Yb(III) catalysed *syn*-Thioallylation of Ynamides

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SUPPORTING INFORMATION

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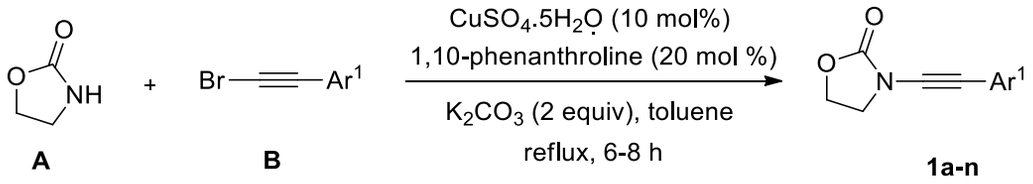
General Experimental

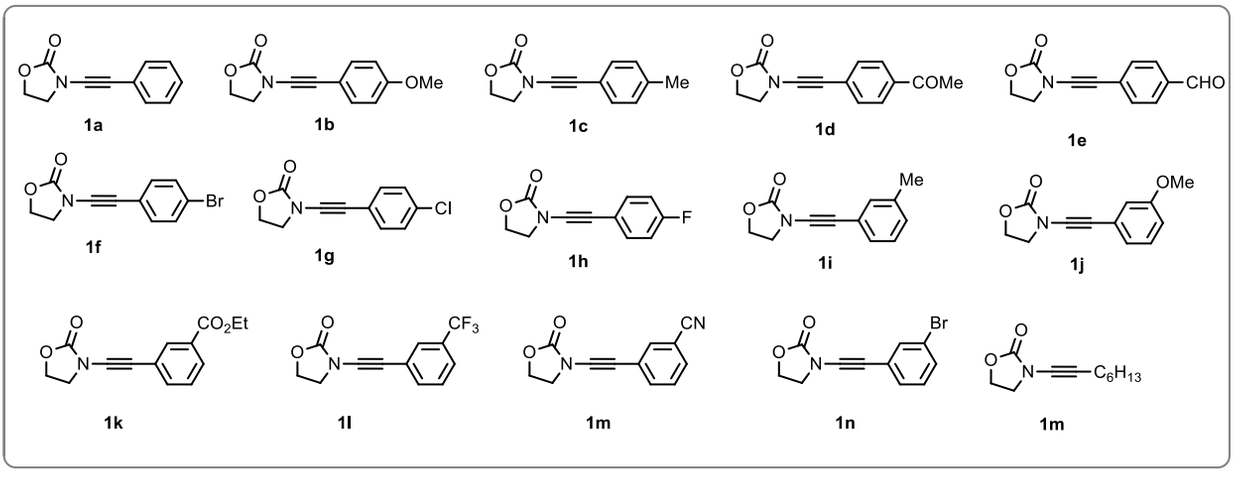
All the reactions were performed in an oven-dried Schlenk flask. Commercial grade solvents were distilled prior to use. Column chromatography was performed using silica gel (100−200 Mesh) eluting with hexanes and ethyl acetate mixture. Thin layer chromatography (TLC) was performed on silica gel GF254 plates. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over I_2 chamber. Proton, carbon and fluorine nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C NMR and ^{19}F NMR) were recorded based on 400 MHz (^{1}H NMR, 400 MHz; ^{13}C NMR, 101 MHz; ^{19}F NMR, 376 MHz) spectrometer and 500 MHz (1H NMR, 500 MHz; ^{13}C NMR, 126 MHz; ^{19}F NMR, 470 MHz) spectrometer having solvent resonance as internal standard (^{1}H NMR, $CHCl_3$ at 7.26 ppm; ^{13}C NMR, $CDCl_3$ at 77.0 ppm). Few cases tetramethylsilane (TMS) at 0.00 ppm was used as reference standard. Data for ^{1}H NMR are reported as follows: chemical shift (ppm), the abbreviations were used to explain the multiplicities: s = singlet; d = doublet; t = triplet; q = quartet; dd = doublet of doublet; m = multiplet; br = broad; coupling constants *J*, in (Hz). ^{13}C NMR, ^{19}F NMR were reported in terms of chemical shift (ppm). IR spectra were recorded on FT/IR spectrometer and reported in cm^{-1}. High resolution mass spectra (HRMS) were obtained in ESI mode. Melting points were determined by electro-thermal heating and are uncorrected. LC-MS spectra were obtained with a Shimadzu 2010A (EI-positive/ negative mode) with ionization voltage of 70ev; data was reported in the form of m/z (intensity relative to base peak = 100). X−ray data was collected at 298 K on a Bruker D8 Quest CCD diffractometer using Mo-Kα radiation (0.71073 Å).

Materials: Unless otherwise noted, all the reagents and intermediates were obtained commercially and used without purification. 1,4-dioxane, dichloromethane (CH_2Cl_2; DCM), toluene, acetonitrile (CH_3CN), 1,2-dichloroethane (1,2-DCE), CH_3NO_2 and acetone were distilled over CaH_2. THF was freshly distilled over sodium/benzophenone ketyl under dry nitrogen. $Ph_3PAuNTf_2$, $In(OTf)_2$, $Pd(OAc)_2$, $PdCl_2(PPh_3)_2$, $Sc(OTf)_3$, $Fe(OTf)_3$ and $Cu(OTf)_2$ were purchased from Sigma Aldrich Ltd. and used as received. Silver salts such as AgOTf was purchased from Aldrich Ltd. and used as received. Thiols, Allyl methyl sulfide, diallyl sulfide and phenyl acetylene were purchased and used as received. $CuSO_4 \cdot 5H_2O$, 1.10-phenanthroline, K_2CO_3, were directly purchased. The aryl iodides were purchased from Aldrich and used. Analytical and spectral data of all those known compounds are exactly matching with the reported values.

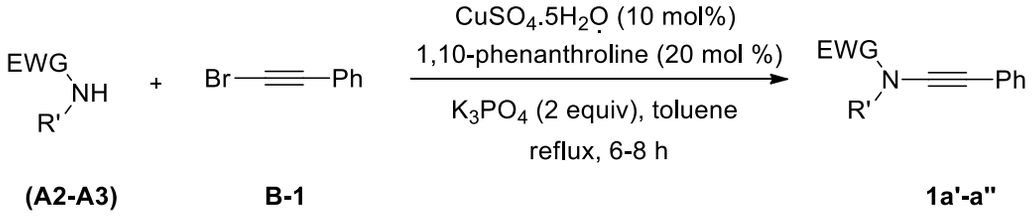
General procedure for the synthesis of ynamides 1 (GP-1)[1-4]



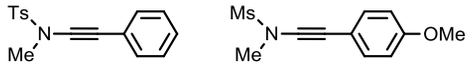
A mixture of 2-oxazolidinone (**A**) (1.0 mmol), $CuSO_4 \cdot 5H_2O$ (0.10 mmol, 25mg), 1,10-phenanthroline (0.20 mmol, 36 mg), and K_3CO_3 (2.0 mmol, 425 mg) in dry toluene (5.0 mL) was taken in a Schlenk tube. Subsequently, 1-bromo-2-arylacetylene(**B**) was introduced, and the resulting mixture was heated to 80 °C under a nitrogen atmosphere for 24 h. The progress of the reaction was monitored by TLC. Upon completion, the reaction mixture was cooled to room temperature and diluted with dichloromethane (10 mL). The crude mixture was filtered through a small pad of Celite and concentrated under reduced pressure. The crude residue was purified using column chromatography on silica gel to provide **1a-n**. Analytical and spectral data of all the known compounds **1a-n** are exactly matching with the reported values.



General procedure for the synthesis of ynamides 1 (GP-2)[5-6]

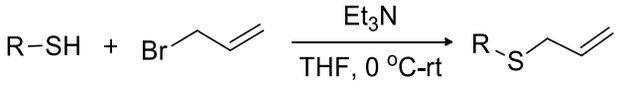


A mixture of amide (**A2-A3**) (1.0 mmol), $CuSO_4 \cdot 5H_2O$ (0.10 mmol, 25mg), 1,10-phenanthroline (0.20 mmol, 36 mg), and K_3PO_4 (2.0 mmol, 425 mg) in dry toluene (5.0 mL) was taken in a Schlenk tube. Subsequently, 1-bromo-2-phenylacetylene (**B-1**) was introduced, and the resulting mixture was heated to 80 °C under a nitrogen atmosphere for 24 h. The progress of the reaction was monitored by TLC. Upon completion, the reaction mixture was cooled to room temperature and diluted with dichloromethane (10 mL). The crude mixture was filtered through a small pad of Celite and concentrated under reduced pressure. The crude residue was purified using column chromatography on silica gel to provide **1a'-a"**. Analytical and spectral data of all the known compounds **1a'-a"** are exactly matching with the reported values.



1a' **1a"**

General procedure for the synthesis of allyl sulfides (GP-3)[7-8]



2' **2"** **2**

To a cooled solution of thiol (**2'**) (0.6 mmol) and triethylamine (1.5 mmol) in dry THF (5.0 mL) was added allyl bromide (**2"**) (123μL, 1.5 mmol) and the reaction mixture was stirred for 30 min at room temperature. Solvent was removed in vacuo. The compounds were purified by silica gel column chromatography eluting with hexane-ethyl acetate solvent to give allyl sulfides (**2a-w**), **2'a** and **6**. Analytical and spectral data of all the known compounds **2a-w, 2'a, 2x, 2y** and **2z** are exactly matching with the reported values.

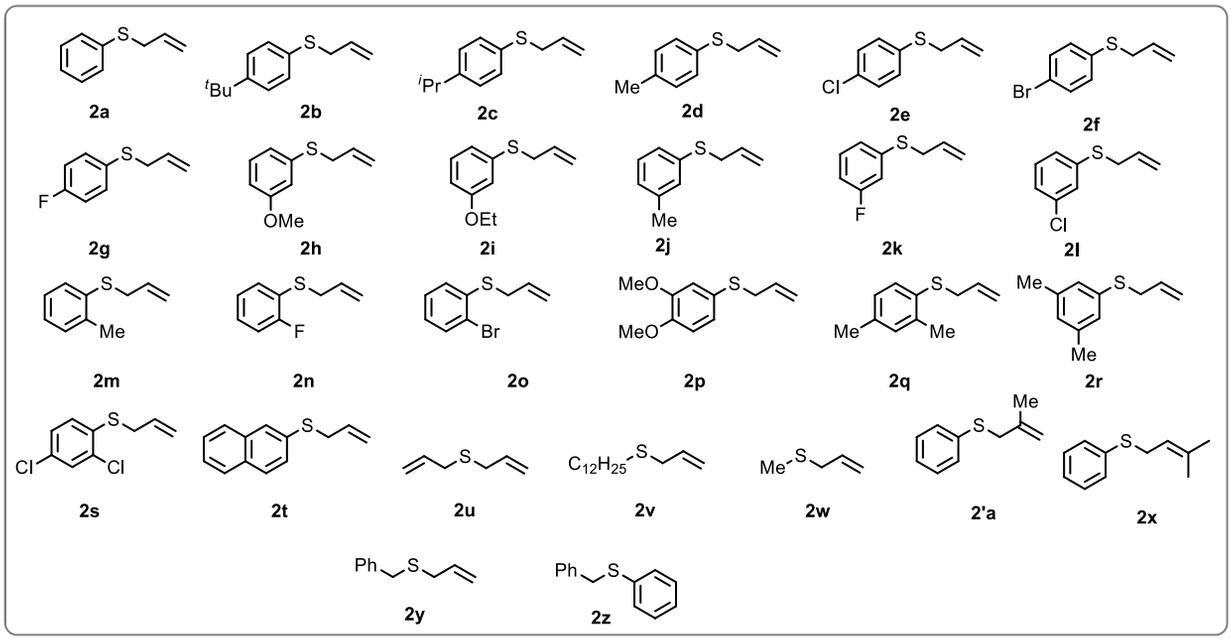
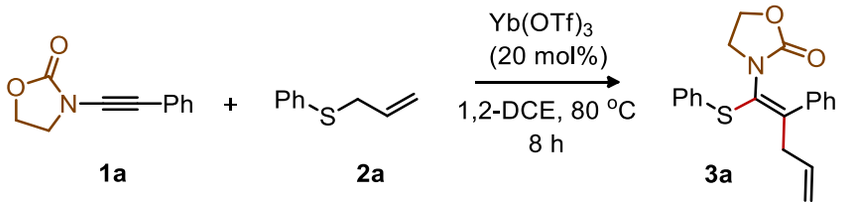


Table S1. Optimization of the thioallylation of ynamides

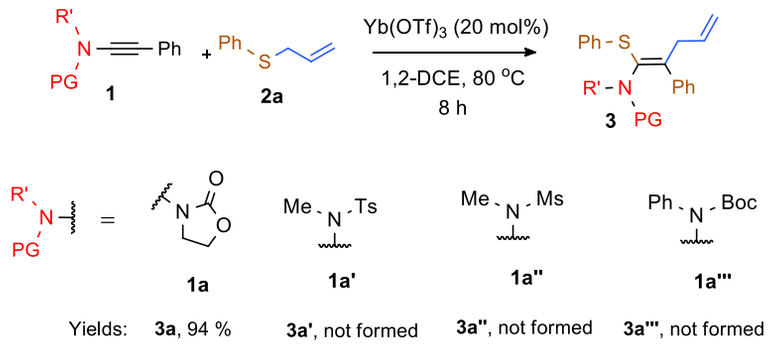


Entry	Catalyst	Catalyst (x mol%)	Solvent	**3a**[a]
1	$Yb(OTf)_3$	20 mol%	1,2-DCE	94
2	$Sc(OTf)_3$	20 mol%	1,2-DCE	72
3	$Fe(OTf)_3$	20 mol%	1,2-DCE	45
4	$Cu(OTf)_3$	20 mol%	1,2-DCE	10
5	$In(OTf)_3$	20 mol%	1,2-DCE	64
6	AgOTf	20 mol%	1,2-DCE	ND
7	$Ph_3PAuNTf_2$	5 mol%	1,2-DCE	ND
8	Ph_2NTf_2	10 mol%	1,2-DCE	ND
9	TfOH	10 mol%	1,2-DCE	ND
10	$Yb(OTf)_3$	20 mol%	THF	41
11	$Yb(OTf)_3$	20 mol%	CH_3NO_2	34
12	$Yb(OTf)_3$	20 mol%	toluene	20

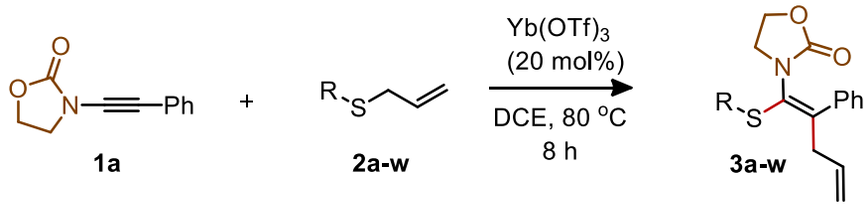
13	$Yb(OTf)_3$	20 mol%	EtOAc	15
14	$Yb(OTf)_3$	20 mol%	acetone	24
15	$Yb(OTf)_3$	20 mol%	DCM	63
16	$Yb(OTf)_3$	20 mol%	$CHCl_3$	52
17[b]	$Yb(OTf)_3$	20 mol%	1,2-DCE	ND
18[c]	$Yb(OTf)_3$	20 mol%	1,2-DCE	85

[a]Isolated yield. [b]Reaction carried out at room temperature. [c]Reaction carried out at 100 °C; ND = not detected.

Table S2. Screening of N-protecting groups



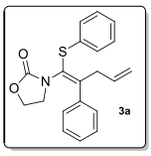
General procedure for the Yb-catalyzed thioallylation of ynamides (GP–4):



A solution of **1a** (0.6 mmol) and $Yb(OTf)_3$ (74 mg, 0.12 mmol) in 1,2-DCE (4.0 mL) was placed in a screw capped tube under an argon atmosphere. Allyl sulfide (**2a-w**) (0.9 mmol) was next introduced. The reaction mixture was stirred for the specified time shown in the respective schemes at 80 °C. The progress of the reaction was periodically monitored by TLC. After 8 h, the reaction mixture was diluted with dichloromethane (10 mL), and filtered over a small pad of Celite. The solvent was evaporated under the reduced pressure and the residue was purified by flash

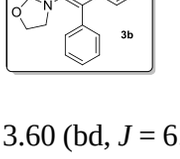
chromatography on silica gel eluting with hexane/EtOAc mixture to afford the expected product **3a-w**.

(*E*)-3-(2-Phenyl-1-(phenylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (3a): Following the general procedure GP–4, compound **3a** (190 mg) was obtained in 94% yield as yellow solid; mp = 120–122 °C; R_f = 0.32 (5:1 hexane/EtOAc); [Silica, UV and I_2]; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.49 (d, J = 8.0 Hz, 2H), 7.38–7.22 (m, 8H), 5.81–5.69 (m, 1H), 5.11 (dt, J = 16.8, 1.6 Hz, 1H), 5.03 (d, J = 9.6 Hz, 1H), 3.79 (t, J = 7.6 Hz, 2H), 3.61 (bd, J = 6.0 Hz, 2H), 3.35 (t, J = 8.0 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.2, 144.2, 139.8, 133.9, 131.9, 131.4, 129.2, 128.4, 127.8, 127.7, 127.4, 126.8, 116.9, 61.8, 46.1, 40.6; **IR** (Neat)ν_{max} 3056, 1752, 1477, 1395, 1218, 1036, 698 cm^{-1}; **HRMS** (ESI) for $C_{20}H_{20}NO_2S^+$ $(M+H)^+$: calcd 338.1209 found 338.1209



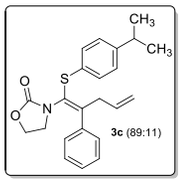
(*E*)-3-(1-((4-(*tert*-Butyl)phenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3b):

Following the general procedure GP–4, compound **3b** (198 mg) was obtained in 84% yield as a gummy brown solid; R_f = 0.40 (5:1 hexane/EtOAc); [Silica, UV and I_2];]; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.41 (d, J = 8.0 Hz, 2H), 7.37–7.22 (m, 7H), 5.81–5.69 (m, 1H), 5.09 (d, J = 16.8 Hz, 1H), 5.02 (d, J = 10 Hz, 1H), 3.74 (bt, J = 7.2 Hz, 2H), 3.60 (bd, J = 6.0 Hz, 2H), 3.31 (t, J = 7.6 Hz, 2H), 1.29 (s, 9H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.2, 151.3, 143.5, 140.0, 134.0, 131.5, 128.4, 128.0, 127.6, 127.4, 127.3, 126.2, 116.8, 61.8, 46.2, 40.5, 34.6, 31.2; **IR** (Neat)ν_{max} 2960, 1751, 1595, 1489, 1394, 1217, 1035, 700 cm^{-1}; **HRMS** (ESI) for $C_{24}H_{28}NO_2S^+$ $(M+H)^+$: calcd 394.1835 found 394.1834

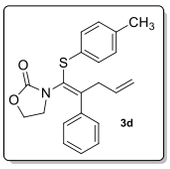


(*E*)-3-(1-((4-Isopropylphenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3c):

Following the general procedure GP–4, compound **3c** (182 mg) was obtained in 80% yield with inseparable minor isomer (89:11) as pale brown gummy liquid; R_f = 0.30 (5:1 hexane/EtOAc); [Silica, UV and I_2]; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.42 (dt, J = 9.0, 2.5 Hz, 2H), 7.36–7.29 (m, 3H), 7.27–7.24 (m, 2H), 7.21–7.17 (m, 2H), 5.80–5.70 (m, 1H), 5.11 (dq, J = 17, 1.5 Hz, 1H), 5.03 (dq, J = 10, 1.5 Hz, 1H), 3.74 (bt, J = 7.0 Hz, 2H), 3.60 (d, J = 6.5 Hz, 2H), 3.30 (t, J = 8.0 Hz, 2H), 2.93–2.83 (m, 1H), 1.23 (s, 3H), 1.22 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.2, 149.0, 143.2, 139.9, 133.9, 131.9, 128.4, 128.3, 127.5, 127.4, 127.3, 116.7, 61.8, 46.2, 40.4, 33.7, 23.8; **IR** (Neat)ν_{max} 2961, 1756, 1397, 1264, 1039, 735 cm^{-1}; **HRMS** (ESI) for $C_{23}H_{26}NO_2S+$ $(M+H)^+$: calcd 380.1679, found 380.1679.

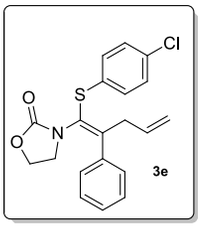


(*E*)-3-(2-Phenyl-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (3d):



Following the general procedure GP–4, compound **3d** (194 mg) was obtained in 92% yield as yellow solid; mp = 128–130°C; R_f = 0.36 (5:1 hexane/EtOAc); [Silica, UV and I_2]; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.43–7.36 (m, 2H), 7.35–7.29 (m, 2H), 7.28–7.22 (m, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 5.82–5.69 (m, 1H), 5.11 (dt, *J* = 16.8, 1.6 Hz, 1H), 5.03 (d, *J* = 10 Hz, 1H), 3.77 (t, *J* = 7.6 Hz, 2H), 3.61 (d, *J* = 6.4 Hz, 2H), 3.32 (t, *J* = 7.6 Hz, 2H), 2.33 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.2, 143.1, 139.9, 138.1, 134.0, 132.0, 129.9, 128.3, 128.0, 127.6, 127.5, 127.4, 116.7, 61.8, 46.2, 40.5, 21.1; **IR** (Neat)ν_{max} 2917, 1751, 1636, 1491, 1395, 1294, 1036 cm^{-1}; **HRMS** (ESI) for $C_{21}H_{22}NO_2S$+ $(M+H)^+$: calcd 352.1366 found 352.1366.

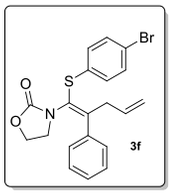
(*E*)-3-(1-((4-Chlorophenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3e):



Following the general procedure GP–4, compound **3e** (185 mg) was obtained in 83% yield as yellow solid; mp = 142–144 °C; R_f = 0.40 (5:1 hexane/EtOAc); [Silica, UV and I_2]; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.44–7.39 (m, 2H), 7.37–7.21 (m, 7H), 5.78–5.64 (m, 1H), 5.09 (dd, *J* = 17.2, 1.6 Hz, 1H), 5.03 (dd, *J* = 10.0, 1.2 Hz, 1H), 3.87 (t, *J* = 8.0 Hz, 2H), 3.59 (d, *J* = 6.4 Hz, 2H), 3.39 (t, *J* = 8.0 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.1, 145.2, 139.6, 133.8, 133.7, 132.3, 130.6, 129.3, 128.4, 127.8, 127.2, 126.1, 117.0, 61.8, 46.0, 40.6; **IR** (Neat)ν_{max} 2977, 1749, 1636, 1475, 1393, 1090, 700 cm^{-1}; **HRMS** (ESI) $C_{20}H_{19}ClNO_2S^+$ $(M+H)^+$: calcd 372.0820 found 372.0822.

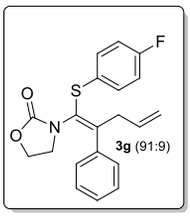
(*E*)-3-(1-((4-Bromophenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3f):

Following the general procedure GP–4, compound **3f** (209 mg) was obtained in 84% yield as yellow



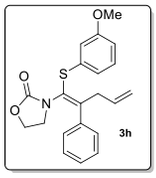
gummy solid; R_f = 0.42 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.44 (d, *J* = 8.5 Hz, 2H), 7.37–7.22 (m, 7H), 5.77–5.68 (m, 1H), 5.08 (dd, *J* = 17.5, 1.5 Hz, 1H), 5.03 (bd, *J* = 10.0, 1H), 3.87 (t, *J* = 7.5 Hz, 2H), 3.59 (d, *J* = 6.5 Hz, 2H), 3.40 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 145.7, 139.6, 133.7, 132.5, 132.3, 131.4, 128.4, 127.8, 127.3, 126.0, 121.8, 117.0, 61.8, 46.1, 40.6; IR (Neat)ν_{max} 2917, 1752, 1472, 1394, 1250, 1007, 699 cm^{-1}; HRMS (ESI) for $C_{20}H_{19}BrNO_2S^+$ $(M+H)^+$: calcd 416.0314 found 416.0317

(*E*)-3-(1-((4-Fluorophenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3g):



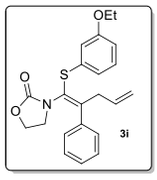
Following the general procedure GP–4, compound **3g** (181 mg) was obtained in 85% yield with inseparable minor isomer (91:9) as yellow gummy solid; R_f = 0.39 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.52–7.46 (m, 2H), 7.36–7.29 (m, 2H), 7.28–7.21 (m, 3H), 7.06–7.00 (m, 2H), 5.80–5.68 (m, 1H), 5.10 (dq, *J* = 17.0, 1.5 Hz, 1H), 5.03 (dq, *J* = 11.0, 1.0 Hz, 1H), 3.81 (t, *J* = 8.0 Hz, 2H), 3.59 (d, *J* = 6.5 Hz, 2H), 3.32 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.6 (d, *J* = 250 Hz, 1C), 155.2, 143.9, 139.6, 134.0 (d, *J* = 7.6 Hz, 1C), 133.7, 128.4, 127.7, 127.3, 127.0, 126.8 (d, *J* = 2.5 Hz, 1C), 116.9, 116.3 (d, *J* = 22 Hz, 1C), 61.8, 46.1, 40.4; ^{19}F NMR (376 MHz) δ −112.9; IR (Neat)ν_{max} 2921, 1754, 1588, 1489, 1396, 1223, 1036, 833 cm^{-1}; HRMS (ESI) for $C_{20}H_{19}FNO_2S^+$ $(M+H)^+$: calcd 356.1115 found 356.1115

(*E*)-3-(1-((3-Methoxyphenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3h):



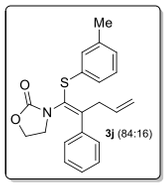
Following the general procedure GP–4, compound **3h** (181 mg) was obtained in 82% yield as yellow gummy solid; R_f = 0.35 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35–7.30 (m, 2H), 7.28–7.19 (m, 5H) (1H from $CDCl_3$) 7.06–7.00 (m, 2H), 6.82–6.78 (m, 1H), 5.80–5.70 (m, 1H), 5.11 (dq, *J* = 17.0, 1.5 Hz, 1H), 5.04 (dq, *J* = 10.0, 1.5 Hz, 1H), 3.83 (t, *J* = 8.0 Hz, 2H), 3.79 (s, 3H), 3.60 (d, *J* = 6.5 Hz, 2H), 3.41 (bt, *J* = 8.0 Hz, 2H),; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 155.1, 144.7, 139.8, 133.9, 133.3, 129.9, 128.3, 127.6, 127.3, 126.4, 122.8, 116.8, 115.4 114.2, 61.8, 55.4, 46.1, 40.5; IR (Neat)ν_{max} 2910, 1754, 1588, 1477, 1395, 1248, 1037, 700 cm^{-1}; HRMS (ESI) for $C_{21}H_{21}NNaO_3S+$ $(M+Na)^+$: calcd 390.1134 found 390.1134

(*E*)-3-(1-((3-Ethoxyphenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3i):



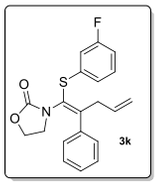
Following the general procedure GP–4, compound **3i** (146 mg) was obtained in 64% yield as yellow gummy solid; R_f = 0.30 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35–7.30 (m, 2H), 7.28–7.23 (m, 3H), 7.21 (t, *J* = 8.0 Hz, 1H), 7.05–6.99 (m, 2H), 6.82–6.78 (m, 1H), 5.79–5.70 (m, 1H), 5.11 (dq, *J* = 17.0, 1.5 Hz, 1H), 5.03 (dq, *J* = 10.0, 1.0 Hz, 1H), 4.01 (q, *J* = 7.0 Hz, 2H), 3.82 (t, *J* = 7.5 Hz, 2H), 3.60 (d, *J* = 6.0 Hz, 2H), 3.39 (t, *J* = 8.0 Hz, 2H), 1.39 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.4, 155.1, 144.5, 139.9, 133.9, 133.2, 129.9, 128.3, 127.6, 127.3, 126.6, 123.0, 116.8, 116.2 114.8, 63.6, 61.8, 46.1, 40.5, 14.7; IR (Neat)ν_{max} 2910, 1754, 1588, 1477, 1395, 1248, 1037, 700 cm^{-1}; HRMS (ESI) for $C_{22}H_{24}NO_3S+$ $(M+H)^+$: calcd 382.1477 found 382.1475

(*E*)-3-(2-Phenyl-1-(*m*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (3j):



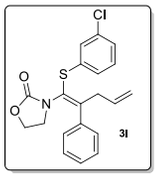
Following the general procedure GP–4, compound **3j** (169 mg) was obtained in 80% yield with inseparable minor isomer (84:16) as yellow gummy solid; R_f = 0.41 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.35–7.24 (m, 6H), 7.20 (t, *J* = 8.0 Hz, 1H), 7.07 (d, *J* = 7.5 Hz, 1H), 5.80–5.70 (m, 1H), 5.10 (dq, *J* = 17.0, 1.5 Hz, 1H), 5.03 (dq, *J* = 10.0, 1.5 Hz, 1H), 3.79 (t, *J* = 8.0 Hz, 2H), 3.61 (d, *J* = 6.0 Hz, 2H), 3.35 (br t, *J* = 7.5 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 144.0, 139.9, 139.1, 134.0, 132.0, 131.6, 128.9, 128.5, 128.3, 127.6, 127.4, 126.9, 116.8, 61.8, 46.1, 40.5, 21.2; IR (Neat)ν_{max} 2916, 1751, 1591, 1475, 1393, 1035, 694 cm^{-1}; HRMS (ESI) for $C_{21}H_{22}NO_2S^+$ $(M+H)^+$: calcd 352.1366 found 352.1365

(*E*)-3-(1-((3-Fluorophenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3k):



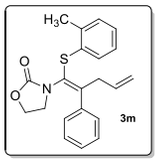
Following the general procedure GP–4, compound **3k** (173 mg) was obtained in 81% yield as yellow gummy solid; R_f = 0.40 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38–7.22 (m, 7H), 7.19 (dt, *J* = 8.8, 2.0 Hz, 1H), 6.98–6.92 (m, 1H), 5.78–5.65 (m, 1H), 5.08 (dd, *J* = 16.8, 1.6 Hz, 1H), 5.03 (dd, *J* = 12.0, 1.2 Hz, 1H), 3.89 (t, *J* = 8.0 Hz, 2H), 3.60 (d, *J* = 6.4 Hz, 2H), 3.43 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.7 (d, *J* = 251 Hz, 1C), 155.1, 146.4, 139.5, 134.6 (d, *J* = 7.1 Hz, 1C), 133.7, 130.5 (d, *J* = 9.1 Hz, 1C), 128.4, 127.8, 127.3, 126.2 (d, *J* = 3.0 Hz, 1C), 125.6, 117.2 (d, *J* = 24 Hz, 1C), 117.0, 114.5 (d, *J* = 21.2 Hz, 1C), 61.8, 46.1, 40.6; ^{19}F NMR (376 MHz) δ −111.2; IR (Neat)ν_{max} 2911, 1750, 1596, 1474, 1395, 1215, 1116, 877 cm^{-1}; HRMS (ESI) for $C_{20}H_{19}FNO_2S^+$ $(M+H)^+$: calcd 356.1115 found 356.1116.

(*E*)-3-(1-((3-Chlorophenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3l):



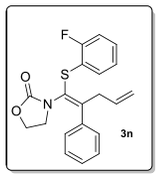
Following the general procedure GP–4, compound **3l** (174 mg) was obtained in 78% yield as yellow solid; mp = 154–156 °C; R_f = 0.43 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47–7.45 (m, 1H), 7.39–7.31 (m, 4H), 7.29–7.23 (m, 4H), 5.78–5.66 (m, 1H), 5.09 (dq, *J* = 17.2, 1.6 Hz, 1H), 5.03 (dq, *J* = 10.0, 1.2 Hz, 1H), 3.88 (t, *J* = 8.0 Hz, 2H), 3.59 (dt, *J* = 6.4, 1.6 Hz, 2H), 3.40 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2, 146.5, 139.5, 134.8, 134.5, 133.7, 130.3, 130.2, 128.9, 128.5, 127.9, 127.7, 127.3, 125.8, 117.1, 61.8, 46.2, 40.7; IR (Neat)ν_{max} 2917, 1755, 1574, 1396, 1219, 1036, 777 cm^{-1}; HRMS (ESI) for $C_{20}H_{19}ClNO_2S^+$ $(M+H)^+$: calcd 372.0820 found 372.0822

(*E*)-3-(2-Phenyl-1-(*o*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (3m):



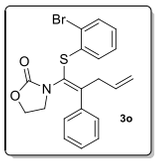
Following the general procedure GP–4, compound **3m** (200 mg) was obtained in 95% yield(with inseparable minor isomer) as pale yellow gummy liquid; R_f = 0.27 (9:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52–7.48 (m, 1H), 7.36–7.30 (m, 2H), 7.28–7.23 (m, 3H), 7.22–7.19 (m, 2H), 7.19–7.12 (m, 2H), 5.82–5.69 (m, 1H), 5.10 (dd, *J* = 16.8, 1.6 Hz, 1H), 5.03 (dd, *J* = 10.0, 1.6 Hz, 1H), 3.75 (t, *J* = 7.6 Hz, 2H), 3.63 (d, *J* = 6.8 Hz, 2H), 3.24 (t, *J* = 8.0 Hz, 2H), 2.50 (s, 3H) (1H from CDCl3); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2, 144.4, 139.8, 139.7, 134.0, 132.7, 131.0, 130.6, 128.4, 128.2, 127.7, 127.4, 126.7, 117.0, 61.9, 46.2, 40.5, 20.6; IR (Neat)ν_{max} 2974, 1749, 1392, 1249, 1216, 1035, 748; HRMS (ESI) for $C_{21}H_{22}NO_2S+$ $(M+H)^+$: calcd 352.1366, found 352.1376.

(*E*)-3-(1-((2-Fluorophenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3n):



Following the general procedure GP–4, compound **3n** (147 mg) was obtained in 69% yield (with inseparable minor isomer) as yellow gummy solid; R_f = 0.37 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (td, 7.6, 1.6 Hz 1H), 7.35–7.21 (m, 6H), 7.16–7.05 (m, 2H), 5.80–5.68 (m, 1H), 5.10 (dq, *J* = 17.2, 1.6 Hz, 1H), 5.03 (dq, *J* = 10.0, 1.6 Hz, 1H), 3.83 (t, *J* = 8.0 Hz, 2H), 3.63 (dt, *J* = 6.4, 1.2 Hz, 2H), 3.36 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.6 (d, *J* = 248 Hz, 1C), 155.1, 145.5, 139.6, 134.8, 133.7, 130.3 (d, *J* = 8.1 Hz, 1C), 128.4, 128.1, 127.7, 127.3, 125.8, 124.9 (d, *J* = 4.0 Hz, 1C), 119.0 (d, *J* = 17.2 Hz, 1C), 117.0, 115.7 (d, *J* = 22.2 Hz, 1C), 61.9, 46.0, 40.5; ^{19}F NMR (376 MHz) δ −108.9; IR (Neat)ν_{max} 2919, 2125, 1755, 1473, 1396, 1222, 916, 757 cm^{-1}; HRMS (ESI) for $C_{20}H_{19}FNO_2S+$ $(M+H)^+$: calcd 356.1115 found 356.1116.

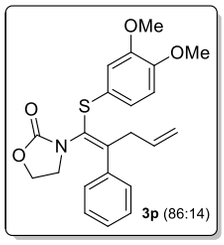
(*E*)-3-(1-((2-Bromophenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3o):



Following the general procedure GP–4, compound **3o** (112 mg) was obtained in 45% yield as pale brown gummy liquid; R_f = 0.25 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (600 MHz, DMSO-d_6): δ 7.64 (d, *J* = 7.2 Hz, 1H), 7.40 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.34-7.28 (m, 5H), 7.27-7.20 (m, 1H), 7.17 (td, *J* = 8.4, 1.2 Hz, 1H), 5.67–5.58 (m, 1H), 5.01 (dd, *J* = 17.4, 1.2 Hz, 1H), 4.95 (dd, *J* = 10.2, 1.2 Hz, 1H), 3.92 (t, *J* = 7.2 Hz, 2H), 3.53 (d, *J* = 6.0 Hz, 2H), 3.49 (t, *J* = 8.4 Hz, 2H); ^{13}C NMR (151 MHz, DMSO-d_6) δ 155.0, 147.4, 139.7, 134.7, 134.5, 133.7, 131.1, 129.3, 128.9, 128.8, 128.3, 127.9, 125.1, 123.0, 117.5, 62.4, 46.1, 40.6; IR

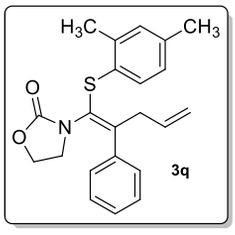
(Neat)ν_{max} 2975, 1748, 1477, 1391, 1216, 1018, 747; HRMS (ESI) for $C_{20}H_{19}BrNO_2S$+ $(M+H)^+$: calcd 416.0314, found 416.0320.

(*E*)-3-(1-((3,4-Dimethoxyphenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3p):



Following the general procedure GP–4, compound **3p** (207 mg) was obtained in 87% yield with inseparable minor isomer (86:14) as pale yellow gummy solid; R_f = 0.30 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.33–7.28 (m, 2H), 7.25–7.21 (m, 3H), 7.06 (dd, J = 8.3, 2.0 Hz, 1H), 7.02 (d, J = 1.9 Hz, 1H), 6.80 (d, J = 8.3 Hz, 1H), 5.81–5.71 (m, 1H), 5.12 (dd, J = 17.1, 1.4 Hz, 1H), 5.04 (dd, J = 10.1, 1.1 Hz, 1H), 3.86 (s, 3H), 3.85 (s, 3H), 3.80–3.72 (m, 2H), 3.58 (d, J = 6.1 Hz, 2H), 3.33–3.25 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 149.3, 142.2, 140.0, 133.9, 128.5, 128.3, 128.0, 127.8, 127.5, 127.3, 125.0, 116.7, 115.6, 111.4, 61.8, 56.1, 55.9, 46.1, 40.3; IR (Neat)ν_{max} 2915, 1753, 1503 1396, 1254, 1023, 701 cm^{-1}; HRMS (ESI) for $C_{22}H_{24}NO_4S^+$ $(M+H)^+$: calcd 398.1421 found 398.1421.

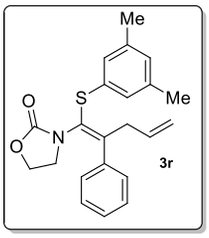
(*E*)-3-(1-((2,4-Dimethylphenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3q):



Following the general procedure GP–4, compound **3q** (195 mg) was obtained in 89% yield as yellow solid; R_f = 0.42 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 (d, J = 8.0 Hz, 1H), 7.36–7.29 (m, 3H), 7.28–7.21 (m, 2H), 7.04 (br s, 1H), 6.97 (d, J = 8.0 Hz, 1H), 5.82–5.69 (m, 1H), 5.10 (d, J = 16.8 Hz, 1H), 5.03 (d, J = 10.0 Hz, 1H), 3.74 (t, J = 7.6 Hz, 2H), 3.63 (d, J = 6.4 Hz, 2H), 3.21 (t, J = 8.0 Hz, 2H), 2.46 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.1, 143.2, 140.1, 139.9, 138.5, 134.0, 133.4, 131.4, 128.3, 128.0, 127.5, 127.4, 127.2, 127.0, 116.8, 61.8, 46.2, 40.4, 21.0, 20.5; IR (Neat)ν_{max} 2918, 1755, 1600, 1477, 1396, 1218, 1036, 701 cm^{-1}; HRMS (ESI) for $C_{22}H_{24}NO_2S^+$ $(M+H)^+$: calcd 366.1522 found 366.1522.

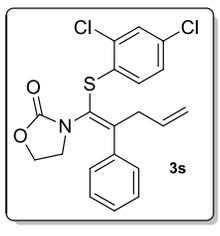
(*Z*)-3-(1-(3,5-Dimethylphenyl)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3r):

Following the general procedure GP–4, compound **3r** (213 mg) was obtained in 97% yield as pale yellow semi solid; R_f = 0.30 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36–7.29 (m, 3H), 7.28-7.24 (m, 2H), 7.10 (br s, 2H), 6.89 (br s, 1H), 5.82–5.68 (m, 1H), 5.09 (dd, J = 17.2, 1.6 Hz, 1H), 5.03 (dd, J = 10.0, 1.6 Hz, 1H), 3.80 (t, J = 7.6 Hz, 2H), 3.61 (d, J = 6.4 Hz, 2H), 3.35 (t, J = 7.6 Hz, 2H), 2.28 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2, 143.8, 140.0, 138.9, 134.1, 131.4, 129.5, 128.9, 128.4, 127.6, 127.5, 116.8, 61.8, 46.2, 40.6, 21.2; IR (Neat)ν_{max} 2912, 1746, 1635, 1475, 1394, 1210, 842; HRMS (ESI) for $C_{22}H_{24}NO_2S^+$ $(M+H)^+$: calcd 366.1522, found 366.1528.



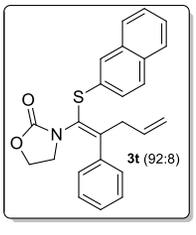
(*E*)-3-(1-((2,4-Dichlorophenyl)thio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3s):

Following the general procedure GP–4, compound **3s** (199 mg) was obtained in 82% yield as white solid; mp = 162–164 °C; R_f = 0.32 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.53 (d, J = 8.5 Hz, 1H), 7.41 (d, J = 2.5 Hz, 1H), 7.35 (t, J = 7.2 Hz, 2H), 7.31–7.20 (m, 4H), 5.79–5.66 (m, 1H), 5.08 (dd, J = 17.1 1.5 Hz, 1H), 5.02 (dd, J = 10.1, 1.5 Hz, 1H), 3.94 (t, J = 7.9 Hz, 2H), 3.61 (d, J = 6.5 Hz, 2H), 3.46 (t, J = 7.9 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 148.0, 139.3, 134.7, 133.8, 133.6, 133.0, 130.6, 129.6, 128.5, 128.0, 127.9, 127.2, 124.5, 117.2, 61.8, 46.0, 40.7; IR (Neat)ν_{max} 2961, 1740, 1475, 1395, 1247, 805; HRMS (ESI) for $C_{20}H_{18}Cl_2NO_2S^+$ $(M+H)^+$: calcd 406.0430, found 406.0430.

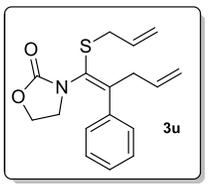


(*E*)-3-(1-(Naphthalen-2-ylthio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3t):

Following the general procedure GP–4, compound **3t** (177 mg) was obtained in 76% yield with inseparable minor isomer (92:8) as pale yellow solid; mp = 154–157 °C; R_f = 0.35 (5:1 hexane/EtOAc); [Silica, UV and I_2]; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.96 (br s, 1H), 7.83–7.76 (m, 3H), 7.54 (dd, J = 8.5, 1.5 Hz, 1H), 7.51–7.44 (m, 2H), 7.36–7.24 (m, 5H), 5.84–5.73 (m, 1H), 5.13 (dd, J = 17.5, 2.0 Hz, 1H), 5.05 (dd, J = 10.0, 1.0 Hz, 1H), 3.74–3.64 (m, 4H), 3.35 (t, J = 8.0 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.1, 144.8, 139.9, 133.9, 133.6, 132.5, 130.1, 129.5, 128.8, 128.4, 127.71, 127.66, 127.5, 127.4, 126.8, 126.7, 126.4, 116.9, 61.7, 46.1, 40.6; **IR** (Neat)ν_{max} 2923, 1756, 1396, 1264, 1039, 734, 701; **HRMS** (ESI) for $C_{24}H_{21}NNaO_2S^+$ $(M+Na)^+$: calcd 410.1191, found 410.1185.

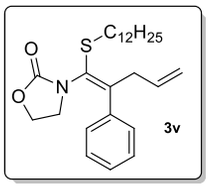


(*E*)-3-(1-(Allylthio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3u):



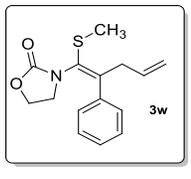
Following the general procedure GP–4, compound **3u** (159 mg) was obtained in 88% yield as yellow gummy solid; R_f = 0.30 (5:1 hexane/EtOAc); [Silica, UV and I_2]; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.34–7.14 (m, 5H), 5.99–5.87 (m, 1H), 5.78–5.63 (m, 1H), 5.24 (dd, *J* = 16.8, 1.2 Hz, 1H), 5.12 (dd, *J* = 10.4, 1.2 Hz, 1H), 5.08–4.96 (m, 2H) 4.09 (t, *J* = 8.0 Hz, 2H), 3.62–3.47 (m, 4H), 3.37–3.31 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.9, 146.3, 139.6, 134.0, 133.9, 128.6, 128.2, 127.5, 127.1, 117.6, 116.7, 61.9, 45.9, 40.6, 35.4; **IR** (Neat)ν_{max} 2916, 1751, 1591, 1475, 1393, 1216, 694 cm^{-1}; **HRMS** (ESI) for $C_{17}H_{20}NO_2S^+$ $(M+H)^+$: calcd 302.1209 found 302.1209

(*E*)-3-(1-(Dodecylthio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3v):



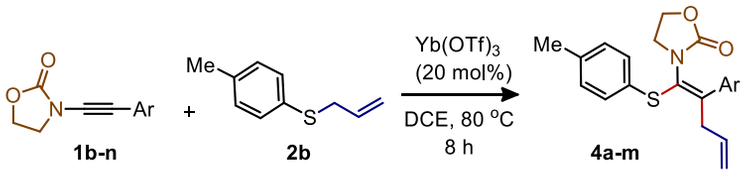
Following the general procedure GP–4, compound **3v** (221 mg) was obtained in 86% yield as yellow gummy solid; R_f = 0.32 (5:1 hexane/EtOAc); [Silica, UV and I_2]; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.33–7.28 (m, 2H), 7.26–7.21 (m, 1H), 7.20–7.17 (m, 2H), 5.75–5.65 (m, 1H), 5.04 (dd, *J* = 17.0, 1.5 Hz, 1H), 4.99 (dd, *J* = 10.0, 1.5 Hz, 1H), 4.11 (t, *J* = 8.0 Hz, 2H), 3.59 (br s, 2H), 3.50 (d, *J* = 6.5 Hz, 2H), 2.64 (t, *J* = 7.5 Hz, 2H), 1.72–1.61 (m, 3H), 1.44–1.34 (m, 2H), 1.31–1.20 (m, 15 H), 0.88 (t, *J* = 7.0 Hz, 3 H)**; ^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.9, 145.6, 139.9, 134.0, 128.6, 128.2, 127.4, 127.2, 116.6, 61.9, 46.0, 40.6, 32.2, 31.9, 29.7, 29.6, 29.58, 29.54, 29.49, 29.3, 29.1, 28.8, 22.6, 14.1; **IR** (Neat)ν_{max} 2921, 2851, 1751, 1395, 1248, 1036, 699 cm^{-1}; **HRMS** (ESI) for $C_{26}H_{40}NO_2S^+$ $(M+H)^+$: calcd 430.2774 found 430.2774

(*E*)-3-(1-(Methylthio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (3w):



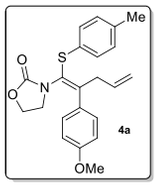
Following the general procedure GP–4, compound **3w** (149 mg) was obtained in 90% as yellow gummy solid; R_f = 0.36 (4:1 hexane/EtOAc); [Silica, UV and I_2]; **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.34–7.29 (m, 2H), 7.26–7.23 (m, 1H), 7.21–7.18 (m, 2H), 5.78–5.67 (m, 1H), 5.07 (dd, *J* = 17.0, 1.5 Hz, 1H), 5.01 (dd, *J* = 10.5, 1.5 Hz, 1H), 4.13 (t, *J* = 8.0 Hz, 2H), 3.56 (br s, 2H), 3.47 (d, *J* = 6.5 Hz, 2H), 2.23 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 156.3, 144.2, 139.8, 133.9, 128.5, 128.2, 127.5, 127.2, 116.7, 62.1, 46.0, 40.3, 14.9; **IR (Neat)ν_{max}** 2921, 2091, 1745, 1695, 1401, 1218, 1033, 757 cm^{-1}; **HRMS** (ESI) for $C_{15}H_{18}NO_2S^+$ $(M+H)^+$: calcd 276.1053 found 276.1055.

General procedure for the Yb-catalyzed thioallylation of ynamides (GP–5):



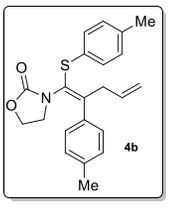
A solution of **1b-n** (0.6 mmol) and $Yb(OTf)_3$ (74 mg, 0.12 mmol) in 1,2-DCE (4.0 mL) was placed in a screw capped tube under an argon atmosphere. Allyl sulfide, **2b** (0.9 mmol) was next introduced. The reaction mixture was stirred for the specified time shown in the respective schemes at 80 °C. The progress of the reaction was periodically monitored by TLC. After 8 h, the reaction mixture was diluted with dichloromethane (10 mL), and filtered over a small pad of Celite. The solvent was evaporated under the reduced pressure and the residue was purified by flash chromatography on silica gel eluting with hexane/EtOAc mixture to afford the expected product **4a-m.**

(*E*)-3-(2-(4-Methoxyphenyl)-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (4a)



Following the general procedure GP–5, compound **4a** (151 mg) was obtained in 66% yield as yellow gummy solid; R_f = 0.35 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 8.4 Hz, 2H), 7.21–7.09 (m, 4H), 6.87–6.82 (m, 2H), 5.82–5.68 (m, 1H), 5.09 (dd, J = 16.8, 1.6 Hz, 1H), 5.02 (dd, J = 10.4, 1.6 Hz, 1H), 3.90–3.70 (m, 5H), 3.59 (d, J = 6.4 Hz, 2H), 3.32 (t, J = 8.0 Hz, 2H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.8, 155.3, 142.9, 138.0, 134.2, 132.0, 131.9, 130.4, 129.9, 128.6, 128.2, 126.8, 116.6, 113.8, 61.8, 55.1, 46.1, 40.5, 21.1; IR (Neat) ν_{max} 2918, 1753, 1636, 1597,1489, 1395, 915 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{24}NO_3S$ $(M+H)^+$: calcd. 382.1477, found 382.1483.

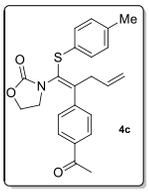
(*E*)-3-(2-(*p*-Tolyl)-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (4b):



Following the general procedure GP–5, compound **4b** (140 mg) was obtained in 64% yield as yellow gummy solid; R_f = 0.41 (5:1 hexane/EtOAc); [Silica, UV and I_2];^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, J = 8.0 Hz, 2H), 7.17–7.10 (m, 6H), 5.80–5.70 (m, 1H), 5.10 (dq, J = 17.0, 1.5 Hz, 1H), 5.03 (dd, J = 6.5, 1.5 Hz, 1H), 3.79 (t, J = 7.5 Hz, 2H), 3.60 (d, J = 6.0 Hz, 2H), 3.33 (t, J = 7.5 Hz, 2H), 2.31 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 143.3, 138.0, 137.3, 136.9, 134.1, 131.9, 130.6, 129.9, 129.1, 128.2, 127.2, 116.6, 61.8, 46.2,

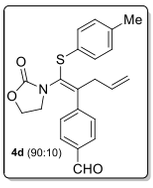
40.5, 21.2, 21.1; IR (Neat) ν_{max} 2918, 1751, 1604, 1491, 1393, 1113, 809 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{24}NO_2S$ $(M+H)^+$: calcd. 366.1528, found 366.1531.

(*E*)-3-(2-(4-Acetylphenyl)-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (4c):



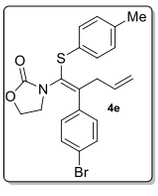
Following the general procedure GP–5, compound **4c** (104 mg) was obtained in 44% yield as light yellow solid; mp = 120–122 °C; R_f = 0.22 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90 (d, J = 8.4 Hz, 2H), 7.38–7.30 (m, 4H), 7.13 (d, J = 8.0 Hz, 2H), 5.78–5.66 (m, 1H), 5.08 (dd, J = 17.2, 1.2 Hz, 1H), 5.03 (dd, J = 10.0, 1.2 Hz, 1H), 3.79 (br t, J = 7.2 Hz, 2H), 3.61 (br d, J = 5.6 Hz, 2H), 3.42 (br t, J = 6.8 Hz, 2H), 2.57 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.5, 155.0, 145.2, 141.6, 138.3, 135.9, 133.6, 131.8, 130.0, 128.5, 128.4, 127.7, 127.4, 117.0, 61.8, 45.9, 40.2, 26.5, 21.1; IR (Neat)ν_{max} 2915, 1750, 1670, 1597, 1400, 1258, 1027, 811 cm^{-1}; HRMS (ESI) for $C_{23}H_{24}NO_3S^+$ $(M+H)^+$: calcd 394.1471 found 394.1479

(*E*)-4-(1-(2-Oxooxazolidin-3-yl)-1-(*p*-tolylthio)penta-1,4-dien-2-yl)benzaldehyde (4d)



Following the general procedure GP–5, compound **4d** (143 mg) was obtained in 63% yield with inseparable minor isomer (90:10) as yellow gummy solid; R_f = 0.40 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.97 (s, 1H), 7.84 (d, J = 8.0 Hz, 2H), 7.41 (d, J = 8.5 Hz, 2H), 7.35 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 8.0 Hz, 2H), 5.80–5.69 (m, 1H), 5.10 (dd, J = 17.0, 1.5 Hz, 1H), 5.05 (dd, J = 10.0, 1.0 Hz, 1H), 3.90–3.38 (m, 6H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.7, 155.0, 146.7, 141.5, 138.4, 135.3, 133.6, 131.9, 130.1, 129.8, 129.5, 128.3, 127.4, 117.2, 61.8, 46.0, 40.2, 21.1; IR (Neat) ν_{max} 2918, 1750, 1698, 1600, 1491, 1392, 915 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{22}NO_3S$ $(M+H)^+$: calcd. 380.1320, found 380.1318.

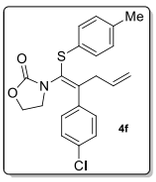
(*E*)-3-(2-(4-Bromophenyl)-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (4e):



Following the general procedure GP–5, compound **4e** (157 mg) was obtained in 61% yield as yellow gummy solid; R_f = 0.67 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46–7.41 (m, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.15–7.09 (m, 4H), 5.78–5.67 (m, 1H), 5.08 (dd, J = 17.2, 1.6 Hz, 1H), 5.03 (dd, J = 10.0, 1.2 Hz, 1H), 3.79 (br t, J = 8.0 Hz, 2H), 3.57 (d, J = 6.4 Hz, 2H), 3.36 (br t, J = 7.6 Hz, 2H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.1, 141.6, 138.9, 138.2, 133.7, 132.0, 131.5, 130.0, 129.1, 128.0, 127.6,

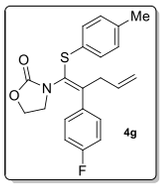
121.5, 117.0, 61.8, 46.0, 40.3, 21.1; IR (Neat)ν_{max} 2908, 1745, 1478, 1396, 1223, 1035, 807 cm^{-1}; HRMS (ESI) for $C_{21}H_{21}BrNO_2S^+$ $(M+H)^+$: calcd 430.0471 found 430.0475

(*E*)-3-(2-(4-Chlorophenyl)-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (4f):



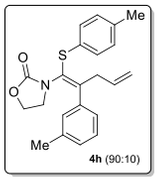
Following the general procedure GP–5, compound **4f** (171 mg) was obtained in 74% yield as yellow gummy solid; R_f = 0.43 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, J = 8.0 Hz, 2H), 7.31–7.27 (m, 2H), 7.20–7.16 (m, 2H), 7.13 (d, J = 8.0 Hz, 2H), 5.80–5.67 (m, 1H), 5.08 (dq, J = 17.0, 1.5 Hz, 1H), 5.04 (dq, J = 10.0, 1.5 Hz, 1H), 5.04 3.80 (br s, 2H), 3.57 (d, J = 5.5 Hz, 2H), 3.37 (br s, 2H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.1, 141.8, 138.5, 138.3, 133.7, 133.4, 132.0, 130.0, 128.9, 128.6, 128.1, 127.7, 117.0, 61.8, 46.0, 40.4, 21.1; IR (Neat) ν_{max} 2917, 1744, 1638, 1479, 1397, 1034, 807 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{21}ClNO_2S$ $(M+H)^+$: calcd. 386.0982, found 386.0977.

(*E*)-3-(2-(4-Fluorophenyl)-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (4g):



Following the general procedure GP–5, compound **4g** (142 mg) was obtained in 64% yield as yellow gummy solid; R_f = 0.47 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.34 (m, 2H), 7.24–7.19 (m, 2H), 7.13 (d, J = 8.0 Hz, 2H), 7.04–6.98 (m, 2H), 5.80–5.68 (m, 1H), 5.09 (dq, J = 17.2, 1.6 Hz, 1H), 5.04 (dq, J = 10.0, 1.6 Hz, 1H), 3.80 (t, J = 7.6 Hz, 2H), 3.57 (d, J = 6.4 Hz, 2H), 3.35 (t, J = 7.2 Hz, 2H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.0 (d, J = 249 Hz, 1C), 155.2, 142.1, 138.2, 135.8 (d, J = 4.0 Hz, 1C), 133.8, 132.0, 130.0, 129.2 (d, J = 8.1 Hz, 2C), 127.8, 116.9, 115.4 (d, J = 21.2 Hz, 2C), 61.8, 46.0, 40.5, 21.1; ^{19}F NMR (376 MHz) δ −114.2; IR (Neat) ν_{max} 2919, 1744, 1637, 1597, 1502, 1398, 839 cm^{-1}; **HRMS (ESI)** for $C_{21}H_{21}FNO_2S$ $(M+H)^+$: calcd. 370.1277, found 370.1283.

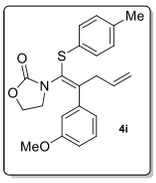
(*E*)-3-(2-(*m*-Tolyl)-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (4h):



Following the general procedure GP–5, compound **4h** (131 mg) was obtained in 60% yield with inseparable minor isomer (90:10) as yellow gummy solid; R_f = 0.41 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.36 (m, 1H), 7.24–7.16 (m, 2H), 7.15–7.00 (m, 5H), 5.82–5.70 (m, 1H), 5.11 (dq, J = 17.2, 1.6 Hz, 1H), 5.03 (dq, J = 10.4, 1.6 Hz, 1H), 3.78 (t, J = 8.0 Hz, 2H), 3.60 (d, J = 6.4 Hz, 2H), 3.33 (t, J = 7.6 Hz, 2H), 2.33 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 143.5, 139.9, 138.1, 137.9, 134.1, 132.0, 130.8, 129.9, 128.4, 128.1, 128.0, 127.3, 124.5, 116.7, 61.8, 46.2, 40.5, 21.5, 21.1; IR (Neat) ν_{max} 2917,

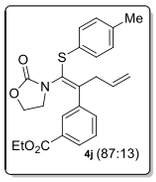
1751, 1600, 1490, 1394, 1036, 808 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{24}NO_2S$ $(M+H)^+$: calcd. 366.1528, found 366.1531.

(*E*)-3-(2-(3-Methoxyphenyl)-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (4i):



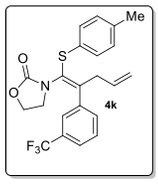
Following the general procedure GP–5, compound **4i** (151 mg) was obtained in 66% yield as yellow solid; R_f = 0.35 (5:1 hexane/EtOAc); [Silica, UV and I_2]; Yellow gummy solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41–7.37 (m, 2H), 7.24–7.20 (m, 1H), 7.13 (d, J = 8.0 Hz, 2H), 6.85–6.76 (m, 3H), 5.83–5.70 (m, 1H), 5.11 (dq, J = 17.2, 1.6 Hz, 1H), 5.04 (dq, J = 10.0, 1.2 Hz, 1H), 3.87–3.70 (m, 5H). 3.58 (d, J = 6.4 Hz, 2H), 3.30 (t, J = 8.0 Hz, 2H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4, 155.4, 142.9, 141.3, 138.2, 134.0, 132.3, 129.9, 129.3, 127.9, 127.7, 119.7, 116.8, 113.2, 113.0, 61.8, 55.2, 46.2, 40.4, 21.1; IR (Neat) ν_{max} 2894, 1742, 1637, 1592, 1488, 1396, 805 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{24}NO_3S$ $(M+H)^+$: calcd. 382.1477, found 382.1479.

(*E*)-Ethyl 3-(1-(2-oxooxazolidin-3-yl)-1-(*p*-tolylthio)penta-1,4-dien-2-yl)benzoate (4j):



Following the general procedure GP–5, compound **4j** (150 mg) was obtained in 59% yield with inseparable minor isomer (87:13). as light yellow liquid; R_f = 0.51 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.93–7.88 (m, 2H), 7.49 (dt, J = 8.0, 1.5 Hz, 1H), 7.42–7.37 (m, 1H), 7.34 (d, J = 8.5 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 5.78–5.68 (m, 1H), 5.09 (dd, J = 17.0, 1.5 Hz, 1H), 5.02 (dd, J = 10.0, 1.5 Hz, 1H), 4.34 (q, J = 7.0 Hz, 2H), 3.80 (br t, J = 7.5 Hz, 2H), 3.61 (d, J = 5.0 Hz, 2H), 3.44 (br t, J = 7.0 Hz, 2H), 2.30 (s, 3H), 1.37 (t, J = 7.0 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.2, 155.8, 141.7, 140.1, 138.0, 133.7, 132.1, 131.5, 130.6, 130.4, 129.9, 128.47, 128.45, 128.4, 128.1, 127.6, 61.7, 60.9, 45.9, 40.1, 21.0, 14.2; IR (Neat)ν_{max} 2978, 1753, 1713,1491, 1392, 1239, 1084, 808 cm^{-1}; HRMS (ESI) for $C_{24}H_{26}NO_4S^+$ $(M+H)^+$: calcd 424.1577 found 424.1585.

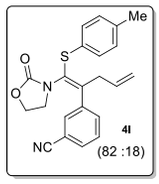
(*E*)-3-(1-(*p*-Tolylthio)-2-(3-(trifluoromethyl)phenyl)penta-1,4-dien-1-yl)oxazolidin-2-one (4k):



Following the general procedure GP–5, compound 4**k** (111 mg) was obtained in 44% yield as colorless liquid; R_f = 0.68 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53–7.43 (m, 4H), 7.37 (d, J = 8.4 Hz, 2H), 7.13 (d, J = 8.0 Hz, 2H), 5.81–5.69 (m, 1H), 5.11 (dd, J = 16.8, 1.6 Hz, 1H) 5.06 (dd, J = 10.0, 1.6 Hz, 1H), 3.88–3.73 (m, 2H), 3.62 (br d, J = 4.0 Hz, 2H), 3.44 (br s, 2H), 2.31 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 141.2, 140.8, 138.2, 133.5, 131.7, 131.1, 130.3 (q, J = 32.3 Hz, 1C), 130.0, 128.9,

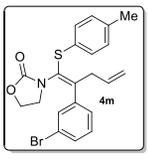
128.7, 127.4, 124.0 (q, J = 273 Hz, 1C), 124.1 (q, J = 4.0 Hz, 1C), 117.1, 61.7, 45.9, 40.2, 21.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ −62.5; IR (Neat)ν_{max} 2917, 1751, 1491, 1393, 1332, 1118, 805; HRMS (ESI) for $C_{22}H_{21}F_3NO_2S^+$ $(M+H)^+$: calcd 420.1240 found 420.1244**.**

(*E*)-3-(1-(2-Oxooxazolidin-3-yl)-1-(*p*-tolylthio)penta-1,4-dien-2-yl)benzonitrile (4l)



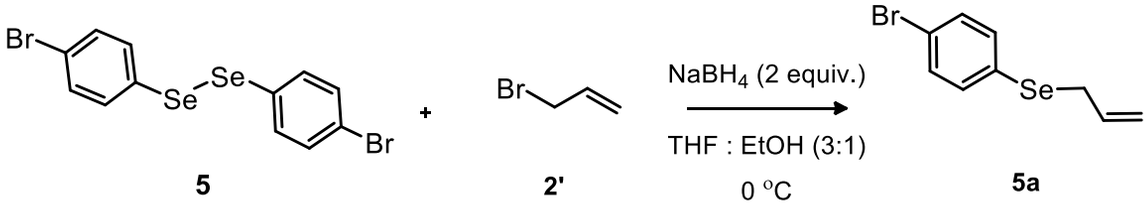
Following the general procedure GP–5, compound **4l** (165 mg) was obtained in 73% yield with inseparable minor isomer (82 :18) as yellow gummy solid; R_f = 0.37 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57–7.48 (m, 3H), 7.45–7.41 (m, 1H), 7.32 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 7.6 Hz, 2H), 5.77–5.65 (m, 1H), 5.12–5.03 (m, 2H), 3.81 (br s, 2H), 3.57 (br s, 2H), 3.48 (br s, 2H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.8, 141.5, 138.4, 133.3, 132.3, 131.7, 130.98, 130.93, 130.1, 129.2, 127.2, 117.4, 112.4, 61.8, 45.8, 40.2, 21.1; IR (Neat) ν_{max} 2916, 2227, 1749, 1596, 1477, 1392, 804 cm^{-1}; **HRMS (ESI)** for $C_{22}H_{21}N_2O_2S$ $(M+H)^+$: calcd. 377.1318, found 377.1324.

(*E*)-3-(2-(3-Bromophenyl)-1-(*p*-tolylthio)penta-1,4-dien-1-yl)oxazolidin-2-one (4m)



Following the general procedure GP–5, compound **4m** (149 mg) was obtained in 58% yield as yellow gummy compound; R_f = 0.67 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.33 (m, 4H), 7.22–7.18 (m, 2H), 7.13 (d, J = 8.0 Hz, 2H), 5.80–5.67 (m, 1H), 5.11 (dq, J = 17.2, 1.6 Hz, 1H), 5.05 (dq, J = 10.0, 1.6 Hz, 1H), 3.83 (t, J = 7.2 Hz, 2H), 3.58 (d, J = 6.0 Hz, 2H), 3.41 (t, J = 7.6 Hz, 2H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.0, 142.1, 141.3, 138.3, 133.6, 131.9, 130.5, 130.2, 130.00, 129.95, 128.5, 127.6, 126.3, 122.1, 117.1, 61.8, 46.0, 40.3, 21.1; IR (Neat)ν_{max} 2908, 1745, 1478, 1396, 1223, 1035, 807 cm^{-1}; HRMS (ESI) for $C_{21}H_{21}BrNO_2S^+$ $(M+H)^+$: calcd 430.0471 found 430.0475

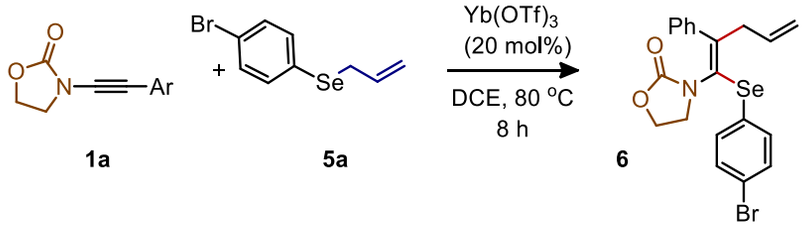
Synthesis of allyl(4-bromophenyl)selane (5a)[9]



To a suspension of $NaBH_4$ (2.0 eq.) in EtOH (20 mL) was added a solution of diselenide **5** (5.0 mmol, 1.0 eq.) in THF (40.0 mL) dropwise under an argon atmosphere. The mixture was kept under agitation

at 0 ºC and allyl bromide (10.0 mmol, 2.0 eq.) in THF (20 mL) was added. After 25 minutes, the reaction mixture was quenched with water and the organic phase was extracted with diethyl ether. The organic layers were combined, dried over Na_2SO_4, and concentrated under vacuum. The residue was purified by flash chromatography on silica gel using n-hexane as the eluent to afford the desire product **5a** in 60% yield.

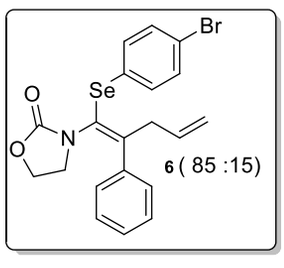
General procedure for the Yb-catalyzed selenoallylation of ynamides (GP–6):



A solution of **1a** (0.6 mmol) and $Yb(OTf)_3$ (74 mg, 0.12 mmol) in 1,2-DCE (4.0 mL) was placed in a Schlenk flask under an argon atmosphere. Allyl senenide (**5a**) (0.9 mmol) was next introduced. The reaction mixture was stirred for the specified time shown in the respective schemes at 80 °C. The progress of the reaction was periodically monitored by TLC. After 8 h, the reaction mixture was diluted with dichloromethane (10 mL), and filtered over a small pad of Celite. The solvent was evaporated under the reduced pressure and the residue was purified by flash chromatography on silica gel eluting with hexane/EtOAc mixture to afford the expected product **6.**

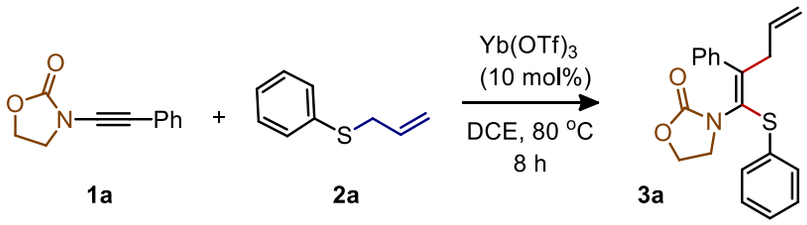
***(E)*-3-(1-((4-Bromophenyl)selanyl)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (6)**

Following the general procedure GP–6 compound **6** (136 mg) was obtained in 49% yield with



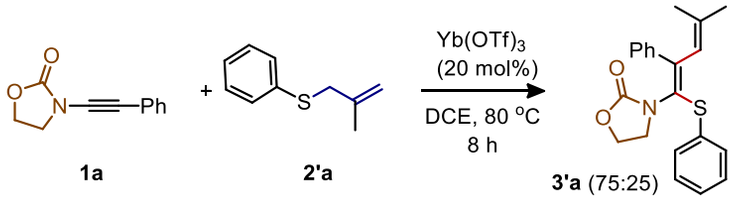
inseparable minor isomer (85 :15) as yellow gummy compound; R_f = 0.67 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, J = 8.5 Hz, 2H), 7.41 (d, J = 8.0 Hz, 2H), 7.42–7.32 (m, 5H), 7.31–7.28 (m, 1H), 7.25 (d, *J* = 7.0 Hz, 1H), 5.78–5.67 (m, 1H), 5.12 (d, *J* = 17.0 Hz, 1H), 5.06 (d, *J* = 10.0 Hz, 1H), 3.78 (t, *J* = 6.5 Hz, 2H), 3.54 (d, *J* = 6.5 Hz, 2H), 3.26 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 145.8, 139.6, 135.9, 133.4, 132.4, 128.4, 127.7, 127.2, 126.5, 124.7, 122.7, 117.1, 61.8, 46.5, 41.9; IR (Neat)ν_{max} 2908, 1745, 1478, 1396, 1223, 1035, 807 cm^{-1}; HRMS (ESI) for $C_{20}H_{19}BrNO_2Se^+$ $(M+H)^+$: calcd 463.9759 found 463.9757

General procedure for gram scale synthesis of 3a (GP–7):



A solution of **1a** (1g, 5.3 mmol) and $Yb(OTf)_3$ (331mg, 0.53 mmol) in 1,2-DCE (35 mL) was placed in a sealed tube under an argon atmosphere. Allyl sulfide (**2a**) (1.2g, 7.95 mmol) was next introduced. The reaction mixture was stirred at 80 °C in an oil bath. The progress of the reaction was periodically monitored by TLC. After 10 h, the reaction mixture was diluted with dichloromethane (30 mL), and filtered over a small pad of Celite. The solvent was evaporated under the reduced pressure and the residue was purified by flash chromatography on silica gel eluting with hexane/EtOAc mixture to afford the expected product **3a** (1.4 g, 75%).

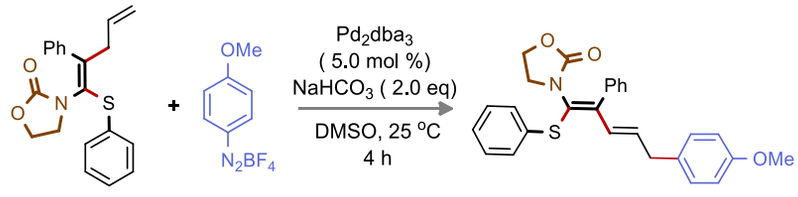
Synthesis of (*E*)-3-(4-Methyl-2-phenyl-1-(phenylthio)penta-1,3-dien-1-yl)oxazolidin-2-one (3'a):



A solution of **1a** (0.6 mmol) and $Yb(OTf)_3$ (74 mg, 0.12 mmol) in 1,2-DCE (4.0 mL) was placed in a Schlenk flask under an argon atmosphere. Allyl sulfide (**2'a**) (147 mg, 0.9 mmol) was next introduced. The reaction mixture was stirred at 80 °C. The progress of the reaction was periodically monitored by TLC. After 8 h, the reaction mixture was diluted with dichloromethane (10 mL), and filtered over a small pad of Celite. The solvent was evaporated under the reduced pressure and the residue was purified by flash chromatography on silica gel eluting with hexane/EtOAc mixture to afford the expected product **3'a** (177 mg) in 84% yield as yellow gummy compound (in 75:25 ratio of cisoid and transoid isomers); R_f = 0.67 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52–7.47 (m, 2H), 7.37 (br d, J = 7.6 Hz, 1.4H), 7.34–7.37 (m, 8H), 7.25–7.20 (m, 2H), 6.40 (d, J = 1.2 Hz, 1H), 5.96 (d, J = 1.2 Hz, 0.34H), 4.09 (br s, 0.73H), 3.80–3.65 (m, 3H), 3.26 (t, J = 7.5 Hz, 2H), 1.82 (s, 3H), 1.81 (s, 1H), 1.32 (s, 1.1H), 1.24 (s, 3H); ^{13}C NMR (126 MHz,

$CDCl_3$) δ 155.4, 155.1, 143.2, 141.8, 141.7, 140.2, 140.0, 139.9, 138.8, 133.8, 132.2, 132.0, 131.7, 129.5, 129.2, 129.1, 129.0, 128.4, 128.1, 128.0, 127.8, 127.5, 127.4, 126.8, 123.9, 123.1, 62.0, 61.8, 46.3, 44.9, 27.0, 26.8, 20.2, 19.9; IR (Neat)ν_{max} 2916, 1751, 1951, 1475, 1393, 1216, 1035, 694cm^{-1}; HRMS (ESI) for $C_{21}H_{22}NO_2S$+ $(M+H)^+$: calcd 352.1366 found 352.1368.

Synthesis of 3-((1*E*,3*E*)-5-(4-Methoxyphenyl)-2-phenyl-1-(phenylthio)penta-1,3-dien-1-yl)oxazolidin-2-one (11):

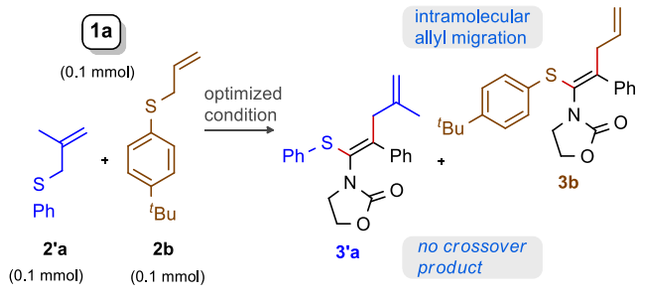


3a **9** **10**

The compound **3a** (0.2 mmol), aryldiazonium salt **9** (89 mg, 0.4 mmol), $Pd_2(dba)_3$ (9.16 mg, 0.01 mmol) and $NaHCO_3$ (33.6 mg, 0.4 mmol) and DMSO (2.0 mL) were added in a reaction tube. The resulting solution was stirred vigorously at room temperature. The progress of the reaction was periodically monitored by TLC. After 4 h, the reaction mixture was quenched with water (10 mL), and extracted with ethyl acetate (3 × 10 mL). The combined organic layer was dried over Na_2SO_4 and evaporated under the reduced pressure and the residue was purified by flash chromatography on silica gel eluting with hexane/EtOAc mixture to afford the expected product **10** (54 mg, 62%) as yellow gummy compound; R_f = 0.67 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55–7.48 (m, 2H), 7.37–7.27 (m, 8H), 7.24–7.19 (m, 2H), 6.81 (d, J = 8.8 Hz, 2H), 6.37 (d, J = 16.0 Hz, 1H), 6.00–5.91 (m, 1H), 3.81–3.76 (m, 5H), 3.73 (br dd, J = 6.8, 1.2 Hz, 1H), 3.37 (t, J = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 155.2, 144.9, 139.9, 132.1, 131.4, 130.2, 129.2, 128.4, 127.8, 127.7, 127.4, 127.3, 126.7, 123.4, 113.8, 61.8, 55.3, 46.2, 39.9; IR (Neat)ν_{max} 2921, 2851, 1752, 1396, 1249, 1091, 1037, 700 cm^{-1}; HRMS (ESI) for $C_{27}H_{26}NO_3S$+ $(M+H)^+$: calcd 444.1628 found 444.1629

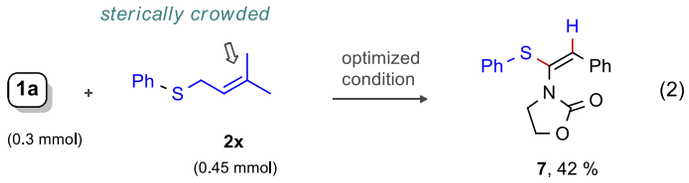
Mechanistic Studies

General procedure for cross-over experiment (GP–8):



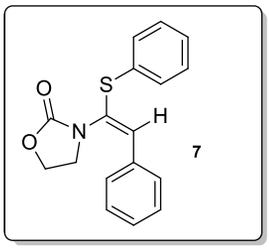
A solution of **1a** (18.7 mg, 0.1 mmol) and $Yb(OTf)_3$ (12.3 mg, 0.02 mmol) in 1,2-DCE (0.67 mL) was placed in a Schlenk flask under an argon atmosphere. Allyl sulfide **2'a** (16.3 mg, 0.1 mmol) and **2b** (20.1 mg, 0.1 mmol) were next introduced. The reaction mixture was stirred at 80 °C. The progress of the reaction was periodically monitored by TLC. After 8 h, the reaction mixture was diluted with dichloromethane (2 mL), and filtered over a small pad of Celite. The solvent was evaporated under the reduced pressure and the residue analyzed through HRMS. The formation of products **3'a** and **3b** was observed. No cross-over products were observed.

General procedure for the experiment of thioallylation by terminally disubstituted allyl sulfide (GP–9):



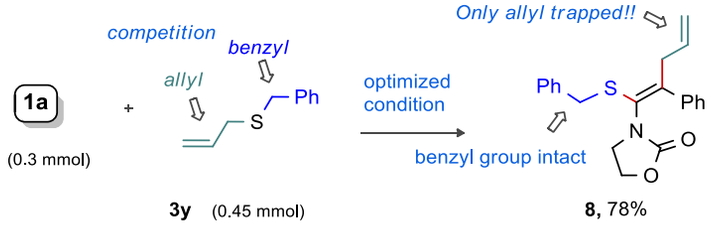
A solution of **1a** (56 mg, 0.3 mmol) and $Yb(OTf)_3$ (37 mg, 0.06 mmol) in 1,2-DCE (2.0 mL) was placed in a Schlenk flask under an argon atmosphere. The allyl sulfide **2x** (80 mg, 0.45 mmol) was next introduced. The reaction mixture was stirred at 80 °C. The progress of the reaction was periodically monitored by TLC. After 8 h, the reaction mixture was diluted with dichloromethane (10 mL), and filtered over a small pad of Celite. The solvent was evaporated under the reduced pressure and the residue was purified by flash chromatography on silica gel eluting with hexane/EtOAc mixture to afford the product **7** (42%).

(*E*)-3-(2-Phenyl-1-(phenylthio)vinyl)oxazolidin-2-one (7)



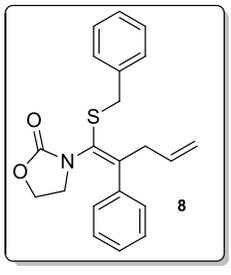
Following the general procedure GP−12, compound **7** (37 mg) was obtained in 42% yield as yellow gummy compound; R_f = 0.67 (5:1 hexane/EtOAc); [Silica, UV and I_2]; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.47 (m, 2H), 7.37-7.32 (m, 6H), 7.30-7.27 (m, 2H), 6.88 (s, 1H), 4.11 (t, J = 7.5 Hz, 2H), 3.67 (t, J = 8.0 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.8, 134.7, 132.0, 131.5, 131.3, 129.5, 129.4, 129.2, 128.7, 128,3, 128.0, 62.2, 45.2; IR (Neat)ν_{max} 2920, 1773, 1697, 1386, 1364, 1221, 704 cm^{-1}; HRMS (ESI) for $C_{17}H_{16}NO_2S$+ $(M+H)^+$: calcd 298.0896 found 298.0891

General procedure for competitive experiment to trap allyl vs benzyl (GP−10):



A solution of **1a** (56 mg, 0.3 mmol) and Yb(OTf)$_3$ (37 mg, 0.06 mmol) in 1,2-DCE (2.0 mL) was placed in a Schlenk flask under an argon atmosphere. Allyl benzyl sulfide **3y** (74 mg, 0.45 mmol) was next introduced. The reaction mixture was stirred at 80 °C. The progress of the reaction was periodically monitored by TLC. After 8 h, the reaction mixture was diluted with dichloromethane (10 mL), and filtered over a small pad of Celite. The solvent was evaporated under the reduced pressure and the residue was purified by flash chromatography on silica gel eluting with hexane/EtOAc mixture to afford the product **8** (78%) and no benzyl migration product was observed.

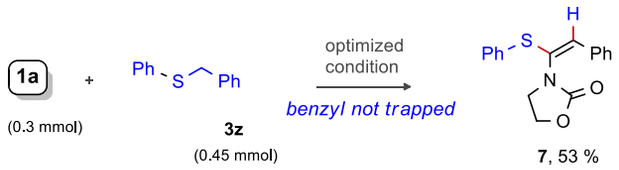
(*E*)-3-(1-(Benzylthio)-2-phenylpenta-1,4-dien-1-yl)oxazolidin-2-one (8):



Following the general procedure GP−10, compound **8** (82 mg) was obtained in 78% yield as pale yellow gummy liquid; R_f = 0.20 (5:1 hexane/EtOAc); [Silica, UV and I_2]; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.44–7.40 (m, 2H), 7.36–7.22 (m, 7H) (1H from $CDCl_3$), 7.19–7.15 (m, 2H), 5.69–5.57 (m, 1H), 5.05–4.95 (m, 2H), 3.93 (s, 2H), 3.84 (t, J = 8.0 Hz, 2H), 3.42–3.38 (m, 2H), 3.28 (t, J = 8.0 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.0, 146.6, 139.7, 138.2, 134.0, 128.8, 128.6, 128.3, 127.6,

127.3, 127.2, 116.8, 61.9, 45.8, 40.5, 37.2; **IR** (Neat)ν_{max} 2912, 1744, 1490, 1395, 1218, 1033, 914; **HRMS** (ESI) for $C_{21}H_{22}NO_2S+$ $(M+H)^+$: calcd 352.1366, found 352.1370.

General procedure for experiment to trap benzyl in absence of allyl(GP–11):



A solution of **1a** (56 mg, 0.3 mmol) and $Yb(OTf)_3$ (37 mg, 0.06 mmol) in 1,2-DCE (2.0 mL) was placed in a Schlenk flask under an argon atmosphere. Phenyl benzyl sulfide **3z** (90 mg, 0.45 mmol) was next introduced. The reaction mixture was stirred at 80 °C. The progress of the reaction was periodically monitored by TLC. After 8 h, the reaction mixture was diluted with dichloromethane (10 mL), and filtered over a small pad of Celite. The solvent was evaporated under the reduced pressure and the residue was purified by flash chromatography on silica gel eluting with hexane/EtOAc mixture to afford the hydrothiolation product **7** (53%) and no benzyl migration product was observed.

DFT computations

The calculations were carried out with the Gaussian 09 program[10] using the hybrid functional B3PW91[11] (following a rare recent theoretical study on Yb-catalyzed reactions).[12] Ytterbium was treated with a large-core Stuttgart Dresden relativistic effective core potential (RECP). For the +3 oxidation state, the MWB RECP is recommended and it was used in combination with its optimized basis set augmented by a f polarization function.[13] Hydrogen, carbon, oxygen, and nitrogen atoms were described with the 6-31+G(d,p) double–ζ quality basis set. Electronic energies were computed at T = 353.15 K in gas phase. Geometry optimizations were performed without symmetry constraints and analytical frequency calculations allowed to verify the nature of the extrema. Transition states were optimized using the TS keyword and characterized by a frequency calculation showing a single imaginary frequency (noted in the Energies and Cartesian coordinates section). Intrinsic Reaction Coordinates (IRC)[14] were carried out to verify the connections of the optimized transition states. The values presented are $\Delta G_{353.15}$ (kcal/mol). The three-dimensional images of the optimized structures were prepared using CYLview.[15]

The $Yb(OTf)_3$-catalyzed *syn*-thioallylation of ynamide **1a** with allylmethylsulfane **2a** was first studied (Figure S1). Coordination of the reactants to the Yb(III) center gives **intA$_0$**, lying 26.9 kcal/mol above the reactants. Subsequently, a *syn* insertion of the alkyne moiety into the S-Yb

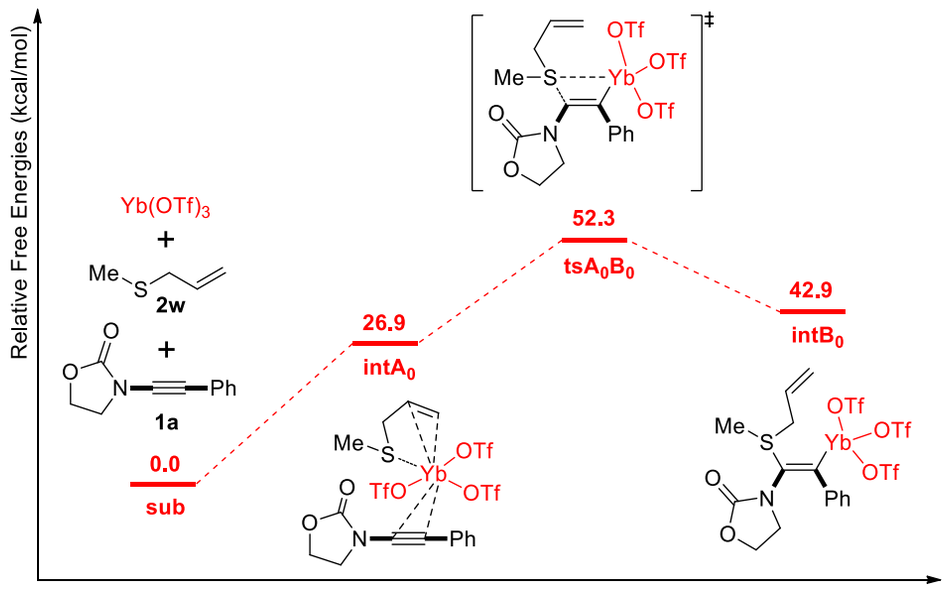


Figure S1. Partial Gibbs free energy profile for the *syn*-thioallylation of ynamides catalyzed by $Yb(OTf)_3$.

proceeds through transition state **tsA$_0$B$_0$**, resulting in the vinyl-Yb complex **intB$_0$** (42.9 kcal/mol; with *trans* orientation of the phenyl and sulfide groups). This step requires 52.3 kcal/mol of free activation energy, which is not possible at 353.15 K.

Repeated efforts for computing the thioallylation of ynamides using $Yb(OTf)_3$ as active species all failed. This prompted us to examine another potentially active species. The true nature of the catalytically active species in lanthanide-catalyzed reactions remains unknown. However, Eberlin, Roithová et al have recently shown that, owing to the poor coordinating ability of the triflate anion, $Ln(OTf)_3$ Lewis acids easily form ion pairs with Lewis bases and that the corresponding charged metal species (Ln^{2+} or Ln^{3+}) are much more active than the neutral one.[16] This ability of $Ln(OTf)_3$

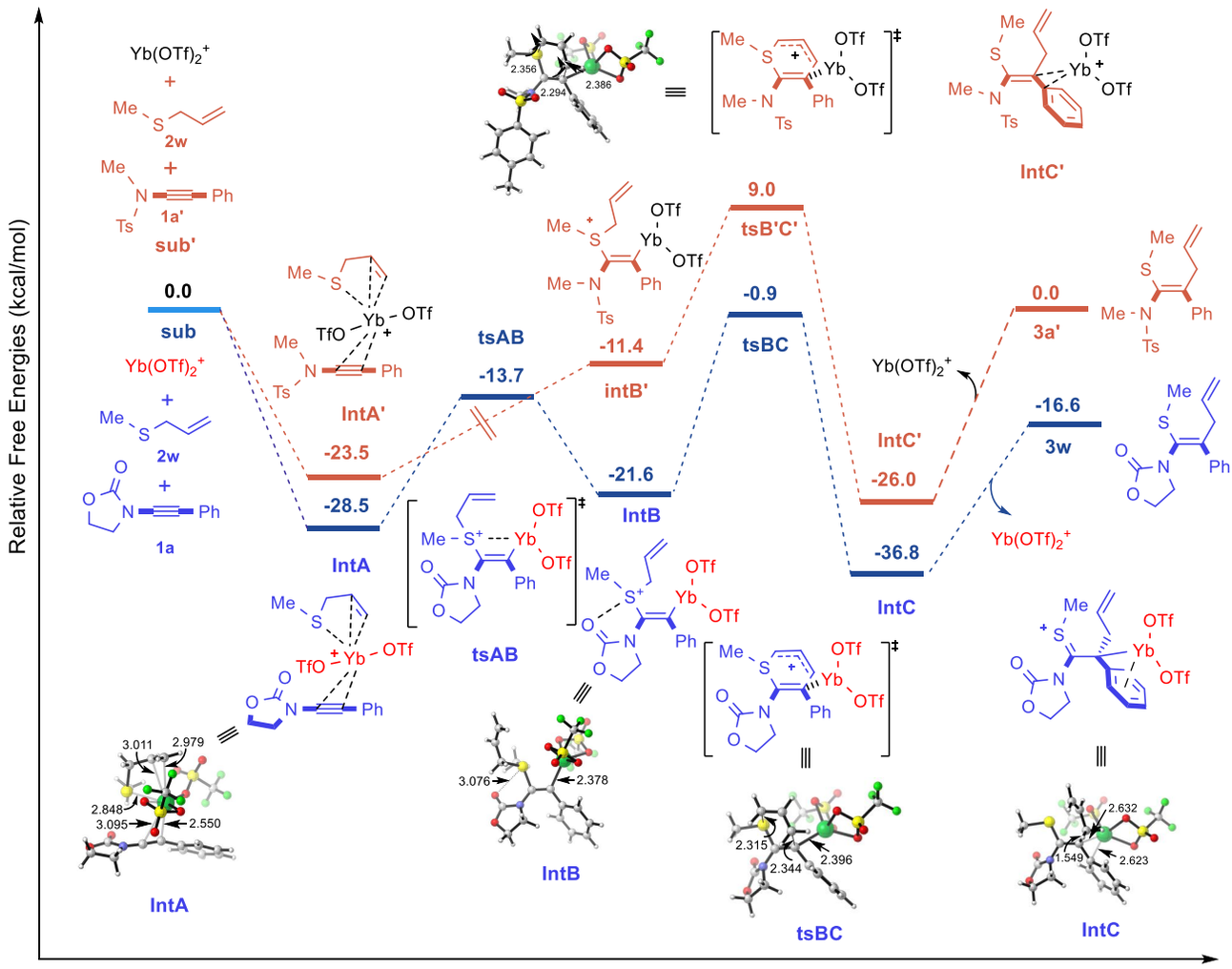


Figure S2. DFT analysis: comparison of N-oxazolidinone and N-sulfonyl ynamides (free energy profile, $\Delta G_{353.15}$ (kcal/mol); selected distances in Å).

Lewis acids to form charged species would be the reason why triflates are privileged catalysts in lanthanide chemistry. Consistently, the experimental results could be rationalized when $Yb(OTf)^{2+}$ was used as active species, as discussed in the manuscript and with more details below (Figure S2).

The transformation begins with the barrierless coordination of ynamide **1a** and allyl-methylsulfide (**2w**) to $Yb(OTf)^{2+}$ to provide the pentavalent species **intA**. This process is highly exergonic by 28.5 kcal/mol. Next, *syn*-insertion of the alkyne into the S-Yb bond proceeds through transition state **tsAB** (see Fig S3 for IRC plot), found at -13.7 kcal/mol on the free energy surface, and gives the vinyl-Yb complex **intB** (-21.6 kcal/mol) with *trans*-orientation of phenyl and sulfide groups. The sulfonium cation is stabilized by a non-covalent interaction with one oxazolidinone oxygen (nonbonding O···S distance 3.076 Å, which agrees well with a previous report (3.32 Å)[17] and the NCI analysis of **intB** shown in Figure S4). Next, a suprafacial [3,3]-sigmatropic shift promotes the migration of the allyl-group from the sulfonium to the C=C bond of **intB** via the 6-membered ring transition state **tsBC** (see Fig S3 for IRC plot), spanning a barrier of 20.7 kcal/mol (27.6 kcal/mol from **intA**). This step generates the very stable $Yb(III)^{+}$ intermediate **intC**, lying at -36.8 kcal/mol. Of note, it was not possible to locate a transition state corresponding to a [1,3]-sigmatropic shift. Finally, the catalyst is regenerated with concomitant release of the desired product **3w**, which is 16.6 kcal/mol more stable than the reactants. Thus, the rate-determining step is the allyl migration.

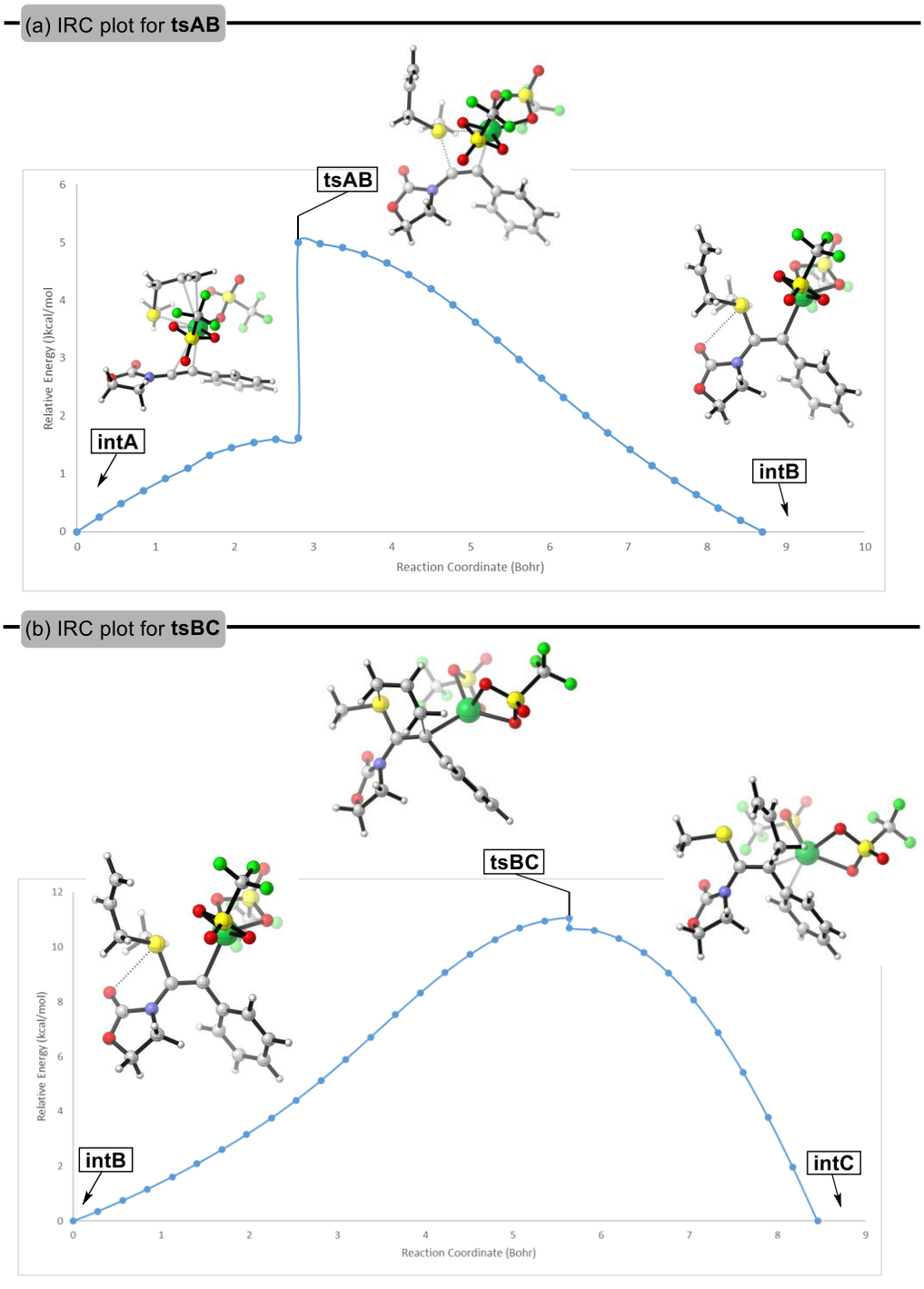


Figure S3. IRC plots of **tsAB** (a) and **tsBC** (b).

Based on the experimental findings, the N-sulfonyl protected ynamides was reluctant to undergo the *syn*-thioallylation process. To understand the contrasting reactivity of such substrates, further DFT calculations were performed (red lines; Fig S2). The coordination of N-tosyl ynamide **1a'**

and **2w** to $Yb(OTf)_2^+$ at first gives **intA'**, lying at -23.5 kcal/mol. Complex **intA'** should then undergo a *syn* insertion to give the vinyl-Yb complex **intB'**, but the corresponding transition state could not be found. Of note, NCI analysis of **intB'** (see Figure S4) reveals that the noncovalent interaction between the vinylic S and one O of the SO_2 moiety is virtually inexistent (O···S distance 3.720 Å). There is also a steric hindrance between the Ts and the Ph groups. These two features explain why **intB'** is much less stable than **intB**. The formation of **C'** through the [3,3]-sigmatropic transition state **tsB'C'** requires 31.5 kcal/mol of free energy of activation from **intA'**, which is significantly higher than the one required for forming **intC** (27.6 kcal/mol). Moreover, the final product **3a'** as the same free energy as the reactants. This is again likely due to a steric clash between the large Ts and the Ph group. Therefore, the *syn*-thioallylation of oxazolidinone-derived ynamides is favored kinetically and thermodynamically.

We plotted a space of nonbonding O···S interactions based on the electron density (ρ) and its derivative, namely the reduced electron density gradient (RDG),[18] to characterize the nature of this interaction. In this study, the surface is colored on a blue-green-red scale, ranging from -3.0 to 3.0 (see the color bar). Blue, green and red denote a strong attraction, weak vdW interactions and repulsive steric, respectively. Taking the dispersion effect into account, we performed B3PW91-D3 calculation including Grimme's dispersion correction[19] on the intermediates **intB** and **intB'**. After dispersion correction, the O···S distance of **intB** is shorter (3.042 Å). In addition, there is a blue area of noncovalent interactions located between O and S of **intB** in the NCI plot, indicating that there is a strong attraction. In contrast, there is no obvious interaction between O and S of **intB'** in the NCI plot, and the main interaction comes from the hydrogen bond, which is also proved by the 3D structure.

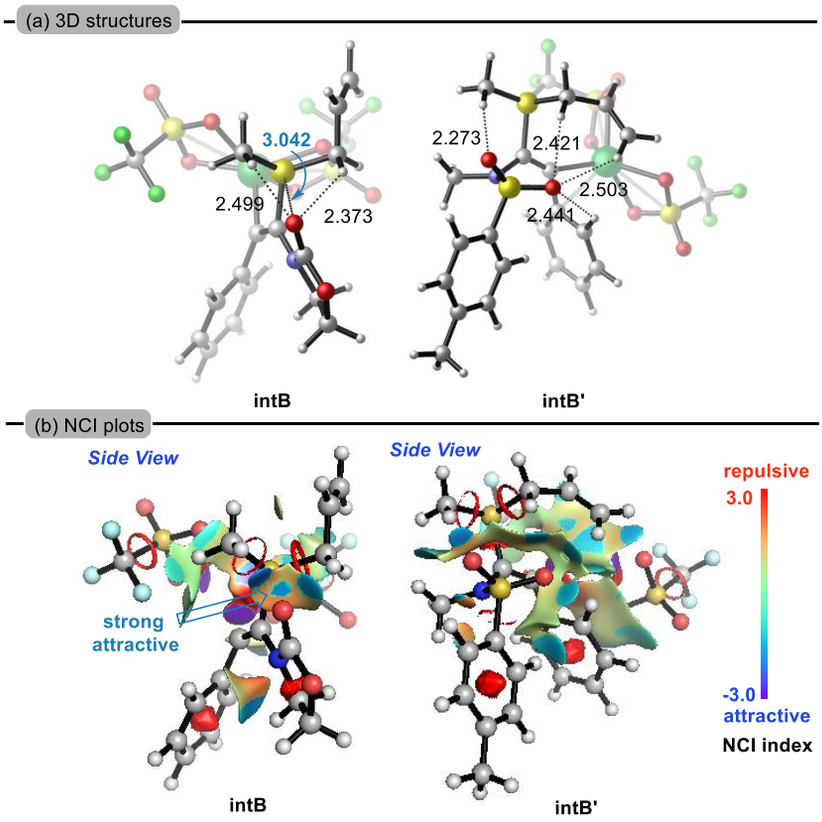
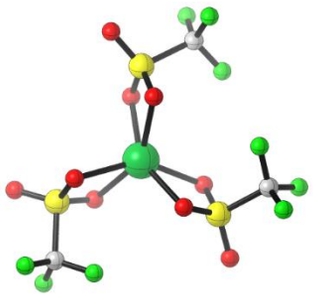


Figure S4. 3D structures (a) and NCI plots (b) of **intB** and **intB'**. Bond distances are in Å.

Energies and Cartesian coordinates for all the intermediates and transition states

$Yb(OTf)_3$



Zero-point correction= 0.086213 (Hartree/Particle)

Thermal correction to Energy= 0.122577

Thermal correction to Enthalpy= 0.123727

Thermal correction to Gibbs Free Energy= 0.001018

Sum of electronic and zero-point Energies= -2923.167982

Sum of electronic and thermal Energies= -2923.131618

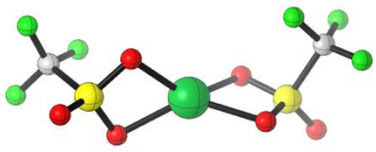
Sum of electronic and thermal Enthalpies= -2923.130468

Sum of electronic and thermal Free Energies= -2923.253177

E(RB3PW91) = -2923.25419522

Atom	X	Y	Z
Yb	-0.208715000000	0.263090000000	-0.041281000000
O	1.457502000000	1.138489000000	1.277911000000
O	-0.313312000000	-1.845325000000	0.878863000000
O	-2.102818000000	0.650715000000	-1.277374000000
S	-2.937425000000	1.244731000000	-0.154282000000
S	1.883250000000	2.248617000000	0.330505000000
S	0.269898000000	-2.594101000000	-0.307164000000
O	-0.452958000000	-3.738832000000	-0.804972000000
O	0.605709000000	-1.485430000000	-1.291697000000
O	-2.013314000000	1.153316000000	1.050533000000
O	-3.604850000000	2.499534000000	-0.397798000000
O	0.995896000000	2.030549000000	-0.883716000000
O	1.987493000000	3.585103000000	0.861939000000
C	3.589720000000	1.744475000000	-0.248150000000
C	1.931451000000	-3.204799000000	0.298953000000
C	-4.257373000000	-0.040826000000	0.174434000000
F	3.534944000000	0.524016000000	-0.782954000000
F	4.011404000000	2.610897000000	-1.160216000000
F	4.418057000000	1.738699000000	0.789169000000
F	-5.054598000000	-0.124561000000	-0.883222000000
F	-3.679522000000	-1.220894000000	0.395489000000
F	-4.957332000000	0.320795000000	1.242477000000
F	2.623813000000	-2.183013000000	0.802413000000
F	1.739221000000	-4.119333000000	1.241007000000
F	2.597451000000	-3.735748000000	-0.719299000000

$Yb(OTf)_2^+$



Zero-point correction= 0.057388 (Hartree/Particle)

Thermal correction to Energy= 0.081590

Thermal correction to Enthalpy= 0.082740

Thermal correction to Gibbs Free Energy= -0.010629

Sum of electronic and zero-point Energies= -1961.649665

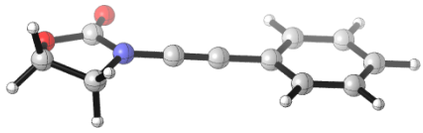
Sum of electronic and thermal Energies= -1961.625463

Sum of electronic and thermal Enthalpies= -1961.624313

Sum of electronic and thermal Free Energies= -1961.717682

Atom	**X**	**Y**	**Z**
Yb	-0.002599000000	-0.388011000000	-0.003221000000
O	-1.633386000000	0.445425000000	1.216527000000
O	1.981587000000	-1.245612000000	0.411479000000
S	-2.772120000000	-0.399050000000	0.601655000000
S	2.767732000000	-0.388120000000	-0.604864000000
O	3.641493000000	-1.065723000000	-1.516739000000
O	1.630614000000	0.471377000000	-1.201755000000
O	-1.986736000000	-1.242739000000	-0.426411000000
O	-3.653786000000	-1.086289000000	1.498384000000
C	-3.715803000000	0.836792000000	-0.465144000000
C	3.725149000000	0.825068000000	0.476130000000
F	-2.810705000000	1.425792000000	-1.257008000000
F	-4.599943000000	0.185368000000	-1.185787000000
F	-4.285516000000	1.724158000000	0.318207000000
F	2.830434000000	1.407262000000	1.283324000000
F	4.610400000000	0.156158000000	1.179296000000
F	4.295081000000	1.720465000000	-0.298144000000

1a oxazolidinone ynamide



Zero-point correction= 0.178624 (Hartree/Particle)

Thermal correction to Energy= 0.190358

Thermal correction to Enthalpy= 0.191302

Thermal correction to Gibbs Free Energy= 0.138068

Sum of electronic and zero-point Energies= -629.343337

Sum of electronic and thermal Energies= -629.331603

Sum of electronic and thermal Enthalpies= -629.330659

Sum of electronic and thermal Free Energies= -629.383892

E(RB3PW91) = -629.521960606

Atom	**X**	**Y**	**Z**
O	-4.117416000000	0.464683000000	-0.085635000000
C	-4.186621000000	-0.948281000000	0.148352000000
C	-2.770956000000	-1.465540000000	-0.125964000000
N	-2.007738000000	-0.237243000000	0.065527000000
C	-2.828151000000	0.892155000000	-0.021818000000
O	-2.488651000000	2.043280000000	-0.045151000000
C	-0.667371000000	-0.179839000000	0.039966000000
C	0.546674000000	-0.156577000000	0.031433000000
C	1.969359000000	-0.092229000000	0.016254000000
C	2.620539000000	1.155712000000	0.029390000000
C	4.010391000000	1.220238000000	0.015778000000
C	4.773598000000	0.051507000000	-0.012179000000
C	4.134359000000	-1.189293000000	-0.025911000000
C	2.744858000000	-1.266062000000	-0.011270000000
H	-4.487527000000	-1.111865000000	1.188571000000
H	-4.939289000000	-1.367767000000	-0.520587000000
H	-2.458184000000	-2.238260000000	0.580368000000
H	-2.646368000000	-1.840931000000	-1.149255000000

H 2.025672000000 2.063536000000 0.050023000000

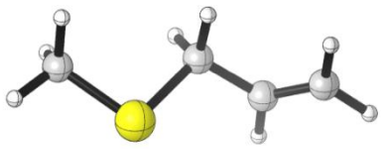
H 4.500211000000 2.190039000000 0.026534000000

H 5.858355000000 0.107349000000 -0.023205000000

H 4.720785000000 -2.103808000000 -0.047792000000

H 2.248983000000 -2.232034000000 -0.021256000000

2w allylmethylsulfane



Zero-point correction= 0.109564 (Hartree/Particle)

Thermal correction to Energy= 0.119119

Thermal correction to Enthalpy= 0.120269

Thermal correction to Gibbs Free Energy= 0.069442

Sum of electronic and zero-point Energies= -555.202770

Sum of electronic and thermal Energies= -555.193214

Sum of electronic and thermal Enthalpies= -555.192064

Sum of electronic and thermal Free Energies= -555.242892

E(RB3PW91) = -555.312333411

Atom X Y Z

S 0.931043000000 -0.637589000000 -0.093412000000

C -0.371992000000 0.634563000000 0.132882000000

C 2.403807000000 0.421267000000 -0.036815000000

C -1.676777000000 -0.021387000000 0.455370000000

C -2.754937000000 0.017946000000 -0.330975000000

H -0.456059000000 1.245216000000 -0.772424000000

H -0.061069000000 1.282147000000 0.962435000000

H 3.269952000000 -0.232515000000 -0.165270000000

H 2.401322000000 1.156897000000 -0.846565000000

H 2.492987000000 0.932812000000 0.926382000000

H -1.715854000000 -0.567194000000 1.397743000000

H -3.681379000000 -0.472228000000 -0.046129000000

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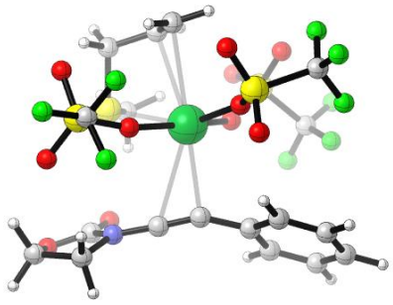
intA0



Zero-point correction= 0.377059 (Hartree/Particle)

Thermal correction to Energy= 0.444962

Thermal correction to Enthalpy= 0.446112

Thermal correction to Gibbs Free Energy= 0.246157

Sum of electronic and zero-point Energies= -4107.706087

Sum of electronic and thermal Energies= -4107.638184

Sum of electronic and thermal Enthalpies= -4107.637034

Sum of electronic and thermal Free Energies= -4107.836989

E(RB3PW91) = -4108.08314612

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Yb	-0.086738000000	-0.138539000000	-0.345118000000
O	1.740503000000	-1.231458000000	-0.759318000000
O	0.803015000000	1.752677000000	0.007083000000
O	-2.140149000000	0.588183000000	-0.159175000000
S	-3.612216000000	0.717320000000	-0.564086000000
S	2.923138000000	-1.305328000000	-1.742872000000
S	0.646315000000	3.274144000000	0.231931000000
O	-0.100045000000	3.896237000000	-0.851820000000
O	0.305530000000	3.553474000000	1.622058000000
O	-3.765084000000	0.814303000000	-2.013105000000
O	-4.451057000000	-0.224181000000	0.177251000000
O	2.735106000000	-2.392037000000	-2.702362000000
O	3.301841000000	0.014781000000	-2.230291000000
C	4.286585000000	-1.862054000000	-0.595793000000

C	2.422879000000	3.809786000000	0.010385000000
C	-4.031041000000	2.402346000000	0.126439000000
F	3.960503000000	-3.019766000000	-0.013564000000
F	5.404623000000	-2.031480000000	-1.301665000000
F	4.501399000000	-0.946148000000	0.348746000000
F	-3.307833000000	3.343472000000	-0.466802000000
F	-5.327118000000	2.640132000000	-0.083203000000
F	-3.793655000000	2.421778000000	1.441775000000
F	2.837988000000	3.541462000000	-1.226743000000
F	2.504041000000	5.125021000000	0.222469000000
F	3.213692000000	3.181188000000	0.883423000000
S	-1.501791000000	-2.174073000000	-1.913689000000
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C	-0.384240000000	-3.539425000000	-2.350982000000
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C	-0.245581000000	1.092958000000	-3.014734000000
H	-2.363891000000	-0.500588000000	-3.363172000000
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H	-0.816170000000	-4.083577000000	-3.193886000000
H	0.623314000000	-3.189751000000	-2.580185000000
H	0.724407000000	-0.679650000000	-3.611819000000
H	0.670623000000	1.676722000000	-3.000961000000
H	-1.177659000000	1.617169000000	-2.808723000000
O	-3.671920000000	-3.957309000000	1.420127000000
C	-4.496843000000	-2.897873000000	1.958848000000
C	-3.516733000000	-1.906665000000	2.594586000000
N	-2.277999000000	-2.284919000000	1.898387000000
C	-2.405420000000	-3.559166000000	1.286078000000
O	-1.517317000000	-4.171078000000	0.755336000000
C	-1.111520000000	-1.688405000000	2.041917000000
C	-0.064135000000	-1.042459000000	2.161063000000
C	1.190468000000	-0.719041000000	2.808751000000

C 2.064528000000 -1.761458000000 3.169671000000

C 3.245782000000 -1.468796000000 3.841123000000

C 3.563007000000 -0.146709000000 4.163773000000

C 2.698522000000 0.886586000000 3.803488000000

C 1.518173000000 0.611099000000 3.116804000000

H -5.044974000000 -2.443750000000 1.131501000000

H -5.182503000000 -3.349681000000 2.675648000000

H -3.783846000000 -0.873737000000 2.372691000000

H -3.392671000000 -2.055677000000 3.672081000000

H 1.809852000000 -2.786398000000 2.918120000000

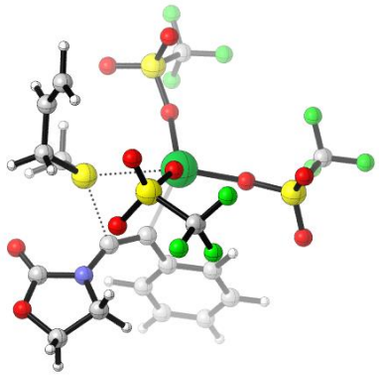
H 3.919912000000 -2.275154000000 4.115329000000

H 4.486554000000 0.076077000000 4.690499000000

H 2.942633000000 1.916160000000 4.046688000000

H 0.855213000000 1.423376000000 2.833924000000

$ts\mathbf{A}_0\mathbf{B}_0$



Frequency -134.4057

Zero-point correction= 0.375877 (Hartree/Particle)

Thermal correction to Energy= 0.442735

Thermal correction to Enthalpy= 0.443885

Thermal correction to Gibbs Free Energy= 0.245593

Sum of electronic and zero-point Energies= -4107.666292

Sum of electronic and thermal Energies= -4107.599434

Sum of electronic and thermal Enthalpies= -4107.598284

Sum of electronic and thermal Free Energies= -4107.796577

E(RB3PW91) = -4108.04216964

Atom	X	Y	Z
S	-1.785165000000	-1.959018000000	0.374379000000
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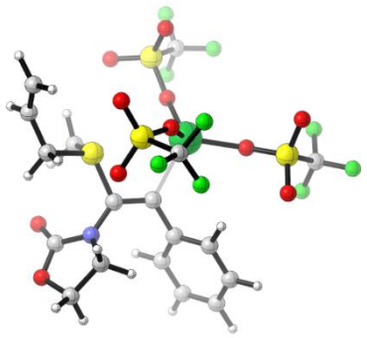
Yb	0.411200000000	-0.106483000000	-0.184093000000
O	1.704648000000	-1.744694000000	0.228441000000
O	1.751669000000	1.531228000000	-0.171672000000
O	-0.582414000000	0.164429000000	-2.079973000000
C	-1.516682000000	-3.927871000000	-2.788866000000
C	-1.101789000000	0.491609000000	1.708374000000
S	2.266208000000	-3.146862000000	-0.099750000000
S	2.373365000000	2.847321000000	-0.704513000000
S	-1.958225000000	0.297316000000	-2.745601000000
O	-2.101209000000	-0.562470000000	-3.908537000000
O	-3.019322000000	0.285267000000	-1.727322000000
C	-1.873640000000	2.056323000000	-3.370228000000
O	1.415166000000	-4.191801000000	0.463296000000
O	2.706499000000	-3.234524000000	-1.482715000000
C	3.803152000000	-3.113629000000	0.962008000000
O	2.325177000000	2.908078000000	-2.155908000000
O	1.925343000000	3.976716000000	0.100598000000
C	4.157852000000	2.542757000000	-0.240227000000
F	3.473307000000	-2.920419000000	2.242836000000
F	4.434997000000	-4.281486000000	0.847726000000
F	4.617360000000	-2.133891000000	0.571127000000
F	4.614234000000	1.450018000000	-0.853888000000
F	4.891186000000	3.591966000000	-0.611773000000
F	4.271264000000	2.378160000000	1.080697000000
F	-0.898630000000	2.188661000000	-4.258218000000
F	-3.040519000000	2.368199000000	-3.937684000000
F	-1.657367000000	2.885136000000	-2.342363000000
C	-2.722793000000	-3.048784000000	-0.796705000000

C	-1.394592000000	-3.068097000000	1.748555000000
C	-1.821066000000	-4.016011000000	-1.490084000000
H	-3.200318000000	-2.352007000000	-1.489790000000
H	-3.489545000000	-3.528655000000	-0.180796000000
H	-0.929368000000	-2.454699000000	2.522578000000
H	-2.323814000000	-3.496506000000	2.125684000000
H	-0.678664000000	-3.818862000000	1.410262000000
H	-1.403649000000	-4.819940000000	-0.887124000000
H	-0.861176000000	-4.657728000000	-3.254743000000
H	-1.901430000000	-3.129515000000	-3.419327000000
N	-3.592157000000	0.179468000000	1.592539000000
C	-4.223338000000	1.395316000000	1.050903000000
C	-5.681031000000	1.156473000000	1.457413000000
O	-5.778560000000	-0.262132000000	1.701615000000
C	-4.566477000000	-0.806402000000	1.866114000000
H	-6.392937000000	1.406902000000	0.670741000000
H	-5.951246000000	1.674343000000	2.382025000000
H	-4.076494000000	1.422464000000	-0.031942000000
H	-3.792715000000	2.284837000000	1.513929000000
O	-4.348633000000	-1.949570000000	2.170070000000
C	-0.814674000000	1.422479000000	2.825683000000
C	-1.412531000000	1.233585000000	4.087079000000
C	0.063708000000	2.504029000000	2.650475000000
C	-1.146331000000	2.108876000000	5.135840000000
H	-2.063508000000	0.378282000000	4.249422000000
C	-0.290584000000	3.196104000000	4.943359000000
H	-1.604115000000	1.938651000000	6.106573000000
C	0.308174000000	3.389793000000	3.698909000000
H	-0.082781000000	3.878789000000	5.762399000000
H	0.981061000000	4.226409000000	3.535218000000
H	0.552309000000	2.673977000000	1.697014000000

intB$_0$



Zero-point correction= 0.377656 (Hartree/Particle)

Thermal correction to Energy= 0.444602

Thermal correction to Enthalpy= 0.445752

Thermal correction to Gibbs Free Energy= 0.247460

Sum of electronic and zero-point Energies= -4107.681415

Sum of electronic and thermal Energies= -4107.614469

Sum of electronic and thermal Enthalpies= -4107.613319

Sum of electronic and thermal Free Energies= -4107.811611

E(RB3PW91) = -4108.05907094

Atom	X	Y	Z
S	2.321082000000	1.304097000000	0.500273000000
C	2.212648000000	-0.353137000000	1.229736000000
Yb	-0.672010000000	0.262409000000	-0.217936000000
O	-0.989684000000	2.245488000000	0.513996000000
O	-2.477253000000	-0.829721000000	-0.105211000000
O	0.210488000000	-0.024059000000	-2.154461000000
C	3.797572000000	3.234239000000	-2.172571000000
C	0.934704000000	-0.795595000000	1.260318000000
S	-1.055981000000	3.748693000000	0.149924000000
S	-3.443449000000	-1.878453000000	-0.717251000000
S	1.497120000000	-0.317635000000	-2.943323000000
O	1.836219000000	0.757904000000	-3.861751000000
O	2.543238000000	-0.836210000000	-2.053194000000
C	0.931980000000	-1.768945000000	-3.975392000000

O 0.159245000000 4.434316000000 0.578156000000

O -1.567716000000 3.940047000000 -1.198247000000

C -2.399260000000 4.292545000000 1.329168000000

O -4.109675000000 -1.355639000000 -1.898039000000

O -2.815602000000 -3.194142000000 -0.743637000000

C -4.723319000000 -1.928890000000 0.643632000000

F -2.030661000000 4.046481000000 2.589976000000

F -2.603690000000 5.600318000000 1.182544000000

F -3.531841000000 3.638471000000 1.072623000000

F -5.280301000000 -0.727380000000 0.801060000000

F -5.668409000000 -2.810228000000 0.316631000000

F -4.161894000000 -2.301064000000 1.797253000000

F -0.069480000000 -1.406094000000 -4.769281000000

F 1.955405000000 -2.194557000000 -4.716095000000

F 0.527934000000 -2.759669000000 -3.176710000000

C 3.949486000000 1.550995000000 -0.340610000000

C 2.361511000000 2.475497000000 1.879446000000

C 4.037165000000 2.940173000000 -0.891313000000

H 3.946955000000 0.784899000000 -1.120072000000

H 4.711590000000 1.346934000000 0.415158000000

H 1.494726000000 2.234940000000 2.496941000000

H 3.289883000000 2.351873000000 2.435553000000

H 2.218262000000 3.467834000000 1.448095000000

H 4.327317000000 3.723829000000 -0.194235000000

H 3.889613000000 4.254809000000 -2.532220000000

H 3.497253000000 2.478585000000 -2.894821000000

N 3.381791000000 -1.056239000000 1.541534000000

C 3.666976000000 -2.377348000000 0.974336000000

C 4.918931000000 -2.759476000000 1.772059000000

O 5.416217000000 -1.519725000000 2.312902000000

C 4.460124000000 -0.571949000000 2.251216000000

H 5.707171000000 -3.198783000000 1.159489000000

H 4.689770000000 -3.424401000000 2.609822000000

H 3.844121000000 -2.292694000000 -0.102857000000

H 2.839994000000 -3.068613000000 1.148024000000

O 4.578099000000 0.536421000000 2.731652000000

C 0.613944000000 -2.019493000000 2.025340000000

C 1.041350000000 -2.167412000000 3.360088000000

C -0.174400000000 -3.038598000000 1.462559000000

C 0.699792000000 -3.298523000000 4.096670000000

H 1.622251000000 -1.375164000000 3.825266000000

C -0.061325000000 -4.314966000000 3.513816000000

H 1.024128000000 -3.384496000000 5.130424000000

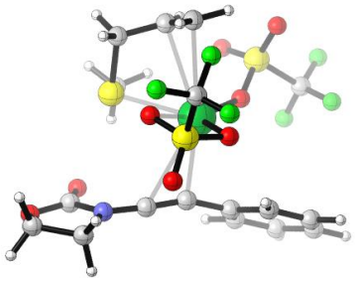
C -0.494698000000 -4.180806000000 2.194767000000

H -0.327737000000 -5.196657000000 4.089822000000

H -1.102185000000 -4.953486000000 1.732880000000

H -0.546593000000 -2.955368000000 0.444598000000

intA



Zero-point correction= 0.349108 (Hartree/Particle)

Thermal correction to Energy= 0.404277

Thermal correction to Enthalpy= 0.405427

Thermal correction to Gibbs Free Energy= 0.240022

Sum of electronic and zero-point Energies= -3146.280721

Sum of electronic and thermal Energies= -3146.225552

Sum of electronic and thermal Enthalpies= -3146.224402

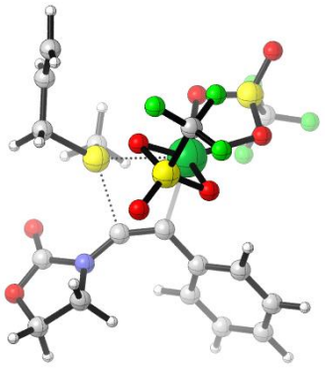
Sum of electronic and thermal Free Energies= -3146.389808

E(RB3PW91) = -3146.62982951

Atom	X	Y	Z
Yb	0.018189000000	-0.313644000000	-0.131253000000
O	-2.080971000000	-0.262787000000	-0.259606000000
O	0.918423000000	-1.633410000000	1.498318000000
S	-3.308571000000	-0.694155000000	-1.121206000000
S	2.369318000000	-1.618887000000	1.029146000000
O	2.280876000000	-1.017351000000	-0.358929000000
O	3.347037000000	-1.046044000000	1.928443000000
O	-3.363633000000	0.119117000000	-2.332107000000
O	-3.374448000000	-2.145068000000	-1.213809000000
C	-4.711360000000	-0.138620000000	-0.016479000000
C	2.828572000000	-3.424637000000	0.808994000000
F	-4.645003000000	1.179282000000	0.165613000000
F	-5.857643000000	-0.451819000000	-0.604769000000
F	-4.625454000000	-0.754005000000	1.160398000000
F	1.914703000000	-4.029835000000	0.050951000000
F	4.012448000000	-3.484504000000	0.216364000000
F	2.875512000000	-3.995821000000	1.999268000000
S	0.879579000000	0.944587000000	-2.536737000000
C	0.771502000000	-0.654135000000	-3.451712000000
C	-0.495976000000	1.919494000000	-3.229740000000
C	-0.333105000000	-1.485610000000	-2.882086000000
C	-0.147147000000	-2.556110000000	-2.085672000000
H	1.751470000000	-1.124253000000	-3.334184000000
H	0.617821000000	-0.419555000000	-4.509203000000
H	-0.443451000000	2.890064000000	-2.732500000000
H	-0.310916000000	2.057525000000	-4.296868000000
H	-1.466337000000	1.449984000000	-3.057309000000
H	-1.348220000000	-1.169140000000	-3.123550000000
H	-1.003507000000	-3.110202000000	-1.706773000000
H	0.847627000000	-2.949813000000	-1.891571000000
O	3.869781000000	3.858952000000	-1.117234000000
C	4.825855000000	3.105117000000	-0.339527000000

C	4.024538000000	2.509743000000	0.827287000000
N	2.660836000000	2.613957000000	0.283732000000
C	2.618586000000	3.507558000000	-0.830150000000
O	1.618975000000	3.865531000000	-1.388523000000
C	1.563606000000	2.179677000000	0.857082000000
C	0.545713000000	1.686922000000	1.359317000000
C	-0.634348000000	1.654586000000	2.200075000000
C	-1.601539000000	2.671754000000	2.077490000000
C	-2.725348000000	2.650404000000	2.893737000000
C	-2.900174000000	1.627098000000	3.830441000000
C	-1.945642000000	0.618096000000	3.951734000000
C	-0.816164000000	0.617618000000	3.135052000000
H	5.251999000000	2.337287000000	-0.990102000000
H	5.606630000000	3.794068000000	-0.018340000000
H	4.280962000000	1.470947000000	1.041123000000
H	4.103939000000	3.105481000000	1.741445000000
H	-1.456450000000	3.470191000000	1.356289000000
H	-3.466640000000	3.438716000000	2.803958000000
H	-3.779672000000	1.620959000000	4.467273000000
H	-2.074302000000	-0.171125000000	4.686153000000
H	-0.060095000000	-0.153386000000	3.248591000000

tsAB



Frequency -149.8792

Zero-point correction= 0.348030 (Hartree/Particle)

Thermal correction to Energy= 0.401903

Thermal correction to Enthalpy= 0.403053

Thermal correction to Gibbs Free Energy= 0.239255

Sum of electronic and zero-point Energies= -3146.257485

Sum of electronic and thermal Energies= -3146.203612

Sum of electronic and thermal Enthalpies= -3146.202462

Sum of electronic and thermal Free Energies= -3146.366260

E(RB3PW91) = -3146.60551490

Atom	**X**	**Y**	**Z**
S	-1.253082000000	0.567015000000	-1.933087000000
C	-2.411489000000	-0.201001000000	-0.144901000000
Yb	0.749721000000	0.053558000000	0.064700000000
O	2.402988000000	-1.432169000000	0.582953000000
O	0.685534000000	2.34465000000	-0.015177000000
C	0.673879000000	3.107958000000	-3.846905000000
C	-1.470453000000	-0.801827000000	0.540919000000
S	2.808520000000	-1.783781000000	-0.841545000000
S	0.851357000000	2.590491000000	1.483314000000
O	-0.120658000000	3.454055000000	2.110246000000
O	1.025334000000	1.191559000000	2.045025000000
C	2.543639000000	3.381978000000	1.640493000000
O	1.839655000000	-0.956959000000	-1.681605000000
O	4.206499000000	-1.728394000000	-1.181254000000
C	2.216095000000	-3.546142000000	-1.067512000000
F	0.908691000000	-3.594885000000	-0.784738000000
F	2.410657000000	-3.912374000000	-2.325404000000
F	2.880354000000	-4.340036000000	-0.245737000000
F	2.517698000000	4.564623000000	1.044557000000
F	2.840369000000	3.514751000000	2.921473000000
F	3.436812000000	2.593081000000	1.042741000000
C	-1.425547000000	2.107416000000	-2.959091000000
C	-1.467729000000	-0.781758000000	-3.119412000000

C -0.332558000000 2.236714000000 -3.967749000000

H -1.404798000000 2.916826000000 -2.224663000000

H -2.422423000000 2.039839000000 -3.404529000000

H -1.473415000000 -1.708326000000 -2.542881000000

H -2.424168000000 -0.656673000000 -3.627121000000

H -0.622650000000 -0.784361000000 -3.809063000000

H -0.400261000000 1.602582000000 -4.849562000000

H 1.432332000000 3.197926000000 -4.618609000000

H 0.763086000000 3.767460000000 -2.986698000000

N -3.626286000000 0.333386000000 -0.059903000000

C -4.114441000000 1.088037000000 1.107927000000

C -5.585159000000 1.269061000000 0.718138000000

O -5.606563000000 1.126185000000 -0.719175000000

C -4.514994000000 0.494941000000 -1.152675000000

H -5.981058000000 2.255175000000 0.959252000000

H -6.229419000000 0.494761000000 1.142923000000

H -3.576376000000 2.038398000000 1.190366000000

H -3.982389000000 0.510194000000 2.023947000000

O -4.291611000000 0.159498000000 -2.285909000000

C -1.728283000000 -1.823707000000 1.574936000000

C -2.818189000000 -2.709722000000 1.484649000000

C -0.852467000000 -1.937568000000 2.669158000000

C -3.025243000000 -3.674361000000 2.466124000000

H -3.482971000000 -2.661396000000 0.626094000000

C -2.159092000000 -3.764576000000 3.558657000000

H -3.861739000000 -4.361426000000 2.376549000000

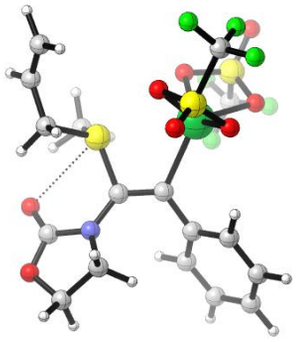
C -1.076193000000 -2.890978000000 3.659699000000

H -2.323125000000 -4.518672000000 4.322543000000

H -0.398231000000 -2.955391000000 4.505486000000

H -0.008919000000 -1.258381000000 2.775768000000

intB



Zero-point correction= 0.349821 (Hartree/Particle)

Thermal correction to Energy= 0.403798

Thermal correction to Enthalpy= 0.404948

Thermal correction to Gibbs Free Energy= 0.240215

Sum of electronic and zero-point Energies= -3146.269231

Sum of electronic and thermal Energies= -3146.215254

Sum of electronic and thermal Enthalpies= -3146.214104

Sum of electronic and thermal Free Energies= -3146.378837

E(RB3PW91) = -3146.61905193

Atom	**X**	**Y**	**Z**
S	-1.269557000000	-0.721638000000	1.774805000000
C	-2.245330000000	-0.429016000000	0.274699000000
Yb	0.888217000000	0.185183000000	-0.214074000000
O	1.963069000000	2.165744000000	-0.572242000000
O	1.455136000000	-1.982641000000	0.267476000000
C	0.451959000000	-3.175204000000	3.788241000000
C	-1.452908000000	0.200004000000	-0.630307000000
S	2.134334000000	2.560629000000	0.887428000000
S	1.911118000000	-2.371227000000	-1.137519000000
O	1.351703000000	-3.577992000000	-1.694729000000
O	1.743259000000	-1.080176000000	-1.922990000000
C	3.766979000000	-2.586711000000	-0.980041000000
O	1.430912000000	1.428381000000	1.633742000000
O	3.447329000000	2.942078000000	1.337707000000
C	0.989633000000	4.026918000000	1.105421000000

F -0.238693000000 3.673504000000 0.706265000000

F 0.956496000000 4.362848000000 2.386926000000

F 1.424559000000 5.035586000000 0.372421000000

F 4.010102000000 -3.613924000000 -0.180104000000

F 4.280290000000 -2.799871000000 -2.178592000000

F 4.278152000000 -1.472363000000 -0.454761000000

C -1.558733000000 -2.386559000000 2.546032000000

C -1.740281000000 0.477027000000 3.048813000000

C -0.722292000000 -2.537150000000 3.776427000000

H -1.269877000000 -3.084404000000 1.755239000000

H -2.631139000000 -2.439053000000 2.746851000000

H -1.665887000000 1.459561000000 2.580086000000

H -2.754600000000 0.270770000000 3.387174000000

H -0.992491000000 0.391382000000 3.840037000000

H -1.135217000000 -2.129972000000 4.696932000000

H 1.012119000000 -3.296528000000 4.710392000000

H 0.882731000000 -3.606014000000 2.887555000000

N -3.542893000000 -0.916189000000 0.135535000000

C -4.013200000000 -1.560063000000 -1.097985000000

C -5.497242000000 -1.746451000000 -0.767486000000

O -5.568143000000 -1.672266000000 0.670698000000

C -4.461794000000 -1.102507000000 1.160626000000

H -5.894635000000 -2.714042000000 -1.074007000000

H -6.119008000000 -0.945353000000 -1.176415000000

H -3.485914000000 -2.509253000000 -1.249576000000

H -3.860892000000 -0.921853000000 -1.969433000000

O -4.293328000000 -0.832458000000 2.330792000000

C -1.973915000000 0.805781000000 -1.868542000000

C -3.084740000000 1.672274000000 -1.847678000000

C -1.303400000000 0.605029000000 -3.090708000000

C -3.509004000000 2.309686000000 -3.010603000000

H -3.597459000000 1.864616000000 -0.908570000000

C -2.847413000000 2.083154000000 -4.220088000000

H -4.357228000000 2.987432000000 -2.973426000000

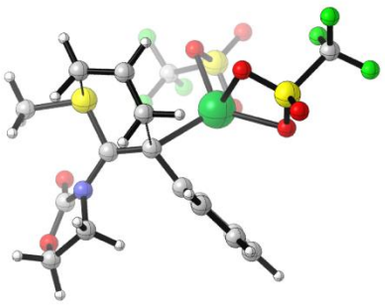
C -1.747806000000 1.225088000000 -4.257326000000

H -3.182628000000 2.579194000000 -5.125981000000

H -1.228208000000 1.043722000000 -5.193601000000

H -0.449675000000 -0.069102000000 -3.142260000000

tsBC



Frequency -315.6671

Zero-point correction= 0.348947 (Hartree/Particle)

Thermal correction to Energy= 0.401747

Thermal correction to Enthalpy= 0.402897

Thermal correction to Gibbs Free Energy= 0.244736

Sum of electronic and zero-point Energies= -3146.241696

Sum of electronic and thermal Energies= -3146.188895

Sum of electronic and thermal Enthalpies= -3146.187745

Sum of electronic and thermal Free Energies= -3146.345907

E(RB3PW91) = -3146.59064244

Atom X Y Z

S 2.641406000000 0.668777000000 -1.844230000000

C 2.543325000000 -0.585390000000 -0.623622000000

Yb -0.829101000000 0.069124000000 0.108877000000

O -0.894310000000 1.837507000000 1.560010000000

O -2.301903000000 -0.787559000000 -1.398379000000

C 0.615952000000 -2.059394000000 -2.353712000000

C 1.262187000000 -0.999239000000 -0.366137000000

S -0.917216000000 2.937880000000 0.507413000000

S -3.230133000000 -1.481916000000 -0.401677000000

O -3.550165000000 -2.863931000000 -0.665399000000

O -2.607941000000 -1.139275000000 0.939009000000

C -4.812112000000 -0.478153000000 -0.471322000000

O -0.760157000000 2.160505000000 -0.796595000000

O -1.970589000000 3.917483000000 0.575712000000

C 0.714461000000 3.828917000000 0.736817000000

F 1.703486000000 2.931924000000 0.743041000000

F 0.888589000000 4.677603000000 -0.266119000000

F 0.690221000000 4.475324000000 1.890328000000

F -5.350838000000 -0.610058000000 -1.672944000000

F -5.641644000000 -0.919184000000 0.459766000000

F -4.511229000000 0.800718000000 -0.245780000000

C 1.949179000000 -0.550032000000 -3.686456000000

C 4.373587000000 0.831317000000 -2.342899000000

C 0.701623000000 -1.039717000000 -3.279919000000

H 2.812823000000 -1.210871000000 -3.651588000000

H 2.002053000000 0.242559000000 -4.429535000000

H 4.887265000000 1.448432000000 -1.604704000000

H 4.851495000000 -0.146128000000 -2.428893000000

H 4.362049000000 1.332195000000 -3.313753000000

H -0.193480000000 -0.475553000000 -3.534101000000

H -0.357445000000 -2.423571000000 -2.039697000000

H 1.453014000000 -2.735193000000 -2.208623000000

N 3.733953000000 -1.112211000000 -0.107995000000

C 3.944935000000 -2.515558000000 0.254338000000

C 5.394161000000 -2.449630000000 0.748413000000

O 5.572456000000 -1.083419000000 1.161412000000

C 4.645126000000 -0.299625000000 0.587910000000

H 6.116677000000 -2.664980000000 -0.044968000000

H 5.589751000000 -3.090922000000 1.607766000000

H 3.827735000000 -3.173676000000 -0.609889000000

H 3.257555000000 -2.833522000000 1.044329000000

O 4.608918000000 0.902762000000 0.665304000000

C 0.912132000000 -1.846805000000 0.803336000000

C 0.867736000000 -1.188217000000 2.061210000000

C 0.390209000000 -3.155317000000 0.732528000000

C 0.352547000000 -1.827146000000 3.194265000000

H 1.300952000000 -0.191429000000 2.162448000000

C -0.139594000000 -3.126869000000 3.101722000000

H 0.343166000000 -1.300627000000 4.144235000000

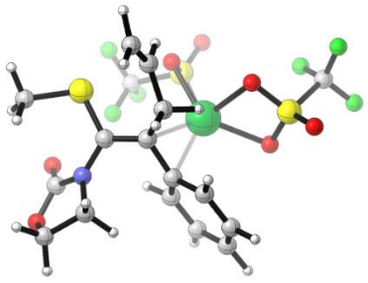
C -0.111913000000 -3.785076000000 1.870117000000

H -0.548410000000 -3.621498000000 3.977019000000

H -0.499391000000 -4.796495000000 1.788131000000

H 0.389687000000 -3.691729000000 -0.210468000000

intC



Zero-point correction= 0.350855 (Hartree/Particle)

Thermal correction to Energy= 0.404116

Thermal correction to Enthalpy= 0.405266

Thermal correction to Gibbs Free Energy= 0.244446

Sum of electronic and zero-point Energies= -3146.296752

Sum of electronic and thermal Energies= -3146.243491

Sum of electronic and thermal Enthalpies= -3146.242341

Sum of electronic and thermal Free Energies= -3146.403161

E(RB3PW91) = -3146.64760708

Atom X Y Z

S -2.835369000000 0.620474000000 1.841008000000

C -2.557931000000 -0.684282000000 0.741887000000

Yb	0.752747000000	0.002816000000	-0.086962000000
O	0.981861000000	1.872051000000	-1.331558000000
O	2.394835000000	-0.721717000000	1.269283000000
C	-0.696809000000	-1.899149000000	2.093910000000
C	-1.319765000000	-1.370691000000	0.777727000000
S	0.748988000000	2.883812000000	-0.209242000000
S	3.316672000000	-1.300961000000	0.192442000000
O	3.778714000000	-2.653268000000	0.383815000000
O	2.564111000000	-0.980762000000	-1.088921000000
C	4.801507000000	-0.153176000000	0.189089000000
O	0.379330000000	1.982074000000	0.966352000000
O	1.756374000000	3.888575000000	0.008277000000
C	-0.845755000000	3.744982000000	-0.687006000000
F	-1.760008000000	2.822248000000	-0.980307000000
F	-1.257214000000	4.480665000000	0.333983000000
F	-0.615404000000	4.505253000000	-1.744214000000
F	5.427644000000	-0.266014000000	1.348255000000
F	5.600496000000	-0.496862000000	-0.807264000000
F	4.370189000000	1.094888000000	0.021133000000
C	-1.221091000000	-1.509720000000	4.506942000000
C	-4.631980000000	0.744543000000	2.057004000000
C	-0.748387000000	-1.064573000000	3.341087000000
H	-1.674048000000	-2.494195000000	4.604601000000
H	-1.162368000000	-0.905749000000	5.407187000000
H	-5.065623000000	1.384164000000	1.287318000000
H	-5.094390000000	-0.244281000000	2.055938000000
H	-4.770617000000	1.197953000000	3.041055000000
H	-0.288173000000	-0.076846000000	3.300889000000
H	0.363159000000	-2.129822000000	1.903990000000
H	-1.158365000000	-2.874135000000	2.310881000000
N	-3.549790000000	-1.058492000000	-0.143314000000
C	-3.855132000000	-2.443071000000	-0.522241000000
C	-5.266721000000	-2.265425000000	-1.085131000000

O -5.298858000000 -0.896847000000 -1.528534000000

C -4.366032000000 -0.174052000000 -0.890119000000

H -6.043023000000 -2.400385000000 -0.325621000000

H -5.476173000000 -2.902304000000 -1.944249000000

H -3.820615000000 -3.102567000000 0.346804000000

H -3.161837000000 -2.811878000000 -1.285243000000

O -4.231610000000 1.016163000000 -0.979594000000

C -0.854850000000 -2.033029000000 -0.472805000000

C -0.950529000000 -1.334605000000 -1.714481000000

C -0.139493000000 -3.250067000000 -0.479999000000

C -0.404363000000 -1.854825000000 -2.890521000000

H -1.519603000000 -0.401798000000 -1.769114000000

C 0.275740000000 -3.073935000000 -2.867690000000

H -0.505168000000 -1.298448000000 -3.818073000000

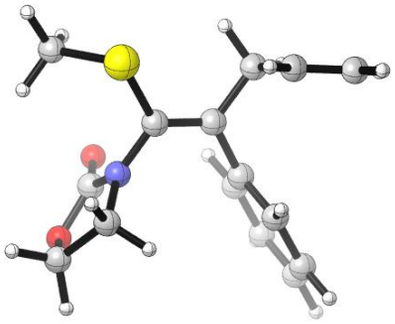
C 0.402680000000 -3.761750000000 -1.661364000000

H 0.713762000000 -3.473851000000 -3.776477000000

H 0.940030000000 -4.705046000000 -1.629593000000

H -0.021330000000 -3.816476000000 0.437968000000

3aw



Zero-point correction= 0.291872 (Hartree/Particle)

Thermal correction to Energy= 0.319003

Thermal correction to Enthalpy= 0.320153

Thermal correction to Gibbs Free Energy= 0.224370

Sum of electronic and zero-point Energies= -1184.585691

Sum of electronic and thermal Energies= -1184.558561

Sum of electronic and thermal Enthalpies= -1184.557410

Sum of electronic and thermal Free Energies= -1184.653194

E(RB3PW91) = -1184.87756348

Atom	X	Y	Z
S	1.823911000000	2.232675000000	-0.183015000000
C	0.771725000000	0.803093000000	-0.023343000000
C	-1.190069000000	2.191448000000	0.737333000000
C	-0.535856000000	0.896345000000	0.299127000000
C	-3.176564000000	3.162436000000	-0.474188000000
C	3.267752000000	1.734327000000	0.806056000000
C	-1.865791000000	2.921695000000	-0.393739000000
H	-3.866246000000	2.824249000000	0.296367000000
H	-3.602699000000	3.708604000000	-1.311358000000
H	2.986793000000	1.557400000000	1.845489000000
H	3.741436000000	0.841320000000	0.393092000000
H	3.973690000000	2.566716000000	0.750941000000
H	-1.206673000000	3.273369000000	-1.188614000000
H	-0.420654000000	2.841743000000	1.171882000000
H	-1.928243000000	1.962530000000	1.514571000000
N	1.363408000000	-0.439998000000	-0.356061000000
C	1.538914000000	-0.907448000000	-1.719589000000
C	2.385760000000	-2.168842000000	-1.485922000000
O	2.274867000000	-2.451000000000	-0.084821000000
C	1.757118000000	-1.374194000000	0.573661000000
H	3.443363000000	-2.006243000000	-1.720230000000
H	2.024059000000	-3.037588000000	-2.039315000000
H	2.055624000000	-0.160251000000	-2.330848000000
H	0.567357000000	-1.130833000000	-2.178615000000
O	1.688913000000	-1.303518000000	1.778575000000
C	-1.425447000000	-0.301343000000	0.223183000000
C	-2.200519000000	-0.537613000000	-0.921345000000
C	-1.541958000000	-1.173503000000	1.314223000000

C -3.065575000000 -1.631470000000 -0.977773000000

H -2.130940000000 0.143878000000 -1.764818000000

C -3.171622000000 -2.498171000000 0.110243000000

H -3.659037000000 -1.802471000000 -1.872257000000

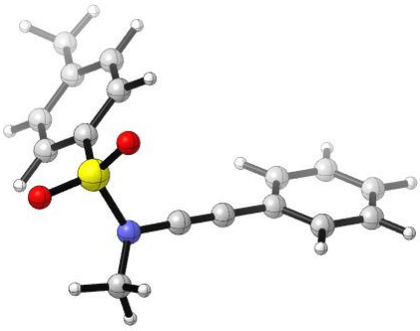
C -2.407817000000 -2.265438000000 1.254884000000

H -3.845014000000 -3.349968000000 0.066304000000

H -2.478277000000 -2.939561000000 2.104320000000

H -0.931527000000 -1.007475000000 2.196864000000

1a’ N-sulfonyl ynamides



Zero-point correction= 0.273734 (Hartree/Particle)

Thermal correction to Energy= 0.301150

Thermal correction to Enthalpy= 0.302300

Thermal correction to Gibbs Free Energy= 0.204527

Sum of electronic and zero-point Energies= -1221.399957

Sum of electronic and thermal Energies= -1221.372540

Sum of electronic and thermal Enthalpies= -1221.371390

Sum of electronic and thermal Free Energies= -1221.469163

E(RB3PW91) = -1221.67369039

Atom X Y Z

C 0.645768000000 -1.376826000000 -0.467732000000

C 1.702495000000 -0.787222000000 -0.339417000000

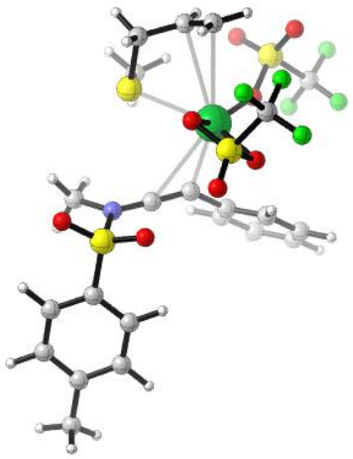
C 2.942195000000 -0.098959000000 -0.186427000000

N -0.525321000000 -2.011129000000 -0.661771000000

C 3.017655000000 1.293078000000 -0.381930000000

C	4.228708000000	1.961098000000	-0.228715000000
C	5.385691000000	1.255322000000	0.107315000000
C	5.322562000000	-0.126580000000	0.297294000000
C	4.112503000000	-0.799879000000	0.160292000000
C	-0.499925000000	-3.357435000000	-1.255241000000
C	-2.055882000000	0.045454000000	0.250722000000
C	-2.805935000000	0.471226000000	-0.847061000000
C	-3.031589000000	1.831223000000	-1.018064000000
C	-2.521886000000	2.772619000000	-0.109109000000
C	-1.777255000000	2.312020000000	0.982254000000
C	-1.538766000000	0.951487000000	1.171767000000
C	-2.784328000000	4.240890000000	-0.308905000000
S	-1.779563000000	-1.694842000000	0.492814000000
O	-2.925379000000	-2.453557000000	-0.007074000000
O	-1.282197000000	-1.896151000000	1.851188000000
H	2.118667000000	1.837373000000	-0.655089000000
H	4.272135000000	3.036557000000	-0.378972000000
H	6.330841000000	1.778870000000	0.220501000000
H	6.218958000000	-0.681240000000	0.560984000000
H	4.058122000000	-1.872463000000	0.319809000000
H	0.050125000000	-3.291316000000	-2.196099000000
H	-0.014045000000	-4.083103000000	-0.593990000000
H	-1.526467000000	-3.666234000000	-1.453840000000
H	-3.211363000000	-0.254838000000	-1.544466000000
H	-3.618794000000	2.170526000000	-1.868046000000
H	-1.378596000000	3.025163000000	1.699170000000
H	-0.968331000000	0.591094000000	2.021436000000
H	-3.858588000000	4.454867000000	-0.282667000000
H	-2.302779000000	4.843431000000	0.465287000000
H	-2.411085000000	4.579257000000	-1.281817000000

intA’



Zero-point correction= 0.443812 (Hartree/Particle)

Thermal correction to Energy= 0.509957

Thermal correction to Enthalpy= 0.511107

Thermal correction to Gibbs Free Energy= 0.314914

Sum of electronic and zero-point Energies= -3738.338267

Sum of electronic and thermal Energies= -3738.272122

Sum of electronic and thermal Enthalpies= -3738.270972

Sum of electronic and thermal Free Energies= -3738.467165

E(RB3PW91) = -3738.78207892

Atom	**X**	**Y**	**Z**
Yb	1.061557000000	0.414456000000	-0.202051000000
O	2.624113000000	-0.984683000000	-0.111518000000
O	0.732790000000	1.266918000000	1.881824000000
S	4.068498000000	-1.357667000000	-0.558709000000
S	0.354637000000	2.691048000000	1.484242000000
O	0.485737000000	2.658206000000	-0.031977000000
O	-0.837534000000	3.259742000000	2.055375000000
O	4.055471000000	-1.753362000000	-1.964819000000
O	5.024762000000	-0.367331000000	-0.089245000000

C	4.324146000000	-2.912689000000	0.448420000000
C	1.806082000000	3.719834000000	2.074791000000
F	3.403844000000	-3.817656000000	0.117321000000
F	5.534372000000	-3.392046000000	0.190340000000
F	4.219289000000	-2.629182000000	1.744477000000
F	2.942281000000	3.144801000000	1.670322000000
F	1.713695000000	4.935254000000	1.552210000000
F	1.781987000000	3.781973000000	3.395075000000
S	0.497123000000	0.598342000000	-3.012844000000
C	1.835013000000	1.827206000000	-3.328760000000
C	1.200333000000	-0.931416000000	-3.719447000000
C	3.003317000000	1.565487000000	-2.430654000000
C	3.362238000000	2.359558000000	-1.408472000000
H	1.377696000000	2.803593000000	-3.144434000000
H	2.094551000000	1.759650000000	-4.389900000000
H	0.480121000000	-1.728439000000	-3.523419000000
H	1.299869000000	-0.799643000000	-4.798831000000
H	2.160289000000	-1.196898000000	-3.270859000000
H	3.594084000000	0.675525000000	-2.646677000000
H	4.227584000000	2.111360000000	-0.799391000000
H	2.840411000000	3.290056000000	-1.199646000000
N	-2.840753000000	-0.294805000000	-1.439989000000
C	-1.881270000000	-0.785189000000	-0.746436000000
C	-0.898460000000	-1.109837000000	-0.014549000000
C	-0.595194000000	-2.212849000000	0.910862000000
C	-0.752094000000	-3.547346000000	0.498613000000
C	-0.439496000000	-4.586153000000	1.369952000000
C	0.023520000000	-4.311280000000	2.658907000000
C	0.176449000000	-2.988986000000	3.072789000000
C	-0.118818000000	-1.939468000000	2.203187000000
H	-1.108554000000	-3.764897000000	-0.504120000000
H	-0.560535000000	-5.614512000000	1.041942000000
H	0.264794000000	-5.125600000000	3.335444000000

H 0.529200000000 -2.767306000000 4.075649000000

H -0.019342000000 -0.913212000000 2.546217000000

C -3.172447000000 -0.674889000000 -2.822794000000

H -4.188146000000 -1.077686000000 -2.852435000000

H -3.103528000000 0.203305000000 -3.466472000000

H -2.473228000000 -1.444347000000 -3.150045000000

S -3.883840000000 1.009812000000 -0.668304000000

O -3.097577000000 1.391341000000 0.489847000000

O -4.153439000000 1.887763000000 -1.794935000000

C -5.340178000000 0.146544000000 -0.191479000000

C -5.362975000000 -0.519946000000 1.038222000000

C -6.447818000000 0.162919000000 -1.043641000000

C -6.522422000000 -1.191157000000 1.404406000000

H -4.500266000000 -0.494994000000 1.696425000000

C -7.596638000000 -0.515572000000 -0.650101000000

H -6.415896000000 0.715974000000 -1.977029000000

C -7.655134000000 -1.201489000000 0.572585000000

H -6.555157000000 -1.707638000000 2.359874000000

H -8.467286000000 -0.501984000000 -1.299949000000

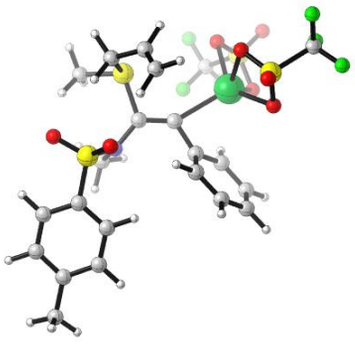
C -8.912043000000 -1.900971000000 1.003883000000

H -9.538849000000 -2.167887000000 0.149518000000

H -8.690450000000 -2.810394000000 1.569296000000

H -9.504234000000 -1.247733000000 1.656331000000

intB’



Zero-point correction= 0.444706 (Hartree/Particle)

Thermal correction to Energy= 0.509280

Thermal correction to Enthalpy= 0.510430

Thermal correction to Gibbs Free Energy= 0.321418

Sum of electronic and zero-point Energies= -3738.324546

Sum of electronic and thermal Energies= -3738.259972

Sum of electronic and thermal Enthalpies= -3738.258822

Sum of electronic and thermal Free Energies= -3738.447833

E(RB3PW91) = -3738.76925167

Atom	**X**	**Y**	**Z**
S	-0.919011000000	1.762356000000	2.096923000000
C	-1.565336000000	0.870988000000	0.620017000000
Yb	1.783184000000	-0.062842000000	-0.258017000000
O	2.782880000000	1.339169000000	-1.765421000000
O	2.722077000000	-1.287478000000	1.419762000000
C	-0.386130000000	-1.752005000000	3.318915000000
C	-0.565283000000	0.281115000000	-0.049816000000
S	3.286336000000	2.373463000000	-0.765752000000
S	2.931090000000	-2.575391000000	0.631501000000
O	2.466651000000	-3.801437000000	1.233657000000
O	2.410399000000	-2.221467000000	-0.751123000000
C	4.788864000000	-2.689785000000	0.420531000000
O	2.761381000000	1.856039000000	0.561616000000
O	4.668722000000	2.768396000000	-0.844922000000
C	2.241440000000	3.885222000000	-1.118453000000
F	0.945429000000	3.539679000000	-1.073345000000
F	2.479511000000	4.807275000000	-0.197180000000
F	2.529292000000	4.351936000000	-2.322659000000
F	5.350743000000	-2.858042000000	1.607123000000
F	5.071361000000	-3.710531000000	-0.373599000000
F	5.223797000000	-1.554066000000	-0.129738000000
C	-1.140382000000	0.603212000000	3.540568000000
C	-2.104718000000	3.063063000000	2.518174000000

C -0.098506000000 -0.462215000000 3.522856000000

H -2.159079000000 0.213185000000 3.504824000000

H -1.027775000000 1.273483000000 4.400602000000

H -2.048722000000 3.829419000000 1.743593000000

H -3.111025000000 2.647660000000 2.612015000000

H -1.771915000000 3.491117000000 3.466725000000

H 0.924635000000 -0.153404000000 3.733022000000

H 0.390979000000 -2.509183000000 3.363716000000

H -1.402249000000 -2.081927000000 3.120140000000

N -2.931070000000 0.914098000000 0.283746000000

C -0.749614000000 -0.628765000000 -1.193154000000

C -0.084238000000 -0.325262000000 -2.406092000000

C -1.335076000000 -1.903140000000 -1.050063000000

C -0.049294000000 -1.250804000000 -3.454667000000

H 0.325430000000 0.674236000000 -2.569379000000

C -0.637444000000 -2.503110000000 -3.296551000000

H 0.439005000000 -0.986307000000 -4.387998000000

C -1.276778000000 -2.822164000000 -2.094288000000

H -0.592462000000 -3.231906000000 -4.099888000000

H -1.725621000000 -3.803461000000 -1.966018000000

H -1.814683000000 -2.158762000000 -0.109744000000

C -3.453452000000 2.082344000000 -0.441259000000

H -4.323724000000 1.777712000000 -1.027016000000

H -3.744649000000 2.906448000000 0.218505000000

H -2.679802000000 2.420180000000 -1.132916000000

S -4.031893000000 0.048341000000 1.272311000000

O -3.293851000000 -1.154263000000 1.664553000000

C -5.364826000000 -0.336127000000 0.173649000000

C -6.620434000000 0.218395000000 0.426282000000

C -5.156940000000 -1.217773000000 -0.891089000000

C -7.682211000000 -0.120886000000 -0.408510000000

H -6.758854000000 0.892314000000 1.265400000000

C -6.230307000000 -1.536997000000 -1.713000000000

H -4.175793000000 -1.642768000000 -1.073803000000

C -7.508986000000 -1.000336000000 -1.485752000000

H -8.663515000000 0.303797000000 -0.215319000000

H -6.077447000000 -2.220018000000 -2.544490000000

C -8.666639000000 -1.387354000000 -2.361964000000

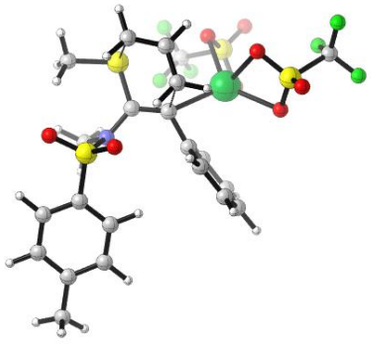
H -9.471304000000 -0.649428000000 -2.315763000000

H -8.359449000000 -1.498629000000 -3.405825000000

H -9.082462000000 -2.349901000000 -2.040311000000

O -4.541095000000 0.941561000000 2.322096000000

tsB'C'



Frequency -311.8374

Zero-point correction= 0.444423 (Hartree/Particle)

Thermal correction to Energy= 0.507683

Thermal correction to Enthalpy= 0.508833

Thermal correction to Gibbs Free Energy= 0.326694

Sum of electronic and zero-point Energies= -3738.297724

Sum of electronic and thermal Energies= -3738.234464

Sum of electronic and thermal Enthalpies= -3738.233314

Sum of electronic and thermal Free Energies= -3738.415453

E(RB3PW91) = -3738.74214752

Atom X Y Z

S -0.927676000000 2.349082000000 1.724168000000

C -1.571516000000 1.012706000000 0.764859000000

Yb 1.659565000000 -0.125737000000 -0.090449000000

O	2.385279000000	1.057025000000	-1.911029000000
O	3.001743000000	-1.071275000000	1.488878000000
C	-0.142681000000	-0.875267000000	2.565552000000
C	-0.640787000000	0.038242000000	0.520806000000
S	2.883805000000	2.282324000000	-1.157587000000
S	3.321596000000	-2.362132000000	0.737097000000
O	3.162901000000	-3.598869000000	1.462093000000
O	2.555051000000	-2.197941000000	-0.562822000000
C	5.123598000000	-2.178236000000	0.256147000000
O	2.496943000000	1.982658000000	0.281989000000
O	4.225227000000	2.737251000000	-1.416360000000
C	1.713645000000	3.640691000000	-1.692640000000
F	0.450144000000	3.224440000000	-1.514997000000
F	1.925363000000	4.722465000000	-0.958321000000
F	1.910304000000	3.906669000000	-2.973643000000
F	5.865290000000	-2.170947000000	1.351910000000
F	5.465155000000	-3.188084000000	-0.528026000000
F	5.269318000000	-1.025210000000	-0.398929000000
C	-0.498867000000	1.198484000000	3.734484000000
C	-2.328787000000	3.316220000000	2.349482000000
C	0.358152000000	0.179309000000	3.310407000000
H	-1.555579000000	0.980325000000	3.870184000000
H	-0.106627000000	2.031071000000	4.313913000000
H	-2.560681000000	4.108791000000	1.635899000000
H	-3.200066000000	2.683126000000	2.534167000000
H	-1.990580000000	3.771657000000	3.283346000000
H	1.433900000000	0.314280000000	3.408072000000
H	0.518963000000	-1.684530000000	2.262900000000
H	-1.203046000000	-1.107115000000	2.596482000000
N	-2.917765000000	0.990347000000	0.346973000000
C	-0.854605000000	-1.075779000000	-0.435658000000
C	-0.503805000000	-0.812119000000	-1.785115000000
C	-1.137450000000	-2.409521000000	-0.081414000000

C -0.463218000000 -1.835433000000 -2.738395000000

H -0.337696000000 0.217758000000 -2.108188000000

C -0.749355000000 -3.145536000000 -2.364626000000

H -0.206751000000 -1.598134000000 -3.766800000000

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C -3.470061000000 2.103340000000 -0.436937000000

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H -3.964903000000 2.861517000000 0.177714000000

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O -3.272349000000 -0.946536000000 1.934158000000

C -5.228174000000 -0.478954000000 0.169922000000

C -6.532846000000 0.015130000000 0.210821000000

C -4.851602000000 -1.474544000000 -0.735433000000

C -7.472432000000 -0.503773000000 -0.676161000000

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C -5.806167000000 -1.974224000000 -1.612708000000

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O -4.723719000000 1.108138000000 2.203501000000

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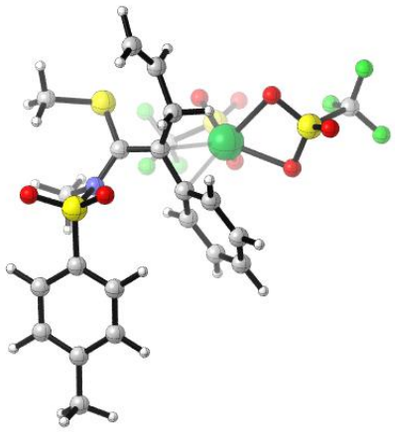

Zero-point correction= 0.446236 (Hartree/Particle)

Thermal correction to Energy= 0.510002

Thermal correction to Enthalpy= 0.511152

Thermal correction to Gibbs Free Energy= 0.325906

Sum of electronic and zero-point Energies= -3738.350868

Sum of electronic and thermal Energies= -3738.287102

Sum of electronic and thermal Enthalpies= -3738.285952

Sum of electronic and thermal Free Energies= -3738.471197

E(RB3PW91) = -3738.79710374

Atom	**X**	**Y**	**Z**
S	-0.899272000000	2.624402000000	1.807534000000
C	-1.497672000000	1.089147000000	1.232207000000
Yb	1.493996000000	-0.087701000000	-0.018003000000
O	2.030109000000	0.901737000000	-1.991784000000
O	3.120575000000	-0.878738000000	1.322395000000
C	-0.051018000000	-0.443984000000	2.738696000000
C	-0.692922000000	-0.056661000000	1.386757000000
S	2.406350000000	2.267832000000	-1.428851000000
S	3.456696000000	-2.139631000000	0.521562000000
O	3.493615000000	-3.387299000000	1.242422000000
O	2.516038000000	-2.033539000000	-0.667900000000
C	5.165435000000	-1.800480000000	-0.175118000000
O	2.075285000000	2.121773000000	0.049956000000
O	3.687645000000	2.818011000000	-1.784494000000

C	1.087628000000	3.412780000000	-2.102653000000
F	-0.118271000000	2.868462000000	-1.871687000000
F	1.165687000000	4.583455000000	-1.492155000000
F	1.260353000000	3.555763000000	-3.405384000000
F	6.033143000000	-1.763036000000	0.821937000000
F	5.476051000000	-2.764851000000	-1.026237000000
F	5.141959000000	-0.626845000000	-0.804527000000
C	-0.151931000000	0.689829000000	4.958165000000
C	-2.342552000000	3.429029000000	2.577624000000
C	0.360412000000	0.606859000000	3.728039000000
H	-0.960756000000	0.040920000000	5.287072000000
H	0.227721000000	1.407316000000	5.679542000000
H	-2.651504000000	4.294275000000	1.988673000000
H	-3.167398000000	2.722139000000	2.685433000000
H	-2.022568000000	3.755201000000	3.569655000000
H	1.181067000000	1.266758000000	3.449501000000
H	0.826949000000	-1.088831000000	2.557353000000
H	-0.786276000000	-1.101825000000	3.224013000000
N	-2.718870000000	1.032569000000	0.593022000000
C	-0.834410000000	-1.185115000000	0.418130000000
C	-0.894972000000	-0.909044000000	-0.978434000000
C	-0.672062000000	-2.535011000000	0.793896000000
C	-0.827027000000	-1.927756000000	-1.930840000000
H	-1.062840000000	0.115544000000	-1.316065000000
C	-0.685165000000	-3.256650000000	-1.525896000000
H	-0.878763000000	-1.676765000000	-2.986349000000
C	-0.614771000000	-3.549853000000	-0.165008000000
H	-0.615172000000	-4.050017000000	-2.263285000000
H	-0.497871000000	-4.578668000000	0.163016000000
H	-0.620886000000	-2.803877000000	1.842879000000
C	-3.256208000000	2.159483000000	-0.179592000000
H	-3.803304000000	1.763722000000	-1.039810000000
H	-3.928179000000	2.787801000000	0.410003000000

H -2.421141000000 2.760272000000 -0.540329000000

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O -3.283454000000 -1.006240000000 2.082894000000

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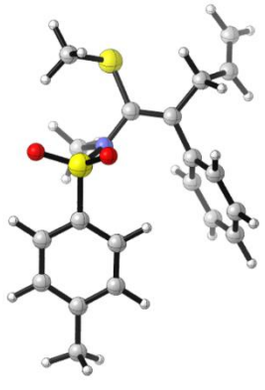

Zero-point correction= 0.387727 (Hartree/Particle)

Thermal correction to Energy= 0.424856

Thermal correction to Enthalpy= 0.426006

Thermal correction to Gibbs Free Energy= 0.308785

Sum of electronic and zero-point Energies= -1776.633039

Sum of electronic and thermal Energies= -1776.595909

Sum of electronic and thermal Enthalpies= -1776.594759

Sum of electronic and thermal Free Energies= -1776.711980

E(RB3PW91) = -1777.02076542

Atom	**X**	**Y**	**Z**
S	3.022973000000	-1.918900000000	0.541973000000
C	1.761629000000	-0.690848000000	0.241433000000
C	3.473858000000	0.919722000000	-0.667771000000
C	2.086932000000	0.556402000000	-0.177801000000
C	5.426468000000	1.356058000000	0.855500000000
C	2.530273000000	-3.300060000000	-0.538398000000
C	4.249909000000	1.724273000000	0.343748000000
H	5.902828000000	0.420535000000	0.570437000000
H	5.948990000000	1.976538000000	1.578578000000
H	3.240829000000	-4.104279000000	-0.330069000000
H	1.518124000000	-3.646802000000	-0.320842000000
H	2.602531000000	-3.015255000000	-1.590141000000
H	3.797080000000	2.664056000000	0.661348000000
H	3.359444000000	1.522867000000	-1.579830000000
H	4.029931000000	0.016570000000	-0.929453000000
N	0.408865000000	-1.018710000000	0.568163000000
C	1.113945000000	1.682383000000	-0.145865000000
C	0.547506000000	2.105679000000	1.065791000000
C	0.812362000000	2.403242000000	-1.311403000000
C	-0.294738000000	3.215513000000	1.112180000000
H	0.784644000000	1.565888000000	1.977899000000
C	-0.590430000000	3.922700000000	-0.054543000000
H	-0.715819000000	3.531442000000	2.063075000000
C	-0.037535000000	3.508508000000	-1.267654000000
H	-1.242141000000	4.791621000000	-0.018282000000
H	-0.265596000000	4.047045000000	-2.183805000000
H	1.225547000000	2.081618000000	-2.263423000000

C	0.156588000000	-1.654847000000	1.863189000000
H	-0.914621000000	-1.614234000000	2.079016000000
H	0.494882000000	-2.695609000000	1.902094000000
H	0.683803000000	-1.080424000000	2.627927000000
S	-0.600183000000	-1.582573000000	-0.690792000000
O	-0.099891000000	-0.983374000000	-1.925157000000
C	-2.184313000000	-0.871246000000	-0.274708000000
C	-3.193269000000	-1.701174000000	0.209180000000
C	-2.407083000000	0.491658000000	-0.478850000000
C	-4.441384000000	-1.151300000000	0.501936000000
H	-3.000934000000	-2.761718000000	0.336119000000
C	-3.658090000000	1.020056000000	-0.182637000000
H	-1.616409000000	1.124896000000	-0.867674000000
C	-4.693665000000	0.211943000000	0.313025000000
H	-5.231632000000	-1.796974000000	0.876977000000
H	-3.834805000000	2.080979000000	-0.342282000000
C	-6.042559000000	0.805724000000	0.619213000000
H	-6.727850000000	0.057455000000	1.026112000000
H	-5.959621000000	1.619837000000	1.347986000000
H	-6.500676000000	1.225689000000	-0.283543000000
O	-0.763066000000	-3.039567000000	-0.585796000000

X-ray crystallography:[20]

X-ray reflections for 5ag were collected on Bruker D8 Quest CCD diffractometer using Mo-Kα, radiation. Data reduction was performed using CrysAlisPro (version 1.171.33.55). Apex 2 and SHELXL 97 program were used to solve and refine the data. All non-hydrogen atoms were refined anisotropically,and C−H hydrogens were fixed.

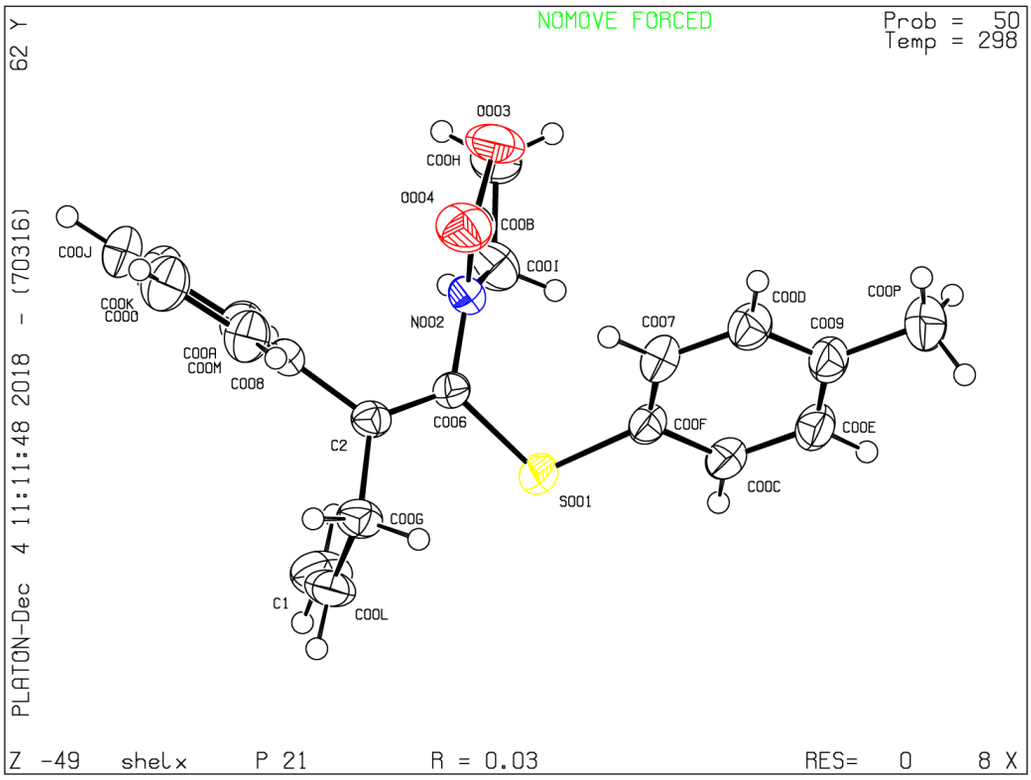

Figure S3. Molecular structure of compound **3d**, {oxygen (red), nitrogen (blue), and Sulphur (yellow)}

Table S3. Crystallographic Data for Compound **3d**

Compound	**3d**
Formula	351.45
Formula weight	$C_{21}H_{21}NO_2S$
Crystal system	Monoclinic
Space group	P 21
T (K)	298 K

a [Å]	6.1683 (9)
b [Å]	18.221 (3)
C [Å]	8.3375 (14)
α [°]	90
β [°]	100.838 (5)
γ [°]	90
V [Å^3]	920.4 (3)
Z	2
ρ_{calcd} [gcm^{-3}]	1.268
μ [mm^{-1}]	0.189
Total reflns	16985
Unique reflns	4130
observed	3877
R_1[I>2σ(I)]	0.0287 (3877)
wR2 [all]	0.0744 (4130)
GOF	1.056
Diffractometer	Bruker D8 Quest CCD
CCDC Number	2064571

References:

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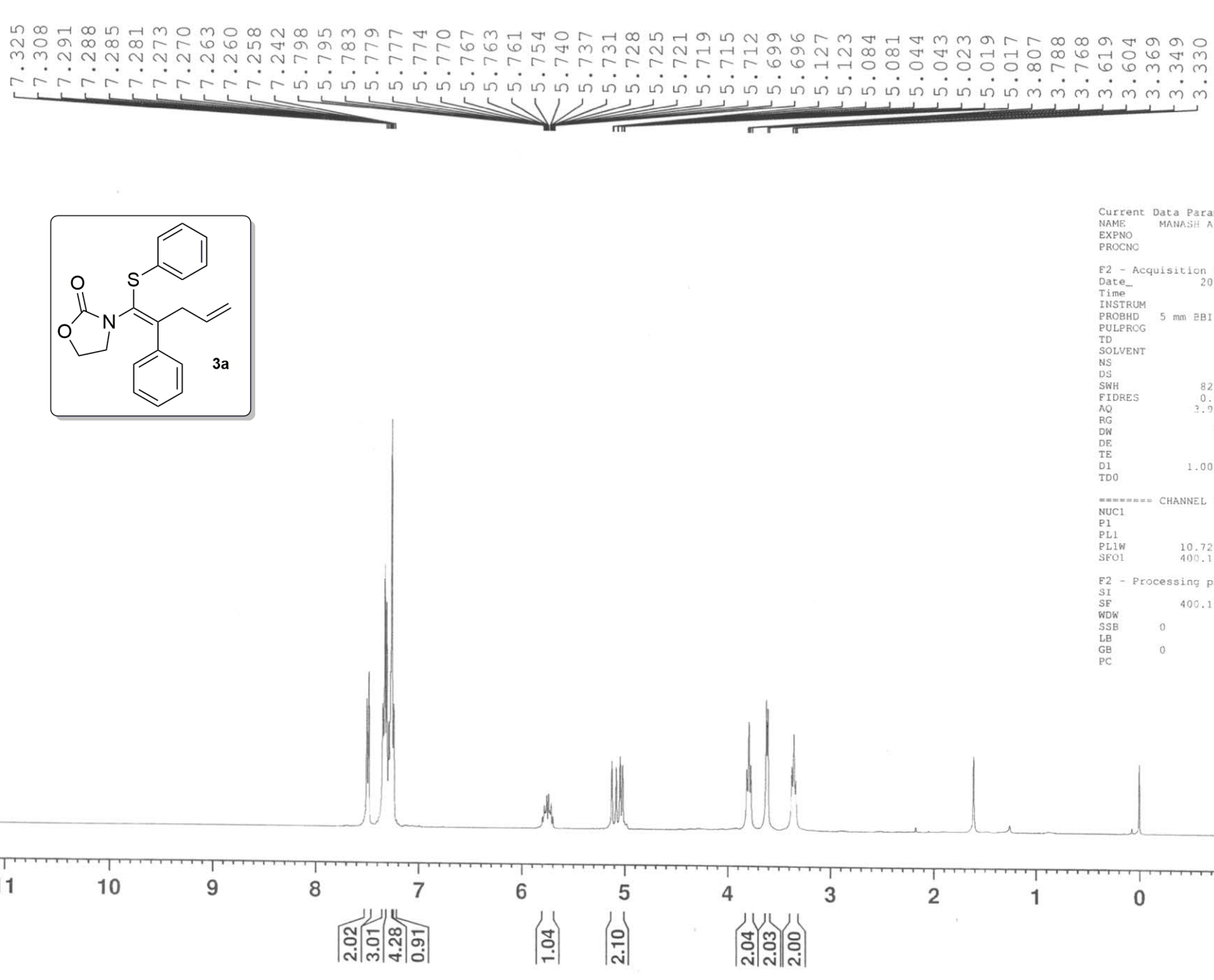
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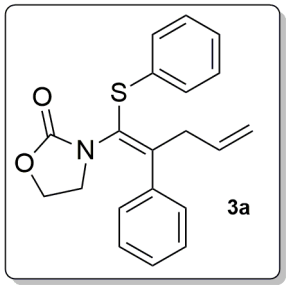

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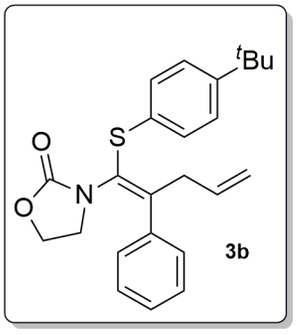
TE                   673.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                    30.00 usec
PL1                    4.50 dB
PL1W           94.86473846 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                     1H
PCPD2                 90.00 usec
PL2                    1.00 dB
PL12                  18.81 dB
PL13                 120.00 dB
PL2W           10.72012138 W
PL12W           0.11199529 W
PL13W       0 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF            100.6127745 MHz
WDW                       EM
SSB         0
LB                     1.00 Hz
GB          0
PC                     1.40
```

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



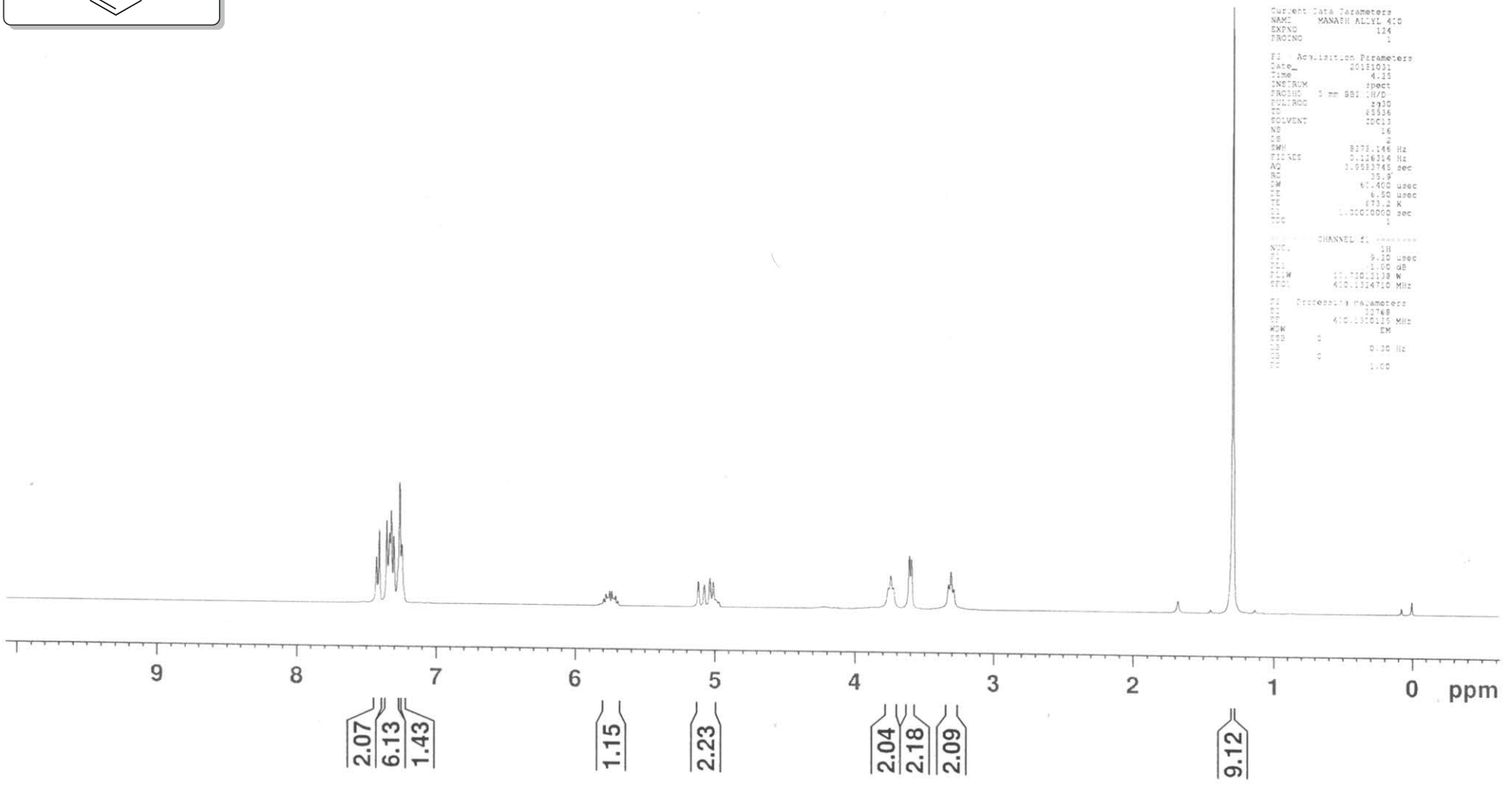
7.425
7.405
7.351
7.330
7.319
7.302
7.272
7.260
7.244
5.794
5.778
5.768
5.762
5.752
5.736
5.726
5.720
5.710
5.694
5.117
5.075
5.035
5.010
3.759
3.741
3.722
3.606
3.591
3.324
3.305
3.285
1.289

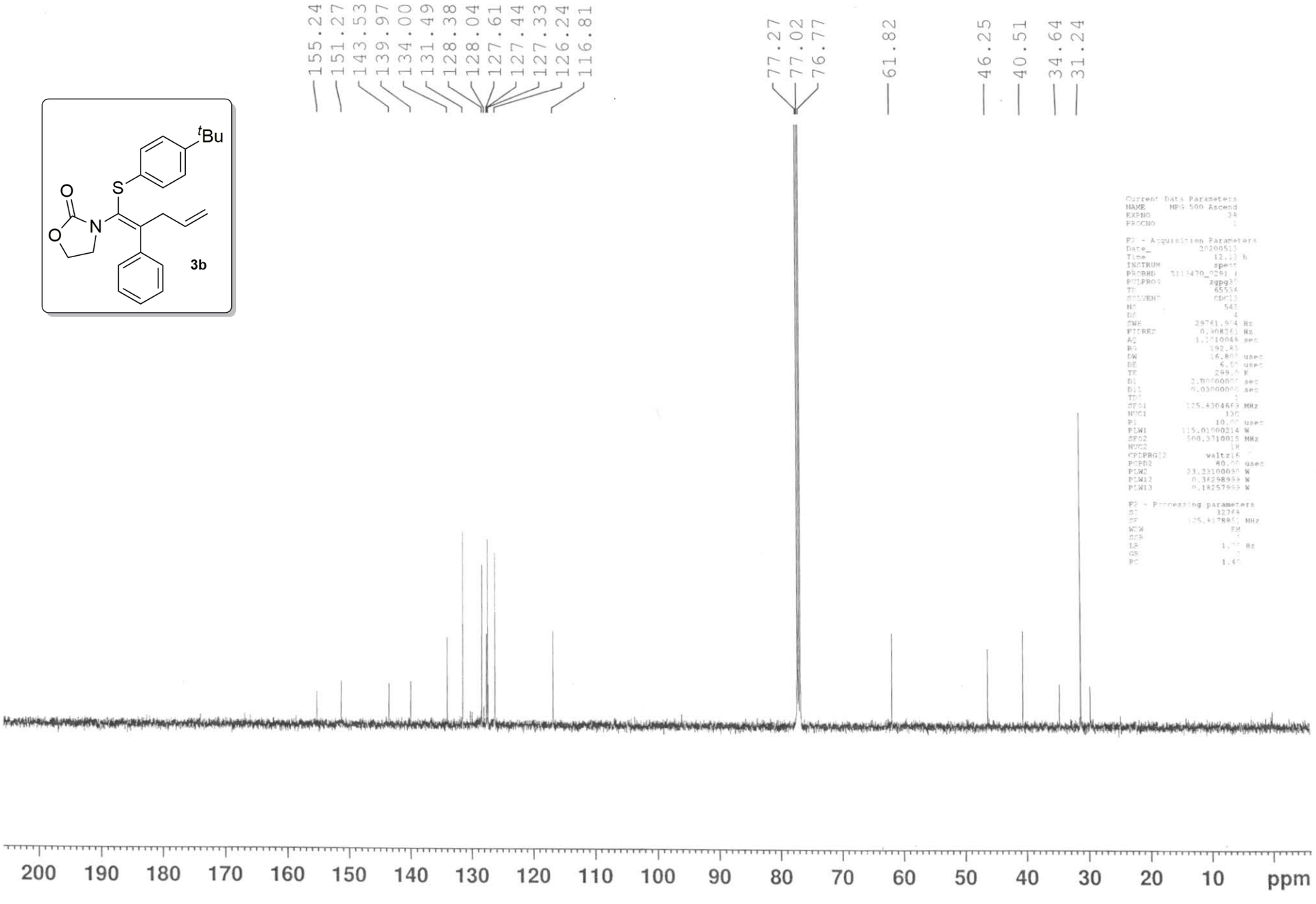
Current Data Parameters
NAME MANASH ALLYL 4CO
EXPNO 124
PROCNO 1

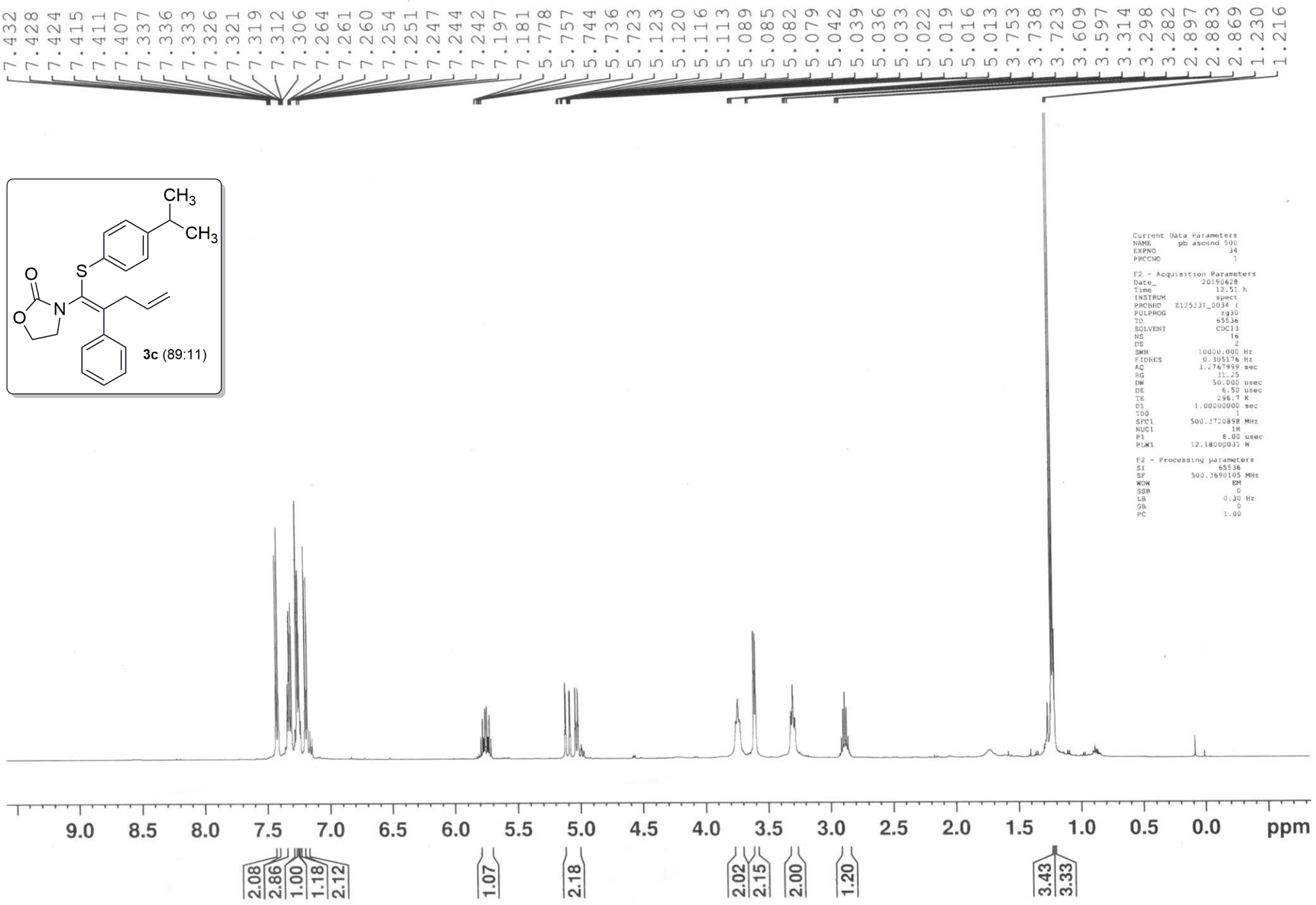
F1 Acquisition Parameters
Date_ 20181031
Time 4.25
INSTRUM spect
PROBHD 5 mm BBI 1H/D
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.95833745 sec
RG 35.9
DW 60.400 usec
DE 6.50 usec
TE 273.2 K
D1 1.00000000 sec
TD0 1

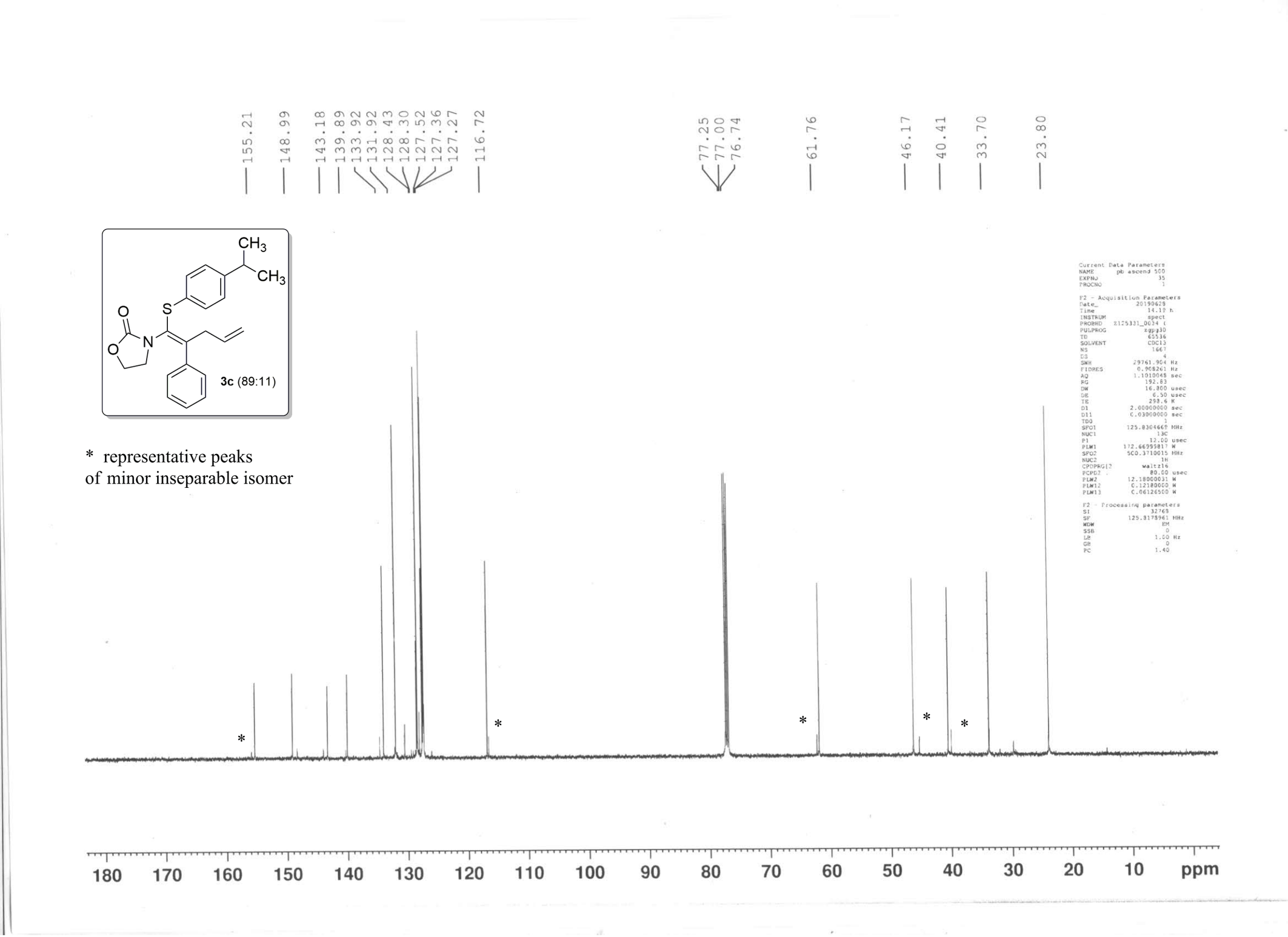
CHANNEL f1
NUC1 1H
P1 9.20 usec
PL1 1.00 dB
PL1W 11.72012138 W
SFO1 400.1324710 MHz

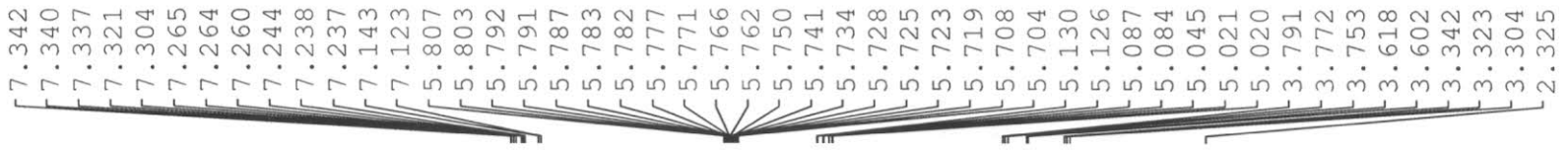
F2 Processing parameters
SI 32768
SF 400.1300135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

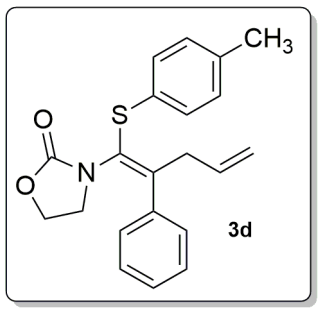



155.24
151.27
143.53
139.97
134.00
131.49
128.38
128.04
127.61
127.44
127.33
126.24
116.81
77.27
77.02
76.77
61.82
46.25
40.51
34.64
31.24
tBu
S
O
N
O
3b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.432
7.428
7.424
7.415
7.411
7.407
7.337
7.336
7.333
7.326
7.321
7.319
7.312
7.306
7.264
7.261
7.260
7.254
7.251
7.247
7.244
7.242
7.197
7.181
5.778
5.757
5.744
5.736
5.723
5.123
5.120
5.116
5.113
5.089
5.085
5.082
5.079
5.042
5.039
5.036
5.033
5.022
5.019
5.016
5.013
3.753
3.738
3.723
3.609
3.597
3.314
3.298
3.282
2.897
2.883
2.869
1.230
1.216
CH3
CH3
S
O
N
O
3c (89:11)
Current Data Parameters
NAME pb ascend 500
EXPNO 34
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190628
Time 12.51 h
INSTRUM spect
PROBHD Z125331_0034 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1
SFO1 500.2720898 MHz
NUC1 1H
P1 8.00 usec
PLW1 12.18000031 W
F2 - Processing parameters
SI 65536
SF 500.3690105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.08
2.86
1.00
1.18
2.12
1.07
2.18
2.02
2.15
2.00
1.20
3.43
3.33


155.21
148.99
143.18
139.89
133.92
131.92
128.43
128.30
127.52
127.36
127.27
116.72
77.25
77.00
76.74
61.76
46.17
40.41
33.70
23.80
CH3
CH3
S
O
N
O
3c (89:11)
* representative peaks
of minor inseparable isomer
Current Data Parameters
NAME pb ascend 500
EXPNO 35
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190629
Time 14.19 h
INSTRUM spect
PROBHD Z125331_0034 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1667
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.83
DW 16.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8304669 MHz
NUC1 13C
P1 12.00 usec
PLW1 172.66955817 W
SFO2 500.3710015 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.18000031 W
PLW12 0.12180000 W
PLW13 0.06126500 W
F2 - Processing parameters
SI 32768
SF 125.8178961 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



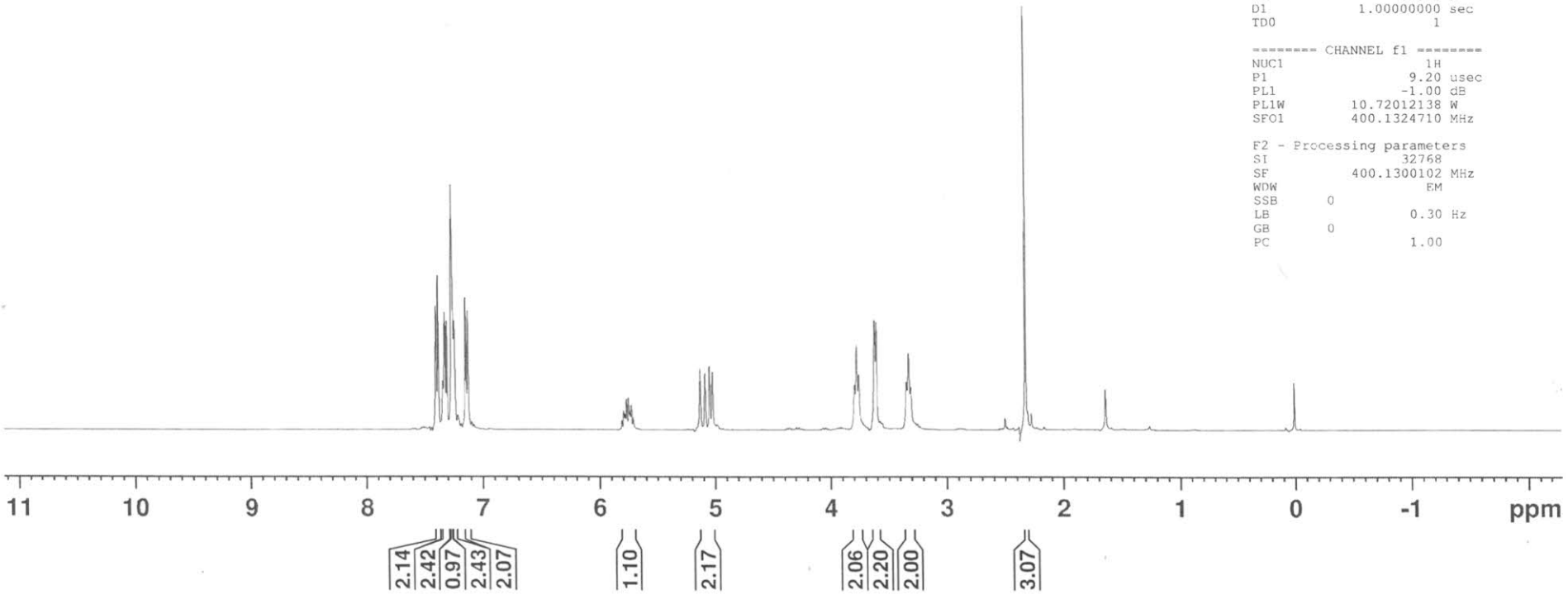


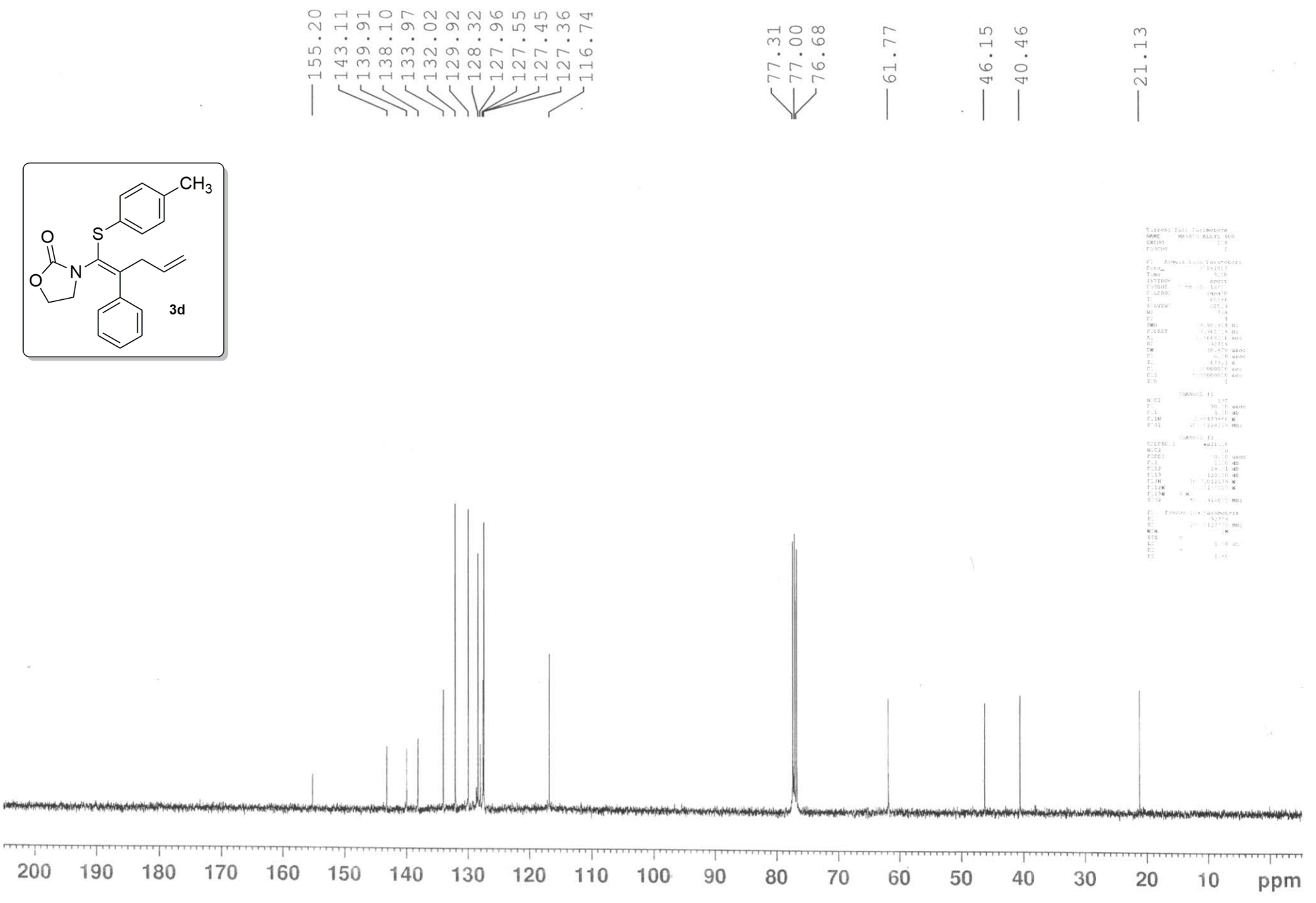

```
Current Data Parameters
NAME      MANASH ALLYL 400
EXPNO                 113
PROCNO                  1

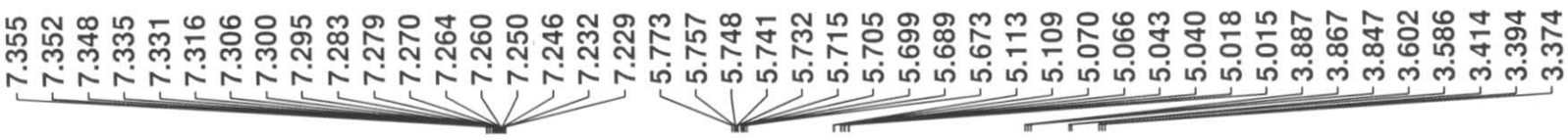
F2 - Acquisition Parameters
Date_           20181027
Time                2.51
INSTRUM            spect
PROBHD   5 mm BBI 1H/D-
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9583745 sec
RG                 71.8
DW                60.400 usec
DE                 6.50 usec
TE                673.2 K
D1             1.00000000 sec
TD0                    1

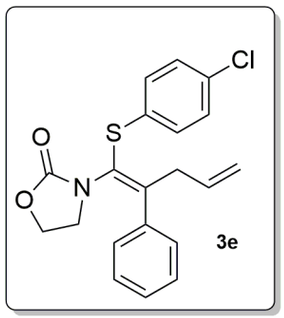
======== CHANNEL f1 ========
NUC1                  1H
P1                 9.20 usec
PL1               -1.00 dB
PL1W        10.72012138 W
SFO1        400.1324710 MHz

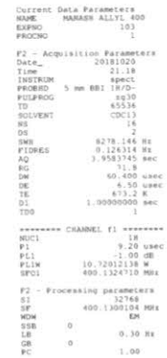
F2 - Processing parameters
SI                 32768
SF          400.1300102 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

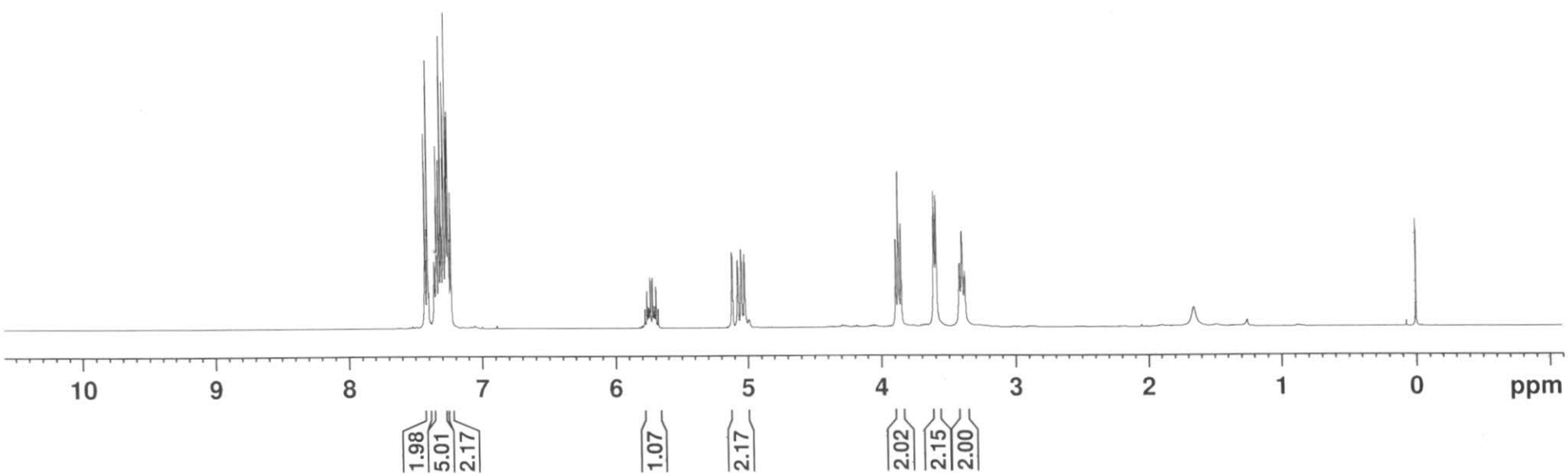


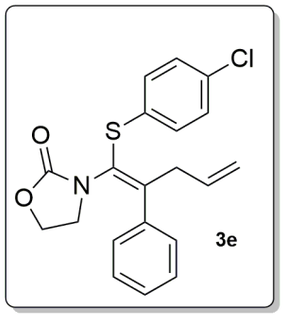

155.20
143.11
139.91
138.10
133.97
132.02
129.92
128.32
127.96
127.55
127.45
127.36
116.74
77.31
77.00
76.68
61.77
46.15
40.46
21.13
CH3
S
O
N
O
3d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.355
7.352
7.348
7.335
7.331
7.316
7.306
7.300
7.295
7.283
7.279
7.270
7.264
7.260
7.250
7.246
7.232
7.229
5.773
5.757
5.748
5.741
5.732
5.715
5.705
5.699
5.689
5.673
5.113
5.109
5.070
5.066
5.043
5.040
5.018
5.015
3.887
3.867
3.847
3.602
3.586
3.414
3.394
3.374


Cl
S
O
O
N
3e


Current Data Parameters
NAME MARASH ALLYL 400
EXPNO 103
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181020
Time 21.18
INSTRUM spect
PROBHD 5 mm BBI 1H/D-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.20 usec
PL1 1.00 dB
PLW 10.72012138 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


10
9
8
7
6
5
4
3
2
1
0
ppm
1.98
5.01
2.17
1.07
2.17
2.02
2.15
2.00

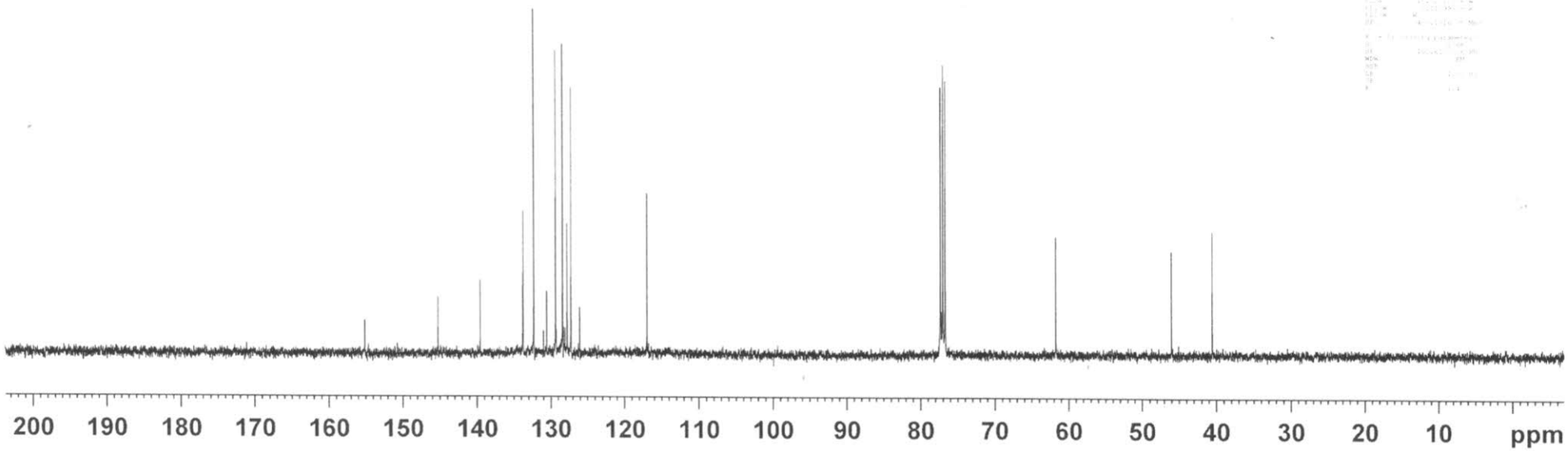


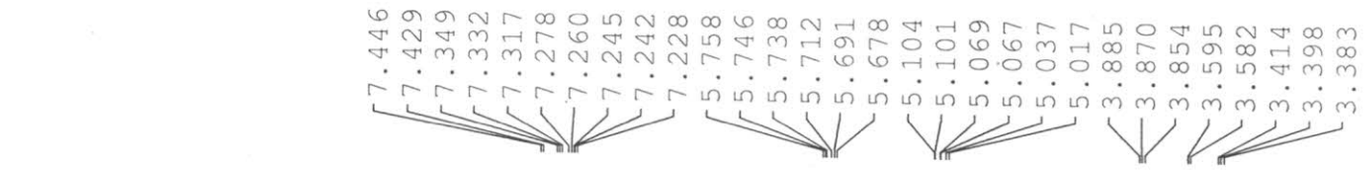
155.13
145.23
139.56
133.79
133.74
132.31
130.56
129.34
128.40
127.79
127.24
126.09
116.97

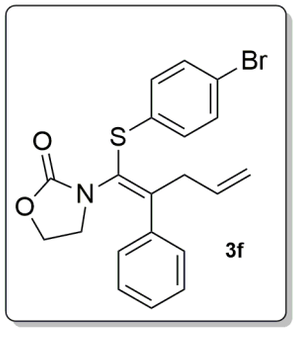
77.31
77.00
76.68

61.76

46.04
40.57





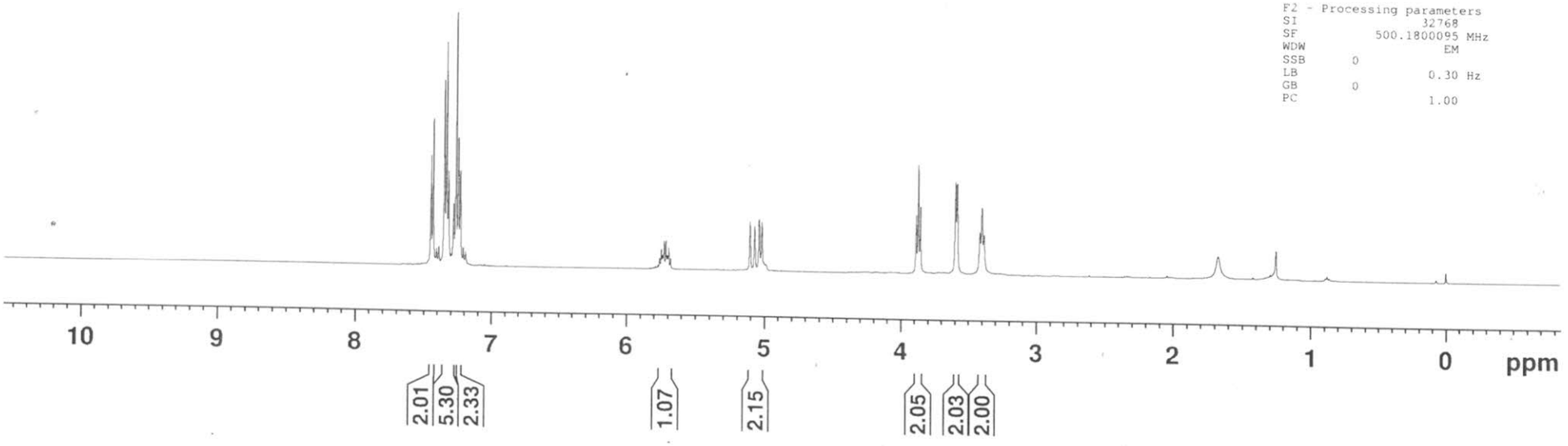


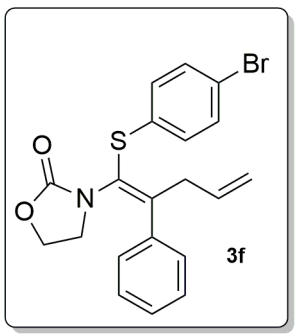

```
Current Data Parameters
NAME                  MPG 500
EXPNO                      66
PROCNO                      1

F2 - Acquisition Parameters
Date_               20191003
Time                   12.00
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                10330.578 Hz
FIDRES             0.157632 Hz
AQ                 3.1719425 sec
RG                      144
DW                   48.400 usec
DE                    6.50 usec
TE                   296.6 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                    14.90 usec
PL1                    2.00 dB
PL1W             12.85348415 W
SFO1             500.1830888 MHz

F2 - Processing parameters
SI                        32768
SF               500.1800095 MHz
WDW                          EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```





155.16
145.67
139.58
133.72
132.46
132.28
131.41
128.39
127.79
127.26
126.00
121.78
117.00

77.25
77.00
76.74

61.76

46.07

40.57

Current Data Parameters
NAME MPG 500
EXPNO 67
PROCNO 1

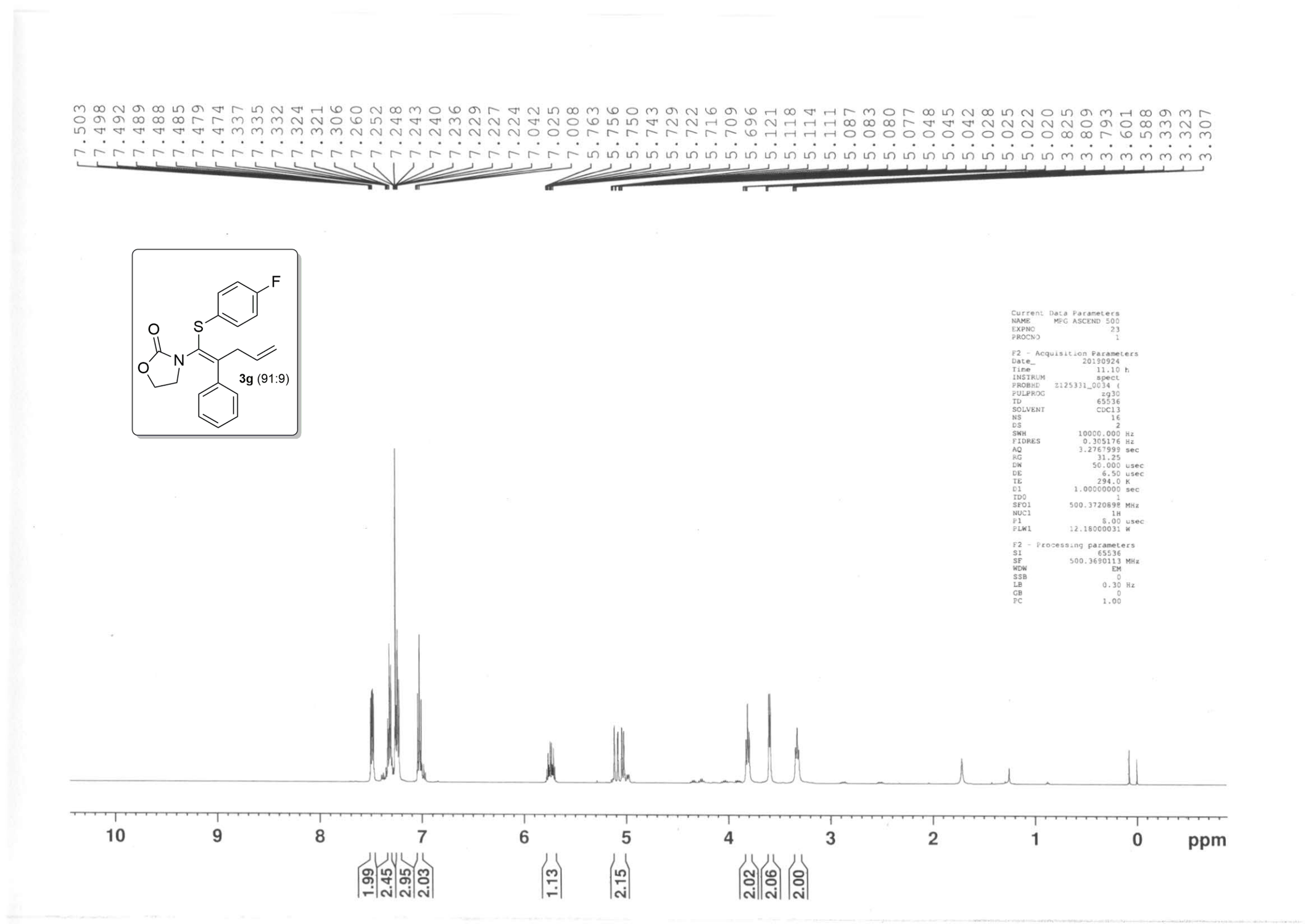
F2 Acquisition Parameters
Date_ 20191003
Time 12.05
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 322
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
ID0 1

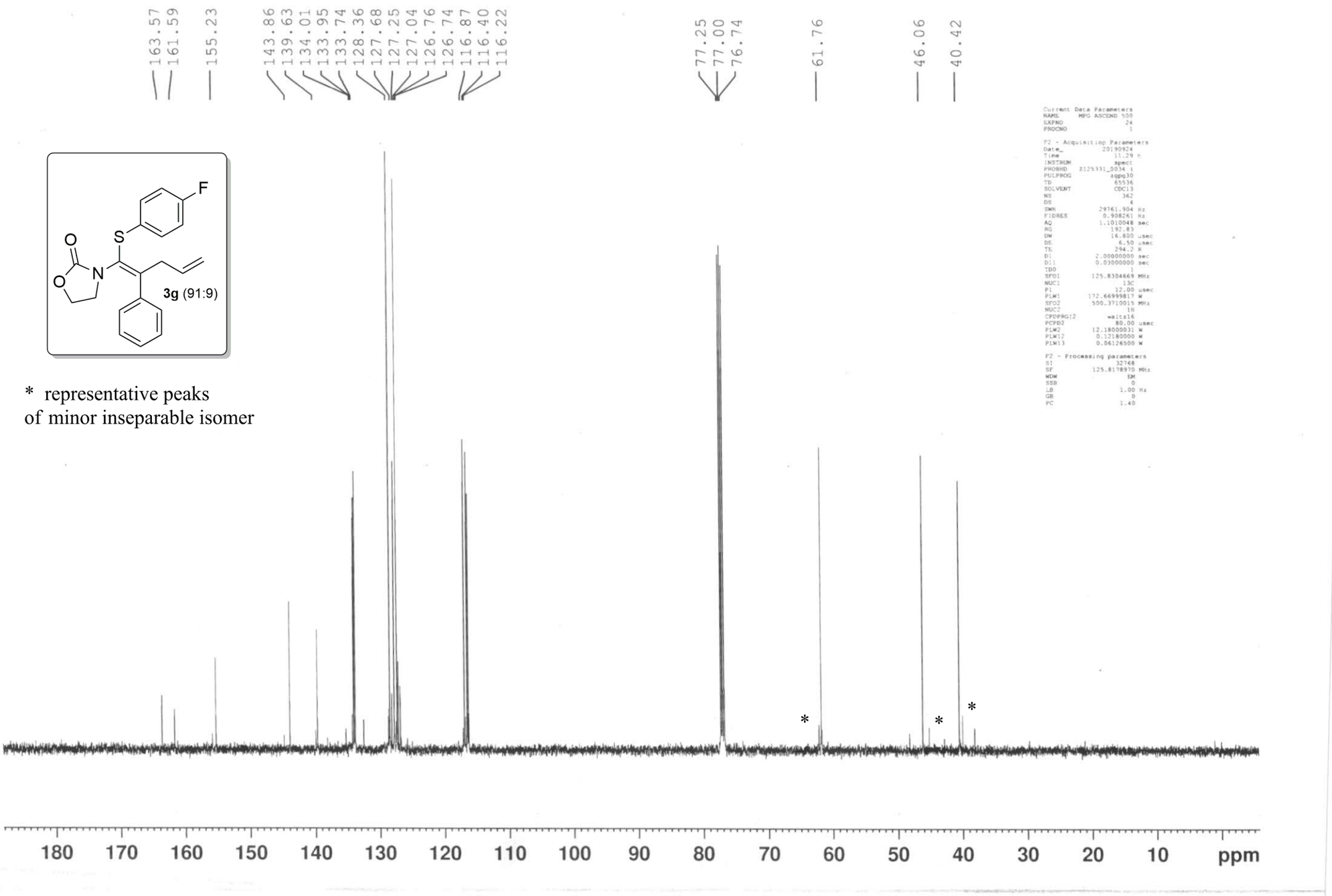
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 0 dB
PL1W 76.36138101 W
SFO1 125.7829381 MHz

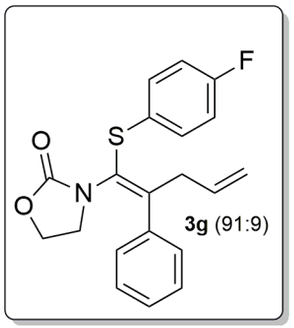
======== CHANNEL f2 ========
CPDPRG 2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
PL2W 12.85348415 W
PL12W 0.45605880 W
PL13W 0.45605880 W
SFO2 500.1820007 MHz

F2 Processing parameters
SI 32768
SF 125.7702664 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

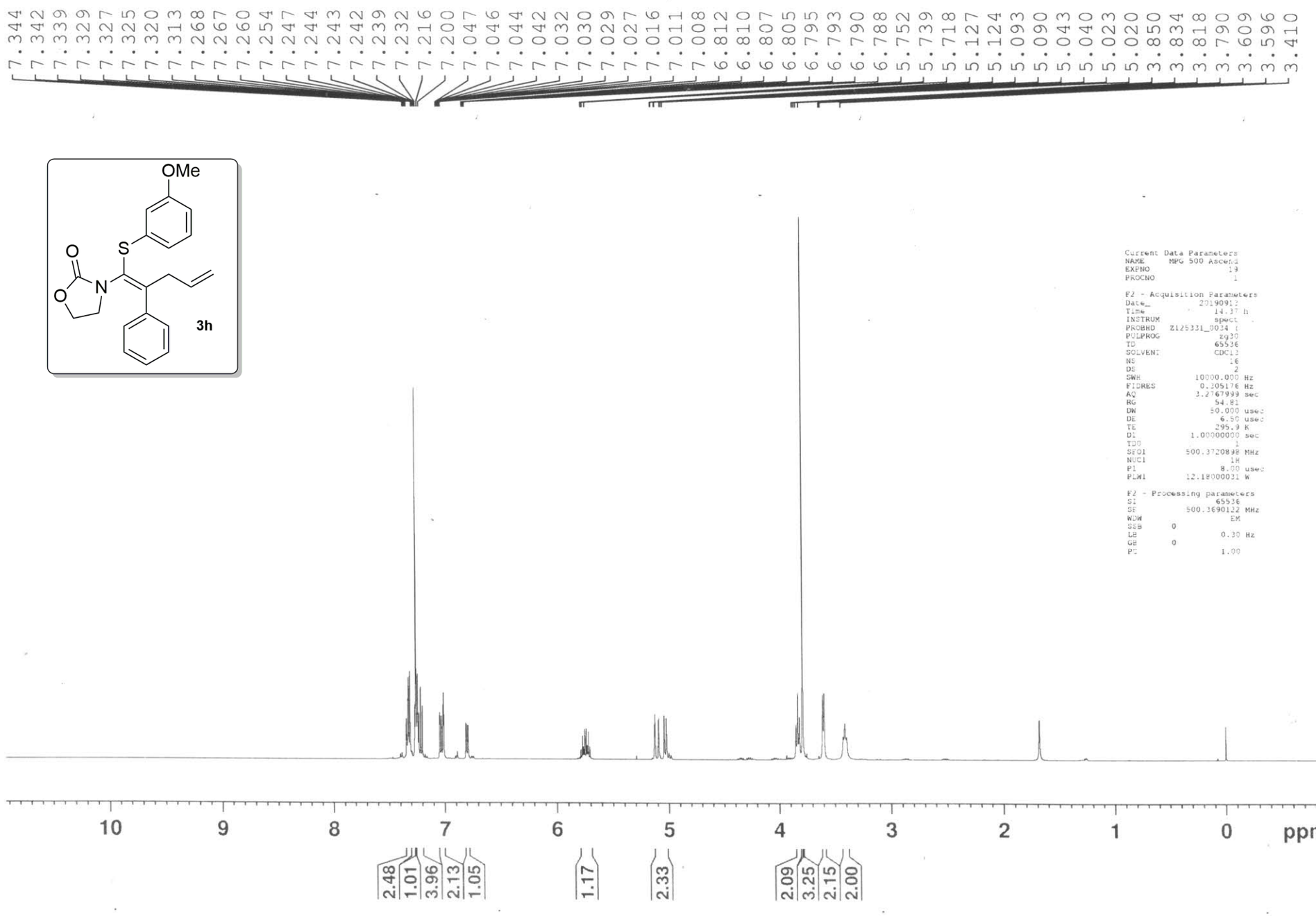
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

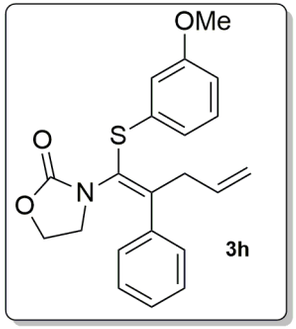

7.503
7.498
7.492
7.489
7.488
7.485
7.479
7.474
7.337
7.335
7.332
7.324
7.321
7.306
7.260
7.252
7.248
7.243
7.240
7.236
7.229
7.227
7.224
7.042
7.025
7.008
5.763
5.756
5.750
5.743
5.729
5.722
5.716
5.709
5.696
5.121
5.118
5.114
5.111
5.087
5.083
5.080
5.077
5.048
5.045
5.042
5.028
5.025
5.022
5.020
3.825
3.809
3.793
3.601
3.588
3.339
3.323
3.307
F
S
O
N
O
3g (91:9)
Current Data Parameters
NAME MPG ASCEND 500
EXPNO 23
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190924
Time 11.10 h
INSTRUM spect
PROBHD 2125331_0034 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 31.25
DW 50.000 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 8.00 usec
PLW1 12.18000031 W
F2 - Processing parameters
SI 65536
SF 500.3690113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.45
2.95
2.03
1.13
2.15
2.02
2.06
2.00


163.57
161.59
155.23
143.86
139.63
134.01
133.95
133.74
128.36
127.68
127.25
127.04
126.76
126.74
116.87
116.40
116.22
77.25
77.00
76.74
61.76
46.06
40.42
F
S
O
N
O
3g (91:9)
* representative peaks
of minor inseparable isomer
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

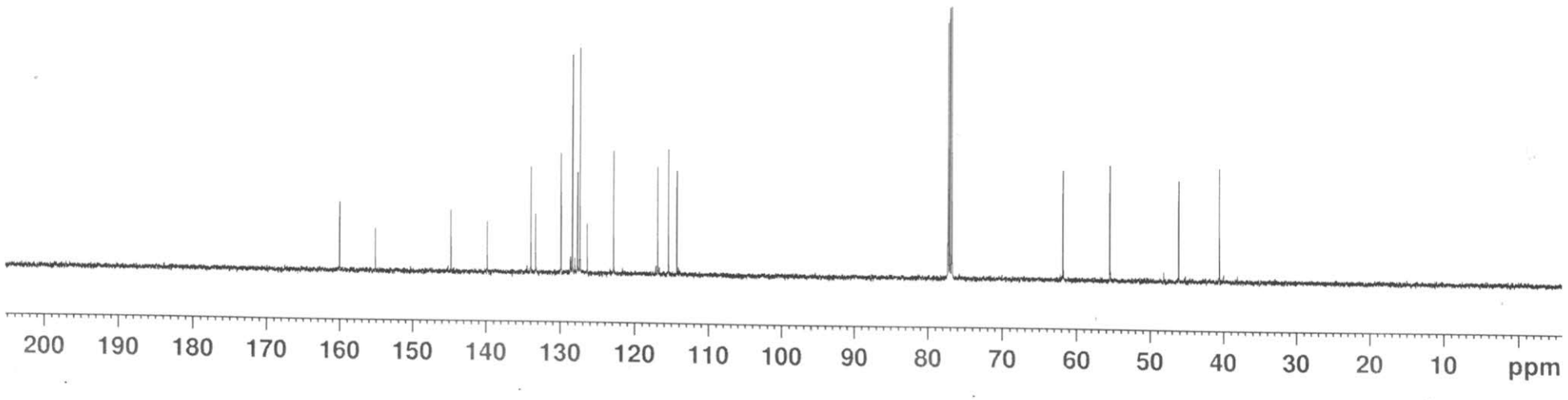

F
S
O
N
O
3g (91:9)

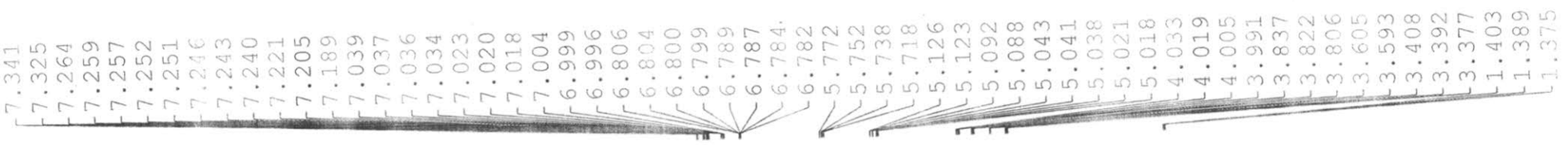
-112.89
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

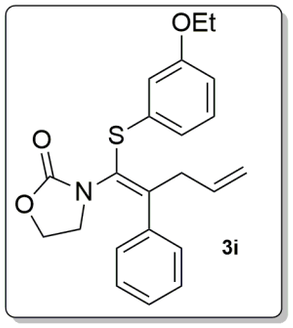

7.344
7.342
7.339
7.329
7.327
7.325
7.320
7.313
7.268
7.267
7.260
7.254
7.247
7.244
7.243
7.242
7.239
7.232
7.216
7.200
7.047
7.046
7.044
7.042
7.032
7.030
7.029
7.027
7.016
7.011
7.008
6.812
6.810
6.807
6.805
6.795
6.793
6.790
6.788
5.752
5.739
5.718
5.127
5.124
5.093
5.090
5.043
5.040
5.023
5.020
3.850
3.834
3.818
3.790
3.609
3.596
3.410
OMe
S
O
N
O
3h
Current Data Parameters
NAME MPG 500 Ascend
EXPNO 19
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190912
Time 14.37 h
INSTRUM spect
PROBHD Z125331_0034 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767949 sec
RG 54.81
DW 50.000 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 8.00 usec
PLW1 12.18000031 W
F2 - Processing parameters
SI 65536
SF 500.3690122 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.48
1.01
3.96
2.13
1.05
1.17
2.33
2.09
3.25
2.15
2.00

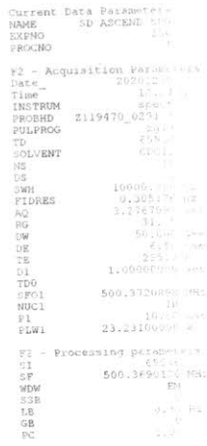


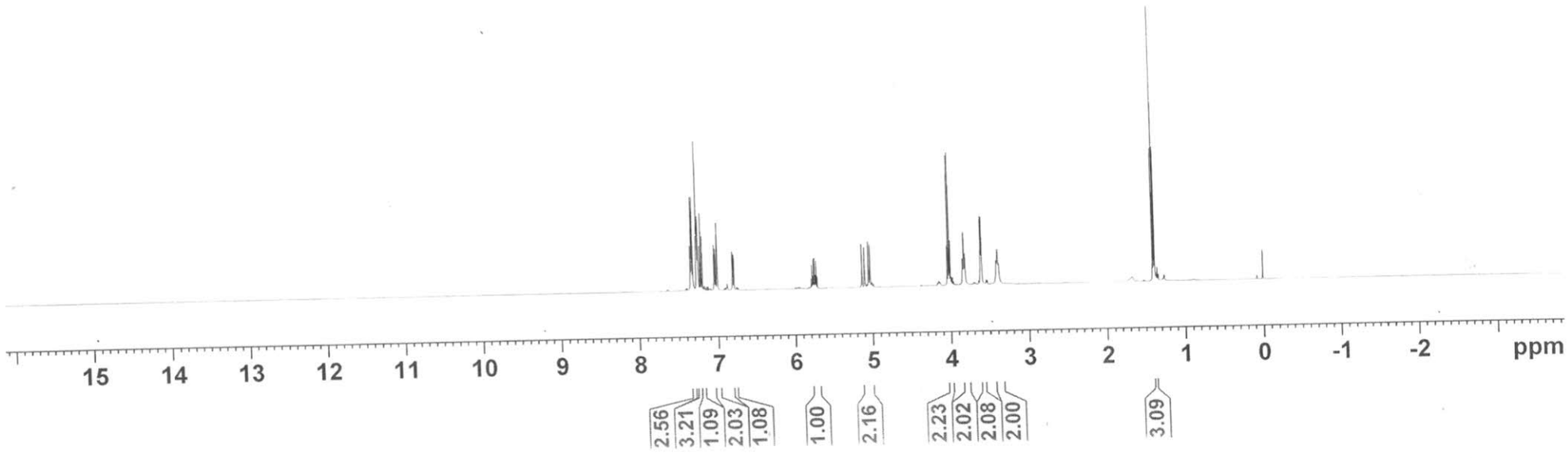
160.00
155.11
144.74
139.82
133.93
133.30
129.87
128.32
127.62
127.33
126.36
122.81
116.83
115.36
114.23
77.25
77.00
76.74
61.77
55.43
46.08
40.54




7.341
7.325
7.264
7.259
7.257
7.252
7.251
7.246
7.243
7.240
7.221
7.205
7.189
7.039
7.037
7.036
7.034
7.023
7.020
7.018
7.004
6.999
6.996
6.806
6.804
6.800
6.799
6.789
6.787
6.784
6.782
5.772
5.752
5.738
5.718
5.126
5.123
5.092
5.088
5.043
5.041
5.038
5.021
5.018
4.033
4.019
4.005
3.991
3.837
3.822
3.806
3.605
3.593
3.408
3.392
3.377
1.403
1.389
1.375


OEt
O
S
O
N
3i


Current Data Parameters
NAME SD ASCEND
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD Z119470_0291
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
TD0
SFO1
NUC1
P1
PLW1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC


15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
ppm
2.56
3.21
1.09
2.03
1.08
1.00
2.16
2.23
2.02
2.08
2.00
3.09

SD-P-OET

159.41
155.11
144.47
139.87
133.94
133.15
129.85
128.31
127.59
127.34
126.61
122.96
116.80
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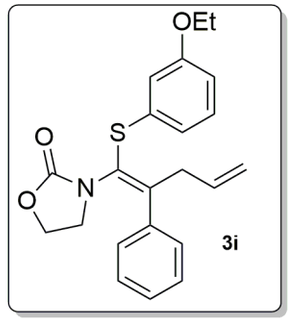
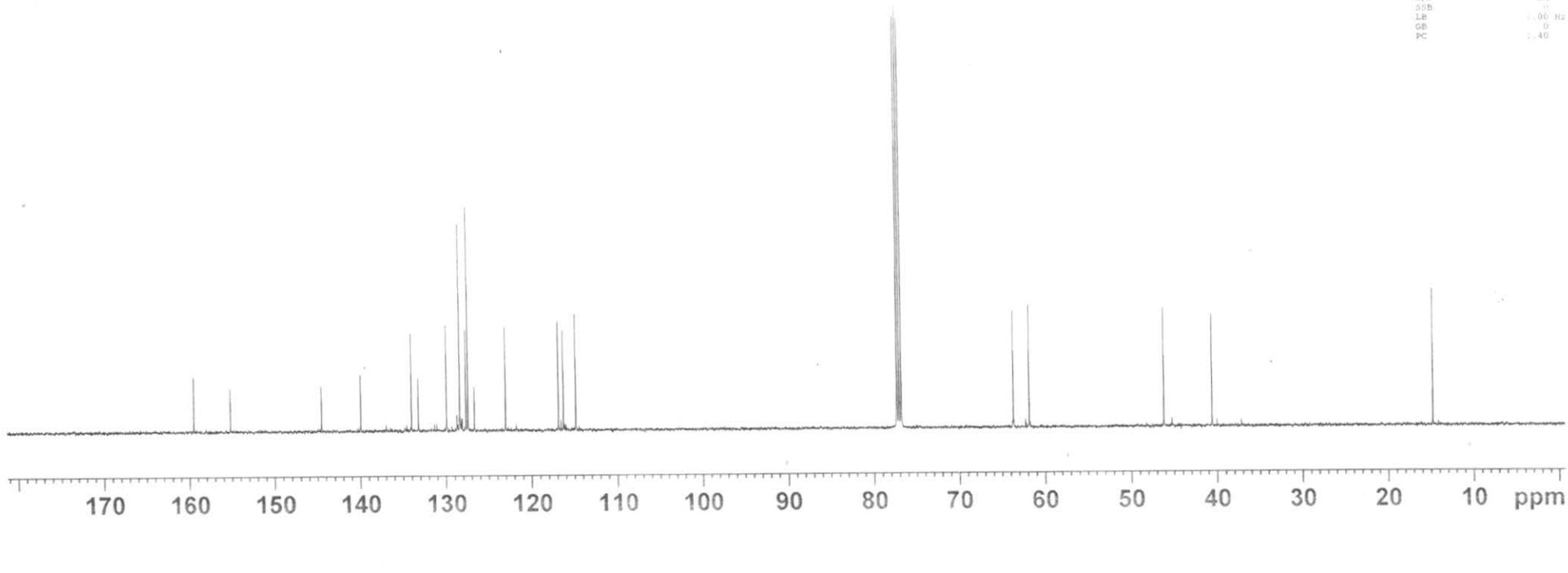
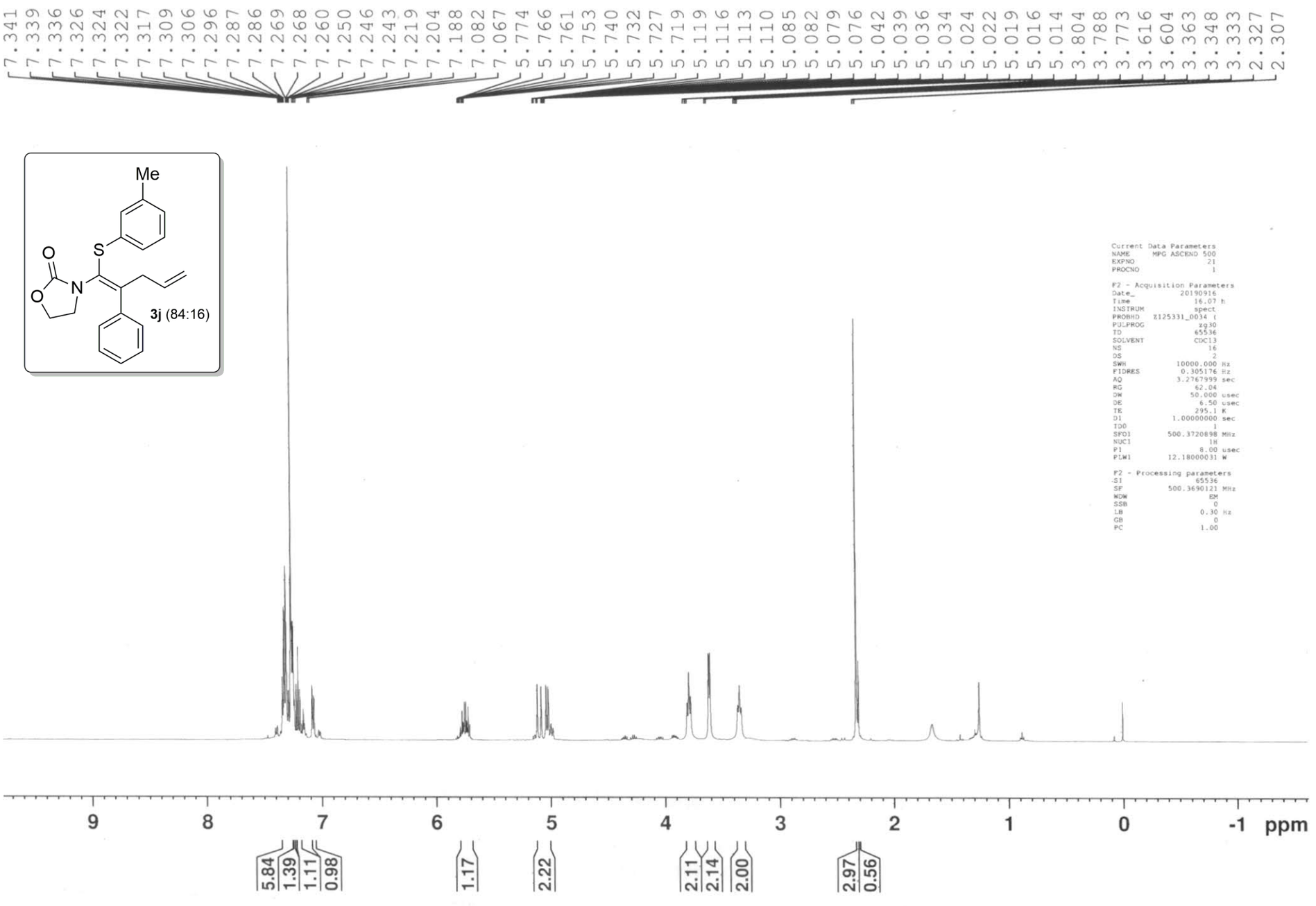
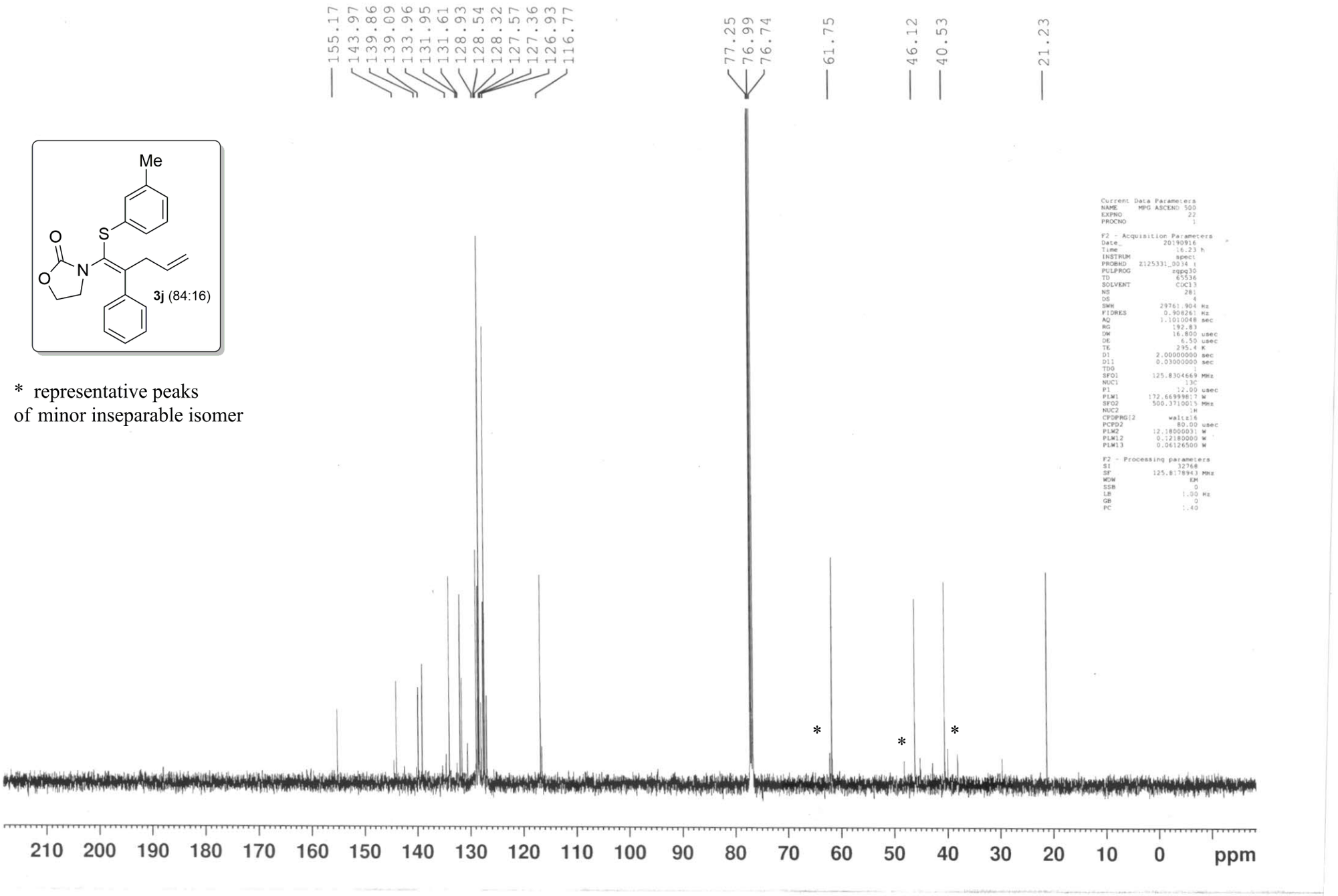
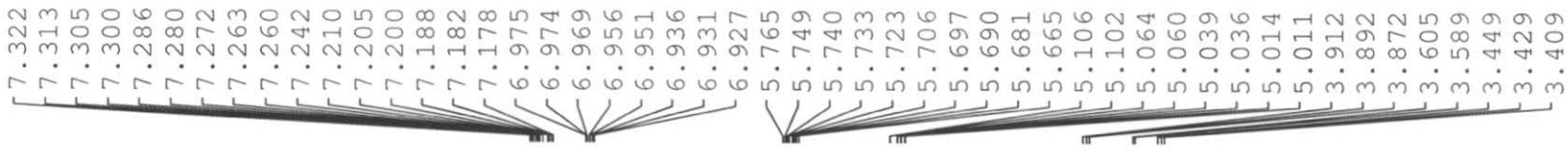
114.79
77.25
77.00
76.74
63.63
61.77
46.11
40.51
14.71

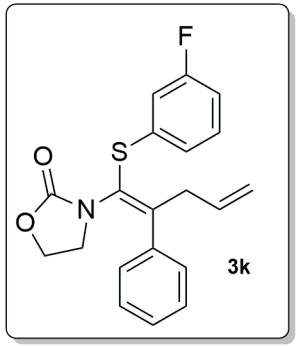





7.341
7.339
7.336
7.326
7.324
7.322
7.317
7.309
7.306
7.296
7.287
7.286
7.269
7.268
7.260
7.250
7.246
7.243
7.219
7.204
7.188
7.082
7.067
5.774
5.766
5.761
5.753
5.740
5.732
5.727
5.719
5.119
5.116
5.113
5.110
5.085
5.082
5.079
5.076
5.042
5.039
5.036
5.034
5.024
5.022
5.019
5.016
5.014
3.804
3.788
3.773
3.616
3.604
3.363
3.348
3.333
2.327
2.307
Me
S
O
N
O
3j (84:16)
Current Data Parameters
NAME MPG ASCEND 500
EXPNO 21
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190916
Time 16.07 h
INSTRUM spect
PROBHD Z125331_0034 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 62.04
DW 50.000 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.3720898 MHz
NUC1 1H
P1 8.00 usec
PLW1 12.18000031 W
F2 - Processing parameters
SI 65536
SF 500.3690121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
-1 ppm
5.84
1.39
1.11
0.98
1.17
2.22
2.11
2.14
2.00
2.97
0.56


155.17
143.97
139.86
139.09
133.96
131.95
131.61
128.93
128.54
128.32
127.57
127.36
126.93
116.77
77.25
76.99
76.74
61.75
46.12
40.53
21.23
Me
S
O
N
O
3j (84:16)
* representative peaks
of minor inseparable isomer
Current Data Parameters
NAME MPG ASCEND 500
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190916
Time 16.23 h
INSTRUM spect
PROBHD Z125331_0034 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 281
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.83
DW 16.800 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.8304669 MHz
NUC1 13C
P1 12.00 usec
PLW1 172.66999817 W
SFO2 500.3710015 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 12.18000031 W
PLW12 0.12180000 W
PLW13 0.06126500 W
F2 - Processing parameters
SI 32768
SF 125.8178943 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
*
*
*
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



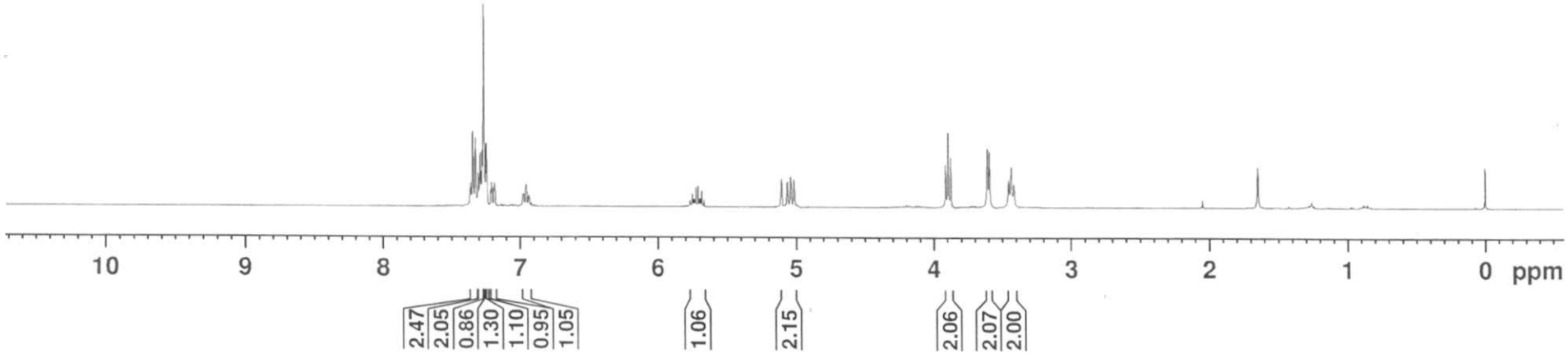


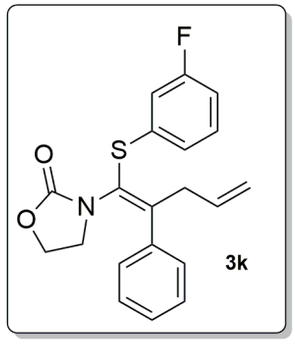

```
Current Data Parameters
NAME      MANASH ALLYL 400
EXPNO              101
PROCNO               1

F2 - Acquisition Parameters
Date_          20181020
Time              19.59
INSTRUM           spect
PROBHD   5 mm BBI 1H/D-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.9583745 sec
RG                71.8
DW               60.400 usec
DE                6.50 usec
TE               673.2 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                9.20 usec
PL1              -1.00 dB
PL1W        10.72012138 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300107 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





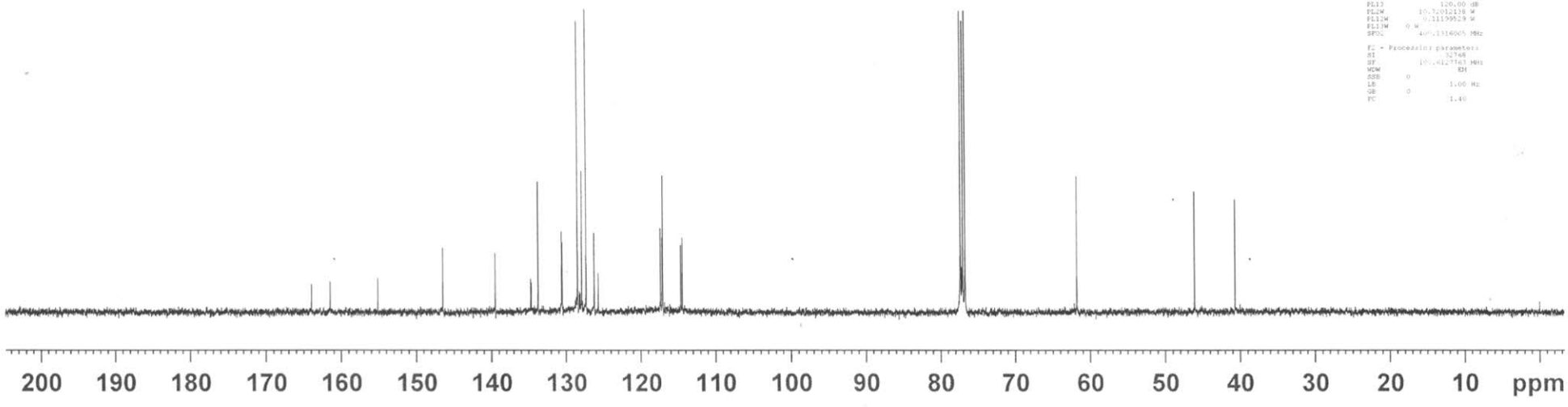
163.92
161.44
155.10
146.42
139.46
134.68
134.61
133.69
130.56
130.47
128.41
127.84
127.25
126.20
126.17
125.63
117.34
117.11
117.04
114.62
114.41

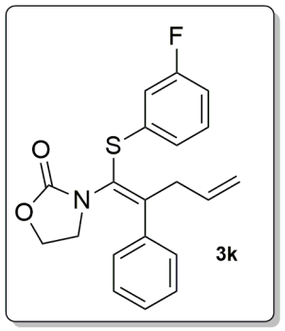
77.31
77.00
76.68

61.77

46.06

40.64





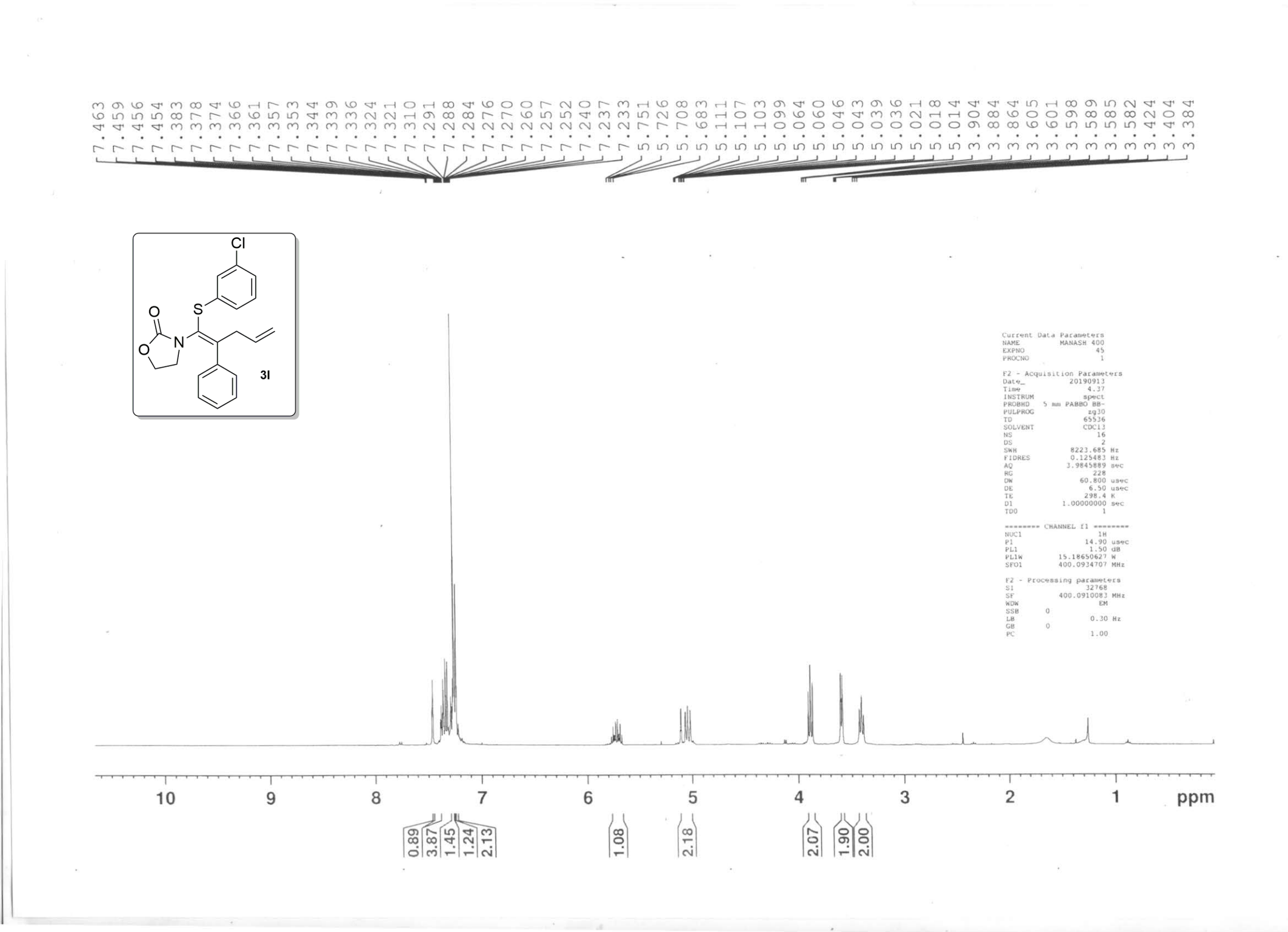

```
Current Data Parameters
NAME      MANASH ALLYL 400 operator
EXPNO                 25
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181027
Time                4.15
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG         zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                    16
DS                     4
SWH           89285.711 Hz
FIDRES        0.681196 Hz
AQ            0.7340032 sec
RG                  2050
DW                 5.600 usec
DE                 6.50 usec
TE                296.3 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  19F
P1                 14.80 usec
PL1                -1.20 dB
PL1W         18.11287308 W
SFO1         376.4240234 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 1.50 dB
PL12               17.18 dB
PL2W         15.18650627 W
PL12W         0.41063678 W
SFO2         400.0926004 MHz

F2 - Processing parameters
SI                 65536
SF           376.4616700 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```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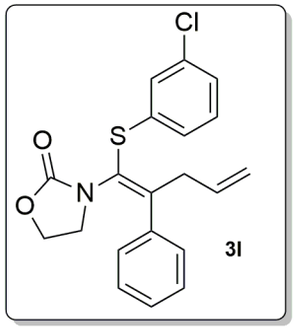
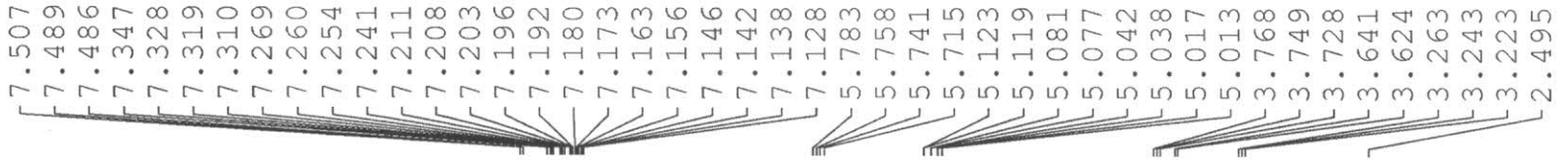
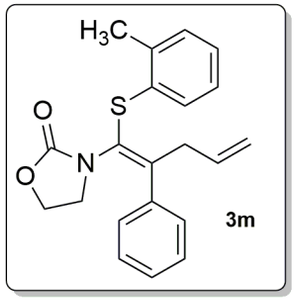
7.454
7.383
7.378
7.374
7.366
7.361
7.357
7.353
7.344
7.339
7.336
7.324
7.321
7.310
7.291
7.288
7.284
7.276
7.270
7.260
7.257
7.252
7.240
7.237
7.233
5.751
5.726
5.708
5.683
5.111
5.107
5.103
5.099
5.064
5.060
5.046
5.043
5.039
5.036
5.021
5.018
5.014
3.904
3.884
3.864
3.605
3.601
3.598
3.589
3.585
3.582
3.424
3.404
3.384
Cl
S
O
O
N
3l
Current Data Parameters
NAME MANASH 400
EXPNO 45
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190913
Time 4.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 228
DW 60.800 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 1.50 dB
PL1W 15.18650627 W
SFO1 400.0934707 MHz
F2 - Processing parameters
SI 32768
SF 400.0910083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
0.89
3.87
1.45
1.24
2.13
1.08
2.18
2.07
1.90
2.00


Cl
S
O
N
O
3l

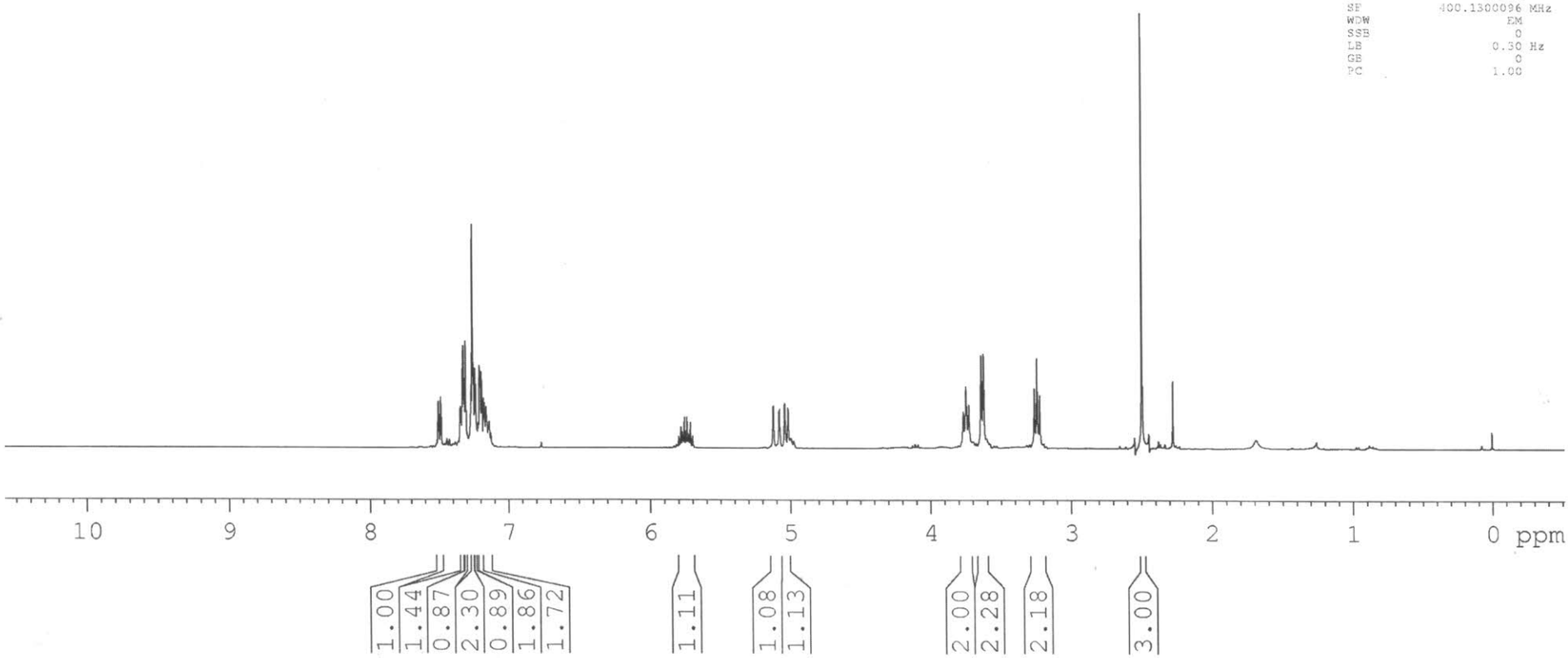
155.19
146.45
139.53
134.80
134.49
133.71
130.31
130.20
128.91
128.46
127.89
127.70
127.33
125.81
117.12
77.36
77.04
76.73
61.83
46.15
40.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

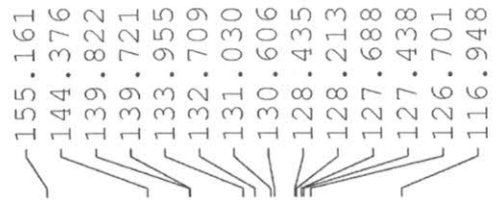


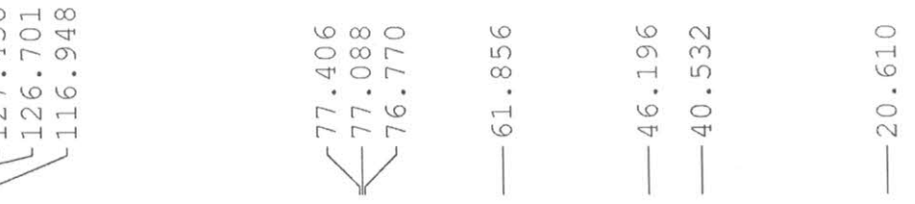


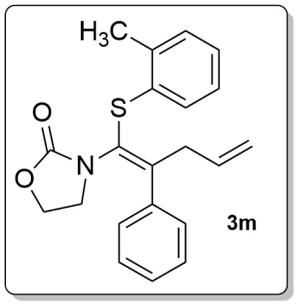

```
NAME                Praba
EXPNO                 265
PROCNO                  1
Date_            20181230
Time                11.24
INSTRUM             spect
PROBHD   5 mm BBI 1H/D-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                     57
DW                 60.400 usec
DE                  6.50 usec
TE                 673.2 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                   9.20 usec
PL1                 -1.00 dB
PL1W          10.72012138 W
SFO1         400.1324710 MHz
SI                  32768
SF           400.1300096 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```





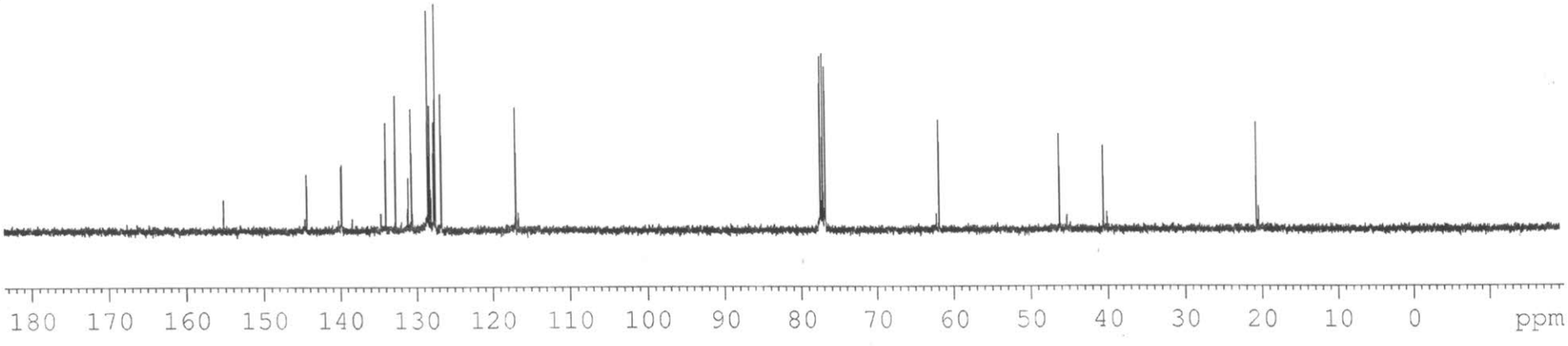


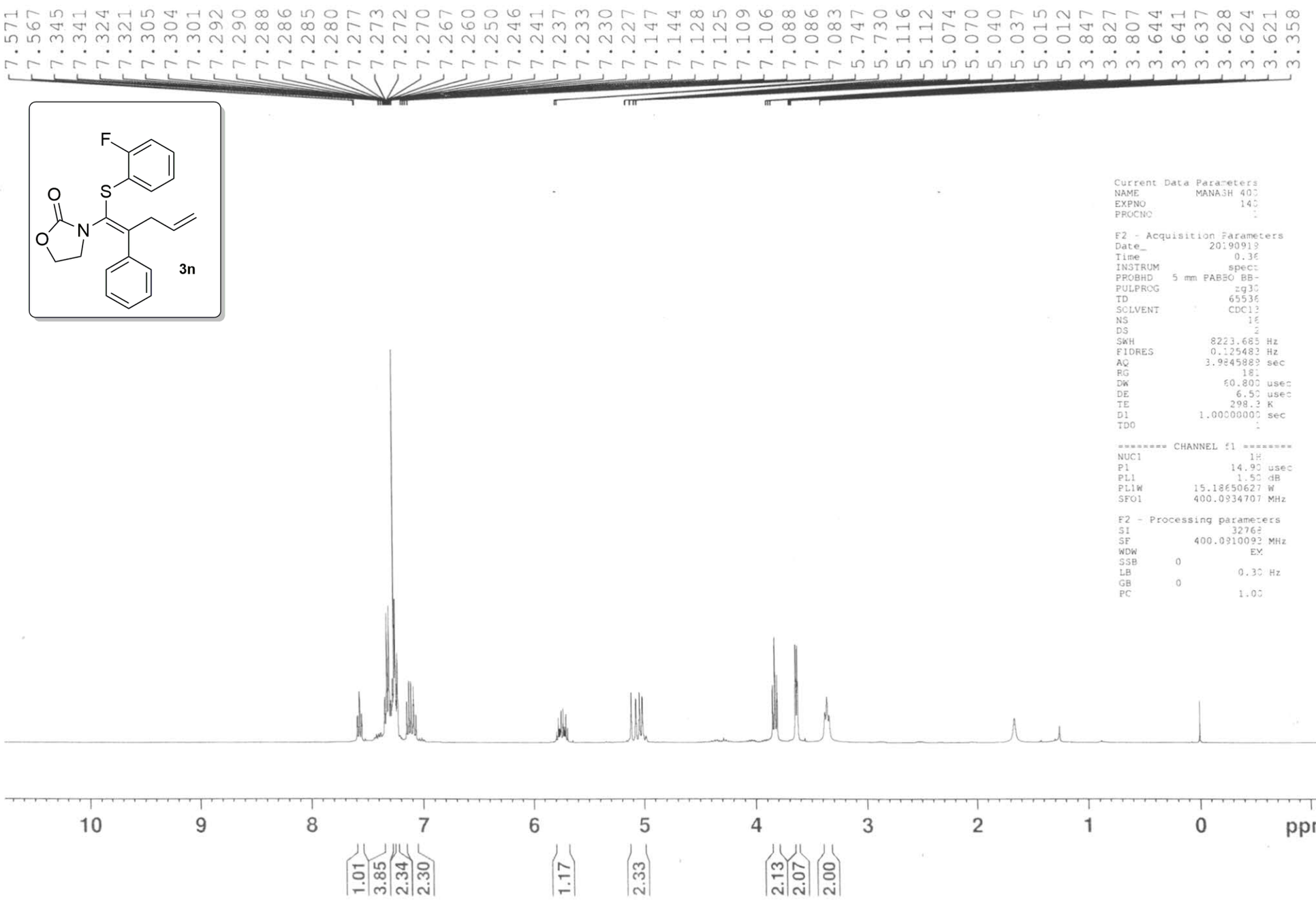


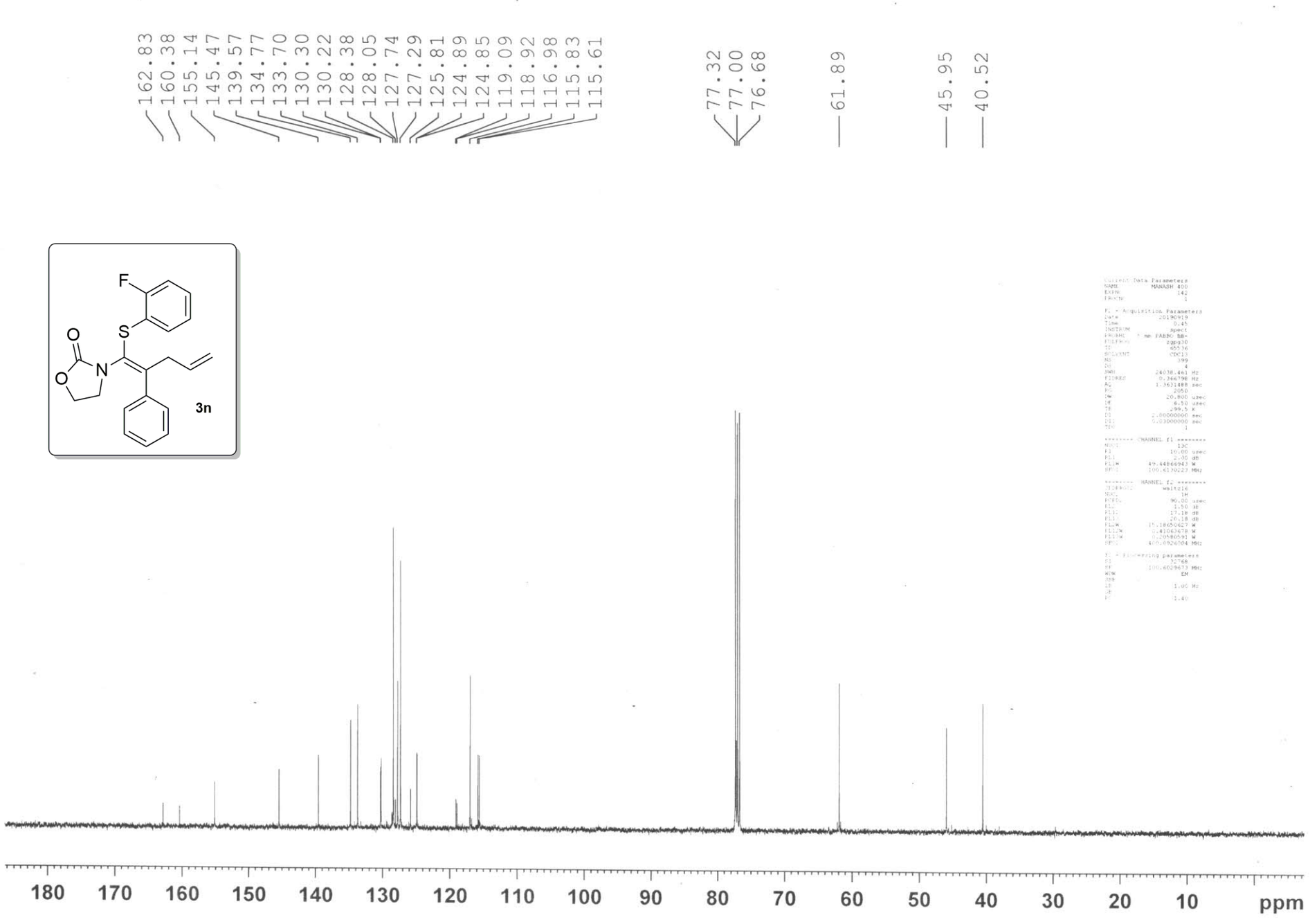

```
NAME                 Praba
EXPNO                  266
PROCNO                   1
Date_             20181230
Time                 11.42
INSTRUM              spect
PROBHD   5 mm BBI 1H/D-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      400
DS                        4
SWH               23980.814 Hz
FIDRES            0.365918 Hz
AQ                1.3664756 sec
RG                    32768
DW                   20.850 usec
DE                    6.50 usec
TE                   673.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

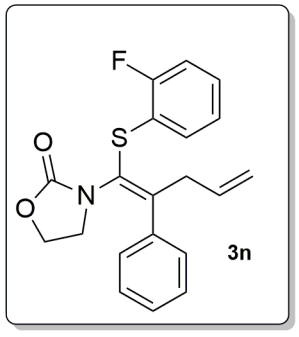
======== CHANNEL f1 ========
NUC1                    13C
P1                    30.00 usec
PL1                   -4.50 dB
PL1W          94.86473846 W
SFO1          100.6229298 MHz

======== CHANNEL f2 ========
CPDPRGZ            waltz16
NUC2                    1H
PCPD2                 90.00 usec
PL2                   -1.00 dB
PL12                  18.81 dB
PL13                 120.00 dB
PL2W          10.72012138 W
PL12W         0.11199529 W
PL13W         0.00000000 W
SFO2          400.1316005 MHz
SI                    32768
SF            100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```




7.571
7.567
7.345
7.341
7.324
7.321
7.305
7.304
7.301
7.292
7.290
7.288
7.286
7.285
7.280
7.277
7.273
7.272
7.270
7.267
7.260
7.250
7.246
7.241
7.237
7.233
7.230
7.227
7.147
7.144
7.128
7.125
7.109
7.106
7.088
7.086
7.083
5.747
5.730
5.116
5.112
5.074
5.070
5.040
5.037
5.015
5.012
3.847
3.827
3.807
3.644
3.641
3.637
3.628
3.624
3.621
3.358
F
S
O
N
O
3n
Current Data Parameters
NAME MANA3H 400
EXPNO 140
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190919
Time 0.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 181
DW 60.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 1.50 dB
PL1W 15.18650627 W
SFO1 400.0834707 MHz
F2 - Processing parameters
SI 32768
SF 400.0810093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
3.85
2.34
2.30
1.17
2.33
2.13
2.07
2.00


162.83
160.38
155.14
145.47
139.57
134.77
133.70
130.30
130.22
128.38
128.05
127.74
127.29
125.81
124.89
124.85
119.09
118.92
116.98
115.83
115.61
77.32
77.00
76.68
61.89
45.95
40.52
F
S
O
N
O
3n
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



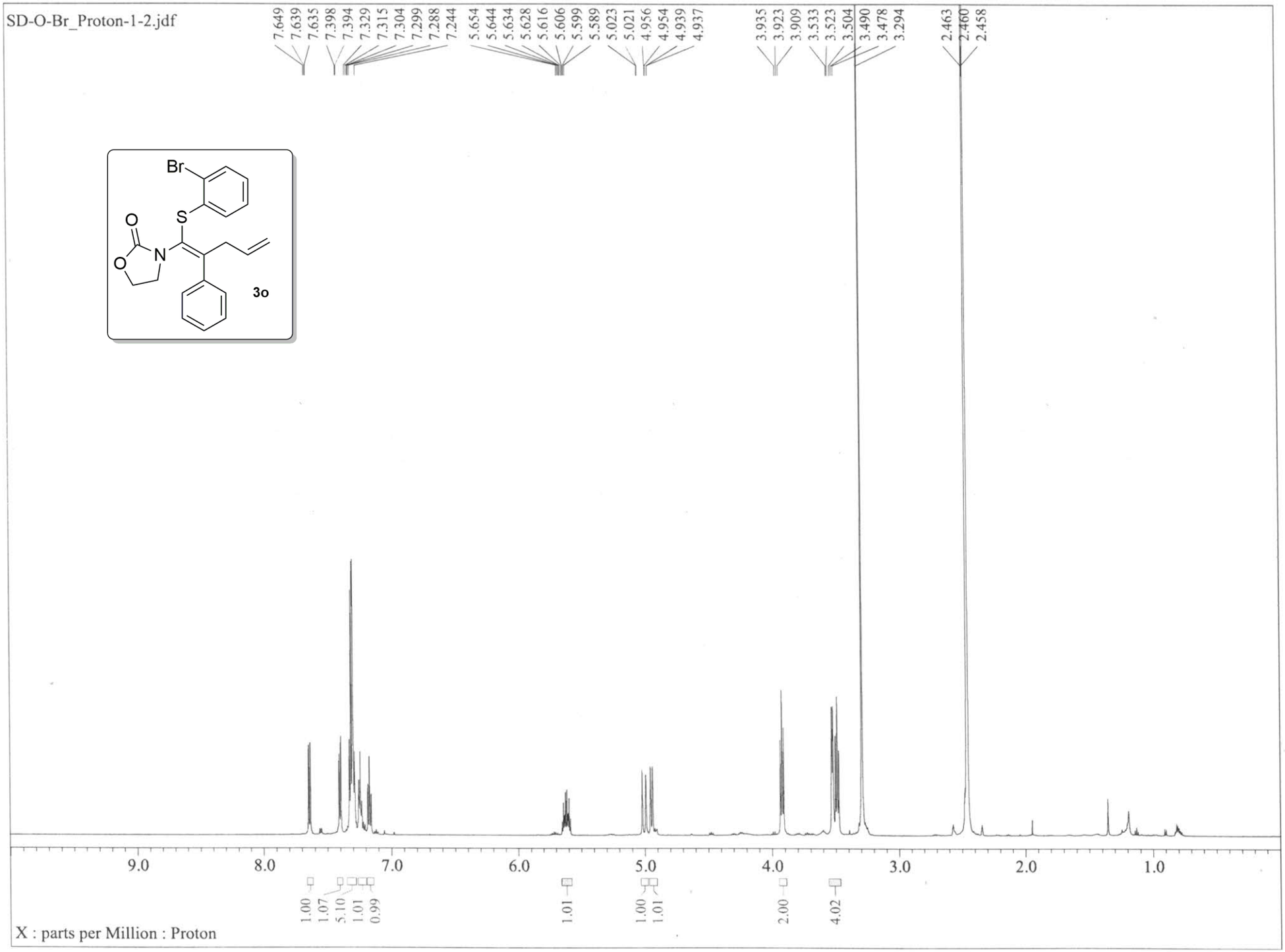

```
Current Data Parameters
NAME          MANASH 400
EXPNO                141
PROCNO                 1

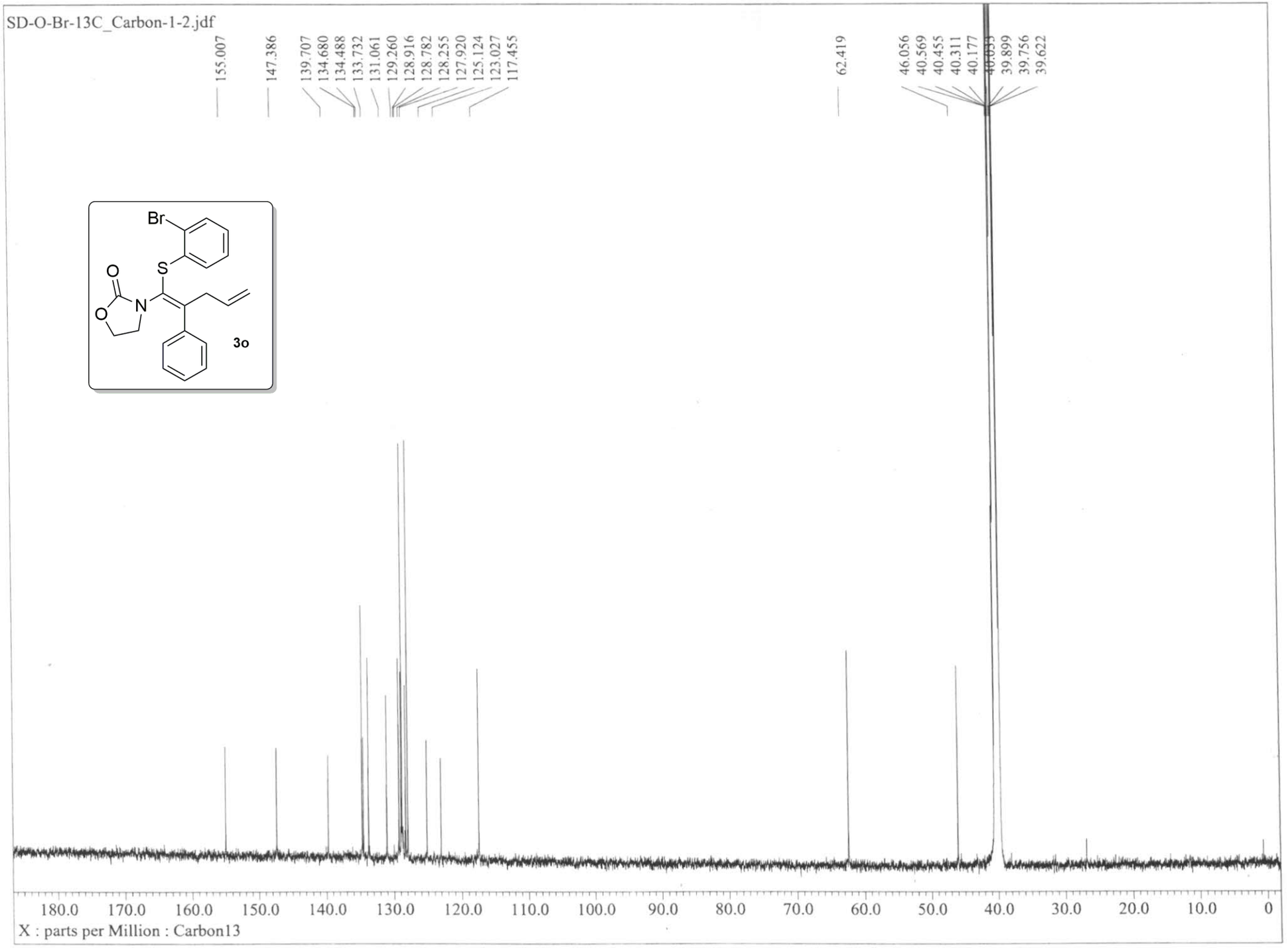
F2 - Acquisition Parameters
Date_           20190919
Time                0.38
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG         zgfhigqn
TD                131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH             89285.711 Hz
FIDRES          0.681196 Hz
AQ              0.7340032 sec
RG                   2050
DW                5.600 usec
DE                6.50 usec
TE                298.4 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1

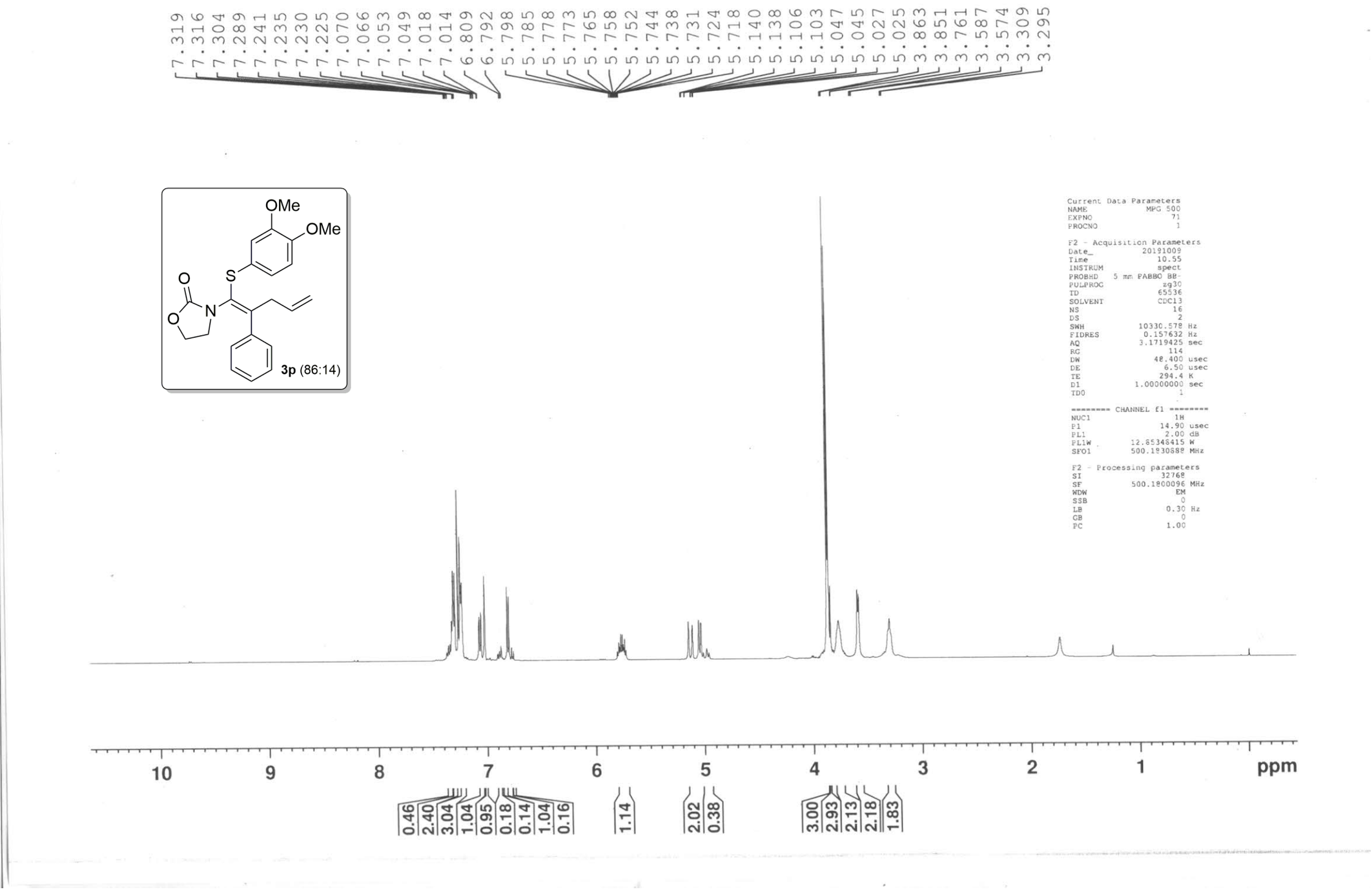
======== CHANNEL f1 ========
NUC1                  19F
P1                 14.80 usec
PL1                -1.20 dB
PL1W         18.11287308 W
SFO1         376.4240234 MHz

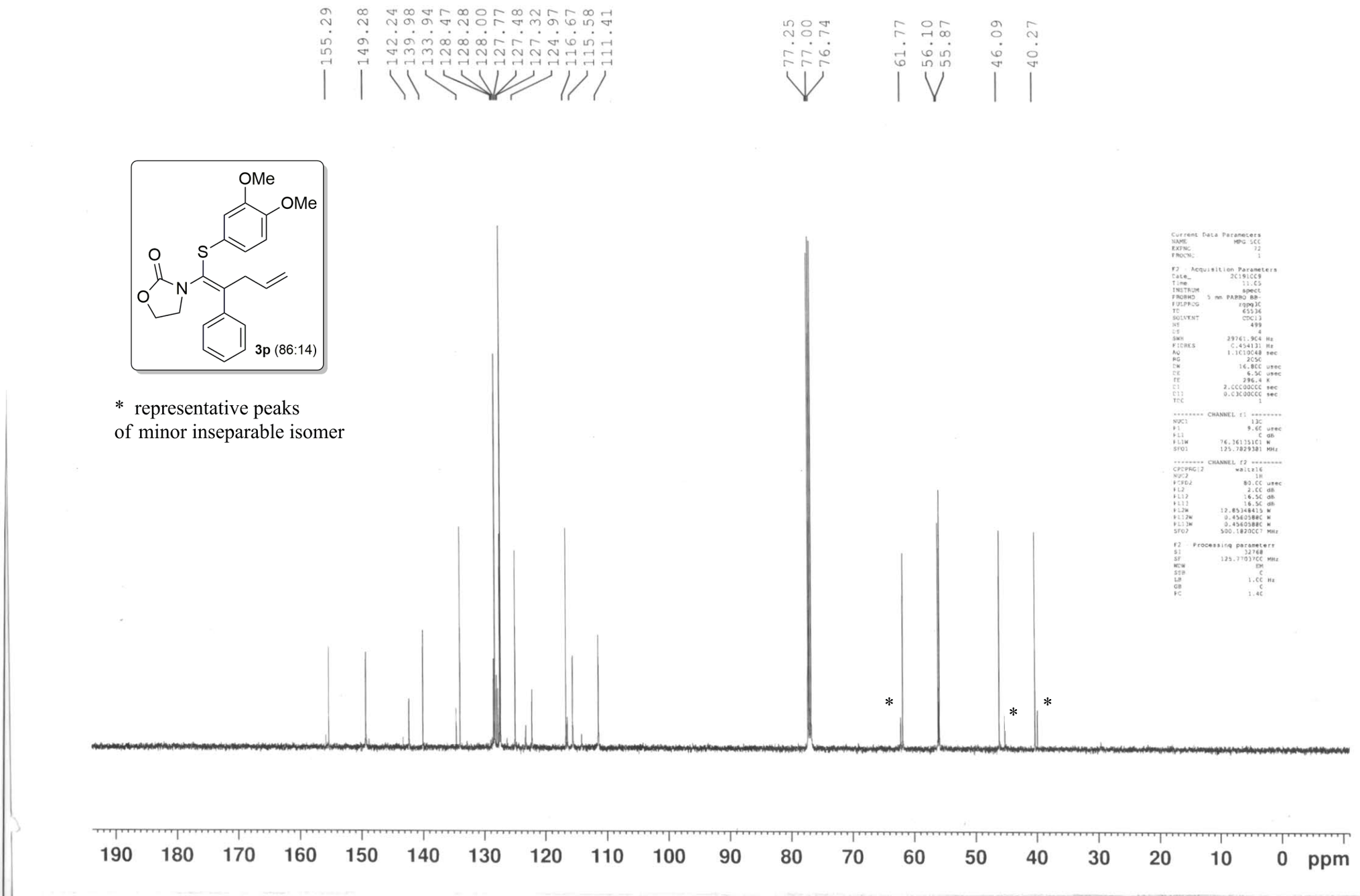
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                 1.50 dB
PL12               17.18 dB
PL2W         15.18650627 W
PL12W         0.41063678 W
SFO2         400.0926004 MHz

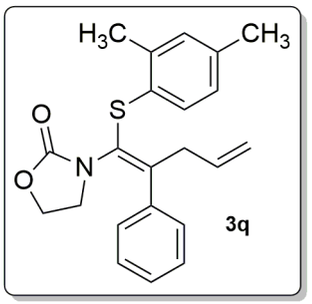
F2 - Processing parameters
SI                   65536
SF          376.4616700 MHz
WDW                     EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

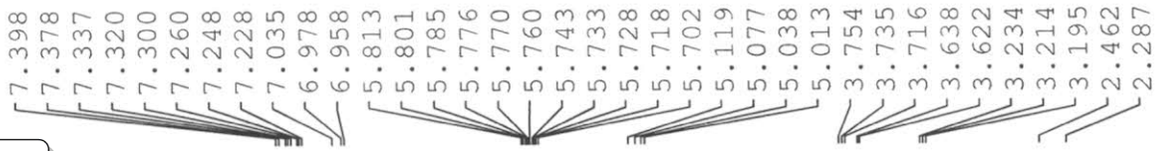

SD-O-Br_Proton-1-2.jdf
7.649
7.639
7.635
7.398
7.394
7.329
7.315
7.304
7.299
7.288
7.244
5.654
5.644
5.634
5.628
5.616
5.606
5.599
5.589
5.023
5.021
4.956
4.954
4.939
4.937
3.935
3.923
3.909
3.533
3.523
3.504
3.490
3.478
3.294
2.463
2.460
2.458
Br
S
O
N
O
3o
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
1.00
1.07
5.10
1.01
0.99
1.01
1.00
1.01
2.00
4.02
X : parts per Million : Proton


SD-O-Br-13C_Carbon-1-2.jdf
155.007
147.386
139.707
134.680
134.488
133.732
131.061
129.260
128.916
128.782
128.255
127.920
125.124
123.027
117.455
62.419
46.056
40.569
40.455
40.311
40.177
40.033
39.899
39.756
39.622
Br
S
O
N
O
3o
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
X : parts per Million : Carbon13


7.319
7.316
7.304
7.289
7.241
7.235
7.230
7.225
7.070
7.066
7.053
7.049
7.018
7.014
6.809
6.792
5.798
5.785
5.778
5.773
5.765
5.758
5.752
5.744
5.738
5.731
5.724
5.718
5.140
5.138
5.106
5.103
5.047
5.045
5.027
5.025
3.863
3.851
3.761
3.587
3.574
3.309
3.295
OMe
OMe
S
O
N
O
3p (86:14)
Current Data Parameters
NAME MPG 500
EXPNO 71
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191009
Time 10.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 114
DW 48.400 usec
DE 6.50 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 2.00 dB
PL1W 12.85348415 W
SFO1 500.1830888 MHz
F2 - Processing parameters
SI 32768
SF 500.1800096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
0.46
2.40
3.04
1.04
0.95
0.18
0.14
1.04
0.16
1.14
2.02
0.38
3.00
2.93
2.13
2.18
1.83


155.29
149.28
142.24
139.98
133.94
128.47
128.28
128.00
127.77
127.48
127.32
124.97
116.67
115.58
111.41
77.25
77.00
76.74
61.77
56.10
55.87
46.09
40.27
OMe
OMe
S
O
N
O
3p (86:14)
* representative peaks
of minor inseparable isomer
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



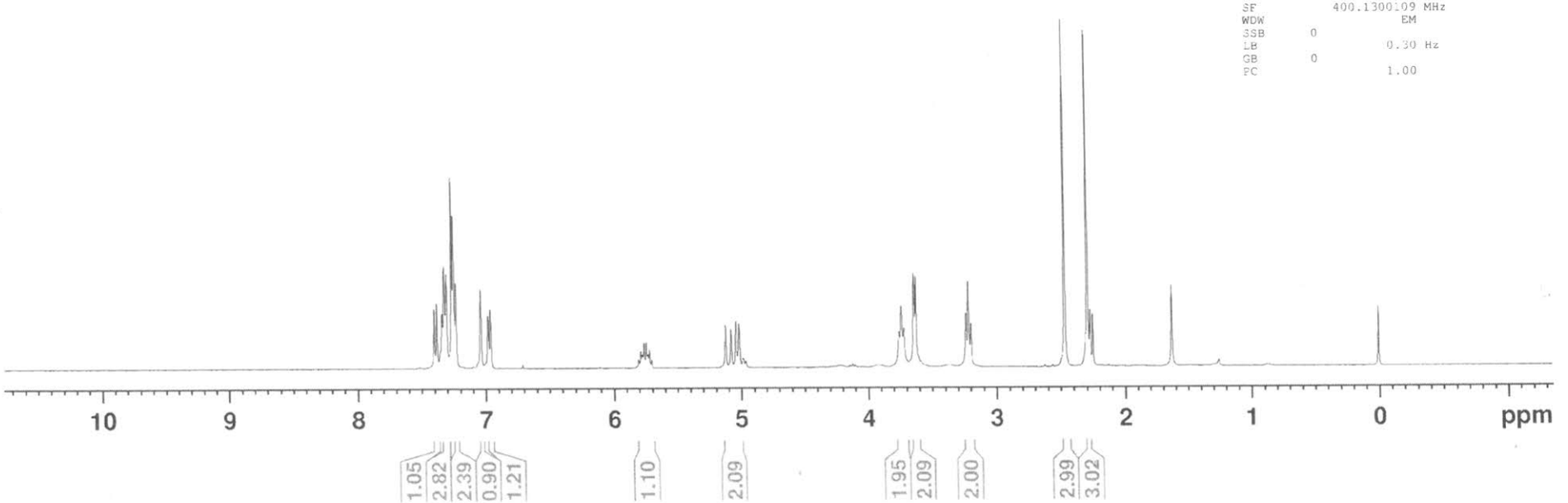


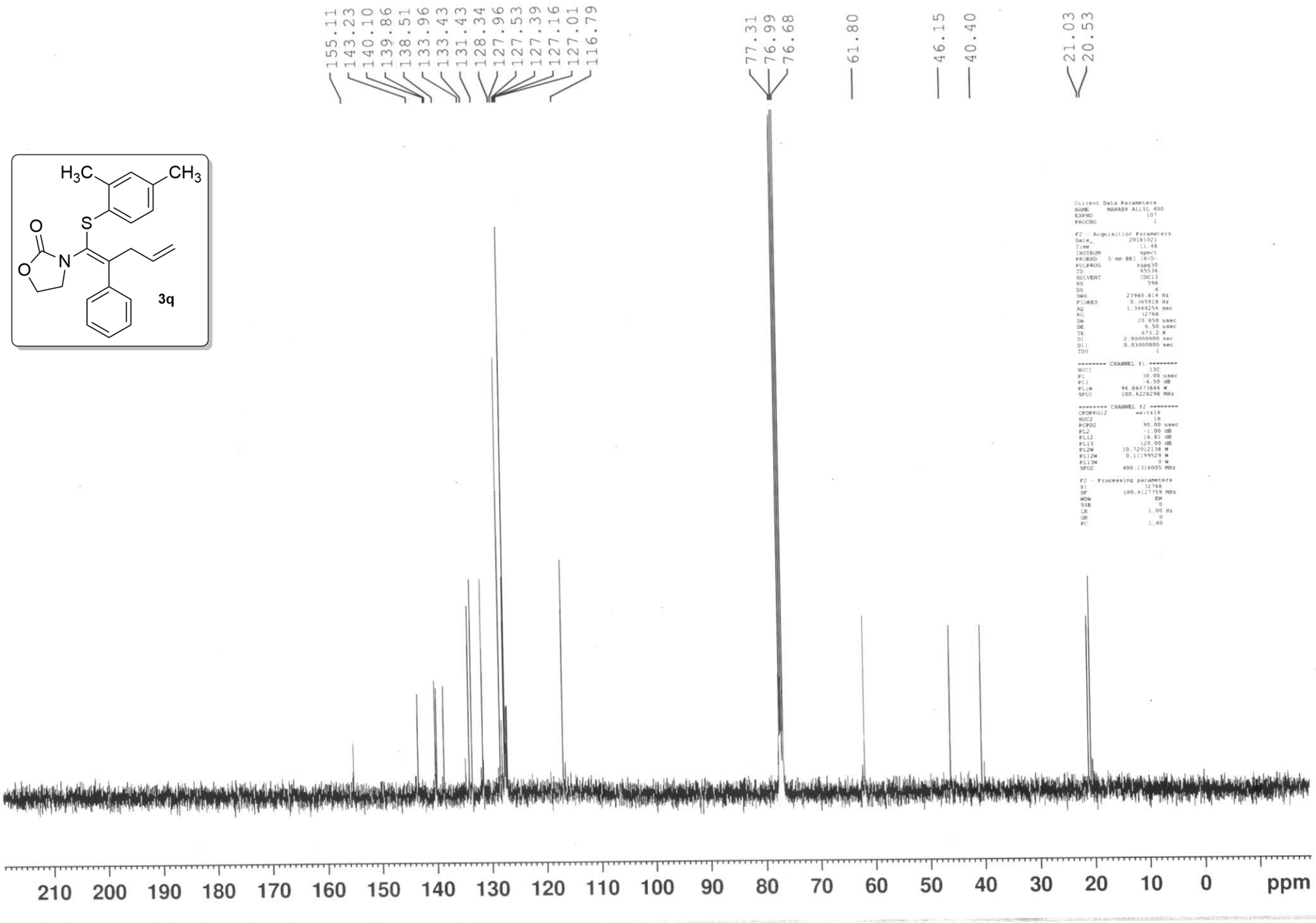

```
Current Data Parameters
NAME      MANASH ALLYL 400
EXPNO                 106
PROCNO                  1

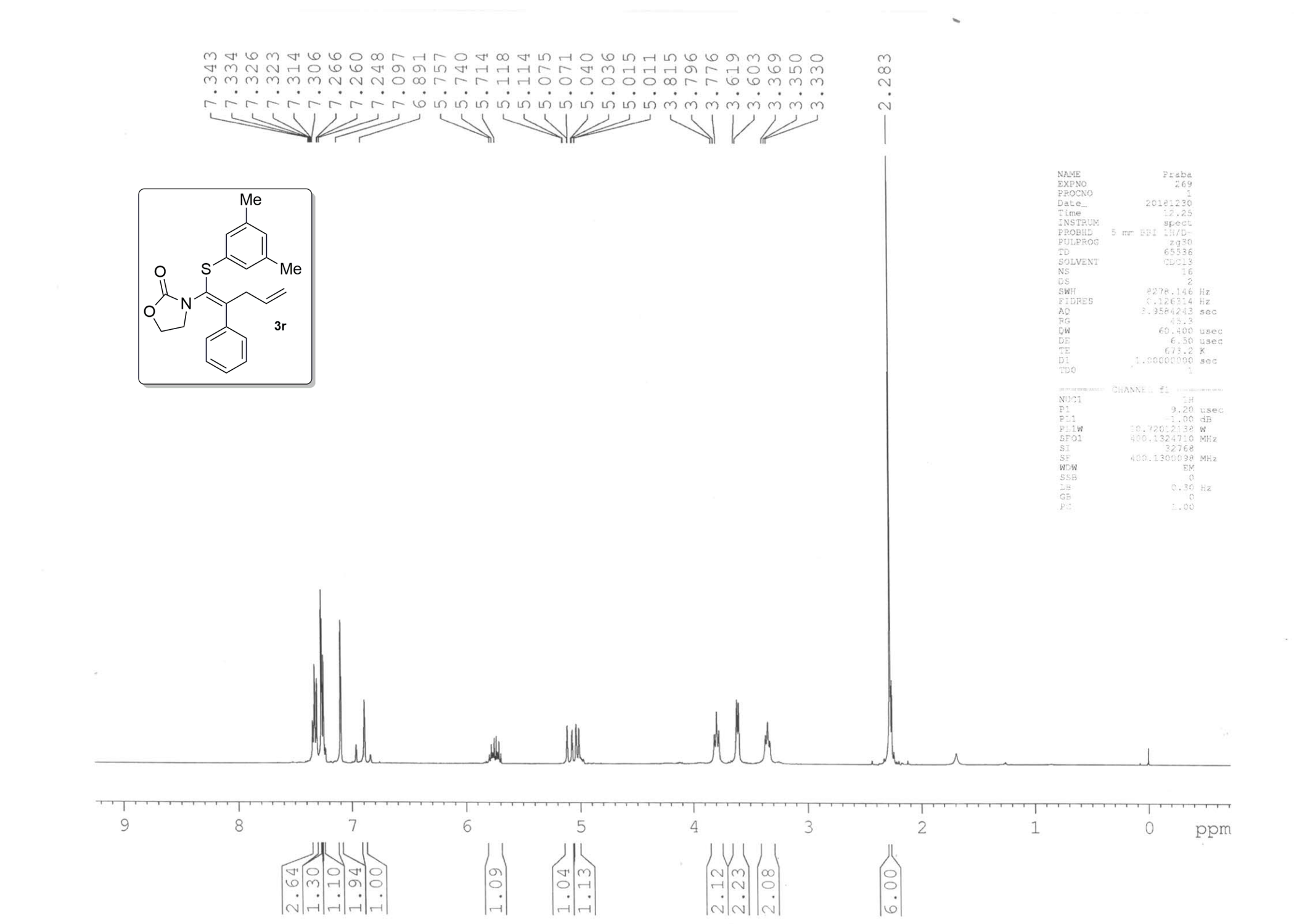
F2 - Acquisition Parameters
Date_           20181021
Time              11.37
INSTRUM           spect
PROBHD   5 mm BBI 1H/D-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.9583745 sec
RG                 90.5
DW               60.400 usec
DE                6.50 usec
TE                673.2 K
D1           1.00000000 sec
D0                   1

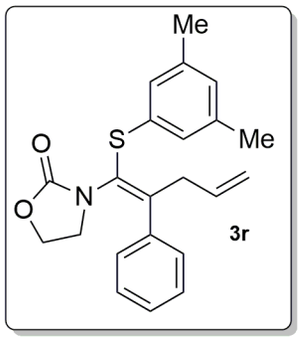
======== CHANNEL f1 ========
NUC1                1H
P1               9.20 usec
PL1             -1.00 dB
PL1W        10.72012138 W
SFO1       400.1324710 MHz

F2 - Processing parameters
SI                32768
SF         400.1300109 MHz
WDW                EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```



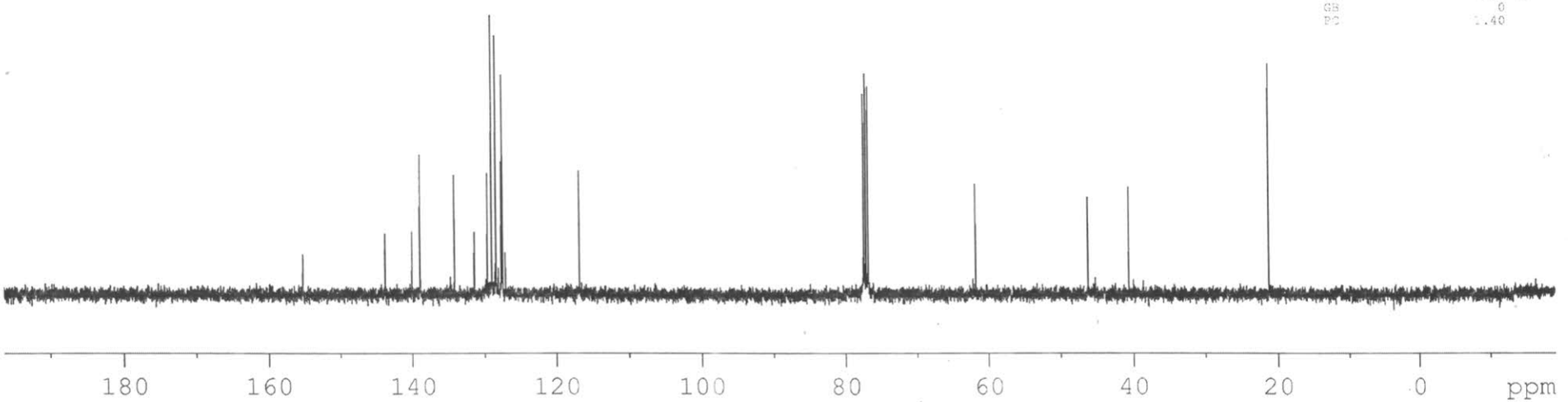

155.11
143.23
140.10
139.86
138.51
133.96
133.43
131.43
128.34
127.96
127.53
127.39
127.16
127.01
116.79
77.31
76.99
76.68
61.80
46.15
40.40
21.03
20.53
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

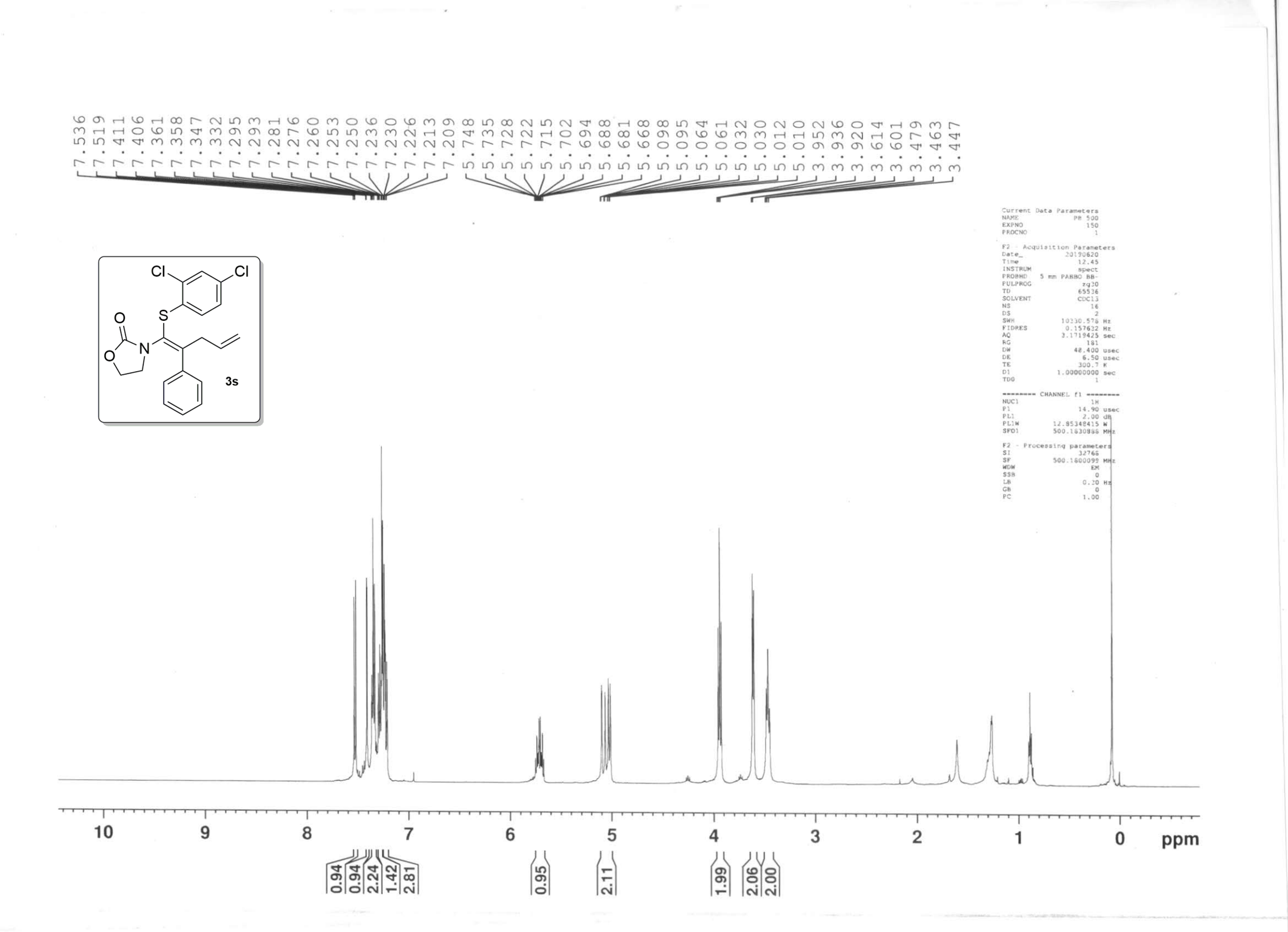

7.343
7.334
7.326
7.323
7.314
7.306
7.266
7.260
7.248
7.097
6.891
5.757
5.740
5.714
5.118
5.114
5.075
5.071
5.040
5.036
5.015
5.011
3.815
3.796
3.776
3.619
3.603
3.369
3.350
3.330
2.283
Me
Me
S
O
N
O
3r
NAME Praba
EXPNO 269
PROCNO 1
Date_ 20181230
Time 12.25
INSTRUM spect
PROBHD 5 mm BBI 1H/D-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 45.3
DW 60.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 9.20 usec
PL1 -1.00 dB
PL1W 10.72012138 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.64
1.30
1.10
1.94
1.00
1.09
1.04
1.13
2.12
2.23
2.08
6.00

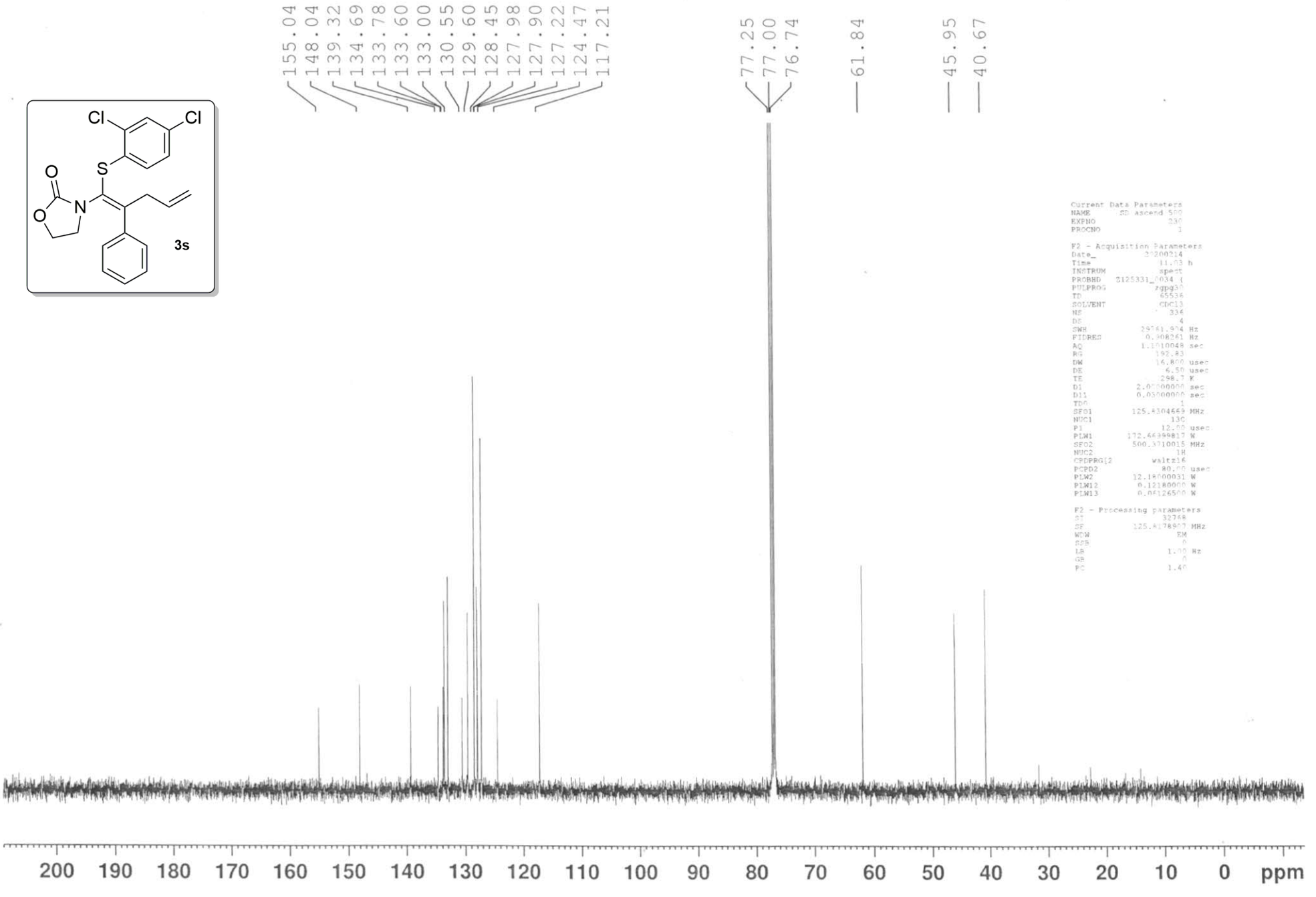


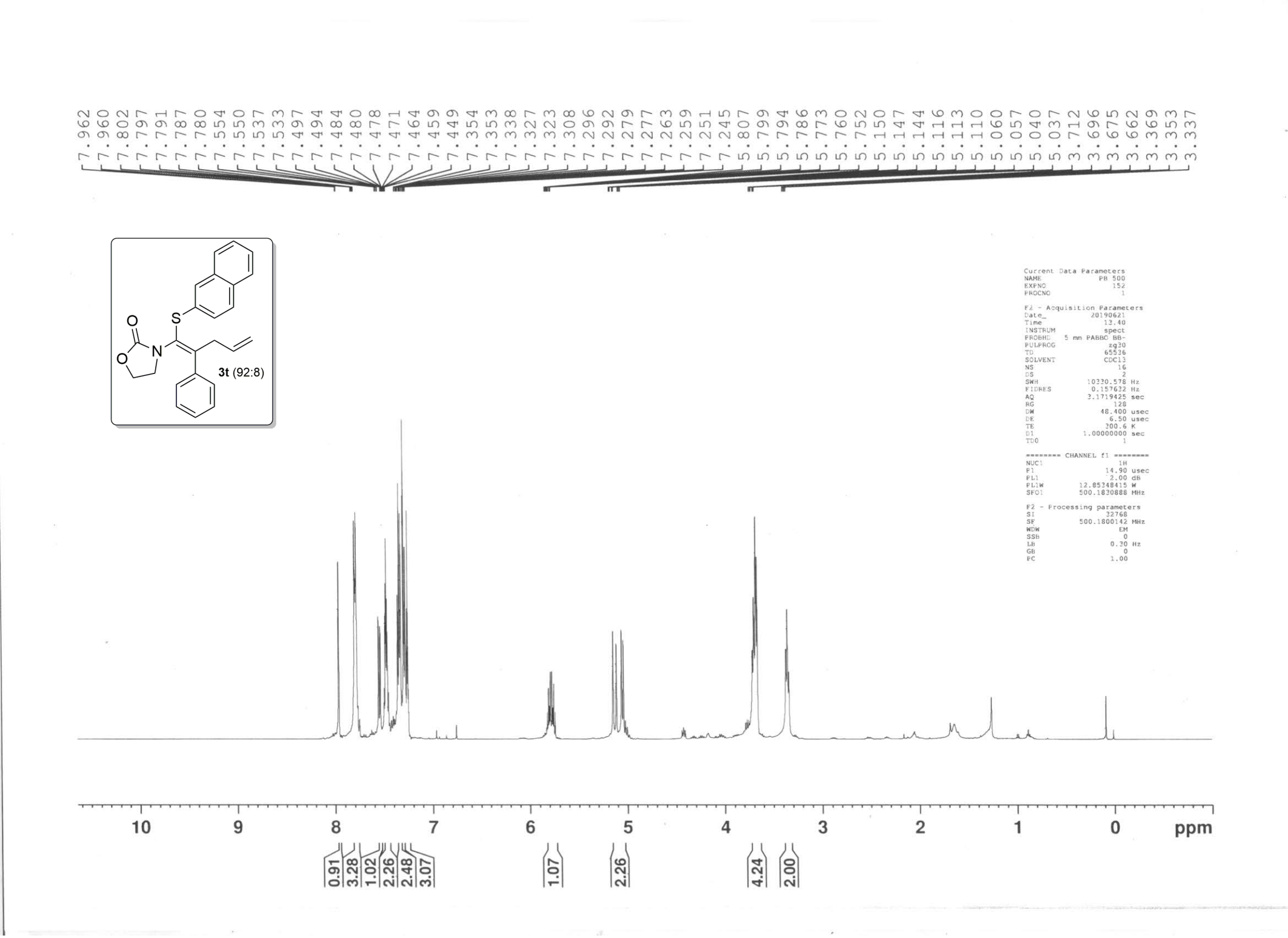
155.243
143.788
139.992
138.894
134.105
131.385
129.544
128.934
128.375
127.603
127.461
116.796
77.403
77.085
76.767
61.820
46.208
40.600
21.204

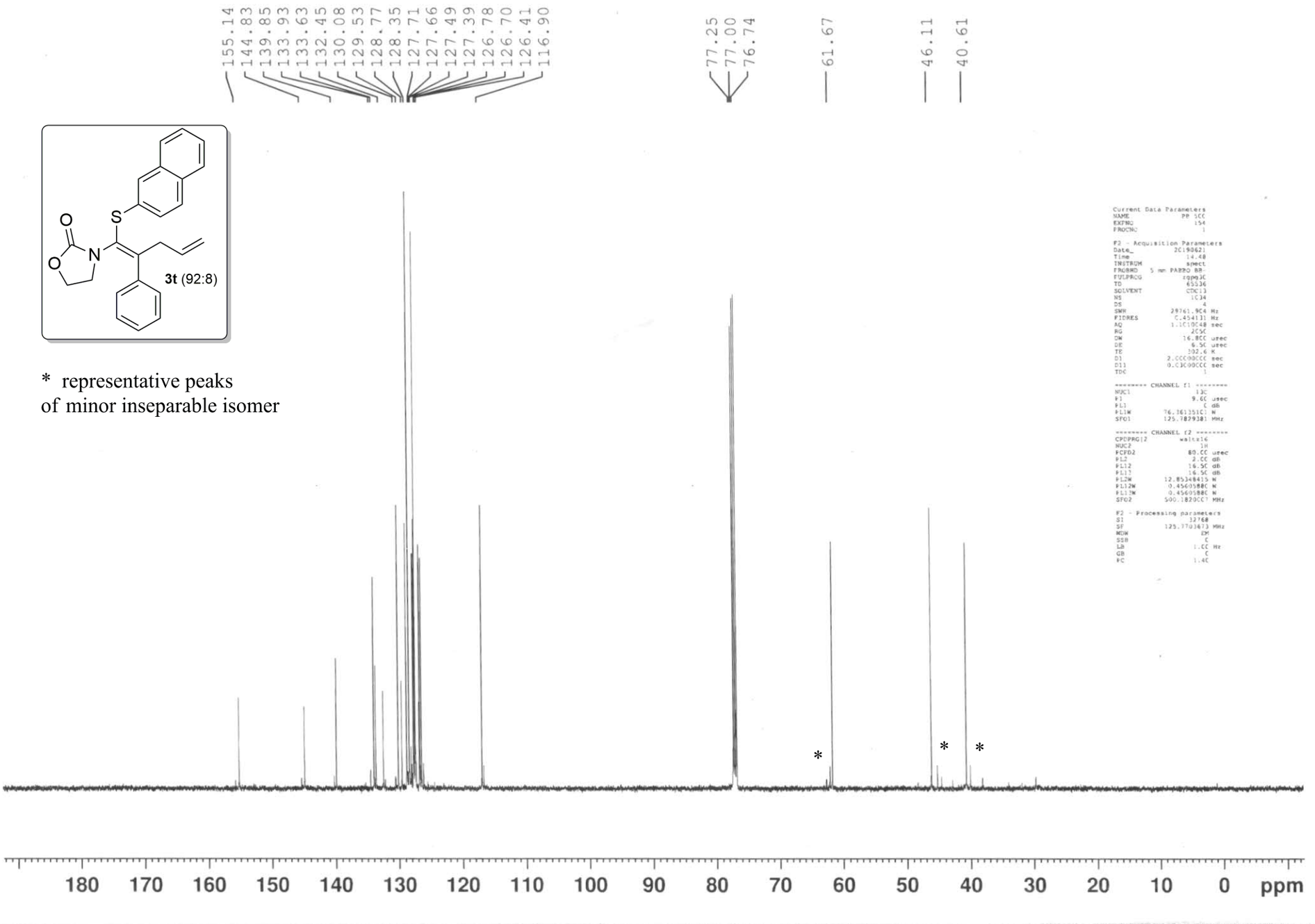
NAME	Praba
EXPNO	270
PROCNO	1
Date_	20181230
Time	12.26
INSTRUM	spect
PROBHD	5 mm BBI 1H/D-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	137
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	32768
DW	20.850 usec
DE	6.50 usec
TE	673.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	30.00 usec
PL1	-4.50 dB
PL1W	94.86473846 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	18.81 dB
PL13	120.00 dB
PL2W	10.72012138 W
PL12W	0.11199529 W
PL13W	0.00000000 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

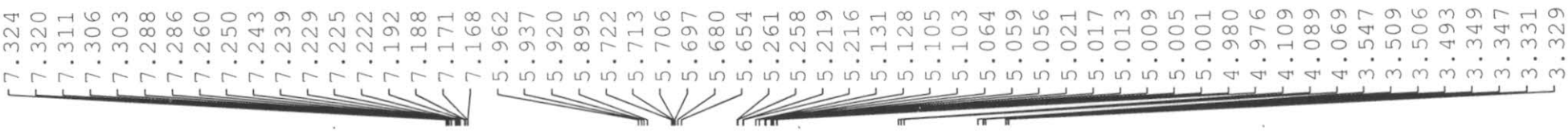


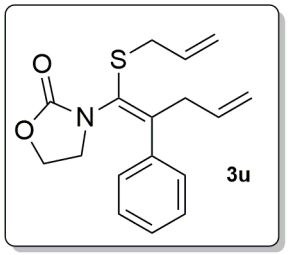

7.536
7.519
7.411
7.406
7.361
7.358
7.347
7.332
7.295
7.293
7.281
7.276
7.260
7.253
7.250
7.236
7.230
7.226
7.213
7.209
5.748
5.735
5.728
5.722
5.715
5.702
5.694
5.688
5.681
5.668
5.098
5.095
5.064
5.061
5.032
5.030
5.012
5.010
3.952
3.936
3.920
3.614
3.601
3.479
3.463
3.447
Cl
Cl
S
O
O
N
3s
Current Data Parameters
NAME PB 500
EXPNO 150
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190620
Time 12.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157622 Hz
AQ 3.1719425 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 300.7 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.90 usec
PL1 2.00 dB
PL1W 12.85348415 W
SFO1 500.1830988 MHz
F2 - Processing parameters
SI 32766
SF 500.1800099 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
0.94
0.94
2.24
1.42
2.81
0.95
2.11
1.99
2.06
2.00

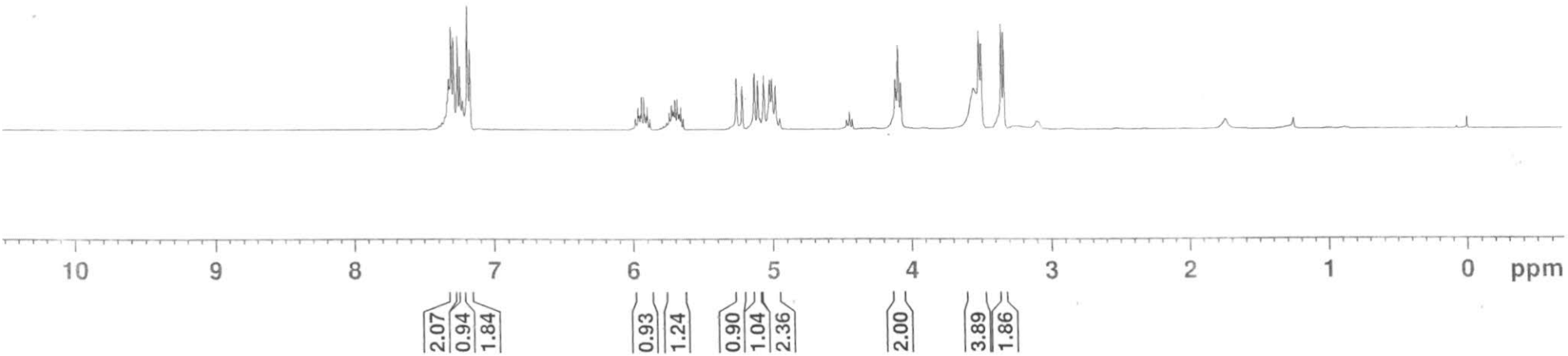

155.04
148.04
139.32
134.69
133.78
133.60
133.00
130.55
129.60
128.45
127.98
127.90
127.22
124.47
117.21
77.25
77.00
76.74
61.84
45.95
40.67
Cl
Cl
S
O
N
O
3s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

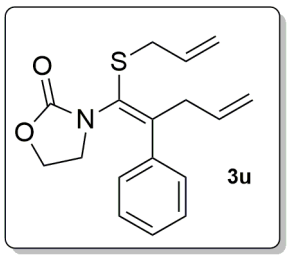

7.962
7.960
7.802
7.797
7.791
7.787
7.780
7.554
7.550
7.537
7.533
7.497
7.494
7.484
7.480
7.478
7.471
7.464
7.459
7.449
7.354
7.353
7.338
7.327
7.323
7.308
7.296
7.292
7.279
7.277
7.263
7.259
7.251
7.245
5.807
5.799
5.794
5.786
5.773
5.760
5.752
5.150
5.147
5.144
5.116
5.113
5.110
5.060
5.057
5.040
5.037
3.712
3.696
3.675
3.662
3.369
3.353
3.337
O
S
N
O
3t (92:8)
Current Data Parameters
NAME PB 500
EXPNO 152
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190621
Time 12.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 200.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 2.00 dB
PL1W 12.85348415 W
SFO1 500.1830888 MHz
F2 - Processing parameters
SI 32768
SF 500.1800142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
0.91
3.28
1.02
2.26
2.48
3.07
1.07
2.26
4.24
2.00


155.14
144.83
139.85
133.93
133.63
132.45
130.08
129.53
128.77
128.35
127.71
127.66
127.49
127.39
126.78
126.70
126.41
116.90
77.25
77.00
76.74
61.67
46.11
40.61
3t (92:8)
* representative peaks
of minor inseparable isomer
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.324
7.320
7.311
7.306
7.303
7.288
7.286
7.260
7.250
7.243
7.239
7.229
7.225
7.222
7.192
7.188
7.171
7.168
5.962
5.937
5.920
5.895
5.722
5.713
5.706
5.697
5.680
5.654
5.261
5.258
5.219
5.216
5.131
5.128
5.105
5.103
5.064
5.059
5.056
5.021
5.017
5.013
5.009
5.005
5.001
4.980
4.976
4.109
4.089
4.069
3.547
3.509
3.506
3.493
3.349
3.347
3.331
3.329


O
S
N
O
3u


10
9
8
7
6
5
4
3
2
1
0
ppm
2.07
0.94
1.84
0.93
1.24
0.90
1.04
2.36
2.00
3.89
1.86



155.88
146.33
139.64
134.00
133.92
128.58
128.19
127.50
127.14
117.61
116.70
77.31
77.00
76.68
61.88
45.88
40.56
35.36

Current Data Parameters
NAME 67-furan-2018
EXPNO 723
PROCNO 1

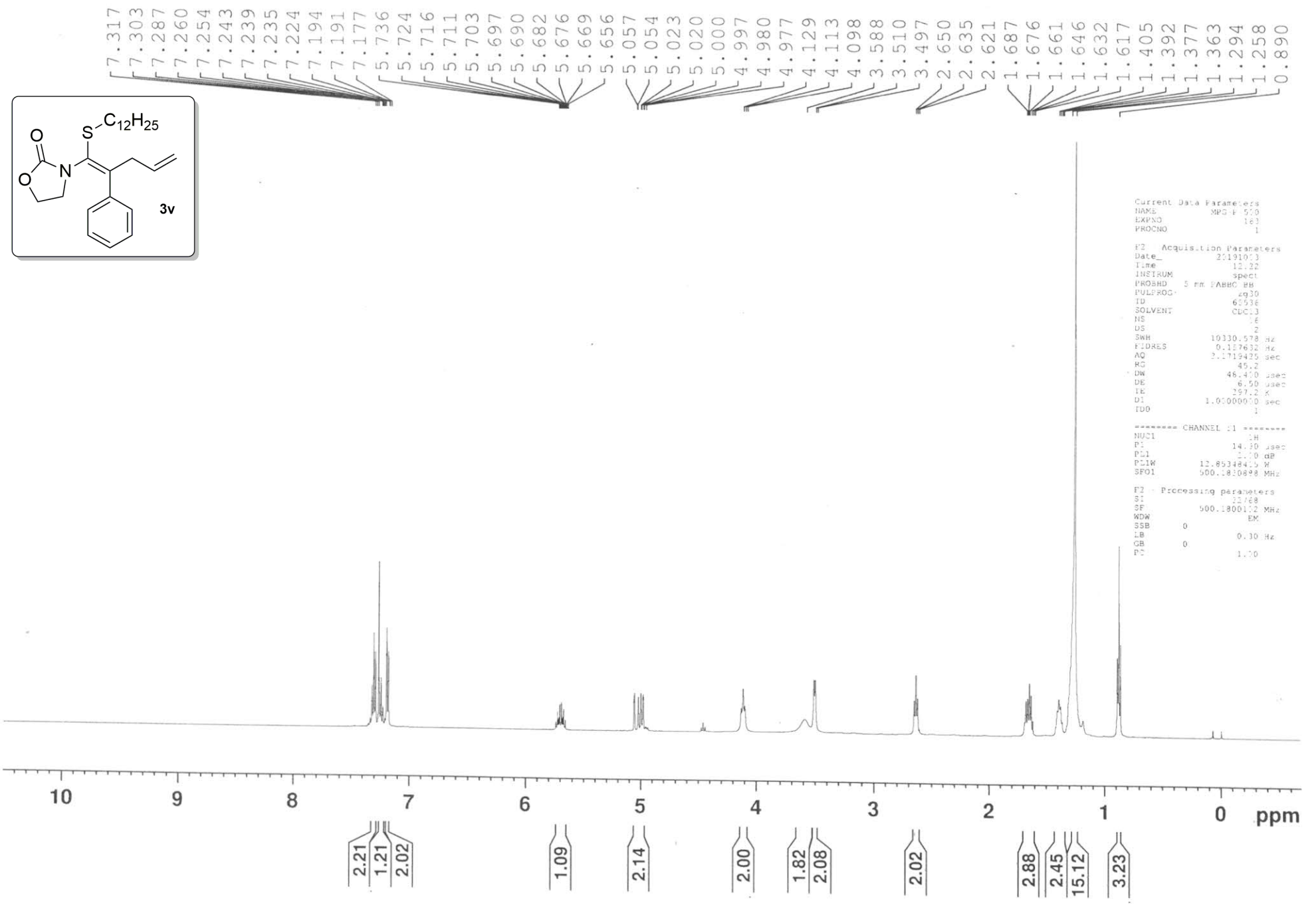
F2 - Acquisition Parameters
Date_ 20180808
Time 2.22
INSTRUM spect
PROBHD 5 mm DBI 1H/D
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 32768
DW 20.850 usec
DE 6.50 usec
TE 293.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

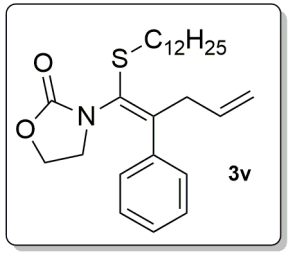
CHANNEL f1
NUC1 13C
P1 10.60 usec
PL1 -6.50 dB
PL1W 34.86473846 W
SFO1 100.6232758 MHz

CHANNEL f2
CPDPRG[2 waltz16
NUC2 1H
PCPD2 96.60 usec
PL2 1.60 dB
PL12 18.80 dB
PL13 20.00 dB
PL2W 16.72112136 W
PL12W 0.11195523 W
PL13W 0 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127752 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.317
7.303
7.287
7.260
7.254
7.243
7.239
7.235
7.224
7.194
7.191
7.177
5.736
5.724
5.716
5.711
5.703
5.697
5.690
5.682
5.676
5.669
5.656
5.057
5.054
5.023
5.020
5.000
4.997
4.980
4.977
4.129
4.113
4.098
3.588
3.510
3.497
2.650
2.635
2.621
1.687
1.676
1.661
1.646
1.632
1.617
1.405
1.392
1.377
1.363
1.294
1.258
0.890
O
S
$C_{12}H_{25}$
O
N
O
3v
Current Data Parameters
NAME MPS-F-509
EXPNO 163
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191013
Time 12.32
INSTRUM spect
PROBHD 5 mm DABBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 45.2
DW 48.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.30 usec
PL1 1.10 dB
PL1W 12.85348415 W
SFO1 500.1810898 MHz
F2 - Processing parameters
SI 32768
SF 500.1800112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.21
1.21
2.02
1.09
2.14
2.00
1.82
2.08
2.02
2.88
2.45
15.12
3.23

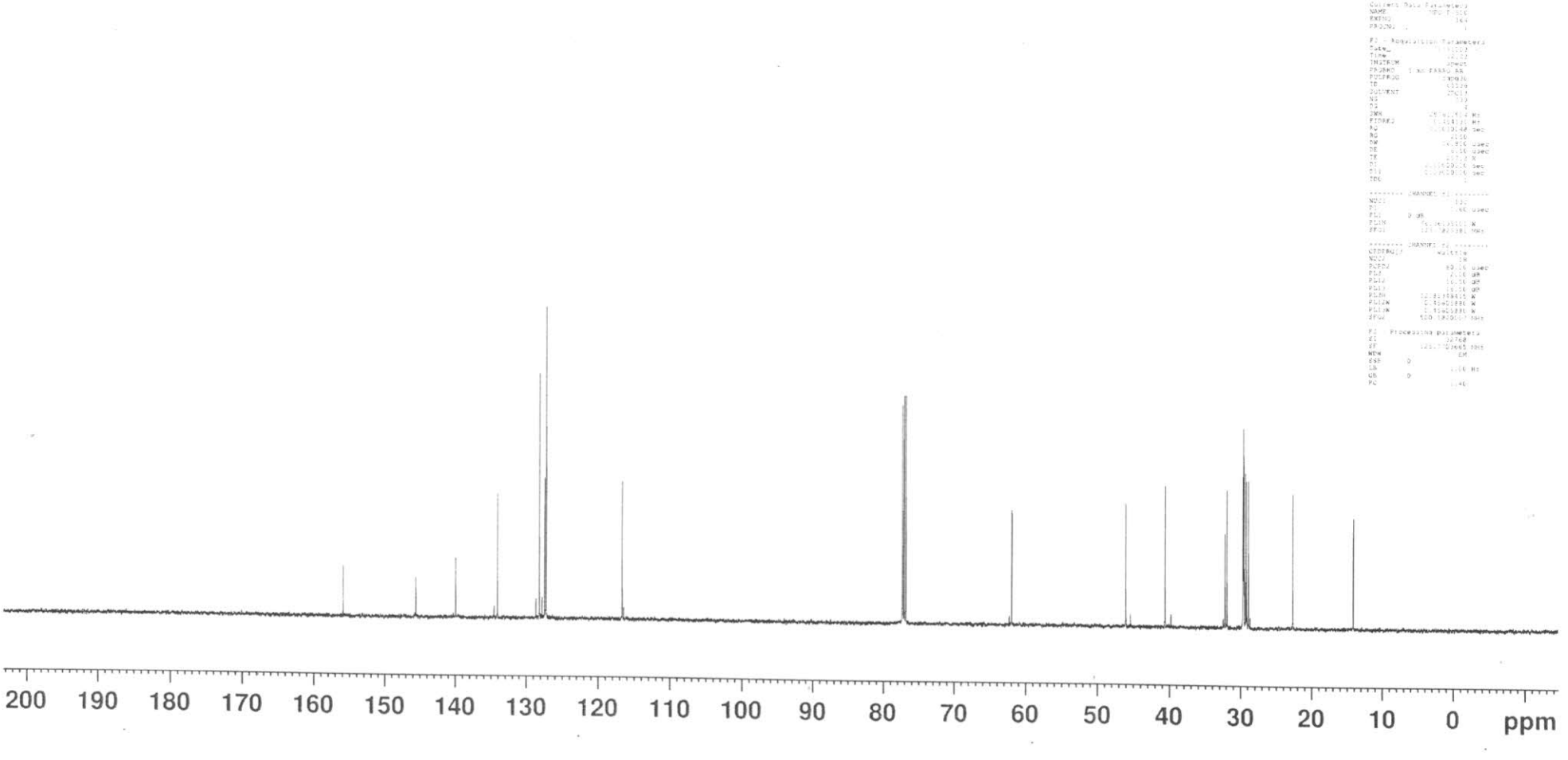


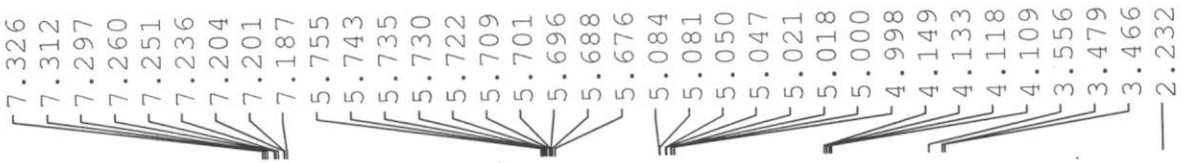
155.85
145.57
139.91
134.04
128.61
128.16
127.41
127.21
116.61

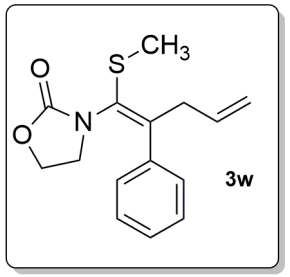
77.25
77.00
76.74

61.89

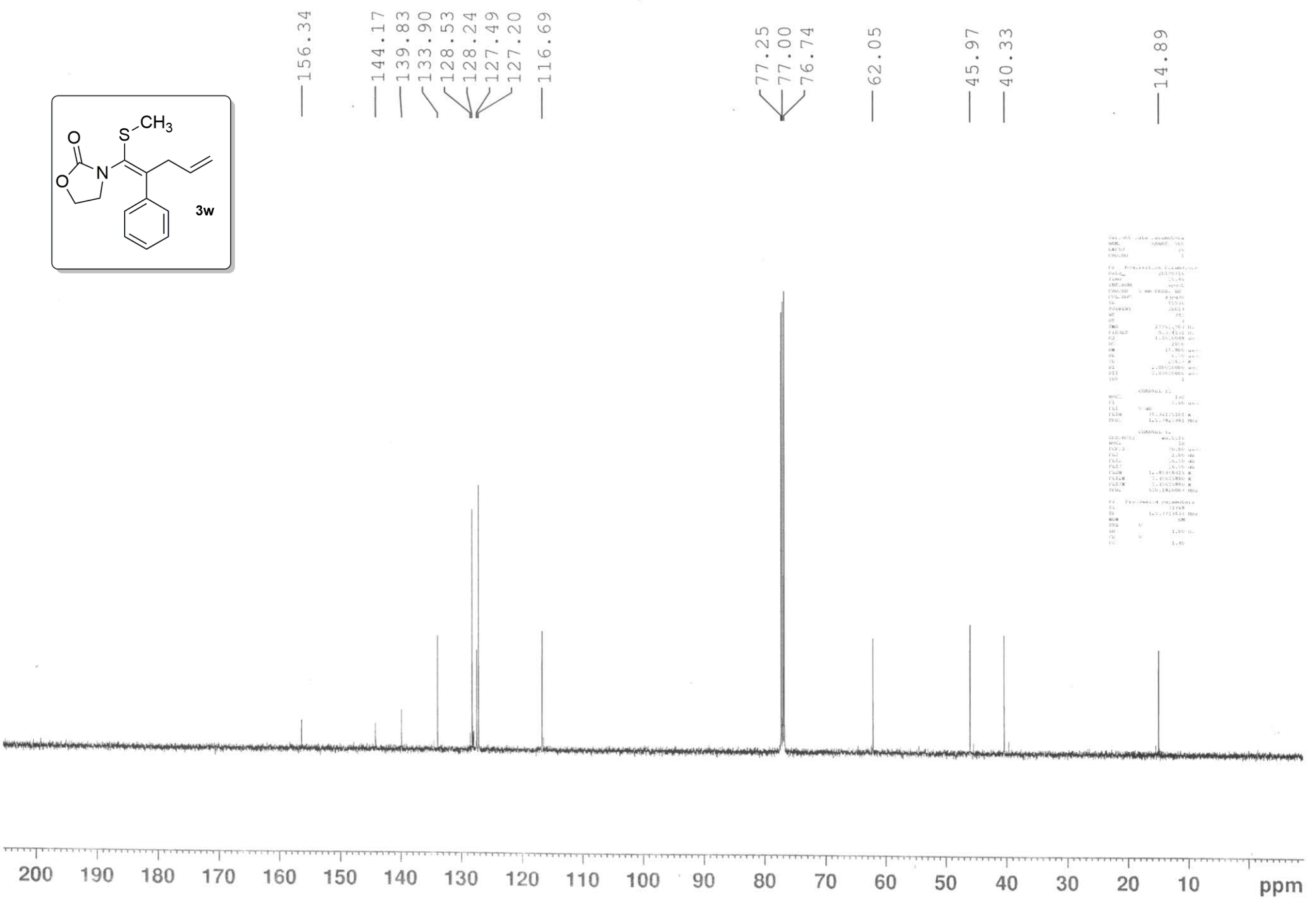
46.01
40.55
32.16
31.87
29.65
29.60
29.58
29.54
29.49
29.29
29.13
28.84
22.63
14.05

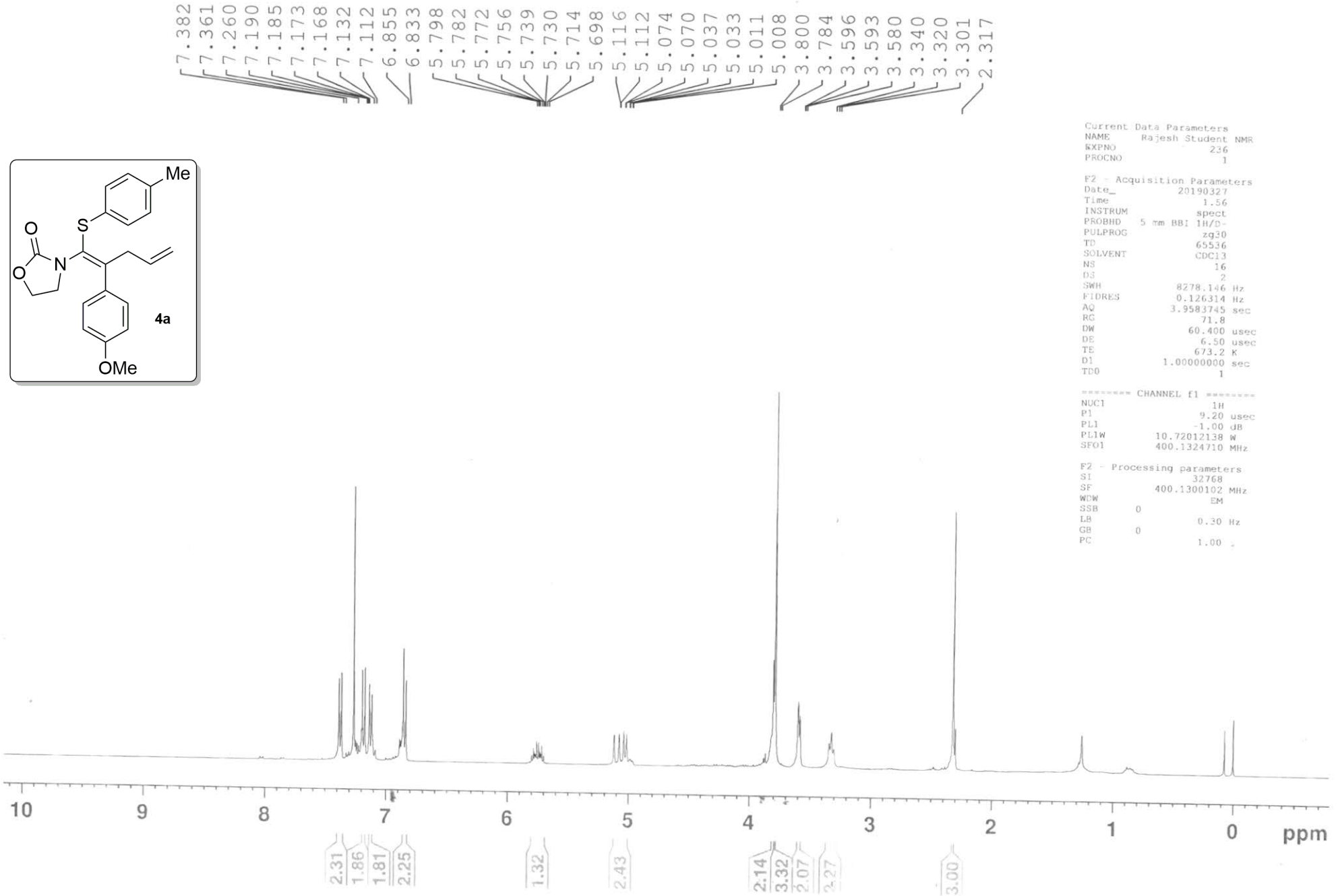


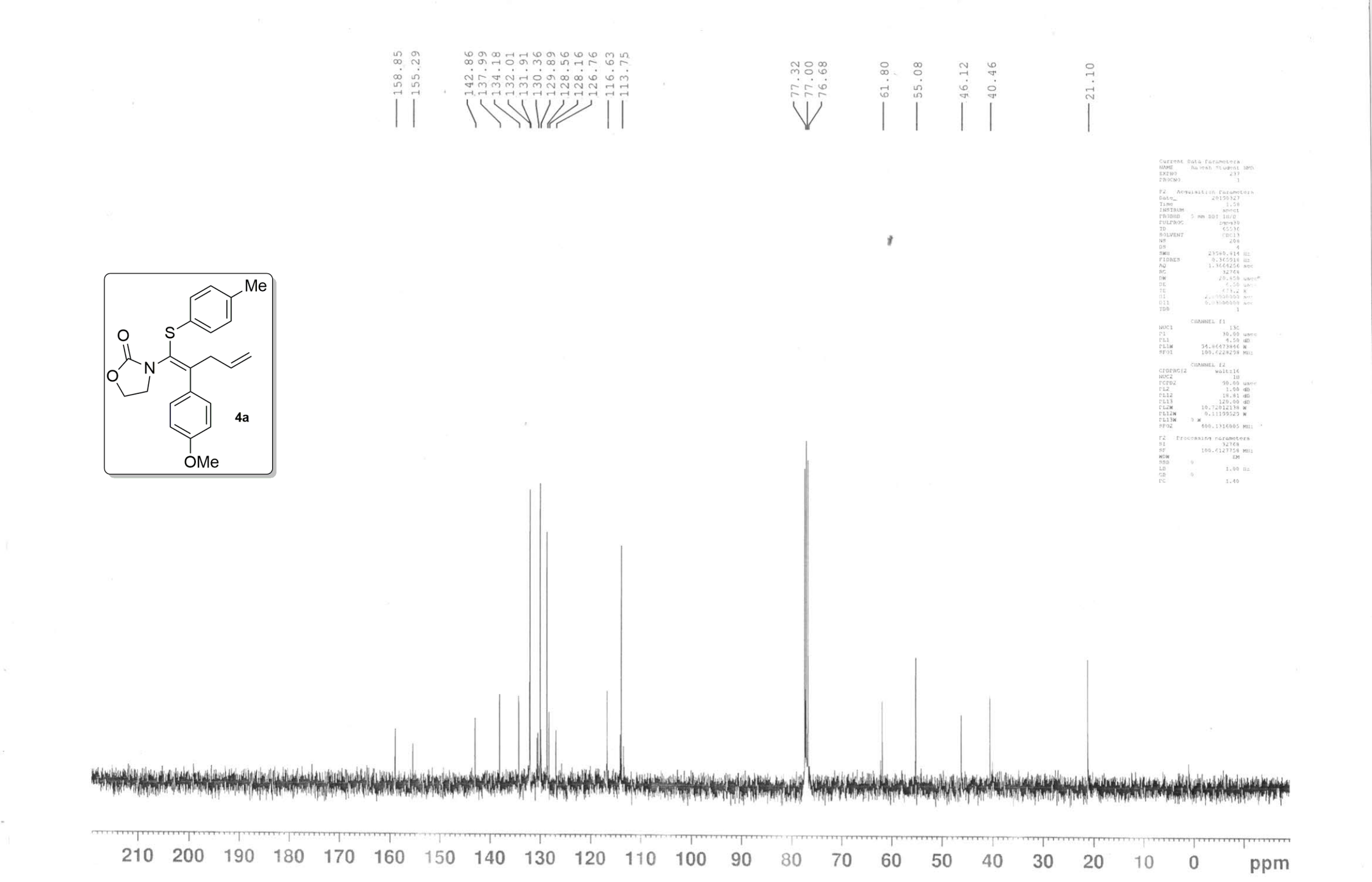

7.326
7.312
7.297
7.260
7.251
7.236
7.204
7.201
7.187
5.755
5.743
5.735
5.730
5.722
5.709
5.701
5.696
5.688
5.676
5.084
5.081
5.050
5.047
5.021
5.018
5.000
4.998
4.149
4.133
4.118
4.109
3.556
3.479
3.466
2.232

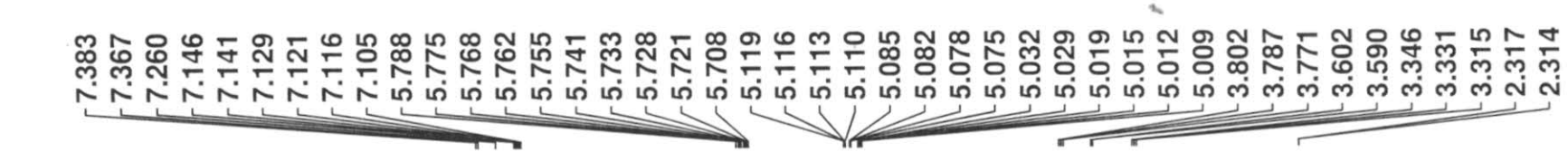

O
S
CH3
O
N
3w

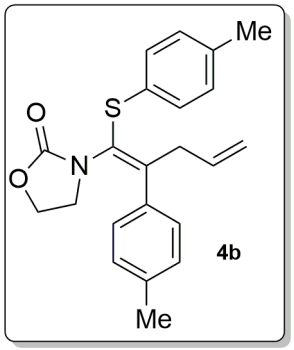
Current Data Parameters
NAME MANASH 500
EXPNO 24
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180716
Time 15.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1715425 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.90 usec
PL1 2.00 dB
PL1W 12.85348415 W
SFO1 500.1330888 MHz
F2 - Processing parameters
SI 32768
SF 500.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.15
0.83
2.00
1.07
1.00
1.07
2.00
1.86
2.12
3.05


156.34
144.17
139.83
133.90
128.53
128.24
127.49
127.20
116.69
77.25
77.00
76.74
62.05
45.97
40.33
14.89
O
S
CH3
N
O
3w
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

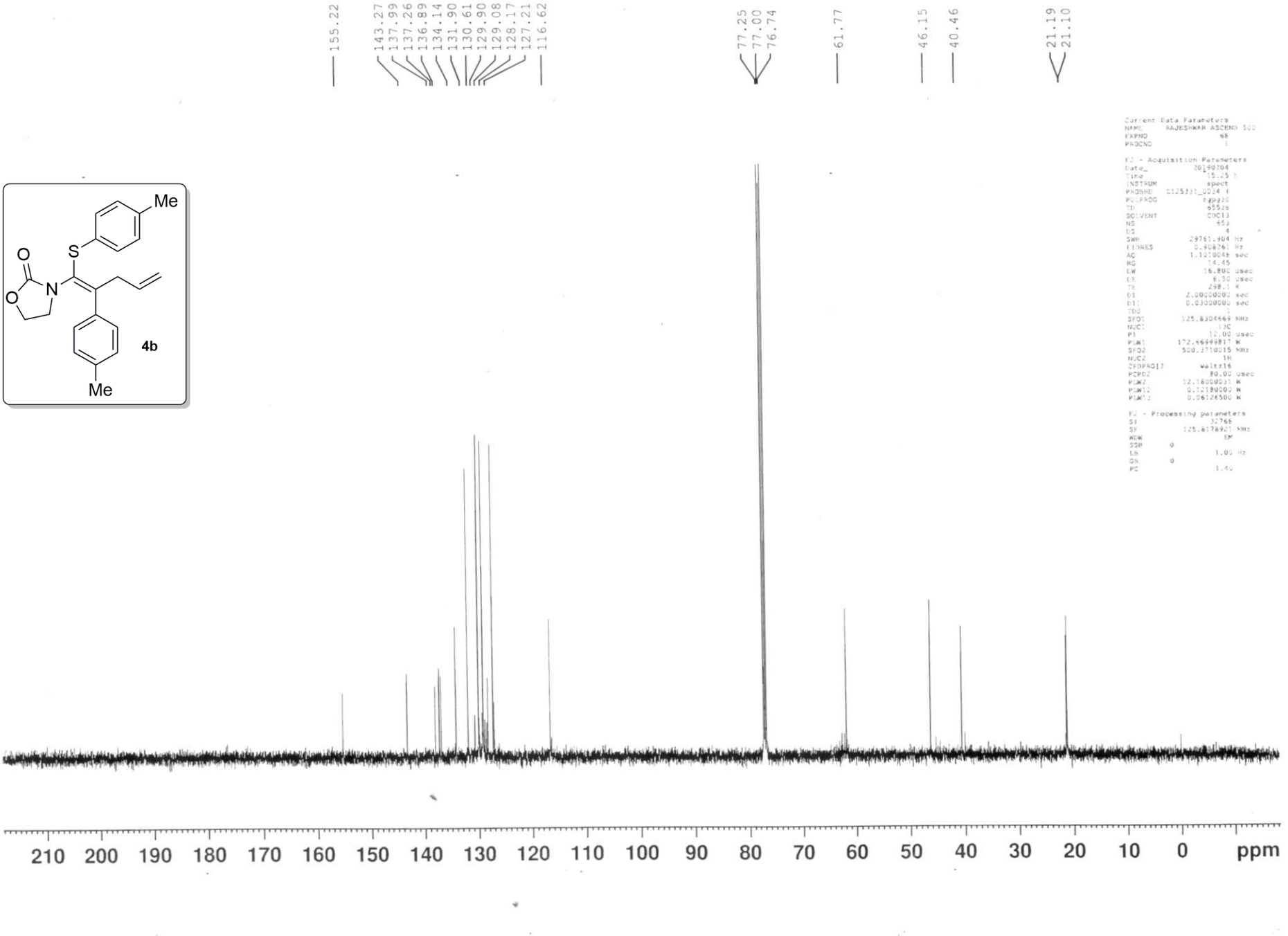

7.382
7.361
7.260
7.190
7.185
7.173
7.168
7.132
7.112
6.855
6.833
5.798
5.782
5.772
5.756
5.739
5.730
5.714
5.698
5.116
5.112
5.074
5.070
5.037
5.033
5.011
5.008
3.800
3.784
3.596
3.593
3.580
3.340
3.320
3.301
2.317
Me
S
O
N
O
4a
OMe
Current Data Parameters
NAME Rajesh Student NMR
EXPNO 236
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190327
Time 1.56
INSTRUM spect
PROBHD 5 mm BBI 1H/D-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 9.20 usec
PL1 -1.00 dB
PL1W 10.72012138 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.31
1.86
1.81
2.25
1.32
2.43
2.14
3.32
2.07
2.27
3.00

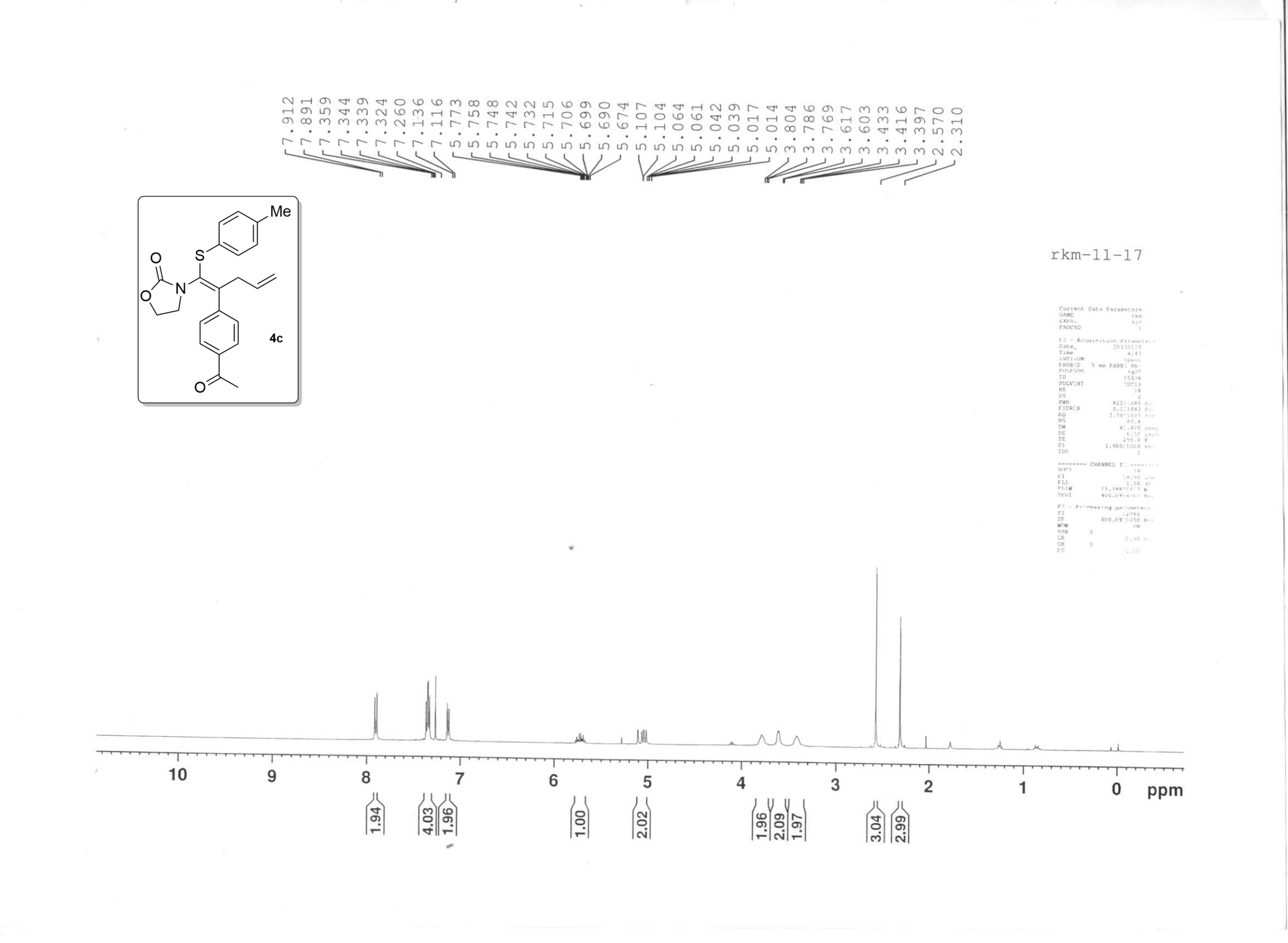

158.85
155.29
142.86
137.99
134.18
132.01
131.91
130.36
129.89
128.56
128.16
126.76
116.63
113.75
77.32
77.00
76.68
61.80
55.08
46.12
40.46
21.10
Me
S
O
N
O
4a
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

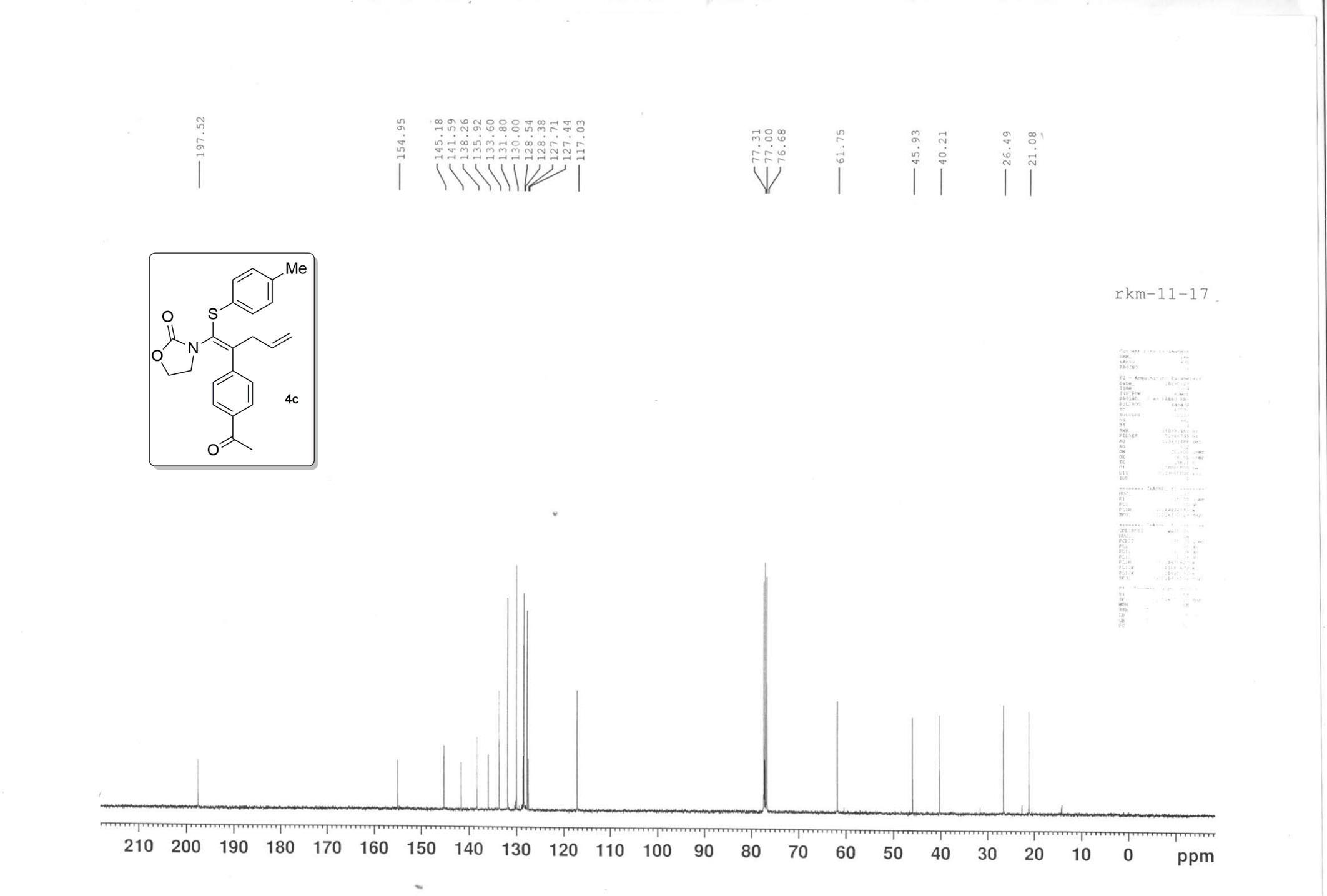

7.383
7.367
7.260
7.146
7.141
7.129
7.121
7.116
7.105
5.788
5.775
5.768
5.762
5.755
5.741
5.733
5.728
5.721
5.708
5.119
5.116
5.113
5.110
5.085
5.082
5.078
5.075
5.032
5.029
5.019
5.015
5.012
5.009
3.802
3.787
3.771
3.602
3.590
3.346
3.331
3.315
2.317
2.314

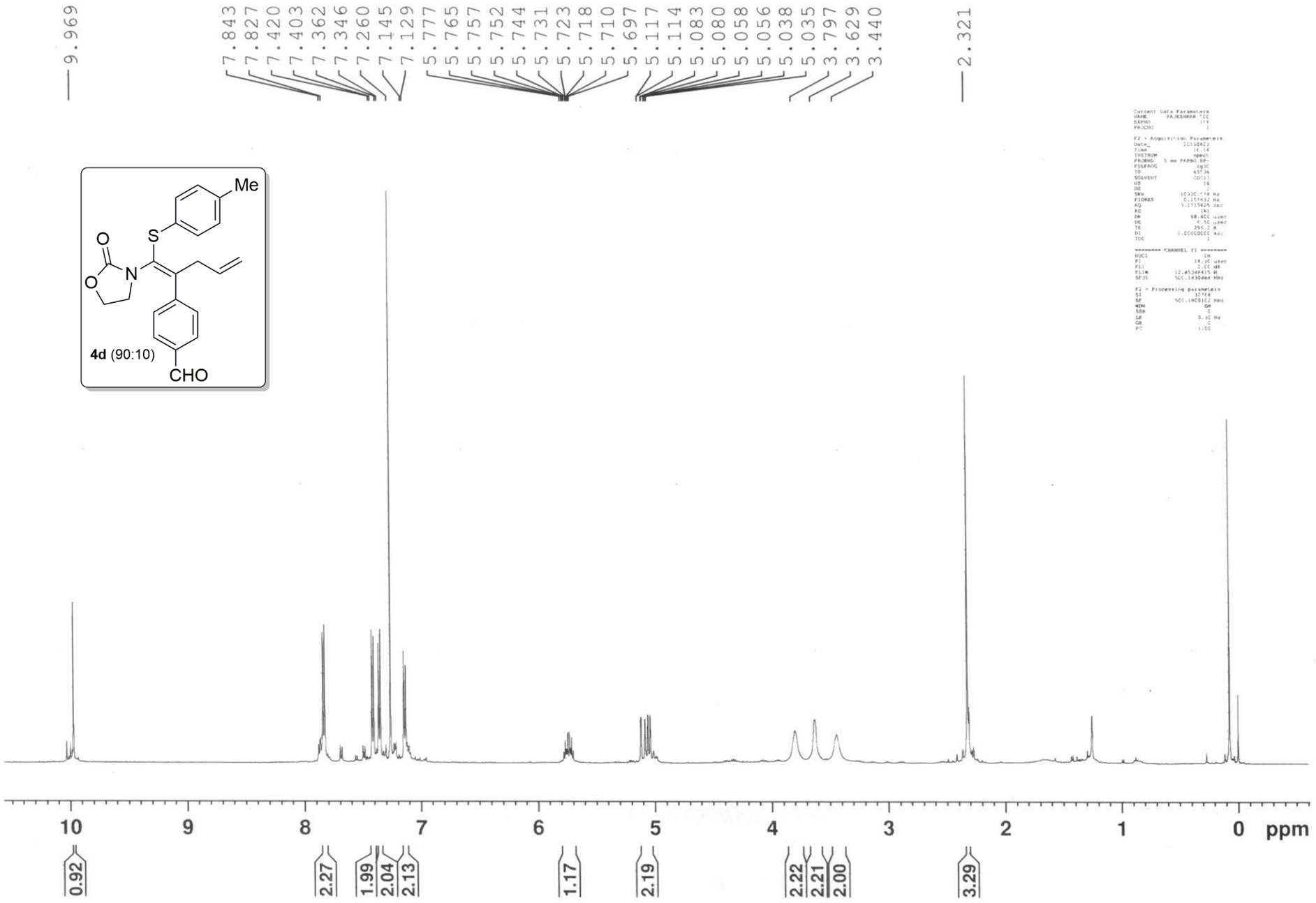

Me
S
O
N
O
4b
Me

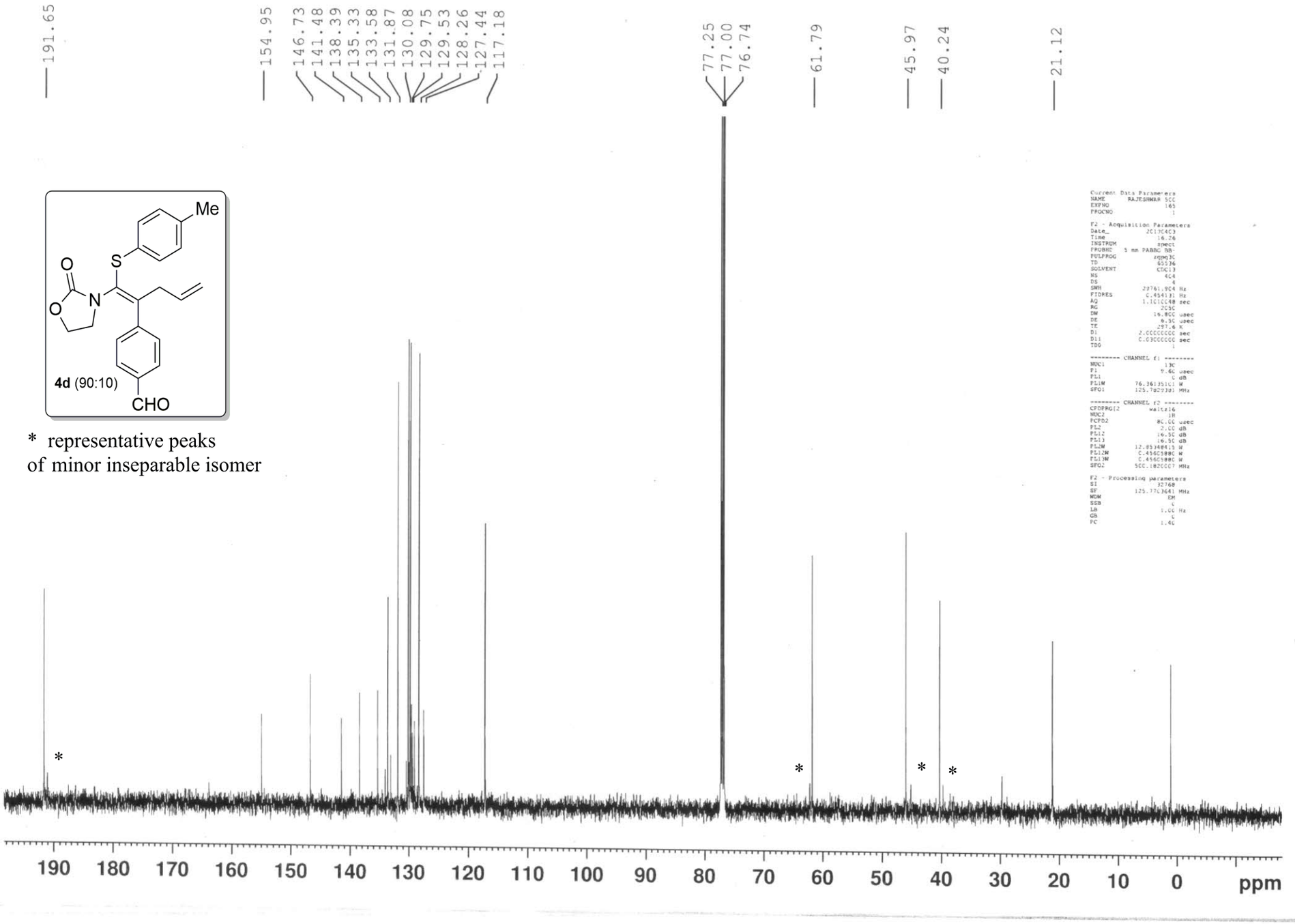
10
9
8
7
6
5
4
3
2
1
0
ppm
2.03
6.42
1.10
2.26
2.18
2.05
2.00
6.08


155.22
143.27
137.99
137.26
136.89
134.14
131.90
130.61
129.90
129.08
128.17
127.21
116.62
77.25
77.00
76.74
61.77
46.15
40.46
21.19
21.10
Me
S
O
N
O
4b
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

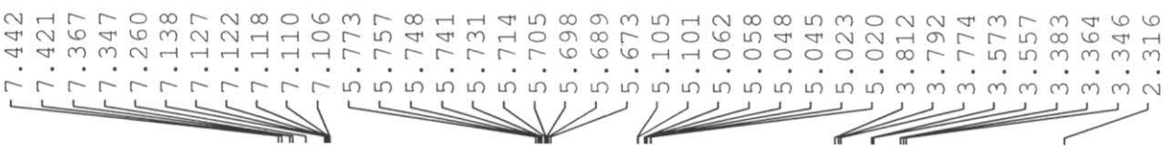

7.912
7.891
7.359
7.344
7.339
7.324
7.260
7.136
7.116
5.773
5.758
5.748
5.742
5.732
5.715
5.706
5.699
5.690
5.674
5.107
5.104
5.064
5.061
5.042
5.039
5.017
5.014
3.804
3.786
3.769
3.617
3.603
3.433
3.416
3.397
2.570
2.310
Me
S
O
N
O
O
4c
rkm-11-17
10
9
8
7
6
5
4
3
2
1
0
ppm
1.94
4.03
1.96
1.00
2.02
1.96
2.09
1.97
3.04
2.99

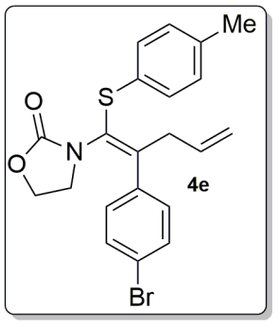

197.52
154.95
145.18
141.59
138.26
135.92
133.60
131.80
130.00
128.54
128.38
127.71
127.44
117.03
77.31
77.00
76.68
61.75
45.93
40.21
26.49
21.08
Me
S
O
N
O
O
4c
rkm-11-17
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


9.969
7.843
7.827
7.420
7.403
7.362
7.346
7.260
7.145
7.129
5.777
5.765
5.757
5.752
5.744
5.731
5.723
5.718
5.710
5.697
5.117
5.114
5.083
5.080
5.058
5.056
5.038
5.035
3.797
3.629
3.440
2.321
Me
S
O
O
N
4d (90:10)
CHO
10
9
8
7
6
5
4
3
2
1
0
ppm
0.92
2.27
1.99
2.04
2.13
1.17
2.19
2.22
2.21
2.00
3.29



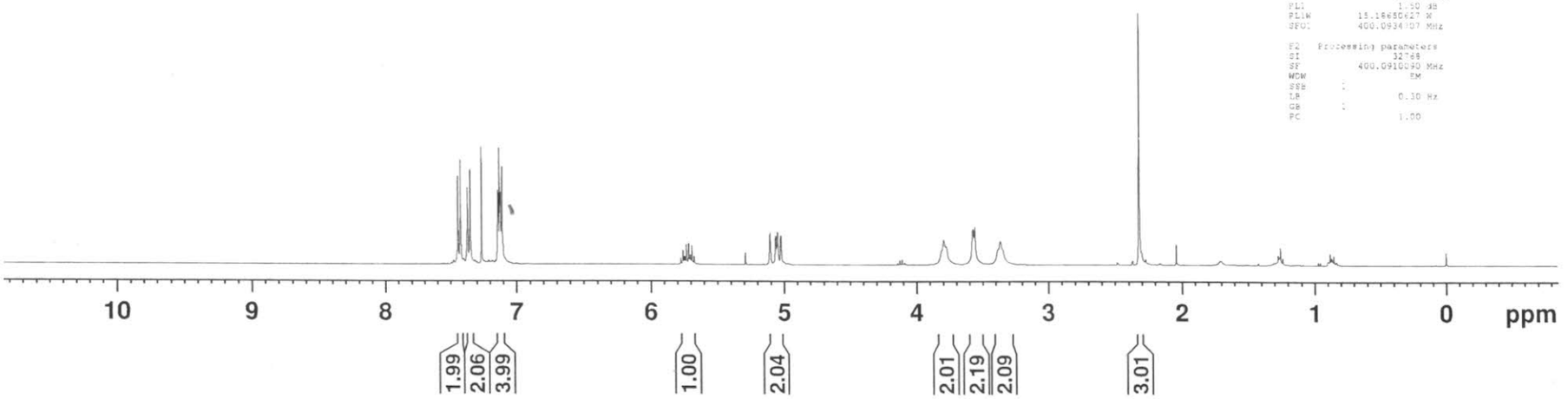
* representative peaks
of minor inseparable isomer

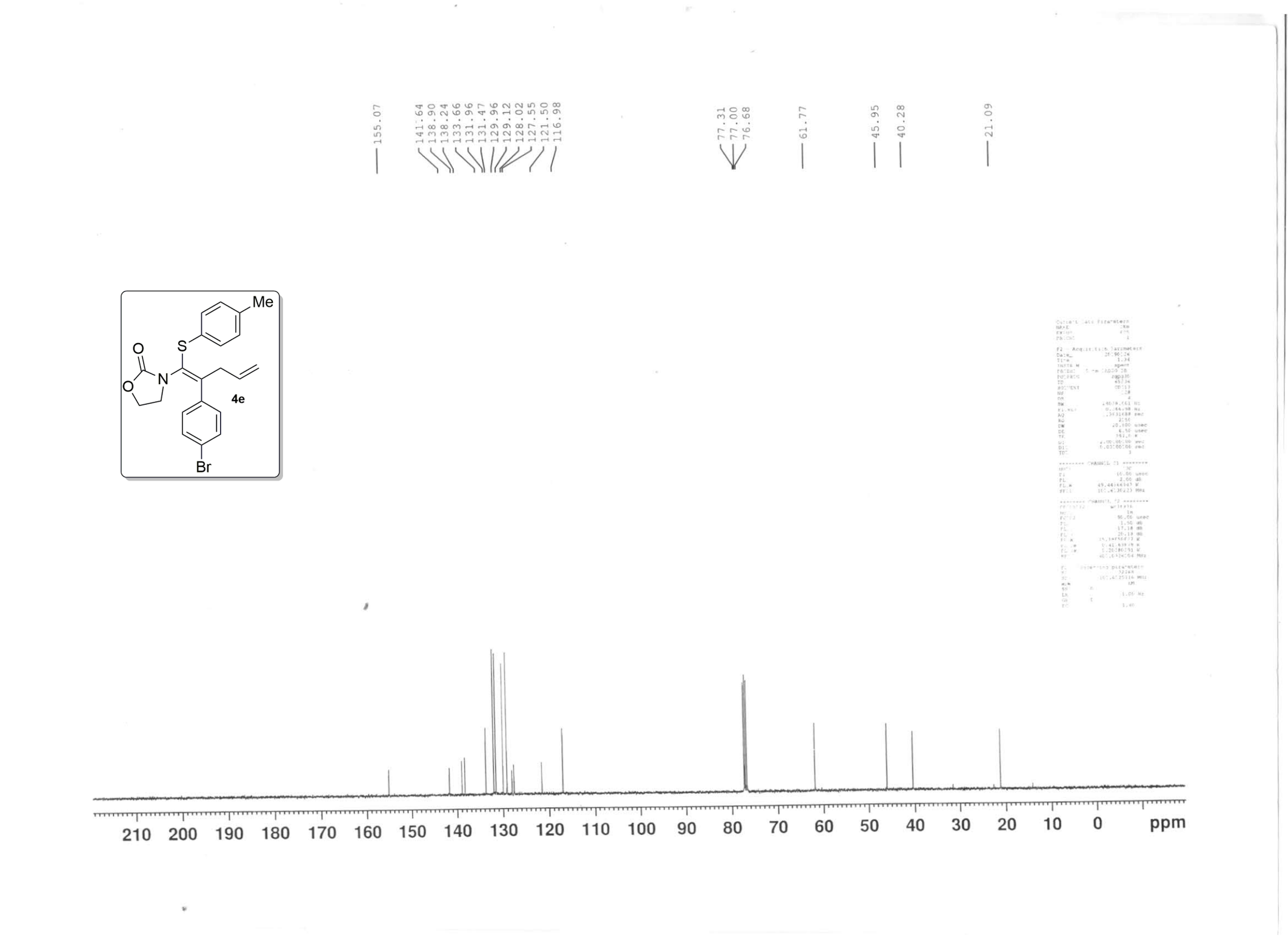

7.442
7.421
7.367
7.347
7.260
7.138
7.127
7.122
7.118
7.110
7.106
5.773
5.757
5.748
5.741
5.731
5.714
5.705
5.698
5.689
5.673
5.105
5.101
5.062
5.058
5.048
5.045
5.023
5.020
3.812
3.792
3.774
3.573
3.557
3.383
3.364
3.346
2.316

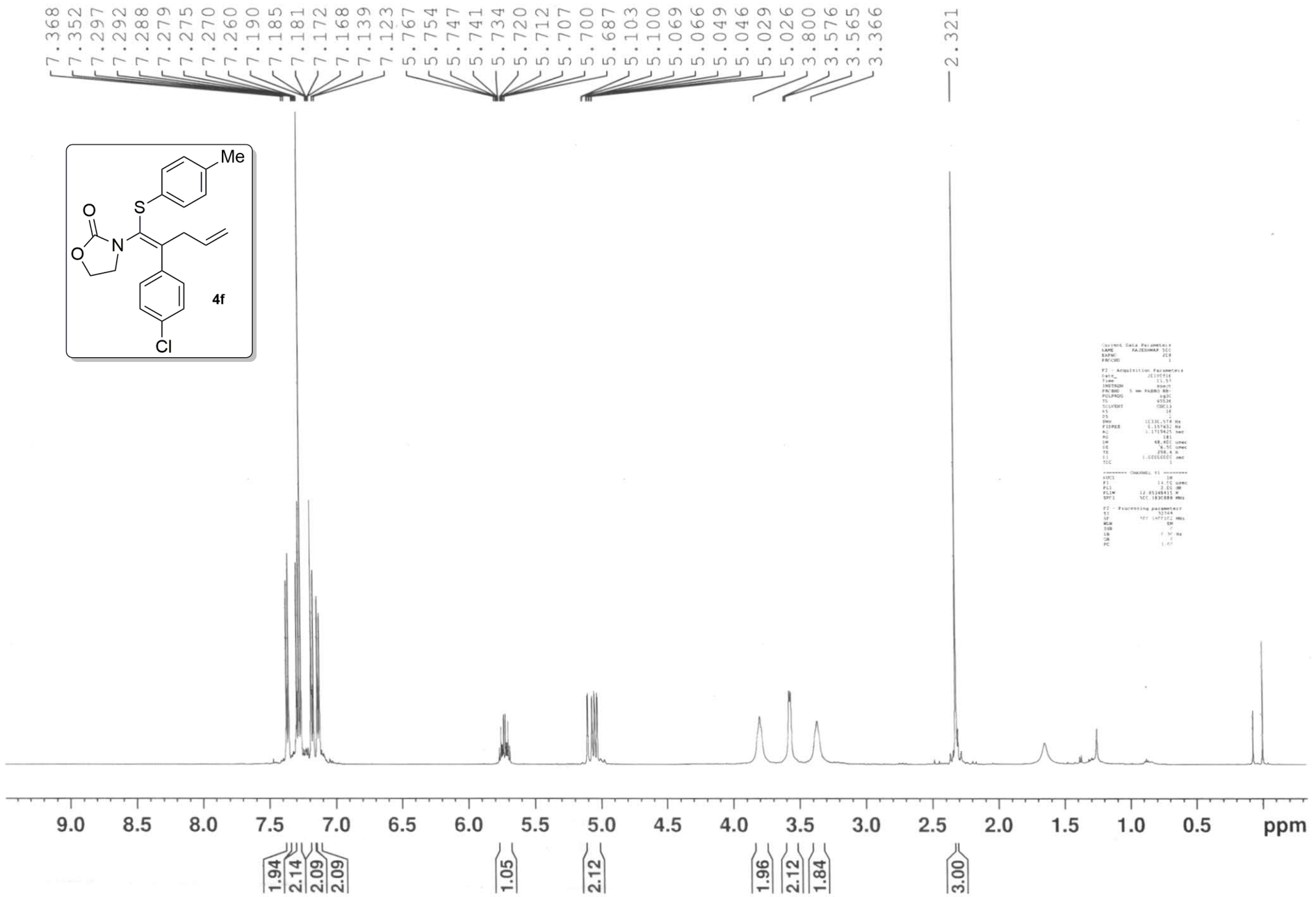

Me
S
O
N
O
4e
Br

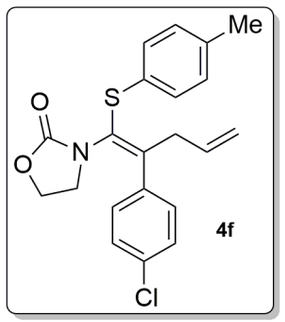
rkm-11-28


Current Data Parameters
NAME rkm
EXPNO 424
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190126
Time 1.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 80.6
DW 60.800 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 1.50 dB
PL1W 15.18650627 W
SFO1 400.0934707 MHz
F2 - Processing parameters
SI 32768
SF 400.0910000 MHz
WDW EM
SSB 1
LB 0.30 Hz
GB 1
PC 1.00


10
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.06
3.99
1.00
2.04
2.01
2.19
2.09
3.01

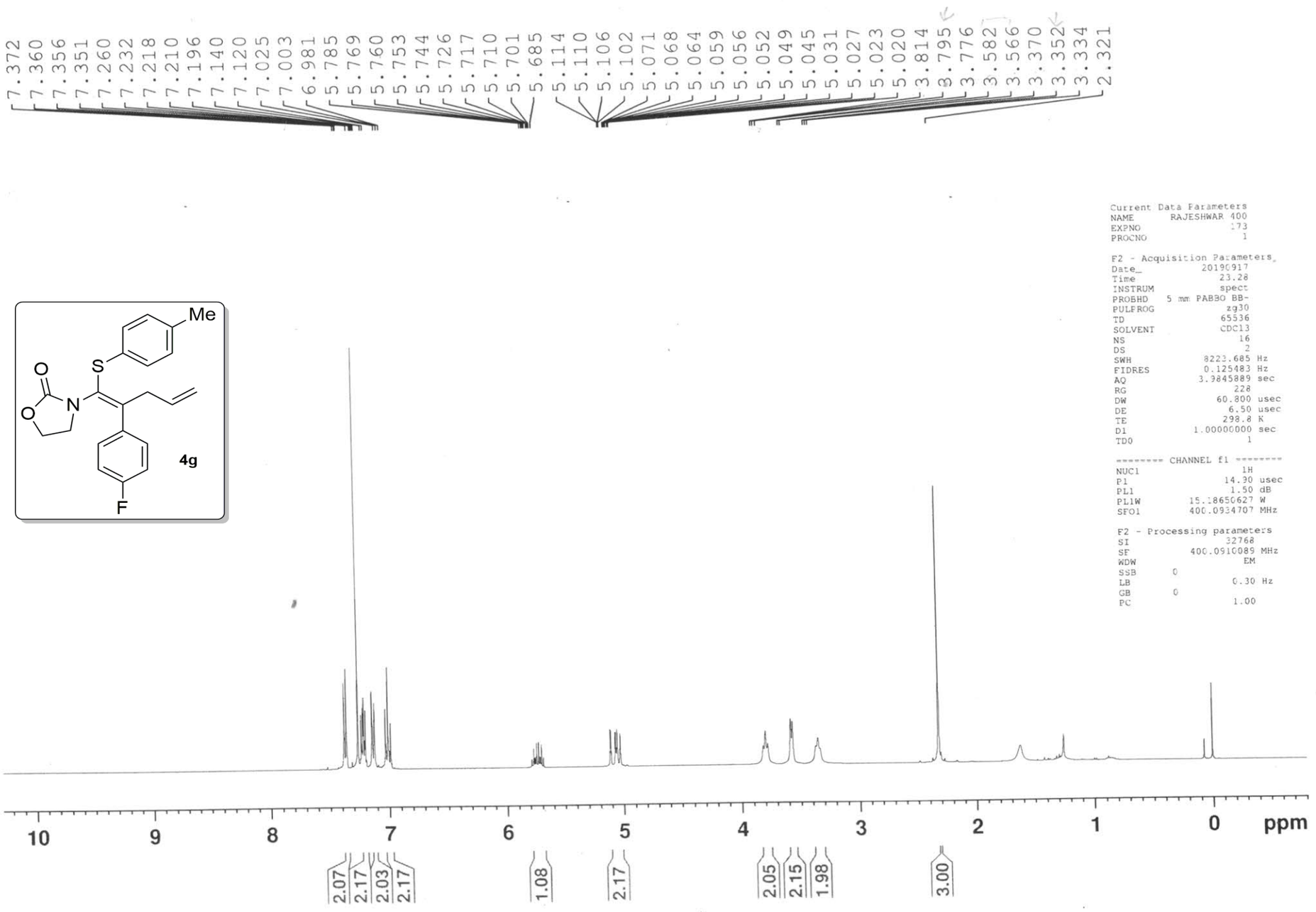

155.07
141.64
138.90
138.24
133.66
131.96
131.47
129.96
129.12
128.02
127.55
121.50
116.98
77.31
77.00
76.68
61.77
45.95
40.28
21.09
Me
S
O
N
O
4e
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

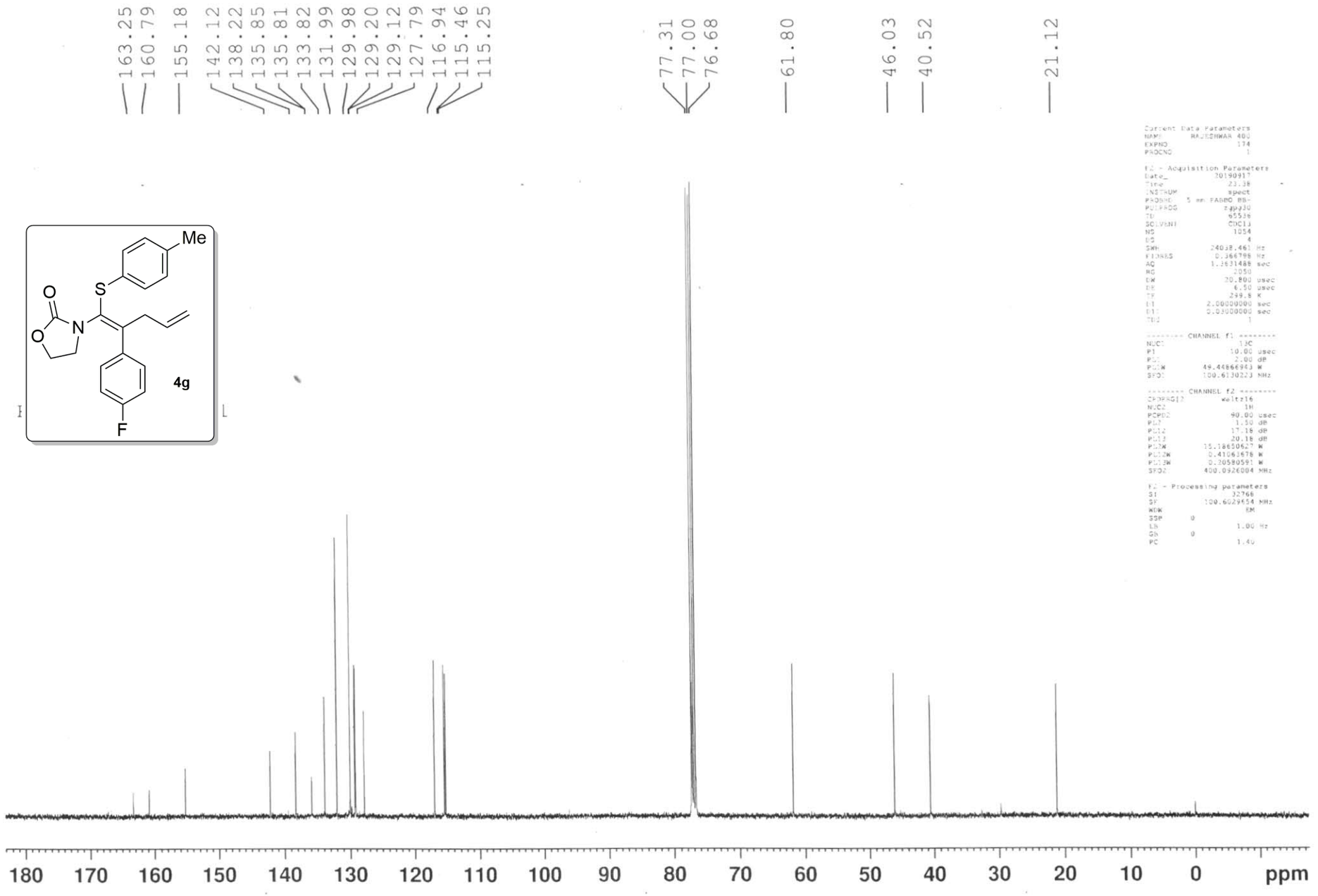

7.368
7.352
7.297
7.292
7.288
7.279
7.275
7.270
7.260
7.190
7.185
7.181
7.172
7.168
7.139
7.123
5.767
5.754
5.747
5.741
5.734
5.720
5.712
5.707
5.700
5.687
5.103
5.100
5.069
5.066
5.049
5.046
5.029
5.026
3.800
3.576
3.565
3.366
2.321
Me
S
O
O
N
Cl
4f
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.94
2.14
2.09
2.09
1.05
2.12
1.96
2.12
1.84
3.00

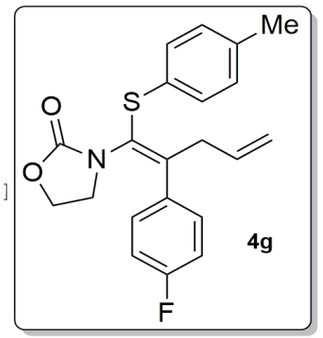

Me
S
O
O
N
Cl

4f

155.13
141.82
138.45
138.29
133.73
133.36
132.02
130.00
128.85
128.59
128.09
127.68
117.02
77.25
77.00
76.74
61.80
46.01
40.37
21.12
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.372
7.360
7.356
7.351
7.260
7.232
7.218
7.210
7.196
7.140
7.120
7.025
7.003
6.981
5.785
5.769
5.760
5.753
5.744
5.726
5.717
5.710
5.701
5.685
5.114
5.110
5.106
5.102
5.071
5.068
5.064
5.059
5.056
5.052
5.049
5.045
5.031
5.027
5.023
5.020
3.814
3.795
3.776
3.582
3.566
3.370
3.352
3.334
2.321
Me
S
O
O
N
F
4g
Current Data Parameters
NAME RAJESHWAR 400
EXPNO 173
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190917
Time 23.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULFROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 228
DW 60.800 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.30 usec
PL1 1.50 dB
PL1W 15.18650627 W
SFO1 400.0934707 MHz
F2 - Processing parameters
SI 32768
SF 400.0910089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.07
2.17
2.03
2.17
1.08
2.17
2.05
2.15
1.98
3.00


163.25
160.79
155.18
142.12
138.22
135.85
135.81
133.82
131.99
129.98
129.20
129.12
127.79
116.94
115.46
115.25
77.31
77.00
76.68
61.80
46.03
40.52
21.12
Me
S
O
N
O
F
4g
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



4g

-114.21

```
Current Data Parameters
NAME       RAJESHWAR 400
EXPNO             105
PROCNO              1

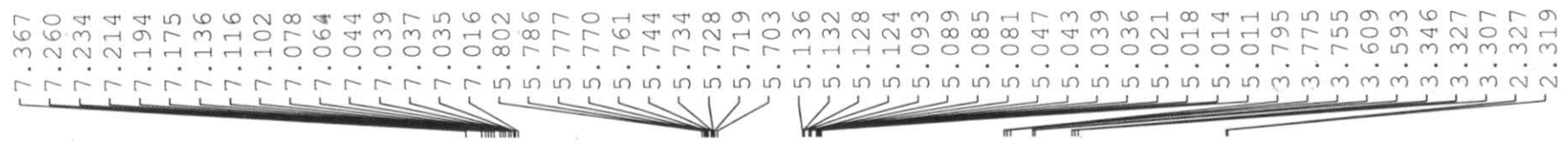
F2 - Acquisition Parameters
Date_          20190330
Time              3.12
INSTRUM          spect
PROBHD  5 mm PABBO BB-
PULPROG      zgfhigqn
TD             131072
SOLVENT           CDCl3
NS                  16
DS                   4
SWH          89285.711 Hz
FIDRES       0.681196 Hz
AQ           0.7340032 sec
RG                2050
DW               5.600 usec
DE               6.50 usec
TE              298.1 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                 1

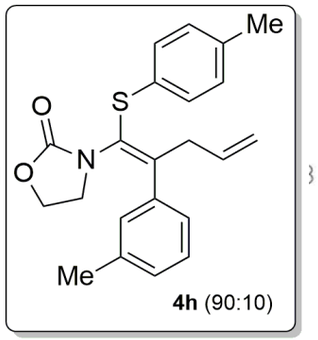
======== CHANNEL f1 ========
NUC1               19F
P1               14.80 usec
PL1              -1.20 dB
PL1W       18.11287308 W
SFO1       376.4240234 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2            90.00 usec
PL2               1.50 dB
PL12             17.18 dB
PL2W       15.18650627 W
PL12W       0.41063678 W
SFO2       400.0926004 MHz

F2 - Processing parameters
SI                65536
SF         376.4616700 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

-40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 ppm


7.367
7.260
7.234
7.214
7.194
7.175
7.136
7.116
7.102
7.078
7.064
7.044
7.039
7.037
7.035
7.016
5.802
5.786
5.777
5.770
5.761
5.744
5.734
5.728
5.719
5.703
5.136
5.132
5.128
5.124
5.093
5.089
5.085
5.081
5.047
5.043
5.039
5.036
5.021
5.018
5.014
5.011
3.795
3.775
3.755
3.609
3.593
3.346
3.327
3.307
2.327
2.319


Me
S
O
N
O
Me

4h (90:10)

Current Data Parameters
NAME RAJESHWAR 400
EXPNO 101
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190328
Time 2.58
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 71.8
DW 60.800 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.30 usec
PL1 1.50 dB
PL1W 15.18650627 W
SFO1 400.0934707 MHz
F2 - Processing parameters
SI 32768
SF 400.0910099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.33
1.86
2.19
1.99
1.33
1.23
2.35
2.09
2.31
2.03
3.00
2.97

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155.23
143.54
139.89
138.05
137.88
134.09
132.02
130.82
129.91
128.37
128.14
127.96
127.30
124.45
116.67

77.25
77.00
76.74

61.78

46.24

40.49

21.46
21.10

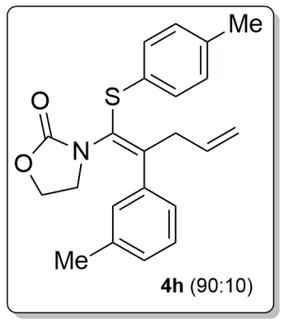
```
Current Data Parameters
NAME       RAJESHWAR 500
EXPNO               211
PROCNO                1

F2 - Acquisition Parameters
Date_          20190917
Time              14.30
INSTRUM           spect
PROBHD   5 mm PABBO BB
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                  492
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG                 2050
DW               16.800 usec
DE                6.50 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.60 usec
PL1       0 dB
PL1W       76.36135101 W
SFO1      125.7829381 MHz

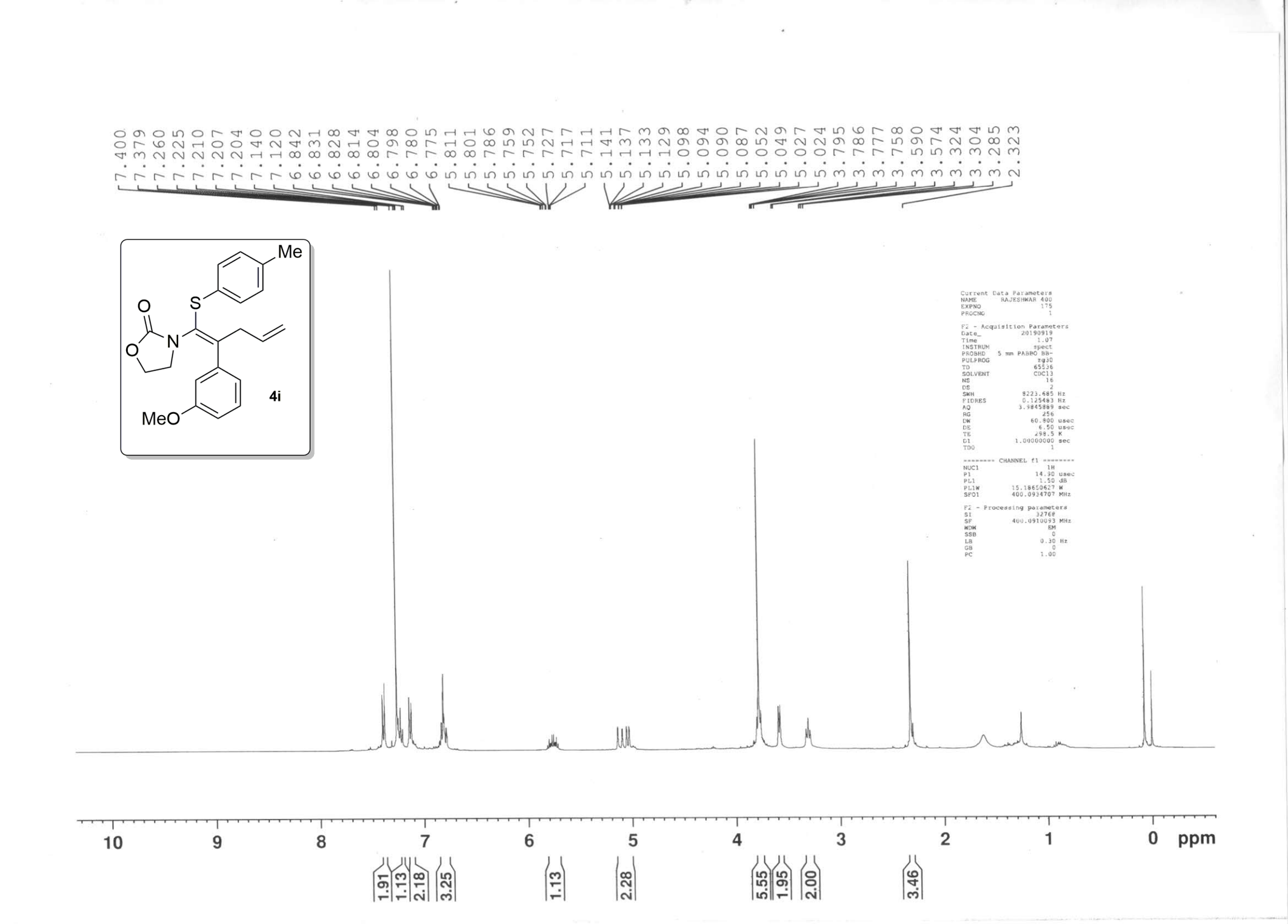
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 2.00 dB
PL12               16.50 dB
PL13               16.50 dB
PL2W       12.85348415 W
PL12W       0.45605880 W
PL13W       0.45605880 W
SFO2      500.1820007 MHz

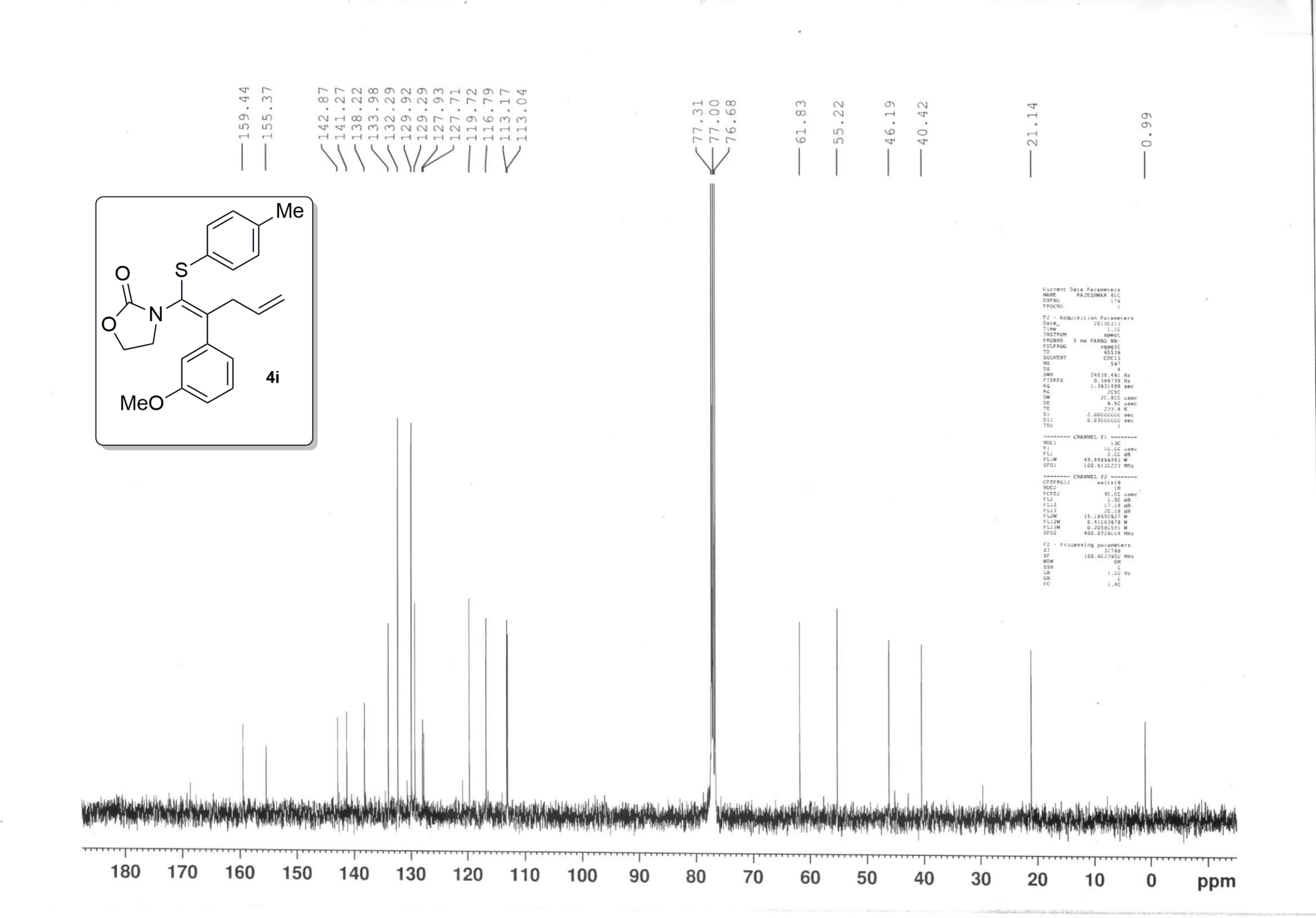
F2 - Processing parameters
SI                 32768
SF          125.7703635 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

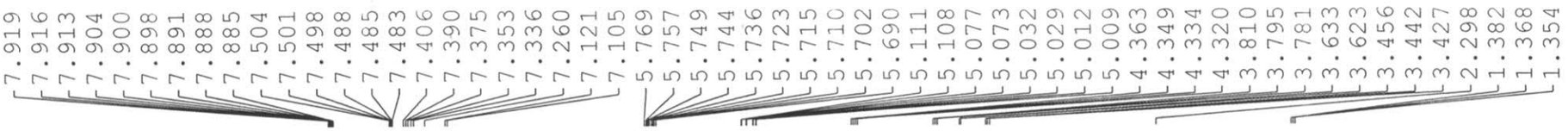


4h (90:10)

* representative peaks
of minor inseparable isomer


7.400
7.379
7.260
7.225
7.210
7.207
7.204
7.140
7.120
6.842
6.831
6.828
6.814
6.804
6.798
6.780
6.775
5.811
5.801
5.786
5.759
5.752
5.727
5.717
5.711
5.141
5.137
5.133
5.129
5.098
5.094
5.090
5.087
5.052
5.049
5.027
5.024
3.795
3.786
3.777
3.758
3.590
3.574
3.324
3.304
3.285
2.323
Me
S
O
N
O
4i
MeO
Current Data Parameters
NAME RAJESHWAR 400
EXPNO 175
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190919
Time 1.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 256
DW 60.800 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 1.50 dB
PL1W 15.18650627 W
SFO1 400.0934707 MHz
F2 - Processing parameters
SI 32768
SF 400.0910093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.91
1.13
2.18
3.25
1.13
2.28
5.55
1.95
2.00
3.46


159.44
155.37
142.87
141.27
138.22
133.98
132.29
129.92
129.29
127.93
127.71
119.72
116.79
113.17
113.04
77.31
77.00
76.68
61.83
55.22
46.19
40.42
21.14
0.99
Me
S
O
N
O
MeO
4i
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

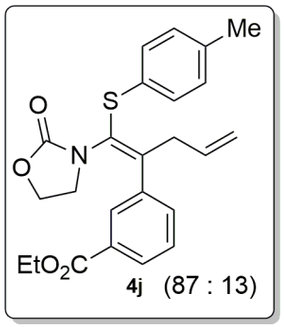


RKM-11-27

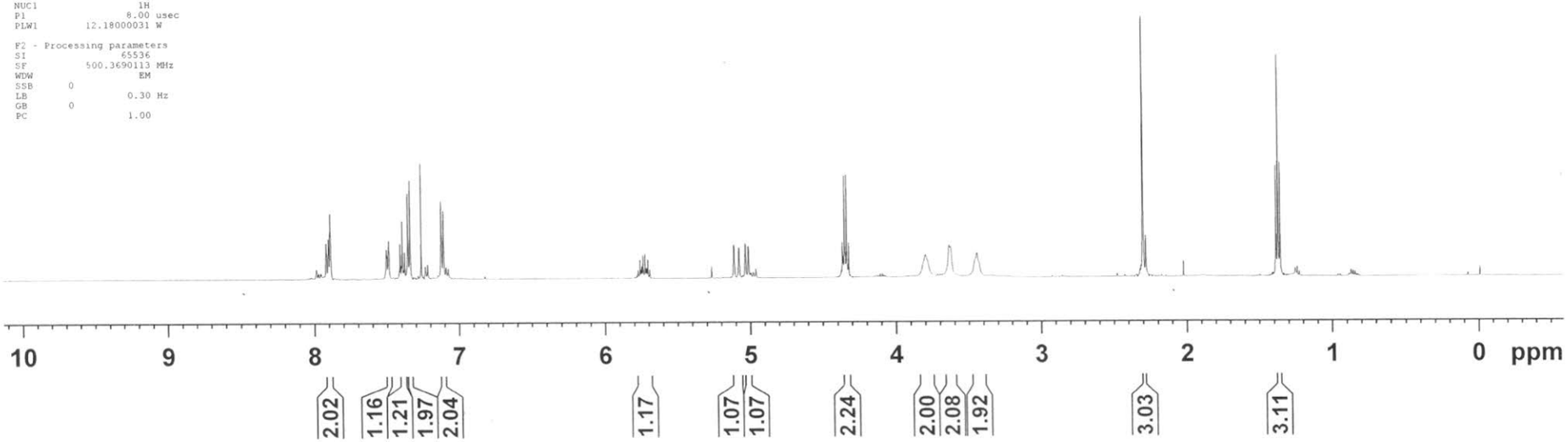
```
Current Data Parameters
NAME      old nmr upto apr 19
EXPNO                    409
PROCNO                     1

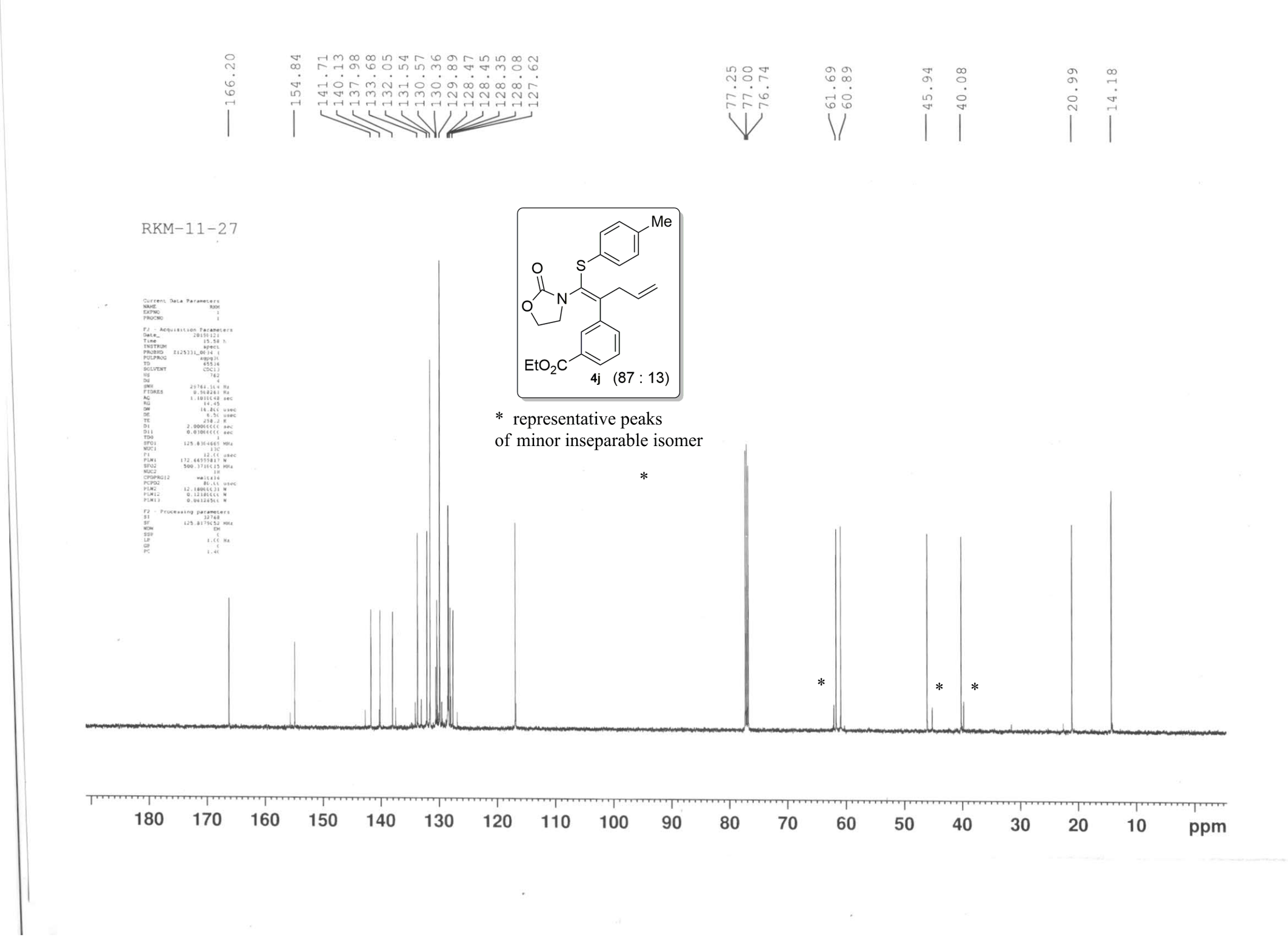
F2 - Acquisition Parameters
Date_              20190121
Time                 15.18 h
INSTRUM                spect
PROBHD    Z125331_0034 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES                0.305176 Hz
AQ                3.2767999 sec
RG                     31.25
DW                    50.000 usec
DE                     6.50 usec
TE                    298.1 K
D1              1.00000000 sec
TD0                       1
SFO1           500.3720898 MHz
NUC1                     1H
P1                     8.00 usec
PLW1           12.18000031 W

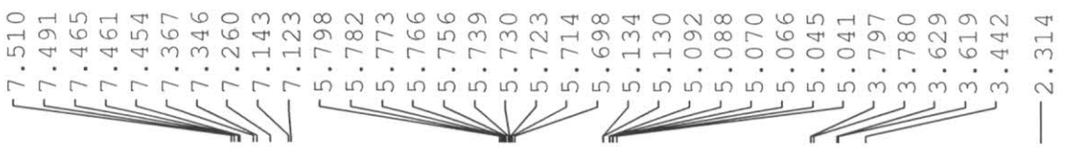
F2 - Processing parameters
SI                    65536
SF             500.3690113 MHz
WDW                      EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```



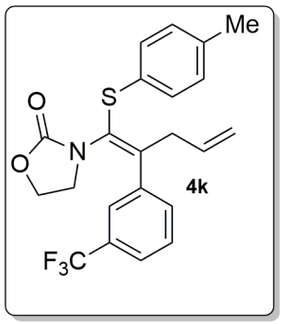
4j (87 : 13)




166.20
154.84
141.71
140.13
137.98
133.68
132.05
131.54
130.57
130.36
129.89
128.47
128.45
128.35
128.08
127.62
77.25
77.00
76.74
61.69
60.89
45.94
40.08
20.99
14.18
RKM-11-27
Me
S
O
N
O
EtO2C
4j (87 : 13)
* representative peaks
of minor inseparable isomer
*
*
*
*
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



rkm-11-26

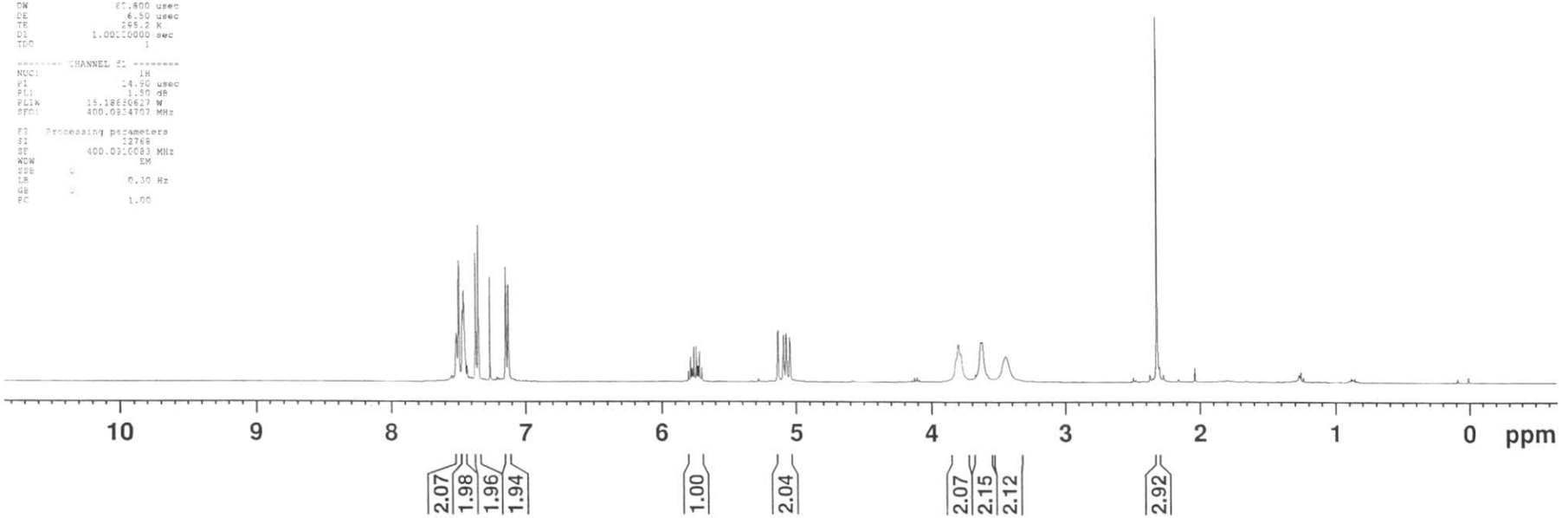


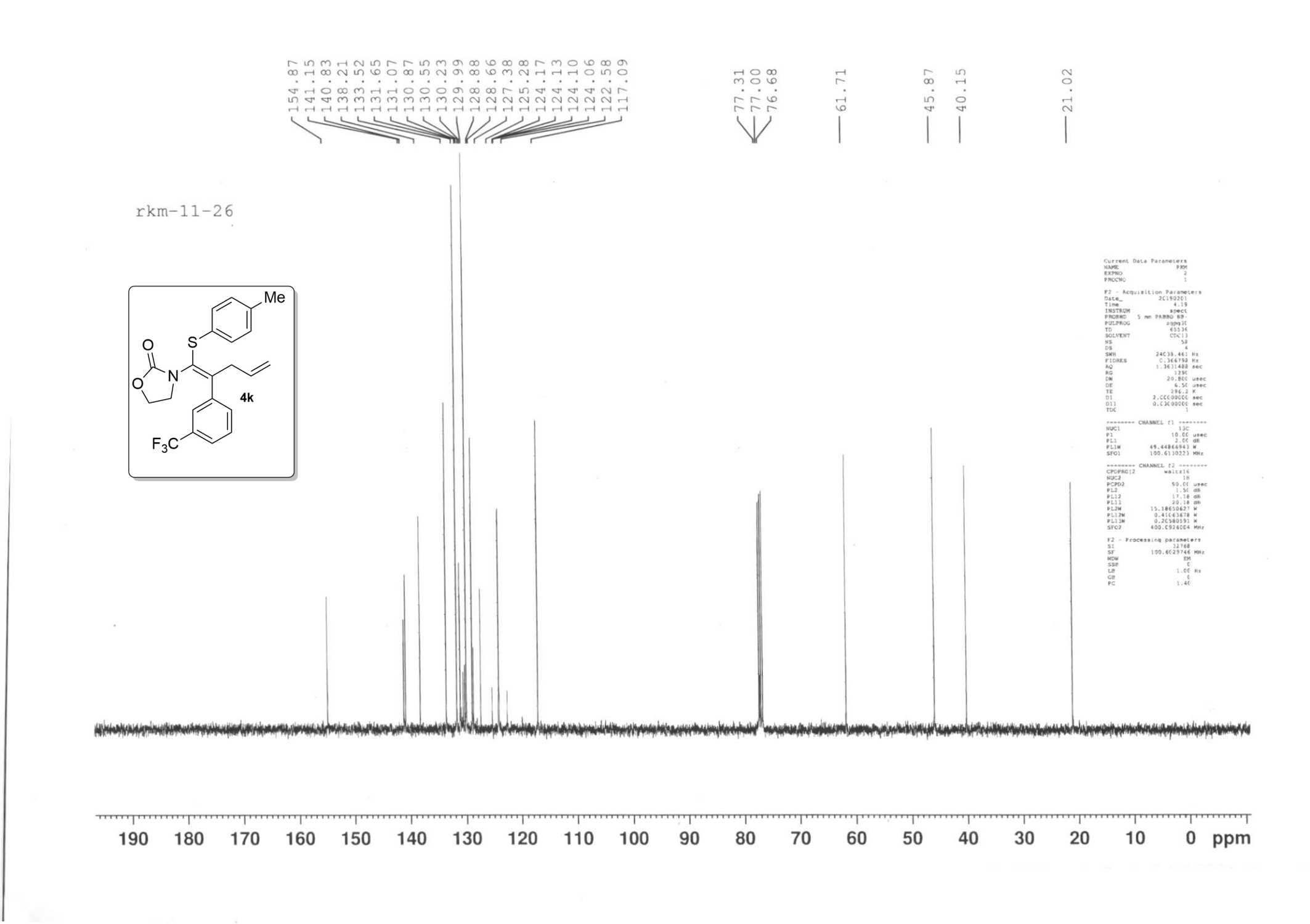

```
Current Data Parameters
NAME                  rkm
EXPNO                 435
PROCNO                  1

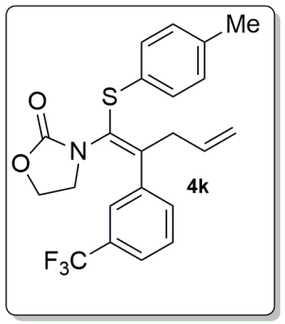
F1 - Acquisition Parameters
Date_           20190201
Time                4.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845885 sec
RG                    64
DW                60.800 usec
DE                 6.50 usec
TE                295.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.90 usec
PL1                1.50 dB
PL1W         15.18650627 W
SFO1         400.0834767 MHz

F2 - Processing parameters
SI                 32768
SF           400.0910083 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

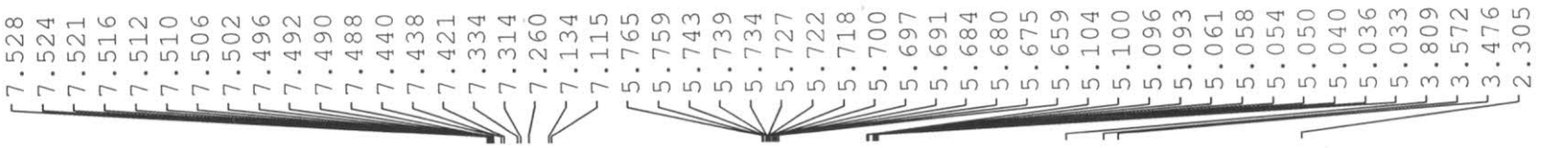



154.87
141.15
140.83
138.21
133.52
131.65
131.07
130.87
130.55
130.23
129.99
128.88
128.66
127.38
125.28
124.17
124.13
124.10
124.06
122.58
117.09
77.31
77.00
76.68
61.71
45.87
40.15
21.02
rkm-11-26
Me
S
O
O
N
4k
F_3C
Current Data Parameters
NAME PRM
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 2C190201
Time 4.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 58
DS 4
SWH 24038.461 Hz
FIDRES 0.366790 Hz
AQ 1.3631488 sec
RG 1298
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 2.00 dB
PL1W 49.44866943 W
SFO1 100.6130223 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 1.50 dB
PL12 17.18 dB
PL13 20.18 dB
PL2W 15.18650627 W
PL12W 0.41663678 W
PL13W 0.26580591 W
SFO2 400.0926004 MHz
F2 - Processing parameters
SI 32768
SF 100.6029746 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

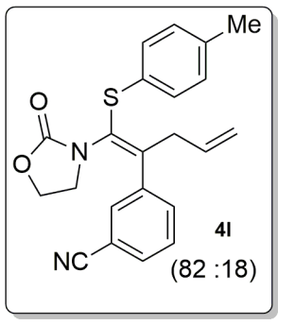


-62.54

rkm-11-26



RKM- 11-18

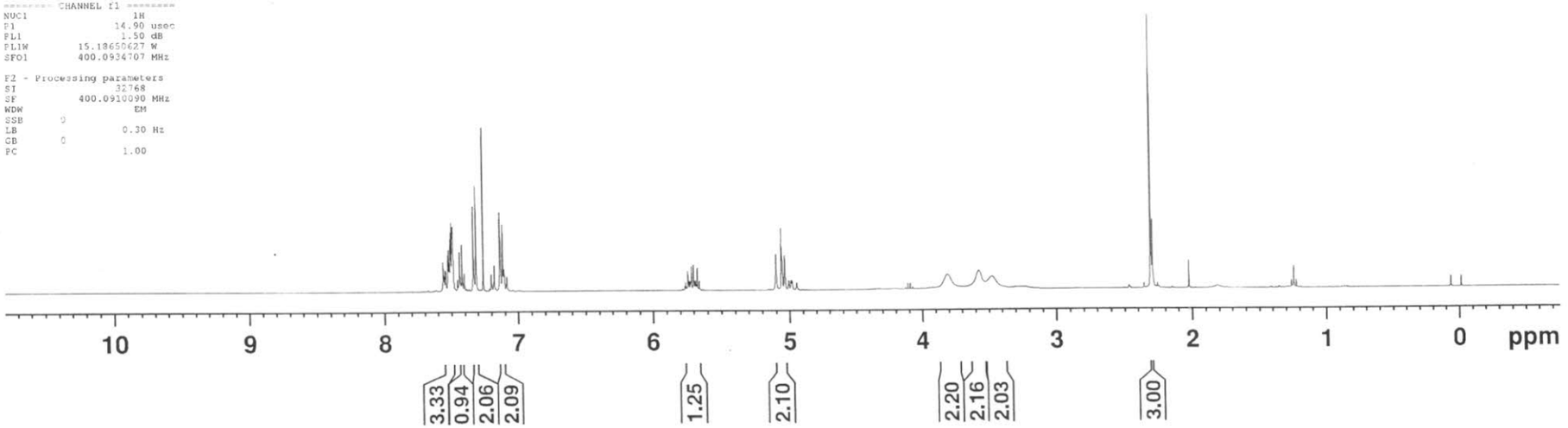


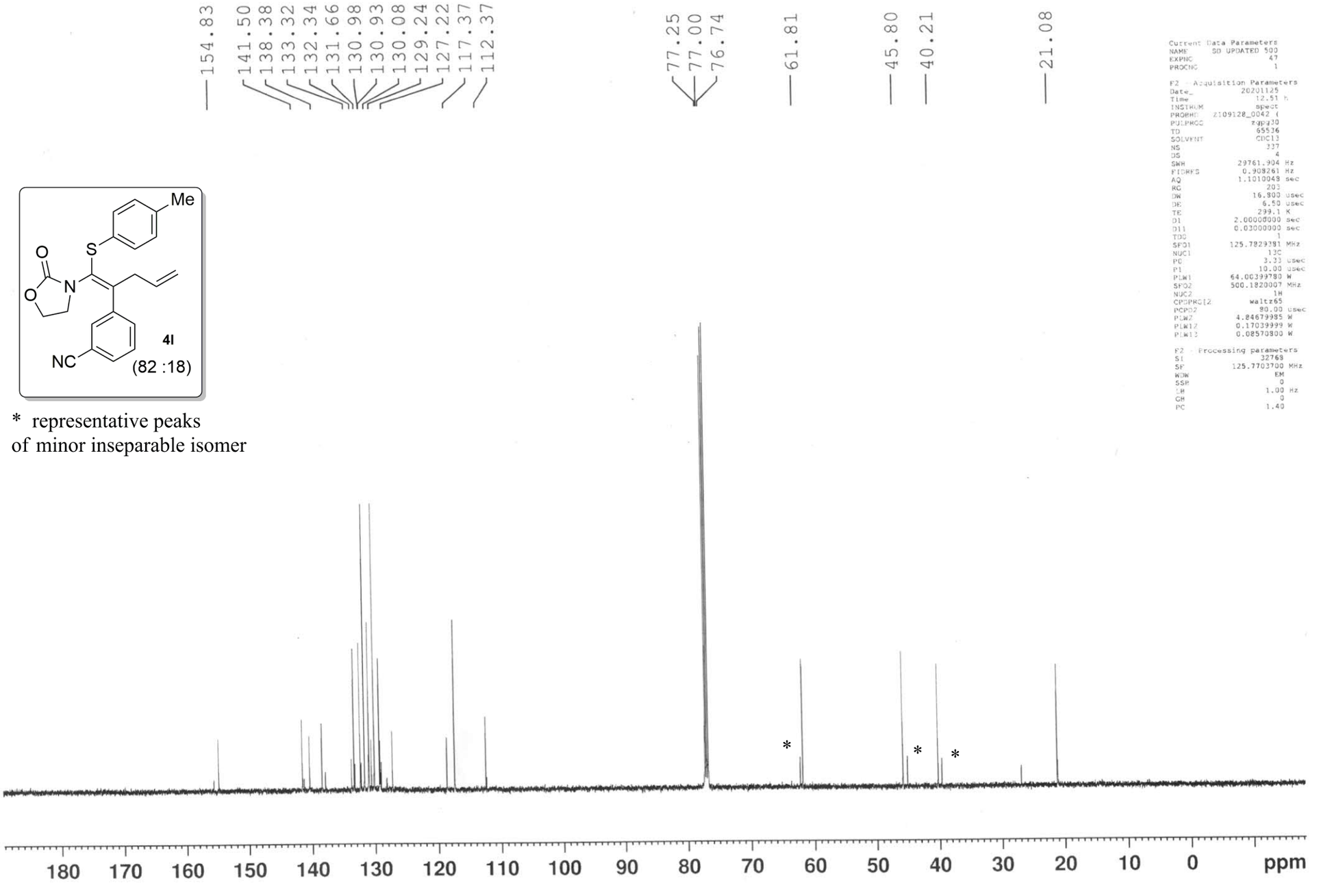

```
Current Data Parameters
NAME                  zkm
EXPNO                 400
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190118
Time                1.09
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                    57
DW                 60.800 usec
DE                  6.50 usec
TE                 293.0 K
D1              1.00000000 sec
TD0                    1

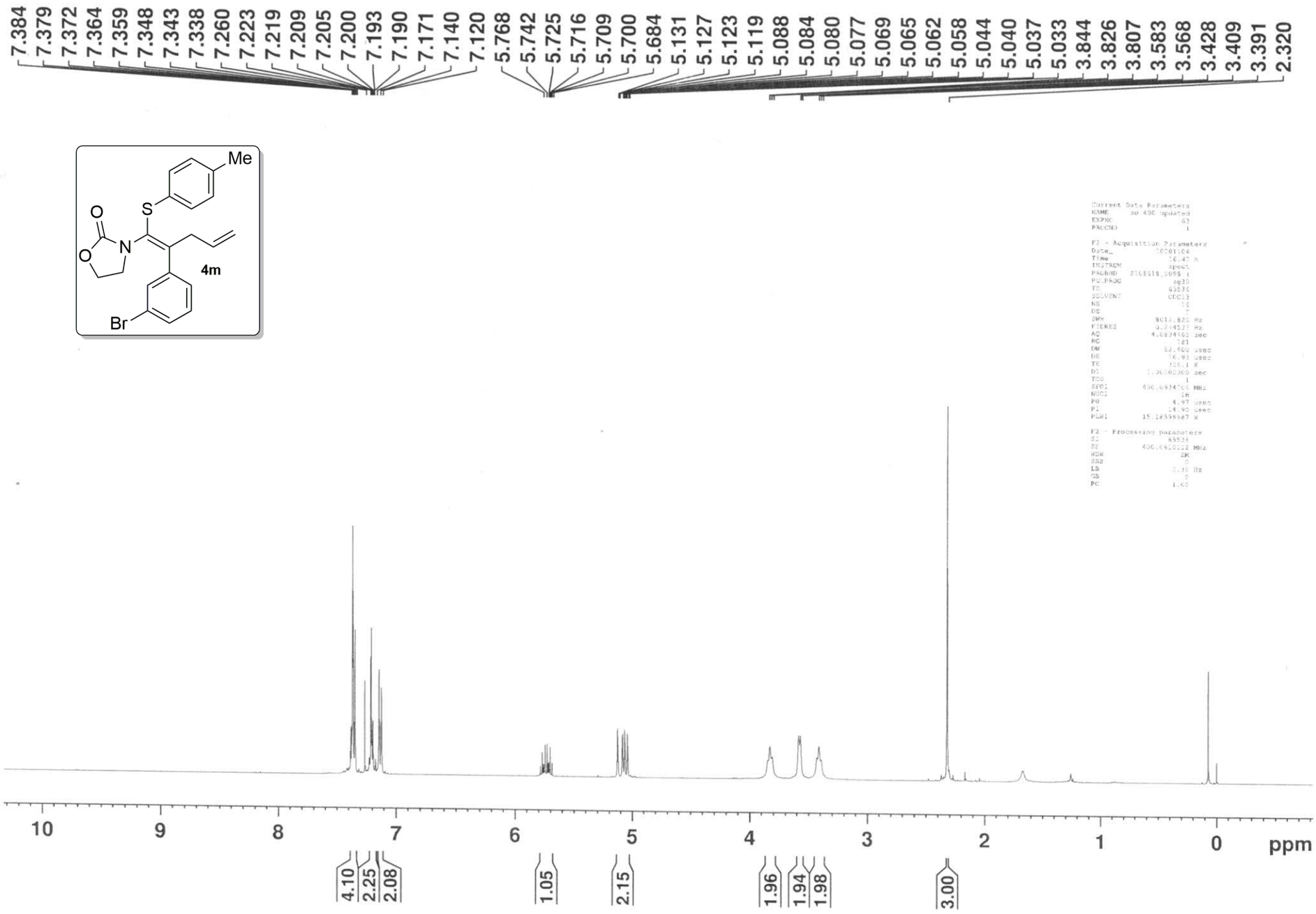
======== CHANNEL f1 ========
NUC1                  1H
P1                 14.90 usec
PL1                 1.50 dB
PL1W         15.18650627 W
SFO1         400.0934707 MHz

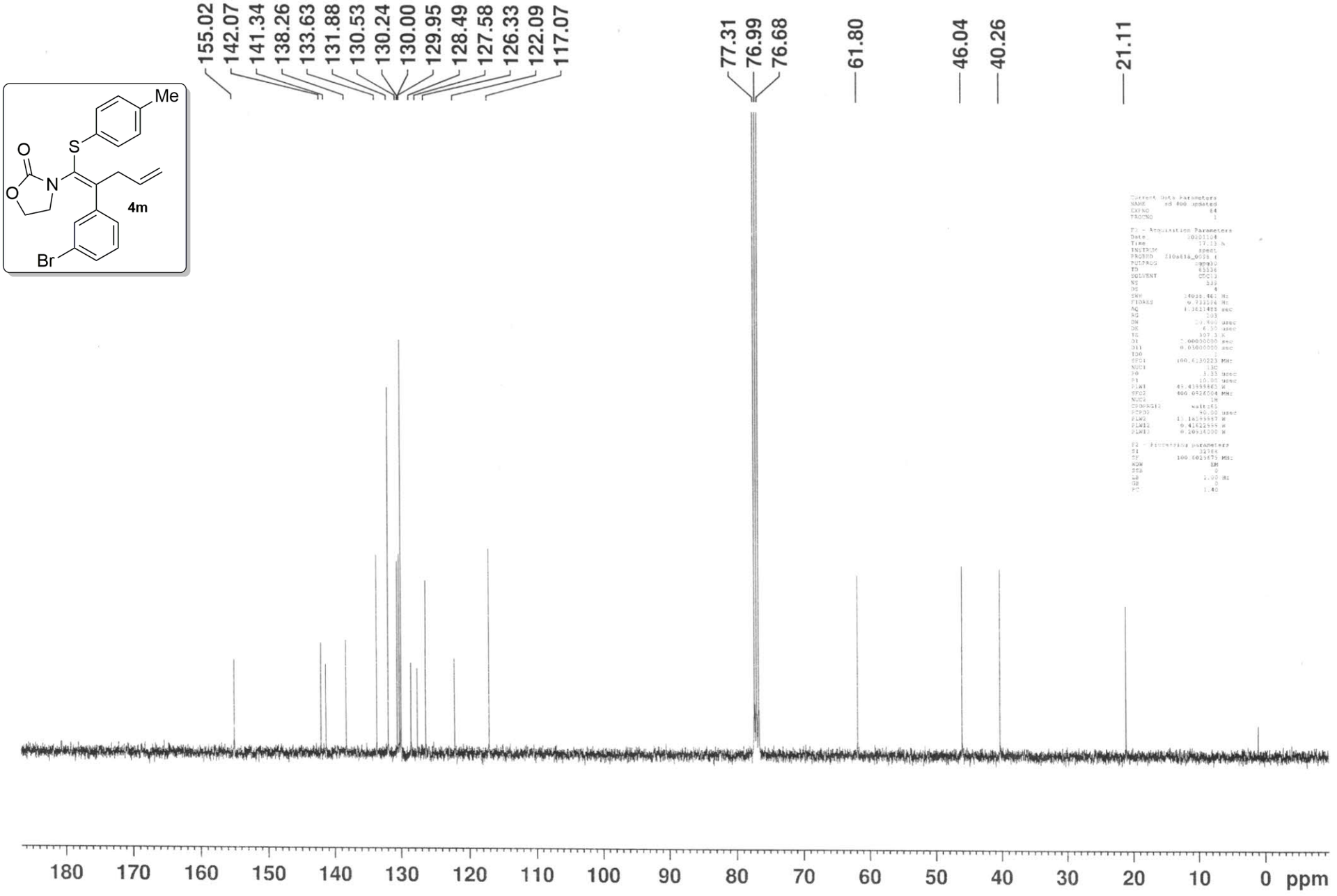
F2 - Processing parameters
SI                 32768
SF           400.0910090 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

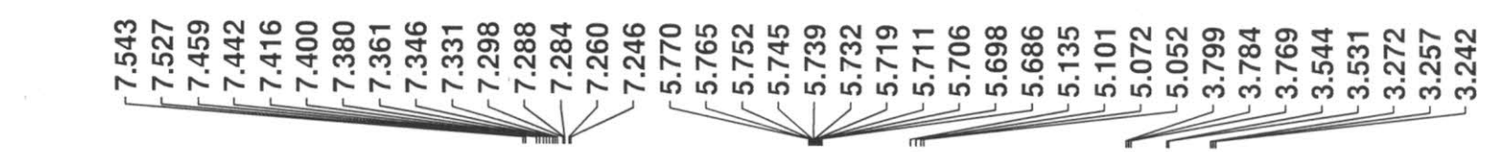


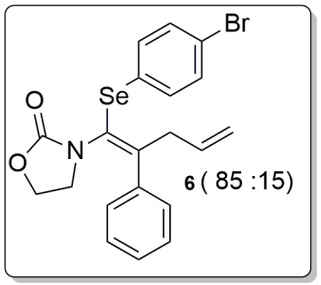


* representative peaks
of minor inseparable isomer

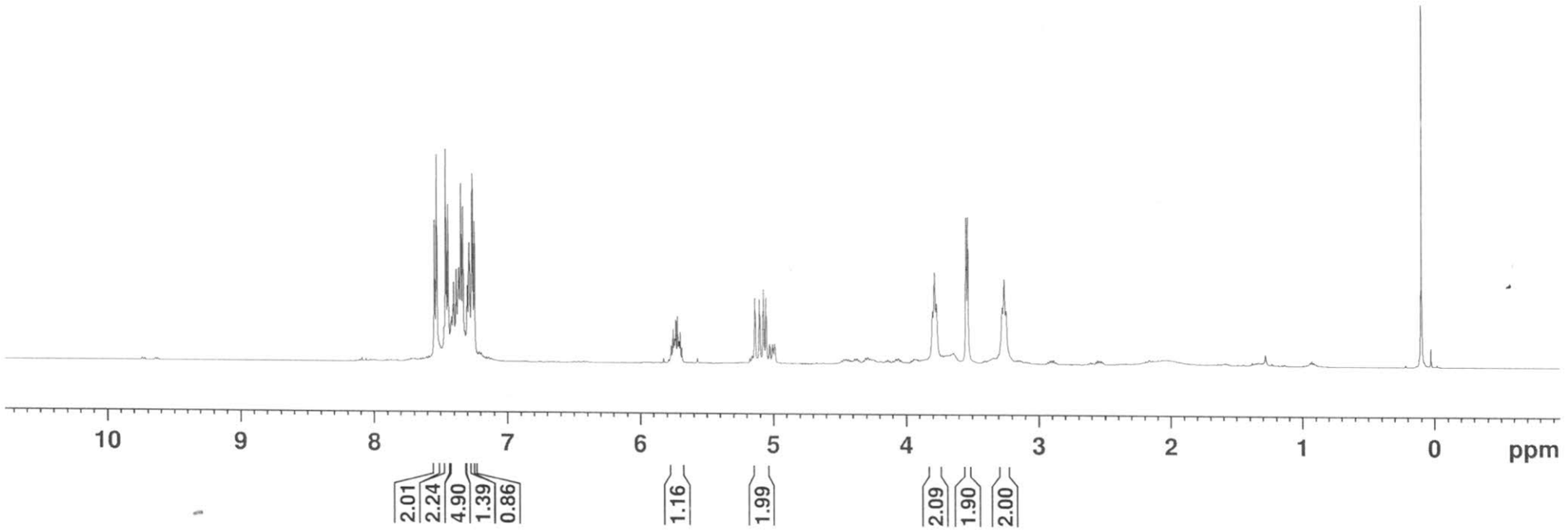

7.384
7.379
7.372
7.364
7.359
7.348
7.343
7.338
7.260
7.223
7.219
7.209
7.205
7.200
7.193
7.190
7.171
7.140
7.120
5.768
5.742
5.725
5.716
5.709
5.700
5.684
5.131
5.127
5.123
5.119
5.088
5.084
5.080
5.077
5.069
5.065
5.062
5.058
5.044
5.040
5.037
5.033
3.844
3.826
3.807
3.583
3.568
3.428
3.409
3.391
2.320
Me
S
O
N
O
4m
Br
10
9
8
7
6
5
4
3
2
1
0
ppm
4.10
2.25
2.08
1.05
2.15
1.96
1.94
1.98
3.00

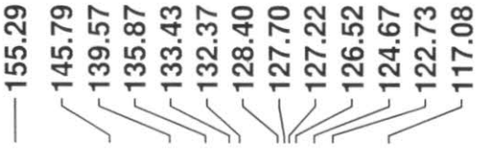

155.02
142.07
141.34
138.26
133.63
131.88
130.53
130.24
130.00
129.95
128.49
127.58
126.33
122.09
117.07
77.31
76.99
76.68
61.80
46.04
40.26
21.11
Me
S
O
N
O
4m
Br
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

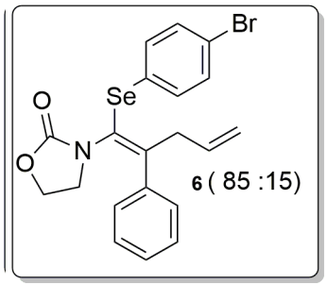

7.543
7.527
7.459
7.442
7.416
7.400
7.380
7.361
7.346
7.331
7.298
7.288
7.284
7.260
7.246
5.770
5.765
5.752
5.745
5.739
5.732
5.719
5.711
5.706
5.698
5.686
5.135
5.101
5.072
5.052
3.799
3.784
3.769
3.544
3.531
3.272
3.257
3.242


Br
Se
O
O
N

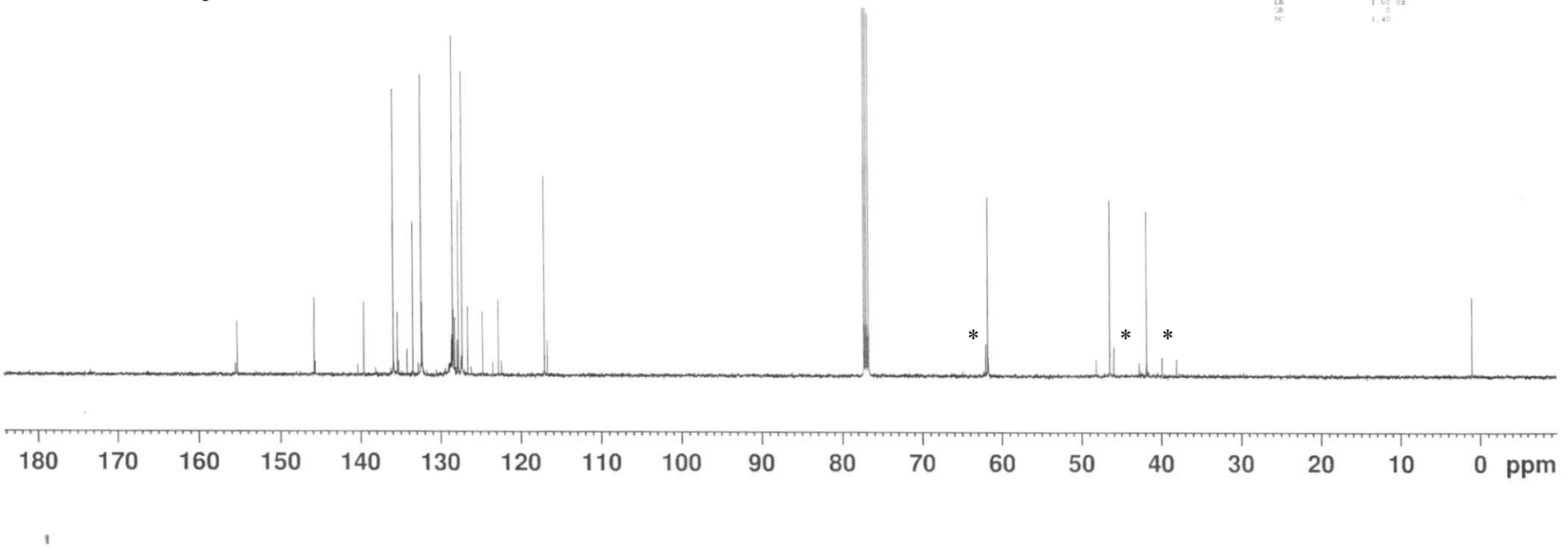
6 (85 :15)

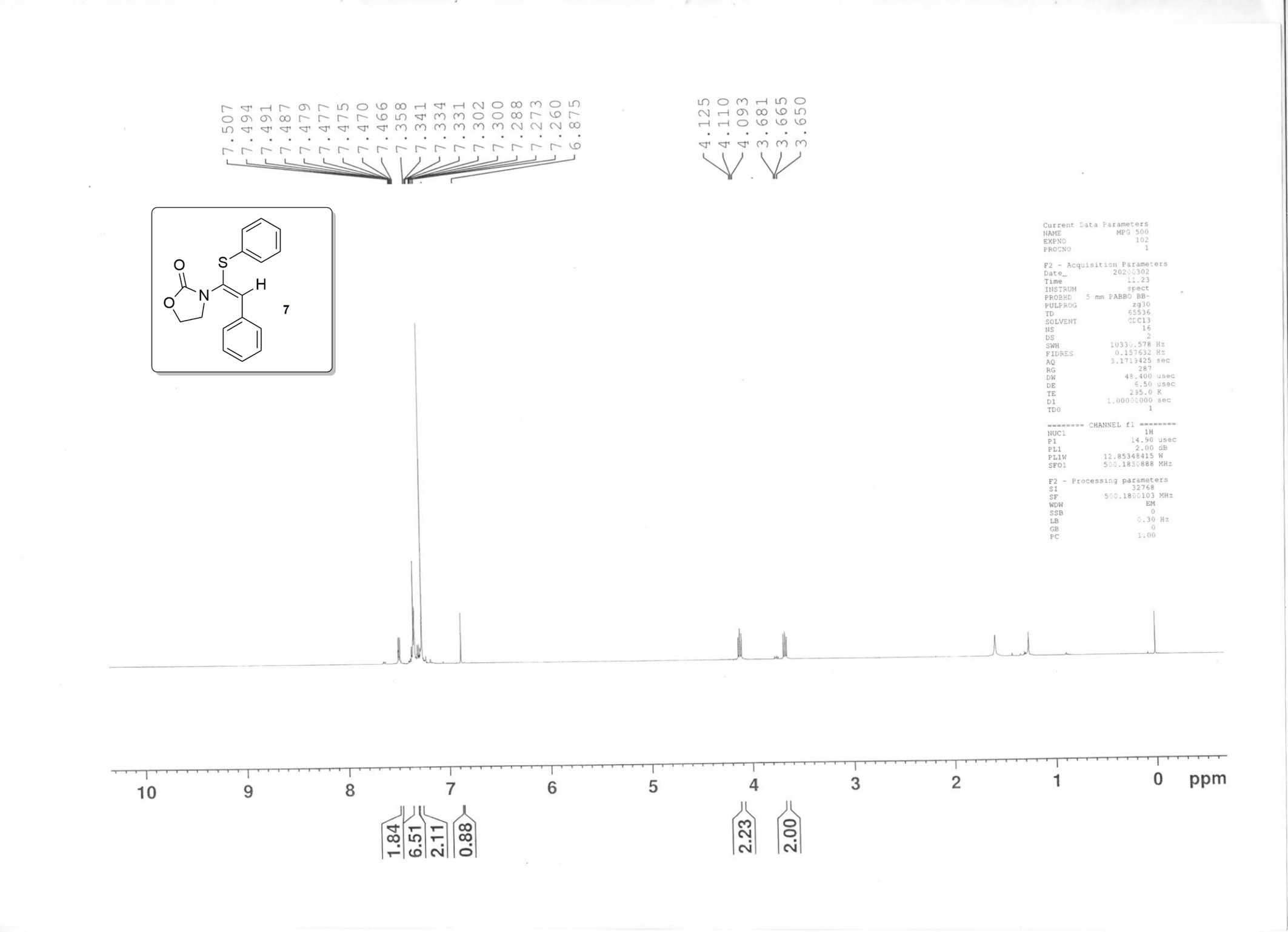

10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.24
4.90
1.39
0.86
1.16
1.99
2.09
1.90
2.00

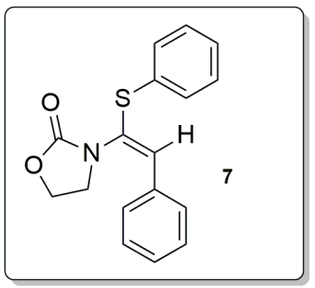




* representative peaks
of minor inseparable isomer

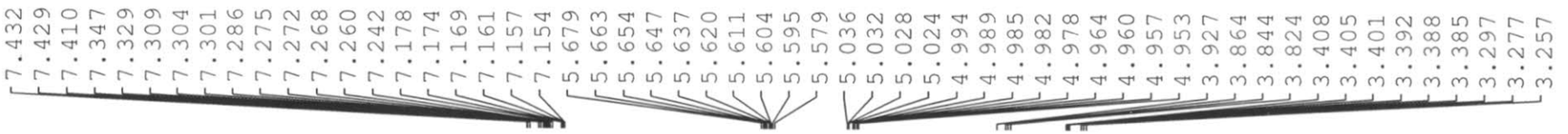


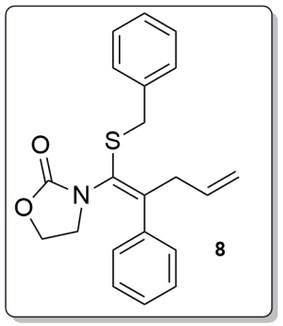

7.507
7.494
7.491
7.487
7.479
7.477
7.475
7.470
7.466
7.358
7.341
7.334
7.331
7.302
7.300
7.288
7.273
7.260
6.875
4.125
4.110
4.093
3.681
3.665
3.650
O
S
H
O
N
7
Current Data Parameters
NAME MPG 500
EXPNO 102
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200302
Time 11.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 287
DW 48.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 2.00 dB
PL1W 12.85348415 W
SFO1 500.1830888 MHz
F2 - Processing parameters
SI 32768
SF 500.1800103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.84
6.51
2.11
0.88
2.23
2.00


O
S
O
N
H

7

154.84
134.70
131.98
131.50
131.32
129.46
129.37
129.20
128.70
128.28
128.18
127.99
77.25
77.00
76.74
62.21
45.19
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



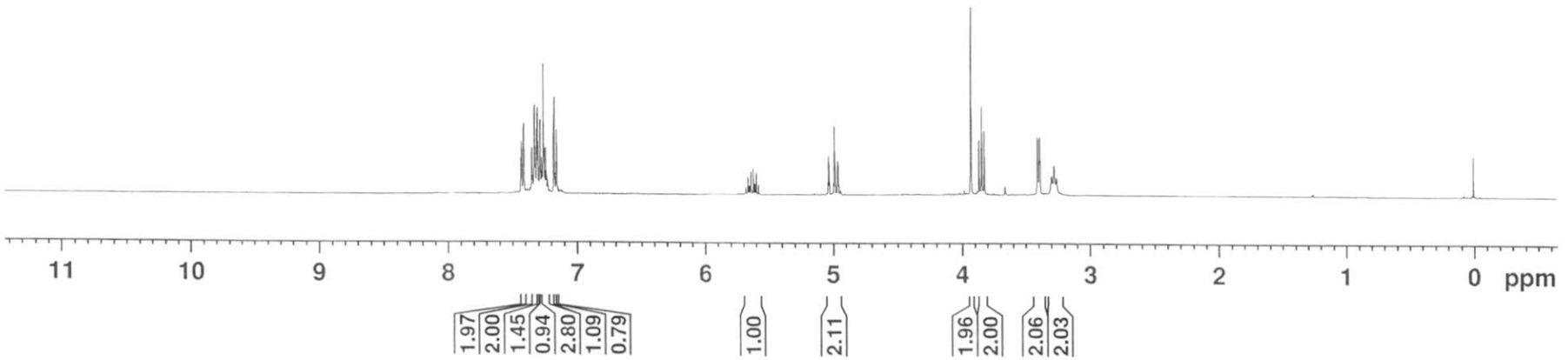



```
Current Data Parameters
NAME                  PB 400
EXPNO                    128
PROCNO                     1

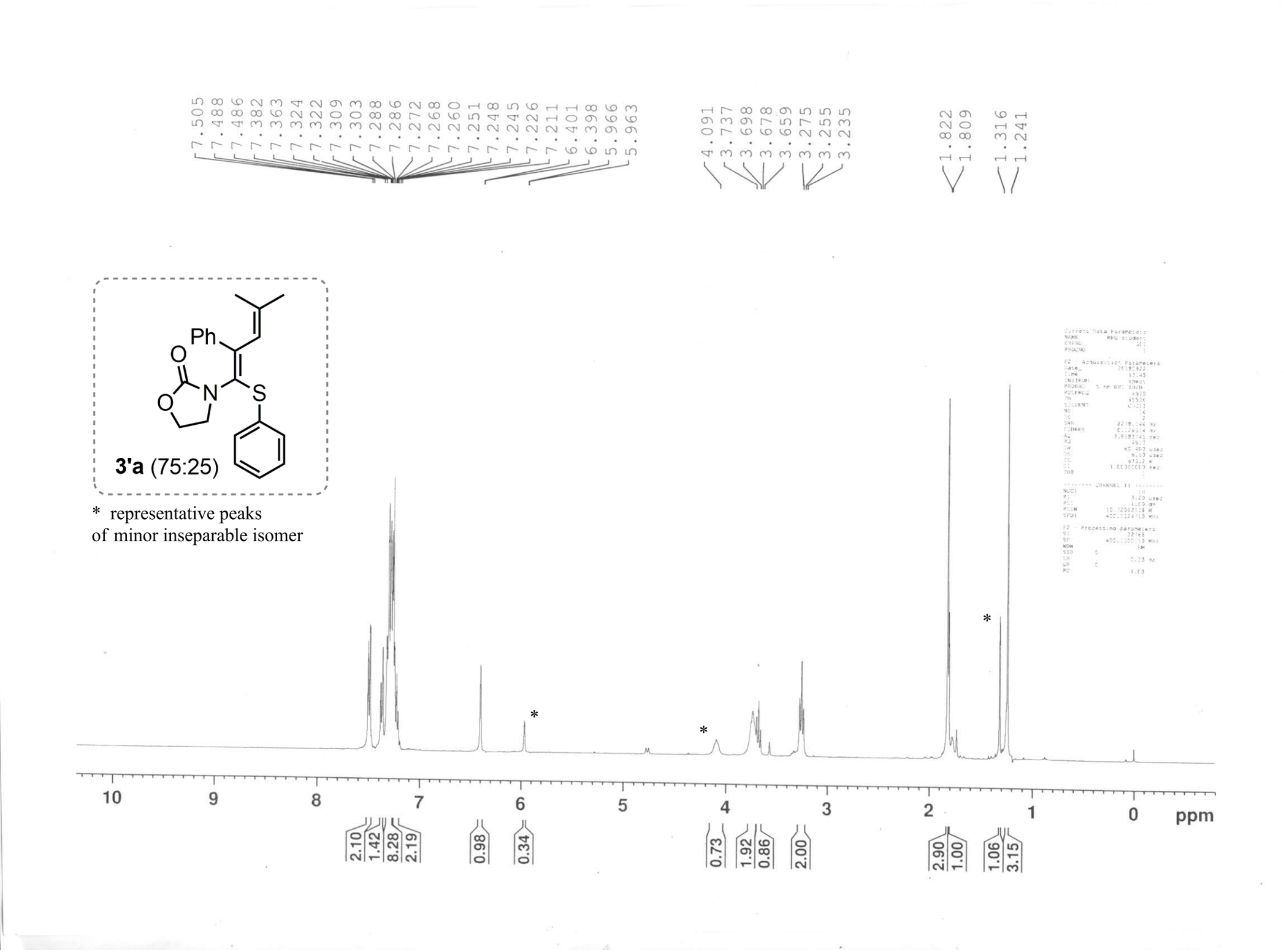
F2 - Acquisition Parameters
Date_              20190220
Time                   0.32
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                      128
DW                   60.800 usec
DE                    6.50 usec
TE                   297.8 K
D1                1.00000000 sec
TD0                        1

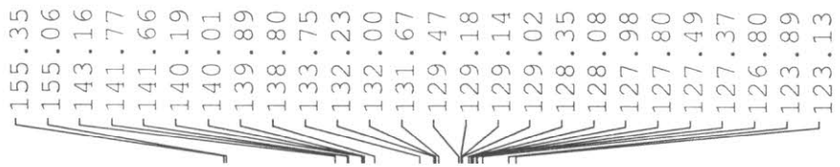
======== CHANNEL f1 ========
NUC1                      1H
P1                    14.90 usec
PL1                    1.50 dB
PL1W          15.18650627 W
SFO1          400.0934707 MHz

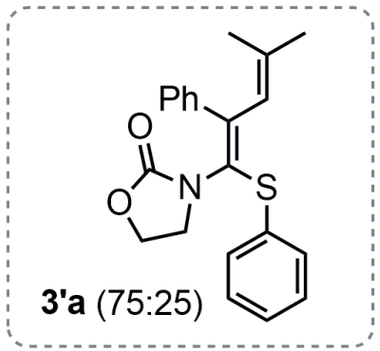
F2 - Processing parameters
SI                        32768
SF             400.0910089 MHz
WDW                          EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```



156.01
146.59
139.67
138.17
133.96
128.80
128.58
128.25
127.58
127.33
127.20
116.77
77.39
77.07
76.75
61.89
45.76
40.50
37.20
O
S
N
O
8
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

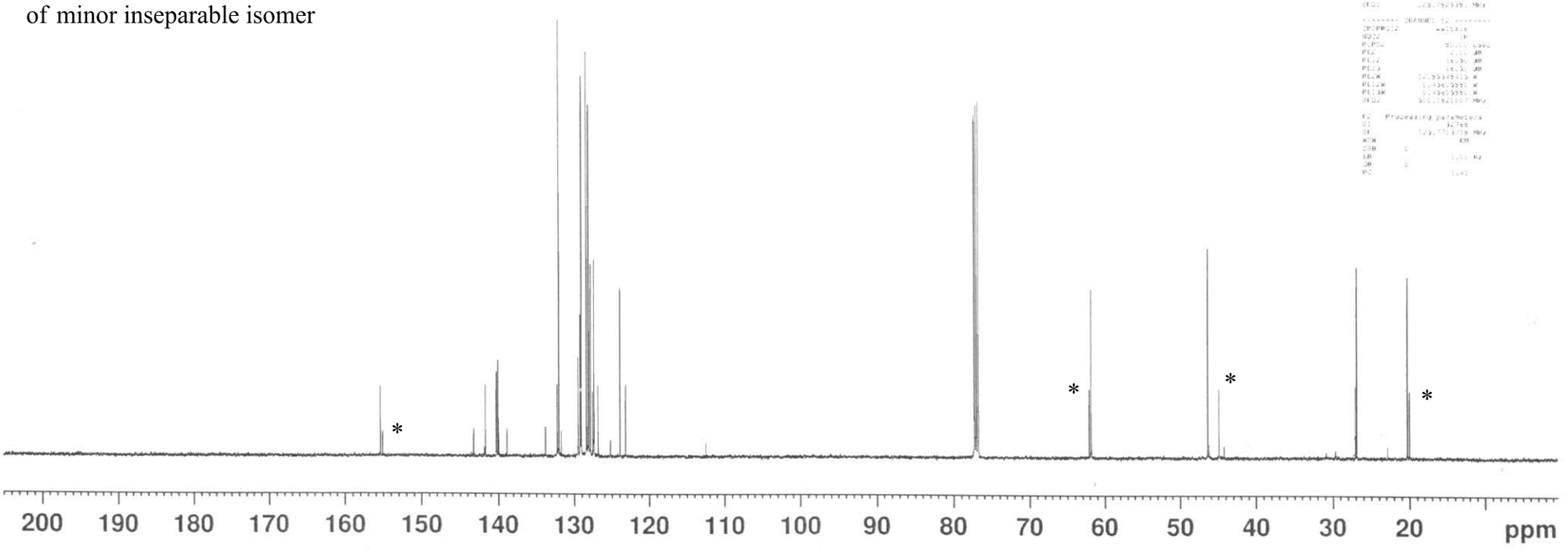

7.505
7.488
7.486
7.382
7.363
7.324
7.322
7.309
7.303
7.288
7.286
7.272
7.268
7.260
7.251
7.248
7.245
7.226
7.211
6.401
6.398
5.966
5.963
4.091
3.737
3.698
3.678
3.659
3.275
3.255
3.235
1.822
1.809
1.316
1.241
Ph
O
N
O
S
3'a (75:25)
* representative peaks
of minor inseparable isomer
*
*
*
10
9
8
7
6
5
4
3
2
1
0
ppm
2.10
1.42
8.28
2.19
0.98
0.34
0.73
1.92
0.86
2.00
2.90
1.00
1.06
3.15

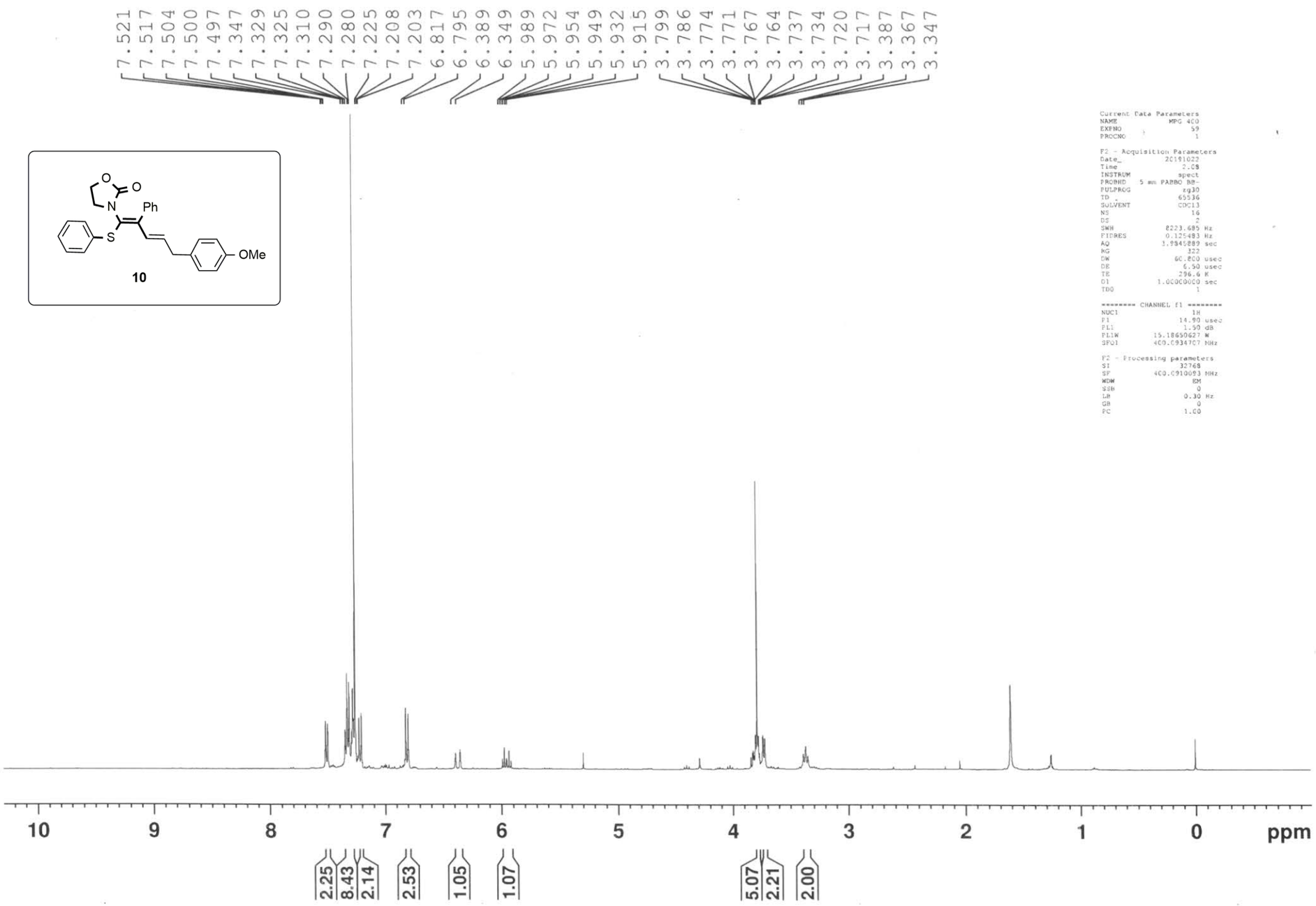


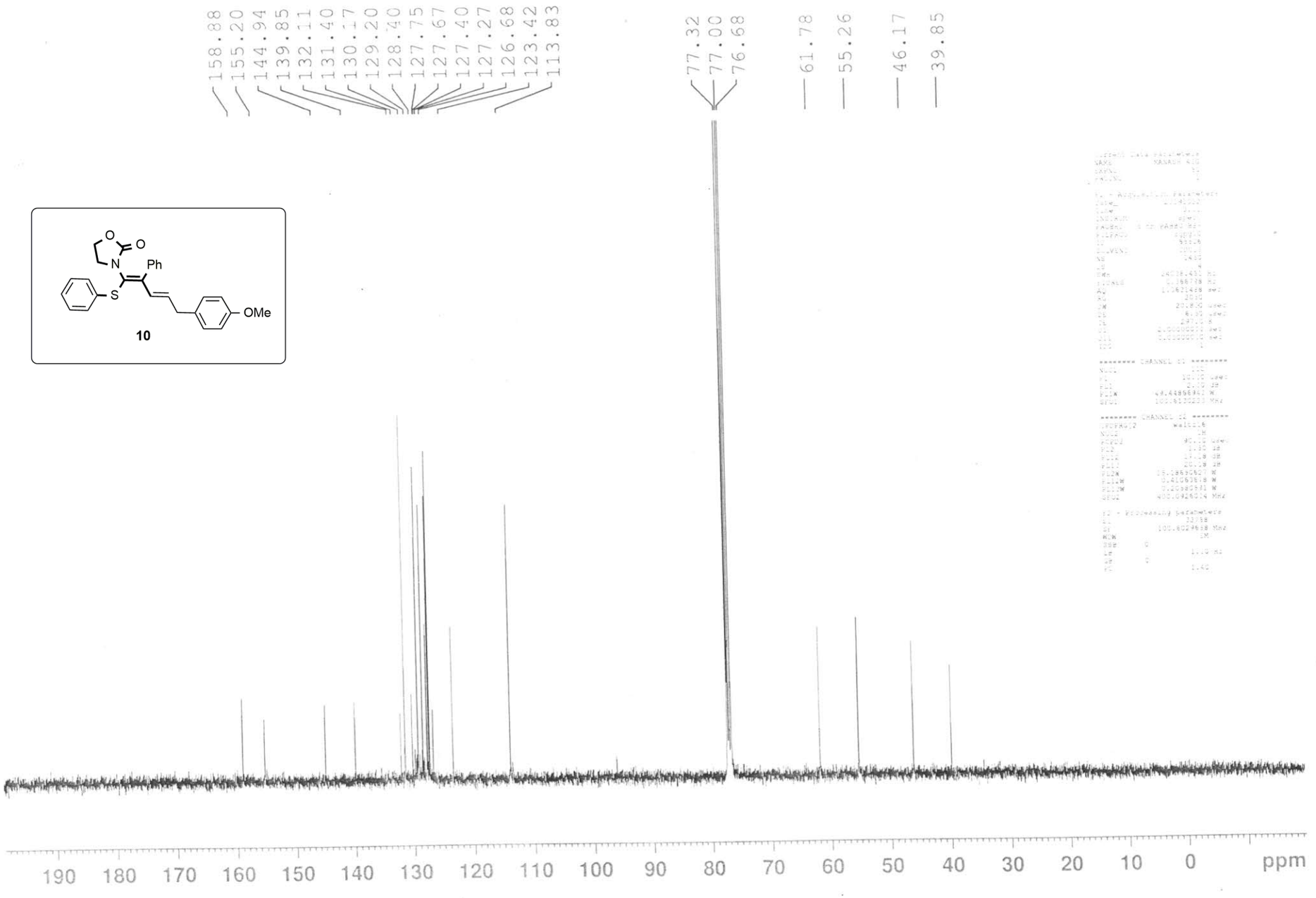


3'a (75:25)

* representative peaks
of minor inseparable isomer




7.521
7.517
7.504
7.500
7.497
7.347
7.329
7.325
7.310
7.290
7.280
7.225
7.208
7.203
6.817
6.795
6.389
6.349
5.989
5.972
5.954
5.949
5.932
5.915
3.799
3.786
3.774
3.771
3.767
3.764
3.737
3.734
3.720
3.717
3.387
3.367
3.347
O
O
N
Ph
S
OMe
10
Current Data Parameters
NAME MPG 4C0
EXPNO 59
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191022
Time 2.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 322
DW 60.800 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.90 usec
PL1 1.90 dB
PL1W 15.18650627 W
SFO1 400.0934707 MHz
F2 - Processing parameters
SI 32768
SF 400.0910093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
2.25
8.43
2.14
2.53
1.05
1.07
5.07
2.21
2.00


158.88
155.20
144.94
139.85
132.11
131.40
130.17
129.20
128.40
127.75
127.67
127.40
127.27
126.68
123.42
113.83
77.32
77.00
76.68
61.78
55.26
46.17
39.85
O
O
N
Ph
S
OMe
10
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm