Supplementary Information

"On water" reaction of deactivated anilines with 4-methoxy-3-buten-2-one, an effective butynone surrogate

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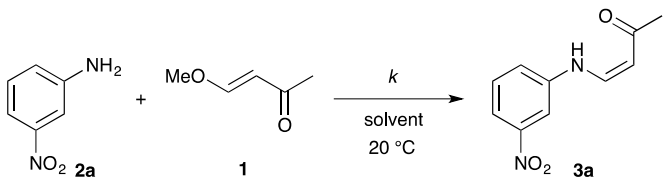
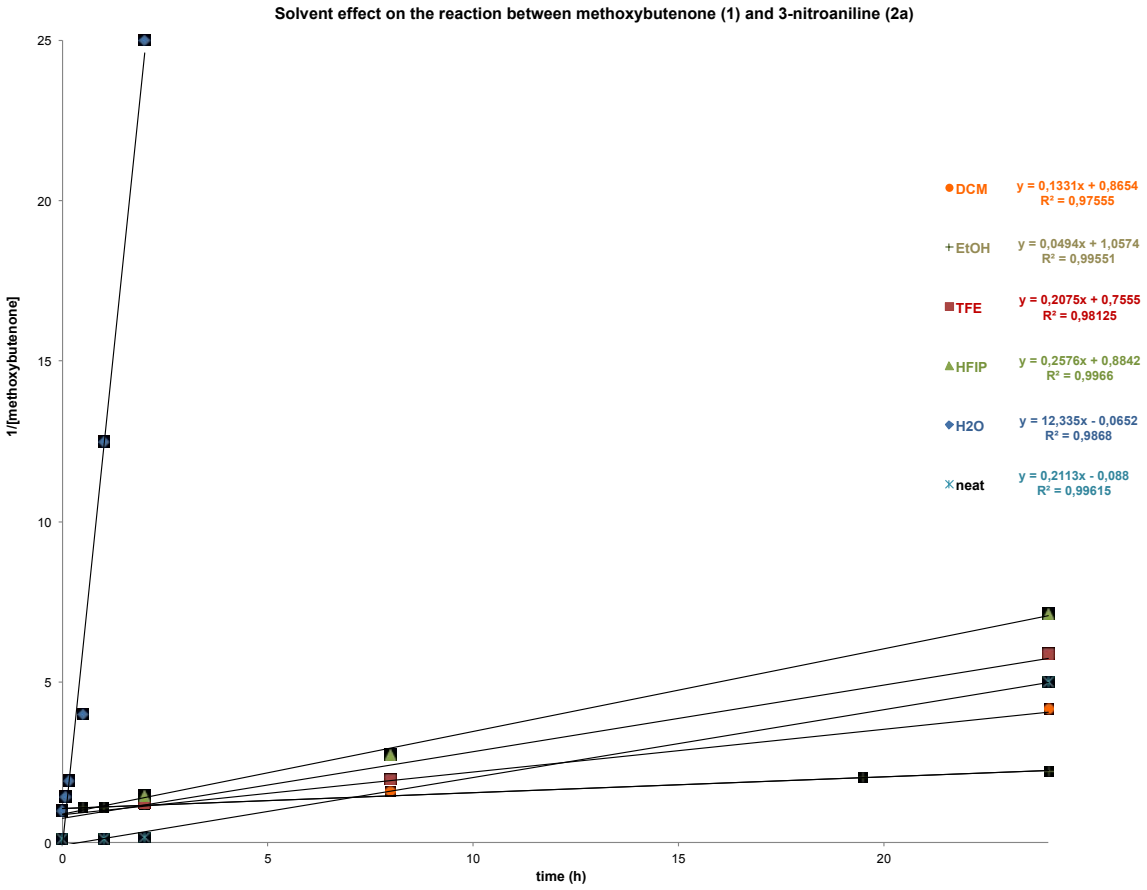
Kinetics measurements of the reaction between 1 and 2a in various solvents



Reactions were performed at 20 °C with butenone **1** (0.5 mmol), aniline **2a** (0.6 mmol) and solvent (0.5 mL) under vigorous stirring (1400 rpm).

							k **(L/mol/h)**
DCM Time (h)	0	2	8	24			
[methoxybutenone]	1	0,81	0,63	0,24			
1/[methoxybutenone]	1	1,2345679	1,58730159	4,16666667			**0,13**
EtOH Time (h)	0	0,5	1	2	19,5	24	
[methoxybutenone]	1	0,92	0,9	0,83	0,49	0,45	
1/[methoxybutenone]	1	1,08695652	1,11111111	1,20481928	2,04081633	2,22222222	**0,05**
TFE Time (h)	0	2	8	24			
[methoxybutenone]	1	0,81	0,51	0,17			
1/[methoxybutenone]	1	1,2345679	1,96078431	5,88235294			**0,21**
HFIP Time (h)	0	2	8	24			
[methoxybutenone]	1	0,69	0,37	0,14			
1/[methoxybutenone]	1	1,44927536	2,7027027	7,14285714			**0,26**
H2O Time (h)	0	0,083	0,166	0,5	1	2	
[methoxybutenone]	1	0,7	0,52	0,25	0,08	0,04	
1/[methoxybutenone]	1	1,42857143	1,92307692	4	12,5	25	**12,33**
neat Time (h)	0	1	2	24			
[methoxybutenone]	10	10	6,5	0,2			
1/[methoxybutenone]	0,1	0,1	0,15384615	5			**0,21**


Solvent effect on the reaction between methoxybutenone (1) and 3-nitroaniline (2a)
1/[methoxybutenone]
time (h)
0
5
10
15
20
25
DCM
y = 0,1331x + 0,8654
R² = 0,97555
EtOH
y = 0,0494x + 1,0574
R² = 0,99551
TFE
y = 0,2075x + 0,7555
R² = 0,98125
HFIP
y = 0,2576x + 0,8842
R² = 0,9966
H2O
y = 12,335x - 0,0652
R² = 0,9868
neat
y = 0,2113x - 0,088
R² = 0,99615

Experimental Section

Silica gel used for chromatography was 40 μm diameter. ^{1}H and ^{13}C spectra were recorded at 300 and 75 MHz, respectively, for solution in $CDCl_3$. Chemical shift (δ) in ppm are reported using residual chloroform (7.26 for ^{1}H and 77.16 for ^{13}C) as internal reference. Micromass Q-TQF (Quadrupole time-of-flight) instrument with an electrospray source in the EI or ESI mode.

General Procedure for the "on water" reaction between *trans*-4-methoxy-3-buten-2-one 1 and anilines

In a capped vial, water (0.5 mL) was added to *trans*-4-methoxy-3-buten-2-one **1** (0.5 mmol) under vigorous stirring (1400 rpm) followed by aromatic amine **2a-p** (0.6 mmol). The mixture was kept at room temperature or warmed to 60 °C according to Table 2. After completion of the reaction (^{1}H NMR monitoring), the aqueous phase was extracted with dichloromethane (2x1.5 mL). The combined organic layers were dried over anhydrous $MgSO_4$, filtered, and the solvent was evaporated under vacuum. The product was isolated in pure form by column chromatography (cyclohexane/AcOEt, 95:05 to 70:30).

(*Z*)-4-((3-Nitrophenyl)amino)-but-3-en-2-one (3a): yellow crystals, 89 mg, (86%), mp (°C): 113; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 2.18 (s, 3 H), 5.41 (d, *J* = 8.03 Hz, 1 H), 7.19-7.29 (m, 2H), 7.45 (t, *J* = 8.0 Hz, 1 H), 7.88-7.81 (m, 2H), 11.68 (d, *J* = 10.5, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.9, 99.5, 109.8, 117.6, 122.1, 130.6, 141.5, 141.8, 149.4, 200.0 ppm; IR (neat) ν (cm^{-1}) 1350, 1621; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{11}N_2O_3$ 207.0770; found 207.0771.

(*Z*)-4-((4-Nitrophenyl)amino)-but-3-en-2-one (3b):[1] yellow crystals, 79 mg, (77%), mp (°C): 174; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 2.21 (s, 3 H), 5.47 (d, *J* = 8.0 Hz, 1 H), 7.07 (d, *J* = 9 Hz, 2 H), 7.22 (dd, *J* = 11.9, 8.0 Hz, 1 H), 8.20 (d, *J* = 9 Hz, 2 H), 11.72 (d, J = 10.8 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 30.2, 100.9, 115.1, 126.2, 140.5, 142.8, 146.1, 200.4 ppm; IR (neat) ν (cm^{-1}) 1324.97, 1648.2; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{11}N_2O_3$ 207.0770; found 207.0773.

***(Z)*-4-((4-(Trifluoromethyl)phenyl)amino)-but-3-en-2-one (3c):** white crystals, 113 mg, (98%), mp (°C): 127; ^{1}H NMR ($CDCl_3$, 300 MHz): δ= 2.16 (s, 3 H), 5.36 (dd, *J* = 7.5, 1.4 Hz, 1 H), 7.05 (d, *J* = 7.5 Hz, 2 H), 7.14-7.25 (m, 1 H), 7.53 (d, *J* = 7.5, 2 H), 11.60 (d, *J* = 9.7 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.8, 99.2, 115.6, 124.2 (q, $^{1}J_{C\text{-}F}$ = 270 Hz), 124.9 (q, $^{2}J_{C\text{-}F}$ = 32 Hz), 127.09 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 141.7, 143.4, 199.8 ppm; IR (neat) ν (cm^{-1}) 1648; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{11}H_{11}F_3NO$ 230.0793; found 230.0792.

***(Z)*-4-((3-(Trifluoromethyl)phenyl)amino)-but-3-en-2-one (3d):** white crystals, 108 mg, (94%), mp (°C): 73; ^{1}H NMR ($CDCl_3$, 300 MHz): δ= 2.18 (s, 3 H), 5.32-5.44 (m, 1 H), 7.11-7.32 (m, 4 H), 7.35-7.49 (m, 1 H), 11.67 (d, *J* = 9.3 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.6, 98.6, 112.3 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 119.1, 119.6, 123.8 (q, $^{1}J_{C\text{-}F}$ = 271 Hz), 130.2, 132.1 (q, $^{2}J_{C\text{-}F}$ = 32 Hz), 141.0, 142.0, 199.5 ppm; IR (neat) ν (cm^{-1}) 1665.52 (C=C) $_{cis}$, 3047 (CH_3); HRMS (ES+) *m/z* [M + H]+ calcd for $C_{11}H_{11}F_3NO$ 230.0793; found 230.0801.

***(Z)*-4-((2-(Trifluoromethyl)phenyl)amino)-but-3-en-2-one (3e):** white crystals, 96 mg, (83%), mp (°C): 40; ^{1}H NMR ($CDCl_3$, 300 MHz): δ= 2.16 (s, 3 H), 5.39 (d, *J* = 7.8 Hz, 1 H), 7.04-7.26 (m, 3 H), 7.48 (t, *J*= 7.8 Hz, 1 H), 7.57 (d, *J* = 7.8 Hz), 12.07 (d, *J* = 9 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.6, 99.7, 116.3, 118.6 (q, $^{2}J_{C\text{-}F}$ = 31 Hz), 122.7, 124.0 (q, $^{1}J_{C\text{-}F}$ = 273 Hz), 127.0 (q, $^{3}J_{C\text{-}F}$ = 5.5 Hz), 133.3, 138.9, 142.4, 199.5 ppm; IR (neat) ν (cm^{-1}) (C-F), 1646.61; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{11}H_{11}F_3NO$ 230.0793; found 230.0788.

***(Z)*-4-((4-Chlorophenyl)amino)-but-3-en-2-one (3f):**[1] white crystals, 96 mg, (98%), mp (°C): 113; ^{1}H NMR ($CDCl_3$, 300 MHz): δ= 2.17 (s, 3 H), 5.33 (d, *J* = 7.8 Hz, 1 H), 6.95 (d, *J* = 8.4 Hz, 2H), 7.15 (dd, *J* = 12.3, 7.8 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 2H), 11.59 (d, *J* = 10 Hz, 1H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.6, 98.0, 117.2, 128.3, 129.7, 139.0, 142.6, 199.2 ppm; IR (neat) ν (cm^{-1}) 1643; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{11}ClNO$ 196.0529; found 196.0528.

***(Z)*-4-((3-Chlorophenyl)amino)-but-3-en-2-one (3g):** white crystals, 90 mg, (92%), mp (°C): 85; ^{1}H NMR ($CDCl_3$, 300 MHz): δ= 2.21 (s, 3 H), 5.38 (d, *J* = 8 Hz), 6.92 (d, *J* = 8 Hz, 1 H), 7.02-7.08 (m, 2 H), 7.16-7.31 (m, 2H), 11.58 (d, *J* = 12 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.8, 98.5, 114.5, 116.0, 123.3, 130.8, 135.6, 141.8, 142.3, 199.4 ppm; IR (neat) ν (cm^{-1}) 1648; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{11}ClNO$ 196.0529; found 196.0529.

***(Z)*-4-((2-Chlorophenyl)amino)-but-3-en-2-one (3h):** white crystals, 92 mg, (94%), mp (°C): 70; ^{1}H NMR ($CDCl_3$, 300 MHz): δ= 2.22 (s, 3 H), 5.44 (d, *J* = 7.8 Hz, 1 H), 6.98 (t, *J* = 7.8 Hz, 1 H), 7.11-7.33 (m, 3H), 7.40 (d, *J* = 7.8 Hz, 1H), 11.99 (br s, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.6, 99.1, 114.0, 122.4, 123.3, 127.9, 130.1, 137.4, 141.3, 199.2 ppm; IR (neat) ν (cm^{-1}) 1644.03; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{11}ClNO$ 196.0529; found 196.0527.

***(Z)*-4-((4-Chloro-2-fluorophenyl)amino)-but-3-en-2-one (3i):** white crystals, 99 mg, (93%), mp (°C): 102; ^{1}H NMR (300 MHz, $CDCl_3$): δ= 2.11 (s, 3 H), 5.34 (d, *J* = 7.84 Hz, 1 H), 6.95-7.15 (m, 4H), 11.56 (d, *J* = 11.7, 1H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.7, 99.2, 115.7, 116.8 (d, $^2J_{C\text{-}F}$ = 22 Hz), 125.0 (d, $^3J_{C\text{-}F}$ = 3.8 Hz), 127.5 (d, $^3J_{C\text{-}F}$ = 9.3 Hz), 128.0 (d, $^2J_{C\text{-}F}$ = 11 Hz), 141.5, 151.7 (d, $^1J_{C\text{-}F}$ = 252 Hz), 199.4 ppm; IR (neat) ν (cm^{-1}) 1643; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{10}ClFNO$ 214.0435; found 214.0432.

***(Z)*-4-((3-Chloro-4-fluorophenyl)amino)-but-3-en-2-one (3j):** brown crystals, 92 mg, (86%), mp (°C): 85; ^{1}H NMR ($CDCl_3$, 300 MHz): δ= 2.15 (s, 3 H), 5.31 (d, *J* = 7.8 Hz, 1 H), 6.81-6.88 (m, 1 H), 7.01-7.11 (m, 3 H), 11.53 (d, J = 11 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.7, 98.4, 115.8 (d, $^3J_{C\text{-}F}$ = 7 Hz), 117.5 (d, $^2J_{C\text{-}F}$ = 23 Hz), 117.9, 122.1 (d, $^2J_{C\text{-}F}$ = 20 Hz), 137.5 (d, $J_{C\text{-}F}$ = 2 Hz), 142.8, 154.4 (d, $^1J_{C\text{-}F}$ = 245 Hz), 199.4 ppm; IR (neat) ν (cm^{-1}); HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{10}ClN_2FNO$ 214.0435; found 214.0436.

***(Z)*-4-((2,4-Difluorophenyl)amino)-but-3-en-2-one (3k):** white crystals, 82 mg (83%), mp (°C): 95; ^{1}H NMR ($CDCl_3$, 300 MHz): δ= 2.14 (s, 3 H), 5.35 (d, *J* = 7.6 Hz, 1 H), 6.77-6.92 (m, 2H), 7.00-7.18 (m, 2H), 11.58 (d, *J* = 10.7 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.6, 98.7, 104.8 (dd, $J_{C\text{-}F}$ = 27, 22 Hz), 111.6 (dd, $J_{C\text{-}F}$ = 23, 3.2 Hz), 116.2 (dd, $J_{C\text{-}F}$ = 9.4, 2.9 Hz), 125.8 (dd, $J_{C\text{-}F}$ = 11, 3.4 Hz), 142.6, 152.1 (dd, $J_{C\text{-}F}$ = 246, 11 Hz), 158.1 (dd, $J_{C\text{-}F}$ = 246, 11 Hz), 199.3 ppm; IR (neat) ν 1635 1733; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{10}F_2NO$ 198.0730; found 198.0736.

***(Z)*-4-((3-Fluorophenyl)amino)-but-3-en-2-one (3l):** white crystals, 78 mg (87%), mp (°C): 58; ^{1}H NMR ($CDCl_3$, 300 MHz): δ= 2.14 (s, 3 H), 5.31 (d, *J* = 7.8 Hz, 1 H), 6.63-6.84 (m, 3 H), 7.07-7.29 (m, 2 H), 11.52 (d, *J* = 10 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.7, 98.3, 103.0 (d, $^2J_{C\text{-}F}$ = 25Hz), 109.9 (d, $^2J_{C\text{-}F}$ = 20 Hz), 111.8 (d, $^4J_{C\text{-}F}$ = 2.8 Hz), 131.0 (d, $^3J_{C\text{-}F}$ = 10 Hz), 142.2 (d, $^3J_{C\text{-}F}$ = 10 Hz), 142.3, 163.7 (d, $^1J_{C\text{-}F}$ = 247 Hz), 199.3 ppm; IR (neat) ν (cm^{-1}) 1641.6; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{11}FNO$ 180.0825; found 183.0577.

***(Z)*-4-((Phenylamino)-but-3-en-2-one (3m):**[1] white crystals, 71 mg, (89%), mp (°C): 85; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 2.16 (s, 3 H), 5.30 (d, *J* = 7.8 Hz, 1H), 7.00-7.04 (m, 3H), 7.23 (dd, *J* = 12.5,

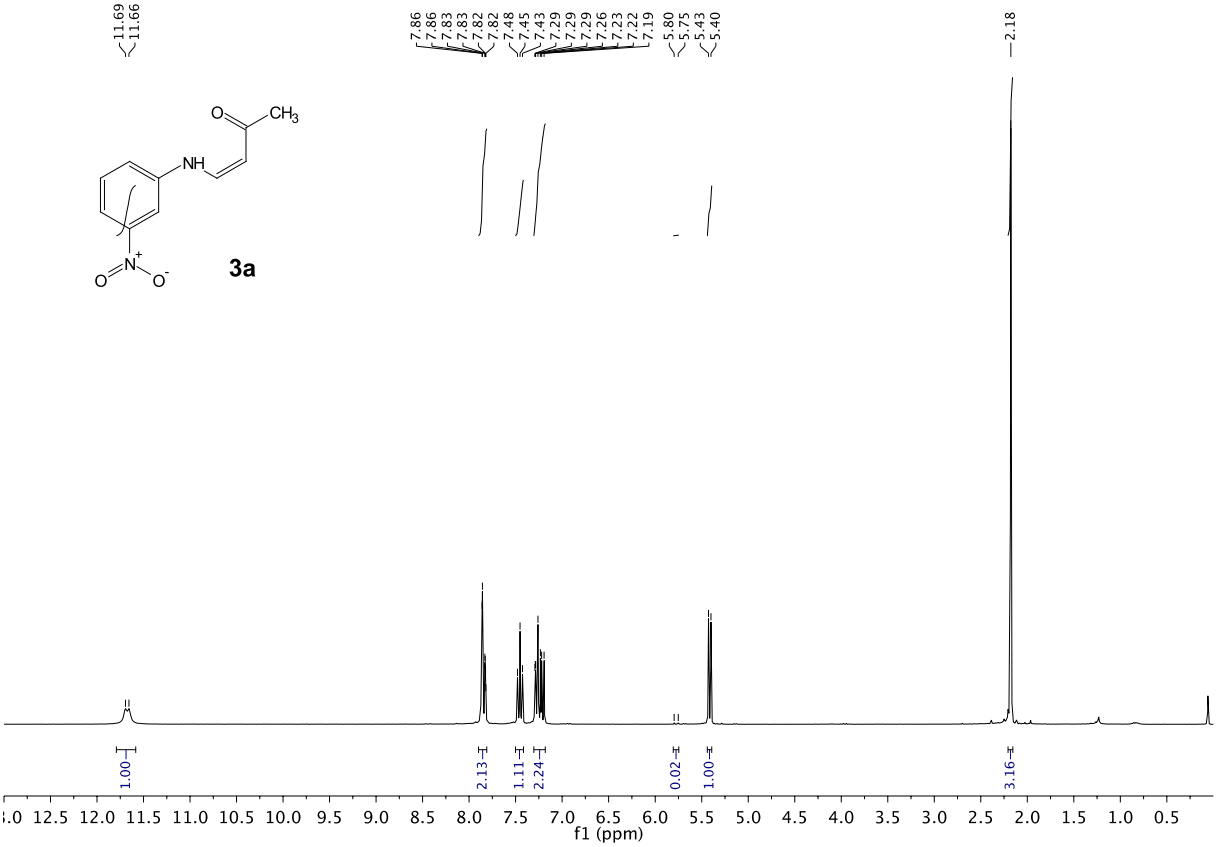
7.9 Hz, 1H), 7.32 (t, *J* = 7.9 Hz, 2H), 11.62 (d, *J* = 12.5, 1H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.6, 97.5, 116.1, 123.4, 129.7, 140.4, 143.0, 199.0 ppm; IR (neat) ν (cm^{-1}) 1666, 3231 ; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{10}H_{12}NO$ 162.0919; found 162.0916.

(*Z*)-4-((4-Methoxyphenyl)amino)-but-3-en-2-one (3n):[1] Brown crystals, 93 mg, (97%), mp (°C): 65; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 2.14 (s, 3 H), 3.78 (s, 3 H), 5.24 (d, *J* = 7.4 Hz, 1 H), 6.85 (d, *J* = 9.03 Hz, 2H), 6.97 (dd, *J* = 9.03 Hz, 2H), 7.13 (dd, J = 11.4, 7.6 Hz, 1 H), 11.61 (d, *J* =11.5 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 29.5, 55.7, 96.7, 115.0, 117.8, 134.2, 144.1, 156.8, 198.5 ppm; IR (neat) ν (cm^{-1}) 1635; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{11}H_{14}NO_2$ 192.1025; found 192.1024.

(*E*)-4-(Methyl(phenyl)amino)but-3-en-2-one (3o):[1] pink oil, 85 mg, (98%), ^{1}H NMR ($CDCl_3$, 300 MHz,): δ= 2.17 (s, 3 H), 3.26 (s, 3 H), 5.40 (d, *J* = 12.9 Hz, 1 H), 7.10-7.17 (m, 3 H), 7.30-7.39 (m, 2 H), 7.88 (d, *J* = 12.9 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 28.3, 37.0, 101.9, 120.4, 124.8, 129.6, 146.6, 148.5, 196.4 ppm; IR (neat) ν (cm^{-1}) 1611.68; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{11}H_{14}NO$ 176.1075; found 176.1071.

(*E*)-4-((4-Chlorophenyl)(methyl)amino)but-3-en-2-one (3p): brown oil, 87 mg (83%) ^{1}H NMR (300 MHz, $CDCl_3$): δ= 2.10 (s, 3 H), 3.16 (s, 3 H), 5.35 (d, *J* = 13 Hz, 1 H), 6.99 (d, *J* = 8.5 Hz, 2 H), 7.23 (d, *J* = 8.5 Hz, 2 H), 7.74 (d, *J* = 13 Hz, 1 H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ= 28.4, 36.9, 102.2, 121.4, 129.4, 129.9, 145.0, 147.8, 196.3 ppm; IR (neat) ν (cm^{-1}) 1610.64 $(C=C)_{aromatique}$, 1661; HRMS (ES+) *m/z* [M + H]+ calcd for $C_{11}H_{13}ClNO$ 210.0686; found 210.0693.

1 D. R. Chisholm, R. Valentine, E. Pohl and A. Whiting, *J. Org. Chem.*, 2016, **81**, 7557−7565.


11.69
11.66
7.86
7.86
7.83
7.83
7.82
7.82
7.48
7.45
7.43
7.29
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7.29
7.26
7.23
7.22
7.19
5.80
5.75
5.43
5.40
2.18
O
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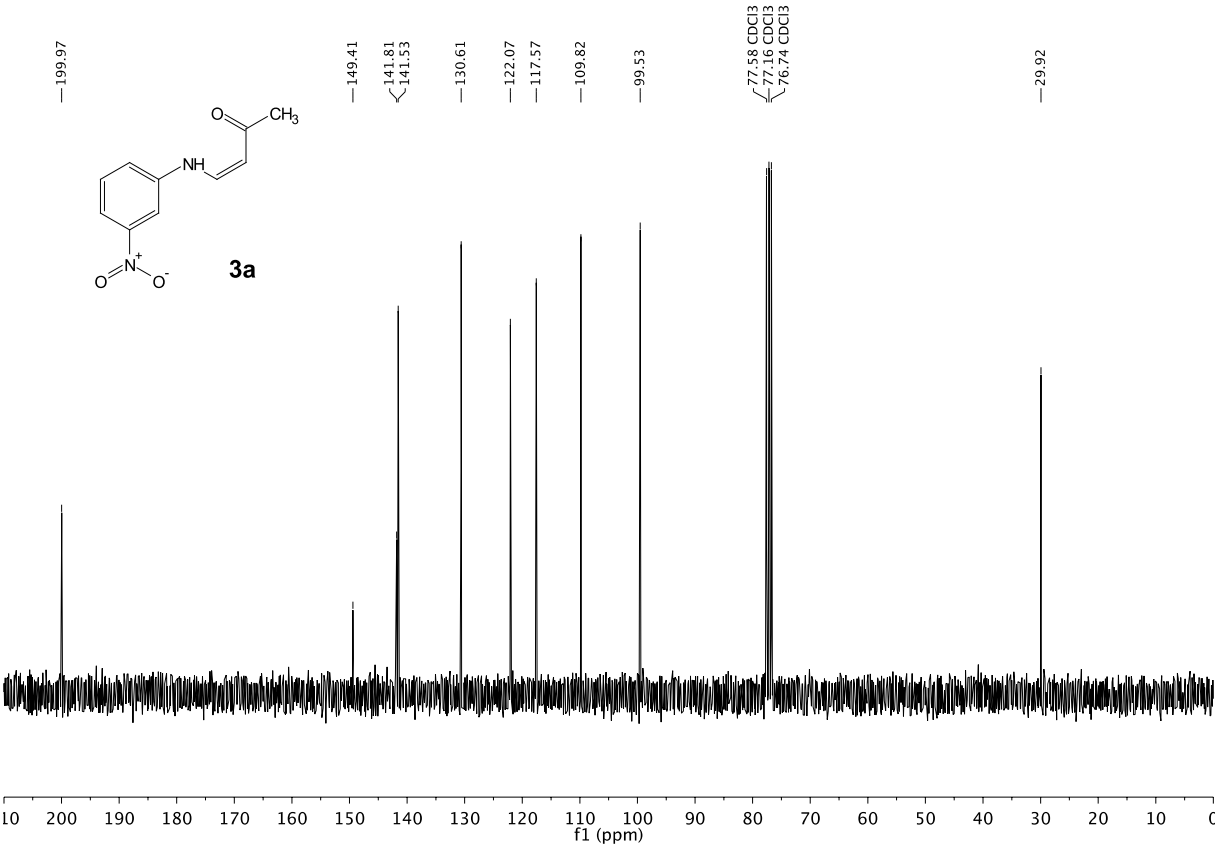
1.11
2.24
0.02
1.00
3.16
f1 (ppm)


199.97
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141.81
141.53
130.61
122.07
117.57
109.82
99.53
77.58 CDCl3
77.16 CDCl3
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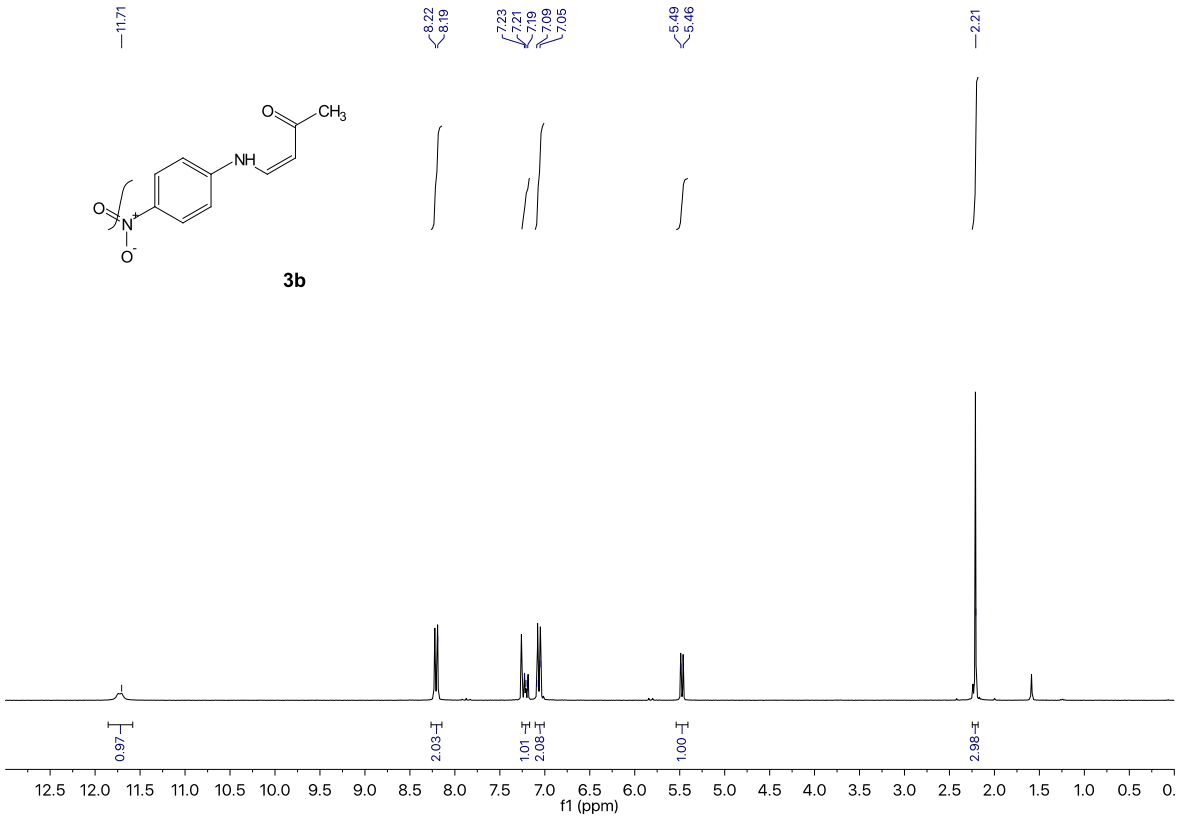
CH3
NH
N+
O
O-
3a
f1 (ppm)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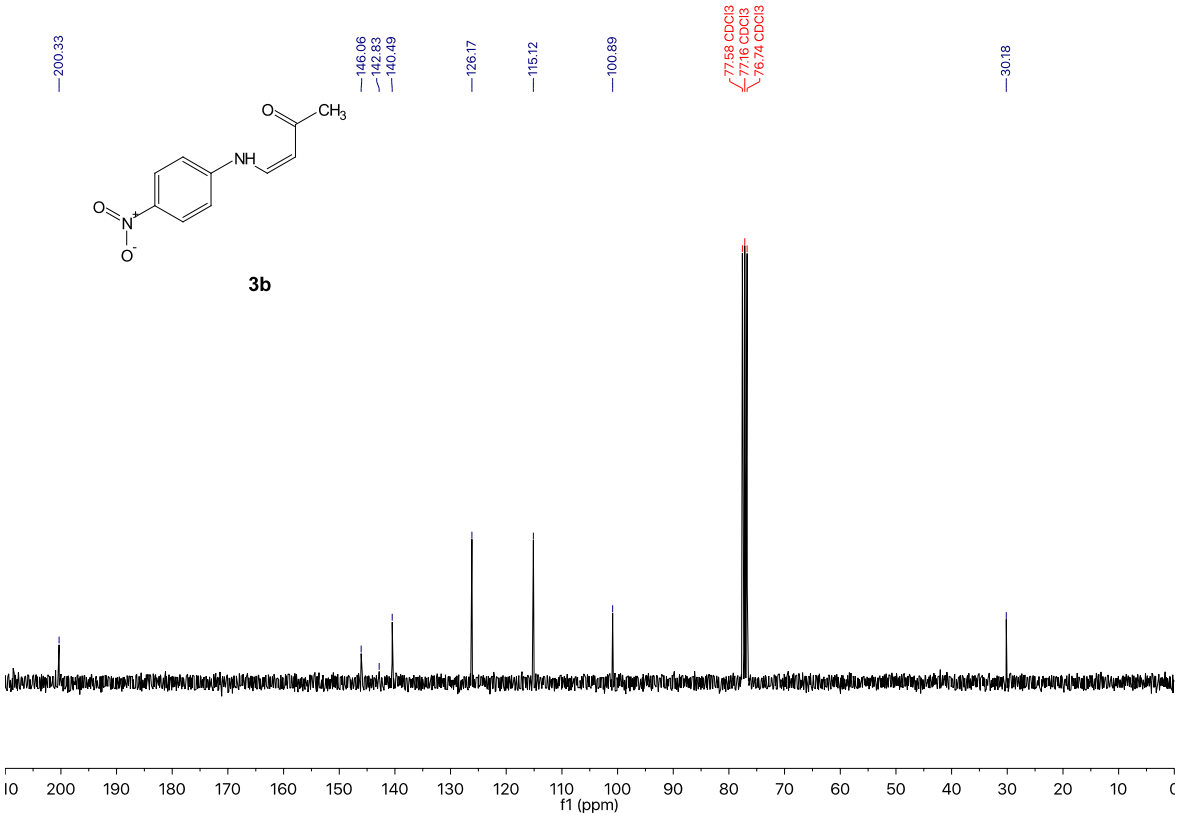
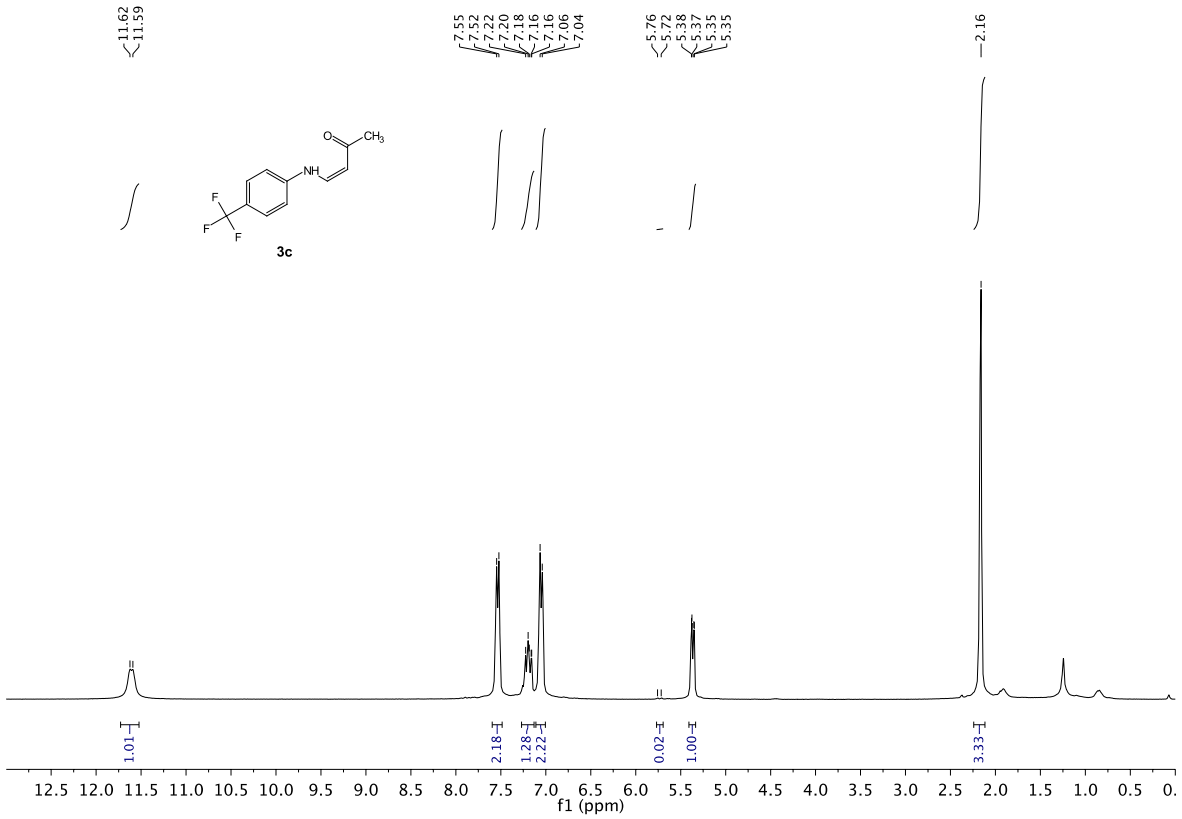
8.22
8.19
7.23
7.21
7.19
7.09
7.05
5.49
5.46
2.21
O
CH3
NH
O
N+
O-
0.97
2.03
1.01
2.08
1.00
2.98
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

3b


200.33
146.06
142.83
140.49
126.17
115.12
100.89
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
30.18
O
CH3
NH
O
N+
O-
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

3b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7.55
7.52
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7.06
7.04
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5.38
5.37
5.35
5.35
2.16
O
CH3
NH
F
F
F
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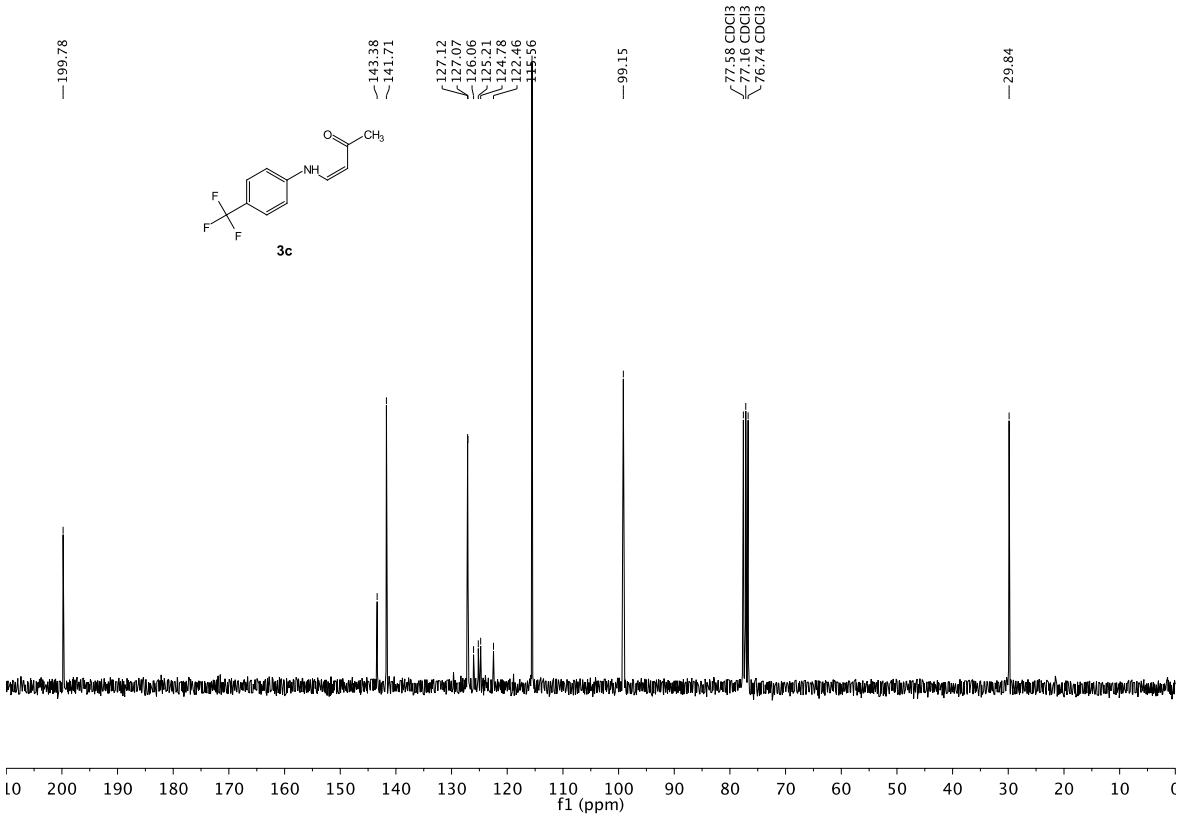
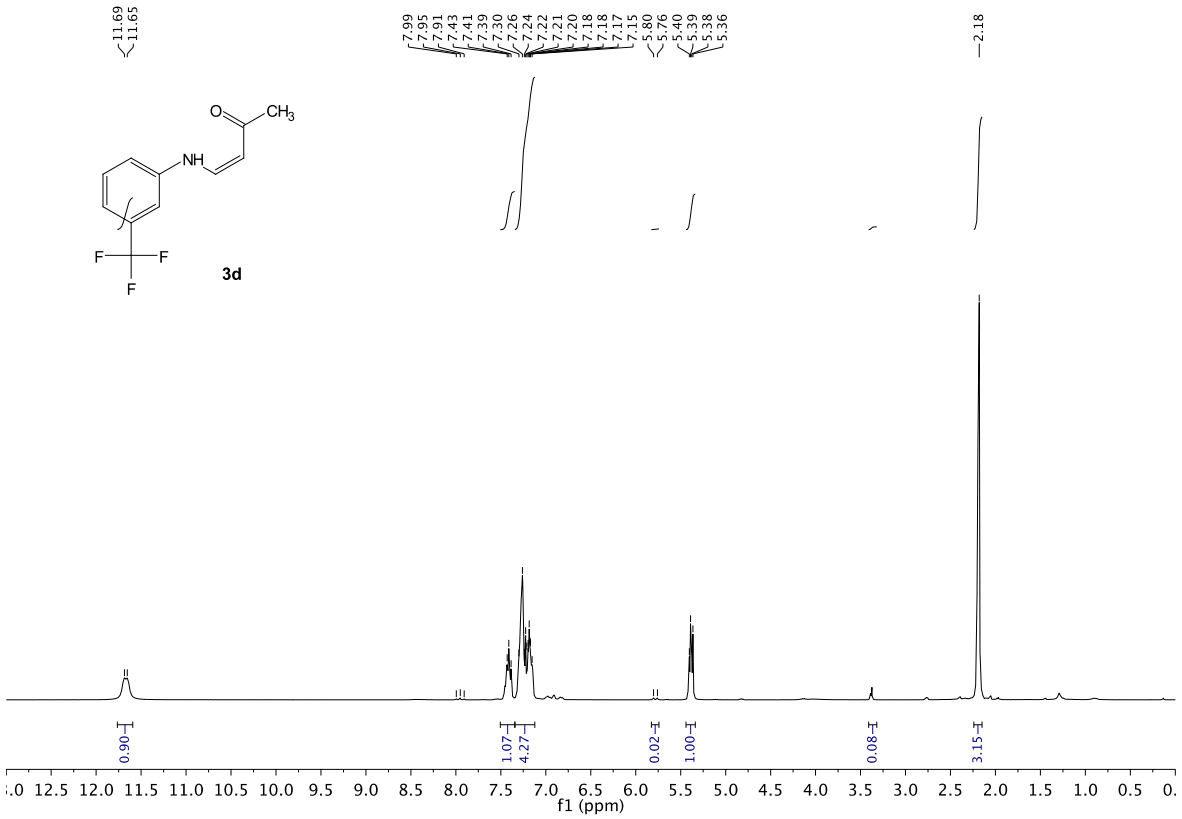
0.02
1.00
3.33
f1 (ppm)


199.78
143.38
141.71
127.12
127.07
126.06
125.21
124.78
122.46
115.56
99.15
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
29.84
O
CH3
NH
F
F
F
3c
f1 (ppm)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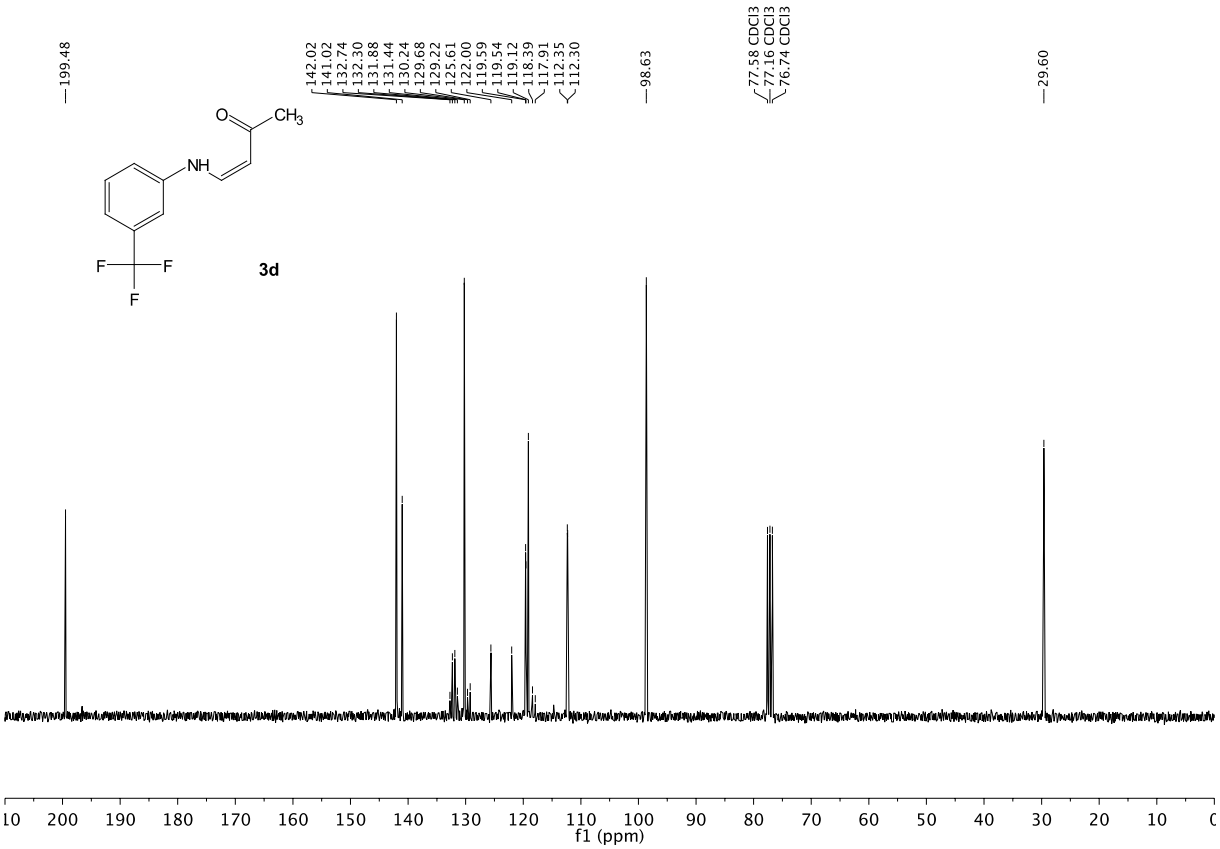
7.95
7.91
7.43
7.41
7.39
7.30
7.26
7.24
7.22
7.21
7.20
7.18
7.18
7.17
7.15
5.80
5.76
5.40
5.39
5.38
5.36
2.18
O
CH3
NH
F
F
F
3d
0.90
1.07
4.27
0.02
1.00
0.08
3.15
f1 (ppm)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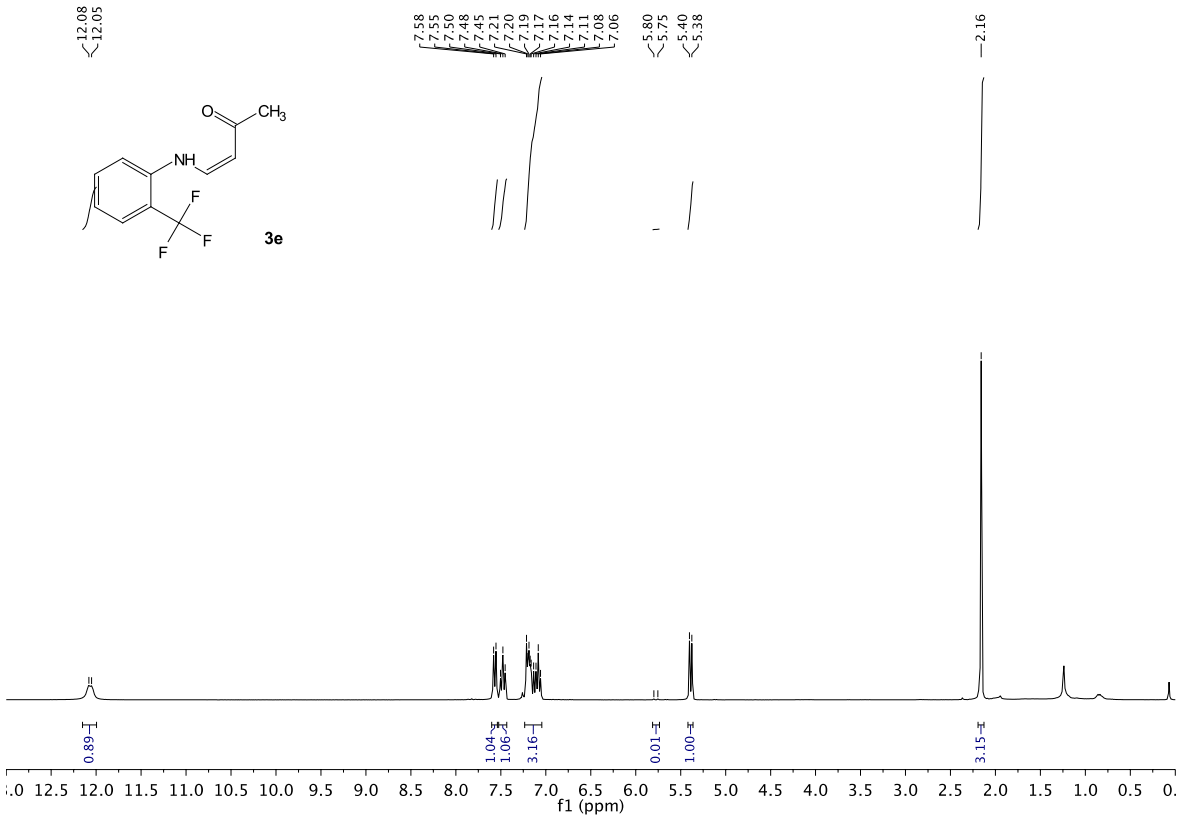
142.02
141.02
132.74
132.30
131.88
131.44
130.24
129.68
129.22
125.61
122.00
119.59
119.54
119.12
118.39
117.91
112.35
112.30
98.63
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
29.60
O
CH3
NH
F
F
F
3d
f1 (ppm)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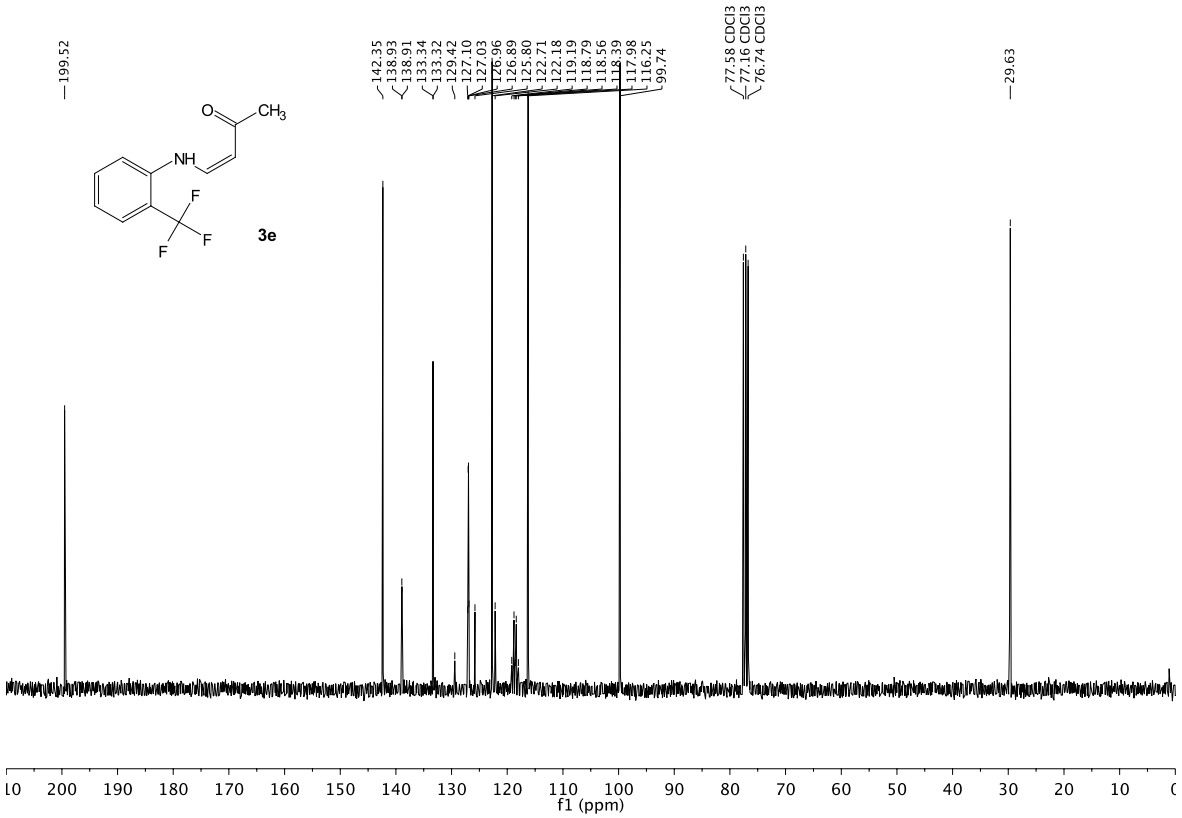
12.05
7.58
7.55
7.50
7.48
7.45
7.21
7.20
7.19
7.17
7.16
7.14
7.11
7.08
7.06
5.80
5.75
5.40
5.38
2.16
O
CH3
NH
F
F
F
3e
0.89
1.04
1.06
3.16
0.01
1.00
3.15
f1 (ppm)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138.91
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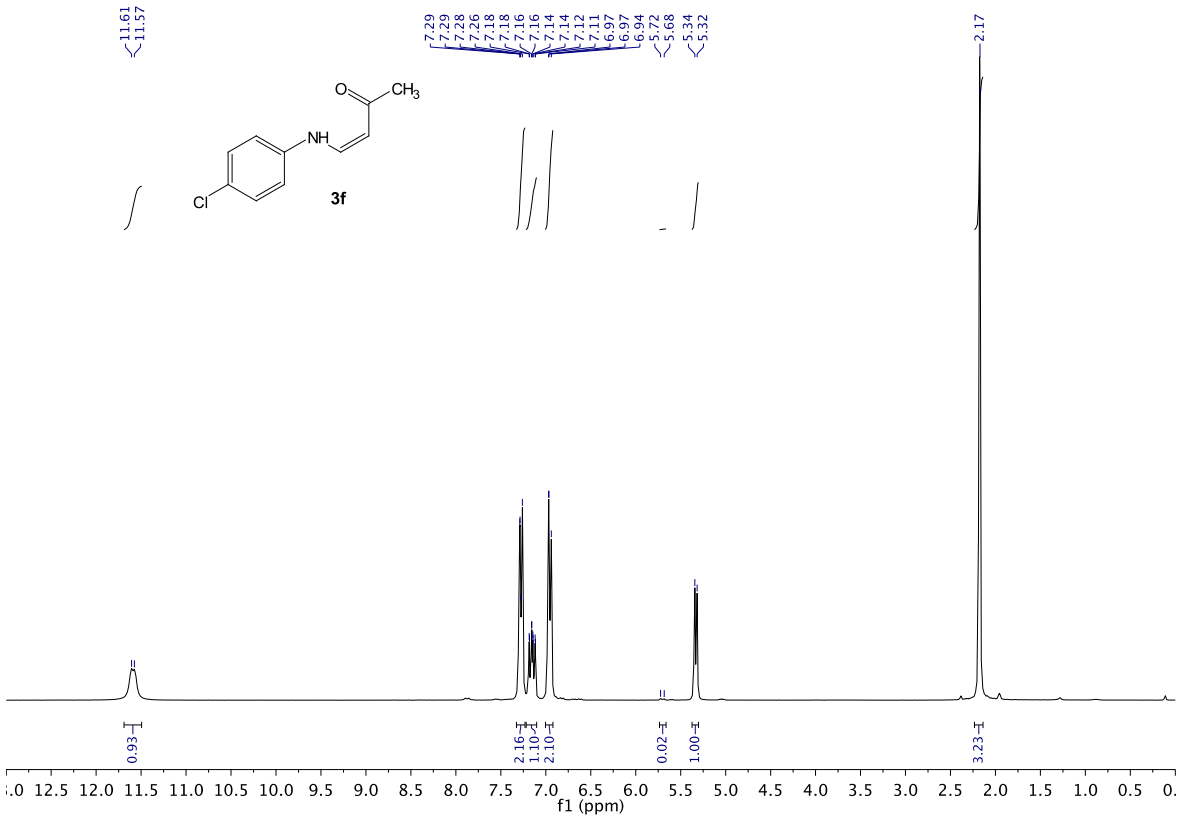
133.32
129.42
127.10
127.03
126.96
126.89
123.80
122.71
122.18
119.19
118.79
118.56
118.39
117.98
116.25
99.74
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
29.63
O
CH3
NH
F
F
F
3e
f1 (ppm)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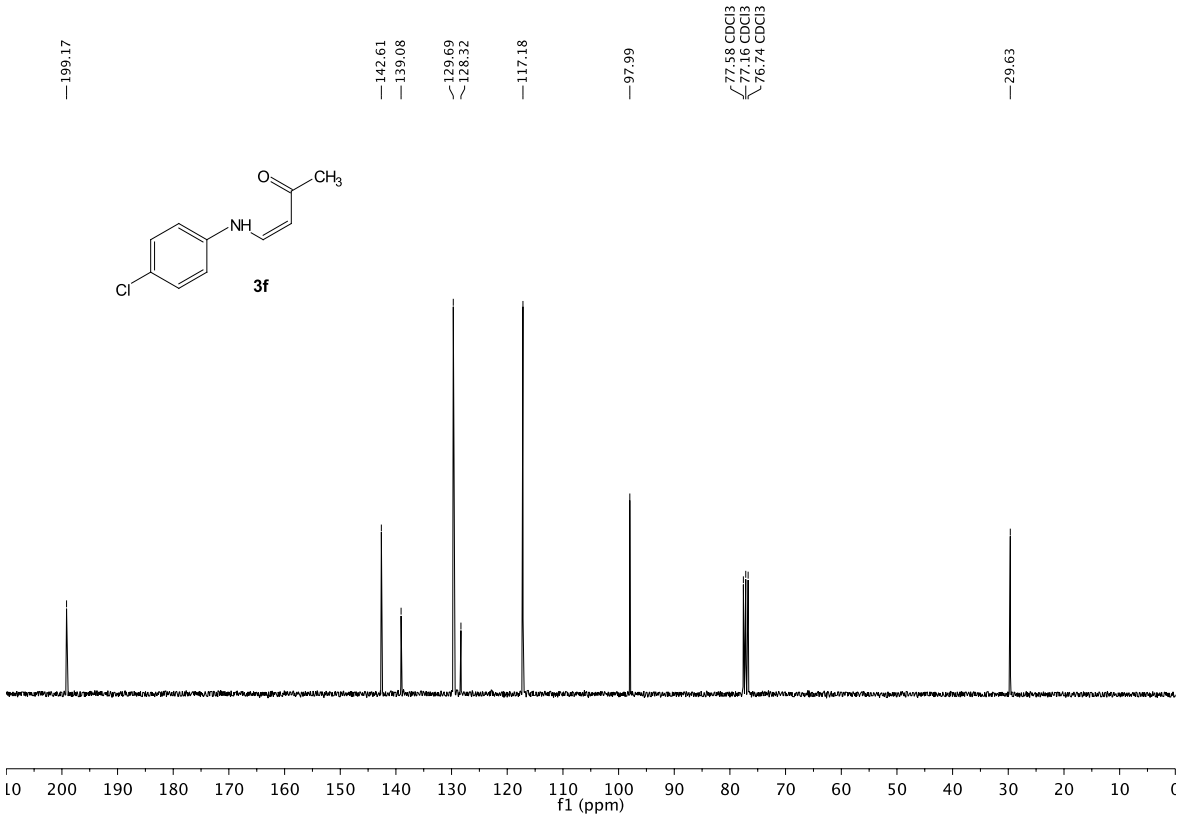
11.57
7.29
7.29
7.28
7.26
7.18
7.16
7.16
7.14
7.14
7.12
7.11
6.97
6.97
6.94
5.72
5.68
5.34
5.32
2.17
O
CH3
NH
Cl
3f
0.93
2.16
1.10
2.10
0.02
1.00
3.23
f1 (ppm)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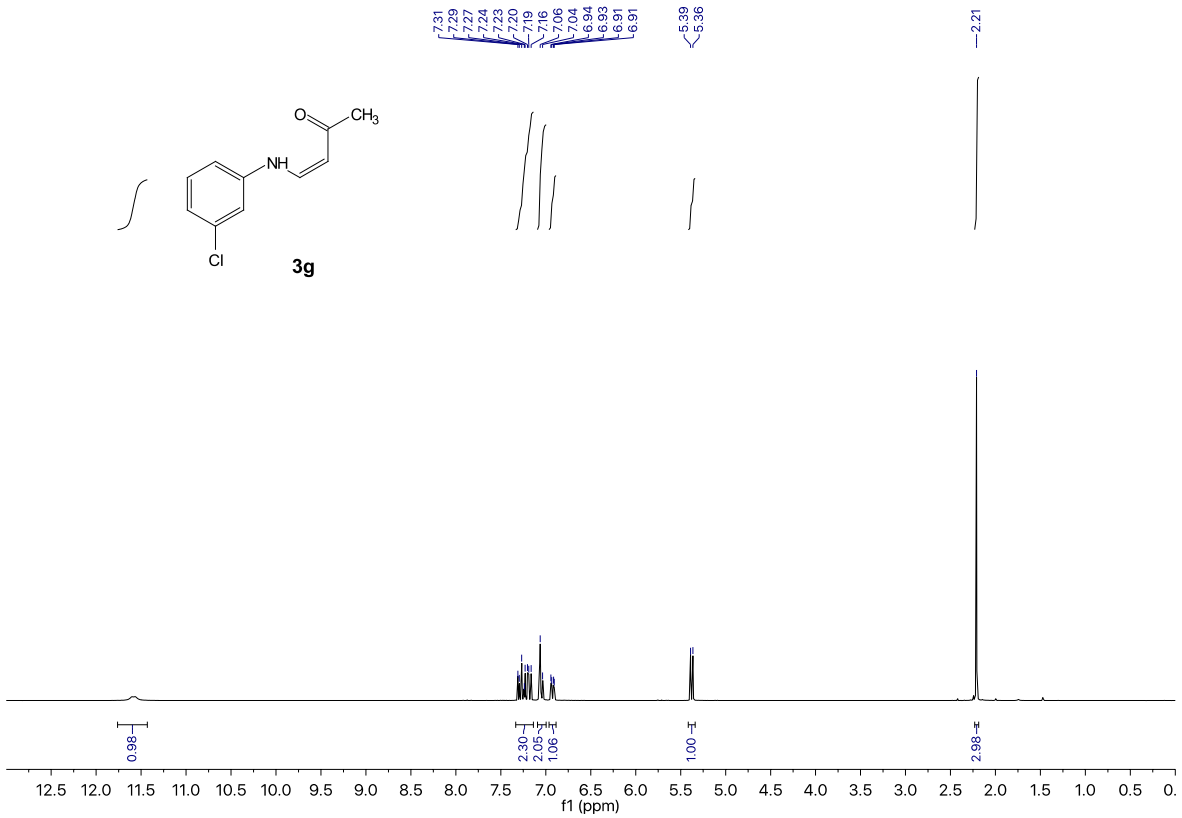
139.08
129.69
128.32
117.18
97.99
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
29.63
O
CH3
NH
Cl
3f
f1 (ppm)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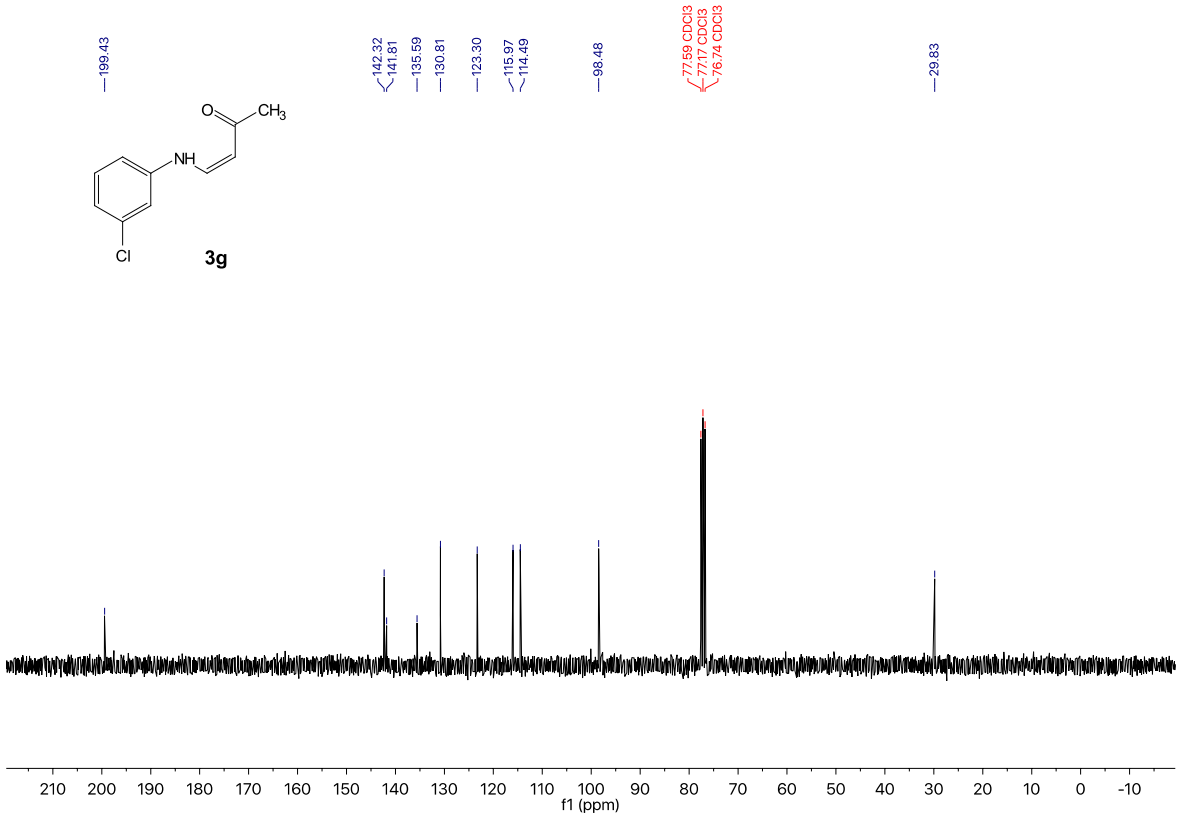
7.29
7.27
7.24
7.23
7.20
7.19
7.16
7.06
7.04
6.94
6.93
6.91
6.91
5.39
5.36
2.21
O
CH3
NH
Cl
3g
0.98
2.30
2.05
1.06
1.00
2.98
f1 (ppm)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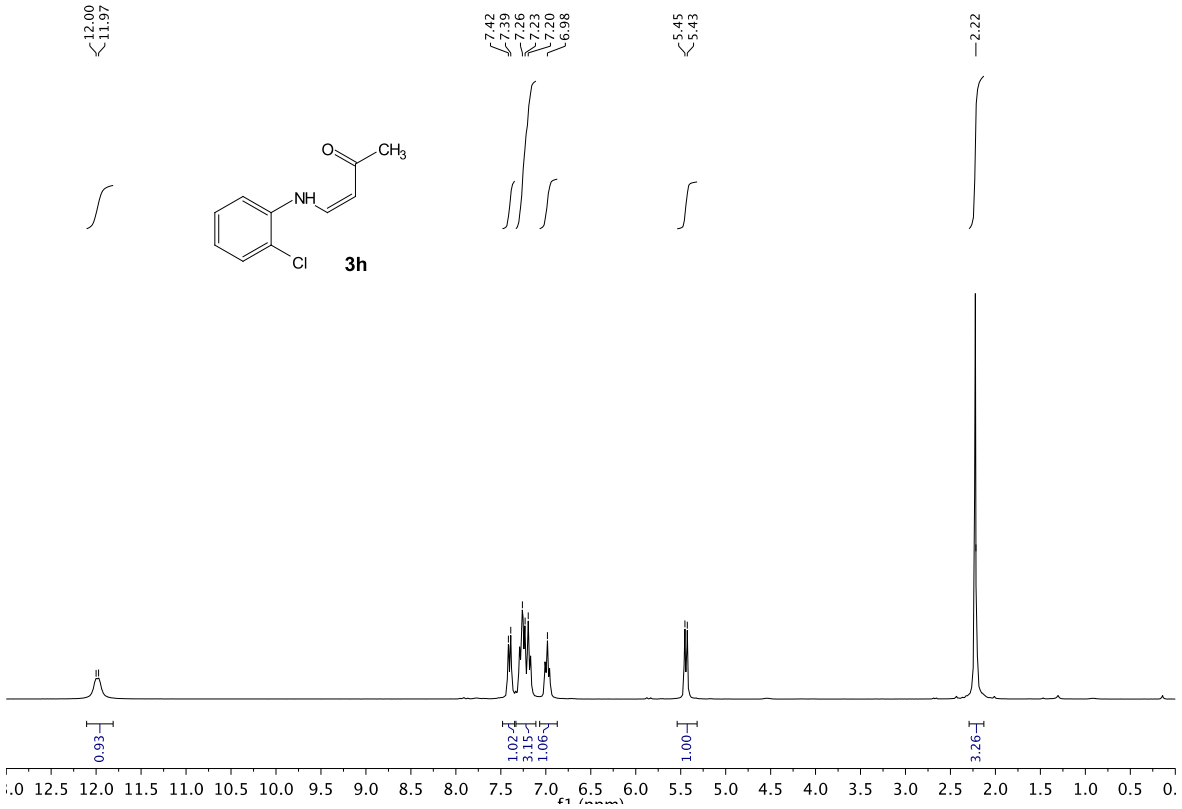
141.81
135.59
130.81
123.30
115.97
114.49
98.48
77.59 CDCl3
77.17 CDCl3
76.74 CDCl3
29.83
O
CH3
NH
Cl
3g
f1 (ppm)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11.97
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7.39
7.26
7.23
7.20
6.98
5.45
5.43
2.22
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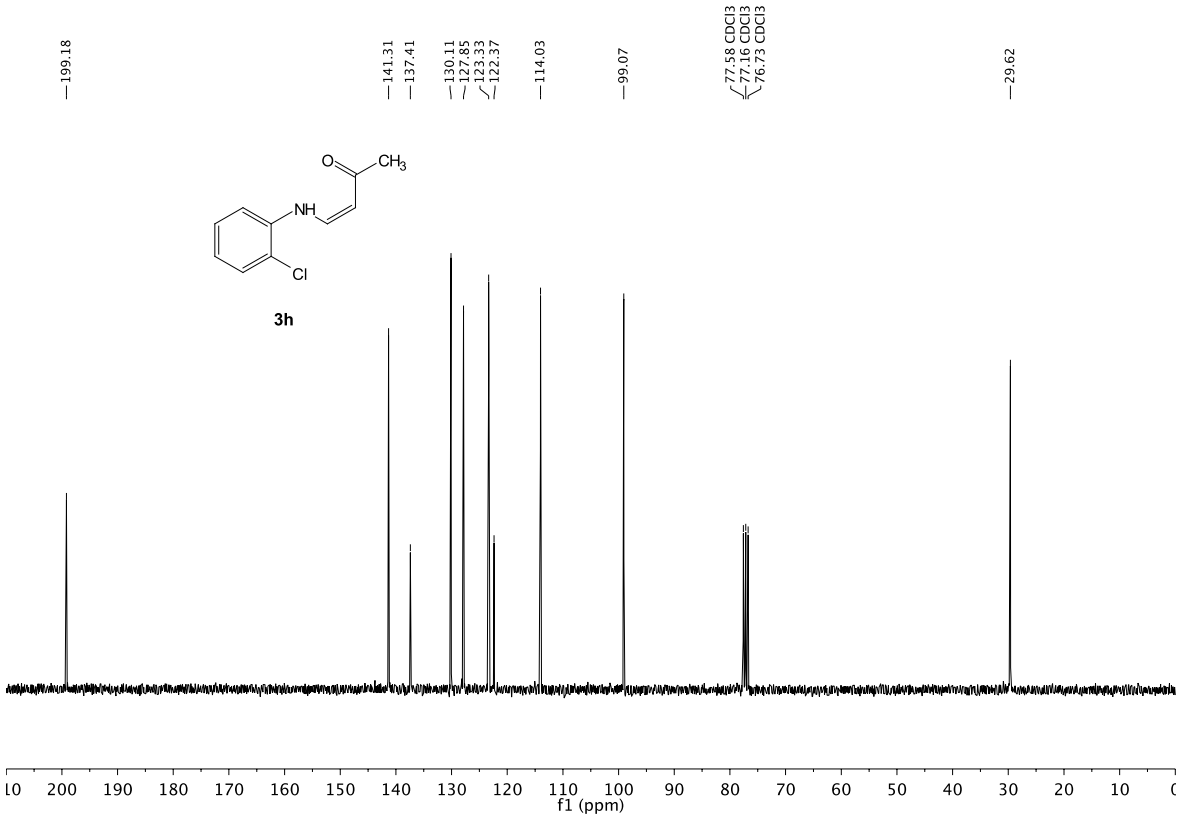
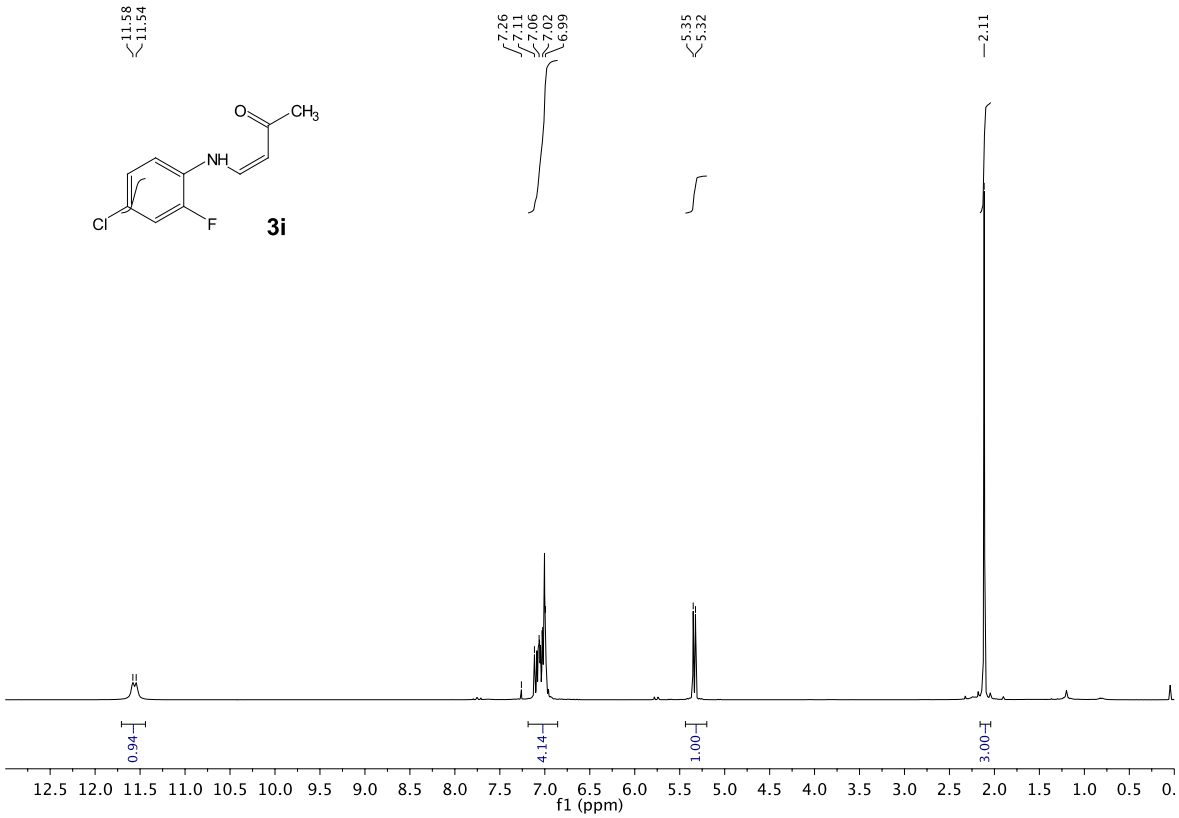
CH3
NH
Cl
3h
0.93
1.02
3.15
1.06
1.00
3.26
f1 (ppm)


199.18
141.31
137.41
130.11
127.85
123.33
122.37
114.03
99.07
77.58 CDCl3
77.16 CDCl3
76.73 CDCl3
29.62
O
CH3
NH
Cl
3h
f1 (ppm)


11.58
11.54
7.26
7.11
7.06
7.02
6.99
5.35
5.32
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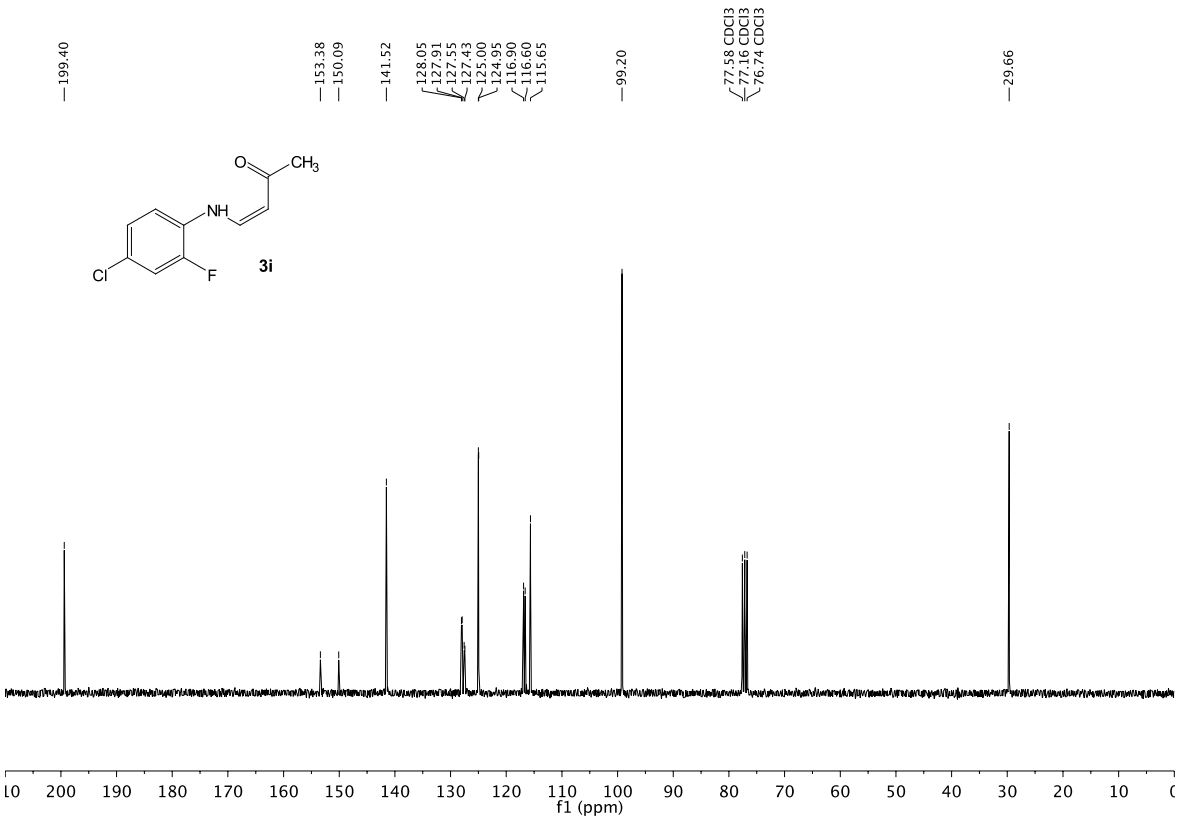
O
CH3
NH
Cl
F
3i
0.94
4.14
1.00
3.00
f1 (ppm)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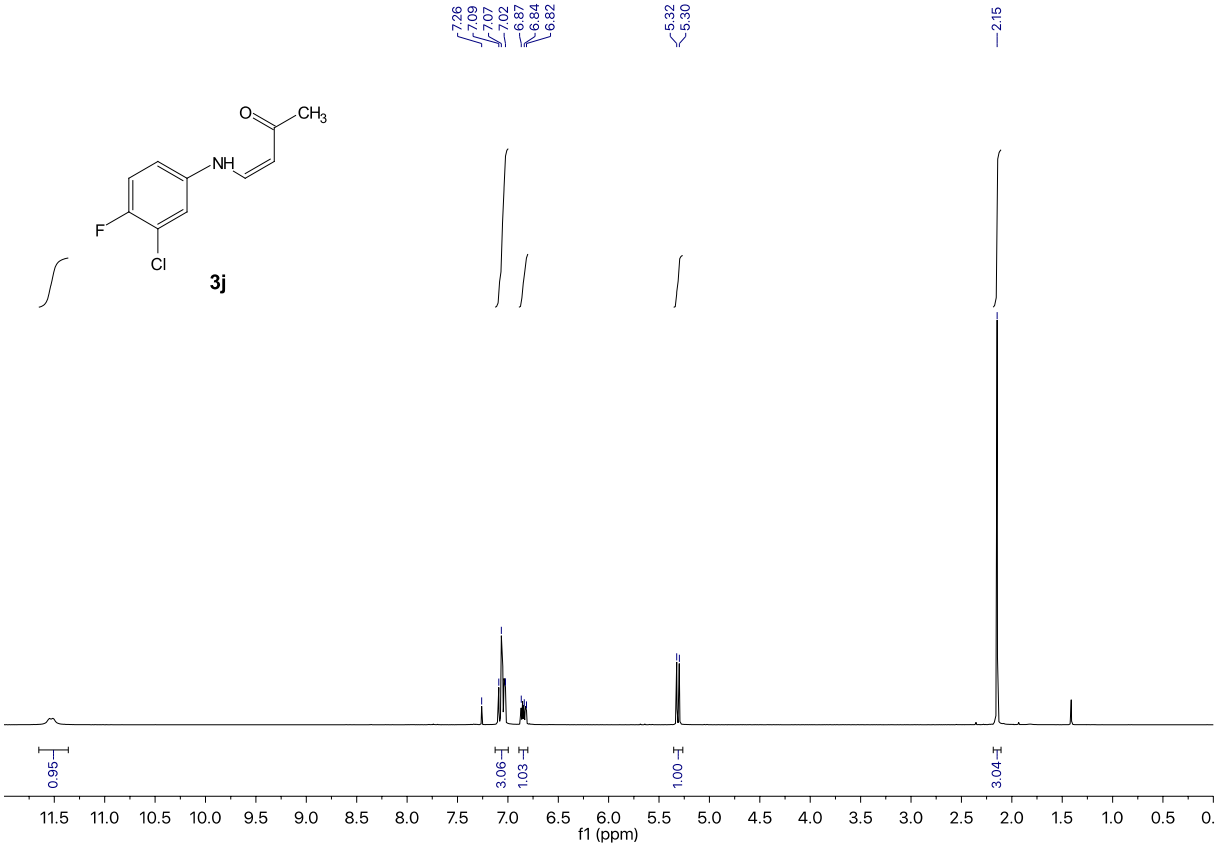
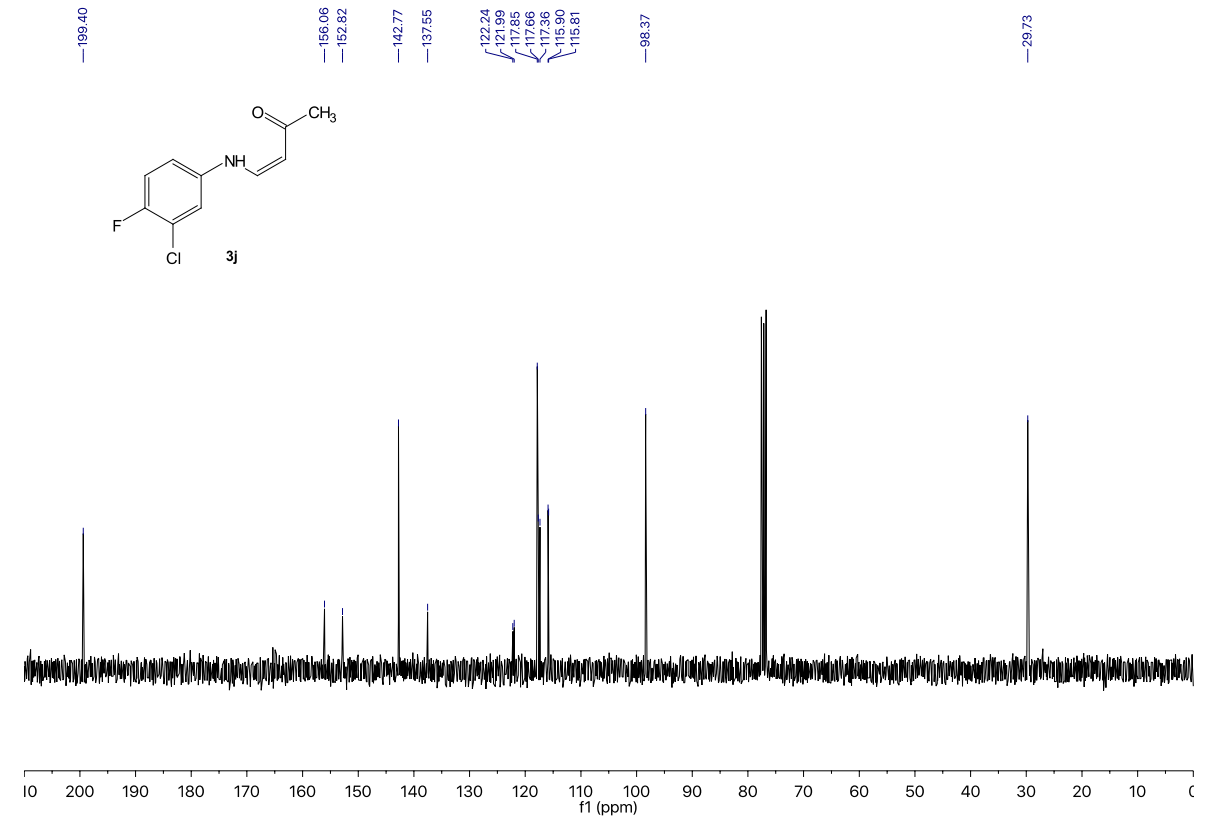
153.38
150.09
141.52
128.05
127.91
127.55
127.43
125.00
124.95
116.90
116.60
115.65
99.20
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
29.66
O
CH3
NH
Cl
F
3i
f1 (ppm)


7.26
7.09
7.07
7.02
6.87
6.84
6.82
5.32
5.30
2.15
O
CH3
NH
F
Cl
3j
0.95
3.06
1.03
1.00
3.04
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)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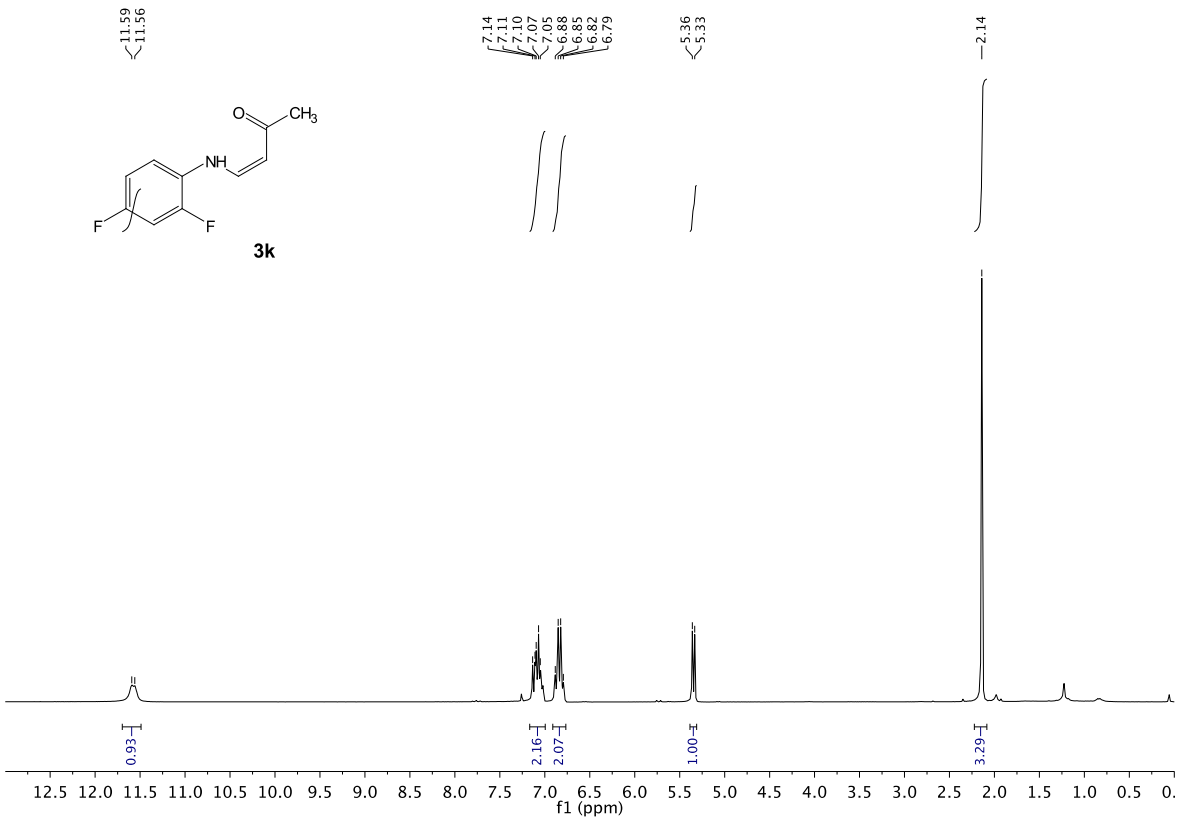
156.06
152.82
142.77
137.55
122.24
121.99
117.85
117.66
117.36
115.90
115.81
98.37
29.73
O
CH3
NH
F
Cl
3j
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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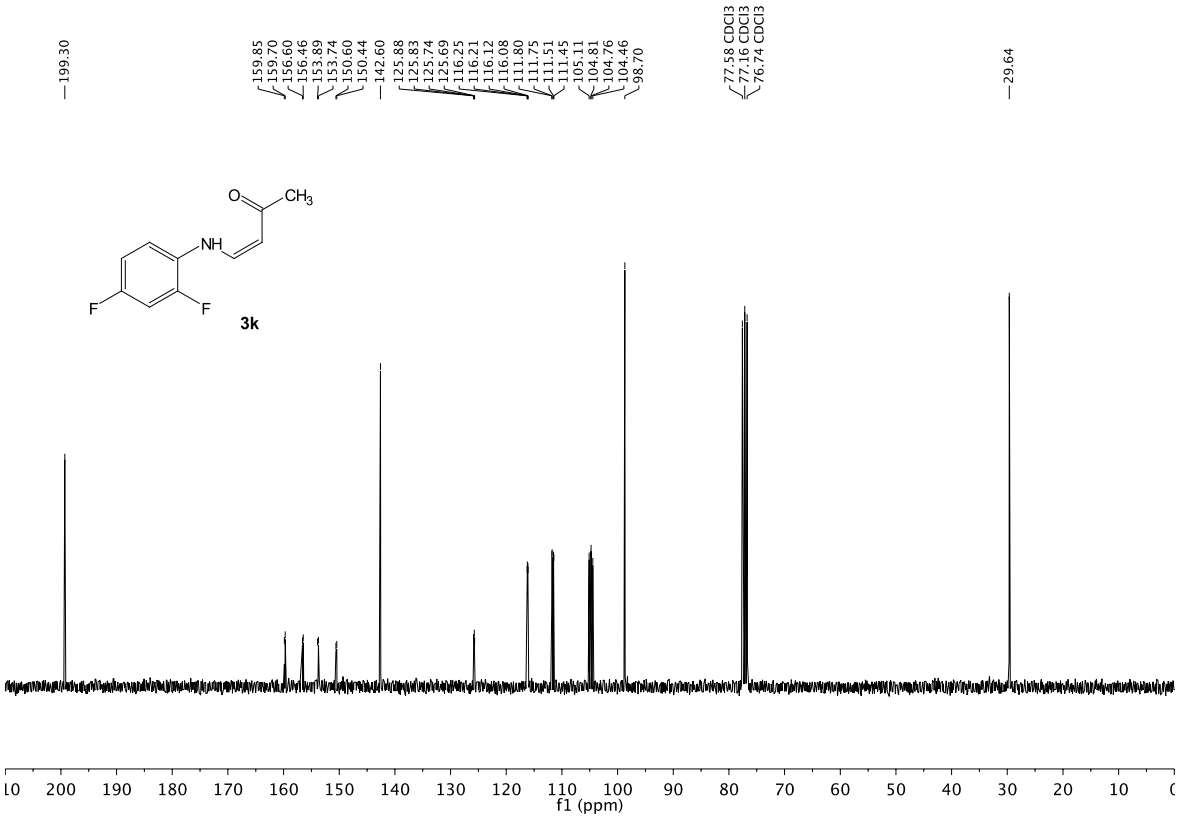
11.56
7.14
7.11
7.10
7.07
7.05
6.88
6.85
6.82
6.79
5.36
5.33
2.14
O
CH3
NH
F
F
3k
0.93
2.16
2.07
1.00
3.29
f1 (ppm)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159.85
159.70
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156.46
153.89
153.74
150.60
150.44
142.60
125.88
125.83
125.74
125.69
116.25
116.21
116.12
116.08
111.80
111.75
111.51
111.45
105.11
104.81
104.76
104.46
98.70
77.58 CDCl3
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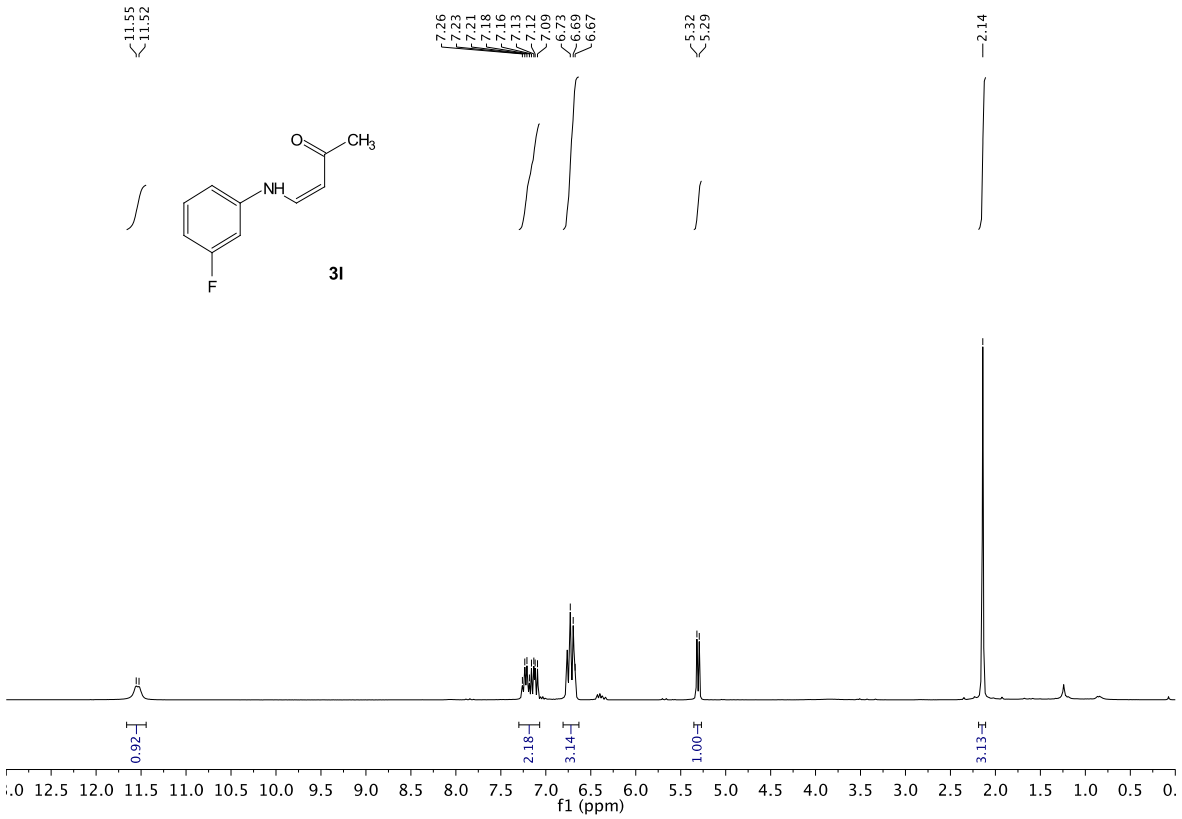
O
CH3
NH
F
F
3k
f1 (ppm)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7.26
7.23
7.21
7.18
7.16
7.13
7.12
7.09
6.73
6.69
6.67
5.32
5.29
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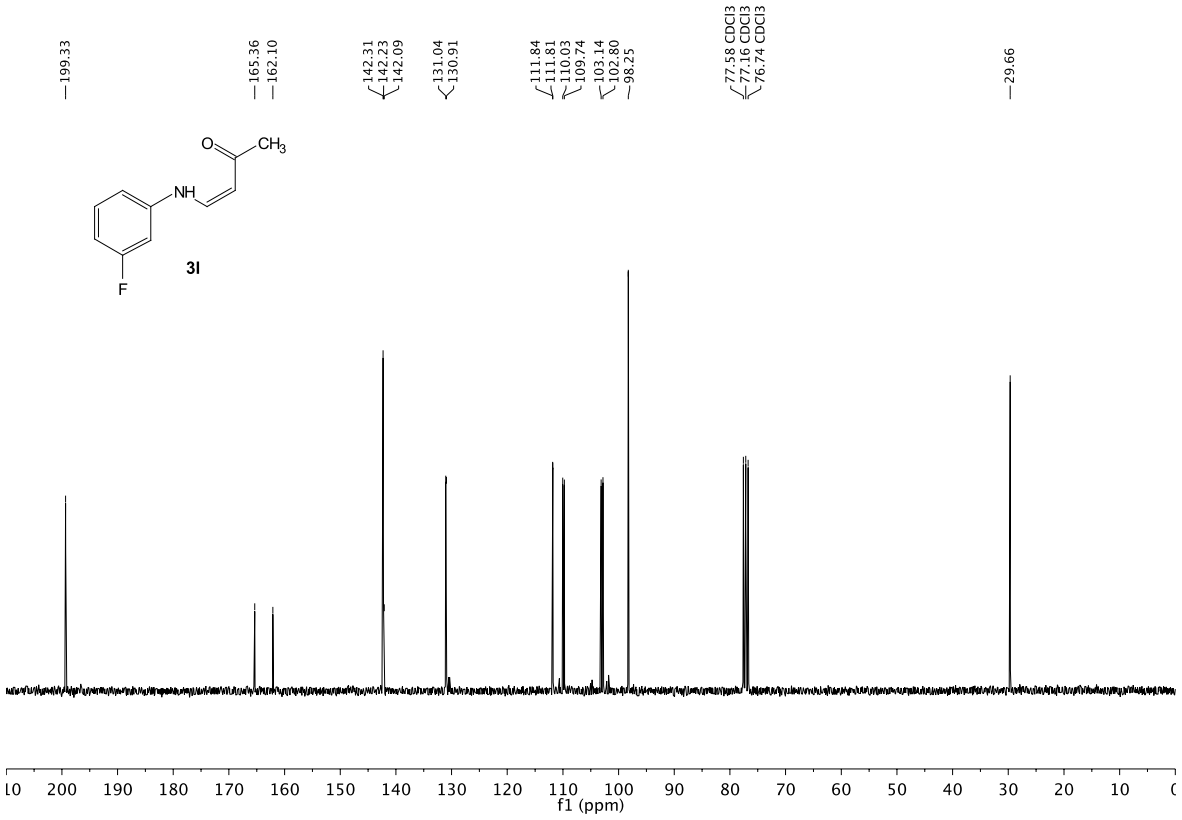
O
CH3
NH
F
3l
0.92
2.18
3.14
1.00
3.13
f1 (ppm)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142.23
142.09
131.04
130.91
111.84
111.81
110.03
109.74
103.14
102.80
98.25
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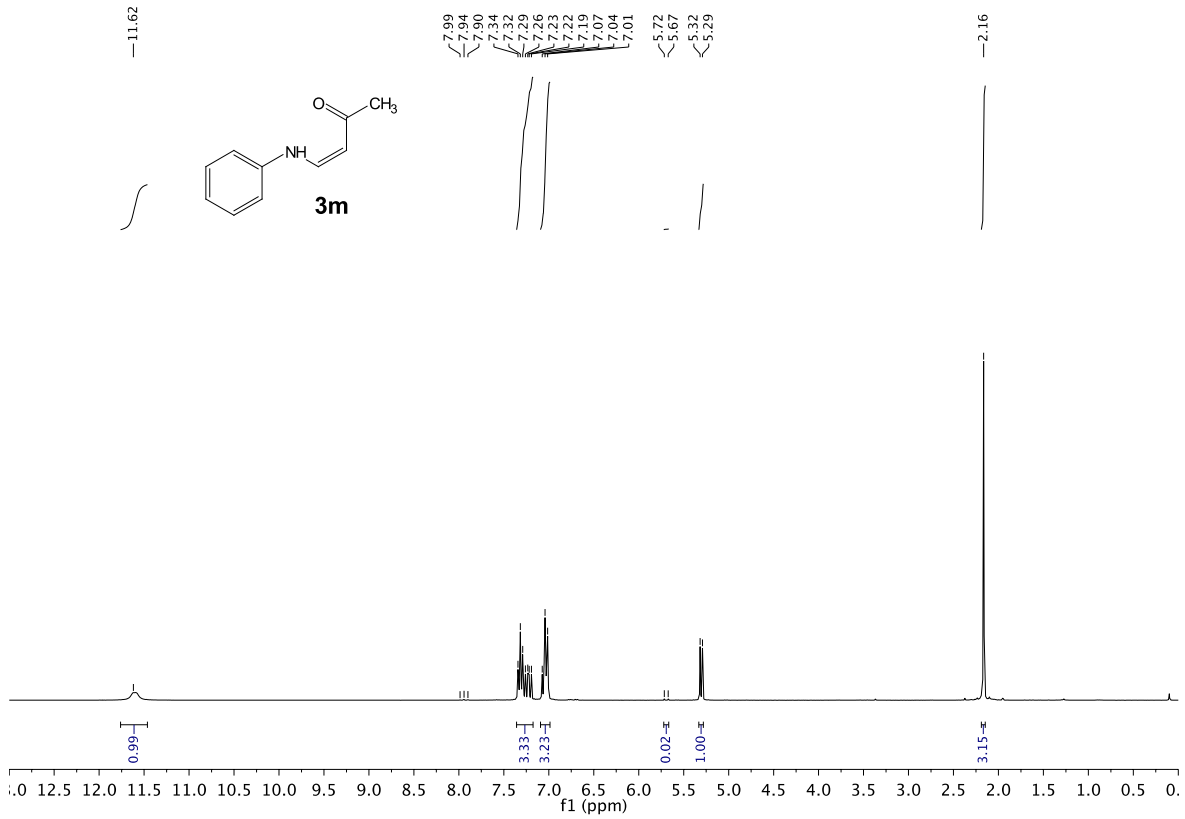
77.16 CDCl3
76.74 CDCl3
29.66
O
CH3
NH
F
3l
f1 (ppm)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7.26
7.23
7.22
7.19
7.07
7.04
7.01
5.72
5.67
5.32
5.29
2.16
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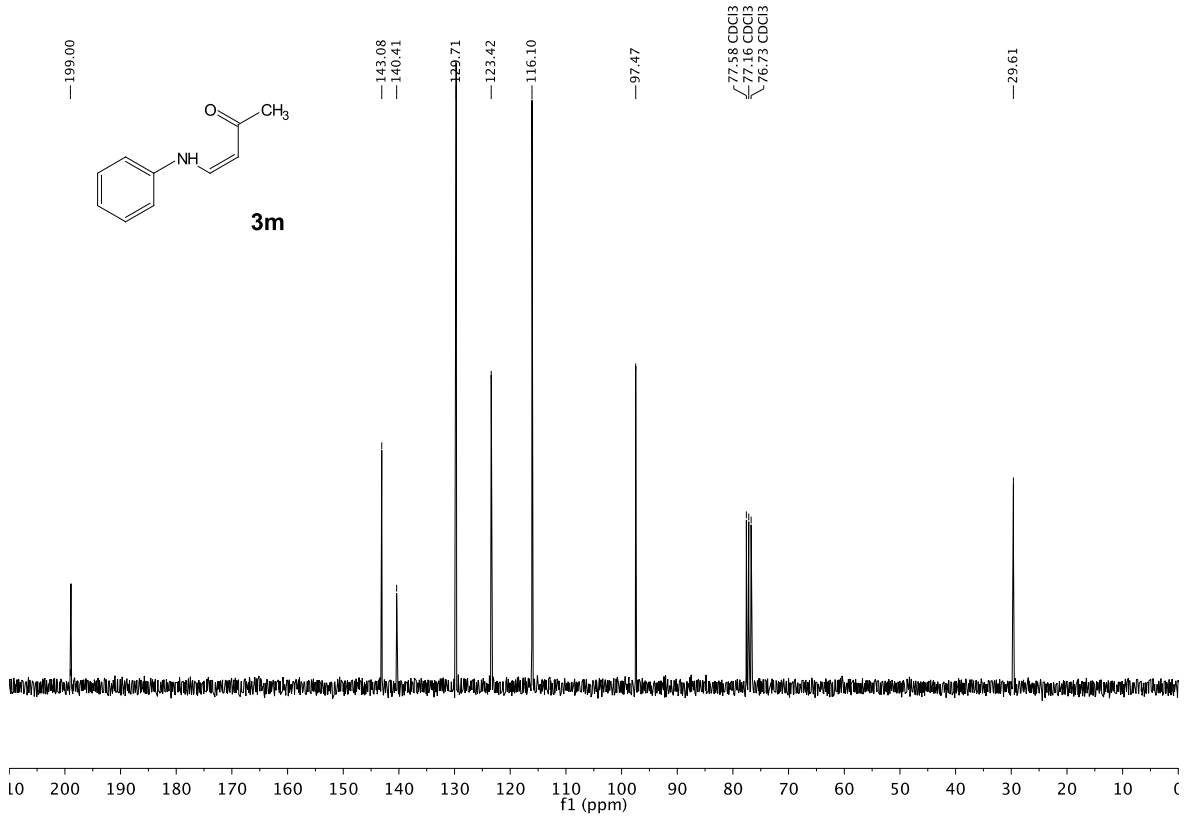
CH3
NH
3m
0.99
3.33
3.23
0.02
1.00
3.15
f1 (ppm)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123.42
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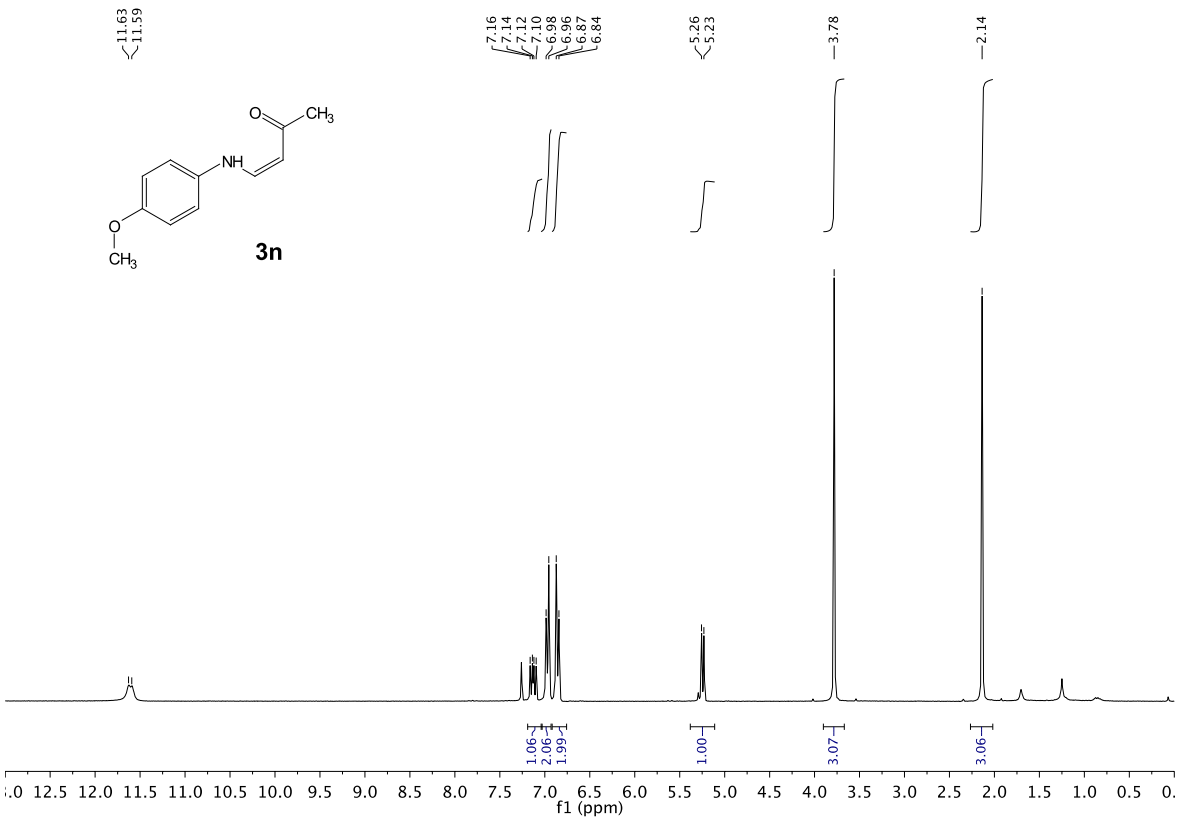
97.47
77.58 CDCl3
77.16 CDCl3
76.73 CDCl3
29.61
O
CH3
NH
3m
f1 (ppm)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7.12
7.10
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6.96
6.87
6.84
5.26
5.23
3.78
2.14
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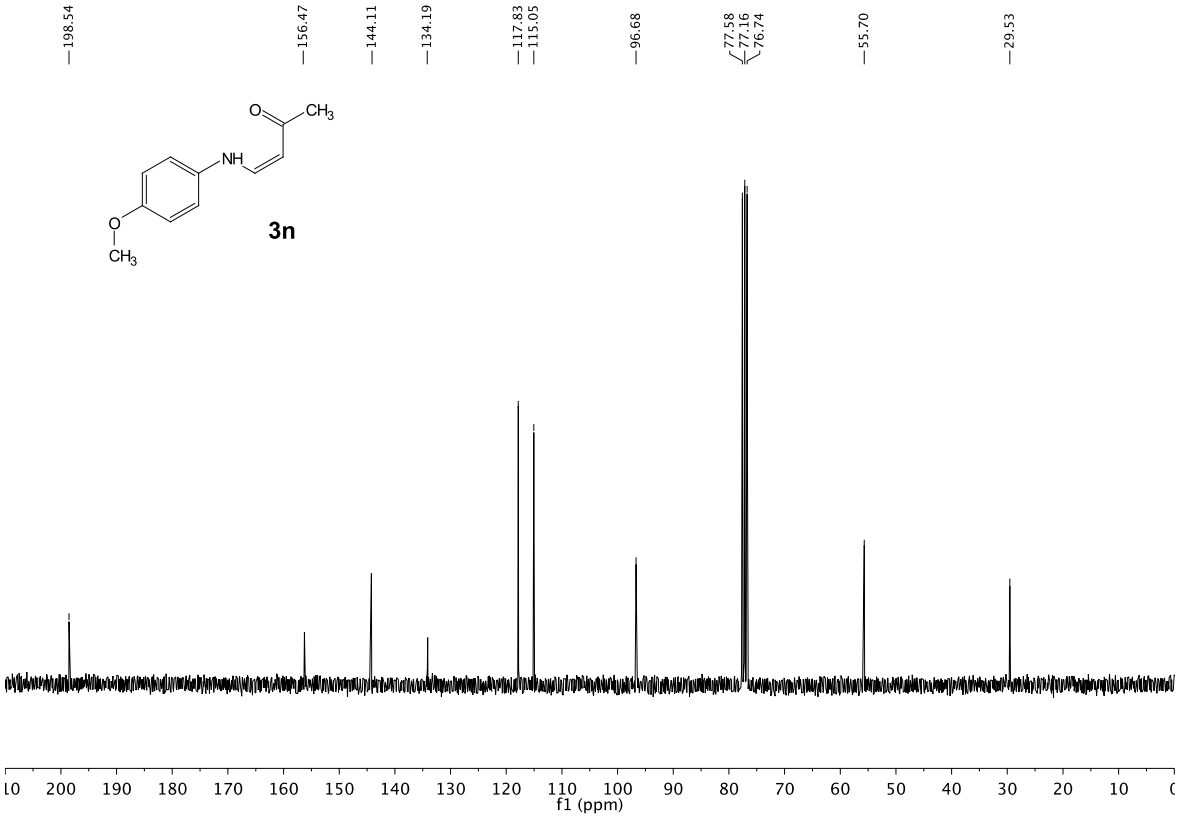
CH3
NH
O
CH3
3n
1.06
2.06
1.99
1.00
3.07
3.06
f1 (ppm)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77.16
76.74
55.70
29.53
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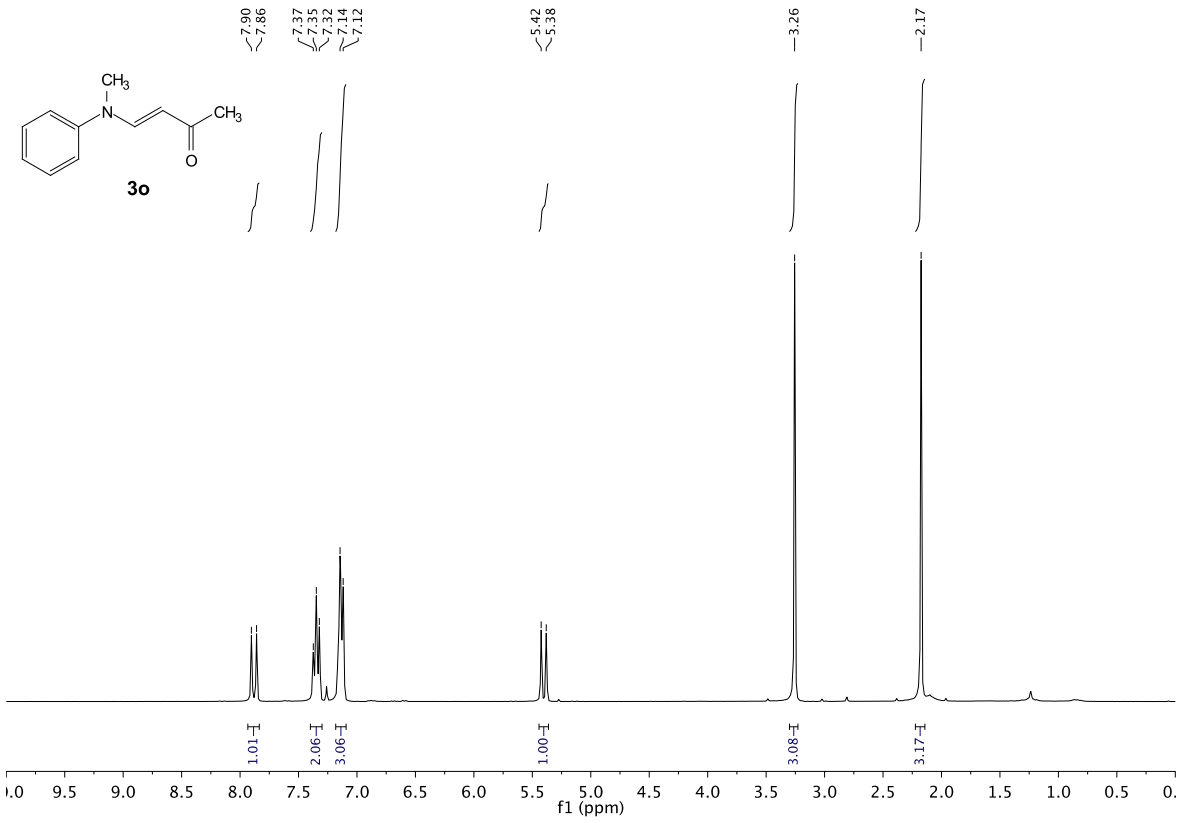
CH3
NH
O
CH3
3n
f1 (ppm)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7.14
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5.42
5.38
3.26
2.17
1.01
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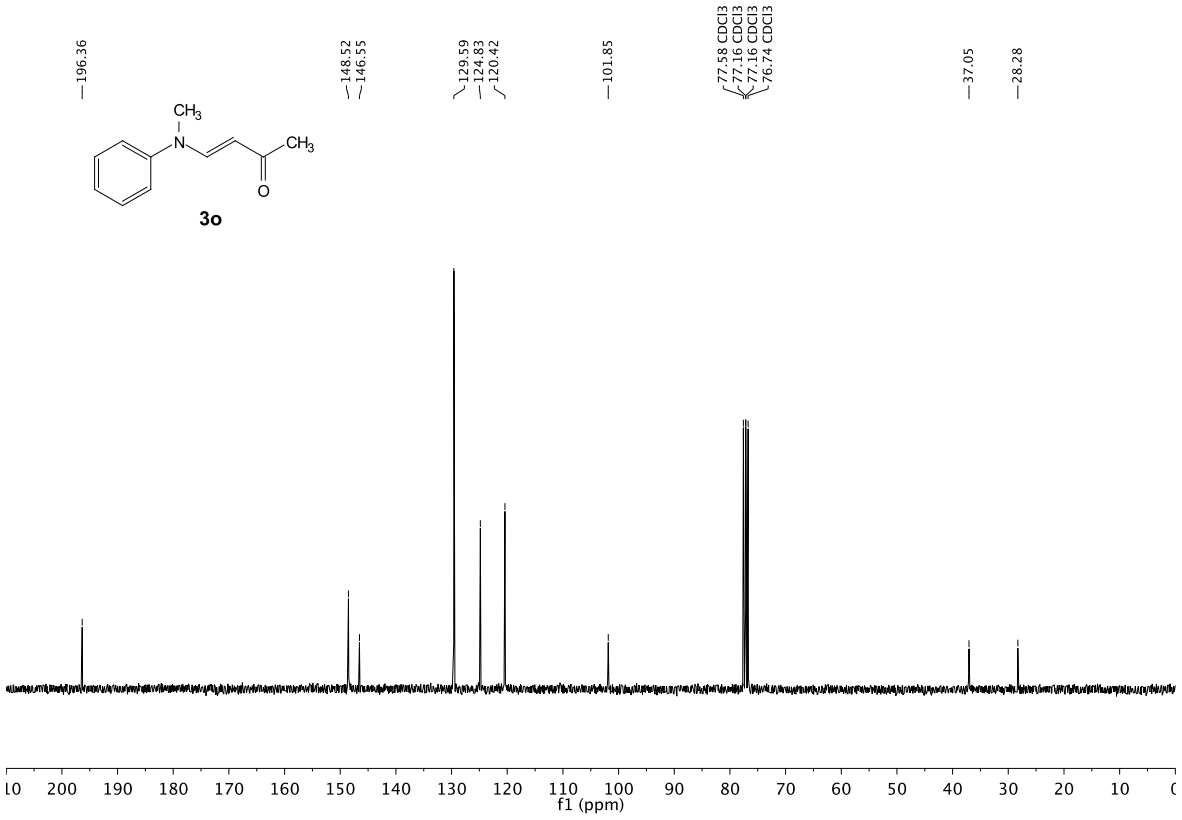
3.06
1.00
3.08
3.17
f1 (ppm)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146.55
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124.83
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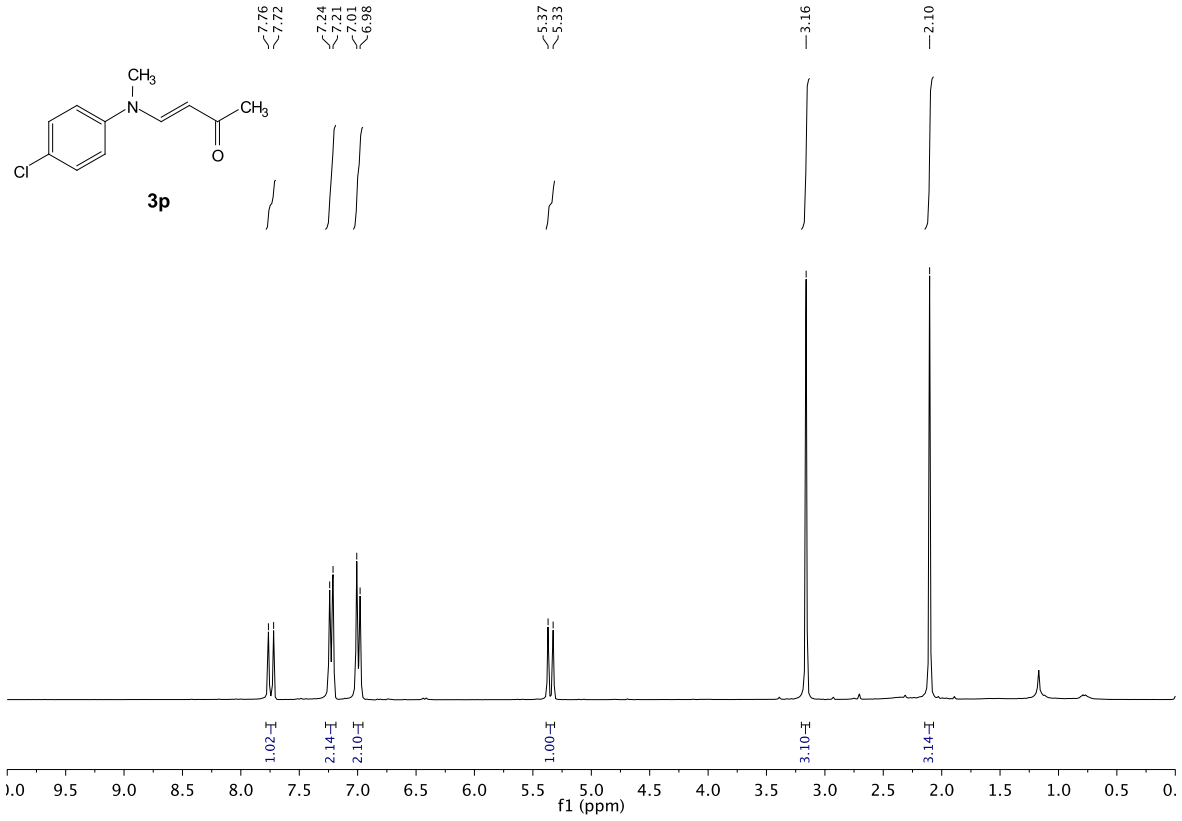
77.58 CDCl3
77.16 CDCl3
77.16 CDCl3
76.74 CDCl3
37.05
28.28
f1 (ppm)


7.76
7.72
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7.21
7.01
6.98
5.37
5.33
3.16
2.10
CH3
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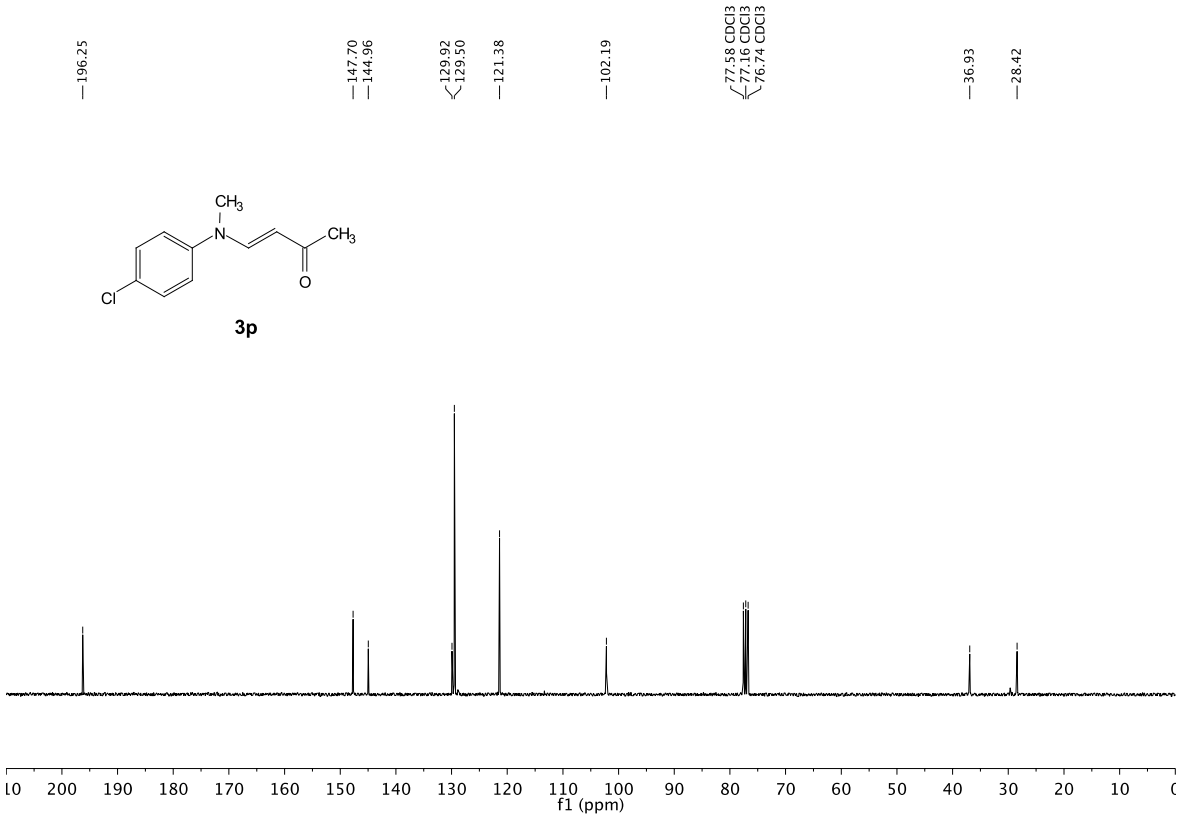
CH3
O
Cl
3p
1.02
2.14
2.10
1.00
3.10
3.14
f1 (ppm)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147.70
144.96
129.92
129.50
121.38
102.19
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
36.93
28.42
CH3
N
CH3
O
Cl
3p
f1 (ppm)