Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

Pd-Catalyzed and CsF-Promoted Reaction of Bromoalkynes with Isocyanides: Regioselective Synthesis of Substituted 5-Iminopyrrolones

Yibiao Li, Jian Zhao, Huoji Chen, Bifu Liu and Huanfeng Jiang*

School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, PRC

Fax: (+86)20-8711-2906

E-mail: jianghf@scut.edu.cn

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I. General

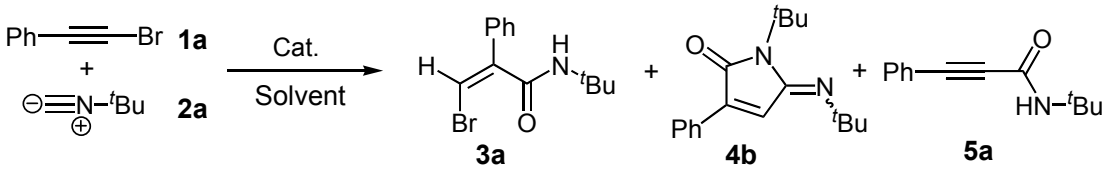
Unless otherwise noted, all commercial materials and solvents were used without further purification. All the reactions were carried out at 90 ^{o}C in a Schlenk tube equipped with magnetic stir bar. ^{1}H NMR spectra were recorded in $CDCl_3$ at 400 MHz and ^{13}C NMR spectra were recorded in $CDCl_3$ at 100 MHz respectively, and ^{1}H and ^{13}C NMR were referenced to $CDCl_3$ at δ 7.260 and 77.0 respectively. The different types of carbon in the structures have been identified by HSQC, HMBC and DEPT techniques. GC–MS was obtained using electron ionization. HRMS was carried out on a MAT 95XP (Thermo). IR spectra were obtained as potassium bromide pellets or as liquid films between two potassium bromide pellets with a Brucker Vector 22 spectrometer. TLC was performed using commercially prepared 100-400 mesh silica gel plates (GF_{254}), and visualization was effected at 254 nm. All the other chemicals were purchased from Aldrich Chemicals. Commercial reagents were used without further purification.

II. Synthesis of Substrates

General procedure for synthesis of bromoalkyne: To a solution of terminal alkyne (10 mmol) in acetone (60 mL) was added NBS (12 mmol) and $AgNO_3$ (5 mol %) at room temperature with magnetic stirring. After 2-4 hours, the reaction mixture was diluted with hexanes (100 mL) and filtered off the crystals formed. The filtrate was concentrated under reduced pressure and passed through a pad of silica gel using hexane as an eluent. The filtrate was collected and evaporated under reduced pressure to afford a pure colorless oil of bromoalkyne.

III. Palladium-Catalyzed or CsF-Promoted Reaction of Bromoalkynes with Isocyanides.

Table 1. Optimization of Reaction Conditions[a]



Entry	Catalyst	Solvent	Base	**2a** (equiv)	Yield (%)[b]		
					3a	4a	5a
1	--	DMSO	--	2.0	<5	--	--
2	--	CH_3CN	CsF	2.0	32	--	<5
3	--	THF	CsF	2.0	41	--	--
4[c]	**--**	**DMSO**	**CsF**	**2.0**	**89 (87)**	**--**	**7**
5[d]	--	DMSO	CsF	2.0	38	--	--
6	--	DMSO	Na_2CO_3	2.0	25	--	13
7	$PdCl_2$	DMSO	CsF	3	<5	81	12
8	$Pd(PPh_3)_4$	DMSO	CsF	3	<5	31	23
9	$Pd_2(dba)_3$	DMSO	CsF	3	<5	71	21
10	$Pd(OAc)_2$	DMF	CsF	3	12	68	9
11[e]	**$Pd(OAc)_2$**	**DMSO**	**CsF**	**3**	**<5**	**88 (85)**	**<5**
12	$Pd(OAc)_2$	DMSO	$(CH_3)_3COK$	3	10	24	<5
13	$Pd(OAc)_2$	DMSO	Et_3N	3	<5	< 5	--
14	$Pd(OAc)_2$	DMSO	--	3	<5	--	--

[a]Reaction conditions: phenylethynyl bromide (1.0 mmol), catalyst (5 mol %), and base (1.5 equiv) in 2 mL of solvent (0.1 mL H_2O) at 90 ^oC for 12 h. [b]Determined by GC. Number in parentheses is isolated yield. [c]Only *Z*-configuration. [d]Room temperature. [e]*Z*/*E* = 20:80. dba = dibenzylideneacetone, DMSO = dimethylsulfoxide, THF = tetrahydrofuran.

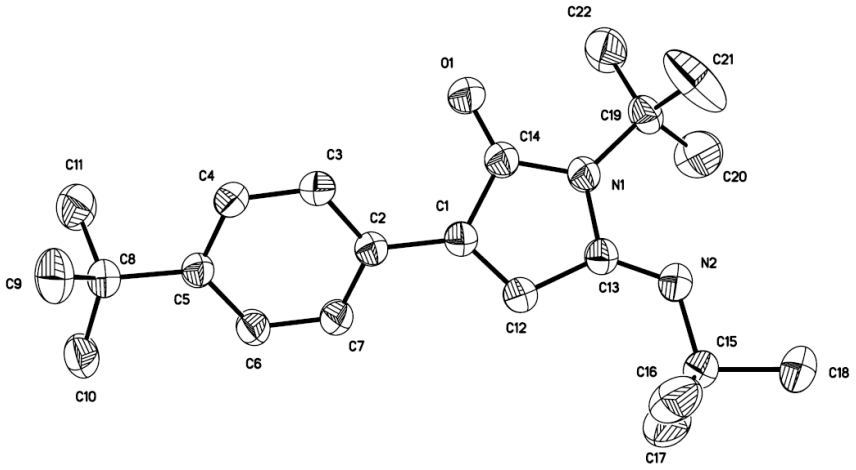
Typical procedure for the palladium-catalyzed reaction of phenylethynyl bromide and 2-isocyano-2-methylpropane:

A mixture of $Pd(OAc)_2$ (12 mg, 0.05 mmol), 0.1 mL H_2O, 2 mL DMSO, 2-isocyano-2-methylpropane (250 mg, 3.0 mmol), phenylethynyl bromide (180 mg, 1 mmol) and CsF (228 mg, 1.5 mmol) was added successively in Schlenk tube. After stirring for 12 h at 90 ^oC the starting materials were completely consumed as monitored by TLC and GC-MS analysis. After the reaction was finished, the reaction mixture was cooled to room temperature, the solution was filtered though a small amount of silica gel. The residue was purified by silica gel preparative TLC (*n*-hexane: EtOAc = 10:1), which furnished **4a** (241 mg, 85%, *Z*/*E* = 1:4) as a pale-yellow solid.

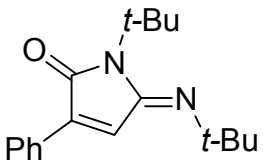
Typical procedure for the CsF-Promoted reaction of phenylethynyl bromide and 2-isocyano-2-methylpropane:

A mixture of CsF (180 mg, 1.2 mmol), 0.1 mL H_2O, 2 mL DMSO, 2-isocyano-2-methylpropane (166 mg, 2.0 mmol), phenylethynyl bromide (180 mg, 1 mmol) was added successively in Schlenk tube. After stirring for 12 h at 90 ^oC the starting materials were completely consumed as monitored by TLC and GC-MS analysis. After the reaction was finished, the reaction mixture was cooled to room temperature, the solution was filtered though a small amount of silica gel. The residue was purified by silica gel preparative TLC (*n*-hexane: EtOAc = 8:1), which furnished **3a** (246 mg, 87%) as a pale-yellow solid.

Figure 1. X-ray crystal structure of complex **4d**. (Thermal ellipsoids set at 50 % probability).

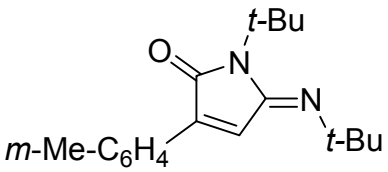


IV. Characterization Data for All Prepared Compounds



(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-phenyl-1*H*-pyrrol-2(5*H*)-one

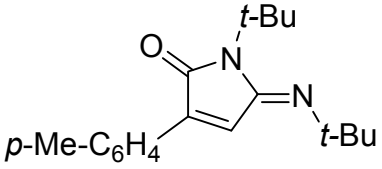
IR (KBr): ν_{max} = 2966, 2928, 1709, 1642, 1353, 1148, 752 cm^{-1}; ^1H NMR (d^6-acetone, 400 MHz) δ 8.01 (q, J = 3.6 Hz, 2H), 7.43–7.40 (m, 4H), 1.69 (s, 9H), 1.45 (s, 9H); ^{13}C NMR (d^6-acetone, 100 MHz) δ 170.1, 154.2, 140.3, 131.7, 130.4, 129.3, 129.3, 129.2, 129.2, 120.5, 58.1, 56.3, 32.7, 32.7, 32.7, 30.2, 30.2, 30.2; MS (EI, 70 eV) m/z (%): 284, 227, 213, 171, 128, 102; HRMS EI (m/z): calcd for $C_{18}H_{24}N_2O$, 284.1889; found, 284.1885.



(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-*m*-tolyl-1*H*-pyrrol-2(5*H*)-one

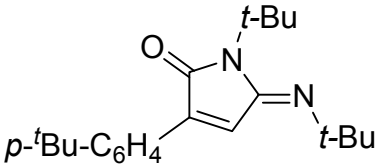
IR (KBr): ν_{max} = 2971, 2928, 1712, 1648, 1346, 1149. 743 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.67 (s, 1H), 7.60 (d, J =

7.7 Hz, 1H), 7.31–7.18 (m, 2H), 6.94 (s, 1H), 2.38 (s, 3H), 1.69 (s, 9H), 1.42 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.70, 152.83, 140.25, 138.11, 130.56, 130.32, 128.82, 128.35, 125.31, 118.87, 57.82, 55.79, 32.52, 32.52, 32.52, 29.84, 29.84, 29.84, 21.42; MS (EI, 70 eV) m/z (%): 298, 241, 227, 185, 171, 142, 115; HRMS EI (m/z): calcd for $C_{19}H_{26}N_2O$, 298.2045; found, 298.2037.



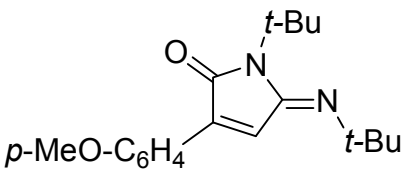
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-*p*-tolyl-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2970, 2928, 1713, 1647, 1346, 1149 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74 (d, J = 8.0 Hz, 2H), 7.20 (d, J = 7.9 Hz, 2H), 6.91 (s, 1H), 2.37 (s, 3H), 1.69 (s, 9H), 1.41 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.78, 153.02, 140.03, 139.76, 129.21, 129.21, 128.14, 128.14, 127.81, 118.11, 57.83, 55.78, 32.51, 32.51, 32.51, 29.86, 29.86, 29.86, 21.41; MS (EI, 70 eV) m/z (%): 298, 241, 227, 186, 171, 142, 105; HRMS EI (m/z): calcd for $C_{19}H_{26}N_2O$, 298.2045; found, 298.2038.



(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-*tert*-butylphenyl)-1*H*-pyrrol-2(5*H*)-one

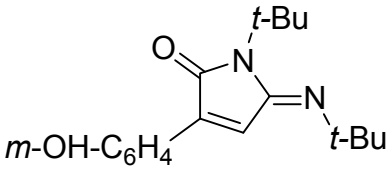
IR (KBr): ν_{max} = 2966, 2870, 1715, 1648, 1460, 1346, 1150, 834 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.76–7.70 (m, 2H), 7.43–7.36 (m, 2H), 6.91 (s, 1H), 1.69 (s, 9H), 1.41 (s, 9H), 1.32 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.77, 152.85, 140.13, 128.00, 128.00, 127.77, 125.44, 125.44, 118.31, 57.81, 55.76, 34.75, 32.49, 32.49, 32.49, 31.16, 31.16, 31.16, 29.84, 29.84, 29.84; MS (EI, 70 eV) m/z (%): 340, 283, 269, 228, 213, 171, 147; HRMS EI (m/z): calcd for $C_{22}H_{32}N_2O$, 340.2515; found, 340.2505.



(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-methoxyphenyl)-1*H*-pyrrol-2(5*H*)-one

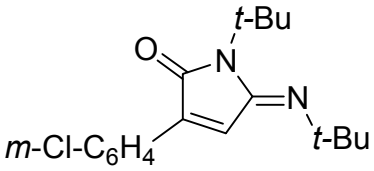
IR (KBr): ν_{max} = 2971, 2929, 1716, 1647, 1346, 1268, 1152, 778 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.84 (d, J = 8.8 Hz, 2H), 6.91 (d, J = 8.8 Hz, 2H), 6.86 (s, 1H), 3.83 (s, 3H), 1.69 (s, 9H), 1.41 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.90,

160.69, 152.97, 139.40, 129.69, 129.69, 123.21, 116.83, 113.91, 113.91, 57.71, 55.63, 55.25, 32.46, 32.46, 32.46, 29.85, 29.85, 29.85; MS (EI, 70 eV) m/z (%): 314, 257, 243, 202, 158; HRMS EI (m/z): calcd for $C_{19}H_{26}N_2O_2$, 314.1994; found, 314.1987.



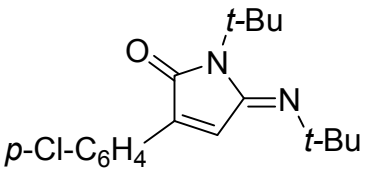
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(3-hydroxyphenyl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 3330, 2968, 2929, 1698, 1652, 1360, 1204 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.52 (s, 1H), 7.21 (t, J = 8 Hz, 1H), 6.88 (q, J = 6.4 Hz, 1H), 6.69–6.73 (m, 2H), 6.22 (s, 1H), 1.66 (s, 9H), 1.09 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.6, 156.3, 146.8, 142.9, 136.0, 132.9, 129.4, 120.3, 116.1, 115.5, 57.8, 56.5, 32.0, 32.0, 32.0, 29.9, 29.9, 29.9; MS (EI, 70 eV) m/z (%): 300, 285, 243, 229, 189, 172, 160, 144, 118; HRMS EI (m/z): calcd for $C_{18}H_{24}N_2O_2$, 300.1838; found, 300.1833.



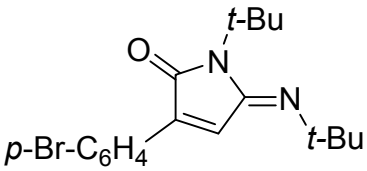
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(3-chlorophenyl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2970, 2930, 1712, 1648, 1348, 1151, 749 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.85 (s, 1H), 7.75–7.72 (m, 1H), 7.37–7.30 (m, 2H), 6.98 (s, 1H), 1.69 (s, 9H), 1.42 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.15, 152.35, 138.78, 134.46, 132.31, 129.70, 129.51, 128.16, 126.37, 119.61, 58.03, 56.03, 32.55, 32.55, 32.55, 29.79, 29.79, 29.79; MS (EI, 70 eV) m/z (%): 320, 318, 261, 247, 207, 162; HRMS EI (m/z): calcd for $C_{18}H_{23}ClN_2O$, 318.1499; found, 318.1499.



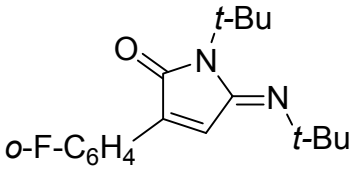
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-chlorophenyl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2970, 2930, 1713, 1648, 1487, 1346, 1209, 1150, 830 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.80 (d, J = 8.3 Hz, 2H), 7.37 (d, J = 8.3 Hz, 2H), 6.95 (s, 1H), 1.68 (s, 9H), 1.42 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.37, 152.46, 138.92, 135.67, 129.53, 129.53, 129.09, 128.73, 128.73, 118.91, 57.97, 55.96, 32.53, 32.53, 32.53, 29.81, 29.81, 29.81; MS (EI, 70 eV) m/z (%): 320, 318, 261, 247, 207, 205, 162; HRMS EI (m/z): calcd for $C_{18}H_{23}ClN_2O$, 318.1499; found, 319.1495.



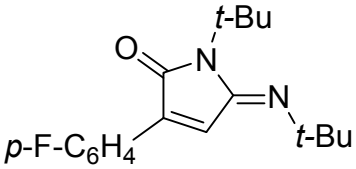
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-bromophenyl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2969, 2929, 1714, 1647, 1345, 1150 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.73 (d, J = 8.5 Hz, 2H), 7.53 (d, J = 8.5 Hz, 2H), 6.97 (s, 1H), 1.68 (s, 9H), 1.42 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.30, 152.46, 138.99, 131.70, 131.70, 129.77, 129.77, 129.53, 124.08, 118.95, 58.00, 55.99, 32.55, 32.55, 32.55, 29.82, 29.82, 29.82; MS (EI, 70 eV) m/z (%): 364, 362, 307, 305, 291, 251, 208, 171, 127, 101; HRMS EI (m/z): calcd for $C_{18}H_{23}BrN_2O$, 362.0994; found, 362.0987.



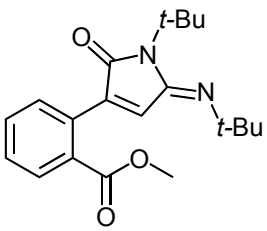
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(2-fluorophenyl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2971, 2931, 1717, 1647, 1346, 1213, 757 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.15–8.19 (m, 1H), 7.31–7.37 (m, 1H), 7.17–7.21 (m, 2H), 7.09–7.14 (m, 1H), 1.69 (s, 9H), 1.42 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.54, 161.29 (d, J = 251.1 Hz, 1C), 153.02, 133.31 (d, J = 1.8 Hz, 1C), 131.26 (d, J = 2.1 Hz, 1C), 130.69 (d, J = 8.9 Hz, 1C), 124.07 (d, J = 3.6 Hz, 1C), 122.94 (d, J = 1.8 Hz, 1C), 118.61 (d, J = 11.4 Hz, 1C), 115.64 (d, J = 22.3 Hz, 1C), 57.89, 55.90, 32.48, 32.48, 32.48, 29.79, 29.79, 29.79; MS (EI, 70 eV) m/z (%): 302, 245, 231, 191, 146, 120; HRMS EI (m/z): calcd for $C_{18}H_{23}FN_2O$, 302.1794; found, 302.1788.



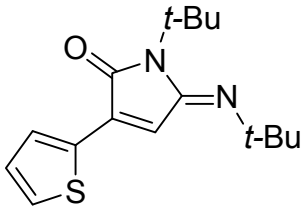
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-fluorophenyl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2970, 2931, 1711, 1648, 1507, 1347, 1231, 1153, 838 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.85 (dd, J = 8.9, 5.5 Hz, 2H), 7.11–7.06 (m, 2H), 6.92 (s, 1H), 1.69 (s, 9H), 1.42 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.52, 163.50 (d, J = 248.9 Hz, 1C), 152.55, 138.99, 130.22 (d, J = 8.2 Hz, 2C), 126.78 (d, J = 3.4 Hz, 1C), 118.42 (d, J = 2.7 Hz, 1C), 115.56 (d, J = 21.5 Hz, 2C), 57.91, 55.86, 32.51, 32.51, 32.51, 29.82, 29.82, 29.82; MS (EI, 70 eV) m/z (%): 302, 245, 231, 190, 140, 120; HRMS EI (m/z): calcd for $C_{18}H_{23}FN_2O$, 302.1794; found, 302.1788.



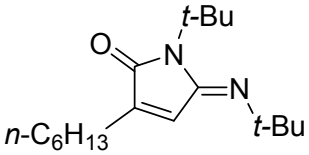
Methyl 2-((5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-2,5-dihydro-2-oxo-1*H*-pyrrol-3-yl)benzoate

IR (KBr): ν_{max} = 2964, 2927, 1720, 1661, 1339, 1263, 716 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.09 (d, J = 8.0 Hz, 1H), 7.55–7.59 (m, 1H), 7.46–7.50 (m, 1H), 7.26–7.29 (m, 1H), 6.08 (s, 1H), 3.81 (s, 3H), 1.70 (s, 9H), 0.96 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.8, 166.1, 143.5, 136.5, 132.1, 131.1, 130.9, 130.7, 130.3, 129.6, 128.9, 57.4, 55.6, 52.3, 31.8, 31.8, 31.8, 29.9, 29.9, 29.9; MS (EI, 70 eV) m/z (%): 342, 285, 271, 253, 231, 215, 199, 171, 156, 129; HRMS EI (m/z): calcd for $C_{20}H_{26}N_2O_3$, 342.1943; found, 342.1939.



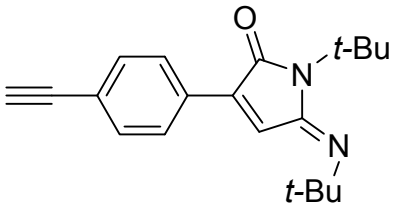
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(thiophen-2-yl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 3106, 2970, 2937, 1714, 1650, 1343, 1145cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.73 (q, J = 3.2 Hz, 1H), 7.48 (q, J = 4.0 Hz, 1H), 7.09 (q, J = 1.2 Hz, 1H), 6.83 (s, 1H), 1.68 (s, 9H), 1.41 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 168.9, 152.9, 134.6, 132.0, 129.8, 128.6, 127.5, 114.2, 58.0, 55.9, 32.4, 32.4, 32.4, 29.8, 29.8, 29.8; MS (EI, 70 eV) m/z (%): 290, 233, 219, 192, 178, 134; HRMS EI (m/z): calcd for $C_{16}H_{22}N_2OS$, 290.1453; found, 290.1449.



(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-hexyl-1*H*-pyrrol-2(5*H*)-one

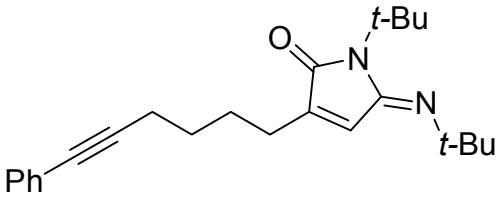
IR (KBr): ν_{max} = 2964, 2928, 2861, 1713, 1652, 1357 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.47 (s, 1H), 2.28 (t, J = 7.7 Hz, 2H), 1.62 (s, 9H), 1.54–1.44 (m, 2H), 1.37–1.25 (m, 15H), 0.88 (t, J = 6.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.99, 153.41, 145.63, 119.70, 57.41, 55.38, 32.38, 32.38, 32.38, 31.50, 29.78, 29.78, 29.78, 29.05, 27.32, 25.36, 22.52, 14.02; MS (EI, 70 eV) m/z (%): 292, 235, 221, 181, 151; HRMS EI (m/z): calcd for $C_{18}H_{32}N_2O$, 292.2515; found, 292.2507.



(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-ethynylphenyl)-1*H*-pyrrol-2(5*H*)-one

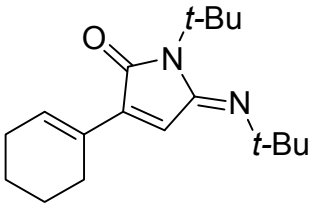
IR (KBr): ν_{max} = 3301, 2969, 2928, 1713, 1648, 1347 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.83 (d, J = 8.5 Hz, 2H), 7.52 (d, J = 8.4 Hz, 2H), 6.99 (s, 1H), 3.17 (s, 1H), 1.69 (s, 9H), 1.43 (s, 9H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.33, 139.26, 132.19, 132.19, 130.92, 128.33, 128.13, 128.13, 123.32, 119.38, 83.32, 78.86, 58.15, 56.12, 32.52, 32.52, 32.52, 29.80, 29.80, 29.80; MS (EI, 70 eV)

m/z (%): 308. 251, 237, 196, 152; HRMS EI (m/z): calcd for $C_{20}H_{24}N_2O$, 308.1889; found, 308.1882.



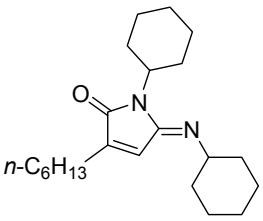
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(6-phenylhex-5-ynyl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2968, 2923, 1710, 1651, 1358, 1213, 1119 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.40–7.38 (m, 2H), 7.28–7.26 (m, 3H), 6.53 (s, 1H), 2.46 (t, J = 6.5 Hz, 2H), 2.37 (t, J = 7.1 Hz, 2H), 1.76–1.66 (m, 4H), 1.63 (s, 9H), 1.34 (s, 9H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.89, 153.30, 145.13, 131.53, 131.53, 128.17, 128.17, 127.56, 123.88, 119.91, 89.77, 80.93, 57.49, 55.46, 32.37, 32.37, 32.37, 29.77, 29.77, 29.77, 28.39, 26.53, 24.90, 19.17 ; MS (EI, 70 eV) m/z (%): 364, 307, 279, 251, 223, 208, 115; HRMS EI (m/z): calcd for $C_{24}H_{32}N_2O$, 364.2515; found, 364.2504.



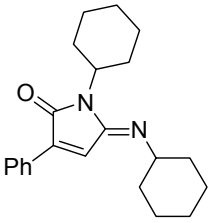
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-cyclohexenyl-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2932, 2865, 1643, 1536, 1222 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.25 (t, J = 4.4 Hz, 1H), 6.44 (s, 1H), 2.24–2.15 (m, 4H), 1.73–1.70 (m, 2H), 1.63–1.60 (m, 11H), 1.35 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.03, 153.22, 139.71, 135.14, 128.39, 115.69, 57.49, 55.44, 32.39, 32.39, 32.39, 29.85, 29.85, 29.85, 26.18, 26.15, 22.38, 21.71; MS (EI, 70 eV) m/z (%): 288, 231, 217, 176, 161, 110; HRMS EI (m/z): calcd for $C_{18}H_{28}N_2O$, 288.2202; found, 288.2195.



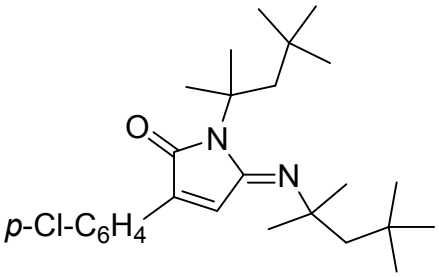
(5*E*)-1-cyclohexyl-5-(cyclohexylimino)-3-hexyl-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2929, 2856, 1712, 1649, 1372 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.12 (s, 1H), 4.12–3.95 (m, 2H), 2.56–2.51 (m, 2H), 2.28–2.17 (m, 2H), 1.84–1.75 (m, 4H), 1.72–1.54 (m, 10H), 1.39–1.26 (m, 12H), 0.89 (d, J = 6.9 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.03, 150.29, 144.98, 127.99, 56.59, 50.73, 35.14, 35.14, 31.59, 30.23, 29.69, 29.64, 29.64, 29.00, 27.86, 26.34, 26.34, 25.67, 25.50, 24.18, 22.53, 14.03; MS (EI, 70 eV) m/z (%): 344, 263, 219, 191, 181, 111, 81; HRMS EI (m/z): calcd for $C_{22}H_{36}N_2O$, 344.2828; found, 344.2821.



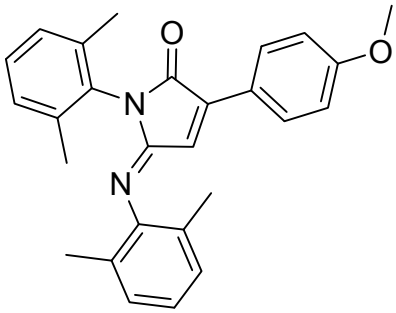
(5*E*)-1-cyclohexyl-5-(cyclohexylimino)-3-phenyl-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2930, 2854, 1713, 1645, 1370, 1184 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.41–7.39 (m, 3H), 7.31–7.27 (m, 2H), 6.22 (s, 1H), 4.20–4.11 (m, 1H), 3.44–3.39 (m, 1H), 2.33–2.23 (m, 2H), 1.83–1.79 (m, 2H), 1.67–1.57 (m, 5H), 1.44–1.31 (m, 9H), 0.84–0.78 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.28, 149.21, 142.66, 134.57, 130.65, 128.64, 128.32, 128.32, 127.32, 127.32, 56.69, 50.99, 34.70, 34.70, 29.59, 29.59, 26.27, 26.27, 25.42, 25.36, 23.92, 23.92; MS (EI, 70 eV) m/z (%): 336, 255, 253, 173, 156, 128, 102; HRMS EI (m/z): calcd for $C_{22}H_{28}N_2O$, 336.2202; found, 336.2200.



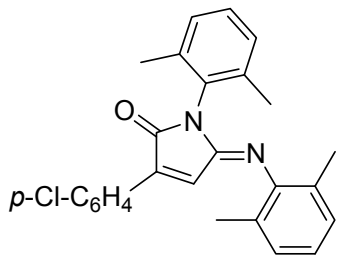
(5*E*)-5-(2,4,4-trimethylpentan-2-ylimino)-3-(4-chlorophenyl)-1-(2,4,4-trimethylpentan-2-yl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2955, 1710, 1643, 1343, 1175, 830 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.81 (d, J = 8.5 Hz, 2H), 7.38 (d, J = 8.5 Hz, 2H), 6.96 (s, 1H), 2.05 (s, 2H), 1.79 (s, 2H), 1.77 (s, 6H), 1.48 (s, 6H), 1.00 (s, 9H), 0.94 (s, 9H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 170.02, 152.94, 138.72, 135.72, 129.60, 129.60, 129.03, 128.74, 128.74, 119.40, 61.54, 60.33, 57.61, 50.65, 33.31, 33.31, 32.11, 32.01, 32.01, 32.01, 31.59, 31.37, 31.37, 31.14, 31.14, 31.14 ; MS (EI, 70 eV) m/z (%): 430, 373, 317, 261, 247, 207, 162, 97; HRMS EI (m/z): calcd for $C_{26}H_{39}ClN_2O$, 430.2751; found, 430. 2746.



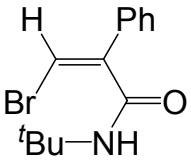
(5*E*)-5-(2,6-dimethylphenylimino)-3-(4-methoxyphenyl)-1-(2,6-dimethylphenyl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 2925, 2847, 2556, 2192, 1727, 1658, 1471, 1254, 1148 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.92–7.19 (m, 5H), 6.58–6.66 (m, 5H), 6.54 (s, 1H), 3.74 (s, 3H), 2.27 (s, 6H), 1.96 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 150.9, 145.2, 137.2, 128.9, 128.2, 127.4, 125.7, 123.3, 122.8, 113.1, 55.3, 18.8, 18.2; MS (EI, 70 eV) m/z (%): 411, 410, 409, 395, 290, 262, 205, 132, 121; HRMS EI (m/z): calcd for $C_{27}H_{26}N_2O_2$, 410.1994; found, 410.1990.



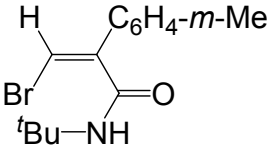
(5*E*)-5-(2,6-dimethylphenylimino)-3-(4-chlorophenyl)-1-(2,6-dimethylphenyl)-1*H*-pyrrol-2(5*H*)-one

IR (KBr): ν_{max} = 3046, 2923, 2858, 1733, 1656, 1592, 1482, 1147, 827, 736 cm^{-1}; ^1H NMR (d^6-acetone, 400 MHz) δ 7.18–7.11 (m, 7H), 6.78 (s, 1H), 6.66–6.59 (m, 3H), 2.27 (s, 6H), 1.97 (s, 6H) ; ^{13}C NMR (d^6-acetone, 100 MHz) δ 151.93, 146.20, 138.38, 133.41, 130.51, 130.26, 129.54, 128.89, 128.89, 128.38, 128.27, 128.27, 126.68, 124.10, 19.05, 19.05, 18.46, 18.46; MS (EI, 70 eV) m/z (%): 415, 414, 412, 399, 294, 259, 231, 207, 136, 121; HRMS EI (m/z): calcd for $C_{26}H_{23}ClN_2O$, 414.1499; found, 414.1490.



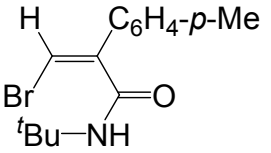
(*Z*)-*N*-*tert*-butyl-3-bromo-2-phenylacrylamide

IR (KBr): ν_{max} = 3278, 3048, 2968, 2926, 1633, 1564, 1539, 1347, 1221 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.42–7.38 (m, 2H), 7.36–7.33 (m, 3H), 6.67 (s, 1H), 5.56 (s, 1H), 1.46 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.95, 144.31, 135.34, 128.86, 128.86, 128.81, 126.08, 126.08, 105.40, 52.28, 28.71, 28.71, 28.71; MS (EI, 70 eV) m/z (%): 283, 281, 266, 226, 209, 202, 181, 102.



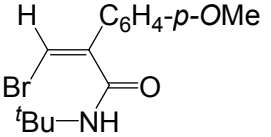
(*Z*)-*N*-*tert*-butyl-3-bromo-2-*m*-tolylacrylamide

IR (KBr): ν_{max} = 3279, 3052, 2968, 2926, 2859, 2215, 1633, 1539, 1221, 786, 692 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.24–7.18 (m, 3H), 7.15 (d, J = 7.1 Hz, 1H), 6.64 (s, 1H), 5.54 (s, 1H), 2.35 (s, 3H), 1.46 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.02, 144.41, 138.53, 135.29, 129.57, 128.70, 126.76, 123.19, 105.16, 52.22, 28.70, 28.70, 28.70, 21.41; MS (EI, 70 eV) m/z (%): 297, 295, 282, 280, 241, 226, 216, 195, 160, 115.



(*Z*)-*N*-*tert*-butyl-3-bromo-2-*p*-tolylacrylamide

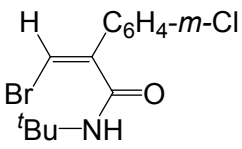
IR (KBr): ν_{max} = 3275, 3067, 2970, 2914, 1643, 1549, 1337, 788 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.28 (d, J = 8.1 Hz, 2H), 7.14 (d, J = 8.2 Hz, 2H), 6.61 (s, 1H), 5.53 (s, 1H), 2.33 (s, 3H), 1.45 (s, 9H) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.09, 144.15, 138.78, 132.49, 129.48, 129.48, 125.91, 125.91, 104.34, 52.13, 28.65, 21.15, 21.15, 21.15 ; MS (EI, 70 eV) m/z (%): 297, 295, 280, 224, 216, 197, 160, 143, 115.



(*Z*)-*N*-*tert*-butyl-3-bromo-2-(4-methoxyphenyl)acrylamide

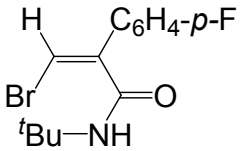
^1H NMR ($CDCl_3$, 400 MHz) δ 7.32 (d, J = 8.8 Hz, 2H), 6.86 (d, J = 8.8 Hz, 2H), 6.53 (s, 1H), 5.55 (s, 1H), 3.80 (s, 3H), 1.45 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.21, 160.01, 143.77, 127.93, 127.38, 127.38, 114.21, 114.21, 103.20,

55.30, 52.18, 28.69, 28.69, 28.69; MS (EI, 70 eV) m/z (%): 313, 311, 232, 211, 176, 148, 132, 117, 89, 57.



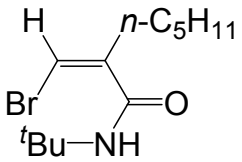
(*Z*)-*N*-*tert*-butyl-3-bromo-2-(3-chlorophenyl)acrylamide

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39 (s, 1H), 7.31–7.26 (m, 3H), 6.70 (s, 1H), 5.59 (s, 1H), 1.46 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.33, 143.15, 137.06, 134.78, 130.05, 128.83, 126.22, 124.30, 106.71, 52.42, 28.69, 28.69, 28.69; MS (EI, 70 eV) m/z (%): 317, 315, 304, 302, 300, 262, 260, 245, 243, 217, 215, 180, 136, 101.



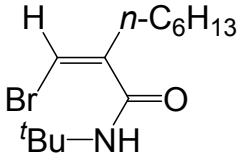
(*Z*)-*N*-*tert*-butyl-3-bromo-2-(4-fluorophenyl)acrylamide

IR (KBr): ν_{max} = 3273, 2969, 2927, 2858, 2217, 1635, 1509, 1231, 837 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39–7.35 (m, 2H), 7.02 (dd, J = 9.5, 7.8 Hz, 2H), 6.59 (s, 1H), 5.62 (s, 1H), 1.45 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.76, 162.93 (d, J = 247.6 Hz, 1C), 143.26, 131.56 (d, J = 3.4 Hz, 1C), 127.93 (d, J = 8.3 Hz, 2C), 115.82 (d, J = 21.7 Hz, 2C), 105.09 (d, J = 1.9 Hz, 1C), 52.30, 28.66, 28.66, 28.66.



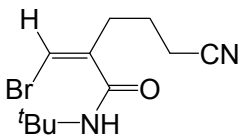
(*Z*)-*N*-*tert*-butyl-2-(bromomethylene)heptanamide

IR (KBr): ν_{max} = 3300, 2961, 2929, 2863, 1650, 1542, 1457, 1329, 1223 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.10 (t, J = 1.3 Hz, 1H), 5.55 (s, 1H), 2.33–2.29 (m, 2H), 1.46–1.39 (m, 11H), 1.33–1.25 (m, 4H), 0.88 (t, J = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.44, 144.59, 101.98, 51.98, 35.16, 31.16, 28.74, 28.74, 28.74, 27.33, 22.32, 13.92; MS (EI, 70 eV) m/z (%): 277, 275, 262, 260, 222, 220, 203, 196, 146, 140, 123, 95.



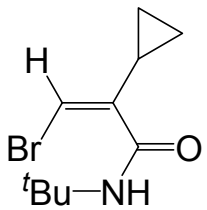
(*Z*)-*N*-*tert*-butyl-2-(bromomethylene)octanamide

IR (KBr): ν_{max} = 3301, 2961, 2930, 2862, 1650, 1542, 1455, 1329, 1223, 833 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.08 (t, J =1.2 Hz, 1H), 5.56 (s, 1H), 2.32–2.28 (m, 2H), 1.42–1.39 (m, 11H), 1.27–1.23 (m, 6H), 0.86 (t, J = 6.8 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.42, 144.55, 101.94, 51.92, 35.16, 31.44, 28.69, 28.69, 28.69, 28.63, 27.58, 22.45, 13.98; MS (EI, 70 eV) m/z (%): 291, 289, 276, 276, 236, 234, 219, 217, 210, 154, 147, 109.



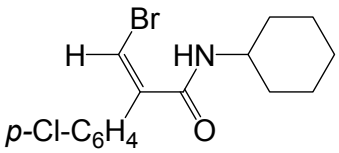
(*Z*)-*N*-*tert*-butyl-2-(bromomethylene)-5-cyanopentanamide

IR (KBr): ν_{max} = 3278, 2965, 2928, 2863, 1711, 1653, 1545, 1329, cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.23 (s, 1H), 5.79 (s, 1H), 2.46–2.42 (m, 2H), 2.36 (t, J = 7.0 Hz, 2H), 1.84–1.77 (m, 2H), 1.36 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.47, 141.56, 119.16, 104.36, 52.02, 33.92, 28.54, 28.54, 28.54, 23.33, 16.20; MS (EI, 70 eV) m/z (%): 274, 272, 259, 257, 202, 200, 177, 145, 92, 51.



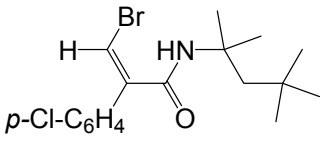
(*Z*)-*N*-*tert*-butyl-3-bromo-2-cyclopropylacrylamide

IR (KBr): ν_{max} = 3275, 3065, 2970, 1653, 1547, 1452, 1223 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 6.06 (s, 1H), 5.44 (s, 1H), 1.64–1.60 (m, 1H), 1.40 (s, 9H), 0.76–0.73 (m, 2H), 0.69–0.66 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.77, 145.27, 101.39, 51.99, 28.71, 28.71, 28.71, 15.56, 5.86, 5.86; MS (EI, 70 eV) m/z (%): 247, 245, 232, 230, 191, 189, 173, 166, 110, 67.



(*Z*)-3-bromo-2-(4-chlorophenyl)-*N*-cyclohexylacrylamide

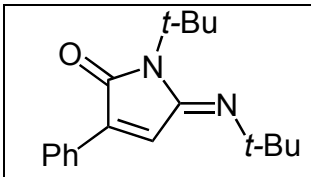
IR (KBr): ν_{max} = 3266, 2933, 2853, 1630, 1446, 1230, 1090, 797, 752 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.34–7.26 (m, 4H), 6.68 (s, 1H), 5.75 (d, J = 7.7 Hz, 1H), 4.00–3.91 (m, 1H), 2.01 (dd, J = 12.2, 2.8 Hz, 2H), 1.75–1.71 (m, 2H), 1.63 (dd, J = 9.0, 3.9 Hz, 1H), 1.44–1.35 (m, 2H), 1.27–1.18 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.39, 142.84, 134.83, 133.71, 129.00, 129.00, 127.42, 127.42, 106.31, 48.65, 32.84, 32.84, 25.40, 24.73, 24.73; MS (EI, 70 eV) m/z (%): 343, 341, 262, 217, 215, 180, 136, 101; HRMS EI (m/z): calcd for $C_{15}H_{17}BrClNO$, 341.0182; found, 341.0173.



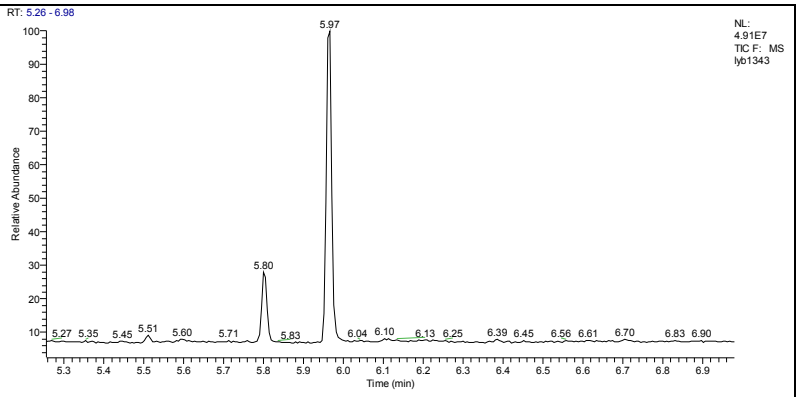
(*Z*)-3-bromo-2-(4-chlorophenyl)-*N*-(2,4,4-trimethylpentan-2-yl)acrylamide

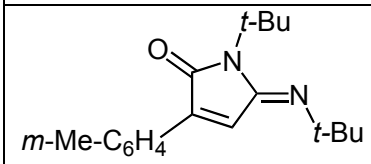
IR (KBr): ν_{max} = 3294, 3070, 2947, 1637, 1550, 1336, 799 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.36–7.30 (m, 4H), 6.63 (s, 1H), 5.58 (s, 1H), 1.74 (s, 2H), 1.54 (s, 6H), 0.99 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 165.25, 143.34, 134.80, 133.96, 129.00, 129.00, 127.56, 127.56, 106.08, 56.59, 53.20, 31.66, 31.57, 31.57, 31.57, 28.47, 28.47; MS (EI, 70 eV) m/z (%): 373, 371, 304, 302, 262, 245, 217, 163, 136, 97; HRMS EI (m/z): calcd for $C_{17}H_{23}BrClNO$, 371.0652; found 371.0648.

V. *Z*/*E* Selectivity Determined by GC Chromatograms.

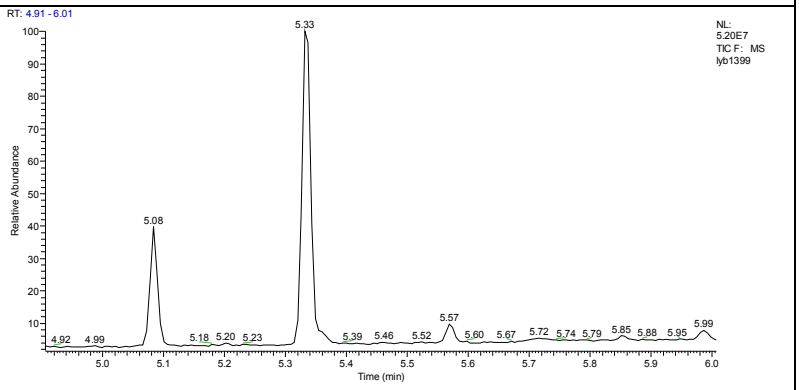


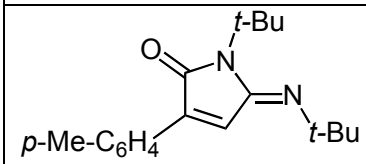
4a, 85 %, Z/E = 20:80



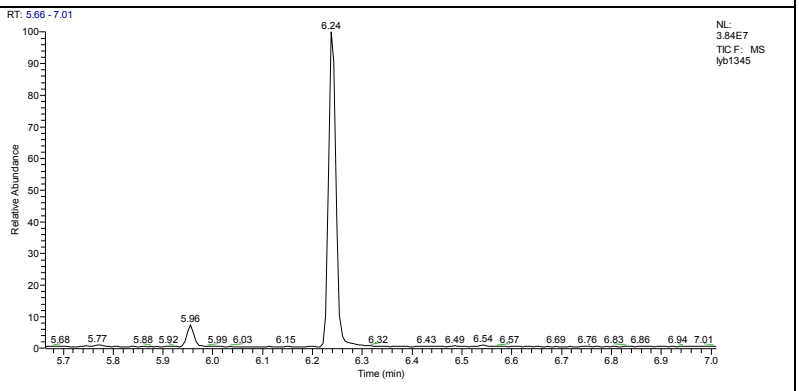


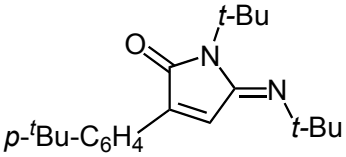
4b, 83 %, Z/E = **24:76**



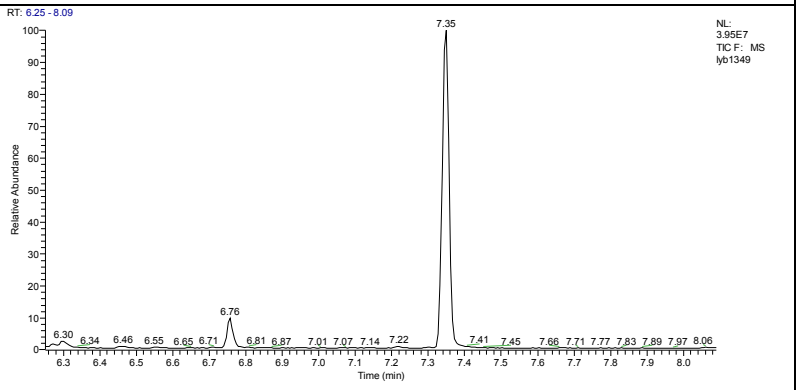


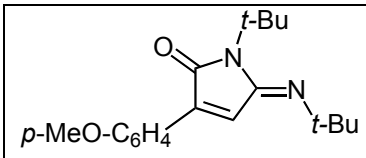
4c, 79 %, Z/E = **7:93**



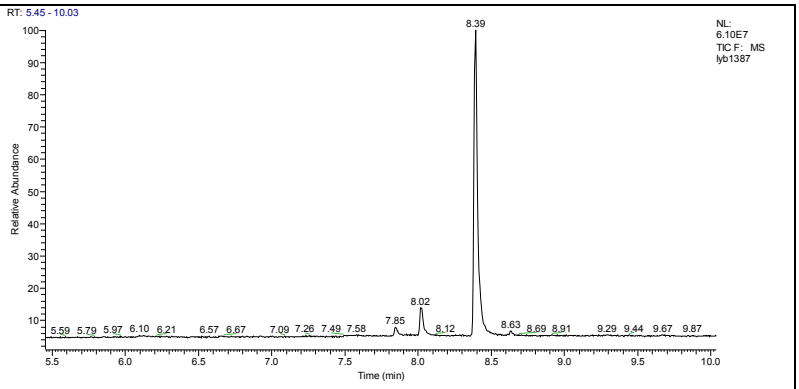


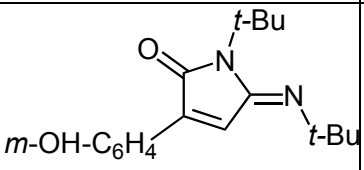
4d, 86 %, Z/E = **8:92**



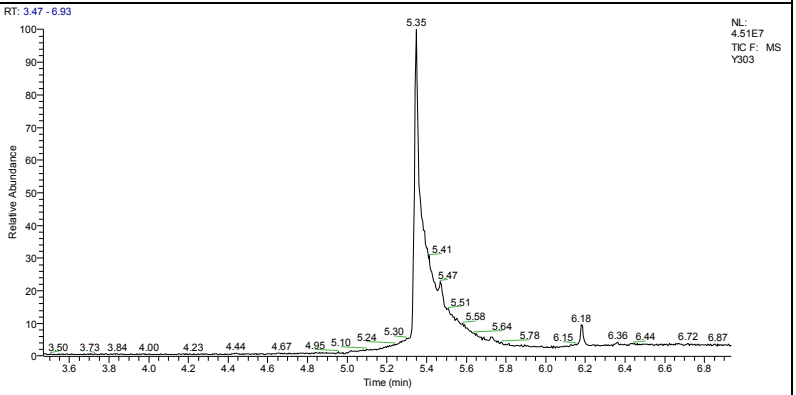


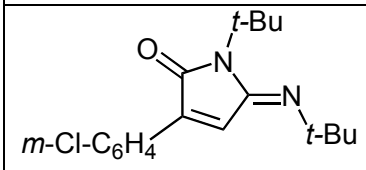
4e, 73 %, Z/E = **9:91**



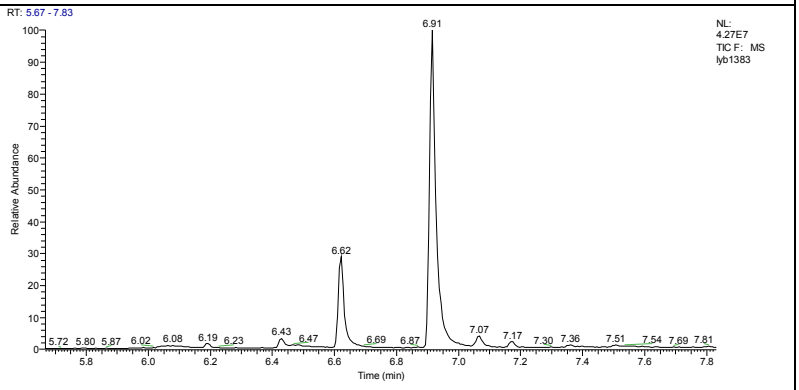


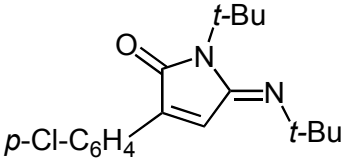
4f, 83 %, E/Z=**6:94**



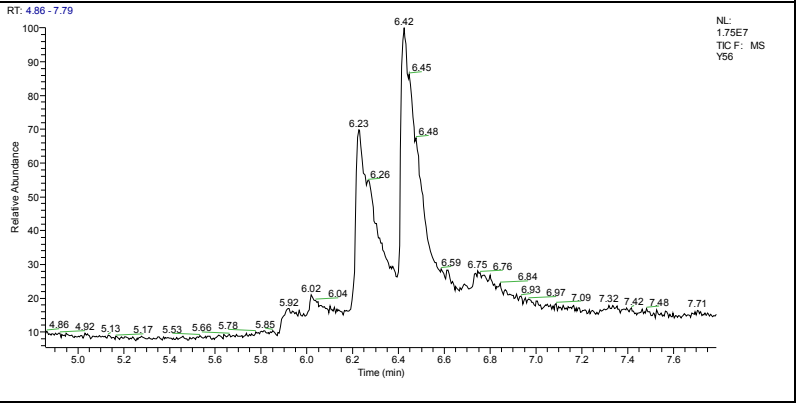


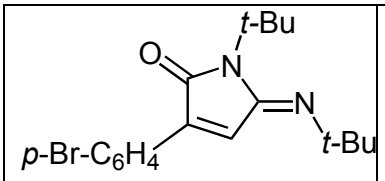
4g, 71 %, E/Z=**20:80**



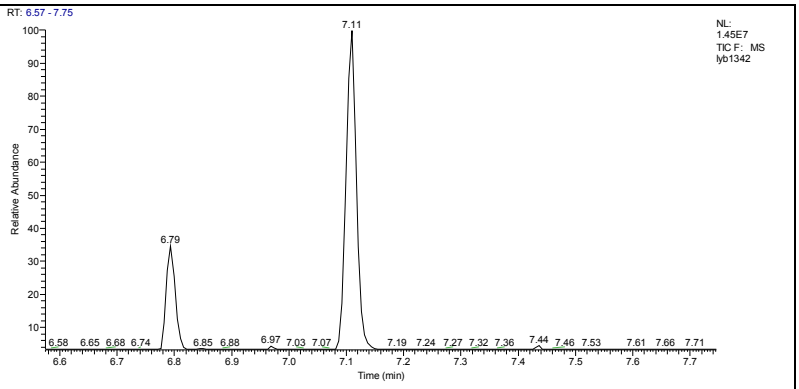


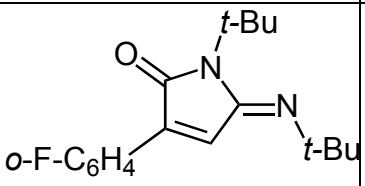
4h, 81 %, E/Z=**40:60**



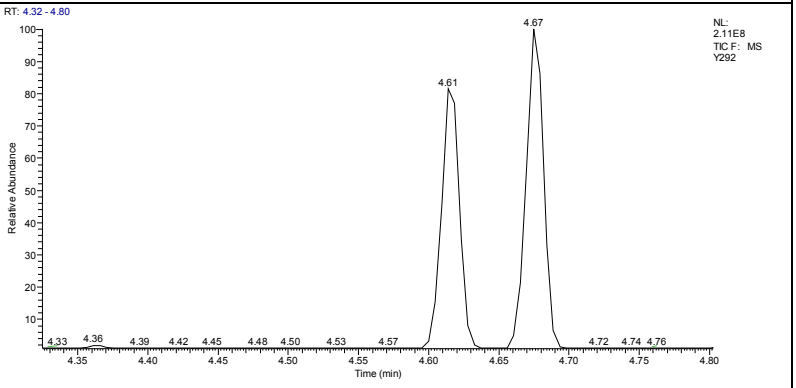


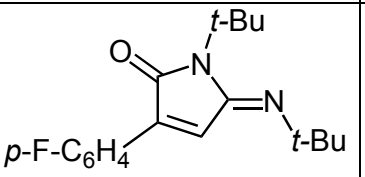
4i, 72 %, Z/E = **23:77**



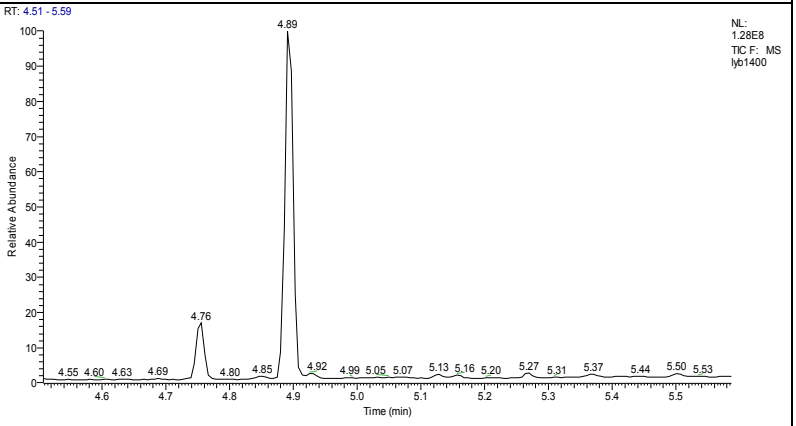


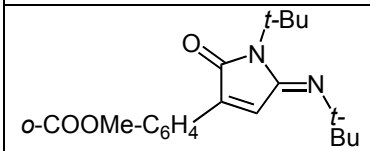
4j, 68%, E/Z= **45:55**



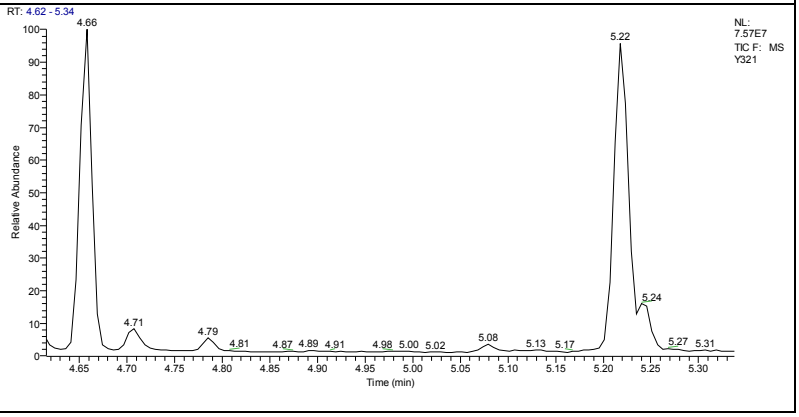


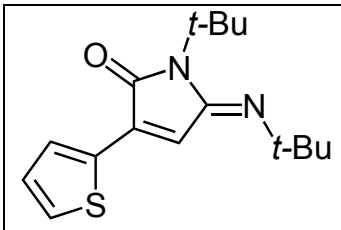
4k, 75 %, Z/E = **14:86**



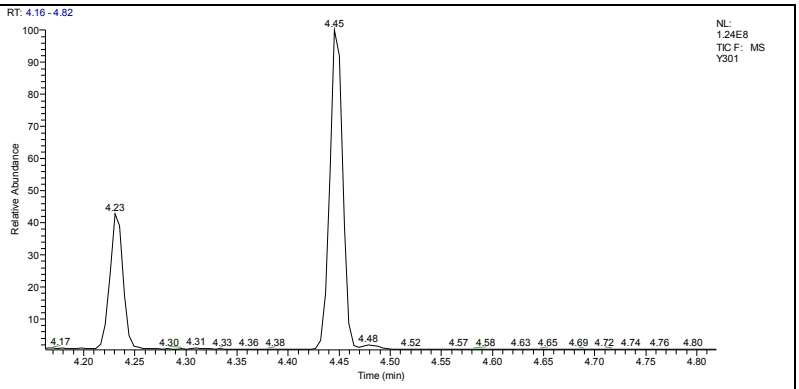


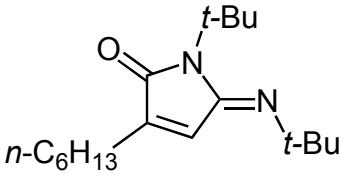
4l, 67%, E/Z= **50:50**



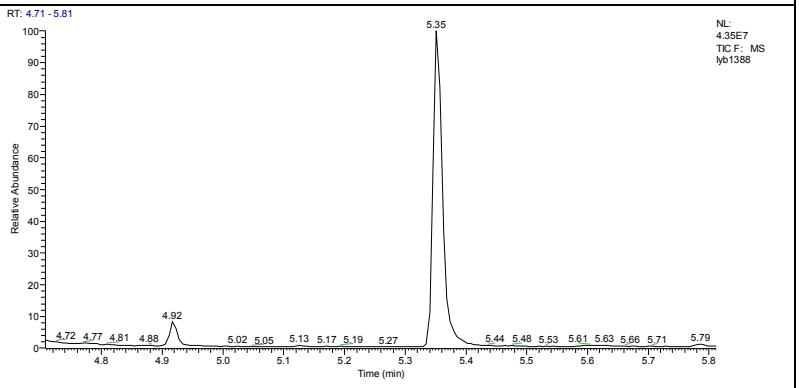


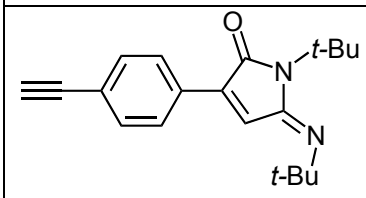
4m, 69 %, E/Z= **31:69**



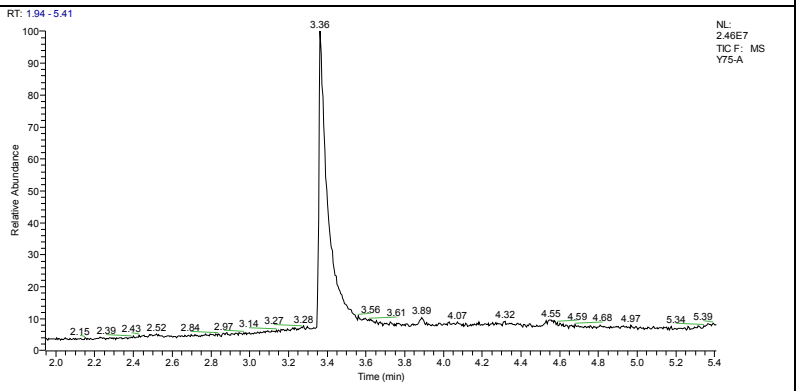


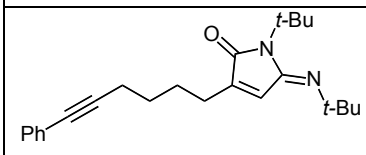
4n, 89 %, Z/E = 6:94



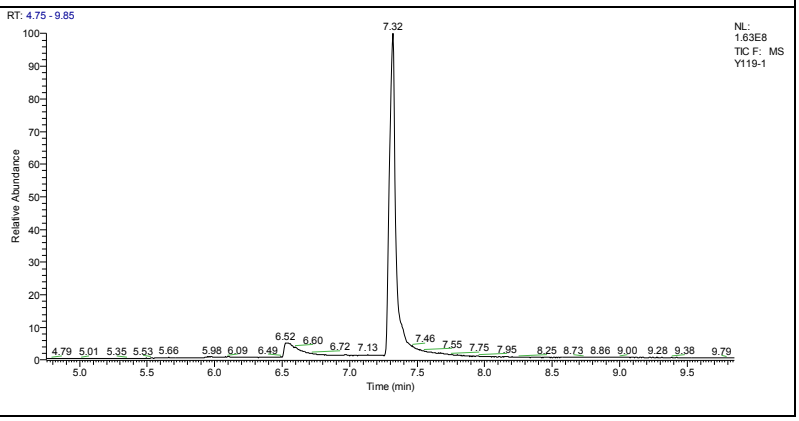


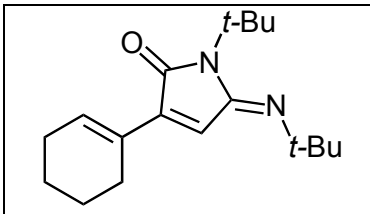
4o, 60 %, only E isomer



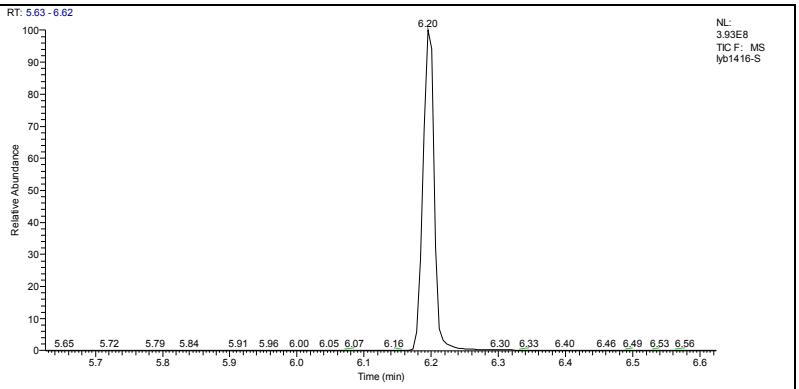


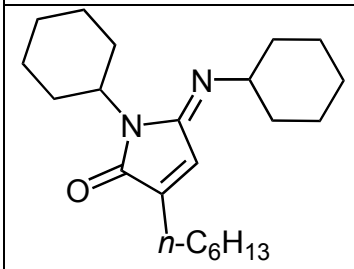
4p, 85 %, Z/E = **9:91**



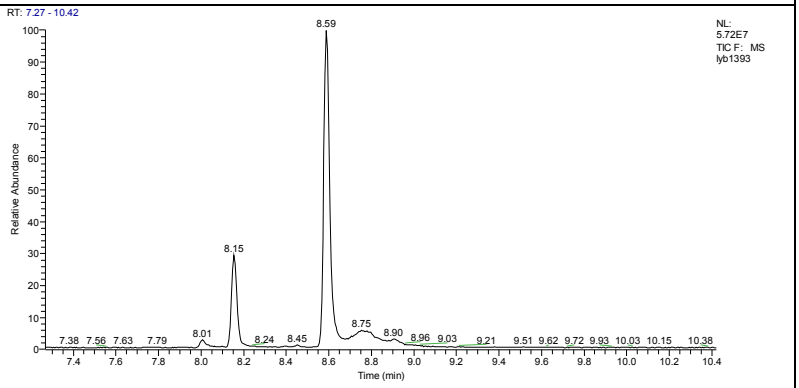


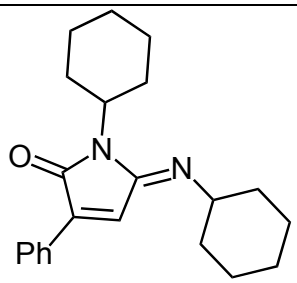
4q, 83 %, only E isomer



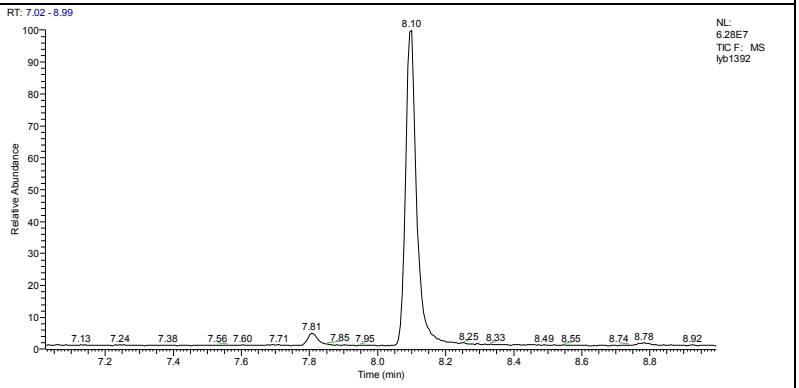


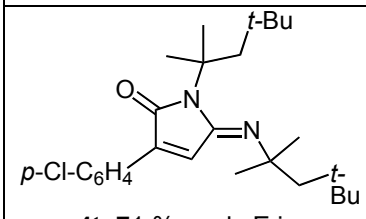
4r, 84 %, Z/E = **19:81**



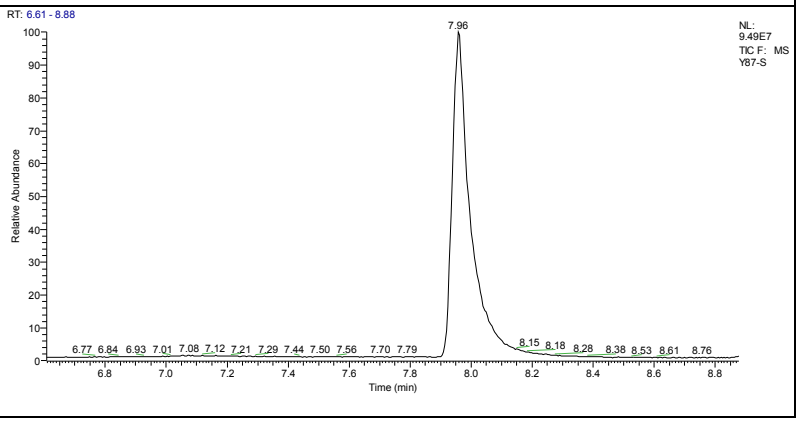


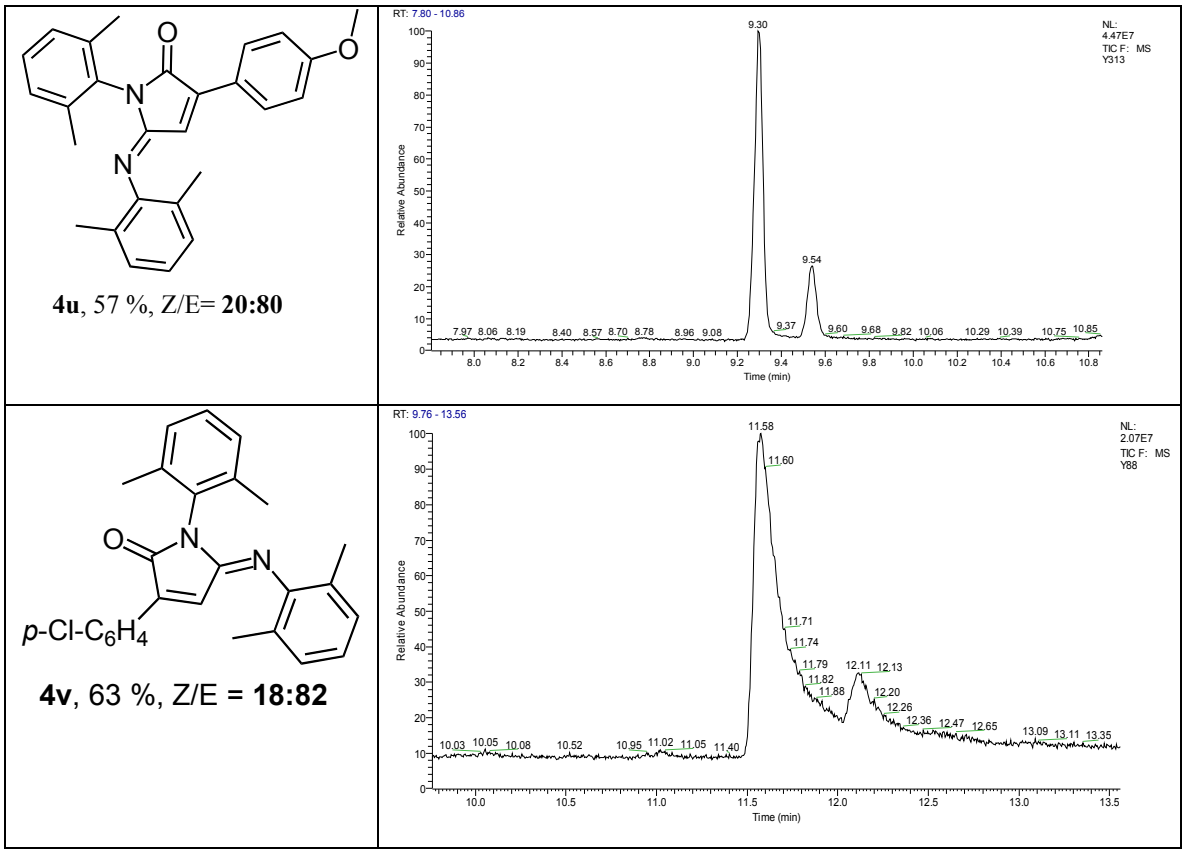
4s, 86 %, Z/E = **4:96**





4t, 71 %, only E isomer





VI. Crystallographic data

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South China University of Technology,
Guangzhou 510640, P. R. China
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School of Chemistry and Chemical Engineering,
South China University of Technology,
Guangzhou 510640, P. R. China
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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H11C H 0.4160 0.0578 0.8471 0.149 Uiso 1 1 calc R . .
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H17B H 0.7936 0.5993 0.4339 0.170 Uiso 1 1 calc R . .
H17C H 0.8722 0.5236 0.4938 0.170 Uiso 1 1 calc R . .
C18 C 0.8634(3) 0.5262(2) 0.2547(3) 0.1105(11) Uani 1 1 d . . .
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H18B H 0.8481 0.5896 0.2390 0.166 Uiso 1 1 calc R . .
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C20 C 0.9922(2) 0.2655(2) 0.4166(4) 0.1220(13) Uani 1 1 d . . .
H20A H 1.0539 0.2396 0.3977 0.183 Uiso 1 1 calc R . .
H20B H 1.0019 0.2725 0.5029 0.183 Uiso 1 1 calc R . .
H20C H 0.9788 0.3240 0.3782 0.183 Uiso 1 1 calc R . .
C21 C 0.8762(3) 0.1947(3) 0.2357(3) 0.1481(18) Uani 1 1 d . . .
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H21B H 0.9376 0.1757 0.2092 0.222 Uiso 1 1 calc R . .
H21C H 0.8537 0.2529 0.2005 0.222 Uiso 1 1 calc R . .
C22 C 0.9323(3) 0.1119(2) 0.4312(4) 0.1123(12) Uani 1 1 d . . .
H22A H 0.8819 0.0662 0.3978 0.168 Uiso 1 1 calc R . .
H22B H 0.9362 0.1171 0.5169 0.168 Uiso 1 1 calc R . .
H22C H 0.9993 0.0947 0.4173 0.168 Uiso 1 1 calc R . .
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N2 N 0.81840(15) 0.38964(13) 0.34428(17) 0.0649(5) Uani 1 1 d . . .
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C6 0.0629(14) 0.0662(14) 0.0713(14) -0.0140(11) 0.0251(11) -0.0087(11)
C7 0.0626(14) 0.0585(13) 0.0776(15) -0.0103(11) 0.0247(12) -0.0122(10)
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C10 0.092(2) 0.099(2) 0.119(2) -0.0253(18) 0.0616(19) -0.0210(16)
C11 0.110(2) 0.092(2) 0.107(2) 0.0310(17) 0.0511(19) 0.0042(17)
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C13 0.0526(12) 0.0603(13) 0.0604(12) 0.0006(10) 0.0145(10) -0.0024(10)
C14 0.0577(13) 0.0600(14) 0.0657(13) 0.0031(11) 0.0171(11) 0.0016(10)
C15 0.0732(16) 0.0584(13) 0.0770(15) 0.0008(11) 0.0278(12) -0.0073(11)
C16 0.091(2) 0.0744(18) 0.130(3) 0.0209(17) 0.0066(19) 0.0036(15)
C17 0.169(3) 0.084(2) 0.092(2) -0.0188(17) 0.039(2) -0.024(2)
C18 0.122(3) 0.083(2) 0.148(3) 0.0272(19) 0.076(2) -0.0021(18)
C19 0.0529(13) 0.0781(15) 0.0694(14) 0.0038(11) 0.0205(11) 0.0100(11)
C20 0.0608(18) 0.109(2) 0.198(4) 0.005(2) 0.031(2) 0.0039(17)
C21 0.124(3) 0.250(5) 0.0722(19) -0.017(3) 0.0259(19) 0.083(3)
C22 0.088(2) 0.097(2) 0.165(3) 0.033(2) 0.058(2) 0.0362(17)
N1 0.0536(10) 0.0608(11) 0.0725(12) 0.0054(9) 0.0235(9) 0.0041(8)
N2 0.0647(12) 0.0630(11) 0.0711(12) 0.0061(9) 0.0238(10) -0.0028(9)
O1 0.0848(13) 0.0578(11) 0.1240(16) 0.0093(10) 0.0476(11) 0.0074(8)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
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 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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C4 C5 1.393(3) . ?
C4 H4 0.9300 . ?
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C6 C7 1.386(3) . ?
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C7 H7 0.9300 . ?
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C8 C9 1.527(4) . ?
C8 C11 1.530(3) . ?
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C12 H12 0.9300 . ?
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C14 O1 1.221(3) . ?
C14 N1 1.377(3) . ?
C15 N2 1.476(3) . ?
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C15 C16 1.516(4) . ?
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C3 C2 C1 121.84(19) . . ?
C4 C3 C2 120.8(2) . . ?
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C3 C4 C5 122.1(2) . . ?
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C5 C6 C7 121.7(2) . . ?
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C2 C7 H7 119.4 . . ?
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C10 C8 C9 109.1(2) . . ?
C5 C8 C11 108.9(2) . . ?
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C10 C8 C11 108.5(2) . . ?
C9 C8 C11 108.4(2) . . ?
C8 C9 H9A 109.5 . . ?
C8 C9 H9B 109.5 . . ?
H9A C9 H9B 109.5 . . ?
C8 C9 H9C 109.5 . . ?
H9A C9 H9C 109.5 . . ?
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H10A C10 H10B 109.5 . . ?
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H10A C10 H10C 109.5 . . ?
H10B C10 H10C 109.5 . . ?
C8 C11 H11A 109.5 . . ?
C8 C11 H11B 109.5 . . ?
H11A C11 H11B 109.5 . . ?
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H11A C11 H11C 109.5 . . ?
H11B C11 H11C 109.5 . . ?
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N2 C15 C17 110.9(2) . . ?
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N2 C15 C18 104.6(2) . . ?
C17 C15 C18 109.4(2) . . ?
C16 C15 C18 107.8(3) . . ?
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C15 C16 H16B 109.5 . . ?
H16A C16 H16B 109.5 . . ?
C15 C16 H16C 109.5 . . ?
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C15 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
C15 C17 H17C 109.5 . . ?
H17A C17 H17C 109.5 . . ?
H17B C17 H17C 109.5 . . ?
C15 C18 H18A 109.5 . . ?
C15 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
C15 C18 H18C 109.5 . . ?
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H18B C18 H18C 109.5 . . ?
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N1 C19 C22 110.8(2) . . ?
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N1 C19 C20 109.6(2) . . ?
C22 C19 C20 104.8(3) . . ?
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C19 C20 H20B 109.5 . . ?
H20A C20 H20B 109.5 . . ?
C19 C20 H20C 109.5 . . ?
H20A C20 H20C 109.5 . . ?
H20B C20 H20C 109.5 . . ?
C19 C21 H21A 109.5 . . ?
C19 C21 H21B 109.5 . . ?
H21A C21 H21B 109.5 . . ?
C19 C21 H21C 109.5 . . ?
H21A C21 H21C 109.5 . . ?
H21B C21 H21C 109.5 . . ?
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C19 C22 H22B 109.5 . . ?
H22A C22 H22B 109.5 . . ?
C19 C22 H22C 109.5 . . ?
H22A C22 H22C 109.5 . . ?
H22B C22 H22C 109.5 . . ?
C14 N1 C13 108.75(17) . . ?
C14 N1 C19 126.26(19) . . ?
C13 N1 C19 124.84(18) . . ?
C13 N2 C15 124.4(2) . . ?

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VII. NMR Data

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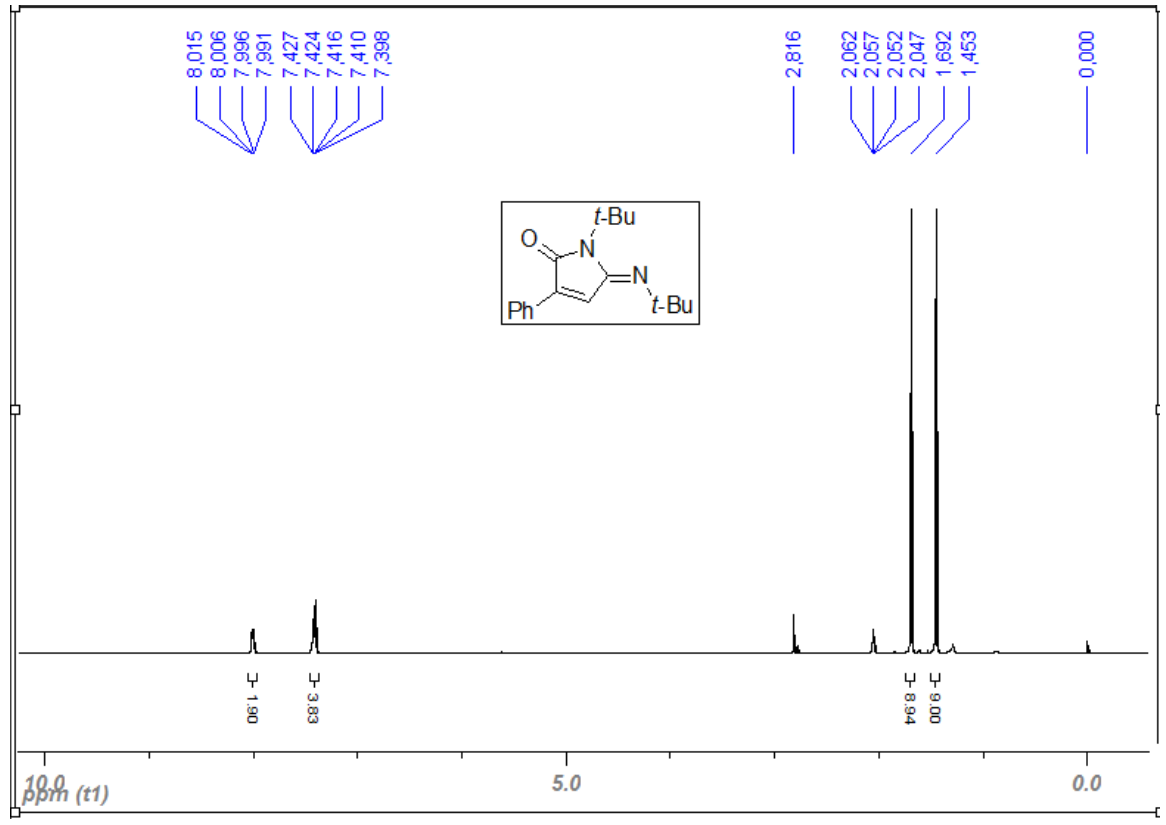

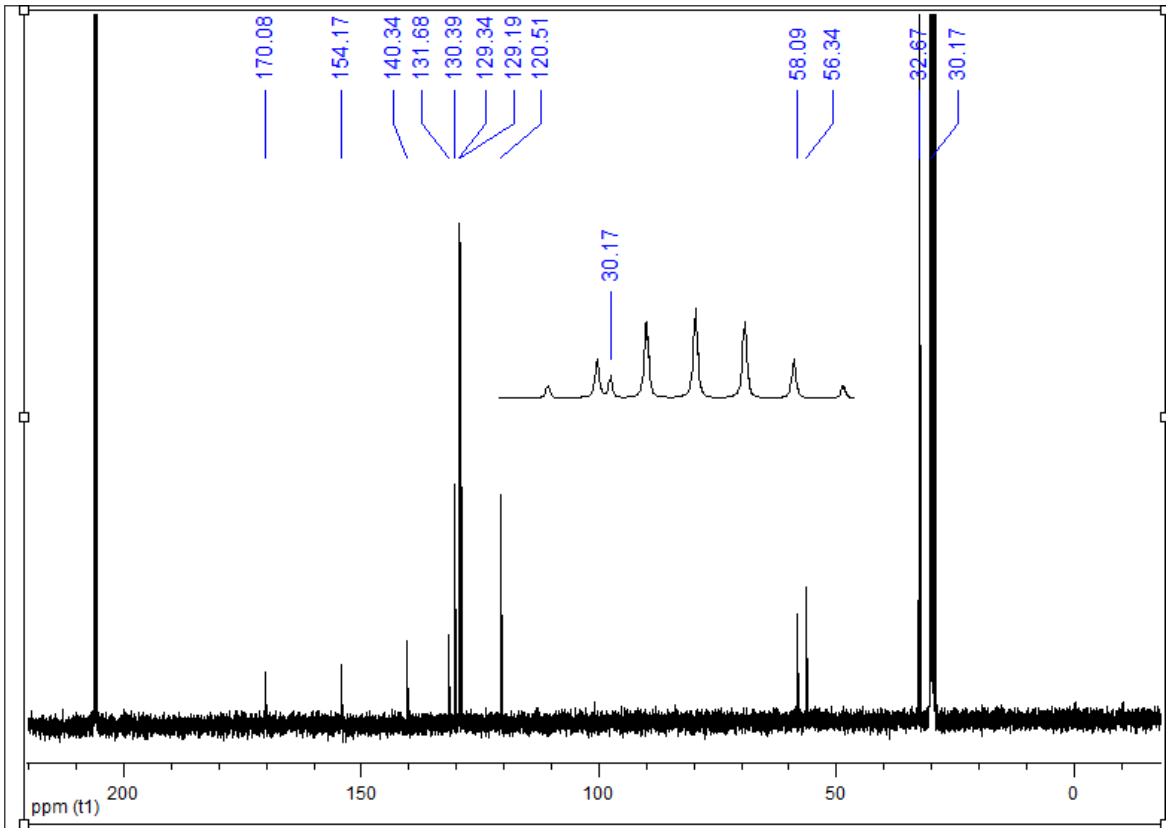

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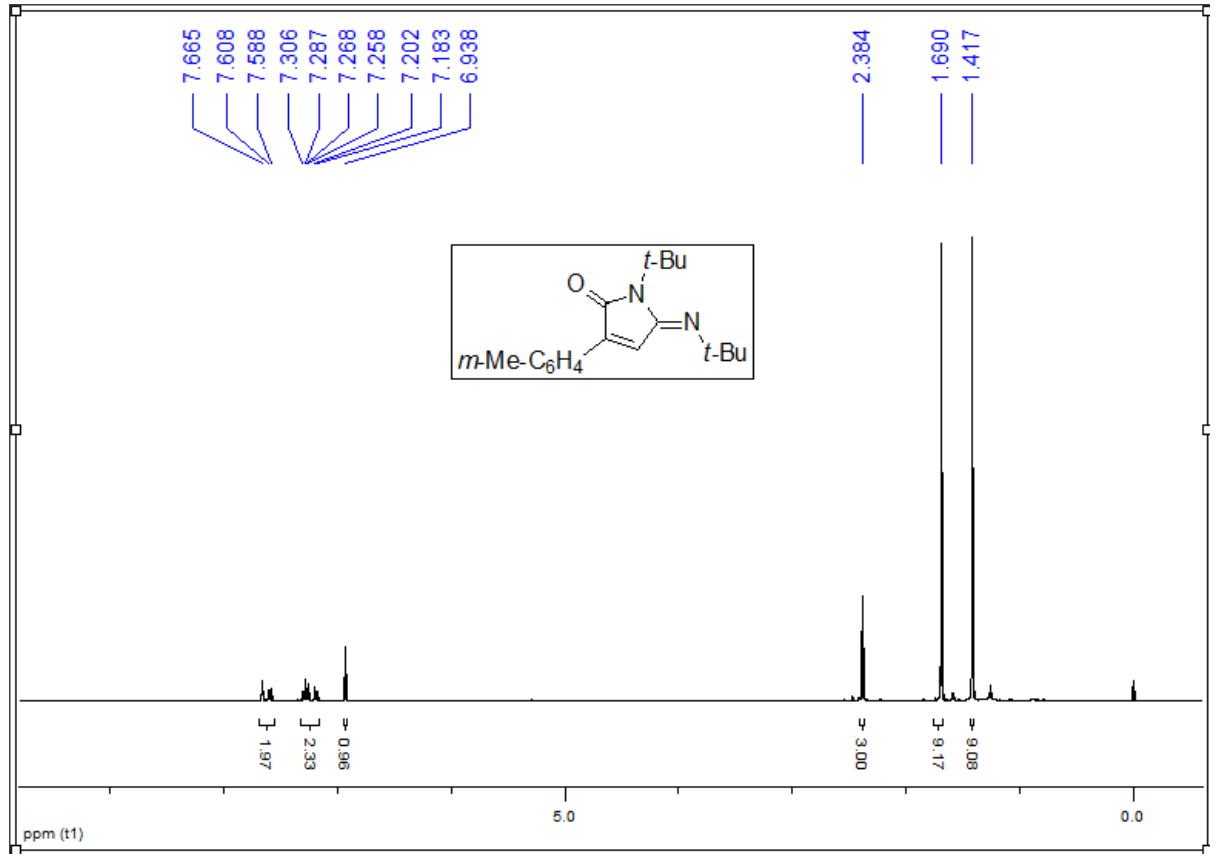
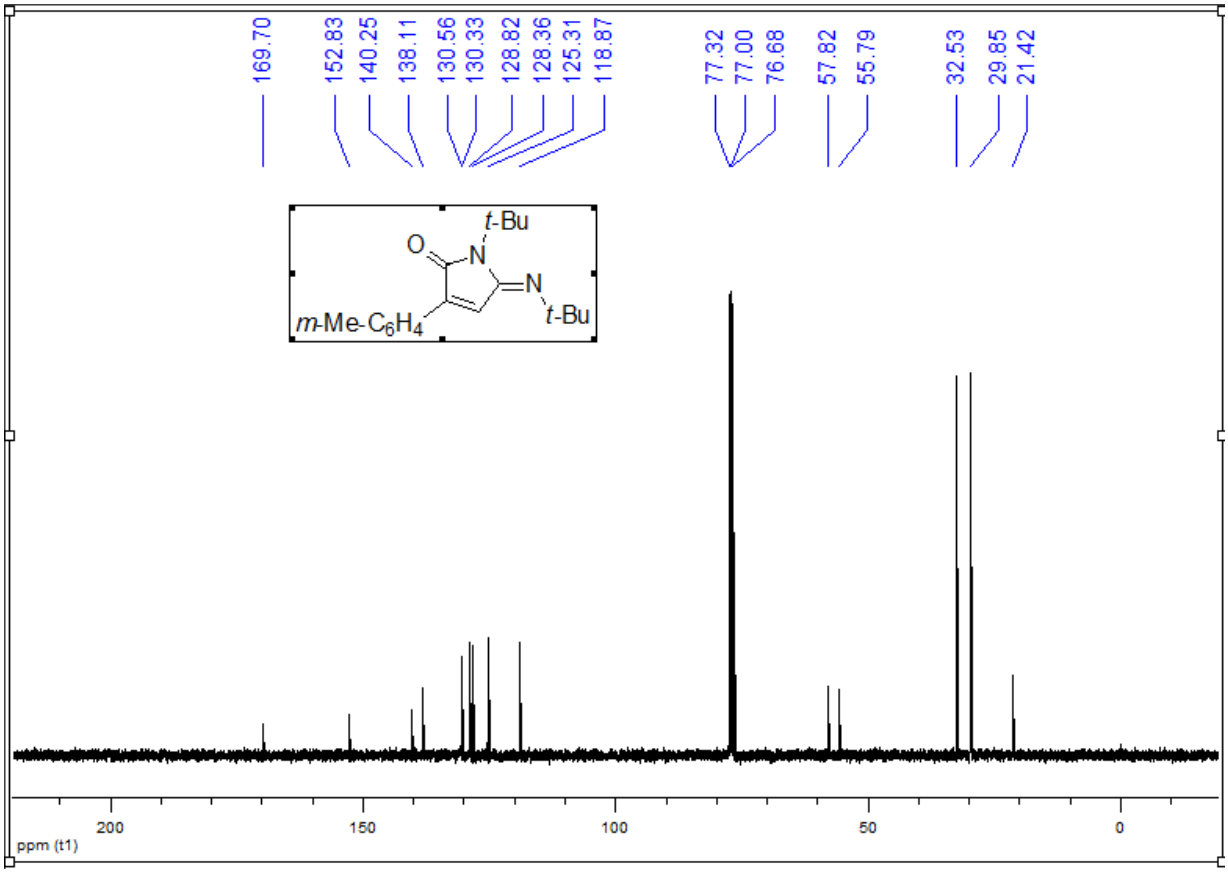
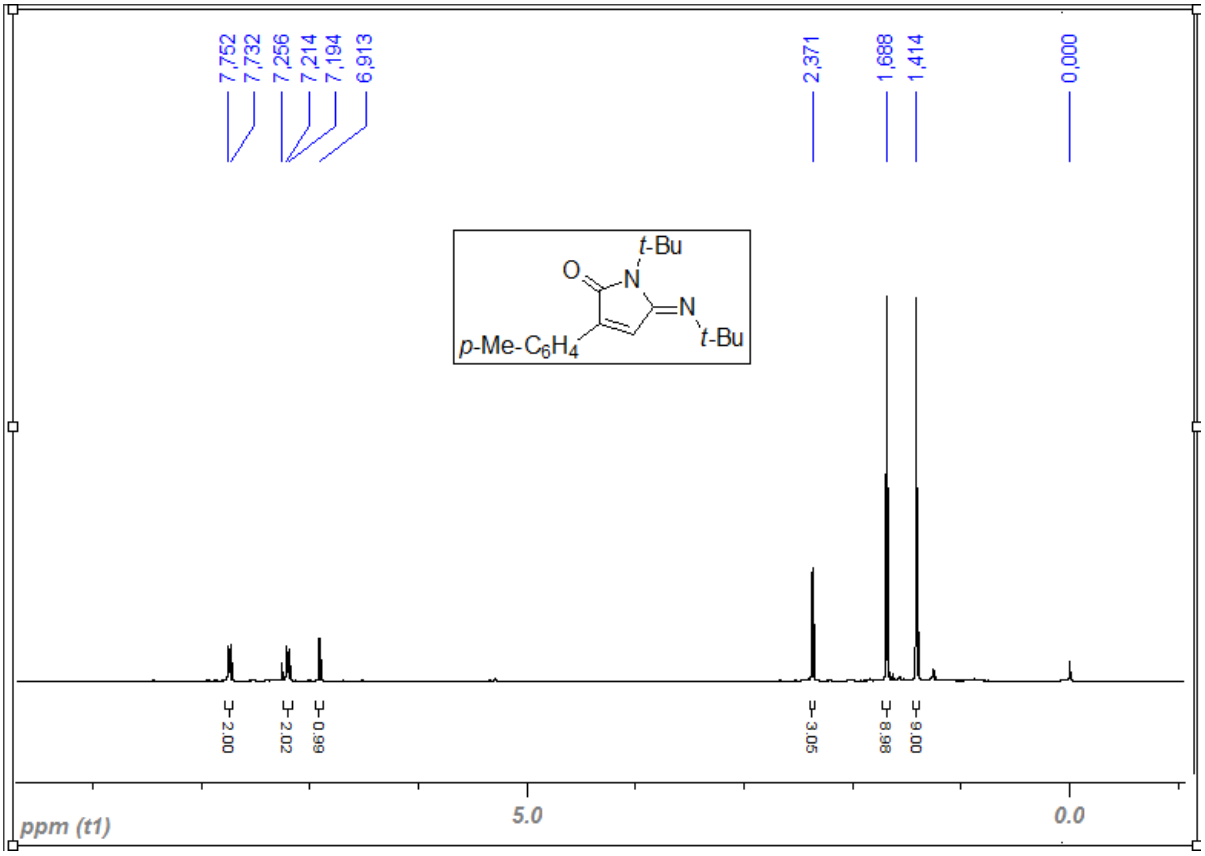
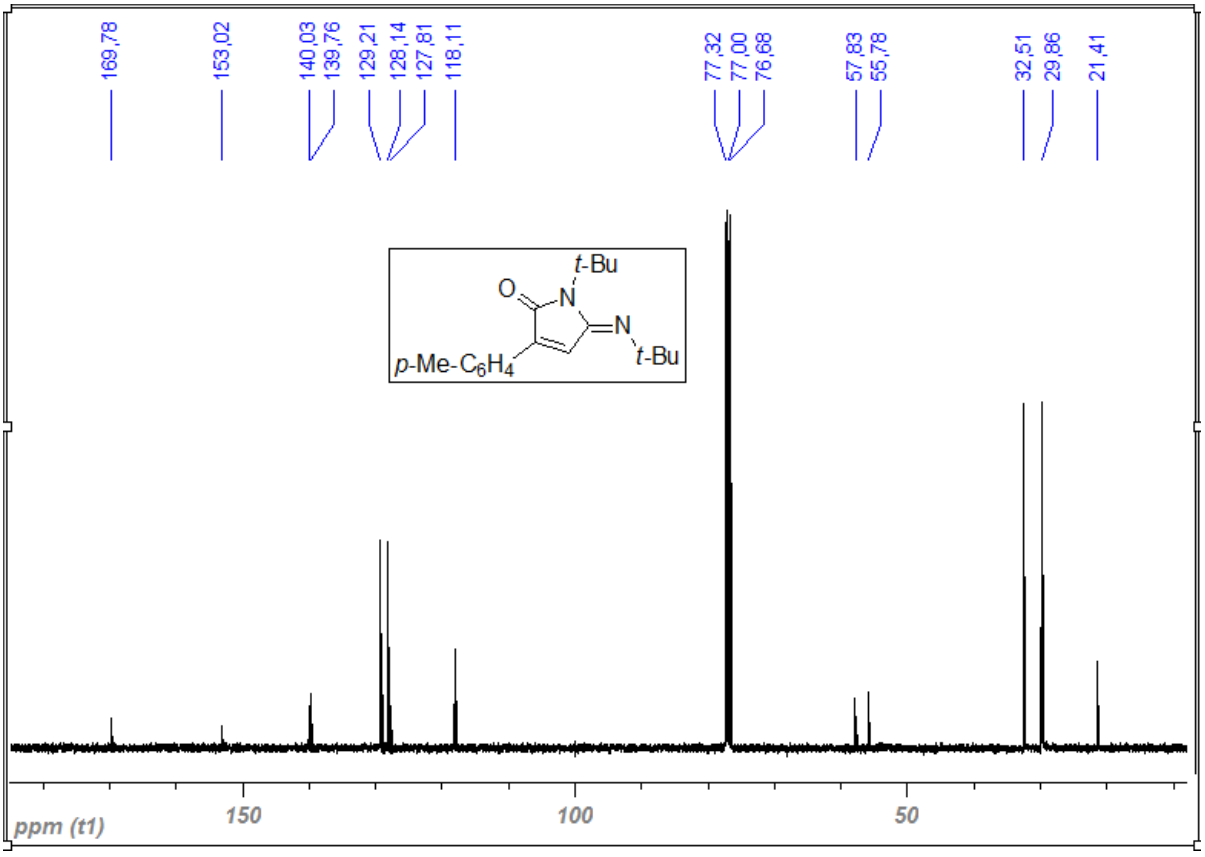


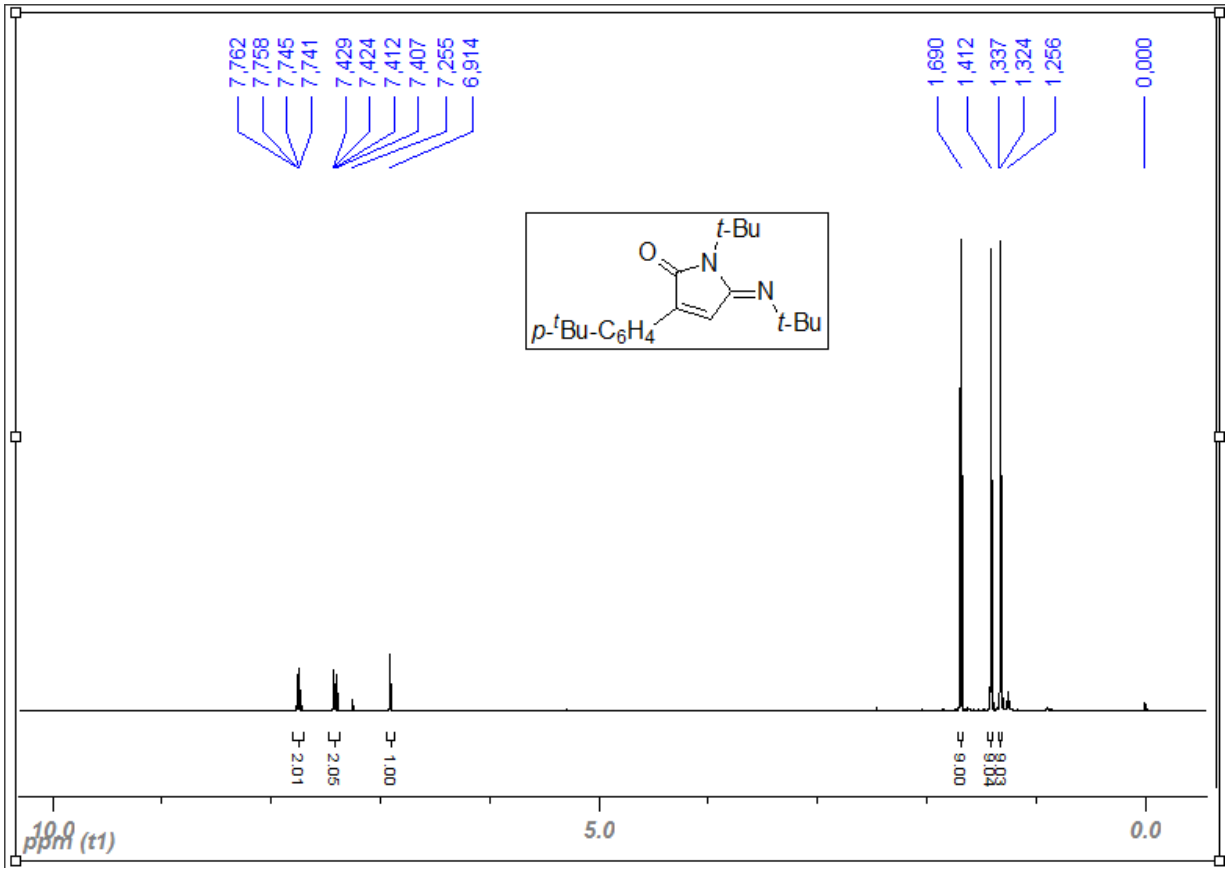


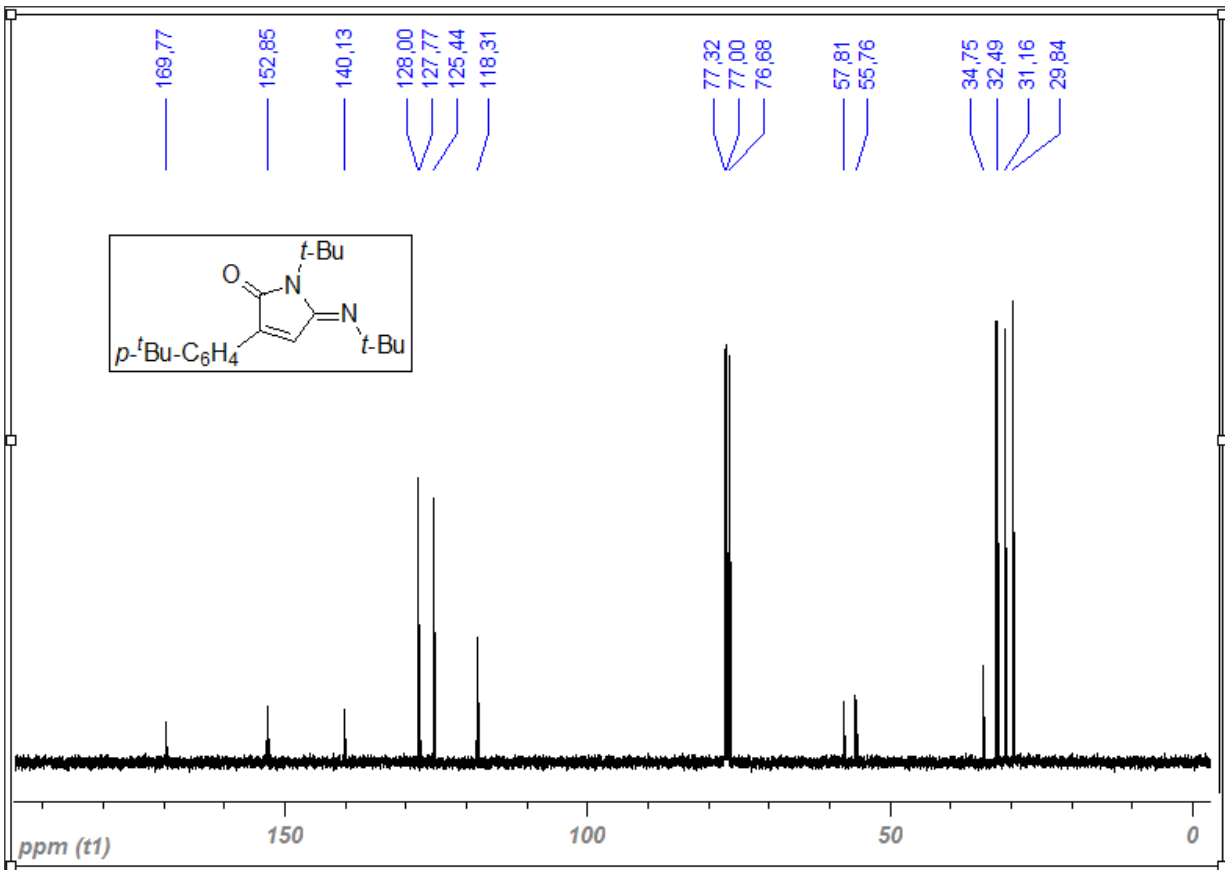
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-*p*-tolyl-1*H*-pyrrol-2(5*H*)-one



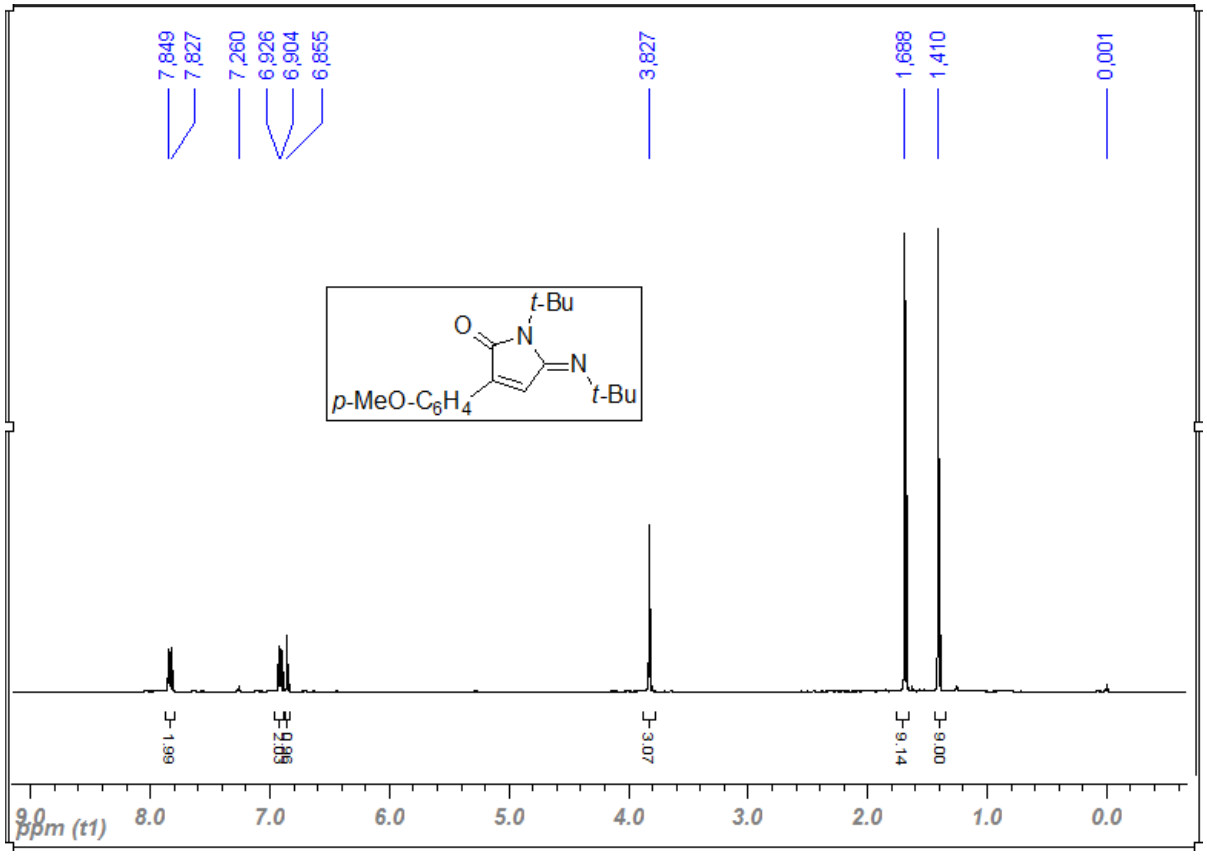


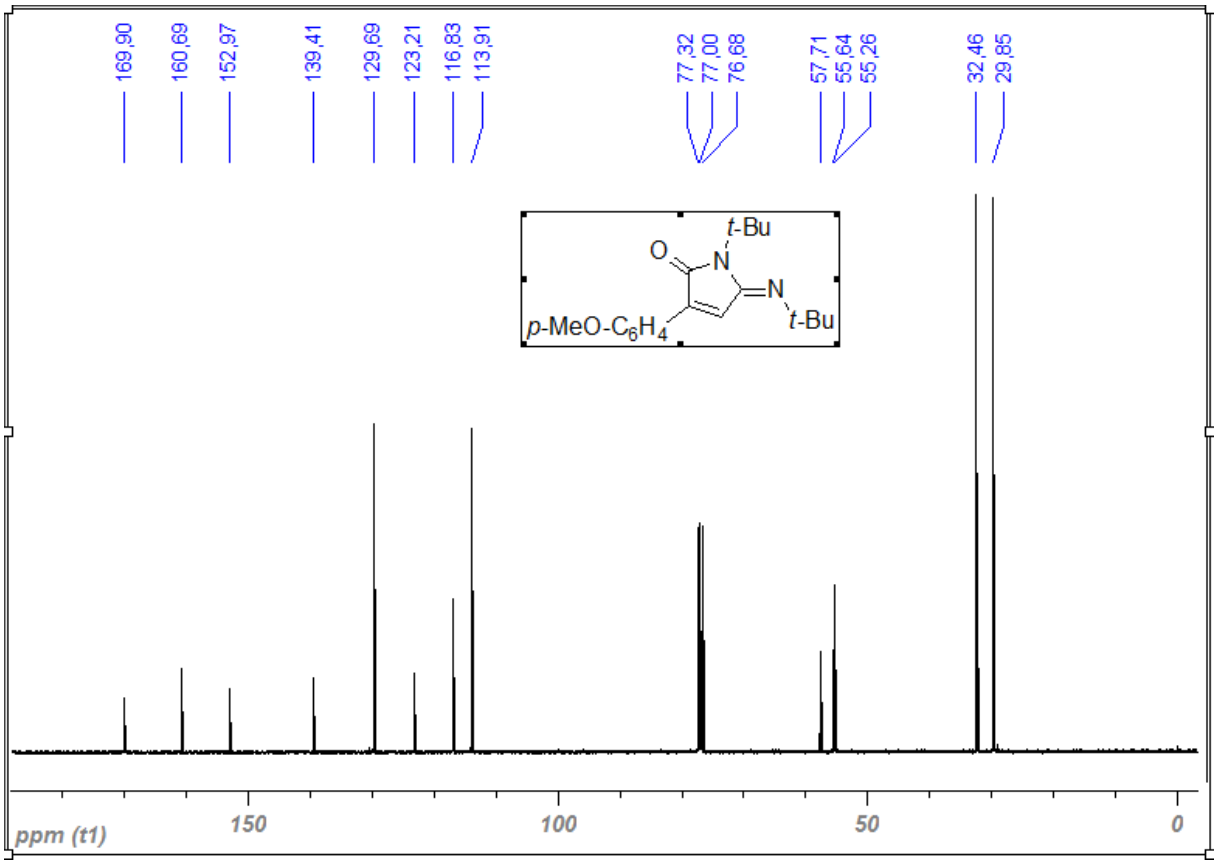
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-*tert*-butylphenyl)-1*H*-pyrrol-2(5*H*)-one



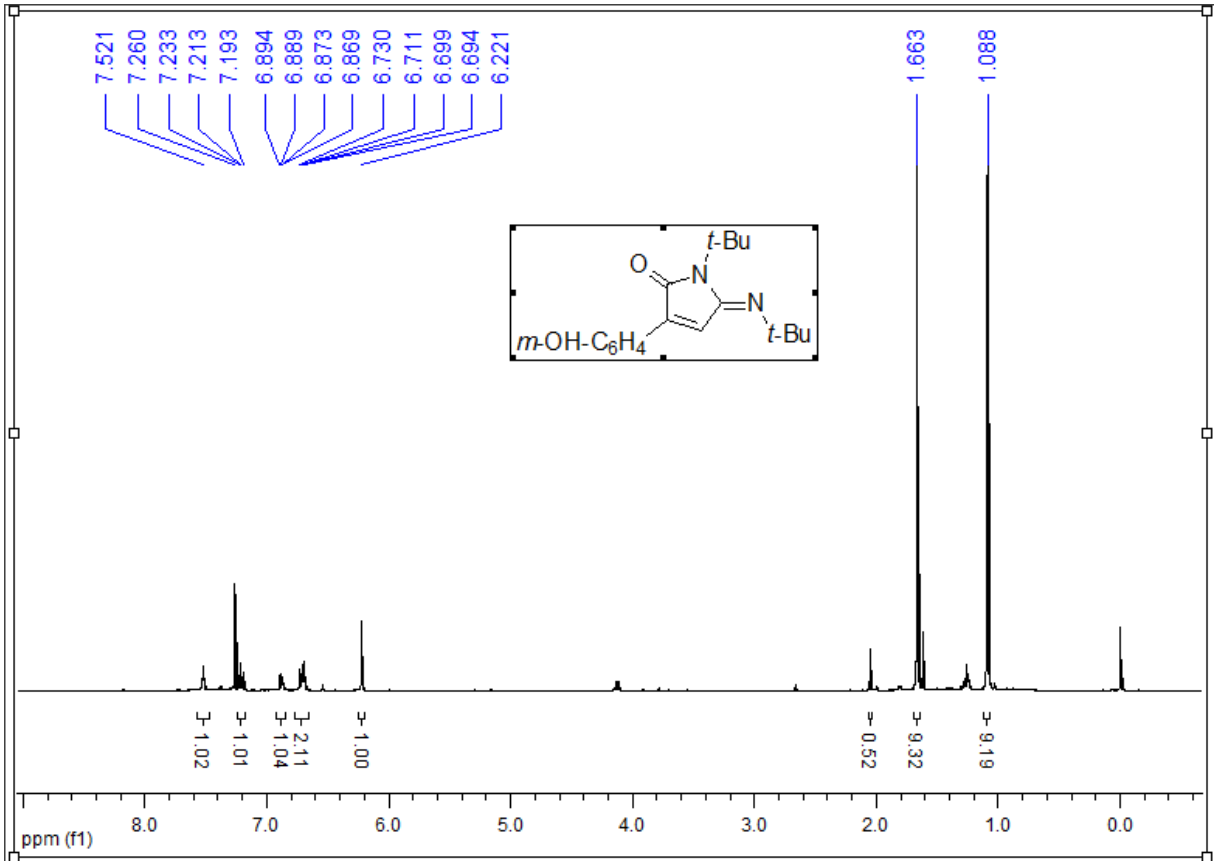


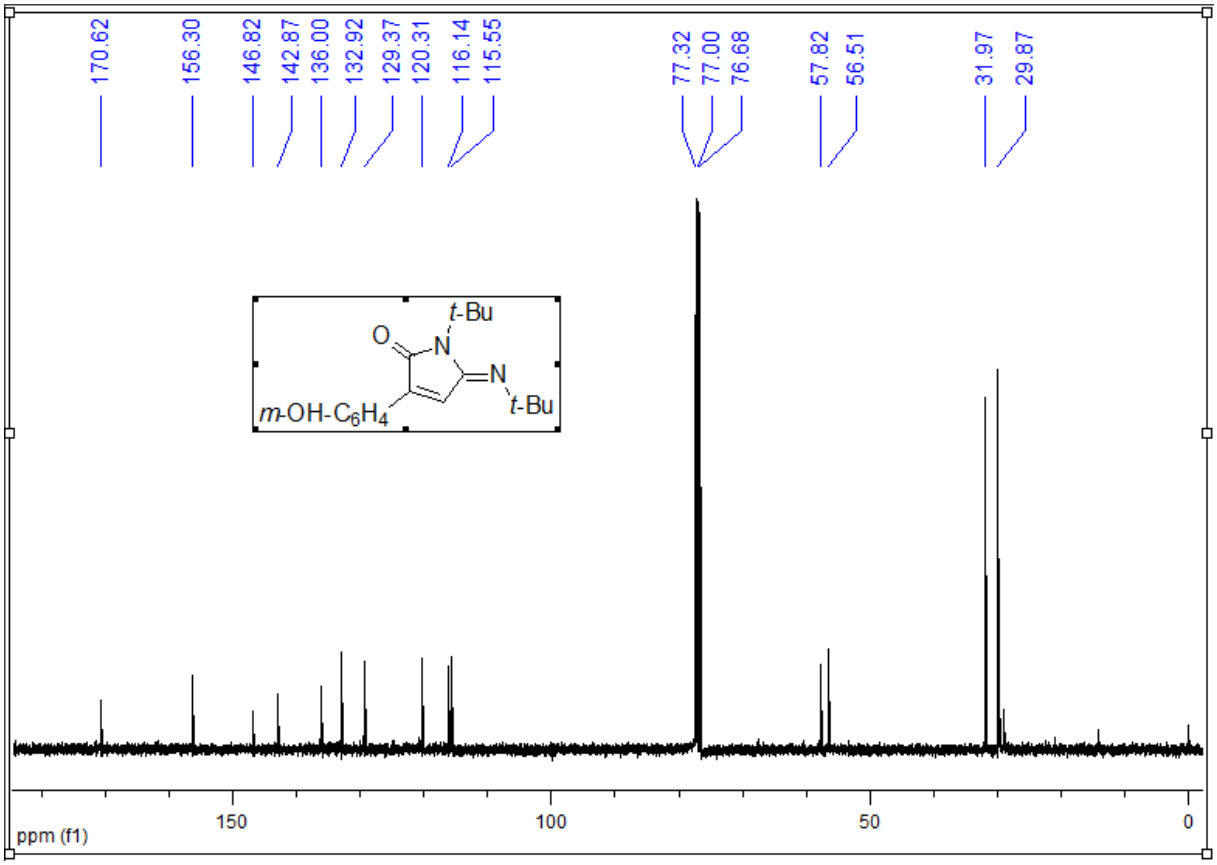
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-methoxyphenyl)-1*H*-pyrrol-2(5*H*)-one



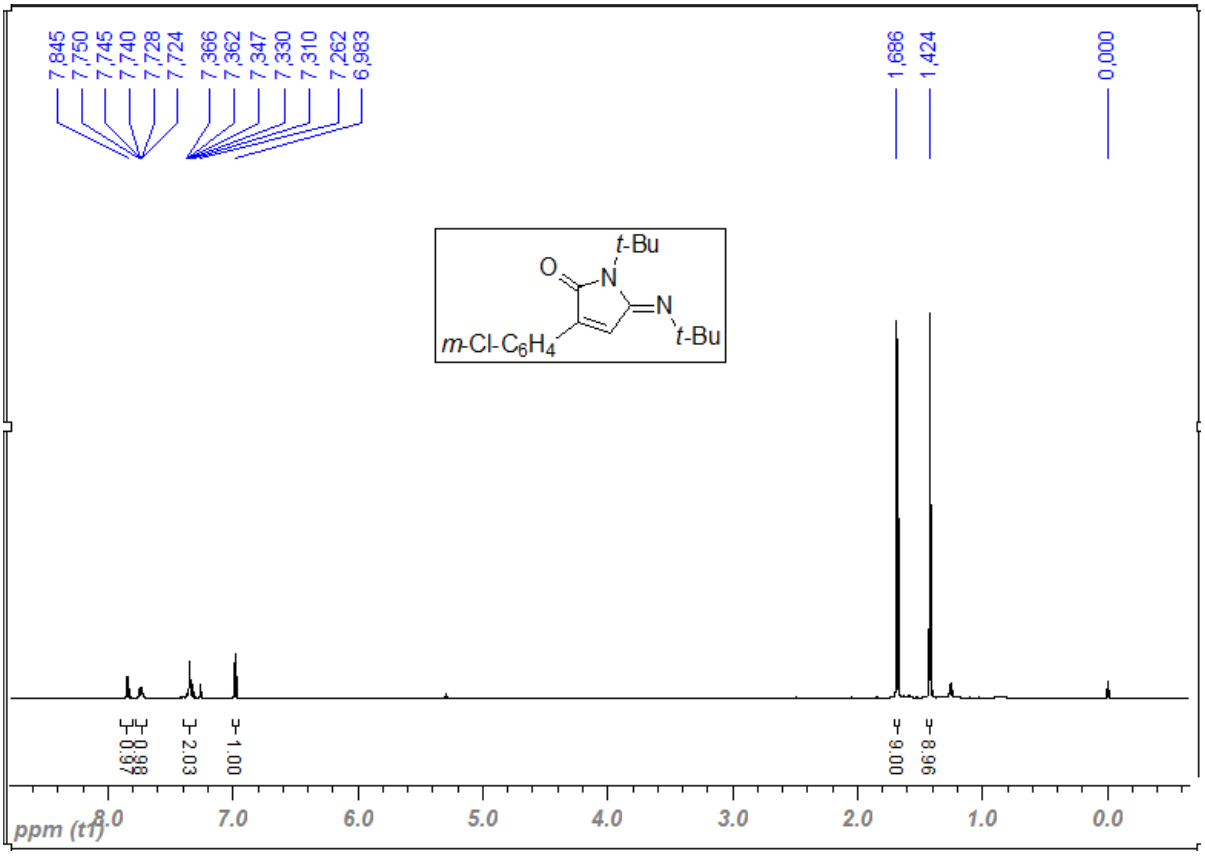


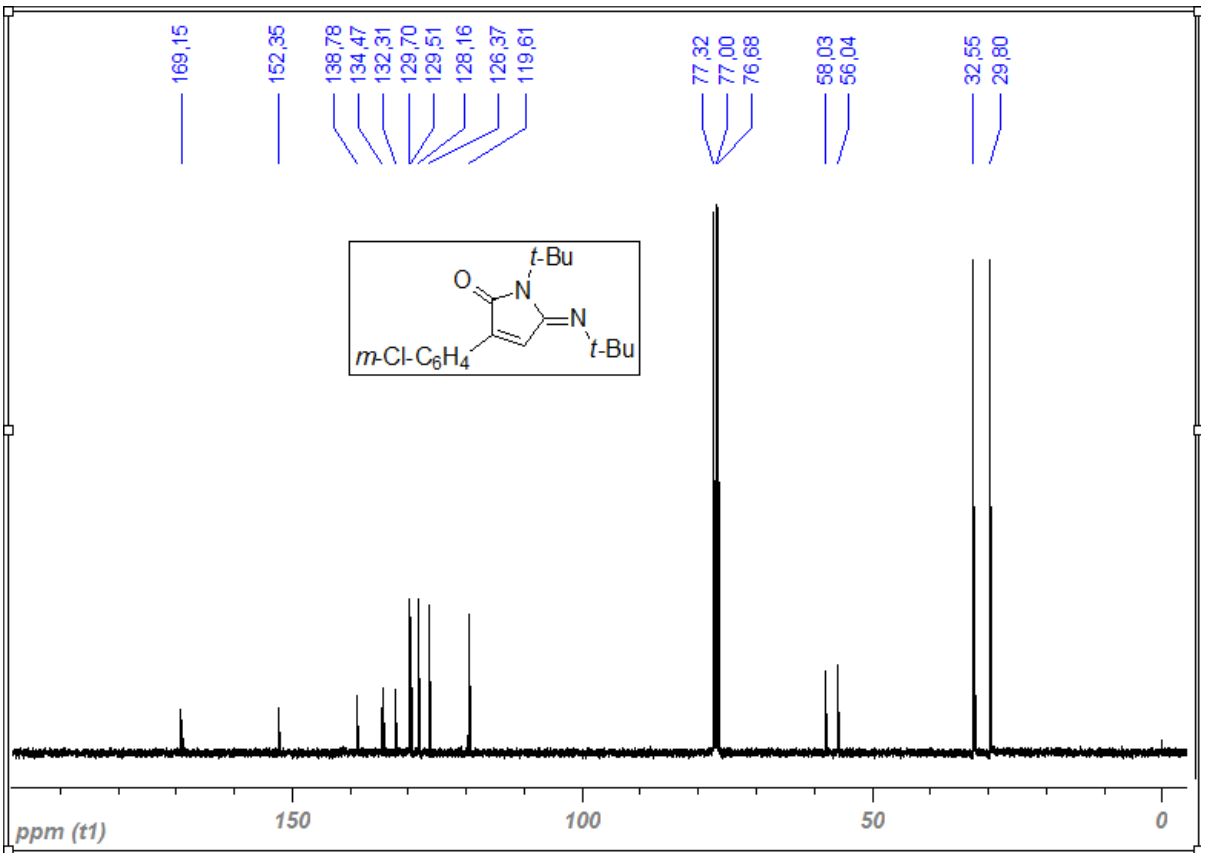
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(3-hydroxyphenyl)-1*H*-pyrrol-2(5*H*)-one



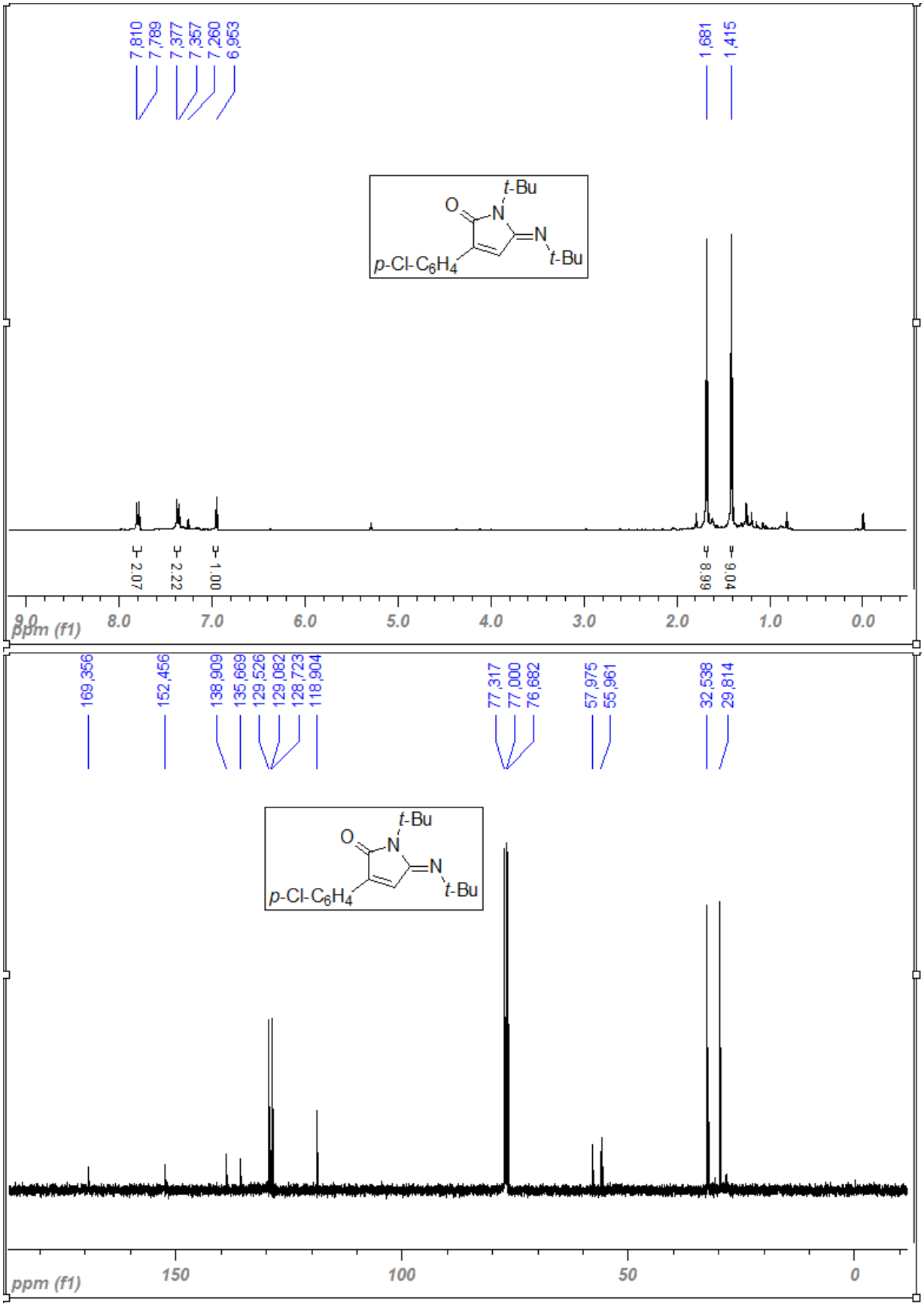


(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(3-chlorophenyl)-1*H*-pyrrol-2(5*H*)-one

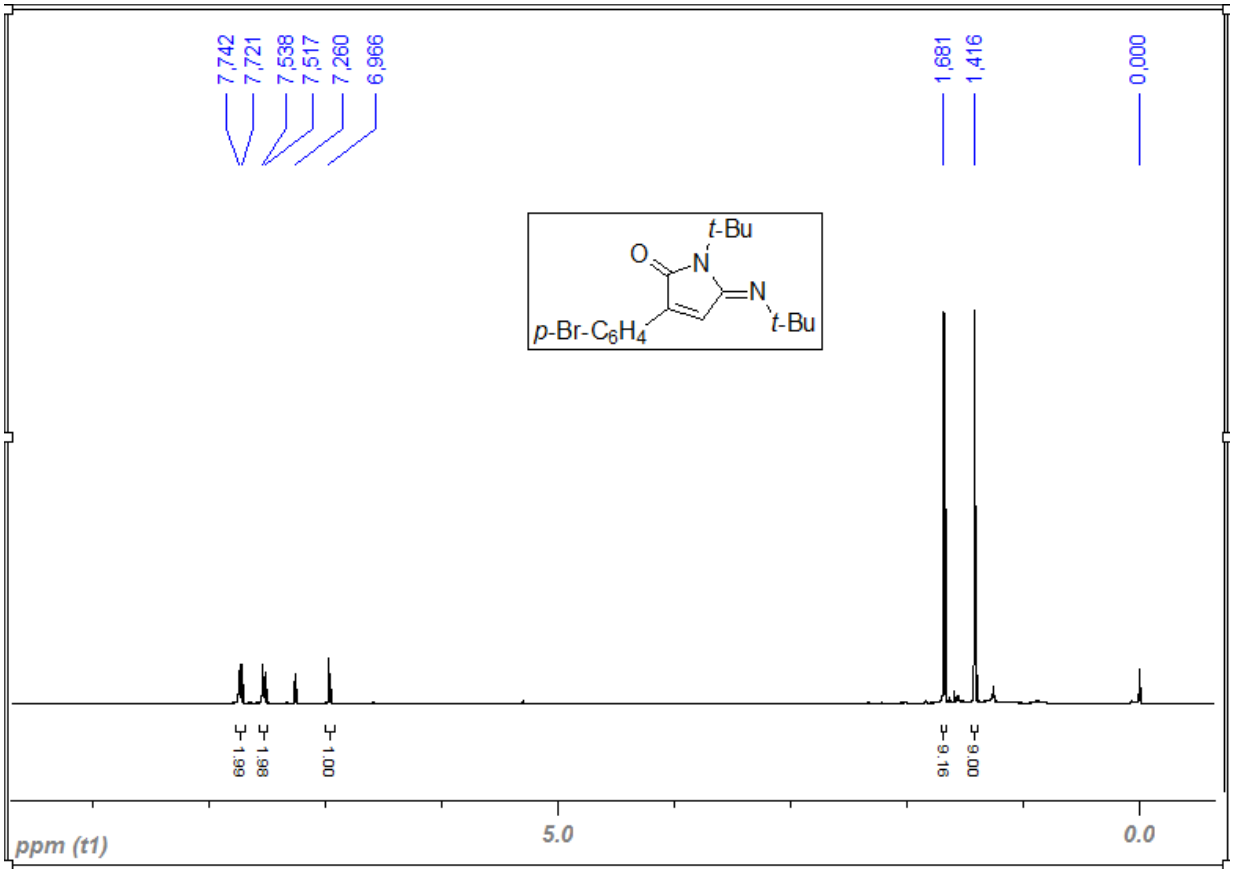


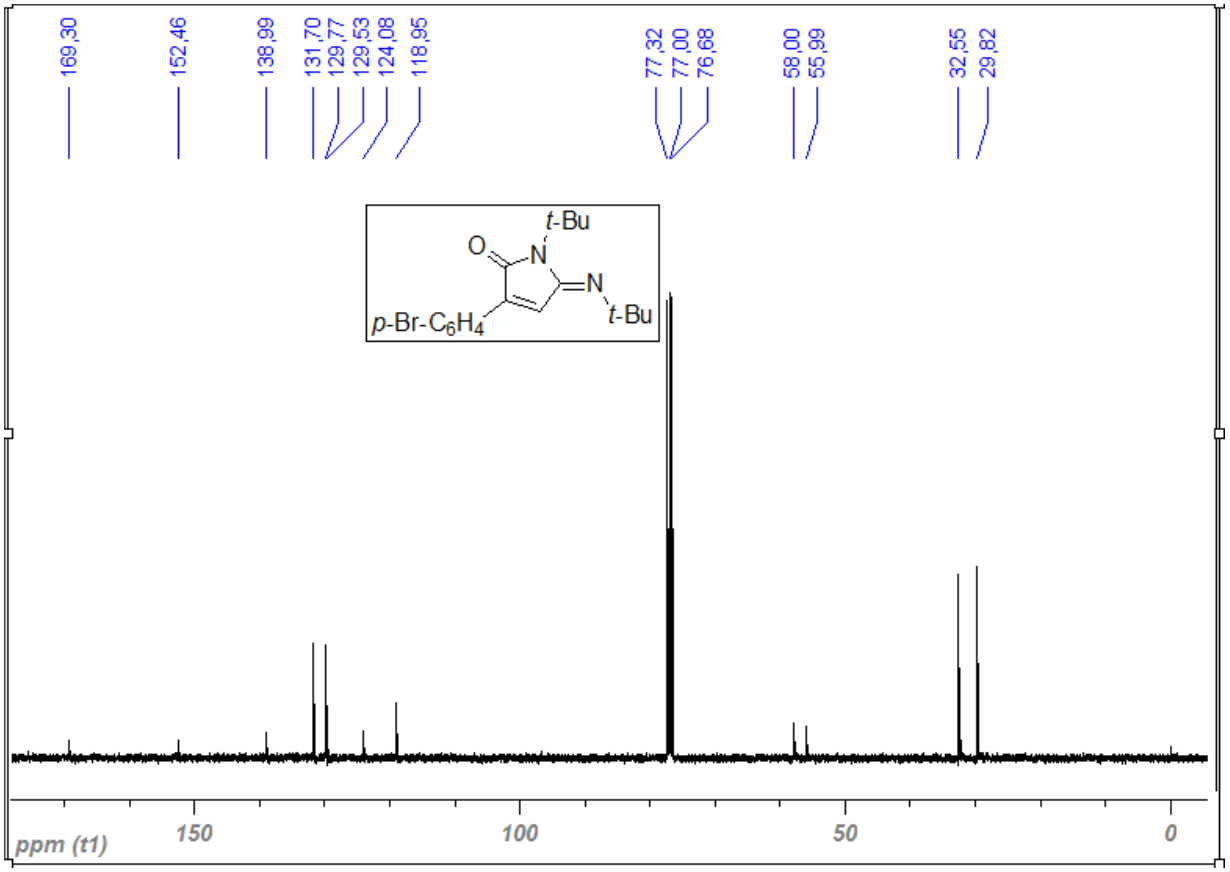


(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-chlorophenyl)-1*H*-pyrrol-2(5*H*)-one

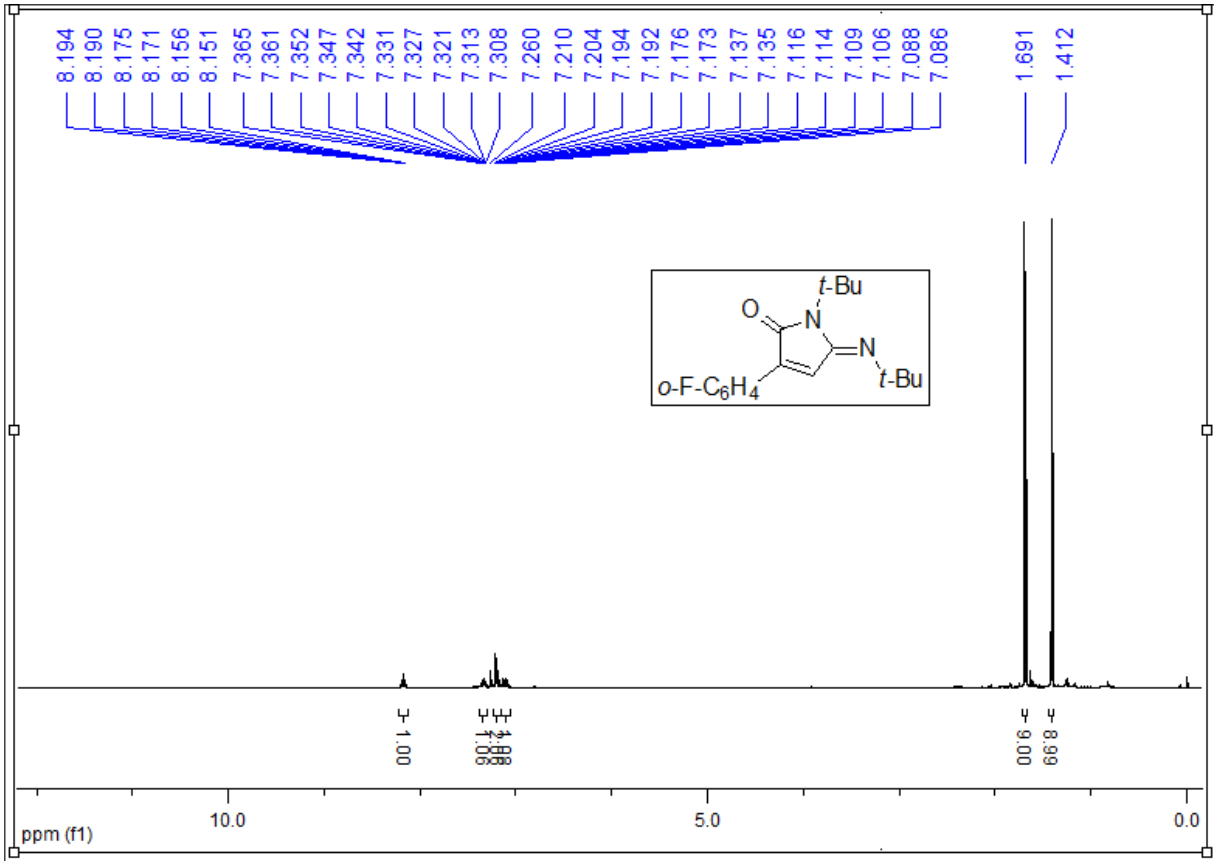


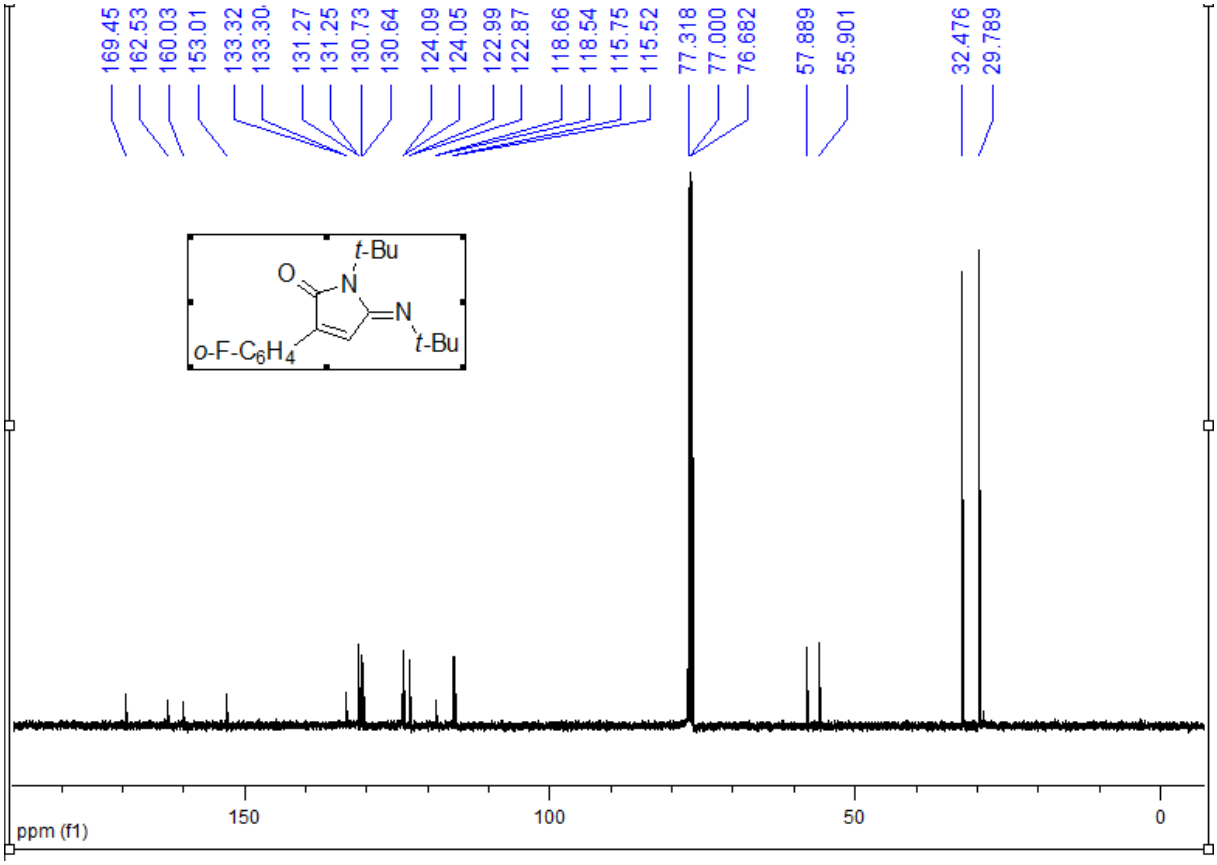
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-bromophenyl)-1*H*-pyrrol-2(5*H*)-one



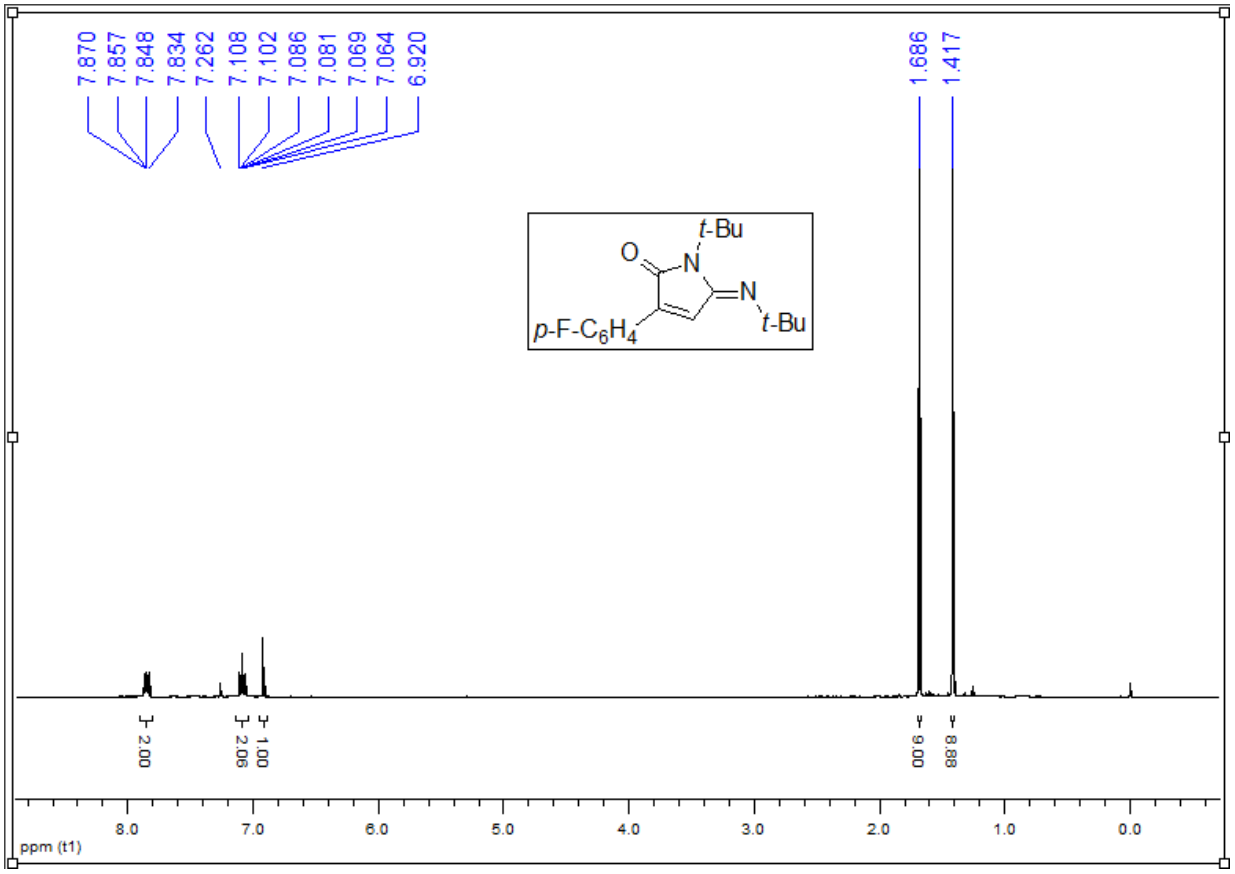


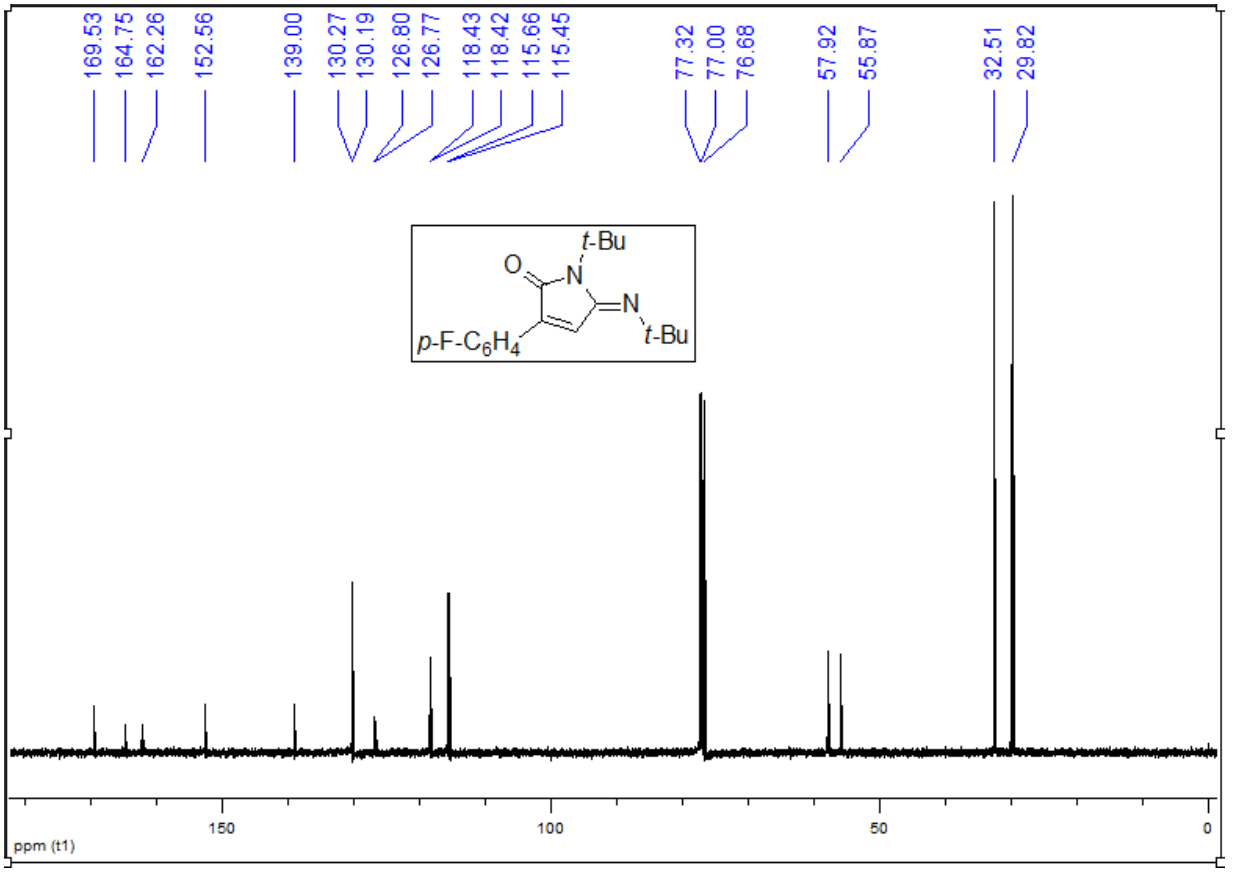
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(2-fluorophenyl)-1*H*-pyrrol-2(5*H*)-one



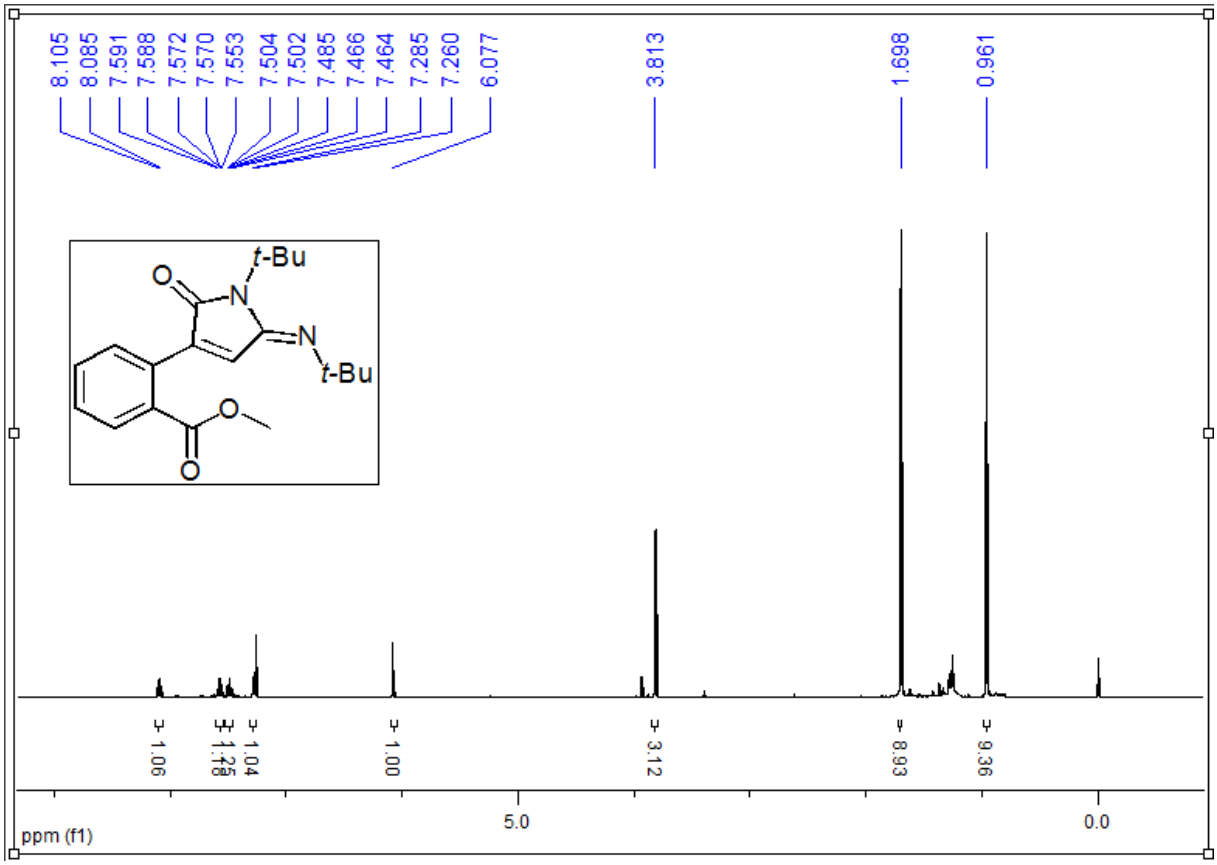


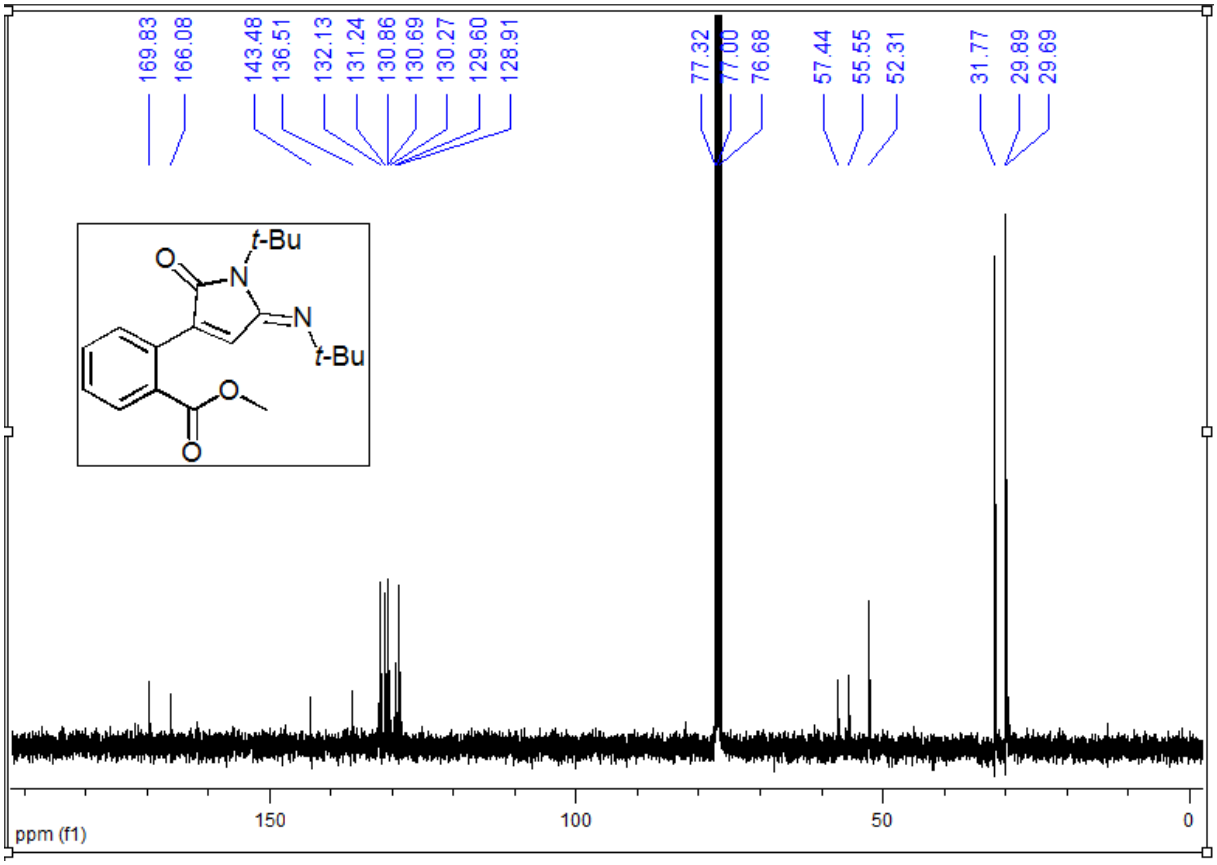
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-fluorophenyl)-1*H*-pyrrol-2(5*H*)-one



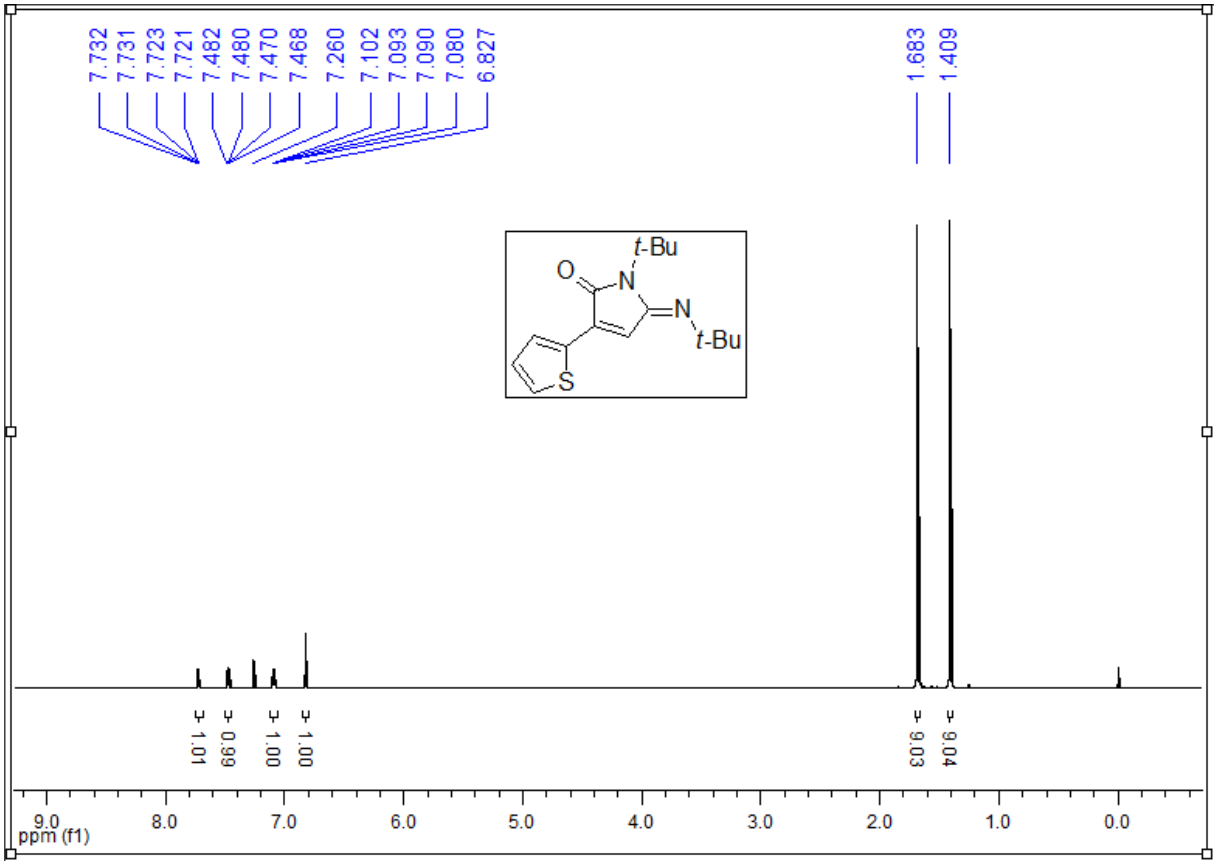


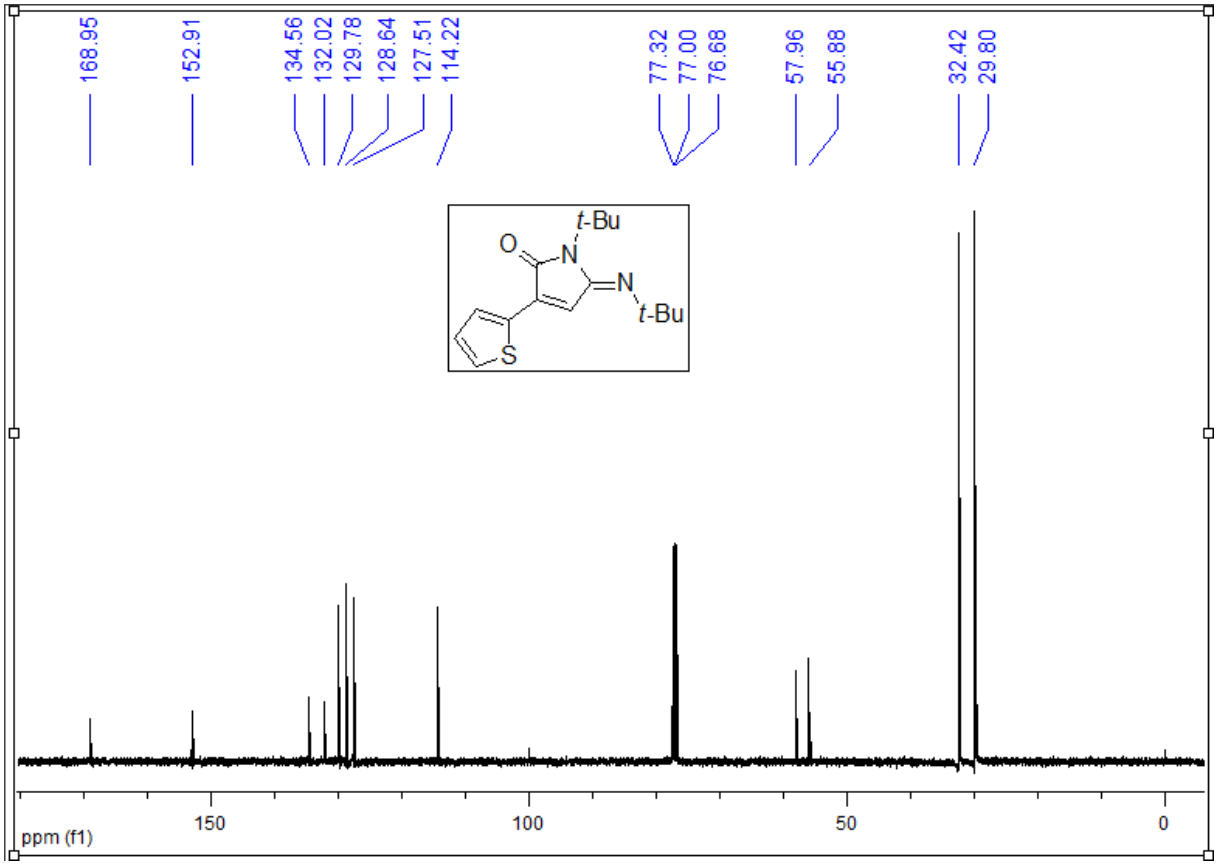
Methyl 2-((5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-2,5-dihydro-2-oxo-1*H*-pyrrol-3-yl)benzoate



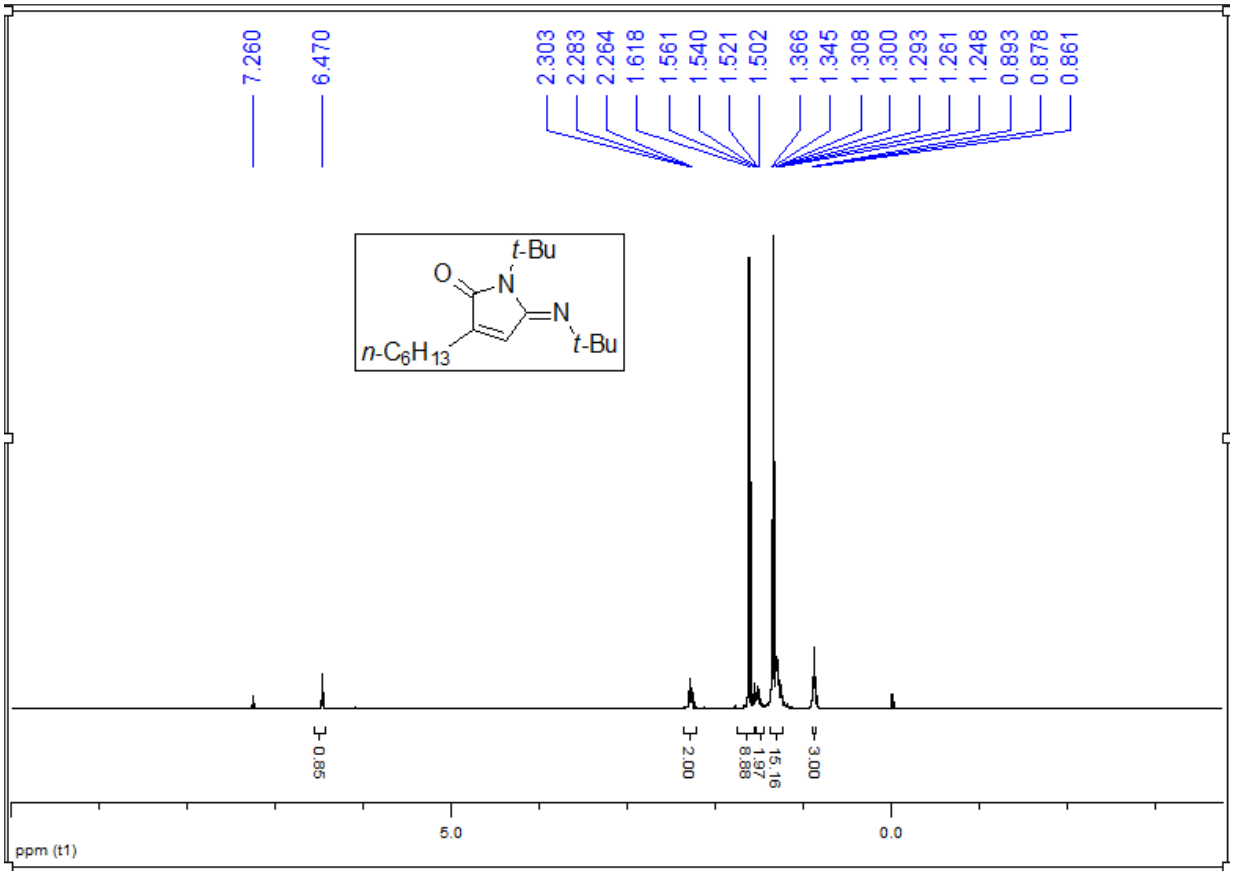


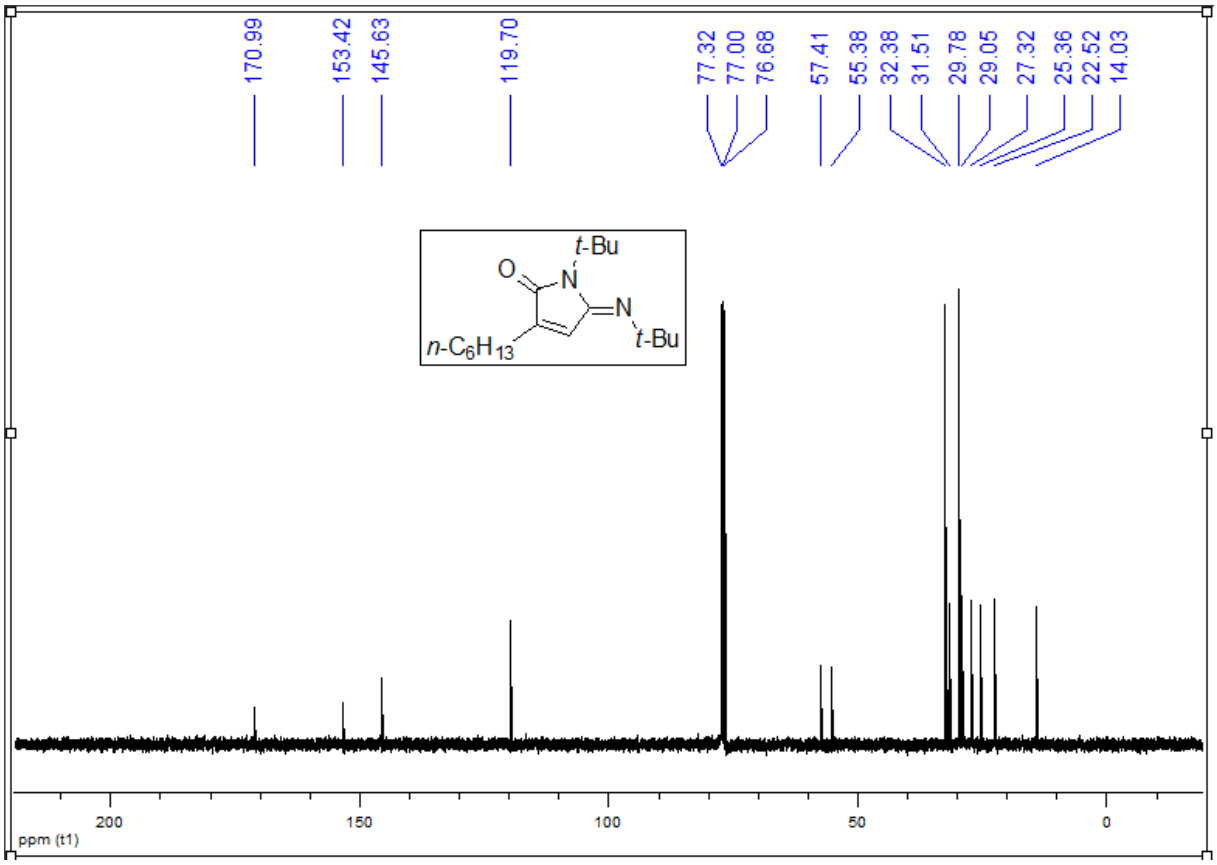
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(thiophen-2-yl)-1*H*-pyrrol-2(5*H*)-one



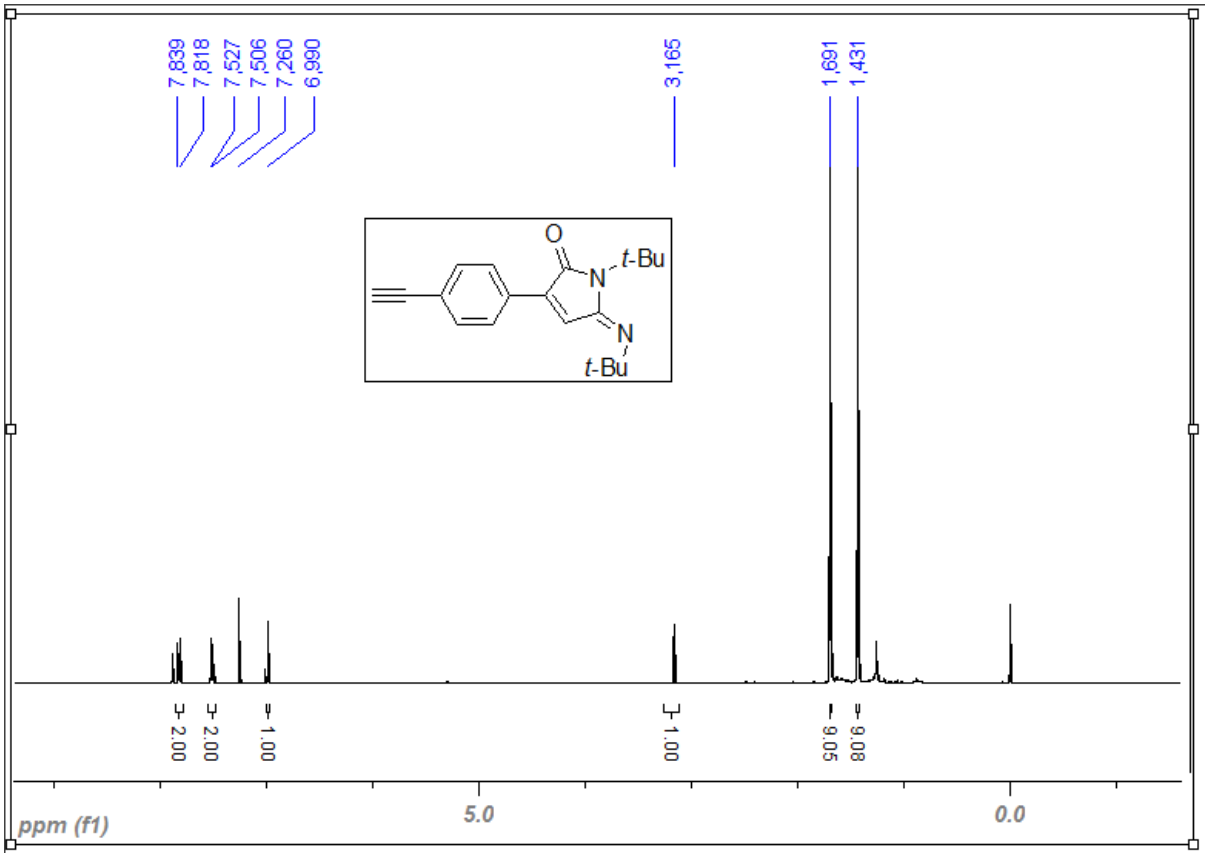


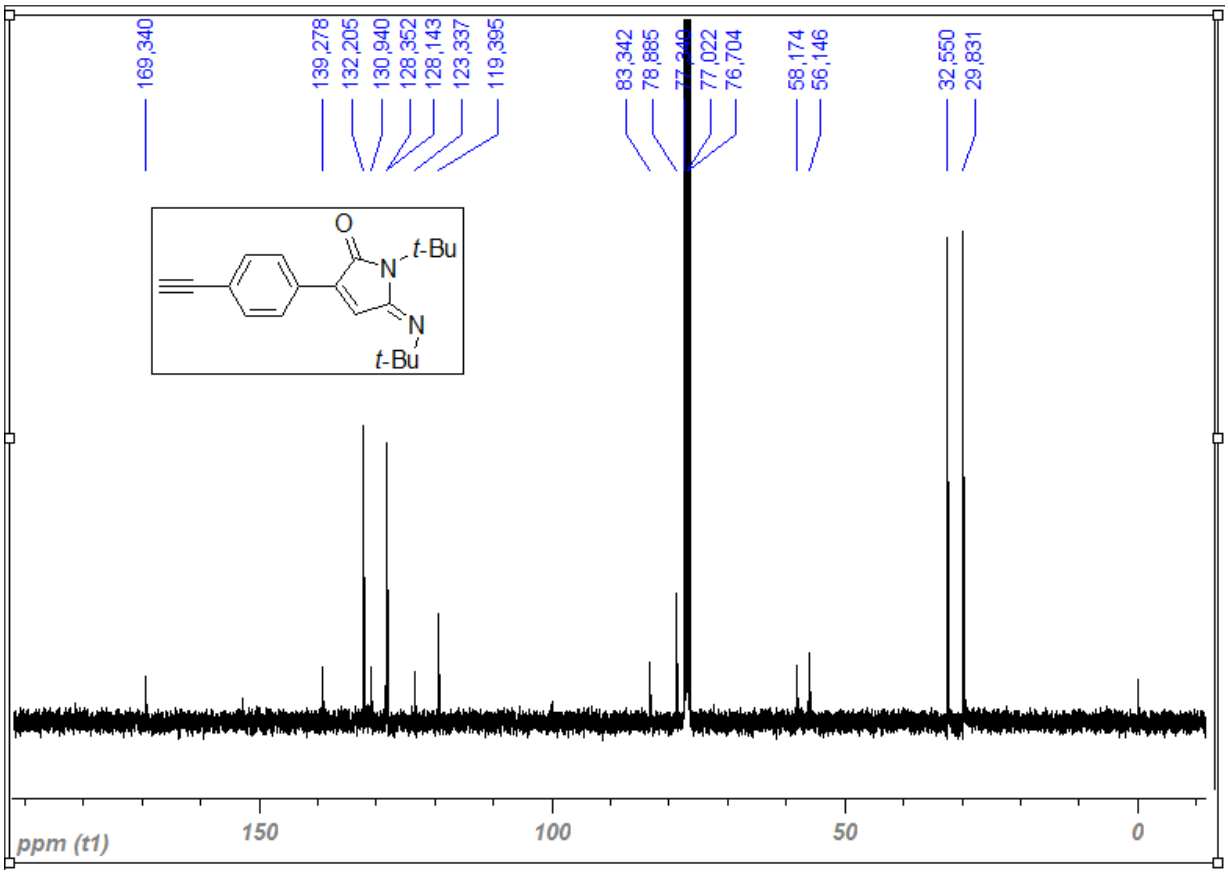
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-hexyl-1*H*-pyrrol-2(5*H*)-one



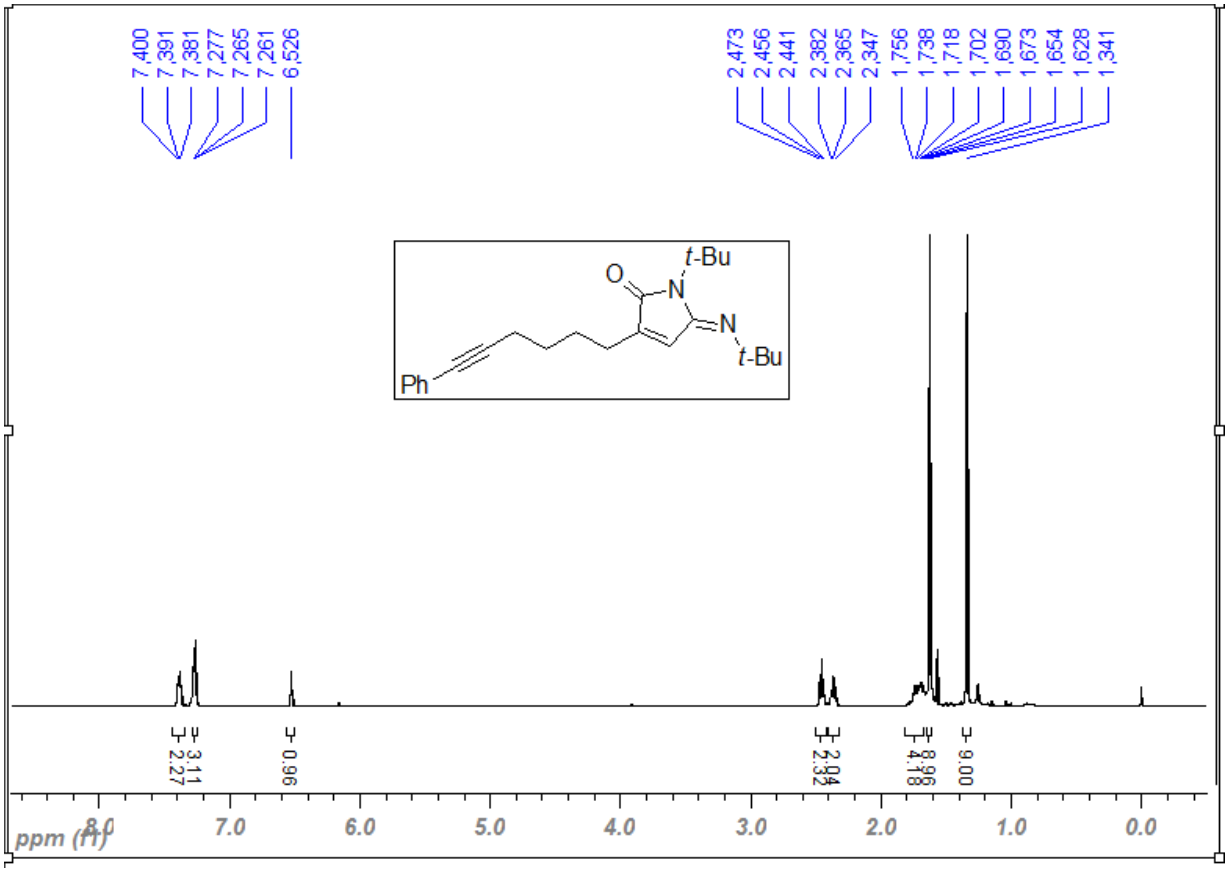


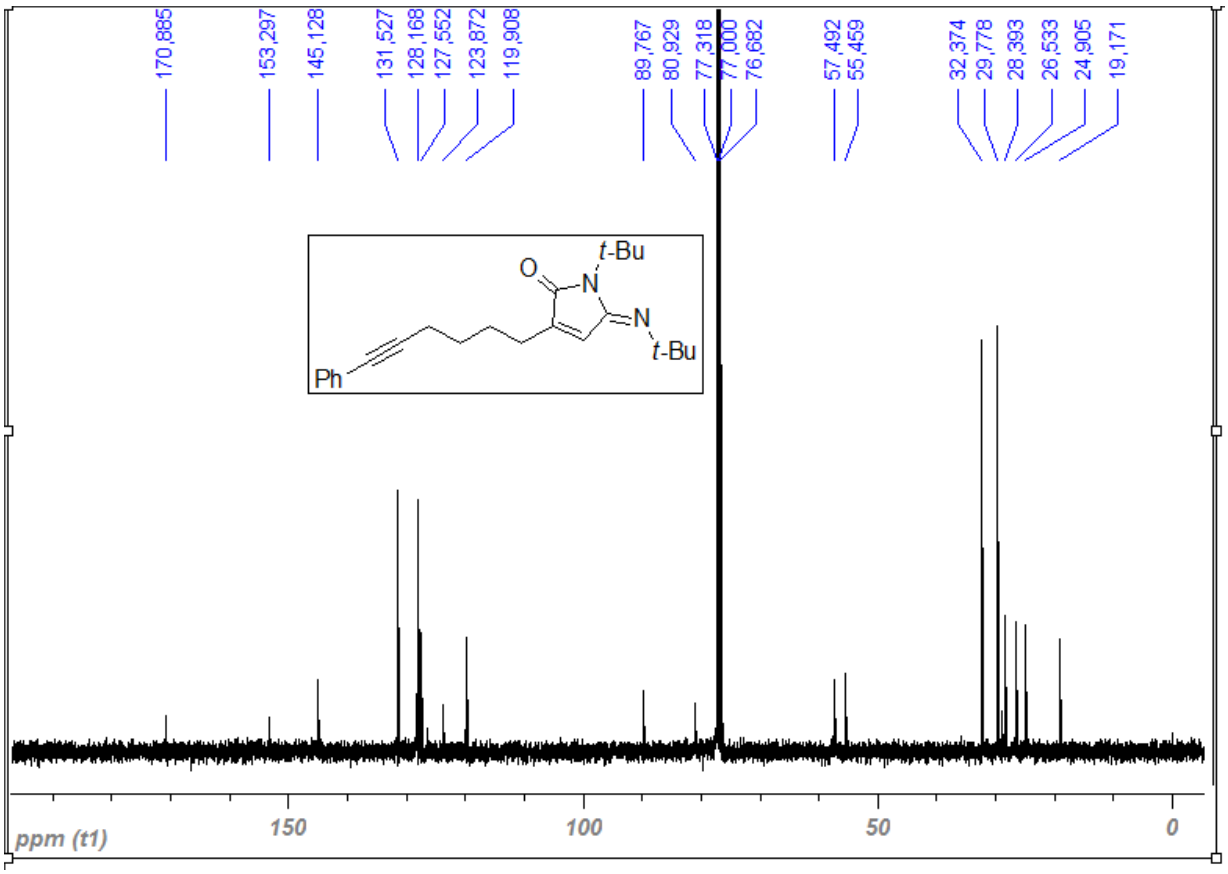
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(4-ethynylphenyl)-1*H*-pyrrol-2(5*H*)-one



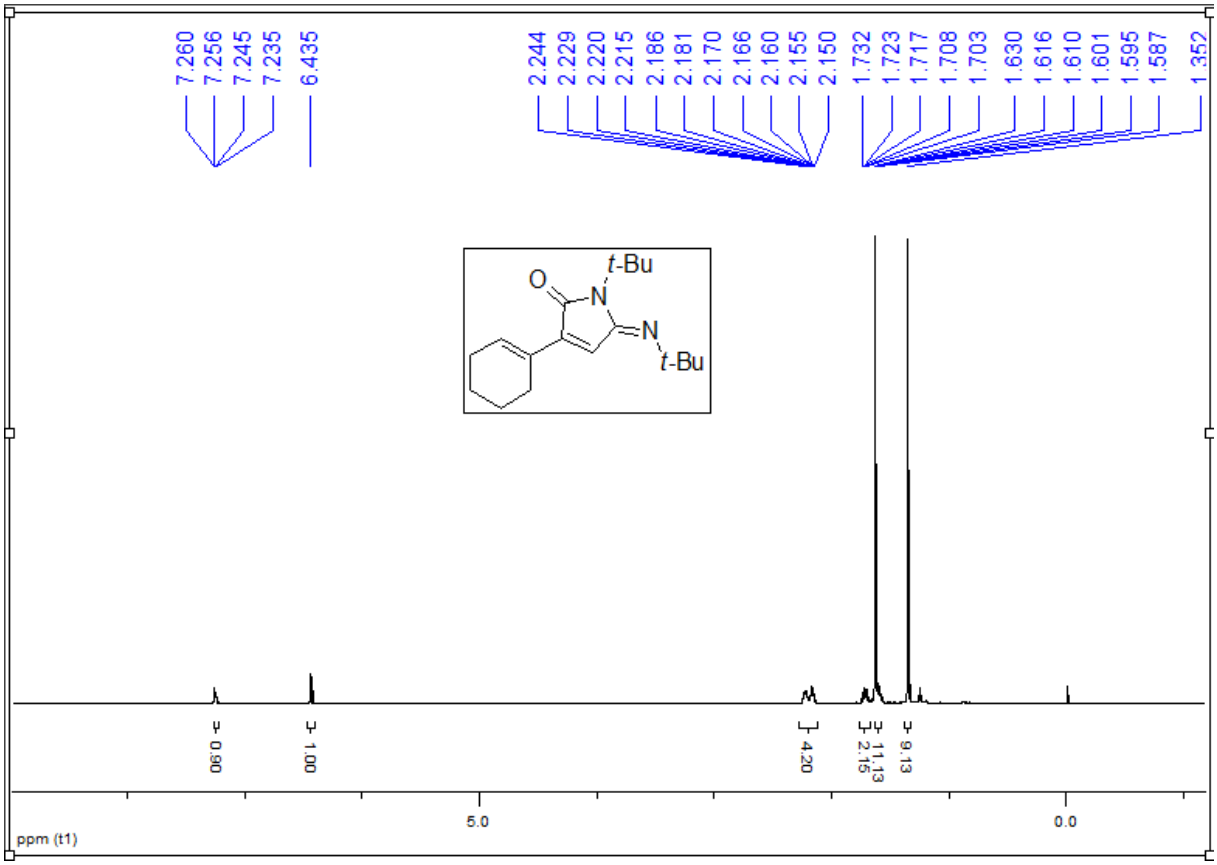


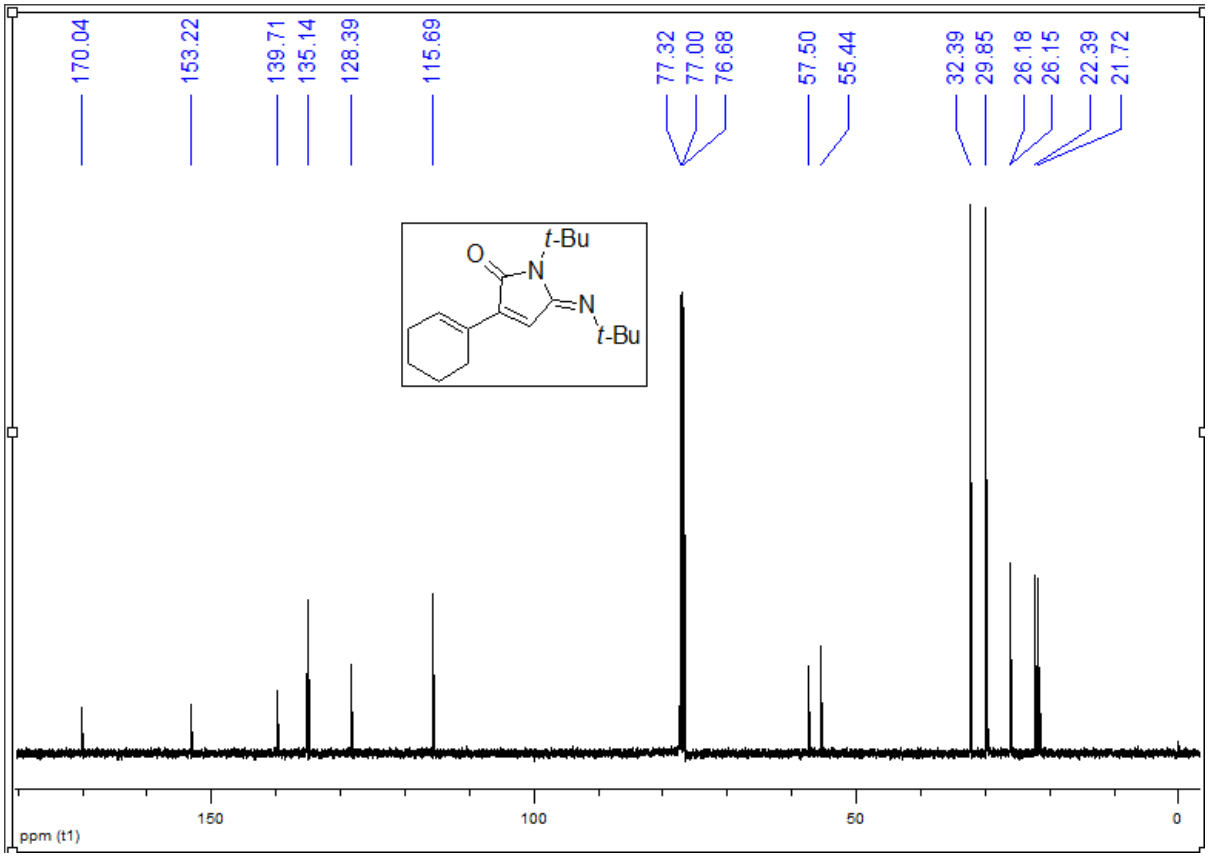
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-(6-phenylhex-5-ynyl)-1*H*-pyrrol-2(5*H*)-one



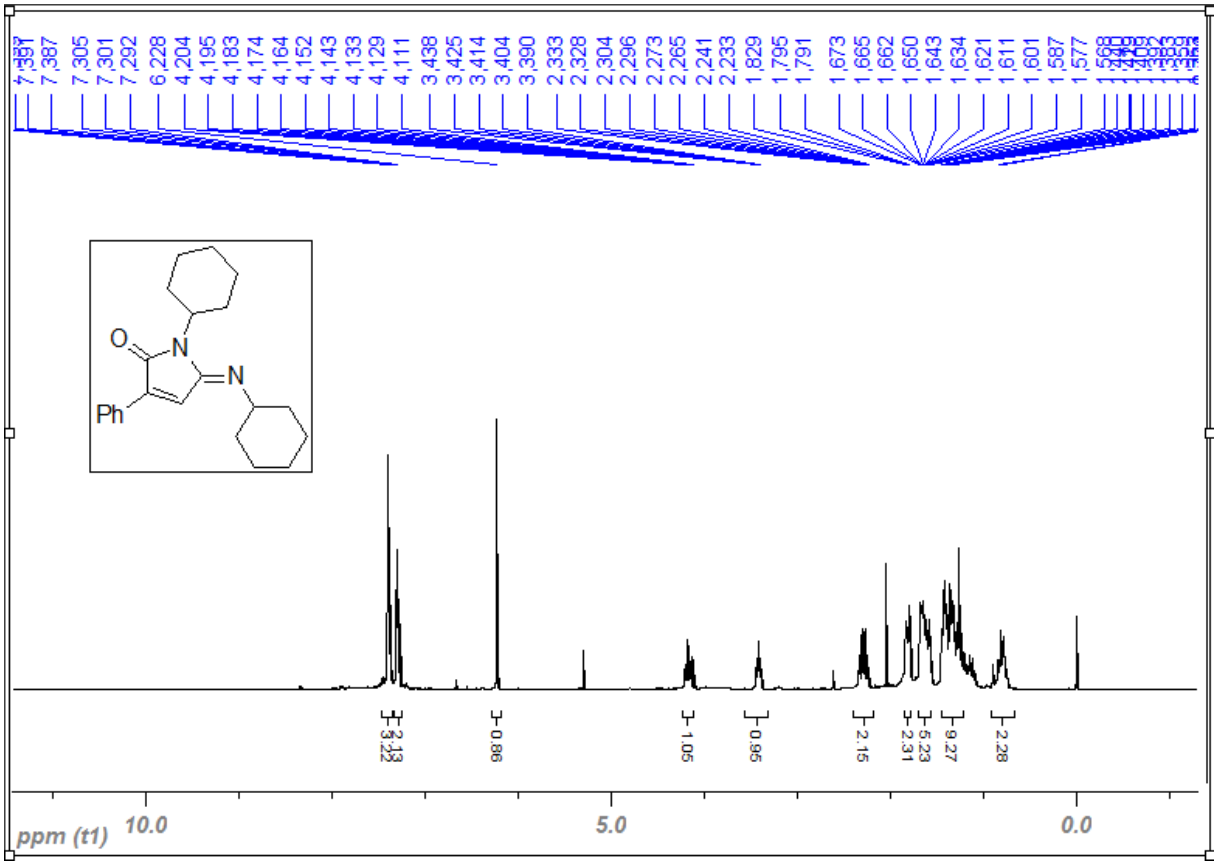


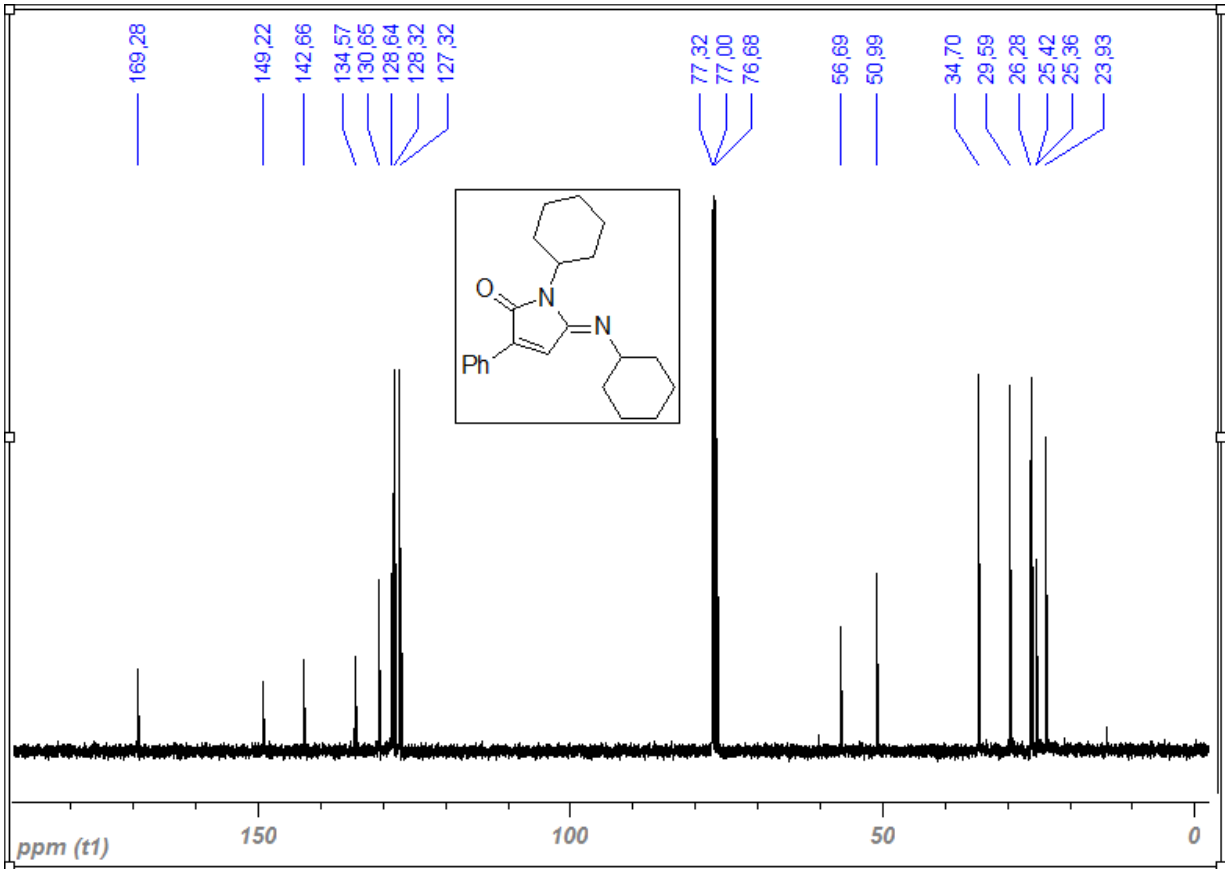
(5*E*)-1-*tert*-butyl-5-(*tert*-butylimino)-3-cyclohexenyl-1*H*-pyrrol-2(5*H*)-one



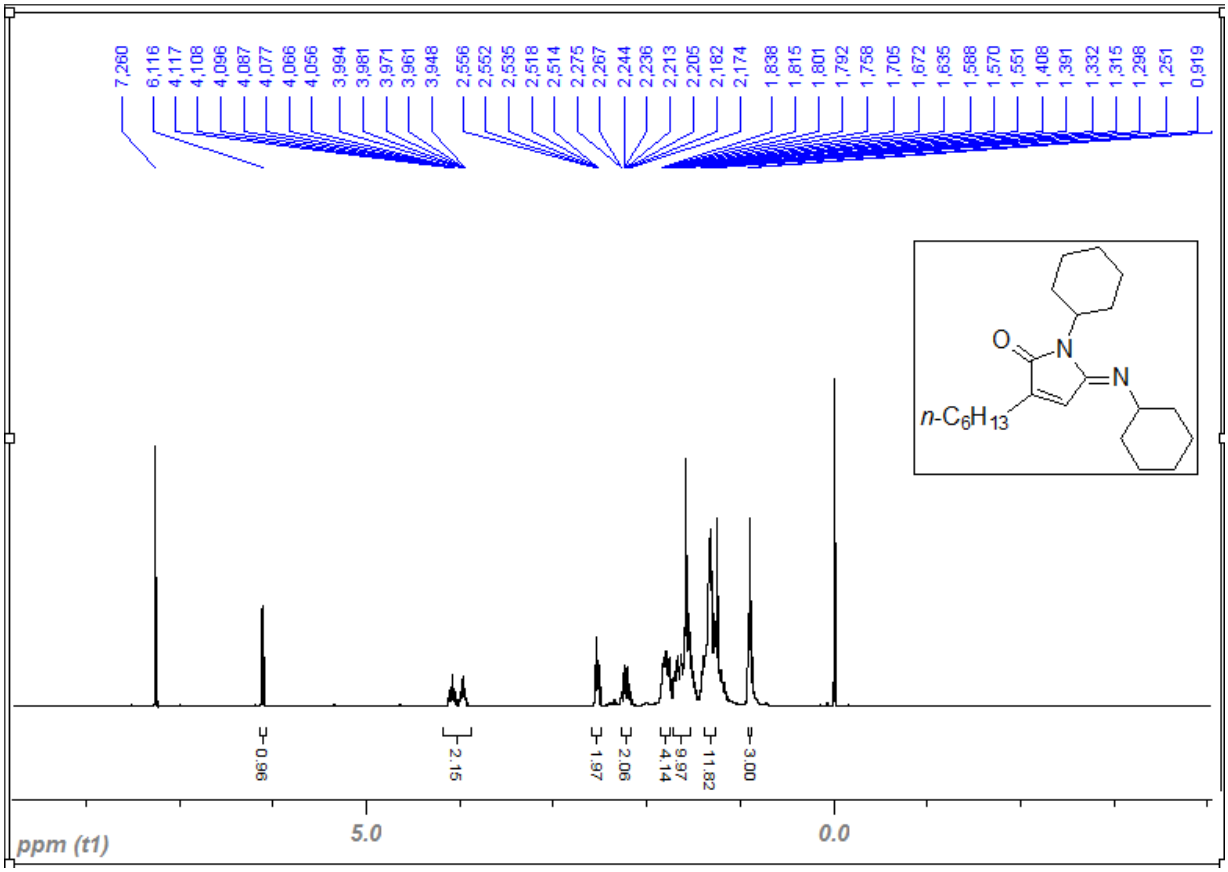


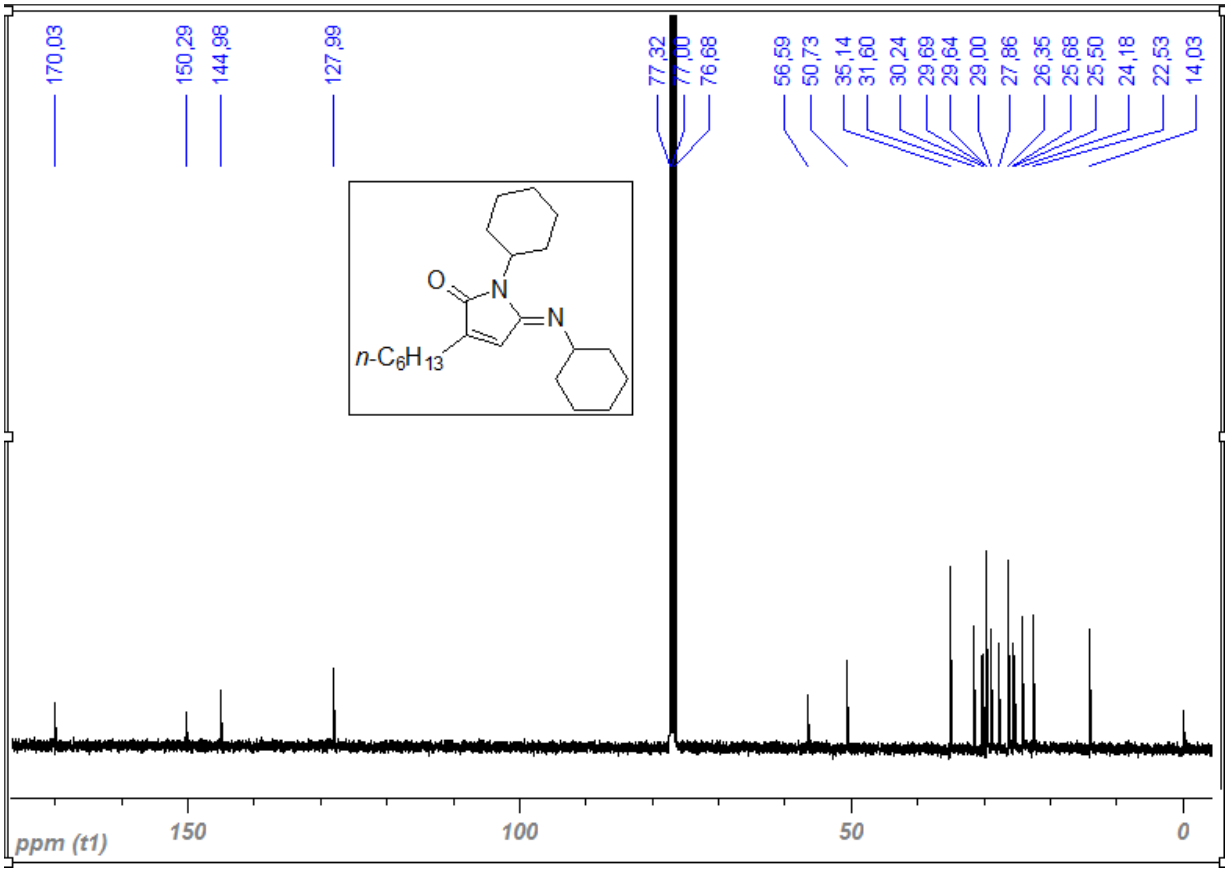
(5*E*)-1-cyclohexyl-5-(cyclohexylimino)-3-phenyl-1*H*-pyrrol-2(5*H*)-one



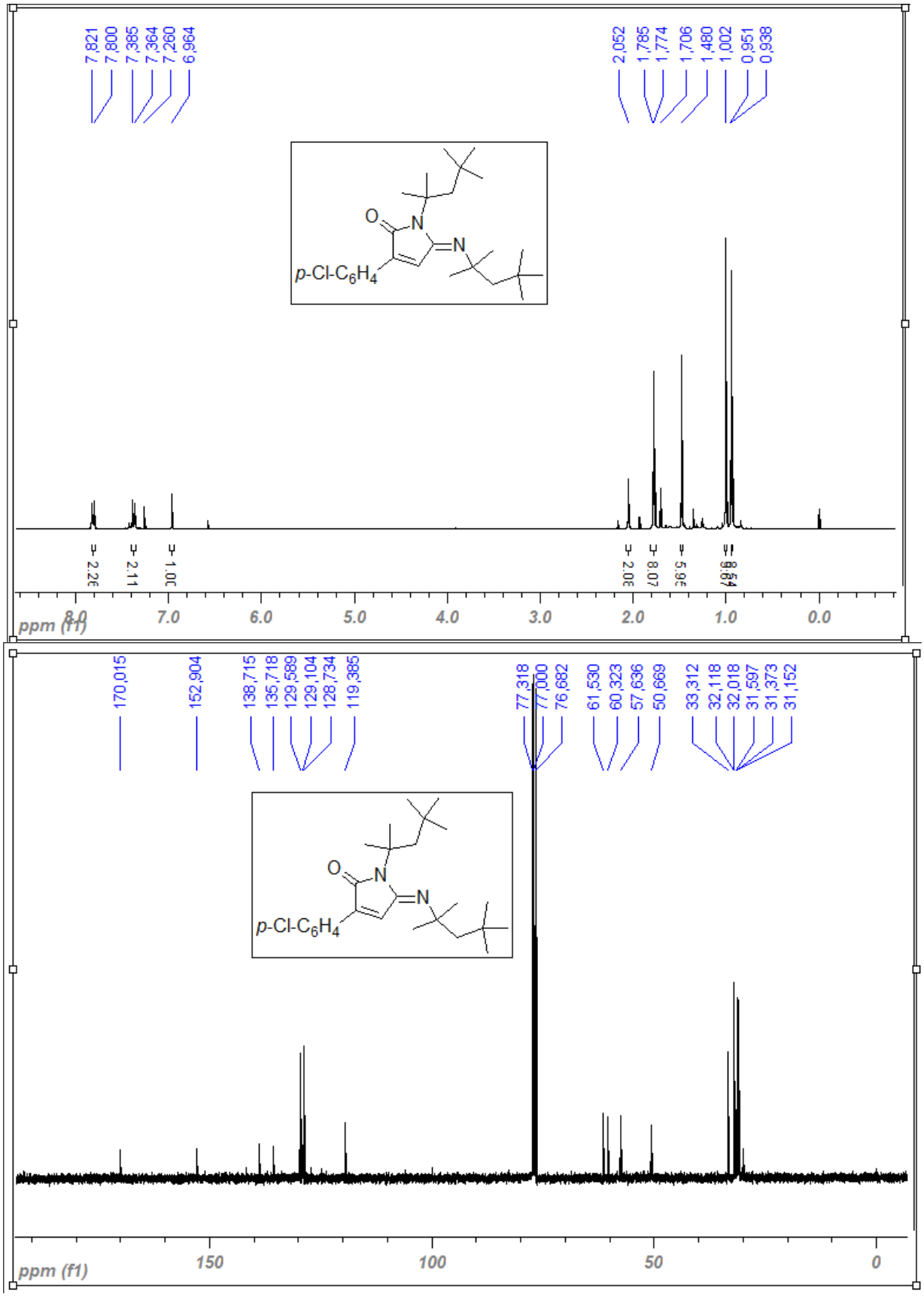


(5*E*)-1-cyclohexyl-5-(cyclohexylimino)-3-hexyl-1*H*-pyrrol-2(5*H*)-one

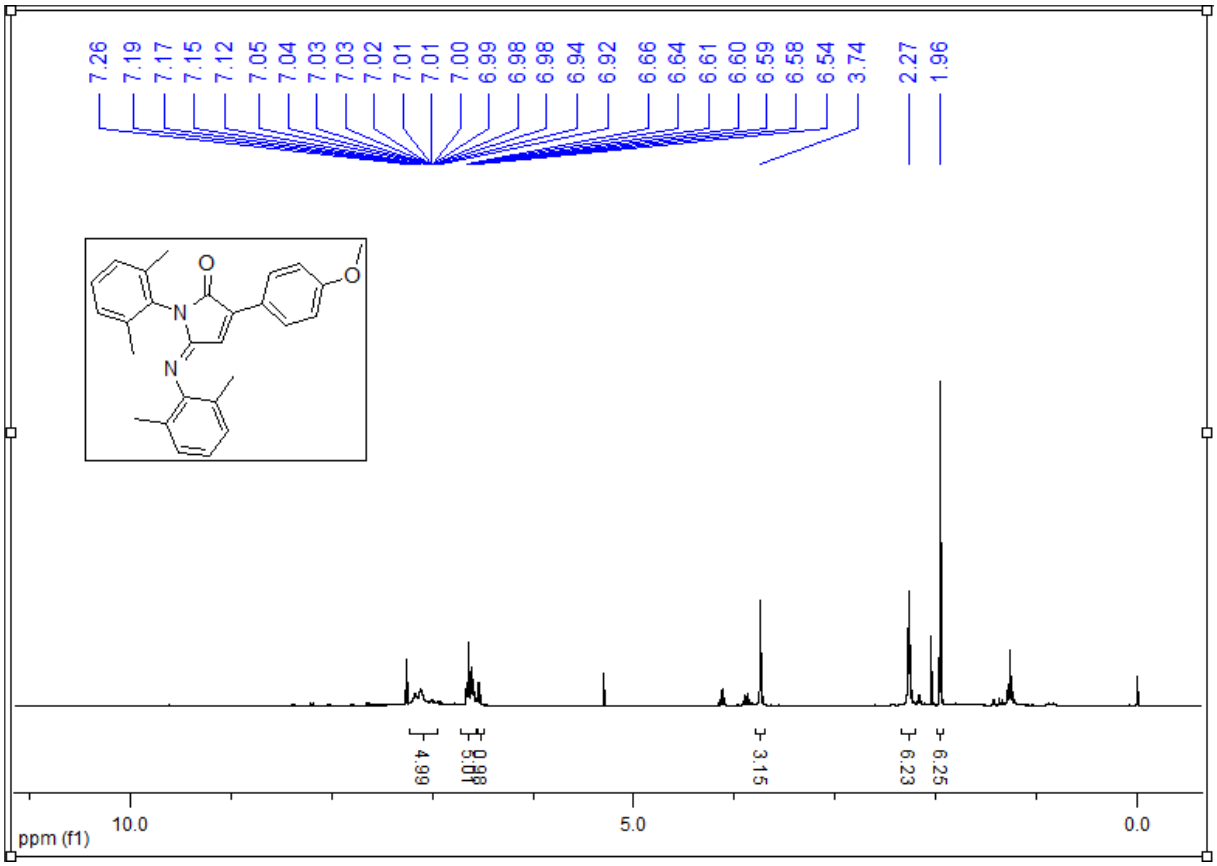


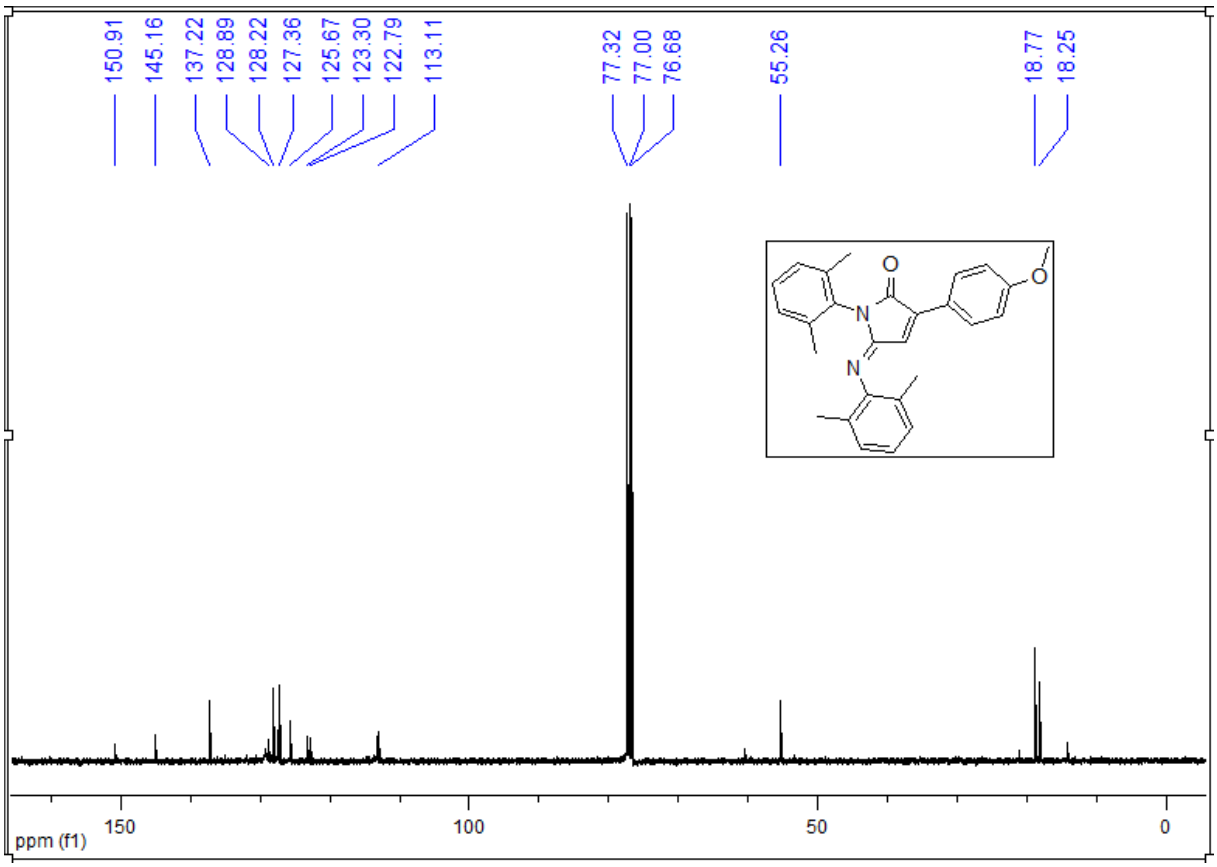


(5*Z*)-5-(2,4,4-trimethylpentan-2-ylimino)-3-(4-chlorophenyl)-1-(2,4,4-trimethylpentan-2-yl)-1*H*-pyrrol-2(5*H*)-one

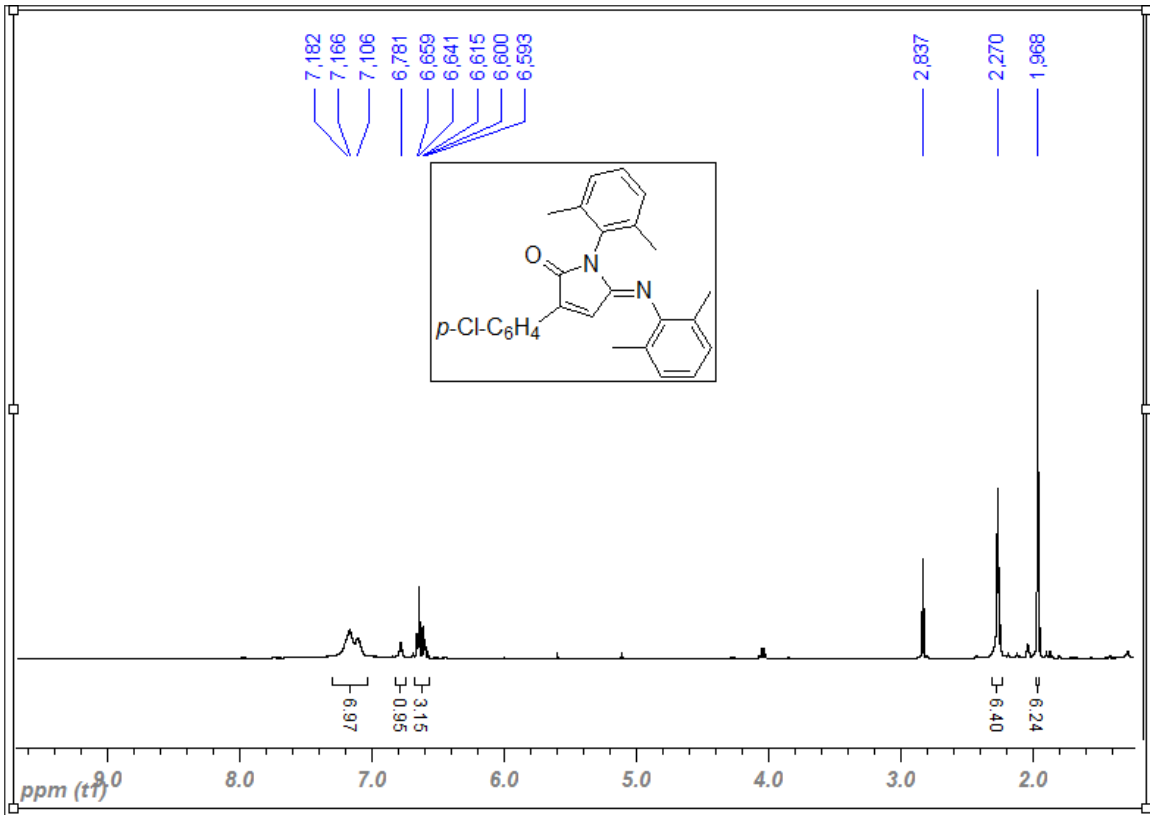


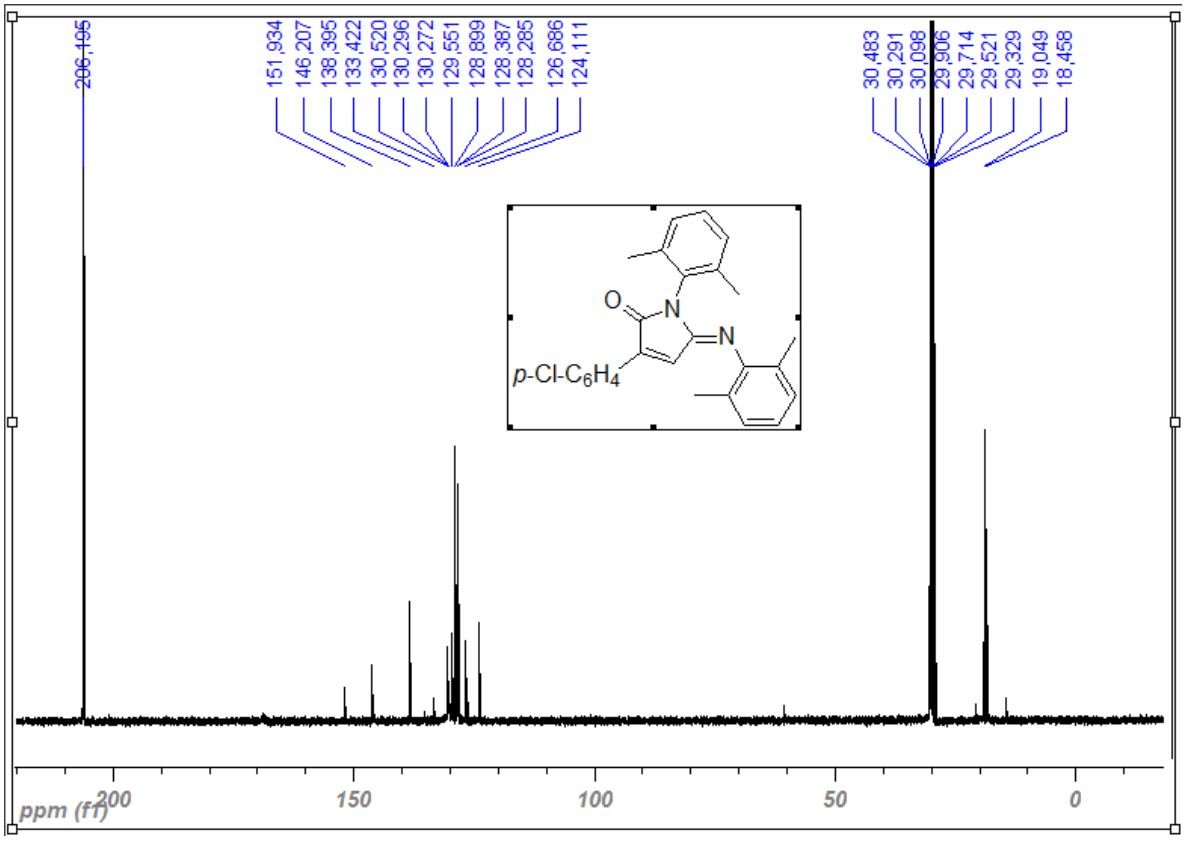
(5*E*)-5-(2,6-dimethylphenylimino)-3-(4-methoxyphenyl)-1-(2,6-dimethylphenyl)-1*H*-pyrrol-2(5*H*)-one



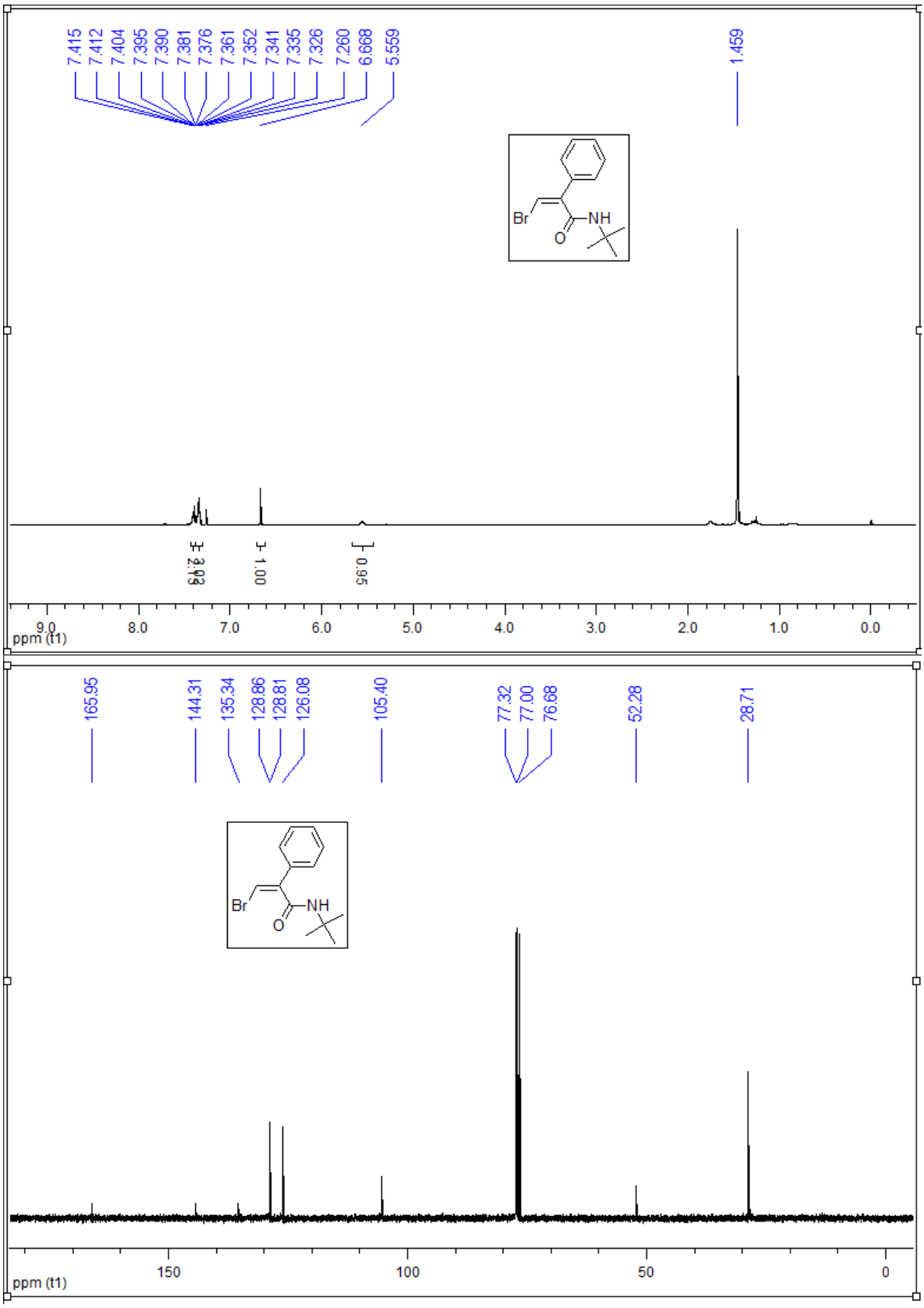


(5*E*)-5-(2,6-dimethylphenylimino)-3-(4-chlorophenyl)-1-(2,6-dimethylphenyl)-1*H*-pyrrol-2(5*H*)-one

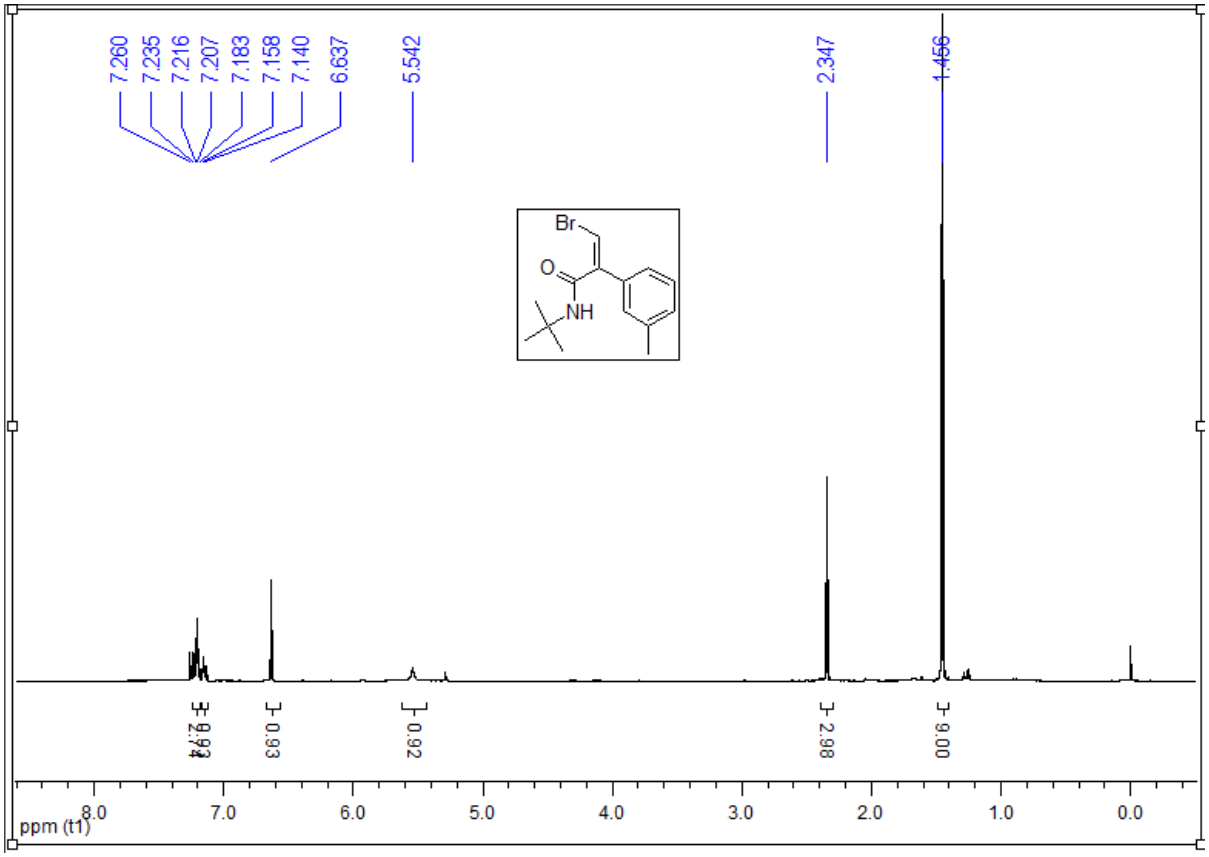


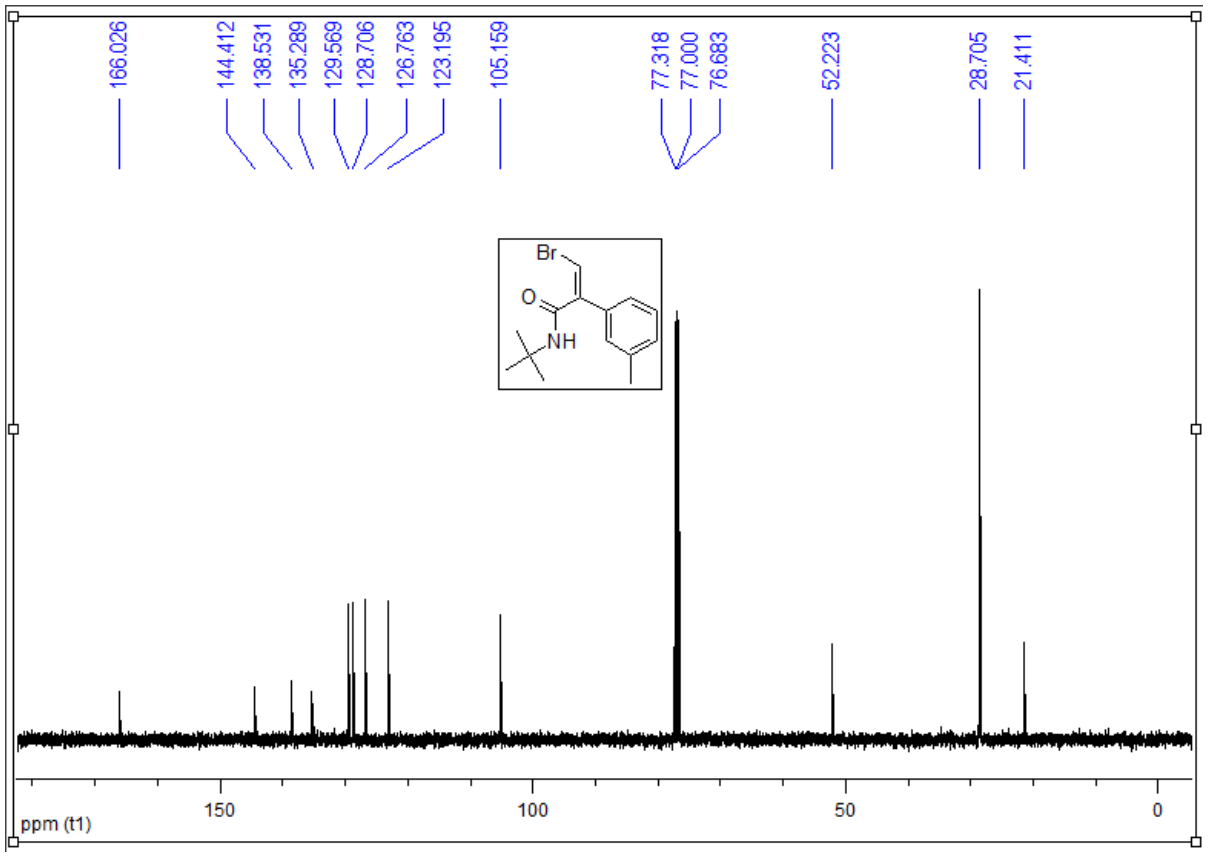


(*Z*)-*N*-*tert*-butyl-3-bromo-2-phenylacrylamide

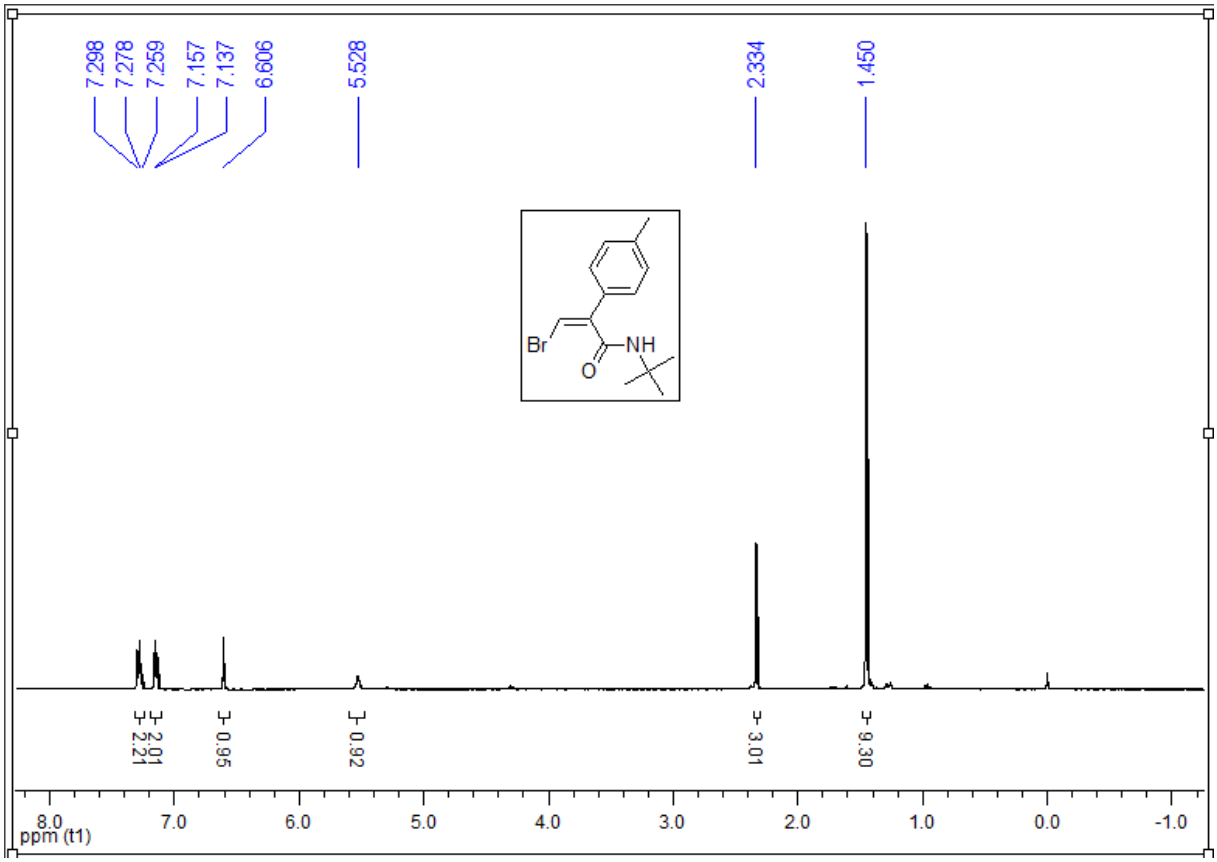


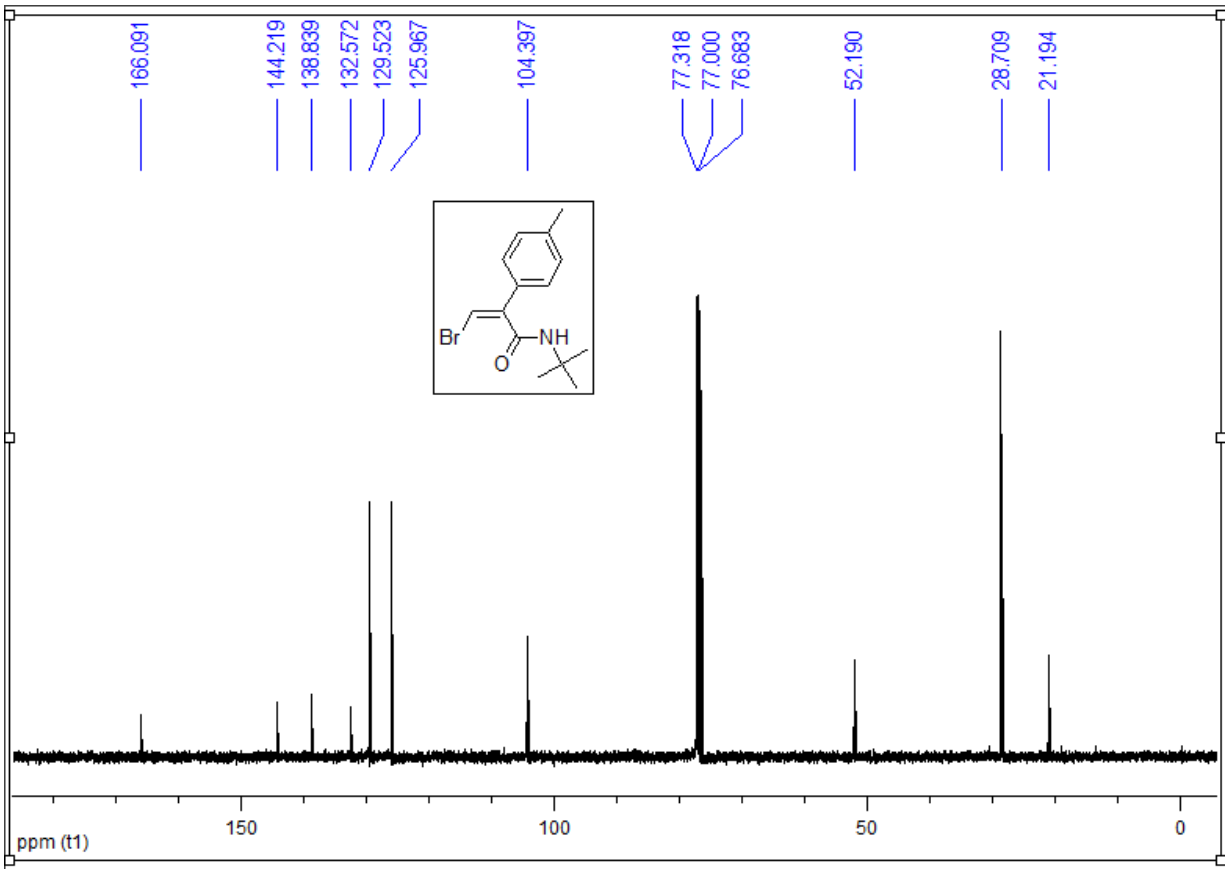
(*Z*)-*N*-*tert*-butyl-3-bromo-2-m-tolylacrylamide



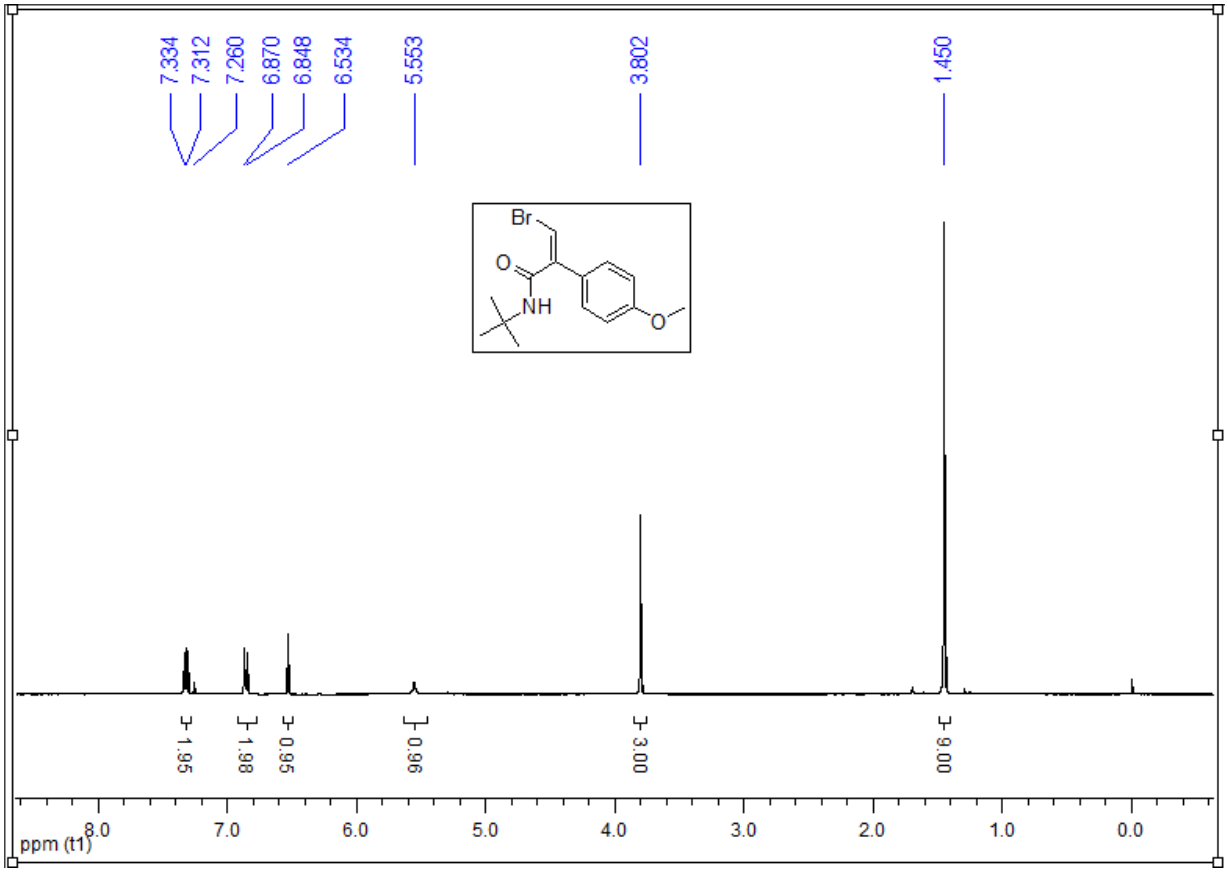


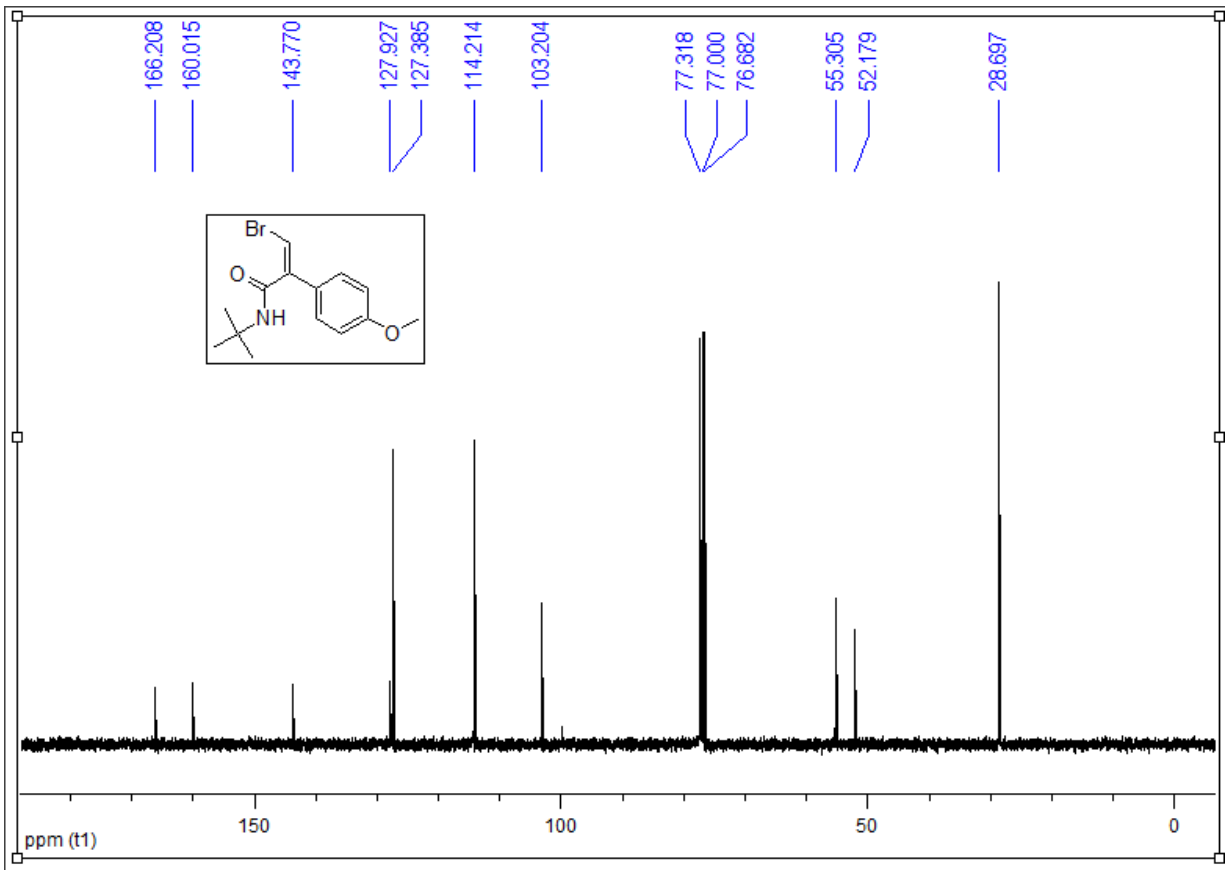
(*Z*)-**N**-*tert*-butyl-3-bromo-2-p-tolylacrylamide



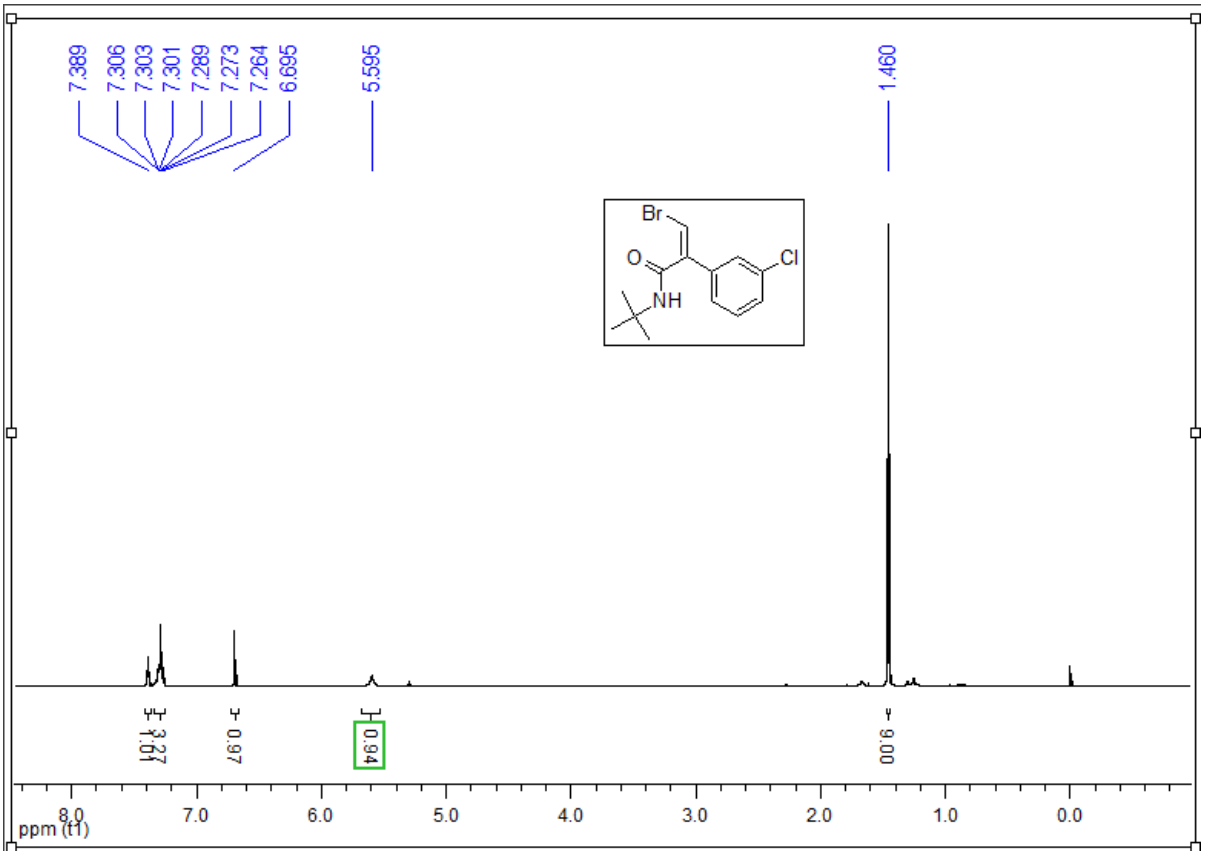


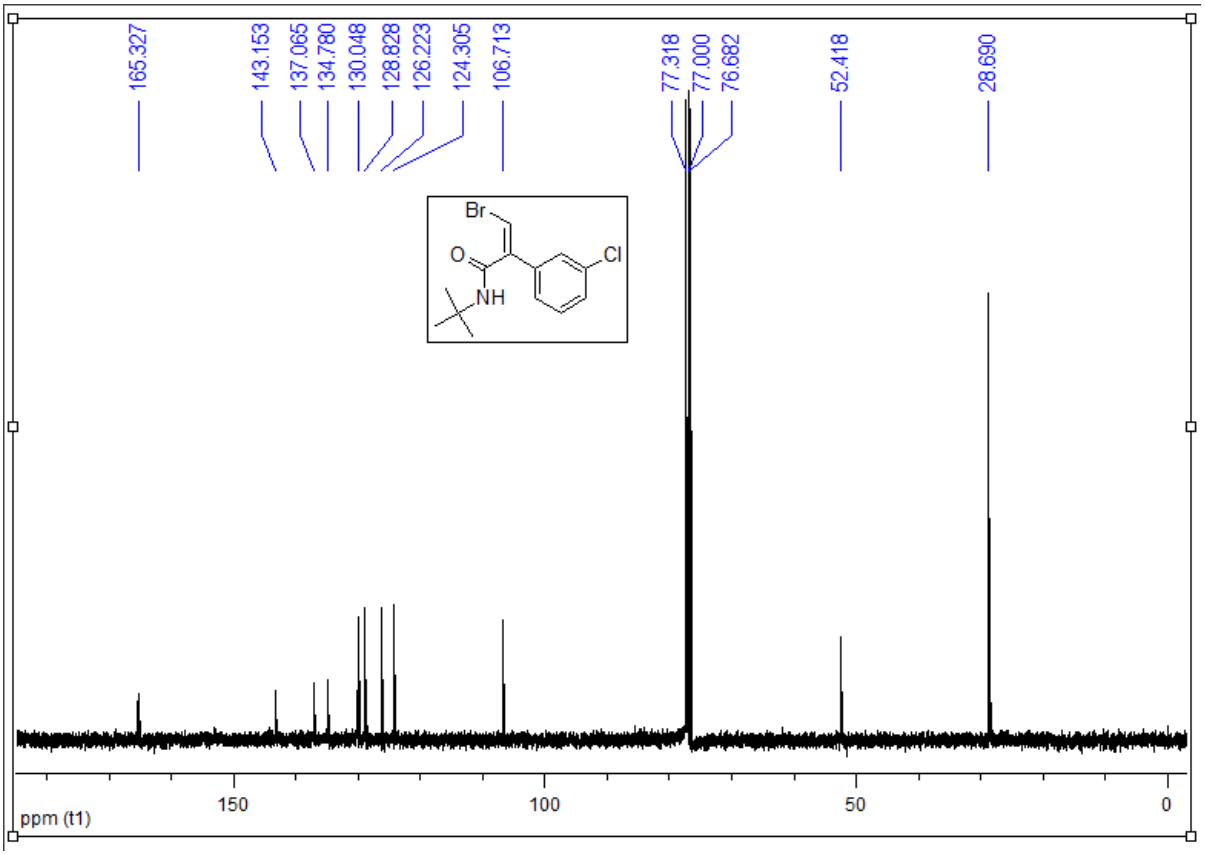
(*Z*)-*N*-*tert*-butyl-3-bromo-2-(4-methoxyphenyl)acrylamide



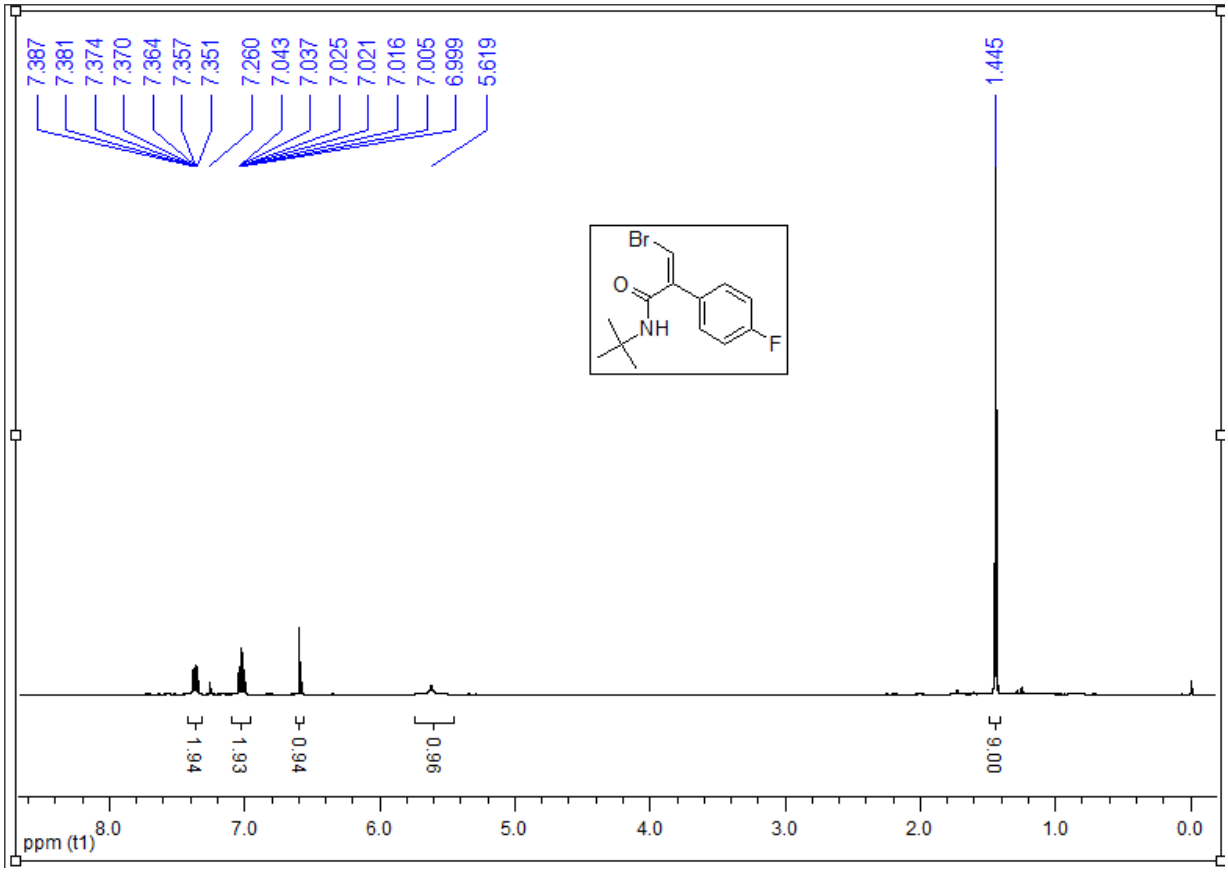


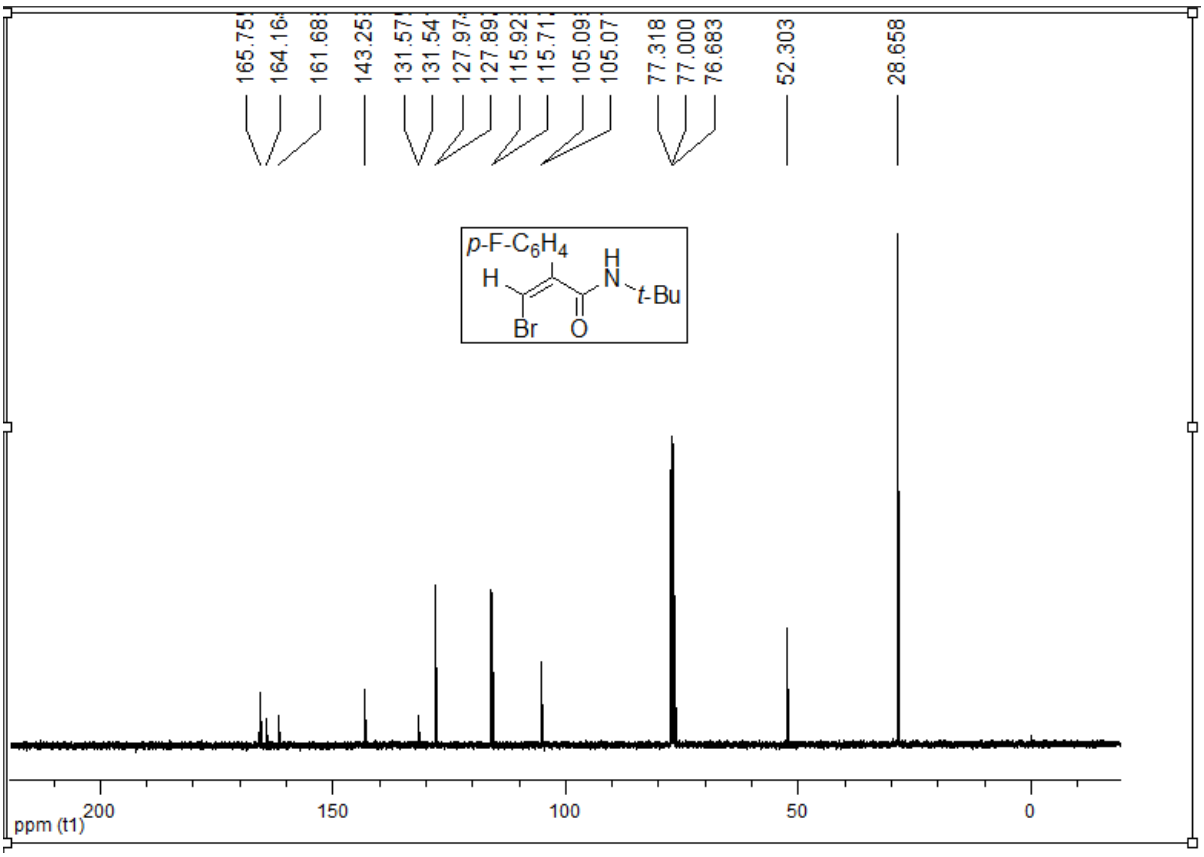
(*Z*)-*N*-*tert*-butyl-3-bromo-2-(4-chlorophenyl)acrylamide



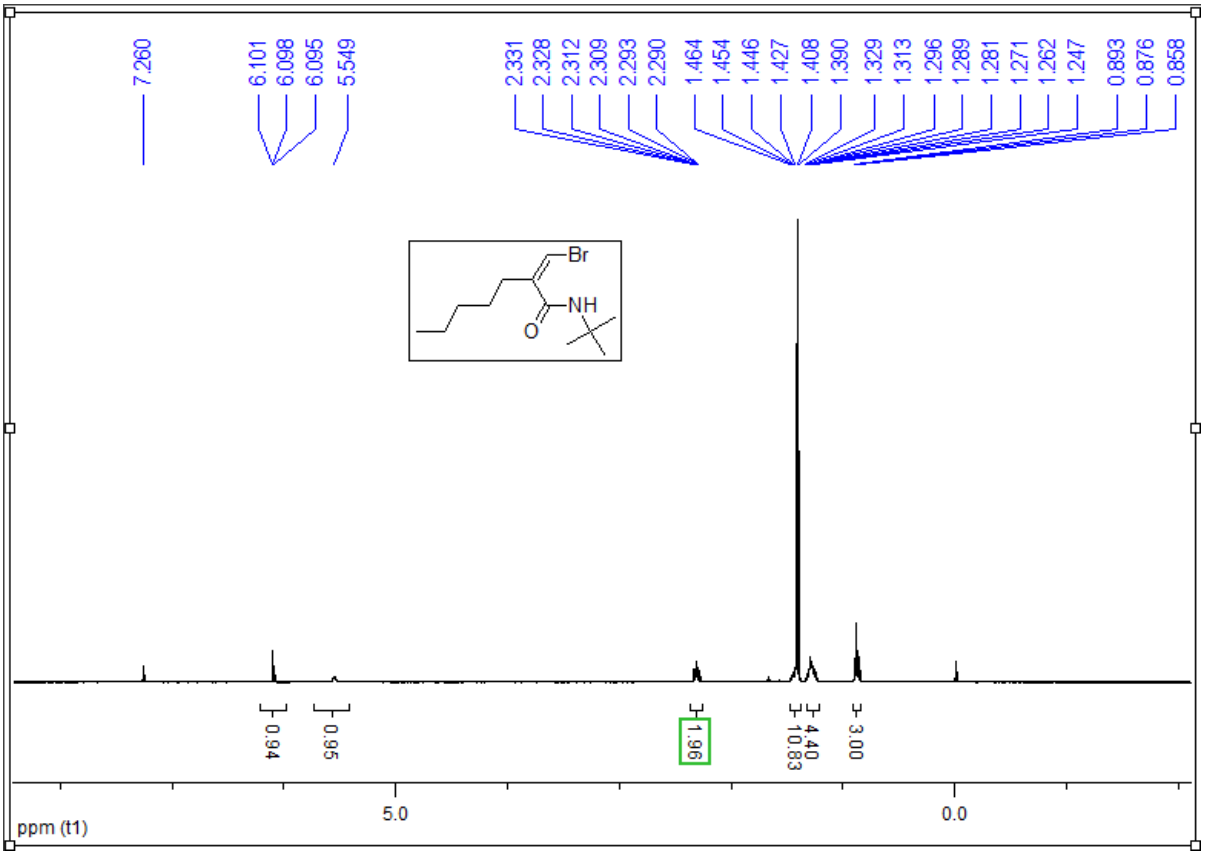


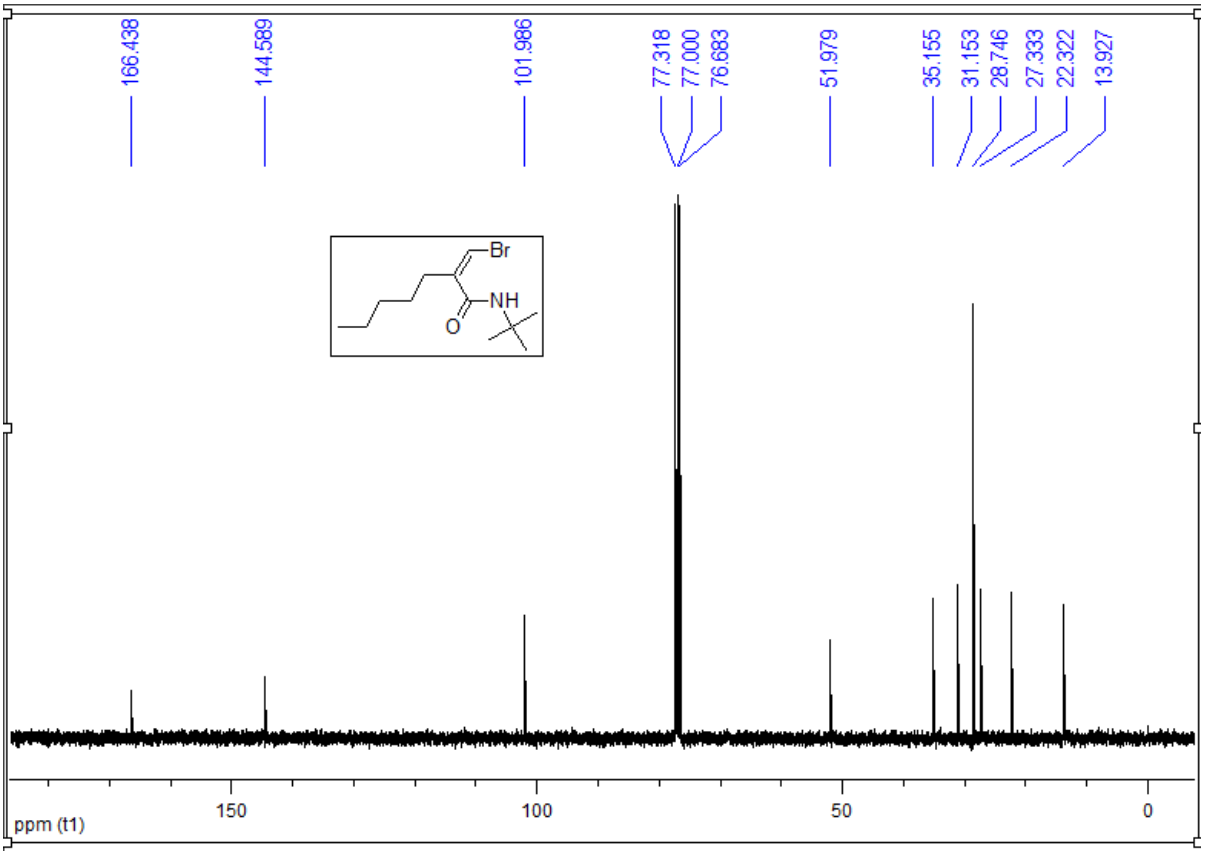
(*Z*)-*N*-*tert*-butyl-3-bromo-2-(4-fluorophenyl)acrylamide



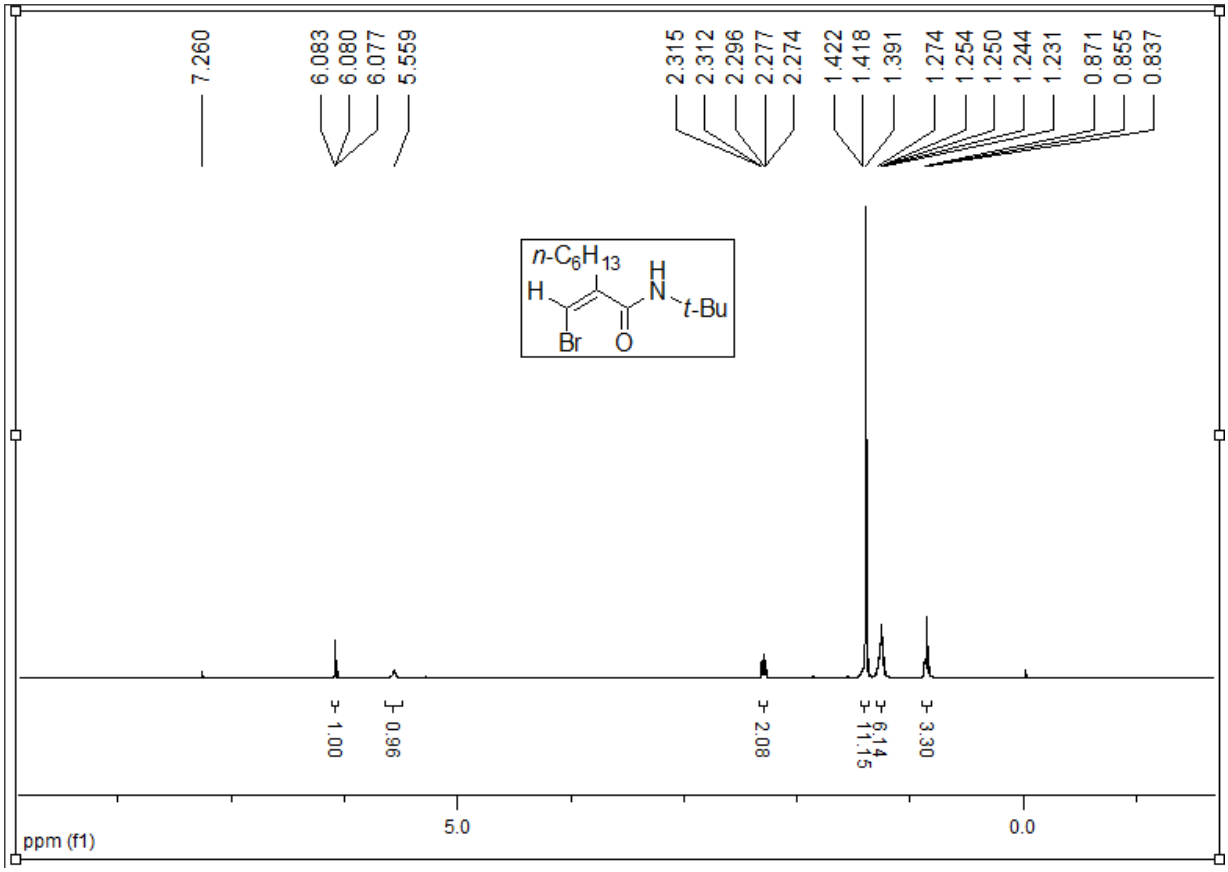


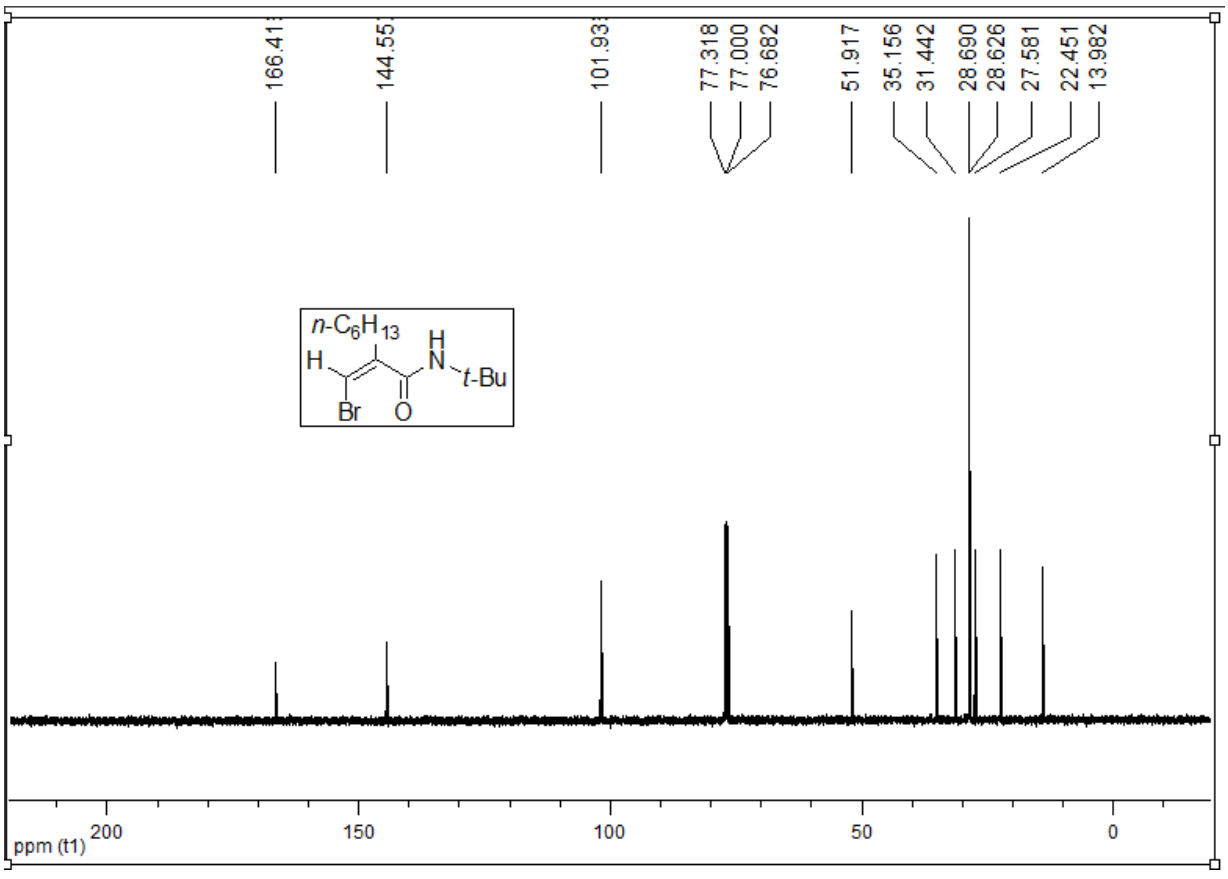
(*Z*)-*N*-*tert*-butyl-2-(bromomethylene)heptanamide



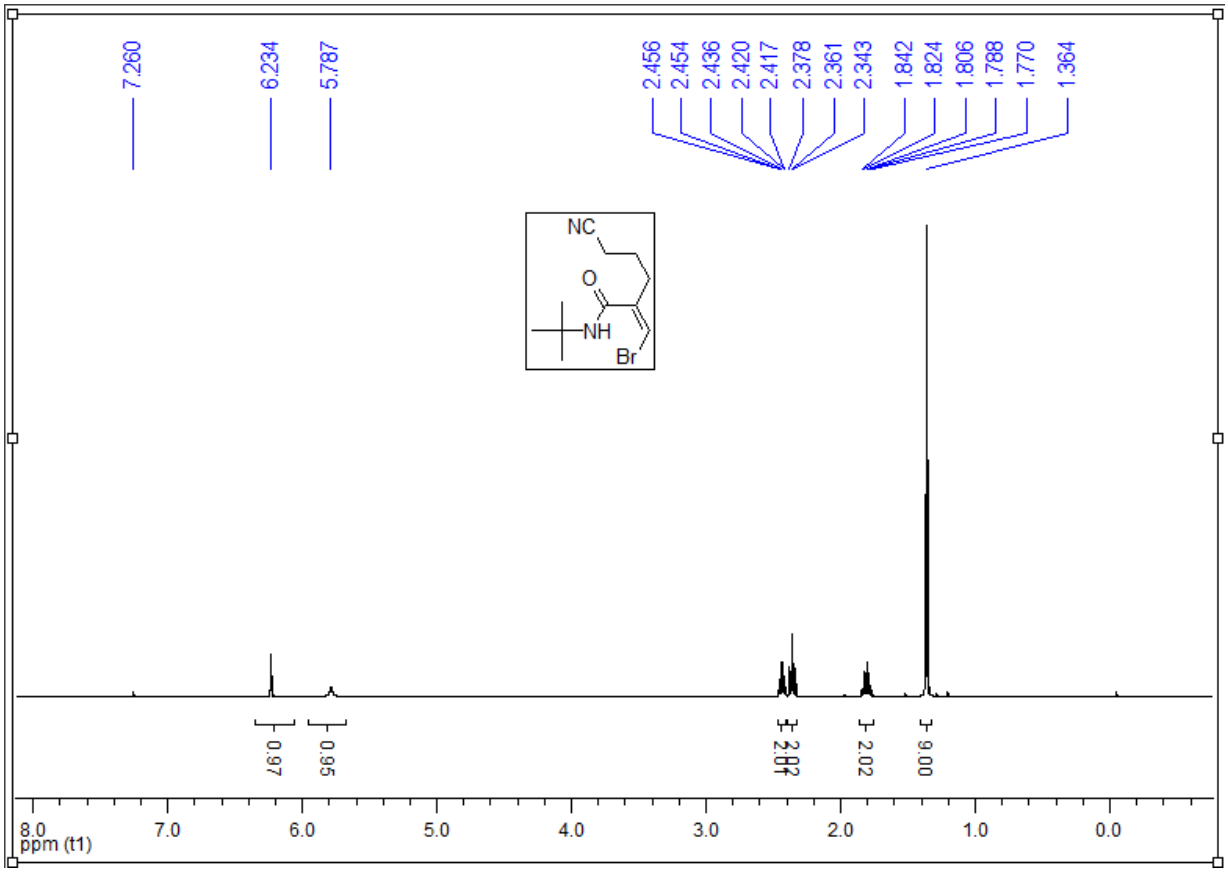


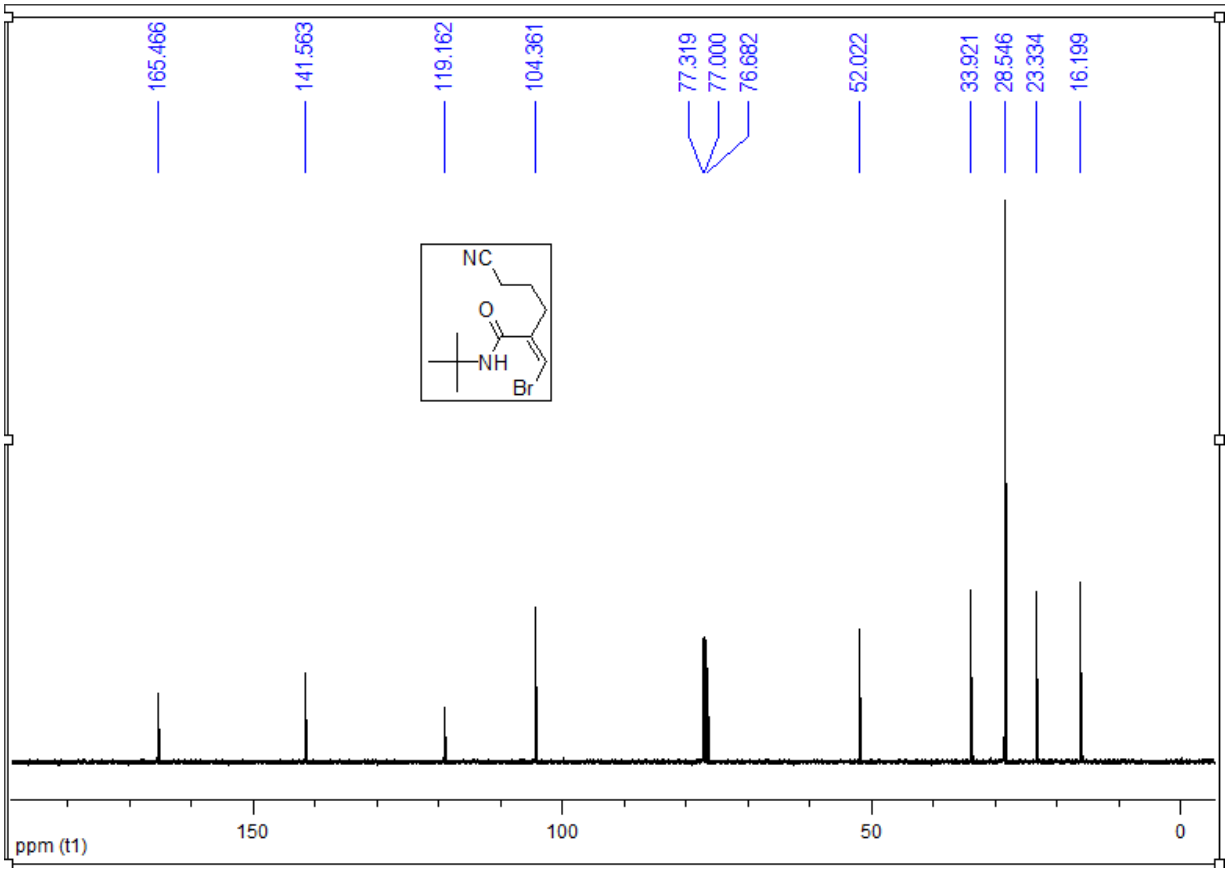
(*Z*)-*N*-*tert*-butyl-2-(bromomethylene)octanamide



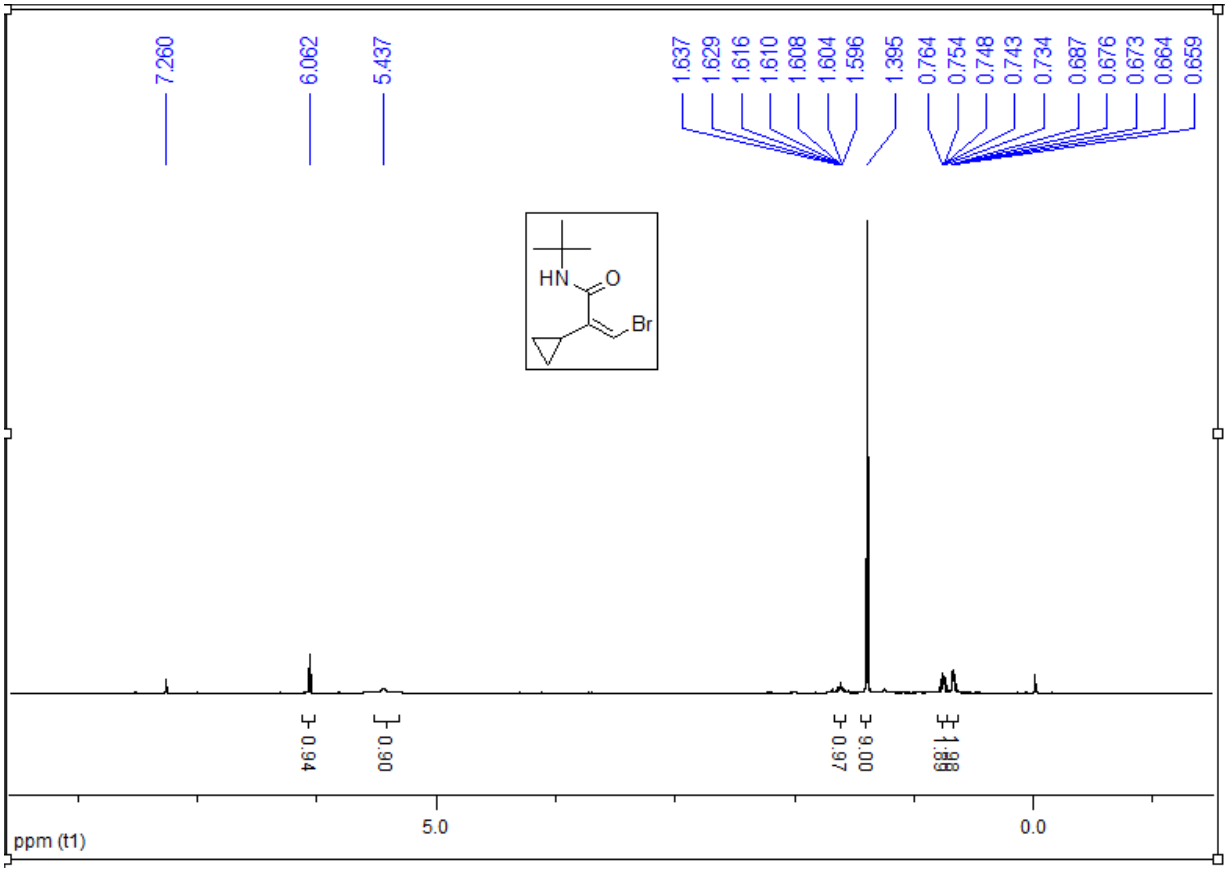


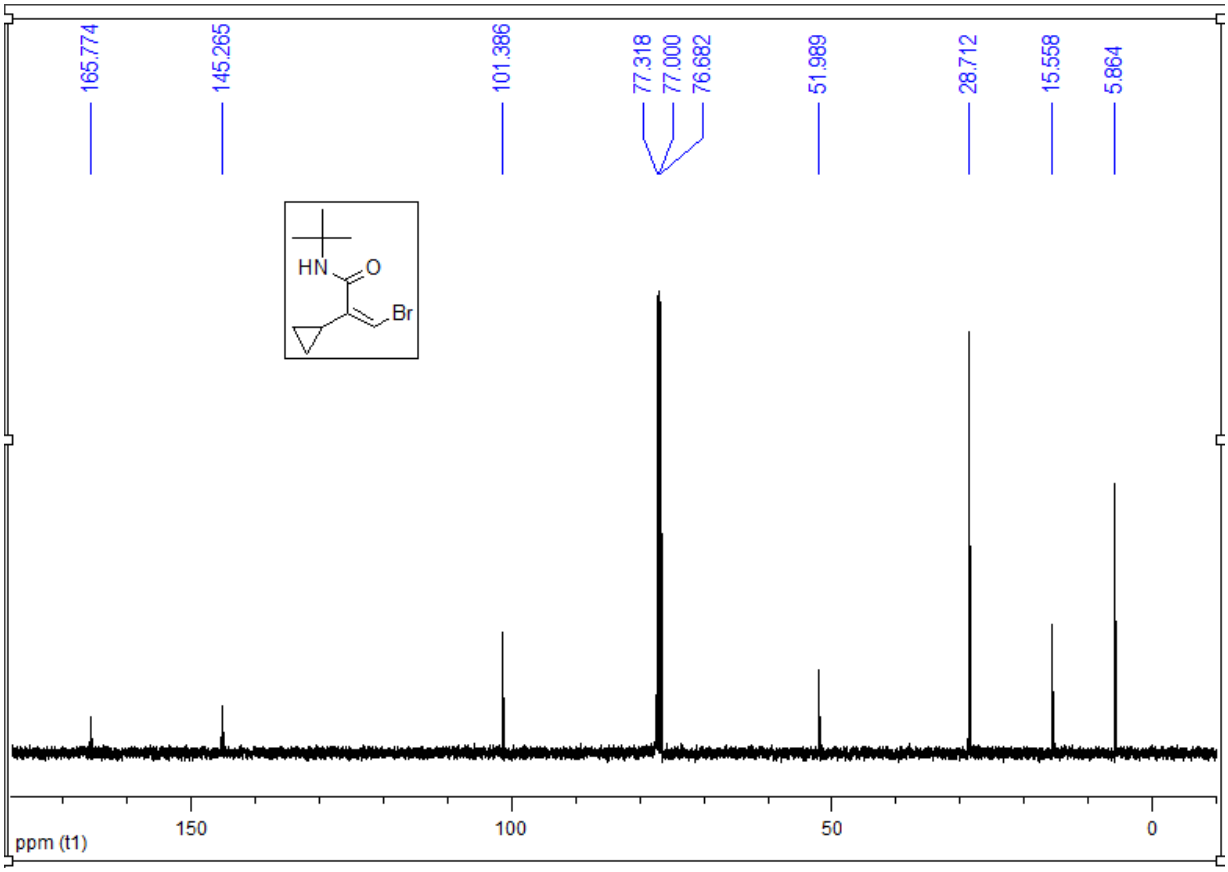
(*Z*)-*N*-*tert*-butyl-2-(bromomethylene)-5-cyanopentanamide



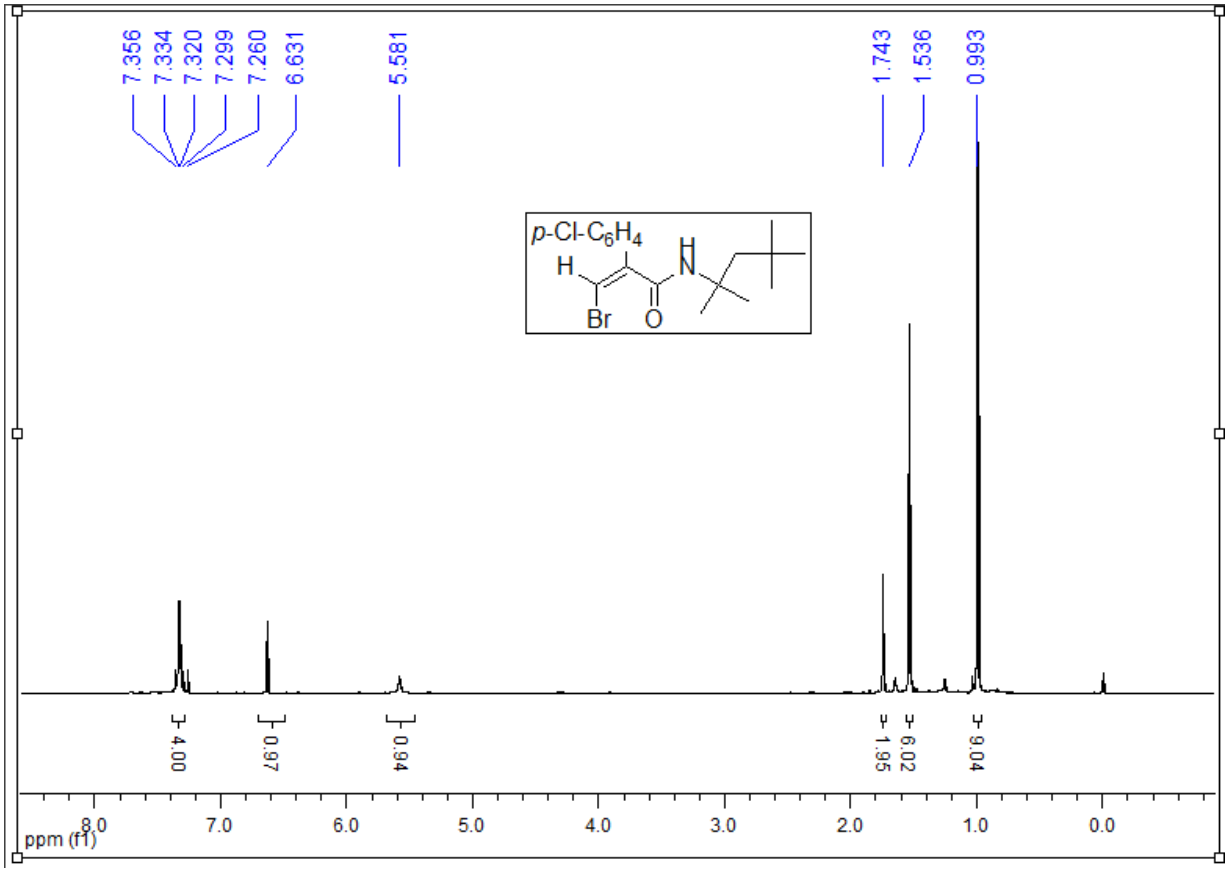


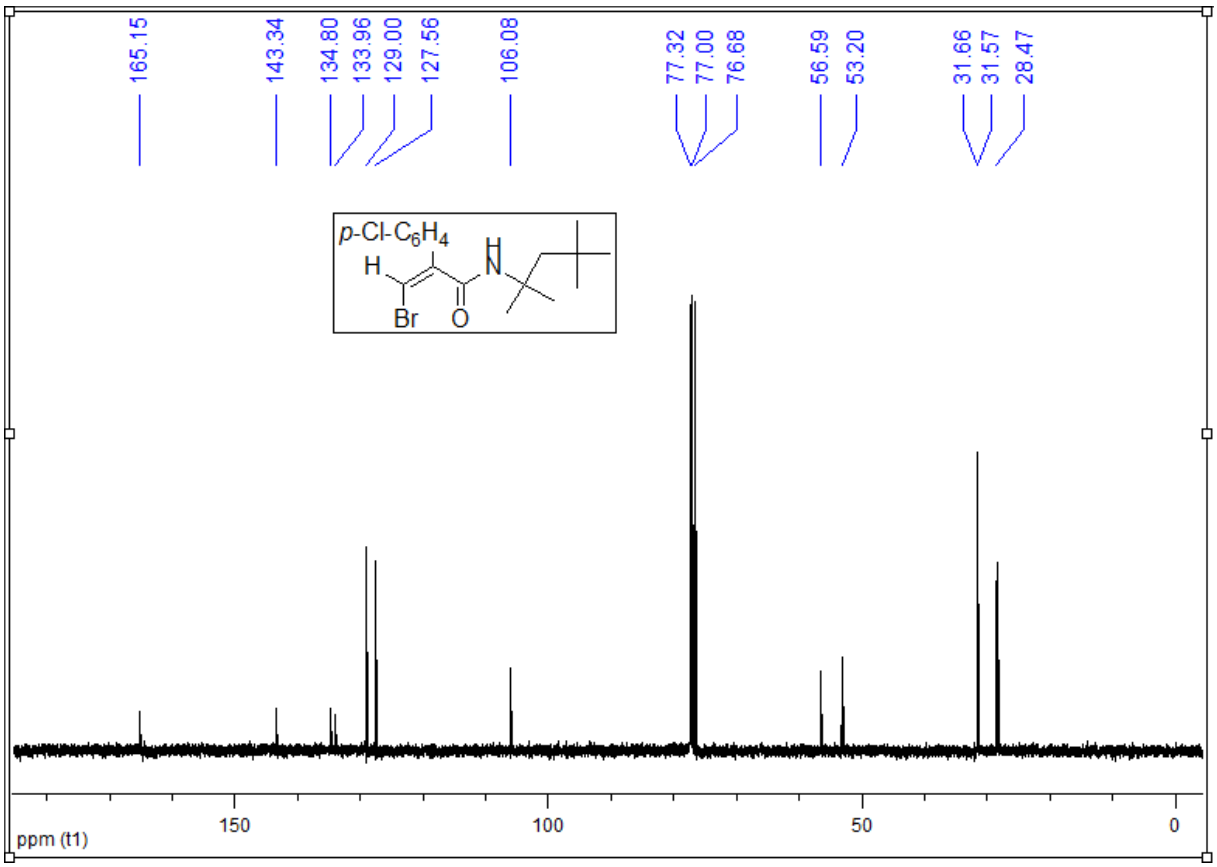
(*Z*)-*N*-*tert*-butyl-3-bromo-2-cyclopropylacrylamide





(*Z*)-3-bromo-2-(4-chlorophenyl)-*N*-(2,4,4-trimethylpentan-2-yl)acrylamide





(*Z*)-3-bromo-2-(4-chlorophenyl)-*N*-cyclohexylacrylamide