Supplementary Information

Direct allylation of aromatic and α,β-unsaturated carboxamides under ruthenium catalysis

Mirim Kim, Satyasheel Sharma, Neeraj Kumar Mishra, Sangil Han, Jihye Park, Minyoung Kim, Youngmi Shin, Jong Hwan Kwak, Sang Hoon Han and In Su Kim*

School of Pharmacy, Sungkyunkwan University, Suwon 440-746, Republic of Korea

* Corresponding author. Tel.: +82-31-290-7788; fax: +82-31-292-8800; e-mail: insukim@skku.edu

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General methods

Commercially available reagents were used without additional purification, unless otherwise stated. Sealed tubes (13 × 100 mm^2) were purchased from Fischer Scientific and dried in oven for overnight and cooled under a stream of nitrogen prior to use. Thin layer chromatography was carried out using plates coated with Kieselgel $60F_{254}$ (Merck). For flash column chromatography, E. Merck Kieselgel 60 (230-400 mesh) was used. Nuclear magnetic resonance spectra (^1H and ^{13}C NMR) were recorded on a Bruker Unity 500 MHz and 700 MHz spectrometer for $CDCl_3$ solutions and chemical shifts are reported as parts per million (ppm) relative to, respectively, residual $CHCl_3$ δ_H (7.24 ppm) and $CDCl_3$ δ_C (77.23 ppm) as internal standards. Resonance patterns are reported with the notations s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). In addition, the notation br is used to indicate a broad signal. Coupling constants (*J*) are reported in hertz (Hz). IR spectra were recorded on a Varian 2000 Infrared spectrophotometer and are reported as cm^{-1}. High-resolution mass spectra (HRMS) were recorded on a JEOL JMS-600 spectrometer.

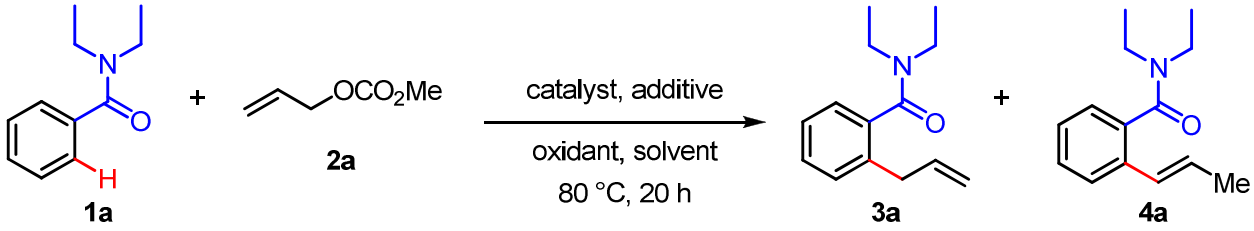
General procedure for the synthesis of amides

To a stirred suspension of carboxylic acid (1.0 equiv.) in dry CH_2Cl_2 (30 mL) was added thionyl chloride (1.5 equiv.) at 0 ^oC and stirred for 1 h at room temperature. To this reaction mixture Et_3N (3 equiv) was added followed by the addition of corresponding amine (1.2 equiv). The reaction mixture was then stirred at room temperature for overnight. The reaction mixture was washed with H_2O and extracted with EtOAc (50 mL). The organic layer was dried over Mg_2SO_4 and concentrated in vacuo. The residue was purified by flash column chromatography.

General procedure for the allylation of amides (3a–3u and 5b–5d)

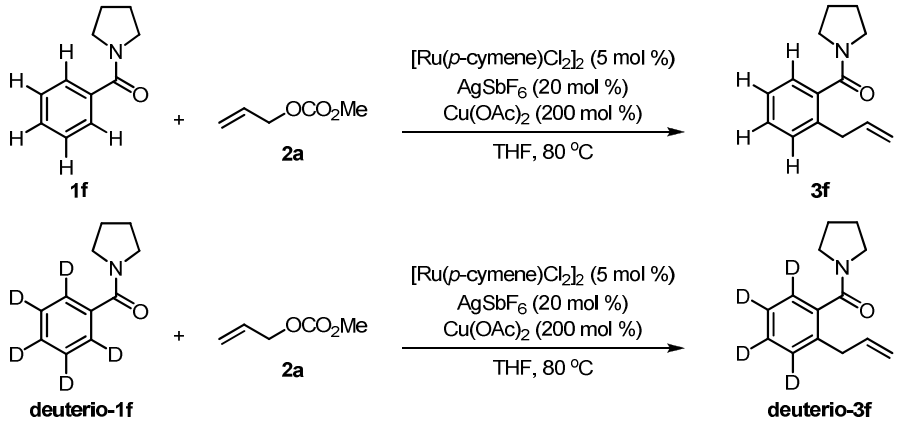
To an oven-dried sealed tube charged with *N*,*N*-diethylbenzamide (**1a**) (53.1 mg, 0.3 mmol, 1.0 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (9.2 mg, 5 mol %), $AgSbF_6$ (20.6 mg, 20 mol %), $Cu(OAc)_2$ (108 mg, 2 equiv.) in THF (1 mL) was added allyl methyl carbonate (**2a**) (69.6 mg, 0.6 mmol, 2 equiv.). The reaction mixture was allowed to stir at 80 °C for 20 h, and cooled to room temperature. The reaction mixture was diluted with EtOAc (3 mL) and concentrated in vacuo. The residue was purified by flash column chromatography (*n*-hexanes/EtOAc) to afford **3a** (35.8 mg) in 55% yield.

Selected optimization of the reaction conditions



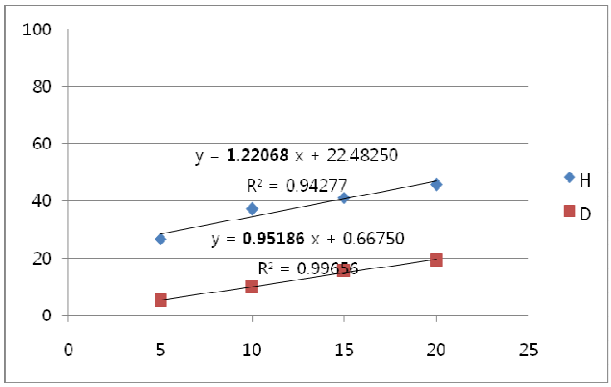
entry	catalyst (mol %)	oxidant (equiv)	additive (mol %)	solvent	yield (%) of (**3a:4a**)
1	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (2)	$AgSbF_6$ (20)	t-AmOH	30 (3:1)
2	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (2)	$AgSbF_6$ (20)	MeOH	traces
3	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (2)	$AgSbF_6$ (20)	MeCN	traces
4	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (2)	$AgSbF_6$ (20)	CH_2Cl_2	20 (4:1)
5	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (2)	$AgSbF_6$ (20)	diglyme	24 (4:1)
6	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (2)	$AgSbF_6$ (20)	DCE	28 (5:1)
7	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (2)	$AgSbF_6$ (20)	toluene	19 (2.4:1)
8	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (2)	$AgSbF_6$ (20)	DMSO	traces
9	**[Ru(*p*-cymene)Cl_2]$_2$ (5)**	**$Cu(OAc)_2$ (2)**	**$AgSbF_6$ (20)**	**THF**	**55 (4.5:1)**
10	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (1)	$AgSbF_6$ (20)	THF	47 (4.3:1)
11	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2$ (0.5)	$AgSbF_6$ (20)	THF	41 (4.2:1)
12	[Ru(*p*-cymene)Cl_2]$_2$ (5)		$AgSbF_6$ (20)	THF	traces
13	[Ru(*p*-cymene)Cl_2]$_2$ (5)	pivalic acid (2)	$AgSbF_6$ (20)	THF	26 (4:1)
14	[Ru(*p*-cymene)Cl_2]$_2$ (5)	CsOAc (2)	$AgSbF_6$ (20)	THF	traces
15	[Ru(*p*-cymene)Cl_2]$_2$ (5)	$Cu(OAc)_2 \cdot H_2O$ (2)	$AgSbF_6$ (20)	THF	42 (3:1)
16	[Ru(*p*-cymene)Cl_2]$_2$ (2.5)	$Cu(OAc)_2$ (2)	$AgSbF_6$ (10)	THF	38 (3.8:1)

Kinetic Isotope Effect (KIE) experiment

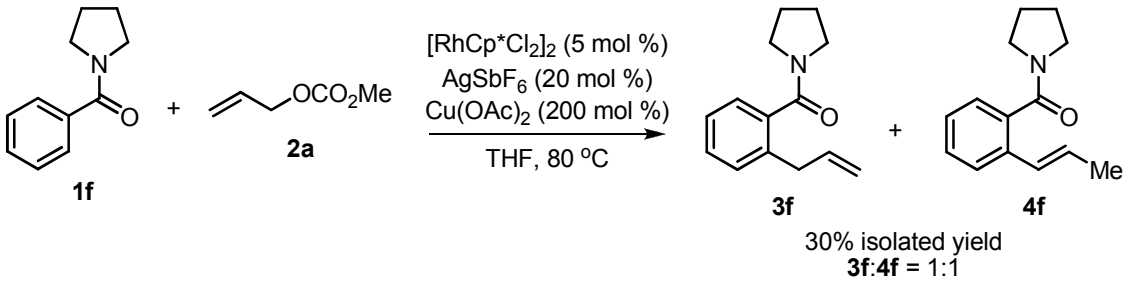


To an oven-dried sealed tube charged with phenyl(pyrrolidin-1-yl)methanone (**1f**) (52.5 mg, 0.3 mmol, 1.0 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (9.2 mg, 5 mol %), $AgSbF_6$ (20.6 mg, 20 mol %), $Cu(OAc)_2$ (108 mg, 2 equiv.) in THF (1 mL) was added allyl methyl carbonate (**2a**) (69.6 mg, 0.6 mmol, 2 equiv.) and tetradecane (59.5 mg, 0.3 mmol) as an internal standard. In another reaction tube, **deuterio-1f** (54.0 mg, 0.3 mmol, 1.0 equiv) was used instead of **1f**. The two reactions were allowed to stir at 80 °C. An aliquot of each reaction mixture was taken at the time of 5 min, 10 min, 15 min, and 20 min. The corresponding yield of each product was determined by GC-MS (tetradecane as an internal standard). A kinetic isotope effect value (k_H/k_D) of 1.28 was observed.

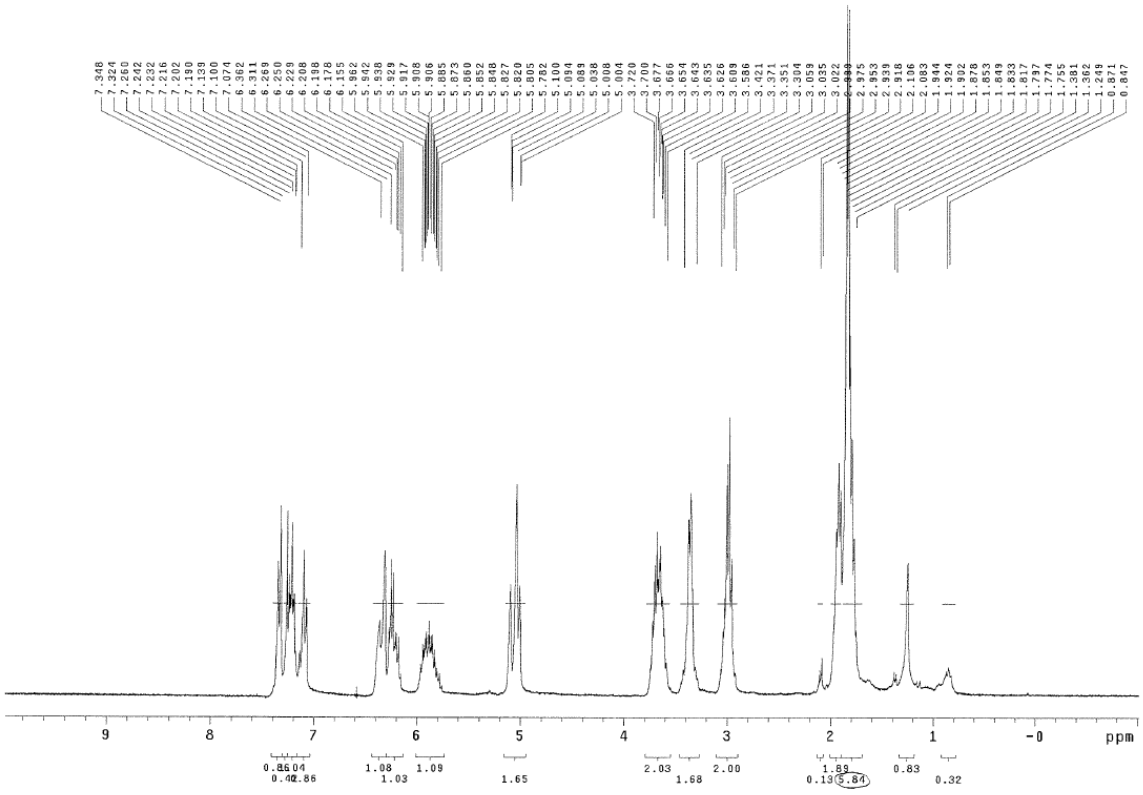
	Relative yield (%) based on tetradecane			
	5 min	10 min	15 min	20 min
3f (H)	26.75	37.246	41.187	45.781
deuterio-3f (D)	5.463	9.884	15.441	19.475


100
80
60
40
20
0
0
5
10
15
20
25
y = 1.22068 x + 22.48250
R² = 0.94277
y = 0.95186 x + 0.66750
H
D

Control experiment using rhodium catalyst

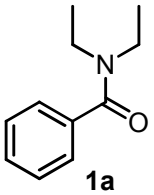


To an oven-dried sealed tube charged with phenyl(pyrrolidin-1-yl)methanone (**1f**) (52.5 mg, 0.3 mmol, 1.0 equiv.), $[RhCp^*Cl_2]_2$ (9.3 mg, 5 mol %), $AgSbF_6$ (20.6 mg, 20 mol %), $Cu(OAc)_2$ (108 mg, 2 equiv.) in THF (1 mL) was added allyl methyl carbonate (**2a**) (69.6 mg, 0.6 mmol, 2 equiv.). The reaction mixture was allowed to stir at 80 °C for 20 h, and cooled to room temperature. The reaction mixture was diluted with EtOAc (3 mL) and concentrated in vacuo. The residue was purified by flash column chromatography (*n*-hexanes/EtOAc) to afford a mixture of **3a** and **4f** in 30% yield with 1:1 ratio.



Characterization data for amides (1a–1u and 6a)

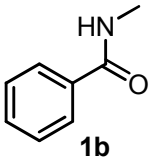
_N_,_N_-Diethylbenzamide (1a)[1]



1a

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.37–7.33 (m, 5H), 3.53 (br s, 2H), 3.22 (br s, 2H), 1.22 (br s, 3H), 1.08 (br s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 171.2, 137.3, 129.0, 128.3, 126.2, 43.2, 39.2, 14.2, 12.9.

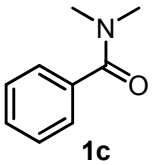
_N_-Methylbenzamide (1b)[2]



1b

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.76–7.75 (m, 2H), 7.47–7.45 (m, 1H), 7.40–7.38 (m, 2H), 6.44 (br s, 1H), 2.98 (d, J = 4.9 Hz, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 168.3, 134.6, 131.3, 128.5, 126.8, 26.8.

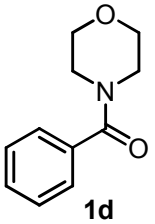
_N_,_N_-Dimethylbenzamide (1c)[1]



1c

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.39–7.35 (m, 5H), 3.09 (s, 3H), 2.95 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 171.6, 136.3, 129.4, 128.3, 127.0, 39.5, 35.3.

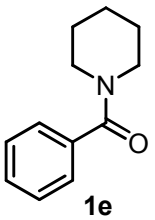
Morpholino(phenyl)methanone (1d)[3]



1d

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.42–7.37 (m, 5H), 3.76–3.43 (m, 8H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 170.4, 135.3, 129.8, 128.5, 127.1, 66.9, 48.2, 42.5.

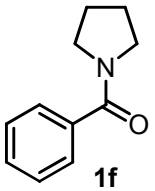
Phenyl(piperidin-1-yl)methanone (1e)[4]



1e

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.38–7.35 (m, 5H), 3.69 (br s, 2H), 3.32 (br s, 2H), 1.66–1.49 (m, 6H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 170.3, 136.5, 129.3, 128.4, 126.7, 48.7, 43.1, 26.5, 25.6, 24.6.

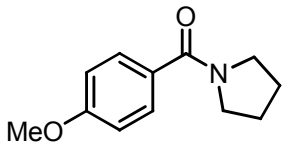
Phenyl(pyrrolidin-1-yl)methanone (1f)[4]



1f

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.41–7.40 (m, 2H), 7.29–7.27 (m, 3H), 3.53 (m, 2H), 3.31 (m, 2H), 1.85–1.83 (m, 2H), 1.76–1.74 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.6, 137.2, 129.6, 128.1, 127.0, 49.5, 46.1, 26.3, 24.3.

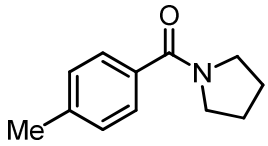
(4-Methoxyphenyl)(pyrrolidin-1-yl)methanone (1g)[4]



1g

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.44–7.43 (m, 2H), 6.82–6.80 (m, 2H), 3.74 (s, 3H), 3.54 (br s, 2H), 3.39 (br s, 2H), 1.85–1.78 (m, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.3, 160.7, 129.3, 129.1, 113.3, 55.2, 49.7, 46.2, 26.4, 24.4.

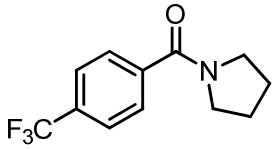
Pyrrolidin-1-yl(*p*-tolyl)methanone (1h)[5]



1h

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.38 (d, J = 7.9 Hz, 2H), 7.13 (d, J = 7.3 Hz, 2H), 3.58 (t, J = 6.4 Hz, 2H), 3.38 (t, J = 6.2 Hz, 2H), 2.32 (s, 3H), 1.90–1.88 (m, 2H), 1.81–1.80 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.7, 139.8, 134.3, 128.7, 127.1, 49.6, 46.1, 26.4, 24.4, 21.3.

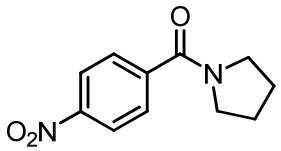
Pyrrolidin-1-yl(4-(trifluoromethyl)phenyl)methanone (1i)[4]



1i

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.61 (d, J = 8.1 Hz, 2H), 7.57 (d, J = 8.0 Hz, 2H), 3.60 (t, J = 7.0 Hz, 2H), 3.34 (t, J = 6.5 Hz, 2H), 1.94–1.90 (m, 2H), 1.86–1.82 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 168.2, 140.7, 131.4 (q, $J_{C\text{-}F}$ = 32.6 Hz), 127.4, 125.3 (q, $J_{C\text{-}F}$ = 4.3 Hz), 124.5 (q, $J_{C\text{-}F}$ = 270.7 Hz), 49.4, 46.2, 26.3, 24.3.

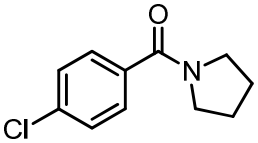
(4-Nitrophenyl)(pyrrolidin-1-yl)methanone (1j)[4]



1j

^{1}H NMR (700 MHz, $CDCl_3$) δ 8.25–8.23 (m, 2H), 7.67–7.65 (m, 2H), 3.64 (t, J = 7.0 Hz, 2H), 3.36 (t, J = 6.6 Hz, 2H), 1.99–1.95 (m, 2H), 1.92–1.88 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 167.3, 148.4, 143.1, 128.1, 123.6, 49.4, 46.3, 26.3, 24.3.

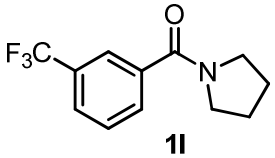
(4-Chlorophenyl)(pyrrolidin-1-yl)methanone (1k)[5]



1k

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.46–7.44 (m, 2H), 7.36–7.34 (m, 2H), 3.61 (t, J = 7.0 Hz, 2H), 3.39 (t, J = 6.6 Hz, 2H), 1.96–1.92 (m, 2H), 1.88–1.84 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 168.5, 135.8, 135.5, 128.6, 128.5, 49.6, 46.2, 26.4, 24.4.

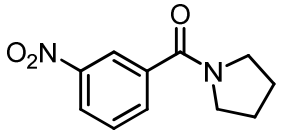
Pyrrolidin-1-yl(3-(trifluoromethyl)phenyl)methanone (1l)



1l

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.69 (d, J = 7.7 Hz, 1H), 7.65 (d, J = 7.2 Hz , 1H), 7.52 (t, J = 7.7 Hz, 1H), 3.64 (t, J = 7.0 Hz, 2H), 3.39 (t, J = 6.6 Hz, 2H), 1.98–1.94 (m, 2H), 1.90–1.87 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 168.0, 137.9, 130.6 (q, $J_{C\text{-}F}$ = 32.1 Hz), 128.9, 126.4 (q, $J_{C\text{-}F}$ = 3.0 Hz), 124.5 (q, $J_{C\text{-}F}$ = 270.7 Hz), 124.1 (q, $J_{C\text{-}F}$ = 4.1 Hz), 49.5, 46.3, 26.4, 24.4; IR (KBr) υ 2974, 2877, 2191, 2620, 1565, 1428, 1399, 1340, 1265, 1203, 1155, 1079, 889, 800, 730 cm^{-1}; HRMS (EI) calcd for $C_{12}H_{12}F_3NO$ $[M]^+$ 243.0871, found 243.0875.

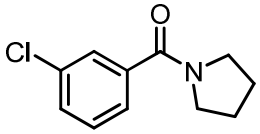
(3-Nitrophenyl)(pyrrolidin-1-yl)methanone (1m)[6]



1m

^{1}H NMR (700 MHz, $CDCl_3$) δ 8.30–8.27 (m, 1H), 8.19–8.15 (m, 1H), 7.80–7.77 (m, 1H), 7.55–7.51 (m, 1H), 3.62–3.57 (m, 2H), 3.41–3.37 (m, 2H), 1.93–1.82 (m, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 166.8, 147.8, 138.6, 133.1, 129.6, 124.4, 122.2, 49.5, 46.4, 26.3, 24.3.

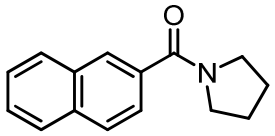
(3-Chlorophenyl)(pyrrolidin-1-yl)methanone (1n)



1n

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.35–7.33 (m, 2H), 7.29 (t, *J* = 7.6 Hz, 1H), 3.59 (t, *J* = 7.0 Hz, 2H), 3.36 (t, *J* = 6.7 Hz, 2H), 1.94–1.90 (m, 2H), 1.86–1.82 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 168.0, 138.9, 134.2, 129.8, 129.6, 127.3, 125.1, 49.5, 46.2, 26.3, 24.4; IR (KBr) υ 2972, 2876, 2162, 1620, 1564, 1476, 1426, 1400, 1339, 1202, 1157, 1078, 916, 888, 800, 768, 741 cm^{-1}; HRMS (EI) calcd for $C_{11}H_{12}ClNO$ $[M]^+$ 209.0607, found 209.0608.

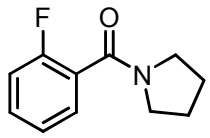
Naphthalen-2-yl(pyrrolidin-1-yl)methanone (1o)[5]



1o

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.79–7.76 (m, 3H), 7.55 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.46–7.42 (m, 2H), 3.63 (t, *J* = 6.5 Hz, 2H), 3.38 (br s, 2H), 1.88 (br s, 2H), 1.77 (br s, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.6, 134.5, 133.7, 132.5, 128.4, 128.0, 127.7, 127.0, 126.9, 126.5, 124.4, 49.6, 46.2, 26.4, 24.4.

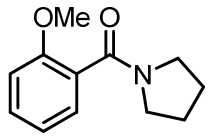
(2-Fluorophenyl)(pyrrolidin-1-yl)methanone (1p)



1p

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.39–7.32 (m, 2H), 7.15 (t, J = 7.5 Hz, 1H), 7.05 (t, J = 8.9 Hz, 1H), 3.61 (t, J = 7.0 Hz, 2H), 3.27 (t, J = 6.7 Hz, 2H), 1.95–1.91 (m, 2H), 1.87–1.83 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 165.1, 157.5 (d, $J_{C\text{-}F}$ = 245.5 Hz), 131.1 (d, $J_{C\text{-}F}$ = 8.6 Hz), 128.8 (d, $J_{C\text{-}F}$ = 3.0 Hz), 125.7 (d, $J_{C\text{-}F}$ = 17.8 Hz), 124.4 (d, $J_{C\text{-}F}$ = 13.6 Hz), 115.8 (d, $J_{C\text{-}F}$ = 22.0 Hz), 47.8, 45.8, 25.8, 24.5; IR (KBr) υ 2975, 2879, 2151, 2040, 1626, 1484, 1453, 1421, 1340, 1268, 1222, 1157, 1098, 1027, 908, 817, 754, 730 cm^{-1}; HRMS (EI) calcd for $C_{11}H_{12}FO$ $[M]^+$ 193.0903, found 193.0902.

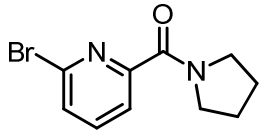
(2-Methoxyphenyl)(pyrrolidin-1-yl)methanone (1q)[7]



1q

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.07–7.05 (m, 1H), 7.00 (dd, J = 7.4, 1.7 Hz, 1H), 6.70 (t, J = 7.4 Hz, 1H), 6.67 (d, J = 8.4 Hz, 1H), 3.55 (s, 3H), 3.36 (t, J = 6.9 Hz, 2H), 2.95 (t, J = 6.6 Hz, 2H), 1.68–1.64 (m, 2H), 1.60–1.56 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 167.4, 155.0, 130.1, 127.4, 127.2, 120.5, 110.9, 55.3, 47.4, 45.2, 25.6, 24.3.

(6-Bromopyridin-2-yl)(pyrrolidin-1-yl)methanone (1r)

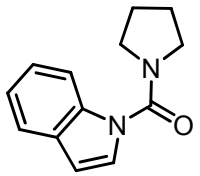


1r

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.87–7.85 (m, 1H), 7.67 (t, J = 7.7 Hz, 1H), 7.55–7.54 (m,

1H), 3.80 (t, *J* = 6.6 Hz, 2H), 3.68 (t, *J* = 6.3 Hz, 2H), 1.97–1.93 (m, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 164.4, 154.9, 140.0, 139.1, 129.2, 123.0, 49.1, 47.1, 26.7, 23.9; IR (KBr) υ 2971, 2877, 2038, 1622, 1549, 1452, 1402, 1337, 1265, 1156, 1119, 1075, 986, 813, 754 cm^{-1}; HRMS (EI) calcd for $C_{10}H_{11}BrN_2O$ $[M]^+$ 254.0055, found 254.0053.

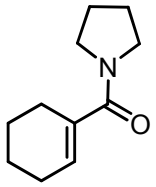
(1*H*-Indol-1-yl)(pyrrolidin-1-yl)methanone (1s)[8]



1s

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.3 Hz, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 3.4 Hz, 1H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 6.56 (s, 1H), 3.53 (br s, 4H), 1.84 (br s, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 153.2, 135.7, 129.2, 125.5, 123.4, 121.7, 120.8, 114.2, 105.4, 48.6, 25.4.

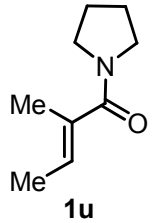
Cyclohexenyl(pyrrolidin-1-yl)methanone (1t)[9]



1t

^{1}H NMR (700 MHz, $CDCl_3$) δ 5.92–5.90 (m, 1H), 3.47–3.43 (m, 4H), 2.23–2.20 (m, 2H), 2.10–2.07 (m, 2H), 1.88–1.83 (m, 4H), 1.68–1.64 (m, 2H), 1.63–1.58 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 171.2, 135.7, 128.5, 48.7, 45.5, 26.2, 25.3, 24.8, 24.4, 22.1, 21.7.

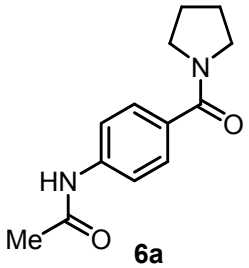
(*E*)-2-Methyl-1-(pyrrolidin-1-yl)but-2-en-1-one (1u)



1u

^{1}H NMR (700 MHz, $CDCl_3$) δ 5.64–5.60 (m, 1H), 3.34–3.31 (m, 4H), 1.75–1.71 (m, 7H), 1.58–1.57 (m, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 171.9, 133.5, 126.2, 48.6, 45.4, 26.1, 24.3, 13.4, 13.1; IR (KBr) υ 2972, 2874, 2057, 1659, 1606, 1418, 1340, 1163, 1037, 913, 837, 730 cm^{-1}; HRMS (EI) calcd for $C_9H_{15}NO$ $[M]^+$ 153.1154, found 153.1152.

***N*-(4-(Pyrrolidine-1-carbonyl)phenyl)acetamide (6a)**

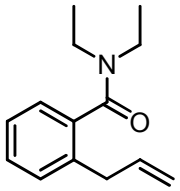


6a

^{1}H NMR (700 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.42 (t, *J* = 8.4 Hz, 2H), 3.62 (t, *J* = 6.9 Hz, 2H), 3.45–3.40 (m, 2H), 2.15 (s, 3H), 1.96–1.93 (m, 2H). 1.87–1.84 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.4, 168.9, 139.8, 132.1, 128.1, 119.2, 49.7, 46.3, 26.4, 24.4, 22.4; IR (KBr) υ 3245, 2973, 2878, 1695, 1602, 1526, 1435, 1310, 1258, 1175, 852 cm^{-1}; HRMS (EI) calcd for $C_{13}H_{16}N_2O_2$ $[M]^+$ 232.1212, found 232.1214.

Characterization data for the allylation of amides (3a–3u, 5b–5d and 7a–7b)

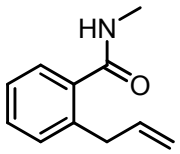
2-Allyl-*N*,*N*-diethylbenzamide (3a)[10]



3a

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.33–7.31 (m, 1H), 7.29–7.26 (m, 1H), 7.25–7.23 (m, 1H), 7.19–7.17 (m, 1H), 5.95 (ddt, *J* = 16.9, 10.0, 6.7 Hz, 1H), 5.12–5.07 (m, 2H), 3.41 (d, *J* = 6.3 Hz, 3H), 3.13–3.10 (m, 2H), 1.30–1.27 (m, 4H), 1.07–1.03 (m, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 170.6, 136.8, 136.5, 136.2, 135.4, 129.6, 128.6, 127.6, 125.9, 116.2, 42.9, 38.6, 37.1, 13.8, 12.8; IR (KBr) υ 2972, 2927, 2191, 2015, 1627, 1427, 1287, 1086, 914, 755 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{19}NO$ $[M]^+$ 217.1467, found 217.1468.

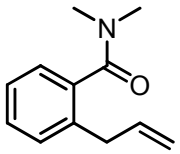
2-Allyl-*N*-methylbenzamide (3b)[11]



3b

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.36–7.32 (m, 2H), 7.22–7.19 (m, 2H), 5.99 (ddt, *J* = 17.0, 10.1, 6.3 Hz, 1H), 5.93 (br s, 1H), 5.05 (dq, *J* = 10.0, 1.4 Hz, 1H), 4.99 (dq, *J* = 17.0, 1.7 Hz, 1H), 3.53–3.52 (m, 2H), 2.92 (d, *J* = 4.9 Hz, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 170.5, 137.6, 137.5, 136.5, 130.4, 129.9, 127.2, 126.3, 115.9, 37.5, 26.5; IR (KBr) υ 3282, 3070, 2922, 2236, 2196, 2015, 1633, 1533, 1441, 1406, 1309, 1157, 996, 911, 745 cm^{-1}; HRMS (EI) calcd for $C_{11}H_{13}NO$ $[M]^+$ 175.0997, found 175.0990.

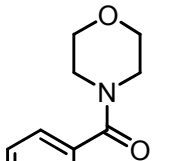
2-Allyl-*N*,*N*-dimethylbenzamide (3c)



3c

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.33–7.30 (m, 1H), 7.29–7.22 (m, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 5.92 (ddt, *J* = 16.9, 10.0, 6.7 Hz, 1H), 5.09–5.05 (m, 2H), 3.41 (br s, 2H), 3.12 (s, 1H), 2.82 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 171.3, 136.6, 136.5, 136.4, 129.8, 128.9, 126.3, 126.0, 116.1, 38.8, 37.3, 34.6; IR (KBr) υ 2925, 2348, 2154, 1982, 1628, 1503, 1441, 1390, 1264, 1187, 1065, 995, 915, 748 cm^{-1}; HRMS (EI) calcd for $C_{12}H_{15}NO$ $[M]^+$ 189.1154, found 189.1158.

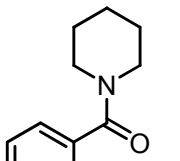
(2-Allylphenyl)(morpholino)methanone (3d)



3d

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.30–7.27 (m, 1H), 7.26–7.19 (m, 2H), 7.15–7.12 (m, 1H), 5.88 (ddt, *J* = 16.8, 10.0, 6.8 Hz, 1H), 5.05–5.04 (m, 2H), 3.84–3.73 (m, 4H), 3.53–3.14 (m, 6H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.8, 136.8, 136.5, 135.4, 130.1, 129.2, 126.3, 126.1, 116.4, 66.9, 66.8, 47.5, 41.9, 37.2; IR (KBr) υ 2913, 2852, 2330, 2186, 1985, 1629, 1424, 1361, 1275, 1254, 1111, 1012, 915, 843, 747 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{17}NO_2$ $[M]^+$ 231.1259, found 231.1264.

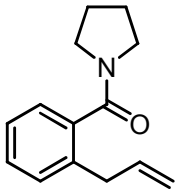
(2-Allylphenyl)(piperidin-1-yl)methanone (3e)



3e

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.28–7.25 (m, 1H), 7.22 (d, *J* = 7.7 Hz, 1H), 7.20–7.17 (m, 1H), 7.14–7.12 (m, 1H), 5.91 (ddt, *J* = 16.8, 10.0, 6.9 Hz, 1H), 5.06–5.03 (m, 2H), 3.84–3.82 (m, 1H), 3.59–3.57 (m, 1H), 3.44–3.40 (m, 1H), 3.36–3.33 (m, 1H), 3.19–3.15 (m, 1H), 3.11–3.07 (m, 1H), 1.66–1.59 (m, 6H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.6, 136.6, 136.5, 136.4, 129.7, 128.7, 126.2, 125.8, 116.2, 48.1, 42.3, 37.2, 26.3, 25.6, 24.5; IR (KBr) υ 2927, 2853, 2338, 2188, 1983, 1626, 1429, 1272, 1120, 997, 912, 852, 746 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{19}NO$ $[M]^+$ 229.1467, found 229.1470.

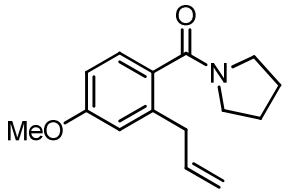
(2-Allylphenyl)(pyrrolidin-1-yl)methanone (3f)



3f

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.32–7.29 (m, 1H), 7.26–7.20 (m, 3H), 5.92 (ddt, *J* = 16.9, 10.0, 6.8 Hz, 1H), 5.08–5.02 (m, 2H), 3.63 (t, *J* = 7.0 Hz, 2H), 3.44 (d, *J* = 6.8 Hz, 2H), 3.14 (t, *J* = 6.7 Hz, 2H), 1.96–1.92 (m, 2H), 1.85–1.81 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.6, 137.6, 136.7, 136.2, 129.8, 128.9, 126.3, 125.9, 115.9, 48.7, 45.4, 37.4, 25.9, 24.5; IR (KBr) υ 2971, 2874, 2329, 2157, 1977, 1622, 1416, 1338, 1251, 1187, 1111, 994, 911, 730 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{17}NO$ $[M]^+$ 215.1310, found 215.1306.

(2-Allyl-4-methoxyphenyl)(pyrrolidin-1-yl)methanone (3g)

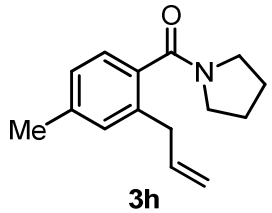


3g

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.14 (d, *J* = 8.4 Hz, 1H), 6.77 (d, *J* = 2.5 Hz, 1H), 6.74 (dd, *J* = 8.3, 2.5 Hz, 1H), 5.90 (ddt, *J* = 16.9, 10.0, 6.8 Hz, 1H), 5.08–5.01 (m, 2H), 3.79 (s, 3H), 3.60

(t, J = 7.0 Hz, 2H), 3.42 (d, J = 6.8 Hz, 2H), 3.15 (t, J = 6.7 Hz, 2H), 1.95–1.91 (m, 2H), 1.83–1.79 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.8, 159.8, 138.4, 136.6, 130.2, 127.4, 116.0, 115.3, 111.4, 55.2, 48.8, 45.4, 37.5, 26.0, 24.6; IR (KBr) υ 2967, 2874, 2157, 1982, 1603, 1500, 1414, 1283, 1242, 1161, 1033, 910 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{19}NO_2$ $[M]^+$ 245.1416, found 245.1412.

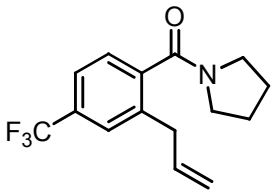
(2-Allyl-4-methylphenyl)(pyrrolidin-1-yl)methanone (3h)



3h

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.07 (d, J = 7.7 Hz, 1H), 7.02 (br s, 1H), 7.00 (d, J = 7.6 Hz, 1H), 5.87 (ddt, J = 16.9, 10.0, 6.8 Hz, 1H), 5.05–4.97 (m, 2H), 3.58 (t, J = 7.2 Hz, 2H), 3.37 (d, J = 6.7 Hz, 2H), 3.11 (t, J = 6.7 Hz, 2H), 2.30 (s, 3H), 1.92–1.88 (m, 2H), 1.80–1.76 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.9, 138.7, 136.9, 136.2, 134.8, 130.5, 126.9, 125.9, 115.7, 48.7, 45.4, 37.4, 25.9, 24.5, 21.2; IR (KBr) υ 2969, 2873, 2186, 2155, 1982, 1624, 1503, 1414, 1338, 1228, 1165, 994, 910, 820, 729 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{19}NO$ $[M]^+$ 229.1467, found 229.1467.

(2-Allyl-4-(trifluoromethyl)phenyl)(pyrrolidin-1-yl)methanone (3i)

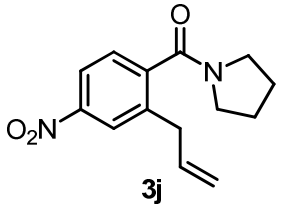


3i

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.53–7.45 (m, 2H), 7.31 (d, J = 7.8 Hz, 1H), 5.88 (ddt, J = 16.9, 10.0, 6.8 Hz, 1H), 5.12–5.06 (m, 2H), 3.64 (t, J = 7.0 Hz, 2H), 3.47 (d, J = 6.7 Hz, 2H), 3.08 (t, J = 6.7 Hz, 2H), 1.96–1.92 (m, 2H), 1.88–1.82 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 168.2, 141.0, 137.5, 135.5, 131.1 (q, $J_{C\text{-}F}$ = 32.2 Hz), 126.7 (q, $J_{C\text{-}F}$ = 4.0 Hz), 126.4, 124.6 (q, $J_{C\text{-}}$

$_F$ = 270.8 Hz), 123.3 (q, J_{C-F} = 4.2 Hz), 117.0, 48.6, 45.5, 37.2, 25.9, 24.5; IR (KBr) υ 2976, 2878, 2187, 2155, 1984, 1628, 1505, 1427, 1328, 1281, 1161, 1118, 1070, 994, 913, 833, 739 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{16}F_3NO$ $[M]^+$ 283.1184, found 283.1181.

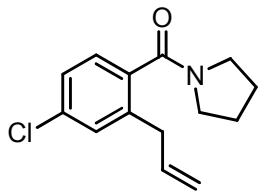
(2-Allyl-4-nitrophenyl)(pyrrolidin-1-yl)methanone (3j)



3j

^{1}H NMR (700 MHz, $CDCl_3$) δ 8.10 (d, *J* = 2.0 Hz, 1H), 8.06 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.36 (d, *J* = 8.3 Hz, 1H), 5.86 (ddt, *J* = 16.4, 10.2, 6.8 Hz, 1H), 5.12–5.09 (m, 2H), 3.61 (t, *J* = 7.1 Hz, 2H), 3.48 (d, *J* = 6.7 Hz, 2H), 3.08 (t, *J* = 6.7 Hz, 2H), 1.97–1.92 (m, 2H), 1.87–1.82 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 167.3, 148.0, 143.5, 138.8, 134.9, 127.1, 124.8, 121.6, 117.6, 48.5, 45.6, 37.1, 25.9, 24.4; IR (KBr) υ 2961, 2873, 2344, 2186, 2152, 1982, 1871, 1635, 1522, 1442, 1346, 1201 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{16}N_2O_3$ $[M]^+$ 260.1161, found 260.1165.

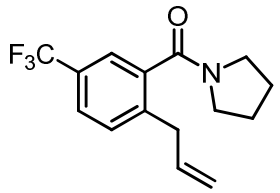
(2-Allyl-4-chlorophenyl)(pyrrolidin-1-yl)methanone (3k)



3k

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.22 (d, *J* = 1.9 Hz, 1H), 7.18 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 1H), 5.84 (ddt, *J* = 17.0, 10.0, 6.7 Hz, 1H), 5.07–5.02 (m, 2H), 3.58 (t, *J* = 7.0 Hz, 2H), 3.37 (d, *J* = 6.8 Hz, 2H), 3.09 (t, *J* = 6.7 Hz, 2H), 1.93–1.89 (m, 2H), 1.82–1.78 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 168.6, 138.5, 135.9, 135.7, 134.6, 129.9, 127.3, 126.5, 116.7, 48.7, 45.5, 37.9, 25.9, 24.5; IR (KBr) υ 2970, 2875, 2344, 2156, 1982, 1624, 1591, 1419, 1338, 1226, 1151, 1106, 994, 911, 864, 822, 766 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{16}ClNO$ $[M]^+$ 249.0920, found 249.0921.

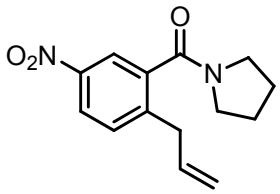
(2-Allyl-5-(trifluoromethyl)phenyl)(pyrrolidin-1-yl)methanone (3l)



3l

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 1H), 7.45 (br s, 1H), 7.36 (d, *J* = 8.0 Hz , 1H), 5.86 (ddt, *J* = 16.8, 10.0, 6.8 Hz, 1H), 5.08–5.04 (m, 2H), 3.61 (t, *J* = 7.0 Hz, 2H), 3.46 (d, *J* = 6.7 Hz, 2H), 3.10 (t, *J* = 6.7 Hz, 2H), 1.95–1.91 (m, 2H), 1.85–1.81 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 168.0, 140.6, 138.1, 135.5, 128.7 (q, $J_{C\text{-}F}$ = 32.7 Hz), 125.7 (q, $J_{C\text{-}F}$ = 3.7 Hz), 125.3 (q, $J_{C\text{-}F}$ = 272.1 Hz), 124.6, 123.0 (q, $J_{C\text{-}F}$ = 3.2 Hz), 116.9, 48.7, 45.5, 37.2, 25.9, 24.4; IR (KBr) υ 2975, 2879, 2185, 2155, 1986, 1630, 1442, 1399, 1324, 1273, 1167, 1118, 1074, 994, 908, 842, 735 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{16}F_3NO$ $[M]^+$ 283.1184, found 283.1185.

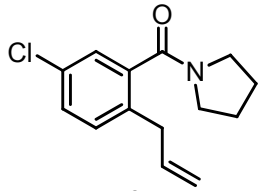
(2-Allyl-5-nitrophenyl)(pyrrolidin-1-yl)methanone (3m)



3m

^{1}H NMR (700 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 8.4, 2.3 Hz, 1H), 8.00 (d, *J* = 2.3 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 5.86 (ddt, *J* = 16.4, 10.6, 6.7 Hz, 1H), 5.10–5.08 (m, 2H), 3.63 (t, *J* = 7.1 Hz, 2H), 3.52 (d, *J* = 6.7 Hz, 2H), 3.14 (t, *J* = 6.7 Hz, 2H), 1.98–1.94 (m, 2H), 1.88–1.84 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 166.9, 146.2, 144.4, 138.6, 134.8, 131.0, 123.8, 121.4, 117.5, 48.8, 45.7, 37.3, 26.0, 24.4; IR (KBr) υ 2971, 2876, 2344, 2155, 1986, 1627, 1520, 1435, 1398, 1339, 1226, 1155, 1075, 995, 909, 844, 739 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{16}N_2O_3$ $[M]^+$ 260.1161, found 260.1163.

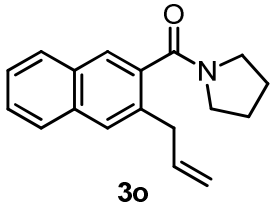
(2-Allyl-5-chlorophenyl)(pyrrolidin-1-yl)methanone (3n)



3n

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.35 (dd, *J* = 7.9, 2.2 Hz, 1H), 7.28–7.26 (m, 2H), 5.94 (ddt, *J* = 16.9, 10.0, 6.6 Hz, 1H), 5.15–5.10 (m, 2H), 3.68 (t, *J* = 7.0 Hz, 2H), 3.47 (d, *J* = 6.7 Hz, 2H), 3.22 (t, *J* = 6.7 Hz, 2H), 2.02–2.00 (m, 2H), 1.92–1.90 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 168.0, 139.0, 136.1, 134.8, 132.1, 131.1, 129.0, 126.0, 116.4, 48.7, 45.5, 36.7, 25.9, 24.5; IR (KBr) υ 2971, 2875, 2186, 1985, 1624, 1427, 1385, 1338, 1253, 1188, 1090, 994, 914, 813 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{16}ClNO$ $[M]^+$ 249.0920, found 249.0923.

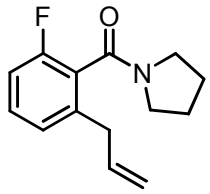
(3-Allylnaphthalen-2-yl)(pyrrolidin-1-yl)methanone (3o)



3o

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.3 Hz, 2H), 7.69 (s, 2H), 7.48–7.42 (m, 2H), 5.97 (ddt, *J* = 17.0, 10.0, 6.8 Hz, 1H), 5.13–5.06 (m, 2H), 3.66 (t, *J* = 7.1 Hz, 2H), 3.60 (d, *J* = 6.7 Hz, 2H), 3.17 (t, *J* = 6.7 Hz, 2H), 1.97–1.93 (m, 2H), 1.83–1.79 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.5, 136.7, 136.1, 134.1, 133.5, 131.6, 128.4, 127.7, 127.4, 126.7, 126.0, 125.0, 116.2, 49.0, 45.5, 37.5, 26.0, 24.6; IR (KBr) υ 2970, 2873, 2330, 2985, 1982, 1617, 1413, 1338, 1190, 995, 911, 809, 749 cm^{-1}; HRMS (EI) calcd for $C_{18}H_{19}NO$ $[M]^+$ 265.1467, found 265.1466.

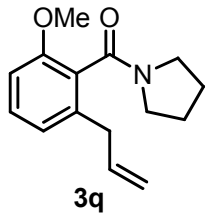
(2-Allyl-6-fluorophenyl)(pyrrolidin-1-yl)methanone (3p)



3p

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.30–7.24 (m, 1H), 7.05 (d, J = 6.8 Hz, 1H), 6.96–6.91 (m, 1H), 5.91–5.85 (m, 1H), 5.09–5.03 (m, 2H), 3.74–3.64 (m, 1H), 3.61–3.57 (m, 1H), 3.52–3.49 (m, 1H), 3.37–3.32 (m, 1H), 3.28–3.24 (m, 1H), 3.12–3.07 (m, 1H), 1.90–1.78 (m, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 164.5, 158.3 (d, $J_{C\text{-}F}$ = 243.8 Hz), 139.1 (d, $J_{C\text{-}F}$ = 4.1 Hz), 136.0, 130.1 (d, $J_{C\text{-}F}$ = 8.8 Hz), 125.6 (d, $J_{C\text{-}F}$ = 19.3 Hz), 125.4 (d, $J_{C\text{-}F}$ = 2.6 Hz), 116.3, 113.4 (d, $J_{C\text{-}F}$ = 22.4 Hz), 47.4, 45.4, 37.2, 25.7, 24.5; IR (KBr) υ 2975, 2878, 2329, 2158, 1986, 1628, 1576, 1459, 1422, 1339, 1242, 1197, 1111, 985, 913, 730 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{16}FNO$ $[M]^+$ 233.1216, found 233.1215.

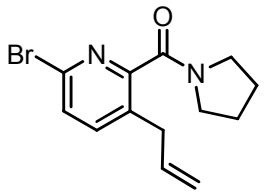
(2-Allyl-6-methoxyphenyl)(pyrrolidin-1-yl)methanone (3q)



3q

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.28–7.24 (m, 1H), 6.86 (d, J = 7.7 Hz, 1H), 6.78 (d, J = 8.3 Hz, 1H), 5.90 (ddt, J = 16.7, 10.0, 6.8 Hz, 1H), 5.09–5.02 (m, 2H), 3.82 (s, 3H), 3.75–3.72 (m, 1H), 3.60–3.57 (m, 1H), 3.43–3.40 (m, 1H), 3.34–3.31 (m, 1H), 3.20–3.17 (m, 1H), 3.07–3.04 (m, 1H), 1.97–1.92 (m, 2H), 1.89–1.77 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 167.2, 155.2, 137.7, 136.6, 129.5, 127.1, 121.9, 115.8, 108.7, 55.7, 47.2, 45.1, 37.3, 25.7, 24.6; IR (KBr) υ 2926, 2874, 2187, 1984, 1624, 1582, 1466, 1421, 1337, 1301, 1259, 1065, 995, 909, 762 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{19}NO_2$ $[M]^+$ 245.1416, found 245.1418.

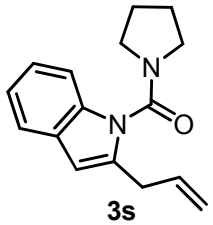
(3-Allyl-6-bromopyridin-2-yl)(pyrrolidin-1-yl)methanone (3r)



3r

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.1 Hz, 1H), 7.44 (d, *J* = 8.1 Hz, 1H), 5.88 (ddt, *J* = 16.9, 10.1, 6.7 Hz, 1H), 5.12–5.07 (m, 2H), 3.66 (t, *J* = 7.0 Hz, 2H), 3.46 (d, *J* = 6.7 Hz, 2H), 3.30 (t, *J* = 6.7 Hz, 2H), 1.99–1.93 (m, 2H), 1.91–1.86 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 165.2, 155.0, 140.9, 140.6, 138.6, 135.2, 131.9, 128.3, 117.2, 48.0, 45.6, 35.3, 26.0, 24.2; IR (KBr) υ 2964, 2877, 2235, 2016, 1626, 1550, 1453, 1405, 1260, 1121, 1076, 985, 916, 816, 756 cm^{-1}; HRMS (EI) calcd for $C_{13}H_{15}BrN_2O$ $[M]^+$ 294.0368, found 294.0365.

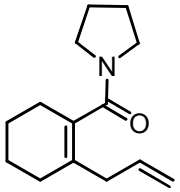
(2-Allyl-1*H*-indol-1-yl)(pyrrolidin-1-yl)methanone (3s)



3s

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.0 Hz, 1H), 7.21–7.17 (m, 2H), 7.13–7.10 (m, 1H), 6.36 (s, 1H), 5.94 (ddt, *J* = 17.0, 10.1, 6.7 Hz, 1H), 5.19–5.08 (m, 2H), 3.66–3.06 (m, 6H), 1.93 (br s, 4H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 152.5, 137.9, 135.1, 135.0, 128.4, 122.2, 120.8, 120.4, 116.8, 48.2, 47.1, 31.7, 25.6, 25.0; IR (KBr) υ 2970, 2881, 2237, 2193, 2018, 1676, 1452, 1399, 1339, 1295, 1188, 994, 915, 791 cm^{-1}; HRMS (EI) calcd for $C_{16}H_{18}N_2O$ $[M]^+$ 254.1419, found 254.1421.

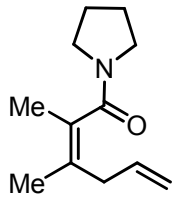
(2-Allylcyclohex-1-enyl)(pyrrolidin-1-yl)methanone (3t)



3t

^{1}H NMR (700 MHz, $CDCl_3$) δ 5.67 (ddt, *J* = 17.0, 10.1, 6.9 Hz, 1H), 4.96–5.90 (m, 2H), 3.42 (t, *J* = 6.8 Hz, 2H), 3.26 (t, *J* = 6.4 Hz, 2H), 2.66 (d, *J* = 6.9 Hz, 2H), 2.09 (br s, 2H), 1.92 (br s, 2H), 1.87–1.75 (m, 8H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 171.5, 135.5, 133.1, 132.1, 129.6, 116.1, 47.2, 45.9, 39.3, 29.6, 27.7, 25.9, 24.4, 22.4; IR (KBr) υ 2924, 2868, 2188, 2018, 1755, 1608, 1423, 1343, 1245, 1175, 1028, 963, 912, 741 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{21}NO$ $[M]^+$ 219.1623, found 219.1623.

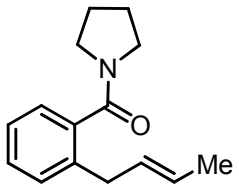
(*Z*)-2,3-Dimethyl-1-(pyrrolidin-1-yl)hexa-2,5-dien-1-one (3u)



3u

^{1}H NMR (700 MHz, $CDCl_3$) δ 5.67 (ddt, *J* = 16.9, 10.1, 6.8 Hz, 1H), 5.09–4.97 (m, 2H), 3.47 (t, *J* = 7.0 Hz, 2H), 3.28 (t, *J* = 6.3 Hz, 2H), 2.73 (d, *J* = 6.7 Hz, 2H), 1.88–1.82 (m, 4H), 1.79 (s, 3H), 1.64 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 171.9, 135.5, 133.3, 130.7, 125.9, 116.1, 47.1, 44.9, 40.3, 25.8, 24.5, 16.5, 15.4; IR (KBr) υ 2972, 2876, 2059, 1725, 1608, 1423, 1339, 1249, 1190, 996, 911, 730 cm^{-1}; HRMS (EI) calcd for $C_{12}H_{19}NO$ $[M]^+$ 193.1467, found 193.1467.

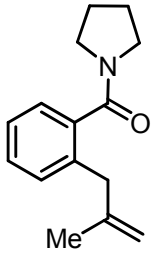
(*E*)-(2-(But-2-enyl)phenyl)(pyrrolidin-1-yl)methanone (5b)



5b

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.29–7.27 (m, 3H), 7.21–7.16 (m, 1H), 5.57–5.46 (m, 2H), 3.63 (t, *J* = 7.0 Hz, 2H), 3.42 (d, *J* = 6.7 Hz, 2H), 3.13 (t, *J* = 6.7 Hz, 2H), 1.95–1.92 (m, 2H), 1.84–1.80 (m, 2H), 1.69–1.68 (m, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.8, 137.6, 137.3, 129.6, 128.9, 128.3, 126.1, 125.8, 125.0, 48.6, 45.3, 30.5, 26.0, 24.6, 12.9; IR (KBr) υ 2969, 2875, 2190, 2108, 1722, 1624, 1486, 1416, 1338, 1251, 1185, 1032, 969, 909, 750 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{19}NO$ $[M]^+$ 229.1467, found 229.1463.

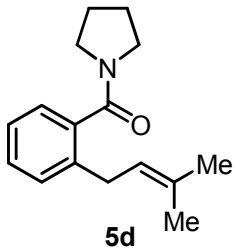
(2-(2-Methylallyl)phenyl)(pyrrolidin-1-yl)methanone (5c)



5c

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.30–7.28 (m, 1H), 7.25–7.19 (m, 3H), 4.77 (s, 1H), 4.68 (s, 1H), 3.61 (t, *J* = 7.0 Hz, 2H), 3.41 (br s, 2H), 3.11 (t, *J* = 6.7 Hz, 2H), 1.94–1.90 (m, 2H), 1.82–1.78 (m, 2H), 1.66 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.7, 144.3, 137.9, 136.0, 130.4, 128.7, 126.2, 126.0, 112.1, 48.7, 45.3, 41.3, 26.0, 24.5, 22.2; IR (KBr) υ 2964, 2876, 2237, 2189, 2016, 1617, 1574, 1415, 1340, 1230, 1027, 923, 789, 714 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{19}NO$ $[M]^+$ 229.1467, found 229.1467.

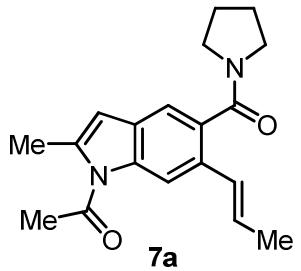
(2-(3-Methylbut-2-enyl)phenyl)(pyrrolidin-1-yl)methanone (5d)[12]



5d

^{1}H NMR (700 MHz, $CDCl_3$) δ 7.28–7.26 (m, 1H), 7.23–7.22 (m, 1H), 7.20–7.16 (m, 2H), 5.23–5.21 (m, 1H), 3.62 (t, *J* = 7.1 Hz, 2H), 3.36 (d, *J* = 6.8 Hz, 2H), 3.12 (t, *J* = 6.7 Hz, 2H), 1.95–1.91 (m, 2H), 1.84–1.81 (m, 2H), 1.70 (s, 3H), 1.68 (s, 3H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.9, 137.9, 137.5, 132.7, 129.6, 128.8, 125.9, 125.8, 122.5, 48.6, 45.3, 31.7, 25.9, 25.8, 24.6, 17.9; IR (KBr) υ 2968, 2875, 2192, 2017, 1618, 1574, 1414, 1339, 1251, 1228, 1160, 1075, 1026, 918, 872, 790, 716, 699 cm^{-1}; HRMS (EI) calcd for $C_{16}H_{21}NO$ $[M]^+$ 243.1623, found 243.1623.

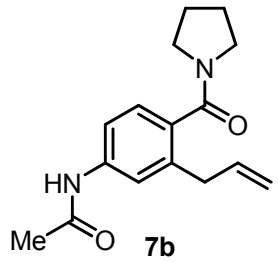
(*E*)-1-(2-methyl-6-(prop-1-enyl)-5-(pyrrolidine-1-carbonyl)-1H-indol-1-yl)ethanone (7a)



7a

^{1}H NMR (700 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.22 (s, 1H), 6.48–6.45 (m, 1H), 6.28 (s, 1H), 6.24–6.19 (m, 1H), 3.64 (t, *J* = 7.0 Hz, 2H), 3.05 (t, *J* = 6.8 Hz, 2H), 2.68 (s, 3H), 2.58 (s, 3H), 1.92–1.87 (m, 2H), 1.83 (d, *J* = 6.7 Hz, 3H), 1.80–1.76 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 170.2, 170.0, 138.1, 137.3, 132.2, 130.4, 128.5, 127.4, 117.2, 116.3, 112.5, 109.7, 48.3, 45.5, 27.4, 25.9, 24.7, 18.7, 17.7; IR (KBr) υ 2923, 2851, 1671, 1594, 1417, 1369, 1264, 1163, 732 cm^{-1}; HRMS (EI) calcd for $C_{19}H_{22}N_2O_2$ $[M]^+$ 310.1681, found 310.1686.

***N*-(3-Allyl-4-(pyrrolidine-1-carbonyl)phenyl)acetamide (7b)**



7b

^{1}H NMR (700 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.21 (s, 1H), 7.03 (d, *J* = 8.1 Hz, 1H), 5.80 (ddt, *J* = 16.9, 10.0, 6.7 Hz, 1H), 5.03–4.97 (m, 2H), 3.59 (t, *J* = 7.1 Hz, 2H), 3.32 (d, *J* = 6.7 Hz, 2H), 3.11 (t, *J* = 6.7 Hz, 2H), 2.11 (s, 3H), 1.94–1.90 (m, 2H), 1.83–1.79 (m, 2H); ^{13}C NMR (175 MHz, $CDCl_3$) δ 169.7, 168.9, 138.8, 137.1, 136.3, 132.9, 126.5, 121.3, 118.1, 116.1, 48.8, 45.5, 37.4, 25.9, 24.5, 24.3; IR (KBr) υ 2922, 2852, 1672, 1592, 1532, 1438, 1255, 1163, 732 cm^{-1}; HRMS (EI) calcd for $C_{16}H_{20}N_2O_2$ $[M]^+$ 272.1525, found 272.1526.

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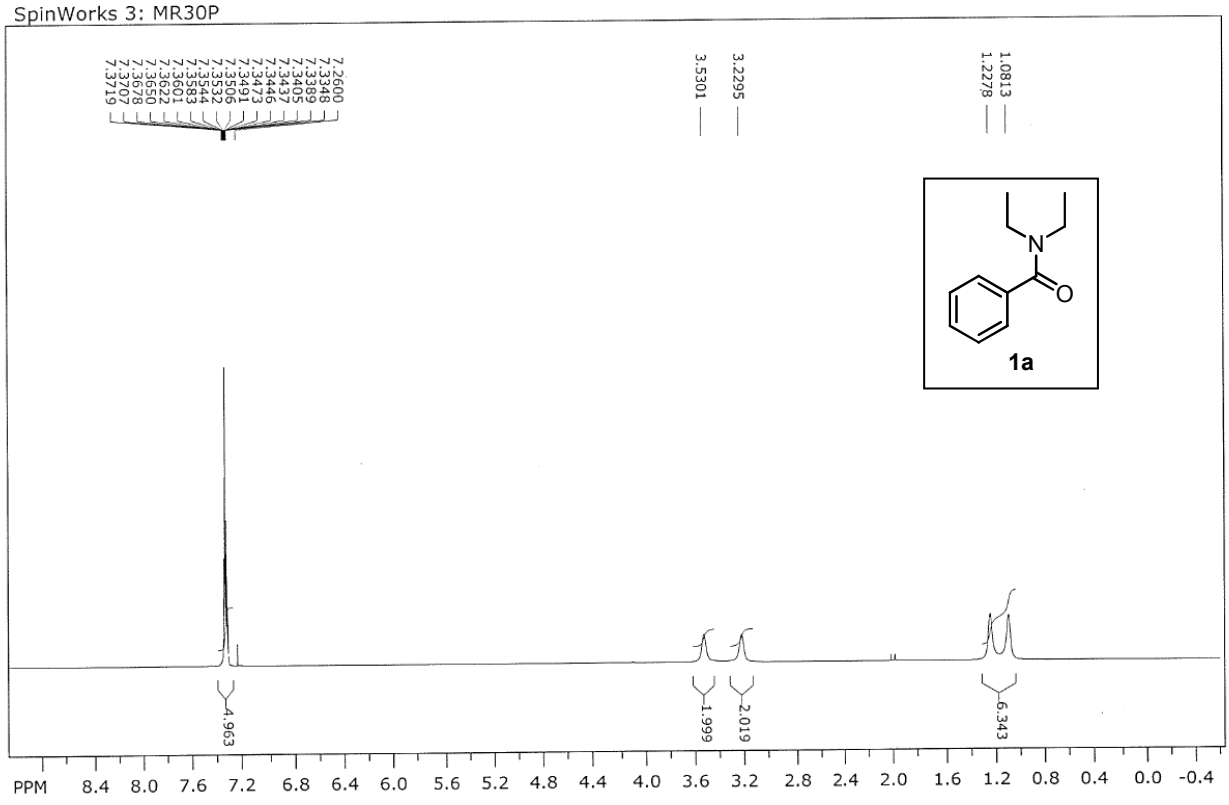
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7.3650
7.3622
7.3601
7.3564
7.3532
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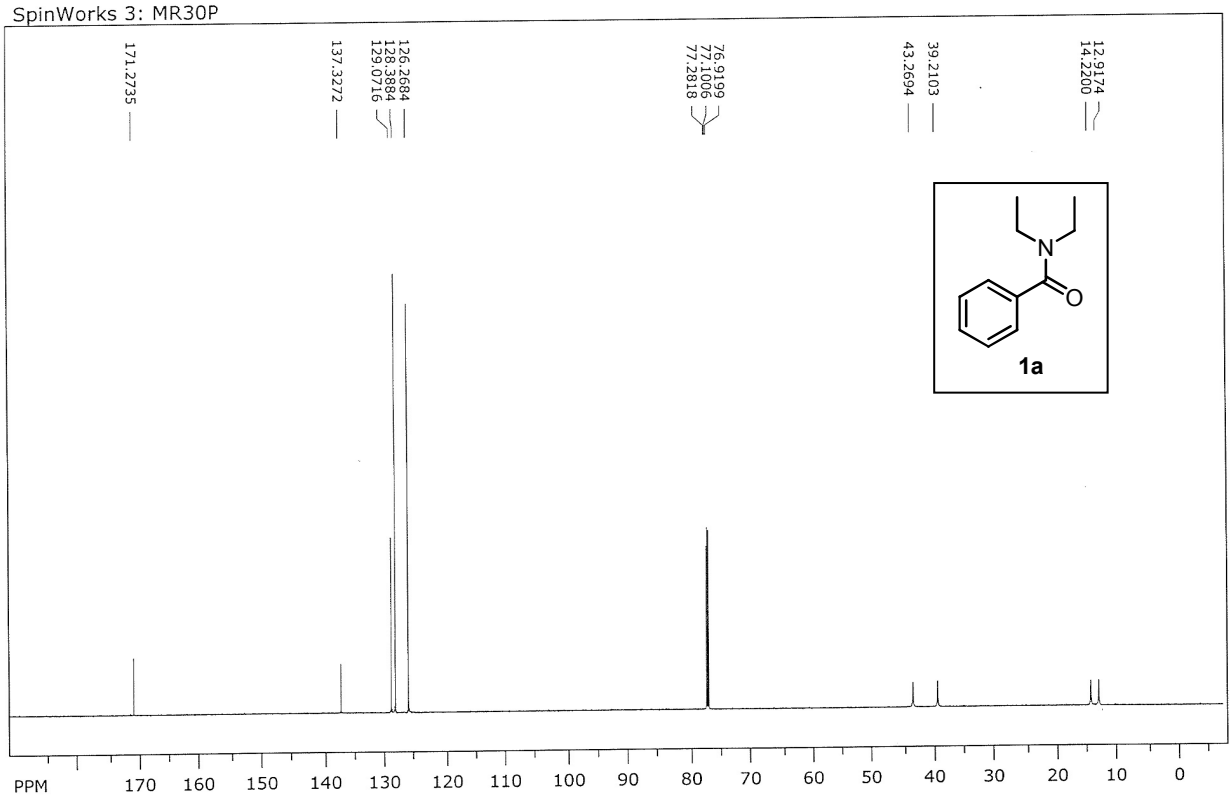
7.3491
7.3473
7.3446
7.3437
7.3405
7.3389
7.3348
7.2600
3.5301
3.2295
1.0813
1.2278
1a
4.963
1.999
2.019
6.343
PPM
8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0 -0.4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128.3884
129.0716
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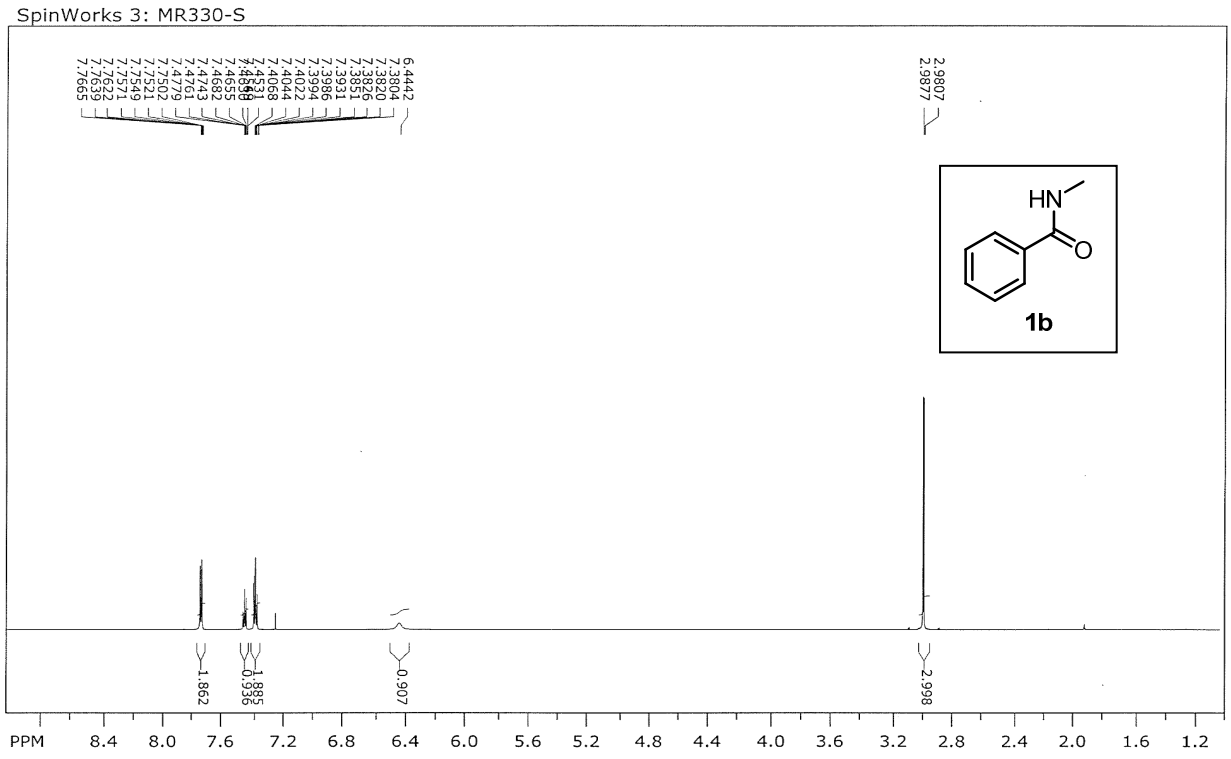
39.2103
14.2200
12.9174
1a
PPM
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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7.7622
7.7571
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7.7502
7.4779
7.4761
7.4743
7.4682
7.4655
7.4068
7.4044
7.4022
7.3994
7.3986
7.3931
7.3851
7.3826
7.3820
7.3804
6.4442
2.9877
2.9807
HN
O
1b
1.862
0.936
1.885
0.907
2.998
PPM
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
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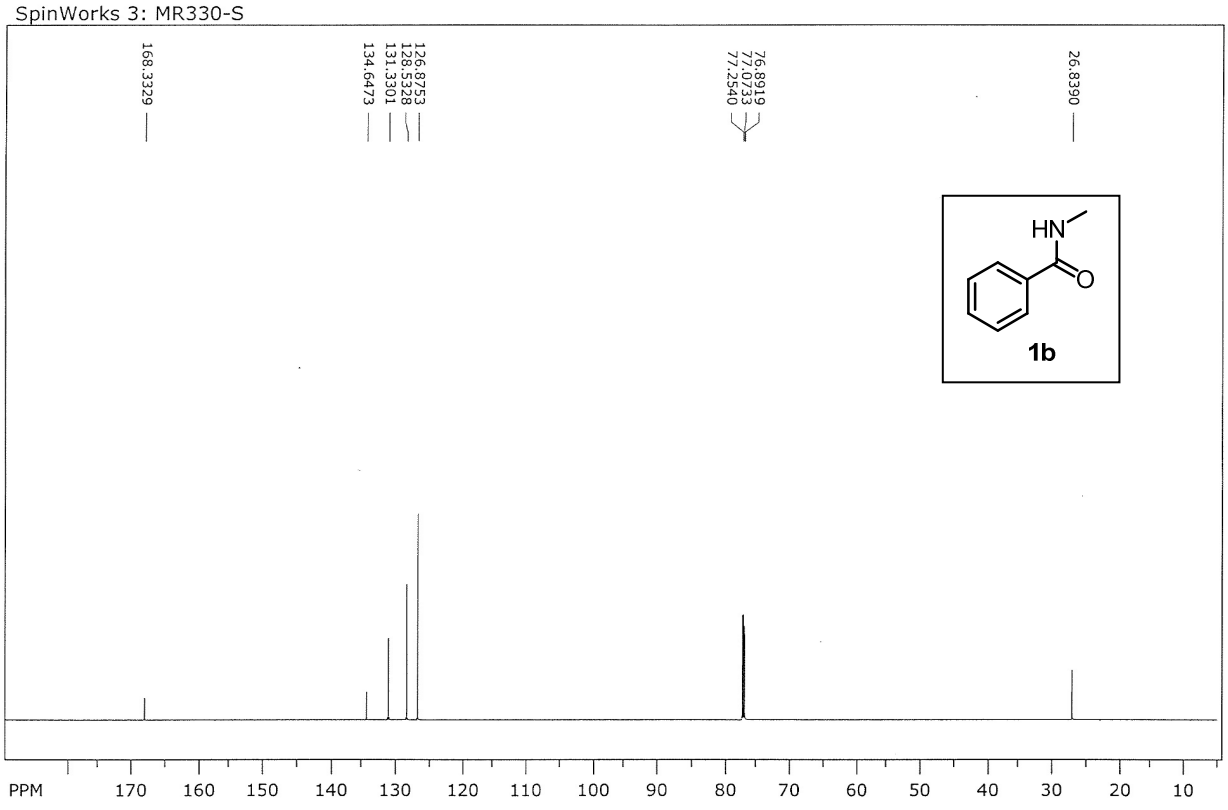
3.2
2.8
2.4
2.0
1.6
1.2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HN
O
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160
150
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130
120
110
100
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80
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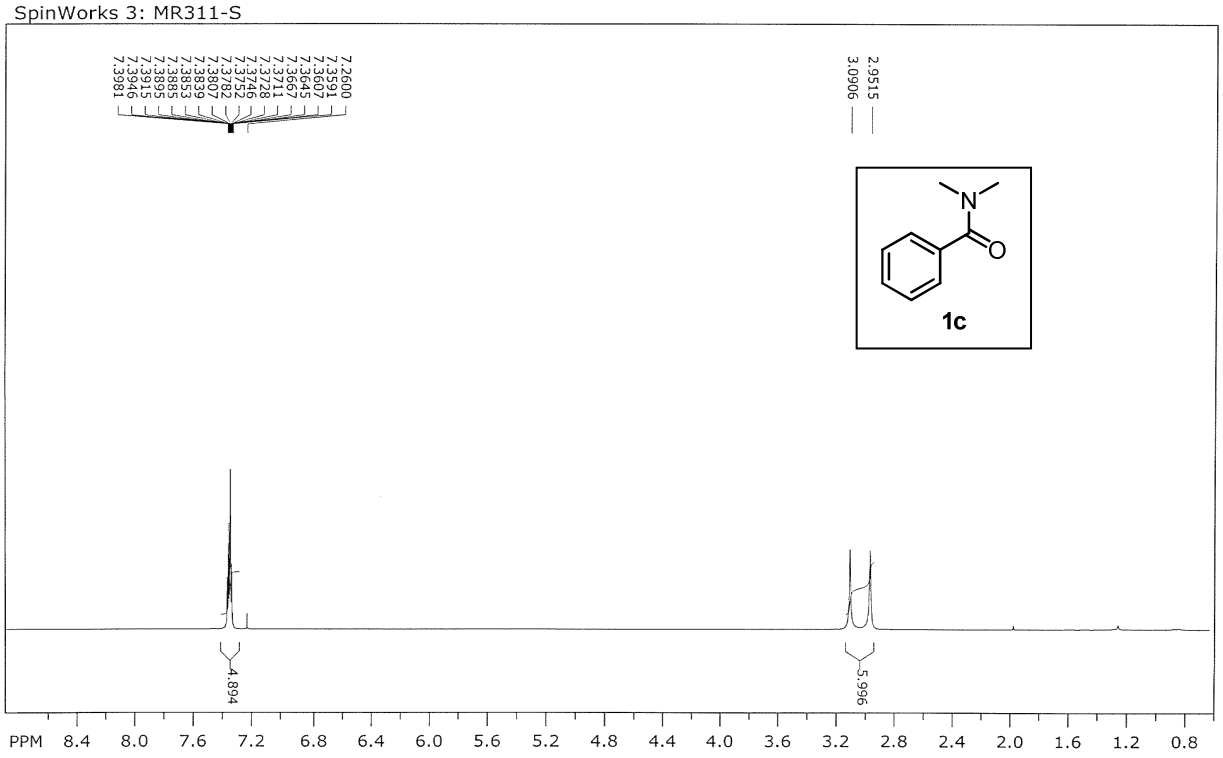
60
50
40
30
20
10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7.3839
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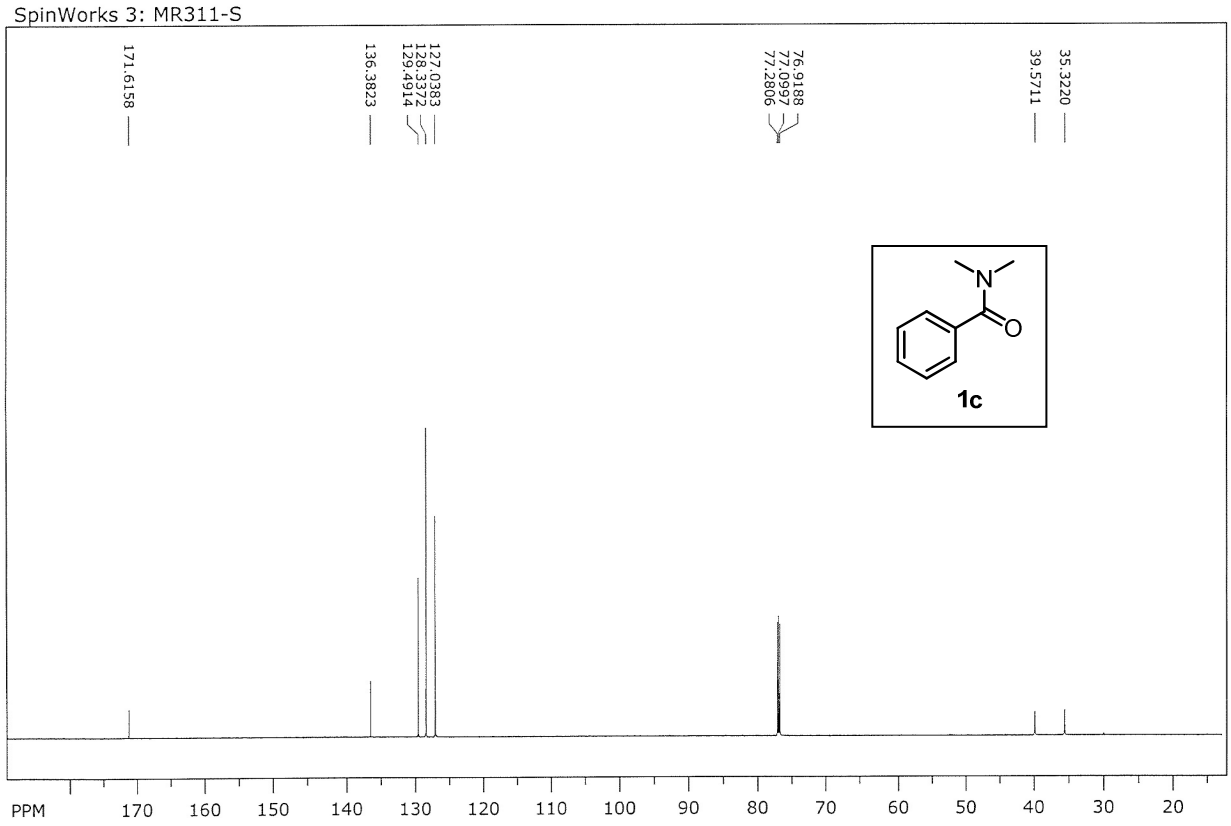
7.3782
7.3752
7.3746
7.3728
7.3711
7.3667
7.3645
7.3607
7.3591
7.2600
3.0906
2.9515
1c
4.894
5.996
PPM 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8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35.3220
1c
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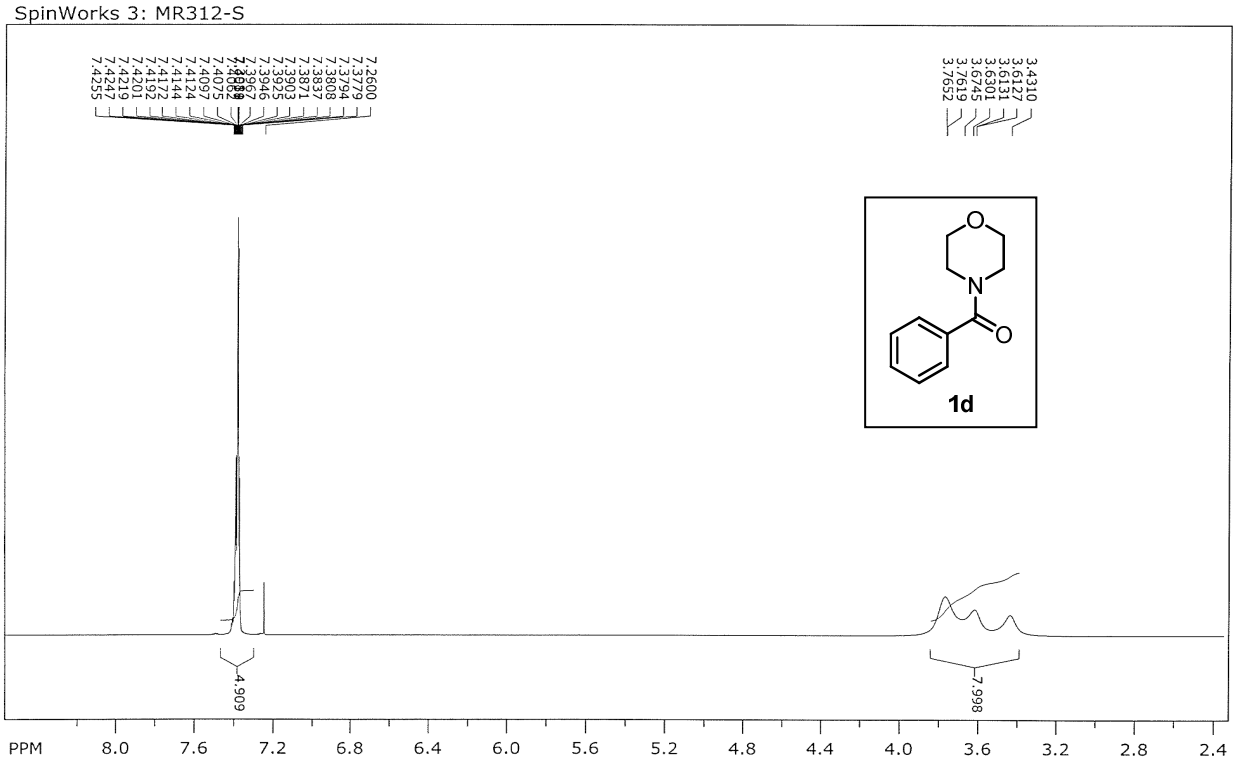
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7.4172
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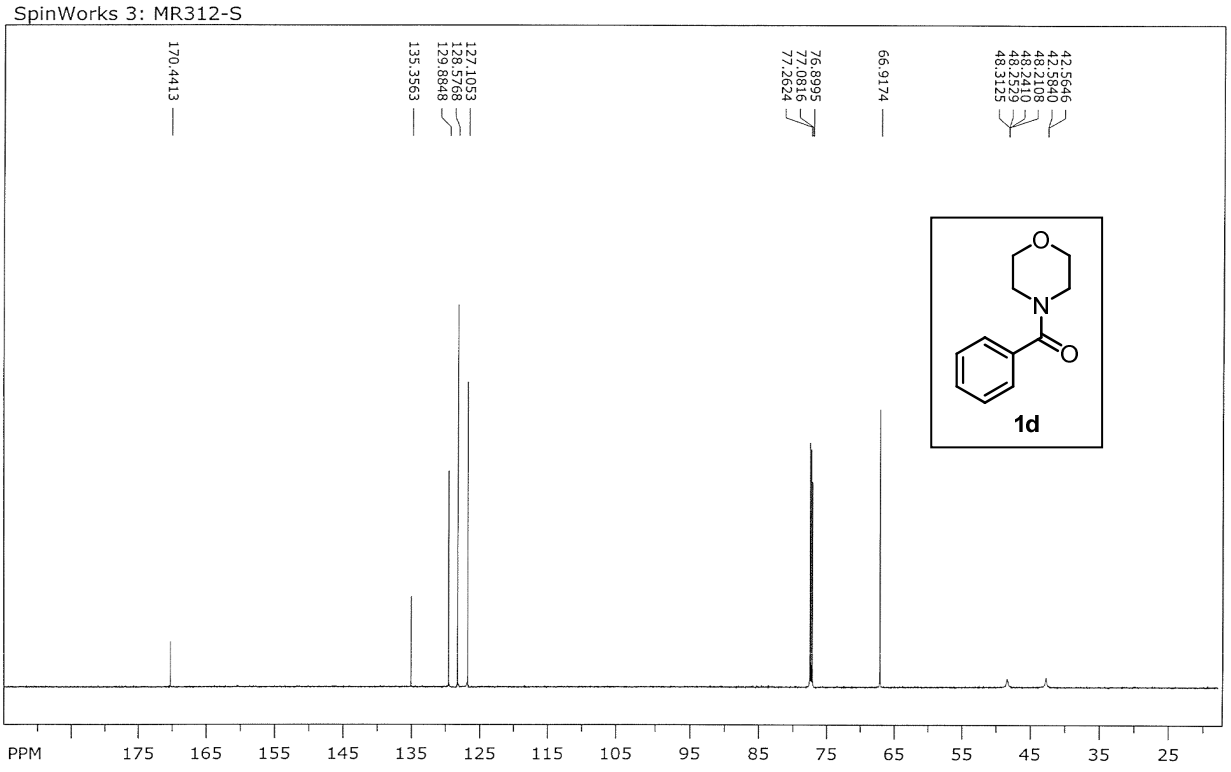
7.4124
7.4097
7.4075
7.3946
7.3925
7.3903
7.3871
7.3837
7.3808
7.3794
7.3779
3.7652
3.7619
3.6745
3.6301
3.6131
3.6127
3.4310
O
N
O
1d
4.909
7.998
PPM
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4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77.0816
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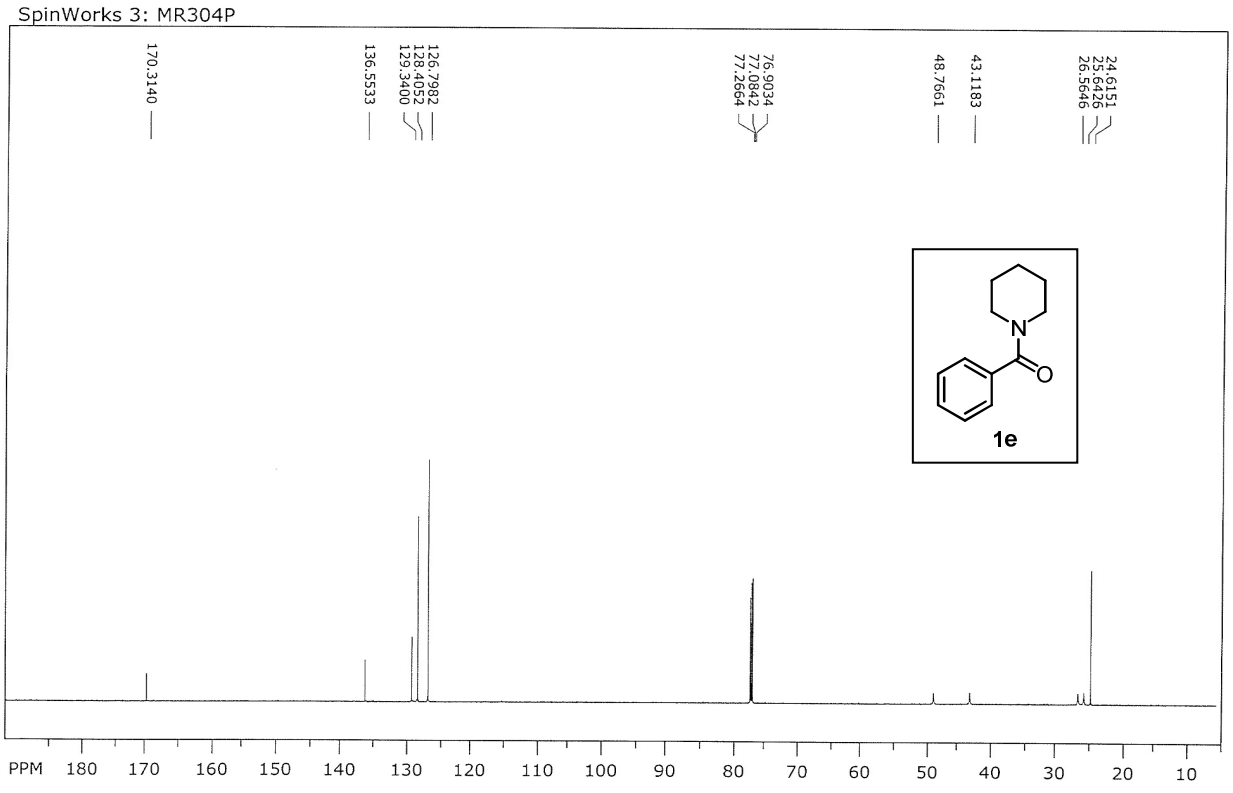
66.9174
48.3125
48.2529
48.2410
48.2108
42.5840
42.5646
O
N
O
1d
PPM
175
165
155
145
135
125
115
105
95
85
75
65
55
45
35
25


SpinWorks 3: MR304P
7.3834
7.3825
7.3724
7.3615
7.3599
7.2600
3.6983
3.3216
1.6621
1.4953
1e
4.915
2.000
2.031
6.040
PPM 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4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77.0842
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26.5646
25.6426
24.6151
1e
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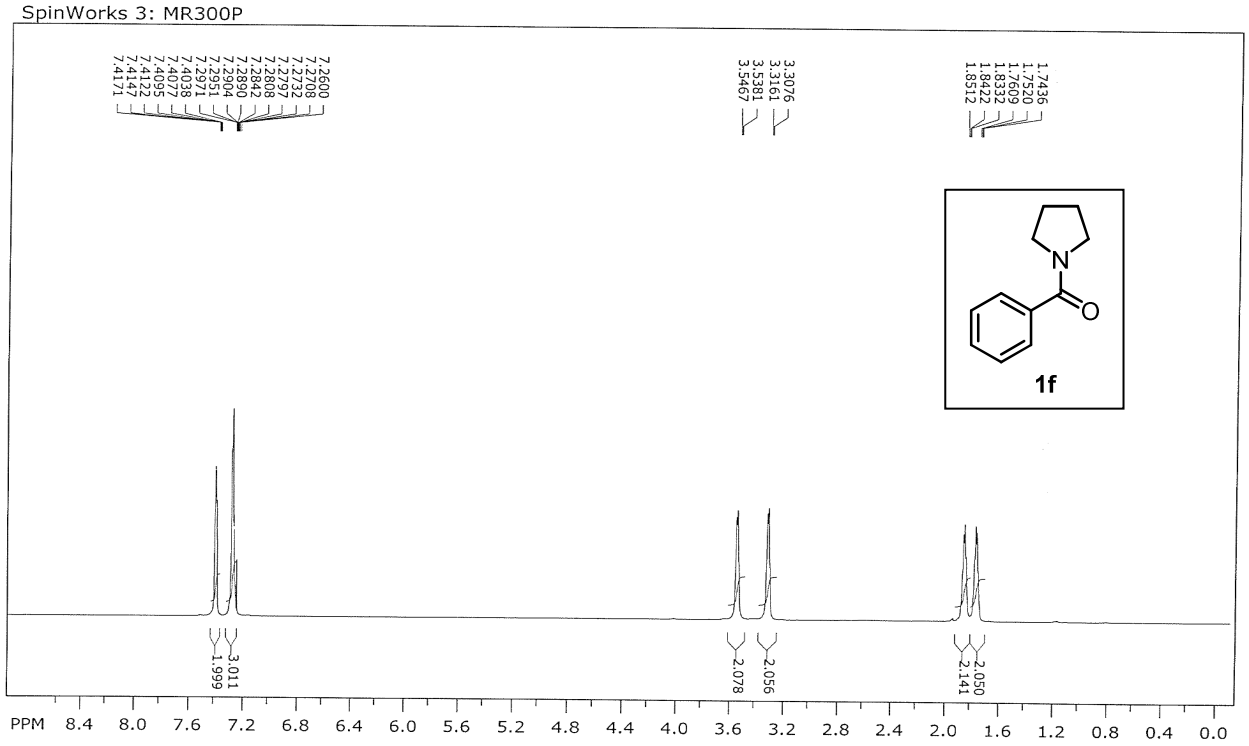
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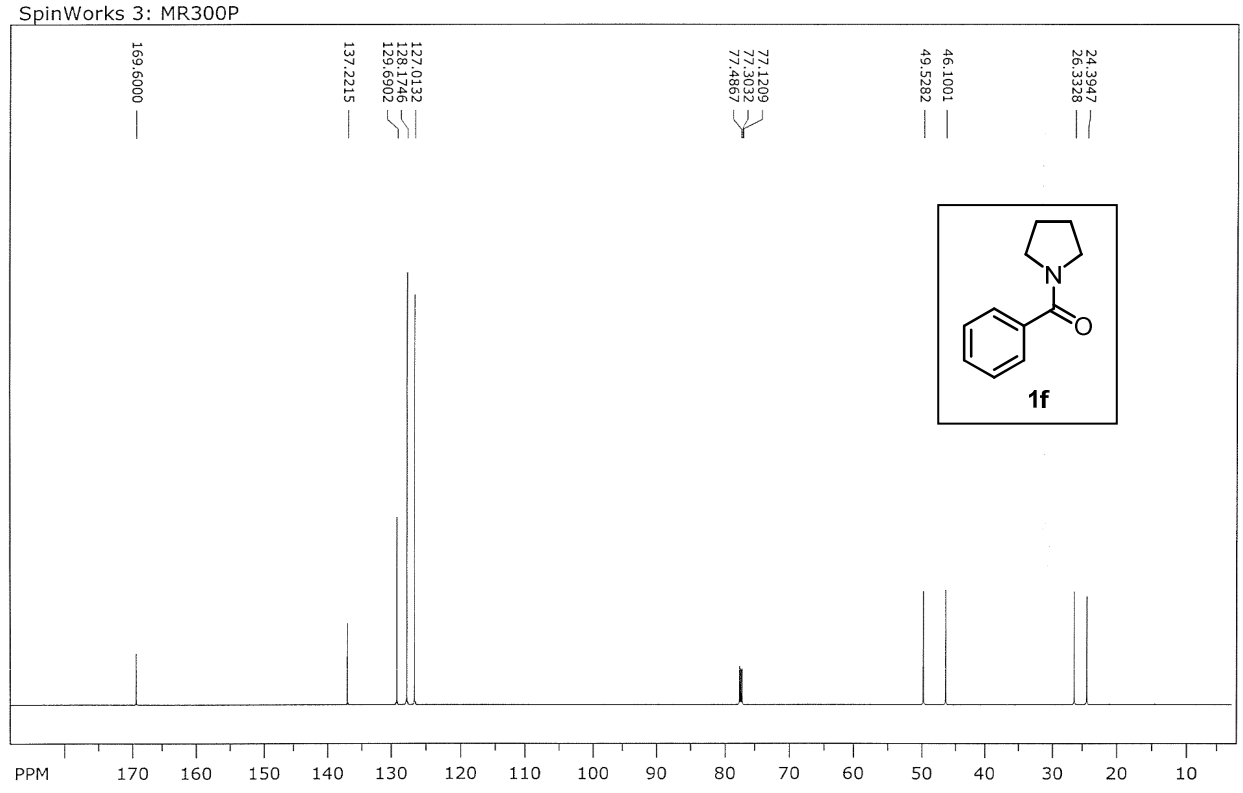
7.4028
7.4077
7.4095
7.4122
7.4147
7.4171
3.3076
3.3161
3.5381
3.5467
1.7436
1.7520
1.7609
1.8332
1.8422
1.8512
1f
1.999
3.011
2.078
2.056
2.141
2.050
PPM 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0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129.6902
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77.3032
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49.5282
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26.3328
1f
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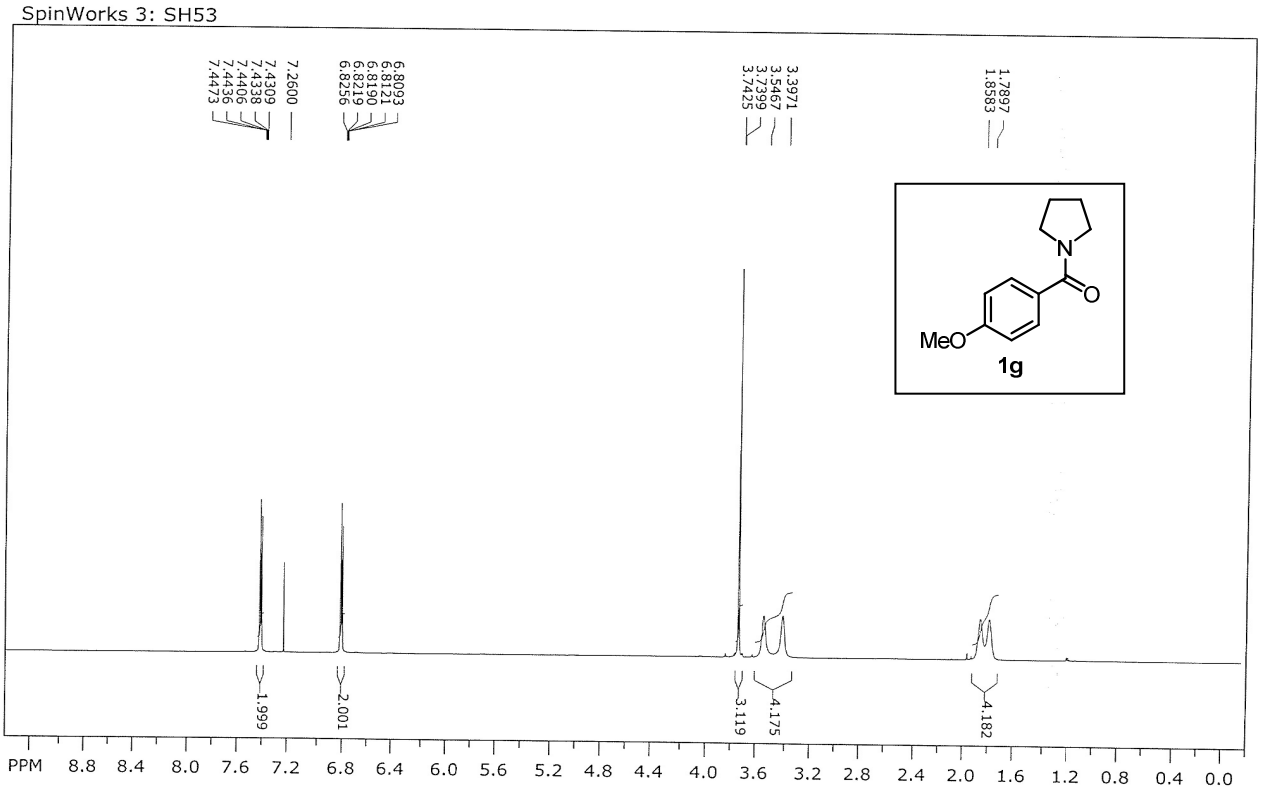
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6.8121
6.8093
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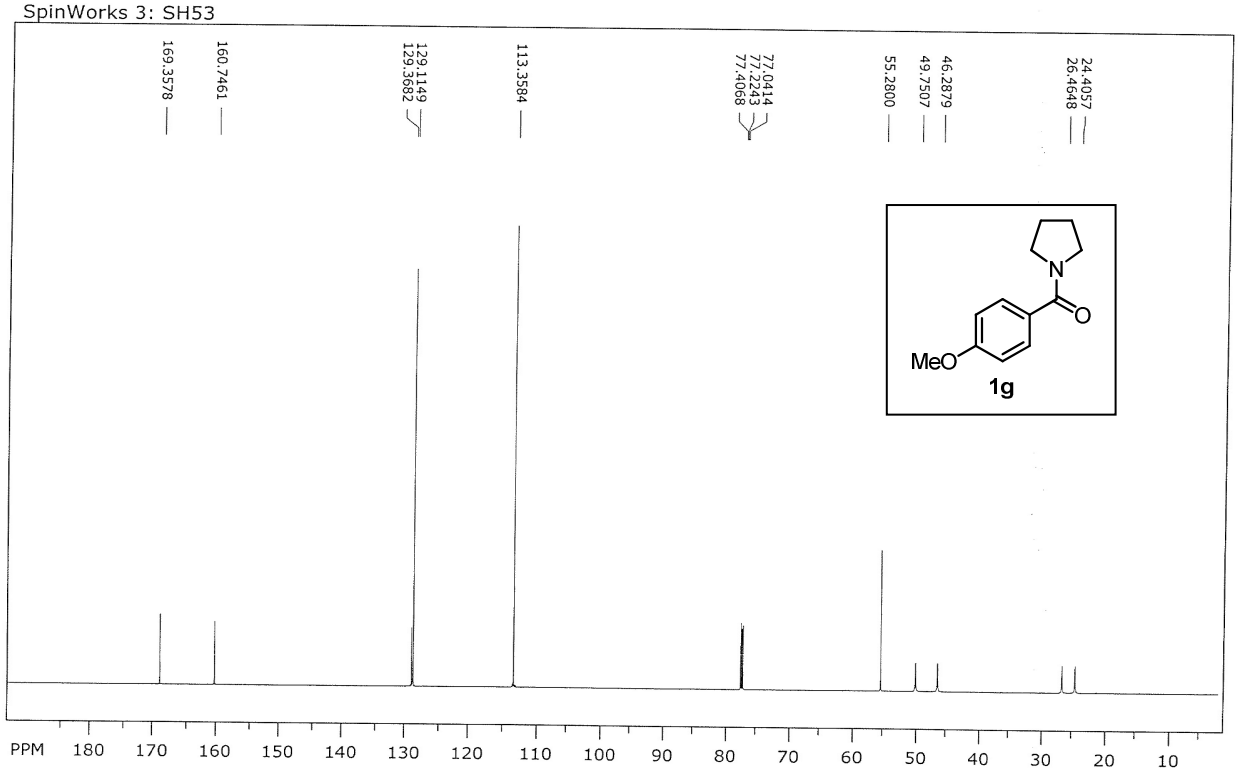
3.7399
3.5467
3.3971
1.8583
1.7897
MeO
1g
1.999
2.001
3.119
4.175
4.182
PPM 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0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1g
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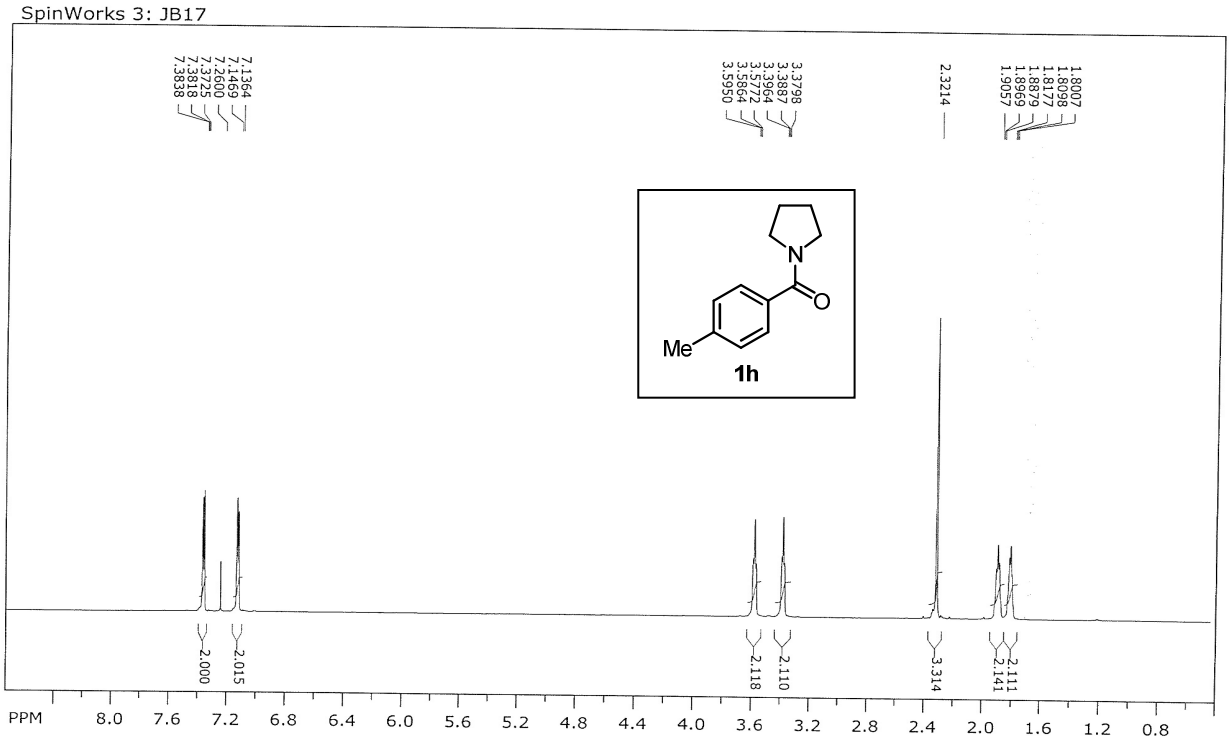
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1.8969
1.8879
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1.8098
1.8007
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O
Me
1h
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2.015
2.118
2.110
3.314
2.111
2.141
PPM
8.0
7.6
7.2
6.8
6.4
6.0
5.6
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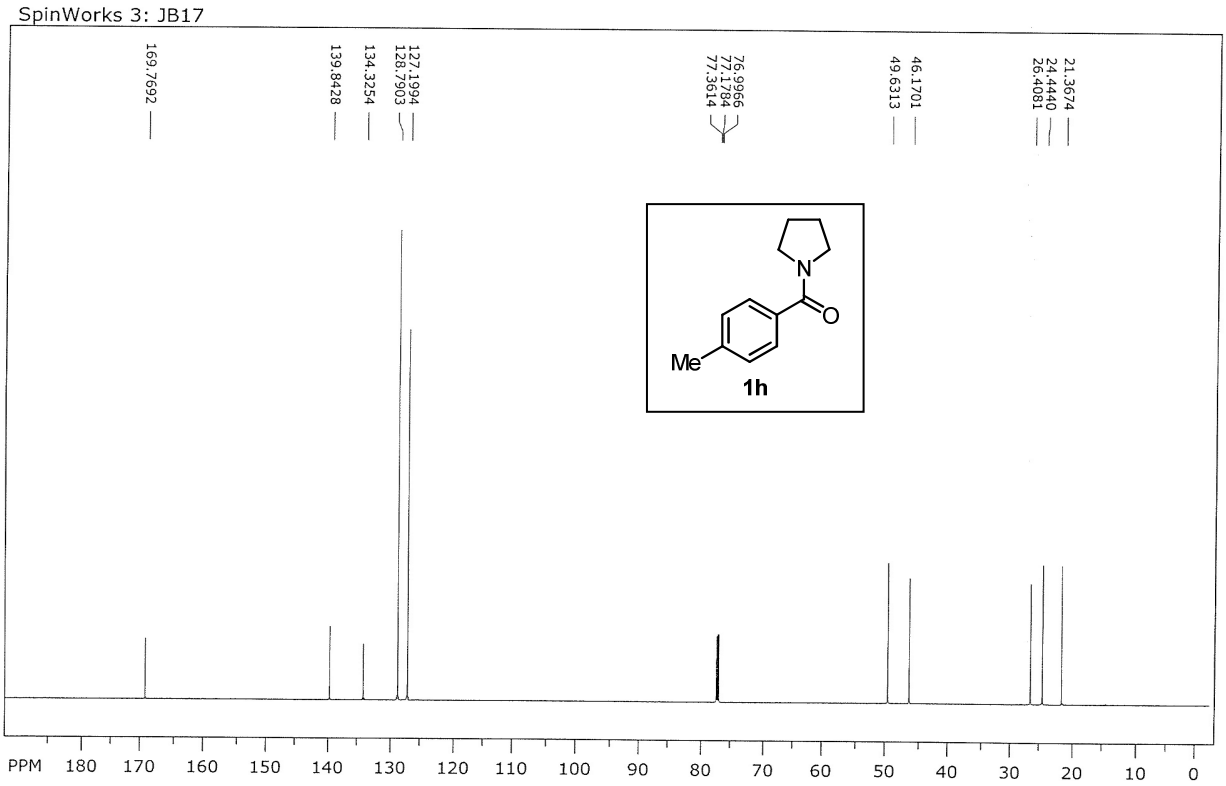
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O
Me
1h
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20
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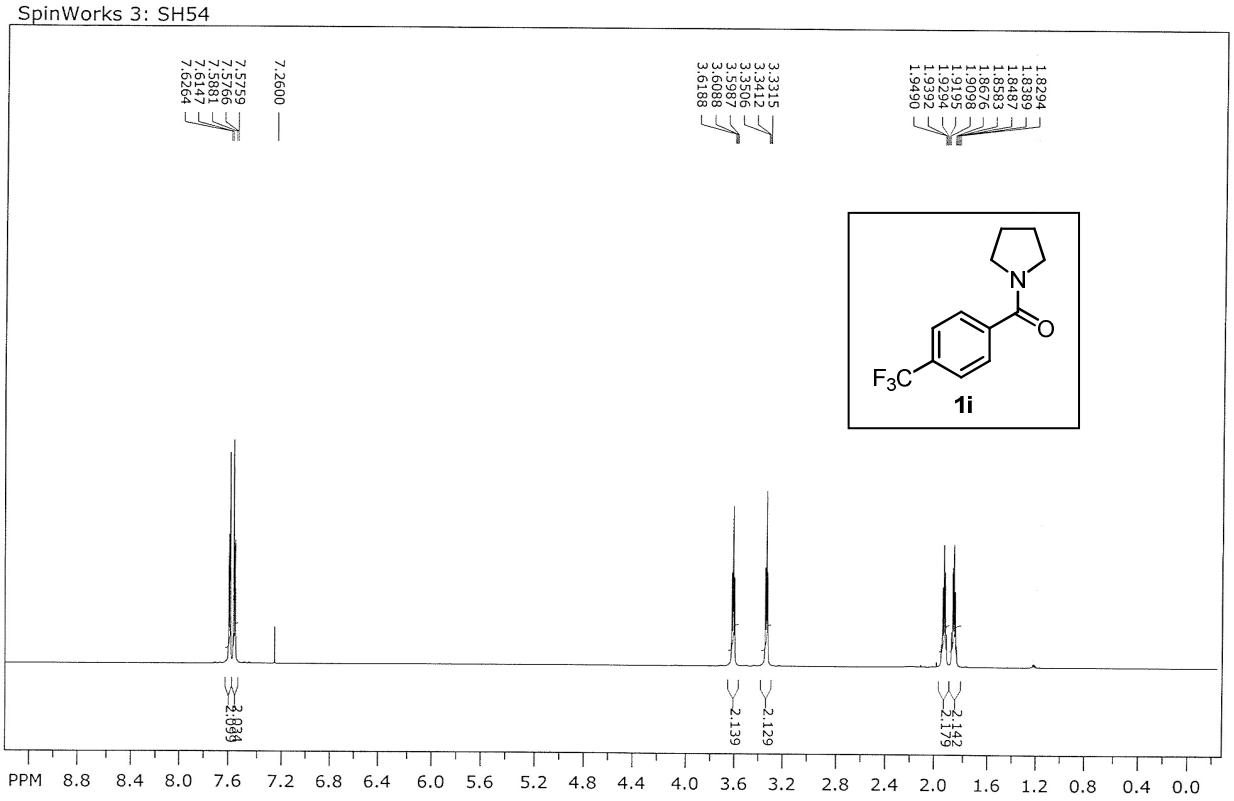
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3.5412
3.3315
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1.9195
1.9098
1.8676
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2.129
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2.179
F3C
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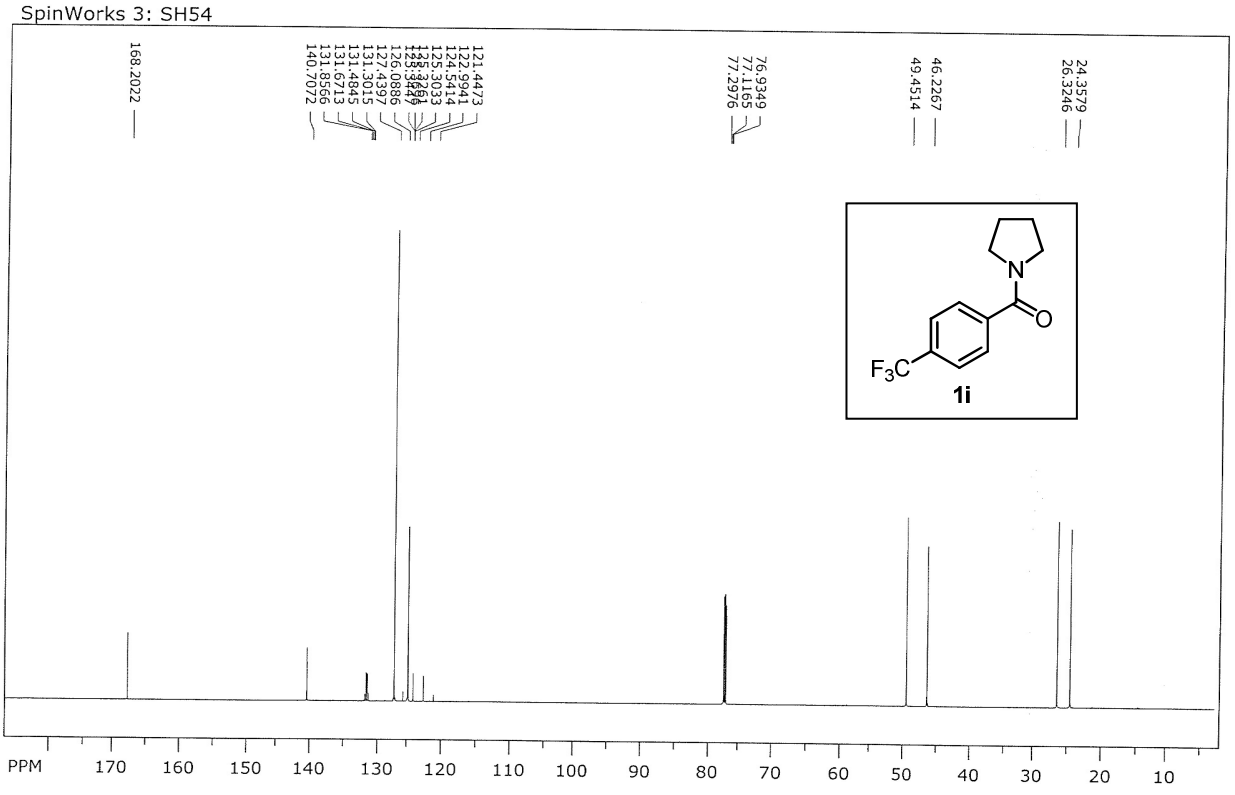
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122.9941
121.4473
77.2976
77.1165
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F3C
1i
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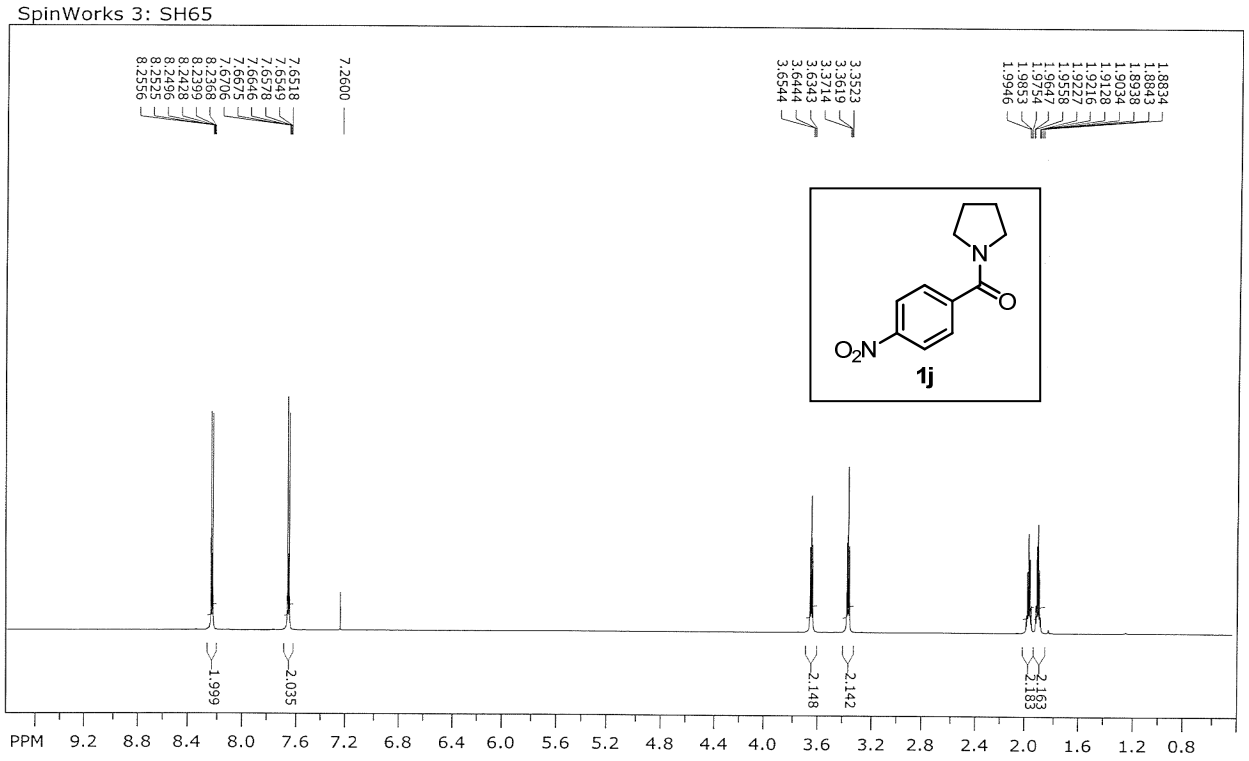
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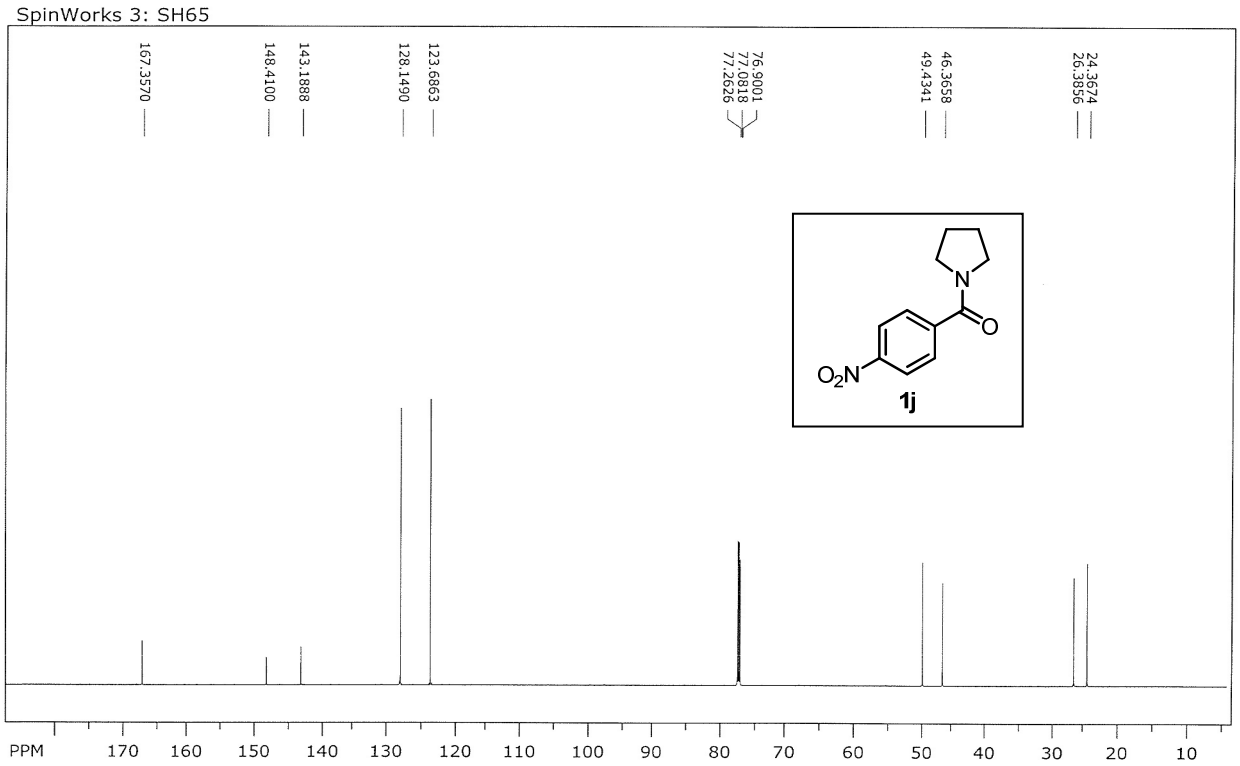
2.183
PPM 9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8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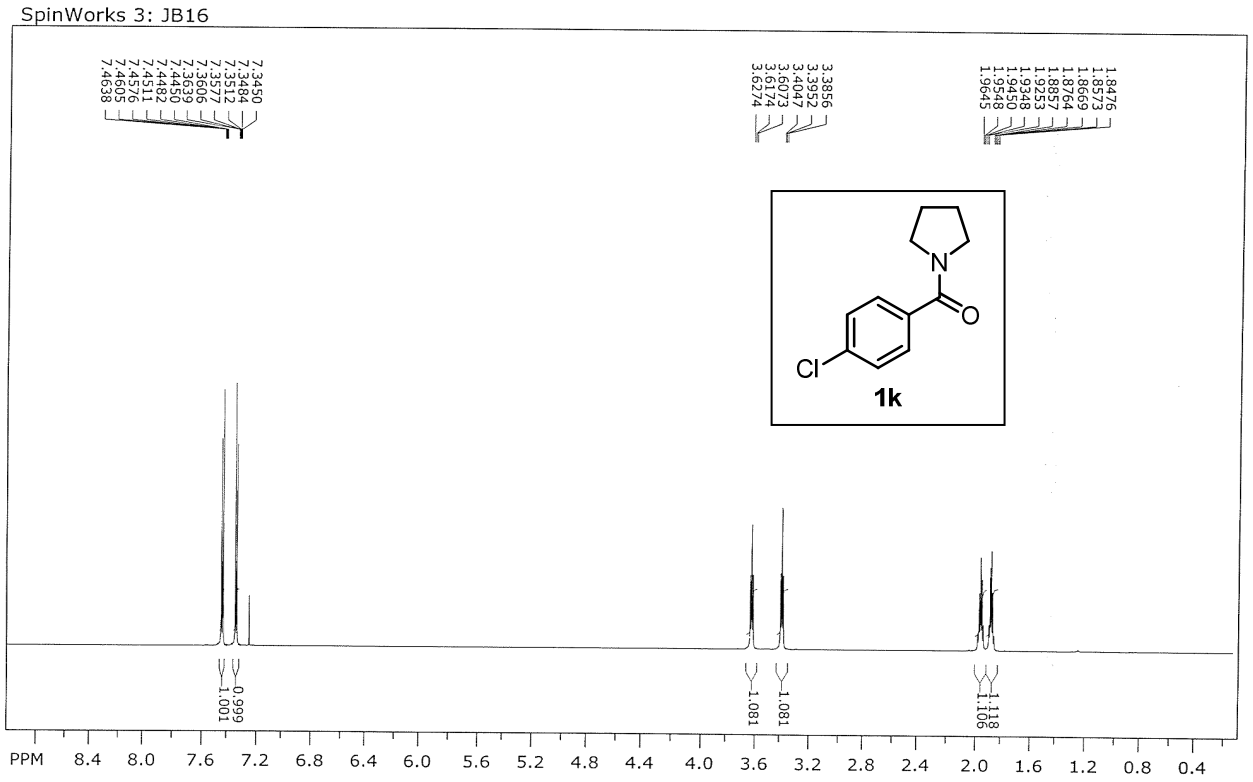
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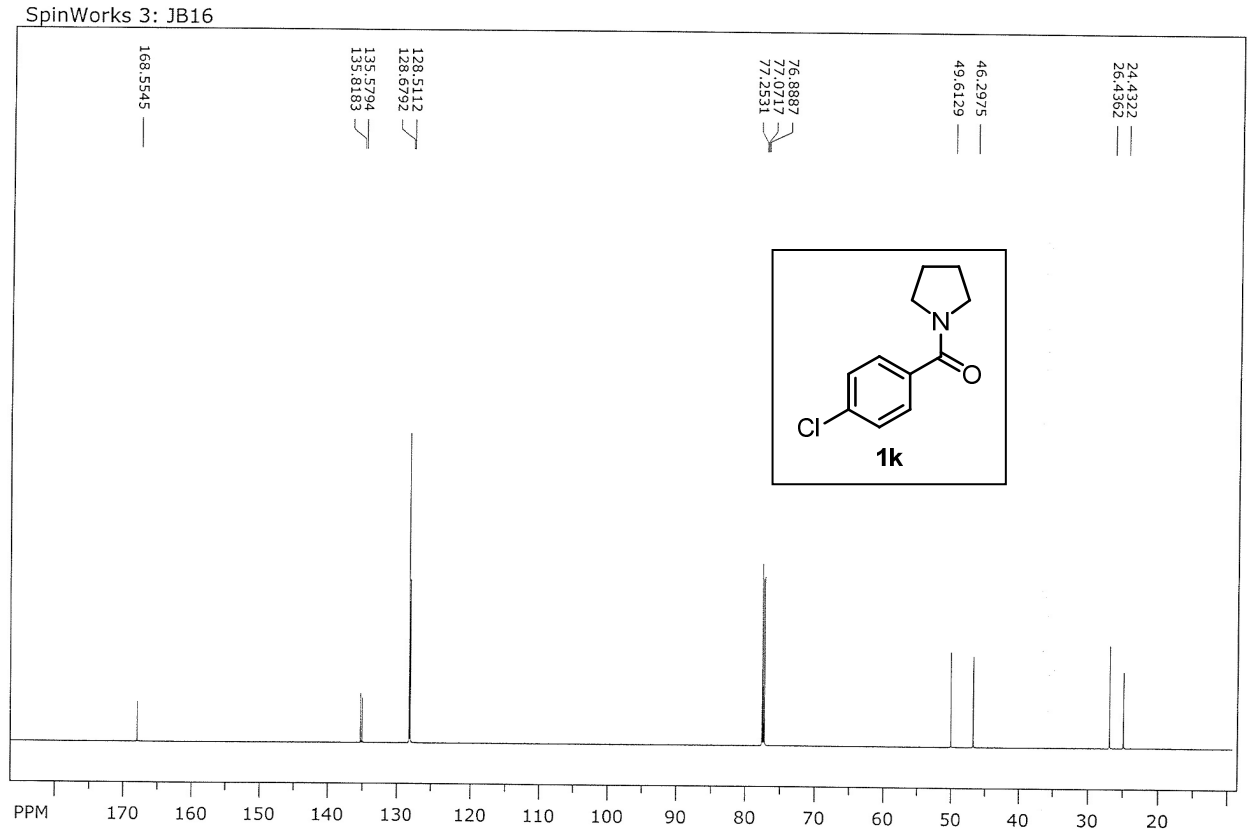
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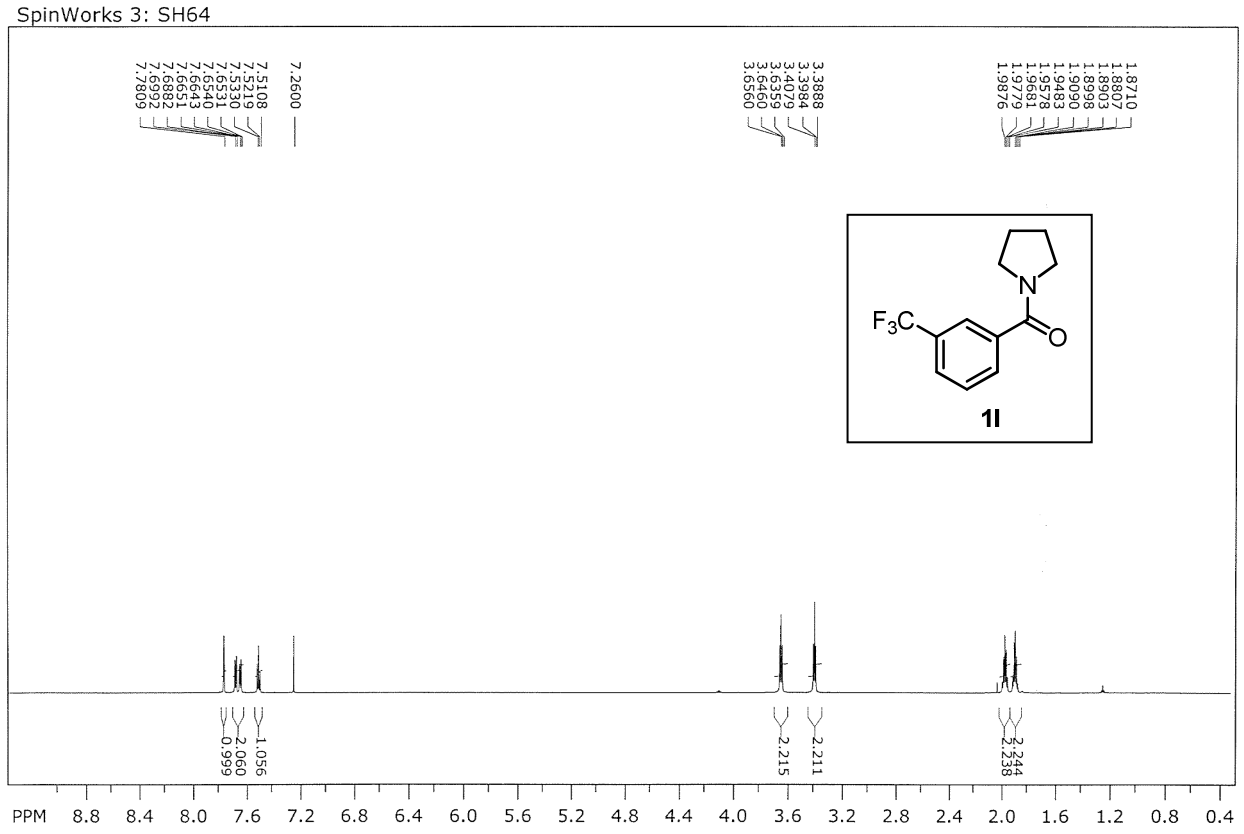
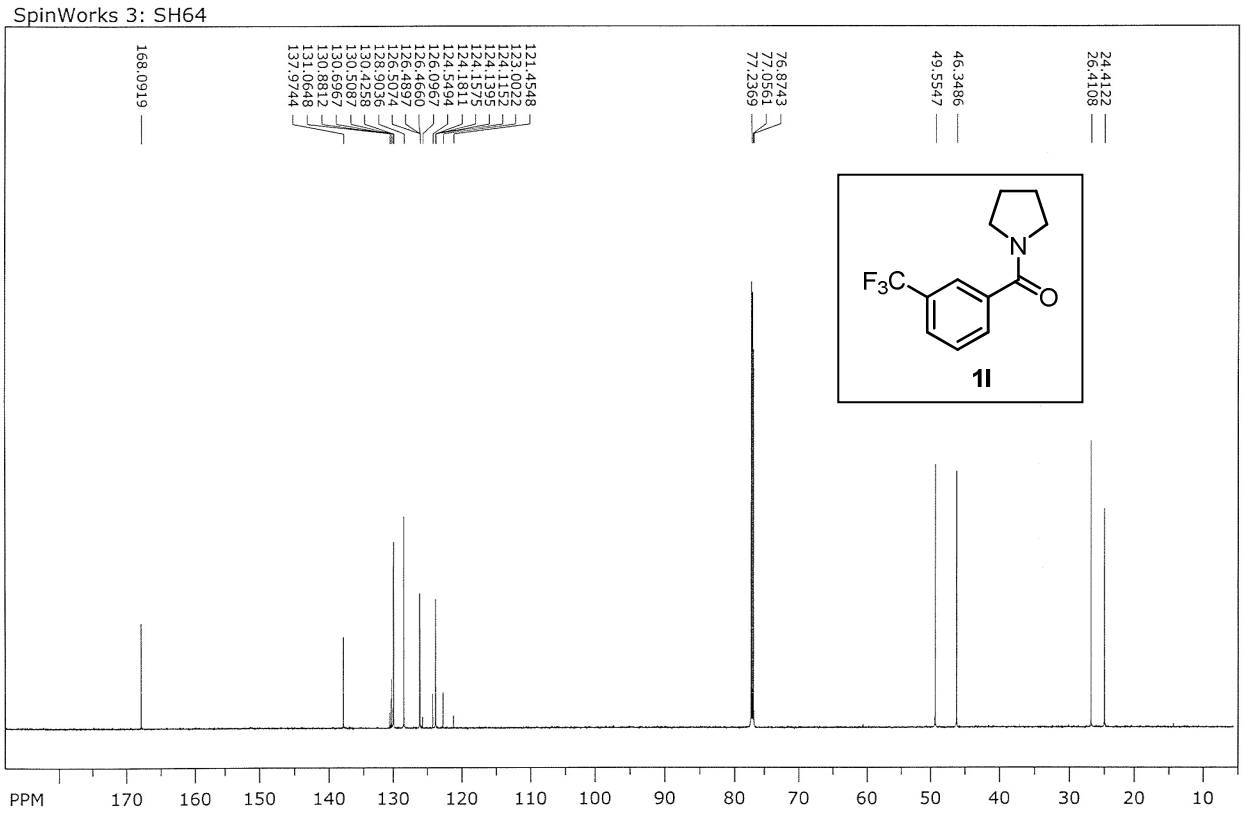
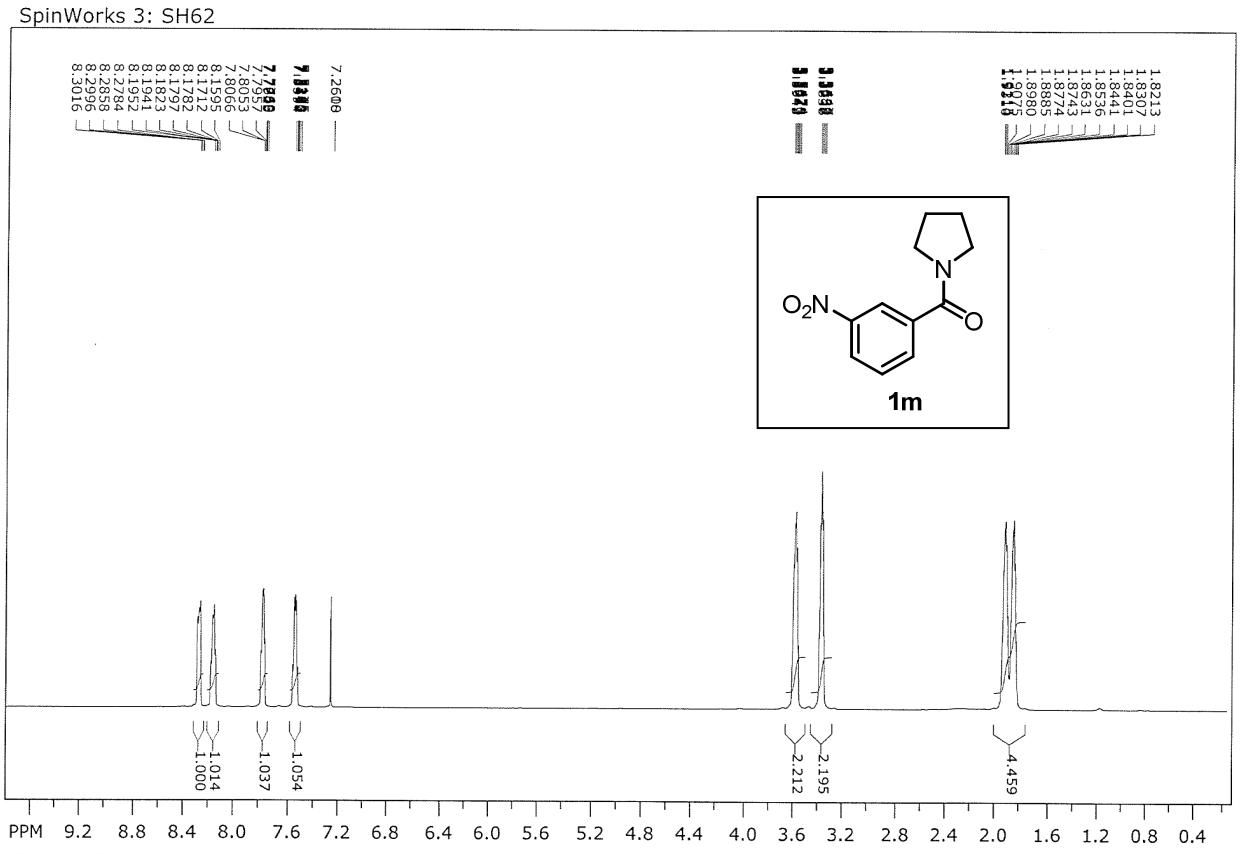
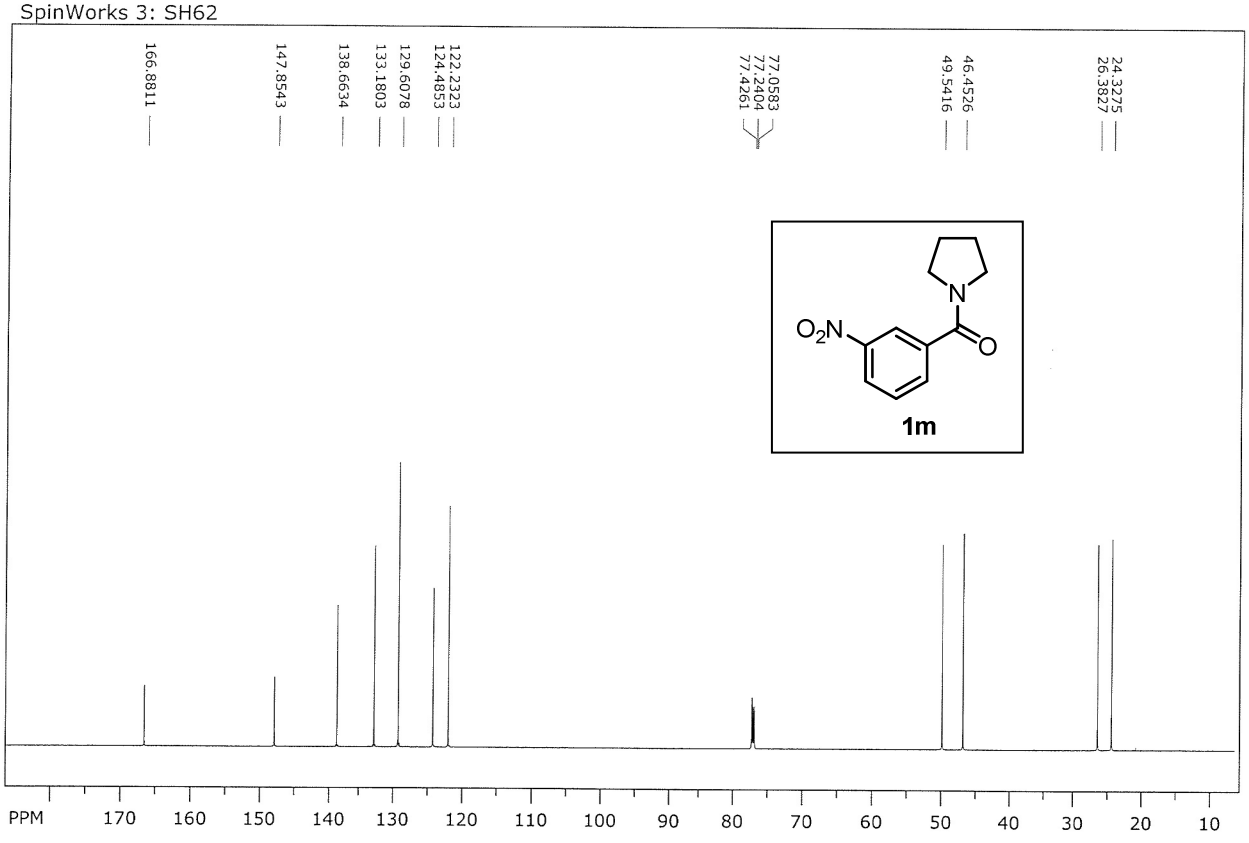
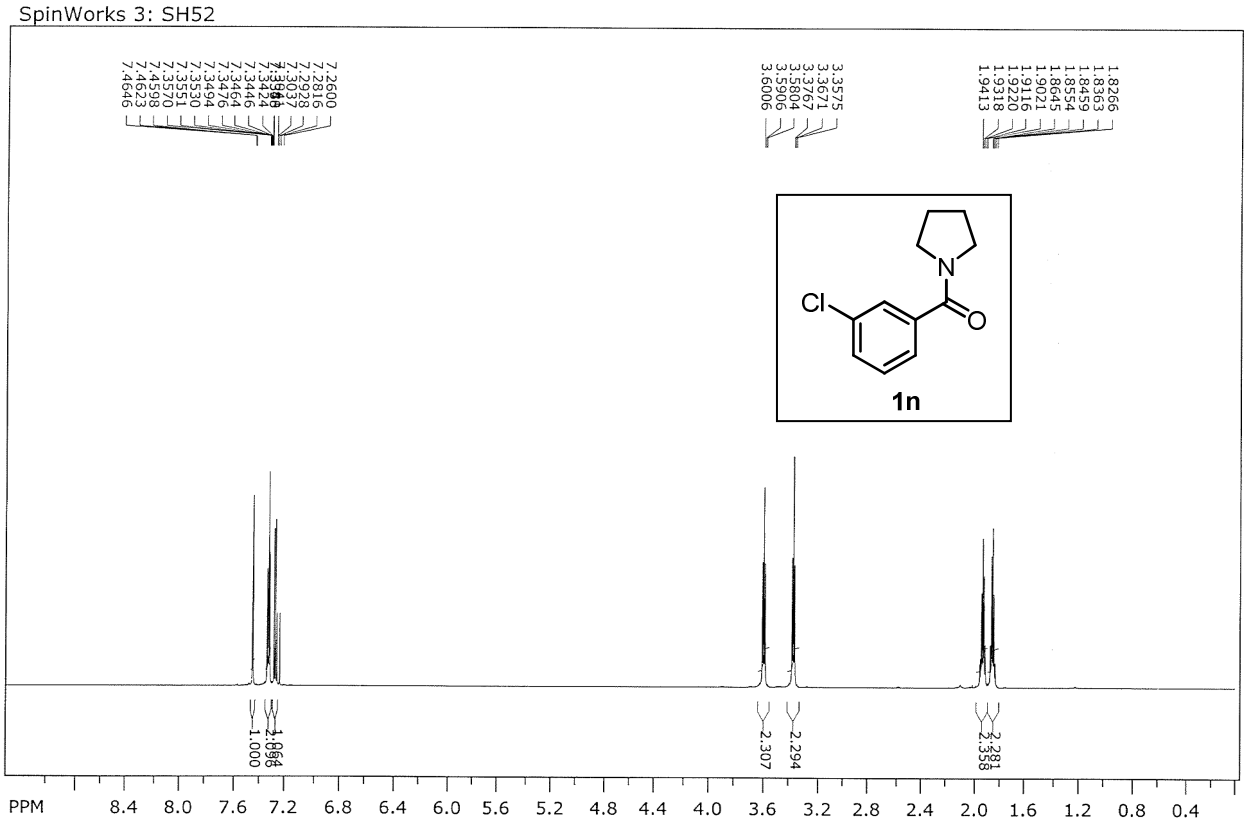
26.4362
24.4322
1k
PPM

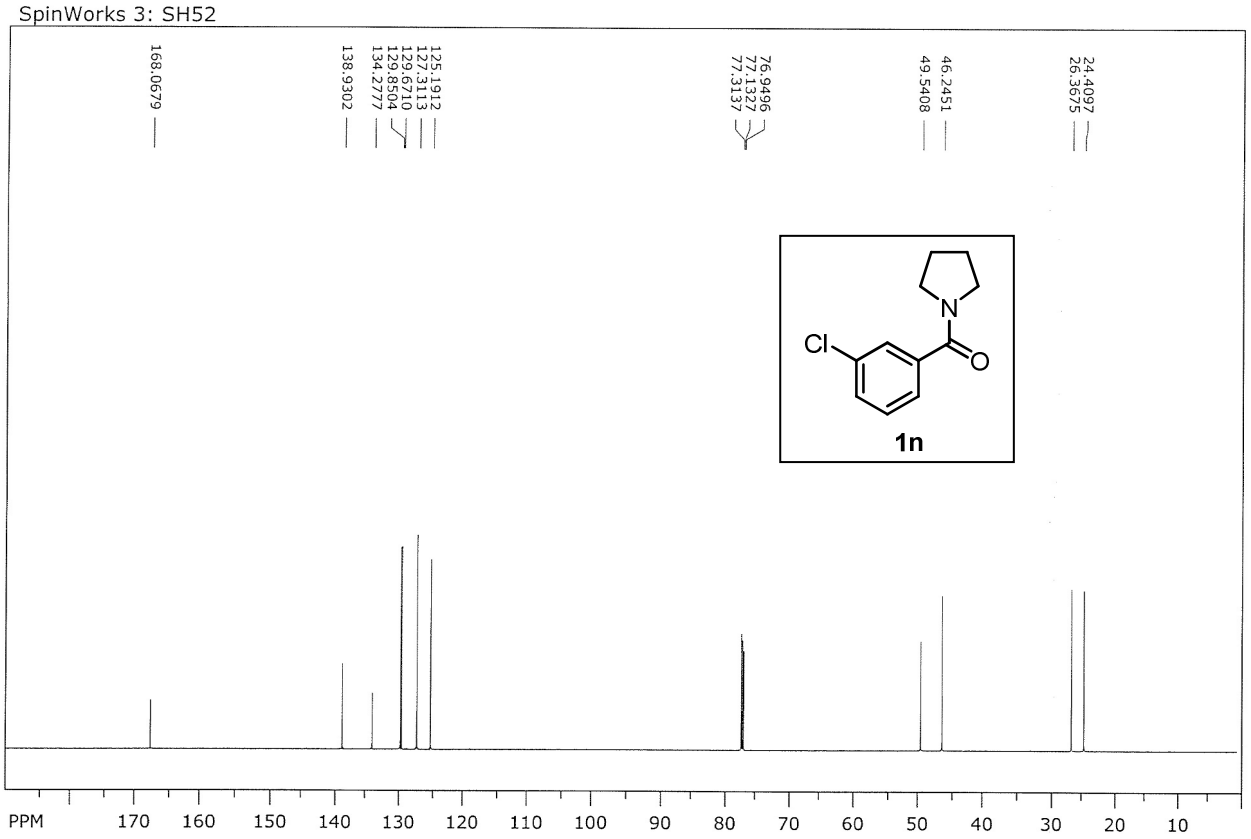

SpinWorks 3: SH64
7.7809
7.7682
7.6882
7.6651
7.6643
7.6540
7.6531
7.5330
7.5219
7.5108
7.2600
3.6560
3.6460
3.6359
3.4079
3.3984
3.3888
1.9876
1.9779
1.9681
1.9578
1.9483
1.9090
1.8998
1.8903
1.8807
1.8710
0.999
2.060
1.056
2.215
2.211
2.238
2.244
PPM 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4
F3C
N
O
1l

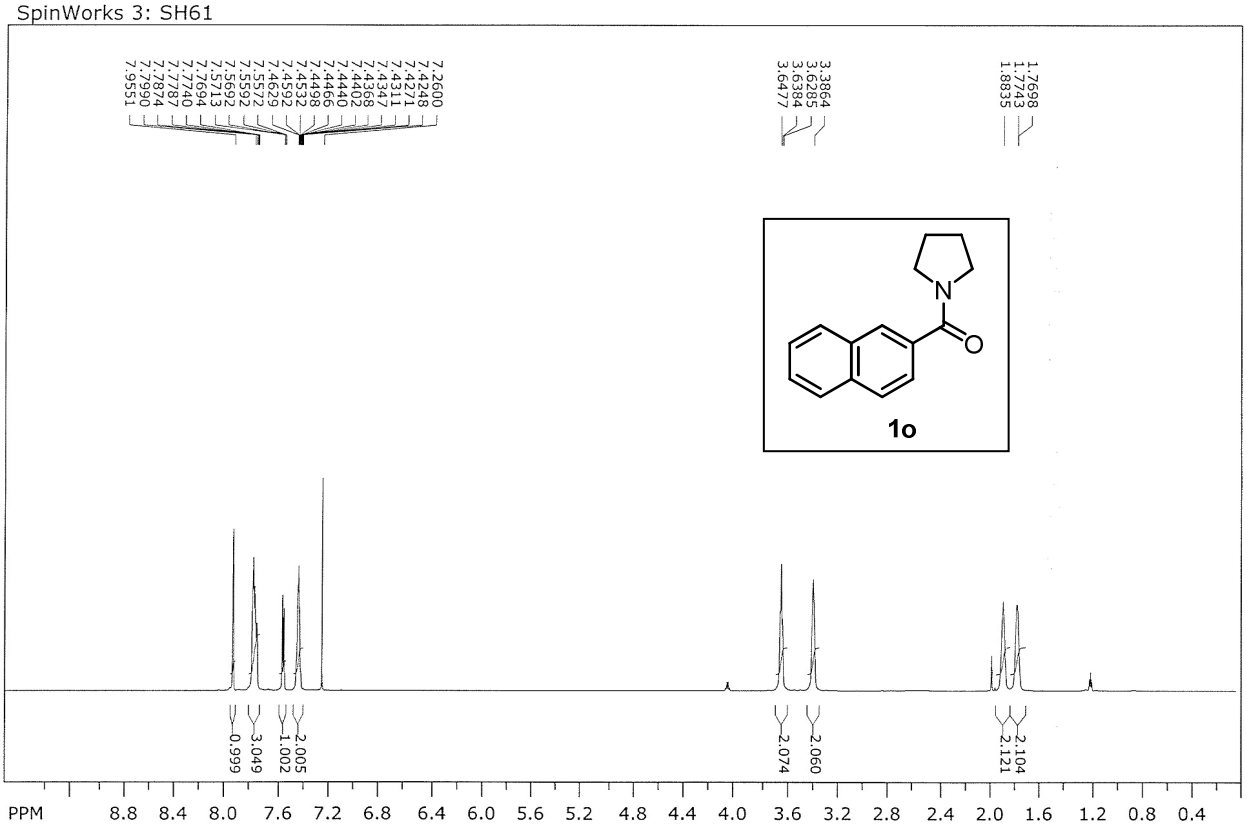

SpinWorks 3: SH64
168.0919
137.9744
131.0648
130.8812
130.6967
130.5087
130.4258
128.9026
126.5892
126.4660
126.0967
124.5494
124.1871
124.1595
124.1152
123.0022
121.4548
77.2369
77.0561
76.8743
49.5547
46.3486
26.4108
24.4122
PPM 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
F3C
N
O
1l

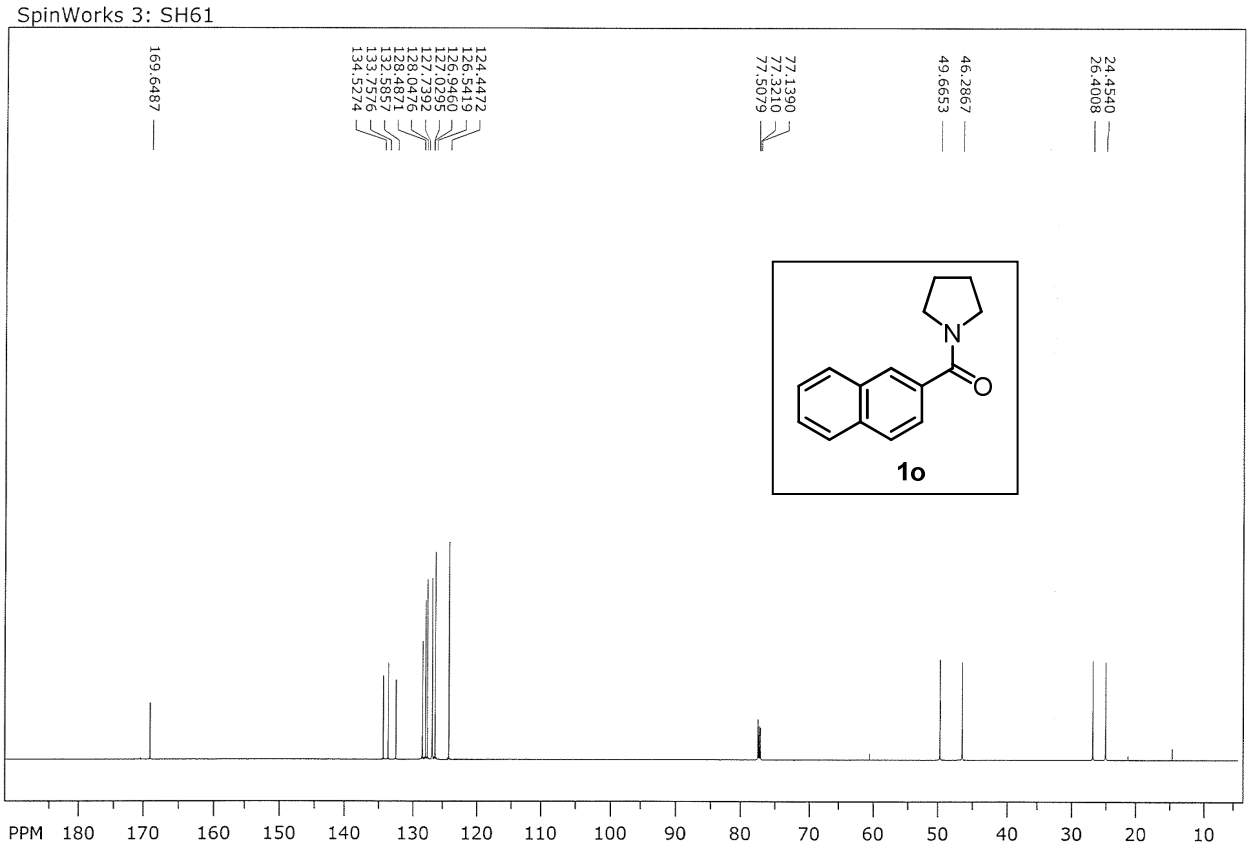

SpinWorks 3: SH62
1m
1.000
1.014
1.037
1.054
2.212
2.195
4.459
PPM

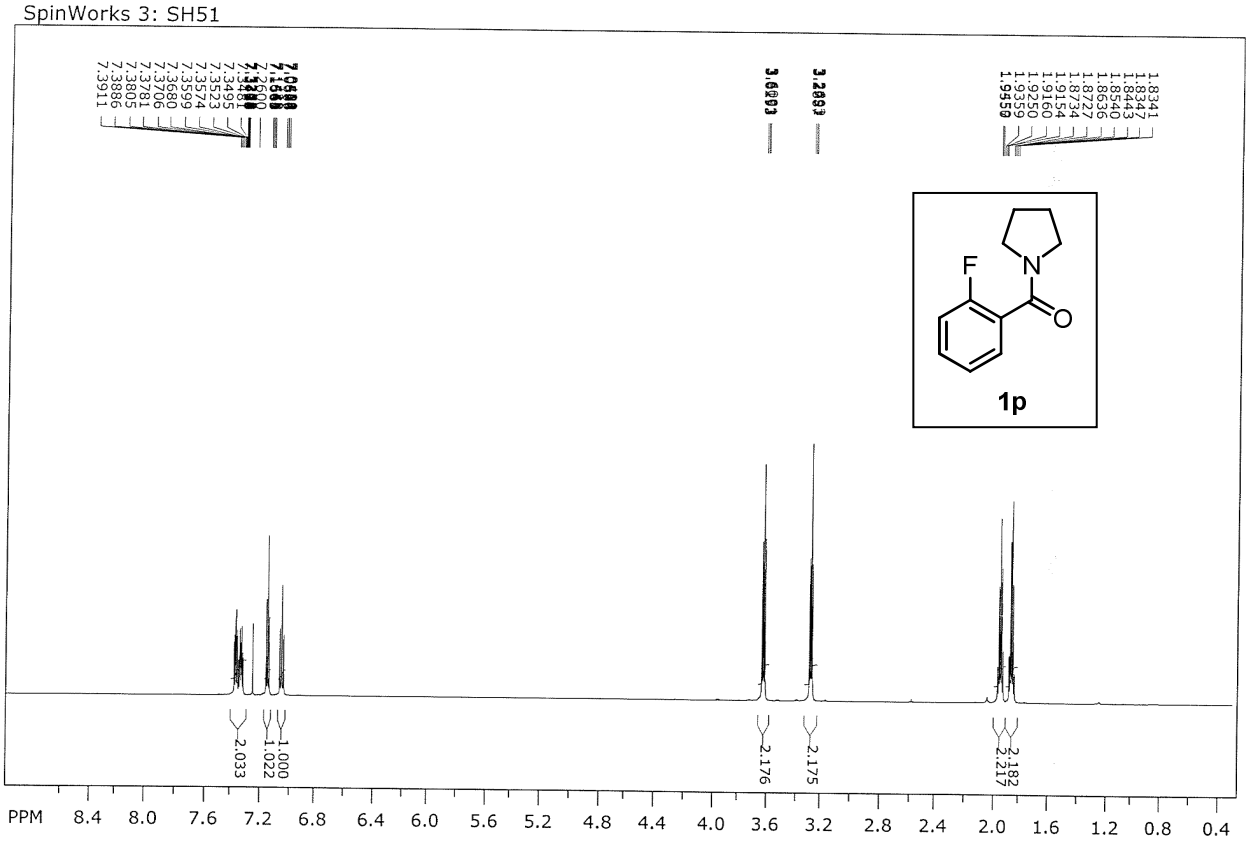

SpinWorks 3: SH62
166.8811
147.8543
138.6634
133.1803
129.6078
124.4853
122.2323
77.0583
77.2404
77.4261
49.5416
46.4526
26.3827
24.3275
1m
PPM

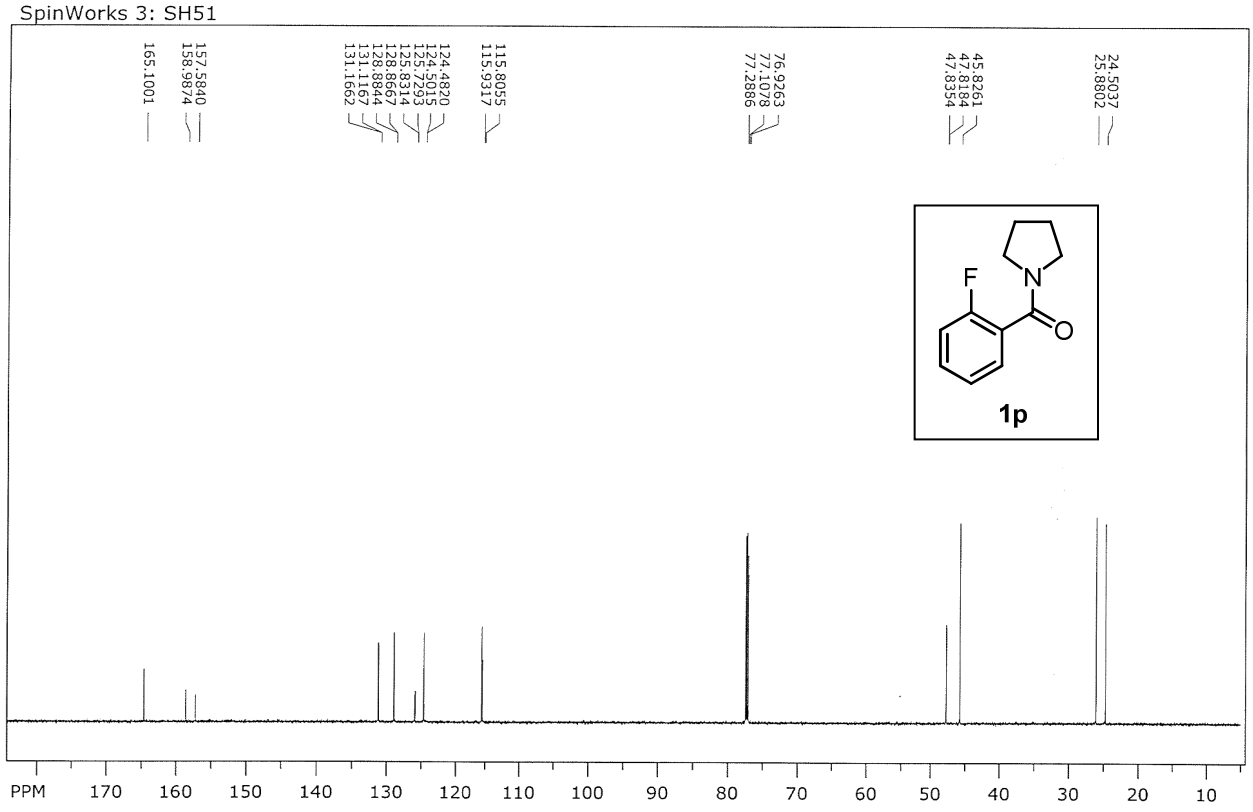

SpinWorks 3: SH52
7.2600
7.2816
7.2928
7.3037
7.3424
7.3446
7.3464
7.3476
7.3494
7.3530
7.3551
7.3570
7.4598
7.4623
7.4646
3.3575
3.3671
3.3767
3.5804
3.5906
3.6006
1.8266
1.8363
1.8459
1.8554
1.8645
1.9021
1.9116
1.9220
1.9318
1.9413
Cl
N
O
1n
1.000
2.307
2.294
2.358
PPM
8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

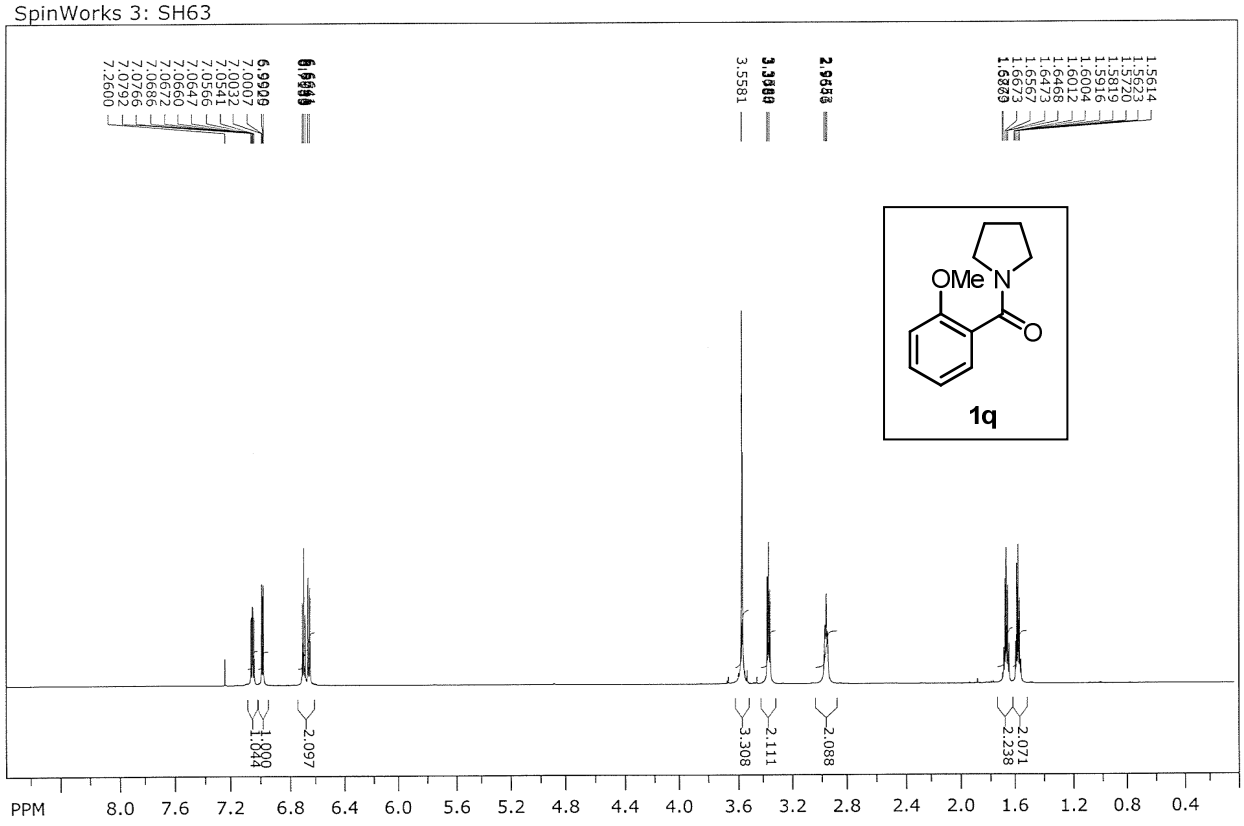

SpinWorks 3: SH52
168.0679
138.9302
134.2777
129.8504
129.6710
127.3113
125.1912
77.3137
77.1327
76.9496
49.5408
46.2451
26.3675
24.4097
Cl
N
O
1n
PPM
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

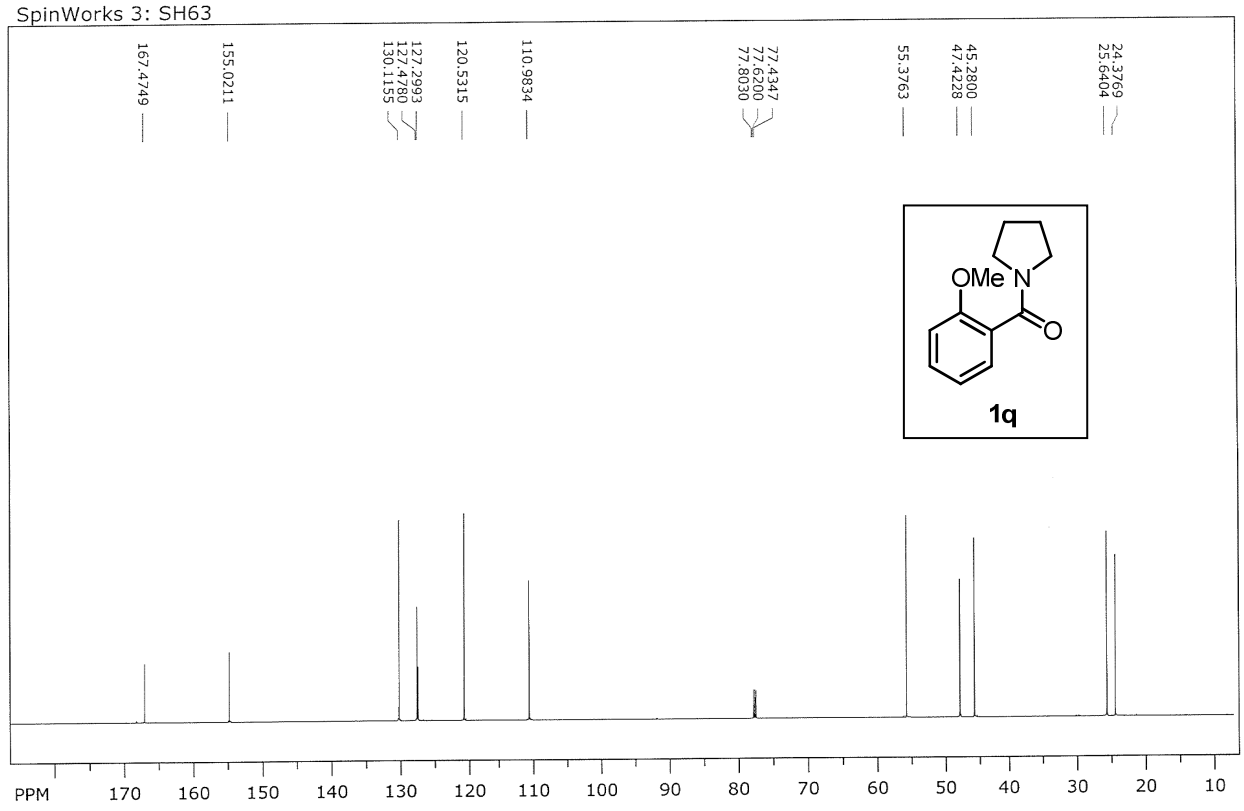

SpinWorks 3: SH61
7.9551
7.7990
7.7874
7.7787
7.7740
7.7694
7.5713
7.5692
7.5572
7.4629
7.4592
7.4532
7.4498
7.4466
7.4440
7.4402
7.4368
7.4347
7.4311
7.4278
7.2600
3.6477
3.6384
3.6285
3.3864
1.8835
1.7743
1.7698
1o
0.999
3.049
1.002
2.005
2.074
2.060
2.121
2.104
PPM 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

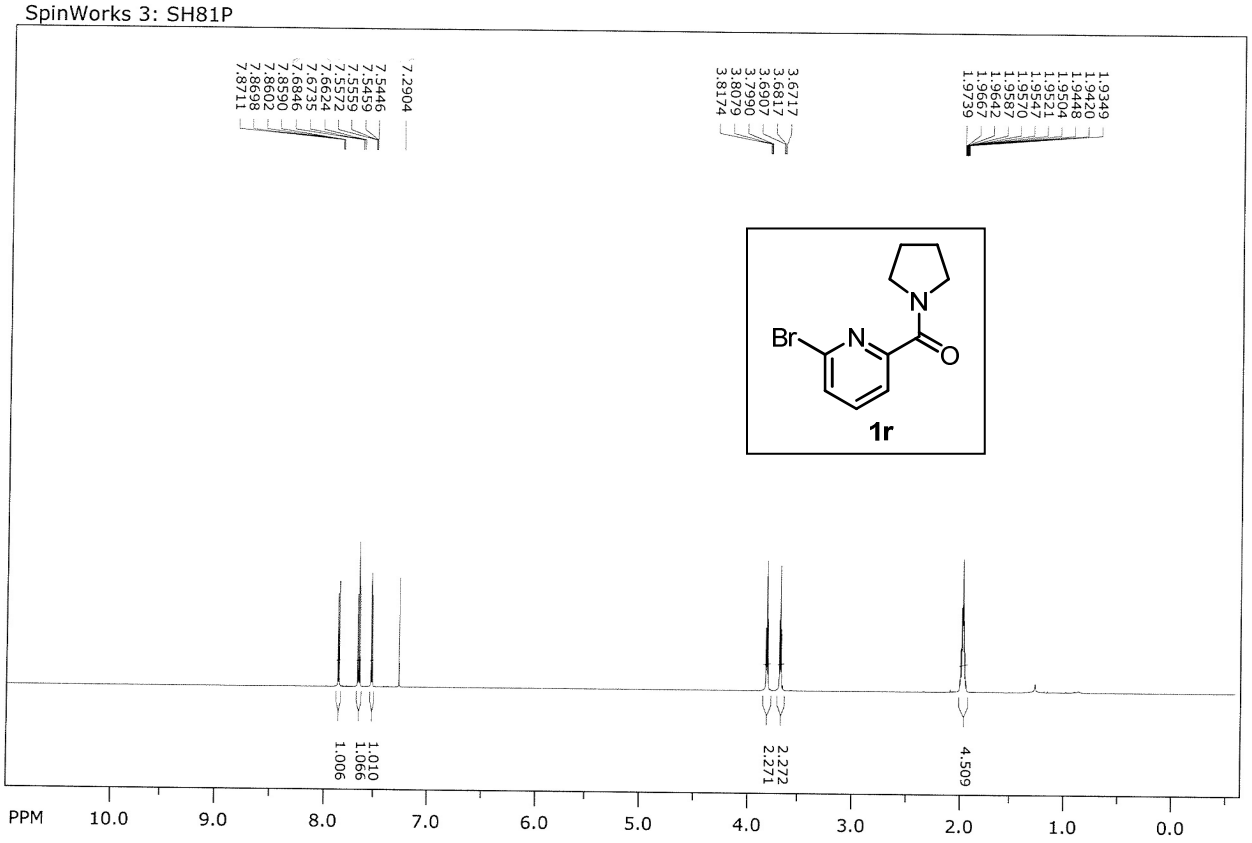

SpinWorks 3: SH61
169.6487
134.5274
133.7576
132.5857
128.4871
128.0476
127.7392
127.0295
126.9460
126.5419
124.4472
77.5079
77.3210
77.1390
49.6653
46.2867
26.4008
24.4540
1o
PPM 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

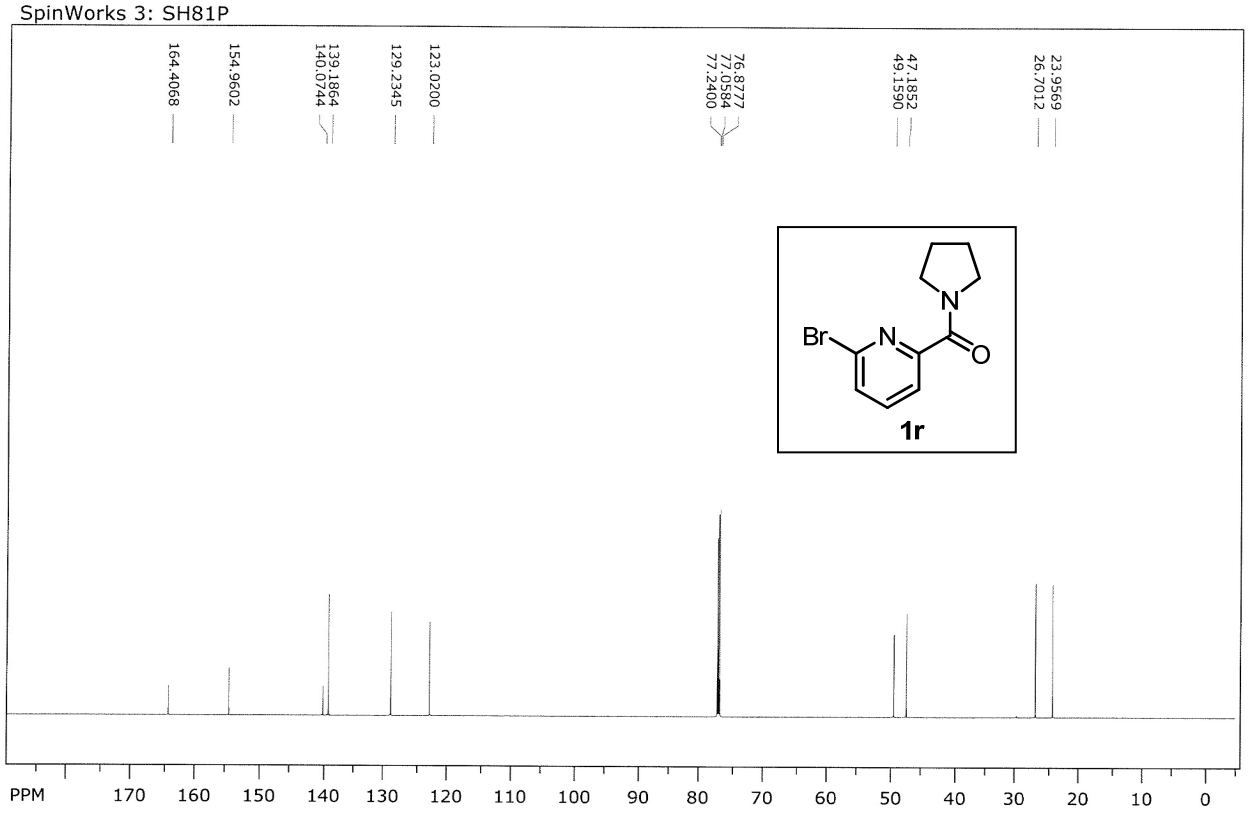

SpinWorks 3: SH51
F
N
O
1p
2.033
1.022
1.000
2.176
2.175
2.182
2.217
PPM 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

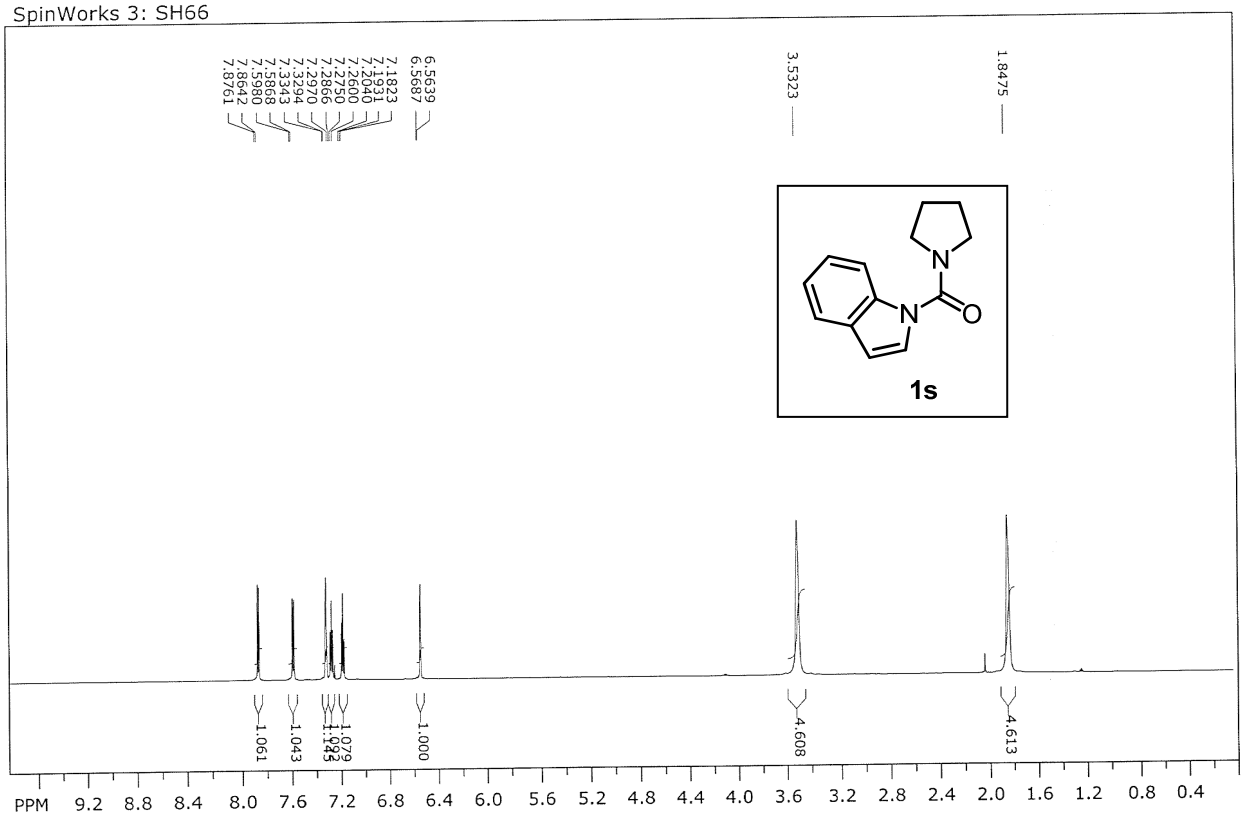

SpinWorks 3: SH51
165.1001
157.5840
158.9874
124.4820
124.5015
125.7293
125.8314
128.8667
128.8844
131.1167
131.1662
115.8055
115.9317
76.9263
77.1078
77.2886
45.8261
47.8184
47.8354
24.5037
25.8802
F
N
O
1p
PPM 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

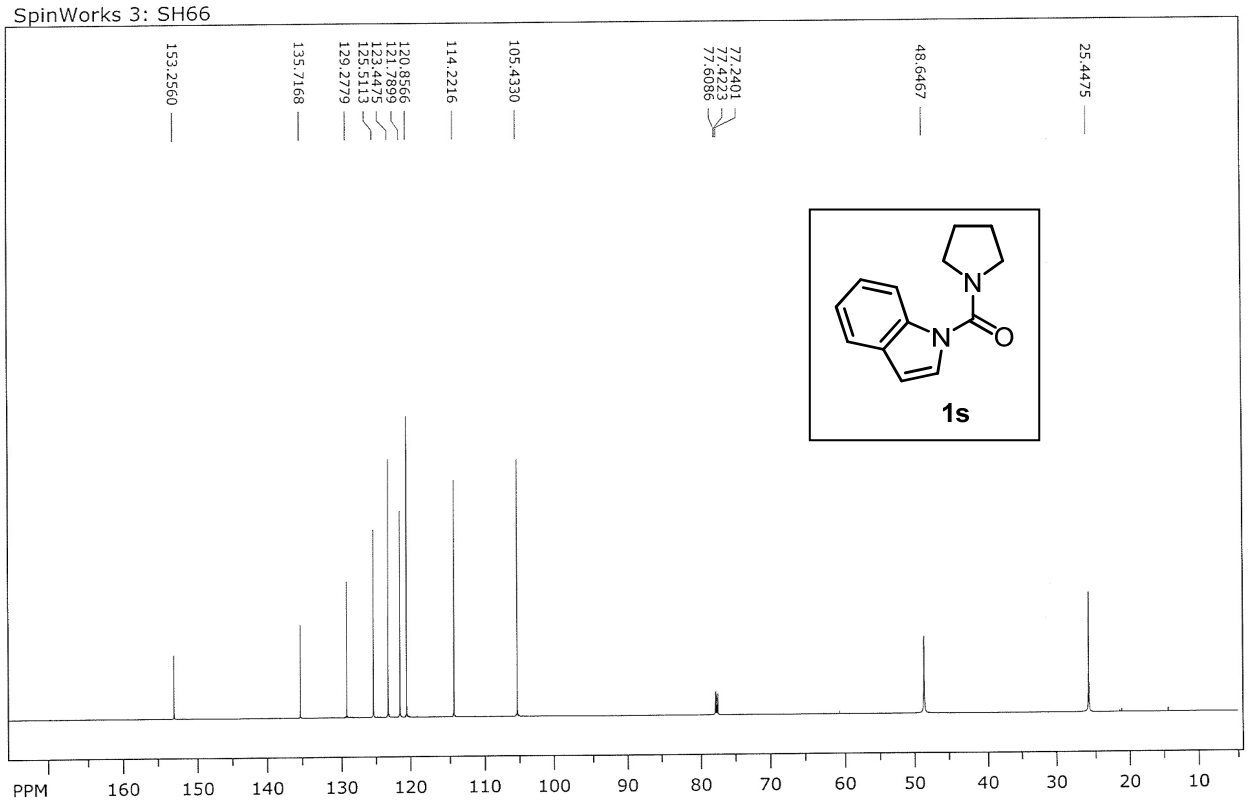

SpinWorks 3: SH63
7.2600
7.0792
7.0766
7.0686
7.0672
7.0660
7.0647
7.0566
7.0541
7.0032
7.0007
6.9909
3.5581
1.5614
1.5623
1.5720
1.5819
1.5916
1.6004
1.6012
1.6468
1.6473
1.6567
1.6673
1.6869
1.044
1.000
2.097
3.308
2.111
2.088
2.238
2.071
OMe
N
O
1q
PPM
8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

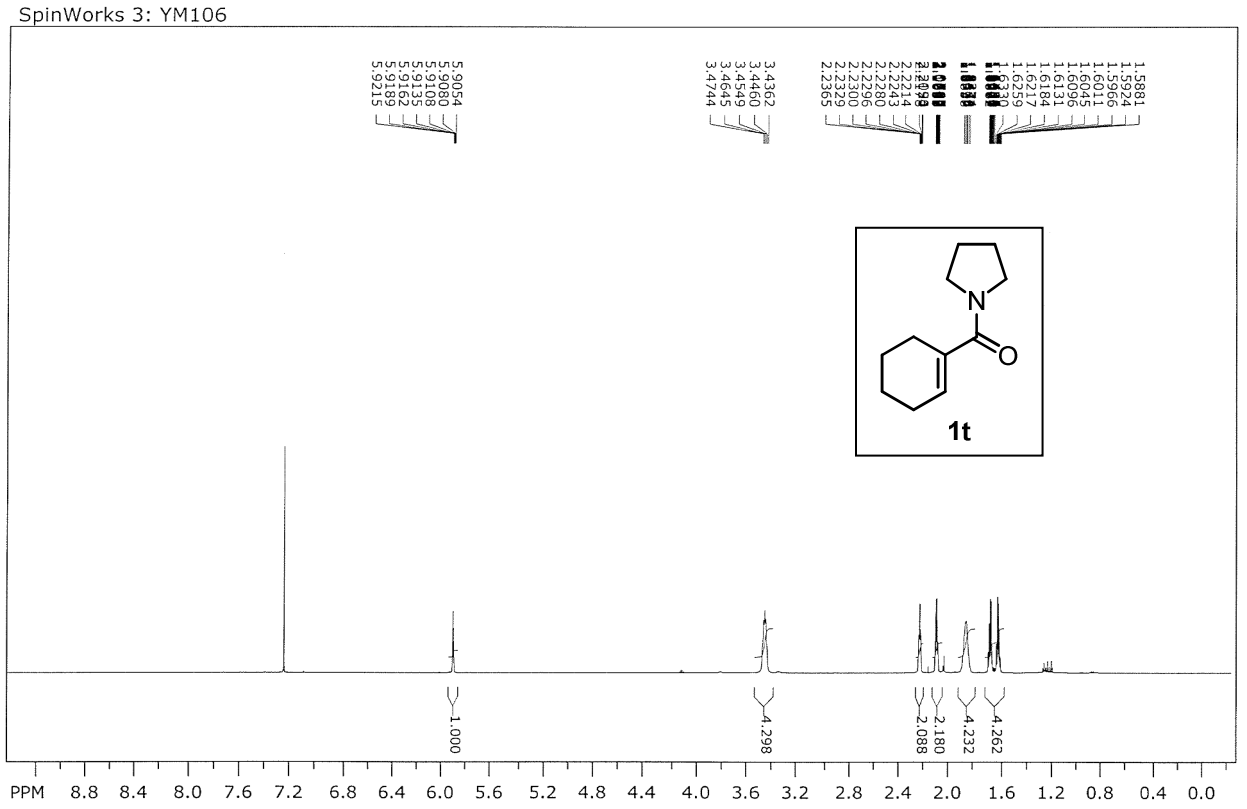

SpinWorks 3: SH63
167.4749
155.0211
130.1155
127.4780
127.2993
120.5315
110.9834
77.8030
77.6200
77.4347
55.3763
47.4228
45.2800
25.6404
24.3769
OMe
N
O
1q
PPM
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

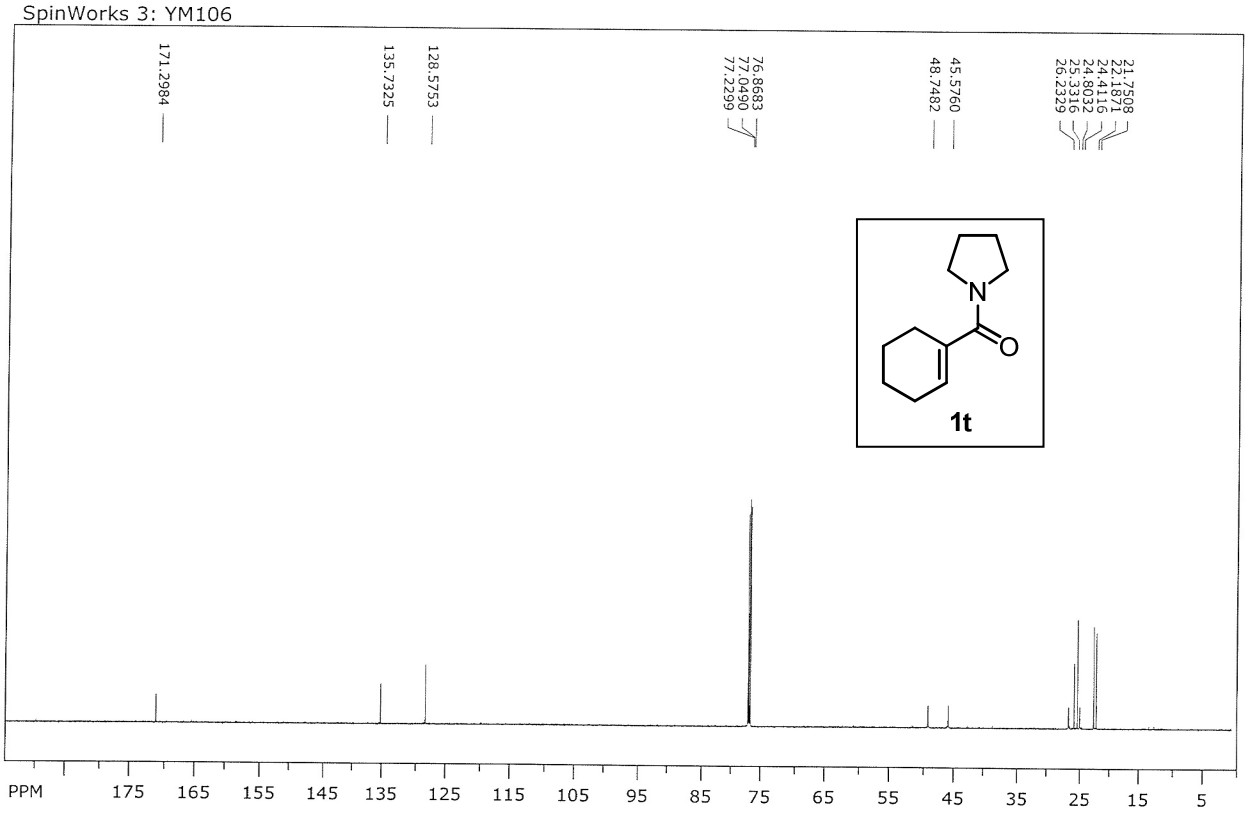

SpinWorks 3: SH81P
7.8711
7.8698
7.8602
7.8590
7.6846
7.6735
7.6624
7.5572
7.5559
7.5459
7.5446
7.2904
3.8174
3.8079
3.7990
3.6907
3.6817
3.6717
1.9739
1.9667
1.9642
1.9587
1.9570
1.9547
1.9521
1.9504
1.9448
1.9420
1.9349
Br
N
N
O
1r
1.006
1.066
1.010
2.271
2.272
4.509
PPM
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

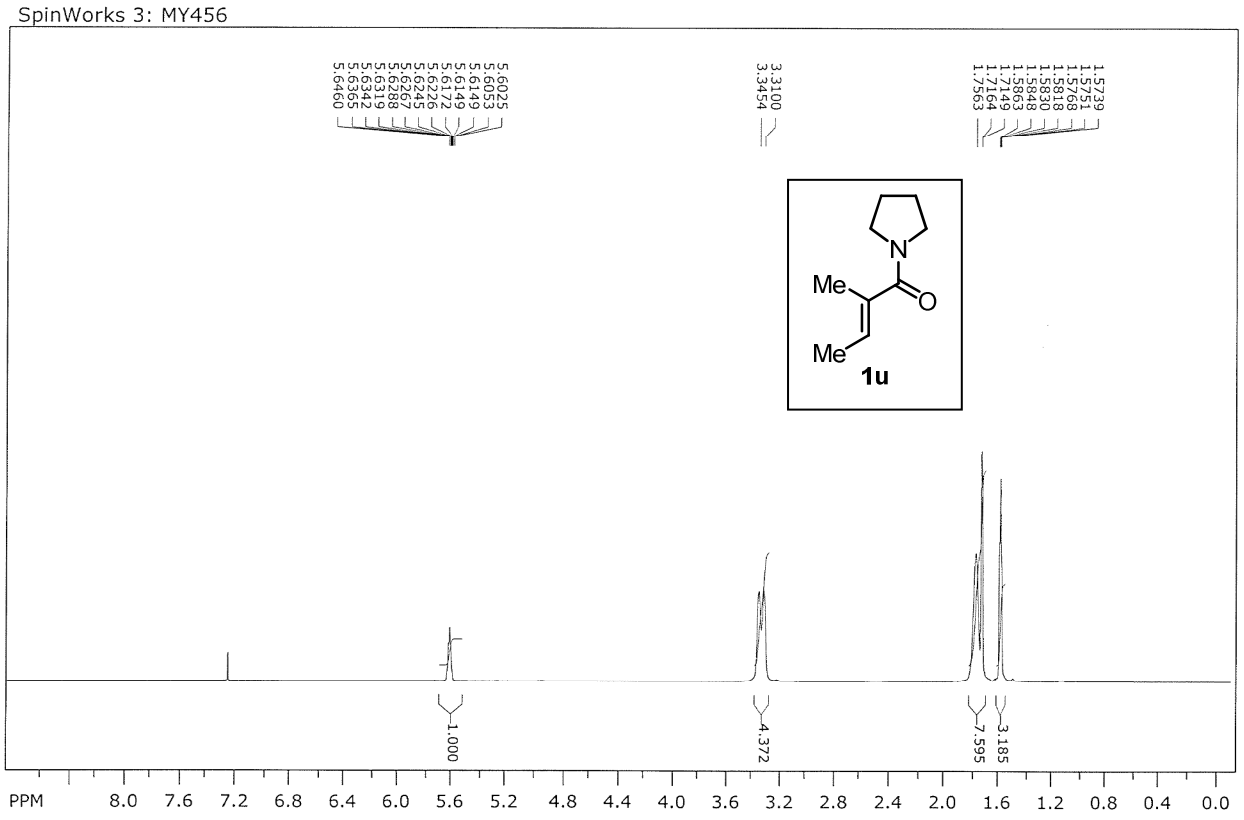

SpinWorks 3: SH81P
164.4068
154.9602
140.0744
139.1864
129.2345
123.0200
77.2400
77.0584
76.8777
49.1590
47.1852
26.7012
23.9569
Br
N
N
O
1r
PPM
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

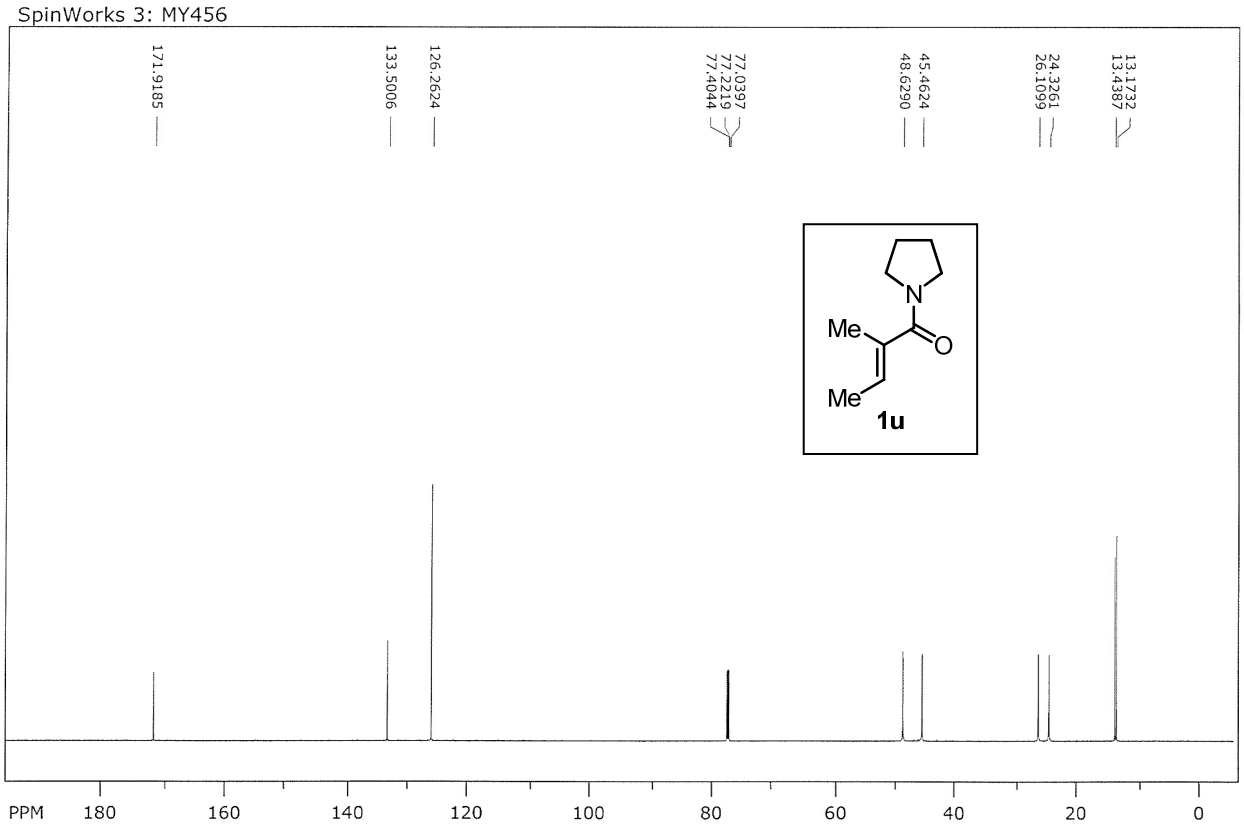

SpinWorks 3: SH66
7.8761
7.8642
7.5980
7.5868
7.3343
7.3294
7.2970
7.2866
7.2750
7.2600
7.2040
7.1823
6.5639
6.5687
3.5323
1.8475
1s
1.061
1.043
1.079
1.000
4.608
4.613
PPM 9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

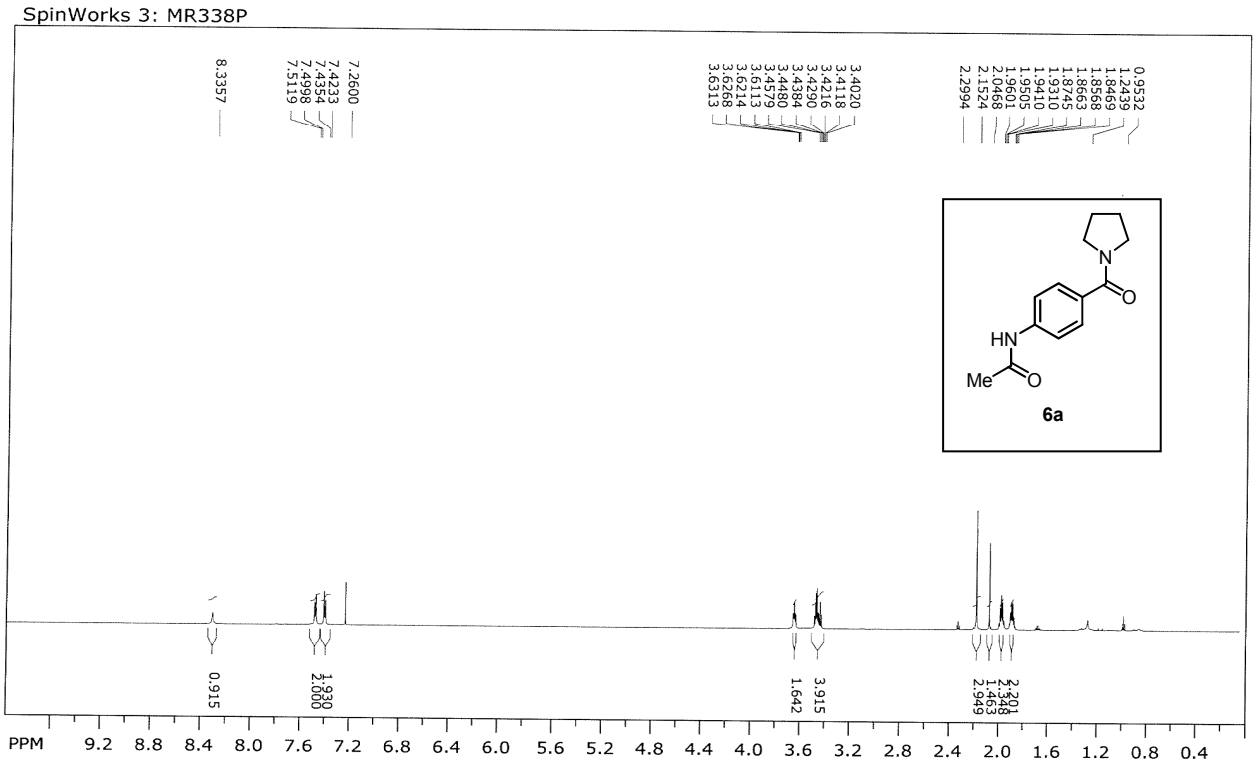

SpinWorks 3: SH66
153.2560
135.7168
129.2779
123.4475
121.7899
120.8566
114.2216
105.4330
77.2401
77.4223
77.6086
48.6467
25.4475
1s
PPM 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

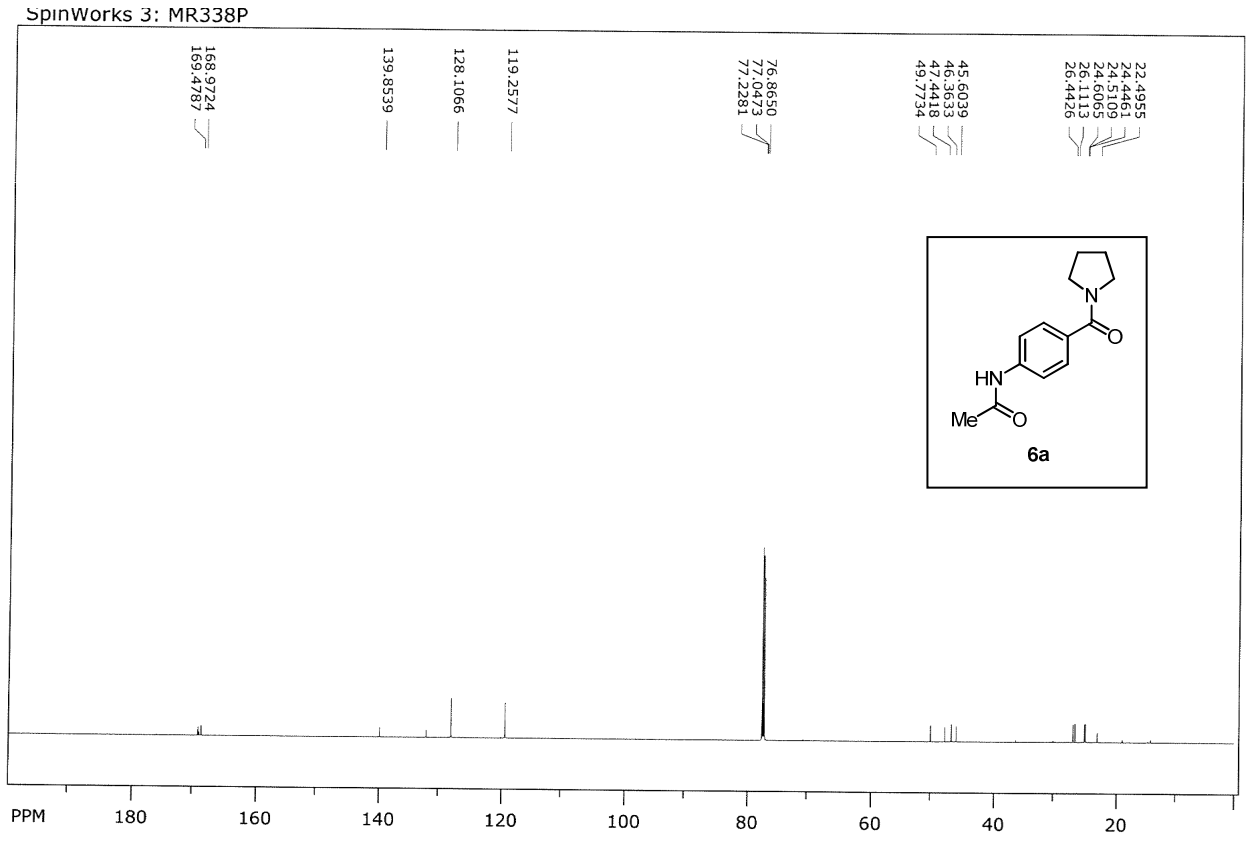

SpinWorks 3: YM106
1t
1.000
4.298
2.088
2.180
4.232
4.262
PPM


SpinWorks 3: YM106
171.2984
135.7325
128.5753
76.8683
77.0490
77.2299
45.5760
48.7482
21.7508
22.1871
24.4116
24.8032
25.3316
26.2329
1t
PPM

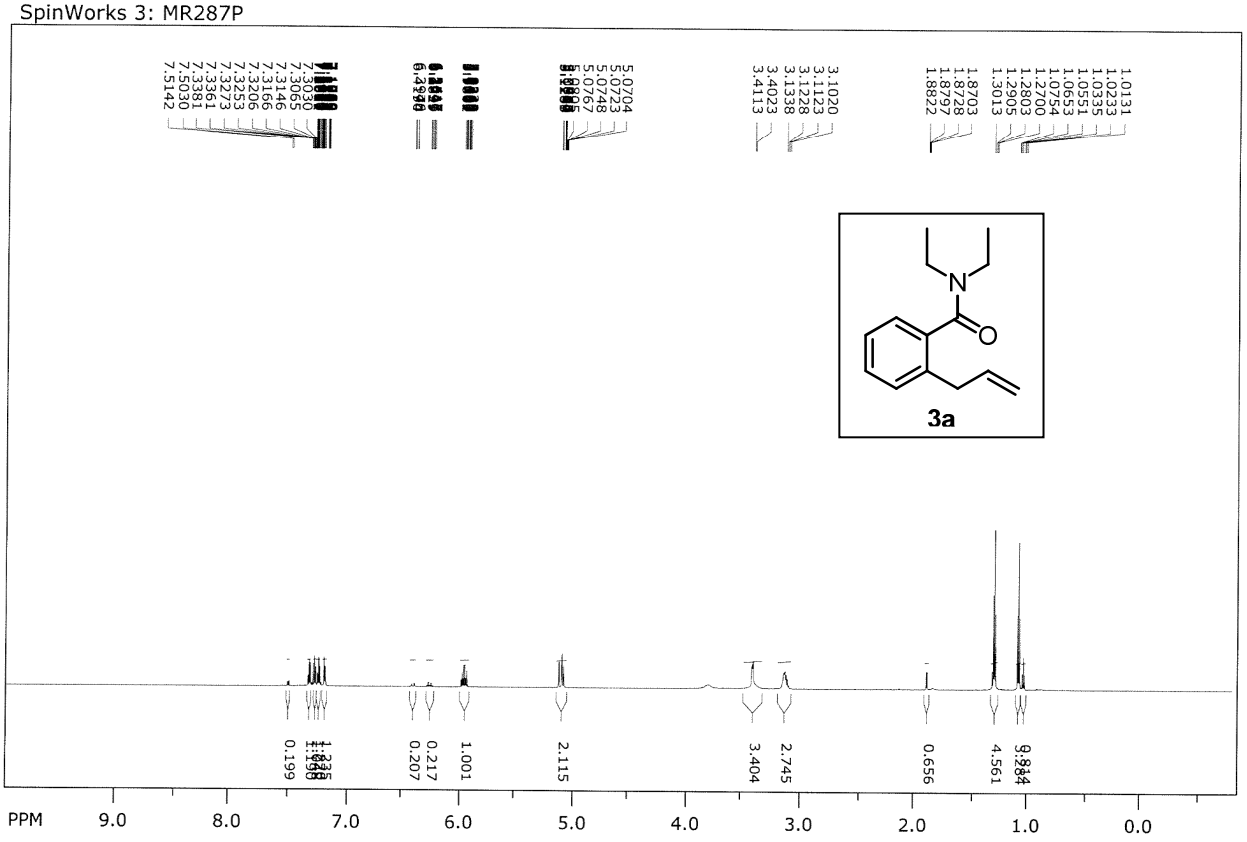

SpinWorks 3: MY456
5.6460
5.6365
5.6342
5.6319
5.6288
5.6245
5.6226
5.6172
5.6149
5.6149
5.6053
5.6025
3.3454
3.3100
1.7563
1.7449
1.7164
1.5863
1.5848
1.5830
1.5818
1.5768
1.5751
1.5739
Me
Me
1u
1.000
4.372
7.595
3.185
PPM
8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0


SpinWorks 3: MY456
171.9185
133.5006
126.2624
77.0397
77.2219
77.4044
48.6290
45.4624
26.1099
24.3261
13.4387
13.1732
Me
Me
1u
PPM
180 160 140 120 100 80 60 40 20 0

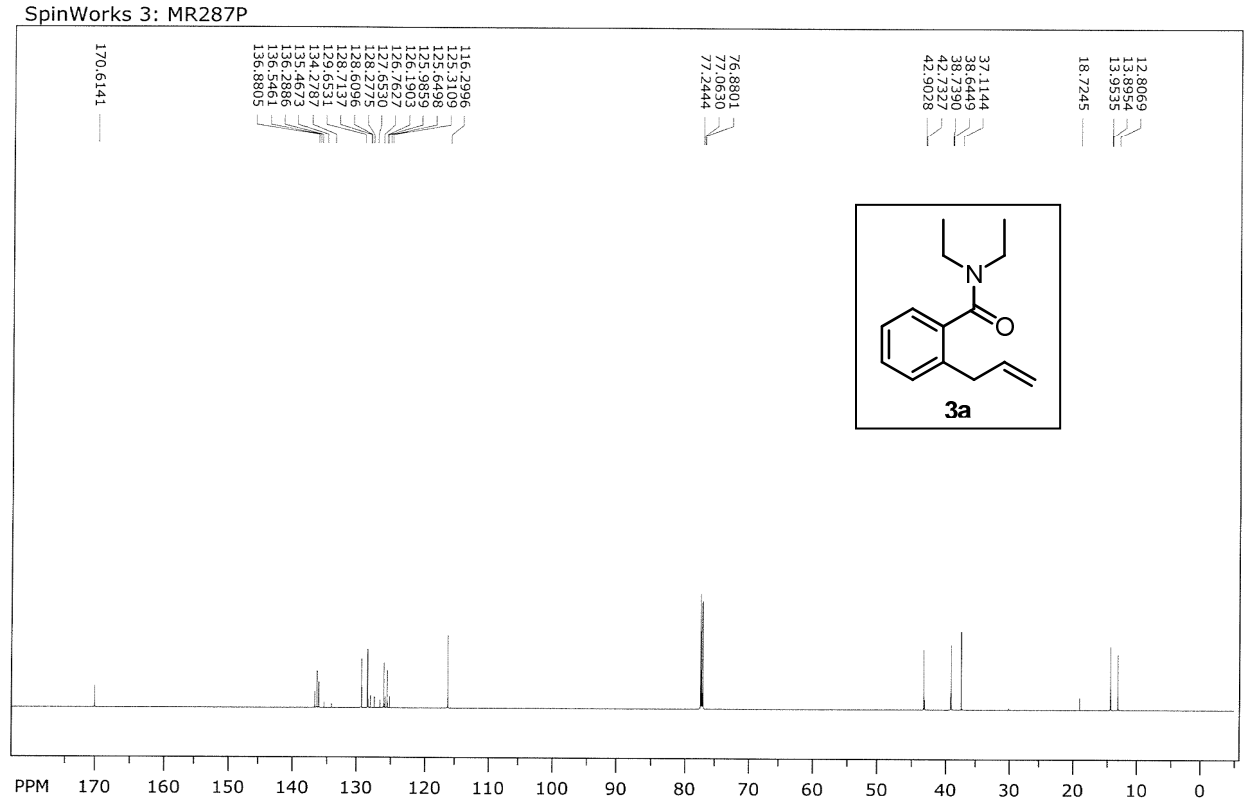

SpinWorks 3: MR338P
8.3357
7.5119
7.4998
7.4354
7.4233
7.2600
3.6313
3.6268
3.6214
3.6113
3.4579
3.4480
3.4384
3.4290
3.4216
3.4118
3.4020
2.2994
2.1524
2.0468
1.9601
1.9505
1.9410
1.9310
1.8745
1.8663
1.8568
1.8469
1.2439
0.9532
HN
Me
O
6a
0.915
2.000
1.930
1.642
3.915
2.949
1.463
1.348
2.201
PPM
9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

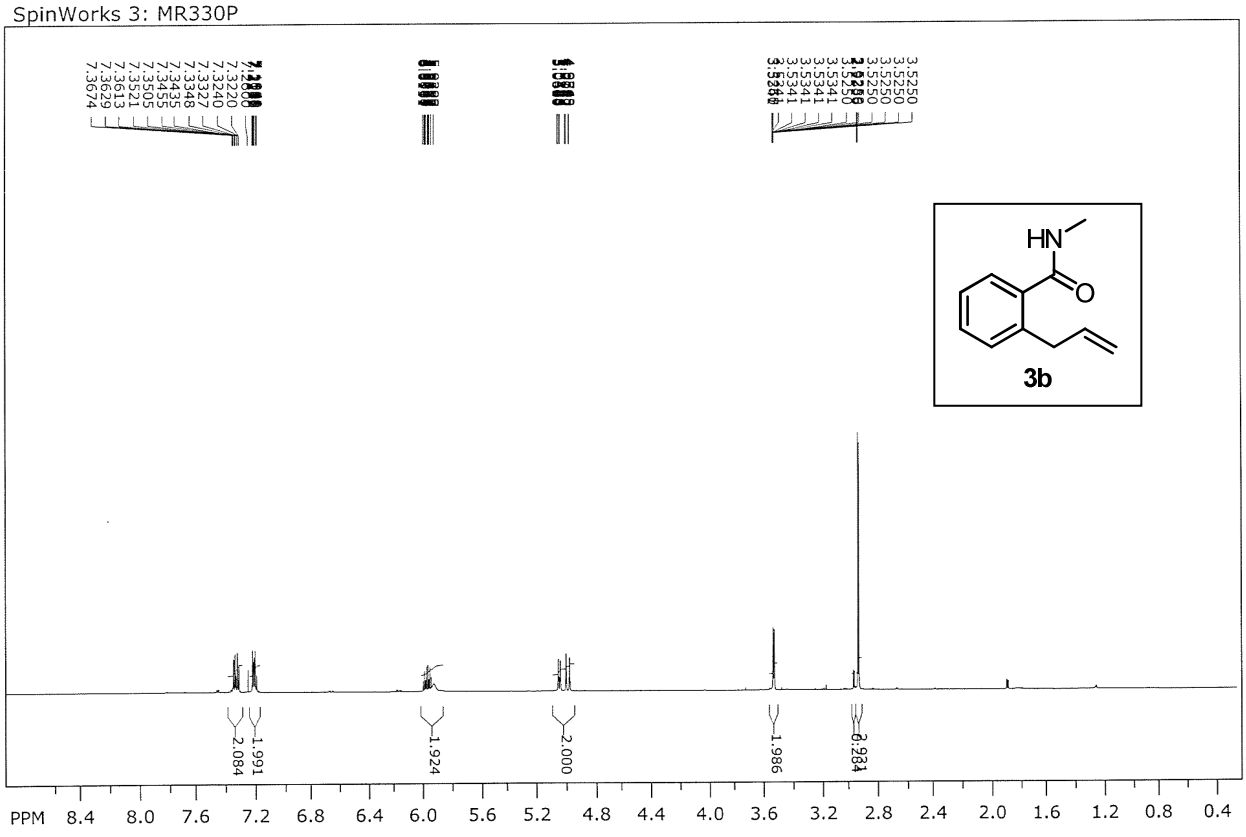

SpinWorks 3: MR338P
169.4787
168.9724
139.8539
128.1066
119.2577
77.2281
77.0473
76.8650
49.7734
47.4418
46.3633
45.6039
26.4426
26.1113
24.6065
24.5109
24.4461
22.4955
HN
Me
O
6a
PPM
180 160 140 120 100 80 60 40 20

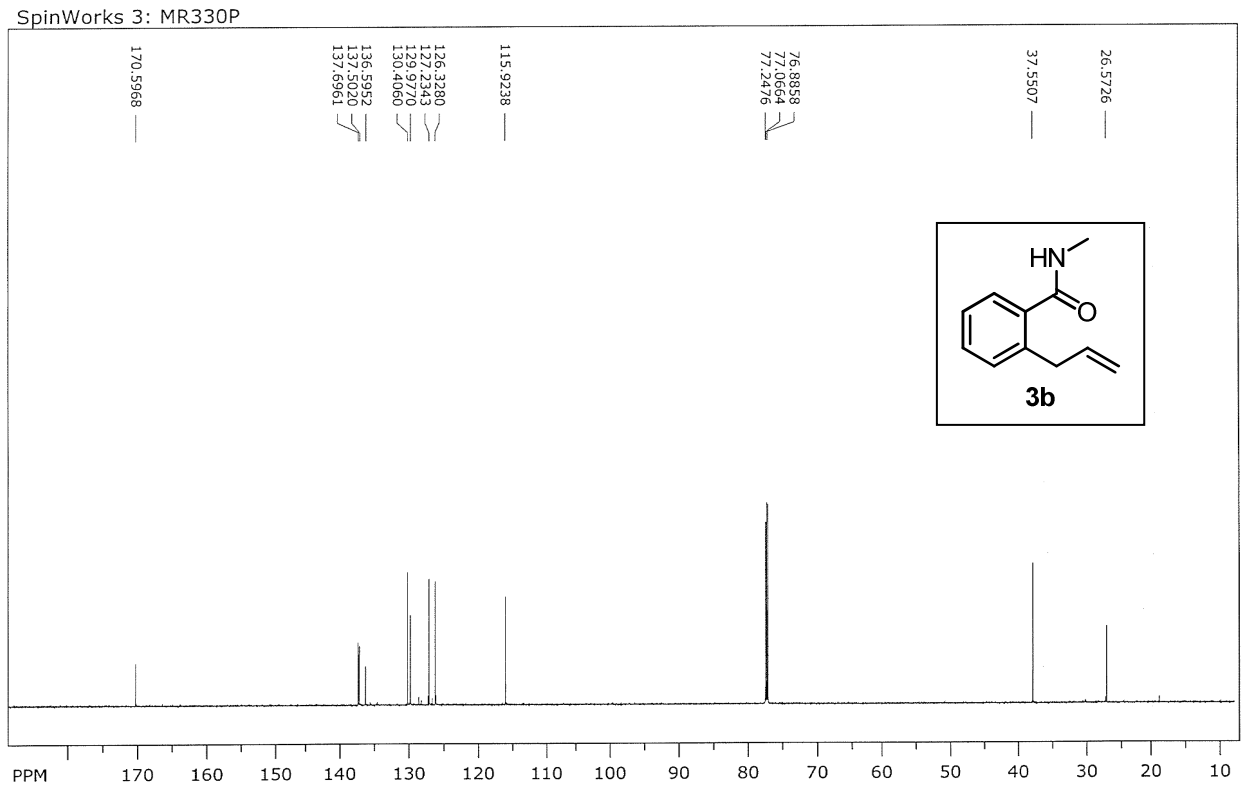
SpinWorks 3: MR287P

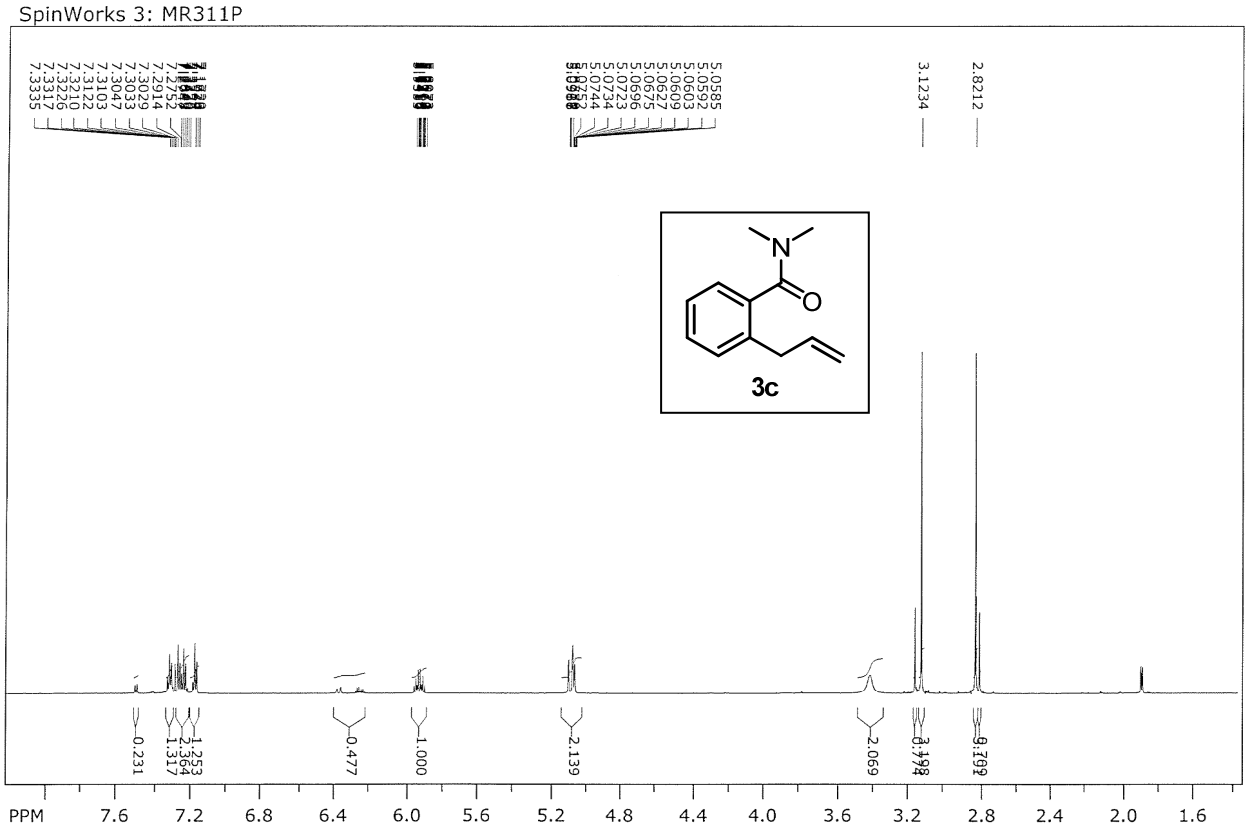


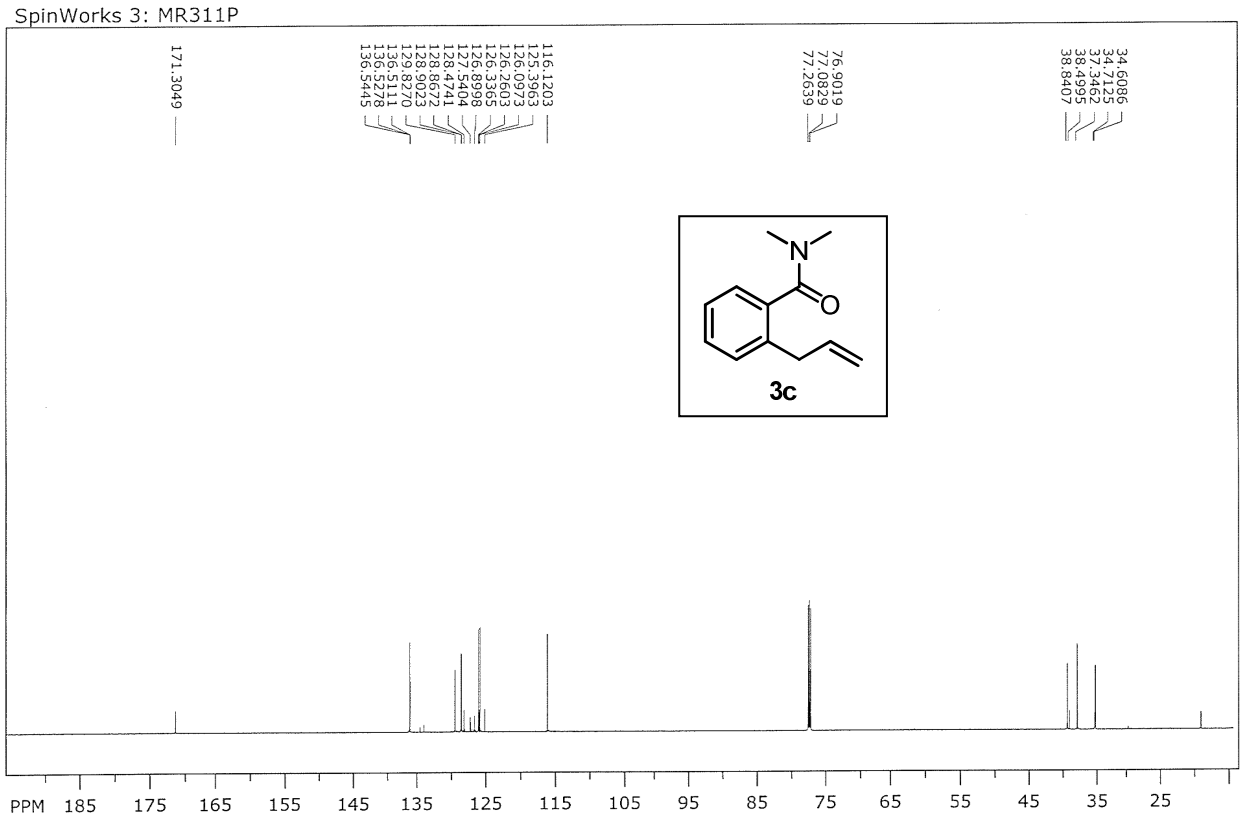
SpinWorks 3: MR287P

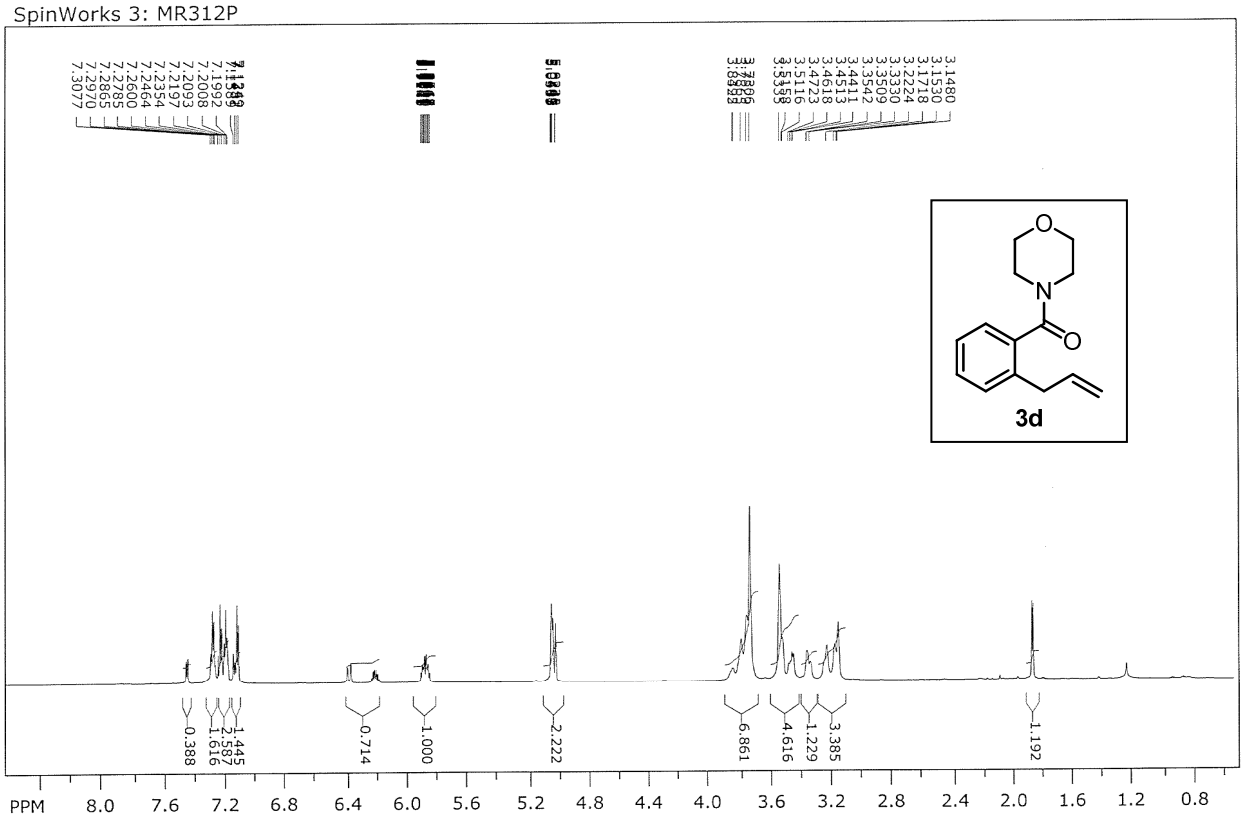


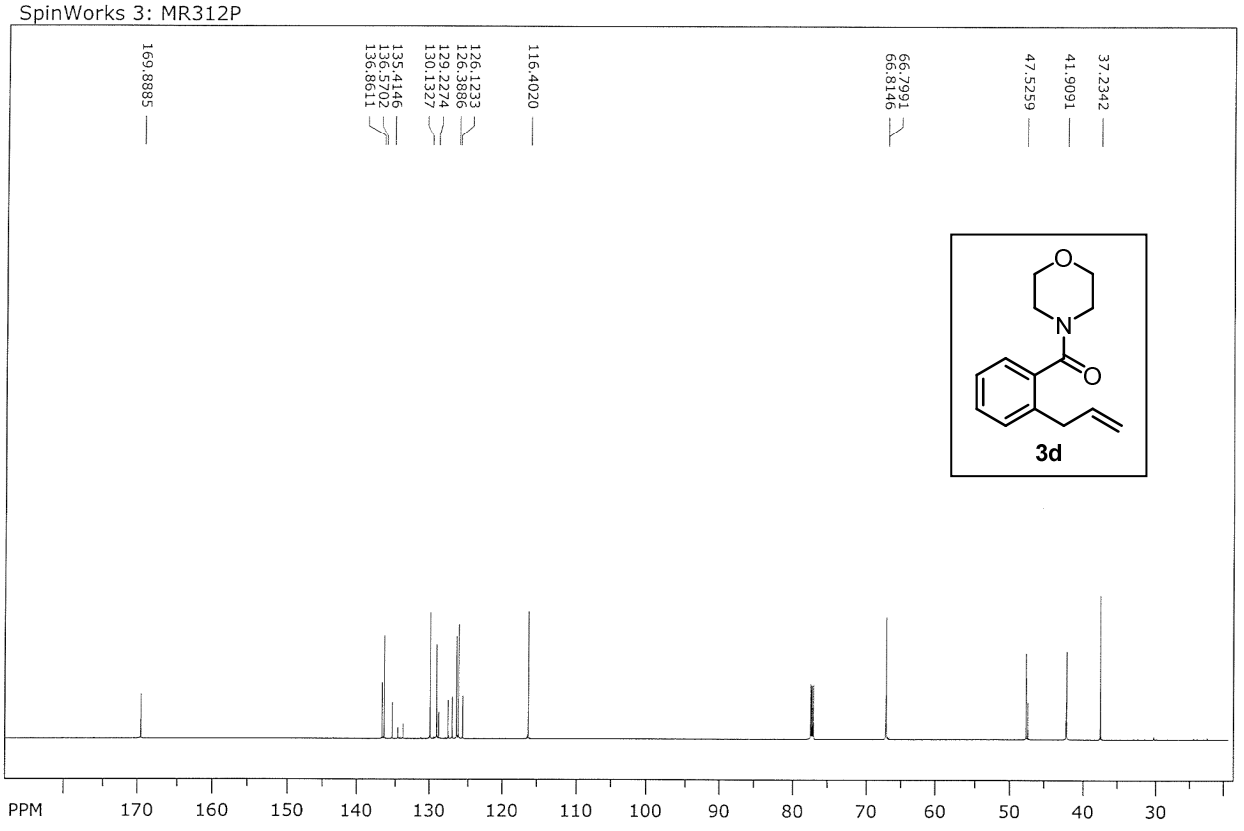

SpinWorks 3: MR330P
HN
O
3b
2.084
1.991
1.924
2.000
1.986
8.934
PPM 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

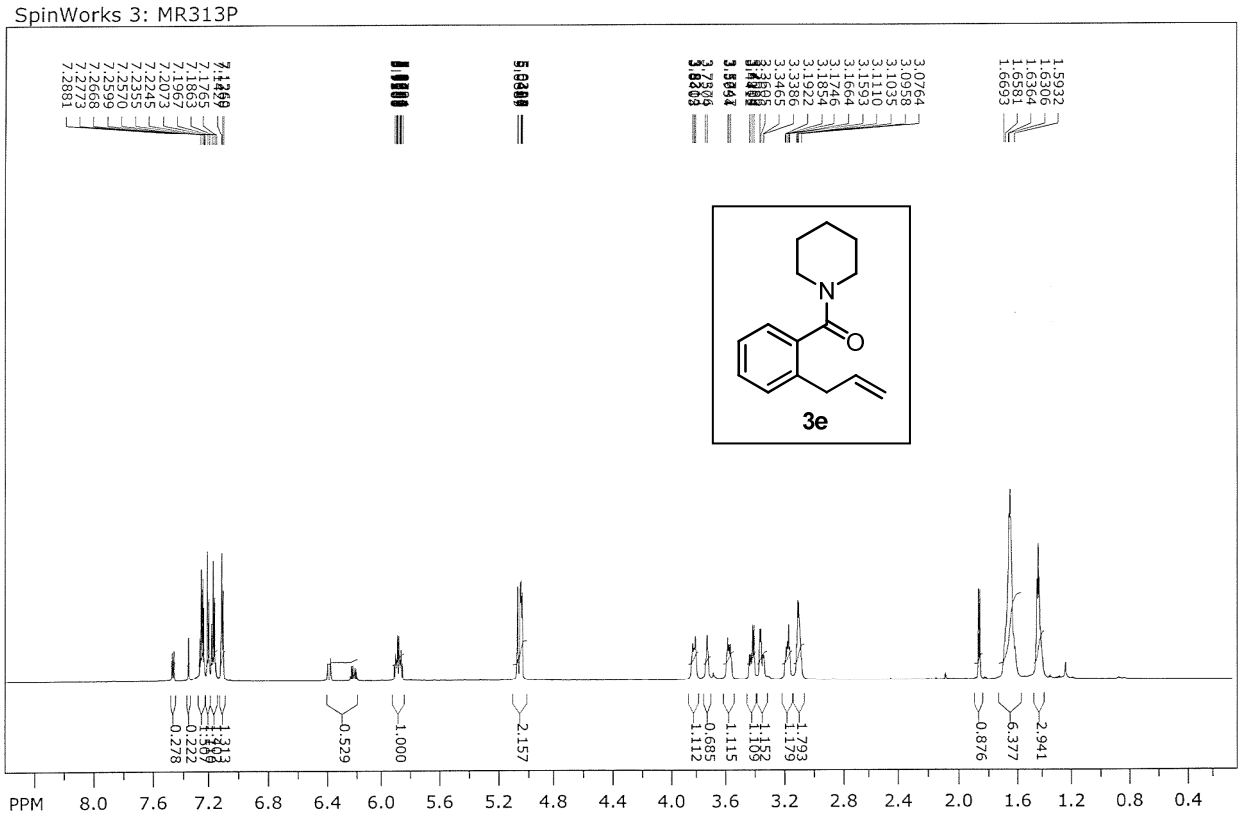

SpinWorks 3: MR330P
170.5968
136.5952
137.5020
137.6961
126.3280
127.2343
129.9770
130.4060
115.9238
76.8858
77.0664
77.2476
37.5507
26.5726
HN
O
3b
PPM 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

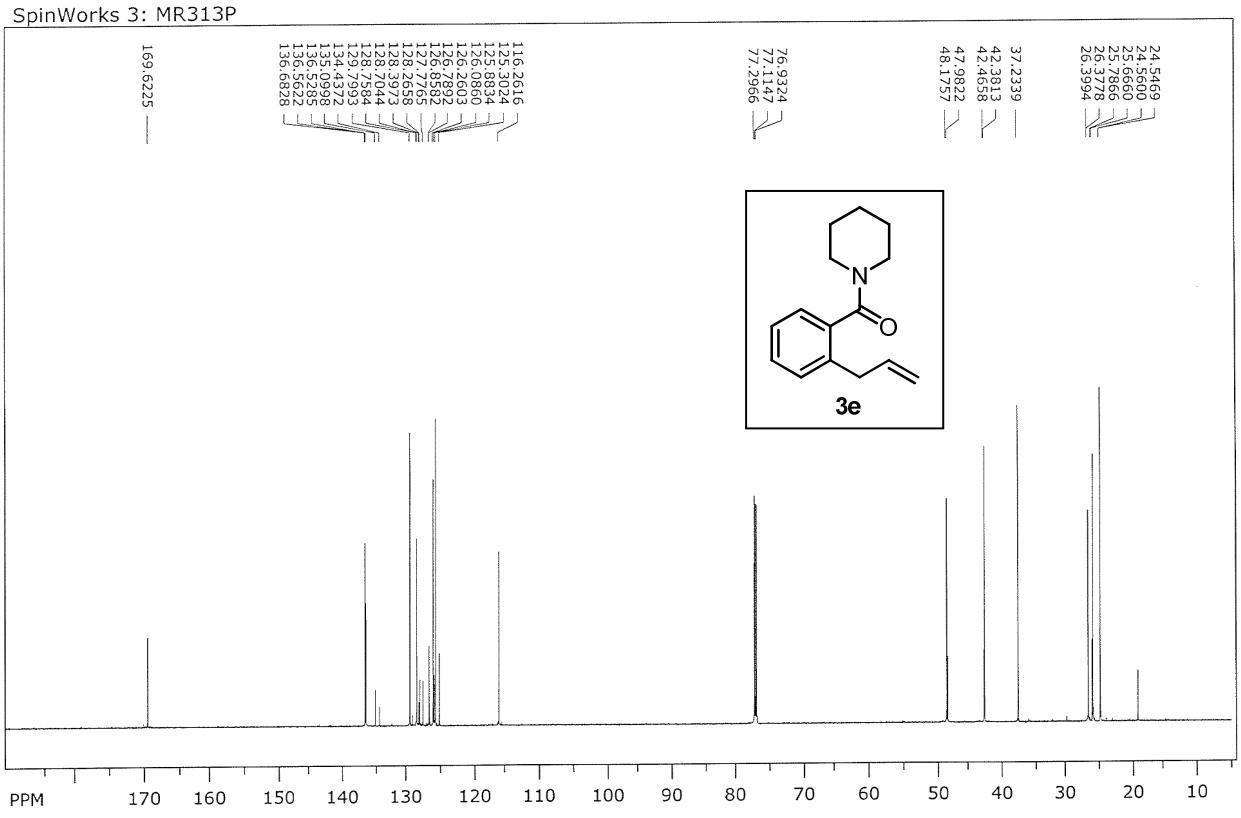

SpinWorks 3: MR311P
3.1234
2.8212
3c
0.231
1.317
2.394
1.253
0.477
1.000
2.139
2.069
PPM

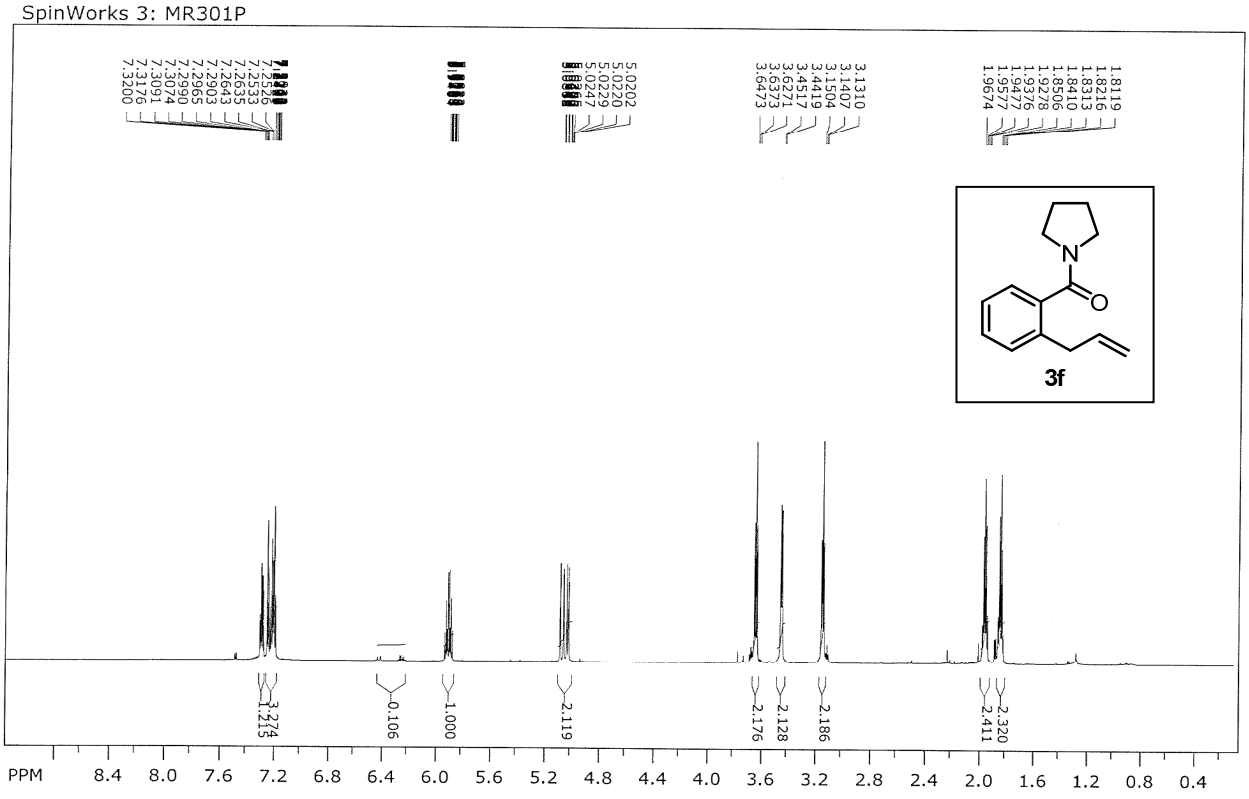

SpinWorks 3: MR311P
171.3049
136.5445
136.5278
136.5211
129.8973
129.8623
128.6741
128.4704
127.5404
126.8998
126.3365
126.2603
126.0973
125.3963
116.1203
77.2639
77.0829
76.9019
38.8407
38.4995
37.3462
34.7125
34.6086
3c
PPM

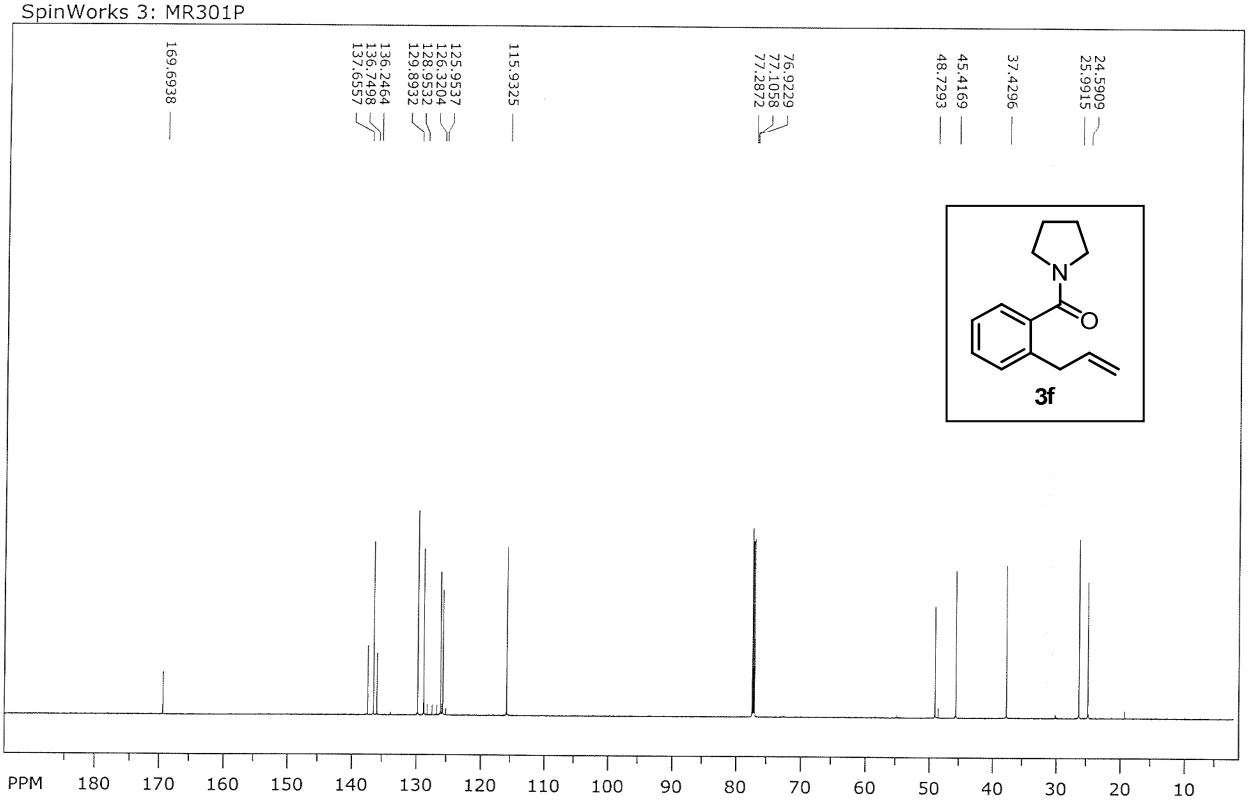

SpinWorks 3: MR312P
3d
0.388
1.616
2.587
1.445
0.714
1.000
2.222
6.861
4.616
1.229
3.385
1.192
PPM

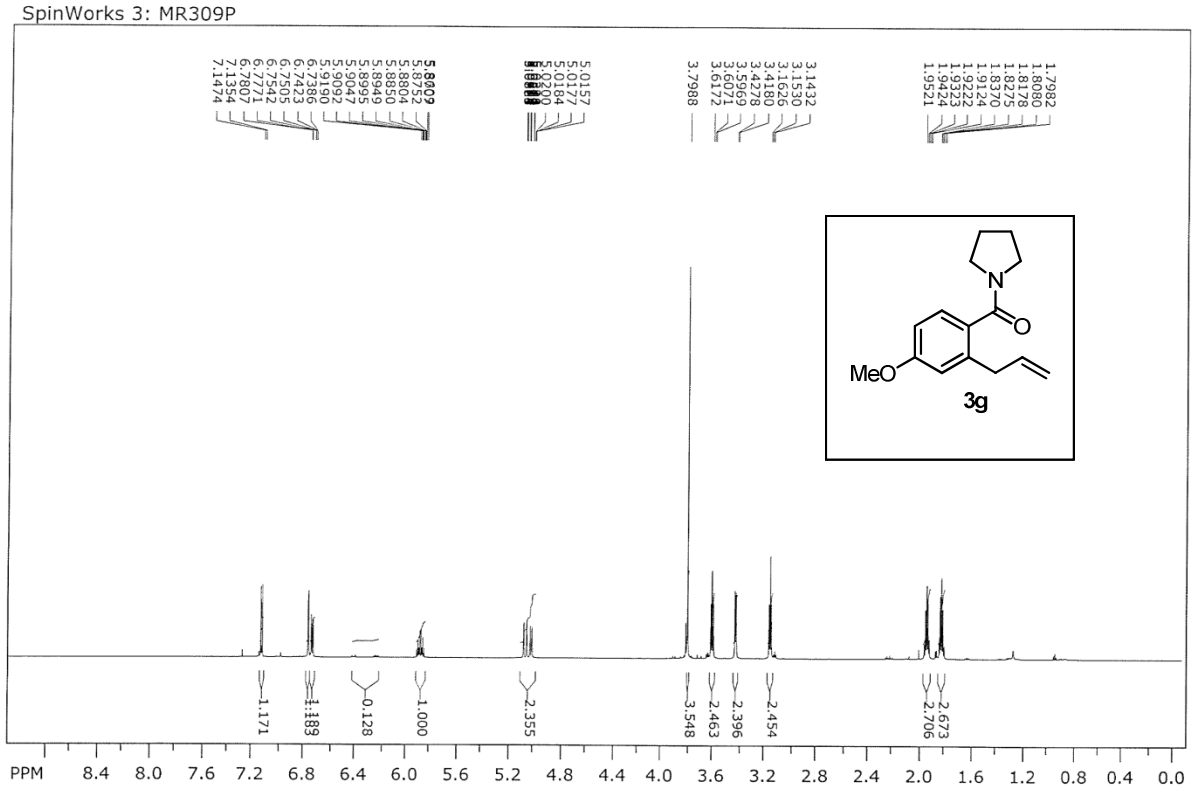

SpinWorks 3: MR312P
169.8885
136.8611
136.5702
135.4146
130.1327
129.2274
126.3886
126.1233
116.4020
66.8146
66.7991
47.5259
41.9091
37.2342
3d
PPM

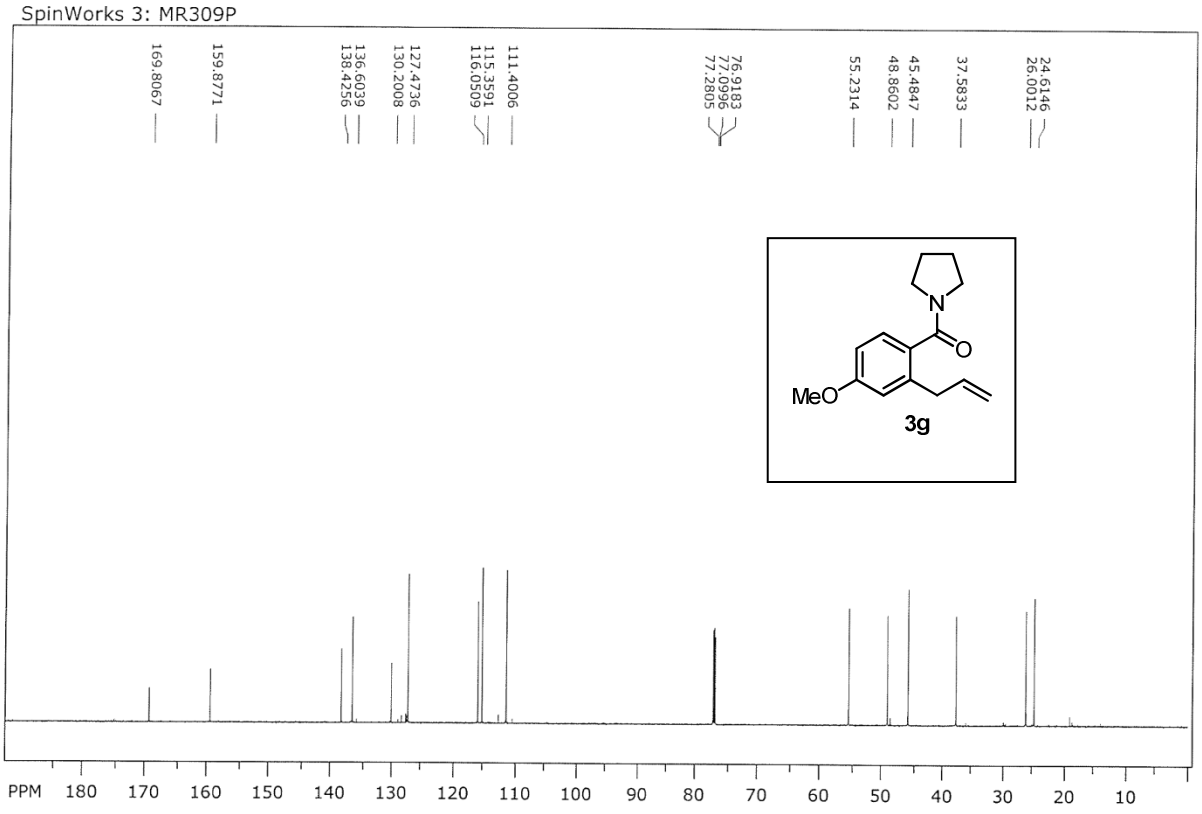

SpinWorks 3: MR313P
3e
PPM

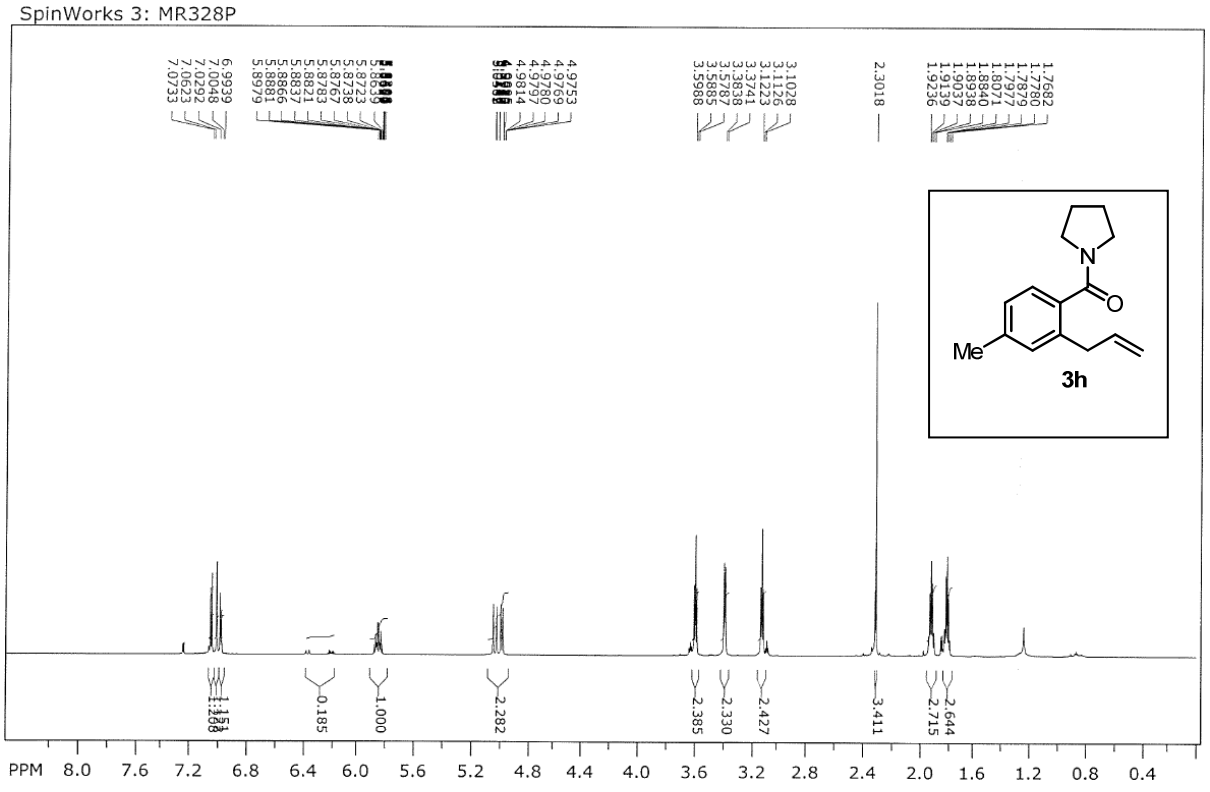

SpinWorks 3: MR313P
3e
PPM

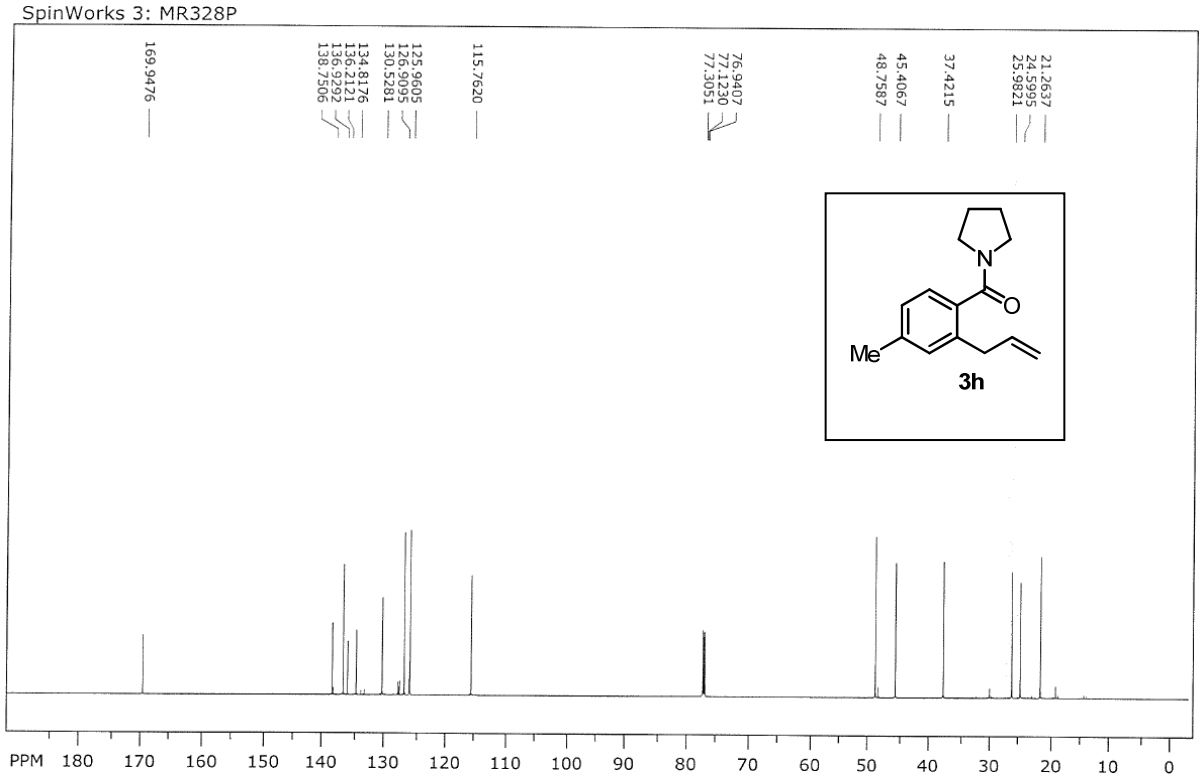

SpinWorks 3: MR301P
7.3200
7.3176
7.3091
7.3074
7.2990
7.2965
7.2903
7.2643
7.2635
7.2533
7.2526
5.0202
5.0220
5.0229
5.0247
3.6473
3.6323
3.6321
3.4517
3.4419
3.1504
3.1407
3.1310
1.9674
1.9577
1.9477
1.9376
1.9278
1.8506
1.8410
1.8313
1.8216
1.8119
3f
3.274
1.215
0.106
1.000
2.119
2.176
2.128
2.186
2.411
2.320
PPM
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4

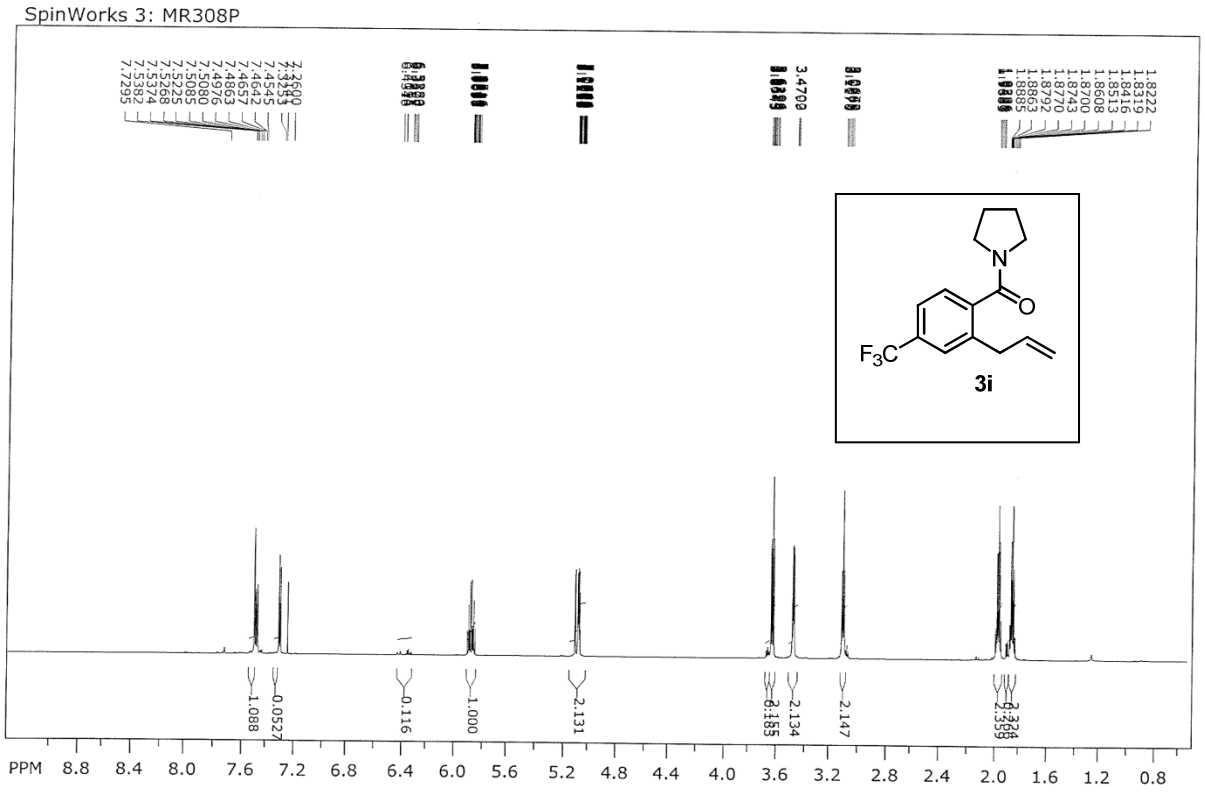

SpinWorks 3: MR301P
169.6938
137.6557
136.2464
136.7498
126.3204
125.9537
128.9532
129.8932
115.9325
77.2872
77.1058
76.9229
48.7293
45.4169
37.4296
25.9915
24.5909
3f
PPM
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

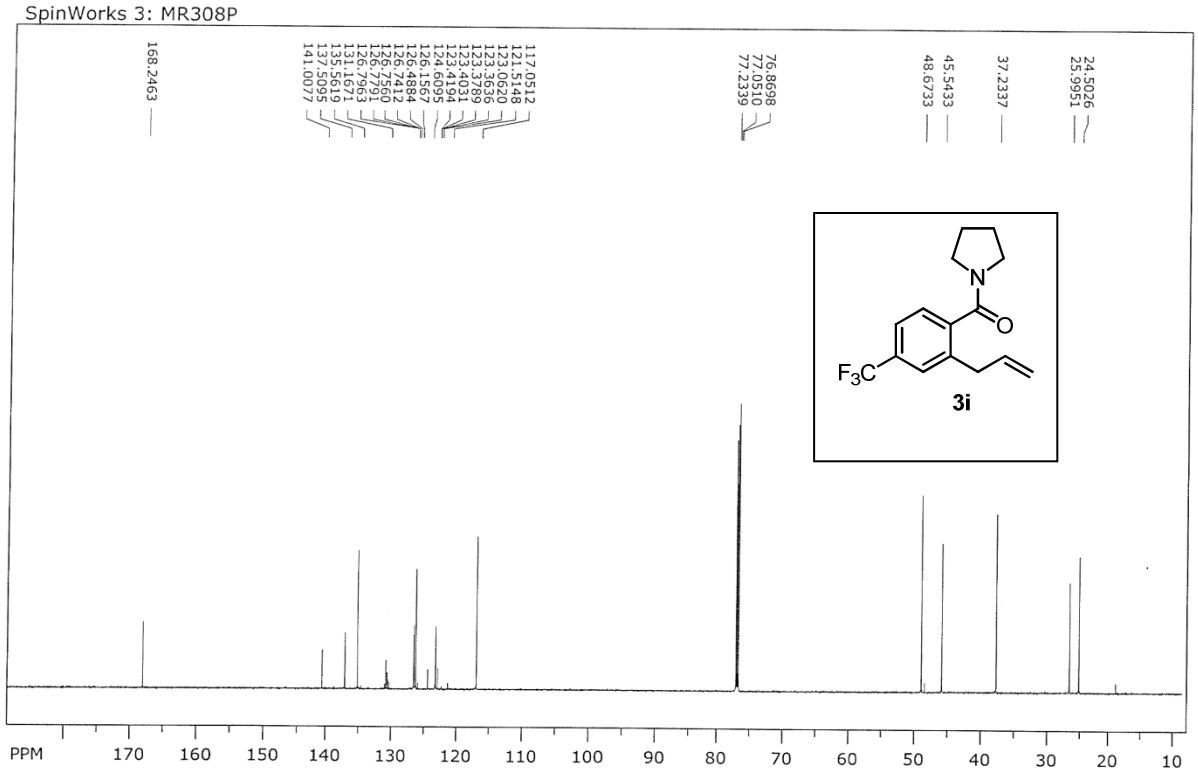

SpinWorks 3: MR309P
MeO
3g
PPM


SpinWorks 3: MR309P
MeO
3g
PPM


SpinWorks 3: MR328P
Me
3h
PPM


SpinWorks 3: MR328P
Me
3h
PPM


SpinWorks 3: MR308P
3.4709
1.088
0.0527
0.116
1.000
2.131
2.155
2.134
2.147
PPM
3i


SpinWorks 3: MR308P
168.2463
141.0077
137.5095
135.5619
131.1671
126.7963
126.7761
126.7412
126.4884
126.1567
124.6095
123.4194
123.4031
123.3789
123.3636
123.0620
121.5148
117.0512
77.2339
77.0510
76.8698
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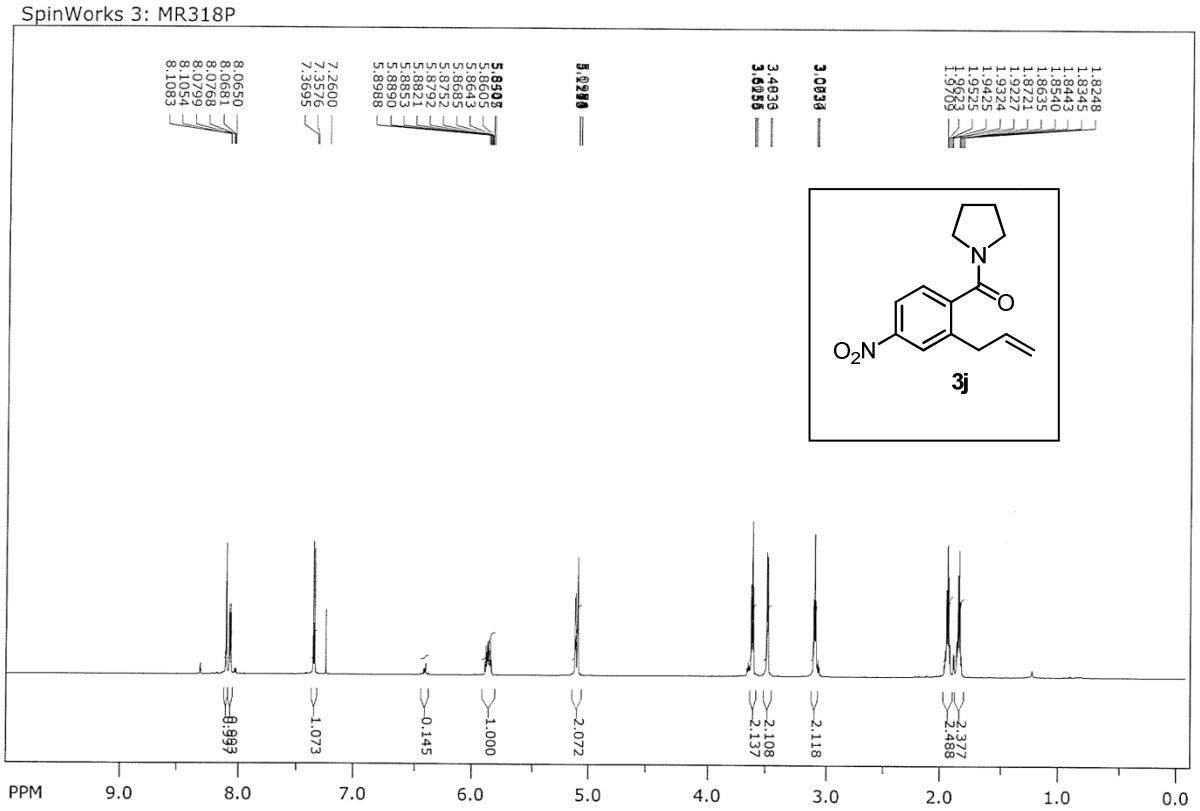
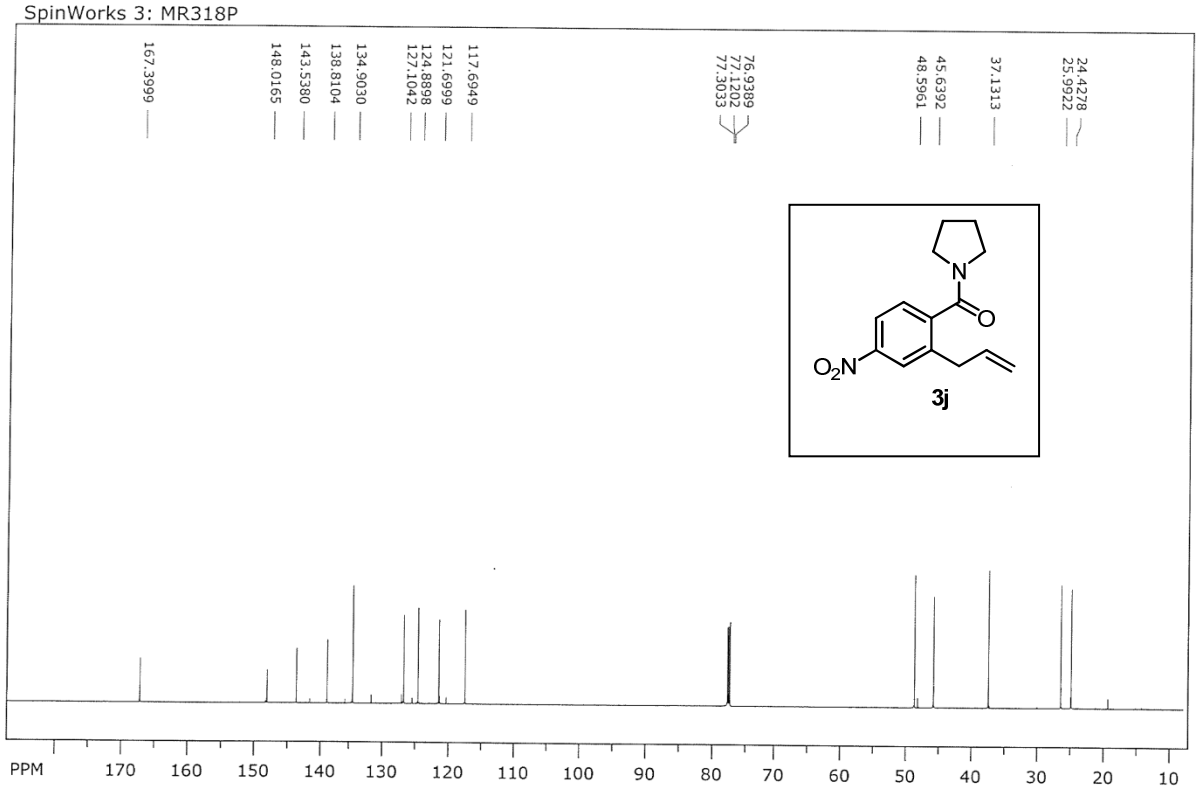
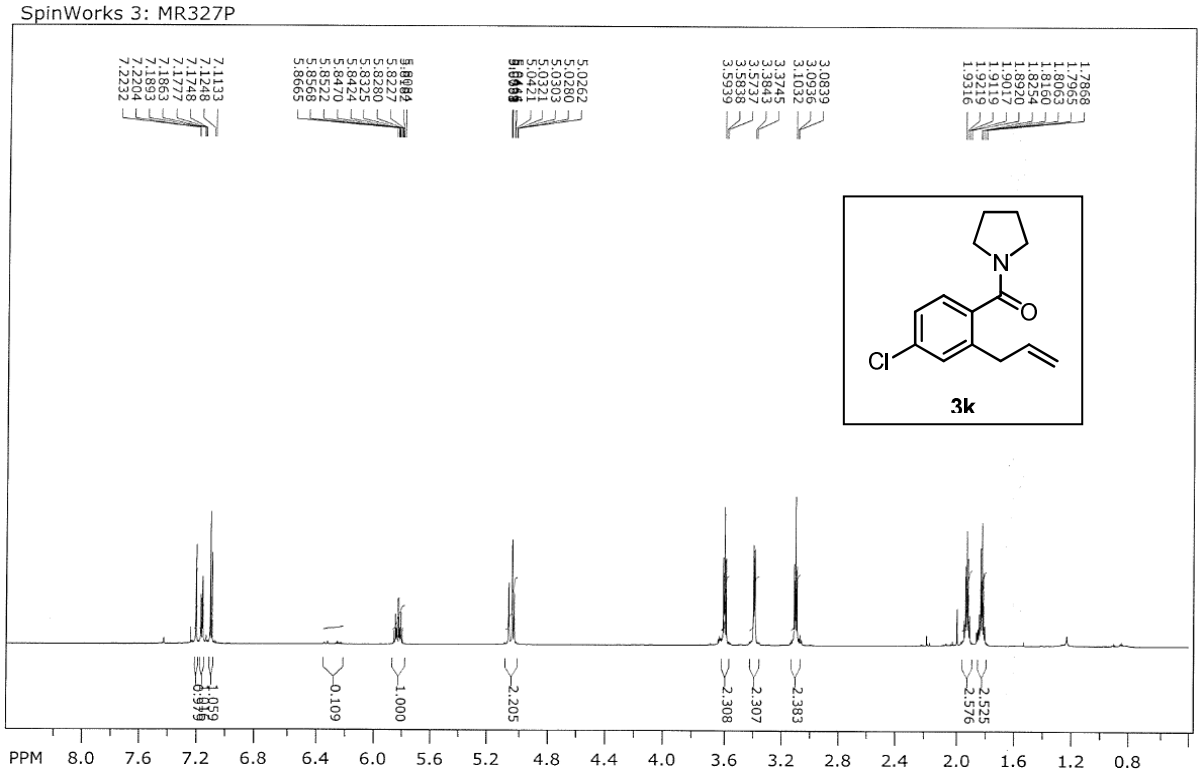
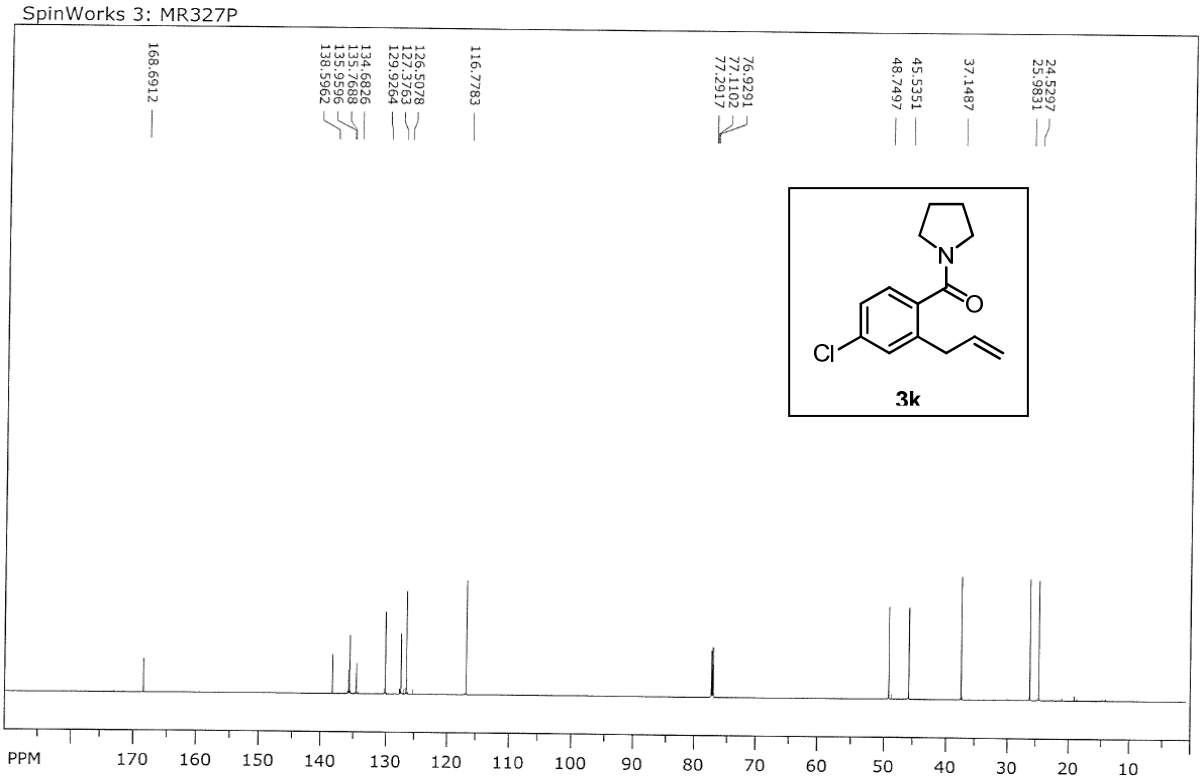
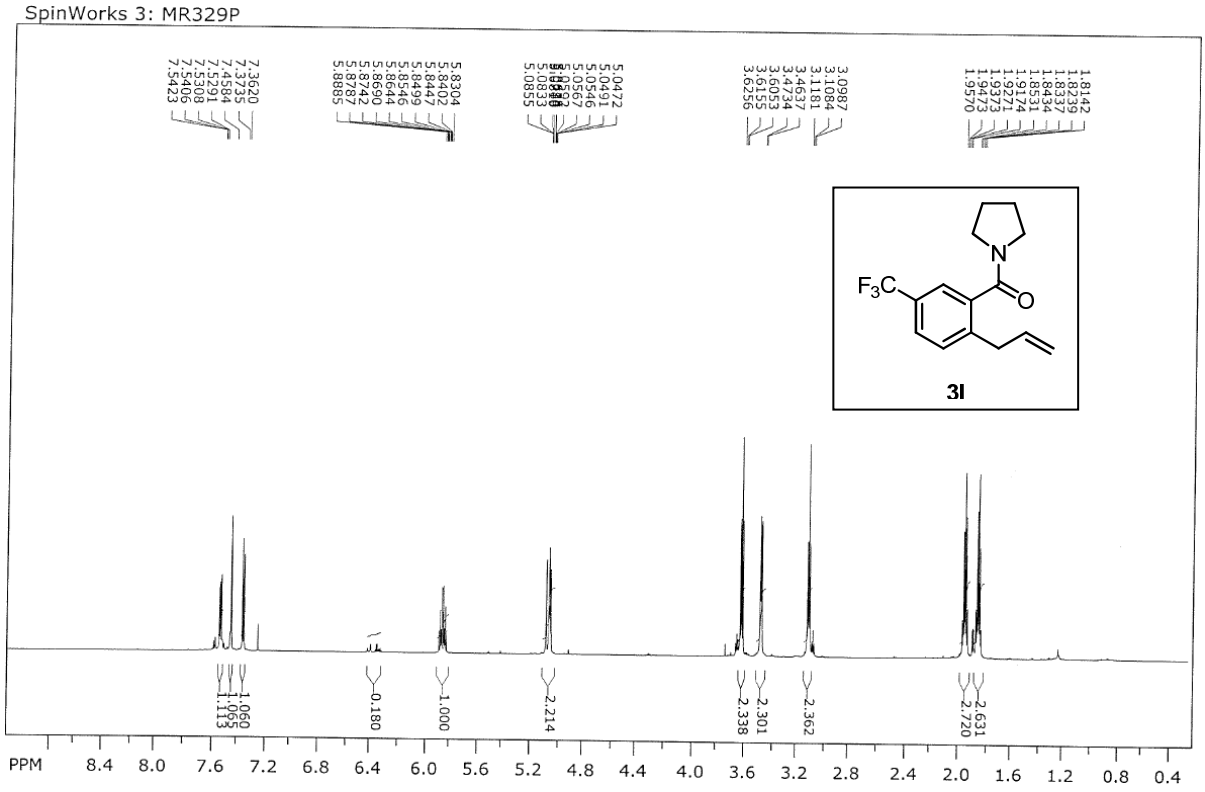
37.2337
25.3951
24.5026
PPM
3i

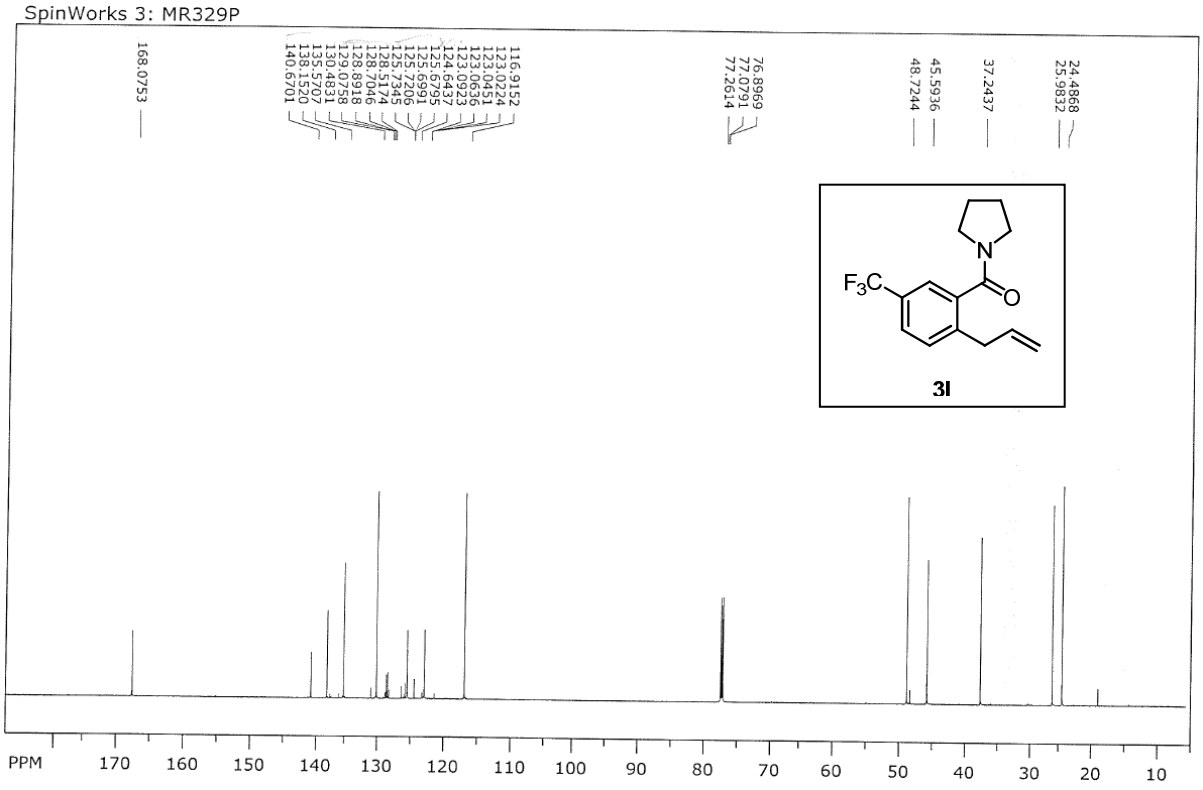

SpinWorks 3: MR318P
8.0650
8.0681
8.0768
8.0799
8.1059
8.1083
7.2600
7.3576
7.3695
5.8968
5.8890
5.8853
5.8821
5.8792
5.8752
5.8685
5.8643
5.8605
1.8248
1.8345
1.8443
1.8540
1.8635
1.8721
1.9227
1.9324
1.9425
1.9525
1.9623
1.9709
O2N
3j
1.073
0.145
1.000
2.072
2.137
2.108
2.118
2.377
2.488
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


SpinWorks 3: MR318P
167.3999
148.0165
143.5380
138.8104
134.9030
127.1042
124.8898
121.6999
117.6949
77.3033
77.1202
76.9389
48.5961
45.6392
37.1313
25.9922
24.4278
O2N
3j
PPM
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


SpinWorks 3: MR327P
7.1133
7.1248
7.1748
7.1777
7.1863
7.1893
7.2204
7.2232
5.8280
5.8424
5.8470
5.8522
5.8668
5.0262
5.0280
5.0303
5.0321
5.0421
3.0839
3.0936
3.1032
3.3745
3.3843
3.5737
3.5838
3.5939
1.7868
1.7965
1.8063
1.8160
1.8254
1.8920
1.9017
1.9119
1.9219
1.9316
1.059
0.977
0.109
1.000
2.205
2.308
2.307
2.383
2.525
2.576
PPM
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
N
O
Cl
3k


SpinWorks 3: MR327P
168.6912
138.5962
135.9596
135.7688
134.6826
129.9264
127.3763
126.5078
116.7783
77.2917
77.1102
76.9291
48.7497
45.5351
37.1487
25.9831
24.5297
PPM
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
N
O
Cl
3k


SpinWorks 3: MR329P
7.3620
7.3735
7.4584
7.5291
7.5308
7.5406
7.5423
5.8304
5.8402
5.8447
5.8499
5.8546
5.8644
5.8690
5.8742
5.8787
5.8885
5.0472
5.0491
5.0546
5.0567
5.0855
3.0987
3.1084
3.1181
3.4637
3.4734
3.6053
3.6236
1.8142
1.8239
1.8337
1.8434
1.8531
1.9174
1.9271
1.9373
1.9473
1.9570
3l
1.060
1.065
1.113
0.180
1.000
2.214
2.338
2.301
2.362
2.631
2.720
PPM
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4


SpinWorks 3: MR329P
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135.4931
129.0758
128.8918
128.7046
128.5174
125.7345
125.7206
125.6991
125.6795
124.6437
123.0923
123.0636
123.0451
123.0224
116.9152
76.8969
77.0791
77.2614
48.7244
45.5936
37.2437
25.9832
24.4868
3l
PPM
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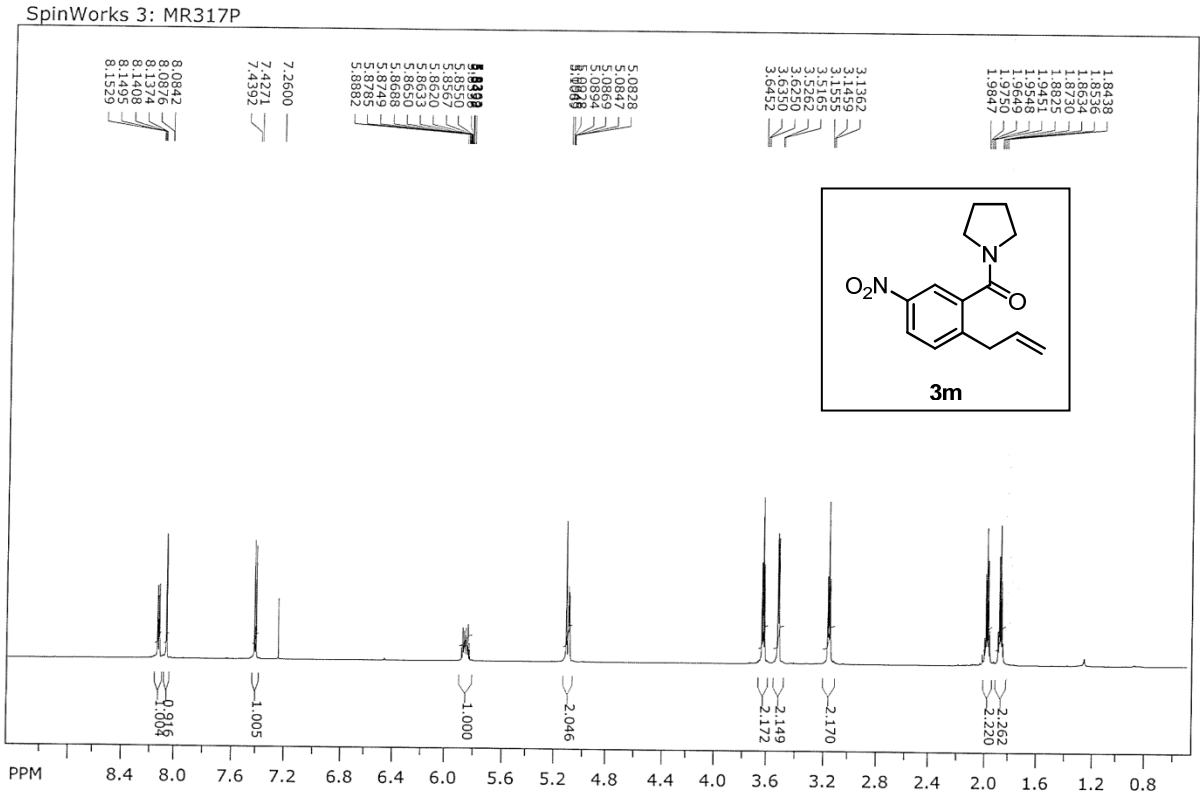
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


SpinWorks 3: MR317P
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8.0876
8.1374
8.1408
8.1495
8.1529
7.2600
7.4271
7.4392
5.8682
5.8749
5.8785
5.8868
5.8903
5.8938
5.8973
5.9008
5.9043
5.9078
5.9113
5.9148
5.9183
5.9218
5.9253
5.9288
5.9323
5.9358
5.9393
5.9428
5.9463
5.9498
5.9533
5.9568
5.9603
5.9638
5.9673
5.9708
5.9743
5.9778
5.9813
5.9848
5.9883
5.9918
5.9953
5.9988
6.0023
6.0058
6.0093
6.0128
6.0163
6.0198
6.0233
6.0268
6.0303
6.0338
6.0373
6.0408
6.0443
6.0478
6.0513
6.0548
6.0583
6.0618
6.0653
6.0688
6.0723
6.0758
6.0793
6.0828
5.0847
5.0884
3.6452
3.6350
3.6250
3.5262
3.5165
3.1555
3.1459
3.1362
1.9847
1.9750
1.9649
1.9548
1.9451
1.8835
1.8734
1.8636
1.8536
1.8438
3m
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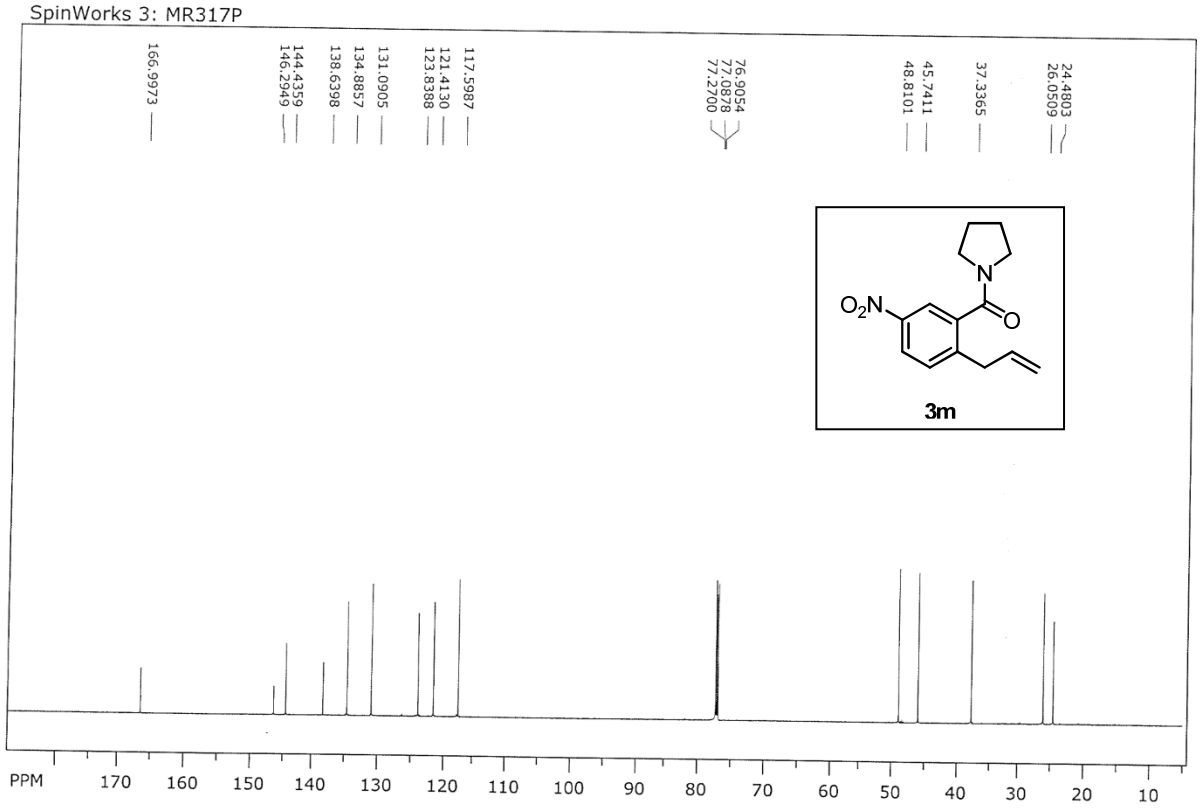
0.816
1.005
1.000
2.046
2.172
2.149
2.170
2.220
2.262
PPM


SpinWorks 3: MR317P
166.9973
146.2949
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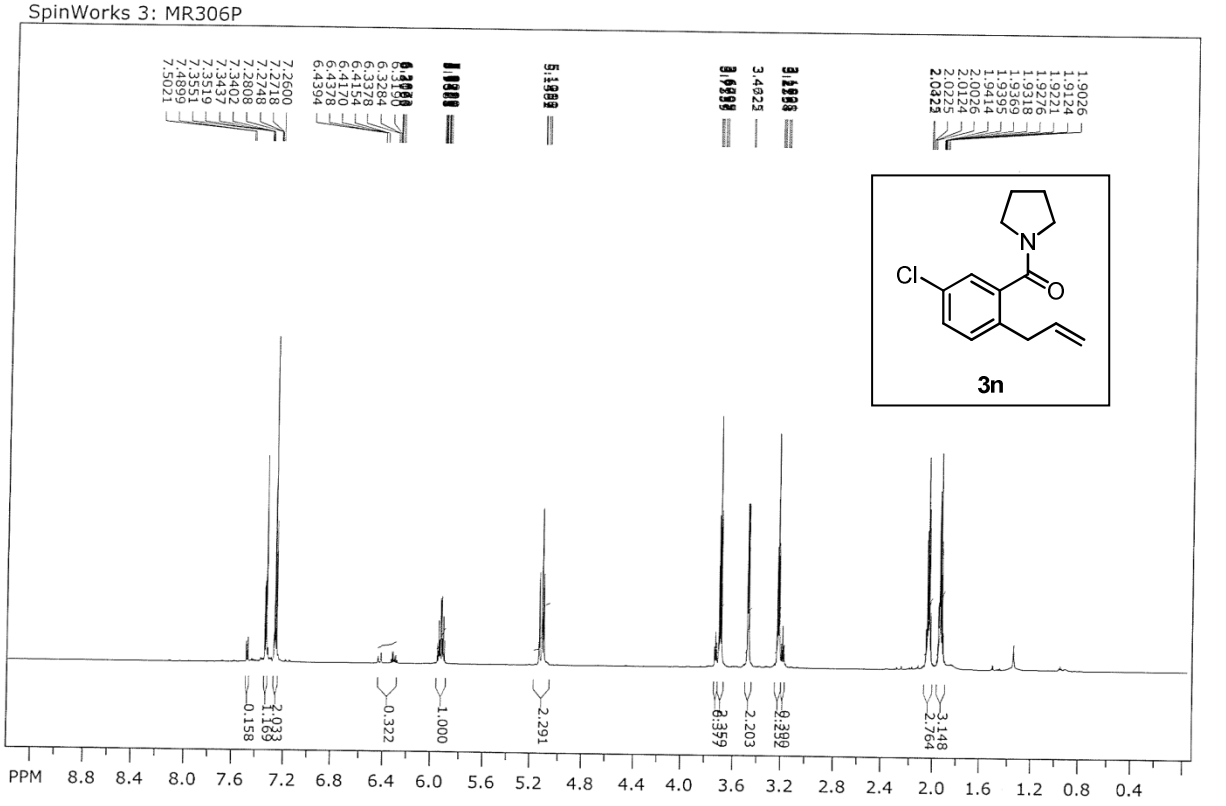
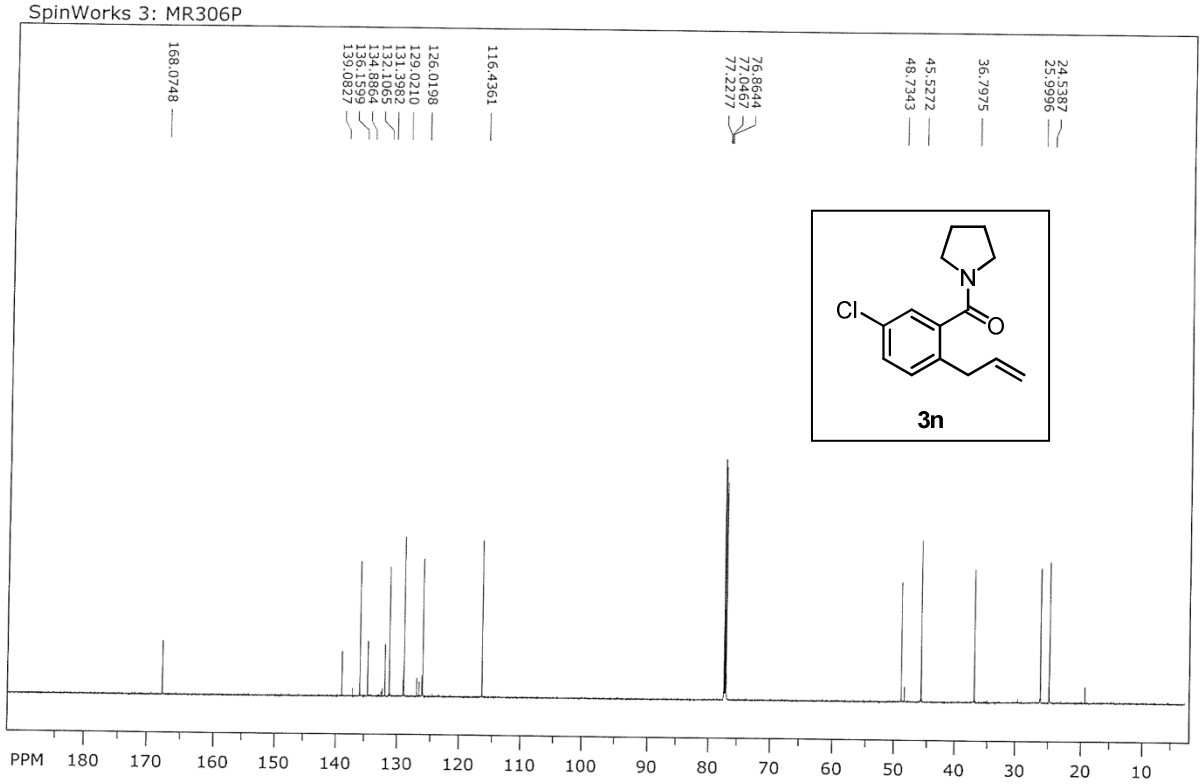
138.6398
134.8857
131.0905
123.8388
121.4130
117.5987
77.2700
77.0878
76.9054
48.8101
45.7411
37.3365
26.0509
24.4803
3m
PPM


SpinWorks 3: MR306P
Cl
N
O
3n
PPM 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4


SpinWorks 3: MR306P
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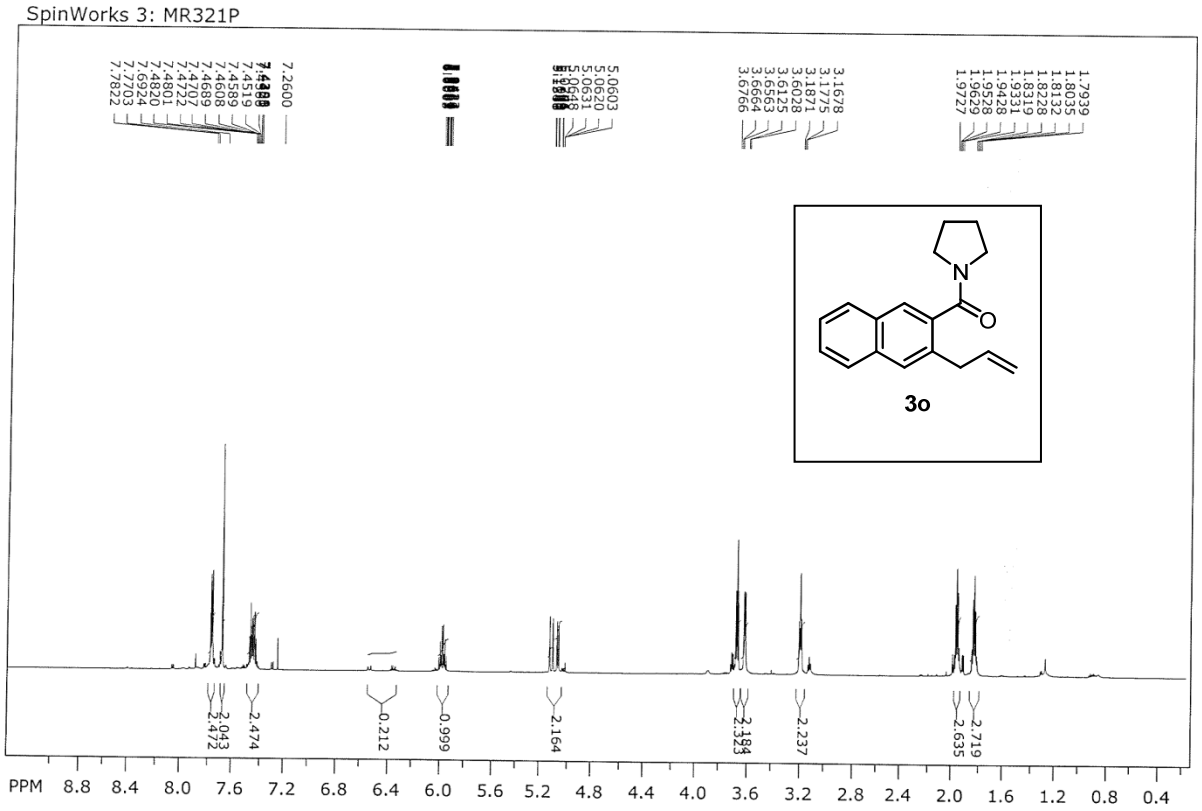
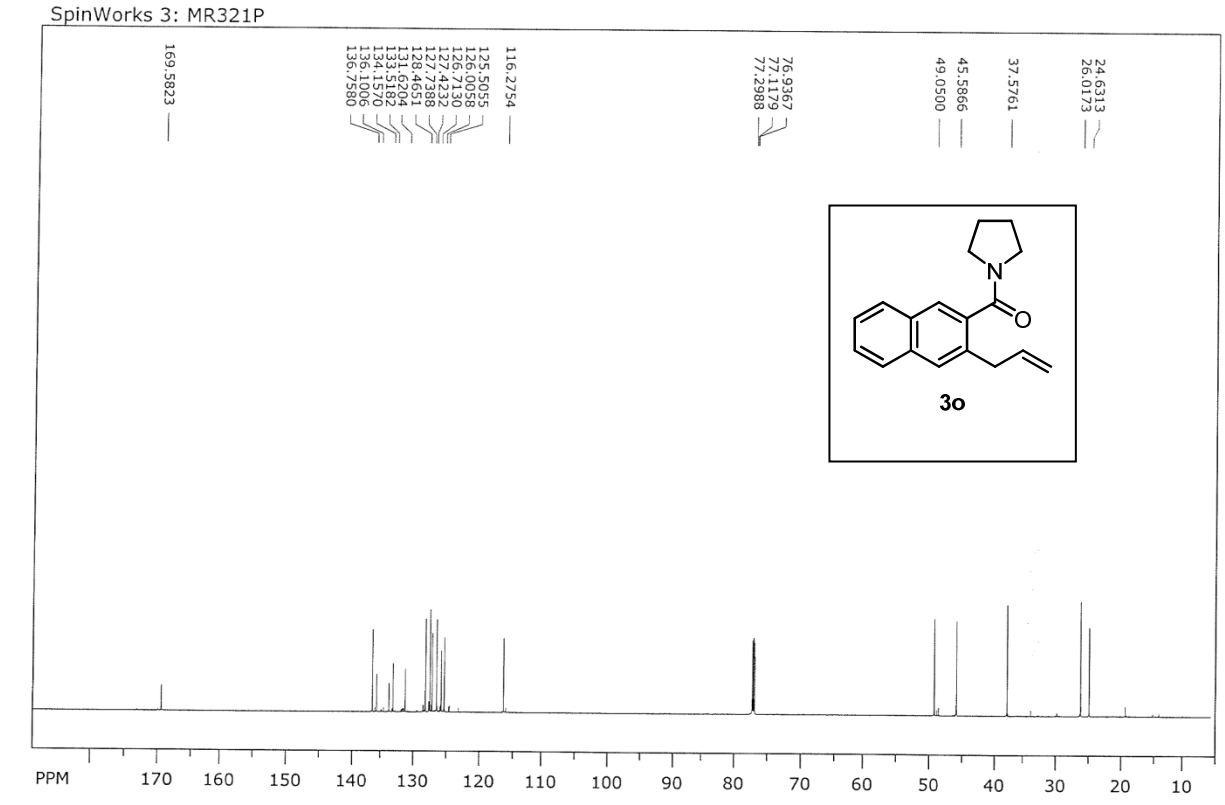
134.8864
132.1065
131.3982
129.0210
126.0198
116.4361
77.2277
77.0467
76.8644
48.7343
45.5272
36.7975
25.9996
24.5387
Cl
N
O
3n
PPM 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


SpinWorks 3: MR321P
7.7822
7.7703
7.6924
7.4820
7.4801
7.4722
7.4707
7.4689
7.4608
7.4589
7.4519
7.2600
5.0603
5.0620
5.0631
3.6766
3.6664
3.6563
3.6125
3.6028
3.1871
3.1775
3.1678
1.9727
1.9629
1.9528
1.9428
1.9331
1.8319
1.8228
1.8132
1.8035
1.7939
3o
2.472
3.043
2.474
0.212
0.999
2.164
2.184
2.193
2.237
2.635
2.719
PPM 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4


SpinWorks 3: MR321P
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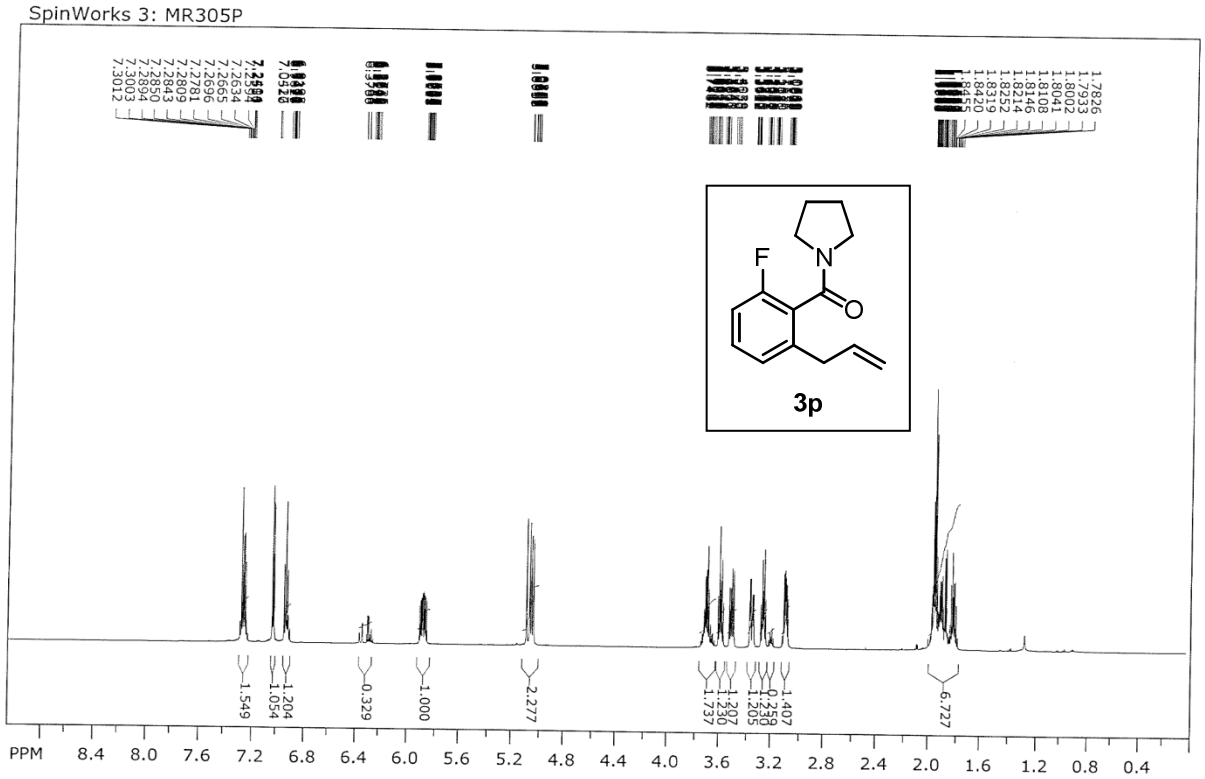
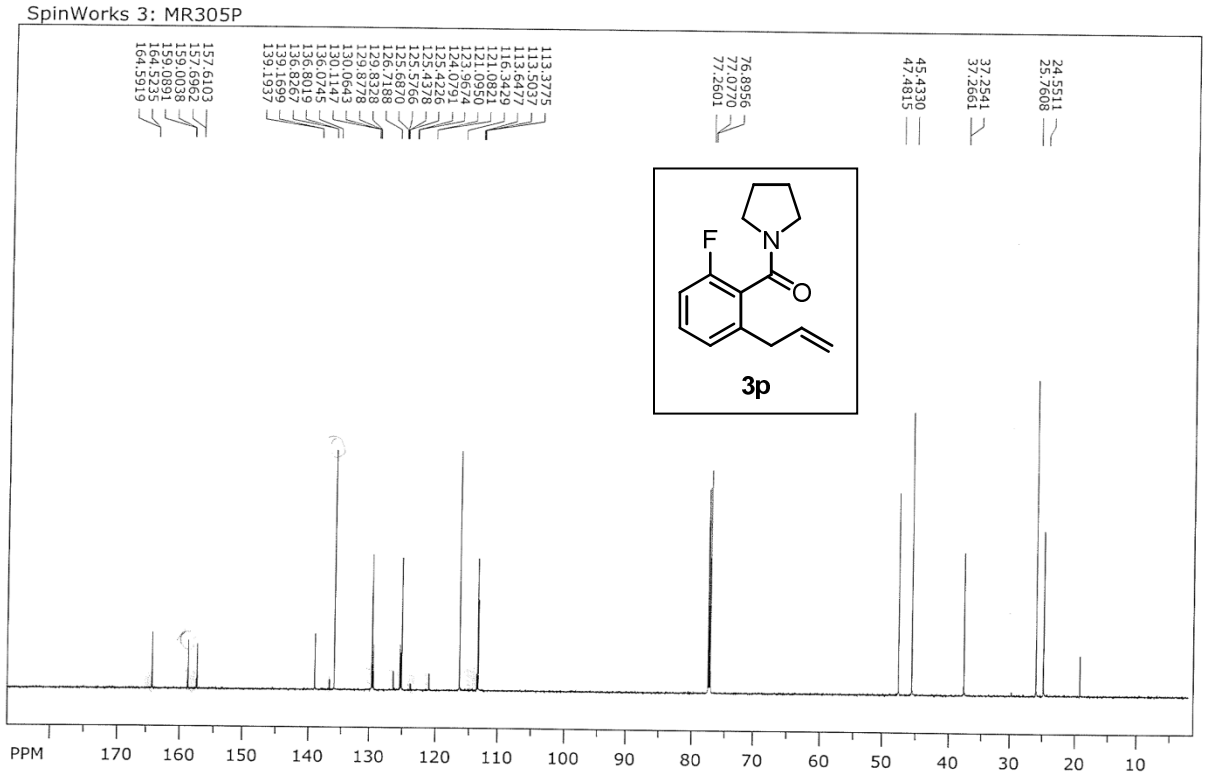
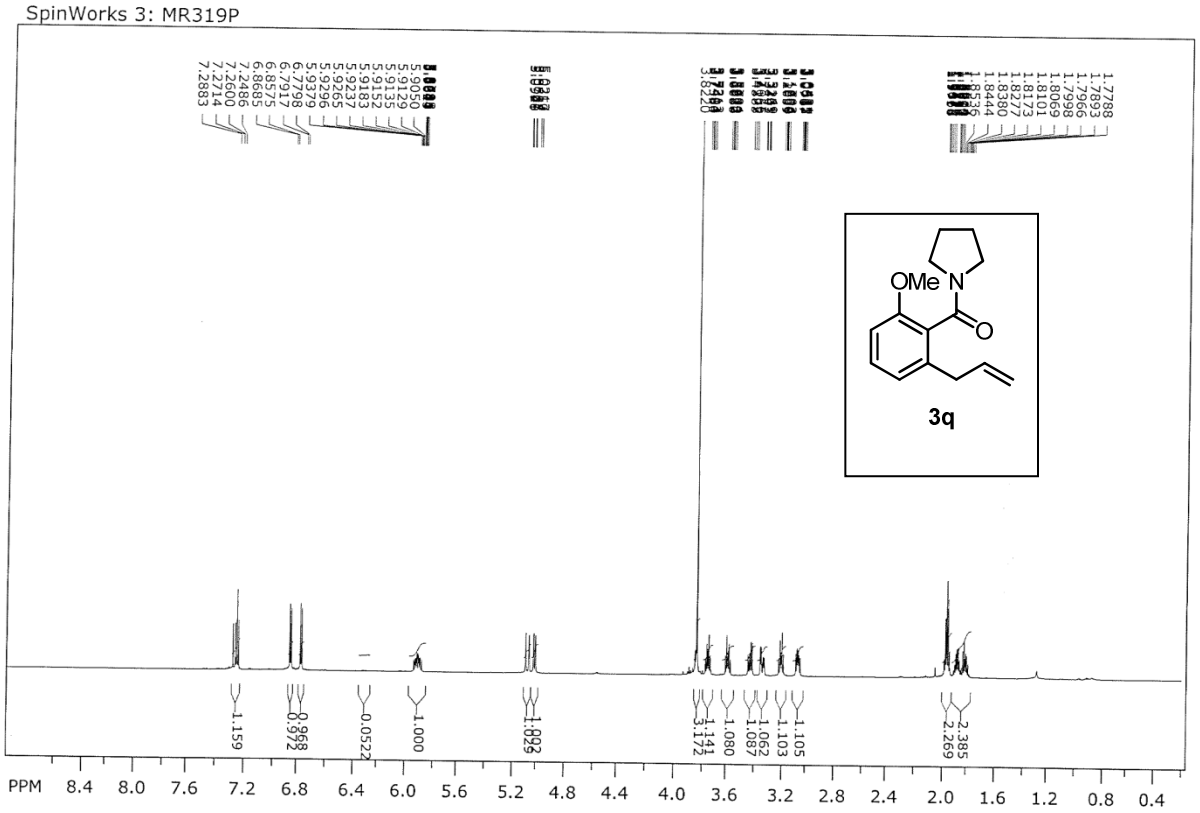
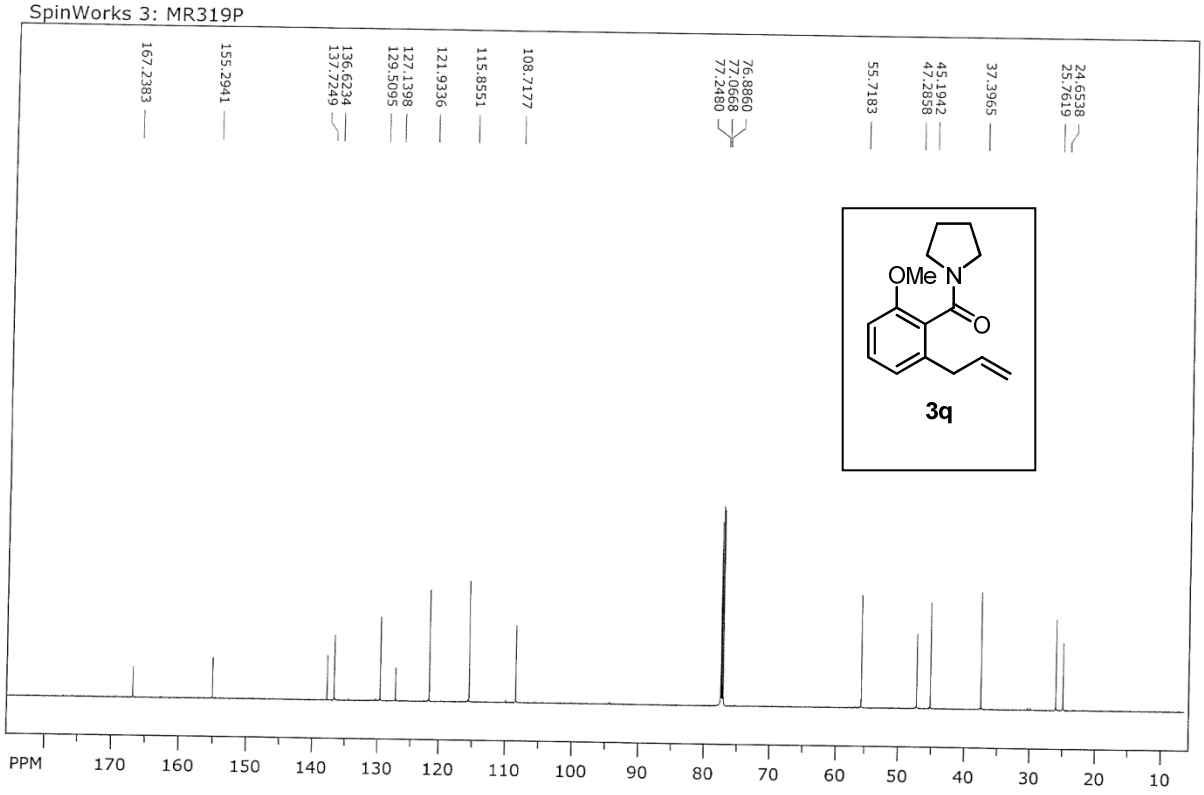
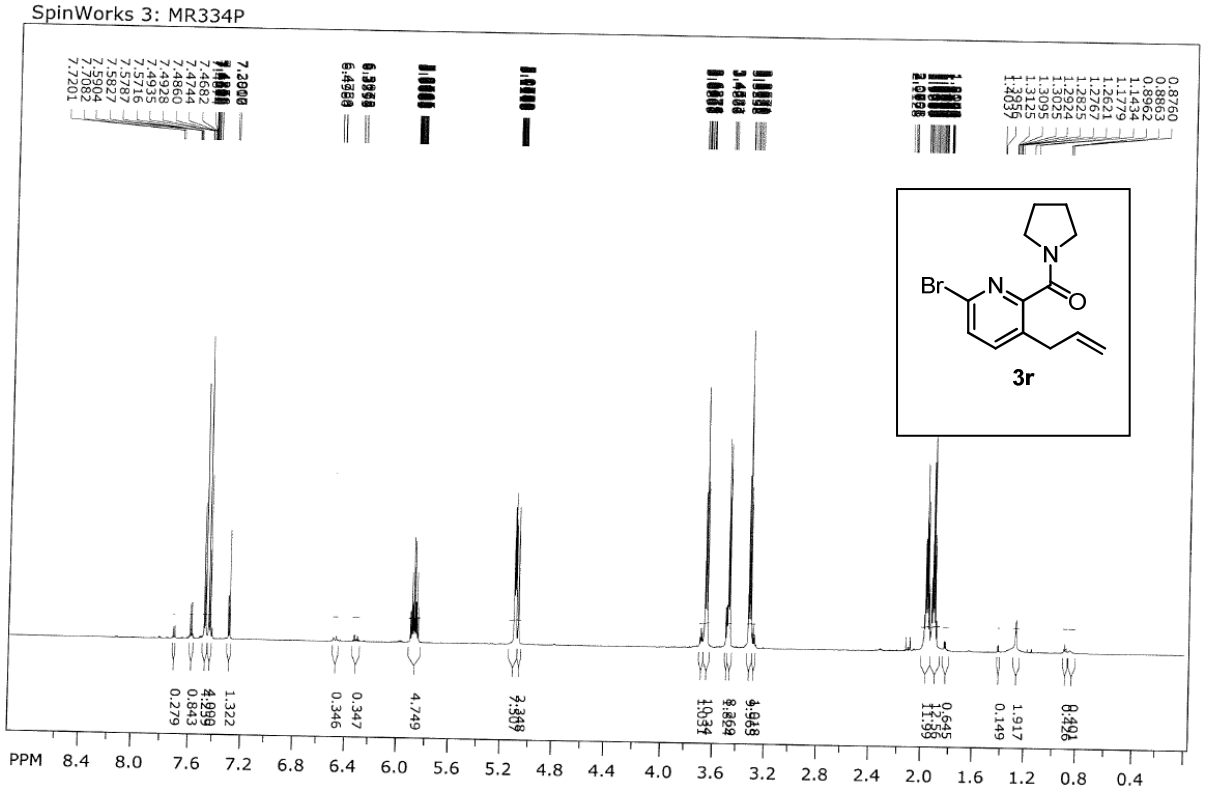
134.1570
133.5182
131.6204
128.4651
127.7388
127.4232
126.7130
126.0058
125.5055
116.2754
77.2988
77.1179
76.9367
49.0500
45.5866
37.5761
26.0173
24.6313
3o
PPM 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

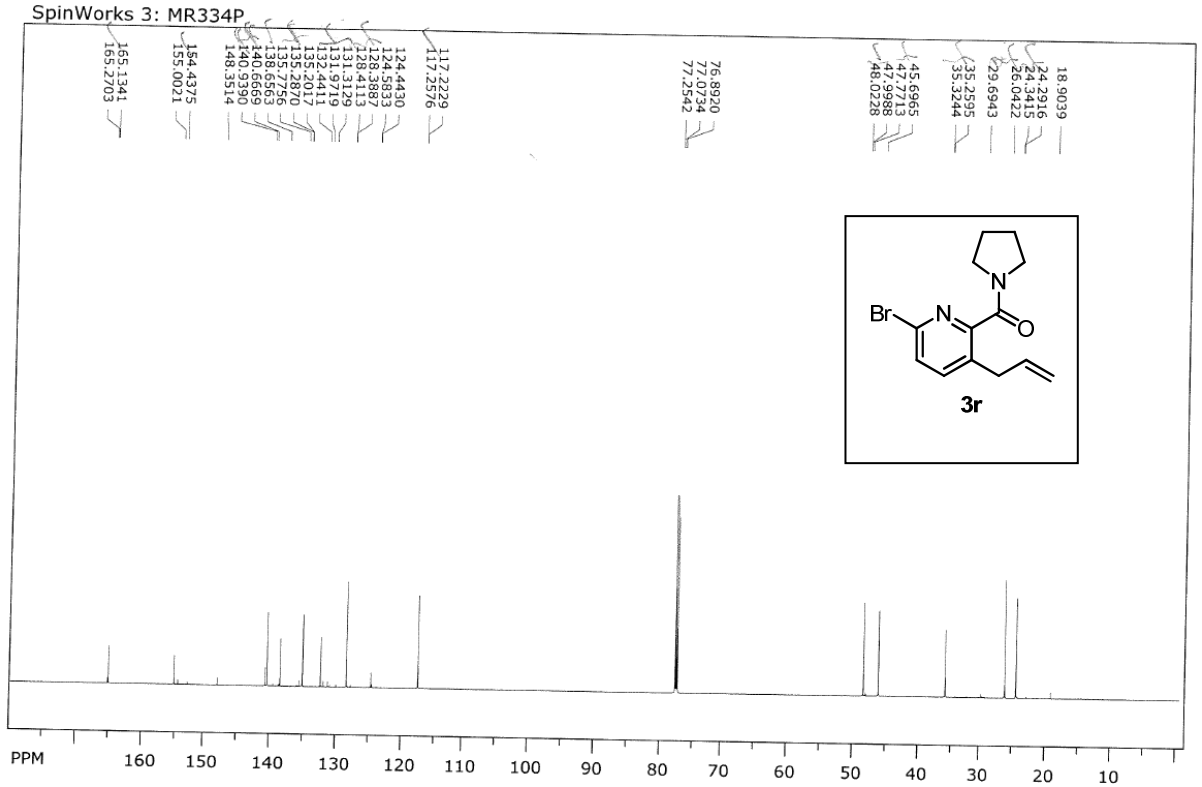

SpinWorks 3: MR305P
F
N
O
3p
1.549
1.054
1.204
0.329
1.000
2.277
1.737
1.307
1.290
1.205
0.259
1.407
6.727
PPM
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4

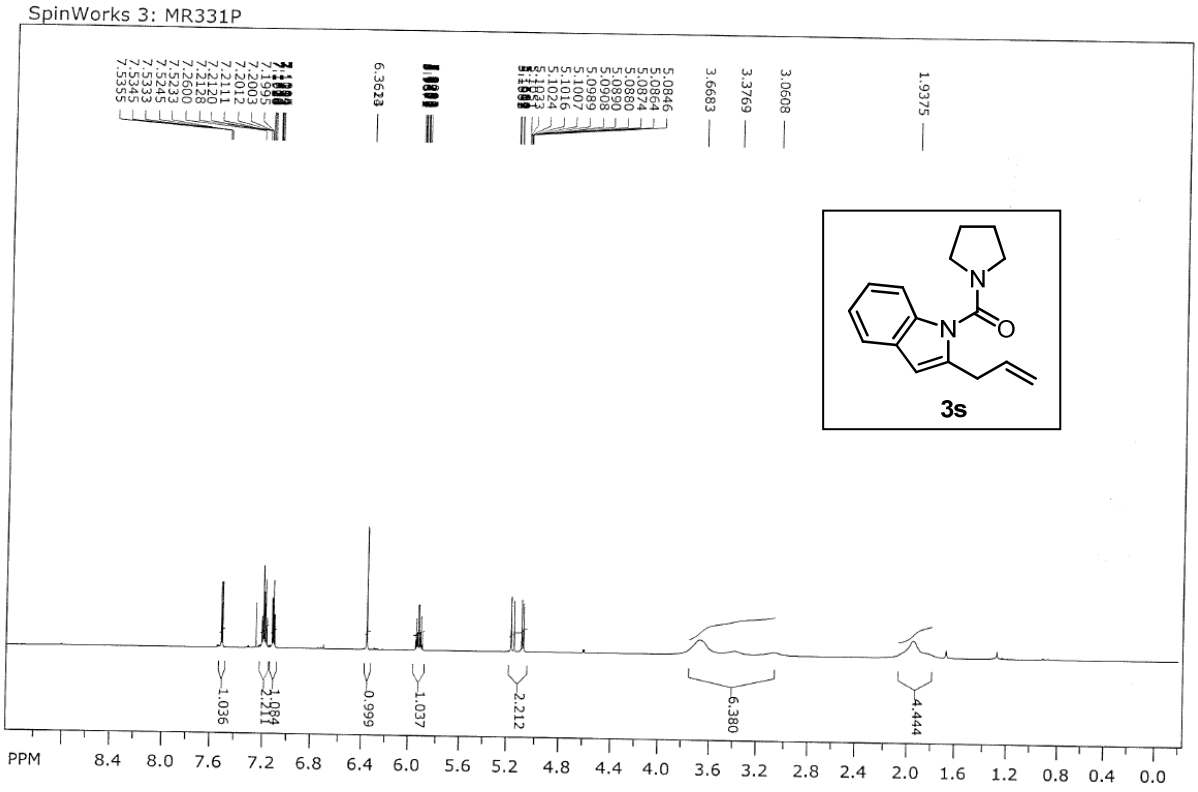

SpinWorks 3: MR305P
F
N
O
3p
PPM
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

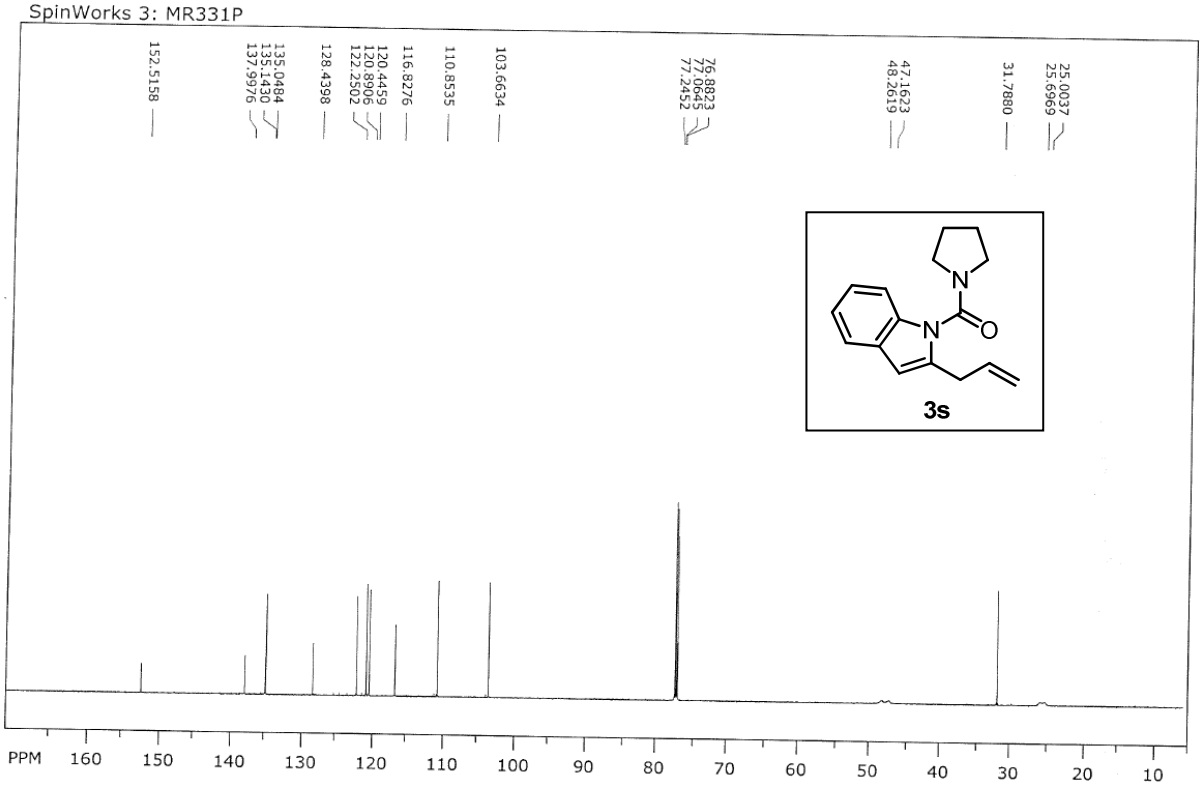

SpinWorks 3: MR319P
OMe
N
O
3q
PPM

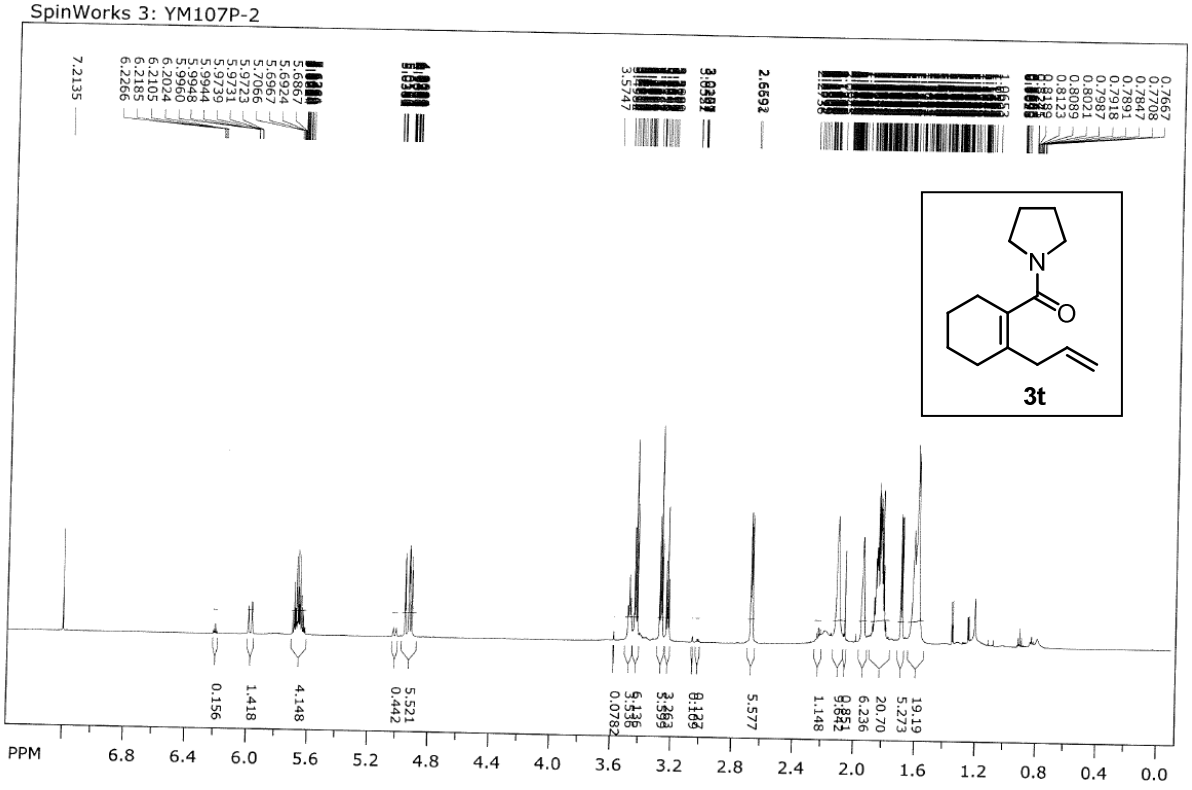

SpinWorks 3: MR319P
OMe
N
O
3q
PPM

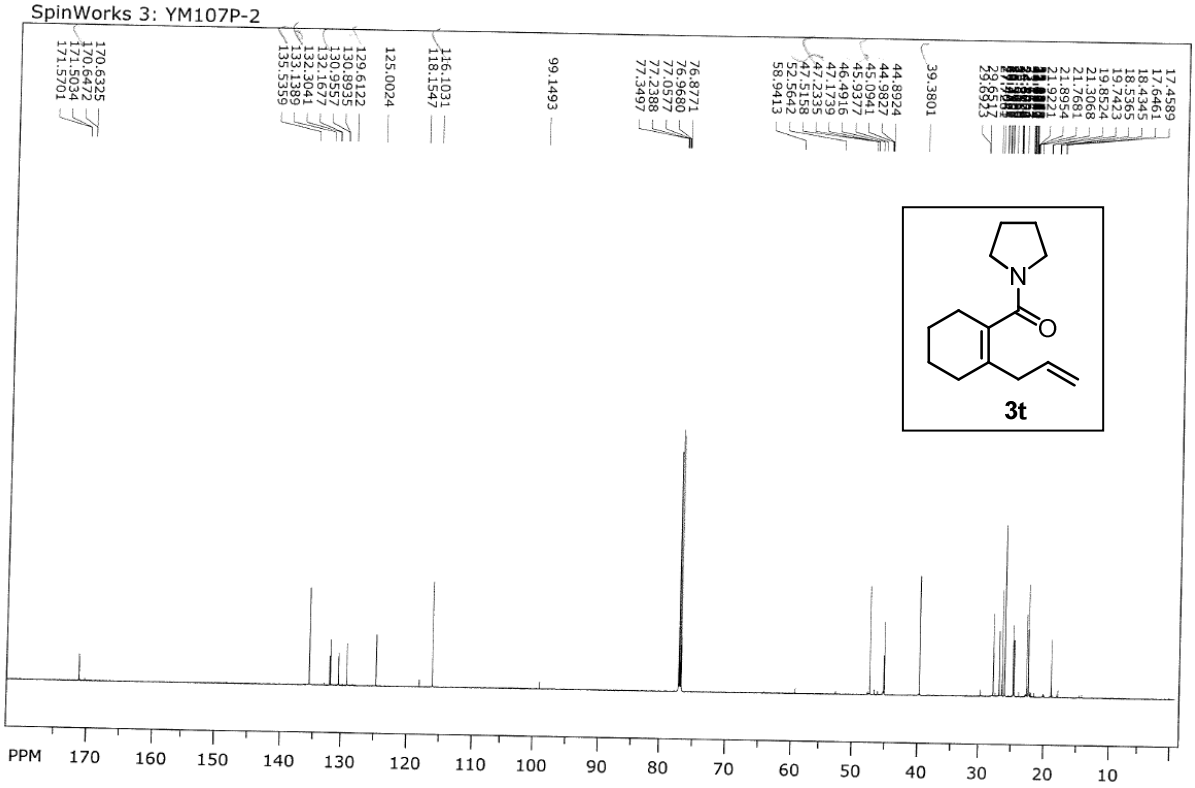

SpinWorks 3: MR334P
Br
N
O
3r
PPM

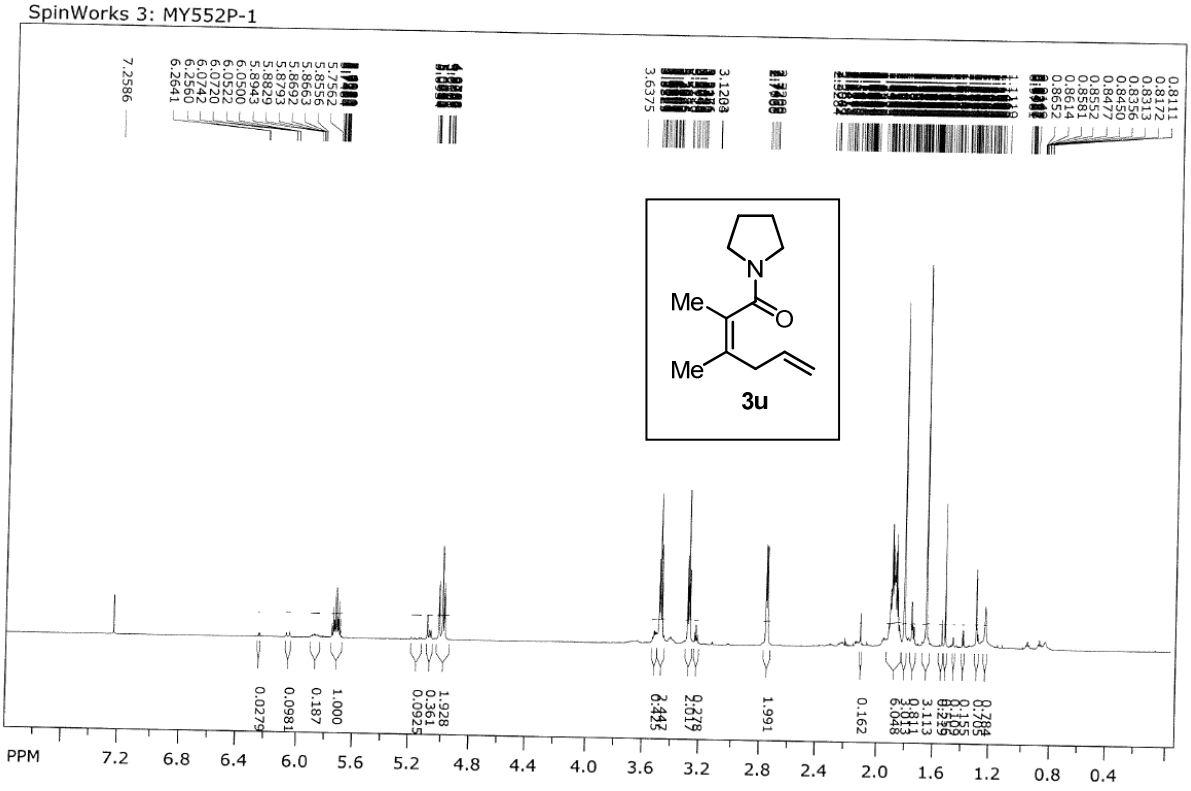

SpinWorks 3: MR334P
Br
N
O
3r
PPM

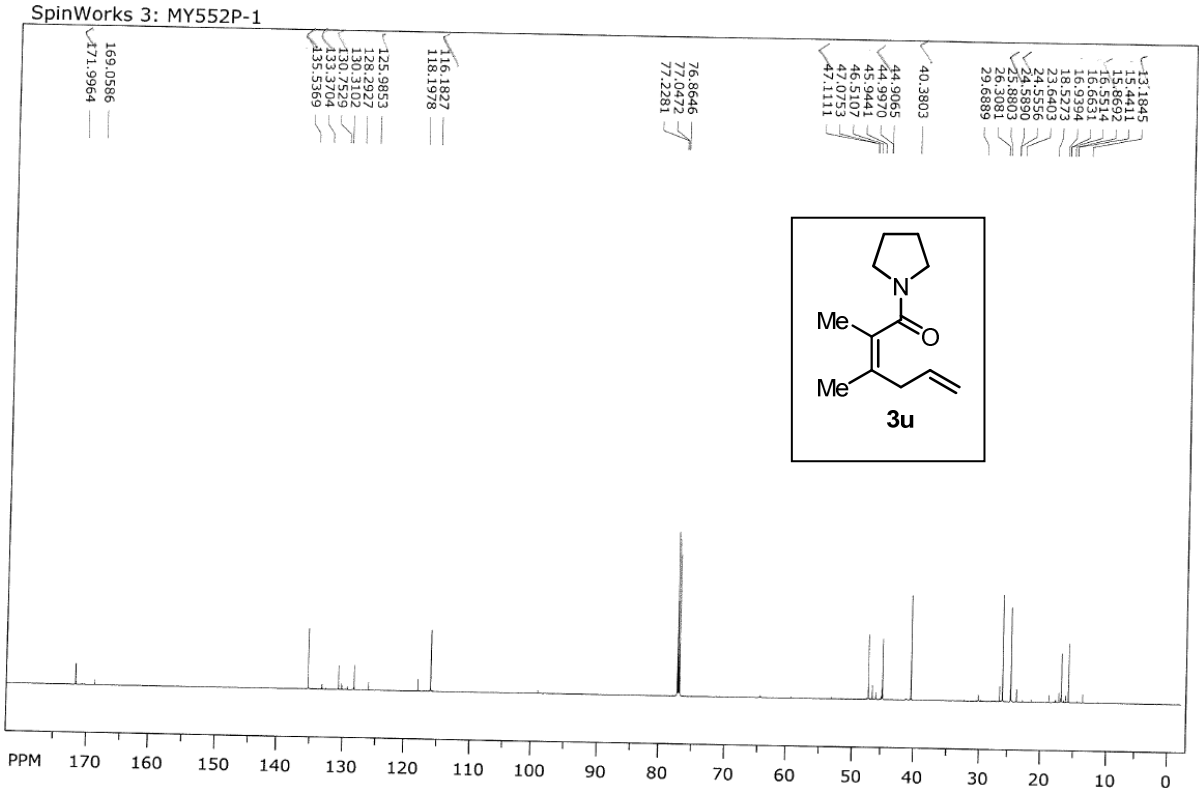

SpinWorks 3: MR331P
7.5355
7.5345
7.5333
7.5245
7.5233
7.2600
7.2128
7.2120
7.2111
7.2012
7.2003
6.3623
5.0846
5.0854
5.0864
5.0880
5.0890
5.0908
5.0989
5.1007
5.1016
5.1024
3.6683
3.3769
3.0608
1.9375
3s
1.036
2.211
2.984
0.999
1.037
2.212
6.380
4.444
PPM
8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0

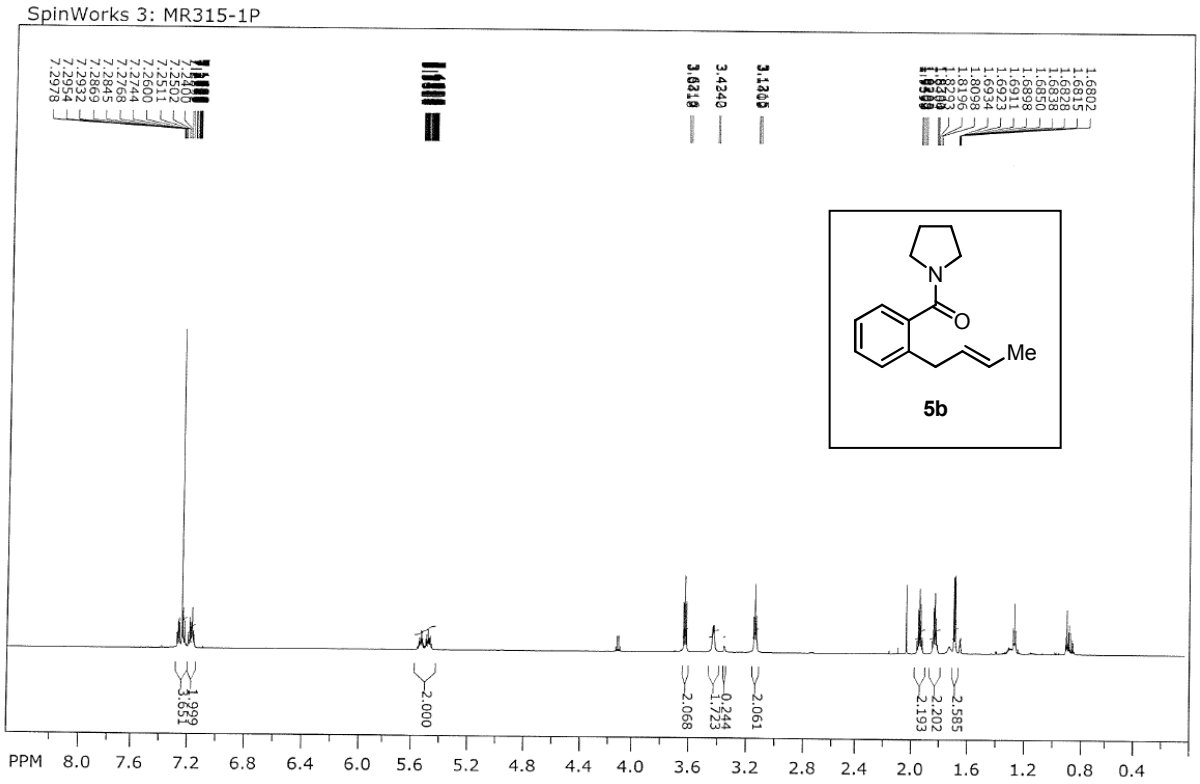

SpinWorks 3: MR331P
152.5158
137.9976
135.1430
135.0484
128.4398
122.2502
120.8906
120.4459
116.8276
110.8535
103.6634
77.2452
77.0645
76.8823
48.2619
47.1623
31.7880
25.6969
25.0037
3s
PPM
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

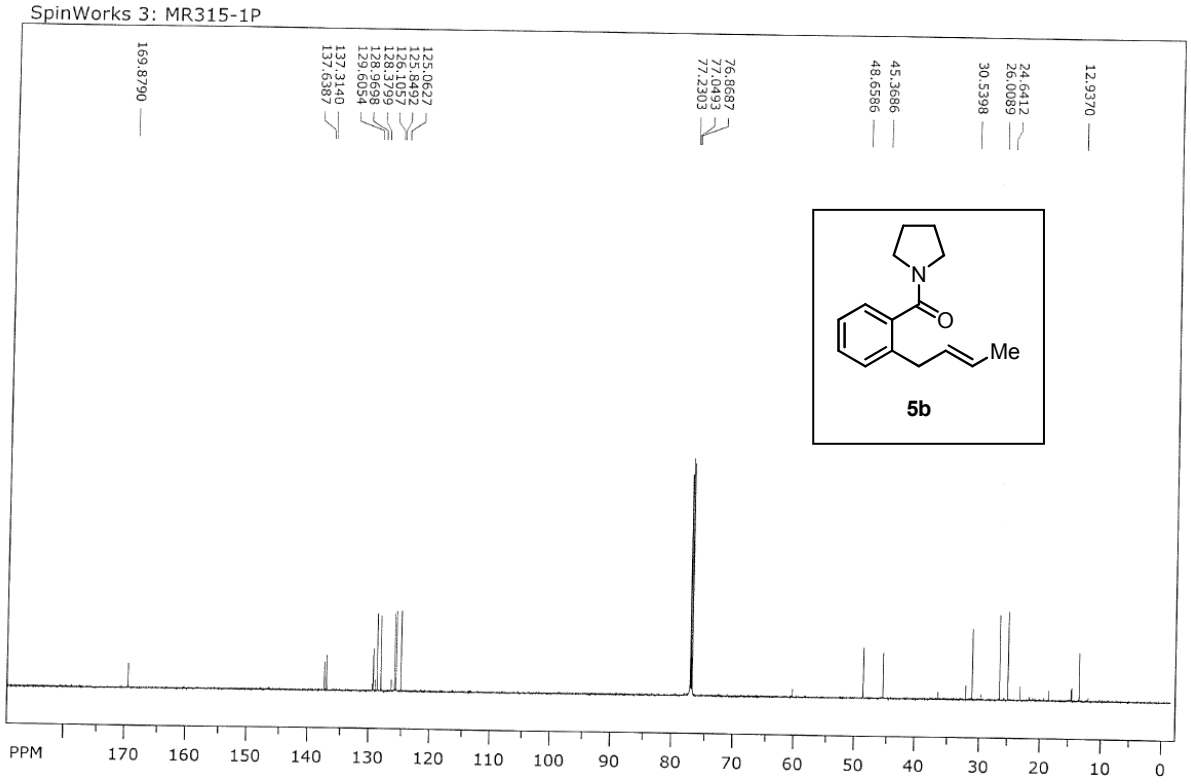

SpinWorks 3: YM107P-2
3t
PPM

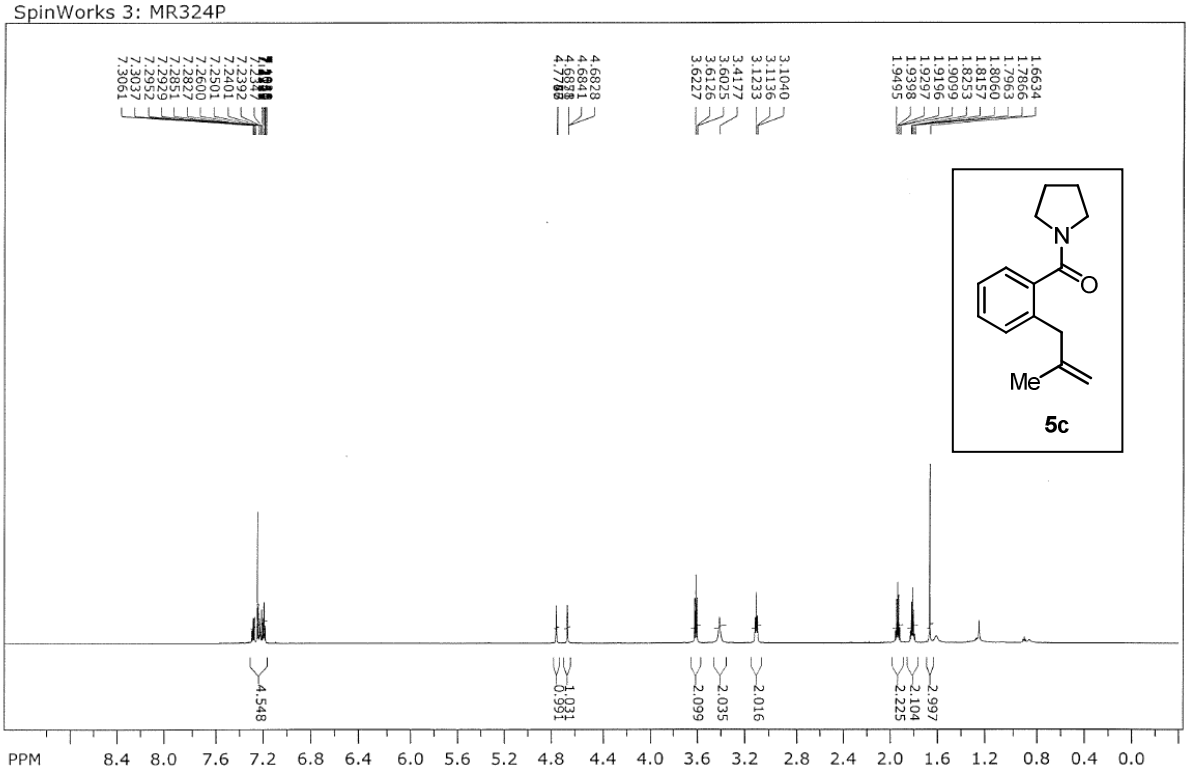

SpinWorks 3: YM107P-2
3t
PPM

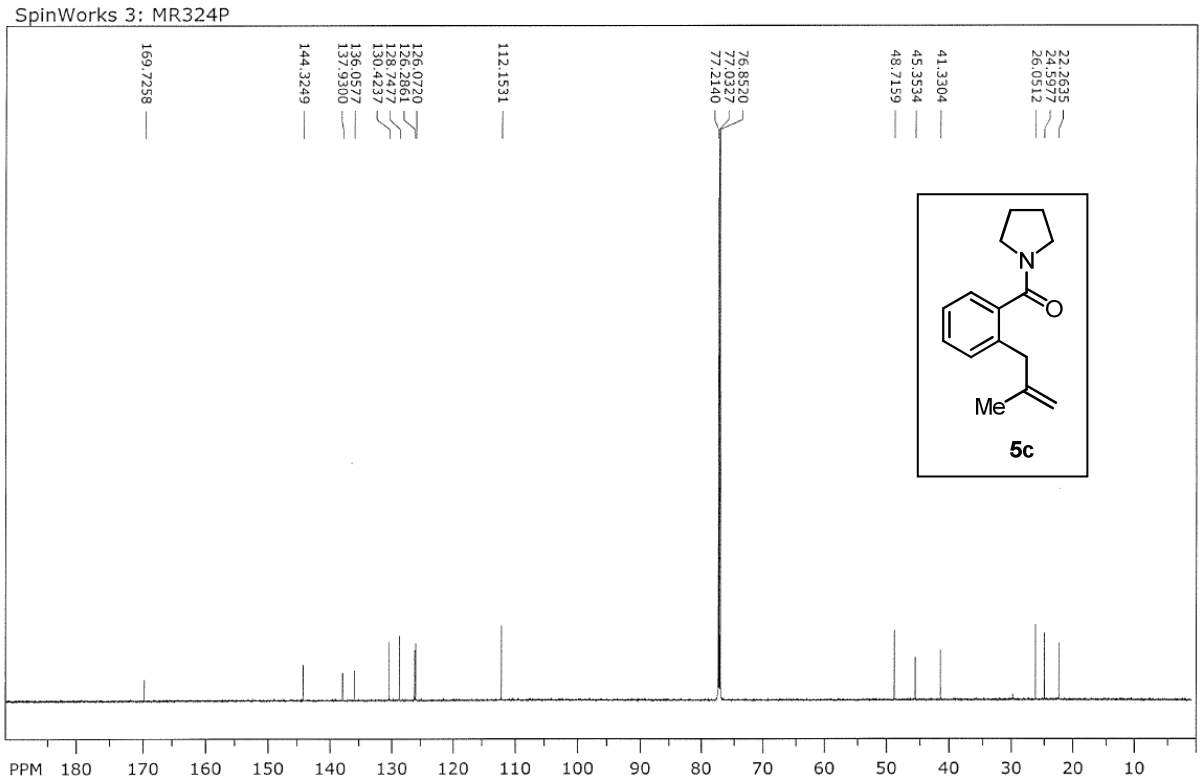

SpinWorks 3: MY552P-1
Me
Me
O
N
3u
PPM

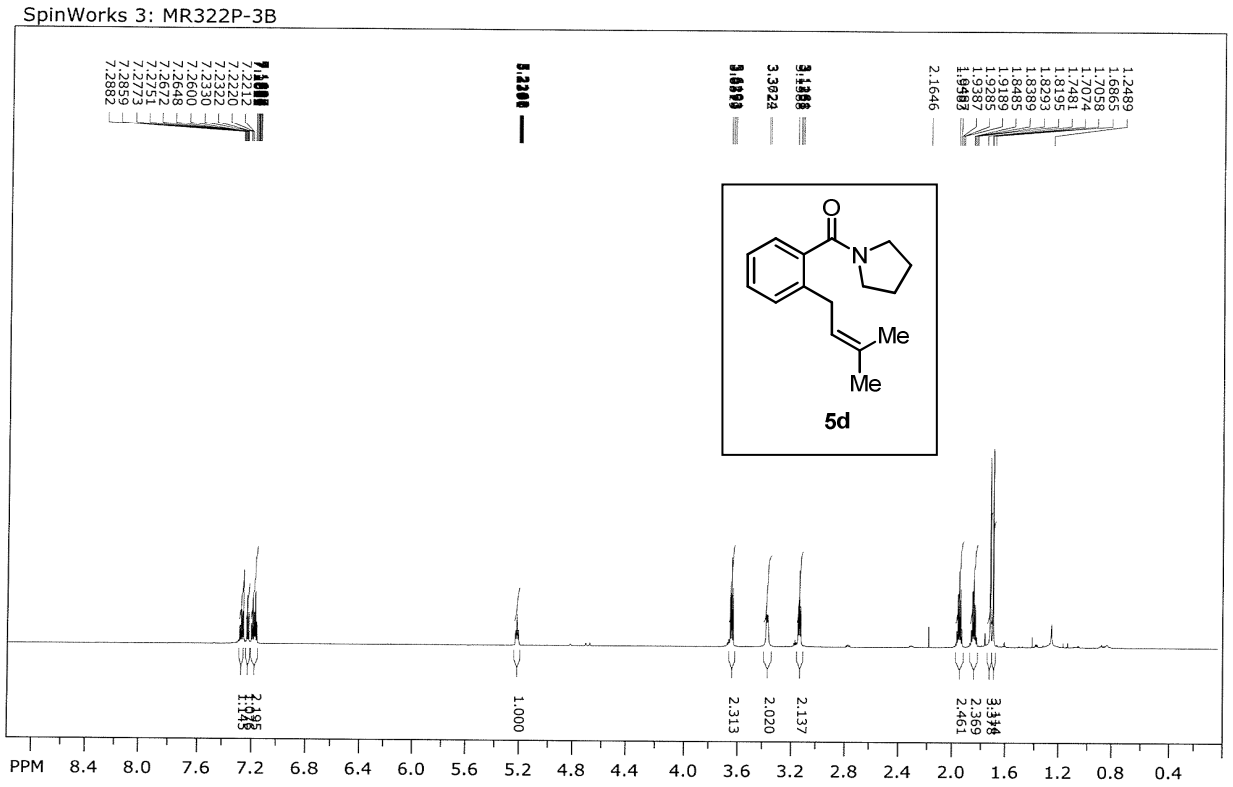

SpinWorks 3: MY552P-1
Me
Me
O
N
3u
PPM

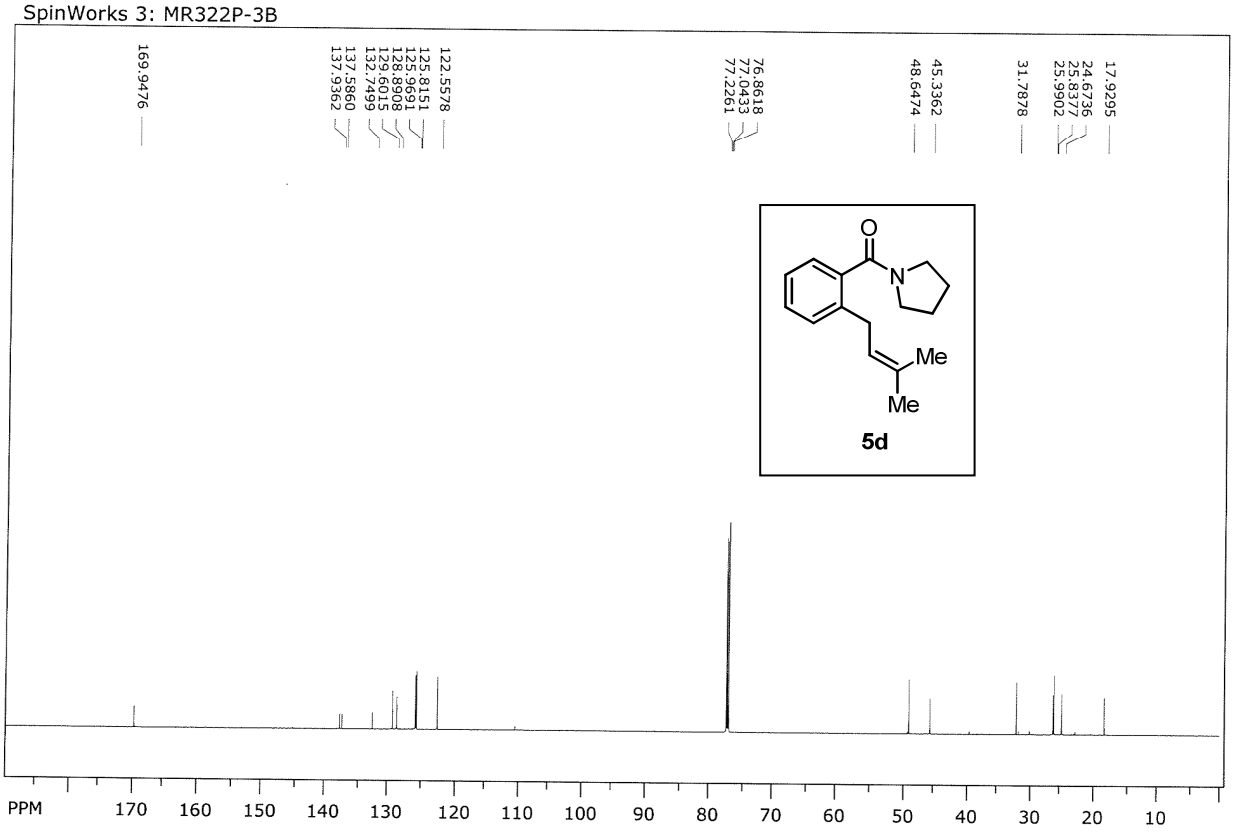

SpinWorks 3: MR315-1P
N
O
Me
5b
PPM 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4

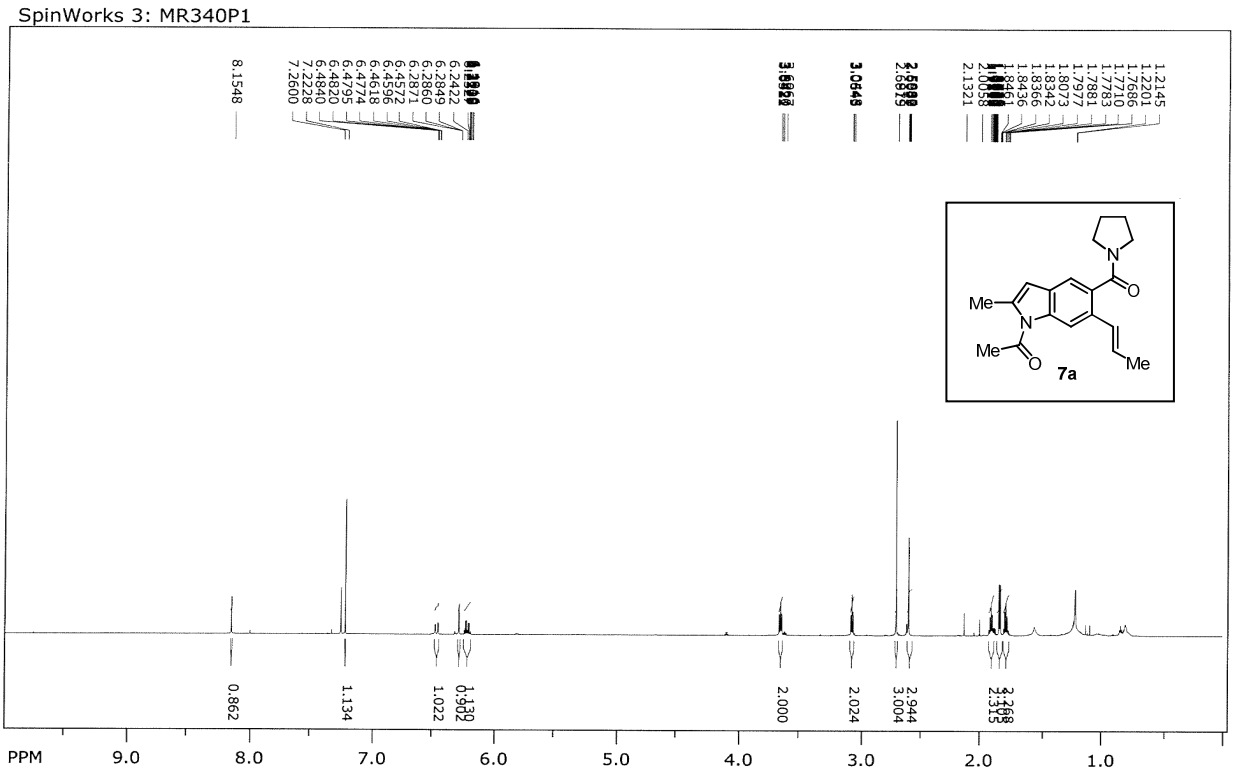

SpinWorks 3: MR315-1P
N
O
Me
5b
PPM 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

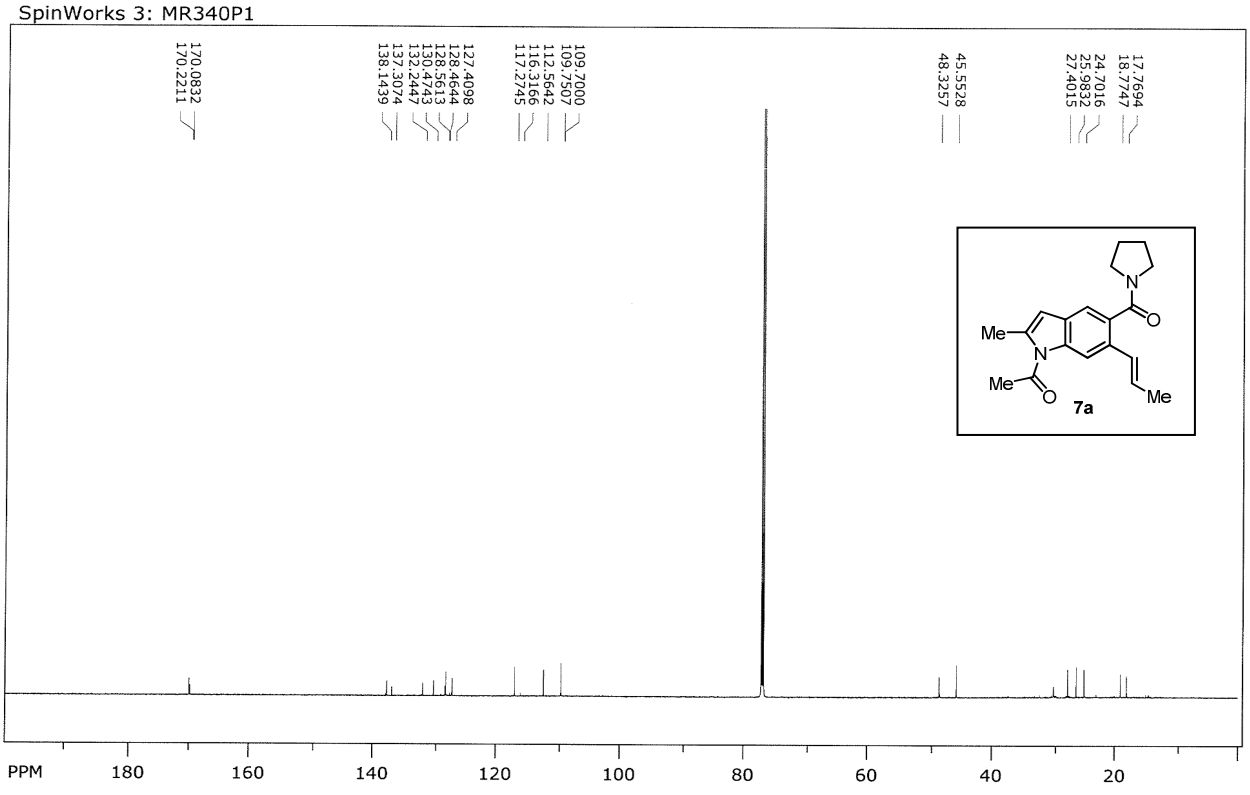

SpinWorks 3: MR324P
7.3061
7.3037
7.2952
7.2929
7.2851
7.2607
7.2501
7.2401
7.2392
4.6828
4.6841
3.6227
3.6126
3.6025
3.4177
3.1233
3.1136
3.1040
1.9495
1.9398
1.9297
1.9196
1.9099
1.8253
1.8157
1.8060
1.7963
1.7866
1.6634
4.548
1.031
0.991
2.099
2.035
2.016
2.225
2.104
2.997
PPM
8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0
N
O
Me
5c

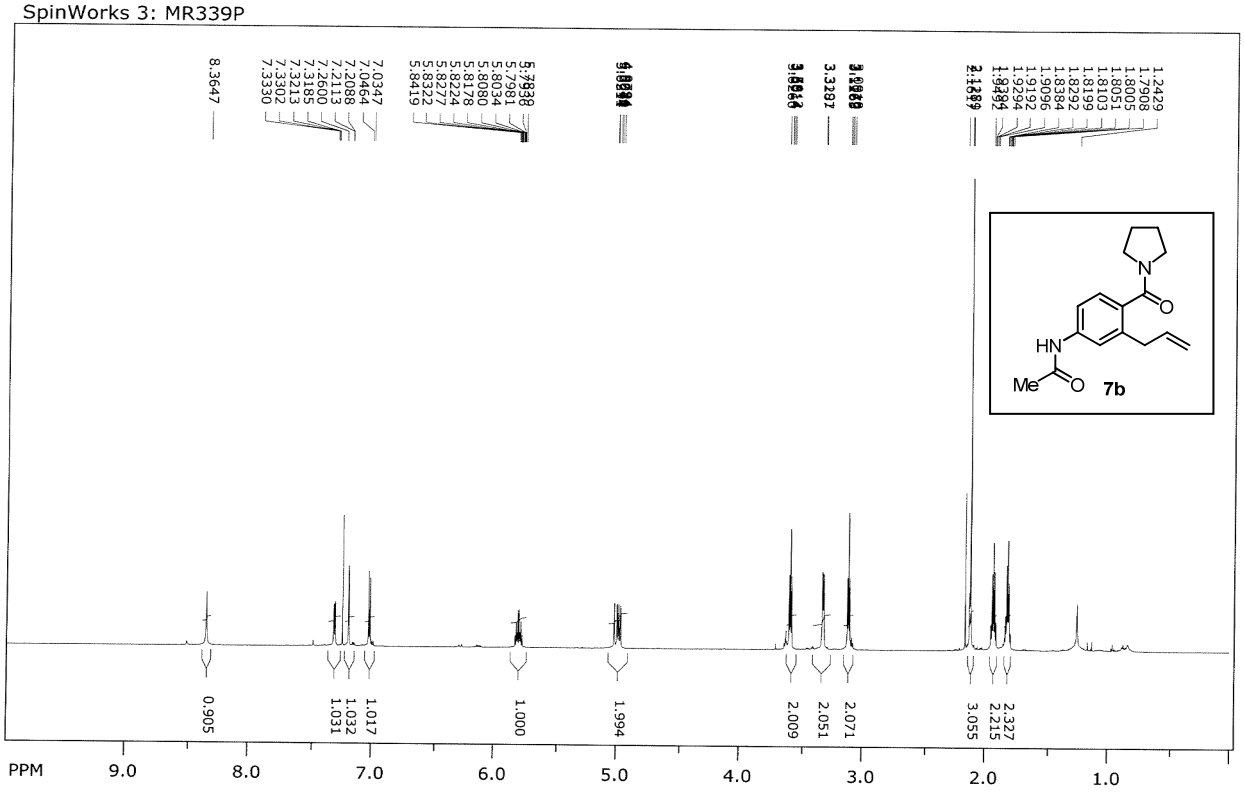

SpinWorks 3: MR324P
169.7258
144.3249
136.0577
137.9300
126.0720
126.2861
128.7477
130.4237
112.1531
76.8520
77.0327
77.2140
48.7159
45.3534
41.3304
26.0512
24.5977
22.2635
PPM
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
N
O
Me
5c

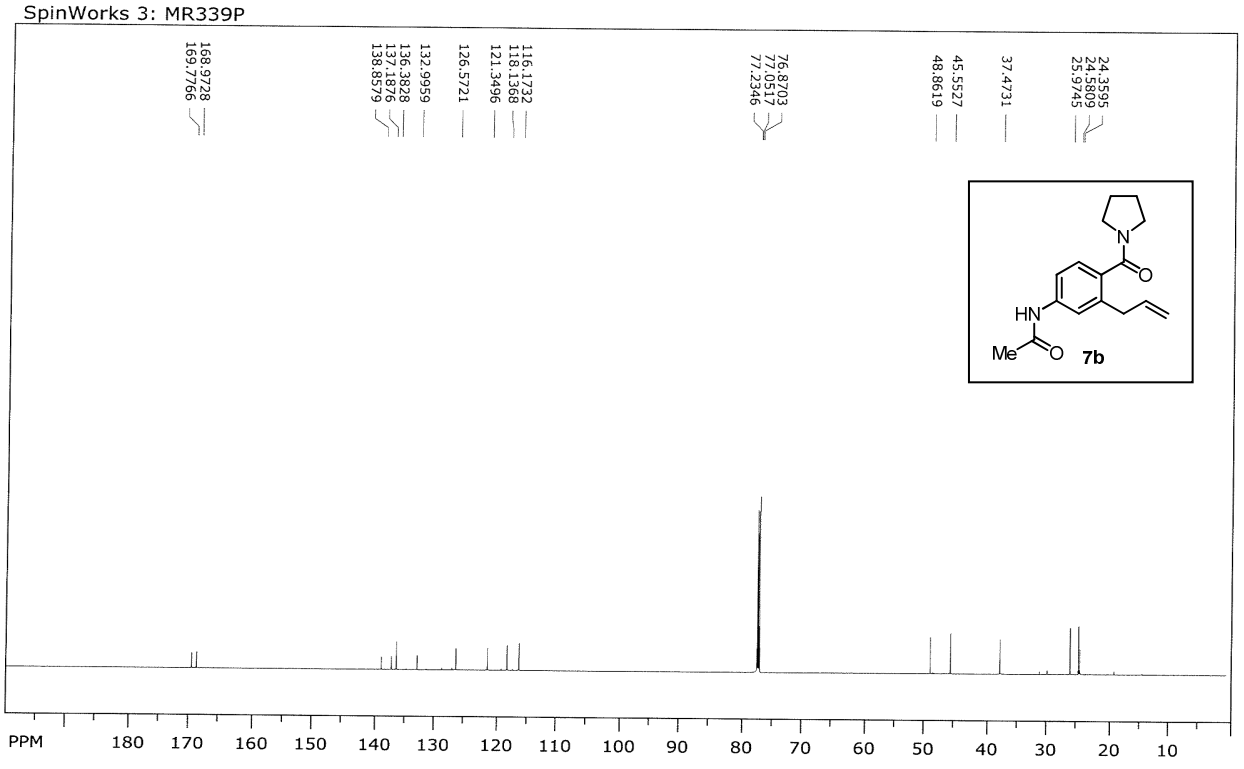

SpinWorks 3: MR322P-3B
5d
1.000
2.313
2.020
2.137
2.461
2.369
PPM


SpinWorks 3: MR322P-3B
169.9476
137.5860
137.9362
122.5578
125.8151
125.9691
128.8908
129.6015
132.7499
76.8618
77.0433
77.2261
45.3362
48.6474
31.7878
24.6736
25.8377
25.9902
17.9295
5d
PPM


SpinWorks 3: MR340P1
8.1548
7.2600
7.2228
6.4840
6.4820
6.4795
6.4774
6.4618
6.4596
6.4572
6.2871
6.2860
6.2849
6.2422
3.0548
2.8819
2.1321
2.0538
1.8436
1.8366
1.8342
1.8073
1.7977
1.7881
1.7783
1.7710
1.7686
1.2201
1.2145
Me
N
O
Me
N
O
Me
7a
0.862
1.134
1.022
2.000
2.024
3.004
2.315
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0


SpinWorks 3: MR340P1
170.0832
170.2211
138.1439
137.3074
132.2447
130.4743
128.5613
128.4644
127.4098
117.2745
112.5642
109.7507
109.7000
48.3257
45.5528
27.4015
25.9832
24.7016
18.7747
17.7694
Me
N
O
Me
N
O
Me
7a
PPM
180
160
140
120
100
80
60
40
20


SpinWorks 3: MR339P
8.3647
7.3330
7.3302
7.3213
7.3185
7.2600
7.2113
7.2088
7.0464
7.0347
5.8419
5.8322
5.8277
5.8224
5.8178
5.8080
5.8034
5.7981
1.2429
1.7908
1.8005
1.8051
1.8103
1.8199
1.8292
1.8384
1.9096
1.9192
1.9294
0.905
1.031
1.032
1.017
1.000
1.994
2.009
2.051
2.071
3.055
2.215
2.327
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
HN
Me
O
7b


SpinWorks 3: MR339P
168.9728
169.7766
138.8579
137.1876
136.3828
132.9959
126.5721
121.3496
118.1368
116.1732
77.2346
77.0517
76.8703
48.8619
45.5527
37.4731
25.9745
24.5809
24.3595
PPM
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
HN
Me
O
7b