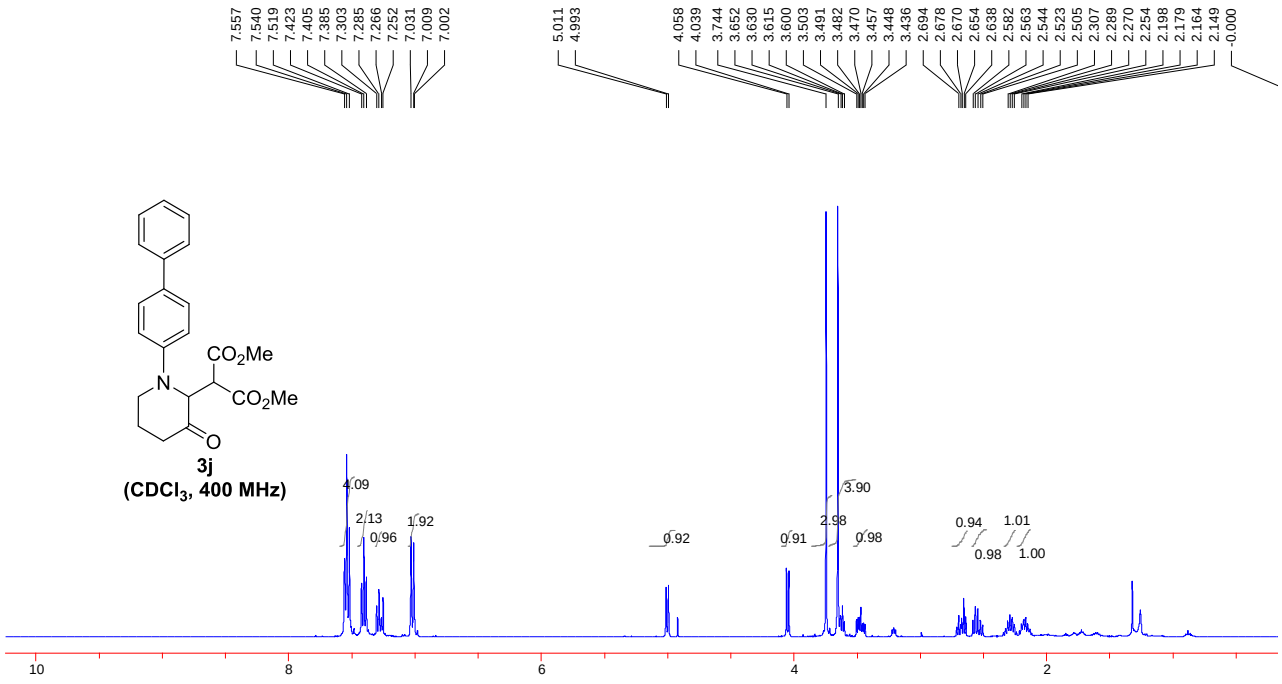
167.648 167.436
145.838
134.477 129.344 128.491 127.455 126.748 126.566 123.685 118.421 110.910
77.280 77.069 76.857
66.576
52.846 52.802 52.773 44.919
37.146
22.847
CO2Me
CO2Me
N
O
3i
(CDCl3, 150 MHz)
200 150 100 50 0 PI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7.540
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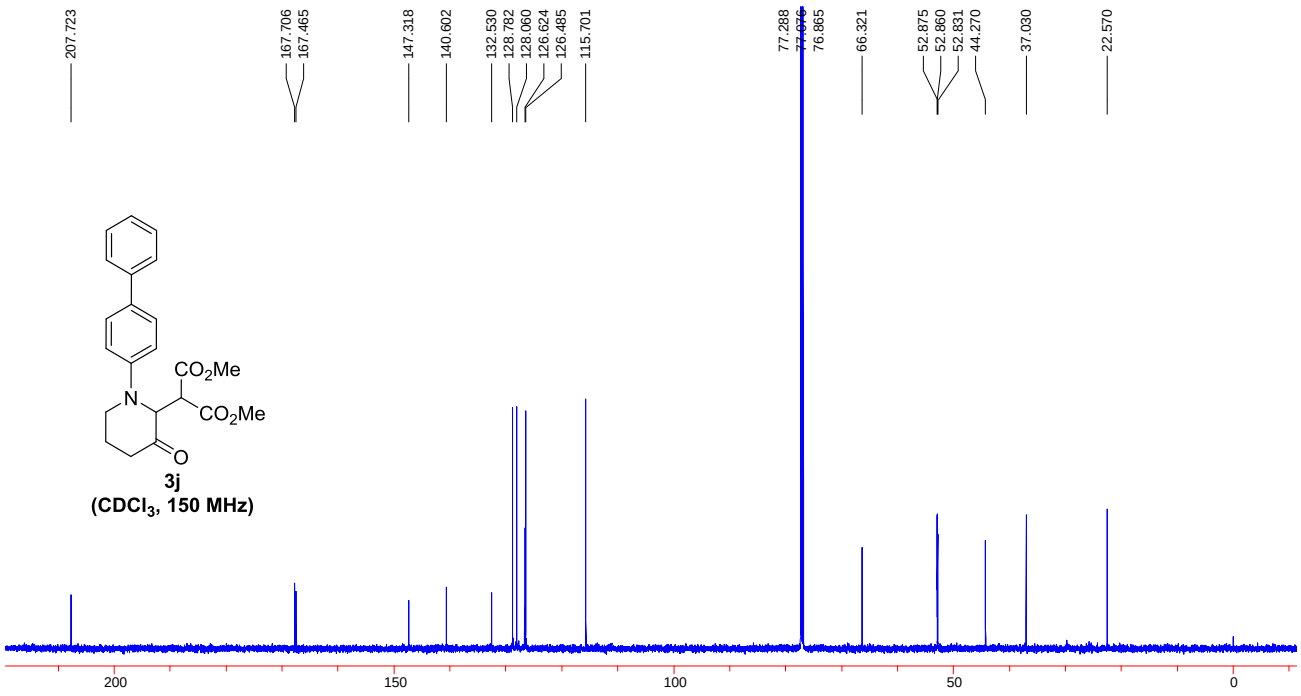
7.423
7.405
7.385
7.303
7.285
7.266
7.252
7.031
7.009
7.002
5.011
4.993
4.058
4.039
3.744
3.652
3.630
3.615
3.600
3.503
3.491
3.482
3.470
3.457
3.448
3.436
2.694
2.678
2.670
2.654
2.638
2.582
2.563
2.544
2.523
2.505
2.307
2.289
2.270
2.254
2.198
2.179
2.164
2.149
-0.000
CO2Me
CO2Me
N
O
3j
(CDCl3, 400 MHz)
4.09
2.13
0.96
1.92
0.92
0.91
3.90
2.98
0.98
0.94
0.98
1.01
1.00
10
8
6
4
2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140.602
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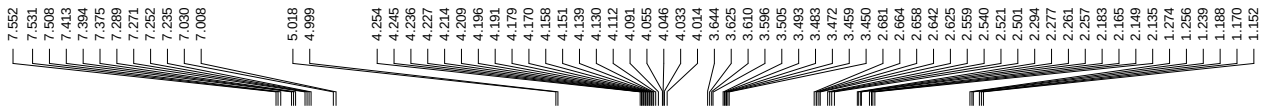
128.060
126.624
126.485
115.701
77.288
77.076
76.865
66.321
52.875
52.860
52.831
44.270
37.030
22.570
CO2Me
CO2Me
N
O
3j
(CDCl3, 150 MHz)
200
150
100
50
0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7.413
7.394
7.375
7.289
7.271
7.252
7.235
7.030
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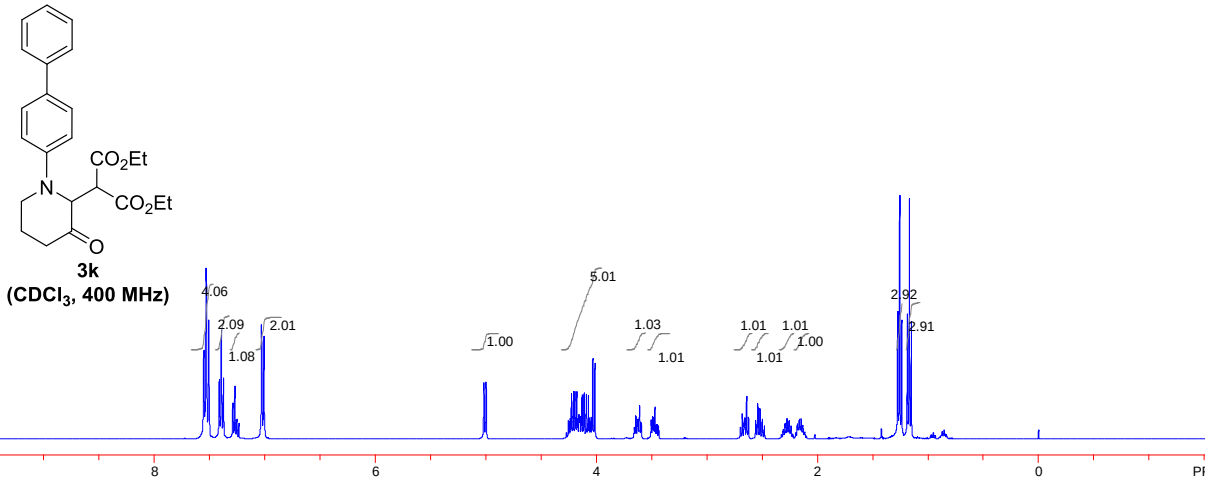
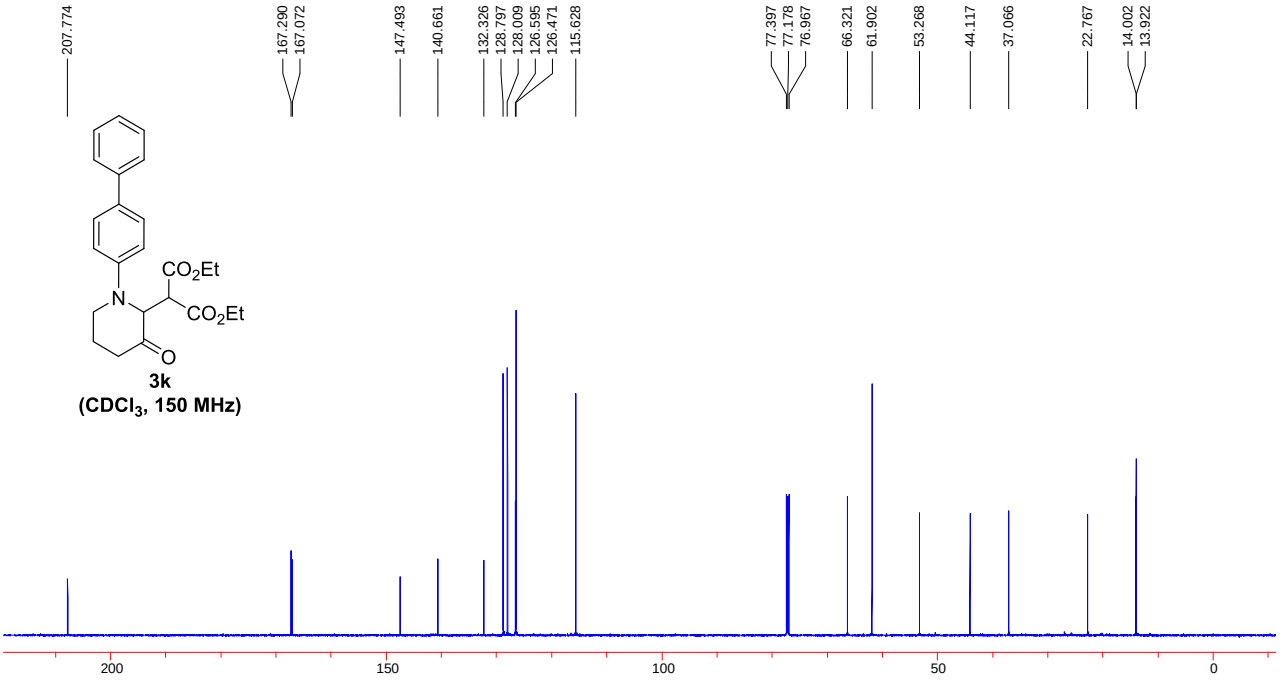
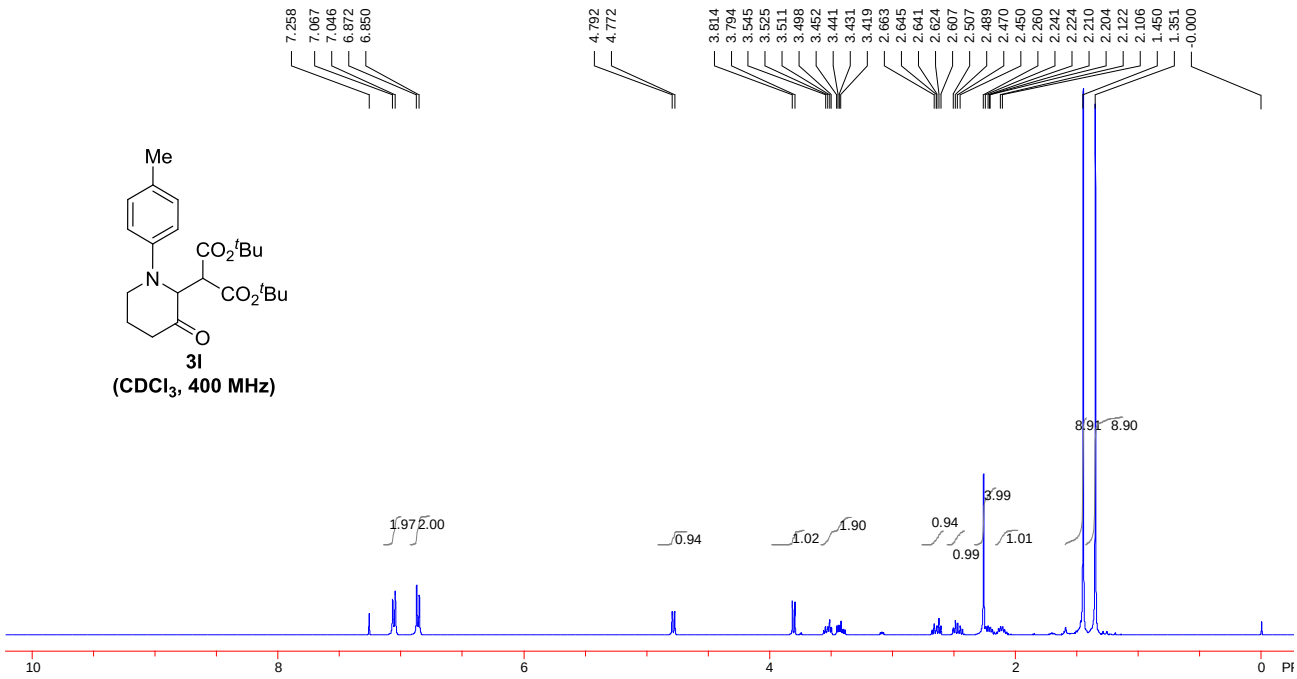
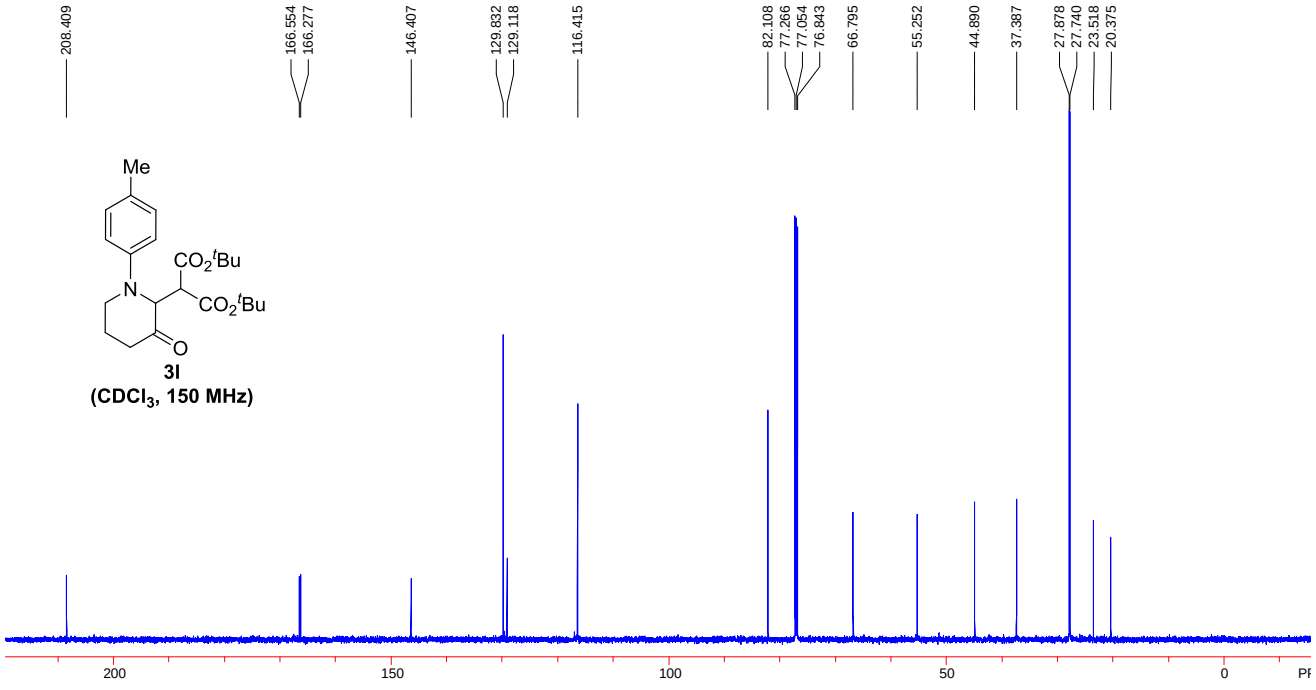
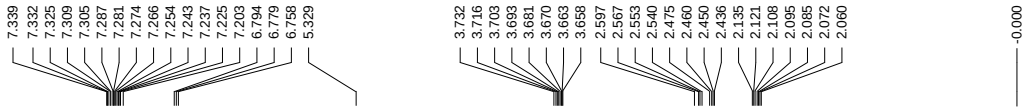
4.999
4.254
4.245
4.236
4.227
4.214
4.209
4.196
4.191
4.179
4.170
4.158
4.151
4.139
4.130
4.112
4.091
4.055
4.046
4.033
4.014
3.644
3.625
3.610
3.596
3.505
3.493
3.483
3.472
3.459
3.450
2.681
2.664
2.658
2.642
2.625
2.559
2.540
2.521
2.501
2.294
2.277
2.261
2.257
2.183
2.165
2.149
2.135
1.274
1.256
1.239
1.188
1.170
1.152

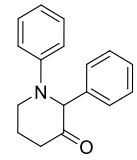

CO2Et
CO2Et
N
O
3k
(CDCl3, 400 MHz)
4.06
2.09
1.08
2.01
1.00
5.01
1.03
1.01
1.01
1.01
1.01
1.00
2.92
2.91
8
6
4
2
0


207.774
167.290
167.072
147.493
140.661
132.326
128.797
128.009
126.595
126.471
115.628
77.397
77.178
76.967
66.321
61.902
53.268
44.117
37.066
22.767
14.002
13.922
CO2Et
CO2Et
N
O
3k
(CDCl3, 150 MHz)
200
150
100
50
0

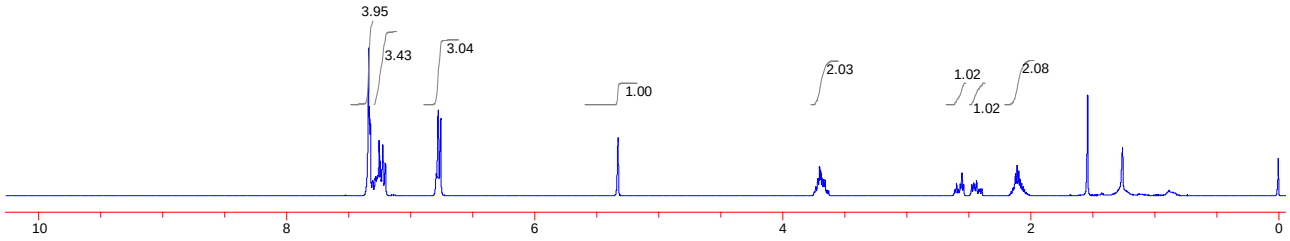

7.258
7.067
7.046
6.872
6.850
4.792
4.772
3.814
3.794
3.545
3.525
3.511
3.498
3.452
3.441
3.431
3.419
2.663
2.645
2.641
2.624
2.607
2.507
2.489
2.470
2.450
2.260
2.242
2.224
2.210
2.204
2.122
2.106
1.450
1.351
0.000
Me
CO2tBu
N
CO2tBu
O
3l
(CDCl3, 400 MHz)
8.91
8.90
3.99
1.97
2.00
0.94
1.02
1.90
0.94
0.99
1.01
10
8
6
4
2
0
PI

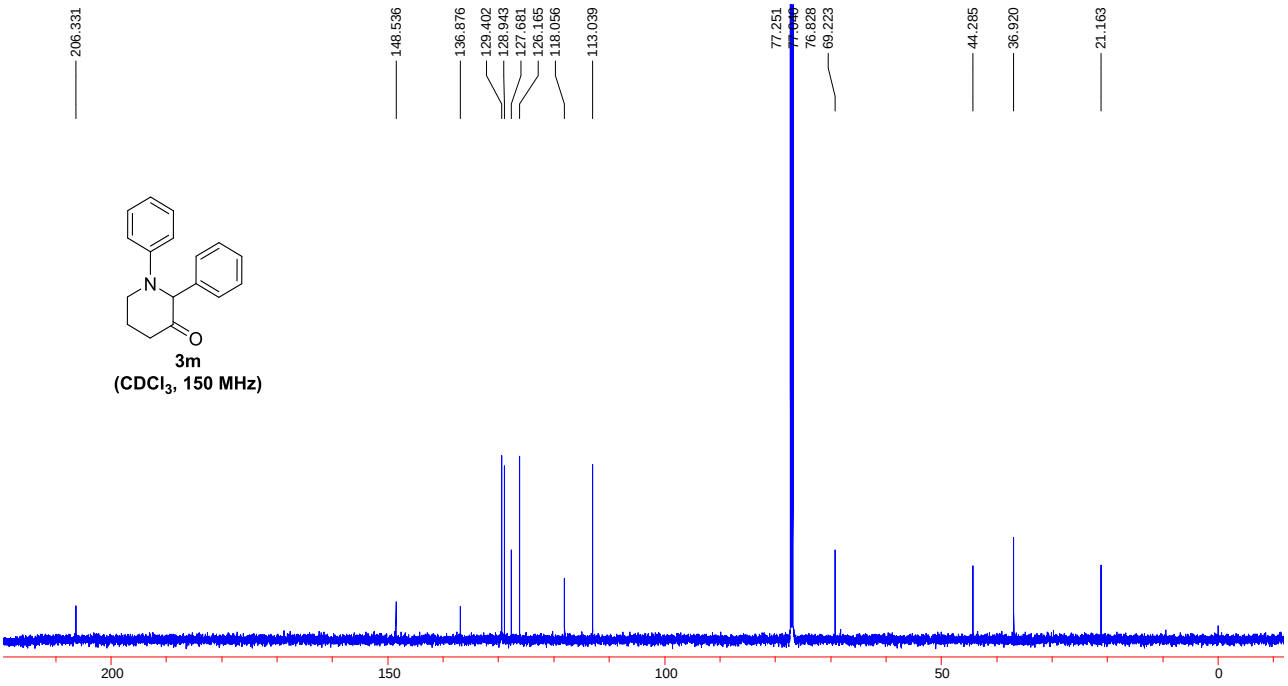

208.409
166.554
166.277
146.407
129.832
129.118
116.415
82.108
77.266
77.054
76.843
66.795
55.252
44.890
37.387
27.878
27.740
23.518
20.375
Me
CO2tBu
N
CO2tBu
O
3l
(CDCl3, 150 MHz)
200
150
100
50
0
PI



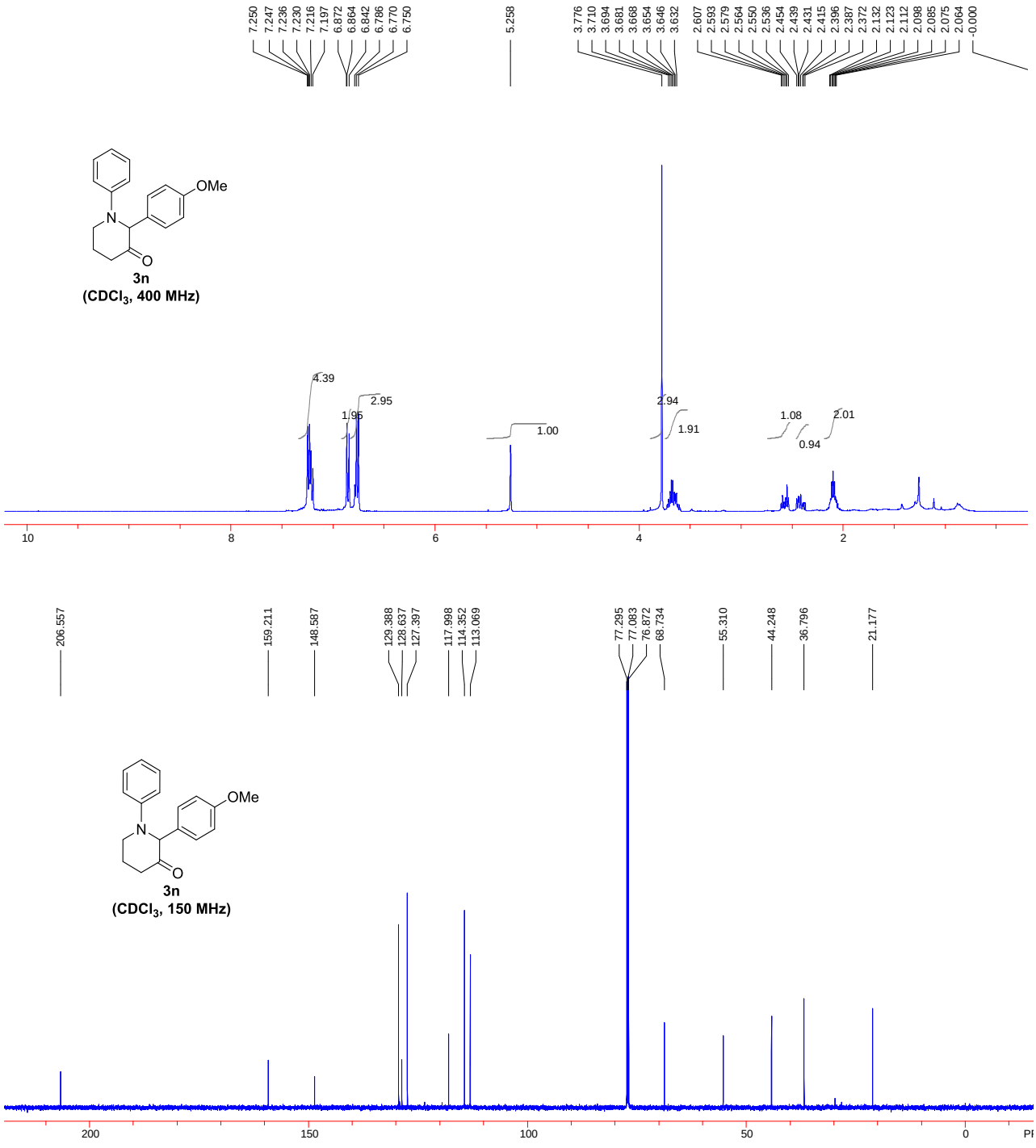


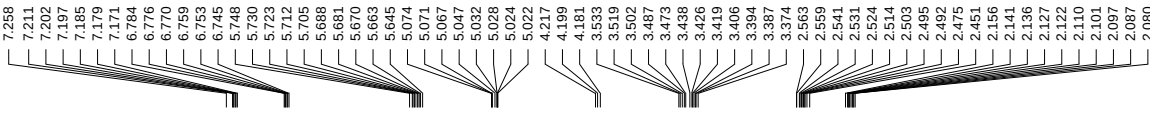
3m
($CDCl_3$, 400 MHz)

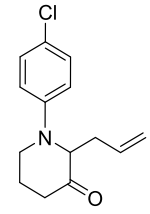




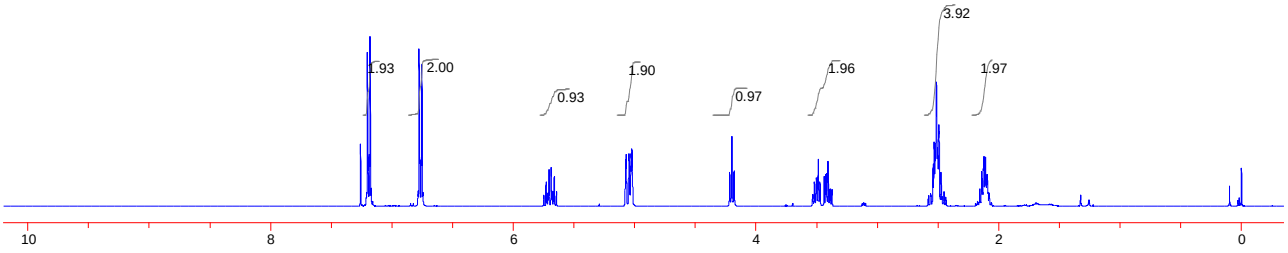
3m
($CDCl_3$, 150 MHz)

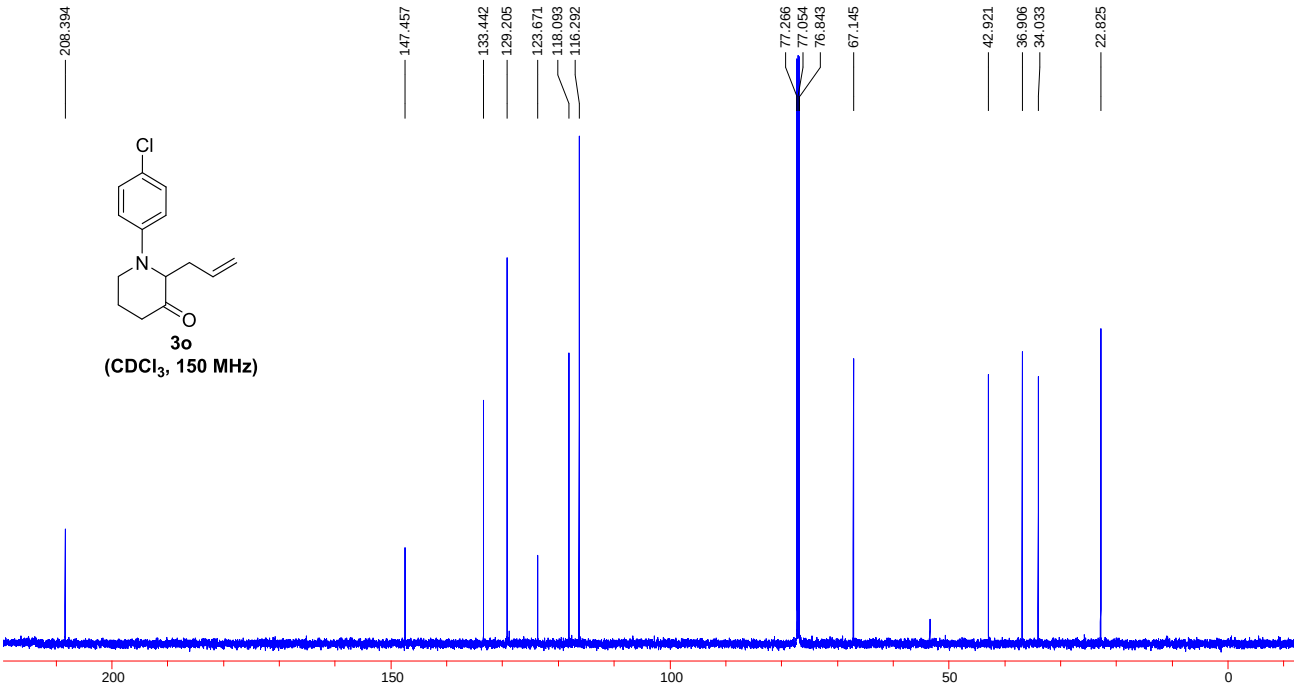

7.250
7.247
7.236
7.230
7.216
7.197
6.872
6.864
6.842
6.786
6.770
6.750
5.258
3.776
3.710
3.694
3.681
3.668
3.654
3.646
3.632
2.607
2.593
2.579
2.564
2.550
2.536
2.454
2.439
2.431
2.415
2.396
2.387
2.372
2.132
2.123
2.112
2.098
2.085
2.075
2.064
-0.000
OMe
N
O
3n
(CDCl3, 400 MHz)
4.39
1.95
2.95
1.00
2.94
1.91
1.08
0.94
2.01
10
8
6
4
2
206.557
159.211
148.587
129.388
128.637
127.397
117.998
114.352
113.069
77.295
77.083
76.872
68.734
55.310
44.248
36.796
21.177
OMe
N
O
3n
(CDCl3, 150 MHz)
200
150
100
50
0



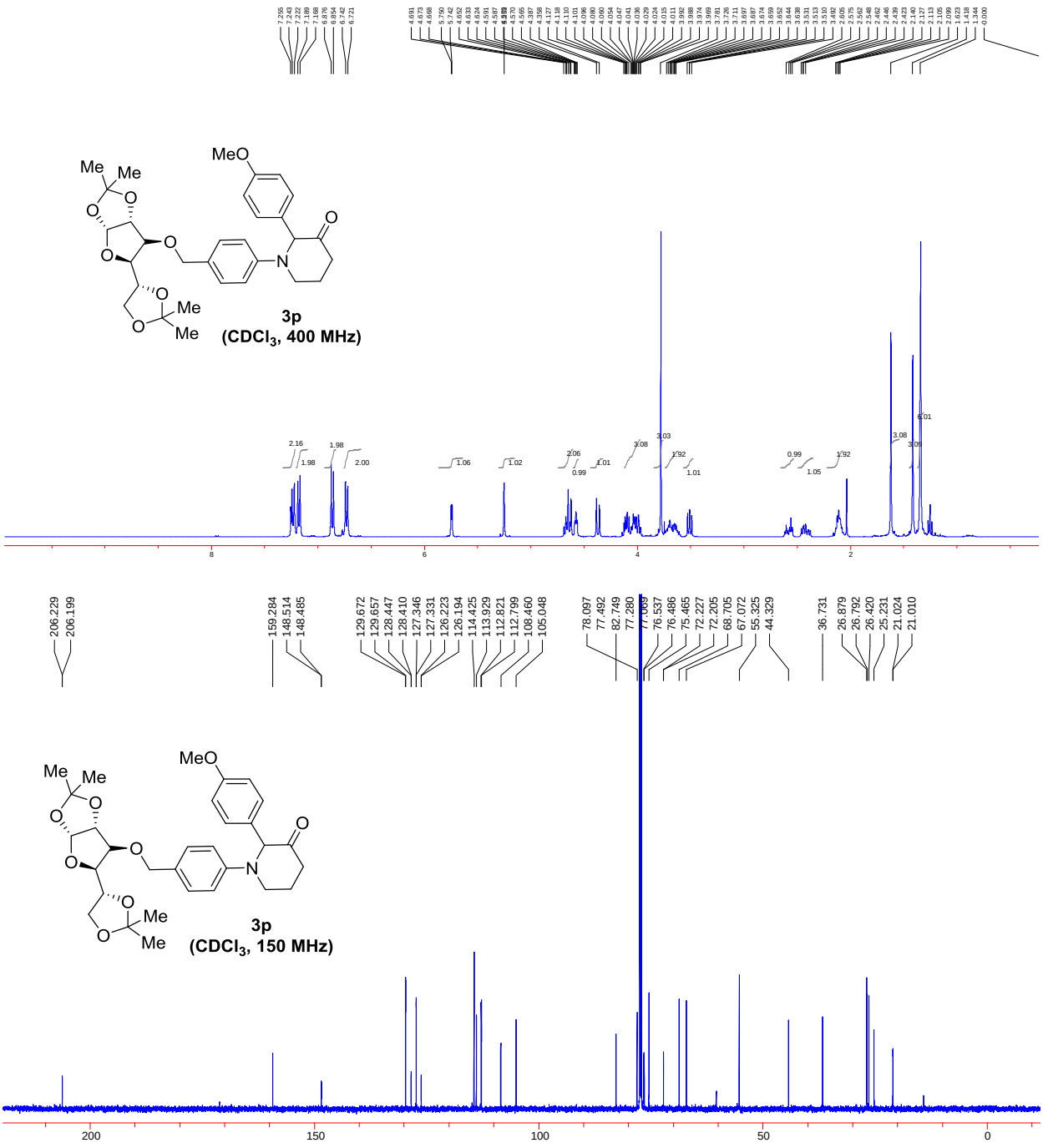


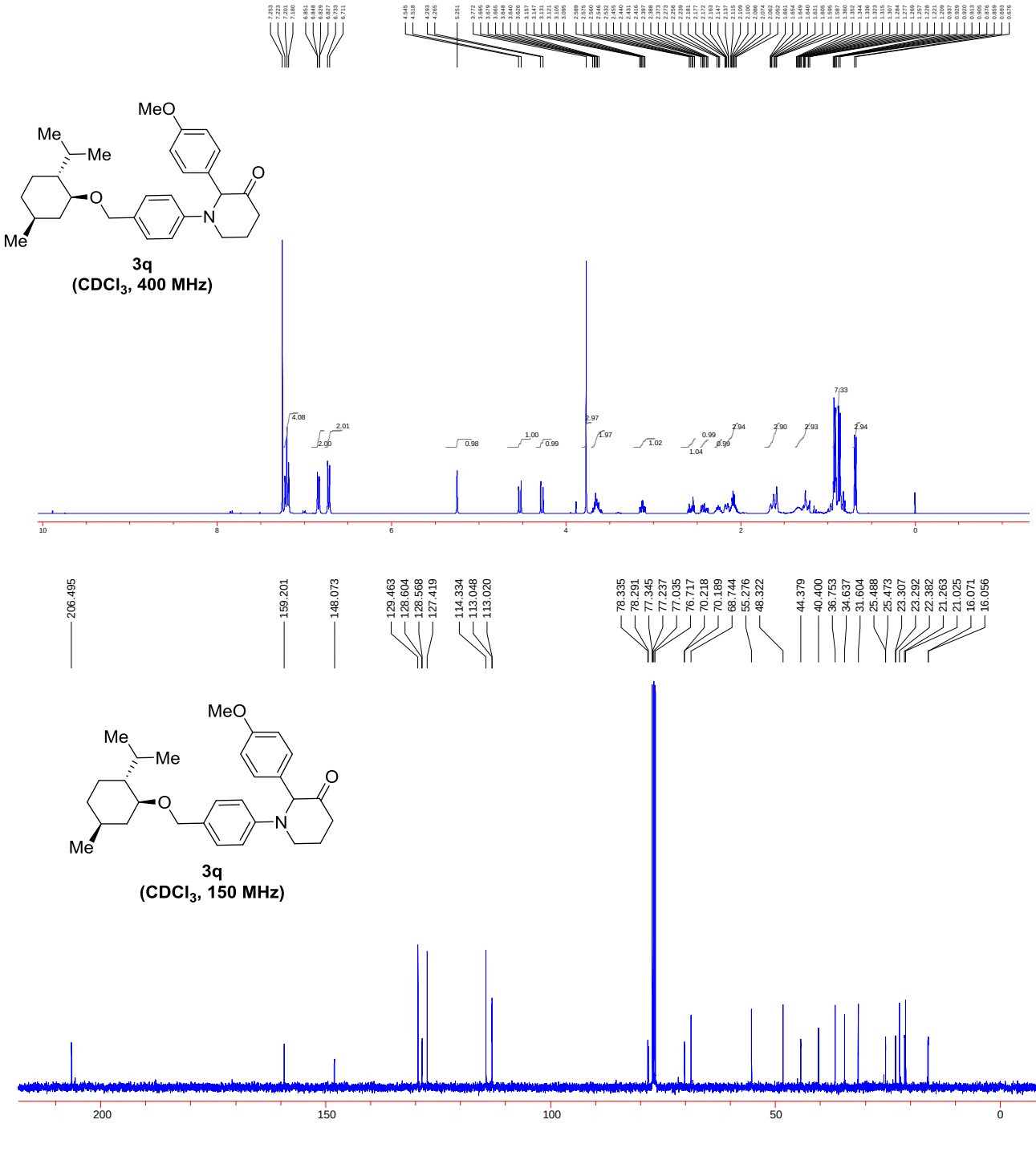
3o
($CDCl_3$, 400 MHz)



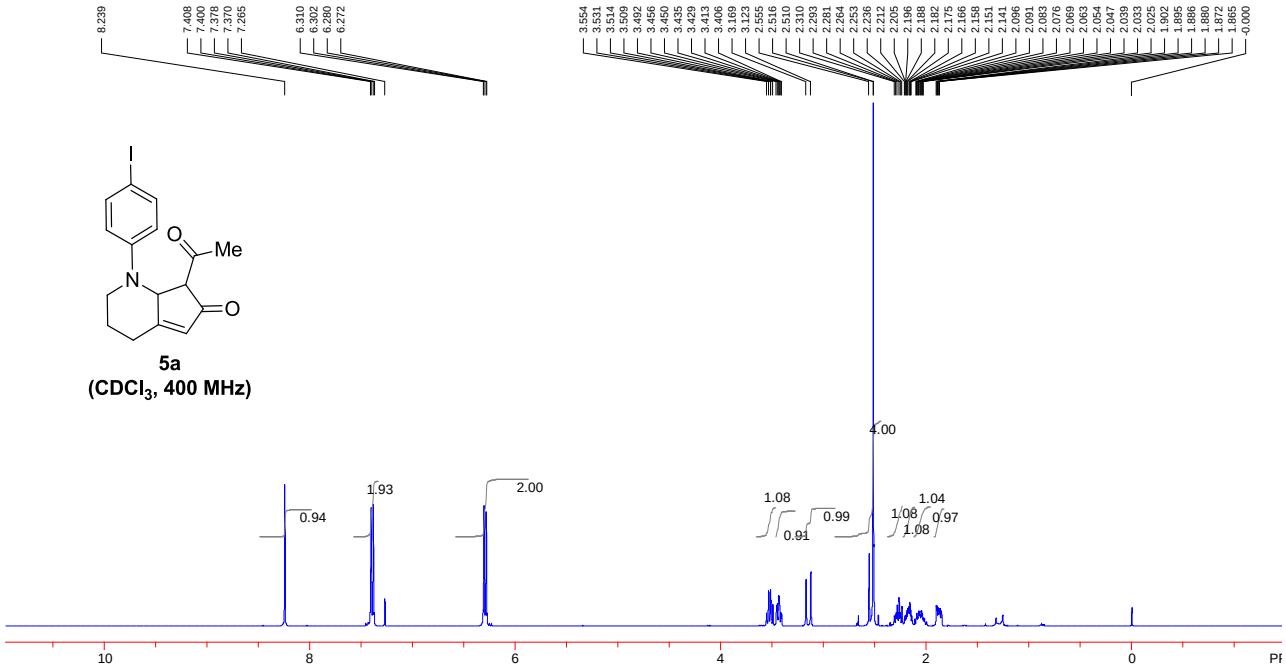


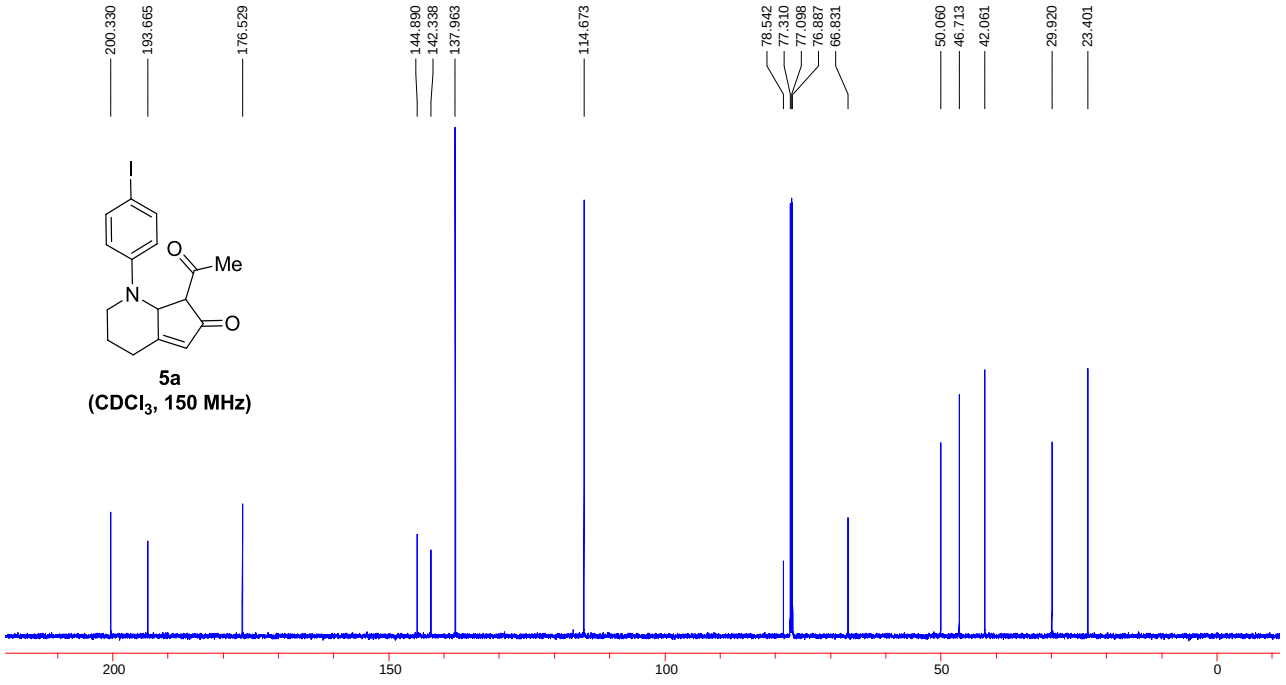
3o
($CDCl_3$, 150 MHz)

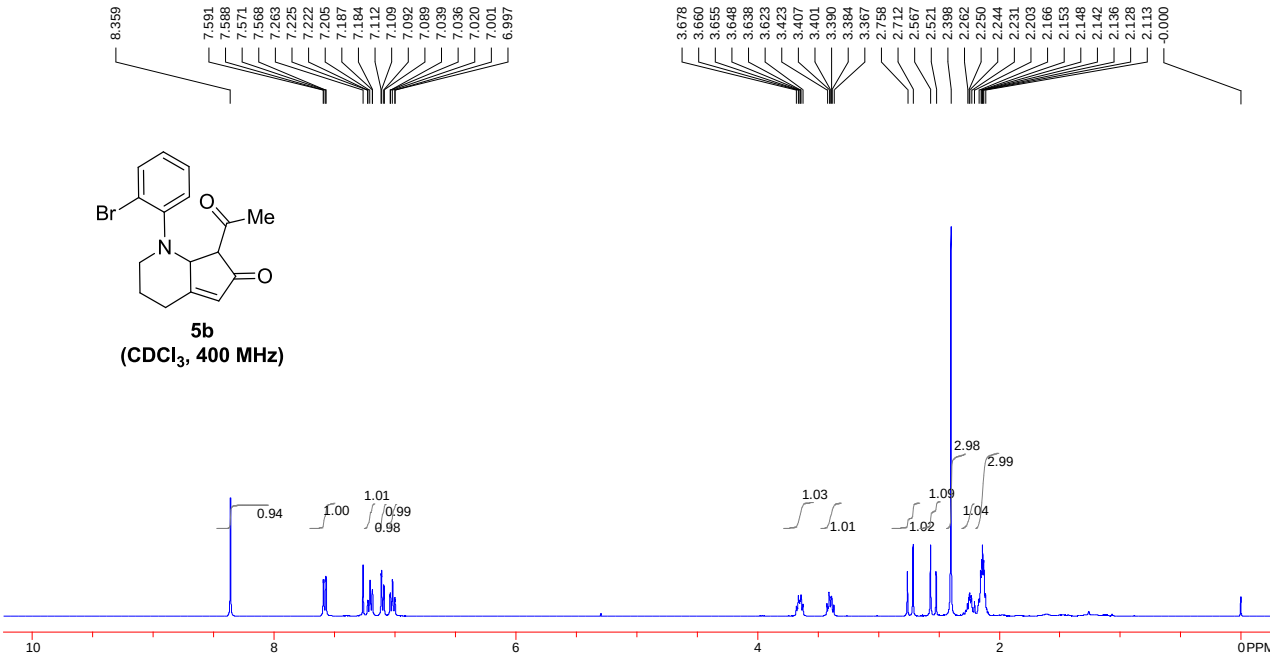

MeO
Me
Me
O
N
Me
Me
3p
(CDCl3, 400 MHz)
3p
(CDCl3, 150 MHz)

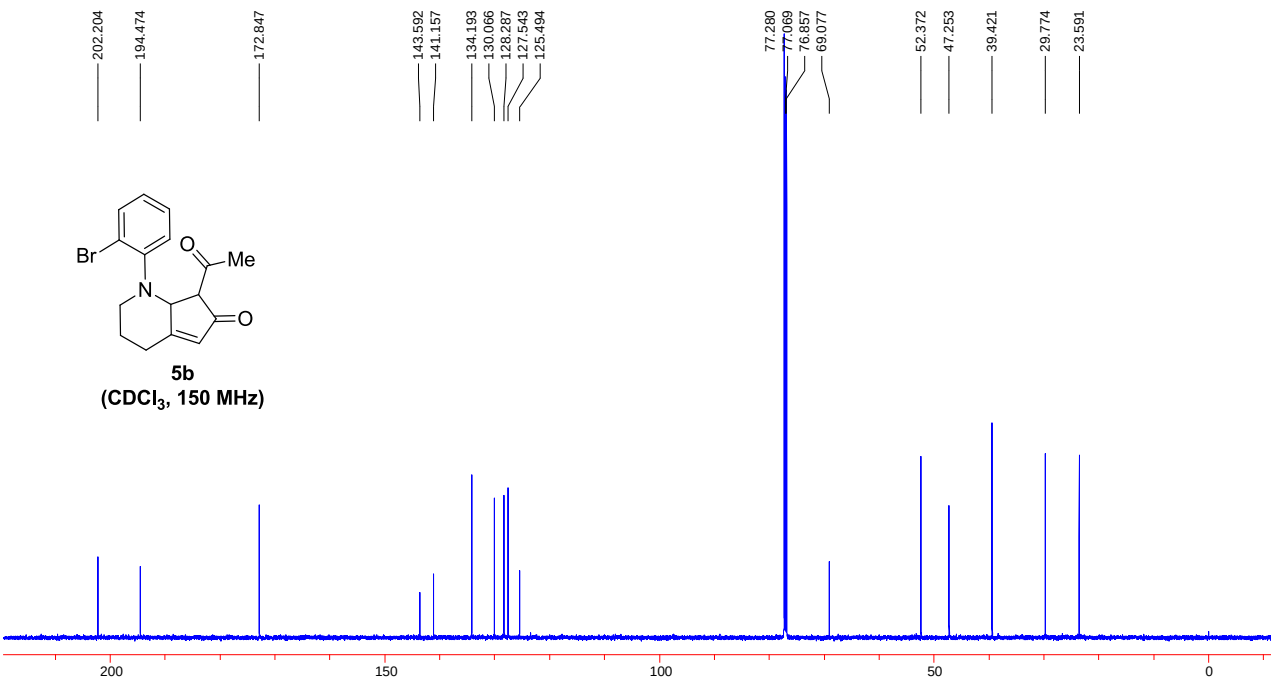

MeO
Me
Me
O
N
Me
3q
(CDCl3, 400 MHz)
4.08
2.01
2.00
0.98
1.00
0.99
2.97
1.97
1.02
0.99
1.04
0.99
2.94
2.90
2.93
7.33
2.94
10
8
6
4
2
0
206.495
159.201
148.073
129.463
128.604
128.568
127.419
114.334
113.048
113.020
78.335
78.291
77.345
77.237
77.035
76.717
70.218
70.189
68.744
55.276
48.322
44.379
40.400
36.753
34.637
31.604
25.488
25.473
23.307
23.292
22.382
21.263
21.025
16.071
16.056
MeO
Me
Me
O
N
Me
3q
(CDCl3, 150 MHz)
200
150
100
50
0

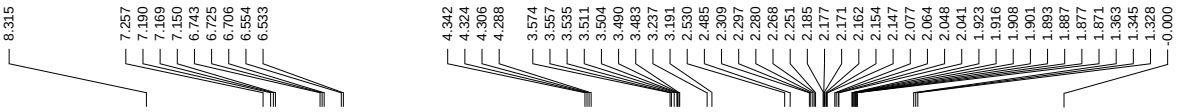
IV. Copies of the NMR Spectra of 5a-5d

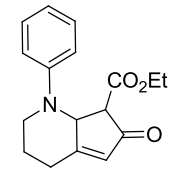




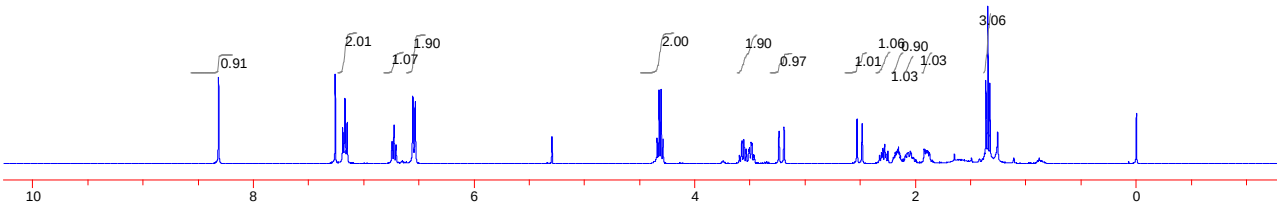

8.359
7.591
7.588
7.571
7.568
7.263
7.225
7.222
7.205
7.187
7.184
7.112
7.109
7.092
7.089
7.039
7.036
7.020
7.001
6.997
3.678
3.660
3.655
3.648
3.638
3.623
3.423
3.407
3.401
3.390
3.384
3.367
2.758
2.712
2.567
2.521
2.398
2.262
2.250
2.244
2.231
2.203
2.166
2.153
2.148
2.142
2.136
2.128
2.113
-0.000
Br
N
O
Me
O
5b
(CDCl3, 400 MHz)
0.94
1.00
1.01
0.99
0.98
1.03
1.01
1.09
1.02
2.98
2.99
1.04
10
8
6
4
2
0PPM

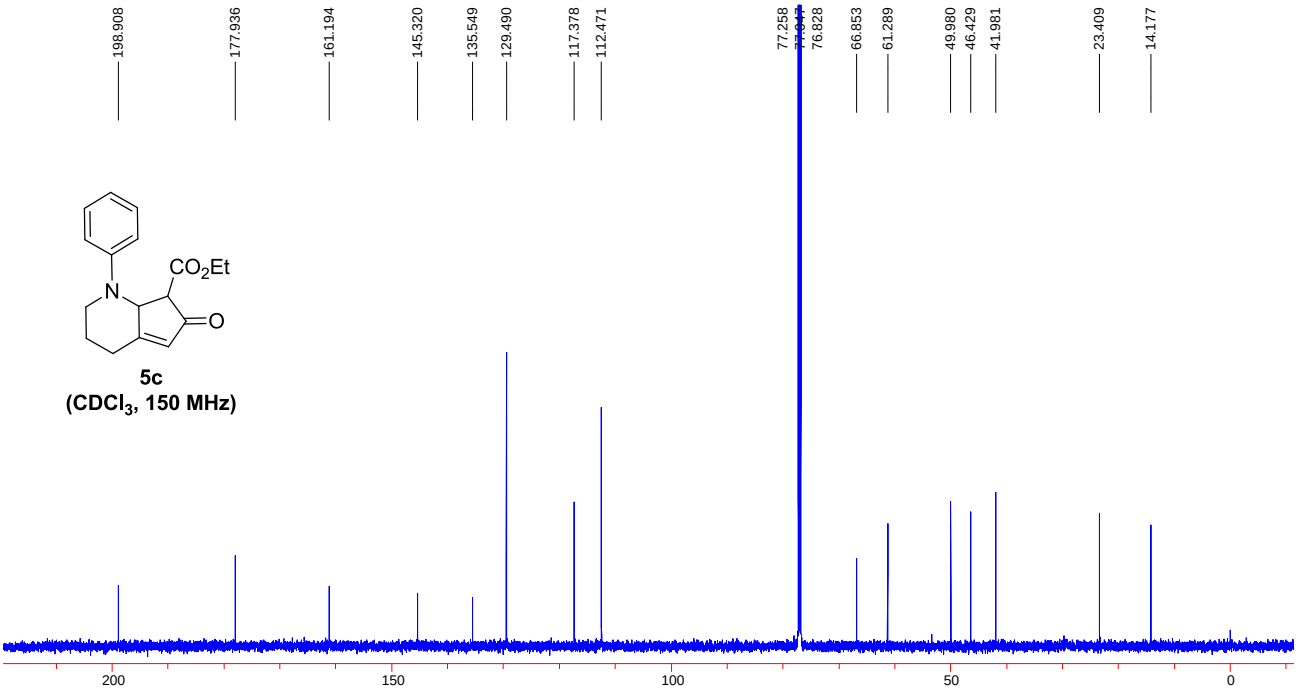

202.204
194.474
172.847
143.592
141.157
134.193
130.066
128.287
127.543
125.494
77.280
77.069
76.857
69.077
52.372
47.253
39.421
29.774
23.591
Br
N
O
Me
O
5b
(CDCl3, 150 MHz)
200
150
100
50
0



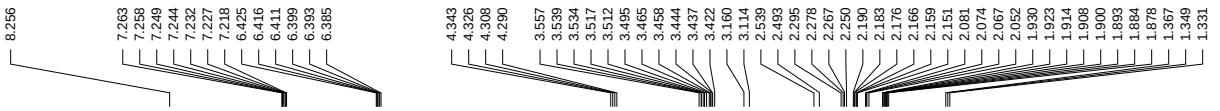


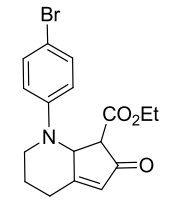
5c
($CDCl_3$, 400 MHz)



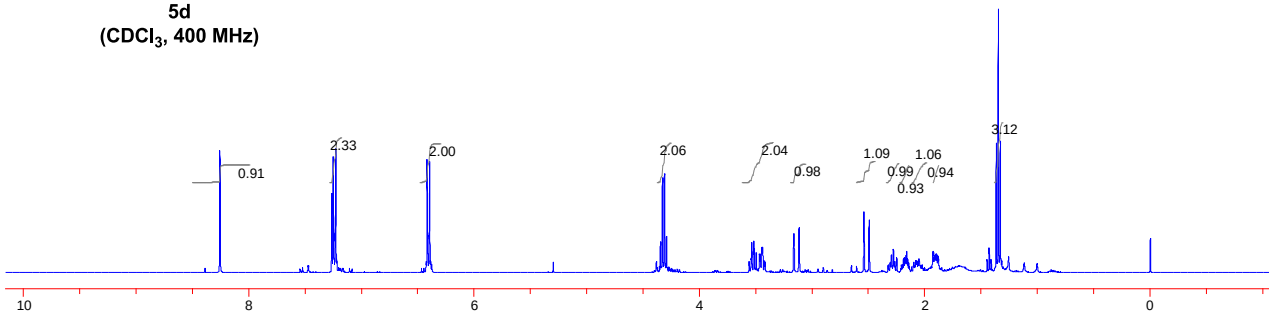


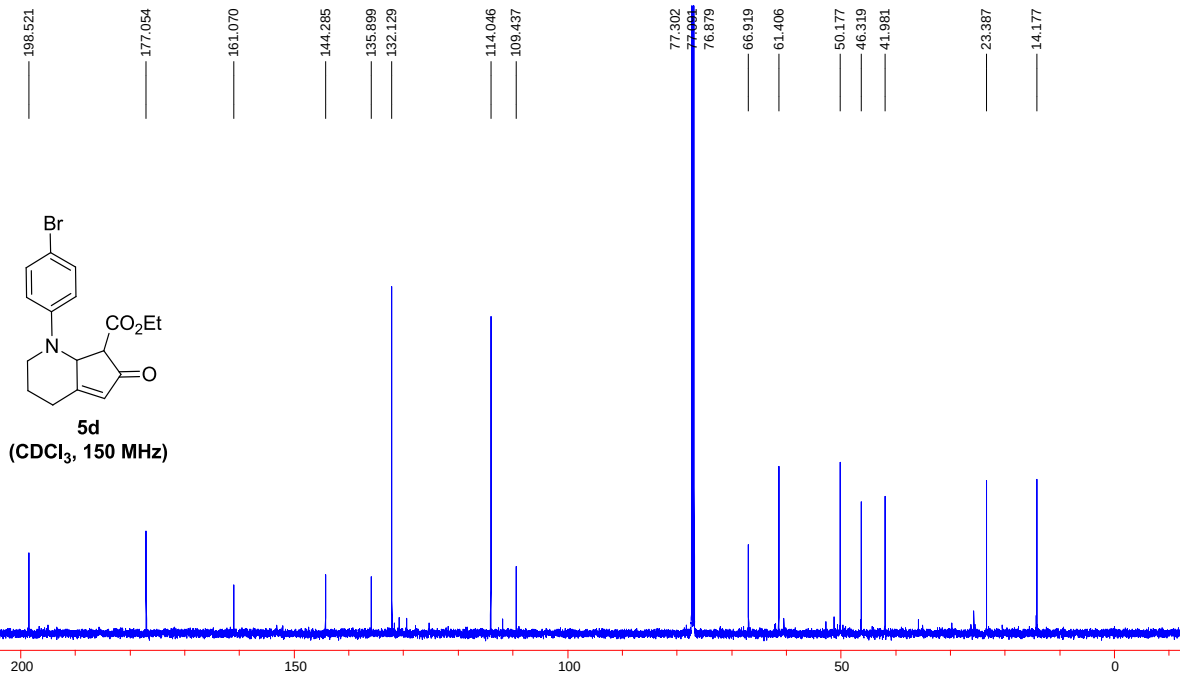
5c
($CDCl_3$, 150 MHz)





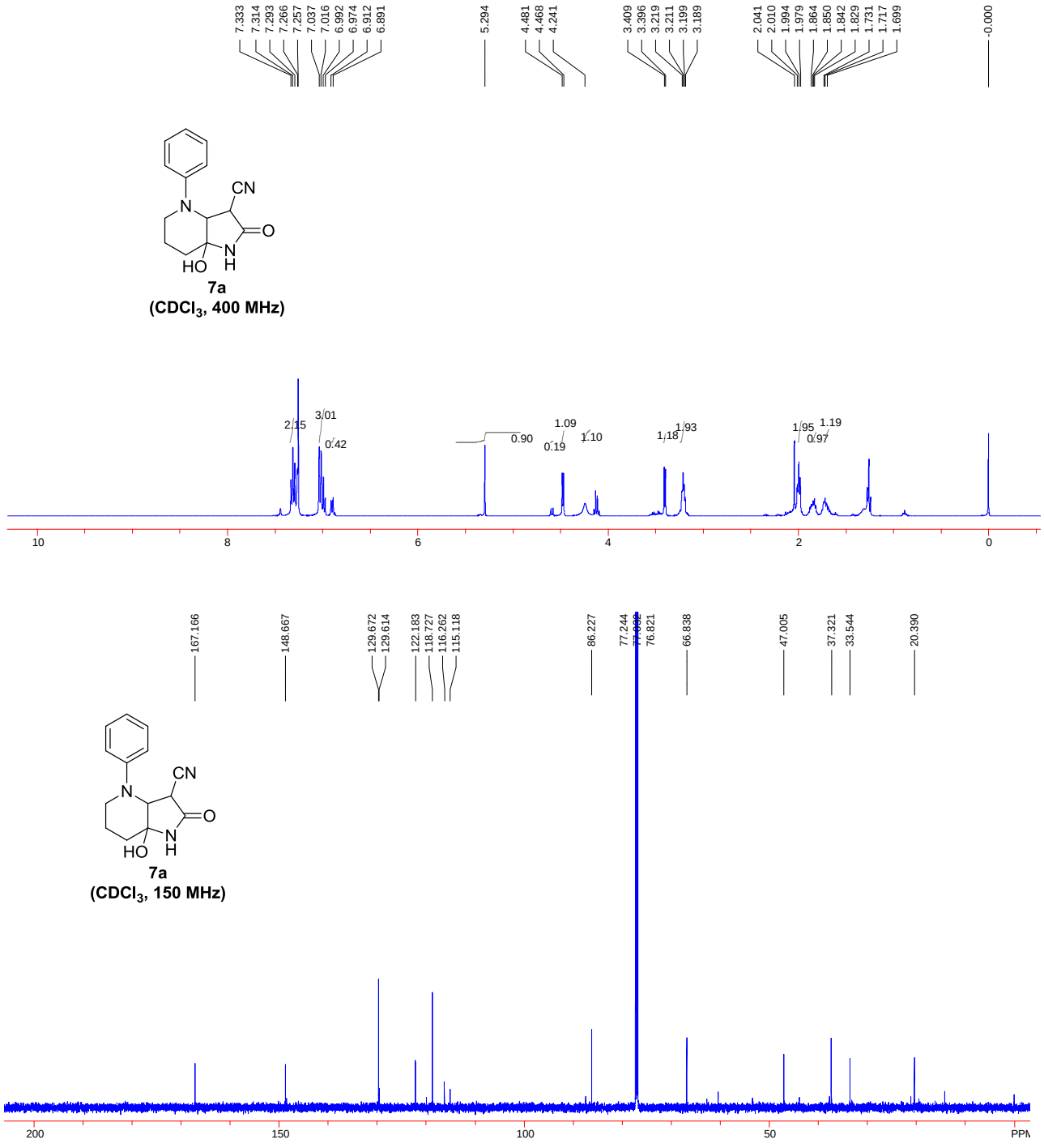
5d
($CDCl_3$, 400 MHz)

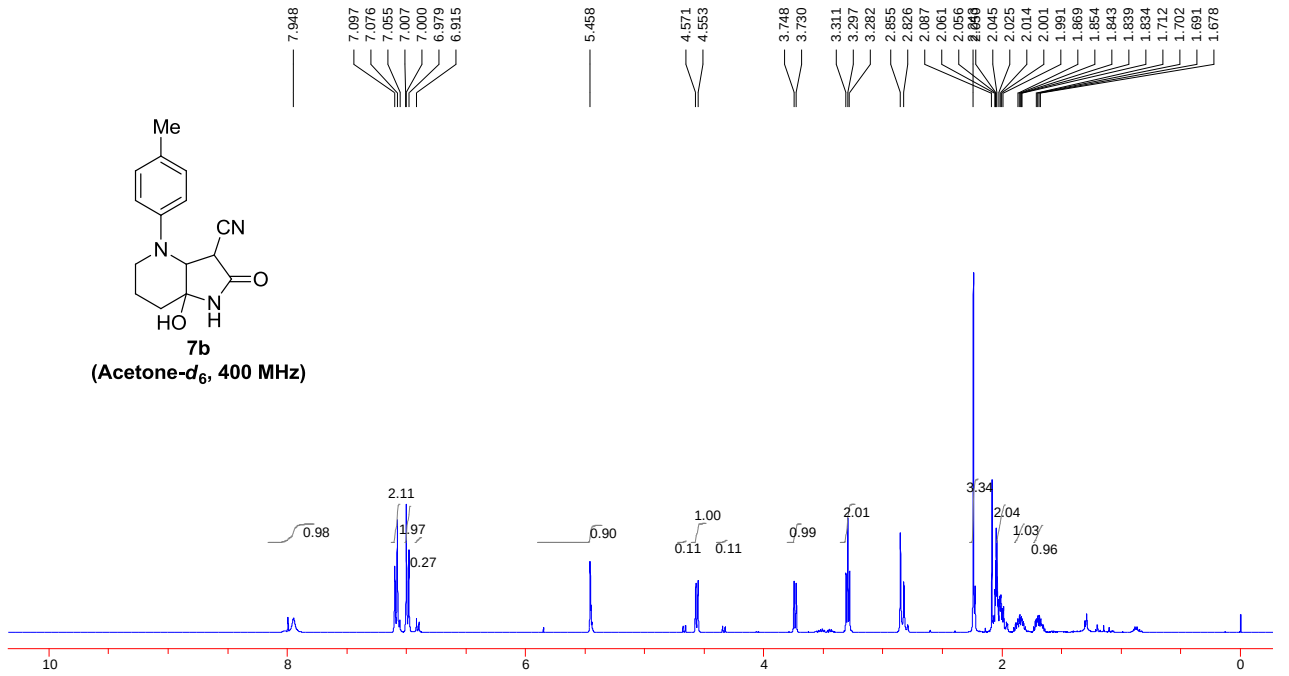


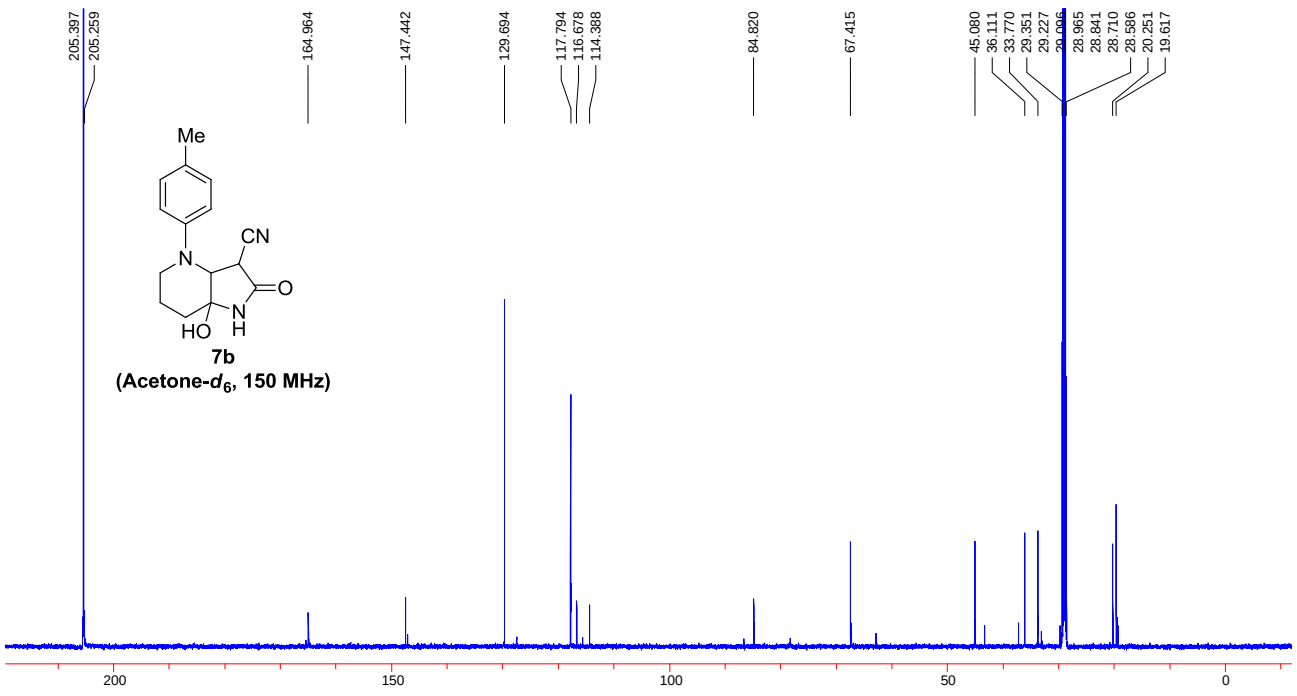


5d
($CDCl_3$, 150 MHz)

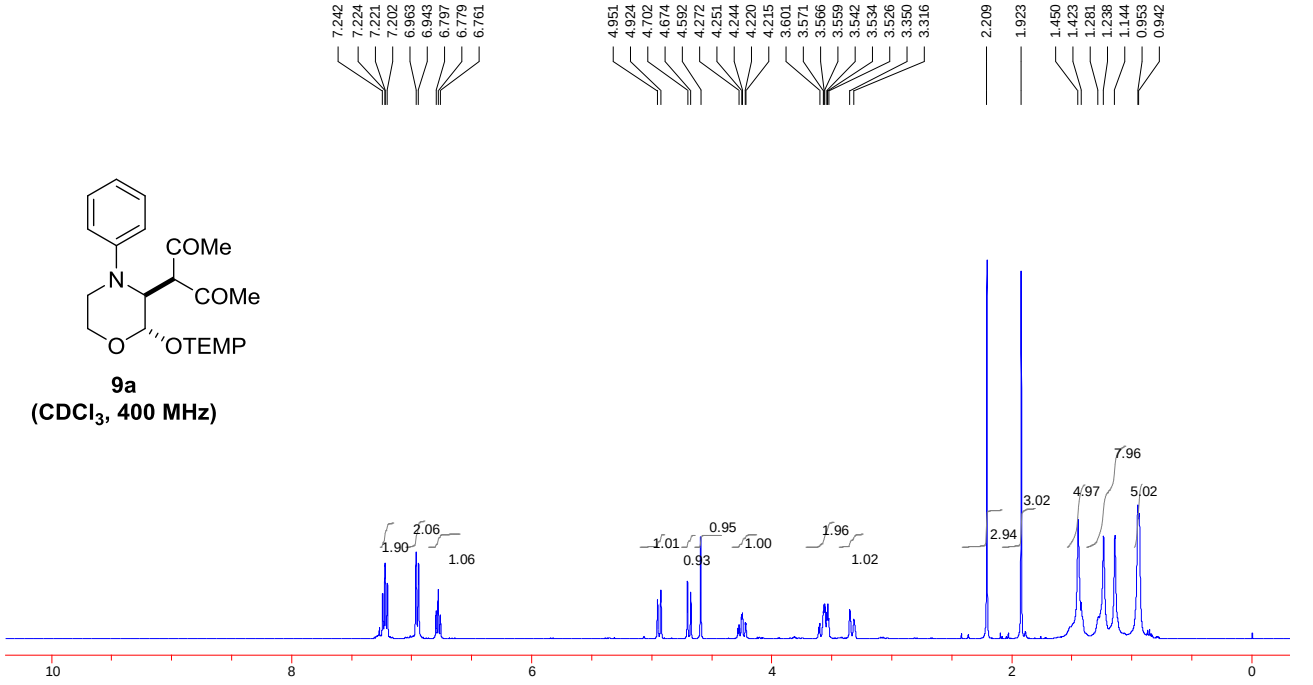
V. Copies of the NMR Spectra of 7a-7b

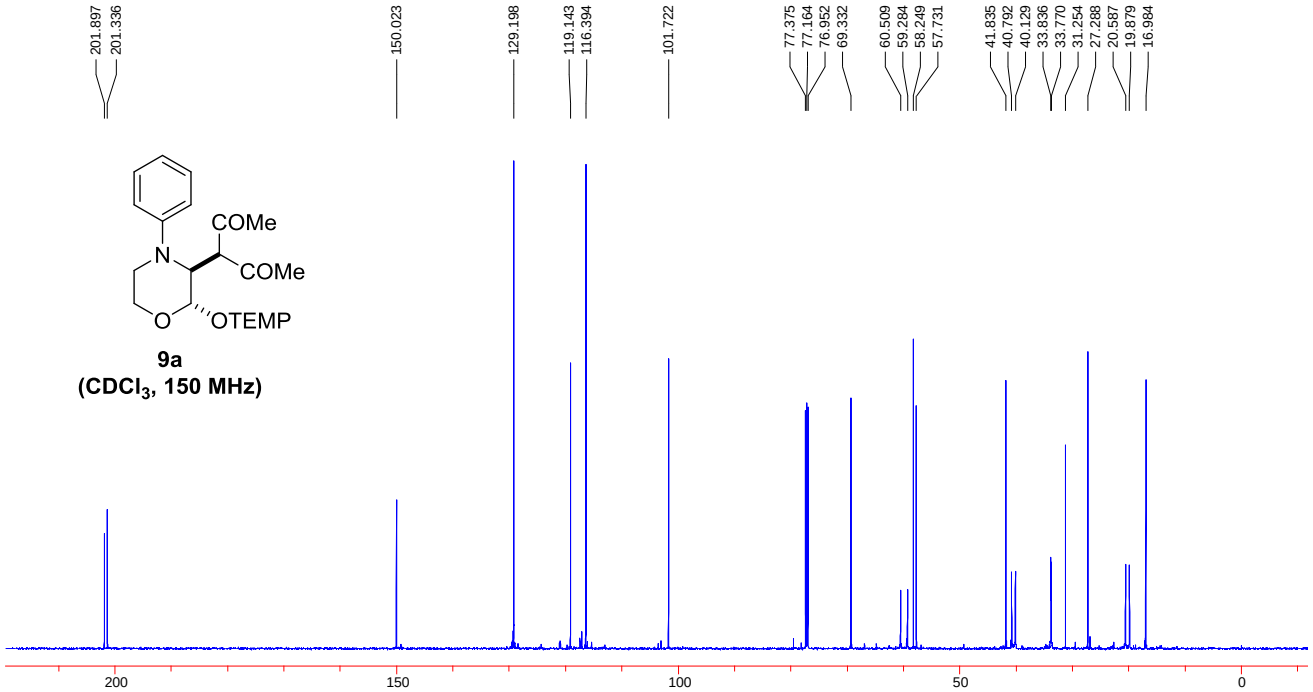


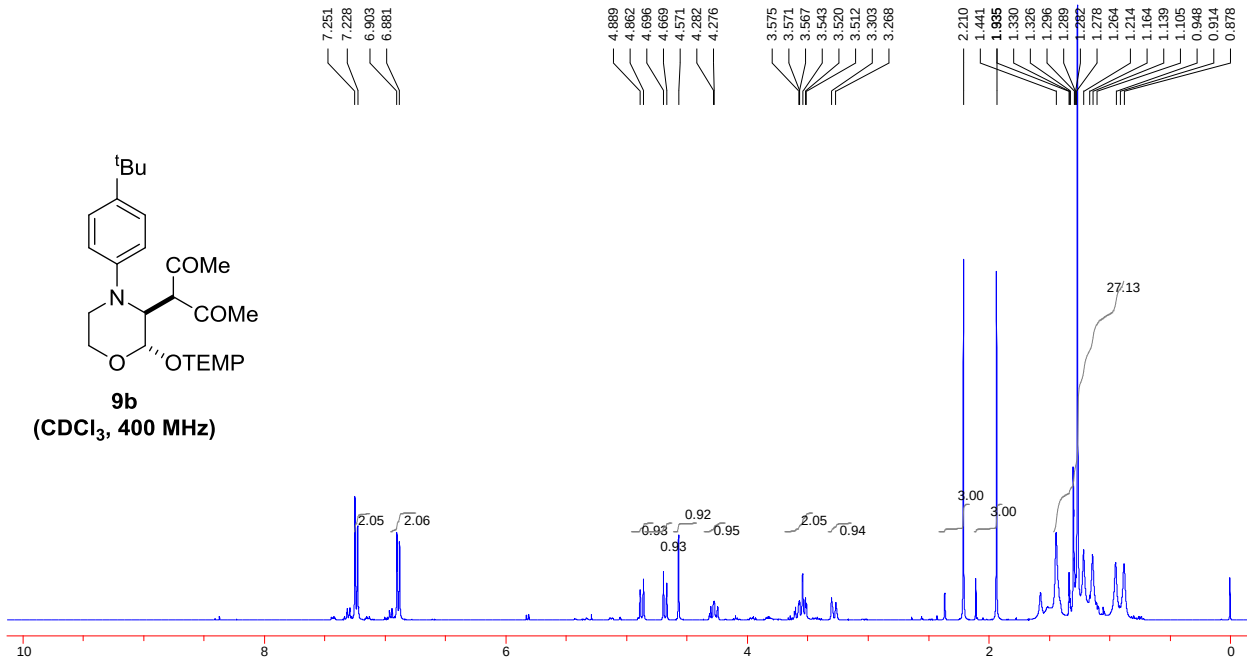

7.948
7.097
7.076
7.055
7.007
7.000
6.979
6.915
5.458
4.571
4.553
3.748
3.730
3.311
3.297
3.282
2.855
2.826
2.087
2.061
2.056
2.045
2.025
2.014
2.001
1.991
1.869
1.854
1.843
1.839
1.834
1.712
1.702
1.691
1.678
Me
CN
N
O
N
H
HO
7b
(Acetone-d6, 400 MHz)
0.98
2.11
1.97
0.27
0.90
1.00
0.11
0.11
0.99
2.01
3.34
2.04
1.03
0.96
10
8
6
4
2
0

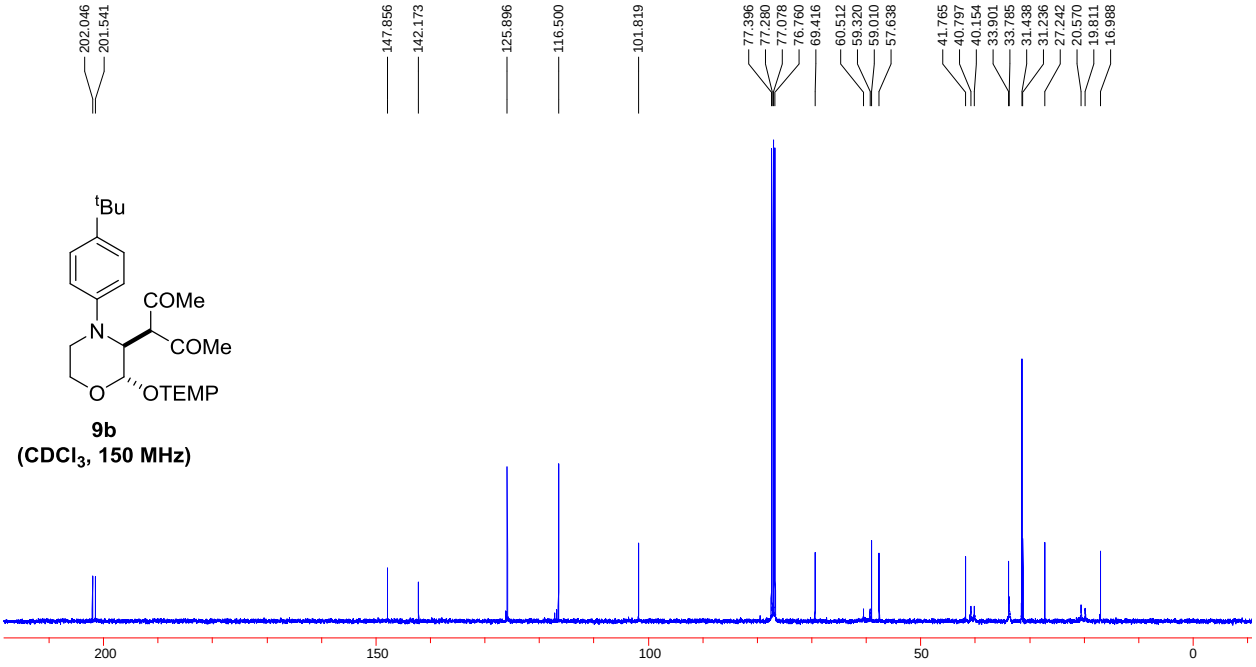

205.397
205.259
164.964
147.442
129.694
117.794
116.678
114.388
84.820
67.415
45.080
36.111
33.770
29.351
29.227
29.006
28.965
28.841
28.710
28.586
20.251
19.617
Me
CN
N
O
N
H
HO
7b
(Acetone-d6, 150 MHz)
200
150
100
50
0

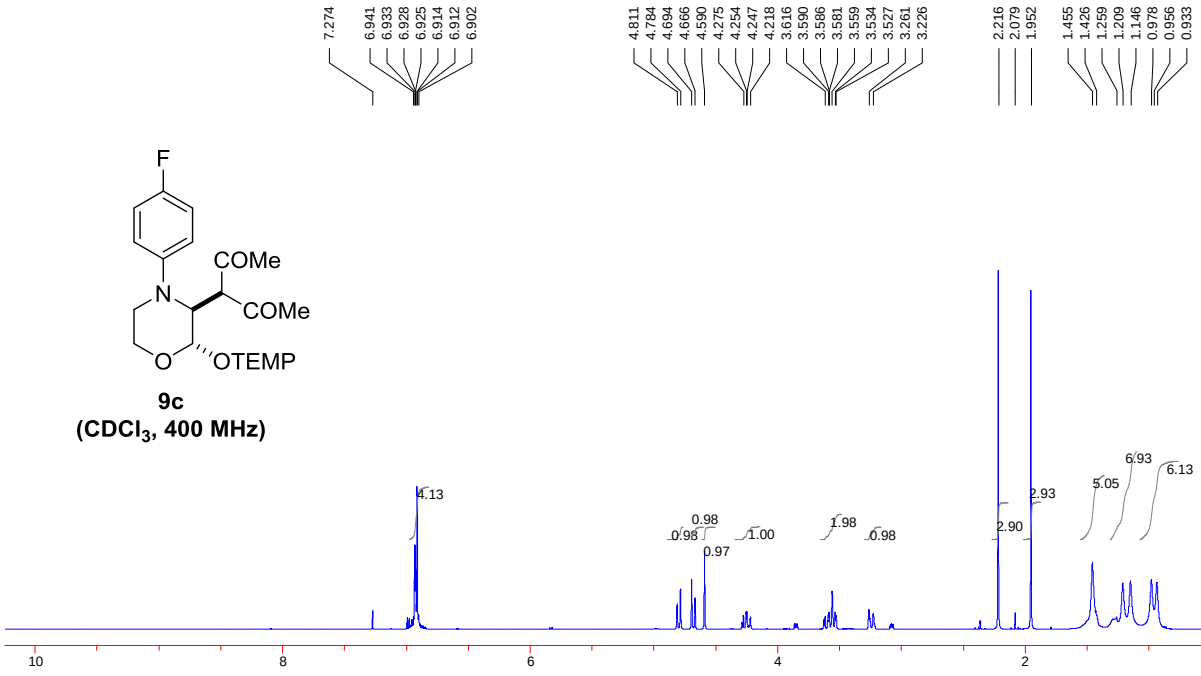
VI. Copies of the NMR Spectra of 9a-9q



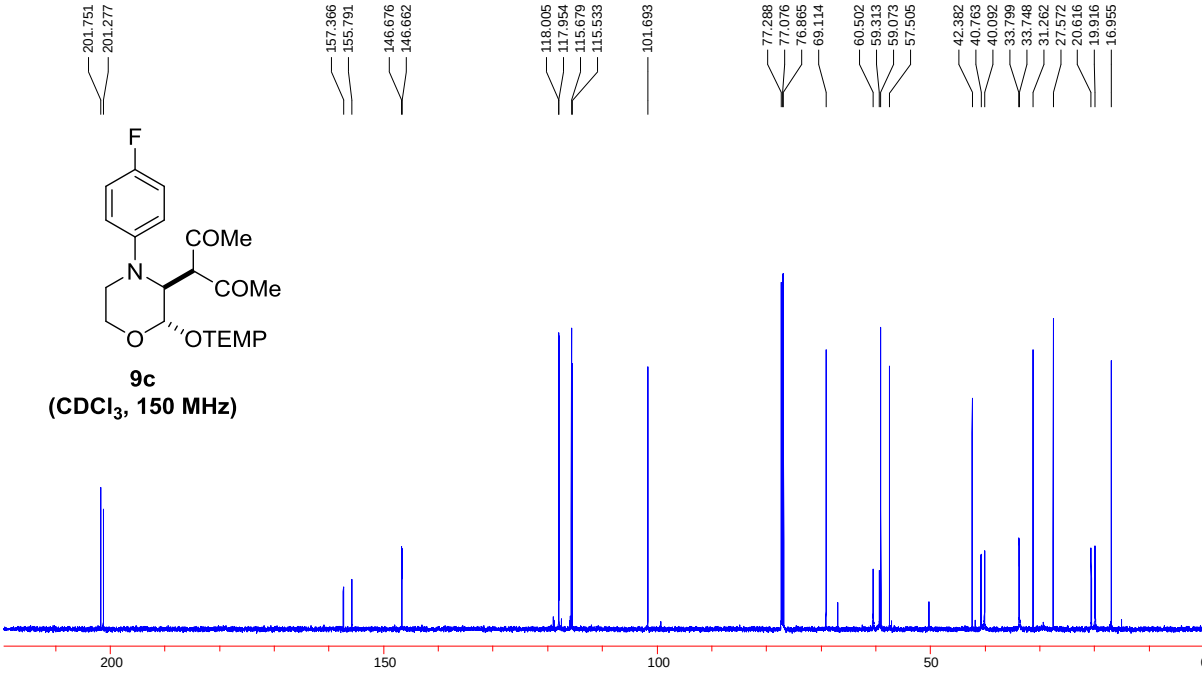



7.251
7.228
6.903
6.881
4.889
4.862
4.696
4.669
4.571
4.282
4.276
3.575
3.571
3.567
3.543
3.520
3.512
3.303
3.268
2.210
1.441
1.335
1.330
1.326
1.296
1.289
1.282
1.278
1.264
1.214
1.164
1.139
1.105
0.948
0.914
0.878
tBu
COMe
COMe
N
O
OTEMP
9b
(CDCl3, 400 MHz)
27.13
2.05
2.06
0.93
0.92
0.95
0.93
2.05
0.94
3.00
3.00
10
8
6
4
2
0

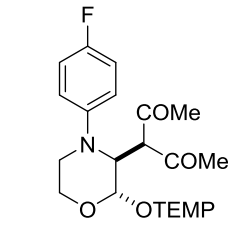

202.046
201.541
147.856
142.173
125.896
116.500
101.819
77.396
77.280
77.078
76.760
69.416
60.512
59.320
59.010
57.638
41.765
40.797
40.154
33.901
33.785
31.438
31.236
27.242
20.570
19.811
16.988
tBu
COMe
COMe
N
O
OTEMP
9b
(CDCl3, 150 MHz)
200
150
100
50
0



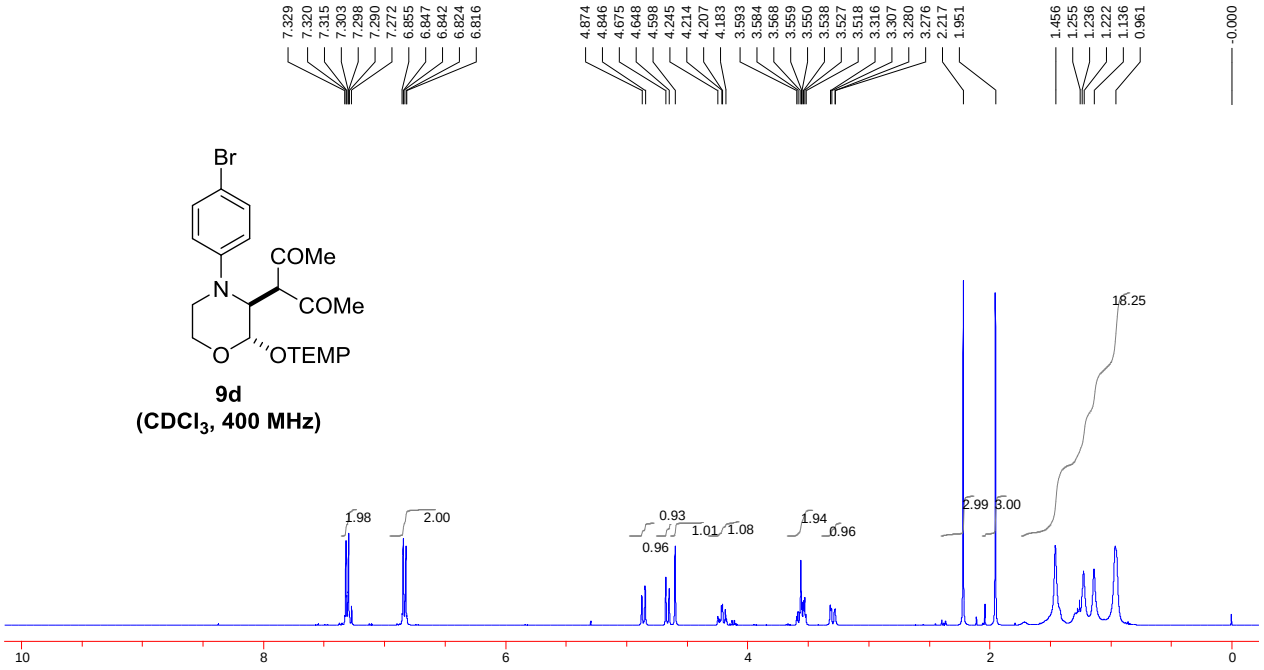
9c
($CDCl_3$, 400 MHz)

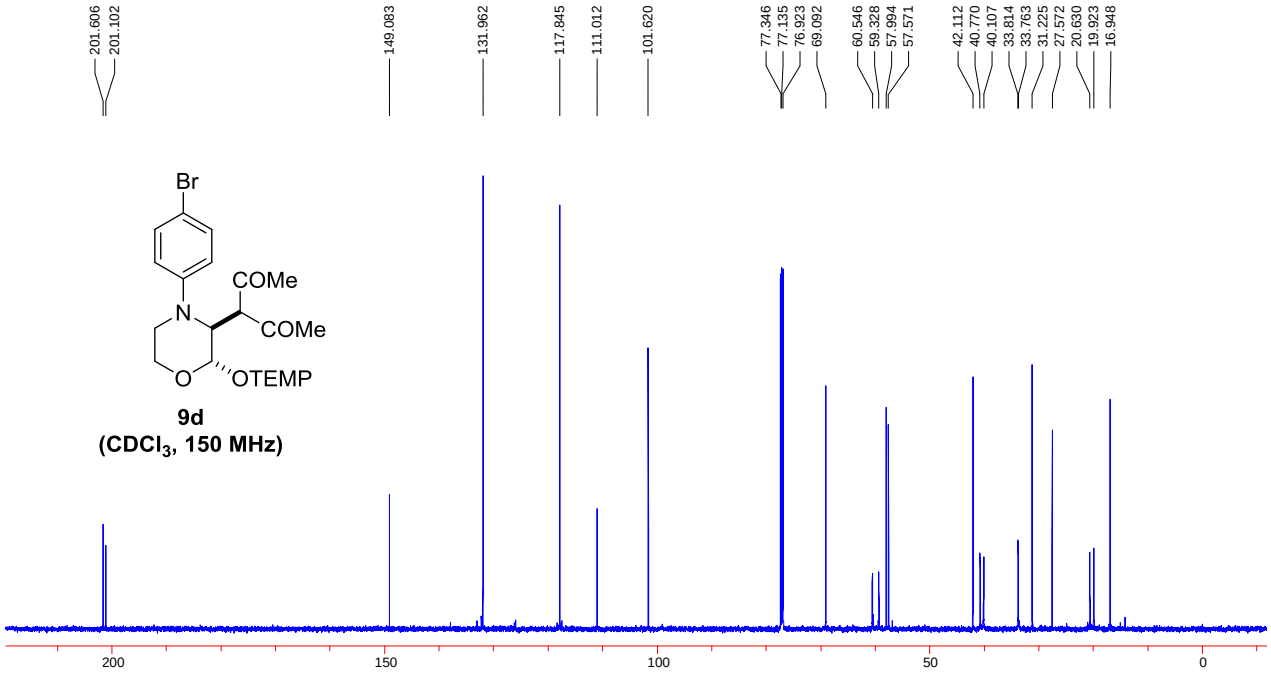


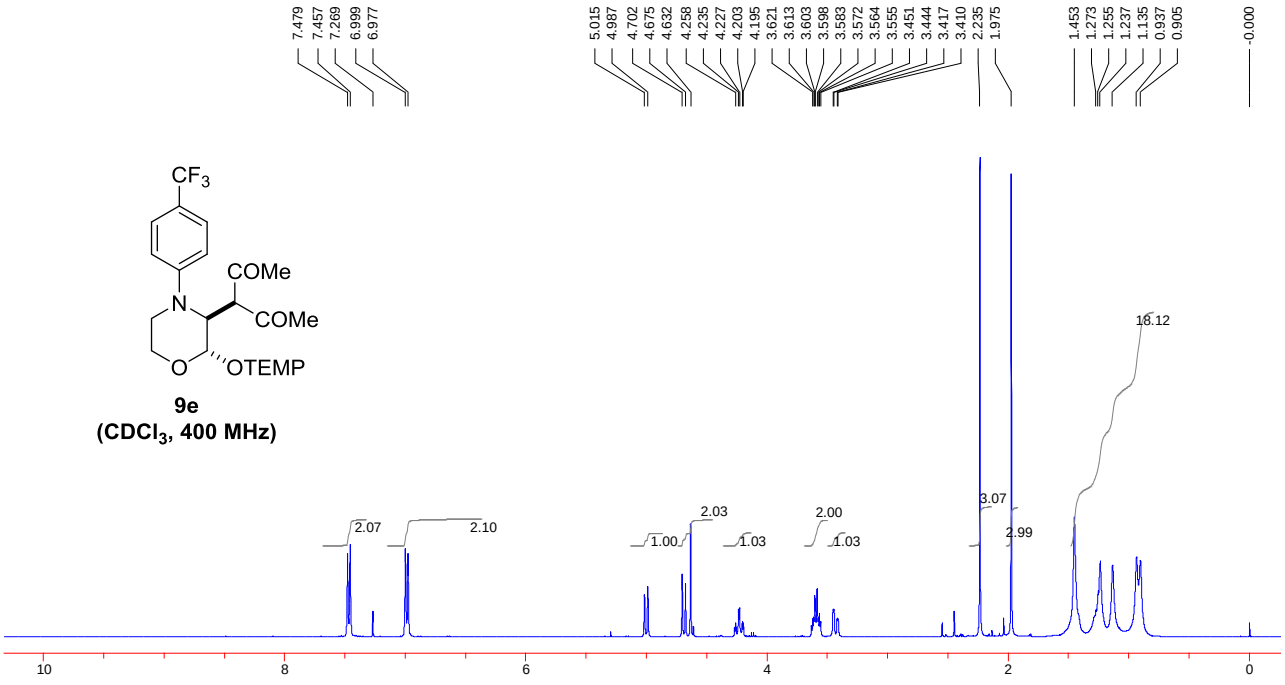
9c
($CDCl_3$, 150 MHz)

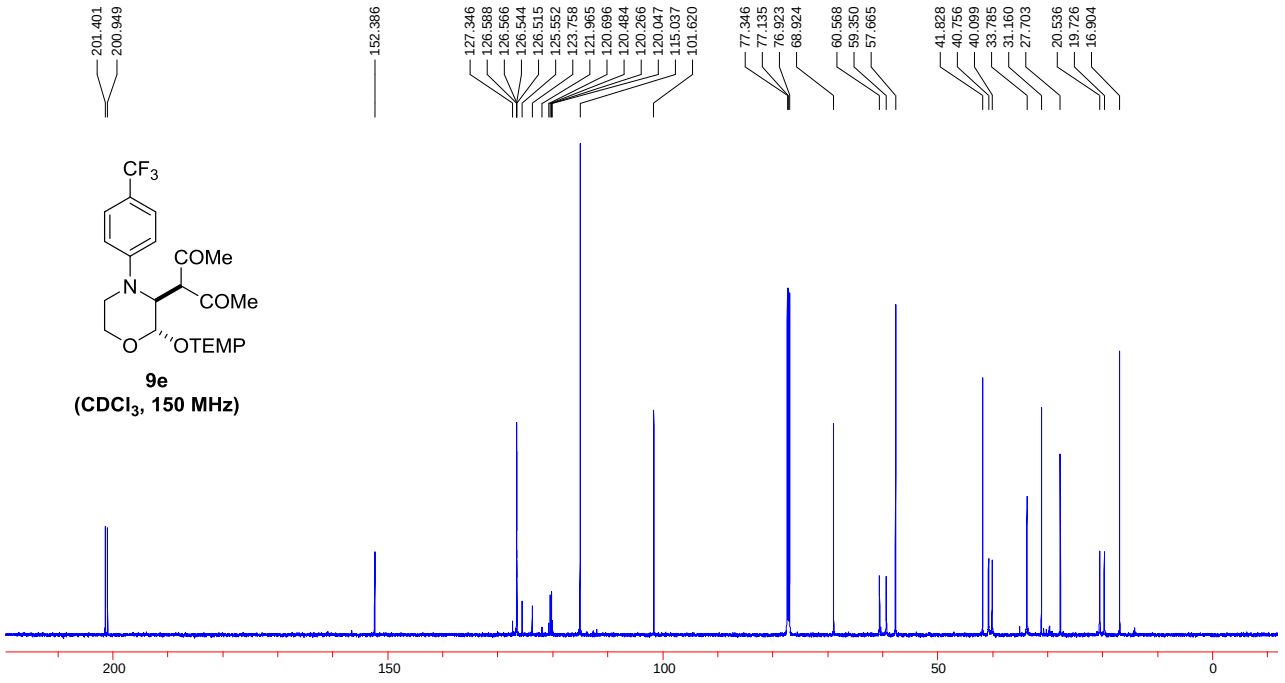


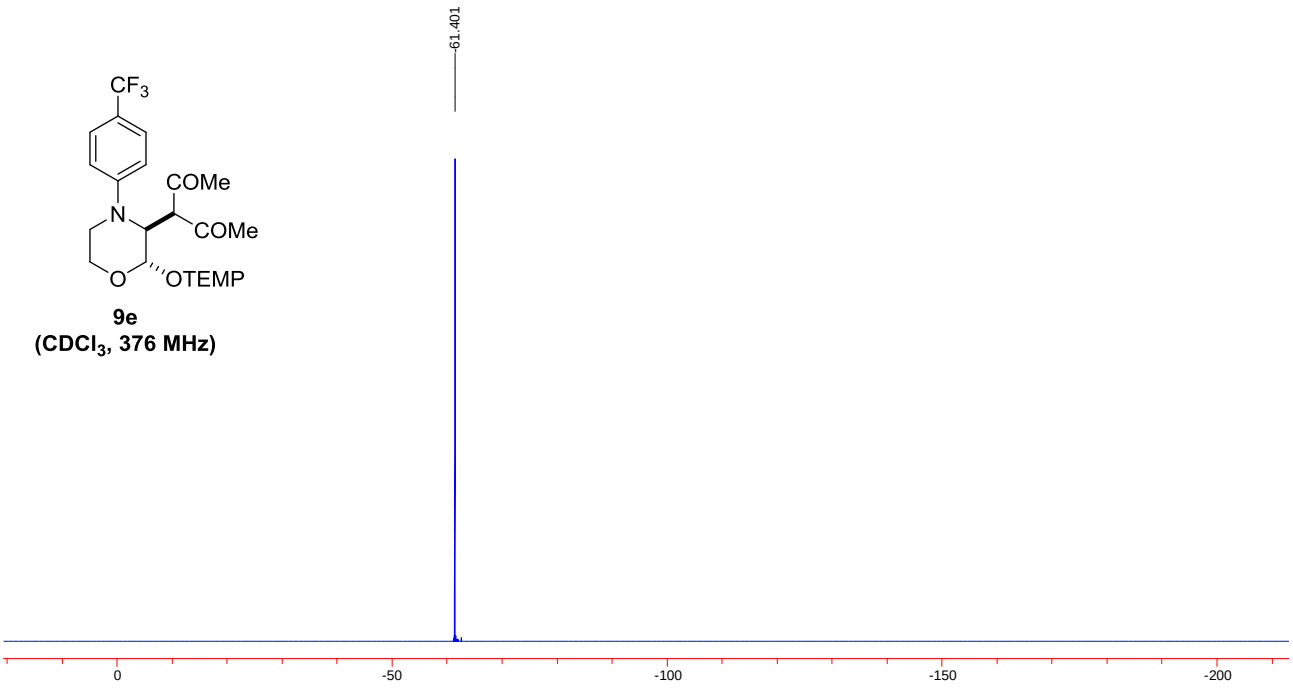
9c
($CDCl_3$, 376 MHz)


7.329
7.320
7.315
7.303
7.298
7.290
7.272
6.855
6.847
6.842
6.824
6.816
4.874
4.846
4.675
4.648
4.598
4.245
4.214
4.207
4.183
3.593
3.584
3.568
3.559
3.550
3.538
3.527
3.518
3.316
3.307
3.280
3.276
2.217
1.951
1.456
1.255
1.236
1.222
1.136
0.961
-0.000
Br
COMe
N
COMe
O
OTEMP
9d
(CDCl3, 400 MHz)
18.25
1.98
2.00
0.93
1.01
1.08
0.96
1.94
0.96
2.99
3.00
10
8
6
4
2
0

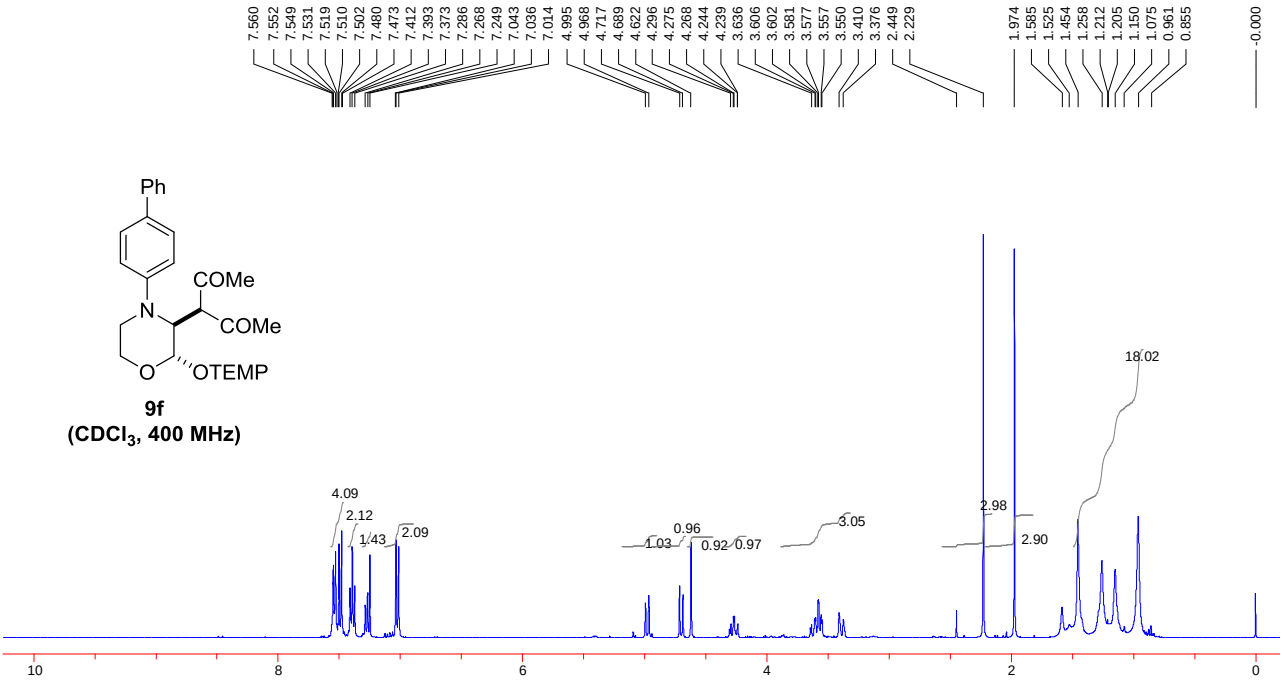

201.606
201.102
149.083
131.962
117.845
111.012
101.620
77.346
77.135
76.923
69.092
60.546
59.328
57.994
57.571
42.112
40.770
40.107
33.814
33.763
31.225
27.572
20.630
19.923
16.948
Br
COMe
N
COMe
O
OTEMP
9d
(CDCl3, 150 MHz)
200
150
100
50
0

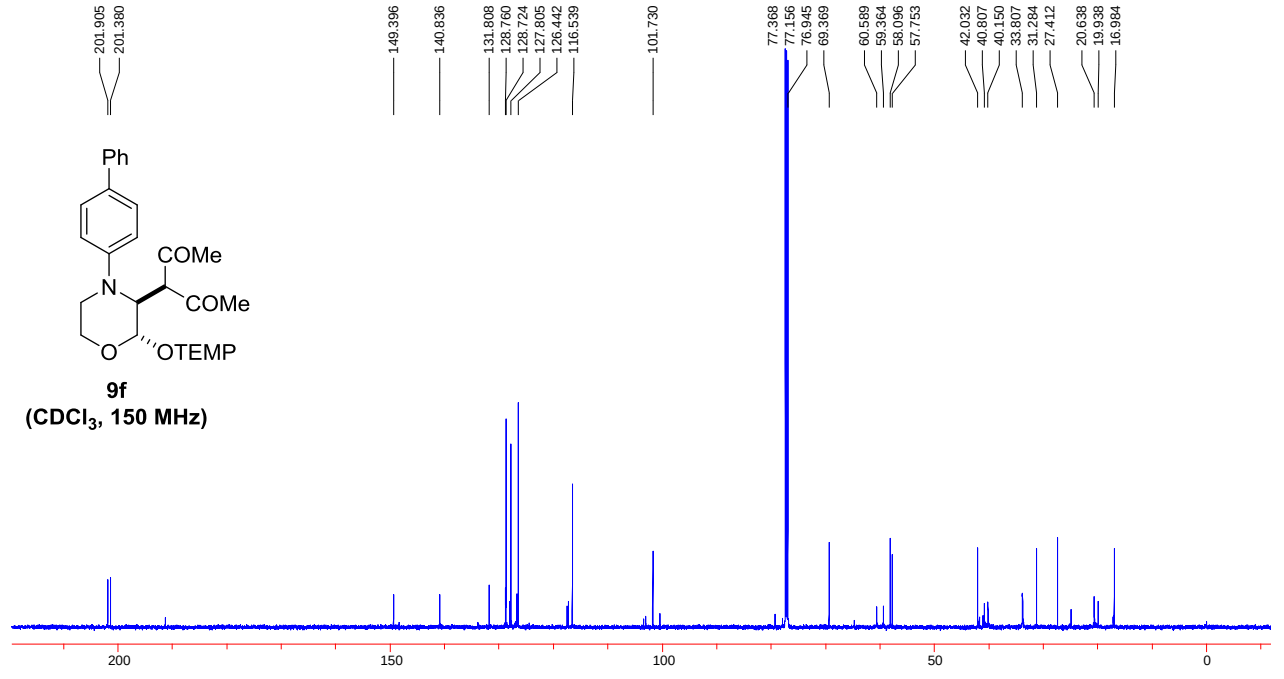

7.479
7.457
7.269
6.999
6.977
5.015
4.987
4.702
4.675
4.632
4.258
4.235
4.227
4.203
4.195
3.621
3.613
3.603
3.598
3.583
3.572
3.564
3.555
3.451
3.444
3.417
3.410
2.235
1.975
1.453
1.273
1.255
1.237
1.135
0.937
0.905
-0.000
CF3
COMe
N
COMe
O
OTEMP
9e
(CDCl3, 400 MHz)
2.07
2.10
1.00
2.03
1.03
2.00
1.03
3.07
2.99
18.12
10
8
6
4
2
0

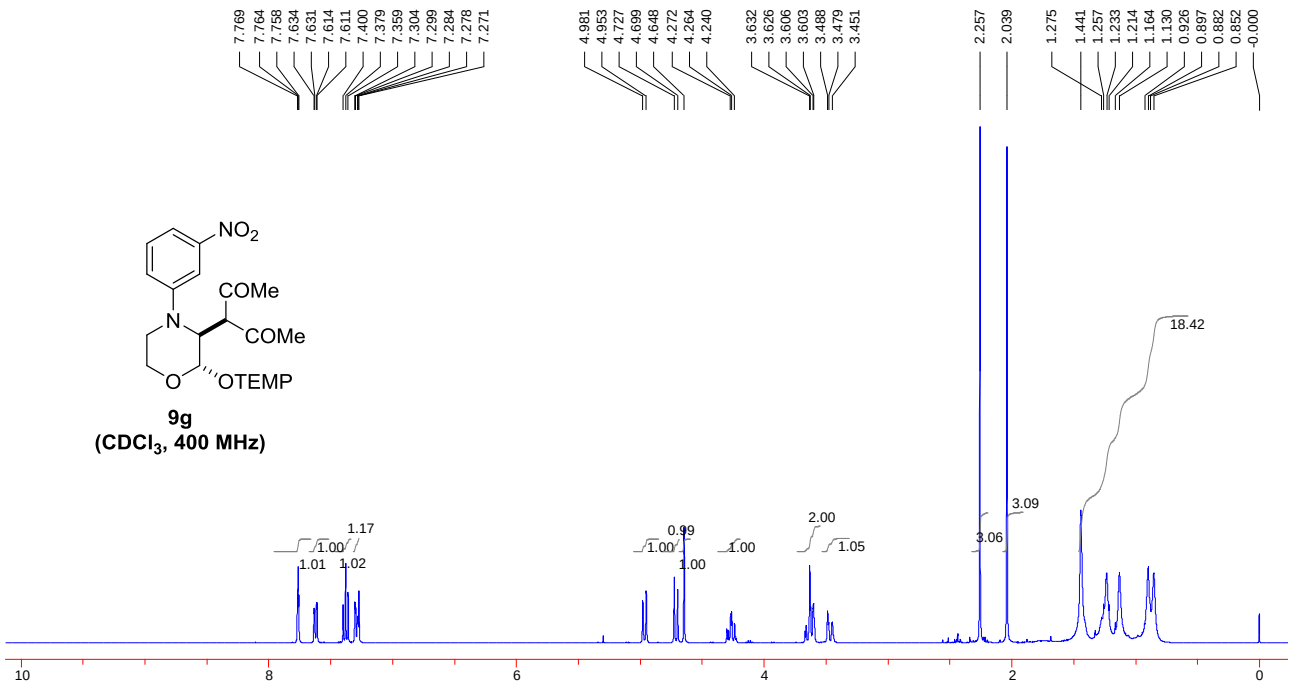

201.401
200.949
152.386
127.346
126.588
126.566
126.544
126.515
125.552
123.758
121.965
120.696
120.484
120.266
120.047
115.037
101.620
77.346
77.135
76.923
68.924
60.568
59.350
57.665
41.828
40.756
40.099
33.785
31.160
27.703
20.536
19.726
16.904
CF3
COMe
N
COMe
O
OTEMP
9e
(CDCl3, 150 MHz)
200
150
100
50
0

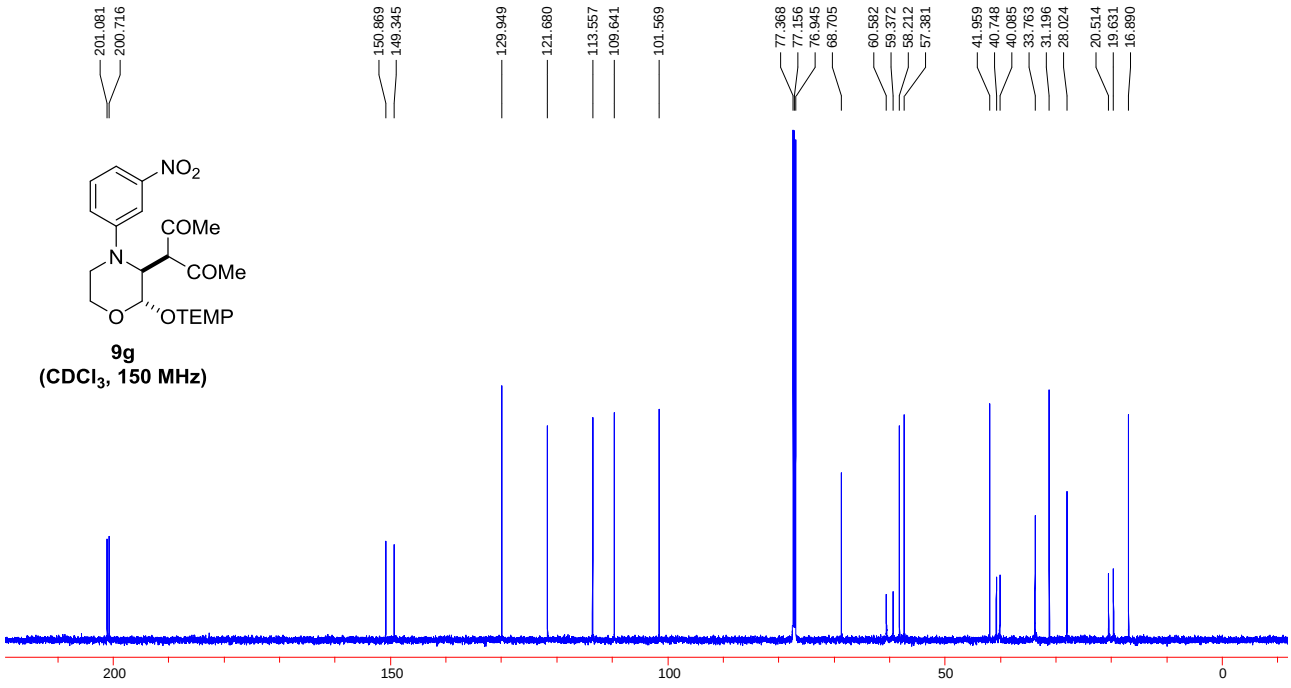


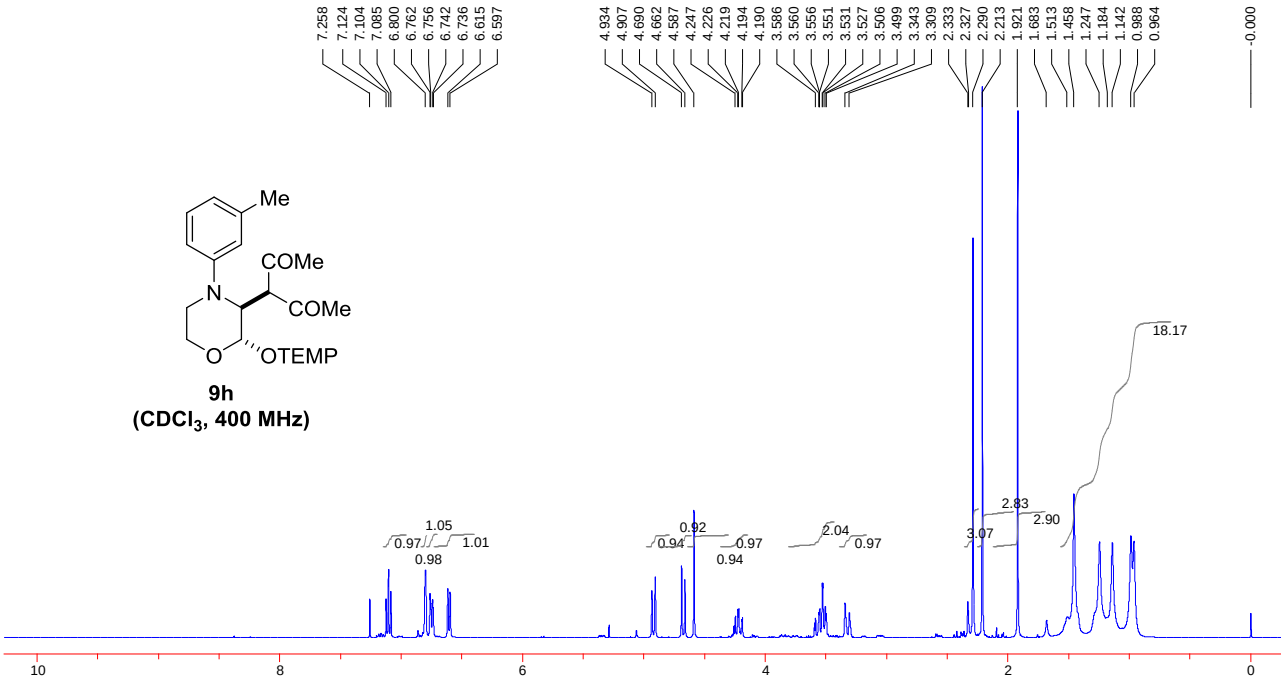
9e
($CDCl_3$, 376 MHz)

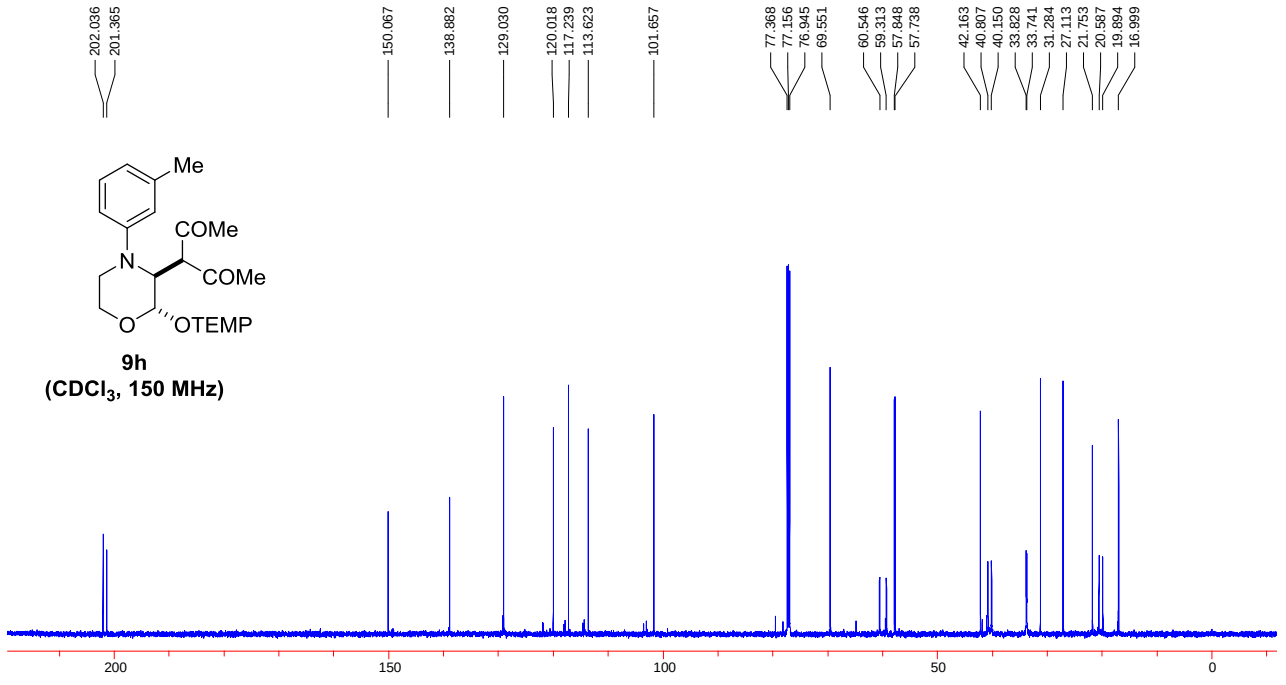

7.560
7.552
7.549
7.531
7.519
7.510
7.502
7.480
7.473
7.412
7.393
7.373
7.286
7.268
7.249
7.043
7.036
7.014
4.995
4.968
4.717
4.689
4.622
4.296
4.275
4.268
4.244
4.239
3.636
3.606
3.602
3.581
3.577
3.557
3.550
3.410
3.376
2.449
2.229
1.974
1.585
1.525
1.454
1.258
1.212
1.205
1.150
1.075
0.961
0.855
-0.000
Ph
COMe
COMe
N
O
OTEMP
9f
(CDCl3, 400 MHz)
4.09
2.12
1.43
2.09
1.03
0.96
0.92
0.97
3.05
2.98
2.90
18.02
10
8
6
4
2
0

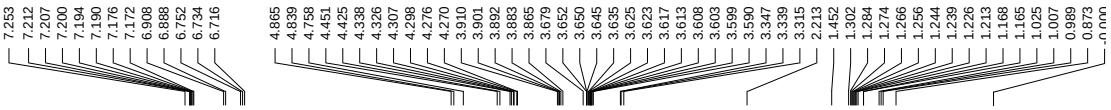

201.905
201.380
149.396
140.836
131.808
128.760
128.724
127.805
126.442
116.539
101.730
77.368
77.156
76.945
69.369
60.589
59.364
58.096
57.753
42.032
40.807
40.150
33.807
31.284
27.412
20.638
19.938
16.984
Ph
COMe
COMe
N
O
OTEMP
9f
(CDCl3, 150 MHz)
200
150
100
50
0

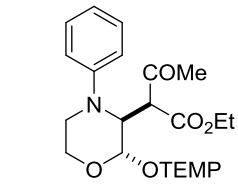

7.769
7.764
7.758
7.634
7.631
7.614
7.611
7.400
7.379
7.359
7.304
7.299
7.284
7.278
7.271
4.981
4.953
4.727
4.699
4.648
4.272
4.264
4.240
3.632
3.626
3.606
3.603
3.488
3.479
3.451
2.257
2.039
1.275
1.441
1.257
1.233
1.214
1.164
1.130
0.926
0.897
0.882
0.852
-0.000
NO2
COMe
COMe
OTEMP
9g
(CDCl3, 400 MHz)
1.17
1.00
1.01
1.02
0.99
1.00
1.00
1.00
2.00
1.05
3.09
3.06
18.42
10
8
6
4
2
0


201.081
200.716
150.869
149.345
129.949
121.680
113.557
109.641
101.569
77.368
77.156
76.945
68.705
60.582
59.372
58.212
57.381
41.959
40.748
40.085
33.763
31.196
28.024
20.514
19.631
16.890
NO2
COMe
COMe
OTEMP
9g
(CDCl3, 150 MHz)
200
150
100
50
0

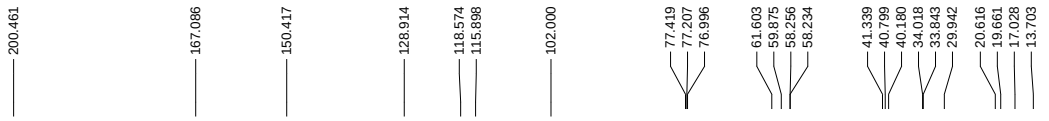

7.258
7.124
7.104
7.085
6.800
6.762
6.756
6.742
6.736
6.615
6.597
4.934
4.907
4.690
4.662
4.587
4.247
4.226
4.219
4.194
4.190
3.586
3.560
3.556
3.551
3.531
3.527
3.506
3.499
3.343
3.309
2.333
2.327
2.290
2.213
1.921
1.683
1.513
1.458
1.247
1.184
1.142
0.988
0.964
-0.000
Me
COMe
COMe
N
O
OTEMP
9h
(CDCl3, 400 MHz)
1.05
0.97
1.01
0.98
0.92
0.94
0.97
0.94
2.04
0.97
18.17
2.83
2.90
3.07
10
8
6
4
2
0

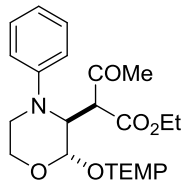

202.036
201.365
150.067
138.882
129.030
120.018
117.239
113.623
101.657
77.368
77.156
76.945
69.551
60.546
59.313
57.848
57.738
42.163
40.807
40.150
33.828
33.741
31.284
27.113
21.753
20.587
19.894
16.999
Me
COMe
COMe
N
O
OTEMP
9h
(CDCl3, 150 MHz)
200
150
100
50
0



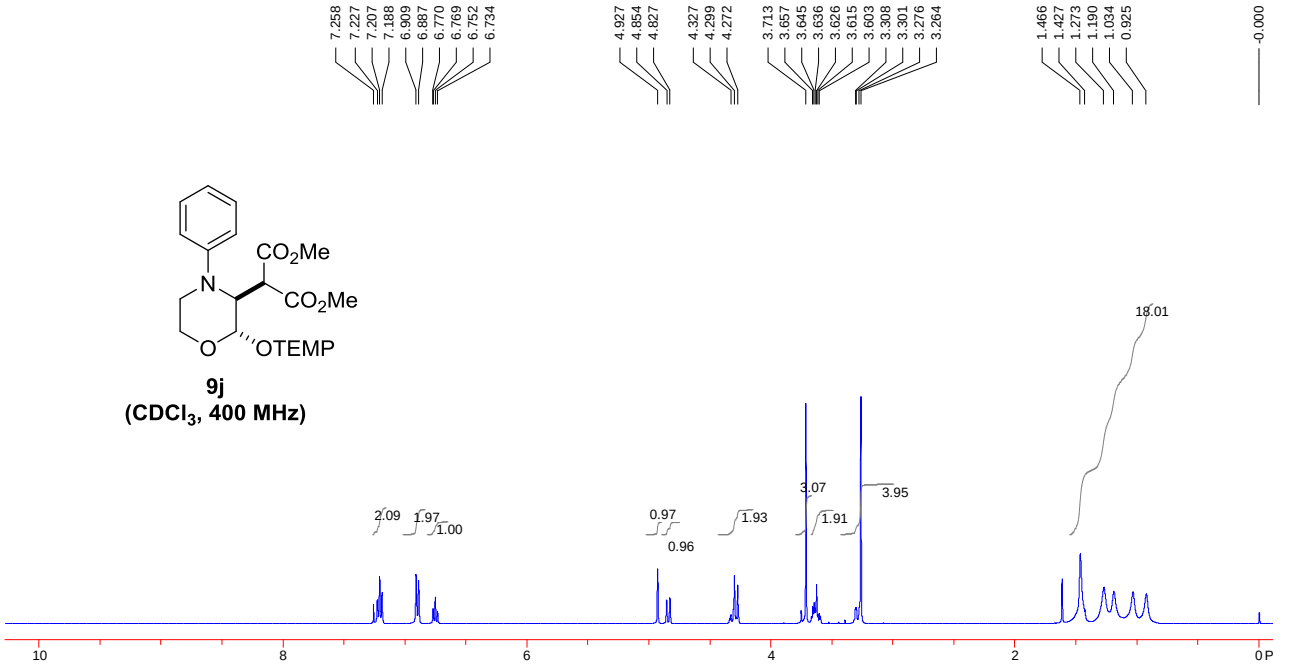


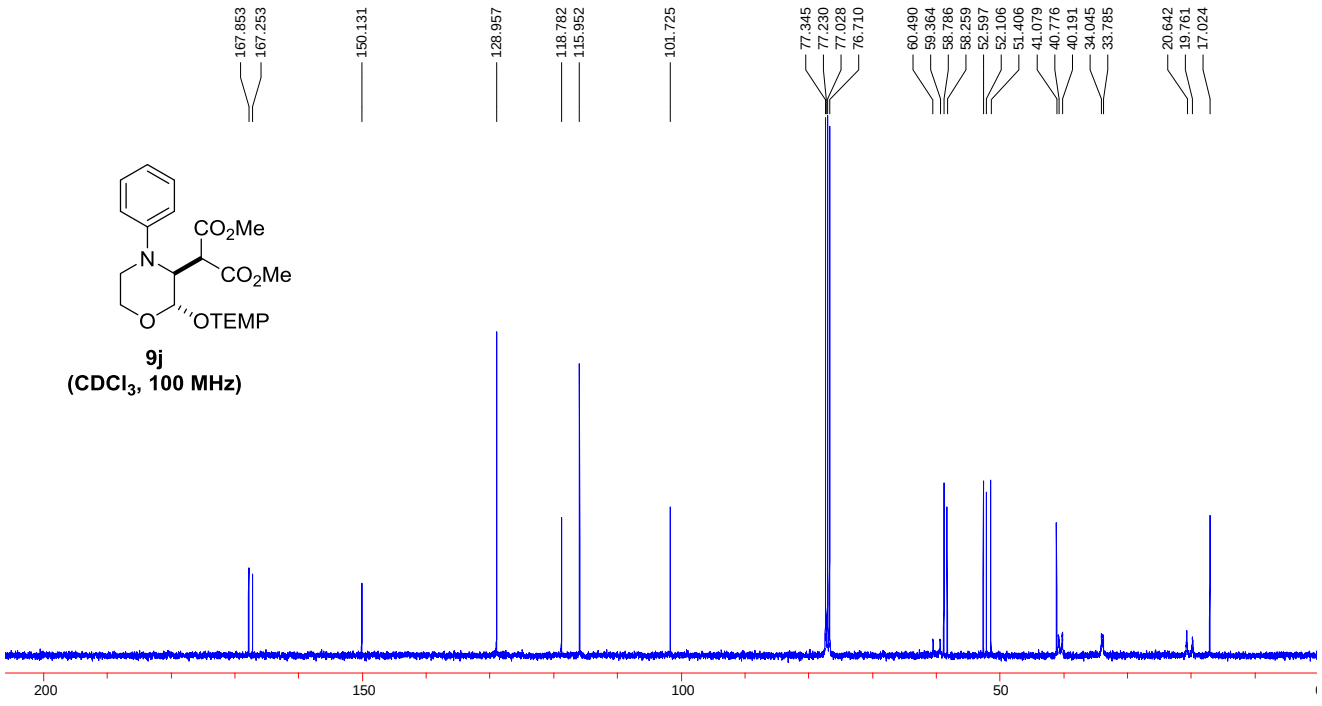
9i
($CDCl_3$, 400 MHz)

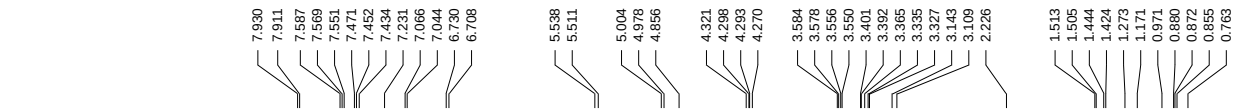


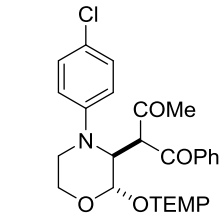


9i
($CDCl_3$, 150 MHz)

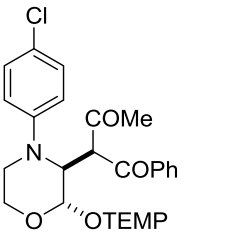

7.258
7.227
7.207
7.188
6.909
6.887
6.770
6.769
6.752
6.734
4.927
4.854
4.827
4.327
4.299
4.272
3.713
3.657
3.645
3.636
3.626
3.615
3.603
3.308
3.301
3.276
3.264
1.466
1.427
1.273
1.190
1.034
0.925
-0.000
CO2Me
CO2Me
N
O
OTEMP
9j
(CDCl3, 400 MHz)
18.01
3.07
3.95
2.09
1.97
1.00
0.97
0.96
1.93
1.91
10
8
6
4
2
0 P


167.853
167.253
150.131
128.957
118.782
115.952
101.725
77.345
77.230
77.028
76.710
60.490
59.364
58.786
58.259
52.597
52.106
51.406
41.079
40.776
40.191
34.045
33.785
20.642
19.761
17.024
CO2Me
CO2Me
N
O
OTEMP
9j
(CDCl3, 100 MHz)
200
150
100
50

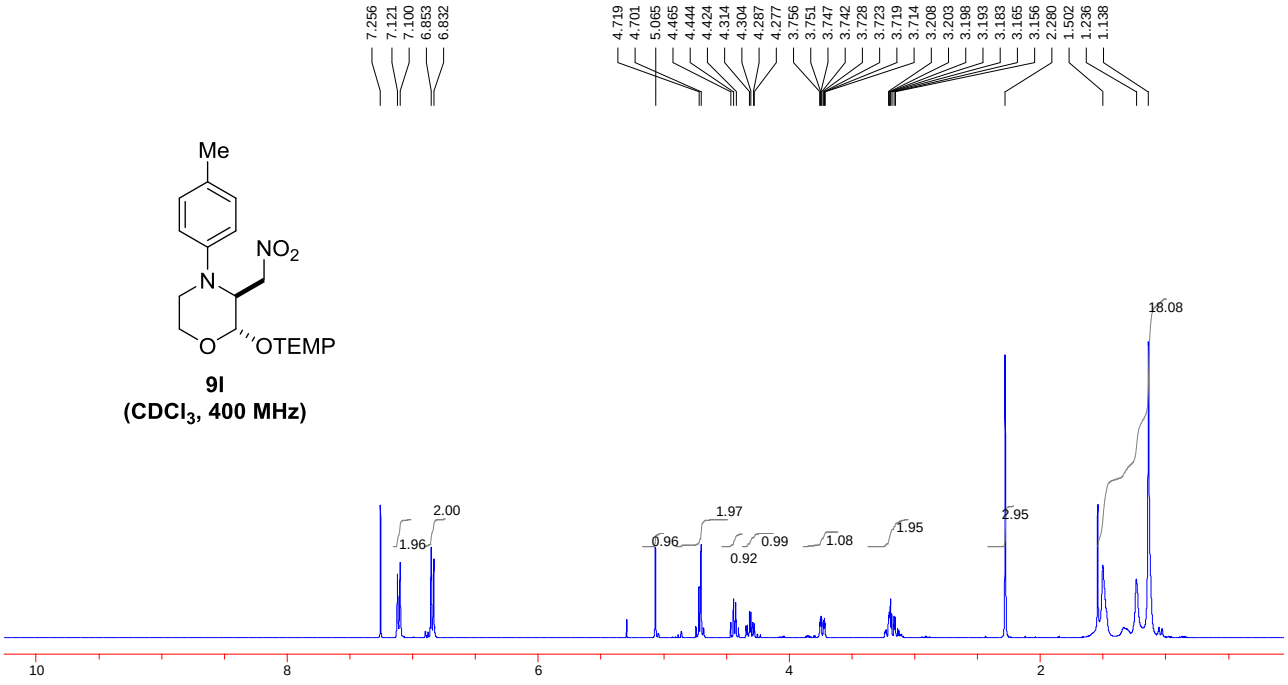


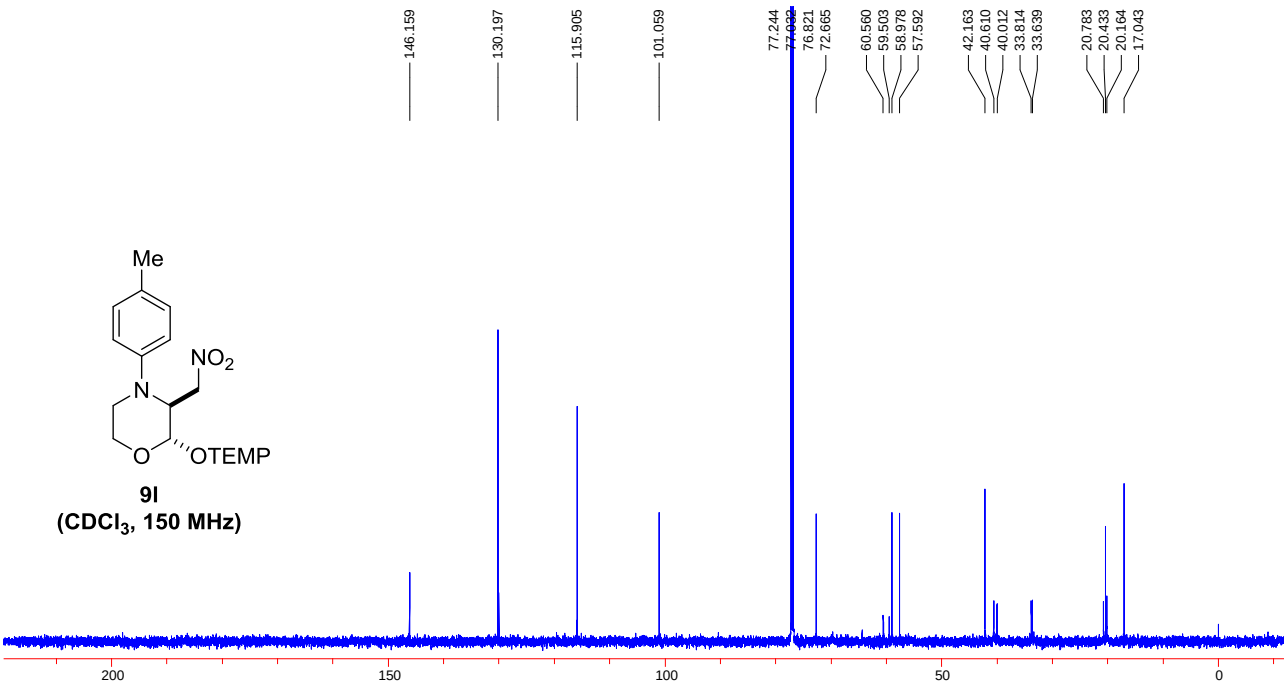


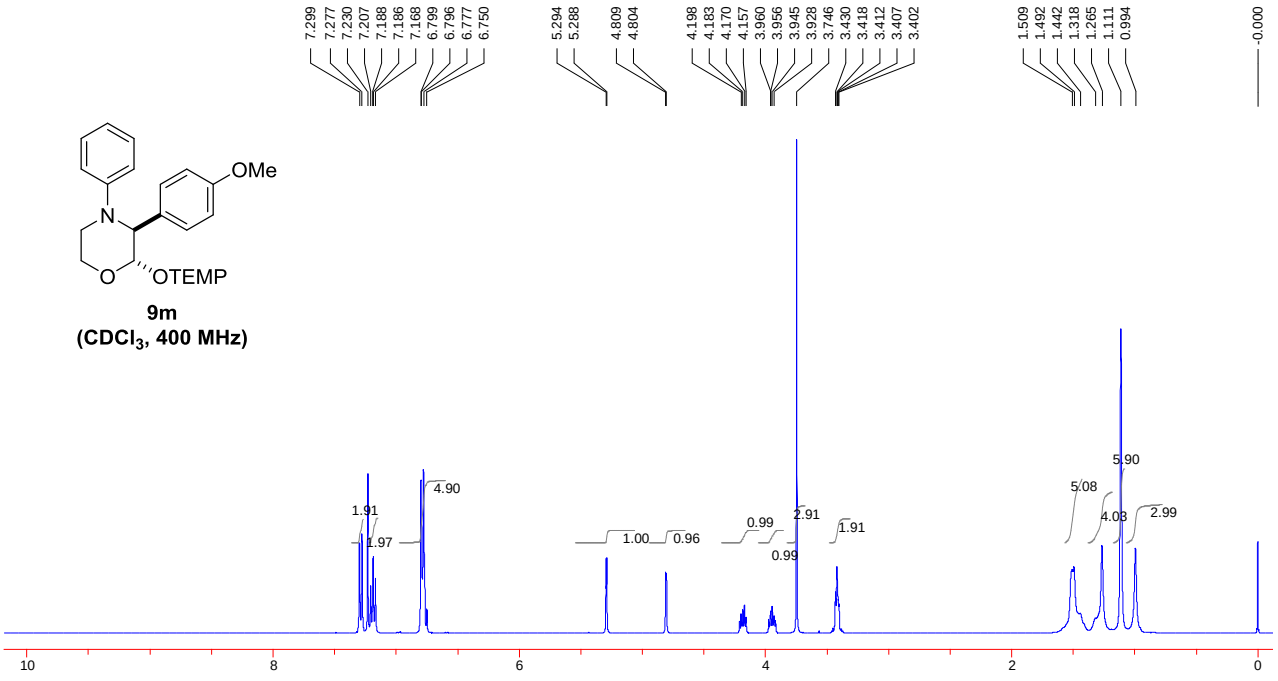
9k
($CDCl_3$, 400 MHz)



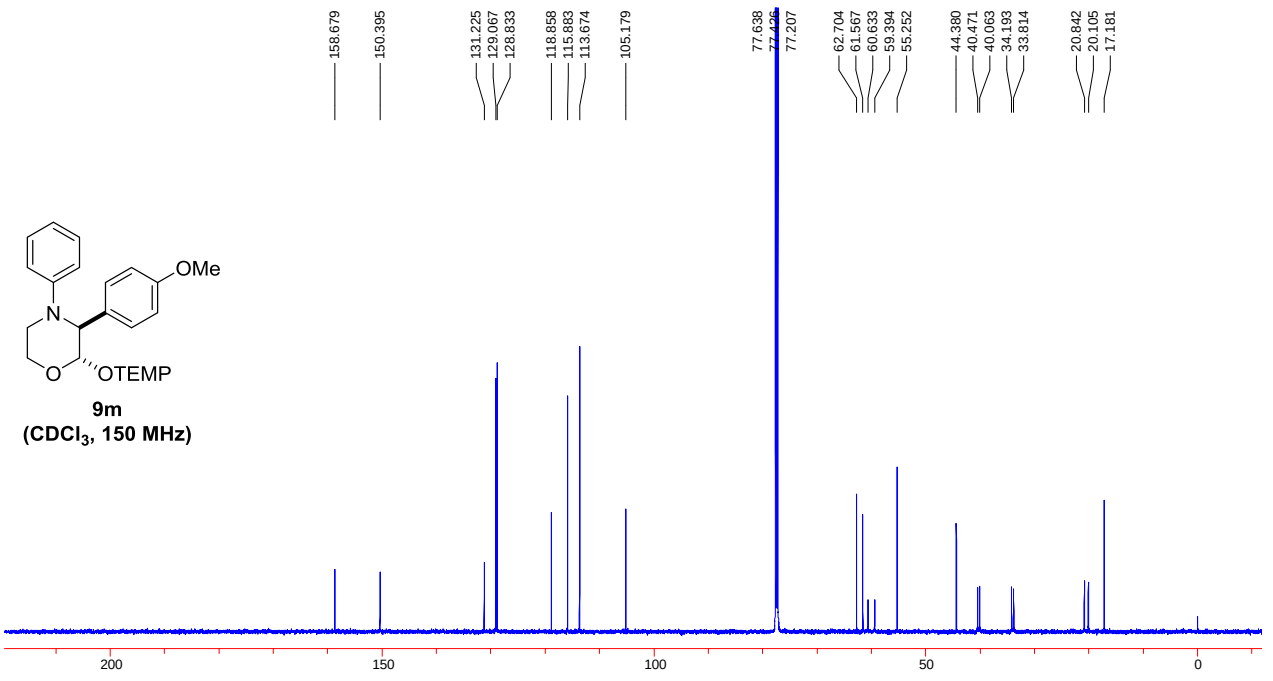
9k
($CDCl_3$, 100 MHz)


7.256
7.121
7.100
6.853
6.832
4.719
4.701
5.065
4.465
4.444
4.424
4.314
4.304
4.287
4.277
3.756
3.751
3.747
3.742
3.728
3.723
3.719
3.714
3.208
3.203
3.198
3.193
3.183
3.165
3.156
2.280
1.502
1.236
1.138
Me
NO2
N
O
OTEMP
9l
(CDCl3, 400 MHz)
18.08
2.00
1.96
1.97
0.96
0.99
0.92
1.08
1.95
2.95
10
8
6
4
2

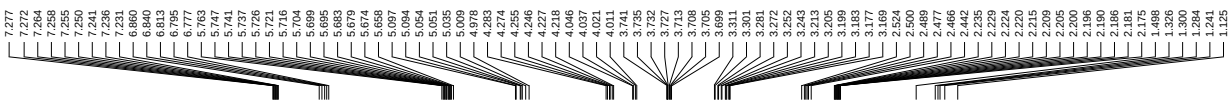

146.159
130.197
115.905
101.059
77.244
77.032
76.821
72.665
60.560
59.503
58.978
57.592
42.163
40.610
40.012
33.814
33.639
20.783
20.433
20.164
17.043
Me
NO2
N
O
OTEMP
9l
(CDCl3, 150 MHz)
200
150
100
50
0

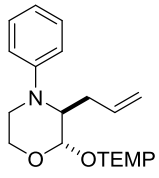


9m
($CDCl_3$, 400 MHz)

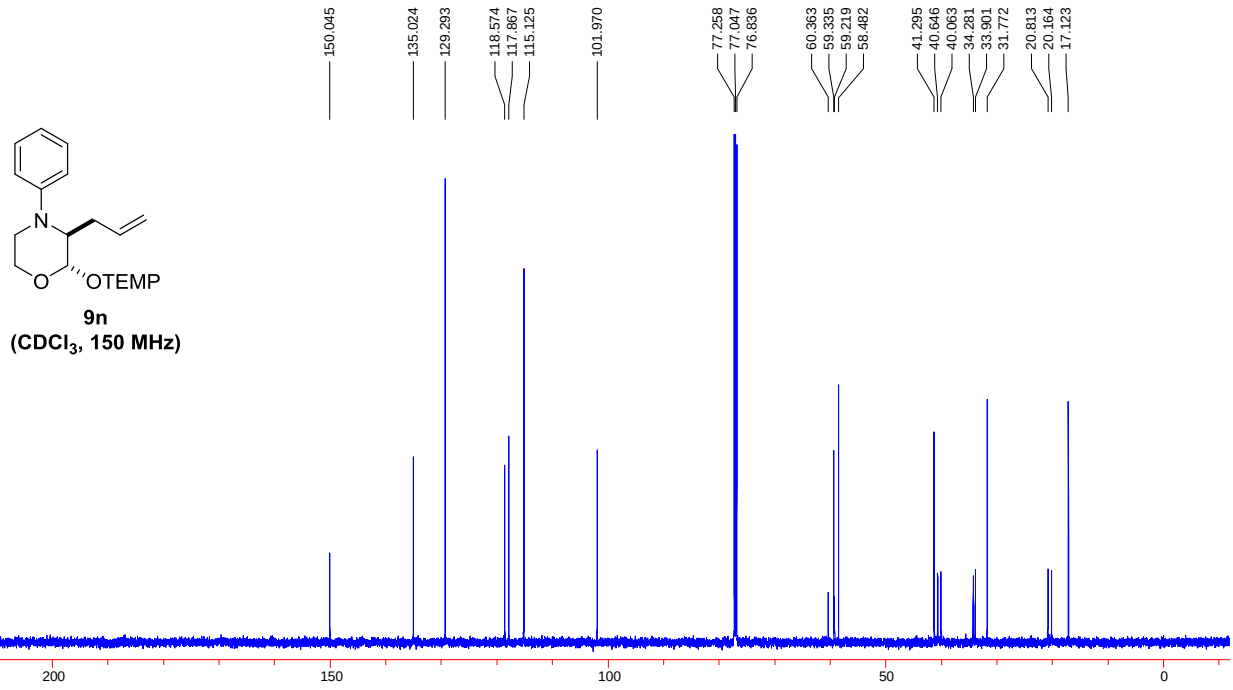


9m
($CDCl_3$, 150 MHz)

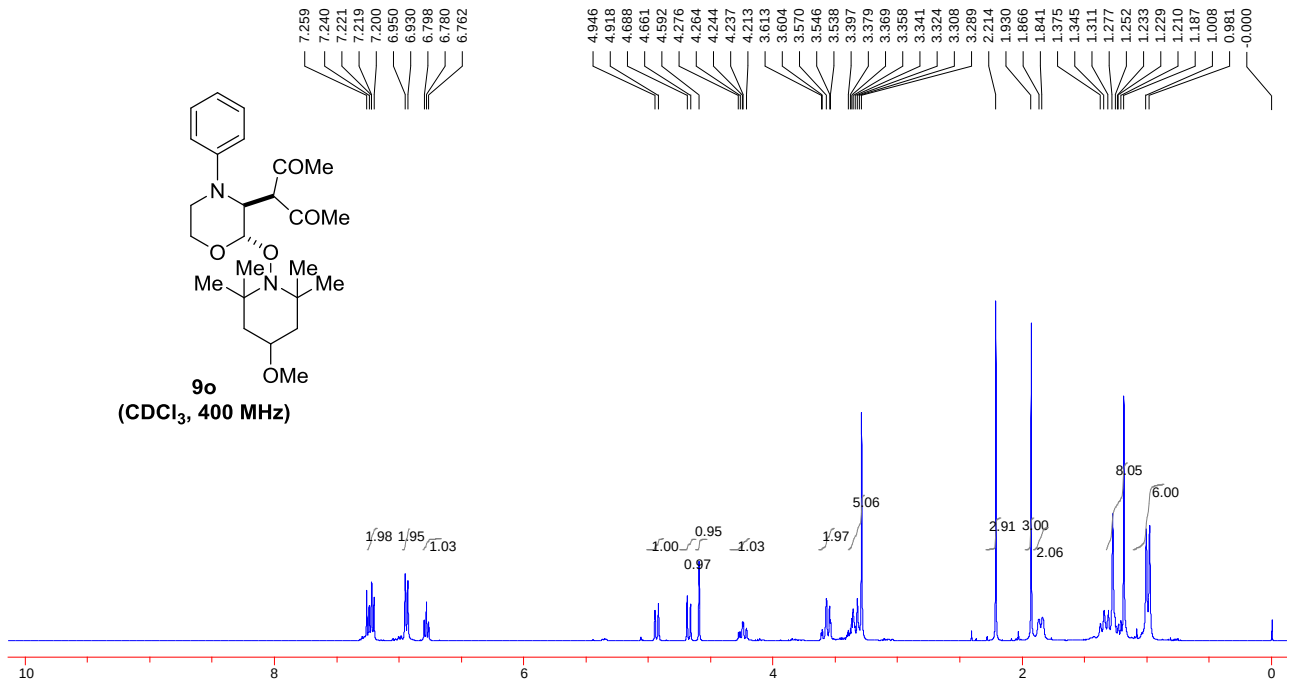


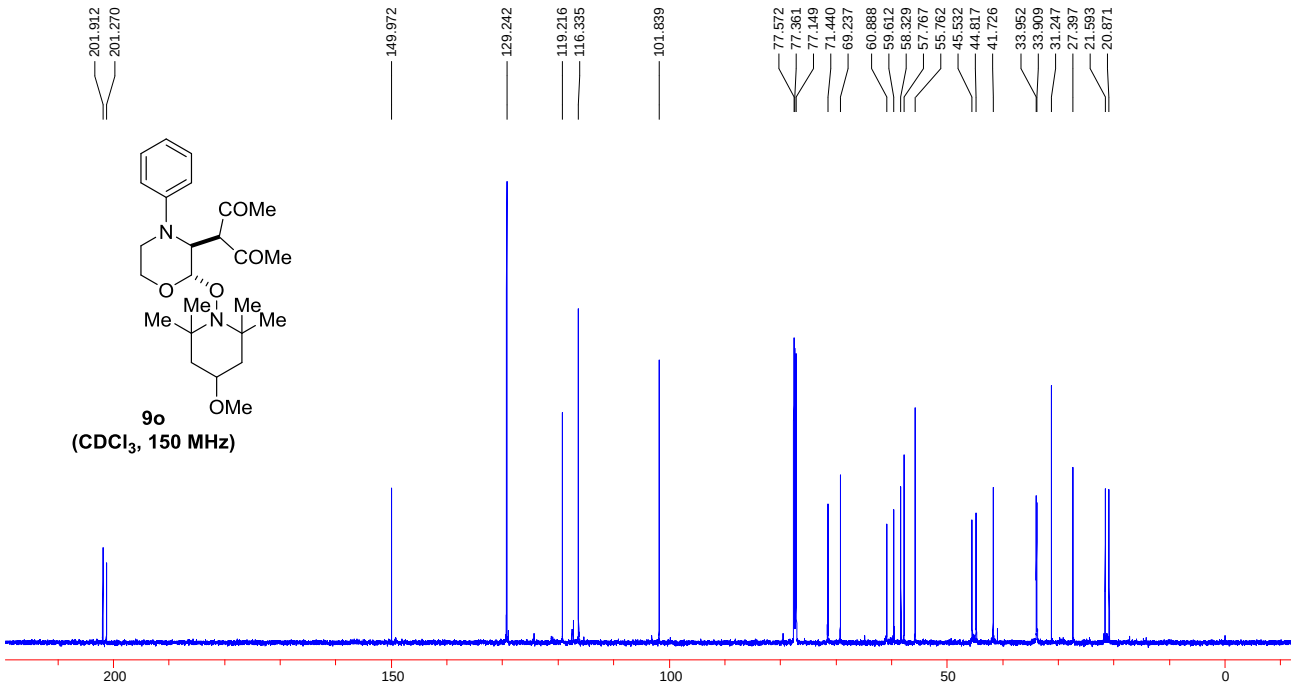


9n
($CDCl_3$, 400 MHz)



9n
($CDCl_3$, 150 MHz)


7.259
7.240
7.221
7.219
7.200
6.950
6.930
6.798
6.780
6.762
4.946
4.918
4.688
4.661
4.592
4.276
4.264
4.244
4.237
4.213
3.613
3.604
3.570
3.546
3.538
3.397
3.379
3.369
3.358
3.341
3.324
3.308
3.289
2.214
1.930
1.866
1.841
1.375
1.345
1.311
1.277
1.252
1.233
1.229
1.210
1.187
1.008
0.981
-0.000
COMe
COMe
N
O
O
Me
Me
Me
N
Me
OMe
9o
(CDCl3, 400 MHz)
1.98
1.95
1.03
1.00
0.95
0.97
1.03
1.97
5.06
2.91
3.00
2.06
8.05
6.00
10
8
6
4
2
0


201.912
201.270
149.972
129.242
119.216
116.335
101.839
77.572
77.361
77.149
71.440
69.237
60.888
59.612
58.329
57.767
55.762
45.532
44.817
41.726
33.952
33.909
31.247
27.397
21.593
20.871
COMe
COMe
N
O
O
Me
Me
Me
N
Me
OMe
9o
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100
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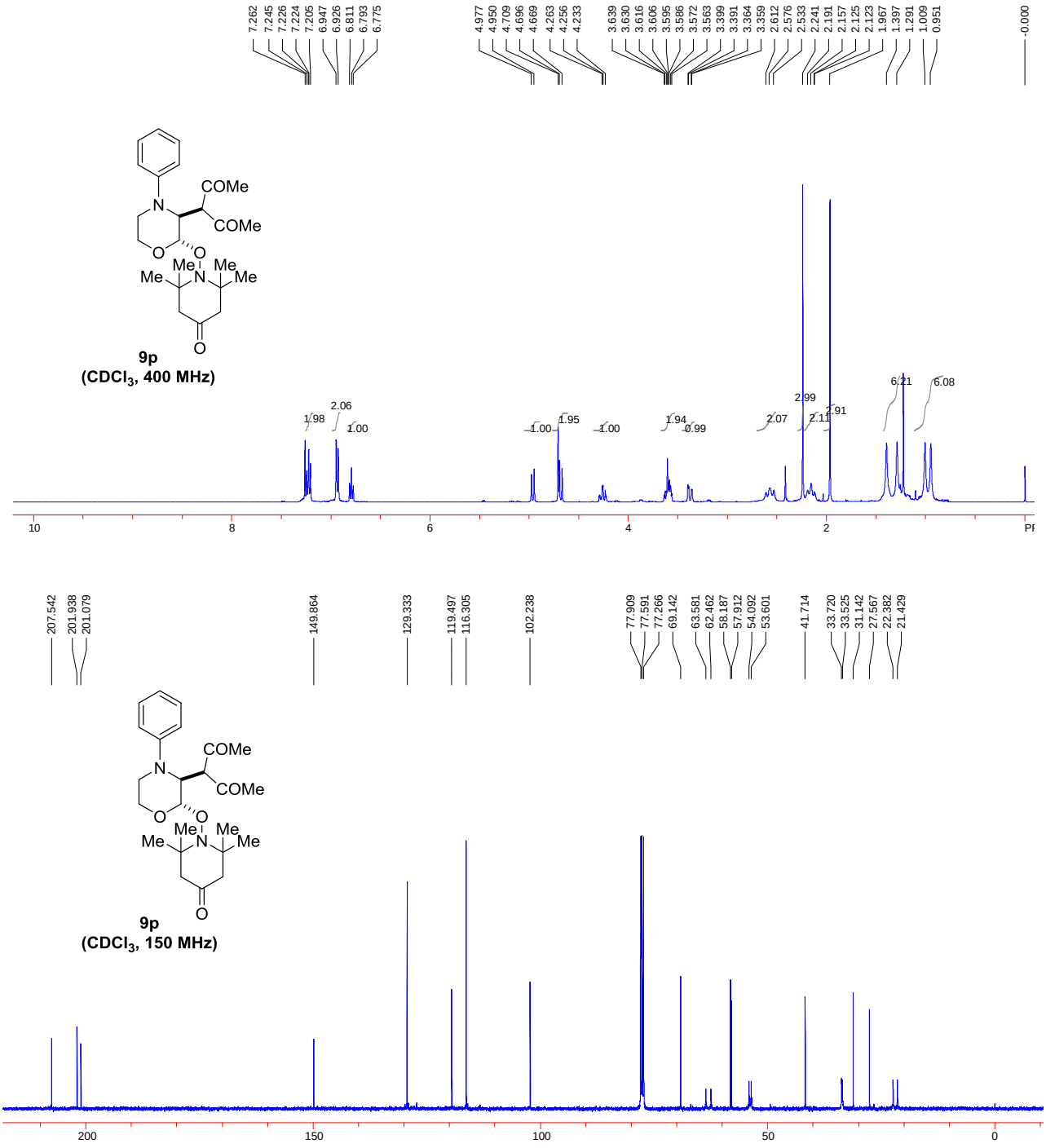
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2.533
2.241
2.191
2.157
2.125
2.123
1.967
1.397
1.291
1.009
0.951
-0.000
COMe
COMe
N
O
O
Me
N
Me
Me
Me
O
9p
(CDCl3, 400 MHz)
1.98
2.06
1.00
1.00
1.95
1.00
1.94
0.99
2.07
2.99
2.11
2.91
6.21
6.08
10
8
6
4
2
Pr
207.542
201.938
201.079
149.864
129.333
119.497
116.305
102.238
77.909
77.591
77.266
69.142
63.581
62.462
58.187
57.912
54.092
53.601
41.714
33.720
33.525
31.142
27.567
22.382
21.429
COMe
COMe
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Me
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Me
Me
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9p
(CDCl3, 150 MHz)
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50
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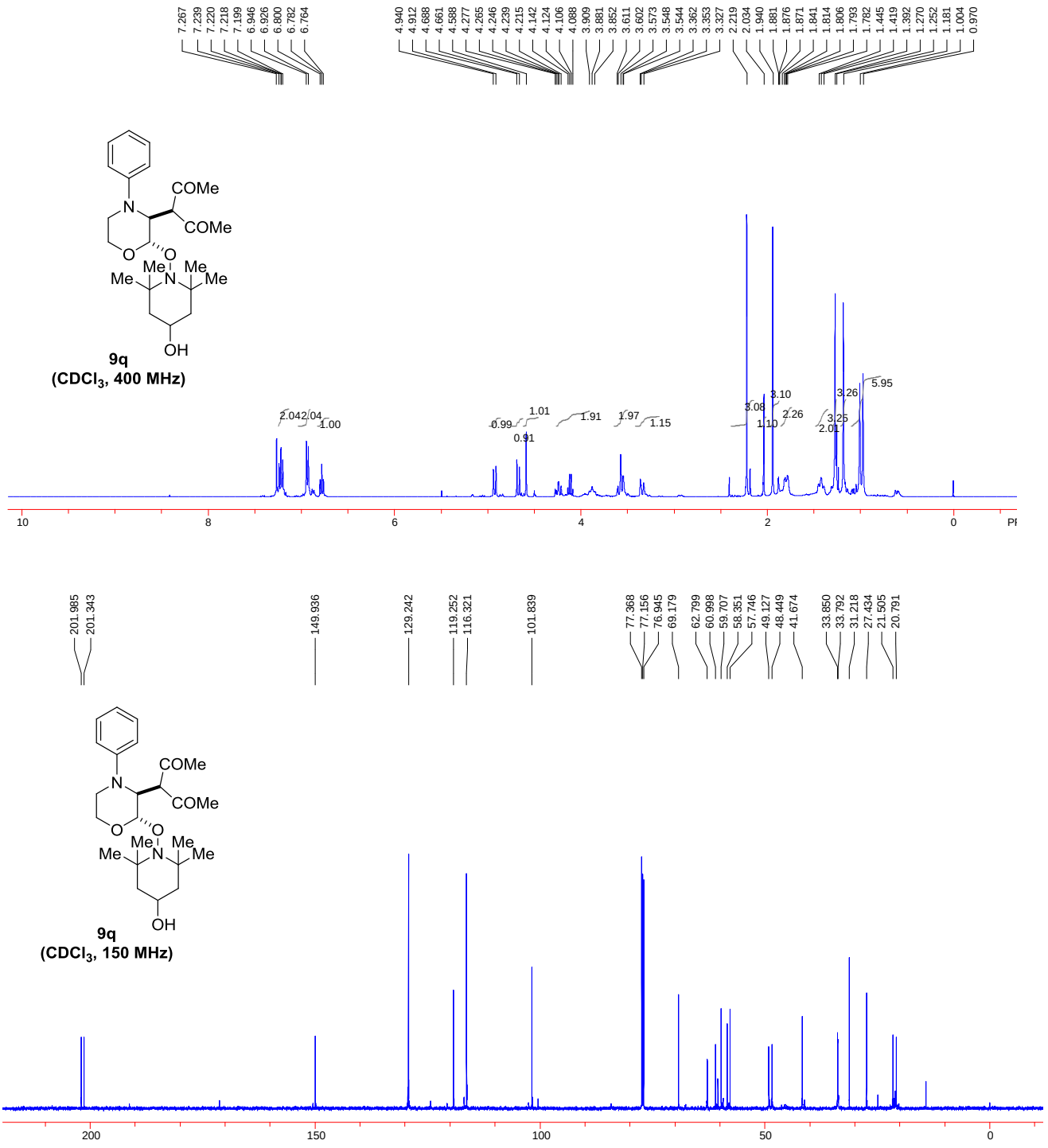
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3.602
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3.327
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1.881
1.876
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1.814
1.806
1.793
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1.392
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COMe
N
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Me
Me
Me
N
Me
OH
9q
(CDCl3, 400 MHz)
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2.04
1.00
0.99
1.01
0.91
1.91
1.97
1.15
3.08
3.10
1.10
2.26
2.01
3.25
3.26
5.95
10
8
6
4
2
0
201.985
201.343
149.936
129.242
119.252
116.321
101.839
77.368
77.156
76.945
69.179
62.799
60.998
59.707
58.351
57.746
49.127
48.449
41.674
33.850
33.792
31.218
27.434
21.505
20.791
COMe
COMe
N
O
O
Me
Me
Me
N
Me
OH
9q
(CDCl3, 150 MHz)
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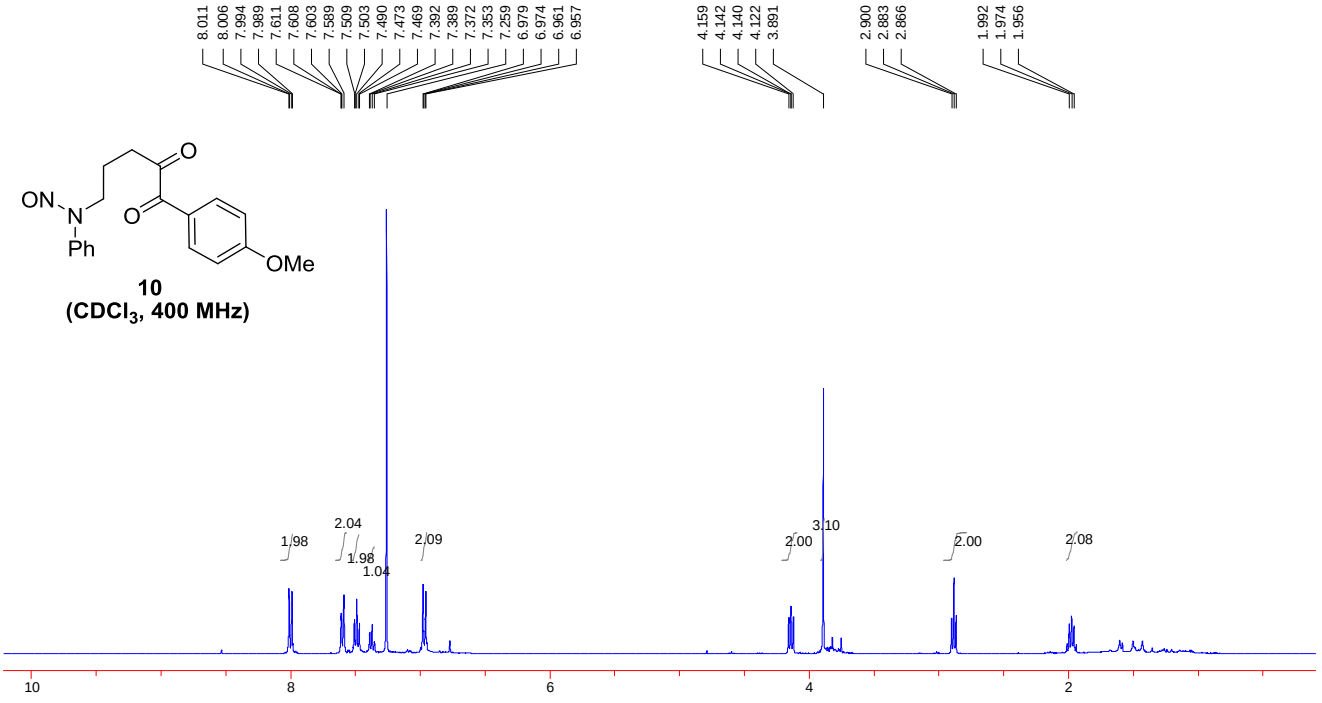
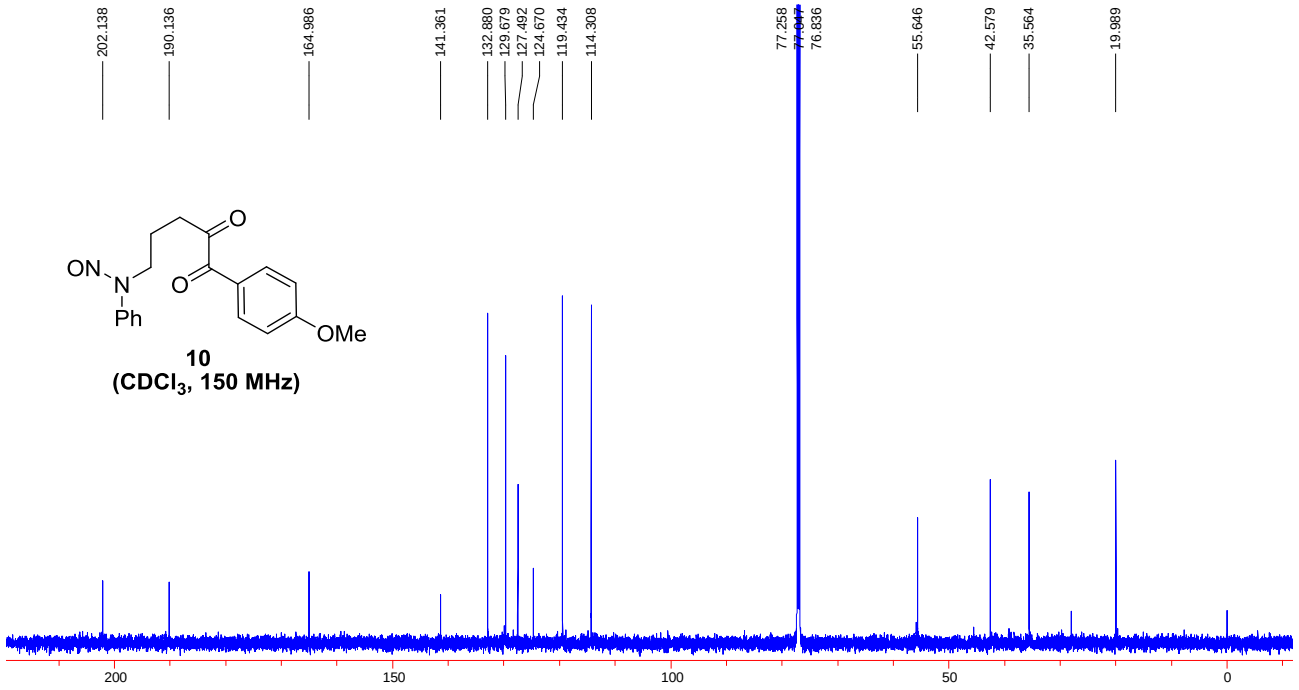
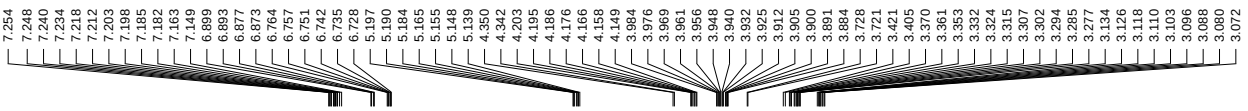
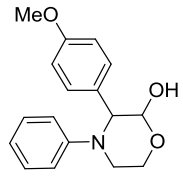
150
100
50
0

VII. Copies of the NMR and HPLC Spectra of 10-13 and 15









11
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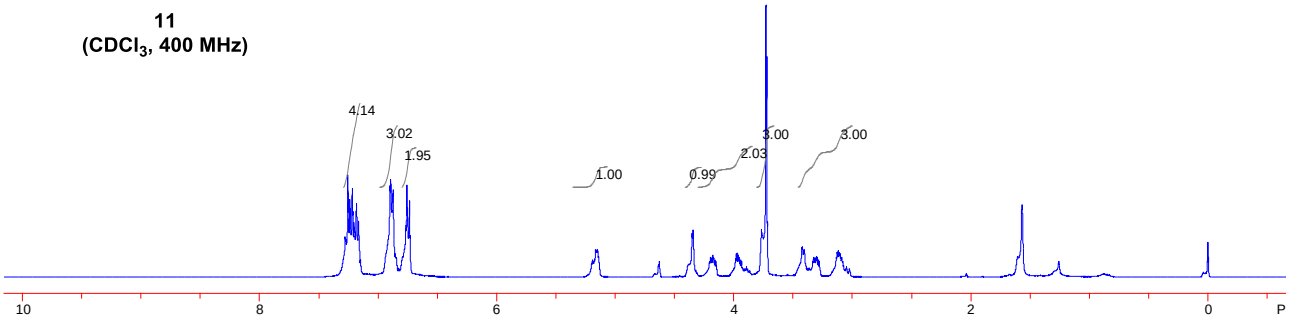

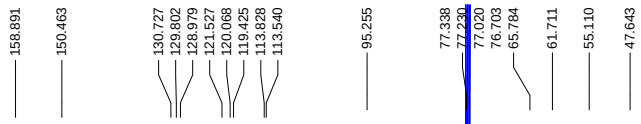

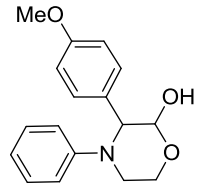

11
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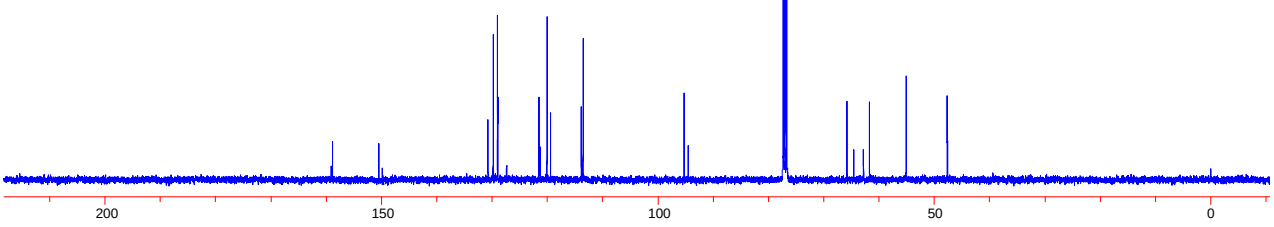

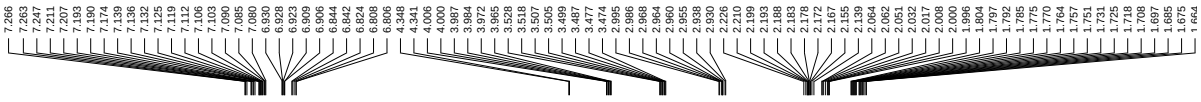

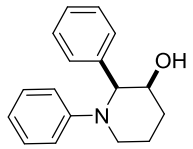

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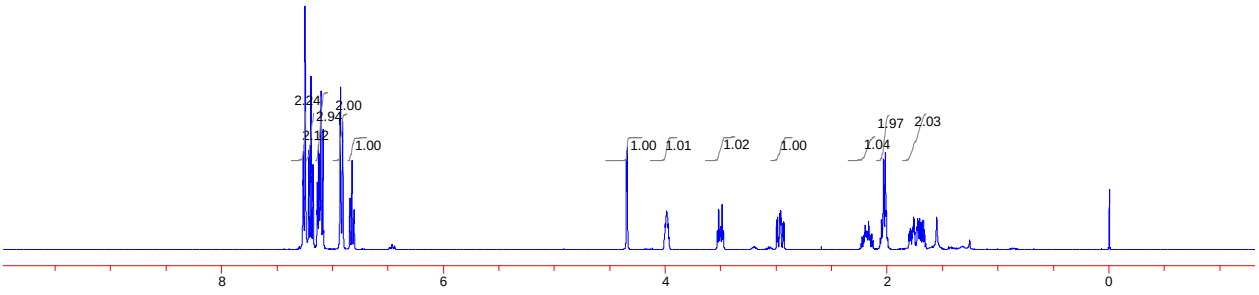

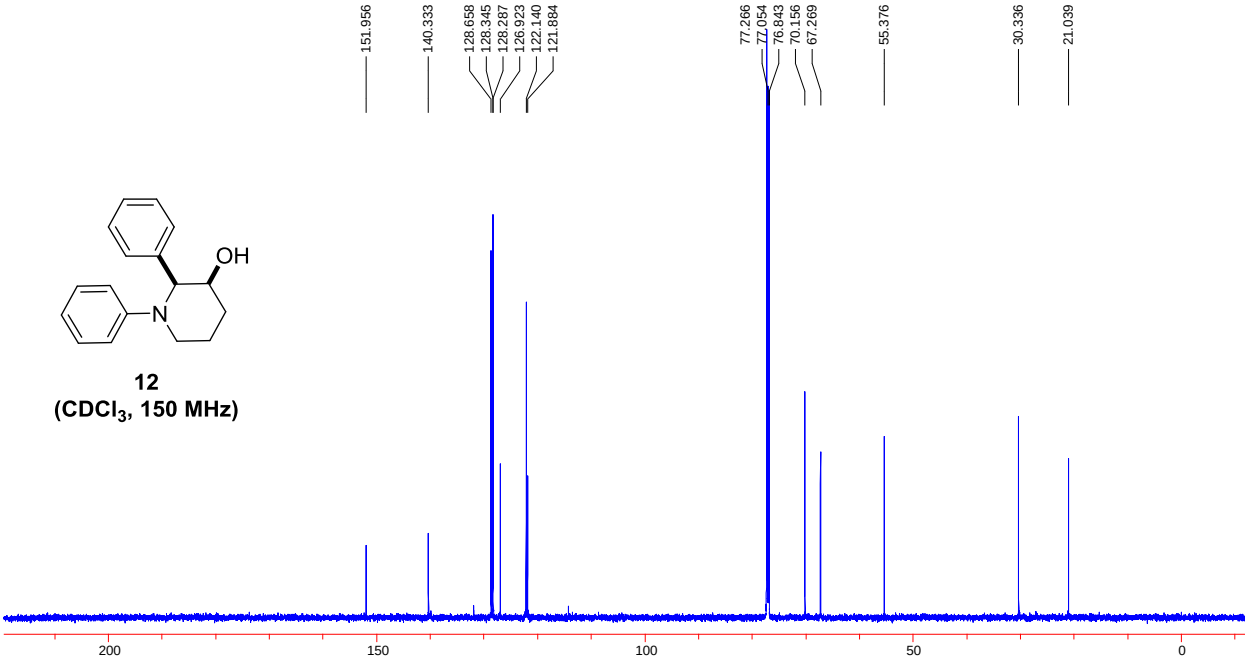

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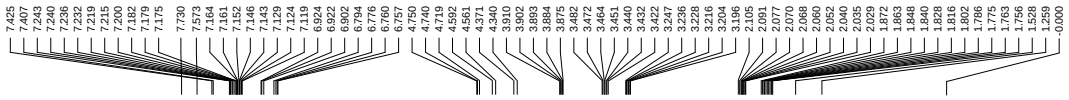

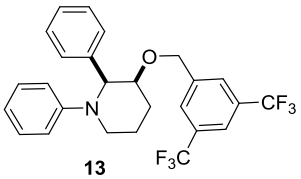

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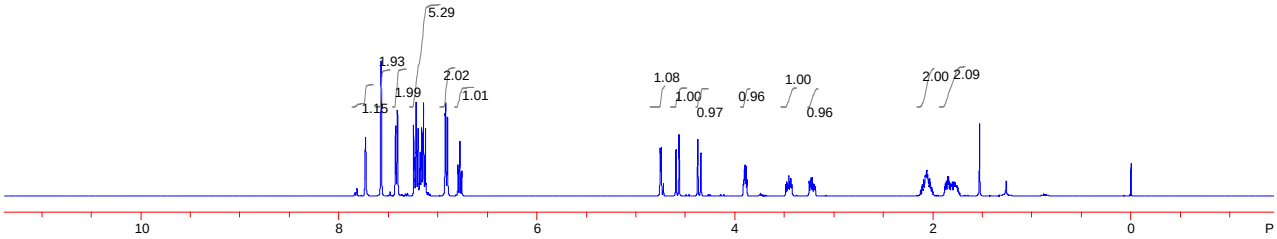

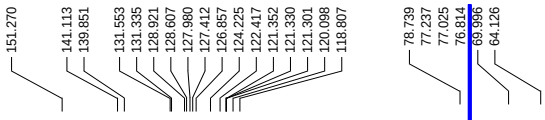

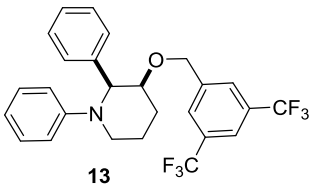

13
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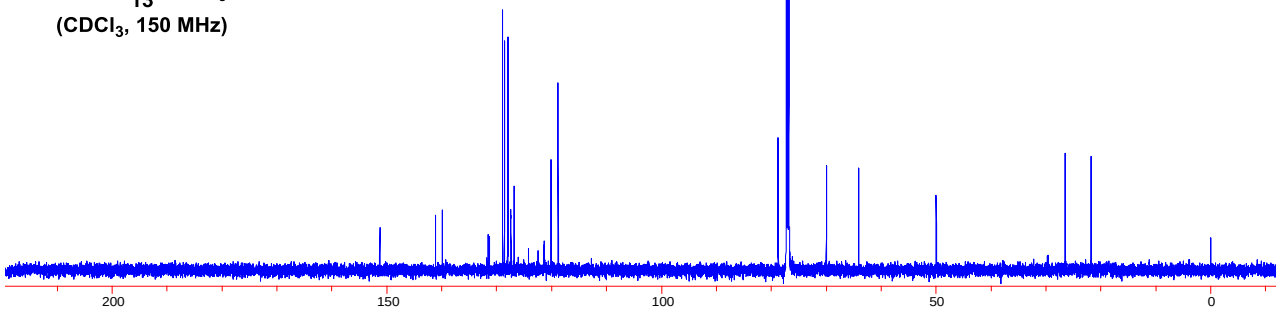

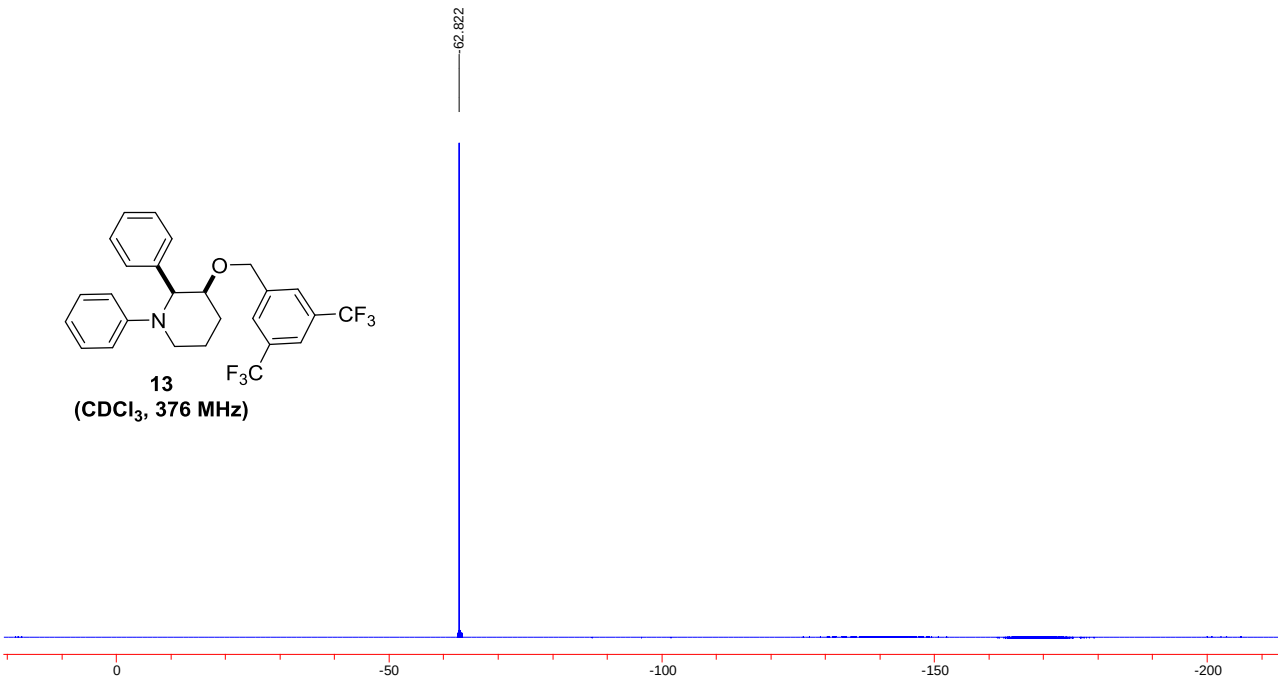

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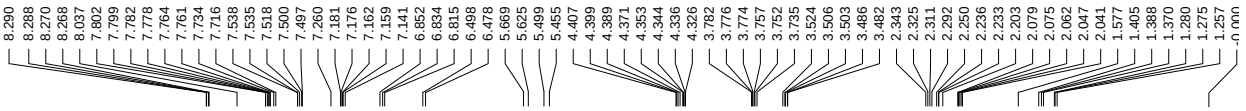
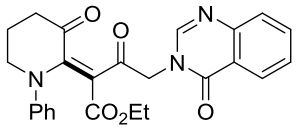
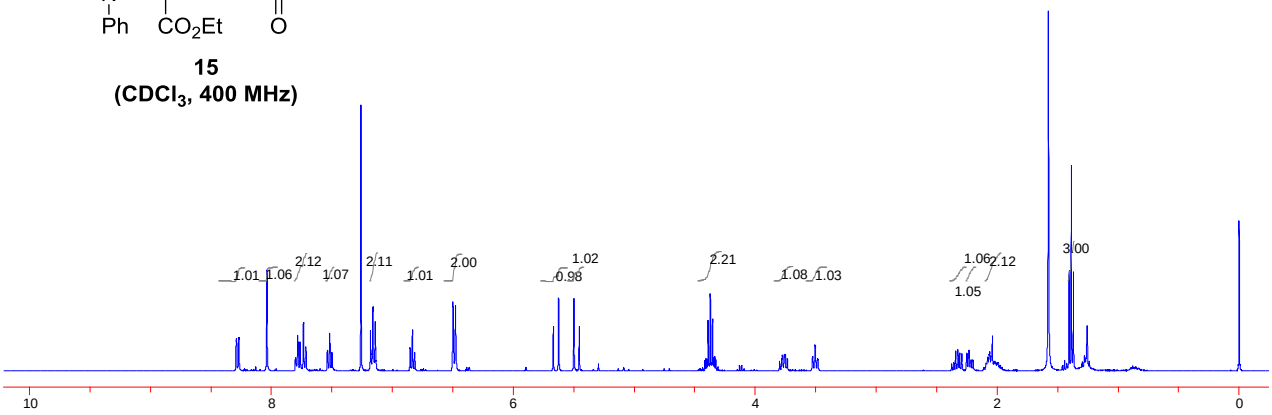
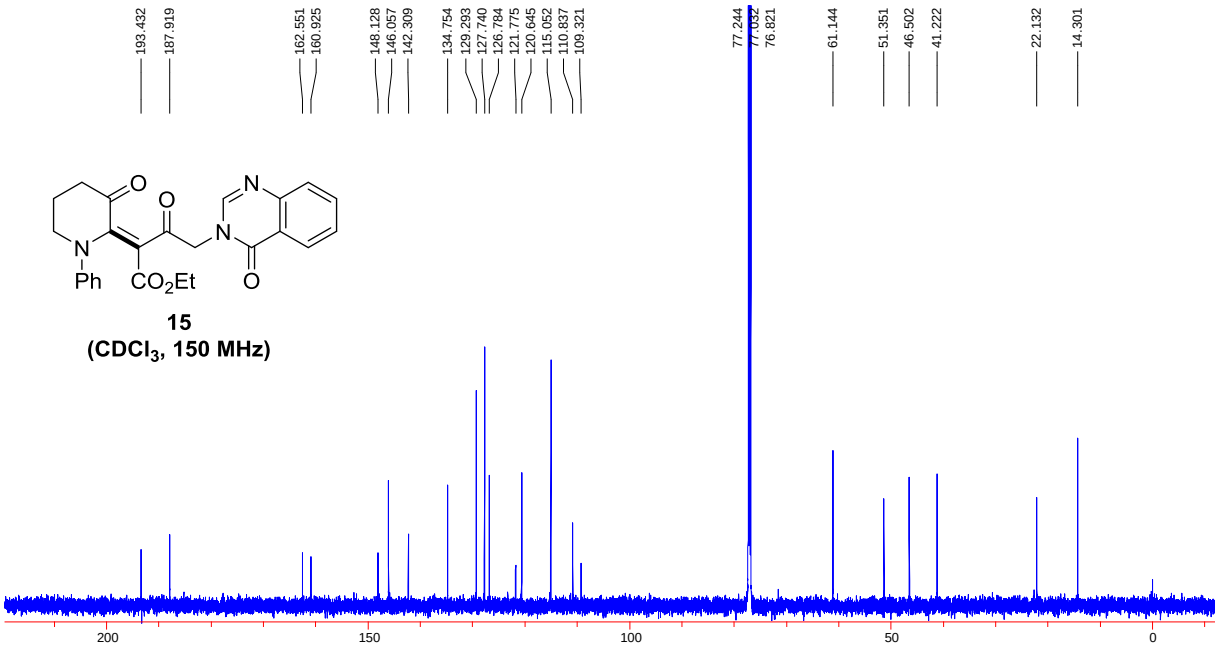




15
($CDCl_3$, 400 MHz)





15
($CDCl_3$, 150 MHz)

VIII. X-ray Crystal Structures and Data of 7b and 9a

1. X-ray Crystal Structure and Data of 7b

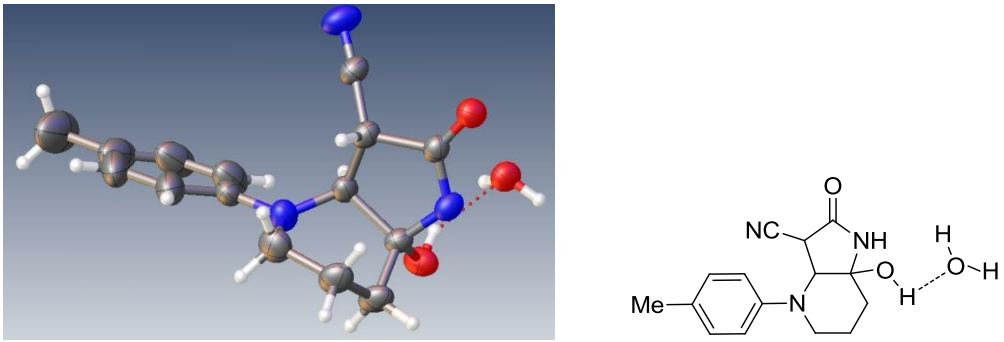


Fig. S6 X-ray structure of **7b**

X-ray structure determination. Single crystals suitable for X-ray diffraction was obtained by slow evaporation of the solvent from a CH_3CN solution of **7b**. Crystal data collection and refinement parameters of **7b** are summarized in Table S1. Intensity data were collected at 293 K on a SuperNova Dual diffractometer using mirror-monochromated Cu Kα radiation, λ = 1.54184 Å. The data were corrected for decay, Lorentz, and polarization effects as well as absorption and beam corrections based on the multi-scan technique. The structure was solved by a combination of direct methods in SHELXTL and the difference Fourier technique, and refined by full-matrix least-squares procedures. Nonhydrogen atoms were refined with anisotropic displacement parameters. The H-atoms were either located or calculated and subsequently treated with a riding model.

Table S1 Crystallographic data and structure refinement results of **7b**

Empirical formula	$C_{15}H_{18}N_3O_3$
Formula weight	288.32
Temp, K	293(2)
Crystal system	monoclinic
Space group	P 2_1/c
a, Å	19.019(4)
b, Å	10.378(2)
c, Å	c=7.6447(13)
α (°)	90

β (°)	100.068(17)
γ (°)	90
Volume, Å^3	1485.7(5)
Z	4
d_{calc}, g cm^{-3}	1.289
λ, Å	1.54184
μ, mm^{-1}	0.752
No. of unique data	2859/12/195
R_{int}	0.0601
Goodness-of-fit on F^2	1.077
R_1, wR_2 ($I > 2\sigma(I)$)	0.1102, 0.3161
R_1, wR_2 (all data)	0.1292, 0.3429

2. X-ray Crystal Structure and Data of 9a

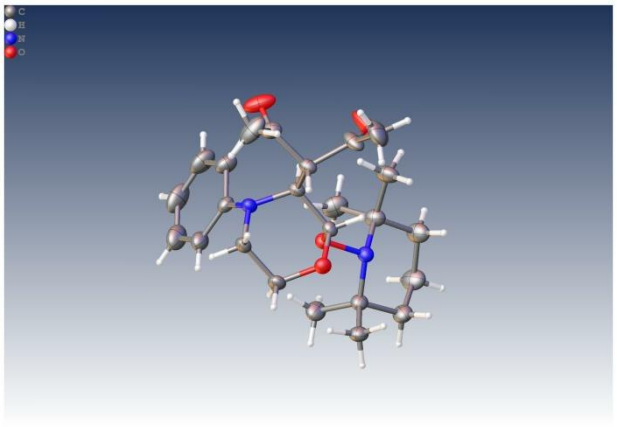


Fig. S7 X-ray structure of **9a**

X-ray structure determination. Single crystals suitable for X-ray diffraction was obtained by slow evaporation of the solvent from a CH_3CN solution of **9a**. Crystal data collection and refinement parameters of **9a** are summarized in Table S2. Intensity data were collected at 293 K on a SuperNova Dual diffractometer using mirror-monochromated Cu Kα radiation, λ = 1.54184 Å. The data were corrected for decay, Lorentz, and polarization effects as well as absorption and beam corrections based on the multi-scan technique. The structure was solved by a combination of direct methods in SHELXTL and the difference Fourier technique, and refined by full-matrix least-squares procedures. Nonhydrogen atoms were refined with anisotropic displacement parameters. The H-atoms were either located or calculated and subsequently treated with a riding model.

Table S2 Crystallographic data and structure refinement results of **9a**

Empirical formula	$C_{24}H_{36}N_2O_4$
Formula weight	416.55
Temp, K	293 (2)
Crystal system	tetragonal
Space group	I 4_1/a
a, Å	33.7249(5)
b, Å	33.7249(5)
c, Å	8.3001(2)
α (°)	90
β (°)	90

γ (°)	90
Volume, Å^3	9440.3(4)
Z	16
d_{calc}, g cm^{-3}	1.172
λ, Å	1.54184
μ, mm^{-1}	0.634
No. of unique data	4404/0/277
R_{int}	0.0156
Goodness-of-fit on F^2	1.053
R_1, wR_2 ($I > 2\sigma(I)$)	0.0508, 0.1304
R_1, wR_2 (all data)	0.0629,0.1411

IX. Details of DFT Calculations

All calculations have been performed using the DFT method implemented in the commercial Gaussian 16[4] program package. Molecular geomtetries of the model complexes were optimized applying the M062X(D3)[5-6] functional with the 6-31G(d)[7] basis set with the SMD[8] continuum solvation model in tetrahydrofuran. As soon as the convergences of optimizations were obtained, the frequency calculations ate the same level have been performed to identify all the stationary points as minima. All transition states were further confirmed by vibrational analysis and characterized by the only one imaginary frequency. Furthermore intrinsic reaction coordinate (IRC)[9] calculations were performed to confirm that the optimized transition states correctly connect the relevant reactants and products. Additionally, the single-point energies for all stationary points have also been calculated at the M062x(D3)/6-311+G(d,p) level in tetrahydrofuran solvent to provide more accurate energy information. All energies discussed in the following parts are Gibbs free energies calculated at 298.15 K unless otherwise stated. All of the optimized geometries mentioned were built by Gaussview 6.0.[10]

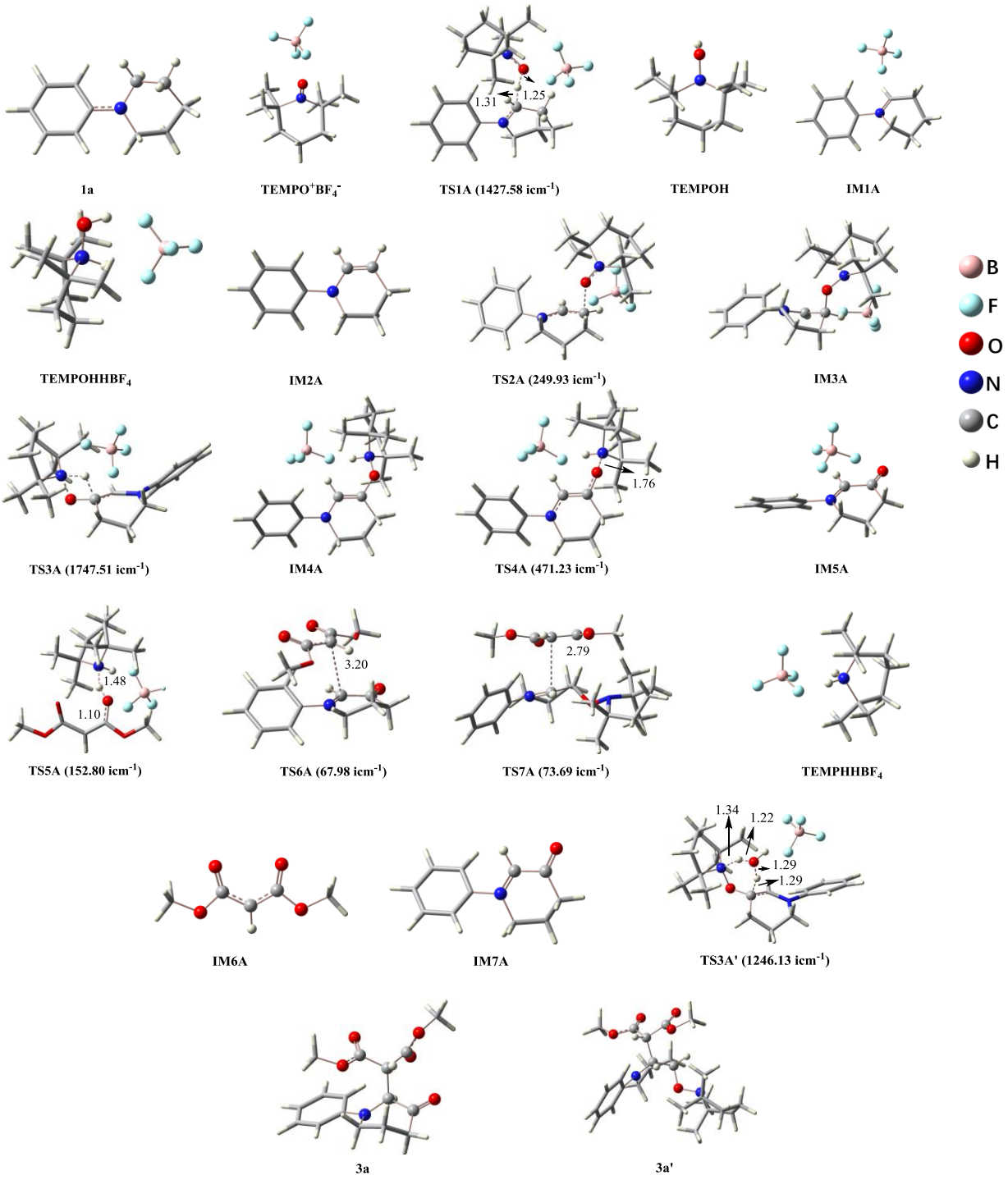


Fig. S8 Optimized structures of key stationary states in Scheme 4

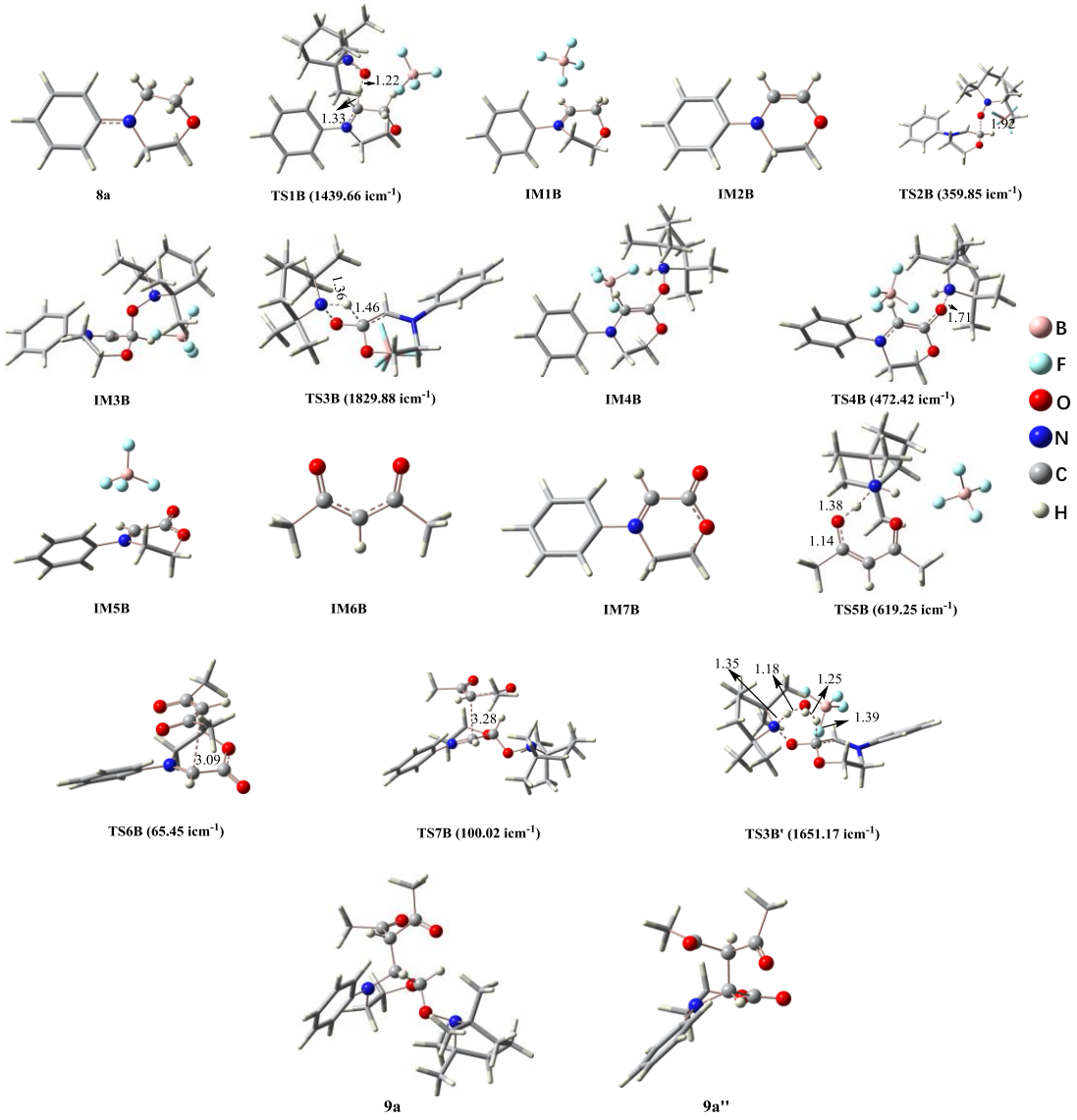


Fig. S9 Optimized structures of key stationary states in Scheme 5

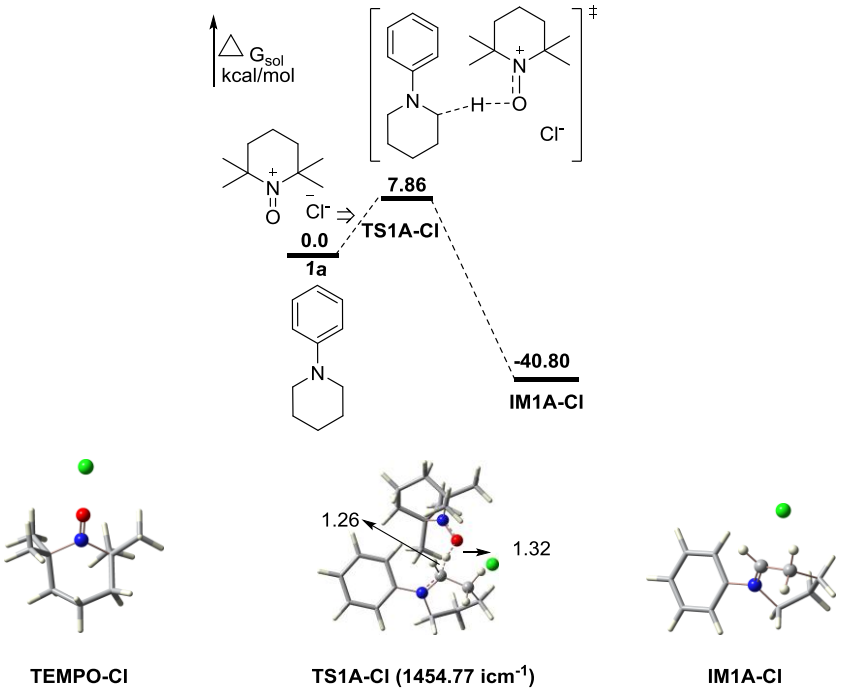


Fig. S10 Computational investigation on the rate determining step for the formation of **3a** (with a chloride ion)

Considering that $CaCl_2$ as additive can improve the yield of the reaction for the formation of **3a**, calculations of the rate determining step (hydride abstraction from α-carbon of piperidine **1a** by $TEMPO^+$ acts as the initial step for the formation of iminium intermediate **IM1A-Cl**) with a chloride ion was conducted. It requires a free energy barrier of 7.86 kcal/mol (**TS1A-Cl**), which is much lower than that with a BF_4^- (23.15 kcal/mol, **TS1A**). The result shows that chloride ion is favorable for rate determining step to further improve the formation of product **3a**.

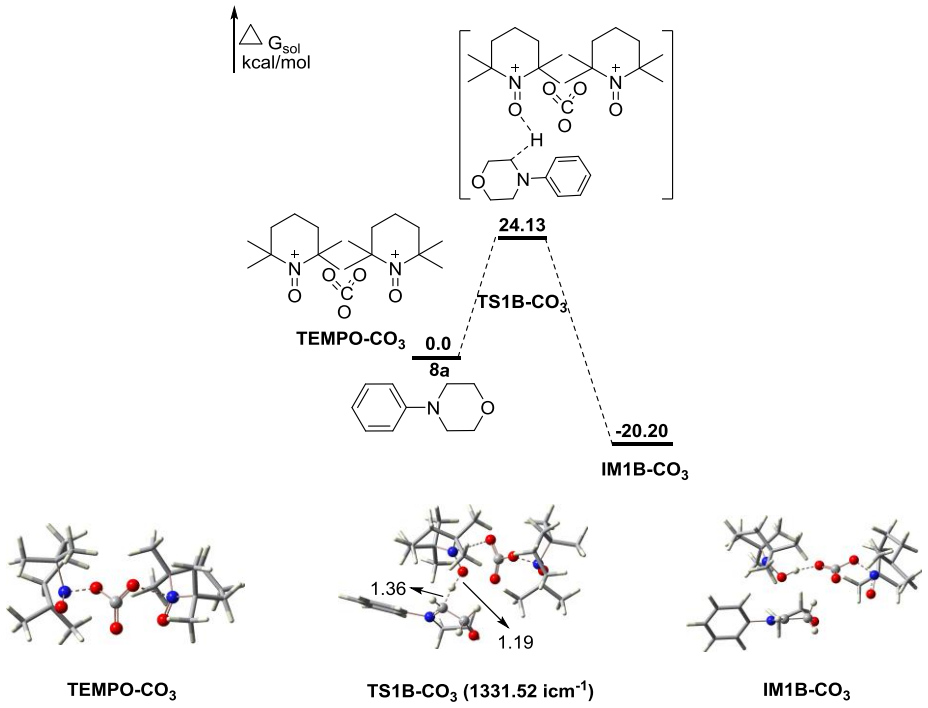


Fig. S11 Computational investigation on the rate determining step for the formation of **9a** (with a carbonate ion)

Considering that Na_2CO_3 as additive can improve the yield of the reaction for the formation of **9a**, calculations of the rate determining step (hydride abstraction from α-carbon of morpholine **8a** by $TEMPO^+$ acts as the initial step for the formation of iminium intermediate **IM1B-CO$_3$**) with a carbonate ion was conducted. It requires a free energy barrier of 24.13 kcal/mol (**TS1B-CO$_3$**), which is a little lower than that with a BF_4^- (24.30 kcal/mol, **TS1B**). In addition, we deduce Na_2CO_3 might act as base to promote the deprotonation of nucleophile acetylacetone to improve the formation of product **9a**. The concrete role of Na_2CO_3 will be further studied in our laboratory.

Coordinates of Stationary Points

Cartesian coordinates (in Å), *E*sol (in kcal/mol), Gibbs free energies (G_{sol}, in kcal/mol) and the number of imaginary vibrational frequencies (N_{imag}) for the stationary points computed at the M062x(D3)/6-311+G(d,p) level in tetrahydrofuran solvent.

Table S3

	G_{sol}	Thermal correction to Gibbs Free Energy (TCG)	E_{sol}	$\triangle G_{sol}=E_{sol}+TCG$	N_{imag}
1a	-482.536329	0.205134	-482.8702751	-482.6651411	0
TEMPOBF$_4$	-907.564217	0.238674	-908.0995694	-907.8608954	0
TS1A	-1390.062088	0.462093	-1390.946769	-1390.484676	-1427.58
IM1A	-906.269569	0.201763	-906.7555742	-906.5538112	0
TEMPOH	-483.861261	0.241587	-484.2491599	-484.0075729	0
TEMPOH$_2$BF$_4$	-908.794307	0.26409	-909.3592486	-909.0951586	0
IM2A	-481.346596	0.182301	-481.657465	-481.475164	0
TS2A	-1388.891123	0.444382	-1389.753162	-1389.30878	-249.93
IM3A	-1388.928629	0.448976	-1389.79415	-1389.345174	0
TS3A	-1388.889361	0.441478	-1389.749217	-1389.307739	-1747.51
TS3A'	-1465.284723	0.468241	-1466.227901	-1465.75966	-1246.13
IM4A	-1388.93773	0.450922	-1389.805724	-1389.354802	0
TS4A	-1388.92543	0.447055	-1389.789809	-1389.342754	-471.23
IM5A	-980.275116	0.182458	-980.7649547	-980.5824967	0
TEMPH	-408.720732	0.239072	-409.0789717	-408.8398997	0
CH$_2$(CO$_2$Me)$_2$	-495.963773	0.098904	-496.2220903	-496.1231863	0
TS5A	-1329.129965	0.366257	-1329.933474	-1329.567217	-152.80
TEMPH$_2$BF$_4$	-833.660814	0.261032	-834.1973714	-833.9363394	0
IM6A	-495.475874	0.086212	-495.734794	-495.648582	0
IM7A	-555.794917	0.175655	-556.1171507	-555.9414957	0
TS6A	-1051.266833	0.285922	-1051.866998	-1051.581076	-67.98
3a	-1051.330498	0.29047	-1051.927167	-1051.636697	0
TS7A	-1459.930457	0.553396	-1460.904556	-1460.35116	-73.69
3a'	-1459.975495	0.554597	-1460.945216	-1460.390619	0

1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.627068	-1.034849	0.728272
2	6	0	-1.290588	-1.248985	0.021580
3	6	0	-1.290582	1.248964	-0.021599
4	6	0	-2.627103	1.034865	-0.728225
5	6	0	-3.499836	-0.000011	0.000022
6	1	0	-0.711261	-1.997745	0.570064
7	1	0	-1.453507	-1.642836	-0.994604
8	1	0	-4.152277	-0.498259	-0.724600
9	1	0	-2.413312	-0.693931	1.747918
10	1	0	-1.453432	1.642786	0.994611
11	1	0	-0.711285	1.997742	-0.570094
12	1	0	-2.413402	0.694002	-1.747900
13	1	0	-3.146437	1.994146	-0.813607
14	1	0	-4.152305	0.498210	0.724638
15	1	0	-3.146399	-1.994125	0.813738
16	7	0	-0.534599	-0.000009	-0.000061
17	6	0	0.841660	-0.000007	-0.000036
18	6	0	1.575784	-1.166974	-0.311524
19	6	0	1.575756	1.166976	0.311478
20	6	0	2.966111	-1.157784	-0.304174
21	1	0	1.055791	-2.077794	-0.587120
22	6	0	2.966080	1.157801	0.304206
23	1	0	1.055728	2.077787	0.587034
24	6	0	3.680838	0.000010	0.000037

25	1	0	3.495996	-2.073318	-0.554153
26	1	0	3.495947	2.073338	0.554209
27	1	0	4.766035	0.000020	0.000070

TEMPOBF$_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.400011	1.062568	1.027451
2	6	0	1.253444	1.310492	0.034073
3	6	0	1.229739	-1.342461	-0.007296
4	6	0	2.756275	-1.350661	0.300077
5	6	0	3.389385	0.038261	0.475678
6	1	0	3.764630	0.392999	-0.491044
7	1	0	2.011398	0.749961	1.999854
8	1	0	3.263341	-1.887787	-0.505581
9	1	0	2.865338	-1.941306	1.214216
10	1	0	4.253434	-0.040657	1.139457
11	1	0	2.890889	2.028075	1.179903
12	7	0	0.935693	-0.009724	-0.654025
13	6	0	0.828030	-2.431609	-0.985501
14	1	0	-0.249643	-2.410462	-1.166238
15	1	0	1.360938	-2.337333	-1.934952
16	1	0	1.095140	-3.388540	-0.530181
17	6	0	0.393890	-1.453332	1.280683
18	1	0	-0.662608	-1.273065	1.083425
19	1	0	0.525949	-2.483502	1.623368
20	1	0	0.741717	-0.793347	2.075072

21	6	0	1.649218	2.296935	-1.063930
22	1	0	0.828874	2.468533	-1.762447
23	1	0	1.888673	3.242434	-0.571990
24	1	0	2.529126	1.955827	-1.616721
25	6	0	-0.050631	1.767455	0.703943
26	1	0	0.181287	2.710005	1.208919
27	1	0	-0.828275	1.940875	-0.042108
28	1	0	-0.419642	1.055446	1.443011
29	8	0	0.465010	0.020391	-1.738275
30	9	0	-3.141095	1.369258	-0.184886
31	9	0	-2.650393	-0.155808	1.453319
32	9	0	-4.044241	-0.732255	-0.268351
33	9	0	-1.808242	-0.430624	-0.655034
34	5	0	-2.922187	0.015152	0.088379

TS1A

Standard orientation:

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

1	6	0	0.376907	3.744804	0.712385
2	6	0	0.949492	2.400483	1.185210
3	6	0	0.342416	1.705709	-1.283683
4	6	0	-0.779672	2.779146	-1.314221
5	6	0	-0.956139	3.554918	-0.002843
6	1	0	-1.646179	3.017648	0.658703
7	1	0	1.090753	4.244677	0.047577
8	1	0	-1.726675	2.297205	-1.579768
9	1	0	-0.539099	3.474857	-2.125272

10	1	0	-1.417213	4.524743	-0.211321
11	1	0	0.265179	4.383138	1.594668
12	7	0	0.709993	1.392224	0.122073
13	6	0	-0.127440	0.421505	-1.962823
14	1	0	0.675057	-0.317132	-2.012822
15	1	0	-0.989579	-0.006162	-1.440587
16	1	0	-0.443622	0.678207	-2.978353
17	6	0	1.621283	2.196555	-1.987417
18	1	0	2.414062	1.453862	-1.863780
19	1	0	1.408475	2.328398	-3.053364
20	1	0	1.965622	3.154830	-1.589025
21	6	0	0.241758	1.926905	2.461659
22	1	0	0.618558	0.950645	2.780566
23	1	0	0.447858	2.646901	3.258628
24	1	0	-0.842789	1.863517	2.328439
25	6	0	2.457335	2.490732	1.442310
26	1	0	2.638691	3.222299	2.236487
27	1	0	2.851285	1.519736	1.751646
28	1	0	2.988181	2.811681	0.541775
29	8	0	0.975271	0.185495	0.420992
30	9	0	2.907124	-1.858771	0.559307
31	9	0	3.638190	0.149961	-0.283747
32	9	0	4.714703	-1.790669	-0.837018
33	9	0	2.627340	-1.376279	-1.665734
34	5	0	3.469871	-1.215626	-0.551140
35	6	0	0.178580	-2.332405	1.943698
36	6	0	-0.820915	-1.331062	1.375431
37	6	0	-1.273801	-2.850496	-0.483021
38	6	0	0.181240	-3.188543	-0.221694
39	1	0	-1.267620	-0.673846	2.124404

40	1	0	0.008718	-0.439861	0.833407
41	1	0	-0.193090	-2.651469	2.923902
42	1	0	-1.895622	-3.728936	-0.280982
43	1	0	-1.431544	-2.534800	-1.519549
44	1	0	0.851813	-2.370515	-0.514458
45	1	0	0.453364	-4.085352	-0.782009
46	1	0	1.144513	-1.830691	2.082797
47	7	0	-1.683713	-1.753673	0.409904
48	6	0	-2.870559	-1.044025	0.113977
49	6	0	-2.995479	0.310898	0.448483
50	6	0	-3.921519	-1.694717	-0.542891
51	6	0	-4.170125	0.993890	0.156548
52	1	0	-2.160459	0.841564	0.897504
53	6	0	-5.090580	-0.997372	-0.833029
54	1	0	-3.838368	-2.742251	-0.810893
55	6	0	-5.225424	0.344345	-0.483135
56	1	0	-4.248629	2.046133	0.413989
57	1	0	-5.902417	-1.514198	-1.335245
58	1	0	-6.138170	0.882578	-0.717269
59	6	0	0.325894	-3.487867	1.155430
60	1	0	-0.417413	-4.224096	1.379844
61	1	0	1.295173	-3.877587	1.386766

IM1A

Standard orientation:

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

1	6	0	-1.335178	2.046256	-0.554550

2	6	0	-0.360888	0.939368	-0.694455
3	6	0	0.846437	2.016695	1.041778
4	6	0	0.685367	3.356421	0.328479
5	6	0	-0.636340	3.421950	-0.461878
6	1	0	-0.481698	0.136948	-1.416452
7	1	0	-0.444541	3.786080	-1.473437
8	1	0	-1.875981	1.840347	0.379409
9	1	0	0.071042	1.866067	1.800811
10	1	0	1.822194	1.908764	1.510996
11	1	0	1.538880	3.483817	-0.343860
12	1	0	0.737954	4.147322	1.080224
13	1	0	-1.335434	4.117479	0.006899
14	1	0	-2.059879	2.001174	-1.365939
15	7	0	0.686288	0.922571	0.056979
16	6	0	1.653096	-0.144397	0.000806
17	6	0	3.007699	0.176734	-0.056869
18	6	0	1.208352	-1.462906	0.000415
19	6	0	3.936979	-0.855521	-0.129442
20	1	0	3.328754	1.214103	-0.065397
21	6	0	2.153366	-2.483829	-0.075593
22	1	0	0.147739	-1.682441	0.072521
23	6	0	3.512072	-2.184134	-0.139193
24	1	0	4.994647	-0.618964	-0.183726
25	1	0	1.820899	-3.516906	-0.073740
26	1	0	4.242250	-2.985433	-0.193703
27	9	0	-1.731034	-0.565098	0.996278
28	9	0	-2.856395	-0.415827	-0.986889
29	9	0	-3.760406	-1.597772	0.757150
30	9	0	-1.922869	-2.404958	-0.345892
31	5	0	-2.580055	-1.252657	0.104749

TEMPOH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.110475	1.408404	0.487161
2	6	0	-1.271409	-0.062506	0.054260
3	6	0	1.282922	-0.030372	0.047960
4	6	0	1.310222	1.513617	-0.133605
5	6	0	-0.075527	2.124933	-0.371653
6	1	0	-0.350249	2.032363	-1.428762
7	1	0	-0.799294	1.457752	1.538715
8	1	0	1.970210	1.773192	-0.968726
9	1	0	1.754369	1.954654	0.766835
10	1	0	-0.054914	3.195084	-0.140879
11	1	0	-2.089974	1.896327	0.425259
12	7	0	0.013777	-0.514630	-0.546599
13	6	0	2.423651	-0.644722	-0.769146
14	1	0	2.512399	-1.719667	-0.589850
15	1	0	2.256785	-0.477281	-1.839153
16	1	0	3.370586	-0.170268	-0.490802
17	6	0	1.482075	-0.425650	1.519291
18	1	0	1.305939	-1.498037	1.652549
19	1	0	2.513612	-0.208764	1.819755
20	1	0	0.821658	0.127421	2.192650
21	6	0	-2.309222	-0.165692	-1.069206
22	1	0	-2.328224	-1.185056	-1.468941
23	1	0	-3.310314	0.076136	-0.695963

24	1	0	-2.067442	0.520261	-1.888170
25	6	0	-1.757036	-0.908251	1.238838
26	1	0	-2.678073	-0.463591	1.633055
27	1	0	-1.977064	-1.932161	0.927565
28	1	0	-1.027880	-0.942118	2.051320
29	8	0	0.013058	-1.939711	-0.528756
30	1	0	0.125752	-2.174719	-1.463605

$TEMPOH_2BF_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.191086	1.102556	1.147940
2	6	0	-1.335850	1.315338	-0.111755
3	6	0	-1.315789	-1.335182	-0.084352
4	6	0	-1.595710	-1.328228	1.441221
5	6	0	-1.571323	0.067383	2.081474
6	1	0	-0.538706	0.352470	2.319497
7	1	0	-3.201329	0.786364	0.864578
8	1	0	-0.865731	-1.970985	1.942317
9	1	0	-2.581075	-1.782437	1.586478
10	1	0	-2.113504	0.039243	3.029964
11	1	0	-2.285422	2.074471	1.642133
12	7	0	-0.611971	-0.014355	-0.412006
13	6	0	-0.329881	-2.446303	-0.437608
14	1	0	-0.171134	-2.522863	-1.516372
15	1	0	0.631145	-2.294266	0.062841
16	1	0	-0.751331	-3.391400	-0.084423

17	6	0	-2.581205	-1.476722	-0.920693
18	1	0	-2.374146	-1.305040	-1.980694
19	1	0	-2.936816	-2.504833	-0.805023
20	1	0	-3.381735	-0.811683	-0.590915
21	6	0	-0.212969	2.320635	0.136527
22	1	0	0.477803	2.347877	-0.711277
23	1	0	-0.653440	3.313769	0.256729
24	1	0	0.352891	2.078729	1.041679
25	6	0	-2.176166	1.759993	-1.301836
26	1	0	-2.711889	2.661891	-0.989450
27	1	0	-1.552068	2.011308	-2.161088
28	1	0	-2.916918	1.016677	-1.599452
29	8	0	-0.180727	0.011730	-1.744187
30	1	0	0.758138	-0.285936	-1.702809
31	1	0	0.235904	-0.009355	0.185324
32	9	0	3.941860	-0.566236	0.531406
33	9	0	1.781311	-0.081871	1.129378
34	9	0	2.257763	-0.682476	-1.018212
35	9	0	2.944547	1.353684	-0.223540
36	5	0	2.767906	0.023582	0.114140

IM2A

Standard orientation:

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

1	6	0	2.624607	1.277026	-0.261151
2	6	0	1.305755	1.130992	-0.457807
3	6	0	1.325843	-1.101075	0.500765

4	6	0	2.768536	-1.180969	0.013921
5	6	0	3.488875	0.149999	0.239317
6	1	0	0.713640	1.931827	-0.889495
7	1	0	4.449803	0.150995	-0.287862
8	1	0	1.310145	-0.892925	1.581761
9	1	0	0.819847	-2.053634	0.337558
10	1	0	2.766855	-1.421595	-1.055576
11	1	0	3.273965	-1.997409	0.538053
12	1	0	3.724601	0.273415	1.305483
13	1	0	3.081388	2.222768	-0.534871
14	7	0	0.596336	-0.041861	-0.205565
15	6	0	-0.807978	-0.006513	-0.091359
16	6	0	-1.558146	-1.169237	-0.332249
17	6	0	-1.490706	1.170184	0.252038
18	6	0	-2.944618	-1.148955	-0.235759
19	1	0	-1.053953	-2.086637	-0.619315
20	6	0	-2.881715	1.184388	0.327487
21	1	0	-0.933556	2.072291	0.482550
22	6	0	-3.619598	0.028261	0.088424
23	1	0	-3.502332	-2.060361	-0.431403
24	1	0	-3.387060	2.108239	0.594504
25	1	0	-4.702820	0.041444	0.155801

TS2A

Standard orientation:

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

1	6	0	-0.316929	-0.644533	-1.434334

2	6	0	-1.428526	-0.075211	-0.801728
3	6	0	-2.779257	-2.047067	-1.228634
4	6	0	-1.984479	-2.161753	-2.520215
5	6	0	-0.503947	-1.905439	-2.239003
6	1	0	-1.377584	0.938026	-0.416964
7	1	0	0.065606	-1.843828	-3.170937
8	1	0	-2.443450	-2.789077	-0.494484
9	1	0	-3.845305	-2.196482	-1.397358
10	1	0	-2.371191	-1.433995	-3.242355
11	1	0	-2.132503	-3.161632	-2.936260
12	1	0	-0.100032	-2.753968	-1.667967
13	1	0	0.472463	0.055113	-1.677032
14	7	0	-2.590481	-0.707429	-0.639345
15	6	0	-3.642627	-0.123347	0.127521
16	6	0	-4.945638	-0.101661	-0.377695
17	6	0	-3.362733	0.434202	1.376625
18	6	0	-5.961434	0.483111	0.370885
19	1	0	-5.159343	-0.513111	-1.359210
20	6	0	-4.386098	1.025070	2.112964
21	1	0	-2.354780	0.385616	1.777042
22	6	0	-5.686844	1.049042	1.615684
23	1	0	-6.970784	0.505301	-0.027897
24	1	0	-4.163570	1.454932	3.084591
25	1	0	-6.483871	1.504683	2.194609
26	6	0	2.994793	0.073845	2.402755
27	6	0	1.594804	-0.338627	1.932886
28	6	0	2.997166	-1.402420	-0.033694
29	6	0	4.090193	-0.323743	0.169979
30	6	0	3.795407	0.701144	1.269422
31	1	0	3.233726	1.536907	0.842865

32	1	0	3.527474	-0.791938	2.813371
33	1	0	4.244343	0.202358	-0.775324
34	1	0	5.019217	-0.857504	0.398874
35	1	0	4.736826	1.106739	1.652499
36	1	0	2.858509	0.781037	3.227928
37	7	0	1.697387	-0.990951	0.588960
38	6	0	2.795193	-1.658336	-1.524638
39	1	0	2.103703	-2.483301	-1.706431
40	1	0	2.445416	-0.757552	-2.032170
41	1	0	3.769356	-1.930386	-1.942770
42	6	0	3.384107	-2.731665	0.643289
43	1	0	2.569731	-3.456318	0.539935
44	1	0	4.274733	-3.132361	0.148525
45	1	0	3.613065	-2.605504	1.704573
46	6	0	0.689586	0.886250	1.809619
47	1	0	-0.257202	0.610272	1.344173
48	1	0	0.474460	1.259146	2.815915
49	1	0	1.148403	1.688584	1.229112
50	6	0	0.966380	-1.350297	2.896655
51	1	0	0.929261	-0.909468	3.897646
52	1	0	-0.052285	-1.600561	2.586663
53	1	0	1.560280	-2.268408	2.942590
54	8	0	0.644888	-1.482491	0.121751
55	5	0	1.510033	2.653421	-1.234404
56	9	0	0.123485	2.471056	-1.115723
57	9	0	2.132390	1.390762	-1.294746
58	9	0	1.986303	3.342496	-0.110576
59	9	0	1.797044	3.374217	-2.391522

IM3A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.061651	-0.232958	-1.367108
2	6	0	-1.311442	0.291011	-0.700124
3	6	0	-2.191659	-1.902900	-1.048982
4	6	0	-1.625154	-1.915694	-2.473328
5	6	0	-0.517944	-0.863798	-2.686677
6	1	0	-1.418329	1.330256	-0.399941
7	1	0	-0.882419	-0.053723	-3.324956
8	1	0	-1.525715	-2.416036	-0.353307
9	1	0	-3.178270	-2.357590	-0.995582
10	1	0	-2.441158	-1.744188	-3.179483
11	1	0	-1.243926	-2.923702	-2.650464
12	1	0	0.355485	-1.297970	-3.177366
13	1	0	0.635077	0.589778	-1.521465
14	7	0	-2.311582	-0.505056	-0.553344
15	6	0	-3.535188	-0.079206	0.081489
16	6	0	-4.748652	-0.339814	-0.551166
17	6	0	-3.470705	0.586702	1.301186
18	6	0	-5.923148	0.093101	0.054497
19	1	0	-4.772441	-0.850880	-1.508733
20	6	0	-4.656286	1.010616	1.896311
21	1	0	-2.512703	0.752022	1.784562
22	6	0	-5.878878	0.765581	1.275870
23	1	0	-6.874356	-0.093321	-0.433122
24	1	0	-4.619204	1.525052	2.850861
25	1	0	-6.800056	1.095745	1.745217

26	6	0	2.577374	-0.993233	2.490474
27	6	0	1.276234	-0.870018	1.671461
28	6	0	2.856532	-1.418344	-0.264074
29	6	0	4.056421	-0.771215	0.474924
30	6	0	3.706578	-0.195671	1.853233
31	1	0	3.394288	0.847279	1.741008
32	1	0	2.871765	-2.044530	2.585989
33	1	0	4.469795	0.027927	-0.150515
34	1	0	4.835761	-1.536841	0.567669
35	1	0	4.591353	-0.198697	2.497936
36	1	0	2.365754	-0.635586	3.504535
37	7	0	1.626630	-0.732506	0.218993
38	6	0	3.006302	-1.121387	-1.758962
39	1	0	2.290632	-1.692074	-2.356815
40	1	0	2.870646	-0.052627	-1.951806
41	1	0	4.013870	-1.406873	-2.080339
42	6	0	2.826433	-2.945853	-0.091908
43	1	0	1.911954	-3.356999	-0.531864
44	1	0	3.681561	-3.383804	-0.618853
45	1	0	2.885668	-3.262898	0.951776
46	6	0	0.568532	0.425897	2.078241
47	1	0	-0.311831	0.603161	1.454213
48	1	0	0.230662	0.360472	3.118709
49	1	0	1.226489	1.290908	1.963389
50	6	0	0.351623	-2.052739	1.980759
51	1	0	0.294738	-2.178202	3.067815
52	1	0	-0.663460	-1.870091	1.613556
53	1	0	0.715231	-2.988321	1.548131
54	8	0	0.537167	-1.238261	-0.556090
55	5	0	1.718492	2.971702	-0.590121

56	9	0	0.402970	2.603021	-0.250872
57	9	0	2.131863	2.219374	-1.702756
58	9	0	2.569481	2.716248	0.492717
59	9	0	1.748585	4.329403	-0.907718

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.734474	0.088480	0.977987
2	6	0	0.472955	-0.490991	0.333443
3	6	0	1.448406	-0.535866	2.507978
4	6	0	0.897047	0.886407	2.739943
5	6	0	-0.160250	1.320883	1.691306
6	1	0	0.599797	-0.546859	-0.747598
7	1	0	0.305494	1.961988	0.934373
8	1	0	0.816949	-1.282709	2.988568
9	1	0	2.462562	-0.645125	2.889952
10	1	0	1.728094	1.596680	2.753079
11	1	0	0.452049	0.871686	3.737495
12	1	0	-0.950540	1.907946	2.163794
13	1	0	-1.501563	0.483495	-0.037572
14	7	0	1.486658	-0.847850	1.057007
15	6	0	2.646577	-1.468438	0.476015
16	6	0	3.915288	-0.968487	0.765227
17	6	0	2.467779	-2.546708	-0.386050
18	6	0	5.021270	-1.561467	0.165776
19	1	0	4.034984	-0.116605	1.427372

20	6	0	3.584805	-3.130350	-0.978839
21	1	0	1.469025	-2.932034	-0.571143
22	6	0	4.859121	-2.640313	-0.703842
23	1	0	6.012833	-1.174040	0.376253
24	1	0	3.454666	-3.975227	-1.647266
25	1	0	5.728028	-3.100059	-1.163906
26	6	0	-4.244518	-1.050159	-1.745665
27	6	0	-3.073233	-1.370647	-0.797947
28	6	0	-3.895625	0.812573	0.353233
29	6	0	-4.477253	1.329558	-0.986954
30	6	0	-4.213222	0.408408	-2.183660
31	1	0	-3.234290	0.635725	-2.622868
32	1	0	-5.200082	-1.271015	-1.257592
33	1	0	-4.070440	2.324293	-1.195453
34	1	0	-5.556349	1.449681	-0.841091
35	1	0	-4.957973	0.592318	-2.963191
36	1	0	-4.165712	-1.723774	-2.604934
37	7	0	-2.758877	-0.123586	0.017269
38	6	0	-3.324690	1.988778	1.143987
39	1	0	-3.027676	1.682864	2.149980
40	1	0	-2.468581	2.439713	0.631700
41	1	0	-4.108862	2.747186	1.231575
42	6	0	-4.938746	0.117148	1.228765
43	1	0	-4.462494	-0.356675	2.090526
44	1	0	-5.634125	0.880988	1.593420
45	1	0	-5.525440	-0.629220	0.689589
46	6	0	-1.825123	-1.702903	-1.620434
47	1	0	-0.983033	-1.975815	-0.978729
48	1	0	-2.045133	-2.569789	-2.250540
49	1	0	-1.522823	-0.871517	-2.265535

50	6	0	-3.396092	-2.557957	0.107424
51	1	0	-3.704403	-3.389506	-0.535779
52	1	0	-2.516561	-2.871282	0.675487
53	1	0	-4.202633	-2.352120	0.812985
54	8	0	-1.969529	-0.497714	1.285194
55	5	0	2.956134	2.472607	-1.016887
56	9	0	4.048165	1.595799	-1.104351
57	9	0	3.312544	3.714336	-1.568751
58	9	0	2.599314	2.643735	0.323652
59	9	0	1.870554	1.941668	-1.729011

TS3A’

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.427322	-1.342016	-0.196124
2	6	0	0.908110	-0.862903	-0.189515
3	6	0	1.737271	-3.101357	-0.528721
4	6	0	0.346492	-3.517127	-0.074670
5	1	0	1.095763	0.194125	-0.015109
6	1	0	1.853168	-3.234006	-1.607851
7	1	0	2.495029	-3.693714	-0.016521
8	1	0	0.288202	-3.498527	1.022244
9	1	0	0.124659	-4.525112	-0.426537
10	1	0	-0.755790	-1.378633	1.155096
11	7	0	1.946178	-1.673765	-0.216593
12	6	0	3.279895	-1.175740	-0.026412
13	6	0	4.166893	-1.863754	0.801294

14	6	0	3.664482	0.001993	-0.664431
15	6	0	5.450629	-1.359855	0.988925
16	1	0	3.856414	-2.768133	1.314661
17	6	0	4.945647	0.504453	-0.454773
18	1	0	2.964923	0.524289	-1.309037
19	6	0	5.843007	-0.176745	0.364369
20	1	0	6.141013	-1.890838	1.636641
21	1	0	5.237544	1.429566	-0.941406
22	1	0	6.844362	0.212864	0.518380
23	6	0	-3.841669	1.823066	0.736645
24	6	0	-2.434545	1.363194	0.305180
25	6	0	-3.752616	-0.701935	-0.548546
26	6	0	-4.880170	-0.448005	0.489104
27	6	0	-4.596339	0.710730	1.453521
28	1	0	-4.003503	0.354605	2.306020
29	1	0	-4.415797	2.154226	-0.135897
30	1	0	-5.052415	-1.364939	1.062698
31	1	0	-5.797541	-0.246931	-0.074757
32	1	0	-5.537156	1.087321	1.864760
33	1	0	-3.717115	2.697778	1.383237
34	7	0	-2.490965	-0.140614	0.060662
35	6	0	-3.575312	-2.208363	-0.731701
36	1	0	-2.874173	-2.438484	-1.535159
37	1	0	-3.222374	-2.689995	0.185680
38	1	0	-4.552768	-2.632650	-0.981182
39	6	0	-4.072392	-0.094143	-1.916530
40	1	0	-3.201749	-0.144287	-2.577210
41	1	0	-4.875311	-0.685057	-2.368867
42	1	0	-4.420230	0.938421	-1.856883
43	6	0	-1.446742	1.588776	1.454287

44	1	0	-0.459813	1.171073	1.234009
45	1	0	-1.315888	2.665775	1.594548
46	1	0	-1.808157	1.158137	2.392813
47	6	0	-1.953909	2.147306	-0.915736
48	1	0	-2.015107	3.211251	-0.662991
49	1	0	-0.915124	1.917910	-1.155963
50	1	0	-2.573076	1.976485	-1.797396
51	8	0	-1.362848	-0.477394	-0.771324
52	5	0	1.772244	2.786096	-0.210538
53	9	0	0.857165	3.806408	0.050313
54	9	0	1.342725	2.046993	-1.334455
55	9	0	1.836515	1.918497	0.895924
56	9	0	3.036564	3.315565	-0.467006
57	8	0	-1.645398	-1.351532	2.032613
58	1	0	-1.989941	-2.262009	2.111862
59	1	0	-2.255191	-0.774372	1.201922
60	6	0	-0.630539	-2.654085	-0.635138
61	1	0	-0.551482	-2.705051	-1.700995
62	1	0	-1.615071	-2.947608	-0.336074

IM4A

Standard orientation:

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

1	6	0	-0.128034	1.891648	0.445637
2	6	0	0.879423	1.013385	0.350846
3	6	0	2.413305	2.795544	-0.310635
4	6	0	1.179201	3.527621	-0.821923

5	6	0	0.011027	3.354642	0.150976
6	1	0	0.751571	-0.046167	0.550626
7	1	0	-0.919318	3.740240	-0.277709
8	1	0	2.735615	3.233788	0.645577
9	1	0	3.231954	2.906375	-1.023110
10	1	0	0.899266	3.125123	-1.802514
11	1	0	1.425110	4.585186	-0.948085
12	1	0	0.193846	3.921979	1.072361
13	1	0	-1.243324	-0.231508	-0.075675
14	7	0	2.140318	1.365260	-0.120609
15	6	0	3.242153	0.523857	0.159024
16	6	0	4.360737	0.546724	-0.687331
17	6	0	3.250050	-0.336321	1.264683
18	6	0	5.455338	-0.271001	-0.430199
19	1	0	4.362906	1.190407	-1.561388
20	6	0	4.343426	-1.165506	1.503171
21	1	0	2.404523	-0.353710	1.944932
22	6	0	5.454126	-1.136311	0.663806
23	1	0	6.309357	-0.240617	-1.100629
24	1	0	4.328040	-1.827074	2.364534
25	1	0	6.307502	-1.778415	0.857915
26	6	0	-3.811441	-1.266975	0.850452
27	6	0	-2.696737	-0.391124	1.443725
28	6	0	-2.840689	0.731650	-0.952545
29	6	0	-3.367241	-0.603994	-1.541159
30	6	0	-3.465467	-1.766983	-0.545129
31	1	0	-2.517053	-2.311697	-0.517983
32	1	0	-4.753966	-0.709424	0.828887
33	1	0	-2.722761	-0.899257	-2.373552
34	1	0	-4.354738	-0.380605	-1.958032

35	1	0	-4.226601	-2.472981	-0.888315
36	1	0	-3.953508	-2.103299	1.542412
37	7	0	-2.003837	0.377334	0.282971
38	6	0	-1.919700	1.395297	-1.975141
39	1	0	-1.635731	2.408136	-1.682945
40	1	0	-1.023645	0.794788	-2.154584
41	1	0	-2.478541	1.463408	-2.913521
42	6	0	-3.956695	1.696610	-0.567178
43	1	0	-3.560102	2.558216	-0.022700
44	1	0	-4.407355	2.059905	-1.495367
45	1	0	-4.746552	1.226415	0.020722
46	6	0	-1.596305	-1.242327	2.071555
47	1	0	-0.740417	-0.622607	2.361689
48	1	0	-1.996012	-1.712204	2.974309
49	1	0	-1.253975	-2.030168	1.393610
50	6	0	-3.258205	0.578507	2.479093
51	1	0	-3.841244	-0.023653	3.183008
52	1	0	-2.465912	1.083849	3.033138
53	1	0	-3.924152	1.325194	2.043413
54	8	0	-1.419933	1.527449	0.867983
55	5	0	0.329194	-2.495590	-0.816001
56	9	0	-0.384979	-1.335361	-1.245925
57	9	0	-0.592536	-3.504343	-0.530711
58	9	0	1.038311	-2.169493	0.344478
59	9	0	1.192950	-2.887368	-1.826931

TS4A

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.141130	1.894688	0.774243
2	6	0	0.967083	1.071666	0.674705
3	6	0	2.365844	2.911874	-0.064863
4	6	0	1.089324	3.534990	-0.617596
5	6	0	-0.070162	3.343384	0.361646
6	1	0	0.872019	0.011377	0.896102
7	1	0	-1.023097	3.659180	-0.073878
8	1	0	2.671498	3.416372	0.860099
9	1	0	3.180808	3.001791	-0.782008
10	1	0	0.852367	3.063096	-1.578239
11	1	0	1.276067	4.596215	-0.800428
12	1	0	0.088886	3.970061	1.248847
13	1	0	-1.312913	-0.337132	-0.055293
14	7	0	2.167647	1.485045	0.241329
15	6	0	3.273653	0.588840	0.214365
16	6	0	4.181212	0.625505	-0.848830
17	6	0	3.442805	-0.342918	1.242940
18	6	0	5.247133	-0.268083	-0.877749
19	1	0	4.043268	1.328339	-1.663990
20	6	0	4.504990	-1.240884	1.195939
21	1	0	2.753957	-0.355447	2.081610
22	6	0	5.413072	-1.206035	0.140038
23	1	0	5.943196	-0.236890	-1.710345
24	1	0	4.627982	-1.960630	1.999396
25	1	0	6.244670	-1.902960	0.110725
26	6	0	-4.057525	-1.277435	0.387708
27	6	0	-2.986064	-0.490558	1.175889
28	6	0	-2.707368	0.755911	-1.081825

29	6	0	-3.243171	-0.495686	-1.854089
30	6	0	-3.521271	-1.715715	-0.968864
31	1	0	-2.595619	-2.286914	-0.829228
32	1	0	-4.955355	-0.662954	0.254011
33	1	0	-2.516255	-0.767111	-2.625557
34	1	0	-4.159221	-0.179709	-2.366240
35	1	0	-4.232832	-2.378603	-1.469470
36	1	0	-4.347370	-2.137211	1.000982
37	7	0	-2.118305	0.253025	0.193200
38	6	0	-1.610570	1.402053	-1.931975
39	1	0	-1.347936	2.397908	-1.575546
40	1	0	-0.713763	0.776489	-1.972674
41	1	0	-1.999748	1.508178	-2.949414
42	6	0	-3.800147	1.787968	-0.814314
43	1	0	-3.427586	2.573001	-0.148167
44	1	0	-4.072957	2.248207	-1.768886
45	1	0	-4.705387	1.353344	-0.385990
46	6	0	-2.059536	-1.457356	1.914409
47	1	0	-1.219062	-0.918528	2.361559
48	1	0	-2.622549	-1.946877	2.714552
49	1	0	-1.667921	-2.229178	1.244577
50	6	0	-3.651312	0.448799	2.184947
51	1	0	-4.368159	-0.148227	2.758214
52	1	0	-2.925205	0.873877	2.878874
53	1	0	-4.199209	1.260674	1.704261
54	8	0	-1.255724	1.371995	1.235665
55	5	0	0.492620	-2.453892	-0.475477
56	9	0	-0.084351	-1.298120	-1.070945
57	9	0	-0.484711	-3.450308	-0.399725
58	9	0	0.923970	-2.117770	0.814647

59	9	0	1.564375	-2.877000	-1.249358

IM5A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.065346	-1.479217	-0.744486
2	6	0	0.607866	-1.080053	-0.830370
3	6	0	0.433495	-0.988745	1.581505
4	6	0	1.554748	-2.012730	1.633732
5	6	0	2.651357	-1.686416	0.622082
6	1	0	0.173462	-0.952709	-1.818397
7	1	0	3.405078	-2.474586	0.558676
8	1	0	0.775803	0.020989	1.827883
9	1	0	-0.394237	-1.262304	2.234675
10	1	0	1.138706	-3.006558	1.437063
11	1	0	1.962256	-2.015589	2.646915
12	1	0	3.154571	-0.750976	0.891521
13	7	0	-0.129045	-0.904714	0.203638
14	6	0	-1.528696	-0.583621	0.063414
15	6	0	-2.311482	-1.358305	-0.786800
16	6	0	-2.054841	0.475757	0.798908
17	6	0	-3.664537	-1.053701	-0.909772
18	1	0	-1.875353	-2.198058	-1.319593
19	6	0	-3.407408	0.766261	0.660778
20	1	0	-1.408163	1.083992	1.421851
21	6	0	-4.211476	0.004313	-0.187767
22	1	0	-4.289477	-1.654126	-1.562539

23	1	0	-3.832445	1.597141	1.214220
24	1	0	-5.267401	0.236178	-0.284002
25	8	0	2.650258	-1.614832	-1.792864
26	5	0	1.102302	2.078329	-0.146142
27	9	0	0.566445	2.160650	1.150656
28	9	0	0.097932	1.717376	-1.049860
29	9	0	2.095866	1.073147	-0.150439
30	9	0	1.666503	3.294978	-0.506742

TEMPH

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.105339	0.997699	-0.822257
2	6	0	1.258901	-0.247407	0.083903
3	6	0	-1.275372	-0.223329	0.095209
4	6	0	-1.326033	1.291789	-0.275718
5	6	0	0.060146	1.946104	-0.242523
6	1	0	0.330619	2.189093	0.793356
7	1	0	0.799157	0.697518	-1.833447
8	1	0	-1.997189	1.822108	0.410570
9	1	0	-1.755220	1.402859	-1.279763
10	1	0	0.042330	2.893865	-0.790790
11	1	0	2.079223	1.491644	-0.923628
12	6	0	-2.394150	-0.547731	1.086711
13	1	0	-2.405009	-1.617096	1.323831
14	1	0	-2.257254	0.011876	2.020097
15	1	0	-3.368090	-0.271958	0.668426

16	6	0	-1.486466	-1.081286	-1.157405
17	1	0	-1.351992	-2.142812	-0.921917
18	1	0	-2.505051	-0.935022	-1.534050
19	1	0	-0.799329	-0.814569	-1.965497
20	6	0	2.275691	0.048083	1.190916
21	1	0	2.307993	-0.782053	1.905747
22	1	0	3.277347	0.179424	0.769694
23	1	0	2.012431	0.960407	1.739336
24	6	0	1.774683	-1.440123	-0.726946
25	1	0	2.726030	-1.185175	-1.208976
26	1	0	1.939997	-2.302270	-0.071251
27	1	0	1.072000	-1.736422	-1.509797
28	7	0	-0.012625	-0.600884	0.764698
29	1	0	-0.016057	-0.118027	1.663828

$CH_2(CO_2Me)_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.061875	0.992395	-0.526233
2	1	0	-0.111434	0.931390	-1.616378
3	1	0	-0.260598	2.023478	-0.222892
4	6	0	-1.121361	0.095428	0.077855
5	8	0	-0.931330	-0.680398	0.984837
6	8	0	-2.303466	0.289299	-0.506418
7	6	0	-3.386270	-0.485939	0.025364
8	1	0	-4.263581	-0.204235	-0.554733
9	1	0	-3.180379	-1.552209	-0.089036

10	1	0	-3.536600	-0.252602	1.081504
11	6	0	1.300927	0.578305	-0.026247
12	8	0	1.943285	1.171897	0.806088
13	8	0	1.707523	-0.546220	-0.620038
14	6	0	2.967824	-1.055028	-0.169466
15	1	0	3.142952	-1.964368	-0.742311
16	1	0	3.761200	-0.328485	-0.357911
17	1	0	2.924876	-1.280566	0.898365

TS5A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.742962	2.581550	-1.448608
2	9	0	-0.631850	2.801004	-2.824094
3	9	0	0.036966	1.445493	-1.088737
4	9	0	-2.090187	2.338615	-1.119113
5	9	0	-0.263958	3.701571	-0.743418
6	6	0	3.019600	0.528055	0.762926
7	1	0	3.759984	1.311927	0.659758
8	1	0	0.095665	-0.695720	1.008634
9	6	0	1.800307	0.864306	1.394172
10	8	0	0.814445	0.138608	1.641009
11	8	0	1.812951	2.178720	1.801608
12	6	0	0.561311	2.781706	2.140449
13	1	0	0.803322	3.692117	2.696959
14	1	0	0.039990	3.045075	1.215847
15	1	0	-0.049344	2.127812	2.766353

16	6	0	3.309350	-0.726520	0.173508
17	8	0	2.628813	-1.759069	0.121687
18	8	0	4.559400	-0.704246	-0.439881
19	6	0	4.907720	-1.878173	-1.172625
20	1	0	5.843395	-1.643394	-1.686505
21	1	0	5.061458	-2.739624	-0.512254
22	1	0	4.140015	-2.137632	-1.908864
23	6	0	-2.383684	-2.311702	-1.384871
24	6	0	-0.999382	-2.102245	-0.698467
25	6	0	-2.337674	-0.781292	1.210546
26	6	0	-3.616263	-1.209832	0.437101
27	6	0	-3.381093	-1.186982	-1.074733
28	1	0	-2.997125	-0.209302	-1.397675
29	1	0	-2.818329	-3.248965	-1.012787
30	1	0	-4.462282	-0.587526	0.746082
31	1	0	-3.868837	-2.242060	0.709371
32	1	0	-4.319879	-1.342685	-1.617107
33	1	0	-2.236959	-2.434148	-2.462769
34	6	0	-2.414413	0.696103	1.611563
35	1	0	-1.499328	1.006101	2.119422
36	1	0	-2.571069	1.339208	0.741247
37	1	0	-3.261846	0.826470	2.292491
38	6	0	-2.114058	-1.640578	2.460263
39	1	0	-1.118269	-1.479181	2.888652
40	1	0	-2.854922	-1.355642	3.215202
41	1	0	-2.246890	-2.706540	2.258426
42	6	0	0.093572	-1.749678	-1.720525
43	1	0	1.072475	-1.755008	-1.229617
44	1	0	0.104809	-2.535655	-2.483934
45	1	0	-0.093282	-0.793437	-2.217458

46	6	0	-0.540606	-3.344714	0.068957
47	1	0	-0.415141	-4.169090	-0.642885
48	1	0	0.432607	-3.158521	0.538741
49	1	0	-1.263177	-3.682224	0.813330
50	7	0	-1.121612	-0.902765	0.259580
51	1	0	-1.122676	-0.063733	-0.339387

$TEMPH_2BF_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.551557	1.315867	-0.027767
2	6	0	1.030670	1.321983	0.186259
3	6	0	1.374059	-1.297719	0.121571
4	6	0	2.691112	-1.121558	-0.670492
5	6	0	2.946792	0.323623	-1.119771
6	1	0	2.375935	0.537338	-2.032359
7	1	0	3.064955	1.060327	0.906907
8	1	0	2.681061	-1.780489	-1.544281
9	1	0	3.512693	-1.453834	-0.027133
10	1	0	4.002745	0.441454	-1.377256
11	1	0	2.854272	2.333996	-0.292139
12	6	0	0.555852	-2.478599	-0.396764
13	1	0	-0.376849	-2.584809	0.167303
14	1	0	0.315962	-2.354271	-1.458265
15	1	0	1.141016	-3.395222	-0.281751
16	6	0	1.615632	-1.460295	1.620015
17	1	0	0.669981	-1.436683	2.173494

18	1	0	2.085151	-2.434590	1.784859
19	1	0	2.286349	-0.697018	2.020968
20	6	0	0.328529	2.241004	-0.813086
21	1	0	-0.758279	2.139662	-0.727123
22	1	0	0.600314	3.277920	-0.598080
23	1	0	0.625154	2.012140	-1.842670
24	6	0	0.631970	1.717708	1.603657
25	1	0	0.982112	2.737474	1.789607
26	1	0	-0.458238	1.703232	1.711868
27	1	0	1.073625	1.064711	2.359322
28	7	0	0.496558	-0.079882	-0.107553
29	1	0	0.191024	-0.107435	-1.088324
30	5	0	-2.761633	-0.084470	-0.115384
31	9	0	-2.047177	-0.551705	1.023058
32	9	0	-2.006090	-0.413655	-1.254221
33	9	0	-4.003969	-0.695654	-0.165161
34	9	0	-2.889089	1.301775	-0.021959
35	1	0	-0.376834	-0.221321	0.427653

IM6A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.007969	-0.568170	0.024161
2	1	0	0.002430	-1.652066	0.015866
3	6	0	-1.255333	0.079815	-0.030207
4	8	0	-1.516637	1.297135	0.095701
5	8	0	-2.289008	-0.803913	-0.120361

6	6	0	-3.585815	-0.250631	0.036813
7	1	0	-4.272468	-1.099104	0.009985
8	1	0	-3.676561	0.275442	0.990248
9	1	0	-3.818433	0.442482	-0.774816
10	6	0	1.256349	0.098470	-0.004822
11	8	0	1.525107	1.291542	-0.101801
12	8	0	2.282648	-0.812806	0.069933
13	6	0	3.586269	-0.254095	0.010701
14	1	0	4.279285	-1.093614	0.087492
15	1	0	3.750455	0.275523	-0.932386
16	1	0	3.757399	0.443327	0.835964

IM7A

Standard orientation:

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

1	6	0	-2.605723	0.780357	-0.305463
2	6	0	-1.093855	0.848069	-0.330492
3	6	0	-0.924393	-1.506388	0.202138
4	6	0	-2.272964	-1.378537	0.890245
5	6	0	-3.238173	-0.529723	0.065409
6	1	0	-0.632057	1.801038	-0.574855
7	1	0	-4.169624	-0.324914	0.598118
8	1	0	-0.995902	-1.998267	-0.772738
9	1	0	-0.201865	-2.033497	0.824002
10	1	0	-2.126586	-0.934735	1.880738
11	1	0	-2.676791	-2.383428	1.030702
12	1	0	-3.484545	-1.035245	-0.875132

13	7	0	-0.346395	-0.157969	-0.061897
14	6	0	1.089915	-0.022405	-0.041329
15	6	0	1.653375	1.024615	0.681177
16	6	0	1.865479	-0.954970	-0.726081
17	6	0	3.040249	1.144791	0.709493
18	1	0	1.019715	1.714061	1.231088
19	6	0	3.248373	-0.816822	-0.688277
20	1	0	1.392516	-1.735411	-1.312099
21	6	0	3.835670	0.226743	0.028084
22	1	0	3.494518	1.951236	1.275577
23	1	0	3.868829	-1.524849	-1.227767
24	1	0	4.916476	0.322147	0.055600
25	8	0	-3.195954	1.799158	-0.576171

TS6A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.784409	2.618248	-0.604888
2	6	0	1.373388	2.037361	1.209491
3	6	0	0.019765	2.507685	1.734424
4	6	0	-0.649187	3.388982	0.684422
5	1	0	-0.035410	4.272847	0.462513
6	1	0	1.855752	1.348205	1.904333
7	1	0	2.054933	2.869457	1.010247
8	1	0	0.156380	3.027022	2.683854
9	1	0	-0.607748	1.623281	1.855363
10	1	0	-1.636132	3.744617	0.992731

11	7	0	1.180364	1.261695	-0.050263
12	6	0	2.207555	0.328774	-0.440661
13	6	0	1.863167	-0.915501	-0.963147
14	6	0	3.539971	0.720946	-0.317626
15	6	0	2.879565	-1.779946	-1.360823
16	1	0	0.821192	-1.217948	-1.007133
17	6	0	4.542915	-0.156879	-0.719176
18	1	0	3.794433	1.705726	0.058227
19	6	0	4.216551	-1.407755	-1.238898
20	1	0	2.618571	-2.756209	-1.757262
21	1	0	5.581172	0.146292	-0.631189
22	1	0	5.002235	-2.090584	-1.546592
23	8	0	-1.426988	2.977399	-1.569610
24	6	0	0.098868	1.415552	-0.759170
25	1	0	-0.016406	0.832868	-1.668824
26	6	0	-1.933172	-0.904164	0.749044
27	1	0	-2.141373	-0.217539	1.521023
28	6	0	-0.811173	-1.770605	0.858635
29	8	0	-0.457877	-2.683076	0.126447
30	8	0	-0.096673	-1.484504	1.998493
31	6	0	-2.949310	-1.127530	-0.262752
32	8	0	-2.910646	-1.825575	-1.269793
33	8	0	-4.076886	-0.437293	0.068010
34	6	0	-5.090372	-0.419374	-0.926166
35	1	0	-5.489468	-1.421460	-1.105134
36	1	0	-5.878161	0.229478	-0.541427
37	1	0	-4.705321	-0.016472	-1.867659
38	6	0	1.115097	-2.218517	2.129226
39	1	0	1.757268	-1.628869	2.785263
40	1	0	0.929688	-3.197263	2.584377

41	1	0	1.593087	-2.364589	1.159154

3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.521393	2.025799	-0.666159
2	6	0	1.065208	2.291415	0.709012
3	6	0	-0.172078	3.131968	0.998520
4	6	0	-0.958000	3.367096	-0.296599
5	1	0	-0.282320	3.719097	-1.086692
6	1	0	1.467888	1.865915	1.638366
7	1	0	1.833420	2.947157	0.282030
8	1	0	0.141097	4.080381	1.441152
9	1	0	-0.817126	2.629777	1.729679
10	1	0	-1.776970	4.079813	-0.181605
11	7	0	0.793010	1.229208	-0.261596
12	6	0	1.830212	0.349105	-0.566384
13	6	0	1.614340	-0.843512	-1.290060
14	6	0	3.148856	0.622646	-0.144895
15	6	0	2.671928	-1.696245	-1.591158
16	1	0	0.619236	-1.138155	-1.604236
17	6	0	4.193611	-0.241668	-0.456832
18	1	0	3.370165	1.514189	0.428163
19	6	0	3.972587	-1.408702	-1.183950
20	1	0	2.463157	-2.605625	-2.147849
21	1	0	5.195187	0.007461	-0.117122
22	1	0	4.790920	-2.081011	-1.420234

23	8	0	-2.682084	1.821101	-0.951883
24	6	0	-0.564644	0.834334	-0.547052
25	1	0	-0.584590	0.370859	-1.537292
26	6	0	-1.243351	-0.183302	0.435802
27	1	0	-1.709316	0.362824	1.262294
28	6	0	-0.283808	-1.184533	1.061434
29	8	0	-0.297675	-2.375645	0.857258
30	8	0	0.556687	-0.577147	1.897601
31	6	0	-2.301893	-0.966742	-0.318823
32	8	0	-2.170797	-1.360681	-1.453842
33	8	0	-3.374030	-1.196497	0.434466
34	6	0	-4.409023	-1.964975	-0.192713
35	1	0	-4.030388	-2.948994	-0.476836
36	1	0	-5.198452	-2.060887	0.550997
37	1	0	-4.779894	-1.444365	-1.078165
38	6	0	1.605320	-1.402050	2.420296
39	1	0	2.242742	-0.737181	3.001566
40	1	0	1.190347	-2.186639	3.056733
41	1	0	2.169784	-1.851903	1.598789

TS7A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.479078	-0.867926	1.065069
2	6	0	-0.471892	0.004826	0.282279
3	6	0	-1.984480	0.301339	2.156840
4	6	0	-0.855878	-0.188839	3.050417

5	6	0	-0.120436	-1.343703	2.375708
6	1	0	-0.246426	0.222089	-0.758460
7	1	0	-0.818815	-2.160772	2.165421
8	1	0	-2.440940	1.213974	2.539435
9	1	0	-2.769888	-0.452552	2.038049
10	1	0	-1.288513	-0.500955	4.004907
11	1	0	-0.158349	0.632706	3.251812
12	1	0	0.688130	-1.722418	3.007059
13	1	0	0.764958	-1.693436	0.418070
14	7	0	-1.506104	0.592034	0.781718
15	6	0	-2.228495	1.591207	0.013438
16	6	0	-2.358611	2.860694	0.577013
17	6	0	-2.693903	1.300539	-1.263438
18	6	0	-2.990512	3.862229	-0.150559
19	1	0	-1.948956	3.074972	1.560127
20	6	0	-3.322250	2.320196	-1.976072
21	1	0	-2.572548	0.296853	-1.662640
22	6	0	-3.478194	3.589572	-1.427059
23	1	0	-3.092852	4.853809	0.277879
24	1	0	-3.699233	2.108122	-2.971117
25	1	0	-3.976073	4.370202	-1.993604
26	6	0	3.910597	1.958015	-0.658356
27	6	0	2.657908	1.686997	0.203351
28	6	0	3.614959	-0.675693	0.253211
29	6	0	4.363943	-0.455095	-1.089467
30	6	0	4.071498	0.899912	-1.740792
31	1	0	3.151108	0.842082	-2.332943
32	1	0	4.808828	1.972722	-0.029526
33	1	0	4.104932	-1.259273	-1.786418
34	1	0	5.438813	-0.544402	-0.890215

35	1	0	4.876258	1.167867	-2.432291
36	1	0	3.819905	2.960789	-1.089046
37	7	0	2.409960	0.206376	0.225109
38	6	0	3.169390	-2.141200	0.307404
39	1	0	2.723858	-2.392388	1.275631
40	1	0	2.459792	-2.380881	-0.490352
41	1	0	4.053152	-2.774498	0.176939
42	6	0	4.531972	-0.441569	1.467009
43	1	0	3.945006	-0.461305	2.390369
44	1	0	5.272968	-1.246125	1.518277
45	1	0	5.081013	0.500988	1.416302
46	6	0	1.448761	2.350903	-0.468252
47	1	0	0.551076	2.261461	0.151099
48	1	0	1.636838	3.421315	-0.599537
49	1	0	1.245198	1.911386	-1.450472
50	6	0	2.829096	2.325769	1.589535
51	1	0	3.066817	3.386754	1.454705
52	1	0	1.908383	2.252562	2.172521
53	1	0	3.635224	1.870527	2.166199
54	8	0	1.621022	-0.066636	1.386385
55	6	0	-1.660785	-2.515319	-0.622820
56	1	0	-1.358413	-3.392955	-0.066704
57	6	0	-0.780462	-2.043147	-1.627154
58	8	0	-0.887218	-1.101380	-2.411561
59	8	0	0.400831	-2.771202	-1.607912
60	6	0	1.417200	-2.275039	-2.459553
61	1	0	2.216691	-3.019157	-2.441956
62	1	0	1.049369	-2.134182	-3.477787
63	1	0	1.800203	-1.315624	-2.085390
64	6	0	-2.881244	-1.900269	-0.258084

65	8	0	-3.421703	-0.883921	-0.688350
66	8	0	-3.459363	-2.563125	0.821106
67	6	0	-4.803513	-2.204512	1.079459
68	1	0	-5.080341	-2.704270	2.008947
69	1	0	-4.926942	-1.121634	1.175392
70	1	0	-5.458265	-2.542455	0.269406

3a’

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.479478	-0.727901	-0.233451
2	6	0	0.696782	0.091018	0.251812
3	6	0	1.165433	0.472295	-2.071746
4	6	0	0.975964	-1.019193	-2.323020
5	6	0	-0.012466	-1.668790	-1.340935
6	1	0	0.460399	0.794754	1.039206
7	1	0	0.439786	-2.533873	-0.854585
8	1	0	0.273960	1.043833	-2.341041
9	1	0	2.014284	0.873695	-2.622478
10	1	0	1.952154	-1.506004	-2.240942
11	1	0	0.641184	-1.140987	-3.356664
12	1	0	-0.900620	-2.031175	-1.854506
13	1	0	-0.968128	-1.291717	0.574369
14	7	0	1.400345	0.720698	-0.627953
15	6	0	2.432754	1.638016	-0.226897
16	6	0	3.704467	1.515496	-0.784864
17	6	0	2.151866	2.618287	0.721401

18	6	0	4.705194	2.394936	-0.383108
19	1	0	3.914263	0.727293	-1.500882
20	6	0	3.163607	3.487467	1.120216
21	1	0	1.147337	2.712983	1.123794
22	6	0	4.437907	3.379280	0.567468
23	1	0	5.698557	2.303537	-0.810453
24	1	0	2.948049	4.258209	1.853111
25	1	0	5.222725	4.063073	0.875129
26	6	0	-4.492112	1.274905	0.988513
27	6	0	-2.965166	1.118312	0.828320
28	6	0	-3.645719	0.065577	-1.397666
29	6	0	-5.050683	-0.307856	-0.840709
30	6	0	-5.192215	-0.036610	0.657626
31	1	0	-4.727600	-0.851922	1.222298
32	1	0	-4.869186	2.066949	0.330074
33	1	0	-5.264921	-1.359628	-1.051936
34	1	0	-5.789507	0.292566	-1.385732
35	1	0	-6.249336	-0.009910	0.941281
36	1	0	-4.695344	1.597312	2.015937
37	7	0	-2.710826	0.089623	-0.234707
38	6	0	-3.206096	-1.036524	-2.361723
39	1	0	-2.266410	-0.782351	-2.858915
40	1	0	-3.095173	-1.986611	-1.833438
41	1	0	-3.975190	-1.152177	-3.133438
42	6	0	-3.689843	1.378384	-2.196957
43	1	0	-2.684237	1.658373	-2.529440
44	1	0	-4.312746	1.233580	-3.086658
45	1	0	-4.115888	2.209961	-1.631841
46	6	0	-2.409507	0.571219	2.149374
47	1	0	-1.354626	0.292387	2.060970

48	1	0	-2.479441	1.341399	2.925022
49	1	0	-2.964770	-0.314469	2.478943
50	6	0	-2.301022	2.474483	0.568127
51	1	0	-2.632719	3.180562	1.337440
52	1	0	-1.211473	2.394179	0.630977
53	1	0	-2.557382	2.890679	-0.407747
54	8	0	-1.391226	0.270776	-0.729997
55	6	0	1.712939	-1.117539	0.831415
56	1	0	2.396476	-0.421834	1.298755
57	6	0	2.429491	-1.960874	-0.051851
58	8	0	2.197486	-3.138239	-0.364198
59	8	0	3.496515	-1.317825	-0.611666
60	6	0	4.236415	-2.091082	-1.552363
61	1	0	5.109609	-1.495152	-1.819143
62	1	0	4.545469	-3.039338	-1.107046
63	1	0	3.638823	-2.301360	-2.445796
64	6	0	0.886728	-1.858179	1.702122
65	8	0	0.367886	-2.959676	1.521851
66	8	0	0.616195	-1.147530	2.842277
67	6	0	-0.153318	-1.832757	3.825651
68	1	0	-0.381514	-1.094048	4.595583
69	1	0	-1.068516	-2.238905	3.396693
70	1	0	0.428650	-2.650385	4.265049

Table S4

	Gsol	Thermal correction to Gibbs Free Energy (TCG)	Esol	△Gsol=Esol+TCG	N_{imag}
8a	-518.444088	0.18331	-518.7723446	-518.5890346	0
TEMPOBF$_4$	-907.564217	0.238674	-908.0995694	-907.8608954	0
TS1B	-1425.968	0.438133	-1426.844874	-1426.406741	-1439.66
IM1B	-942.168961	0.179246	-942.646842	-942.467596	0
TEMPOH	-483.861261	0.241587	-484.2491599	-484.0075729	0
TEMPOH$_2$BF$_4$	-908.794307	0.26409	-909.3592486	-909.0951586	0
IM2B	-517.260351	0.15879	-517.5625698	-517.4037798	0
TS2B	-1424.800746	0.422584	-1425.655158	-1425.232574	-359.85
IM3B	-1424.842128	0.424884	-1425.696686	-1425.271802	0
TS3B	-1424.788530	0.420778	-1425.6423	-1425.221522	-1829.88
H$_2$O	-76.378136	0.003586	-76.42967634	-76.42609034	0
TS3B'	-1501.184865	0.440176	-1502.107236	-1501.66706	-1651.17
IM4B	-1424.853944	0.426031	-1425.710099	-1425.284068	0
TS4B	-1424.84601	0.422463	-1425.699917	-1425.277454	-472.42
IM5B	-1016.198939	0.160879	-1016.680966	-1016.520087	0
TEMPH	-408.720732	0.239072	-409.0789717	-408.8398997	0
CH$_2$(COMe)$_2$	-345.556812	0.092316	-345.762425	-345.670109	0
TS5B	-1178.742368	0.355179	-1179.487127	-1179.131948	-619.25
TEMPH$_2$BF$_4$	-833.660814	0.261032	-834.1973714	-833.9363394	0
IM6B	-345.070962	0.077536	-345.2749306	-345.1973946	0
IM7B	-591.718895	0.153282	-592.0322447	-591.8789627	0
TS6B	-936.799902	0.253792	-937.3299883	-937.0761963	-65.45
9a''	-936.857865	0.256417	-937.3869978	-937.1305808	0
TS7B	-1345.441902	0.516095	-1346.345309	-1345.829214	-100.02
9a	-1345.497156	0.522603	-1346.400619	-1345.878016	0

8a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.659525	-0.982120	0.670825
2	6	0	-1.313932	-1.236292	0.007905
3	6	0	-1.313940	1.236286	-0.007944
4	6	0	-2.659575	0.982117	-0.670779
5	1	0	-0.787779	-1.994656	0.596643
6	1	0	-1.458679	-1.639924	-1.005635
7	1	0	-2.486959	-0.675215	1.712462
8	1	0	-1.458622	1.639894	1.005616
9	1	0	-0.787833	1.994667	-0.596699
10	1	0	-2.487075	0.675231	-1.712433
11	1	0	-3.246859	1.904680	-0.680301
12	1	0	-3.246802	-1.904686	0.680402
13	7	0	-0.545529	0.000000	-0.000063
14	6	0	0.831399	0.000004	-0.000030
15	6	0	1.561419	-1.175920	-0.278684
16	6	0	1.561407	1.175928	0.278655
17	6	0	2.951848	-1.166252	-0.272153
18	1	0	1.039999	-2.094440	-0.525021
19	6	0	2.951837	1.166259	0.272181
20	1	0	1.039980	2.094449	0.524970
21	6	0	3.665567	0.000004	0.000029
22	1	0	3.482196	-2.088261	-0.495383
23	1	0	3.482178	2.088268	0.495434
24	1	0	4.750744	0.000003	0.000052

25	8	0	-3.434351	-0.000012	0.000038

TS1B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.385660	3.742250	0.696225
2	6	0	0.955167	2.399053	1.175913
3	6	0	0.347639	1.693422	-1.289787
4	6	0	-0.772135	2.769093	-1.326096
5	6	0	-0.947490	3.551694	-0.018631
6	1	0	-1.638956	3.019167	0.645257
7	1	0	1.100853	4.237313	0.029269
8	1	0	-1.720056	2.287877	-1.589672
9	1	0	-0.529733	3.460283	-2.140461
10	1	0	-1.406399	4.521464	-0.232083
11	1	0	0.274929	4.385161	1.575305
12	7	0	0.713955	1.386082	0.117654
13	6	0	-0.124681	0.406895	-1.962794
14	1	0	0.676254	-0.333694	-2.008809
15	1	0	-0.987952	-0.016348	-1.438828
16	1	0	-0.439887	0.659266	-2.979712
17	6	0	1.627849	2.178058	-1.995382
18	1	0	2.418984	1.434289	-1.867747
19	1	0	1.415771	2.305102	-3.062057
20	1	0	1.974072	3.137546	-1.601568
21	6	0	0.245886	1.933285	2.454376
22	1	0	0.620461	0.957805	2.778250

23	1	0	0.453193	2.656757	3.247876
24	1	0	-0.838739	1.871562	2.321004
25	6	0	2.463092	2.487342	1.433213
26	1	0	2.645681	3.222424	2.223854
27	1	0	2.854832	1.517042	1.747499
28	1	0	2.995001	2.802714	0.531336
29	8	0	0.976523	0.180276	0.422628
30	9	0	2.903937	-1.867411	0.571843
31	9	0	3.639655	0.135574	-0.280783
32	9	0	4.712242	-1.810057	-0.824024
33	9	0	2.626119	-1.395292	-1.655668
34	5	0	3.468525	-1.230951	-0.541518
35	6	0	0.173805	-2.328380	1.957378
36	6	0	-0.823305	-1.327714	1.383755
37	6	0	-1.278665	-2.855315	-0.467383
38	6	0	0.175539	-3.195181	-0.203769
39	1	0	-1.268916	-0.665861	2.129289
40	1	0	0.008461	-0.440971	0.837704
41	1	0	-0.198958	-2.641815	2.938982
42	1	0	-1.902450	-3.731416	-0.261286
43	1	0	-1.435297	-2.544393	-1.505521
44	1	0	0.847985	-2.380042	-0.500271
45	1	0	0.445977	-4.095321	-0.759542
46	1	0	1.140752	-1.828054	2.094418
47	7	0	-1.686602	-1.753231	0.419951
48	6	0	-2.871801	-1.042512	0.120022
49	6	0	-2.993960	0.314307	0.447795
50	6	0	-3.923877	-1.694184	-0.534084
51	6	0	-4.167019	0.998363	0.151994
52	1	0	-2.157994	0.845391	0.894555

53	6	0	-5.091320	-0.995778	-0.828156
54	1	0	-3.842857	-2.743201	-0.796886
55	6	0	-5.223438	0.347933	-0.484935
56	1	0	-4.243377	2.052027	0.404214
57	1	0	-5.904051	-1.513334	-1.328169
58	1	0	-6.134931	0.886957	-0.722109
59	8	0	0.318975	-3.488025	1.174875

IM1B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.506214	1.880320	-0.738975
2	6	0	-0.420985	0.857123	-0.867840
3	6	0	0.403425	1.899153	1.071118
4	6	0	-0.001919	3.261463	0.507906
5	1	0	-0.384684	0.111248	-1.656207
6	1	0	-2.147786	1.600385	0.108055
7	1	0	-0.371388	1.487502	1.725354
8	1	0	1.340392	1.963715	1.621185
9	1	0	0.879860	3.784877	0.128264
10	1	0	-0.443088	3.848335	1.320848
11	1	0	-2.109357	1.907745	-1.645103
12	7	0	0.547552	0.923773	-0.026474
13	6	0	1.660607	0.008250	-0.042401
14	6	0	2.951527	0.524906	0.030617
15	6	0	1.410641	-1.357596	-0.125764
16	6	0	4.024669	-0.358929	-0.000241

17	1	0	3.111245	1.597616	0.091601
18	6	0	2.498826	-2.227287	-0.156996
19	1	0	0.391166	-1.732058	-0.144754
20	6	0	3.799451	-1.732479	-0.095342
21	1	0	5.037413	0.027762	0.045779
22	1	0	2.323196	-3.296434	-0.218386
23	1	0	4.641072	-2.417601	-0.116269
24	9	0	-1.591643	-0.653161	1.034951
25	9	0	-2.699052	-0.595762	-0.961496
26	9	0	-3.561761	-1.795241	0.791190
27	9	0	-1.672025	-2.523635	-0.278090
28	5	0	-2.392542	-1.401966	0.149989
29	8	0	-0.917254	3.155123	-0.574560

IM2B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.693604	1.144246	-0.336301
2	6	0	-1.355590	1.143461	-0.403665
3	6	0	-1.382199	-1.231294	-0.080834
4	6	0	-2.666167	-0.935406	0.691664
5	1	0	-0.827338	2.029984	-0.730693
6	1	0	-1.629971	-1.613511	-1.080212
7	1	0	-0.820087	-1.995702	0.459448
8	1	0	-2.407942	-0.602310	1.705115
9	1	0	-3.292691	-1.826922	0.752678
10	1	0	-3.290726	2.005797	-0.607668

11	7	0	-0.601254	-0.009267	-0.165021
12	6	0	0.785844	0.005336	-0.070547
13	6	0	1.535322	-1.159360	-0.316870
14	6	0	1.475411	1.184011	0.270272
15	6	0	2.922790	-1.139092	-0.217316
16	1	0	1.035582	-2.076426	-0.610511
17	6	0	2.863589	1.190729	0.348480
18	1	0	0.922812	2.087733	0.504481
19	6	0	3.602626	0.032780	0.109678
20	1	0	3.476493	-2.052825	-0.414619
21	1	0	3.370000	2.113720	0.617122
22	1	0	4.685510	0.043388	0.179351
23	8	0	-3.442625	0.067433	0.051661

TS2B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.213979	0.100143	1.491305
2	6	0	1.308454	0.327453	0.641193
3	6	0	2.506808	-1.268939	1.933399
4	1	0	1.246366	1.057017	-0.159287
5	1	0	1.991992	-2.186216	1.617271
6	1	0	3.543247	-1.490315	2.174878
7	1	0	-0.580251	0.830256	1.409053
8	7	0	2.456342	-0.320762	0.797103
9	6	0	3.580520	-0.118400	-0.056217
10	6	0	4.868609	-0.075493	0.484480

11	6	0	3.387012	0.059547	-1.428608
12	6	0	5.957357	0.137498	-0.354948
13	1	0	5.024122	-0.175511	1.553380
14	6	0	4.483986	0.282697	-2.254695
15	1	0	2.387901	0.013036	-1.849536
16	6	0	5.771911	0.316393	-1.724524
17	1	0	6.955030	0.174784	0.070881
18	1	0	4.326784	0.417503	-3.320186
19	1	0	6.625535	0.482308	-2.373834
20	6	0	-2.641053	-1.212645	-2.288101
21	6	0	-1.439208	-1.669301	-1.444698
22	6	0	-3.063696	-1.041489	0.519777
23	6	0	-3.786518	-0.012559	-0.387803
24	6	0	-3.176609	0.123621	-1.788339
25	1	0	-2.363816	0.854502	-1.756834
26	1	0	-3.432122	-1.970646	-2.268367
27	1	0	-3.772533	0.967297	0.098774
28	1	0	-4.834292	-0.324380	-0.462283
29	1	0	-3.929774	0.517319	-2.477663
30	1	0	-2.302439	-1.139717	-3.326520
31	7	0	-1.693346	-1.311198	-0.015641
32	6	0	-2.969590	-0.511006	1.947904
33	1	0	-2.451572	-1.209359	2.610681
34	1	0	-2.487487	0.467002	1.984516
35	1	0	-3.993567	-0.386716	2.313556
36	6	0	-3.808033	-2.389744	0.556351
37	1	0	-3.238041	-3.120500	1.139592
38	1	0	-4.777677	-2.235826	1.040457
39	1	0	-3.992451	-2.797444	-0.439648
40	6	0	-0.164182	-0.951883	-1.887191

41	1	0	0.695844	-1.323970	-1.323310
42	1	0	0.005535	-1.168379	-2.945822
43	1	0	-0.241485	0.131052	-1.754047
44	6	0	-1.224464	-3.183789	-1.537805
45	1	0	-0.991535	-3.444752	-2.575496
46	1	0	-0.384815	-3.489231	-0.905757
47	1	0	-2.117484	-3.736824	-1.235363
48	8	0	-0.734872	-1.438662	0.787594
49	5	0	-1.591414	3.014120	-0.030484
50	9	0	-0.701194	2.083976	-0.612523
51	9	0	-1.911890	2.579071	1.267826
52	9	0	-2.754397	3.081708	-0.799839
53	9	0	-0.979758	4.264015	0.029827
54	6	0	1.903572	-0.692648	3.042531
55	1	0	2.034643	-1.316250	3.902090
56	1	0	2.391059	0.245877	3.205099
57	8	0	0.503796	-0.521894	2.835432

IM3B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.079589	-0.180700	-1.279503
2	6	0	-1.353401	0.327643	-0.630460
3	6	0	-2.200743	-1.791589	-1.230229
4	6	0	-1.504111	-1.615889	-2.573990
5	1	0	-1.428259	1.327667	-0.213118
6	1	0	-1.612062	-2.394528	-0.535619

7	1	0	-3.181006	-2.245119	-1.364052
8	1	0	-2.209814	-1.212459	-3.305776
9	1	0	-1.153921	-2.593278	-2.913798
10	1	0	0.625321	0.636275	-1.421765
11	7	0	-2.366377	-0.460062	-0.603081
12	6	0	-3.601003	-0.108217	0.052564
13	6	0	-4.806526	-0.310565	-0.613759
14	6	0	-3.544573	0.428226	1.335161
15	6	0	-5.986897	0.048903	0.028078
16	1	0	-4.821874	-0.716723	-1.620428
17	6	0	-4.735773	0.779897	1.963735
18	1	0	-2.588082	0.545113	1.836802
19	6	0	-5.952984	0.591010	1.312894
20	1	0	-6.934526	-0.092390	-0.480970
21	1	0	-4.708480	1.191521	2.967162
22	1	0	-6.879176	0.863030	1.808963
23	6	0	2.791503	-1.005183	2.395750
24	6	0	1.420090	-0.901091	1.698599
25	6	0	2.811681	-1.442707	-0.386818
26	6	0	4.092651	-0.850875	0.262110
27	6	0	3.853411	-0.218729	1.638466
28	1	0	3.520517	0.816675	1.513700
29	1	0	3.097609	-2.055709	2.472026
30	1	0	4.522572	-0.099592	-0.409285
31	1	0	4.827225	-1.660605	0.344864
32	1	0	4.790242	-0.191646	2.204264
33	1	0	2.677175	-0.636176	3.421050
34	7	0	1.655459	-0.732945	0.228579
35	6	0	2.823350	-1.103591	-1.880124
36	1	0	1.990727	-1.575705	-2.409508

37	1	0	2.768660	-0.019956	-2.024060
38	1	0	3.759149	-1.464529	-2.319837
39	6	0	2.754910	-2.971236	-0.246205
40	1	0	1.788587	-3.351579	-0.593717
41	1	0	3.538168	-3.417587	-0.868855
42	1	0	2.918659	-3.309146	0.780024
43	6	0	0.706888	0.369195	2.170138
44	1	0	-0.239857	0.502889	1.634583
45	1	0	0.474655	0.295143	3.238250
46	1	0	1.318891	1.257141	1.992153
47	6	0	0.550592	-2.110020	2.066351
48	1	0	0.540314	-2.210632	3.157407
49	1	0	-0.482198	-1.973085	1.730917
50	1	0	0.931666	-3.042986	1.644882
51	8	0	0.467441	-1.170417	-0.433665
52	5	0	1.671334	2.997407	-0.498818
53	9	0	0.371991	2.581361	-0.147259
54	9	0	2.105361	2.247403	-1.604710
55	9	0	2.534591	2.785753	0.583325
56	9	0	1.646767	4.350511	-0.831260
57	8	0	-0.391986	-0.717099	-2.522343

TS3B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.465279	0.167058	0.813528
2	6	0	-0.751959	-0.273009	0.231692

3	6	0	-1.963286	0.405715	2.180414
4	6	0	-0.598872	0.385055	2.852112
5	1	0	-0.744221	-0.700977	-0.762237
6	1	0	-2.271873	1.426076	1.942420
7	1	0	-2.709427	-0.064597	2.820072
8	1	0	-0.342037	-0.641987	3.145187
9	1	0	-0.605971	1.020765	3.738283
10	1	0	1.482572	-0.883443	0.811809
11	7	0	-1.877793	-0.333422	0.908736
12	6	0	-3.029824	-1.014179	0.392548
13	6	0	-3.751806	-1.865254	1.228696
14	6	0	-3.398908	-0.834589	-0.940218
15	6	0	-4.854501	-2.545441	0.719776
16	1	0	-3.446413	-2.012615	2.259965
17	6	0	-4.497084	-1.530074	-1.438437
18	1	0	-2.843366	-0.137967	-1.558845
19	6	0	-5.228297	-2.382294	-0.613008
20	1	0	-5.414983	-3.212198	1.367479
21	1	0	-4.789569	-1.390904	-2.474575
22	1	0	-6.088350	-2.915477	-1.005831
23	6	0	4.070796	-1.540100	-1.475996
24	6	0	2.625818	-1.025489	-1.335734
25	6	0	3.683176	0.220190	0.686375
26	6	0	4.709968	-0.924458	0.871947
27	6	0	4.605824	-2.061135	-0.150697
28	1	0	3.937225	-2.842237	0.228444
29	1	0	4.724359	-0.752984	-1.864604
30	1	0	4.604743	-1.332586	1.881948
31	1	0	5.700400	-0.459411	0.820014
32	1	0	5.584965	-2.527793	-0.290360

33	1	0	4.053872	-2.333265	-2.230255
34	7	0	2.452642	-0.352186	0.026924
35	6	0	3.305554	0.752791	2.067640
36	1	0	2.688188	1.649631	2.005586
37	1	0	2.769528	-0.003010	2.650461
38	1	0	4.234549	0.998631	2.592014
39	6	0	4.242481	1.387709	-0.136534
40	1	0	3.459274	2.124295	-0.337613
41	1	0	5.022497	1.875810	0.456502
42	1	0	4.690762	1.077528	-1.081294
43	6	0	1.677154	-2.227430	-1.379334
44	1	0	0.630754	-1.931473	-1.307373
45	1	0	1.806313	-2.739414	-2.337246
46	1	0	1.890946	-2.937661	-0.574887
47	6	0	2.287316	-0.062401	-2.473235
48	1	0	2.496480	-0.578932	-3.415723
49	1	0	1.233112	0.223126	-2.461054
50	1	0	2.896922	0.843860	-2.439395
51	8	0	1.433402	0.668520	-0.062125
52	5	0	-1.827135	2.475183	-0.902038
53	9	0	-1.929372	3.699391	-1.565575
54	9	0	-0.913388	2.575067	0.150894
55	9	0	-1.381832	1.490832	-1.811027
56	9	0	-3.078581	2.101942	-0.394188
57	8	0	0.391107	0.904164	1.981067

H_2O

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	0.000000	0.000000	0.110812
2	1	0	-0.000000	0.783976	-0.443248
3	1	0	-0.000000	-0.783976	-0.443248

TS3B’

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.428260	-1.343848	-0.204201
2	6	0	0.906084	-0.861747	-0.195512
3	6	0	1.740415	-3.097175	-0.541922
4	6	0	0.350421	-3.517602	-0.089761
5	1	0	1.091289	0.195111	-0.017499
6	1	0	1.856987	-3.225944	-1.621450
7	1	0	2.499331	-3.689533	-0.031441
8	1	0	0.291708	-3.502810	1.007188
9	1	0	0.130987	-4.524900	-0.445082
10	1	0	-0.757114	-1.385734	1.146772
11	7	0	1.945990	-1.670169	-0.224939
12	6	0	3.278513	-1.169775	-0.032616
13	6	0	4.166774	-1.858556	0.793095
14	6	0	3.660661	0.010954	-0.666549
15	6	0	5.449304	-1.352393	0.982869
16	1	0	3.858160	-2.765349	1.303318
17	6	0	4.940616	0.515599	-0.454753
18	1	0	2.960149	0.533828	-1.309649

19	6	0	5.839227	-0.166314	0.362420
20	1	0	6.140660	-1.883984	1.629048
21	1	0	5.230592	1.442994	-0.938180
22	1	0	6.839646	0.225035	0.518092
23	6	0	-3.850069	1.810377	0.737955
24	6	0	-2.441760	1.355130	0.305451
25	6	0	-3.754868	-0.710095	-0.555658
26	6	0	-4.883353	-0.462189	0.482437
27	6	0	-4.602475	0.693944	1.450832
28	1	0	-4.009133	0.336303	2.302343
29	1	0	-4.424640	2.143163	-0.133676
30	1	0	-5.053727	-1.381427	1.052894
31	1	0	-5.800980	-0.261298	-0.081073
32	1	0	-5.544283	1.067031	1.862996
33	1	0	-3.727715	2.683196	1.387519
34	7	0	-2.494700	-0.147973	0.055876
35	6	0	-3.574100	-2.215497	-0.743796
36	1	0	-2.872164	-2.441341	-1.547772
37	1	0	-3.220394	-2.699403	0.172091
38	1	0	-4.550508	-2.641150	-0.995045
39	6	0	-4.075540	-0.098445	-1.921711
40	1	0	-3.204557	-0.144409	-2.582246
41	1	0	-4.876966	-0.689650	-2.376310
42	1	0	-4.425730	0.933126	-1.858728
43	6	0	-1.454869	1.579089	1.455659
44	1	0	-0.466923	1.164354	1.234333
45	1	0	-1.326496	2.655904	1.599574
46	1	0	-1.815637	1.144492	2.392608
47	6	0	-1.962472	2.144413	-0.912660
48	1	0	-2.026160	3.207364	-0.656373

49	1	0	-0.923088	1.918168	-1.153285
50	1	0	-2.580945	1.975151	-1.795107
51	8	0	-1.365536	-0.479416	-0.776833
52	5	0	1.761984	2.789243	-0.204002
53	9	0	0.844513	3.806607	0.059942
54	9	0	1.334526	2.052943	-1.330541
55	9	0	1.827829	1.918088	0.899570
56	9	0	3.025194	3.322420	-0.458245
57	8	0	-0.628361	-2.654893	-0.647681
58	8	0	-1.647086	-1.363582	2.024059
59	1	0	-1.989600	-2.275095	2.100134
60	1	0	-2.257892	-0.785019	1.195090

IM4B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.013210	-1.517952	0.175253
2	6	0	-1.111373	-0.854036	0.570757
3	6	0	-2.420096	-2.223468	-0.914778
4	6	0	-1.112853	-2.306801	-1.693620
5	1	0	-1.066523	-0.144334	1.382923
6	1	0	-2.589528	-3.159045	-0.366397
7	1	0	-3.241675	-2.073953	-1.618868
8	1	0	-0.970642	-1.394163	-2.280784
9	1	0	-1.107224	-3.180053	-2.345817
10	1	0	1.482199	0.322678	-0.085941
11	7	0	-2.347259	-1.086959	-0.008369

12	6	0	-3.494506	-0.385399	0.382490
13	6	0	-4.760253	-0.980088	0.264386
14	6	0	-3.402027	0.919726	0.893388
15	6	0	-5.901056	-0.282343	0.651096
16	1	0	-4.854730	-1.994009	-0.109761
17	6	0	-4.550192	1.595520	1.291531
18	1	0	-2.440228	1.418784	0.931653
19	6	0	-5.808126	1.005261	1.174013
20	1	0	-6.870328	-0.762594	0.552212
21	1	0	-4.457453	2.605939	1.679454
22	1	0	-6.700288	1.542658	1.479060
23	6	0	3.785959	1.105251	1.584191
24	6	0	2.442230	0.387343	1.800427
25	6	0	3.186618	-0.804806	-0.440430
26	6	0	4.001828	0.455942	-0.834432
27	6	0	3.934906	1.619694	0.160911
28	1	0	3.086250	2.265084	-0.086844
29	1	0	4.615840	0.435991	1.832579
30	1	0	3.663270	0.800050	-1.814786
31	1	0	5.036842	0.116608	-0.947338
32	1	0	4.837314	2.230110	0.072098
33	1	0	3.817992	1.928098	2.304695
34	7	0	2.050818	-0.338733	0.480163
35	6	0	2.568878	-1.408557	-1.698405
36	1	0	2.156513	-2.399639	-1.515223
37	1	0	1.788649	-0.758604	-2.108621
38	1	0	3.368993	-1.492082	-2.440152
39	6	0	4.026622	-1.864850	0.266224
40	1	0	3.395660	-2.669034	0.654784
41	1	0	4.698697	-2.295030	-0.482166

42	1	0	4.643576	-1.464128	1.071740
43	6	0	1.331561	1.399756	2.069372
44	1	0	0.379804	0.903270	2.268962
45	1	0	1.599689	1.968022	2.964030
46	1	0	1.198772	2.097280	1.237557
47	6	0	2.537111	-0.601339	2.957597
48	1	0	2.922705	-0.039686	3.814312
49	1	0	1.561129	-1.008765	3.225466
50	1	0	3.227311	-1.422568	2.756094
51	8	0	1.185378	-1.429677	0.847525
52	5	0	-0.071424	1.891738	-1.658952
53	9	0	1.287183	1.517215	-1.428737
54	9	0	-0.696749	2.002324	-0.413567
55	9	0	-0.676806	0.898780	-2.428015
56	9	0	-0.093880	3.108444	-2.325126
57	8	0	-0.007910	-2.464039	-0.801715

TS4B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.139369	1.895705	0.785578
2	6	0	0.966429	1.069913	0.682198
3	6	0	2.370733	2.909570	-0.048181
4	6	0	1.096148	3.539134	-0.598064
5	1	0	0.868203	0.008843	0.898411
6	1	0	2.677720	3.408651	0.879276
7	1	0	3.186078	3.000577	-0.764755

8	1	0	0.857960	3.072628	-1.561031
9	1	0	1.286050	4.600682	-0.775694
10	1	0	-1.317589	-0.328580	-0.055003
11	7	0	2.168279	1.481857	0.251024
12	6	0	3.271642	0.582536	0.219861
13	6	0	4.179482	0.621704	-0.843005
14	6	0	3.437875	-0.354719	1.243908
15	6	0	5.242769	-0.274872	-0.876117
16	1	0	4.043747	1.328906	-1.654751
17	6	0	4.497416	-1.255574	1.192693
18	1	0	2.748854	-0.369303	2.082403
19	6	0	5.405772	-1.218258	0.137112
20	1	0	5.939059	-0.241675	-1.708445
21	1	0	4.618152	-1.979586	1.992651
22	1	0	6.235316	-1.917481	0.104529
23	6	0	-4.065035	-1.262932	0.382993
24	6	0	-2.991390	-0.483069	1.175162
25	6	0	-2.708645	0.773560	-1.076408
26	6	0	-3.248007	-0.472673	-1.854844
27	6	0	-3.529850	-1.696176	-0.975617
28	1	0	-2.605910	-2.270776	-0.838626
29	1	0	-4.961027	-0.645162	0.252156
30	1	0	-2.521767	-0.742478	-2.627515
31	1	0	-4.163037	-0.151504	-2.365588
32	1	0	-4.243280	-2.354515	-1.479556
33	1	0	-4.357516	-2.124828	0.992026
34	7	0	-2.121279	0.262732	0.196241
35	6	0	-1.609805	1.420600	-1.923232
36	1	0	-1.344295	2.413927	-1.561914
37	1	0	-0.714840	0.792599	-1.966843

38	1	0	-1.998499	1.532829	-2.940201
39	6	0	-3.798420	1.807520	-0.804036
40	1	0	-3.423657	2.588195	-0.134015
41	1	0	-4.069713	2.273207	-1.756395
42	1	0	-4.705009	1.373485	-0.377973
43	6	0	-2.067839	-1.456182	1.909103
44	1	0	-1.225854	-0.922021	2.359001
45	1	0	-2.632426	-1.947934	2.706765
46	1	0	-1.678390	-2.225883	1.235577
47	6	0	-3.654033	0.453318	2.188685
48	1	0	-4.372732	-0.144378	2.758927
49	1	0	-2.926791	0.872866	2.884786
50	1	0	-4.199454	1.269138	1.711879
51	8	0	-1.255576	1.374060	1.244278
52	5	0	0.481764	-2.448583	-0.485224
53	9	0	-0.091697	-1.288227	-1.075140
54	9	0	-0.498513	-3.442470	-0.414477
55	9	0	0.913889	-2.120026	0.806588
56	9	0	1.552396	-2.871074	-1.260995
57	8	0	-0.064061	3.346179	0.380057

IM5B

Standard orientation:

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

1	6	0	2.025202	-1.511921	-0.673839
2	6	0	0.568723	-1.144684	-0.814685
3	6	0	0.431662	-0.934690	1.555921

4	6	0	1.493788	-2.007654	1.576229
5	1	0	0.163206	-1.067334	-1.818728
6	1	0	0.825592	0.063392	1.759710
7	1	0	-0.359683	-1.179955	2.263491
8	1	0	1.048645	-2.997624	1.443062
9	1	0	2.040420	-1.973912	2.516906
10	7	0	-0.169970	-0.896672	0.200136
11	6	0	-1.559987	-0.543502	0.056628
12	6	0	-2.362778	-1.308319	-0.784084
13	6	0	-2.053074	0.539914	0.779522
14	6	0	-3.705982	-0.966144	-0.910311
15	1	0	-1.951671	-2.167260	-1.305518
16	6	0	-3.396812	0.866827	0.637087
17	1	0	-1.389626	1.137469	1.395338
18	6	0	-4.221690	0.116746	-0.201765
19	1	0	-4.348432	-1.556993	-1.554606
20	1	0	-3.798091	1.716096	1.180032
21	1	0	-5.270716	0.376829	-0.300765
22	8	0	2.723454	-1.523863	-1.650487
23	5	0	1.202283	2.013318	-0.139968
24	9	0	0.594447	2.202567	1.113883
25	9	0	0.233411	1.639371	-1.078739
26	9	0	2.140935	0.965642	-0.017571
27	9	0	1.844873	3.176453	-0.540880
28	8	0	2.474224	-1.805679	0.538678

$CH_2(COMe)_2$

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.028224	-0.861503	-0.043642
2	1	0	-0.019233	-1.556434	0.798624
3	6	0	-1.227748	-0.016685	-0.071937
4	6	0	1.240149	0.031937	0.064470
5	8	0	1.210551	1.211737	0.319331
6	6	0	2.535970	-0.762610	-0.182804
7	1	0	3.177370	-0.205428	-0.833229
8	1	0	3.033541	-0.932446	0.749119
9	1	0	2.297341	-1.702010	-0.636106
10	6	0	-2.486882	-0.891364	0.073381
11	1	0	-2.495273	-1.635051	-0.695878
12	1	0	-2.480955	-1.368769	1.030956
13	1	0	-3.359270	-0.278005	-0.013967
14	8	0	-1.250786	1.403550	-0.237168
15	1	0	-0.369917	1.757196	-0.093627

TS5B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-2.991798	1.388749	-0.217271
2	9	0	-4.022404	1.292869	-1.151566
3	9	0	-2.742849	2.730555	0.081778
4	9	0	-1.822973	0.802395	-0.758077
5	9	0	-3.337599	0.690248	0.946988
6	6	0	2.640738	2.148670	-0.070206

7	1	0	3.131981	3.007772	-0.516441
8	1	0	1.518542	-0.455197	0.364880
9	6	0	1.359373	2.362804	0.518909
10	8	0	0.697063	1.516693	1.148142
11	6	0	3.344108	0.931733	-0.057081
12	8	0	2.859662	-0.197862	0.350813
13	6	0	-1.081639	-2.050714	-1.596298
14	6	0	0.333204	-1.515026	-1.270304
15	6	0	-0.049594	-1.894940	1.282744
16	6	0	-1.037226	-2.954697	0.764623
17	6	0	-1.912950	-2.381872	-0.347364
18	1	0	-2.403249	-1.471397	0.016592
19	1	0	-0.962822	-2.947915	-2.214229
20	1	0	-1.647766	-3.285653	1.611469
21	1	0	-0.497731	-3.836673	0.399825
22	1	0	-2.706175	-3.087897	-0.610387
23	1	0	-1.618319	-1.310842	-2.197398
24	6	0	-0.712676	-1.008728	2.338796
25	1	0	-0.030783	-0.212321	2.647571
26	1	0	-1.626301	-0.543529	1.952957
27	1	0	-0.970497	-1.620419	3.208429
28	6	0	1.212993	-2.518081	1.872392
29	1	0	1.910132	-1.739413	2.196666
30	1	0	0.930151	-3.119912	2.742169
31	1	0	1.726712	-3.170920	1.163255
32	6	0	0.699994	-0.342871	-2.181336
33	1	0	1.728307	-0.015008	-2.000053
34	1	0	0.616156	-0.666076	-3.223826
35	1	0	0.020056	0.498783	-2.025446
36	6	0	1.410237	-2.591845	-1.406170

37	1	0	1.527306	-2.824555	-2.469485
38	1	0	2.365982	-2.219217	-1.022928
39	1	0	1.150951	-3.520725	-0.893601
40	7	0	0.329748	-0.968288	0.136972
41	1	0	-0.314586	-0.163977	0.145519
42	6	0	0.773466	3.766667	0.404996
43	1	0	1.139914	4.389543	1.230183
44	1	0	1.047772	4.259450	-0.532228
45	1	0	-0.313556	3.695454	0.486137
46	6	0	4.761071	0.930682	-0.612354
47	1	0	5.102800	1.919597	-0.926963
48	1	0	5.445092	0.542755	0.150234
49	1	0	4.812728	0.246617	-1.467134

IM6B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.001176	-0.598964	-0.024024
2	1	0	0.014596	-1.683501	0.013171
3	6	0	1.280101	0.077645	0.021818
4	8	0	1.421907	1.288459	0.202316
5	6	0	-1.233416	0.009317	-0.037416
6	8	0	-1.483672	1.281496	-0.195667
7	6	0	2.513091	-0.801598	-0.097792
8	1	0	2.768190	-1.205266	0.889839
9	1	0	2.344906	-1.648618	-0.769022
10	1	0	3.351084	-0.200100	-0.455775

11	6	0	-2.483128	-0.819184	0.109464
12	1	0	-2.265905	-1.875405	0.278350
13	1	0	-3.073004	-0.435777	0.949096
14	1	0	-3.098574	-0.714267	-0.791151

IM7B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.622943	-0.707729	-0.291239
2	6	0	1.120494	-0.842945	-0.271364
3	6	0	0.953815	1.495349	0.161367
4	6	0	2.272884	1.319335	0.874706
5	1	0	0.699573	-1.820971	-0.483070
6	1	0	1.056192	1.957914	-0.822722
7	1	0	0.269118	2.073590	0.780935
8	1	0	2.119761	0.924042	1.882784
9	1	0	2.797764	2.271372	0.928972
10	7	0	0.352025	0.155367	-0.048054
11	6	0	-1.082704	0.018171	-0.033851
12	6	0	-1.649006	-1.029371	0.685991
13	6	0	-1.850839	0.950698	-0.726573
14	6	0	-3.035543	-1.149674	0.701980
15	1	0	-1.020127	-1.717421	1.242571
16	6	0	-3.233799	0.810973	-0.700291
17	1	0	-1.374002	1.731587	-1.309069
18	6	0	-3.825398	-0.232532	0.012328
19	1	0	-3.494363	-1.955257	1.265435

20	1	0	-3.850333	1.518106	-1.245196
21	1	0	-4.906279	-0.328623	0.031358
22	8	0	3.287206	-1.614388	-0.713453
23	8	0	3.147975	0.422443	0.161711

TS6B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.376106	1.668127	-1.083067
2	6	0	0.610483	0.482082	-0.500773
3	6	0	-0.738338	2.218601	0.667299
4	6	0	0.633405	2.823788	0.836486
5	1	0	0.376017	-0.138333	-1.365734
6	1	0	-1.316300	2.841030	-0.031708
7	1	0	-1.248833	2.233678	1.636835
8	1	0	1.231516	2.286916	1.580078
9	1	0	0.553789	3.868023	1.136354
10	7	0	-0.625418	0.850171	0.180242
11	6	0	-1.803685	0.158454	-0.124254
12	6	0	-1.776514	-1.127360	-0.701012
13	6	0	-3.059385	0.722383	0.170131
14	6	0	-2.959507	-1.798565	-0.987956
15	1	0	-0.833470	-1.625091	-0.897343
16	6	0	-4.233625	0.031567	-0.118218
17	1	0	-3.132132	1.703382	0.623627
18	6	0	-4.200366	-1.229506	-0.705683
19	1	0	-2.902794	-2.787993	-1.433037

20	1	0	-5.185562	0.498412	0.119026
21	1	0	-5.118829	-1.761442	-0.931774
22	8	0	2.041995	1.566578	-2.083082
23	6	0	1.900212	-0.551544	0.610033
24	1	0	2.499909	0.283611	0.991437
25	6	0	2.465456	-1.437562	-0.504159
26	8	0	1.811410	-1.701281	-1.489406
27	6	0	0.862874	-1.181823	1.561211
28	8	0	0.299014	-2.208997	1.252023
29	8	0	1.332422	2.829379	-0.419274
30	6	0	3.849982	-1.976079	-0.272626
31	1	0	3.928999	-2.405448	0.732419
32	1	0	4.097735	-2.726068	-1.024911
33	1	0	4.564567	-1.146432	-0.327577
34	6	0	0.619127	-0.479848	2.867306
35	1	0	0.285240	0.546966	2.684769
36	1	0	-0.134929	-1.018054	3.443698
37	1	0	1.556922	-0.426082	3.431735

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.410279	1.608424	-1.096862
2	6	0	0.614620	0.443455	-0.511969
3	6	0	-0.655658	2.215319	0.689984
4	6	0	0.738430	2.771727	0.844885
5	1	0	0.343060	-0.159742	-1.378509

6	1	0	-1.221605	2.862557	0.003652
7	1	0	-1.151938	2.240529	1.666725
8	1	0	1.327474	2.209077	1.576697
9	1	0	0.698599	3.815905	1.152744
10	7	0	-0.595720	0.847794	0.192652
11	6	0	-1.798906	0.191676	-0.089395
12	6	0	-1.818238	-1.096474	-0.661521
13	6	0	-3.032625	0.793272	0.222759
14	6	0	-3.024653	-1.734475	-0.925617
15	1	0	-0.892865	-1.620983	-0.872585
16	6	0	-4.230831	0.135280	-0.042908
17	1	0	-3.069255	1.778552	0.671362
18	6	0	-4.243666	-1.128849	-0.624657
19	1	0	-3.004026	-2.726909	-1.367122
20	1	0	-5.164910	0.630419	0.207596
21	1	0	-5.180739	-1.635127	-0.832553
22	8	0	2.053573	1.494279	-2.110195
23	6	0	1.614092	-0.407650	0.330150
24	1	0	2.365240	0.230224	0.811447
25	6	0	2.320456	-1.439858	-0.553397
26	8	0	1.797218	-1.868126	-1.558854
27	6	0	0.871320	-1.175762	1.442457
28	8	0	0.392638	-2.265555	1.214841
29	8	0	1.421589	2.762574	-0.419620
30	6	0	3.667593	-1.902514	-0.072084
31	1	0	3.620899	-2.174947	0.988212
32	1	0	4.013602	-2.749916	-0.665348
33	1	0	4.378328	-1.072678	-0.162403
34	6	0	0.802453	-0.522066	2.793857
35	1	0	0.301936	0.448606	2.715553

36	1	0	0.259735	-1.163623	3.489873
37	1	0	1.818369	-0.340919	3.162633

TS7B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.338823	0.266473	0.751405
2	6	0	0.937746	-0.084262	0.019426
3	6	0	1.528755	-1.397653	1.919065
4	6	0	0.904363	-0.291999	2.742043
5	1	0	1.030872	0.170307	-1.028709
6	1	0	0.865025	-2.262086	1.825564
7	1	0	2.475960	-1.705571	2.361021
8	1	0	1.642497	0.494377	2.933375
9	1	0	0.590491	-0.711202	3.701322
10	1	0	-0.710100	1.246777	0.436313
11	7	0	1.795113	-0.891783	0.550952
12	6	0	2.936644	-1.385987	-0.172897
13	6	0	3.360794	-2.696028	0.041577
14	6	0	3.590799	-0.548365	-1.073743
15	6	0	4.455880	-3.172275	-0.672829
16	1	0	2.838321	-3.344002	0.737302
17	6	0	4.686289	-1.038923	-1.777523
18	1	0	3.262153	0.478394	-1.198367
19	6	0	5.119375	-2.348639	-1.580652
20	1	0	4.786566	-4.194149	-0.518628
21	1	0	5.205174	-0.388645	-2.474257

22	1	0	5.975344	-2.726340	-2.130635
23	6	0	-4.203336	-0.409355	-1.799644
24	6	0	-2.690604	-0.404031	-1.498983
25	6	0	-3.472693	-1.033653	0.852946
26	6	0	-4.864348	-0.383327	0.611317
27	6	0	-4.980500	0.347248	-0.730894
28	1	0	-4.580379	1.363607	-0.640628
29	1	0	-4.573698	-1.440702	-1.854255
30	1	0	-5.082951	0.316240	1.425240
31	1	0	-5.618006	-1.177900	0.666089
32	1	0	-6.033789	0.443113	-1.013519
33	1	0	-4.354931	0.031461	-2.791232
34	7	0	-2.508971	-0.301859	-0.014415
35	6	0	-3.078354	-0.798941	2.311901
36	1	0	-2.164650	-1.336664	2.576185
37	1	0	-2.915357	0.266596	2.500215
38	1	0	-3.891902	-1.149091	2.956531
39	6	0	-3.511939	-2.552223	0.617674
40	1	0	-2.501563	-2.972559	0.656396
41	1	0	-4.104403	-3.021448	1.411121
42	1	0	-3.971673	-2.822782	-0.335976
43	6	0	-2.052754	0.854412	-2.095952
44	1	0	-0.987238	0.904860	-1.851222
45	1	0	-2.145476	0.841066	-3.187809
46	1	0	-2.519430	1.765081	-1.708573
47	6	0	-2.023478	-1.625576	-2.144797
48	1	0	-2.290018	-1.641445	-3.207681
49	1	0	-0.934013	-1.570147	-2.070838
50	1	0	-2.352282	-2.568111	-1.702999
51	8	0	-1.192001	-0.767699	0.279512

52	6	0	1.765559	2.659749	-0.290029
53	1	0	2.623897	2.513935	-0.941928
54	6	0	2.012848	2.631930	1.116406
55	8	0	1.189018	2.841581	2.019411
56	6	0	0.551536	3.057736	-0.926772
57	8	0	-0.530949	3.295463	-0.364442
58	8	0	-0.250399	0.257107	2.134941
59	6	0	3.459970	2.339722	1.521454
60	1	0	3.473975	1.789326	2.465091
61	1	0	4.014934	1.779005	0.762951
62	1	0	3.984966	3.288925	1.686534
63	6	0	0.622263	3.183804	-2.450550
64	1	0	1.255218	4.033451	-2.733612
65	1	0	1.062930	2.289837	-2.906899
66	1	0	-0.380756	3.341354	-2.854315

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.313154	-0.915323	-0.480823
2	6	0	1.044409	-0.479933	0.119083
3	6	0	1.311502	0.361191	-2.208363
4	6	0	0.789086	-1.000036	-2.626575
5	1	0	0.794507	0.142786	0.980416
6	1	0	0.527762	1.122618	-2.325935
7	1	0	2.127212	0.607268	-2.893353
8	1	0	1.617482	-1.708955	-2.727376

9	1	0	0.307912	-0.909283	-3.606302
10	1	0	-0.818640	-1.624369	0.171825
11	7	0	1.810669	0.337839	-0.829471
12	6	0	2.513727	1.459106	-0.358459
13	6	0	2.913715	2.493152	-1.237884
14	6	0	2.876920	1.595992	1.002659
15	6	0	3.646818	3.587075	-0.778697
16	1	0	2.646368	2.461442	-2.286343
17	6	0	3.605007	2.699828	1.446288
18	1	0	2.597086	0.849307	1.735710
19	6	0	4.004016	3.706339	0.565405
20	1	0	3.931683	4.358753	-1.489982
21	1	0	3.861803	2.763960	2.501013
22	1	0	4.572998	4.561927	0.917681
23	6	0	-4.032176	1.367261	1.460675
24	6	0	-2.535481	1.106376	1.143388
25	6	0	-3.500654	0.115814	-1.036606
26	6	0	-4.861223	-0.196406	-0.329826
27	6	0	-4.907667	0.154286	1.166591
28	1	0	-4.570482	-0.702837	1.758646
29	1	0	-4.393631	2.223977	0.878435
30	1	0	-5.086556	-1.261998	-0.442875
31	1	0	-5.645235	0.350145	-0.868389
32	1	0	-5.943508	0.355155	1.467955
33	1	0	-4.108949	1.658397	2.515111
34	7	0	-2.441861	0.092683	0.024766
35	6	0	-3.228287	-1.029632	-2.023781
36	1	0	-2.305554	-0.880396	-2.586467
37	1	0	-3.155388	-1.983415	-1.490401
38	1	0	-4.063035	-1.095817	-2.731970

39	6	0	-3.571214	1.434619	-1.838988
40	1	0	-2.586237	1.698051	-2.238724
41	1	0	-4.255574	1.312843	-2.687461
42	1	0	-3.938751	2.274255	-1.243075
43	6	0	-1.865846	0.462431	2.374736
44	1	0	-0.793955	0.309529	2.206893
45	1	0	-1.966405	1.118771	3.247405
46	1	0	-2.315777	-0.507861	2.606985
47	6	0	-1.842391	2.453822	0.857429
48	1	0	-1.919096	3.085924	1.750798
49	1	0	-0.782645	2.323909	0.627474
50	1	0	-2.310273	2.993578	0.029660
51	8	0	-1.136030	0.252843	-0.594769
52	6	0	1.892485	-1.677069	0.727866
53	1	0	2.779729	-1.196419	1.144810
54	6	0	2.416714	-2.727620	-0.261135
55	8	0	1.822904	-3.767353	-0.511440
56	6	0	1.122533	-2.306317	1.898598
57	8	0	0.217312	-3.103851	1.718364
58	8	0	-0.167578	-1.561642	-1.717204
59	6	0	3.770663	-2.460588	-0.890285
60	1	0	3.675178	-2.461047	-1.981847
61	1	0	4.218126	-1.519227	-0.568208
62	1	0	4.440520	-3.288110	-0.625813
63	6	0	1.515376	-1.847862	3.282969
64	1	0	2.602729	-1.797990	3.399076
65	1	0	1.113511	-0.837130	3.446074
66	1	0	1.081290	-2.510413	4.036298

Table S5

	Gsol	Thermal correction to Gibbs Free Energy (TCG)	Esol	△Gsol=Esol+TCG	N_{imag}
TEMPO-Cl	-932.654097	0.256733	-943.8368671	-943.5801341	0
TS1A-Cl	-1425.925062	0.450571	-1426.683321	-1426.23275	-1454.77
IM1A-Cl	-942.137184	0.192871	-942.4955872	-942.3027162	0

TEMPO-Cl

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.096665	-0.797504	0.716404
2	6	0	-0.783757	-1.266094	0.076990
3	6	0	-0.319907	1.355885	0.030118
4	6	0	-1.848889	1.614302	0.015812
5	6	0	-2.709726	0.350376	-0.079348
6	1	0	-2.811492	0.050321	-1.128840
7	1	0	-1.933322	-0.497888	1.756508
8	1	0	-2.077640	2.279228	-0.821451
9	1	0	-2.079378	2.155530	0.938619
10	1	0	-3.715358	0.571259	0.286535
11	1	0	-2.763300	-1.664665	0.735143
12	7	0	-0.053848	-0.044891	-0.469907
13	6	0	0.437639	2.319534	-0.868702
14	1	0	1.516152	2.158809	-0.798990
15	1	0	0.118611	2.221286	-1.910389
16	1	0	0.202033	3.331066	-0.527632
17	6	0	0.267968	1.392571	1.454934

18	1	0	1.305354	1.044151	1.447775
19	1	0	0.242023	2.441067	1.765578
20	1	0	-0.320401	0.813932	2.168501
21	6	0	-1.027349	-2.189221	-1.119015
22	1	0	-0.085582	-2.510691	-1.567267
23	1	0	-1.554775	-3.070350	-0.746476
24	1	0	-1.644687	-1.707498	-1.882515
25	6	0	0.168864	-1.935934	1.073047
26	1	0	-0.319741	-2.857895	1.401972
27	1	0	1.120557	-2.176715	0.593196
28	1	0	0.356241	-1.309450	1.947143
29	8	0	0.806292	-0.218345	-1.266736
30	17	0	3.284838	-0.251411	0.115552

TS1A-Cl

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.419135	-2.525905	0.839279
2	6	0	-2.269818	-1.026751	1.137590
3	6	0	-1.319054	-1.021792	-1.319973
4	6	0	-0.856109	-2.493776	-1.148930
5	6	0	-1.144136	-3.100151	0.231456
6	1	0	-0.304734	-2.903935	0.909381
7	1	0	-3.265386	-2.692042	0.163181
8	1	0	0.217911	-2.555109	-1.354068
9	1	0	-1.361088	-3.080581	-1.923727
10	1	0	-1.223355	-4.187577	0.143170

11	1	0	-2.665154	-3.024868	1.782074
12	7	0	-1.531443	-0.395741	0.012445
13	6	0	-0.270244	-0.210466	-2.076773
14	1	0	-0.625430	0.801913	-2.279089
15	1	0	0.671497	-0.163423	-1.519908
16	1	0	-0.076165	-0.720033	-3.025394
17	6	0	-2.655368	-0.926503	-2.079780
18	1	0	-2.994722	0.112805	-2.091435
19	1	0	-2.499169	-1.270010	-3.107607
20	1	0	-3.431218	-1.550112	-1.627863
21	6	0	-1.462119	-0.801004	2.422361
22	1	0	-1.334964	0.266991	2.622007
23	1	0	-2.013044	-1.240471	3.258593
24	1	0	-0.475299	-1.272218	2.373914
25	6	0	-3.634519	-0.342099	1.266817
26	1	0	-4.176792	-0.790223	2.105779
27	1	0	-3.509759	0.727691	1.449799
28	1	0	-4.225640	-0.474289	0.356435
29	8	0	-1.177247	0.808271	0.175470
30	6	0	0.703267	2.760014	1.590071
31	6	0	1.099188	1.351752	1.170180
32	6	0	2.371302	2.187967	-0.773156
33	6	0	1.259861	3.224751	-0.805104
34	1	0	1.134366	0.630607	1.990216
35	1	0	-0.016365	0.943655	0.620843
36	1	0	1.160731	2.943497	2.569117
37	1	0	3.329529	2.677779	-0.559130
38	1	0	2.465259	1.664425	-1.730026
39	1	0	0.311311	2.769177	-1.113449
40	1	0	1.525771	3.982912	-1.547761

41	1	0	-0.381011	2.767174	1.735945
42	7	0	2.111664	1.173378	0.265293
43	6	0	2.777052	-0.068808	0.161817
44	6	0	2.135262	-1.258067	0.532337
45	6	0	4.083259	-0.118676	-0.340207
46	6	0	2.804266	-2.472672	0.435004
47	1	0	1.096960	-1.237539	0.852967
48	6	0	4.740246	-1.341531	-0.439177
49	1	0	4.591467	0.793923	-0.632682
50	6	0	4.111105	-2.522076	-0.048561
51	1	0	2.288436	-3.385849	0.718330
52	1	0	5.755900	-1.366344	-0.821941
53	1	0	4.628521	-3.472297	-0.132558
54	6	0	1.107984	3.840602	0.580272
55	1	0	2.063719	4.289416	0.874866
56	1	0	0.356289	4.632040	0.570521
57	17	0	-3.449158	2.039084	-0.764210

IM1A-Cl

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.188617	-0.505201	1.477569
2	6	0	0.889873	0.170359	1.102584
3	6	0	0.676784	-1.600429	-0.552618
4	6	0	2.086307	-1.186694	-0.968314
5	1	0	0.478576	1.002099	1.681019
6	1	0	1.916674	-1.374712	2.091014

7	1	0	0.696535	-2.531582	0.029418
8	1	0	0.044254	-1.752423	-1.428193
9	1	0	2.006098	-0.265259	-1.555242
10	1	0	2.497466	-1.956352	-1.626783
11	1	0	2.764848	0.170215	2.114403
12	7	0	0.074097	-0.533548	0.261061
13	6	0	-1.290843	-0.211553	0.125576
14	6	0	-1.729067	1.101457	0.343460
15	6	0	-2.217375	-1.202376	-0.222176
16	6	0	-3.079151	1.412994	0.235109
17	1	0	-1.005286	1.884109	0.557442
18	6	0	-3.565179	-0.875492	-0.335700
19	1	0	-1.891390	-2.225863	-0.375366
20	6	0	-4.004752	0.427215	-0.105707
21	1	0	-3.402214	2.437419	0.397715
22	1	0	-4.277100	-1.651901	-0.598326
23	1	0	-5.057287	0.674128	-0.199674
24	6	0	2.997400	-0.959309	0.246804
25	1	0	3.530486	-1.879819	0.499570
26	1	0	3.750964	-0.208255	-0.005316
27	17	0	2.336060	1.881600	-0.675802

Table S6

	Gsol	Thermal correction to Gibbs Free Energy (TCG)	Esol	△Gsol=Esol+TCG	N_{imag}
TEMPO-CO_3	-1230.120953	0.499015	-1230.984126	-1230.485111	0
TS1B-CO_3	-1748.518314	0.69871	-1749.729939	-1749.031229	-1331.52
IM1B-CO_3	-1748.595616	0.701989	-1749.808327	-1749.106338	0

TEMPO-CO_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.710447	1.918539	0.340941
2	6	0	2.281281	1.342497	0.118770
3	6	0	3.620357	-0.959259	0.224259
4	6	0	4.937105	-0.227749	-0.207108
5	6	0	4.742647	1.254659	-0.566530
6	1	0	4.418814	1.348450	-1.610659
7	1	0	4.000217	1.800657	1.389456
8	1	0	5.371885	-0.760644	-1.057136
9	1	0	5.627367	-0.322846	0.636637
10	1	0	5.700740	1.774415	-0.489278
11	1	0	3.641857	2.992666	0.142565
12	7	0	2.536098	-0.082705	-0.389891
13	6	0	3.499861	-2.338662	-0.405211
14	1	0	2.509983	-2.749992	-0.192794
15	1	0	3.660428	-2.309902	-1.484130
16	1	0	4.270447	-2.972839	0.041245
17	6	0	3.491125	-1.050293	1.745539
18	1	0	2.497231	-1.413709	2.019850
19	1	0	4.249253	-1.767223	2.072978
20	1	0	3.697153	-0.106409	2.250595
21	6	0	1.543381	2.064101	-0.999095
22	1	0	0.600271	1.560156	-1.230981
23	1	0	1.321110	3.071513	-0.638723
24	1	0	2.142890	2.140565	-1.910495

25	6	0	1.448622	1.402614	1.400418
26	1	0	1.468672	2.451125	1.716828
27	1	0	0.417897	1.096718	1.210998
28	1	0	1.853391	0.792772	2.204865
29	8	0	2.191498	-0.356253	-1.496525
30	6	0	-0.072606	-1.143821	-0.293952
31	8	0	-0.017081	-1.646707	-1.409484
32	8	0	-1.051163	-0.096235	-0.070098
33	8	0	0.705170	-1.289788	0.675207
34	6	0	-3.635530	1.566974	-0.790757
35	6	0	-3.224033	0.142052	-1.202548
36	6	0	-2.891953	-0.082468	1.392681
37	6	0	-2.610009	1.430622	1.510668
38	6	0	-2.653938	2.205193	0.184980
39	1	0	-1.656456	2.218299	-0.266147
40	1	0	-4.640646	1.562725	-0.355164
41	1	0	-1.636583	1.579984	1.988128
42	1	0	-3.363615	1.834336	2.197149
43	1	0	-2.937208	3.245715	0.373285
44	1	0	-3.701618	2.160643	-1.710155
45	7	0	-2.490502	-0.594456	-0.018928
46	6	0	-2.058617	-0.864299	2.399839
47	1	0	-2.312835	-1.925621	2.364092
48	1	0	-0.992107	-0.748306	2.198594
49	1	0	-2.287287	-0.481017	3.399835
50	6	0	-4.364522	-0.424485	1.636446
51	1	0	-4.547670	-1.471882	1.385131
52	1	0	-4.566471	-0.284261	2.703178
53	1	0	-5.064199	0.209106	1.089780
54	6	0	-2.273225	0.182727	-2.394423

55	1	0	-1.754237	-0.771663	-2.495375
56	1	0	-2.865351	0.388328	-3.292544
57	1	0	-1.522990	0.969575	-2.289143
58	6	0	-4.446649	-0.684301	-1.596405
59	1	0	-4.991133	-0.121334	-2.362154
60	1	0	-4.139759	-1.644066	-2.013078
61	1	0	-5.128109	-0.866024	-0.764721
62	8	0	-2.568795	-1.879483	-0.118081

TS1B-CO_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.626890	-3.055104	1.498433
2	6	0	0.489929	-2.051195	1.200120
3	6	0	1.808885	-1.756559	-1.024225
4	6	0	3.136218	-2.220923	-0.349480
5	6	0	2.983234	-2.434165	1.161318
6	1	0	3.067766	-1.466579	1.676197
7	1	0	1.486725	-3.981821	0.931381
8	1	0	3.927424	-1.488124	-0.541501
9	1	0	3.443418	-3.156796	-0.829817
10	1	0	3.800842	-3.058953	1.533570
11	1	0	1.568777	-3.321962	2.558687
12	7	0	0.904025	-1.228486	0.027001
13	6	0	2.043802	-0.652938	-2.048924
14	1	0	1.089366	-0.359397	-2.497527
15	1	0	2.513165	0.223926	-1.595775

16	1	0	2.717360	-1.040432	-2.819837
17	6	0	1.109902	-2.927472	-1.733516
18	1	0	0.120314	-2.607914	-2.070431
19	1	0	1.719030	-3.206075	-2.599651
20	1	0	1.020290	-3.812476	-1.099989
21	6	0	0.285185	-1.122396	2.399591
22	1	0	-0.472901	-0.363947	2.188225
23	1	0	-0.055704	-1.731076	3.241211
24	1	0	1.213772	-0.624040	2.696484
25	6	0	-0.847880	-2.728050	0.872381
26	1	0	-1.554684	-1.972899	0.512438
27	1	0	-0.739326	-3.499017	0.106583
28	1	0	-1.242642	-3.199468	1.779660
29	8	0	0.694791	0.024583	0.072252
30	6	0	-1.663930	0.256794	-1.472999
31	8	0	-1.320635	1.434350	-1.572792
32	8	0	-2.592106	-0.068670	-0.374273
33	8	0	-1.303294	-0.761176	-2.081915
34	6	0	-4.623305	0.569457	1.934456
35	6	0	-4.215729	1.390954	0.697657
36	6	0	-4.795474	-0.865061	-0.506900
37	6	0	-4.468278	-1.663907	0.772764
38	6	0	-3.991642	-0.817393	1.961237
39	1	0	-2.902193	-0.716667	1.928274
40	1	0	-5.714242	0.476393	1.986490
41	1	0	-3.715470	-2.423578	0.540748
42	1	0	-5.382571	-2.202997	1.050068
43	1	0	-4.243477	-1.322367	2.899717
44	1	0	-4.321906	1.144172	2.818238
45	7	0	-3.975620	0.455856	-0.546608

46	6	0	-4.408882	-1.662820	-1.747426
47	1	0	-4.750658	-1.155218	-2.652433
48	1	0	-3.326245	-1.796223	-1.802121
49	1	0	-4.898817	-2.641002	-1.687811
50	6	0	-6.283903	-0.526819	-0.609861
51	1	0	-6.445057	0.183772	-1.424010
52	1	0	-6.821845	-1.451462	-0.843353
53	1	0	-6.710337	-0.128317	0.312419
54	6	0	-2.920366	2.153720	0.953044
55	1	0	-2.501743	2.491116	0.003079
56	1	0	-3.144626	3.010692	1.597828
57	1	0	-2.172844	1.526949	1.446796
58	6	0	-5.300704	2.403695	0.338574
59	1	0	-5.495337	3.009260	1.230643
60	1	0	-4.962248	3.056563	-0.466840
61	1	0	-6.239402	1.937018	0.039196
62	8	0	-4.142448	1.087733	-1.664627
63	6	0	1.426914	2.582243	1.626686
64	6	0	2.419907	1.523453	1.215525
65	6	0	3.039250	3.088324	-0.514968
66	6	0	1.551617	3.102434	-0.857615
67	1	0	2.776564	0.835345	1.984135
68	1	0	1.595437	0.660933	0.621980
69	1	0	1.995505	3.375327	2.131898
70	1	0	3.307494	3.980929	0.066384
71	1	0	3.656581	3.081259	-1.410708
72	1	0	1.304483	2.198785	-1.425655
73	1	0	1.353569	3.960418	-1.506163
74	1	0	0.738057	2.155948	2.360354
75	7	0	3.361180	1.906636	0.302763

76	6	0	4.543067	1.152806	0.099415
77	6	0	5.164904	0.523551	1.187314
78	6	0	5.084072	0.994050	-1.184226
79	6	0	6.276584	-0.286704	0.984142
80	1	0	4.792917	0.678909	2.194665
81	6	0	6.204574	0.191692	-1.372279
82	1	0	4.613652	1.455855	-2.045195
83	6	0	6.799750	-0.463780	-0.295739
84	1	0	6.743512	-0.768851	1.837562
85	1	0	6.602160	0.067319	-2.374827
86	1	0	7.668631	-1.095307	-0.450646
87	8	0	0.676548	3.152767	0.406394

IM1B-CO_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.730603	3.966698	-0.406927
2	6	0	2.040069	2.679295	-0.904185
3	6	0	2.468176	1.892039	1.483206
4	6	0	3.668479	2.865008	1.650117
5	6	0	4.002864	3.643633	0.369639
6	1	0	4.668873	3.045500	-0.263514
7	1	0	2.048544	4.537230	0.235586
8	1	0	4.552975	2.300124	1.967170
9	1	0	3.433234	3.564340	2.461414
10	1	0	4.545060	4.561418	0.620599
11	1	0	2.946683	4.601545	-1.274253

12	7	0	2.386189	1.584582	0.037274
13	6	0	2.778806	0.586371	2.220937
14	1	0	1.911474	-0.080402	2.238243
15	1	0	3.613991	0.063325	1.742899
16	1	0	3.058714	0.814471	3.255331
17	6	0	1.187609	2.482496	2.103540
18	1	0	0.315030	1.865478	1.864148
19	1	0	1.299748	2.510751	3.194098
20	1	0	0.996484	3.506105	1.770087
21	6	0	2.629096	2.267478	-2.259046
22	1	0	2.256773	1.277015	-2.540530
23	1	0	2.341905	2.980766	-3.039530
24	1	0	3.723445	2.226181	-2.213649
25	6	0	0.533440	2.912842	-1.083944
26	1	0	0.387240	3.766656	-1.756361
27	1	0	0.040845	2.040230	-1.523722
28	1	0	0.035014	3.141719	-0.138499
29	8	0	1.587943	0.451619	-0.218008
30	6	0	0.438788	-2.126738	-1.335757
31	6	0	1.907480	-1.911367	-1.293536
32	6	0	2.037824	-2.902891	0.900293
33	6	0	0.563551	-2.543089	0.943477
34	1	0	2.393885	-1.433849	-2.139247
35	1	0	0.634757	0.613378	0.055255
36	1	0	0.214677	-2.641301	-2.277971
37	1	0	2.184237	-3.984671	0.853365
38	1	0	2.579548	-2.498859	1.757853
39	1	0	0.422459	-1.467795	1.111534
40	1	0	0.072524	-3.106204	1.739174
41	1	0	-0.049954	-1.136554	-1.379952

42	7	0	2.643523	-2.304579	-0.315928
43	6	0	4.069281	-2.085233	-0.323383
44	6	0	4.554650	-0.821586	-0.648359
45	6	0	4.914685	-3.138431	0.012735
46	6	0	5.933036	-0.620855	-0.655770
47	1	0	3.860817	-0.004089	-0.835194
48	6	0	6.289365	-2.919153	0.000265
49	1	0	4.508935	-4.113755	0.262921
50	6	0	6.798724	-1.665285	-0.335996
51	1	0	6.326703	0.361128	-0.900027
52	1	0	6.961802	-3.733250	0.250518
53	1	0	7.871665	-1.501037	-0.340886
54	6	0	-1.808742	0.395482	-0.325690
55	8	0	-0.929731	0.428155	0.584583
56	8	0	-3.090926	0.540517	0.196018
57	8	0	-1.639804	0.317116	-1.547251
58	6	0	-6.194531	1.025460	0.090962
59	6	0	-5.267578	0.421823	-0.977843
60	6	0	-4.557946	-1.090829	1.068415
61	6	0	-4.947767	0.029274	2.055547
62	6	0	-5.485768	1.315573	1.408651
63	1	0	-4.658903	2.006811	1.226454
64	1	0	-7.045955	0.358691	0.269583
65	1	0	-4.081654	0.274500	2.676249
66	1	0	-5.708948	-0.393682	2.722127
67	1	0	-6.179166	1.810145	2.096405
68	1	0	-6.609948	1.948599	-0.329838
69	7	0	-4.181242	-0.498379	-0.317776
70	6	0	-3.335859	-1.855139	1.569303
71	1	0	-3.089943	-2.677388	0.893724

72	1	0	-2.472804	-1.191759	1.662502
73	1	0	-3.575047	-2.268563	2.554806
74	6	0	-5.695724	-2.092422	0.854971
75	1	0	-5.448949	-2.775294	0.038197
76	1	0	-5.804014	-2.675814	1.774710
77	1	0	-6.658982	-1.619625	0.654639
78	6	0	-4.542871	1.507396	-1.766993
79	1	0	-3.688629	1.074165	-2.292392
80	1	0	-5.247179	1.935057	-2.488406
81	1	0	-4.178715	2.306233	-1.117193
82	6	0	-6.066194	-0.437815	-1.956377
83	1	0	-6.869601	0.186222	-2.361886
84	1	0	-5.433660	-0.777127	-2.777948
85	1	0	-6.522652	-1.307676	-1.481438
86	8	0	-3.726222	-1.367371	-1.113599
87	8	0	-0.036748	-2.925118	-0.283201

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