

# Supporting Information

## Gold-catalyzed Oxidative Hydroacylation Reactions of $\alpha$ -Imino Alkynes with Aldehydes and O<sub>2</sub>

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### *Contents:*

(1) Experiments for measurement of hydrogen evolved-----	S2
(2) Representative synthetic procedures-----	S4
(3) Standard procedures for catalytic operations-----	S5
(4) Figure S1- <sup>18</sup> O-labeling experiments with a complete oxygen transfer-----	S6
(5) Figure S2-The relative energy (kcal/mol) of <i>E</i> and <i>Z</i> -form of <b>3a</b> at M06-2X/6-31 G (d,p) level of theory -----	S9
(6) Table S1-S2-Geometrical coordinates of <i>E</i> and <i>Z</i> -form of <b>3a</b> at M06-2X/6-31G (d,p) level of theory -----	S9
(7) Spectral data for compounds-----	S11
(8) X-ray crystallographic structure and data for compound <b>3a</b> , <b>3m</b> and <b>3t</b> -----	S30
(9) <sup>1</sup> H, <sup>13</sup> C and <sup>1</sup> H NOE Spectral of key compound-----	S57

## (1) Experiments for measurement of hydrogen evolved

A 100-mL one-neck flask was charged with  $P(t\text{-Bu})_2(o\text{-biphenyl})\text{AuCl}$  (5 mol %) and  $\text{AgNTf}_2$  (5 mol%), and the mixture was charged with  $\text{N}_2/\text{O}_2$  (20:1). This mixture was added dry toluene (0.5 mL), and stirred at room temperature for 5 min. To this mixture was added a dry toluene (2.5 mL) of compound **1a** (50 mg, 0.15 mmol), benzaldehyde (4 equiv, 64 mg, 0.61 mmol) and 1 equiv  $\text{H}_2\text{O}$ . This flask was tightly sealed with a new rubber septum and heated to 70 °C for 24 h. GC analysis was conducted on a MS 5A-column using a 0.5 mL gas syringe, before heating and after the reaction. The calibration of hydrogen volume was done on a 0.5 mL sample of a standard 1%  $\text{H}_2/\text{N}_2$  (volume ratio). We observed no hydrogen before the reaction, and the oxygen content was 5.5 %. The GC  $\text{H}_2/\text{N}_2$  area ratios of the reactions and the calibrated gas are as follows 136/199600 and 1054/192613. With these data, the yield of hydrogen is calculated to be 3.7% according to the following procedure.

$$\frac{\text{H}_2}{\text{N}_2} \text{ (the reaction)} : \text{H}_2 / \text{N}_2 \text{ (1\% standard sample)} = X : 0.005 \text{ mL H}_2$$

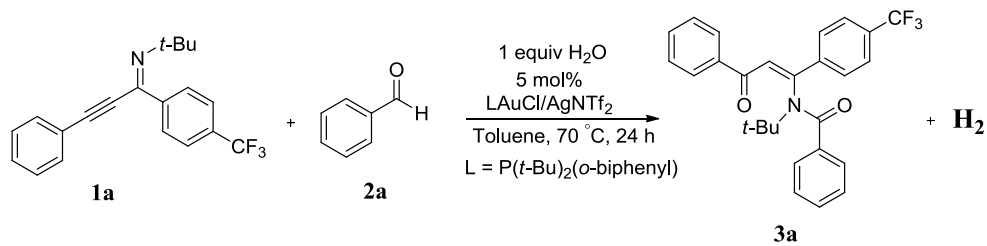
$$\Rightarrow \frac{136}{199600} : \frac{1054}{192613} = X : 0.005$$

$$\Rightarrow X = 0.00062 \text{ mL H}_2$$

The total volume is 100 mL, corresponding to 0.00554 mmol. The yield of the reaction is thus 3.7%.

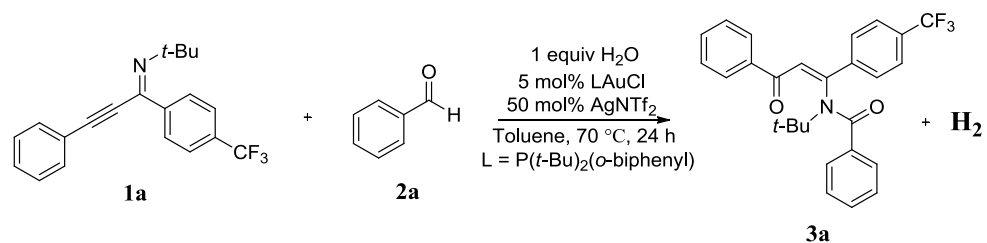
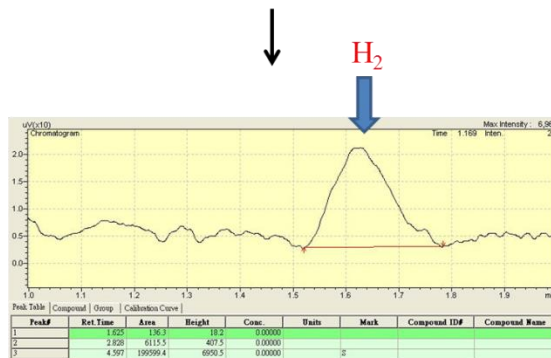
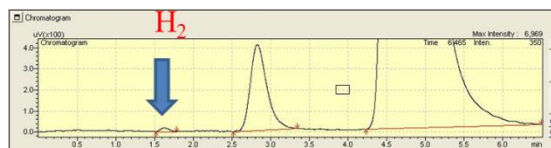
$$\frac{200X}{22400} = \frac{0.124}{22400} = 5.54 \times 10^{-6} \text{ mol}$$

$$\frac{5.54 \times 10^{-6}}{0.1518 \times 10^{-3}} = 0.037$$



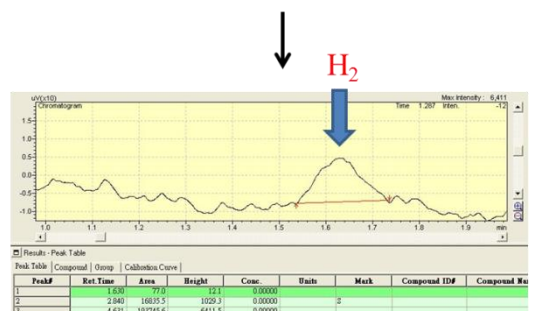
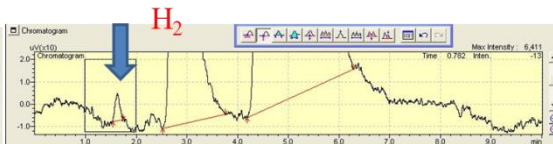
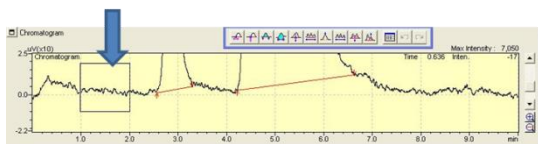
T= 0 (h)

T= 24 (h)



T= 0 (h)

T= 24 (h)



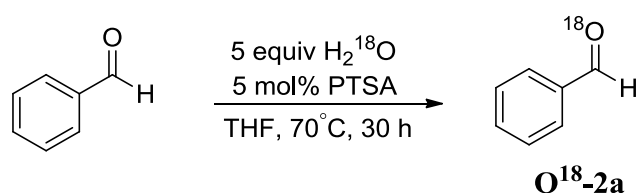
## (2) Representative synthetic procedures:

### (A) General procedure:

Unless otherwise noted, all the reaction for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents, Tetrahydrofuran (THF), toluene and hexane were dried with sodium, benzophenone and distilled before use. Dichloromethane (DCM) were dried over CaH<sub>2</sub> and distilled before use. All other commercial reagents were used without further purification, unless otherwise indicated. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60<sub>f</sub> - 254) using UV light as visualizing agents. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded on a Bruker 400 MHz, 500 MHz, 600MHz, Varian 400 MHz and 700 MHz. Spectrometers using chloroform-*d* (CDCl<sub>3</sub>) as the internal standards.

### (B) Preparation of starting materials:

#### 1. Preparation of <sup>18</sup>O-benzaldehyde (<sup>18</sup>O-2a):

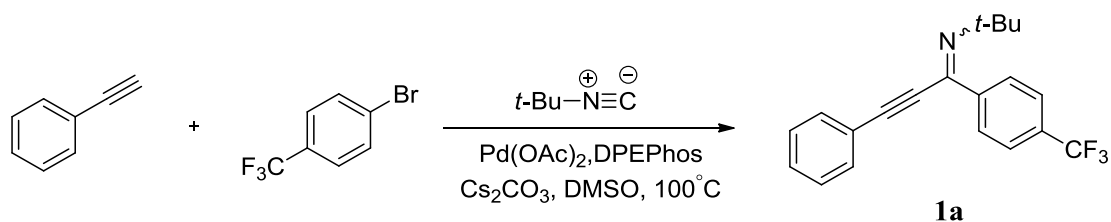


H<sub>2</sub><sup>18</sup>O (189 μL, 9.42 mmol) was added to a solution of benzaldehyde (0.2 g, 1.89 mmol) and *p*-TSA (17.9 mg, 0.0943 mmol) in dry THF (2 mL), and the mixture was stirred for 30 h at 70 °C. Aqueous K<sub>2</sub>CO<sub>3</sub> solution was added and the mixture was extracted with ether. The organic solution concentrated under reduced pressure to get the <sup>18</sup>O-2a (0.22g, 90%, 1.70mmol) and The <sup>18</sup>O content of sample <sup>18</sup>O-2a was estimated peak heights of <sup>16</sup>O- and <sup>18</sup>O-parent peaks in mass spectrum[s<sup>3</sup>].

[s<sup>3</sup>] J.M. Tang, T.A, Liu. R. S. Liu, *J. Org. Chem.* **2008**, 73, 8479–8483

#### 2. Preparation of *N*-(1-(4-(trifluoromethyl)phenyl)-3-phenylprop-2-ynylidene)

##### -2-methylpropan-2-amine (3a):

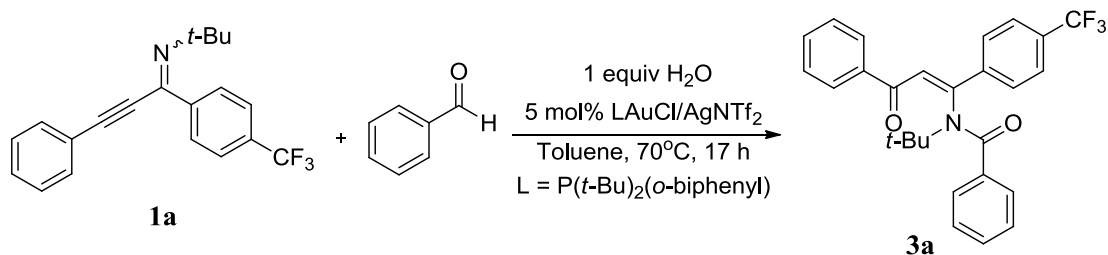


To a flask was added 1-bromo-4-(trifluoromethyl)benzene (0.5 mmol, 112.5 mg), phenylacetylene (0.6 mmol, 61.3mg), *tert*-butyl isocyanide (0.6mmol, 68 $\mu$ L), Pd(OAc)<sub>2</sub> (0.015mmol, 3.37mg), DPEPhos (Bis[(2-diphenylphosphino)phenyl] ether) (0.03 mmol, 16.16 mg), Cs<sub>2</sub>CO<sub>3</sub> (1.0 mmol, 325.82mg), and anhydrous DMSO (2.0mL); this mixture was stirred at 100 °C for 2 h. After a completion of the reaction, as indicated by TLC, the mixture was filtered through a celite bed and the solvent was concentrated under reduced pressure. The residues were purified by an alumina oxide column (10 % EA/hexane, R<sub>f</sub> = 0.53) to give compound **1a** (133 mg, 0.40 mmol, 81%) as orange oil.

All the substrates **1a-1p** were prepared according to literature procedures [s<sup>4</sup>].

[s<sup>4</sup>] T. Tang, X. D. Fei, Z. Y. Ge, Z. Chen, Y. M. Zhu, S. J. Ji, *J. Org. Chem.* **2013**, *78*, 3170-3175

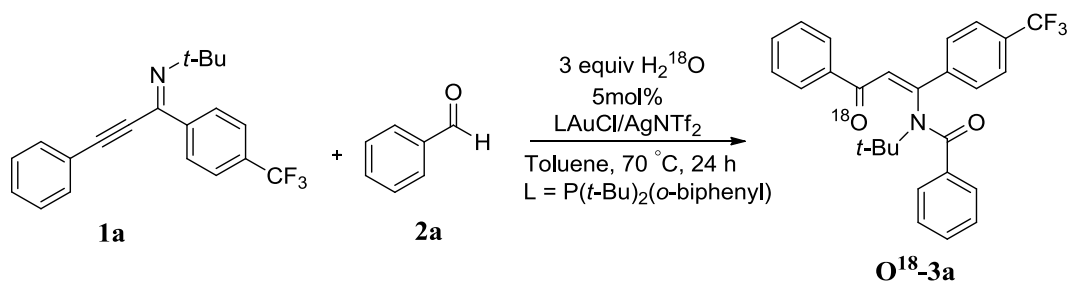
### (3) Standard procedures for catalytic operations:



A reaction flask was charged with chloro[(1,1'-biphenyl-2-yl)di-*tert*-butylphosphine] gold(I) (4.0 mg, 0.008 mmol) and silver bis(trifluoromethane-sulfonyl) imide (2.9 mg, 0.008 mmol), and the mixture was purged with under a mixture of N<sub>2</sub>/O<sub>2</sub> (20:1). This mixture was added dry toluene (0.5 mL) and stirred at room temperature for 5 minutes. To this mixture was added a dry Toluene solution (2.5 mL) of compound **1a** (50 mg, 0.15 mmol), benzaldehyde (64 mg, 0.61 mmol) and H<sub>2</sub>O (2.7  $\mu$ L, 0.15 mmol). The mixture was heated to 70 °C. The solution was monitored by TLC until a complete consumption of starting material (17 h). The mixtures were filtered from a celite bed and purified by a silica column (20%,

EA/hexane,  $R_f = 0.3$ ) to afford **3a** as a yellow solid (57 mg, 0.13 mmol, 83%).

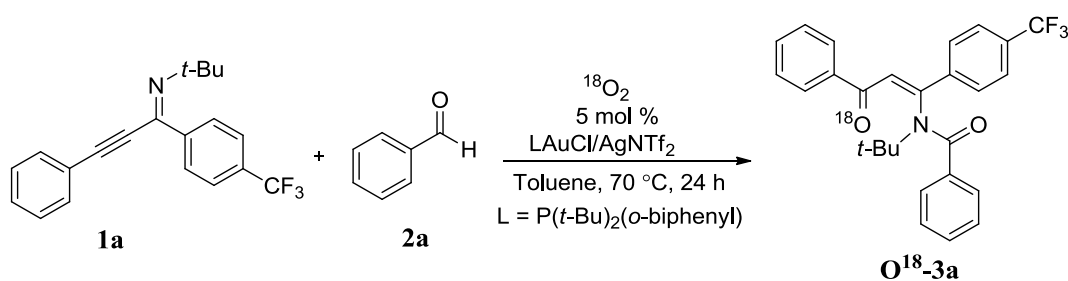
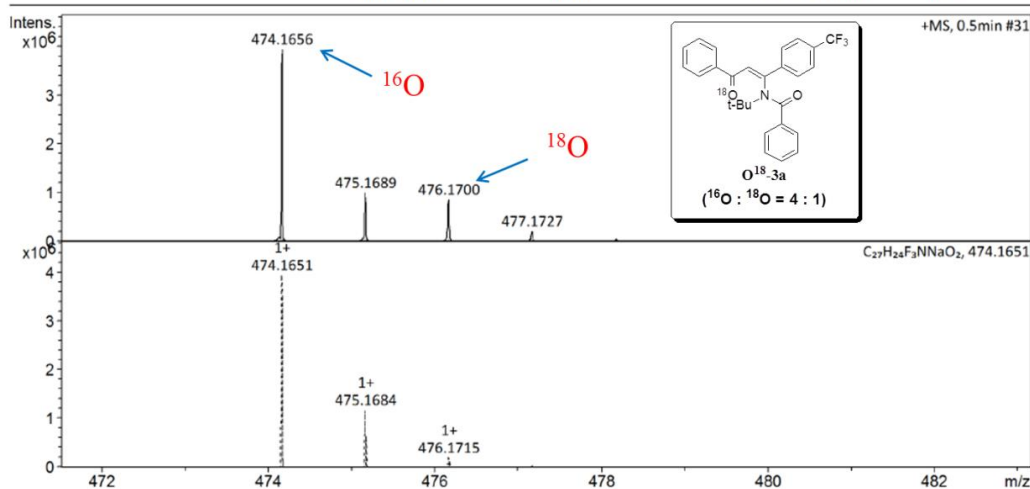
**(4) Figure S1-  $^{18}\text{O}$ -labeling experiments with a complete oxygen transfer**



Display Report

Analysis Info		Acquisition Date	
Analysis Name	D:\Data\nctu service\data\2016\20161223\YU-6-101_GD7_01_12062.d	12/23/2016	9:26:39 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	YU-6-101	Instrument	impact HD
Comment			1819696.00164

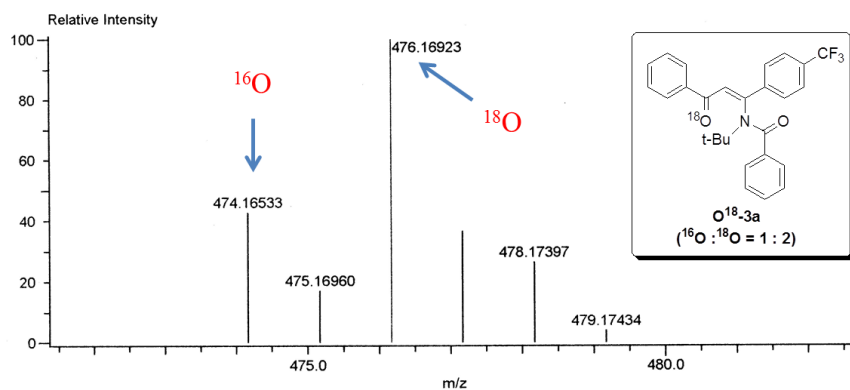
Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



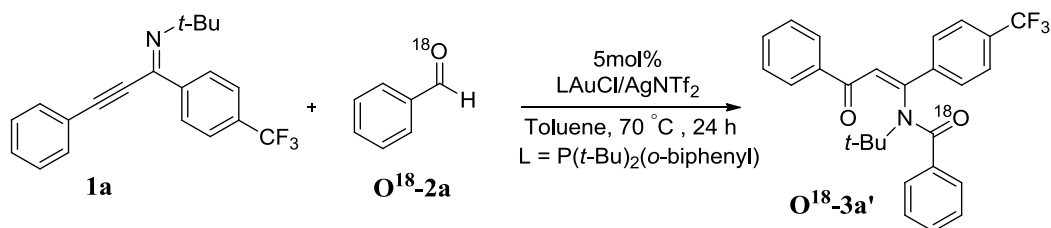
Data: YU-6-106  
 Comment:  
 Description:  
 Ionization Mode: ESI+  
 History: Average(MS[1] 0.77..0.81)

Acquired: 4/18/2017 9:35:31 PM  
 Operator: AccuTOF  
 m/z Calibration File: 20161229TFANA...  
 Created: 4/18/2017 9:39:00 PM  
 Created by: AccuTOF

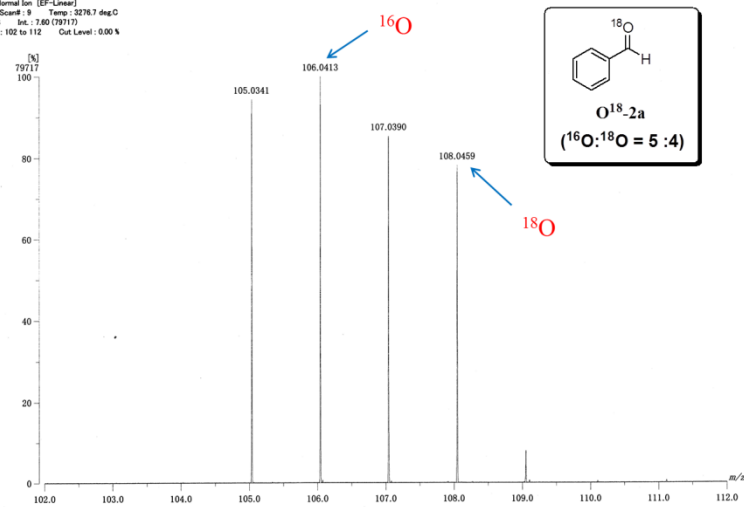
Charge number: 1 Tolerance: 1.50[mDa] Unsaturation Number: -20.0 .. 100.0 (F...  
 Element: <sup>12</sup>C: 27 .. 27, <sup>1</sup>H: 24 .. 24, <sup>18</sup>O: 0 .. 0, <sup>79</sup>Br: 0 .. 0, <sup>35</sup>Cl: 0 .. 0, <sup>19</sup>F: 3 .. 3, <sup>14</sup>N: 1 .. 1, <sup>23</sup>Na: 1 .. 1, <sup>16</sup>O: 1 .. 1, <sup>18</sup>O: 1 .. 1



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
476.16923	16180.07	476.16993	-0.70	-1.46	<sup>12</sup> C <sub>27</sub> <sup>1</sup> H <sub>24</sub> <sup>19</sup> F <sub>3</sub> <sup>14</sup> N <sub>1</sub> <sup>23</sup> Na <sub>1</sub> <sup>16</sup> O <sub>1</sub> <sup>18</sup> O <sub>1</sub>



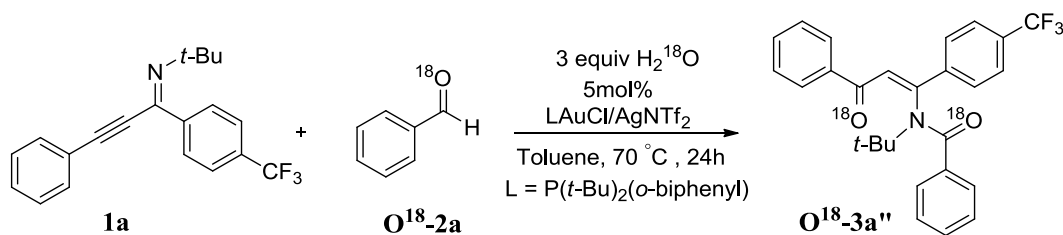
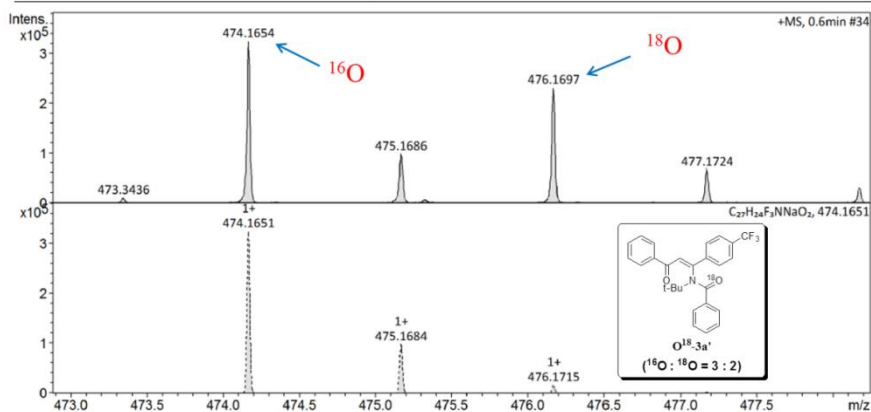
[ Mass Spectrum ]  
 Data : 28002 Data : 28-Dec-2016 11:14  
 Instrument : MDSation  
 Sample : YU-6-91  
 Note :  
 Inlet : Direct Ion Mode : ESI+  
 Spectrum Type : Normal Ion (EF-Linear)  
 RT : 0.39 min Scan# : 9 Temp : 3278.7 deg.C  
 BP : m/z 106.0413 Int. : 7.60 (79717)  
 Output m/z range : 102 to 112 Cut Level : 0.00 %



## Display Report

<b>Analysis Info</b>		Acquisition Date	12/27/2016 9:36:17 AM	
Analysis Name	D:\Data\inctu service\data\2016\20161227\YU-6-102_GE4_01_12068.d	Operator	NCTU	
Method	Small molecule.m	Instrument	impact HD	1819696.00164
Sample Name	YU-6-102	Comment		

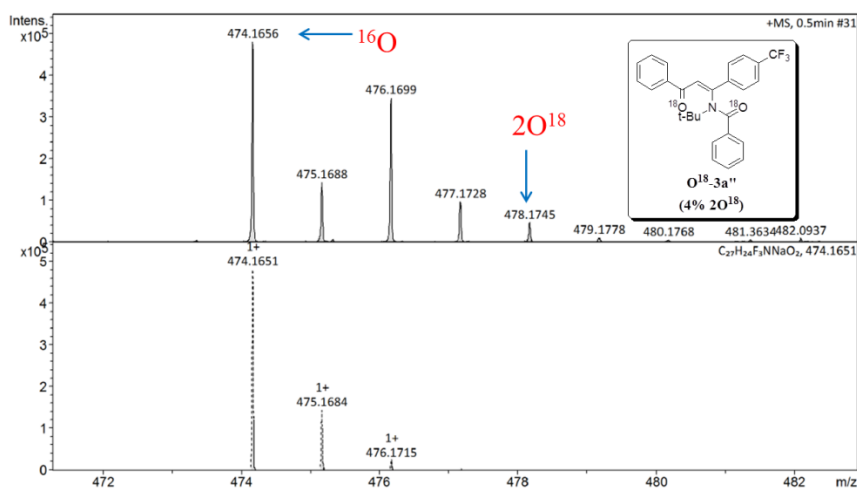
<b>Acquisition Parameter</b>					
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Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



## Display Report

<b>Analysis Info</b>		Acquisition Date	12/30/2016 11:23:22 AM	
Analysis Name	D:\Data\inctu service\report\2016\20161230\YU-6-104_BB7_01_12088.d	Operator	NCTU	
Method	Small molecule.m	Instrument	impact HD	1819696.00164
Sample Name	YU-6-104	Comment		

<b>Acquisition Parameter</b>					
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Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

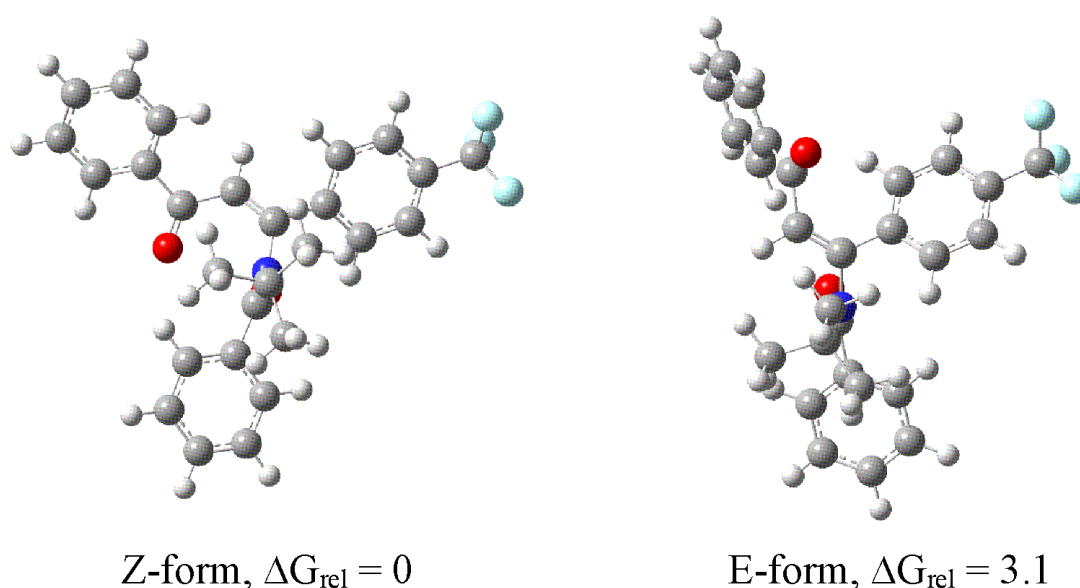




**(5) Figure S2. The relative energy (kcal/mol) of *E* and *Z*-form of 3a at M06-2X/6-31G (d,p) level of theory.**

**Method of calculations:**

In this present work, geometry optimizations were carried out without any symmetry restriction by using M06-2X/6-31G(d,p) level of theory. The vibrational frequency calculations were performed to establish the nature of the stationary points (local minimal states) at the same level of theory. The relative energy are  $\Delta G$  values at 298.15 K and 1 atm.



**Figure S3.** The relative energy (kcal/mol) of *E* and *Z*-form of 3a at M06-2X/6-31G(d,p) level of theory.

**(6) Table S1-S2. Geometrical coordinates of *E* and *Z*-form of 3a at M06-2X/6-31G(d,p) level of theory.**

**Table S1**

**M06-2X/6-31G(d,p)**

**3a-E-form**

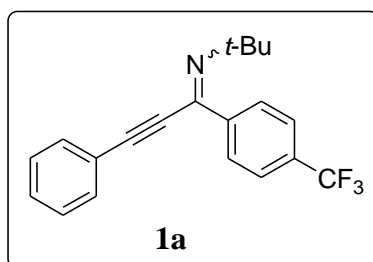
Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-2.042405	-0.553010	0.596275
8	-1.334864	-0.986849	1.489817

6	-3.433627	-0.097827	0.928745
6	-4.396025	-1.021071	1.332914
6	-3.715437	1.268333	0.969965
6	-5.659799	-0.582062	1.718032
1	-4.150917	-2.079173	1.344710
6	-4.970881	1.705913	1.377612
1	-2.948136	1.980153	0.677219
6	-5.948158	0.780201	1.738138
1	-6.415013	-1.302502	2.015100
1	-5.188271	2.768444	1.412583
1	-6.930838	1.121756	2.046628
7	-1.557807	-0.384794	-0.696411
6	-2.377453	-0.534321	-1.953737
6	-0.130300	-0.571806	-0.749999
6	0.378540	-1.787844	-0.965355
1	-0.307849	-2.630764	-1.012256
6	0.663432	0.647730	-0.455210
6	0.173330	1.904221	-0.823556
6	1.885022	0.573759	0.226883
6	0.903700	3.058783	-0.566666
1	-0.790472	1.974887	-1.317384
6	2.616549	1.722047	0.487508
1	2.250432	-0.383138	0.584394
6	2.128398	2.963190	0.082628
1	0.527029	4.029028	-0.869826
1	3.562769	1.660129	1.015560
6	2.930086	4.190691	0.403501
9	4.208234	4.054439	0.020345
9	2.949045	4.434966	1.723514
9	2.440416	5.283887	-0.197756
6	1.825712	-2.132208	-1.137401
8	2.468165	-1.731162	-2.086318
6	2.409852	-3.037437	-0.102335
6	1.756798	-3.241105	1.117446
6	3.635643	-3.657426	-0.359423
6	2.330844	-4.074799	2.073397
1	0.818121	-2.728482	1.322701
6	4.198223	-4.495372	0.593740

1	4.122631	-3.467999	-1.310799
6	3.544041	-4.705089	1.808749
1	1.832877	-4.229747	3.024719
1	5.145877	-4.985782	0.396279
1	3.985987	-5.359863	2.553392
6	-1.455118	-0.380118	-3.171224
1	-0.916858	0.572320	-3.145570
1	-0.718632	-1.179778	-3.247230
1	-2.072871	-0.396135	-4.072106
6	-3.039010	-1.916765	-1.988939
1	-3.706625	-2.050191	-1.132846
1	-3.634538	-2.021352	-2.901106
1	-2.290442	-2.713442	-1.981800
6	-3.463445	0.547397	-2.067778
1	-3.869207	0.521140	-3.083005
1	-4.289716	0.389990	-1.375793
1	-3.047430	1.544465	-1.895073

### (7) Spectral data for compounds:

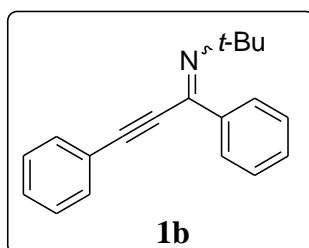
#### Spectral data for *N*-(1-(4-(trifluoromethyl)phenyl)-3-phenylprop-2-ynylidene)-2-methylpropan-2-amine (**1a**)



Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.53$ , 133 mg, 0.40 mmol, 81%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.16(d,  $J = 8.4$  Hz, 2 H), 7.63 (d,  $J = 8.4$  Hz, 2 H), 7.57 (dd,  $J = 8.0$  Hz & 1.2 Hz, 2 H), 7.46 ~ 7.38 (m, 3 H), 1.53 (s, 9 H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  145.7, 142.6, 131.6, 129.9, 128.7, 127.6, 125.1, 125.1, 121.6, 99.5, 83.5, 57.4, 29.4; ESI-MS (M+H) calcd. For  $\text{C}_{20}\text{H}_{19}\text{F}_3\text{N}$ : 330.14700; Found: 330.14700.

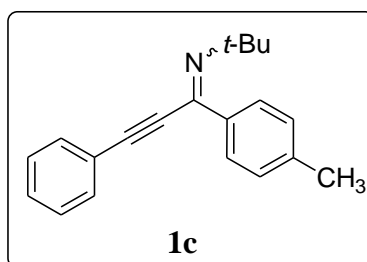
#### Spectral data for 2-methyl-*N*-(1,3-diphenylprop-2-ynylidene)propan-2-amine

(1b)



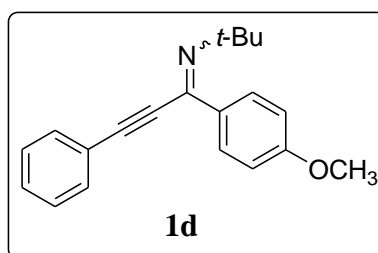
Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.54$ , 118 mg, 0.45 mmol, 90%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.08~8.06 (m, 2H), 7.57 (dd,  $J = 7.5\text{Hz} \ \& \ 2\text{Hz}$ , 2H), 7.42~7.37 (m, 6H), 1.54 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  147.0, 139.5, 131.6, 130.0, 129.6, 128.6, 128.1, 127.2, 122.0, 98.9, 84.1, 57.0, 29.5; EI-MS calcd. for  $\text{C}_{19}\text{H}_{19}\text{N}$ : 261.1517; Found: 261.1516.

**Spectral data for 2-methyl-N-(3-phenyl-1-*p*-tolylprop-2-ynylidene)propan-2-amine (1c)**



Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.62$ , 124 mg, 0.45 mmol, 90%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.97 (d,  $J = 8\text{Hz}$ , 2H), 7.57 (dd,  $J = 7.5\text{Hz} \ \& \ 2\text{Hz}$ , 2H), 7.42~7.38 (m, 3H), 7.19 (d,  $J = 8\text{Hz}$ , 2H), 2.38 (s, 3H), 1.54 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  147.0, 140.2, 136.8, 131.6, 129.6, 128.8, 128.6, 127.2, 122.0, 98.7, 84.2, 56.9, 29.6, 21.3; EI-MS calcd. for  $\text{C}_{20}\text{H}_{21}\text{N}$ : 275.1674; Found: 275.1675.

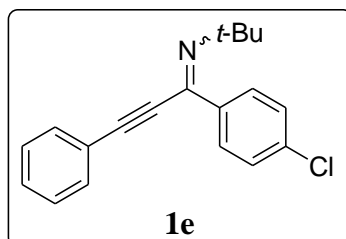
**Spectral data for N-(1-(4-methoxyphenyl)-3-phenylprop-2-ynylidene)-2-methylpropan-2-amine (1d)**



Brown Oil; (10% ethylacetate/hexane,  $R_f = 0.39$ , 108 mg, 0.37 mmol, 74%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.03 (d,  $J = 8.5\text{Hz}$ , 2H), 7.57 (dd,  $J = 7\text{Hz} \ \& \ 2\text{Hz}$ , 2H),

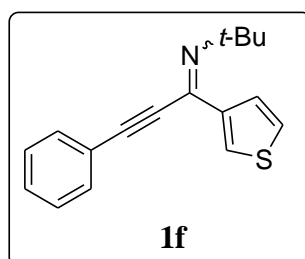
7.42~7.37 (m, 3H), 6.90 (d,  $J = 9\text{Hz}$ , 2H), 3.83 (s, 3H), 1.53 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  161.3, 131.6, 129.5, 128.8, 128.6, 127.0, 122.0, 113.9, 113.4, 98.5, 84.1, 56.7, 55.4, 29.6; EI-MS calcd. for  $\text{C}_{20}\text{H}_{21}\text{NO}$ : 291.1623; Found: 291.1622.

**Spectral data for *N*-(1-(4-chlorophenyl)-3-phenylprop-2-ynylidene)-2-methylpropan-2-amine (1e)**



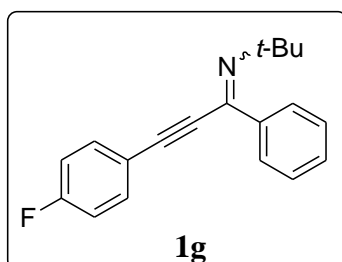
Yellow Oil; (10% ethylacetate/hexane,  $R_f = 0.57$ , 91 mg, 0.31 mmol, 62%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.01 (dd,  $J = 6.5\text{Hz}$  &  $2\text{Hz}$ ), 7.57~7.56 (m, 2H) 7.43~7.40 (m, 3H), 7.35 (dd,  $J = 6.5\text{Hz}$  &  $2\text{Hz}$ , 2H), 1.52 (s, 9H) ;  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  145.8, 137.9, 136.1, 131.6, 129.8, 128.7, 128.6, 128.3, 121.7, 99.1, 83.6, 57.1, 29.5; ESI-MS (M+H) calcd. for  $\text{C}_{19}\text{H}_{19}\text{ClN}$ : 296.1206; Found: 296.12030.

**Spectral data for 2-methyl-*N*-(3-phenyl-1-(thiophen-3-yl)prop-2-ynylidene)propan-2-amine (1f)**



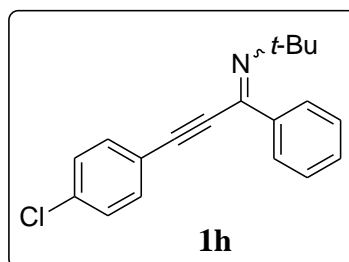
Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.72$ , 120 mg, 0.45 mmol, 90%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.65 (d,  $J = 4.4\text{Hz}$ , 1H), 7.58~7.56 (m, 1H), 7.52~7.50 (m, 2H), 7.43~7.39 (m, 3H), 7.27~7.25 (m, 1H), 1.53 (s, 9H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  143.9, 142.6, 131.6, 129.6, 128.3, 126.5, 125.5, 121.8, 97.2, 84.3, 56.8, 29.6; EI-MS calcd. for  $\text{C}_{17}\text{H}_{17}\text{NS}$ : 267.1082; Found: 267.1084.

**Spectral data for *N*-(3-(4-fluorophenyl)-1-phenylprop-2-ynylidene)-2-methylpropan-2-amine (1g)**



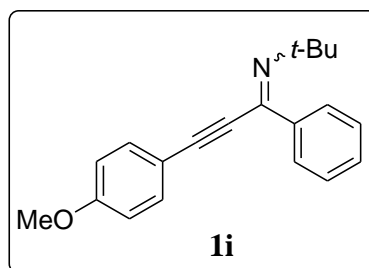
Yellow Oil; (10% ethylacetate/hexane,  $R_f = 0.73$ , 82 mg, 0.29 mmol, 49%);  $^1\text{H}$  NMR (700 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.04 (dd,  $J = 6.3\text{Hz}$  &  $2.8\text{Hz}$ , 2H), 7.56 (dd,  $J = 8.4\text{Hz}$  &  $5.6\text{Hz}$ , 2H), 7.39~7.38 (m, 3H), 7.09 (t,  $J = 8.4\text{Hz}$ , 2H), 1.53 (s, 9H);  $^{13}\text{C}$  NMR (175 MHz,  $\text{CDCl}_3$ ):  $\delta$  164.0, 146.8, 139.4, 133.7, 130.0, 128.2, 127.2, 118.1, 116.1, 97.7, 83.8, 56.9, 29.4; EI-MS calcd. for  $\text{C}_{19}\text{H}_{18}\text{FN}$ : 279.1423; Found: 279.1418.

**Spectral data for *N*-(3-(4-chlorophenyl)-1-phenylprop-2-ynylidene)-2-methylpropan-2-amine (1h)**



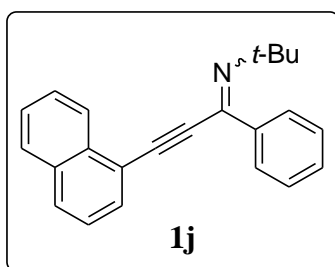
Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.71$ , 131 mg, 0.42 mmol, 88%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.04 (dd,  $J = 6.6\text{Hz}$  &  $1.8\text{Hz}$ , 2H), 7.49 (d,  $J = 9\text{Hz}$ , 2H), 7.39~7.36 (m, 5H), 1.53 (s, 9H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  139.3, 135.9, 132.8, 130.1, 129.0, 128.2, 127.2, 125.3, 120.4, 97.5, 84.8, 57.0, 29.5; EI-MS calcd. for  $\text{C}_{19}\text{H}_{18}\text{ClN}$ : 295.1128; Found: 295.1131.

**Spectral data for *N*-(3-(4-methoxyphenyl)-1-phenylprop-2-ynylidene)-2-methylpropan-2-amine (1i)**



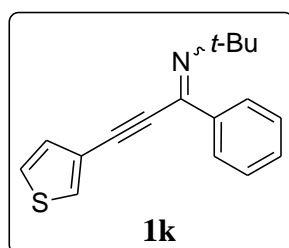
Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.50$ , 122 mg, 0.42 mmol, 84%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.08~8.06 (m, 2H), 7.52 (dt,  $J = 9.6\text{Hz}$  &  $2.4\text{Hz}$ , 2H), 7.40~7.38 (m, 3H), 6.91 (dt,  $J = 9.6\text{Hz}$  &  $2.4\text{Hz}$ , 2H), 3.83 (s, 3H), 1.54 (s, 9H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  160.7, 147.2, 139.6, 133.3, 129.9, 128.1, 127.2, 114.3, 114.0, 99.4, 83.4, 56.8, 55.4, 29.5; ESI-MS (M+H) calcd. for  $\text{C}_{20}\text{H}_{22}\text{NO}$ : 292.1701; Found: 292.1696.

**Spectral data for 2-methyl-*N*-(3-(naphthalen-1-yl)-1-phenylprop-2-ynylidene)propan-2-amine (1j)**



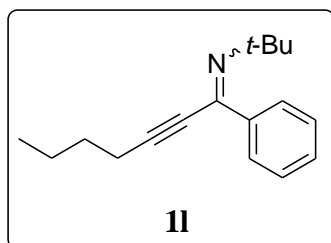
Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.63$ , 138 mg, 0.45 mmol, 89%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.31 (d,  $J = 8.4\text{Hz}$ , 1H), 8.14 (s, 2H), 7.95 (d,  $J = 7.8\text{Hz}$ , 1H), 7.92 (d,  $J = 8.4\text{Hz}$ , 1H), 7.86 (d,  $J = 7.7\text{Hz}$ , 1H), 7.63 (t,  $J = 7.2\text{Hz}$ , 1H), 7.58 (t,  $J = 7.2\text{Hz}$ , 1H), 7.53 (t,  $J = 7.2\text{Hz}$ , 1H), 7.48 (s, 3H), 1.61 (s, 9H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  147.9, 139.0, 132.6, 132.6, 131.3, 130.2, 128.7, 128.4, 128.3, 127.3, 127.1, 126.7, 125.5, 125.2, 118.9, 97.7, 87.9, 56.9, 29.1; EI-MS calcd. for  $\text{C}_{23}\text{H}_{21}\text{N}$ : 311.1674; Found: 311.1672.

**Spectral data for 2-methyl-N-(1-phenyl-3-(thiophen-3-yl)prop-2-ynylidene)propan-2-amine (1k)**



Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.64$ , 125 mg, 0.47 mmol, 93%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.00~7.99 (m, 2H), 7.69 (s, 1H), 7.42 (d,  $J = 4.8\text{Hz}$ , 3H), 7.38 (q,  $J = 2.4\text{Hz}$ , 1H), 7.24 (t,  $J = 4.8\text{Hz}$ , 1H), 1.49 (s, 9H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  147.8, 138.7, 130.8, 130.1, 129.3, 128.2, 126.9, 126.2, 120.3, 94.7, 83.3, 56.7, 29.0; EI-MS calcd. for  $\text{C}_{17}\text{H}_{17}\text{NS}$ : 267.1082; Found: 267.1081.

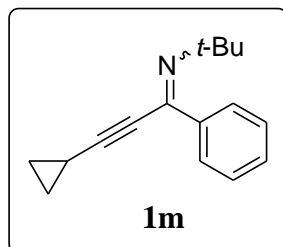
**Spectral data for 2-methyl-N-(1-phenylhept-2-ynylidene)propan-2-amine (1l)**



Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.55$ , 42 mg, 0.17 mmol, 35%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.97~7.96 (m, 2H), 7.38 (d,  $J = 5.4\text{Hz}$ , 3H), 2.49 (t,  $J = 5.4\text{Hz}$ , 2H), 1.64~1.60 (m, 2H), 1.46 (s, 11H), 0.93 (t,  $J = 7.2\text{Hz}$ , 3H);  $^{13}\text{C}$  NMR (150 MHz,

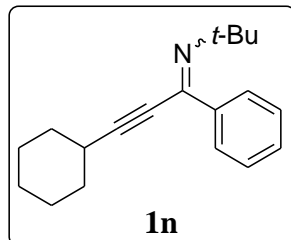
CDCl<sub>3</sub>):  $\delta$  148.0, 139.4, 129.8, 128.0, 126.9, 102.3, 75.7, 56.3, 29.8, 28.9, 22.1, 19.2, 13.7; EI-MS calcd. for C<sub>17</sub>H<sub>23</sub>N: 241.1830; Found: 241.1834.

**Spectral data for *N*-(3-cyclopropyl-1-phenylprop-2-ynylidene)-2-methylpropan-2-amine (1m)**



Orange Oil; (10% ethylacetate/hexane, R<sub>f</sub> = 0.61, 95 mg, 0.42 mmol, 84%); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  7.91~7.90 (m, 2H), 7.37~7.34 (m, 3H), 1.54~1.50 (m, 1H), 1.40 (s, 9H), 0.98~0.95 (m, 2H), 0.91~0.88 (m, 2H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>):  $\delta$  147.9, 139.3, 129.8, 128.0, 126.9, 105.4, 71.3, 56.2, 28.9, 8.8, 0.3; ESI-MS (M+H) calcd. for C<sub>16</sub>H<sub>20</sub>N: 226.1596; Found: 226.15982.

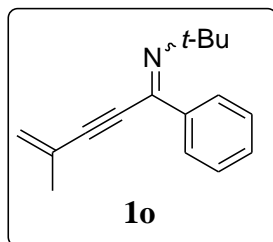
**Spectral data for *N*-(3-cyclohexyl-1-phenylprop-2-ynylidene)-2-methylpropan-2-amine (1n)**



Orange Oil; (10% ethylacetate/hexane, R<sub>f</sub> = 0.68, 101 mg, 0.38 mmol, 75%); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  8.00~7.98 (m, 2H), 7.35~7.34 (m, 3H), 2.70~2.67 (m, 1H), 1.92~1.91 (m, 2H), 1.76~1.74 (m, 2H), 1.62~1.55 (m, 3H), 1.47 (s, 9H), 1.39~1.36 (m, 3H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>):  $\delta$  139.8, 131.5, 129.7, 127.9, 127.2, 105.4, 76.2, 56.5, 31.9, 29.7, 29.3, 25.8, 24.8; ESI-MS (M+H) calcd. for C<sub>19</sub>H<sub>26</sub>N: 268.2065; Found: 268.2061.

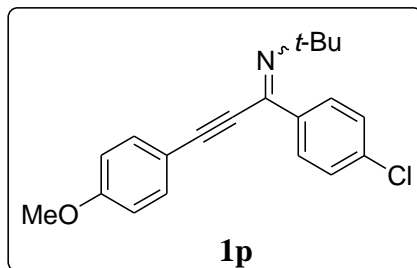
**Spectral data for 2-methyl-*N*-(4-methyl-1-phenylpent-4-en-2-ynylidene)propan-2-amine (1o)**





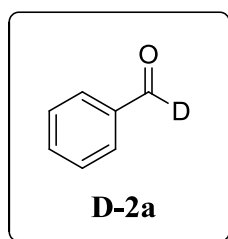
Yellow Oil; (10% ethylacetate/hexane,  $R_f = 0.72$ , 88 mg, 0.39 mmol, 78%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.00~7.98 (m, 2H), 7.38~7.35 (m, 3H), 5.52~5.51 (m, 1H), 5.44~5.43 (m, 1H), 2.02 (s, 3H), 1.49 (s, 9H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  147.0, 139.4, 129.9, 128.1, 127.2, 126.1, 124.1, 100.1, 83.0, 56.8, 29.4, 22.5; EI-MS calcd. for  $\text{C}_{16}\text{H}_{19}\text{N}$ : 225.1517; Found: 225.1511.

**Spectral data for *N*-(1-(4-chlorophenyl)-3-(4-methoxyphenyl)prop-2-ynylidene)-2-methylpropan-2-amine (1p)**



Orange Oil; (10% ethylacetate/hexane,  $R_f = 0.38$ , 114 mg, 0.35 mmol, 70%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  8.01~7.99 (m, 2H), 7.51~7.50 (m, 2H), 7.35~7.33 (m, 2H), 6.92~6.91 (m, 2H), 3.84 (s, 3H), 1.52 (s, 9H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  160.9, 146.0, 138.1, 135.9, 133.3, 128.6, 128.2, 114.4, 113.7, 99.6, 83.0, 56.9, 55.4, 29.5; EI-MS calcd. for  $\text{C}_{20}\text{H}_{20}\text{ClNO}$ : 325.1233; Found: 325.1231.

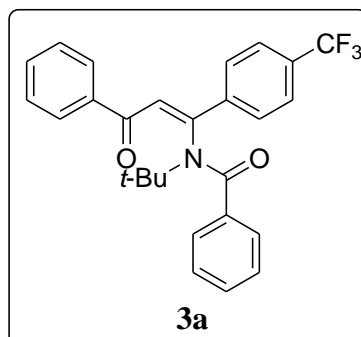
**Spectral data for Benzaldehyde- $\alpha$ - $\text{d}_1$  (D-2a)**



Colorless Oil; (10% ethylacetate/hexane,  $R_f = 0.45$ , 538mg, 5.02 mmol, 50%);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.88~7.86 (m, 2H), 7.63~7.60 (m, 1H), 7.53~7.50 (m, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  192.20, 192.03, 191.85, 136.36, 134.44, 129.72,

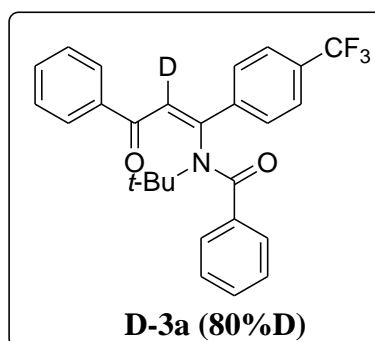
128.99; EI-MS calcd. for C<sub>7</sub>H<sub>5</sub>DO: 107.0481; Found: 107.0480.

**Spectral data for *N*-*tert*-butyl-*N*-((*Z*)-1-(4-(trifluoromethyl)phenyl)-3-oxo-3-phenylprop-1-enyl)benzamide (3a)**



Yellow solid; mp: 149.5°C; (20% ethylacetate/hexane, R<sub>f</sub> = 0.30, 57 mg, 0.13 mmol, 83%); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.80 (d, *J* = 8.5Hz, 2H), 7.72 (d, *J* = 8.5Hz, 2H), 7.51~7.32 (m, 3H), 7.31 (t, *J* = 8Hz, 2H), 7.25~7.23 (m, 2H), 7.07 (s, 1H), 7.04 (t, *J* = 7Hz, 1H), 6.90 (t, *J* = 7.5Hz, 2H), 1.55 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 188.2, 170.6, 150.0, 143.9, 138.3, 138.0, 133.0, 129.3, 128.9, 128.4, 128.0, 127.9, 127.4, 126.7, 126.4, 126.0, 124.7, 61.4, 28.9; ESI-MS (M+H) calcd. for C<sub>27</sub>H<sub>25</sub>F<sub>3</sub>NO<sub>2</sub>: 452.1837; Found: 452.18351.

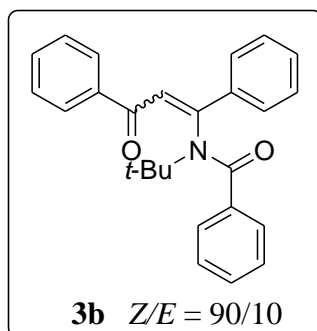
**Spectral data Deuterium-labeling for *N*-*tert*-butyl-*N*-((*Z*)-1-(4-(trifluoromethyl)phenyl)-3-oxo-3-phenylprop-1-enyl)benzamide (D-3a)**



Yellow solid; mp: 149.5°C; (20% ethylacetate/hexane, R<sub>f</sub> = 0.36, 48 mg, 0.11 mmol, 70%); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.81 (d, *J* = 8.5Hz, 2H), 7.72 (d, *J* = 8.5Hz, 2H), 7.51~7.46 (m, 3H), 7.31 (t, *J* = 7.5Hz, 2H), 7.24 (d, *J* = 7.5Hz, 2H), 7.07 (s, 0.2H), 7.04 (t, *J* = 7.5Hz, 1H), 6.89 (t, *J* = 7.5Hz, 2H), 1.55 (s, 9H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 188.2, 170.6, 150.0, 143.9, 138.4, 138.0, 133.0, 132.5, 132.2, 132.0, 131.7, 129.3, 128.9, 128.4, 128.0, 127.9, 127.4, 126.4, 126.0, 126.0, 124.7, 61.4, 28.9;

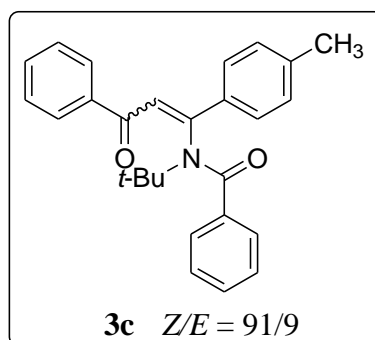
ESI-MS (M+H) calcd. for C<sub>27</sub>H<sub>24</sub>DF<sub>3</sub>NO<sub>2</sub>: 453.1900; Found:453.19009.

**Spectral data for *N*-*tert*-butyl-*N*-(3-oxo-1,3-diphenylprop-1-enyl)benzamide (3b)**



Yellow oil; (20% ethylacetate/hexane, R<sub>f</sub> = 0.32, 66 mg, 0.17 mmol, 90%); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Z/E = 90/10 major isomer: δ 7.72~7.70 (m, 2H), 7.51 (d, J = 7.9Hz, 2H), 7.47~7.41 (m, 4H), 7.31~7.28 (m, 4H), 7.04~7.01 (m, 2H), 6.89 (t, J = 7.7Hz, 2H), 1.55 (s, 9H); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) minor isomer: δ 7.34~7.33 (m, 4H), 7.24~7.23 (m, 2H), 7.15 (d, J = 7.1Hz, 2H), 7.10 (t, J = 7.7Hz, 2H), 6.31 (s, 1H), (remaining peaks merging with major isomer); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 188.4, 170.6, 151.6, 140.3, 138.7, 138.4, 132.7, 130.5, 129.0, 128.6, 128.3, 127.9, 127.7, 127.3, 126.4, 122.9, 61.2, 28.9; ESI-MS (M+H) calcd. for C<sub>26</sub>H<sub>26</sub>NO<sub>2</sub>: 384.1964; Found: 384.19659.

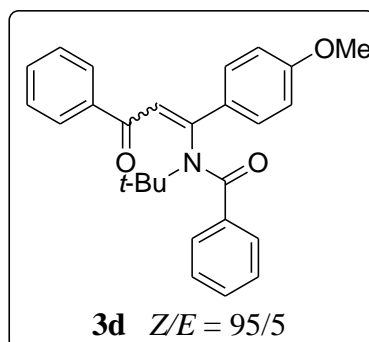
**Spectral data for *N*-*tert*-butyl-*N*-(3-oxo-3-phenyl-1-*p*-tolylprop-1-enyl)benzamide (3c)**



Orange oil; (20% ethylacetate/hexane, R<sub>f</sub> = 0.34, 56 mg, 0.14 mmol, 78%); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) Z/E = 91/9 major isomer: δ 7.61 (d, J = 8.2Hz, 2H), 7.49 (d, J = 7.5Hz, 2H), 7.44 (t, J = 7.3Hz, 2H), 7.31~7.26 (m, 5H), 7.03 (t, J = 7.5Hz, 1H), 6.99 (s, 1H), 6.89 (t, J = 7.8Hz, 2H), 2.43 (s, 3H), 1.54 (s, 9H); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) minor isomer: δ 7.15 (t, J = 7.5Hz, 2H), 7.11 (t, J = 7.1Hz, 1H), 6.24 (s, 1H), 2.40 (s, 3H), 1.53 (s, 9H), (remaining peaks merging with major isomer); <sup>13</sup>C NMR (125 MHz,

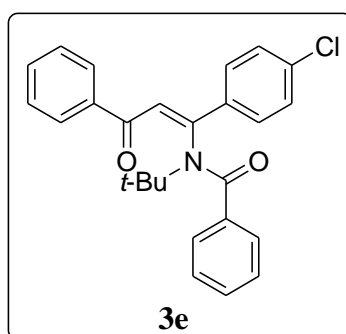
CDCl<sub>3</sub>):  $\delta$  188.4, 170.6, 151.8, 141.0, 138.8, 138.6, 137.5, 132.6, 129.7, 128.6, 128.3, 127.9, 127.7, 127.2, 126.5, 122.1, 61.1, 28.9, 21.4; ESI-MS (M+Na) calcd. for C<sub>27</sub>H<sub>27</sub>NNaO<sub>2</sub>: 420.1939; Found: 420.1937.

**Spectral data for *N*-*tert*-butyl-*N*-(1-(4-methoxyphenyl)-3-oxo-3-phenylprop-1-enyl)benzamide (3d)**



Yellow oil; (20% ethylacetate/hexane,  $R_f$  = 0.22, 41 mg, 0.10 mmol, 59%); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) *Z/E* = 95/5 major isomer:  $\delta$  7.65 (d,  $J$  = 8.9Hz, 2H), 7.52 (d,  $J$  = 7.3Hz, 2H), 7.44 (t,  $J$  = 6.8Hz, 1H), 7.31~7.29 (m, 4H), 7.04 (t,  $J$  = 7.4Hz, 1H), 6.97 (d,  $J$  = 7.0Hz, 2H), 6.95 (s, 1H), 6.90 (t,  $J$  = 7.7Hz, 2H), 3.88 (s, 3H), 1.55 (s, 9H); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) minor isomer:  $\delta$  7.21 (d,  $J$  = 8.9Hz, 2H), 7.16 (t,  $J$  = 7.6Hz, 2H), 7.12 (t,  $J$  = 7.3Hz, 2H), 6.64 (dd,  $J$  = 9Hz & 1.8Hz, 2H), 6.22 (s, 1H), 3.71 (s, 3H), 1.54 (s, 9H), (remaining peaks merging with major isomer); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>):  $\delta$  188.3, 170.6, 161.6, 151.6, 138.9, 138.8, 132.6, 132.5, 129.4, 128.6, 128.3, 127.9, 127.2, 126.4, 120.9, 114.3, 61.1, 55.5, 28.9; ESI-MS (M+H) calcd. for C<sub>27</sub>H<sub>28</sub>NO<sub>3</sub>: 414.2069; Found: 414.20690.

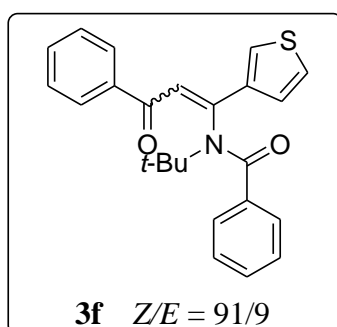
**Spectral data for *N*-*tert*-butyl-*N*-((*Z*)-1-(4-chlorophenyl)-3-oxo-3-phenylprop-1-enyl)benzamide (3e)**



Yellow oil; (20% ethylacetate/hexane,  $R_f$  = 0.32, 56 mg, 0.13 mmol, 80%); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.63 (d,  $J$  = 7.7Hz, 2H), 7.50 (d,  $J$  = 7.5Hz, 2H), 7.48~7.43 (m,

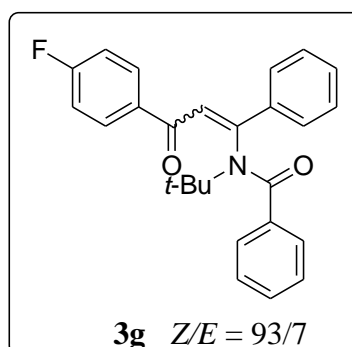
3H), 7.30 (t,  $J = 7.8\text{Hz}$ , 2H), 7.25 (d,  $J = 8.3\text{Hz}$ , 2H), 7.04 (t,  $J = 7.5\text{Hz}$ , 1H), 7.00 (s, 1H), 6.90 (t,  $J = 7.7\text{Hz}$ , 2H), 1.54 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.3, 170.6, 150.5, 138.8, 138.5, 138.2, 136.6, 132.8, 129.3, 128.9, 128.8, 128.3, 127.9, 127.4, 126.4, 123.1, 61.3, 28.9; ESI-MS ( $\text{M}+\text{H}$ ) calcd. for  $\text{C}_{26}\text{H}_{25}\text{ClNO}_2$ : 418.1574; Found: 418.15774.

**Spectral data for *N*-*tert*-butyl-*N*-(3-oxo-3-phenyl-1-(thiophen-3-yl)prop-1-enyl) benzamide (3f)**



Orange oil; (20% ethylacetate/hexane,  $R_f = 0.27$ , 51 mg, 0.13 mmol, 71%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $Z/E = 91/9$  major isomer:  $\delta$  7.70 (m, 1H), 7.60 (d,  $J = 7.9\text{Hz}$ , 2H), 7.48 (t,  $J = 7.4\text{Hz}$ , 1H), 7.36~7.33 (m, 3H), 7.29~7.25 (m, 3H), 7.07 (t,  $J = 7.1\text{Hz}$ , 1H), 7.02 (s, 1H), 6.94 (t,  $J = 7.7\text{Hz}$ , 2H), 1.58 (s, 9H);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  7.16~7.15 (m, 3H), 6.21 (s, 1H), 1.56 (s, 9H), (remaining peaks merging with major isomer);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.5, 170.6, 146.3, 143.5, 138.9, 138.6, 132.7, 130.1, 128.7, 128.4, 127.9, 127.2, 127.2, 126.4, 126.1, 121.3, 60.9, 28.8; ESI-MS ( $\text{M}+\text{Na}$ ) calcd. for  $\text{C}_{24}\text{H}_{23}\text{NNaO}_2\text{S}$ : 412.1347; Found: 412.1346.

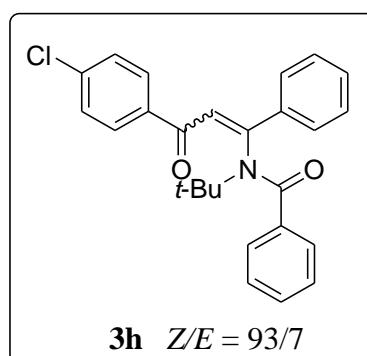
**Spectral data for *N*-*tert*-butyl-*N*-(3-(4-fluorophenyl)-3-oxo-1-phenylprop-1-enyl) benzamide (3g)**



Yellow oil; (20% ethylacetate/hexane,  $R_f = 0.38$ , 48 mg, 0.12 mmol, 68%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $Z/E = 93/7$  major isomer:  $\delta$  7.72~7.70 (m, 2H), 7.50~7.46 (m, 5H),

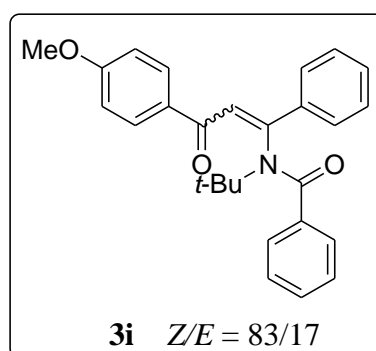
7.27 (d,  $J = 8.2\text{Hz}$ , 2H), 7.03 (t,  $J = 7.6\text{Hz}$ , 1H), 6.96~6.93 (m, 3H), 6.89 (t,  $J = 7.6\text{Hz}$ , 2H), 1.54 (s, 9H);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  7.11 (t,  $J = 7.9\text{Hz}$ , 2H), 6.71 (t,  $J = 8.5\text{Hz}$ , 2H), 1.53 (s, 9H), (remaining peaks merging with major isomer);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.9, 170.4, 166.3, 164.6, 152.0, 140.3, 138.6, 134.7, 130.5, 129.0, 127.7, 127.3, 126.5, 122.9, 115.4, 115.3, 61.2, 28.8; ESI-MS ( $\text{M}+\text{Na}$ ) calcd. for  $\text{C}_{26}\text{H}_{24}\text{FNNaO}_2$ : 424.1689; Found: 424.1682.

**Spectral data for *N-tert-butyl-N-(3-(4-chlorophenyl)-3-oxo-1-phenylprop-1-enyl)benzamide (3h)***



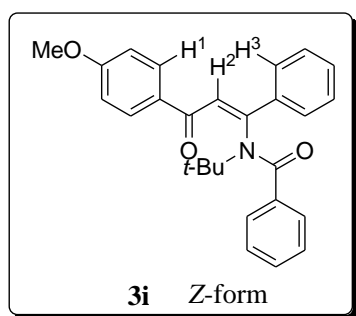
Yellow oil; (20% ethylacetate/hexane,  $R_f = 0.37$ , 47 mg, 0.11 mmol, 67%);  $^1\text{H}$  NMR (700 MHz,  $\text{CDCl}_3$ )  $Z/E = 93/7$  major isomer:  $\delta$  7.71 (d,  $J = 5.6\text{Hz}$ , 2H), 7.49~7.46 (m, 3H), 7.40 (d,  $J = 8.4\text{Hz}$ , 2H), 7.28~7.23 (m, 4H), 7.05 (t,  $J = 7.7\text{Hz}$ , 1H), 6.92 (s, 1H), 6.90 (t,  $J = 7.7\text{Hz}$ , 2H), 1.54 (s, 9H);  $^1\text{H}$  NMR (700 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  7.78 (d,  $J = 7.0\text{Hz}$ , 2H), 7.44~7.43 (m, 3H), 7.12 (t,  $J = 4.2\text{Hz}$ , 1H), 7.00 (d,  $J = 7.0\text{Hz}$ , 2H), 6.24 (s, 1H), 1.52 (s, 9H), (remaining peaks merging with major isomer);  $^{13}\text{C}$  NMR (175 MHz,  $\text{CDCl}_3$ ):  $\delta$  187.2, 170.4, 152.4, 140.2, 139.1, 138.6, 136.7, 130.6, 129.3, 129.1, 128.8, 128.6, 127.7, 127.4, 126.5, 122.6, 61.3, 28.9; ESI-MS ( $\text{M}+\text{H}$ ) calcd. for  $\text{C}_{26}\text{H}_{25}\text{ClNO}_2$ : 418.1574; Found: 418.15716.

**Spectral data for *N-tert-butyl-N-(3-(4-methoxyphenyl)-3-oxo-1-phenylprop-1-enyl)benzamide (3i)***

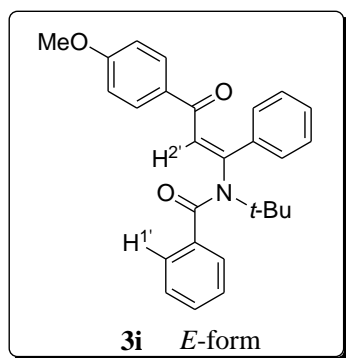


Yellow oil; (20% ethylacetate/hexane,  $R_f = 0.18$ , 67 mg, 0.16 mmol, 95%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $Z/E = 83/17$  major isomer:  $\delta$  7.69~7.68 (m, 2H), 7.51 (d,  $J = 8.8\text{Hz}$ , 2H), 7.46~7.44 (m, 3H), 7.29 (d,  $J = 8.2\text{Hz}$ , 2H), 7.03~7.00 (m, 2H), 6.88 (t,  $J = 7.6\text{Hz}$ , 2H), 6.77 (d,  $J = 8.9\text{Hz}$ , 2H), 3.82 (s, 3H), 1.55 (s, 9H);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  8.07 (d,  $J = 8.3\text{Hz}$ , 2H), 7.43~7.41 (m, 3H), 7.17~7.15 (m, 1H), 7.13~7.09 (m, 2H), 6.56 (d,  $J = 9\text{Hz}$ , 2H), 6.26 (s, 1H), 3.74 (s, 3H), 1.55 (s, 9H), (remaining peaks merging with major isomer);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) major isomer:  $\delta$  187.1, 170.6, 163.3, 150.8, 140.4, 138.8, 140.4, 138.8, 133.5, 131.5, 129.4, 128.7, 128.4, 128.1, 127.2, 126.4, 123.3, 113.5, 61.1, 55.4, 28.8;  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  131.3, 131.0, 130.3, 130.2, 129.0, 128.9, 128.5, 128.1, 127.6, 126.7, 60.5, 55.3, 28.9, (remaining peaks merging with major isomer); ESI-MS ( $M+\text{Na}$ ) calcd. for  $\text{C}_{27}\text{H}_{27}\text{NNaO}_3$ : 436.1889; Found: 436.1892.

### $^1\text{H}$ NOE Data of compound (3i)

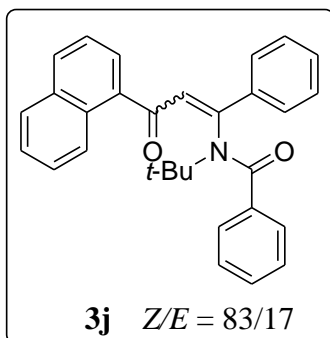


Irradiation	Intensity Increases
$\text{H}^2$ ( $\delta$ 7.00)	$\text{H}^1$ ( $\delta$ 7.51, 7.2%), $\text{H}^3$ ( $\delta$ 7.68, 6.8%)



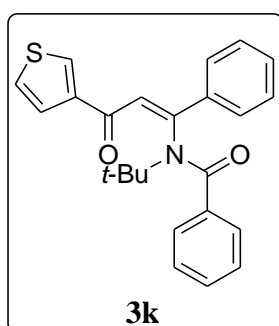
Irradiation	Intensity Increases
$\text{H}^{2'}$ ( $\delta$ 6.26)	$\text{H}^{1'}$ ( $\delta$ 7.10, 3.6%)

### Spectral data for *N*-tert-butyl-*N*-(3-(naphthalen-1-yl)-3-oxo-1-phenylprop-1-enyl)benzamide (3j)



Yellow oil; (20% ethylacetate/hexane,  $R_f = 0.28$ , 60 mg, 0.14 mmol, 87%);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $Z/E = 83/17$  major isomer:  $\delta$  8.08 (dd,  $J = 8.0\text{Hz}$  &  $0.9\text{Hz}$ , 1H), 7.98 (d,  $J = 8.2\text{Hz}$ , 1H), 7.87 (d,  $J = 8.2\text{Hz}$ , 1H), 7.82 (d,  $J = 8.3\text{Hz}$ , 1H), 7.75~7.73 (m, 2H), 7.48~7.44 (m, 6H), 7.27 (t,  $J = 7.7\text{Hz}$ , 1H), 7.19 (t,  $J = 7.4\text{Hz}$ , 1H), 7.04 (t,  $J = 7.8\text{Hz}$ , 3H), 6.92 (s, 1H), 1.60 (s, 9H);  $^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  8.61 (d,  $J = 8.6\text{Hz}$ , 1H), 7.69 (t,  $J = 7.4\text{Hz}$ , 2H), 7.58~7.56 (m, 2H), 7.33 (d,  $J = 1.7\text{Hz}$ , 2H), 7.00~6.97 (m, 2H), 6.89 (td,  $J = 8.0\text{Hz}$  &  $1.8\text{Hz}$ , 3H), 6.40 (s, 1H), 6.38 (dd,  $J = 7.3\text{Hz}$  &  $1.1\text{Hz}$ , 1H), 1.54 (s, 9H), (remaining peaks merging with major isomer);  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ) major isomer:  $\delta$  191.0, 170.7, 151.8, 140.4, 137.6, 133.7, 132.1, 130.7, 130.1, 130.0, 129.0, 128.9, 128.4, 127.9, 127.6, 127.5, 127.3, 126.8, 126.3, 125.4, 125.4, 124.3, 61.6, 29.3;  $^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  195.6, 172.0, 149.7, 139.6, 137.3, 134.4, 133.6, 133.2, 132.8, 129.6, 129.1, 128.8, 128.4, 128.3, 128.1, 127.8, 126.7, 126.3, 123.8, 60.7, 29.0, (remaining peaks merging with major isomer); ESI-MS ( $M+\text{Na}$ ) calcd. for  $\text{C}_{30}\text{H}_{27}\text{NNaO}_2$ : 456.1939; Found: 456.1937.

**Spectral data for *N*-tert-butyl-*N*-((*Z*)-3-oxo-1-phenyl-3-(thiophen-3-yl)prop-1-enyl)benzamide (3k)**

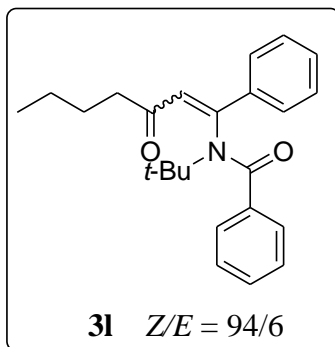


Yellow oil; (20% ethylacetate/hexane,  $R_f = 0.25$ , 47 mg, 0.12 mmol, 65%);  $^1\text{H NMR}$  (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.71~7.70 (m, 2H), 7.54 (d,  $J = 1.7\text{Hz}$ , 1H), 7.47~7.46 (m, 3H), 7.36 (dd,  $J = 5.2\text{Hz}$  &  $1.4\text{Hz}$ , 1H), 7.29 (d,  $J = 7.8\text{Hz}$ , 2H), 7.20 (dd,  $J = 5.1\text{Hz}$  &



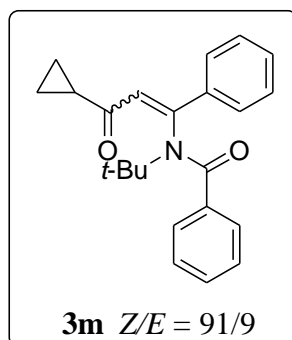
2.8Hz, 1H), 7.02 (t,  $J = 7.4\text{Hz}$ , 1H), 6.90~6.88 (m, 3H), 1.54 (s, 9H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  182.2, 170.6, 151.3, 143.6, 140.3, 138.6, 131.4, 130.5, 129.0, 128.7, 127.7, 127.1, 126.9, 126.5, 126.1, 123.4, 61.2, 28.9; ESI-MS ( $\text{M}+\text{Na}$ ) calcd. for  $\text{C}_{24}\text{H}_{23}\text{NNaO}_2\text{S}$ : 412.1347; Found: 412.1341.

**Spectral data for *N*-tert-butyl-*N*-(3-oxo-1-phenylhept-1-enyl)benzamide (3l)**



Yellow oil; (20% ethylacetate/hexane,  $R_f = 0.30$ , 22 mg, 0.06 mmol, 30%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $Z/E = 94/6$  major isomer:  $\delta$  7.68~7.67 (m, 2H), 7.45~7.44 (m, 3H), 7.35 (d,  $J = 7.8\text{Hz}$ , 2H), 7.17 (t,  $J = 7.4\text{Hz}$ , 1H), 7.07 (t,  $J = 7.7\text{Hz}$ , 2H), 6.33 (s, 1H), 2.18~2.12 (m, 1H), 1.85~1.80 (m, 1H), 1.47 (s, 9H), 1.38~1.32 (m, 2H), 1.19~1.15 (m, 2H), 0.82 (t,  $J = 7.3\text{Hz}$ , 3H);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  7.70~7.69 (m, 2H), 7.40~7.38 (m, 2H), 5.78 (s, 1H), 1.45 (s, 9H), (remaining peaks merging with major isomer);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  197.7, 170.5, 149.5, 140.2, 138.8, 130.4, 128.9, 128.8, 127.7, 127.2, 126.7, 124.6, 61.1, 44.3, 29.0, 25.7, 22.2, 13.8; ESI-MS ( $\text{M}+\text{H}$ ) calcd. for  $\text{C}_{24}\text{H}_{30}\text{NO}_2$ : 364.2277; Found: 364.22775.

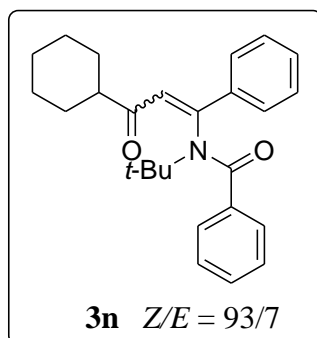
**Spectral data for *N*-tert-butyl-*N*-(3-cyclopropyl-3-oxo-1-phenylprop-1-enyl)benzamide (3m)**



Yellow solid, mp:  $145.5^\circ\text{C}$ ; (20% ethylacetate/hexane,  $R_f = 0.32$ , 63 mg, 0.18 mmol, 82%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ )  $Z/E = 91/9$  major isomer:  $\delta$  7.69~7.68 (m, 2H), 7.45~7.43 (m, 3H), 7.35~7.33 (m, 2H), 7.19~7.15 (m, 1H), 7.07 (d,  $J = 7.9\text{Hz}$ , 2H), 6.51 (s, 1H), 1.61~1.57 (m, 1H), 1.46 (s, 9H), 1.00~0.92 (m, 2H), 0.82~0.68 (m, 2H);

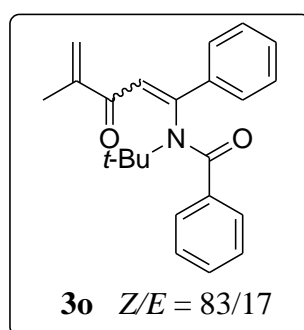
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  7.31~7.30 (m, 3H), 5.85 (s, 1H), 1.51 (s, 9H), 0.46~0.44 (m, 3H), (remaining peaks merging with major isomer);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  197.4, 170.7, 148.9, 140.1, 138.7, 130.4, 128.9, 128.8, 127.8, 127.1, 126.7, 125.1, 61.1, 29.0, 22.7, 11.5, 11.4; ESI-MS ( $\text{M}+\text{H}$ ) calcd. for  $\text{C}_{23}\text{H}_{26}\text{NO}_2$ : 348.1964; Found: 348.19631.

**Spectral data for *N*-tert-butyl-*N*-(3-cyclohexyl-3-oxo-1-phenylprop-1-enyl) benzamide (3n)**



Orange oil; (20% ethylacetate/hexane,  $R_f = 0.40$ , 38 mg, 0.10 mmol, 53%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $Z/E = 93/7$  major isomer:  $\delta$  7.70~7.68 (m, 2H), 7.45~7.44 (m, 3H), 7.36 (d,  $J = 7.6\text{Hz}$ , 2H), 7.17 (t,  $J = 7.5\text{Hz}$ , 1H), 7.05 (t,  $J = 7.7\text{Hz}$ , 2H), 6.45 (s, 1H), 1.96~1.92 (m, 1H), 1.72~1.69 (m, 2H), 1.64~1.58 (m, 4H), 1.46 (s, 9H), 1.21~1.14 (m, 2H), 1.09 (t,  $J = 9.4\text{Hz}$ , 2H);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  7.40 (d,  $J = 7.6\text{Hz}$ , 2H), 7.19 (s, 2H), 5.82 (s, 1H), 1.42 (s, 9H), (remaining peaks merging with major isomer);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) major isomer:  $\delta$  200.0, 170.6, 150.5, 140.4, 138.8, 130.4, 128.9, 128.8, 127.8, 127.0, 126.9, 123.3, 61.2, 52.1, 29.2, 28.3, 27.8, 25.8, 25.7, 25.6;  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  131.1, 129.3, 128.5, 128.0, 126.7, 126.3, 28.9, (remaining peaks merging with major isomer); ESI-MS ( $\text{M}+\text{Na}$ ) calcd. for  $\text{C}_{26}\text{H}_{31}\text{NNaO}_2$ : 412.2252; Found: 412.2250.

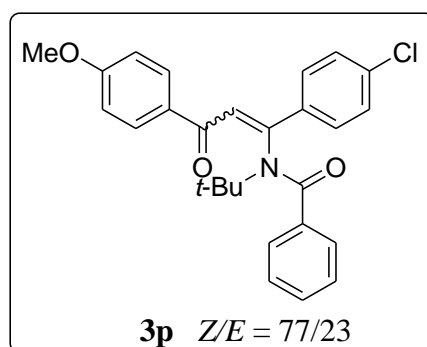
**Spectral data for *N*-tert-butyl-*N*-(4-methyl-3-oxo-1-phenylpenta-1,4-dienyl) benzamide (3o)**



Yellow oil; (20% ethylacetate/hexane,  $R_f = 0.32$ , 21 mg, 0.06 mmol, 28%);  $^1\text{H}$  NMR

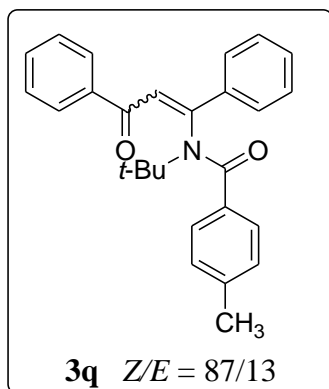
(500 MHz, CDCl<sub>3</sub>) *Z/E* = 83/17 major isomer:  $\delta$  7.66~7.63 (m, 2H), 7.45~7.43 (m, 3H), 7.33~7.31 (m, 2H), 7.12 (t, *J* = 7.5Hz, 1H), 7.03 (t, *J* = 7.7Hz, 2H), 6.79 (s, 1H), 5.41 (s, 1H), 5.28 (s, 1H), 1.77 (s, 3H), 1.50 (s, 9H); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) minor isomer:  $\delta$  7.69 (d, *J* = 7.8Hz, 2H), 7.39 (t, *J* = 7.7Hz, 3H), 6.07 (s, 1H), 5.23 (s, 1H), 4.68 (s, 1H), 1.66 (s, 3H), 1.51 (s, 9H), (remaining peaks merging with major isomer); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) major isomer:  $\delta$  189.9, 170.5, 150.4, 145.7, 140.4, 138.8, 130.2, 128.9, 128.7, 127.6, 127.3, 126.6, 124.1, 122.4, 61.0, 28.8, 17.5; <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) minor isomer:  $\delta$  195.6, 171.8, 147.4, 144.2, 139.4, 138.0, 131.0, 130.7, 129.5, 128.8, 128.5, 128.2, 128.1, 126.5, 60.4, 29.0, 17.0; ESI-MS (M+H) calcd. for C<sub>23</sub>H<sub>26</sub>NO<sub>2</sub>: 348.1964; Found: 348.1958.

**Spectral data for *N-tert-butyl-N-(1-(4-chlorophenyl)-3-(4-methoxyphenyl)-3-oxoprop-1-enyl)benzamide (3p)***



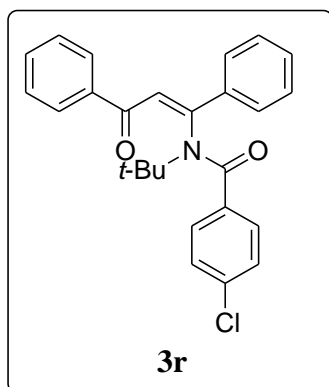
Yellow oil; (20% ethylacetate/hexane, *R<sub>f</sub>* = 0.20, 66 mg, 0.14 mmol, 97%); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) *Z/E* = 77/23 major isomer:  $\delta$  8.08 (d, *J* = 7.3Hz, 1H), 7.61 (d, *J* = 8.6Hz, 2H), 7.51 (d, *J* = 8.6Hz, 1H), 7.43 (t, *J* = 6.8Hz, 2H), 7.25 (d, *J* = 7.5Hz, 2H), 7.23 (t, *J* = 7.4Hz, 1H), 6.97 (s, 1H), 6.89 (t, *J* = 7.7Hz, 2H), 6.78 (d, *J* = 8.8Hz, 2H), 3.82 (s, 3H), 1.54 (s, 9H); <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) minor isomer:  $\delta$  7.57 (t, *J* = 7.5Hz, 2H), 7.45~7.44 (m, 2H), 7.39~7.38 (m, 2H), 7.20 (d, *J* = 8.6Hz, 2H), 7.13 (d, *J* = 8.8Hz, 2H), 7.10 (d, *J* = 8.6Hz, 1H), 6.60 (d, *J* = 8.8Hz, 2H), 6.30 (s, 1H), 3.76 (s, 3H), 1.54 (s, 9H); <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) major isomer:  $\delta$  186.9, 170.7, 163.3, 149.6, 138.8, 136.3, 133.5, 131.2, 130.3, 129.2, 128.7, 128.4, 127.3, 126.3, 123.4, 113.5, 61.2, 55.4, 28.8; <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>) minor isomer;  $\delta$  191.6, 171.2, 163.6, 146.0, 138.5, 131.2, 131.1, 130.1, 129.5, 128.8, 128.7, 128.4, 128.2, 126.6, 113.6, 60.6, 55.4, 28.9, (remaining peaks merging with major isomer); ESI-MS (M+Na) calcd. for C<sub>27</sub>H<sub>26</sub>ClNNO<sub>3</sub>: 470.1499; Found: 470.1498.

**Spectral data for *N-tert-butyl-4-methyl-N-(3-oxo-1,3-diphenylprop-1-enyl)benzamide (3q)***



Yellow oil; (20% ethylacetate/hexane,  $R_f$  = 0.29, 17 mg, 0.04 mmol, 23%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) *Z/E* = 87/13 major isomer:  $\delta$  7.72~7.71 (m, 2H), 7.49~7.45 (m, 6H), 7.28 (t,  $J$  = 7.5Hz, 2H), 7.18 (d,  $J$  = 8.2Hz, 2H), 7.01 (s, 1H), 6.67 (d,  $J$  = 8.0Hz, 2H), 2.09 (s, 3H), 1.54 (s, 9H);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) minor isomer:  $\delta$  6.29 (s, 1H), 2.25 (s, 3H), 1.53 (s, 9H), (remaining peaks merging with major isomer);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.4, 170.7, 151.7, 140.5, 138.6, 138.4, 135.8, 132.6, 130.4, 129.0, 128.1, 128.1, 127.9, 127.7, 126.6, 123.2, 61.1, 28.9, 21.1; ESI-MS (M+H) calcd. for  $\text{C}_{27}\text{H}_{28}\text{NO}_2$ : 398.2120; Found: 398.21163.

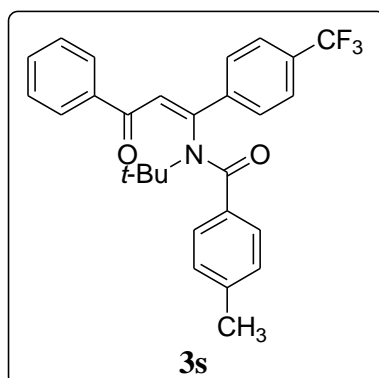
**Spectral data for *N*-tert-butyl-4-chloro-*N*-((*Z*)-3-oxo-1,3-diphenylprop-1-enyl)benzamide (3r)**



Yellow oil; (20% ethylacetate/hexane,  $R_f$  = 0.31, 18 mg, 0.04 mmol, 23%);  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.70~7.69 (m, 2H), 7.54 (d,  $J$  = 7.8Hz, 2H), 7.49~7.47 (m, 3H), 7.34 (t,  $J$  = 8.0Hz, 2H), 7.25~7.23 (m, 3H), 7.07 (s, 1H), 6.85 (d,  $J$  = 8.5Hz, 2H), 1.53 (s, 9H);  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.4, 151.3, 140.1, 138.1, 137.1, 134.8, 133.0, 130.6, 129.1, 128.4, 128.0, 127.9, 127.6, 127.5, 123.1, 61.4, 28.8; ESI-MS (M+H) calcd. for  $\text{C}_{26}\text{H}_{25}\text{ClNO}_2$ : 418.1574; Found: 418.15736.

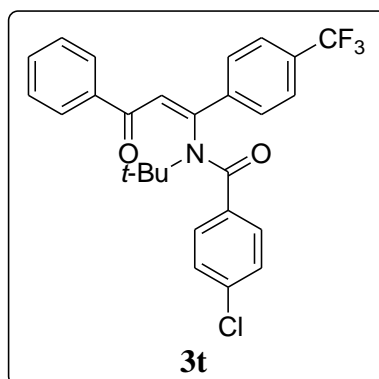
**Spectral data for *N*-tert-butyl-*N*-((*Z*)-1-(4-(trifluoromethyl)phenyl)-3-oxo-3-**

**phenylprop-1-enyl)-4-methylbenzamide (3s)**



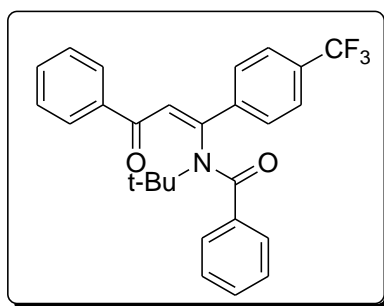
Yellow oil; (20% ethylacetate/hexane,  $R_f = 0.31$ , 20 mg, 0.04 mmol, 29%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.82 (d,  $J = 8.2\text{Hz}$ , 2H), 7.73 (d,  $J = 8.3\text{Hz}$ , 2H), 7.48~7.46 (m, 3H), 7.29 (t,  $J = 7.7\text{Hz}$ , 2H), 7.12 (d,  $J = 8.1\text{Hz}$ , 2H), 7.05 (s, 1H), 6.68 (d,  $J = 7.9\text{Hz}$ , 2H), 2.10 (s, 3H), 1.54 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.2, 170.7, 150.0, 144.1, 138.9, 137.9, 135.4, 132.9, 128.8, 128.4, 128.2, 128.1, 128.0, 127.9, 126.5, 126.0, 125.0, 61.3, 28.9, 21.1; ESI-MS (M+H) calcd. for  $\text{C}_{28}\text{H}_{27}\text{F}_3\text{NO}_2$ : 466.1994; Found: 466.19907.

**Spectral data for *N*-tert-butyl-4-chloro-*N*-((*Z*)-1-(4-(trifluoromethyl)phenyl)-3-oxo-3-phenylprop-1-enyl)benzamide (3t)**



Yellow solid; mp: 186.7°C; (20% ethylacetate/hexane,  $R_f = 0.30$ , 22 mg, 0.05 mmol, 30%);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.81 (d,  $J = 8.3\text{Hz}$ , 2H), 7.74 (d,  $J = 8.4\text{Hz}$ , 2H), 7.53~7.50 (m, 3H), 7.35 (t,  $J = 7.6\text{Hz}$ , 2H), 7.19 (d,  $J = 8.5\text{Hz}$ , 2H), 7.11 (s, 1H), 6.86 (d,  $J = 8.5\text{Hz}$ , 2H), 1.53 (s, 9H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  188.2, 169.5, 149.6, 143.6, 137.7, 136.7, 135.1, 133.3, 132.7, 132.4, 132.1, 131.9, 128.5, 128.0, 127.9, 127.7, 127.7, 126.2, 126.2, 124.9, 61.6, 28.8; ESI-MS (M+H) calcd. for  $\text{C}_{27}\text{H}_{24}\text{ClF}_3\text{NO}_2$ : 486.1448; Found: 486.14469.

**(8) a) X-ray crystallographic structure and data for compound '3a'**



**3a (CCDC 1529471)**

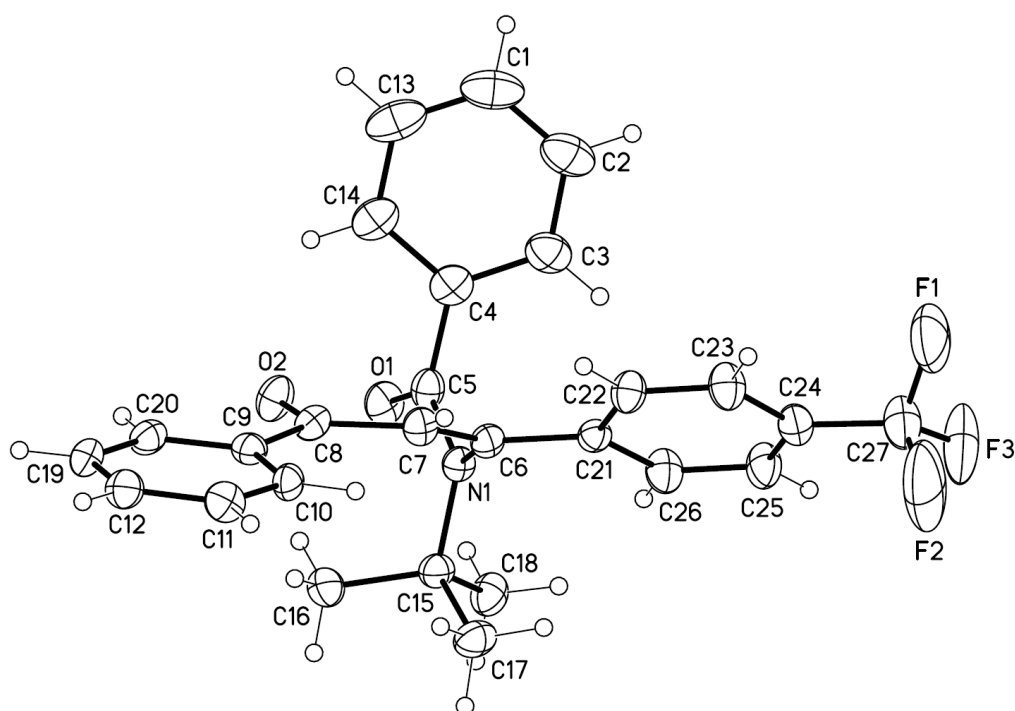


Table 1. Crystal data and structure refinement for 160222lt.

Identification code	160222LT	
Empirical formula	C <sub>27</sub> H <sub>24</sub> F <sub>3</sub> N O <sub>2</sub>	
Formula weight	451.47	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 <sub>1</sub> /c	
Unit cell dimensions	a = 14.9856(13) Å	α = 90°.
	b = 10.6591(8) Å	β = 93.353(4)°.
	c = 14.4299(13) Å	γ = 90°.

Volume	2301.0(3) Å <sup>3</sup>
Z	4
Density (calculated)	1.303 Mg/m <sup>3</sup>
Absorption coefficient	0.098 mm <sup>-1</sup>
F(000)	944
Crystal size	0.15 x 0.08 x 0.02 mm <sup>3</sup>
Theta range for data collection	1.361 to 26.369°.
Index ranges	-18<=h<=18, -13<=k<=13, -18<=l<=10
Reflections collected	17841
Independent reflections	4693 [R(int) = 0.0428]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8372
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4693 / 0 / 301
Goodness-of-fit on F <sup>2</sup>	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0631, wR2 = 0.1869
R indices (all data)	R1 = 0.0947, wR2 = 0.2198
Extinction coefficient	n/a
Largest diff. peak and hole	0.941 and -0.366 e.Å <sup>-3</sup>

Table 2. Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for 160222lt. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	x	y	z	U(eq)
F(1)	10955(2)	1308(2)	4356(2)	86(1)
F(2)	10552(2)	2767(4)	3488(2)	112(1)
F(3)	11244(1)	3182(2)	4757(2)	73(1)
O(1)	6848(1)	3601(2)	8342(1)	31(1)
O(2)	5461(1)	2145(2)	6820(1)	31(1)
N(1)	7093(1)	3556(2)	6789(1)	22(1)
C(1)	8074(3)	-705(3)	8139(2)	47(1)
C(2)	8631(2)	194(3)	7816(2)	44(1)
C(3)	8322(2)	1404(3)	7637(2)	36(1)
C(4)	7434(2)	1702(3)	7777(2)	29(1)
C(5)	7091(2)	3030(3)	7659(2)	26(1)
C(6)	7182(2)	2740(2)	5998(2)	22(1)

C(7)	6483(2)	2086(2)	5627(2)	25(1)
C(8)	5578(2)	2004(2)	5994(2)	25(1)
C(9)	4803(2)	1717(2)	5322(2)	23(1)
C(10)	4894(2)	1615(2)	4371(2)	25(1)
C(11)	4145(2)	1309(2)	3788(2)	30(1)
C(12)	3321(2)	1118(2)	4158(2)	29(1)
C(13)	7196(3)	-415(3)	8295(2)	44(1)
C(14)	6874(2)	799(3)	8123(2)	34(1)
C(15)	6754(2)	4900(2)	6630(2)	25(1)
C(16)	5784(2)	5028(3)	6903(2)	31(1)
C(17)	6791(2)	5239(3)	5606(2)	32(1)
C(18)	7366(2)	5792(3)	7210(2)	32(1)
C(19)	3237(2)	1246(2)	5104(2)	29(1)
C(20)	3968(2)	1540(2)	5685(2)	26(1)
C(21)	8076(2)	2668(2)	5596(2)	22(1)
C(22)	8274(2)	1701(2)	4987(2)	28(1)
C(23)	9097(2)	1622(3)	4615(2)	32(1)
C(24)	9752(2)	2513(3)	4836(2)	30(1)
C(25)	9578(2)	3459(3)	5462(2)	33(1)
C(26)	8748(2)	3531(3)	5836(2)	32(1)
C(27)	10627(2)	2449(3)	4384(2)	42(1)

Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 160222It.

F(1)-C(27)	1.313(4)
F(2)-C(27)	1.335(4)
F(3)-C(27)	1.303(4)
O(1)-C(5)	1.230(3)
O(2)-C(8)	1.224(3)
N(1)-C(5)	1.375(3)
N(1)-C(6)	1.447(3)
N(1)-C(15)	1.533(3)
C(1)-C(2)	1.371(5)
C(1)-C(13)	1.382(5)
C(1)-H(1)	0.9300
C(2)-C(3)	1.390(4)
C(2)-H(21)	0.9300



C(3)-C(4)	1.394(4)
C(3)-H(22)	0.9300
C(4)-C(14)	1.388(4)
C(4)-C(5)	1.512(4)
C(6)-C(7)	1.343(4)
C(6)-C(21)	1.493(3)
C(7)-C(8)	1.486(4)
C(7)-H(16)	0.9300
C(8)-C(9)	1.502(4)
C(9)-C(10)	1.390(4)
C(9)-C(20)	1.396(4)
C(10)-C(11)	1.402(4)
C(10)-H(15)	0.9300
C(11)-C(12)	1.388(4)
C(11)-H(14)	0.9300
C(12)-C(19)	1.385(4)
C(12)-H(2)	0.9300
C(13)-C(14)	1.399(4)
C(13)-H(24)	0.9300
C(14)-H(23)	0.9300
C(15)-C(17)	1.525(4)
C(15)-C(16)	1.534(4)
C(15)-C(18)	1.536(4)
C(16)-H(4)	0.9600
C(16)-H(3)	0.9600
C(16)-H(5)	0.9600
C(17)-H(6)	0.9600
C(17)-H(8)	0.9600
C(17)-H(7)	0.9600
C(18)-H(11)	0.9600
C(18)-H(9)	0.9600
C(18)-H(10)	0.9600
C(19)-C(20)	1.376(4)
C(19)-H(12)	0.9300
C(20)-H(13)	0.9300
C(21)-C(26)	1.393(4)
C(21)-C(22)	1.399(4)
C(22)-C(23)	1.375(4)

C(22)-H(17)	0.9300
C(23)-C(24)	1.389(4)
C(23)-H(20)	0.9300
C(24)-C(25)	1.389(4)
C(24)-C(27)	1.499(4)
C(25)-C(26)	1.387(4)
C(25)-H(19)	0.9300
C(26)-H(18)	0.9300

C(5)-N(1)-C(6)	118.7(2)
C(5)-N(1)-C(15)	120.0(2)
C(6)-N(1)-C(15)	119.21(18)
C(2)-C(1)-C(13)	120.2(3)
C(2)-C(1)-H(1)	119.9
C(13)-C(1)-H(1)	119.9
C(1)-C(2)-C(3)	120.6(3)
C(1)-C(2)-H(21)	119.7
C(3)-C(2)-H(21)	119.7
C(2)-C(3)-C(4)	119.7(3)
C(2)-C(3)-H(22)	120.1
C(4)-C(3)-H(22)	120.1
C(14)-C(4)-C(3)	119.7(3)
C(14)-C(4)-C(5)	118.7(3)
C(3)-C(4)-C(5)	121.2(2)
O(1)-C(5)-N(1)	123.1(2)
O(1)-C(5)-C(4)	119.2(2)
N(1)-C(5)-C(4)	117.7(2)
C(7)-C(6)-N(1)	121.4(2)
C(7)-C(6)-C(21)	121.0(2)
N(1)-C(6)-C(21)	117.6(2)
C(6)-C(7)-C(8)	126.5(2)
C(6)-C(7)-H(16)	116.8
C(8)-C(7)-H(16)	116.8
O(2)-C(8)-C(7)	121.7(2)
O(2)-C(8)-C(9)	120.3(2)
C(7)-C(8)-C(9)	118.0(2)
C(10)-C(9)-C(20)	120.1(2)
C(10)-C(9)-C(8)	122.4(2)

C(20)-C(9)-C(8)	117.5(2)
C(9)-C(10)-C(11)	119.2(2)
C(9)-C(10)-H(15)	120.4
C(11)-C(10)-H(15)	120.4
C(12)-C(11)-C(10)	120.2(2)
C(12)-C(11)-H(14)	119.9
C(10)-C(11)-H(14)	119.9
C(19)-C(12)-C(11)	119.8(2)
C(19)-C(12)-H(2)	120.1
C(11)-C(12)-H(2)	120.1
C(1)-C(13)-C(14)	120.0(3)
C(1)-C(13)-H(24)	120.0
C(14)-C(13)-H(24)	120.0
C(4)-C(14)-C(13)	119.7(3)
C(4)-C(14)-H(23)	120.1
C(13)-C(14)-H(23)	120.1
C(17)-C(15)-N(1)	109.7(2)
C(17)-C(15)-C(16)	108.5(2)
N(1)-C(15)-C(16)	110.8(2)
C(17)-C(15)-C(18)	109.1(2)
N(1)-C(15)-C(18)	108.4(2)
C(16)-C(15)-C(18)	110.4(2)
C(15)-C(16)-H(4)	109.5
C(15)-C(16)-H(3)	109.5
H(4)-C(16)-H(3)	109.5
C(15)-C(16)-H(5)	109.5
H(4)-C(16)-H(5)	109.5
H(3)-C(16)-H(5)	109.5
C(15)-C(17)-H(6)	109.5
C(15)-C(17)-H(8)	109.5
H(6)-C(17)-H(8)	109.5
C(15)-C(17)-H(7)	109.5
H(6)-C(17)-H(7)	109.5
H(8)-C(17)-H(7)	109.5
C(15)-C(18)-H(11)	109.5
C(15)-C(18)-H(9)	109.5
H(11)-C(18)-H(9)	109.5
C(15)-C(18)-H(10)	109.5

H(11)-C(18)-H(10)	109.5
H(9)-C(18)-H(10)	109.5
C(20)-C(19)-C(12)	120.5(3)
C(20)-C(19)-H(12)	119.7
C(12)-C(19)-H(12)	119.7
C(19)-C(20)-C(9)	120.1(2)
C(19)-C(20)-H(13)	120.0
C(9)-C(20)-H(13)	120.0
C(26)-C(21)-C(22)	117.7(2)
C(26)-C(21)-C(6)	121.5(2)
C(22)-C(21)-C(6)	120.8(2)
C(23)-C(22)-C(21)	121.3(2)
C(23)-C(22)-H(17)	119.4
C(21)-C(22)-H(17)	119.4
C(22)-C(23)-C(24)	120.5(2)
C(22)-C(23)-H(20)	119.8
C(24)-C(23)-H(20)	119.8
C(25)-C(24)-C(23)	119.2(3)
C(25)-C(24)-C(27)	121.2(2)
C(23)-C(24)-C(27)	119.6(2)
C(26)-C(25)-C(24)	120.0(2)
C(26)-C(25)-H(19)	120.0
C(24)-C(25)-H(19)	120.0
C(25)-C(26)-C(21)	121.3(2)
C(25)-C(26)-H(18)	119.4
C(21)-C(26)-H(18)	119.4
F(3)-C(27)-F(1)	108.0(3)
F(3)-C(27)-F(2)	105.4(3)
F(1)-C(27)-F(2)	102.5(3)
F(3)-C(27)-C(24)	114.2(3)
F(1)-C(27)-C(24)	113.2(3)
F(2)-C(27)-C(24)	112.6(3)

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 160222It. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

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	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
F(1)	48(1)	58(1)	159(3)	-15(2)	52(2)	3(1)
F(2)	45(1)	231(4)	61(2)	37(2)	24(1)	12(2)
F(3)	35(1)	86(2)	101(2)	-40(1)	30(1)	-22(1)
O(1)	33(1)	40(1)	20(1)	-1(1)	6(1)	3(1)
O(2)	32(1)	40(1)	22(1)	-1(1)	5(1)	-8(1)
N(1)	22(1)	25(1)	19(1)	0(1)	2(1)	-1(1)
C(1)	75(3)	34(2)	31(2)	1(1)	-9(2)	10(2)
C(2)	53(2)	47(2)	33(2)	3(1)	-4(2)	16(2)
C(3)	40(2)	40(2)	27(1)	4(1)	-1(1)	6(1)
C(4)	36(2)	36(2)	14(1)	1(1)	-2(1)	-1(1)
C(5)	23(1)	34(1)	21(1)	-1(1)	3(1)	-2(1)
C(6)	24(1)	26(1)	17(1)	3(1)	3(1)	0(1)
C(7)	25(1)	31(1)	19(1)	0(1)	2(1)	0(1)
C(8)	28(1)	23(1)	23(1)	1(1)	4(1)	-3(1)
C(9)	25(1)	19(1)	26(1)	1(1)	2(1)	1(1)
C(10)	22(1)	25(1)	27(1)	-1(1)	8(1)	0(1)
C(11)	33(2)	32(1)	25(1)	-3(1)	3(1)	2(1)
C(12)	28(1)	28(1)	31(1)	-1(1)	-2(1)	-3(1)
C(13)	74(2)	36(2)	23(1)	4(1)	-5(2)	-11(2)
C(14)	45(2)	38(2)	19(1)	2(1)	1(1)	-6(1)
C(15)	28(1)	23(1)	24(1)	1(1)	6(1)	2(1)
C(16)	29(1)	31(1)	32(1)	2(1)	6(1)	4(1)
C(17)	41(2)	29(1)	26(1)	4(1)	8(1)	1(1)
C(18)	32(2)	30(1)	34(2)	-5(1)	10(1)	-3(1)
C(19)	24(1)	29(1)	34(2)	4(1)	4(1)	-5(1)
C(20)	31(1)	25(1)	24(1)	3(1)	6(1)	-1(1)
C(21)	22(1)	23(1)	21(1)	2(1)	0(1)	-1(1)
C(22)	25(1)	30(1)	29(1)	-5(1)	2(1)	-6(1)
C(23)	28(1)	36(2)	32(2)	-11(1)	6(1)	-1(1)
C(24)	24(1)	34(2)	32(2)	0(1)	3(1)	1(1)
C(25)	24(1)	33(2)	43(2)	-7(1)	3(1)	-6(1)
C(26)	28(2)	30(1)	36(2)	-10(1)	5(1)	-2(1)
C(27)	28(2)	48(2)	52(2)	-8(2)	7(1)	-3(1)

Table 5. Hydrogen coordinates (  $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ )

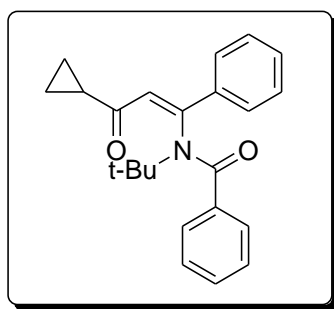
for 160222It.

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	x	y	z	U(eq)
H(1)	8287	-1513	8254	56
H(21)	9222	-8	7715	53
H(22)	8705	2012	7425	43
H(16)	6574	1640	5087	30
H(15)	5446	1749	4125	30
H(14)	4200	1233	3152	36
H(2)	2826	905	3771	35
H(24)	6820	-1027	8515	53
H(23)	6287	1001	8239	41
H(4)	5604	5891	6854	46
H(3)	5740	4748	7531	46
H(5)	5402	4526	6496	46
H(6)	6391	4706	5242	48
H(8)	7390	5126	5417	48
H(7)	6617	6099	5516	48
H(11)	7966	5724	7016	48
H(9)	7356	5572	7855	48
H(10)	7160	6639	7123	48
H(12)	2683	1131	5349	34
H(13)	3907	1621	6319	32
H(17)	7842	1100	4830	33
H(20)	9215	969	4214	38
H(19)	10019	4043	5631	40
H(18)	8638	4168	6255	38

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**b) X-ray crystallographic structure and data for compound '3m'**



**3m (CCDC 1529472)**

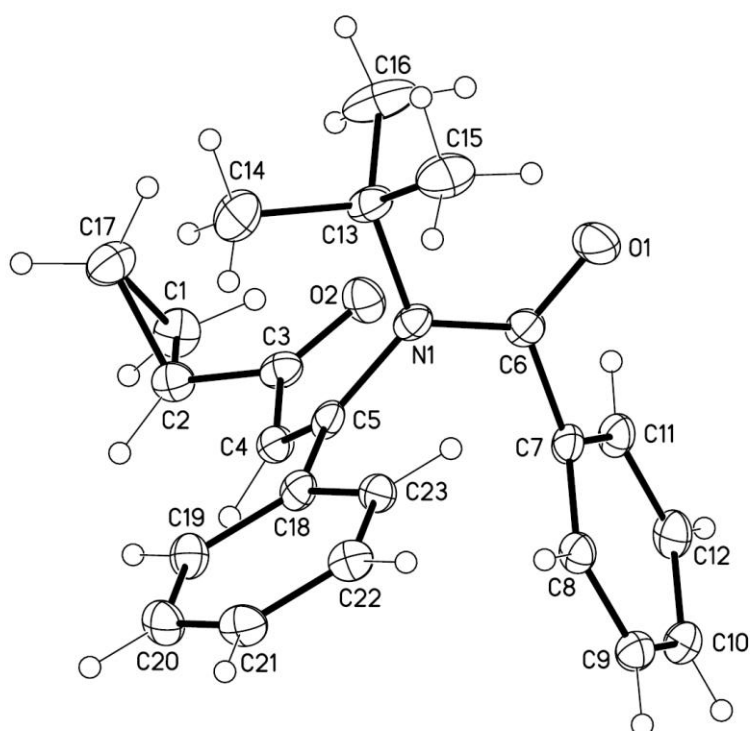


Table 1. Crystal data and structure refinement for 160947LT\_0M.

Identification code	160947lt_0m	
Empirical formula	C <sub>23</sub> H <sub>25</sub> N O <sub>2</sub>	
Formula weight	347.44	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.7947(6) Å	$\alpha = 77.035(2)^\circ$ .
	b = 10.1593(6) Å	$\beta = 75.489(3)^\circ$ .

	$c = 10.2676(6) \text{ \AA}$	$\gamma = 71.193(2)^\circ$ .
Volume	$924.74(10) \text{ \AA}^3$	
Z	2	
Density (calculated)	$1.248 \text{ Mg/m}^3$	
Absorption coefficient	$0.079 \text{ mm}^{-1}$	
F(000)	372	
Crystal size	$0.08 \times 0.05 \times 0.02 \text{ mm}^3$	
Theta range for data collection	$2.074 \text{ to } 26.365^\circ$ .	
Index ranges	$-12 \leq h \leq 12, -12 \leq k \leq 11, -12 \leq l \leq 12$	
Reflections collected	14156	
Independent reflections	3785 [R(int) = 0.0225]	
Completeness to theta = $25.242^\circ$	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8903	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3785 / 0 / 238	
Goodness-of-fit on F <sup>2</sup>	1.120	
Final R indices [I > 2sigma(I)]	R1 = 0.0482, wR2 = 0.1386	
R indices (all data)	R1 = 0.0577, wR2 = 0.1604	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.494 and $-0.368 \text{ e.\AA}^{-3}$	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 160947LT\_0M. U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
O(1)	1328(1)	1400(2)	1501(1)	32(1)
O(2)	1757(1)	4723(1)	1313(1)	24(1)
N(1)	2068(1)	2054(1)	3129(1)	18(1)
C(1)	2163(2)	7515(2)	934(2)	26(1)
C(2)	2165(2)	6477(2)	2234(2)	21(1)
C(3)	1773(2)	5156(2)	2328(2)	19(1)
C(4)	1502(2)	4388(2)	3733(2)	19(1)
C(5)	1717(2)	2988(2)	4109(2)	18(1)
C(6)	1045(2)	2089(2)	2418(2)	20(1)
C(7)	-530(2)	2955(2)	2799(2)	18(1)
C(8)	-1395(2)	2741(2)	4087(2)	19(1)



C(9)	-2893(2)	3412(2)	4311(2)	22(1)
C(10)	-3543(2)	4315(2)	3260(2)	23(1)
C(11)	-1188(2)	3851(2)	1744(2)	21(1)
C(12)	-2679(2)	4532(2)	1977(2)	24(1)
C(13)	3658(2)	1196(2)	2720(2)	22(1)
C(14)	4614(2)	1483(3)	3530(3)	44(1)
C(15)	3760(2)	-365(2)	3020(2)	34(1)
C(16)	4235(2)	1634(3)	1207(2)	42(1)
C(17)	3589(2)	6601(2)	1261(2)	29(1)
C(18)	1646(2)	2321(2)	5559(2)	18(1)
C(19)	1842(2)	2991(2)	6533(2)	22(1)
C(20)	1754(2)	2364(2)	7888(2)	25(1)
C(21)	1485(2)	1069(2)	8308(2)	24(1)
C(22)	1301(2)	383(2)	7364(2)	22(1)
C(23)	1388(2)	1002(2)	6001(2)	18(1)

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Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 160947LT\_0M.

O(1)-C(6)	1.222(2)
O(2)-C(3)	1.224(2)
N(1)-C(6)	1.367(2)
N(1)-C(5)	1.440(2)
N(1)-C(13)	1.525(2)
C(1)-C(17)	1.477(3)
C(1)-C(2)	1.504(2)
C(1)-H(26)	0.9900
C(1)-H(25)	0.9900
C(2)-C(3)	1.487(2)
C(2)-C(17)	1.522(2)
C(2)-H(17)	1.0000
C(3)-C(4)	1.483(2)
C(4)-C(5)	1.349(2)
C(4)-H(18)	0.9500
C(5)-C(18)	1.486(2)
C(6)-C(7)	1.511(2)
C(7)-C(8)	1.394(2)
C(7)-C(11)	1.396(2)

C(8)-C(9)	1.387(2)
C(8)-H(3)	0.9500
C(9)-C(10)	1.391(2)
C(9)-H(24)	0.9500
C(10)-C(12)	1.390(2)
C(10)-H(2)	0.9500
C(11)-C(12)	1.385(2)
C(11)-H(5)	0.9500
C(12)-H(4)	0.9500
C(13)-C(15)	1.521(3)
C(13)-C(14)	1.525(3)
C(13)-C(16)	1.531(2)
C(14)-H(7)	0.9800
C(14)-H(6)	0.9800
C(14)-H(8)	0.9800
C(15)-H(9)	0.9800
C(15)-H(11)	0.9800
C(15)-H(10)	0.9800
C(16)-H(14)	0.9800
C(16)-H(12)	0.9800
C(16)-H(13)	0.9800
C(17)-H(16)	0.9900
C(17)-H(15)	0.9900
C(18)-C(23)	1.397(2)
C(18)-C(19)	1.410(2)
C(19)-C(20)	1.388(2)
C(19)-H(23)	0.9500
C(20)-C(21)	1.378(3)
C(20)-H(22)	0.9500
C(21)-C(22)	1.389(2)
C(21)-H(21)	0.9500
C(22)-C(23)	1.393(2)
C(22)-H(20)	0.9500
C(23)-H(19)	0.9500
C(6)-N(1)-C(5)	120.64(13)
C(6)-N(1)-C(13)	119.48(13)
C(5)-N(1)-C(13)	119.14(12)

C(17)-C(1)-C(2)	61.40(11)
C(17)-C(1)-H(26)	117.6
C(2)-C(1)-H(26)	117.6
C(17)-C(1)-H(25)	117.6
C(2)-C(1)-H(25)	117.6
H(26)-C(1)-H(25)	114.7
C(3)-C(2)-C(1)	120.00(14)
C(3)-C(2)-C(17)	115.83(14)
C(1)-C(2)-C(17)	58.42(12)
C(3)-C(2)-H(17)	116.6
C(1)-C(2)-H(17)	116.6
C(17)-C(2)-H(17)	116.6
O(2)-C(3)-C(4)	123.82(15)
O(2)-C(3)-C(2)	121.92(15)
C(4)-C(3)-C(2)	114.16(13)
C(5)-C(4)-C(3)	126.95(14)
C(5)-C(4)-H(18)	116.5
C(3)-C(4)-H(18)	116.5
C(4)-C(5)-N(1)	122.06(14)
C(4)-C(5)-C(18)	121.51(14)
N(1)-C(5)-C(18)	116.41(13)
O(1)-C(6)-N(1)	122.90(15)
O(1)-C(6)-C(7)	117.05(14)
N(1)-C(6)-C(7)	119.99(14)
C(8)-C(7)-C(11)	119.18(15)
C(8)-C(7)-C(6)	123.08(14)
C(11)-C(7)-C(6)	117.01(14)
C(9)-C(8)-C(7)	120.17(15)
C(9)-C(8)-H(3)	119.9
C(7)-C(8)-H(3)	119.9
C(8)-C(9)-C(10)	120.53(15)
C(8)-C(9)-H(24)	119.7
C(10)-C(9)-H(24)	119.7
C(12)-C(10)-C(9)	119.30(16)
C(12)-C(10)-H(2)	120.4
C(9)-C(10)-H(2)	120.4
C(12)-C(11)-C(7)	120.42(15)
C(12)-C(11)-H(5)	119.8

C(7)-C(11)-H(5)	119.8
C(11)-C(12)-C(10)	120.40(15)
C(11)-C(12)-H(4)	119.8
C(10)-C(12)-H(4)	119.8
C(15)-C(13)-N(1)	109.76(13)
C(15)-C(13)-C(14)	109.24(16)
N(1)-C(13)-C(14)	109.43(14)
C(15)-C(13)-C(16)	110.49(16)
N(1)-C(13)-C(16)	110.15(14)
C(14)-C(13)-C(16)	107.74(17)
C(13)-C(14)-H(7)	109.5
C(13)-C(14)-H(6)	109.5
H(7)-C(14)-H(6)	109.5
C(13)-C(14)-H(8)	109.5
H(7)-C(14)-H(8)	109.5
H(6)-C(14)-H(8)	109.5
C(13)-C(15)-H(9)	109.5
C(13)-C(15)-H(11)	109.5
H(9)-C(15)-H(11)	109.5
C(13)-C(15)-H(10)	109.5
H(9)-C(15)-H(10)	109.5
H(11)-C(15)-H(10)	109.5
C(13)-C(16)-H(14)	109.5
C(13)-C(16)-H(12)	109.5
H(14)-C(16)-H(12)	109.5
C(13)-C(16)-H(13)	109.5
H(14)-C(16)-H(13)	109.5
H(12)-C(16)-H(13)	109.5
C(1)-C(17)-C(2)	60.17(11)
C(1)-C(17)-H(16)	117.8
C(2)-C(17)-H(16)	117.8
C(1)-C(17)-H(15)	117.8
C(2)-C(17)-H(15)	117.8
H(16)-C(17)-H(15)	114.9
C(23)-C(18)-C(19)	117.79(15)
C(23)-C(18)-C(5)	120.96(14)
C(19)-C(18)-C(5)	121.25(15)
C(20)-C(19)-C(18)	120.66(16)

C(20)-C(19)-H(23)	119.7
C(18)-C(19)-H(23)	119.7
C(21)-C(20)-C(19)	120.71(16)
C(21)-C(20)-H(22)	119.6
C(19)-C(20)-H(22)	119.6
C(20)-C(21)-C(22)	119.65(15)
C(20)-C(21)-H(21)	120.2
C(22)-C(21)-H(21)	120.2
C(21)-C(22)-C(23)	120.11(16)
C(21)-C(22)-H(20)	119.9
C(23)-C(22)-H(20)	119.9
C(22)-C(23)-C(18)	121.07(15)
C(22)-C(23)-H(19)	119.5
C(18)-C(23)-H(19)	119.5

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 160947LT\_0M. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
O(1)	24(1)	48(1)	25(1)	-16(1)	-7(1)	-2(1)
O(2)	30(1)	27(1)	17(1)	-1(1)	-7(1)	-9(1)
N(1)	14(1)	24(1)	15(1)	0(1)	-3(1)	-5(1)
C(1)	31(1)	24(1)	22(1)	5(1)	-6(1)	-11(1)
C(2)	22(1)	22(1)	17(1)	-1(1)	-4(1)	-5(1)
C(3)	15(1)	22(1)	18(1)	-1(1)	-4(1)	-2(1)
C(4)	17(1)	24(1)	15(1)	-3(1)	-4(1)	-6(1)
C(5)	13(1)	23(1)	18(1)	-1(1)	-5(1)	-7(1)
C(6)	18(1)	27(1)	13(1)	-1(1)	-3(1)	-7(1)
C(7)	16(1)	24(1)	18(1)	-4(1)	-6(1)	-7(1)
C(8)	21(1)	23(1)	15(1)	-1(1)	-6(1)	-8(1)
C(9)	21(1)	26(1)	19(1)	-4(1)	-3(1)	-9(1)
C(10)	17(1)	28(1)	26(1)	-6(1)	-7(1)	-5(1)
C(11)	22(1)	29(1)	16(1)	-1(1)	-6(1)	-11(1)
C(12)	24(1)	27(1)	22(1)	0(1)	-12(1)	-8(1)
C(13)	14(1)	29(1)	21(1)	-3(1)	-2(1)	-2(1)

C(14)	17(1)	60(1)	61(1)	-29(1)	-12(1)	-1(1)
C(15)	26(1)	30(1)	39(1)	-6(1)	-1(1)	0(1)
C(16)	24(1)	50(1)	30(1)	8(1)	7(1)	-1(1)
C(17)	23(1)	29(1)	33(1)	-4(1)	0(1)	-9(1)
C(18)	16(1)	22(1)	18(1)	-1(1)	-7(1)	-4(1)
C(19)	22(1)	21(1)	24(1)	-2(1)	-9(1)	-6(1)
C(20)	26(1)	31(1)	20(1)	-5(1)	-10(1)	-5(1)
C(21)	24(1)	29(1)	16(1)	0(1)	-6(1)	-4(1)
C(22)	20(1)	22(1)	21(1)	0(1)	-5(1)	-3(1)
C(23)	17(1)	20(1)	18(1)	-3(1)	-6(1)	-3(1)

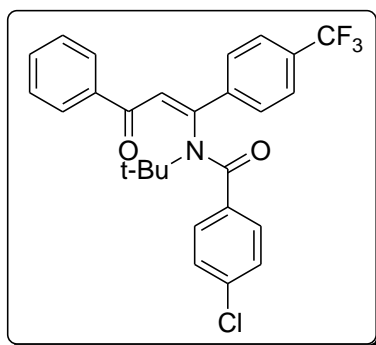
Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 160947LT\_0M.

	x	y	z	U(eq)
H(26)	1823	7317	187	31
H(25)	1903	8525	1008	31
H(17)	1932	6872	3099	25
H(18)	1138	4942	4445	22
H(3)	-959	2135	4814	23
H(24)	-3478	3254	5189	26
H(2)	-4567	4779	3418	28
H(5)	-609	3994	860	26
H(4)	-3114	5152	1255	28
H(7)	4553	2487	3337	67
H(6)	5636	931	3267	67
H(8)	4266	1213	4505	67
H(9)	3473	-648	4004	51
H(11)	4773	-910	2704	51
H(10)	3100	-544	2547	51
H(14)	3687	1395	659	63
H(12)	5281	1137	974	63
H(13)	4105	2652	1020	63
H(16)	4213	7041	1542	35
H(15)	4134	5832	721	35

H(23)	2035	3881	6259	26
H(22)	1881	2833	8534	30
H(21)	1425	648	9237	29
H(20)	1116	-511	7649	26
H(19)	1271	520	5362	22

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c) X-ray crystallographic structure and data for compound '3t'



3t (CCDC 1529475)

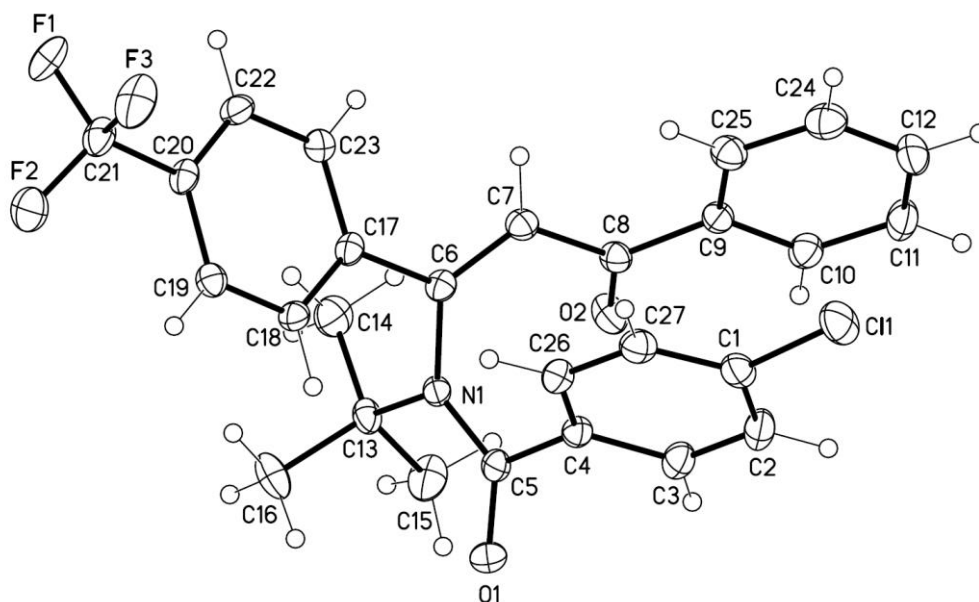


Table 1. Crystal data and structure refinement for 160808lt\_0m.

Identification code	160808LT_0m	
Empirical formula	C <sub>27</sub> H <sub>23</sub> Cl F <sub>3</sub> N O <sub>2</sub>	
Formula weight	485.91	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.3330(4) Å	α = 85.635(2)°.



	$b = 10.1568(4) \text{ \AA}$	$\beta = 69.299(2)^\circ$ .
	$c = 12.9438(5) \text{ \AA}$	$\gamma = 88.318(2)^\circ$ .
Volume	$1144.44(8) \text{ \AA}^3$	
Z	2	
Density (calculated)	1.410 Mg/m <sup>3</sup>	
Absorption coefficient	0.217 mm <sup>-1</sup>	
F(000)	504	
Crystal size	0.20 x 0.18 x 0.15 mm <sup>3</sup>	
Theta range for data collection	1.686 to 26.407°.	
Index ranges	-11<=h<=11, -12<=k<=12, -16<=l<=16	
Reflections collected	19165	
Independent reflections	4667 [R(int) = 0.0240]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8989	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	4667 / 0 / 310	
Goodness-of-fit on F <sup>2</sup>	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0455, wR2 = 0.1212	
R indices (all data)	R1 = 0.0500, wR2 = 0.1282	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.649 and -0.387 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 160808lt\_0m.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Cl(1)	9618(1)	13561(1)	5821(1)	32(1)
F(1)	3589(2)	4406(1)	6215(1)	32(1)
F(2)	1848(1)	5602(1)	7305(1)	34(1)
F(3)	3235(2)	6397(1)	5679(1)	36(1)
O(1)	6474(2)	9664(1)	10468(1)	24(1)
O(2)	10536(2)	8277(1)	8613(1)	25(1)
N(1)	7256(2)	8061(2)	9239(1)	16(1)
C(1)	8765(2)	12405(2)	6923(2)	23(1)
C(2)	9243(2)	12304(2)	7824(2)	25(1)
C(3)	8629(2)	11318(2)	8656(2)	23(1)

C(4)	7565(2)	10422(2)	8586(2)	18(1)
C(5)	7029(2)	9352(2)	9507(2)	18(1)
C(6)	7776(2)	7721(2)	8110(2)	16(1)
C(7)	9205(2)	7952(2)	7403(2)	18(1)
C(8)	10424(2)	8550(2)	7707(2)	18(1)
C(9)	11530(2)	9475(2)	6869(2)	18(1)
C(10)	12643(2)	10064(2)	7171(2)	22(1)
C(11)	13649(2)	10967(2)	6443(2)	26(1)
C(12)	13572(2)	11299(2)	5400(2)	28(1)
C(13)	7022(2)	6928(2)	10128(2)	20(1)
C(14)	7739(3)	5670(2)	9584(2)	27(1)
C(15)	7856(3)	7235(2)	10909(2)	30(1)
C(16)	5309(2)	6720(2)	10761(2)	30(1)
C(17)	6597(2)	7139(2)	7751(1)	16(1)
C(18)	5058(2)	7501(2)	8206(2)	18(1)
C(19)	3974(2)	6989(2)	7836(2)	18(1)
C(20)	4433(2)	6107(2)	7008(2)	18(1)
C(21)	3279(2)	5621(2)	6560(2)	23(1)
C(22)	5951(2)	5717(2)	6564(2)	21(1)
C(23)	7026(2)	6231(2)	6932(2)	19(1)
C(24)	12470(2)	10727(2)	5089(2)	27(1)
C(25)	11452(2)	9815(2)	5828(2)	22(1)
C(26)	7057(2)	10586(2)	7691(2)	21(1)
C(27)	7650(2)	11581(2)	6863(2)	23(1)

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Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 160808lt\_0m.

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Cl(1)-C(1)	1.745(2)
F(1)-C(21)	1.333(2)
F(2)-C(21)	1.342(2)
F(3)-C(21)	1.349(2)
O(1)-C(5)	1.229(2)
O(2)-C(8)	1.224(2)
N(1)-C(5)	1.373(2)
N(1)-C(6)	1.435(2)
N(1)-C(13)	1.527(2)
C(1)-C(27)	1.382(3)

C(1)-C(2)	1.384(3)
C(2)-C(3)	1.387(3)
C(2)-H(23)	0.9500
C(3)-C(4)	1.397(3)
C(3)-H(22)	0.9500
C(4)-C(26)	1.395(3)
C(4)-C(5)	1.506(3)
C(6)-C(7)	1.339(3)
C(6)-C(17)	1.489(2)
C(7)-C(8)	1.487(2)
C(7)-H(15)	0.9500
C(8)-C(9)	1.495(3)
C(9)-C(25)	1.392(3)
C(9)-C(10)	1.396(3)
C(10)-C(11)	1.381(3)
C(10)-H(19)	0.9500
C(11)-C(12)	1.393(3)
C(11)-H(18)	0.9500
C(12)-C(24)	1.385(3)
C(12)-H(1)	0.9500
C(13)-C(14)	1.526(3)
C(13)-C(16)	1.529(3)
C(13)-C(15)	1.531(3)
C(14)-H(2)	0.9800
C(14)-H(4)	0.9800
C(14)-H(3)	0.9800
C(15)-H(6)	0.9800
C(15)-H(5)	0.9800
C(15)-H(7)	0.9800
C(16)-H(8)	0.9800
C(16)-H(10)	0.9800
C(16)-H(9)	0.9800
C(17)-C(18)	1.396(3)
C(17)-C(23)	1.400(3)
C(18)-C(19)	1.391(3)
C(18)-H(14)	0.9500
C(19)-C(20)	1.391(3)
C(19)-H(13)	0.9500

C(20)-C(22)	1.385(3)
C(20)-C(21)	1.502(2)
C(22)-C(23)	1.383(3)
C(22)-H(12)	0.9500
C(23)-H(11)	0.9500
C(24)-C(25)	1.396(3)
C(24)-H(16)	0.9500
C(25)-H(17)	0.9500
C(26)-C(27)	1.388(3)
C(26)-H(20)	0.9500
C(27)-H(21)	0.9500

C(5)-N(1)-C(6)	121.44(15)
C(5)-N(1)-C(13)	121.47(14)
C(6)-N(1)-C(13)	117.05(14)
C(27)-C(1)-C(2)	121.27(18)
C(27)-C(1)-Cl(1)	119.00(16)
C(2)-C(1)-Cl(1)	119.70(15)
C(1)-C(2)-C(3)	118.89(18)
C(1)-C(2)-H(23)	120.6
C(3)-C(2)-H(23)	120.6
C(2)-C(3)-C(4)	121.03(18)
C(2)-C(3)-H(22)	119.5
C(4)-C(3)-H(22)	119.5
C(26)-C(4)-C(3)	118.63(17)
C(26)-C(4)-C(5)	124.71(16)
C(3)-C(4)-C(5)	116.65(16)
O(1)-C(5)-N(1)	122.63(17)
O(1)-C(5)-C(4)	119.01(16)
N(1)-C(5)-C(4)	118.28(15)
C(7)-C(6)-N(1)	122.96(16)
C(7)-C(6)-C(17)	121.54(16)
N(1)-C(6)-C(17)	115.45(15)
C(6)-C(7)-C(8)	124.03(16)
C(6)-C(7)-H(15)	118.0
C(8)-C(7)-H(15)	118.0
O(2)-C(8)-C(7)	120.95(17)
O(2)-C(8)-C(9)	120.76(16)

C(7)-C(8)-C(9)	118.28(16)
C(25)-C(9)-C(10)	119.04(18)
C(25)-C(9)-C(8)	122.92(16)
C(10)-C(9)-C(8)	117.98(17)
C(11)-C(10)-C(9)	120.16(18)
C(11)-C(10)-H(19)	119.9
C(9)-C(10)-H(19)	119.9
C(10)-C(11)-C(12)	120.58(18)
C(10)-C(11)-H(18)	119.7
C(12)-C(11)-H(18)	119.7
C(24)-C(12)-C(11)	119.95(19)
C(24)-C(12)-H(1)	120.0
C(11)-C(12)-H(1)	120.0
C(14)-C(13)-N(1)	109.47(15)
C(14)-C(13)-C(16)	110.03(16)
N(1)-C(13)-C(16)	109.67(15)
C(14)-C(13)-C(15)	106.95(17)
N(1)-C(13)-C(15)	109.56(15)
C(16)-C(13)-C(15)	111.11(17)
C(13)-C(14)-H(2)	109.5
C(13)-C(14)-H(4)	109.5
H(2)-C(14)-H(4)	109.5
C(13)-C(14)-H(3)	109.5
H(2)-C(14)-H(3)	109.5
H(4)-C(14)-H(3)	109.5
C(13)-C(15)-H(6)	109.5
C(13)-C(15)-H(5)	109.5
H(6)-C(15)-H(5)	109.5
C(13)-C(15)-H(7)	109.5
H(6)-C(15)-H(7)	109.5
H(5)-C(15)-H(7)	109.5
C(13)-C(16)-H(8)	109.5
C(13)-C(16)-H(10)	109.5
H(8)-C(16)-H(10)	109.5
C(13)-C(16)-H(9)	109.5
H(8)-C(16)-H(9)	109.5
H(10)-C(16)-H(9)	109.5
C(18)-C(17)-C(23)	118.95(16)

C(18)-C(17)-C(6)	120.95(16)
C(23)-C(17)-C(6)	120.09(16)
C(19)-C(18)-C(17)	120.51(16)
C(19)-C(18)-H(14)	119.7
C(17)-C(18)-H(14)	119.7
C(20)-C(19)-C(18)	119.46(17)
C(20)-C(19)-H(13)	120.3
C(18)-C(19)-H(13)	120.3
C(22)-C(20)-C(19)	120.67(16)
C(22)-C(20)-C(21)	119.91(17)
C(19)-C(20)-C(21)	119.37(17)
F(1)-C(21)-F(2)	107.08(15)
F(1)-C(21)-F(3)	106.00(15)
F(2)-C(21)-F(3)	106.23(16)
F(1)-C(21)-C(20)	112.78(16)
F(2)-C(21)-C(20)	112.76(16)
F(3)-C(21)-C(20)	111.52(15)
C(23)-C(22)-C(20)	119.70(17)
C(23)-C(22)-H(12)	120.2
C(20)-C(22)-H(12)	120.2
C(22)-C(23)-C(17)	120.68(17)
C(22)-C(23)-H(11)	119.7
C(17)-C(23)-H(11)	119.7
C(12)-C(24)-C(25)	119.36(19)
C(12)-C(24)-H(16)	120.3
C(25)-C(24)-H(16)	120.3
C(9)-C(25)-C(24)	120.91(18)
C(9)-C(25)-H(17)	119.5
C(24)-C(25)-H(17)	119.5
C(27)-C(26)-C(4)	120.65(17)
C(27)-C(26)-H(20)	119.7
C(4)-C(26)-H(20)	119.7
C(1)-C(27)-C(26)	119.37(18)
C(1)-C(27)-H(21)	120.3
C(26)-C(27)-H(21)	120.3

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 160808lt\_0m. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Cl(1)	33(1)	22(1)	31(1)	6(1)	-2(1)	-1(1)
F(1)	39(1)	26(1)	40(1)	-10(1)	-23(1)	-6(1)
F(2)	23(1)	45(1)	37(1)	-9(1)	-14(1)	-8(1)
F(3)	51(1)	37(1)	34(1)	8(1)	-33(1)	-13(1)
O(1)	28(1)	28(1)	17(1)	-6(1)	-6(1)	-4(1)
O(2)	19(1)	36(1)	20(1)	3(1)	-9(1)	-4(1)
N(1)	17(1)	20(1)	12(1)	0(1)	-6(1)	-5(1)
C(1)	21(1)	18(1)	24(1)	-1(1)	-2(1)	2(1)
C(2)	21(1)	20(1)	34(1)	-2(1)	-10(1)	-4(1)
C(3)	22(1)	22(1)	26(1)	-3(1)	-11(1)	-3(1)
C(4)	16(1)	17(1)	21(1)	-4(1)	-6(1)	0(1)
C(5)	15(1)	23(1)	18(1)	-3(1)	-7(1)	-4(1)
C(6)	18(1)	17(1)	16(1)	0(1)	-8(1)	-1(1)
C(7)	19(1)	21(1)	16(1)	-2(1)	-7(1)	0(1)
C(8)	15(1)	21(1)	17(1)	-2(1)	-6(1)	1(1)
C(9)	15(1)	19(1)	21(1)	-4(1)	-6(1)	1(1)
C(10)	22(1)	23(1)	23(1)	-3(1)	-9(1)	-1(1)
C(11)	22(1)	24(1)	34(1)	-4(1)	-11(1)	-6(1)
C(12)	26(1)	24(1)	28(1)	2(1)	-3(1)	-6(1)
C(13)	20(1)	25(1)	14(1)	3(1)	-7(1)	-8(1)
C(14)	32(1)	24(1)	25(1)	3(1)	-10(1)	-2(1)
C(15)	42(1)	33(1)	23(1)	6(1)	-21(1)	-11(1)
C(16)	22(1)	35(1)	25(1)	10(1)	-3(1)	-7(1)
C(17)	20(1)	16(1)	15(1)	1(1)	-9(1)	-4(1)
C(18)	22(1)	17(1)	14(1)	-2(1)	-6(1)	-3(1)
C(19)	18(1)	19(1)	18(1)	1(1)	-7(1)	-1(1)
C(20)	23(1)	18(1)	16(1)	2(1)	-12(1)	-5(1)
C(21)	27(1)	24(1)	23(1)	-1(1)	-14(1)	-6(1)
C(22)	26(1)	19(1)	18(1)	-5(1)	-8(1)	-2(1)
C(23)	18(1)	20(1)	19(1)	-2(1)	-6(1)	-2(1)
C(24)	30(1)	32(1)	23(1)	-5(1)	-12(1)	2(1)
C(25)	21(1)	26(1)	20(1)	-2(1)	-7(1)	0(1)
C(26)	20(1)	21(1)	22(1)	-3(1)	-8(1)	-2(1)

C(27) 25(1) 22(1) 20(1) -1(1) -7(1) 1(1)

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Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for 160808lt\_0m.

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	x	y	z	U(eq)
H(23)	9979	12900	7872	30
H(22)	8937	11250	9284	27
H(15)	9455	7720	6662	22
H(19)	12708	9842	7880	26
H(18)	14401	11367	6656	31
H(1)	14275	11916	4902	33
H(2)	7202	5415	9102	41
H(4)	7655	4958	10158	41
H(3)	8822	5829	9143	41
H(6)	8918	7478	10474	46
H(5)	7842	6453	11405	46
H(7)	7341	7970	11347	46
H(8)	4852	7542	11086	44
H(10)	5164	6018	11351	44
H(9)	4815	6469	10251	44
H(14)	4749	8102	8773	22
H(13)	2928	7241	8146	22
H(12)	6251	5100	6010	25
H(11)	8067	5965	6626	23
H(16)	12408	10953	4380	33
H(17)	10695	9422	5617	27
H(20)	6299	10010	7648	25
H(21)	7292	11695	6260	27

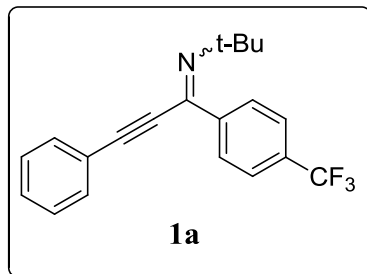
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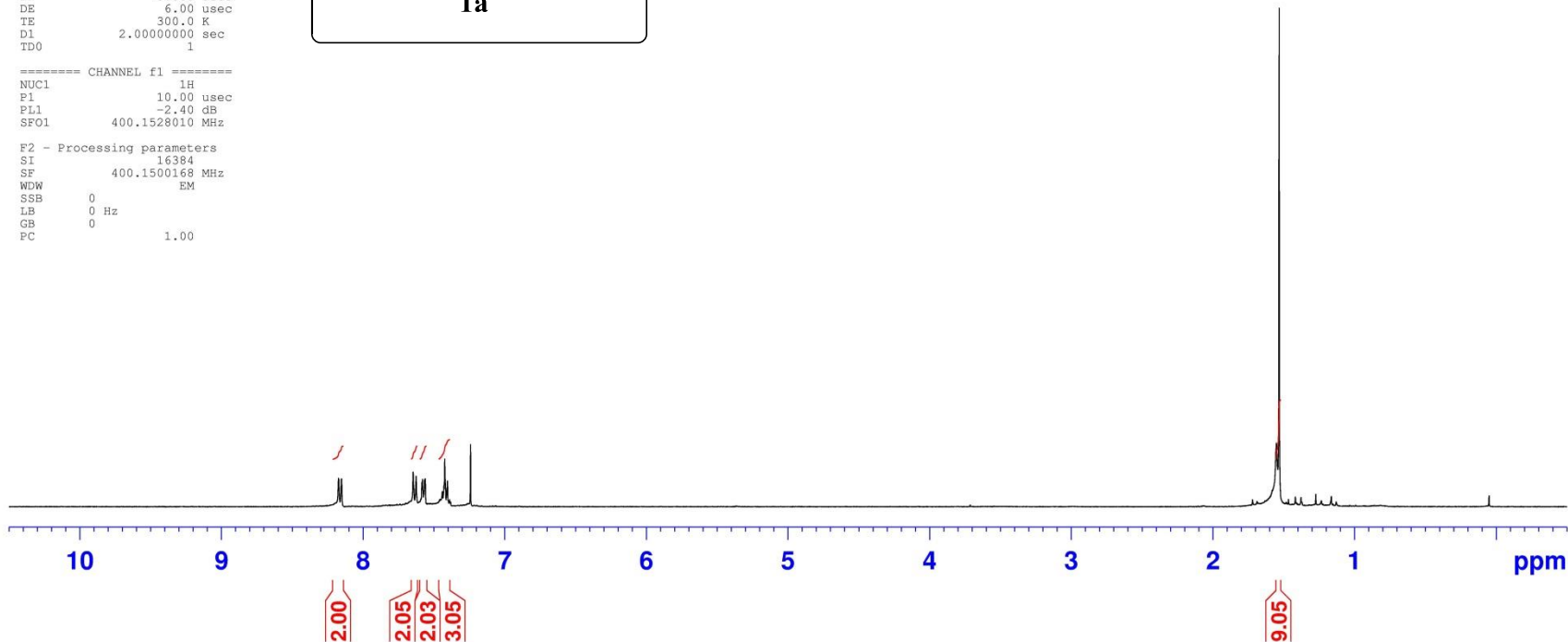
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8.152  
7.645  
7.624  
7.583  
7.580  
7.565  
7.560  
7.458  
7.453  
7.439  
7.427  
7.422  
7.410  
7.403  
7.388  
7.381  
7.240

Current Data Parameters  
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EXPNO 1  
PROCNO 1

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TD 32768  
SOLVENT CDCl3  
NS 11  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 575  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
TD0 1



===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz  
  
F2 - Processing parameters  
SI 16384  
SF 400.1500168 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

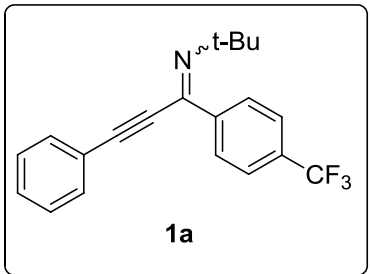


1.532

— 145.73  
 — 142.56  
 — 131.63  
 — 129.90  
 — 128.69  
 — 127.55  
 — 125.08  
 — 125.06  
 — 121.56  
 — 99.51  
 — 83.47  
 — 77.21  
 — 77.00  
 — 76.79  
 — 57.38  
 — 29.42

Current Data Parameters  
 NAME Yu-4  
 EXPNO 2  
 PROCNO 1

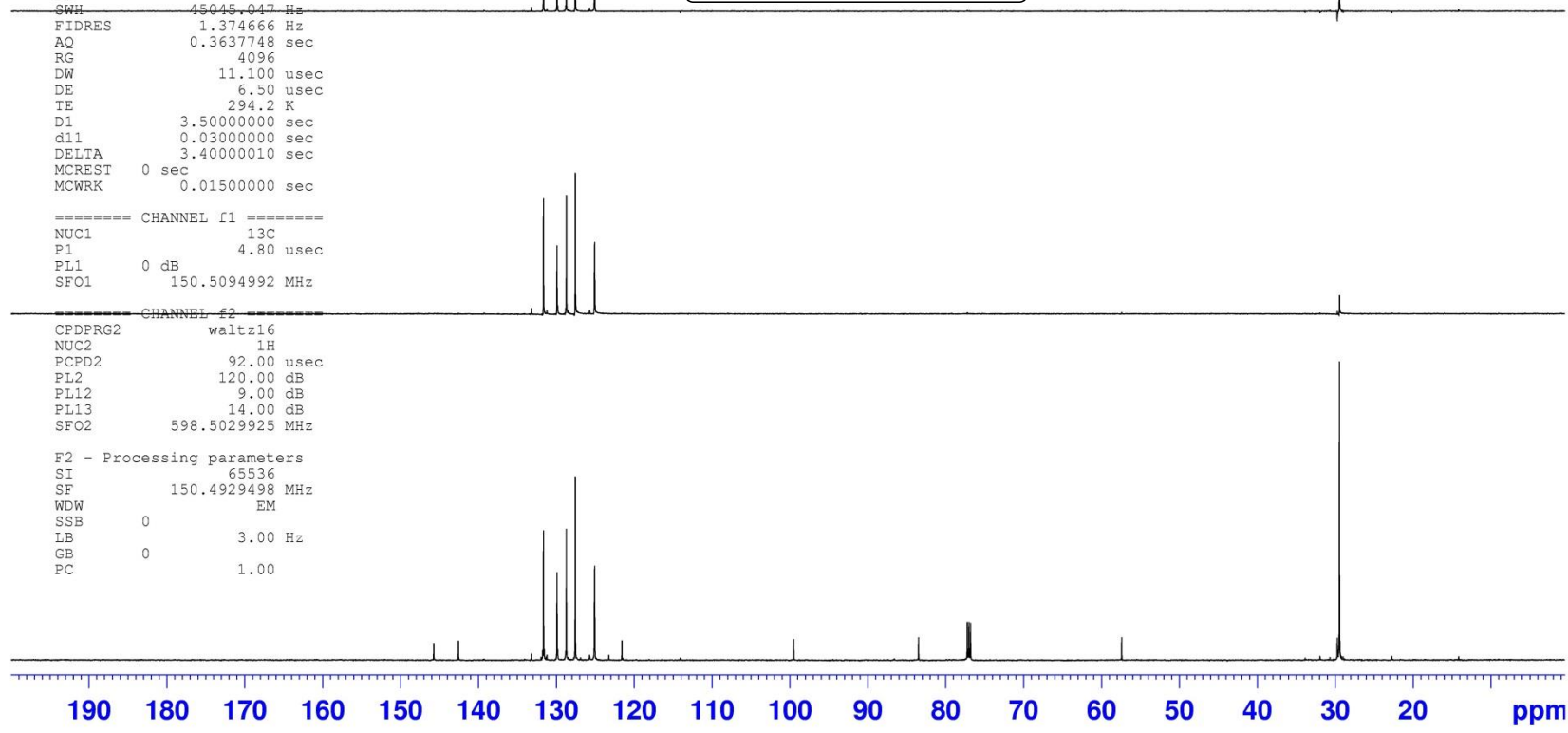
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 SOLVENT CDC13  
 NS 500  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 294.2 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0 sec  
 MCWRK 0.01500000 sec



===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0 dB  
 SFO1 150.5094992 MHz

----- CHANNEL f2 -----  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.5029925 MHz

F2 - Processing parameters  
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 LB 3.00 Hz  
 GB 0  
 PC 1.00

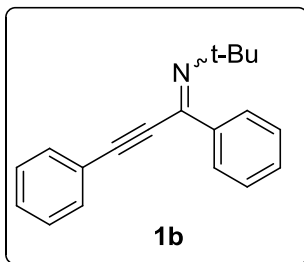


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8.060  
8.057  
7.583  
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7.569  
7.564  
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7.402  
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7.390  
7.382  
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7.240

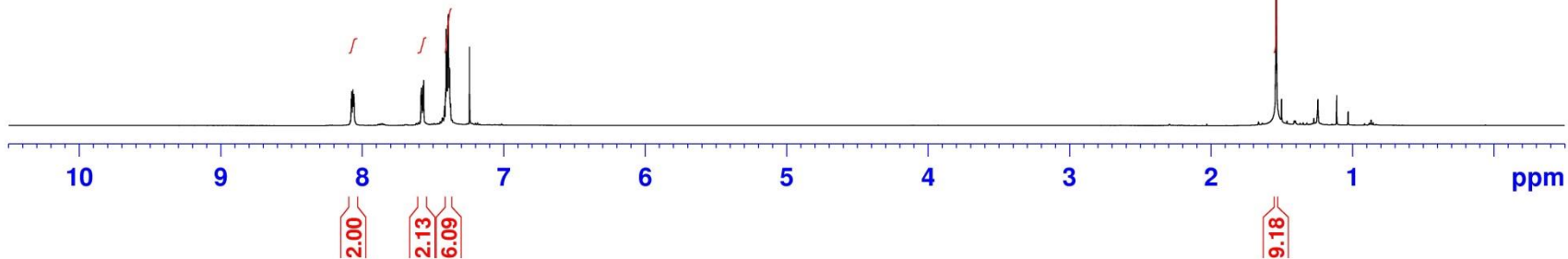
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PROCNO 1

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PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 32  
DS 0  
SWH 10026.738 Hz  
FIDRES 0.305992 Hz  
AQ 1.6340809 sec  
RG 89.22  
DW 49.867 usec  
DE 7.71 usec  
TE 300.0 K  
D1 2.0000000 sec  
TD0 1  
SFO1 500.1630010 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 22.69799995 W



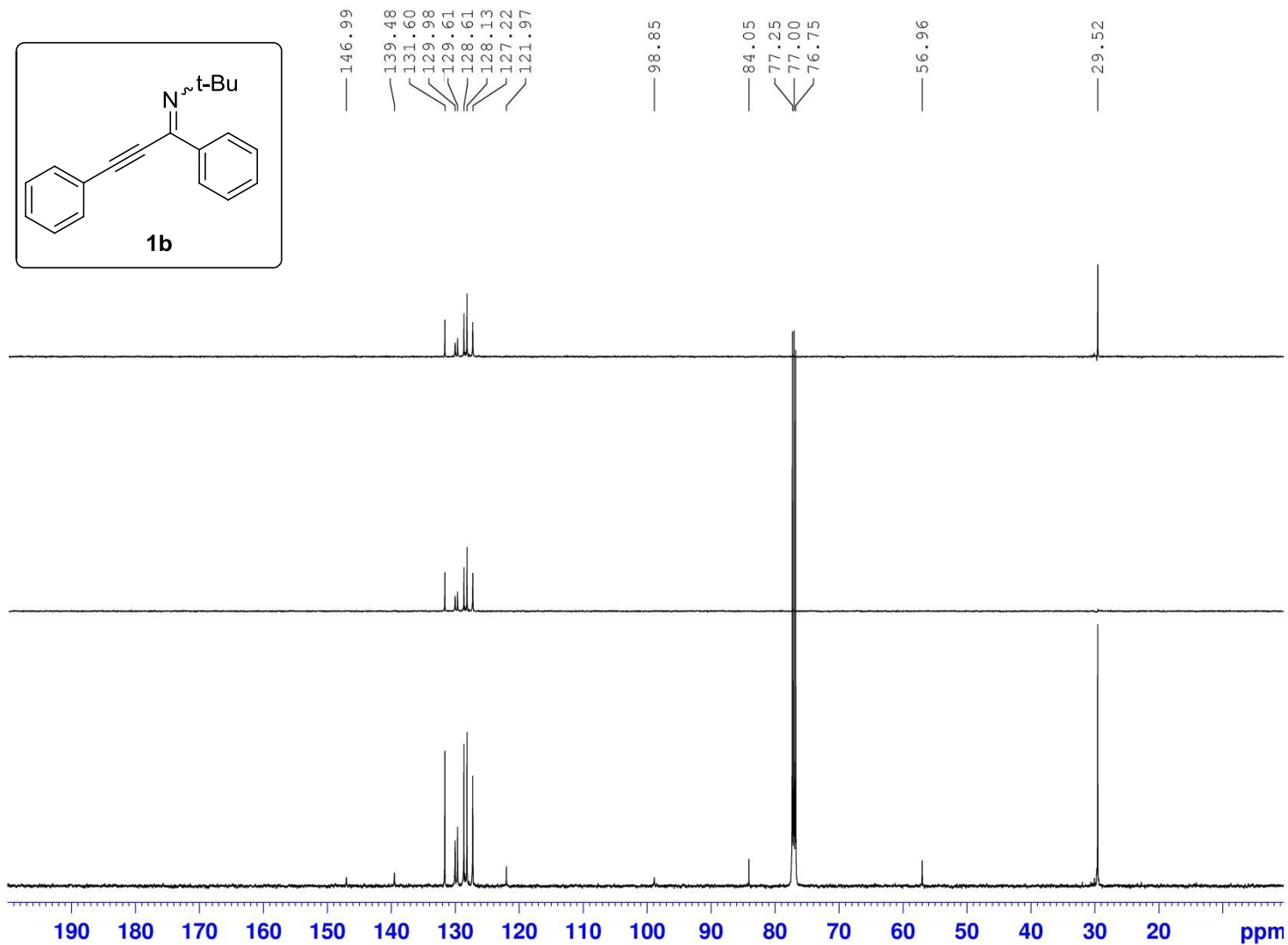
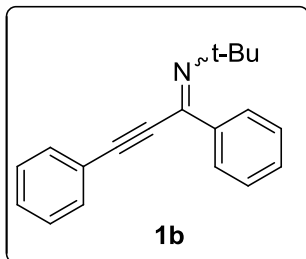
F2 - Processing parameters  
SI 16384  
SF 500.1600214 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME liou0906.001  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160906  
Time 9.49 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 2192  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7785374 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 80.55799866 W  
SFO2 500.1620006 MHz  
NUC2 1H  
CPDPRG[2 bi\_waltz65\_256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W

F2 - Processing parameters  
SI 32768  
SF 125.7653349 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

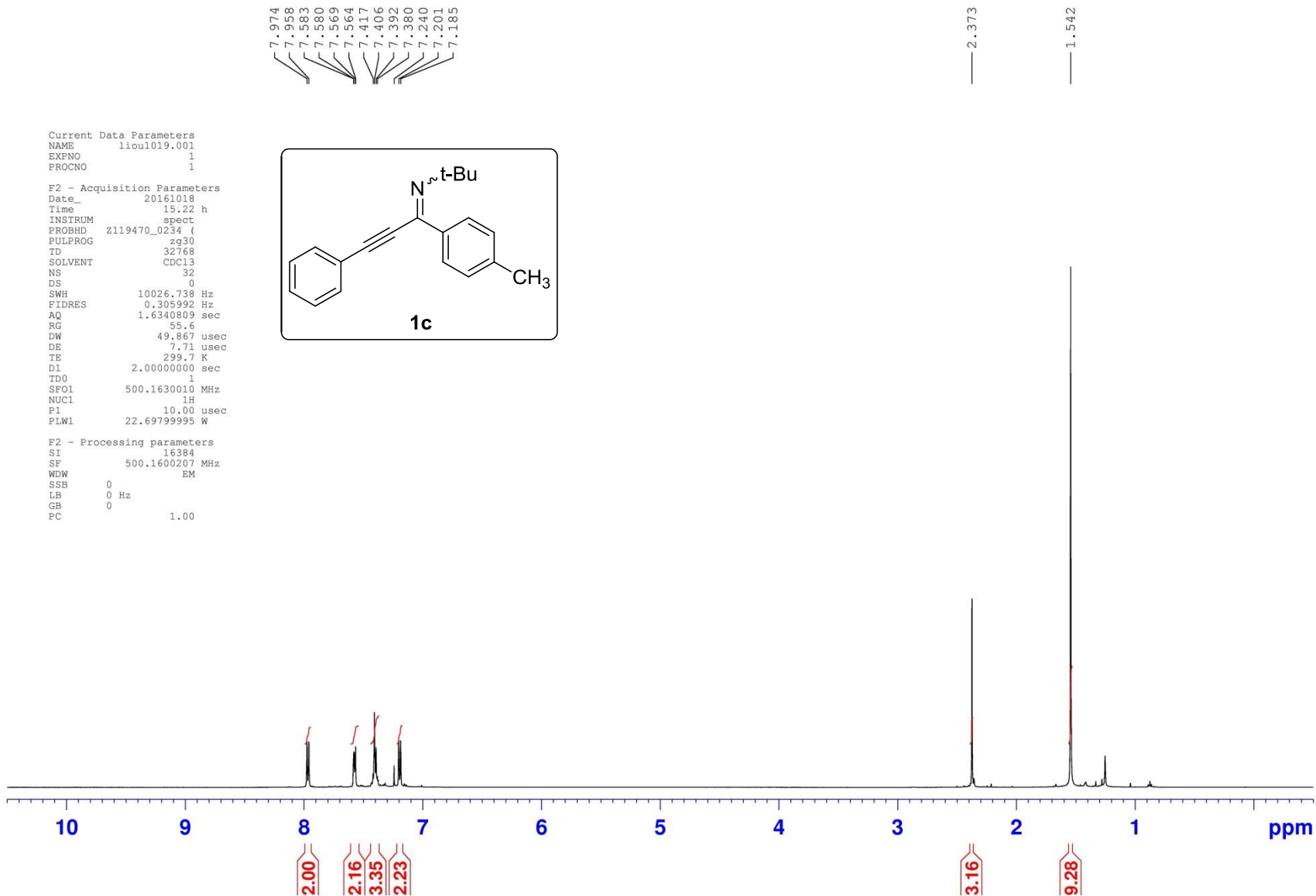
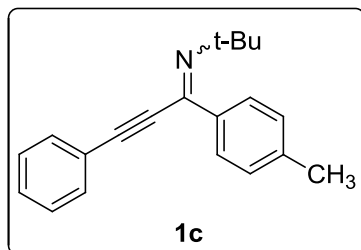


Current Data Parameters  
NAME liou1019.001  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161018  
Time 15.22 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 32  
DS 0  
SWH 10026.738 Hz  
FIDRES 0.305992 Hz  
AQ 1.6340809 sec  
RG 55.6  
DW 49.867 usec  
DE 7.71 usec  
TE 299.7 K  
D1 2.00000000 sec  
TD0 1  
SFO1 500.1630010 MHz  
NUC1 1H  
F1 10.00 usec  
FLM1 22.69799995 W

F2 - Processing parameters  
SI 16384  
SF 500.1600207 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
EC 1.00

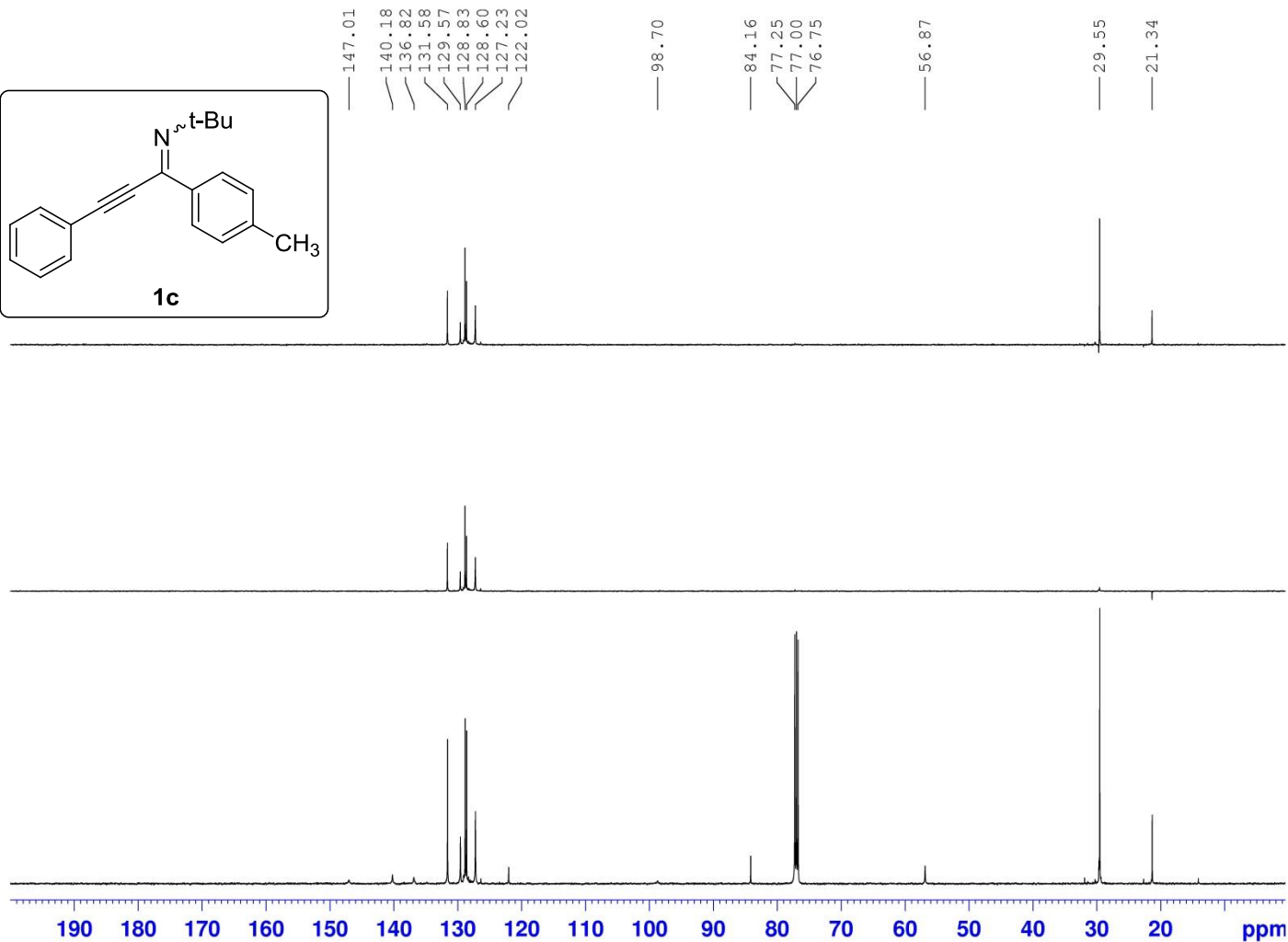
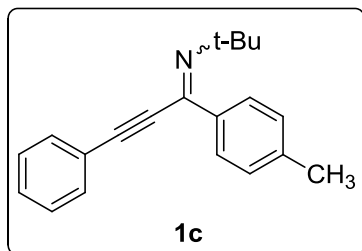
7.974  
7.958  
7.583  
7.580  
7.569  
7.564  
7.417  
7.406  
7.392  
7.380  
7.240  
7.201  
7.185



Current Data Parameters  
NAME liou1019.001  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161018  
Time 16.52 h  
INSTRUM spect  
PROBHD z119470\_0234 ( zpgpg30  
TD 32768  
SOLVENT CDC13  
NS 2048  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 125.7785374 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 80.55799866 W  
SFO2 500.1620006 MHz  
NUC2 1H  
CPDPRG[2 bi\_waltz65\_256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W

F2 - Processing parameters  
SI 32768  
SF 125.7653358 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



8.036  
8.019  
7.578  
7.574  
7.564  
7.559  
7.415  
7.412  
7.402  
7.388  
7.382  
7.377  
7.373  
7.370  
7.240  
6.910  
6.892

3.829

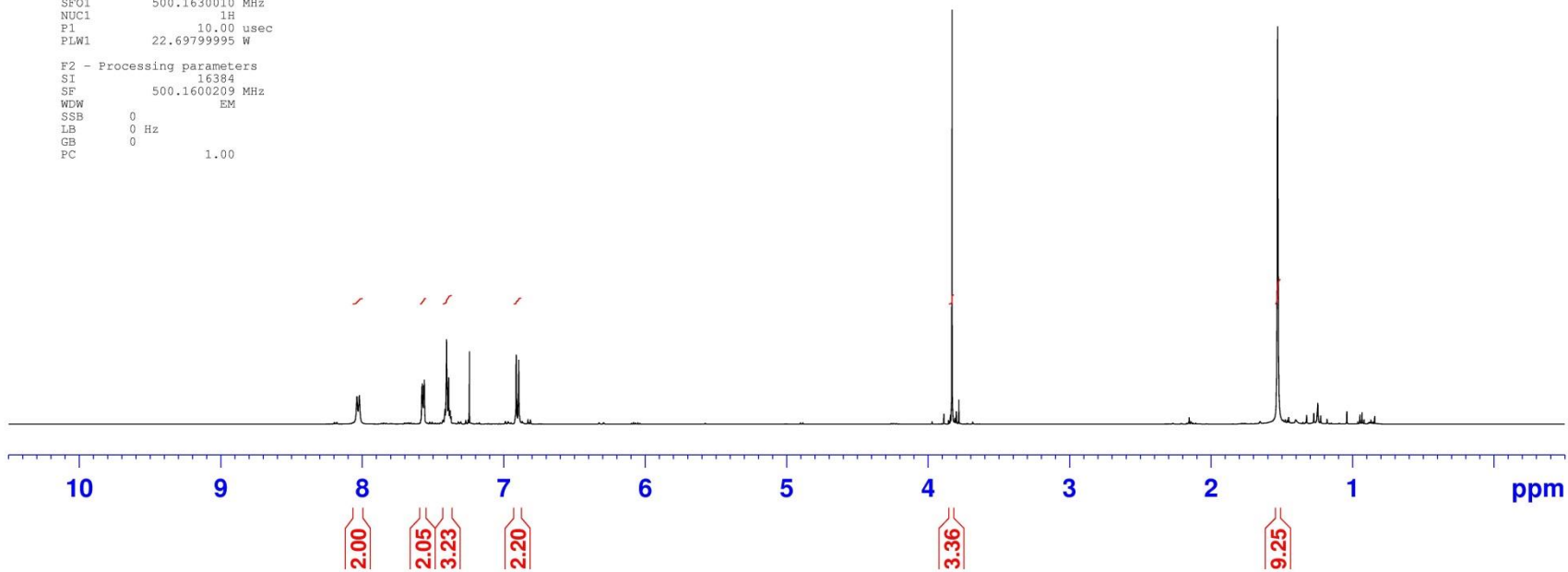
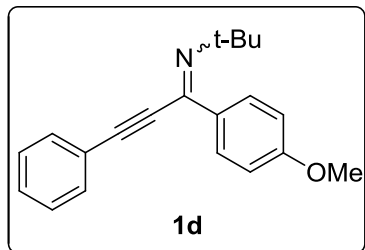
1.527

```

Current Data Parameters
NAME      licu0908.001
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160908
Time     9.17 h
INSTRUM  spect
PROBHD   zg30
PULPROG  zg30
TD        32768
SOLVENT  CDCl3
NS        32
DS        0
SWH       10026.738 Hz
FIDRES    0.305992 Hz
AQ        1.6340809 sec
RG         71.36
DW         49.867 usec
DE         7.71 usec
TE        300.0 K
D1         2.00000000 sec
TDO        1
SFO1      500.1630010 MHz
NUC1       1H
P1         10.00 usec
PLW1      22.69799995 W

F2 - Processing parameters
SI         16384
SF         500.1600209 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         1.00
  
```



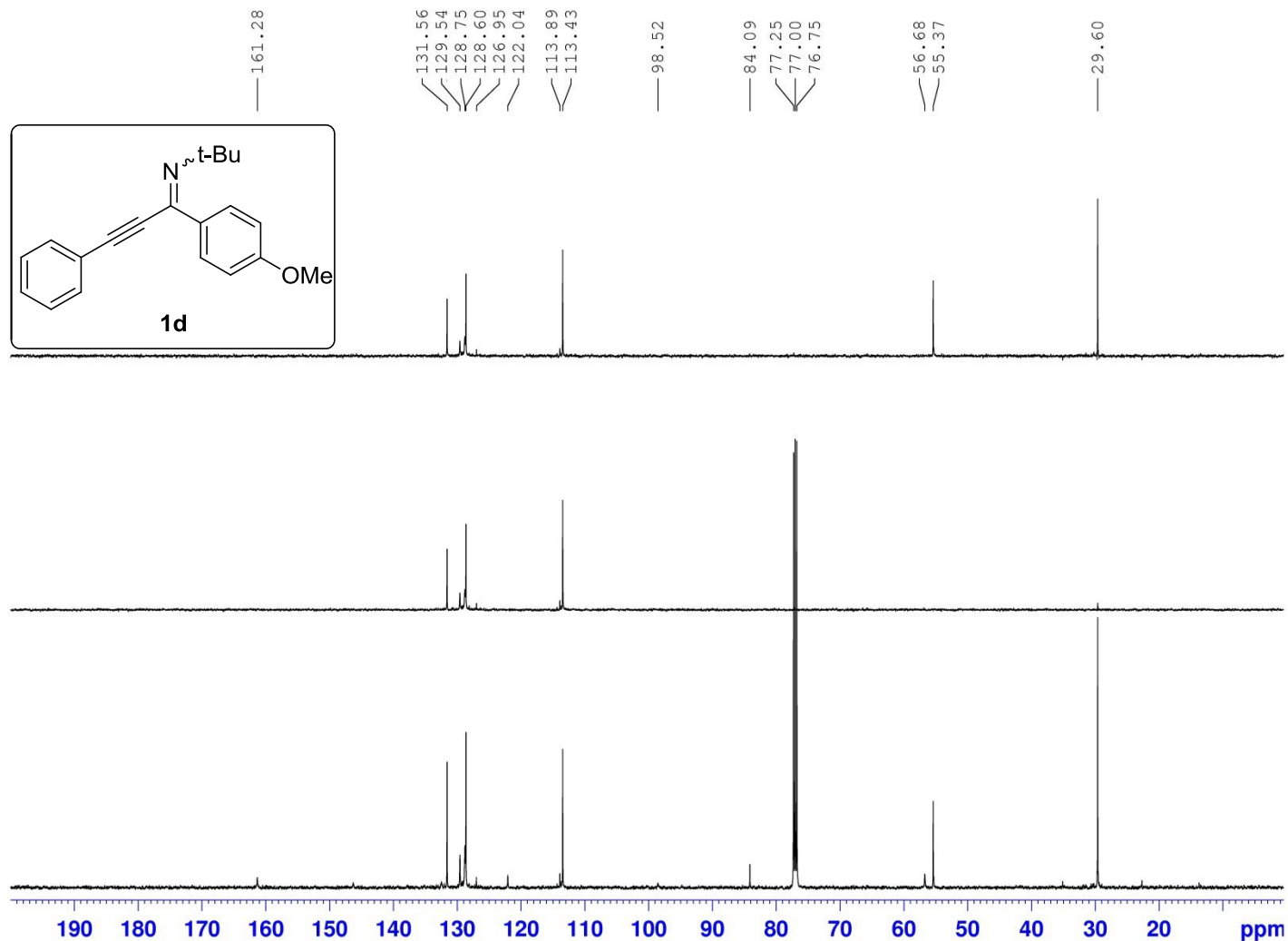
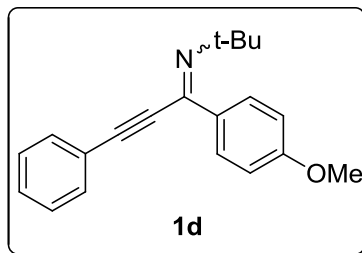
```

Current Data Parameters
NAME      liou0908.001
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20160908
Time      9.40 h
INSTRUM   spect
PROBHD    Z119470_0234 (
PULPROG   zgpg30
TD         32768
SOLVENT   CDC13
NS         1013
DS         0
SWH        29761.904 Hz
FIDRES     0.908261 Hz
AQ         0.5505024 sec
RG         191.01
DW         16.800 usec
DE         6.50 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1       125.7785374 MHz
NUC1       13C
P1         10.00 usec
PLW1       80.55799866 W
SFO2       500.1620006 MHz
NUC2       1H
CPDPRG[2  bi_waltz65 256
PCPD2      . 80.00 usec
PLW2       22.69799995 W
PLW12      0.36415839 W
PLW13      0.18251620 W

F2 - Processing parameters
SI         32768
SF         125.7653348 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00

```





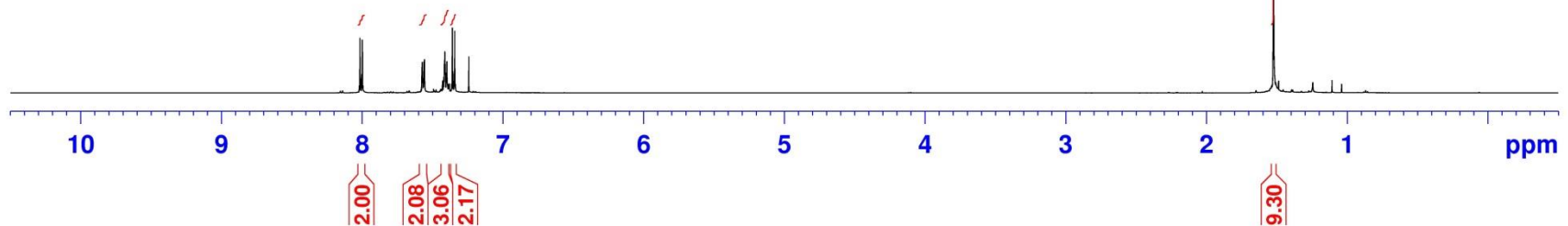
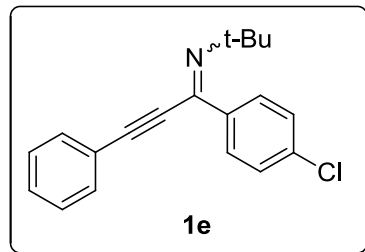
8.014  
8.010  
8.001  
7.997  
7.574  
7.571  
7.563  
7.559  
7.555  
7.426  
7.417  
7.410  
7.401  
7.399  
7.396  
7.362  
7.357  
7.354  
7.344  
7.340  
7.335  
7.240

1.522

Current Data Parameters  
 NAME 11ou0824.002  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160824  
 Time 12.04 h  
 INSTRUM spect  
 PROBHD z119470\_0234 ( )  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 0  
 SWH 10026.738 Hz  
 FIDRES 0.305992 Hz  
 AQ 1.6340309 sec  
 RG 78.62  
 DW 49.867 usec  
 DE 7.71 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 TDO 1  
 SFO1 500.1630010 MHz  
 NUC1 1H  
 P1 10.00 usec  
 PLW1 22.69799995 W

F2 - Processing parameters  
 SI 16384  
 SF 500.1600211 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 FC 1.00

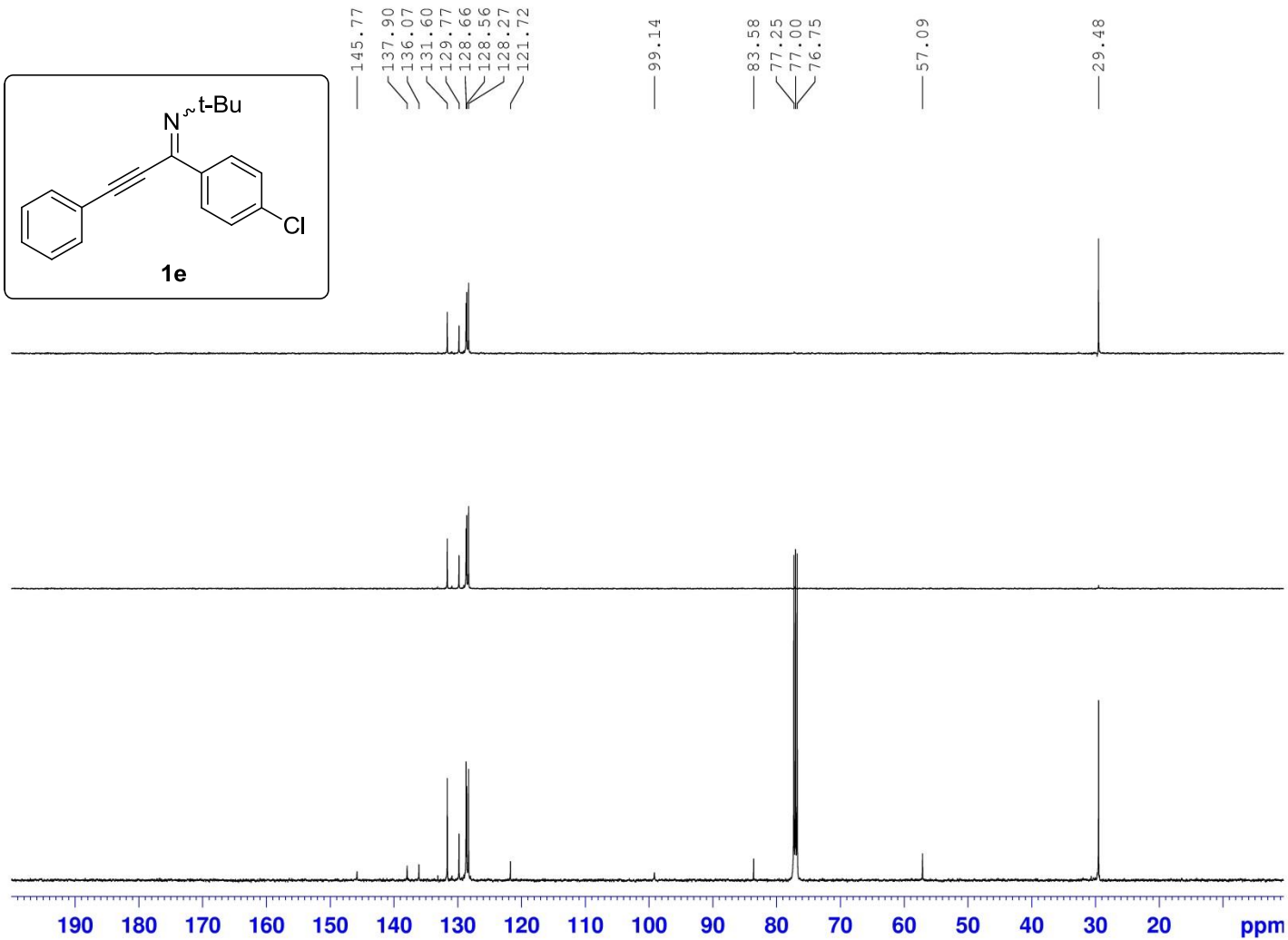
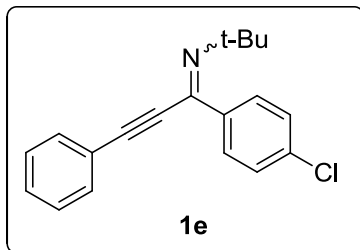


Yu-6-10 / 13C

Current Data Parameters  
NAME liou0824.002  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160824  
Time\_ 15.56 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG \_zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 1436  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7785374 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 80.55799866 W  
SFO2 500.1620006 MHz  
NUC2 1H  
CPDPRG[2 bi\_waltz65\_256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W

F2 - Processing parameters  
SI 32768  
SF 125.7653337 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



7.651  
7.640  
7.578  
7.574  
7.569  
7.565  
7.560  
7.555  
7.524  
7.517  
7.515  
7.510  
7.507  
7.505  
7.500  
7.426  
7.422  
7.410  
7.404  
7.397  
7.393  
7.271  
7.267  
7.263  
7.258  
7.255  
7.250

1.525

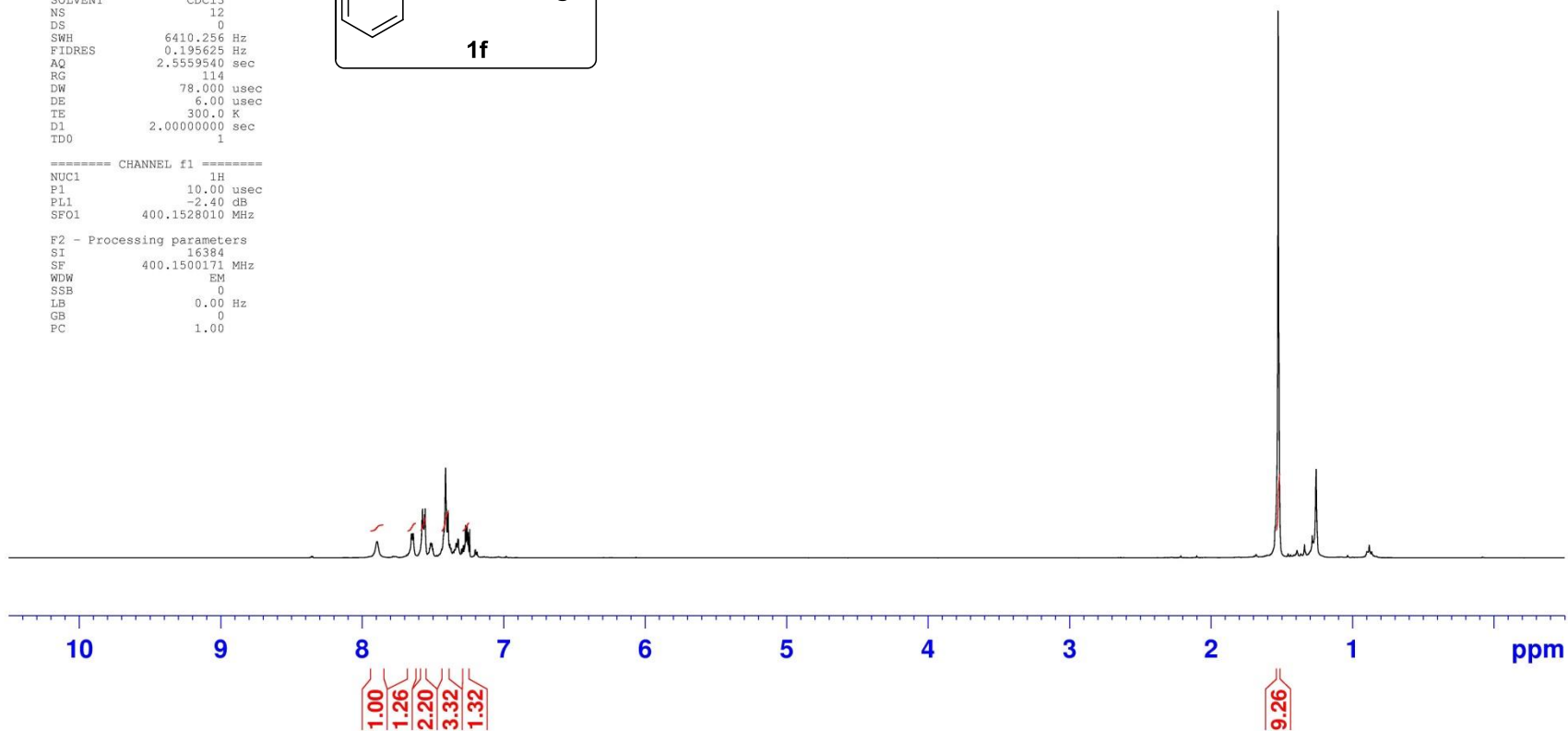
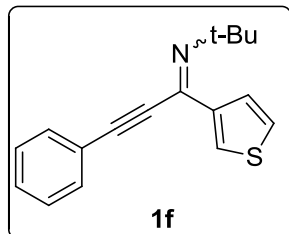
```

Current Data Parameters
NAME      20161018
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    20161018
Time     22.11
INSTRUM spect
PROBHD   5 mm DUL 13C-1
PULPROG zg30
TD       32768
SOLVENT  CDCl3
NS       12
DS       0
SWH      6410.256 Hz
FIDRES   0.195625 Hz
AQ       2.5559540 sec
RG       114
DW       78.000 usec
DE       6.00 usec
TE       300.0 K
D1       2.00000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     1H
P1       10.00 usec
PL1      -2.40 dB
SFO1     400.1528010 MHz

F2 - Processing parameters
SI       16384
SF       400.1500171 MHz
WDW      EM
SSB      0
LB       0.00 Hz
GB       0
PC       1.00
  
```



143.91  
142.57  
131.58  
129.63  
128.61  
128.31  
126.46  
125.50  
121.82

97.15

84.29  
77.32  
77.00  
76.68

56.82

29.59

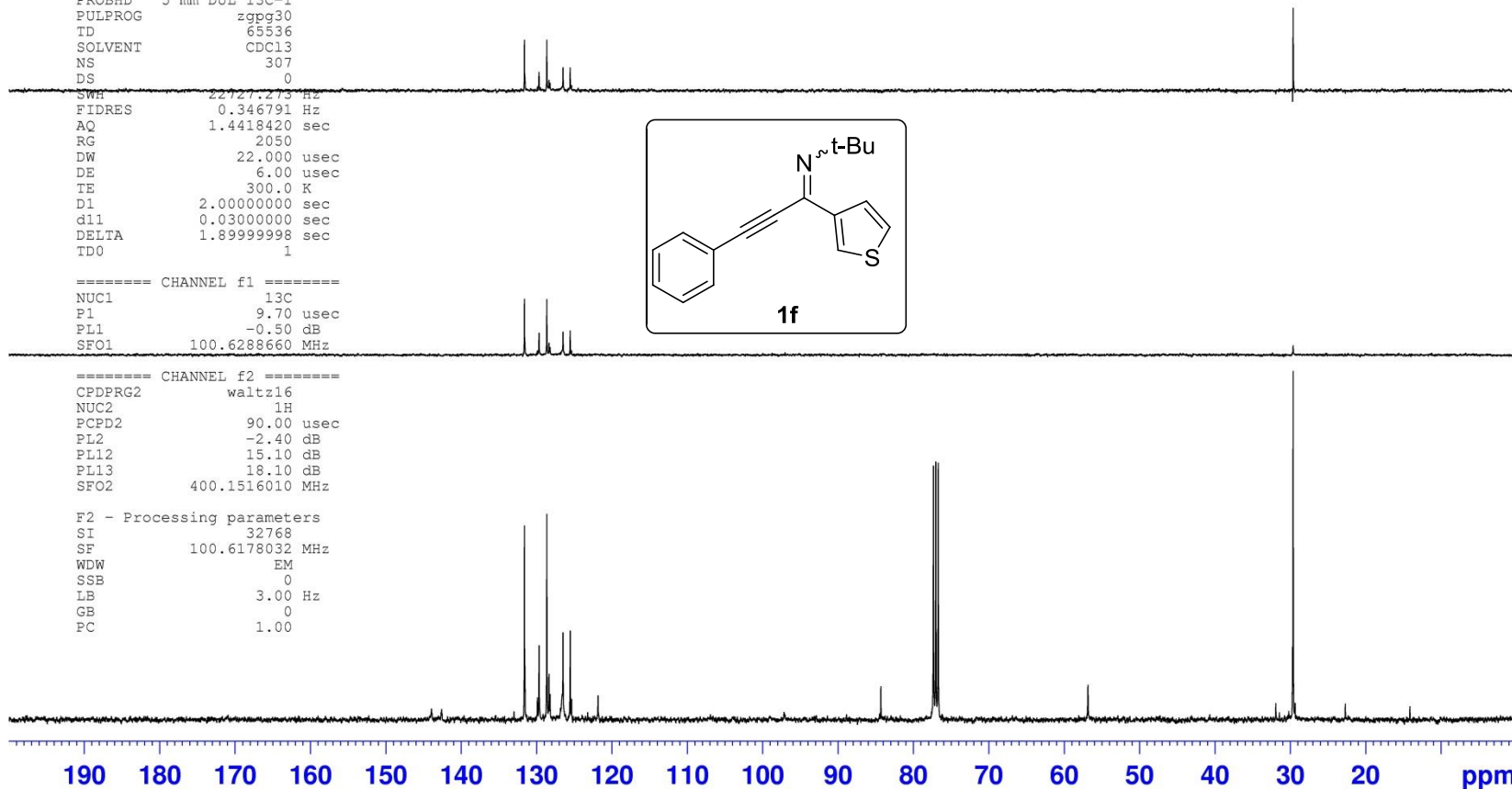
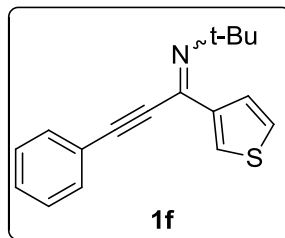
Current Data Parameters  
NAME 20161018  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161018  
Time 22.13  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 307  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 2050  
DW 22.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -0.50 dB  
SFO1 100.6288660 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.40 dB  
PL12 15.10 dB  
PL13 18.10 dB  
SFO2 400.1516010 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6178032 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



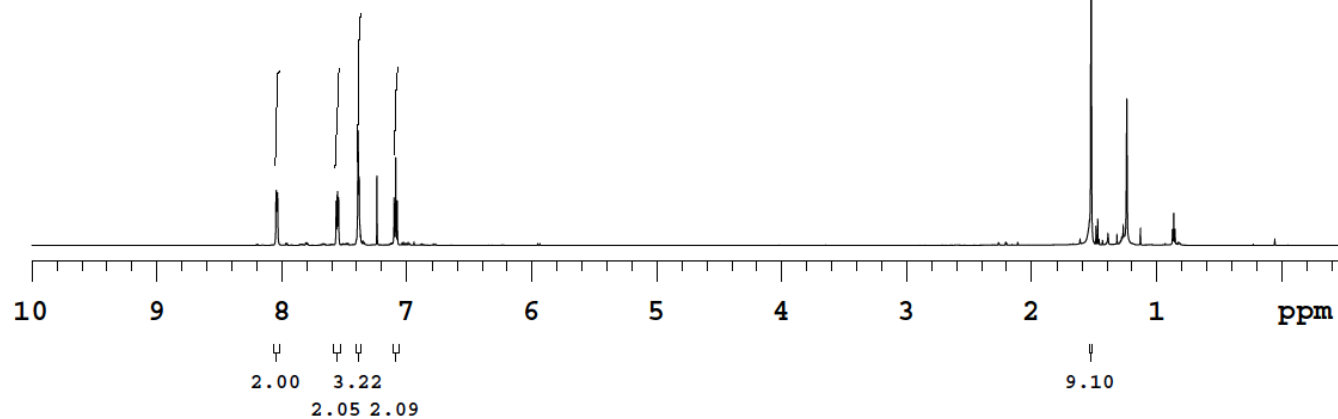
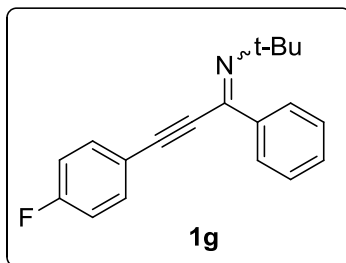
Yu-6-52

8.048  
8.046  
8.039  
8.035  
7.567  
7.559  
7.555  
7.547  
7.392  
7.390  
7.382  
7.240  
7.102  
7.090  
7.078

1.526  
1.240

expl PROTON

SAMPLE		PRESATURATION	
date	Oct 7 2016	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmr1/D-	SPECIAL	
esktop/Yu-6-52-H.f-	temp	25.0	
	id	gain	12
ACQUISITION		spin	
sw	11904.8	hst	0.008
at	2.753	pw90	6.500
np	65536	alfa	10.000
fb	4000	FLAGS	
bs	8	il	n
dl	2.000	in	n
nt	16	dp	y
ct	16	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	699.749	DISPLAY	
tof	349.9	sp	-350.0
tpwr	62	wp	7347.1
pw	3.250	rfl	7174.5
DECOUPLER		rfp	5066.2
dn	C13	rp	-61.1
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_Cold	wc	170
dpwr	40	sc	8
dmf	38462	vs	103
		th	5
		ai	ph

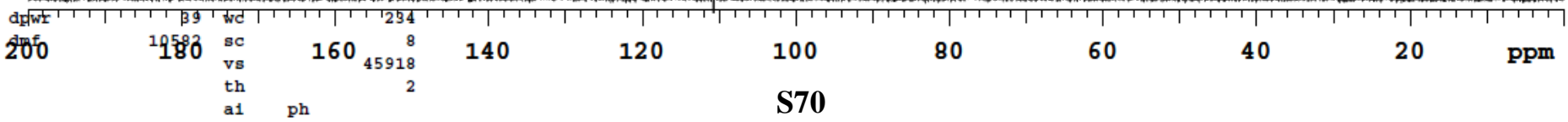
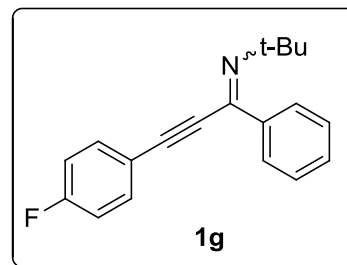


Yu-6-52

164.031  
162.600  
146.821  
139.392  
133.672  
133.624  
130.023  
128.150  
127.164  
118.058  
118.038  
116.121  
115.995  
110.709  
97.731  
83.829  
83.821  
77.181  
77.000  
76.817  
56.948  
31.919  
29.690  
29.650  
29.590  
29.516  
29.355  
22.684  
14.115

exp1 CARBON

SAMPLE		PRESATURATION	
date	Oct 7 2016	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmr1/D-	SPECIAL	
esktop/Yu-6-52-C.f~	temp	25.0	
	id	gain	30
ACQUISITION		not used	
sw	46296.3	hst	0.008
at	1.468	pw90	14.000
np	135926	alfa	10.000
fb	17000	FLAGS	
bs	8	il	n
dl	3.500	in	n
nt	1000	dp	y
ct	760	hs	nn
TRANSMITTER		PROCESSING	
tn	C13	lb	1.00
sfrq	175.972	fn	262144
tof	4438.8	DISPLAY	
tpwr	59	sp	-0.3
pw	7.000	wp	35189.9
DECOUPLER		rfl	15580.6
dn	H1	rfp	13548.2
dof	0	rp	-42.4
dm	nn	lp	0

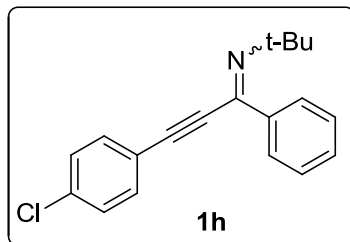


8.046  
8.043  
8.035  
8.031  
7.502  
7.487  
7.394  
7.392  
7.386  
7.383  
7.378  
7.364  
7.240

— 1.525

Current Data Parameters  
NAME Yu-6-51  
EXPNO 1  
PROCNO 1

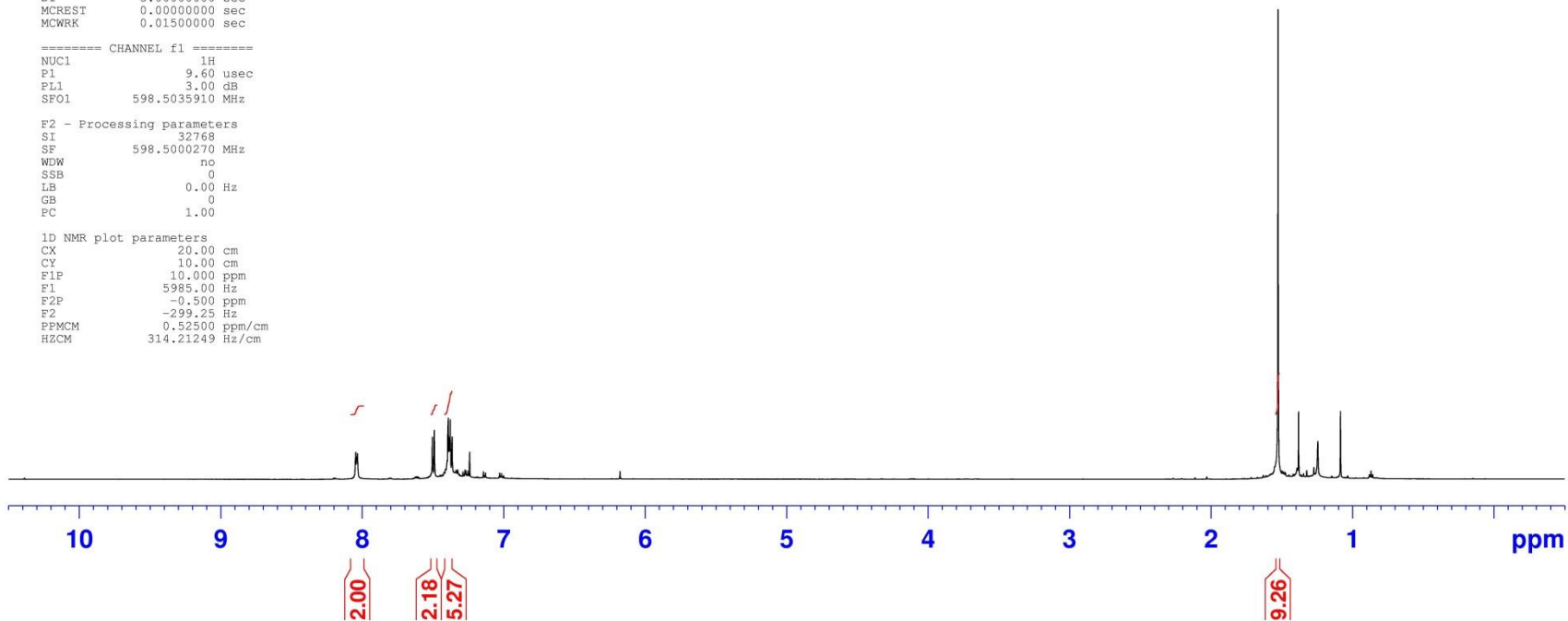
F2 - Acquisition Parameters  
Date\_ 20161005  
Time 8.16  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 512  
DW 41.600 usec  
DE 6.50 usec  
TE 301.5 K  
D1 3.00000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec



===== CHANNEL f1 =====  
NUC1 1H  
P1 9.60 usec  
PL1 3.00 dB  
SFO1 598.5035910 MHz

F2 - Processing parameters  
SI 32768  
SF 598.5000270 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
CY 10.00 cm  
F1P 10.000 ppm  
F1 5985.00 Hz  
F2P -0.500 ppm  
F2 -299.25 Hz  
PPMCM 0.52500 ppm/cm  
HZCM 314.21249 Hz/cm



Current Data Parameters  
NAME Yu-6-51  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161005  
Time 8.34  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 715  
DS 0  
SWH 45045.047 Hz  
FIDRES 1.374666 Hz  
AQ 0.3637748 sec  
RG 4096  
DE 6.50 usec  
TE 301.9 K  
D1 3.50000000 sec  
d11 0.03000000 sec  
DELTA 3.40000010 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 4.80 usec  
PL1 0.00 dB  
SFO1 150.5094992 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 92.00 usec  
PL2 120.00 dB  
PL12 9.00 dB  
PL13 14.00 dB  
SFO2 598.5029925 MHz

F2 - Processing parameters  
SI 65536  
SF 150.4929480 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
CY 4.00 cm  
F1P 200.000 ppm  
F1 30098.59 Hz  
F2P 0.000 ppm  
F2 0.00 Hz  
PPMCM 10.00000 ppm/cm  
HZCM 1504.92944 Hz/cm

139.33  
135.85  
132.78  
130.06  
129.04  
128.16  
127.17  
125.27  
120.40

97.49

84.83

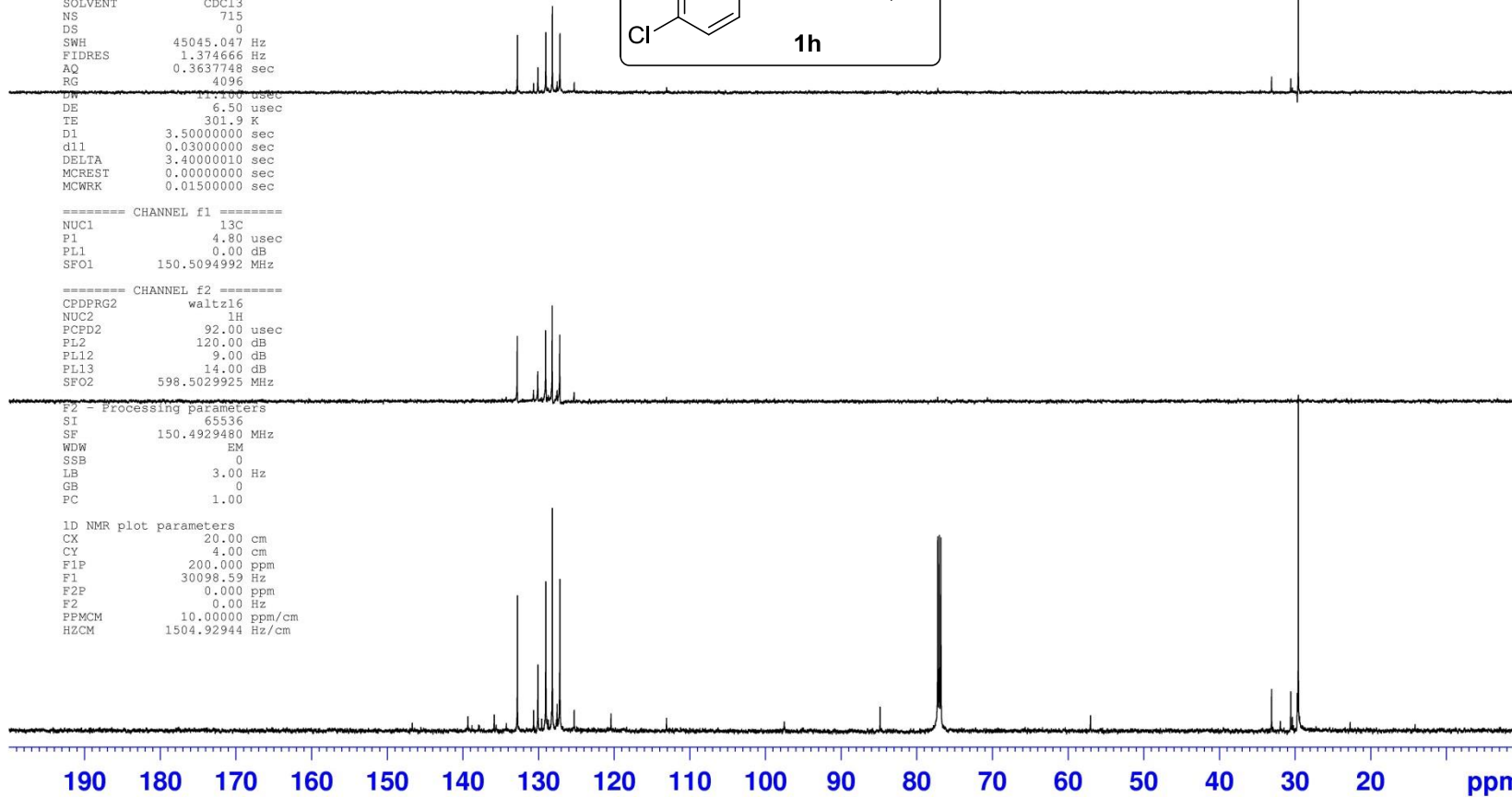
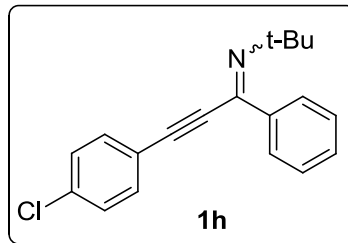
77.21

77.00

76.79

57.02

29.54

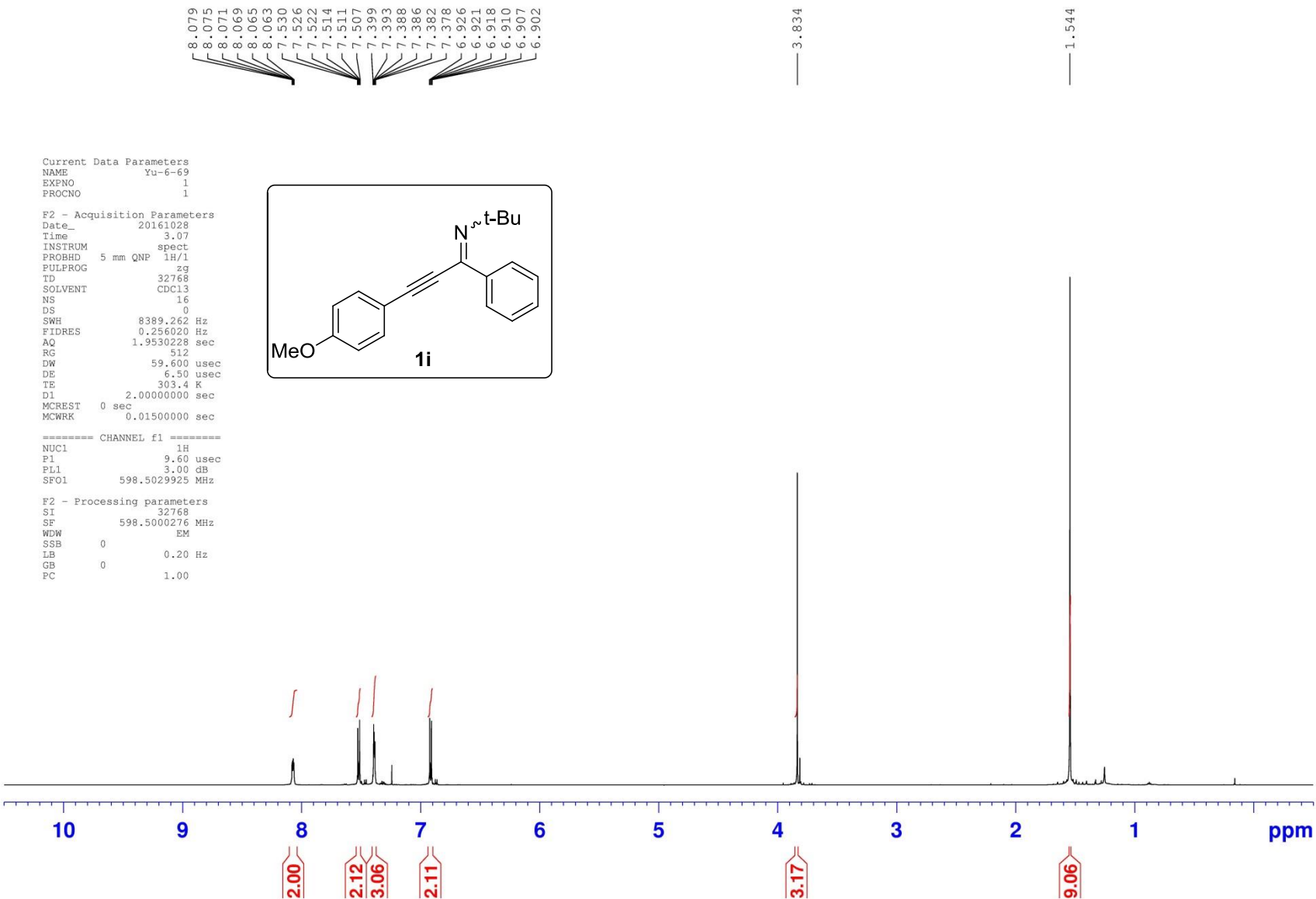
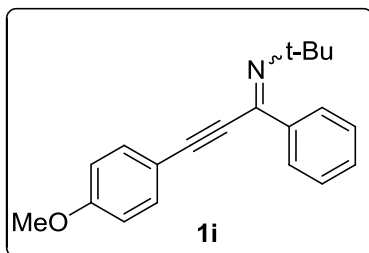


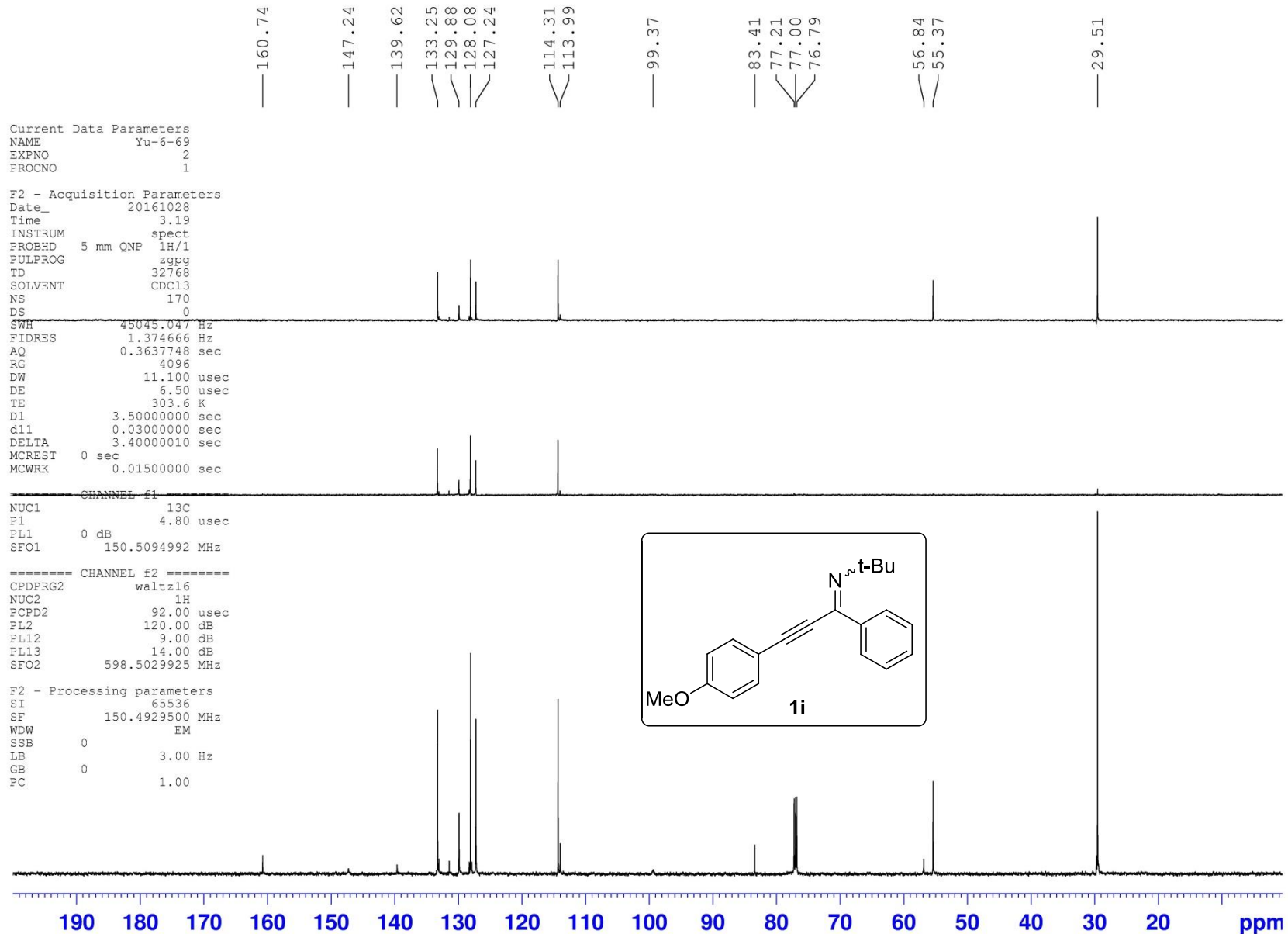


8.079  
8.075  
8.071  
8.069  
8.065  
8.063  
7.530  
7.526  
7.522  
7.514  
7.511  
7.507  
7.399  
7.393  
7.388  
7.386  
7.382  
7.378  
6.926  
6.921  
6.918  
6.910  
6.907  
6.902

Current Data Parameters  
NAME Yu-6-69  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161028  
Time 3.07  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8389.262 Hz  
FIDRES 0.256020 Hz  
AQ 1.9530228 sec  
RG 512  
DW 59.600 usec  
DE 6.50 usec  
TE 303.4 K  
D1 2.0000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

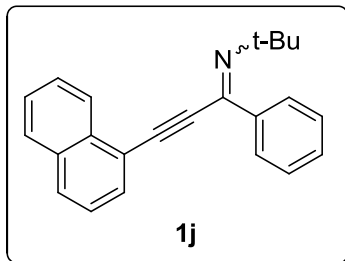




8.320  
8.306  
8.138  
7.959  
7.946  
7.923  
7.909  
7.866  
7.855  
7.644  
7.632  
7.619  
7.595  
7.583  
7.571  
7.541  
7.529  
7.516  
7.476  
7.240

Current Data Parameters  
NAME Yu-6-63-IT  
EXPNO 1  
PROCNO 1

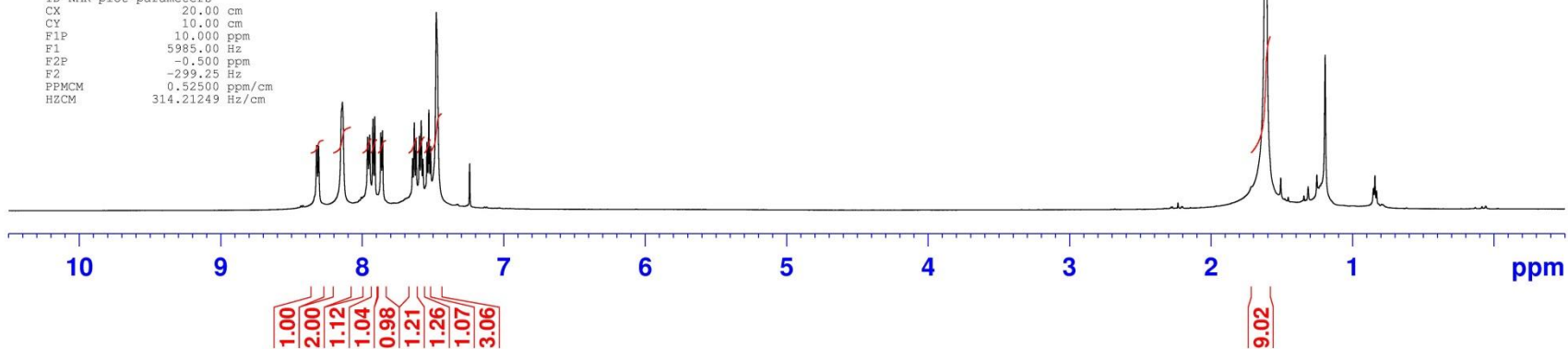
F2 - Acquisition Parameters  
Date\_ 20161012  
Time 9.48  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 16384  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8389.262 Hz  
FIDRES 0.512040 Hz  
AQ 0.9765364 sec  
RG 512  
DW 59.600 usec  
DE 6.00 usec  
TE 256.0 K  
D1 2.00000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec



===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 0.00 dB  
SF01 598.5029925 MHz

F2 - Processing parameters  
SI 32768  
SF 598.5000275 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 0.50

1D NMR plot parameters  
CX 20.00 cm  
CY 10.00 cm  
F1P 10.000 ppm  
F1 5985.00 Hz  
F2P -0.500 ppm  
F2 -299.25 Hz  
PPMCM 0.52500 ppm/cm  
HZCM 314.21249 Hz/cm



147.90  
 139.03  
 132.64  
 132.57  
 131.34  
 130.17  
 128.68  
 128.40  
 128.33  
 127.33  
 127.05  
 126.66  
 125.52  
 125.20  
 118.94

— 97.65

— 87.92

77.21  
 77.00  
 76.79

— 56.86

— 29.12

Current Data Parameters  
 NAME Yu-6-63-LI  
 EXPNO 2  
 PROCNO 1

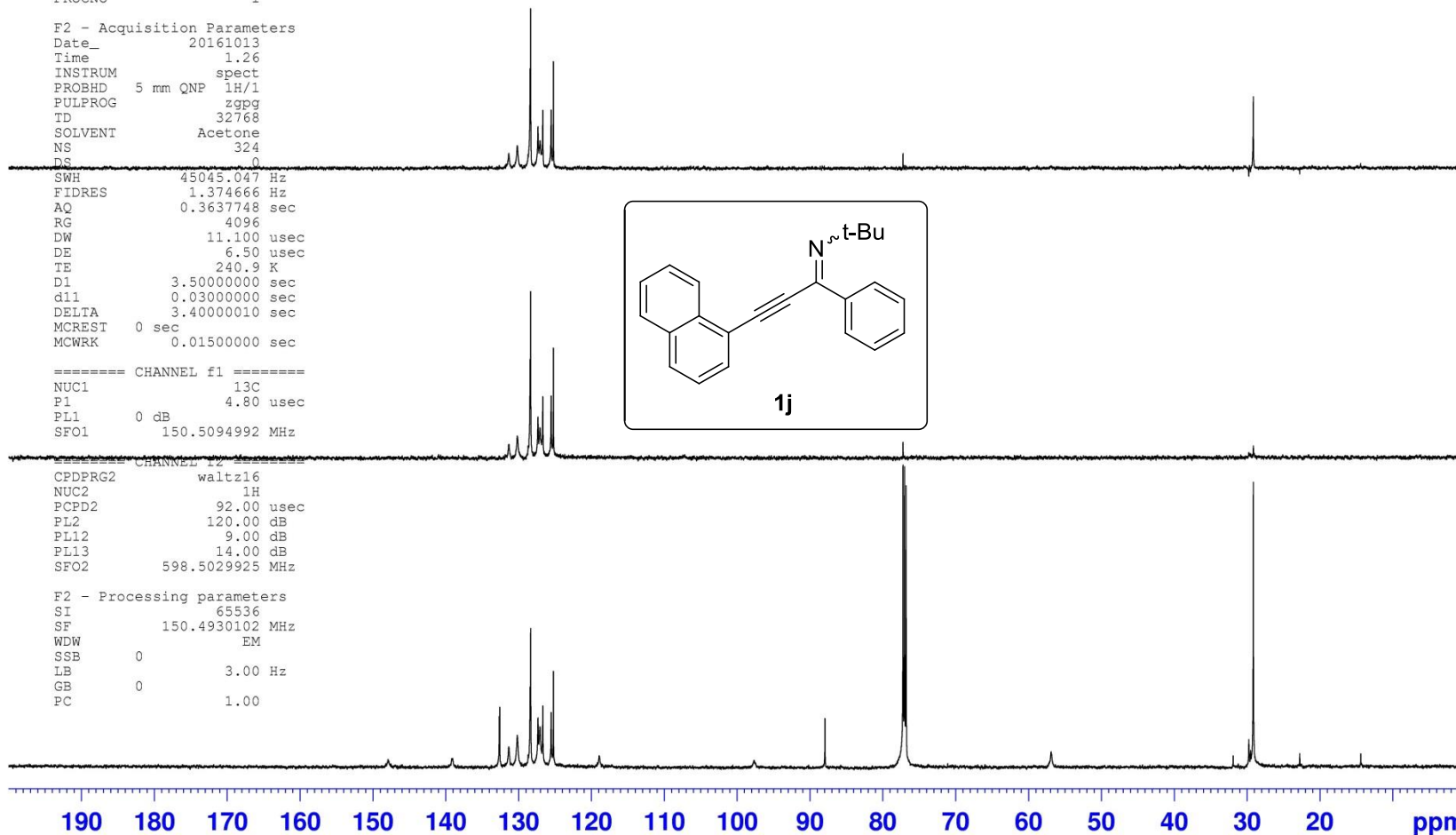
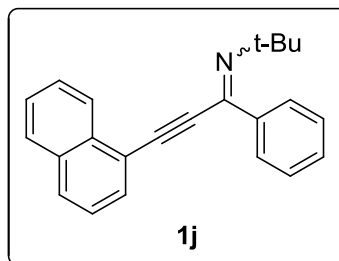
F2 - Acquisition Parameters  
 Date\_ 20161013  
 Time 1.26  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT Acetone  
 NS 324  
 DS 0

SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 240.9 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0 sec  
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0 dB  
 SFO1 150.5094992 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.5029925 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4930102 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00



8.001  
7.998  
7.993  
7.989  
7.687  
7.422  
7.414  
7.388  
7.384  
7.380  
7.376  
7.252  
7.244  
7.240  
7.236

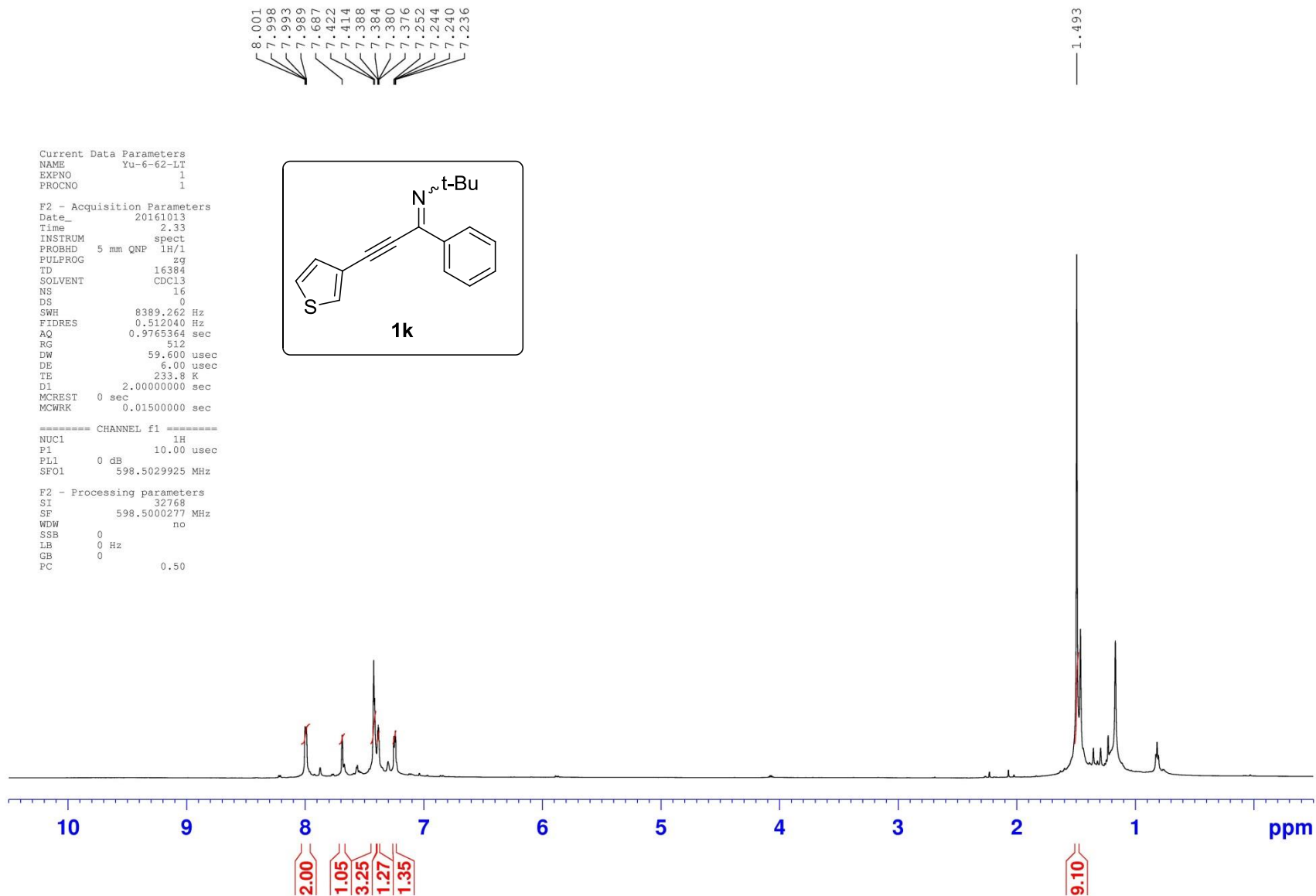
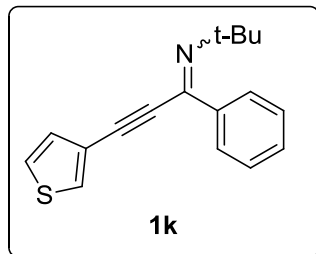
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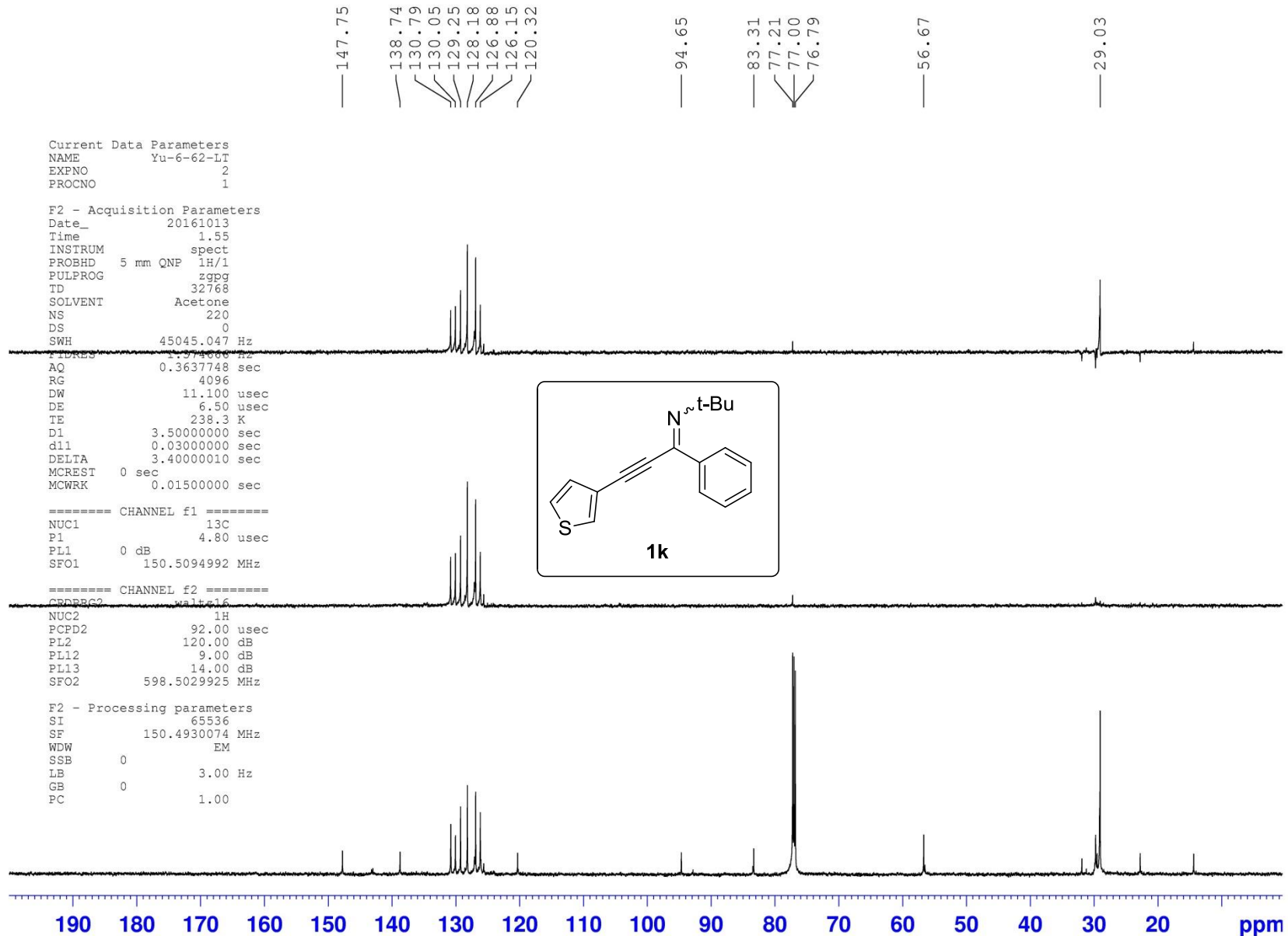
Current Data Parameters
NAME      Yu-6-62-LT
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20161013
Time     2.33
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD        16384
SOLVENT  CDCl3
NS        16
DS        0
SWH       8389.262 Hz
FIDRES    0.512040 Hz
AQ         0.9765364 sec
RG         512
DW         59.600 usec
DE         6.00 usec
TE         233.8 K
D1         2.0000000 sec
MCREST    0 sec
MCNRK     0.0150000 sec

===== CHANNEL f1 =====
NUC1      1H
P1         10.00 usec
PL1        0 dB
SFO1      598.5029925 MHz

F2 - Processing parameters
SI         32768
SF         598.5000277 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0
PC         0.50
  
```



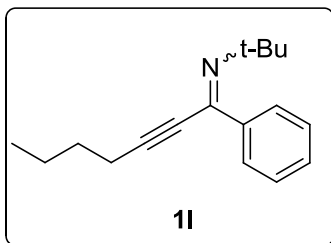


Current Data Parameters  
 NAME Yu-6-33-LT  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160922  
 Time 1.16  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg  
 TD 16384  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8389.262 Hz  
 FIDRES 0.512040 Hz  
 AQ 0.9765364 sec  
 RG 128  
 DW 59.600 usec  
 DE 6.00 usec  
 TE 254.9 K  
 D1 2.00000000 sec  
 MCREST 0 sec  
 MCWRK 0.01500000 sec

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 10.00 usec  
 PL1 0 dB  
 SF01 598.5029925 MHz

F2 - Processing parameters  
 SI 32768  
 SF 598.5000292 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.50

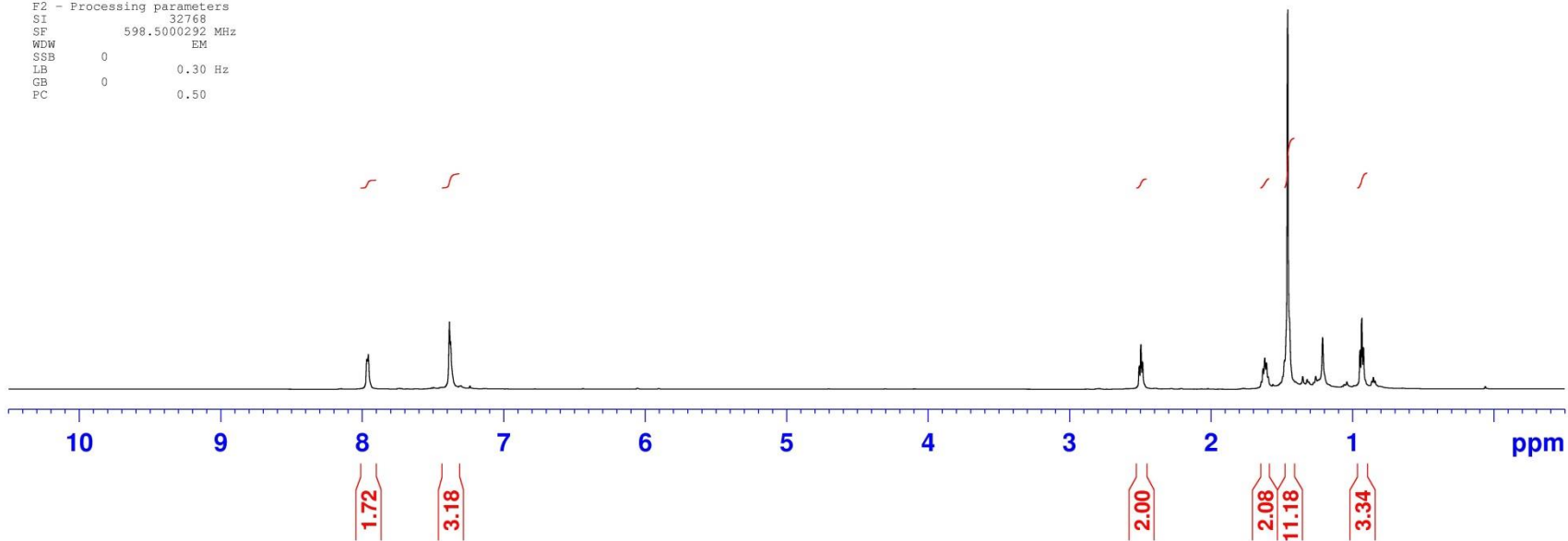


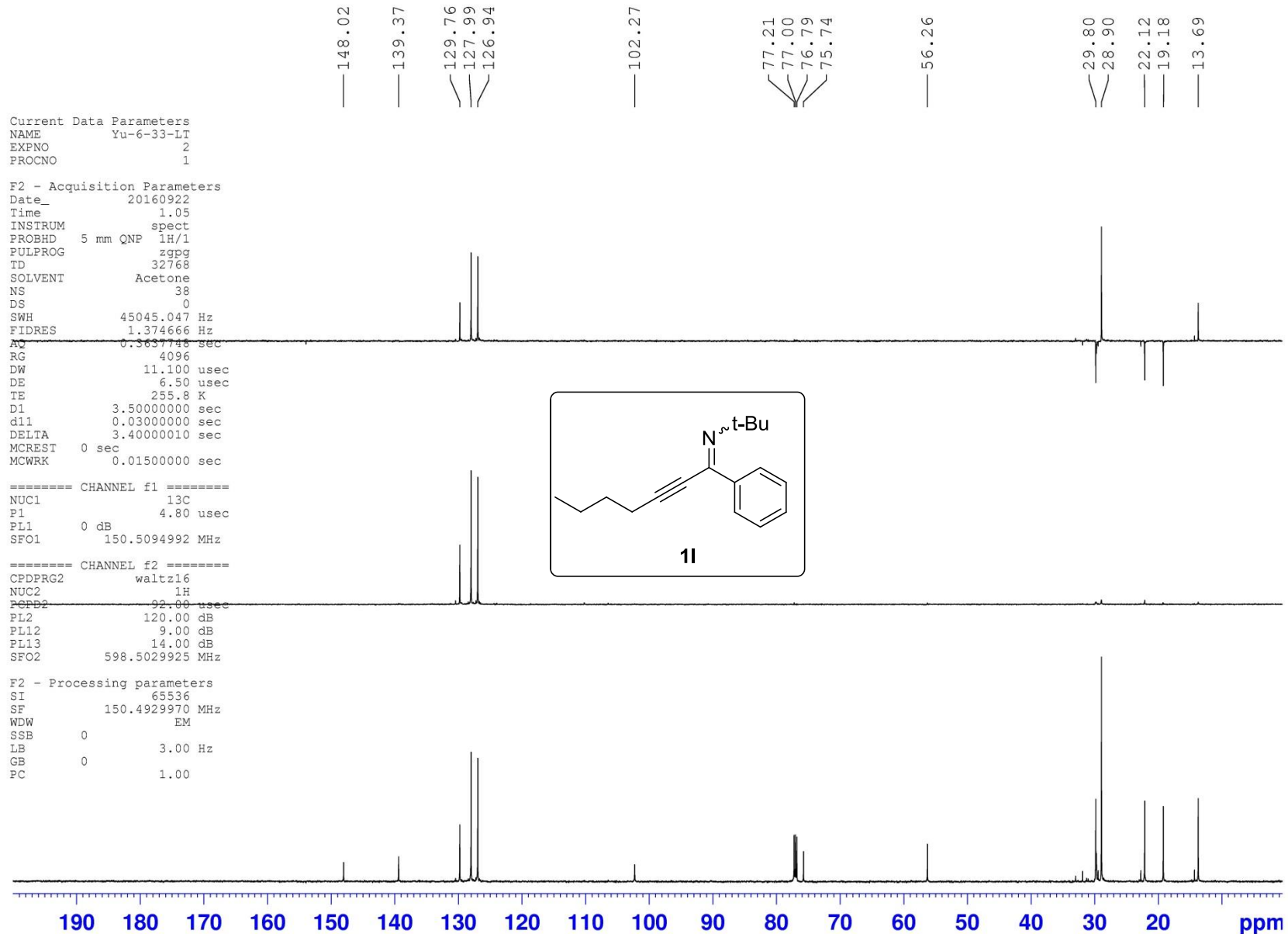
7.969  
7.965  
7.957

7.384  
7.375  
7.240

2.506  
2.497  
2.494  
2.485  
2.482

1.643  
1.631  
1.618  
1.608  
1.596  
1.457  
0.947  
0.945  
0.935  
0.933  
0.923  
0.920







7.912  
7.909  
7.906  
7.899  
7.896  
7.369  
7.362  
7.361  
7.357  
7.350  
7.345  
7.342  
7.336  
7.240

1.539  
1.531  
1.525  
1.522  
1.517  
1.512  
1.508  
1.503  
1.495  
1.404  
0.983  
0.975  
0.970  
0.964  
0.961  
0.957  
0.951  
0.911  
0.905  
0.901  
0.897  
0.893  
0.884

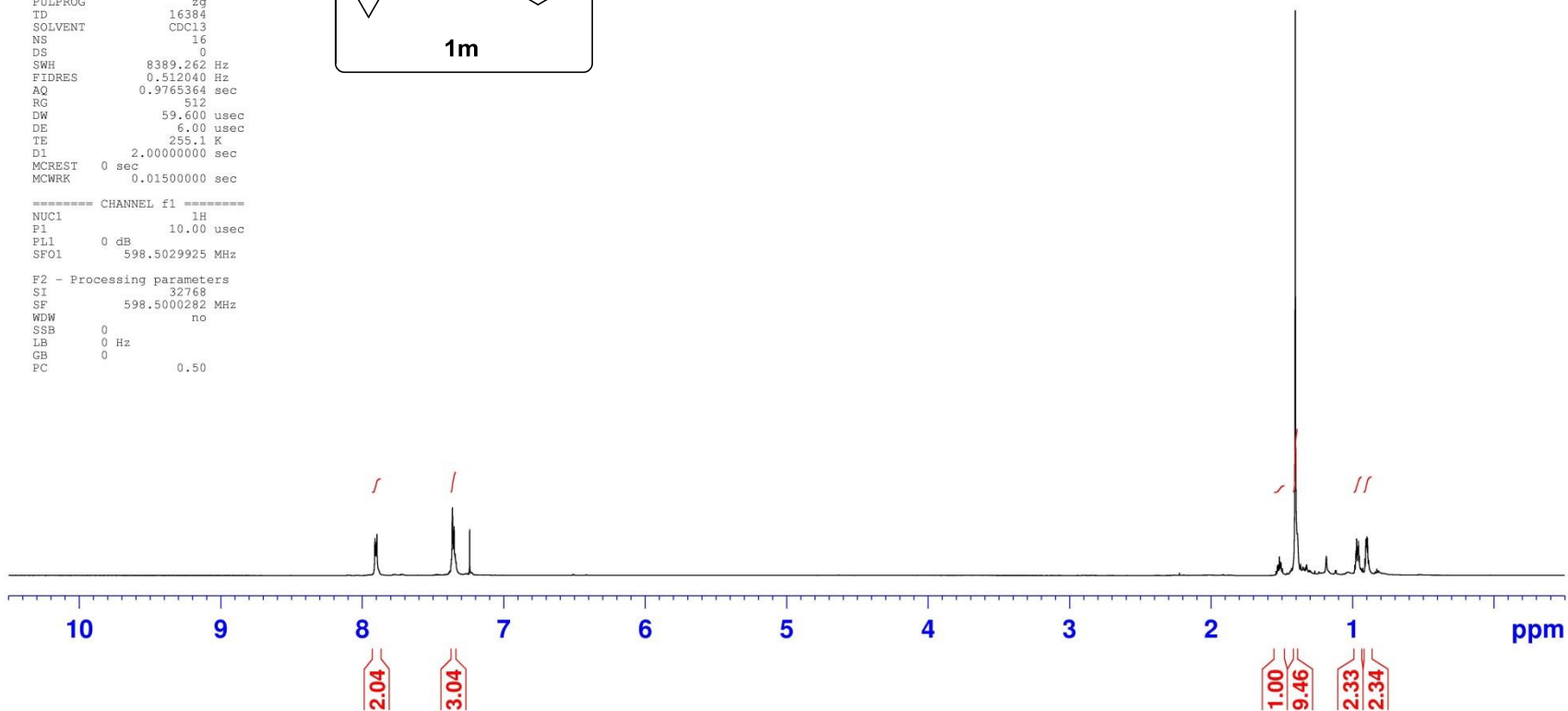
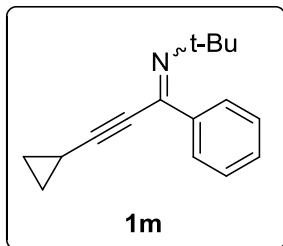
```

Current Data Parameters
NAME      Yu-6-22-LT
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160922
Time     1.22
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD       16384
SOLVENT  CDCl3
NS       16
DS       0
SWH      8389.262 Hz
FIDRES   0.512040 Hz
AQ       0.9765364 sec
RG       512
DW       59.600 usec
DE       6.00 usec
TE       255.1 K
D1       2.00000000 sec
MCREST   0 sec
MCWRK    0.01500000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       10.00 usec
PL1     0 dB
SFO1    598.5029925 MHz

F2 - Processing parameters
SI       32768
SF       598.5000282 MHz
WDW      no
SSB      0
LB       0 Hz
GB       0
PC       0.50
  
```



— 147.92  
 — 139.31  
 \ 129.78  
 \ 128.03  
 \ 126.90  
 — 105.42  
 \ 77.21  
 \ 77.00  
 \ 76.79  
 \ 71.26  
 — 56.24  
 — 28.93  
 — 8.83  
 — 0.30

Current Data Parameters  
 NAME Yu-6-22-LT  
 EXPNO 2  
 PROCNO 1

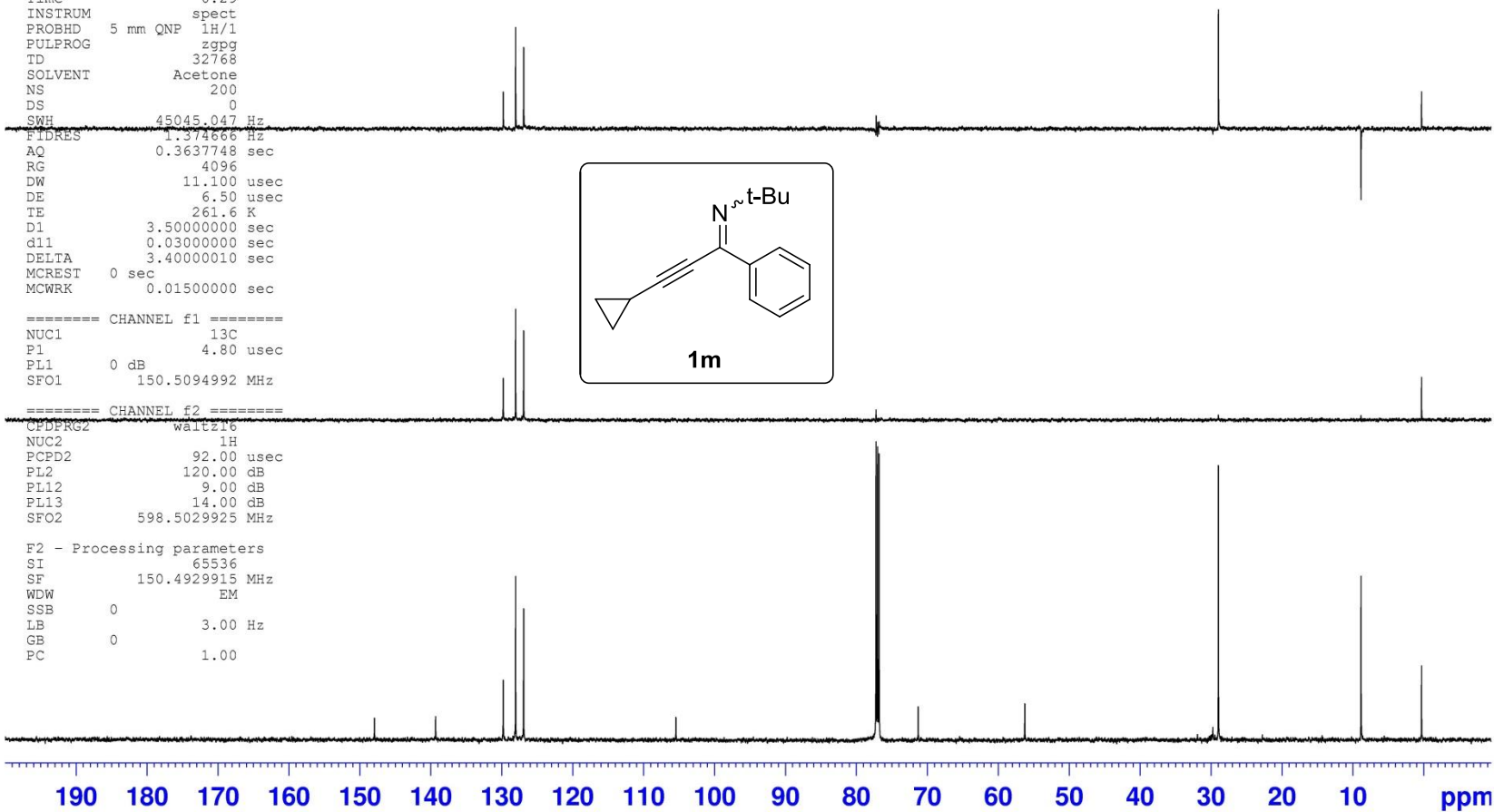
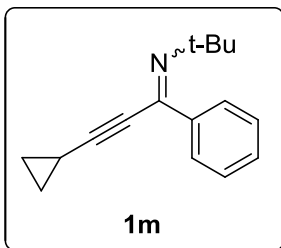
F2 - Acquisition Parameters

Date\_ 20160922  
 Time 0.29  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT Acetone  
 NS 200  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 261.6 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0 sec  
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0 dB  
 SFO1 150.5094992 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.5029925 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4929915 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00



7.996  
7.993  
7.987  
7.984  
7.980  
7.352  
7.348  
7.345  
7.340  
7.338  
7.335  
7.240

2.704  
2.696  
2.689  
2.683  
2.674  
1.924  
1.916  
1.905  
1.761  
1.754  
1.749  
1.745  
1.738  
1.615  
1.599  
1.593  
1.584  
1.577  
1.572  
1.562  
1.554  
1.469  
1.393  
1.378  
1.375  
1.361

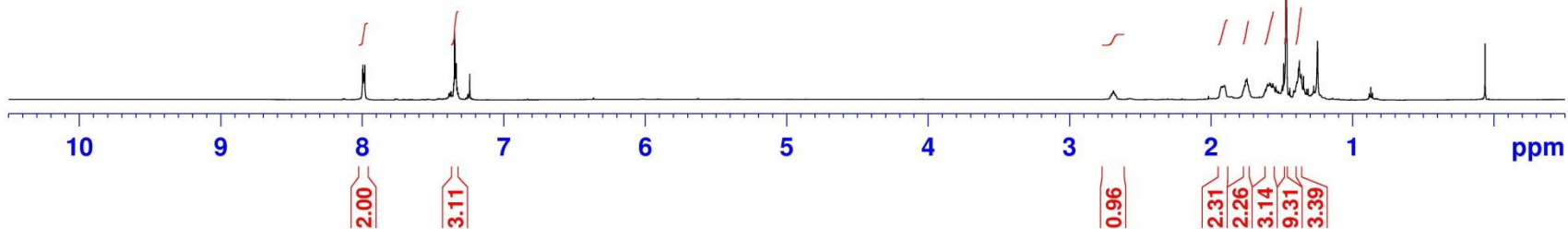
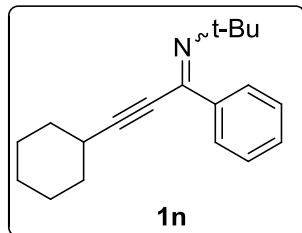
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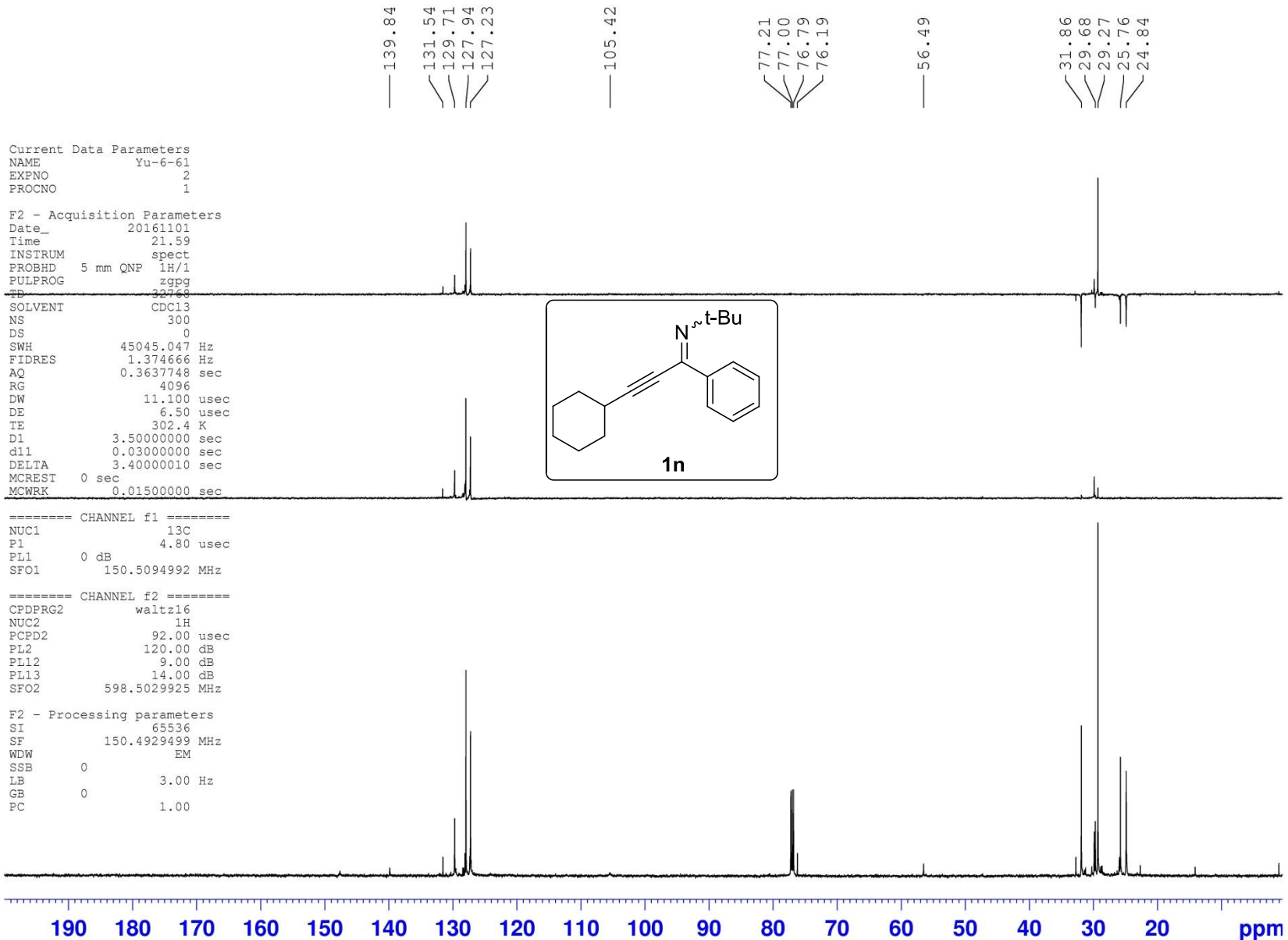
Current Data Parameters
NAME          Yu-6-61
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20161101
Time          21.51
INSTRUM       spect
PROBHD        5 mm QNP 1H/1
PULPROG       zg
TD             32768
SOLVENT       CDC13
NS            16
DS            0
SWH           9541.984 Hz
FIDRES        0.291198 Hz
AQ            1.7170932 sec
RG            512
DW            52.400 usec
DE            6.50 usec
TE            302.3 K
D1            2.0000000 sec
MCREST        0 sec
MCWRK         0.0150000 sec

===== CHANNEL f1 =====
NUC1          1H
P1            9.60 usec
PL1           3.00 dB
SFO1          598.5035910 MHz

F2 - Processing parameters
SI            32768
SF            598.5000278 MHz
WDW           no
SSB           0
LB            0 Hz
GB            0
PC            1.00
  
```



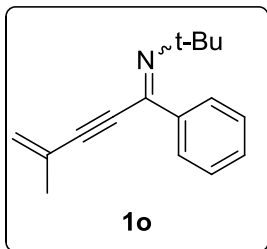


8.000  
7.997  
7.994  
7.993  
7.992  
7.990  
7.989  
7.988  
7.984  
7.981  
7.382  
7.379  
7.378  
7.374  
7.371  
7.370  
7.366  
7.365  
7.363  
7.362  
7.361  
7.360  
7.357  
7.356  
7.354  
7.240  
5.517  
5.515  
5.513  
5.512  
5.511  
5.509  
5.437  
5.434  
5.431  
5.429  
5.426

2.019  
2.018  
2.017  
2.015  
1.486

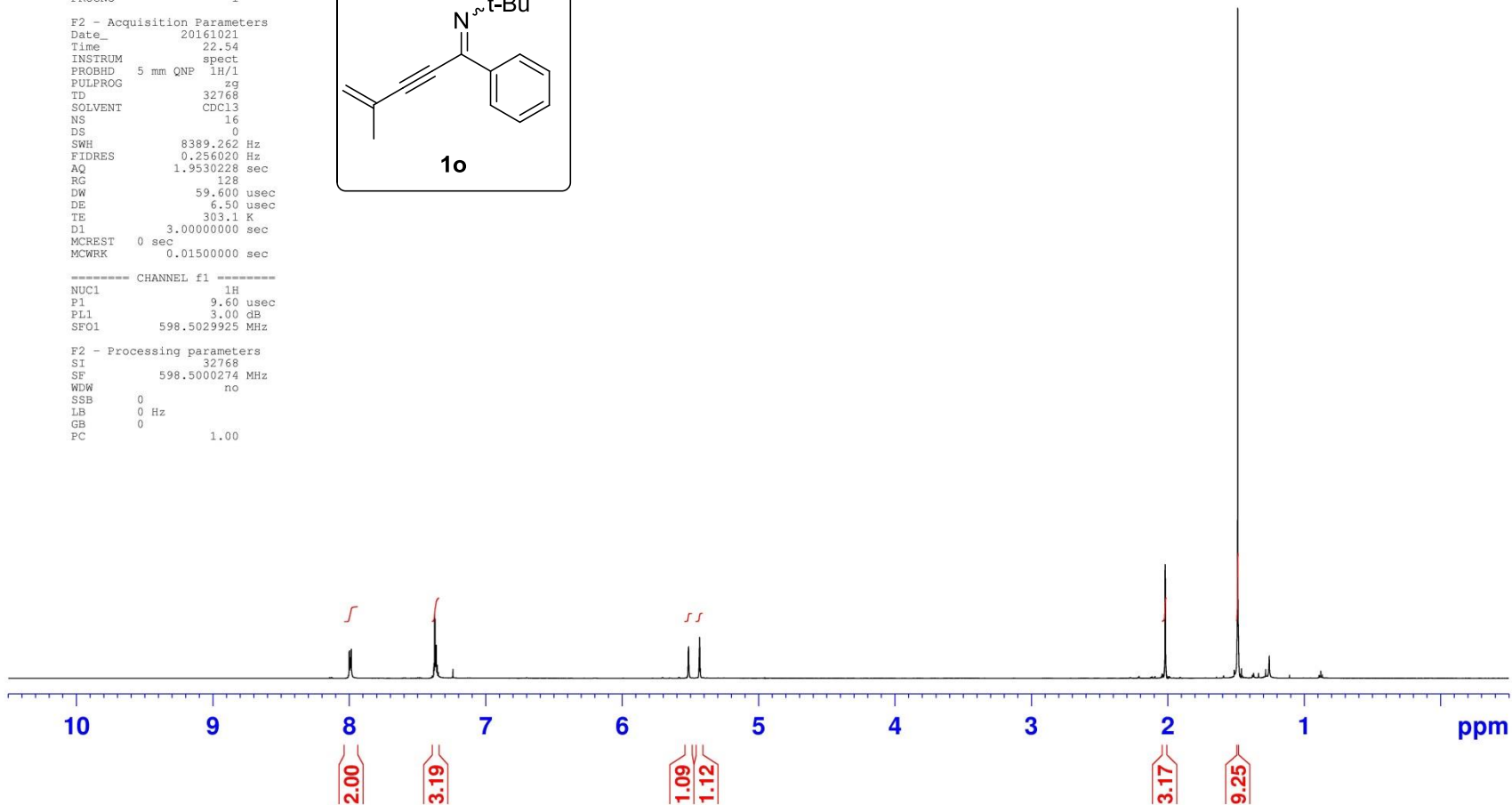
Current Data Parameters  
NAME Yu-6-78  
EXPNO 1  
PROCNO 1

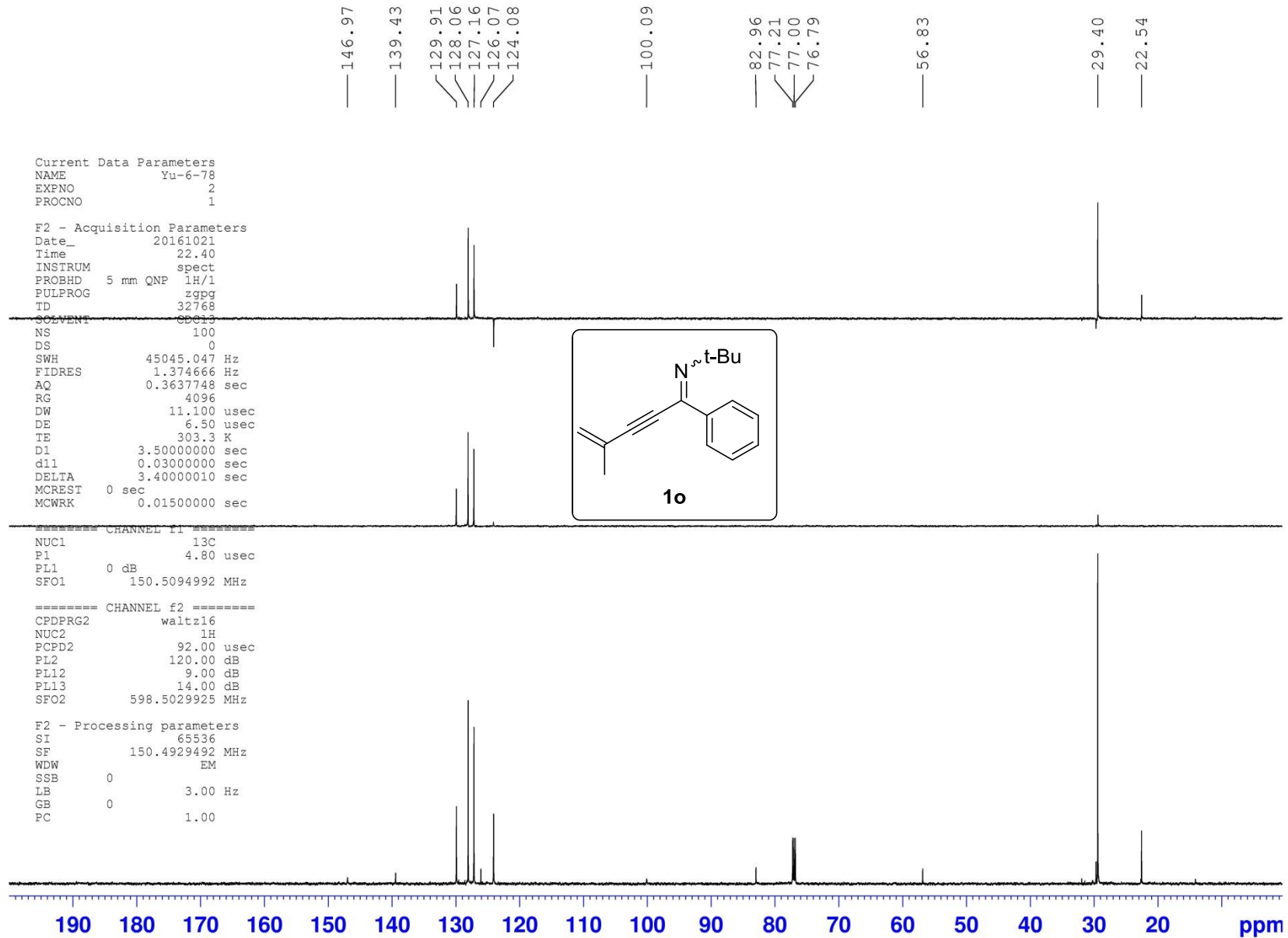
F2 - Acquisition Parameters  
Date\_ 20161021  
Time 22.54  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8389.262 Hz  
FIDRES 0.256020 Hz  
AQ 1.9530228 sec  
RG 128  
DW 59.600 usec  
DE 6.50 usec  
TE 303.1 K  
D1 3.0000000 sec  
MCREST 0 sec  
MCWRK 0.0150000 sec



===== CHANNEL f1 =====  
NUC1 1H  
P1 9.60 usec  
PL1 3.00 dB  
SF01 598.5029925 MHz

F2 - Processing parameters  
SI 32768  
SF 598.5000274 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

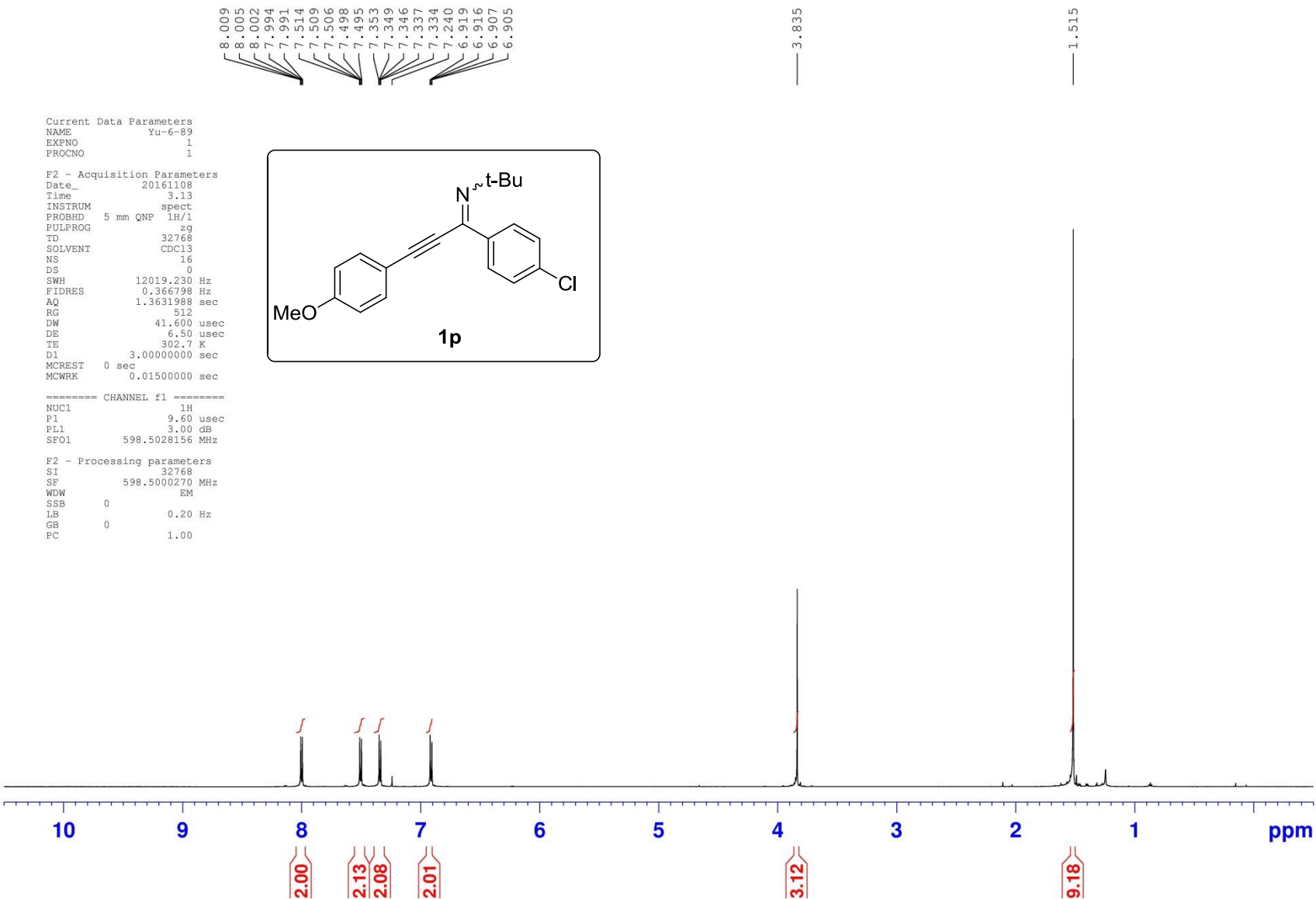
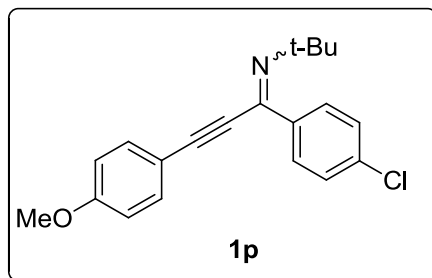


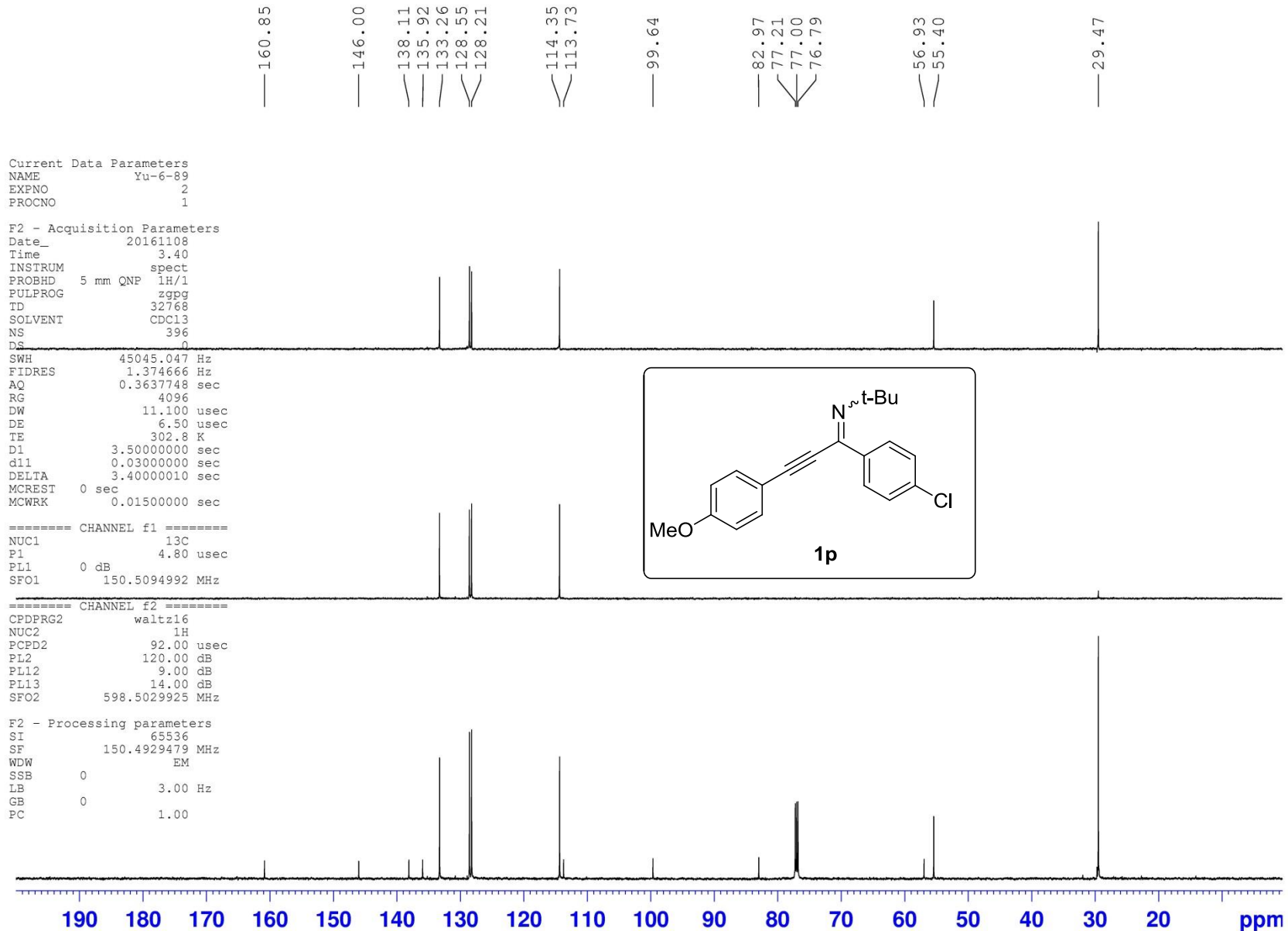


8.009  
8.005  
8.002  
7.994  
7.991  
7.514  
7.509  
7.506  
7.498  
7.495  
7.353  
7.349  
7.346  
7.337  
7.334  
7.240  
6.919  
6.916  
6.907  
6.905

Current Data Parameters  
NAME Yu-6-89  
EXPNO 1  
PROCNO 1

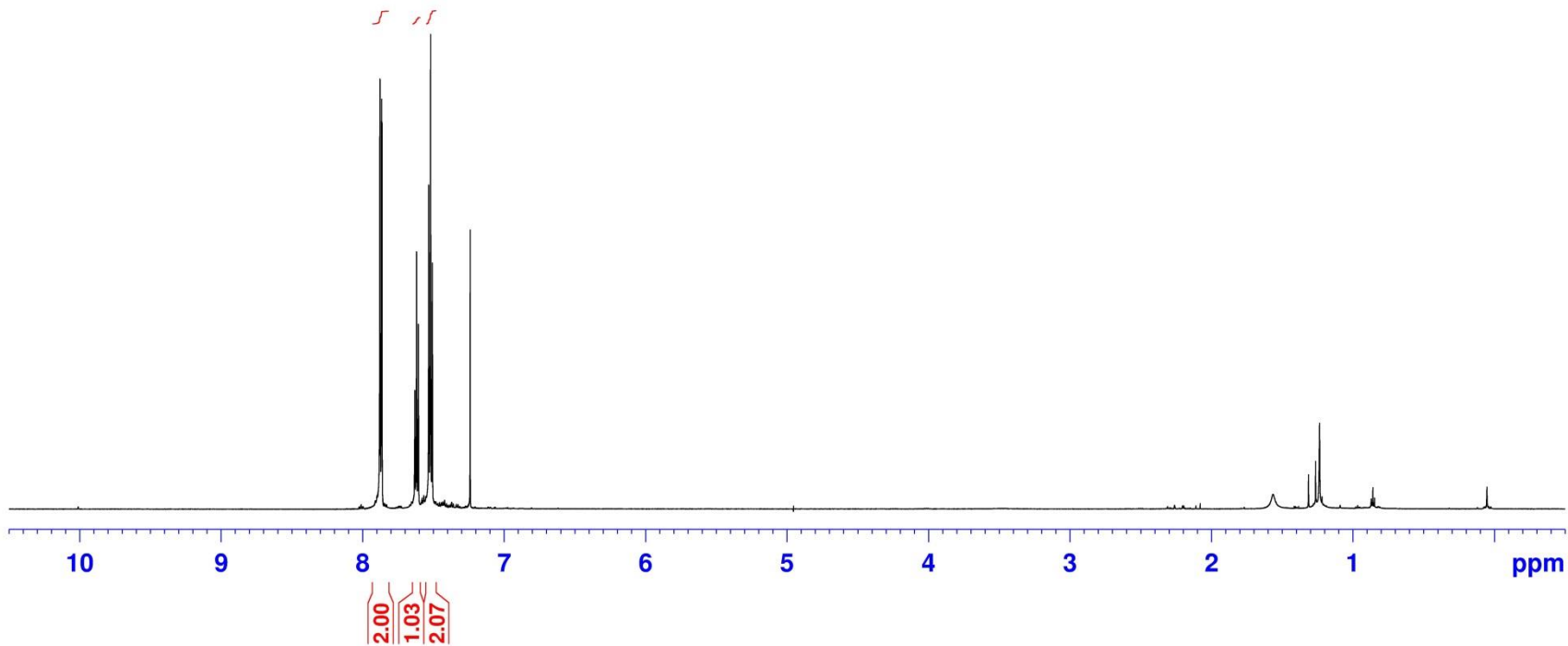
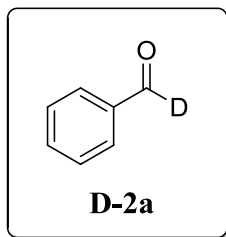
F2 - Acquisition Parameters  
Date\_ 20161108  
Time 3.13  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 512  
DW 41.600 usec  
DE 6.50 usec  
TE 302.7 K  
D1 3.00000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

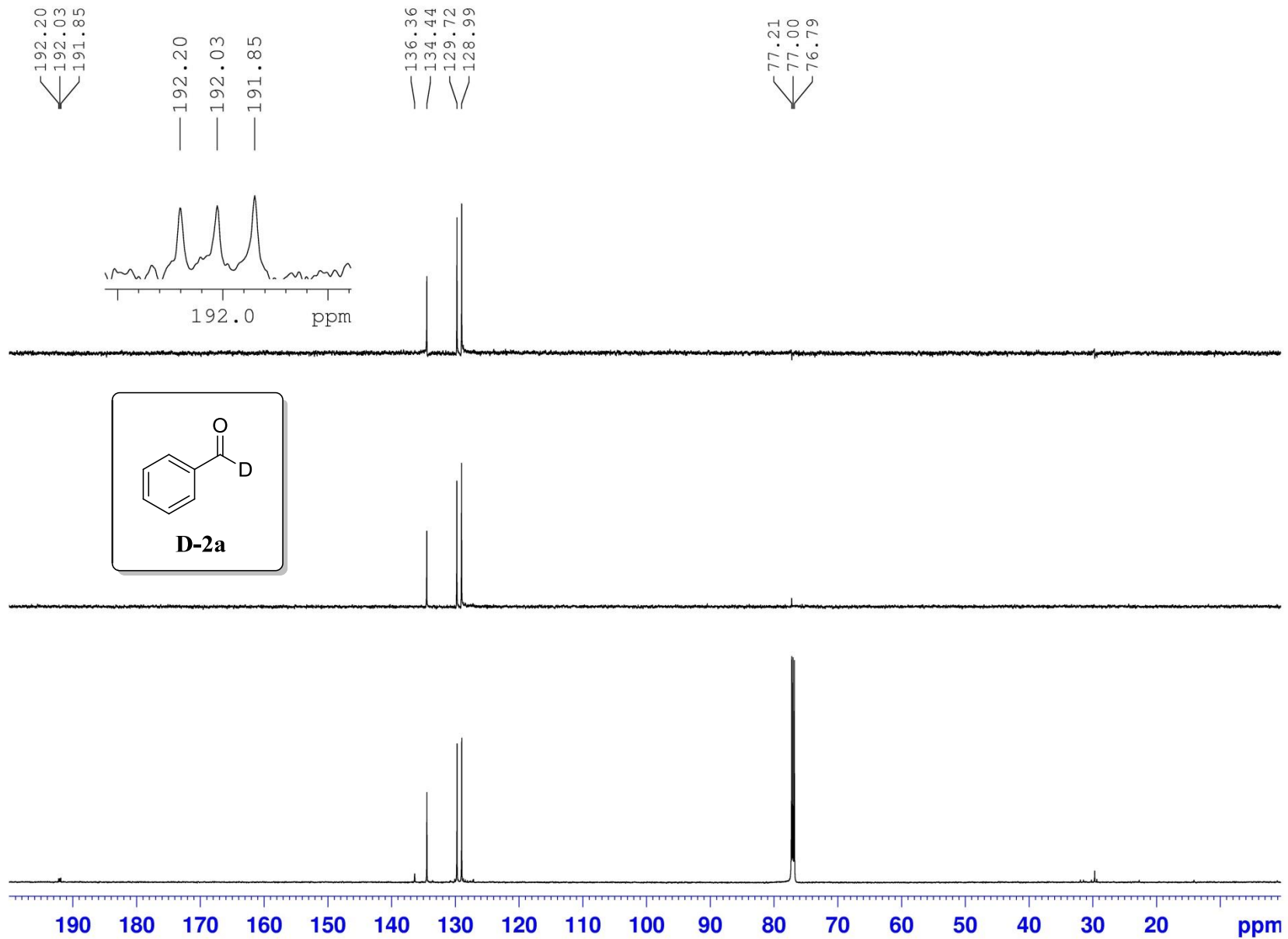






7.879  
7.878  
7.877  
7.869  
7.866  
7.866  
7.864  
7.864  
7.862  
7.862  
7.633  
7.631  
7.630  
7.629  
7.622  
7.620  
7.619  
7.617  
7.616  
7.609  
7.606  
7.605  
7.604  
7.533  
7.533  
7.530  
7.522  
7.520  
7.518  
7.510  
7.508  
7.507  
7.507  
7.240





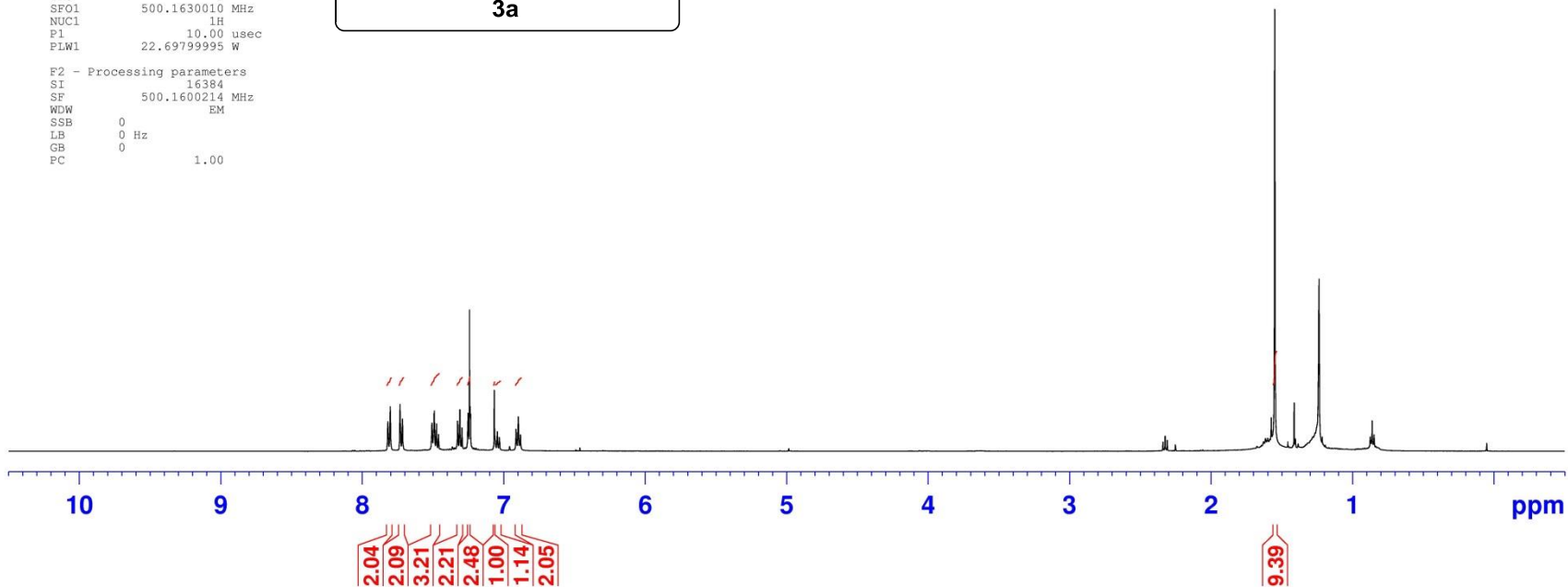
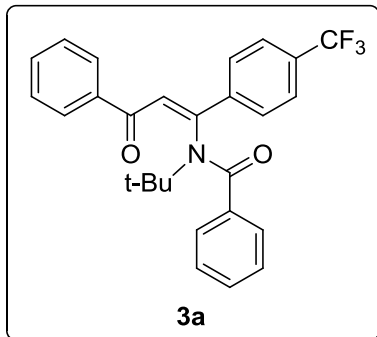
7.817  
7.800  
7.731  
7.714  
7.506  
7.490  
7.489  
7.474  
7.459  
7.324  
7.308  
7.293  
7.250  
7.240  
7.236  
7.233  
7.065  
7.060  
7.043  
7.029  
6.911  
6.896  
6.880

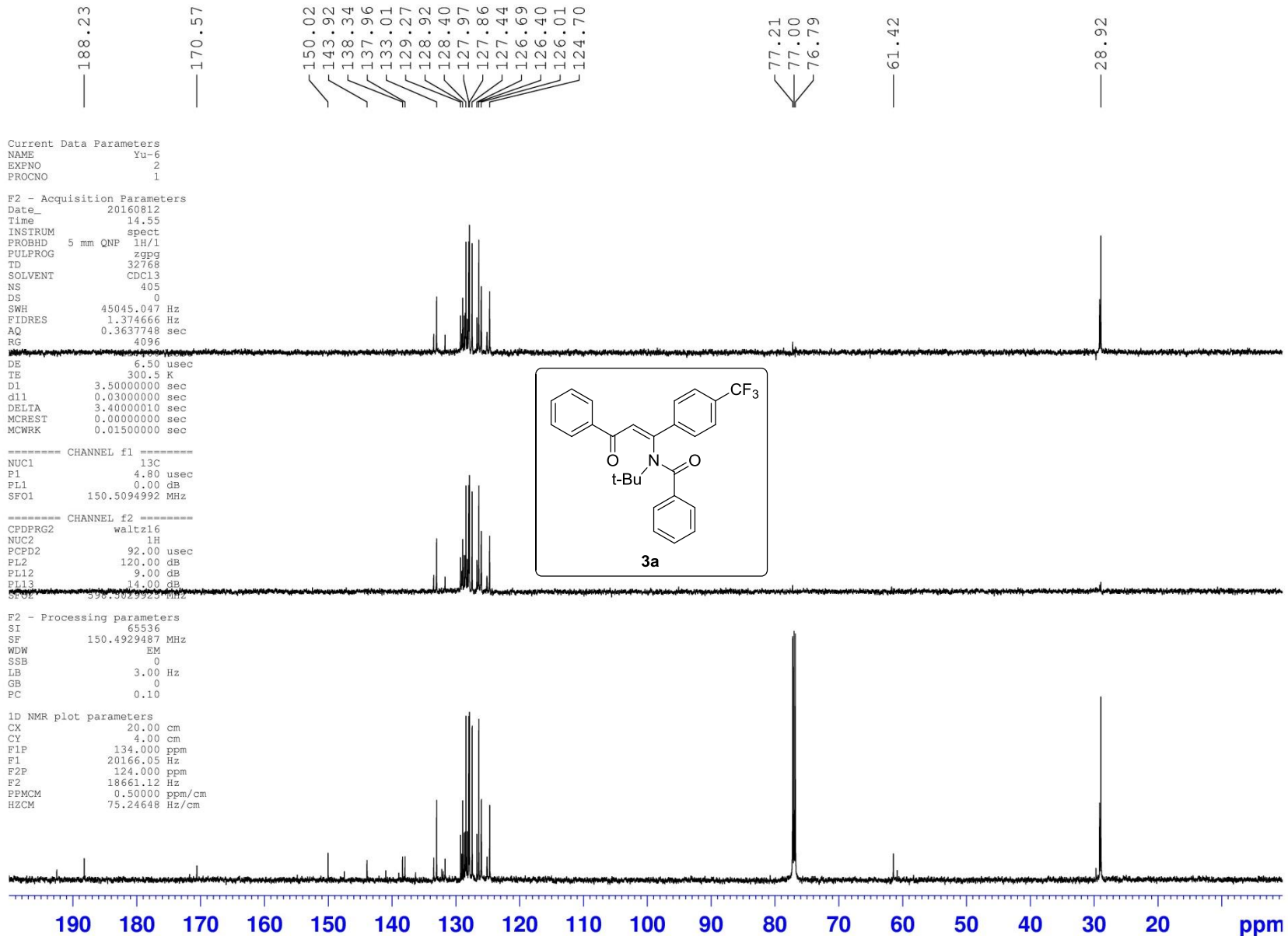
1.548

Current Data Parameters  
NAME liou0817.001  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160816  
Time 16.47 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 10026.738 Hz  
FIDRES 0.305992 Hz  
AQ 1.6340809 sec  
RG 108.84  
DW 49.867 usec  
DE 7.71 usec  
TE 300.0 K  
DL 2.00000000 sec  
TDO 1  
SFO1 500.1630010 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 22.69799995 W

F2 - Processing parameters  
SI 16384  
SF 500.1600214 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



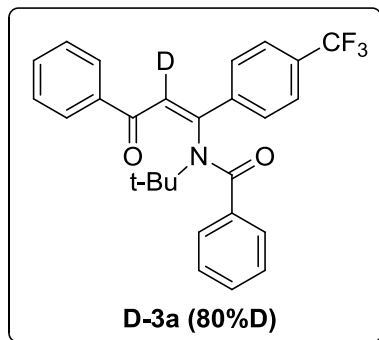


7.816  
7.799  
7.730  
7.713  
7.507  
7.491  
7.474  
7.459  
7.324  
7.309  
7.294  
7.250  
7.240  
7.235  
7.067  
7.057  
7.042  
7.027  
6.910  
6.895  
6.879

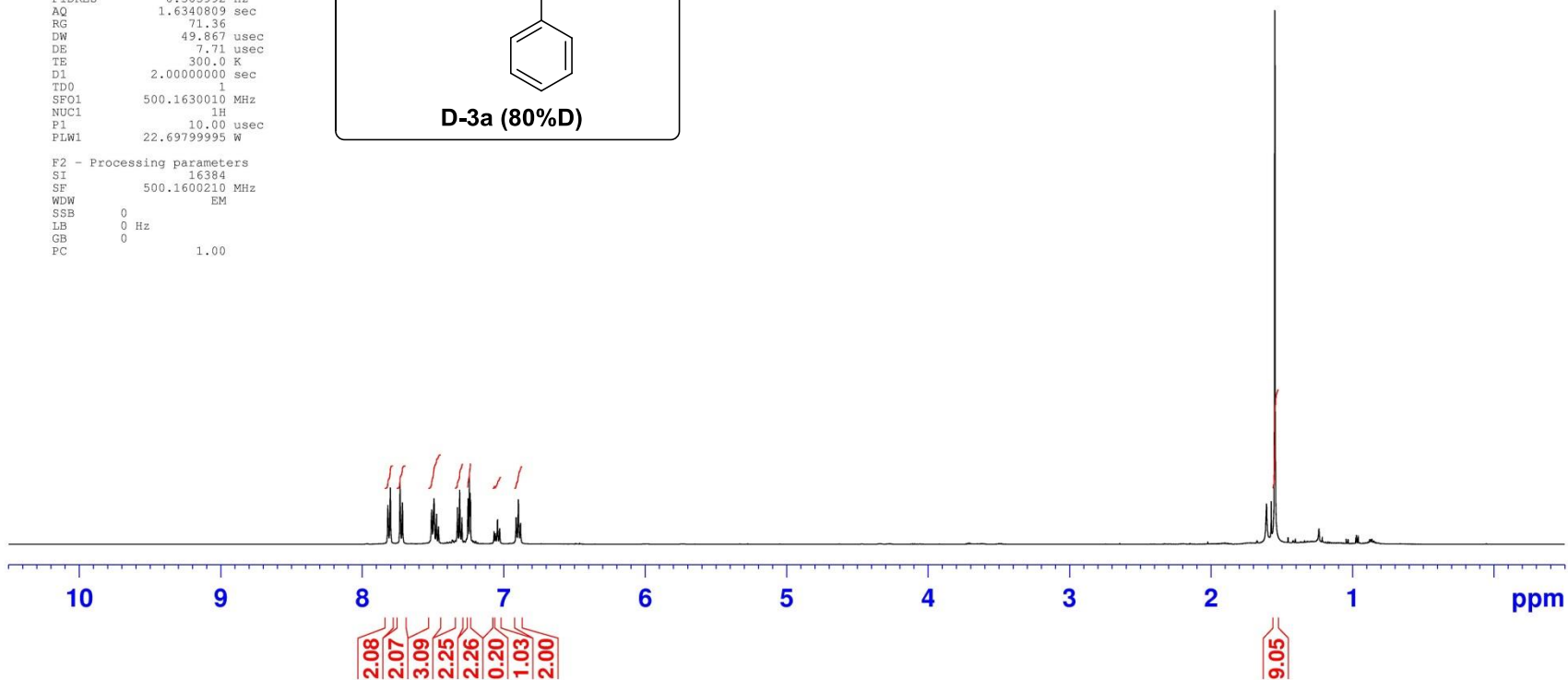
1.547

Current Data Parameters  
NAME liou0818.001  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160817  
Time 16.53 h  
INSTRUM spect  
PROBHD z119470\_0234 (1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 10026.738 Hz  
FIDRES 0.305992 Hz  
AQ 1.6340809 sec  
RG 71.36  
DW 49.867 usec  
DE 7.71 usec  
TE 300.0 K  
D1 2.0000000 sec  
TD0 1  
SFO1 500.1630010 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 22.69799995 W



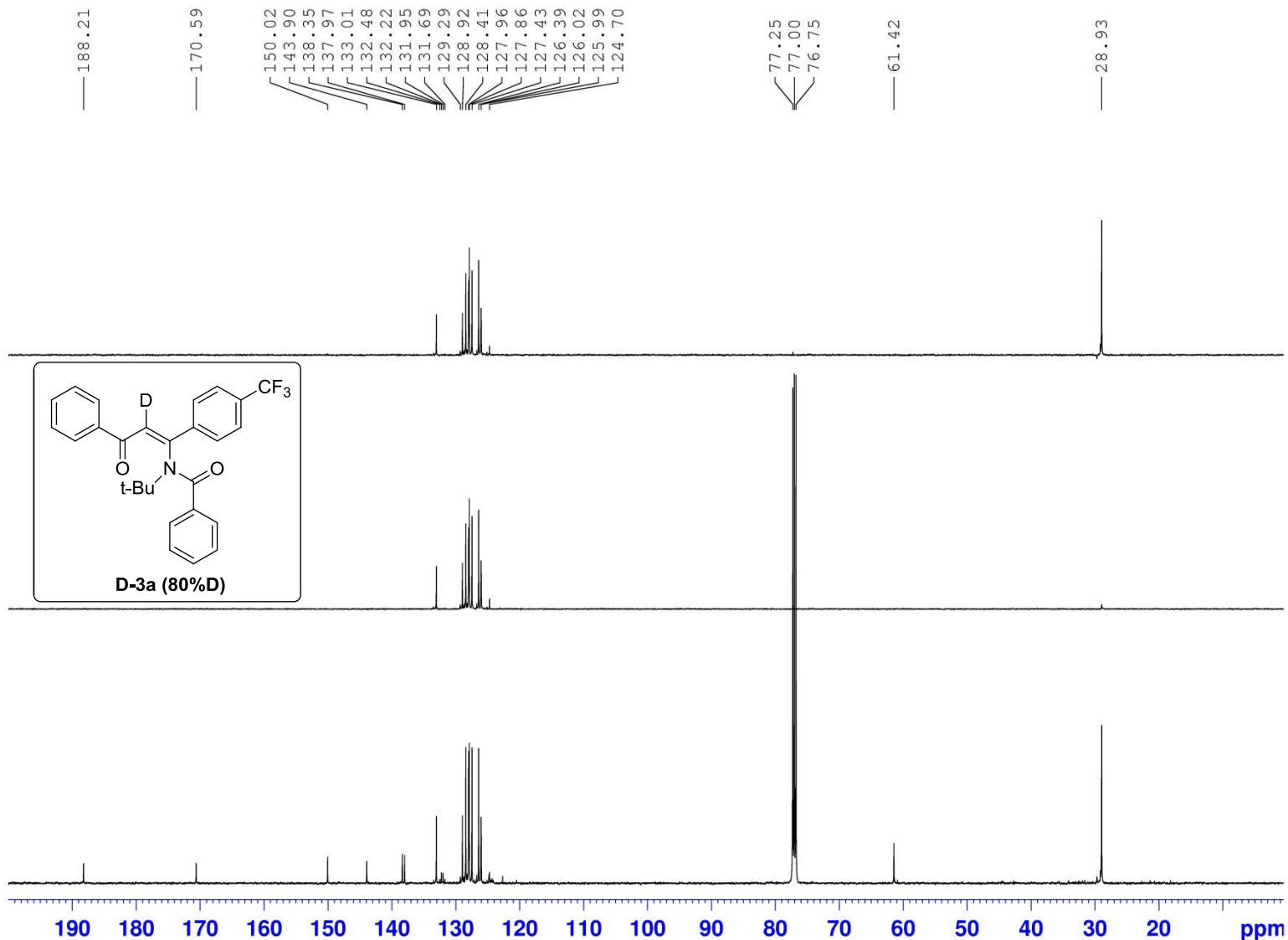
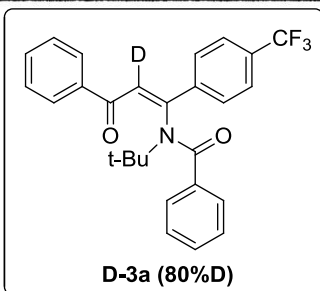
F2 - Processing parameters  
SI 16384  
SF 500.1600210 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



Yu-6-4 / 13C

Current Data Parameters  
NAME liou0818.001  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160817  
Time 17.11 h  
INSTRUM spect  
PROBHD z119470\_0234 (zpgpg30)  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 4098  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7785374 MHz  
NUC1 13C  
F1 10.00 usec  
PLW1 80.55799866 W  
SFO2 500.1620006 MHz  
NUC2 1H  
CPDPRG2 bi\_waltz65\_256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W



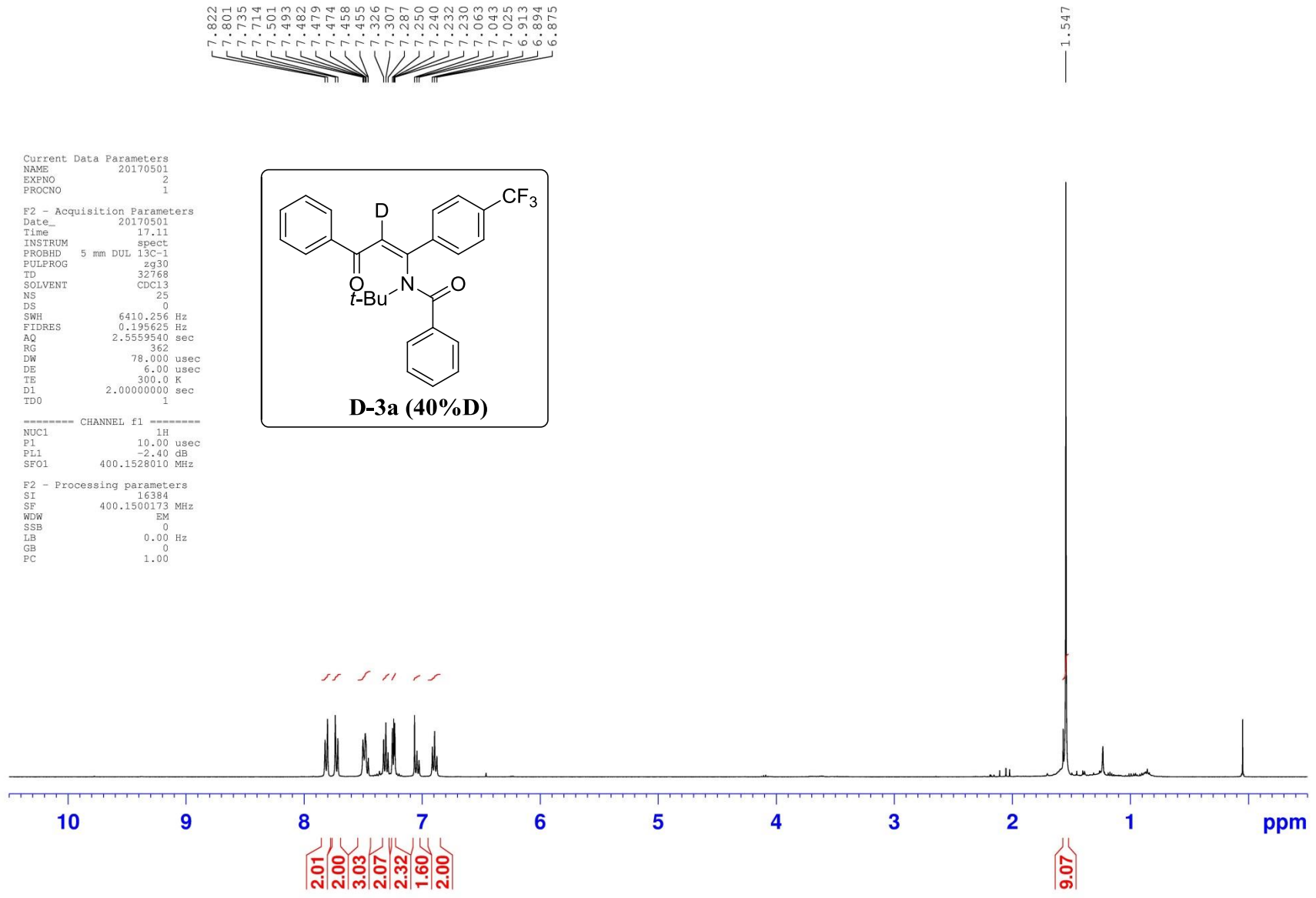
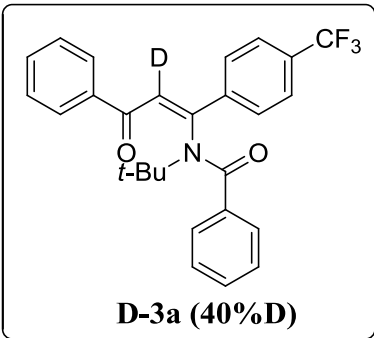
7.822  
7.801  
7.735  
7.714  
7.501  
7.493  
7.482  
7.479  
7.474  
7.458  
7.455  
7.326  
7.307  
7.287  
7.250  
7.240  
7.232  
7.230  
7.063  
7.043  
7.025  
6.913  
6.894  
6.875

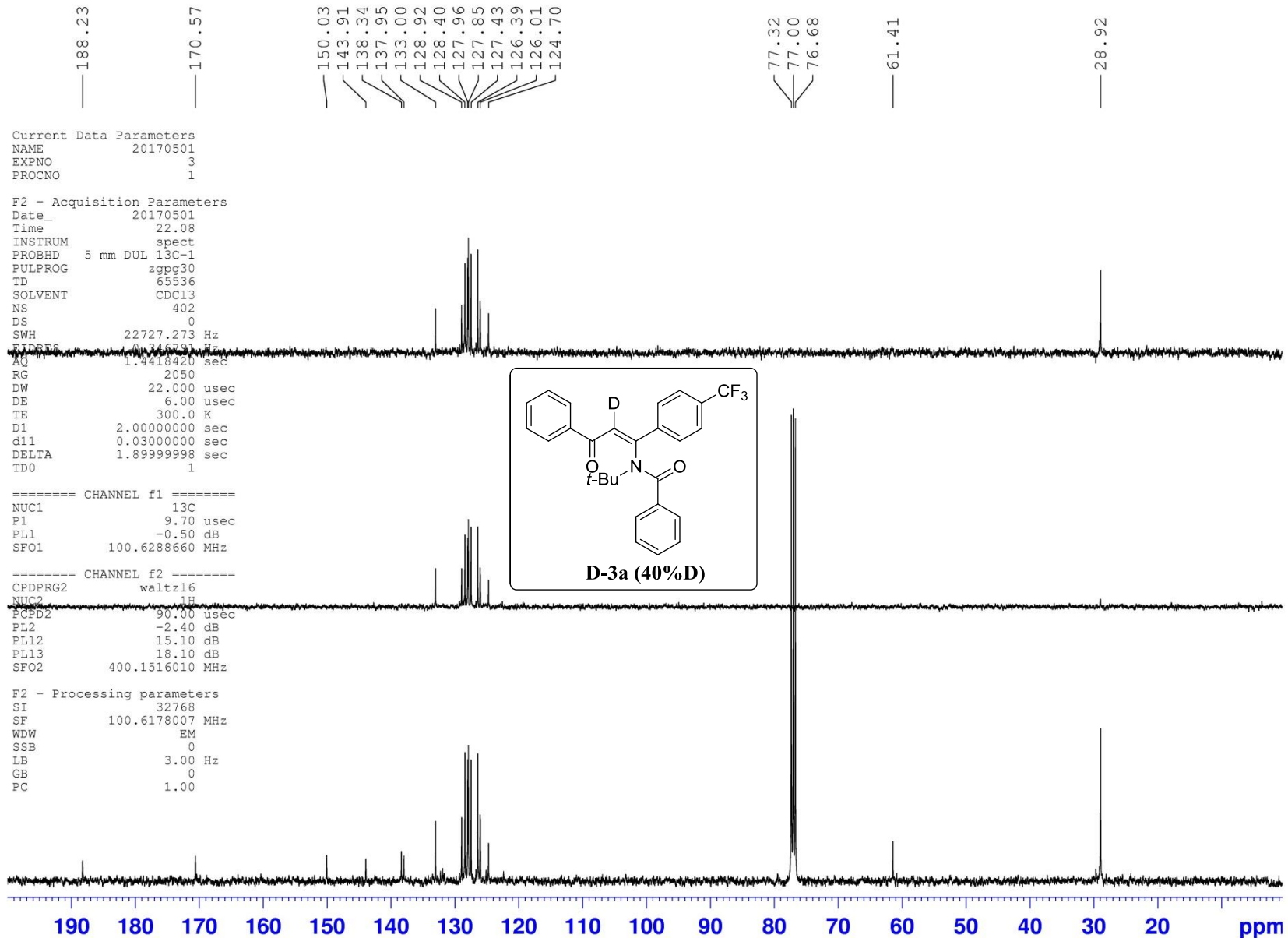
Current Data Parameters  
 NAME 20170501  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20170501  
 Time 17.11  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 25  
 DS 0  
 SWH 6410.256 Hz  
 FIDRES 0.195625 Hz  
 AQ 2.5559540 sec  
 RG 362  
 DW 78.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 DL 2.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 10.00 usec  
 PL1 -2.40 dB  
 SFO1 400.1528010 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1500173 MHz  
 WDW EM  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00



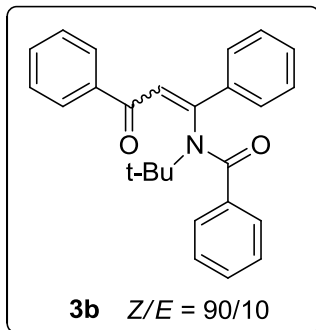




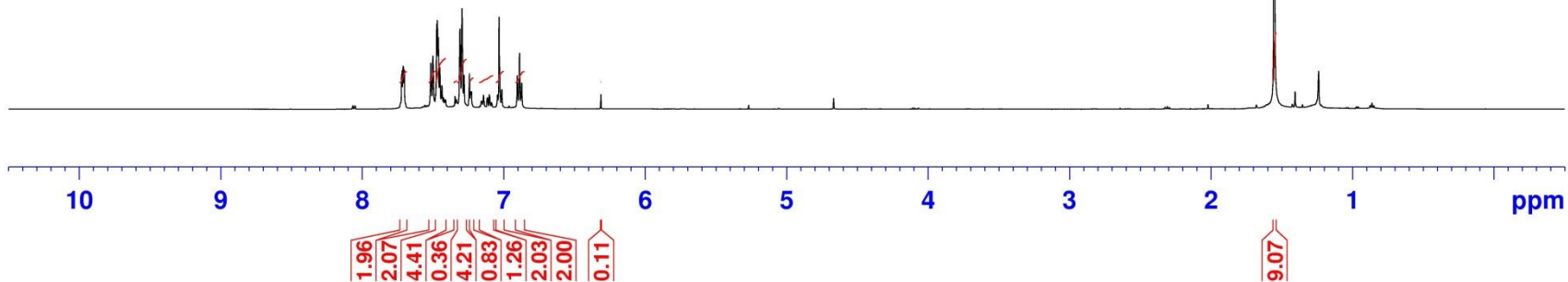
7.720  
7.716  
7.708  
7.701  
7.513  
7.498  
7.472  
7.467  
7.460  
7.450  
7.435  
7.434  
7.426  
7.424  
7.415  
7.409  
7.342  
7.336  
7.331  
7.307  
7.293  
7.279  
7.240  
7.156  
7.152  
7.141  
7.139  
7.115  
7.113  
7.100  
7.098  
7.084  
7.041  
7.031  
7.011  
6.902  
6.886  
6.871  
6.311

Current Data Parameters  
NAME liou0909.001  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160909  
Time 14.31 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 10026.738 Hz  
FIDRES 0.305992 Hz  
AQ 1.6340809 sec  
RG 43.11  
DW 49.867 usec  
DE 7.71 usec  
TE 300.0 K  
D1 2.00000000 sec  
TD0 1  
SFO1 500.1630010 MHz  
NUC1 1H  
F1 10.00 usec  
PLW1 22.69799995 W



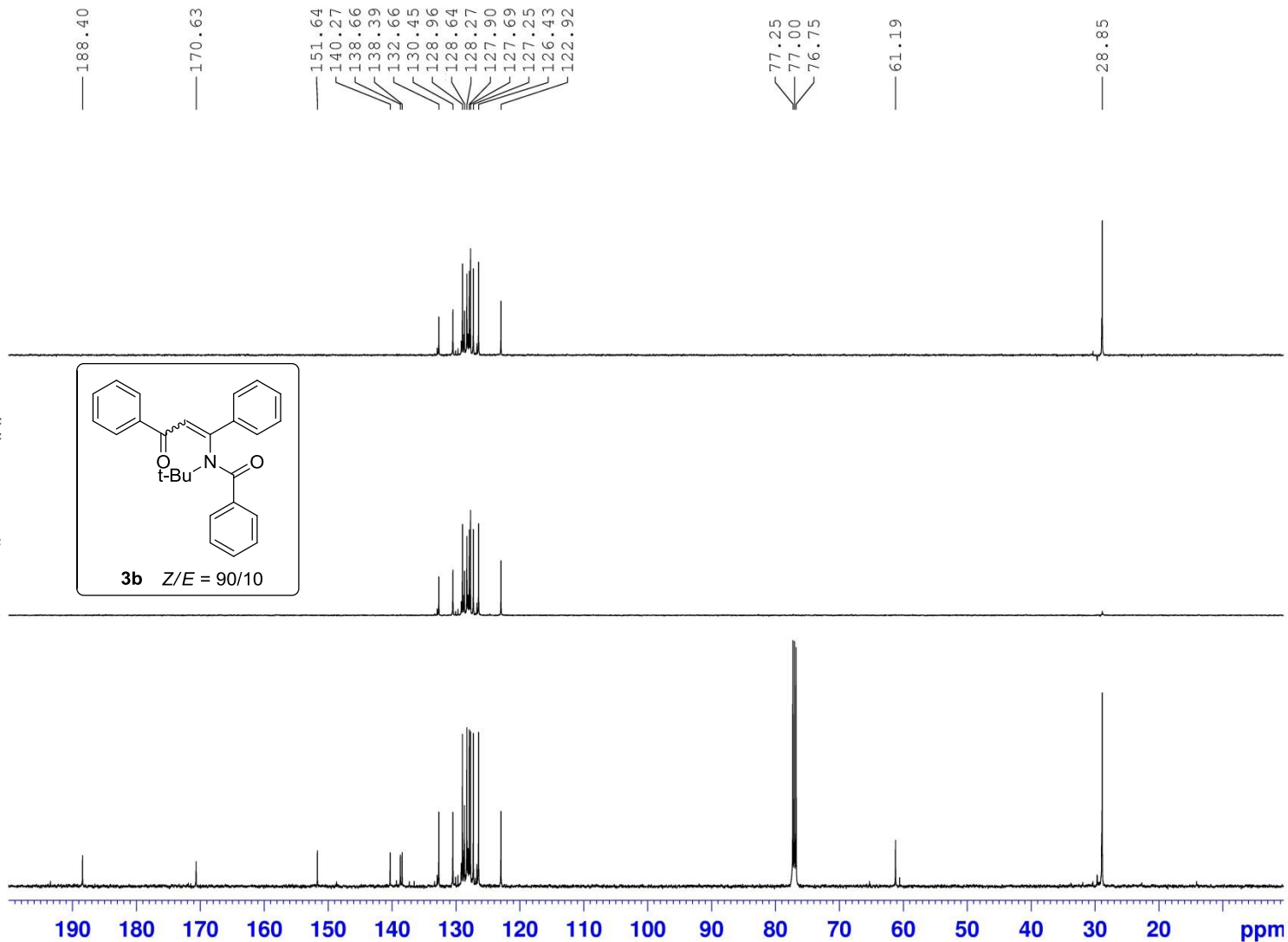
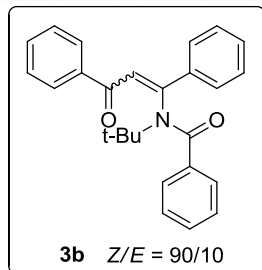
F2 - Processing parameters  
SI 16384  
SF 500.1600210 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



1.552

Current Data Parameters  
NAME liou0909.001  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160909  
Time 14.35 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 465  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7785374 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 80.55799866 W  
SFO2 500.1620006 MHz  
NUC2 1H  
CPDPRG[2] bi\_waltz65 256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W



F2 - Processing parameters  
SI 32768  
SF 125.7653391 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

7.617  
7.601  
7.501  
7.487  
7.485  
7.460  
7.458  
7.456  
7.443  
7.431  
7.428  
7.426  
7.306  
7.290  
7.277  
7.261  
7.240  
7.167  
7.153  
7.150  
7.139  
7.136  
7.123  
7.109  
7.043  
7.029  
7.014  
6.993  
6.906  
6.890  
6.875  
6.240

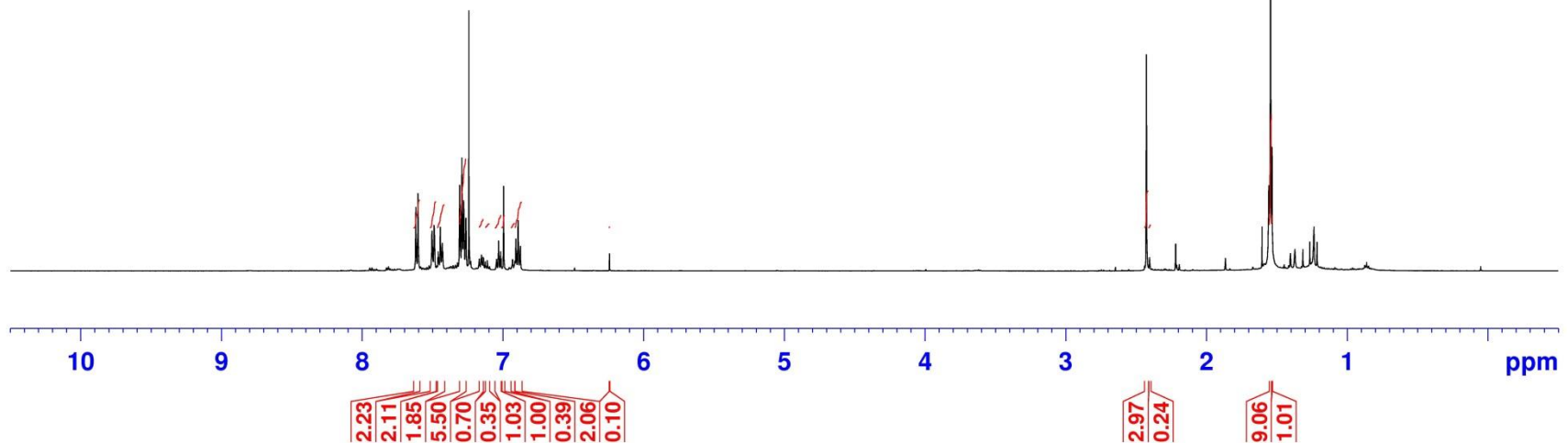
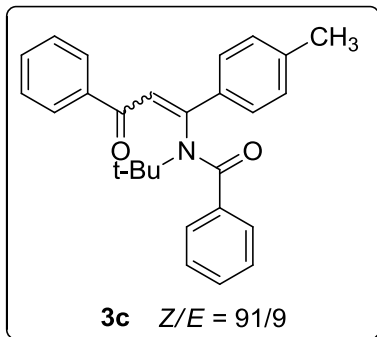
2.426  
2.403

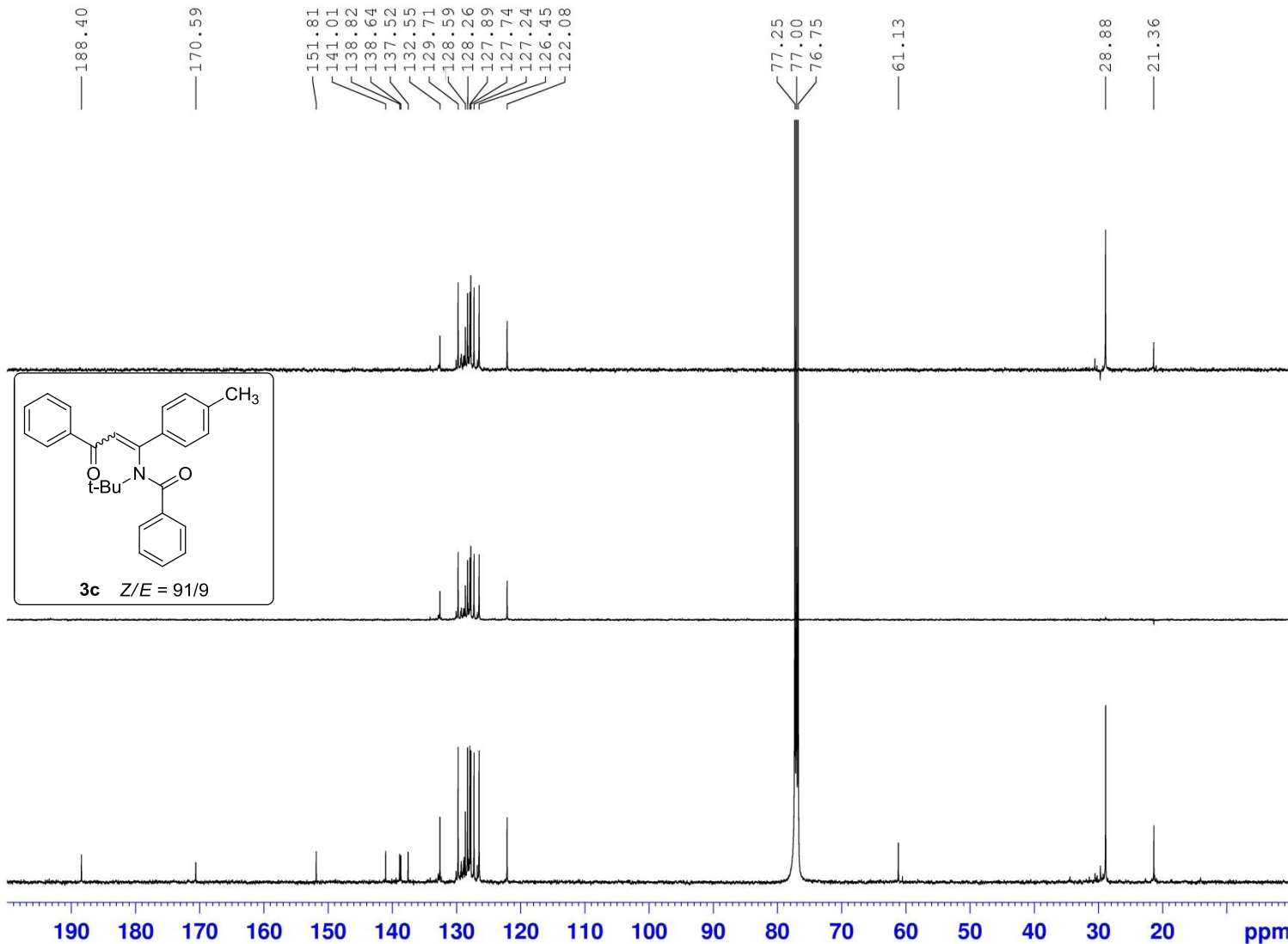
1.544

Current Data Parameters  
 NAME liou1017.001  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161017  
 Time 17.04 h  
 INSTRUM spect  
 PROBHD Z119470\_0234 ( )  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 0  
 SWH 10026.738 Hz  
 FIDRES 0.305992 Hz  
 AQ 1.6340309 sec  
 RG 95.8  
 DW 49.867 usec  
 DE 7.71 usec  
 TE 299.7 K  
 D1 2.00000000 sec  
 TD0 1  
 SFO1 500.1630010 MHz  
 NUC1 1H  
 P1 10.00 usec  
 PLW1 22.69799995 W

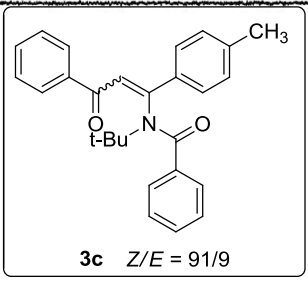
F2 - Processing parameters  
 SI 16384  
 SF 500.1600218 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00





Current Data Parameters  
 NAME liou1017.001  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161017  
 Time 17.11 h  
 INSTRUM spect  
 PROBHD Z119470\_0234 (  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDC13  
 NS 15000  
 DS 0  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 0.5505024 sec  
 RG 191.01  
 DW 16.800 usec  
 DE 6.50 usec  
 TE 300.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 125.7785374 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 80.55799866 W  
 SFO2 500.1620006 MHz  
 NUC2 1H  
 CPDPRG[2 bi\_waltz65 256  
 PCPD2 80.00 usec  
 PLW2 22.69799995 W  
 PLW12 0.36415839 W  
 PLW13 0.18251620 W



F2 - Processing parameters  
 SI 32768  
 SF 125.7653340 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

7.658  
7.647  
7.644  
7.524  
7.512  
7.457  
7.455  
7.444  
7.432  
7.430  
7.312  
7.300  
7.289  
7.287  
7.240  
7.218  
7.213  
7.202  
7.198  
7.189  
7.164  
7.152  
7.150  
7.128  
7.116  
7.102  
7.052  
7.040  
7.027  
6.979  
6.967  
6.964  
6.946  
6.917  
6.904  
6.891  
6.647  
6.644  
6.632  
6.629  
6.221

3.878  
3.709

1.550  
1.541

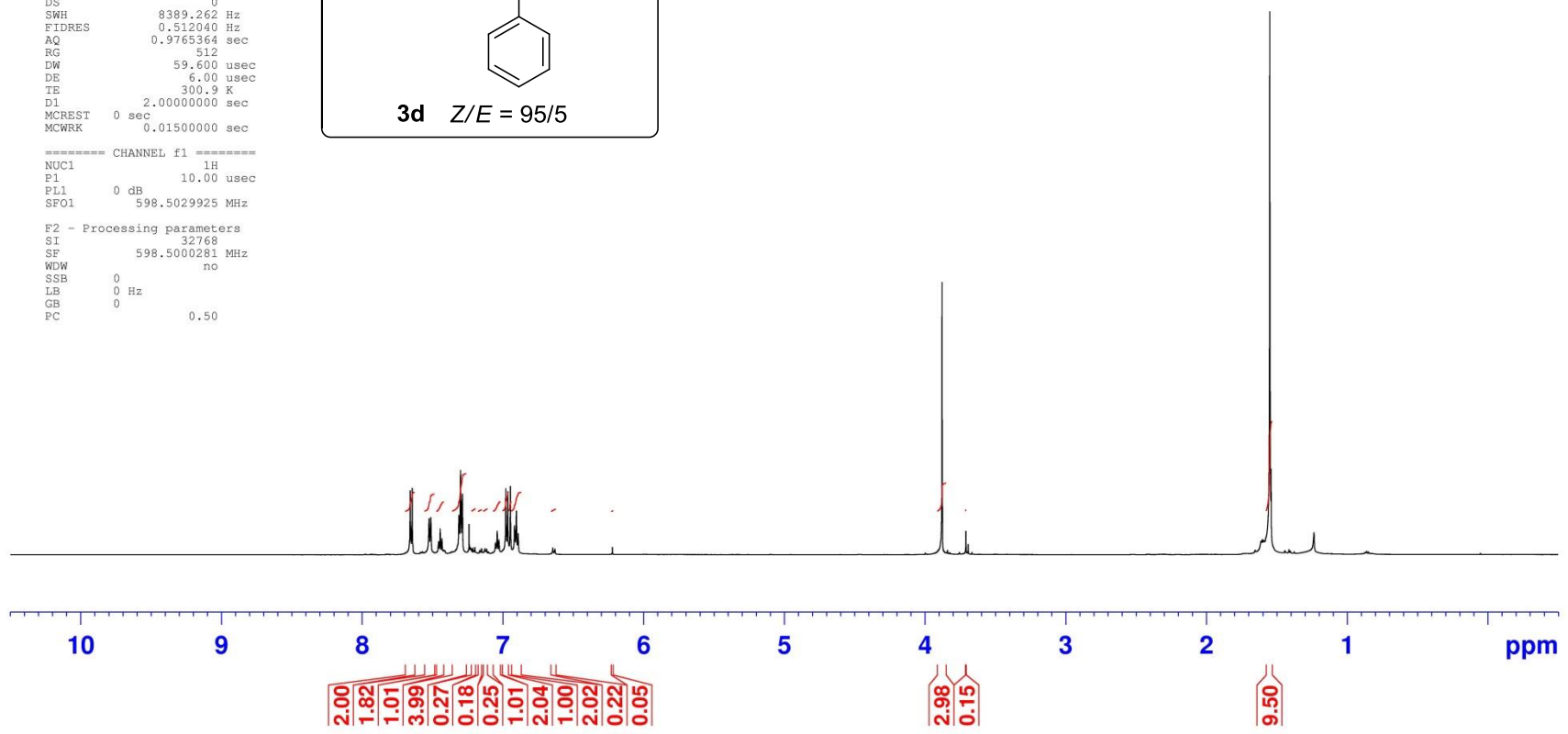
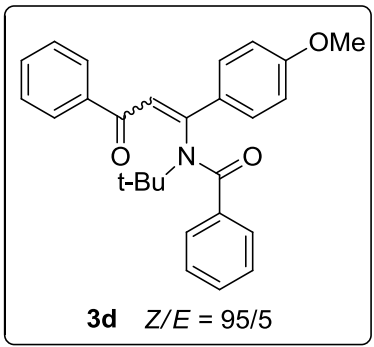
```

Current Data Parameters
NAME      Yu-6-31
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160920
Time     22.46
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD       16384
SOLVENT  CDCl3
NS       16
DS       0
SWH      8389.262 Hz
FIDRES   0.512040 Hz
AQ       0.9765364 sec
RG       512
DW       59.600 usec
DE       6.00 usec
TE       300.9 K
D1       2.00000000 sec
MCREST   0 sec
MCWRK    0.01500000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       10.00 usec
PL1      0 dB
SFO1     598.5029925 MHz

F2 - Processing parameters
SI       32768
SF       598.5000281 MHz
WDW      no
SSB      0
LB       0 Hz
GB       0
PC       0.50
  
```



— 188.30  
 — 170.59  
 — 161.58  
 — 151.60  
 138.89  
 138.81  
 132.59  
 132.47  
 129.35  
 128.58  
 128.25  
 127.85  
 127.22  
 126.35  
 120.93  
 114.33  
 77.21  
 77.00  
 76.79  
 — 61.11  
 — 55.49  
 — 28.89

Current Data Parameters  
 NAME Yu-6-31  
 EXPNO 2  
 PROCNO 1

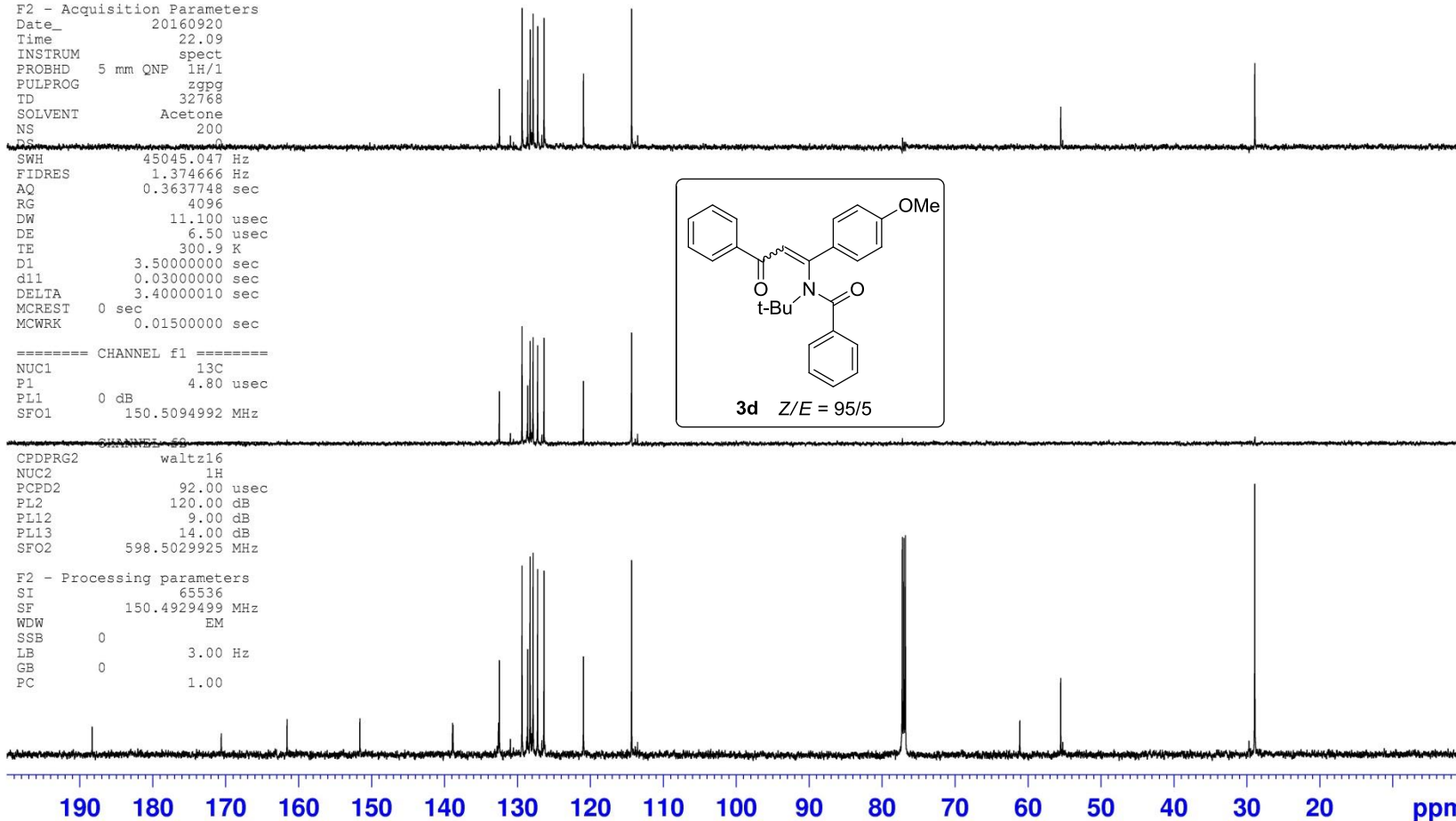
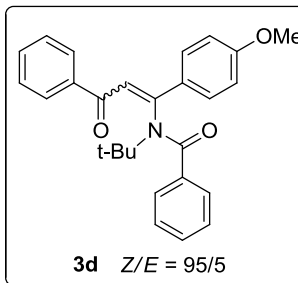
F2 - Acquisition Parameters

Date\_ 20160920  
 Time 22.09  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpgg  
 TD 32768  
 SOLVENT Acetone  
 NS 200  
 DS 4  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 300.9 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0 sec  
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0 dB  
 SFO1 150.5094992 MHz

CHANNELS 50  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.5029925 MHz

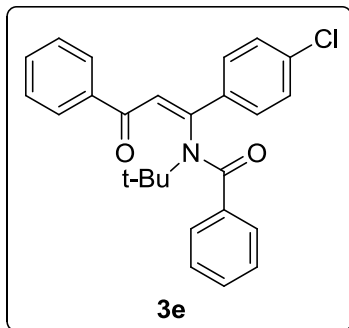
F2 - Processing parameters  
 SI 65536  
 SF 150.4929499 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00



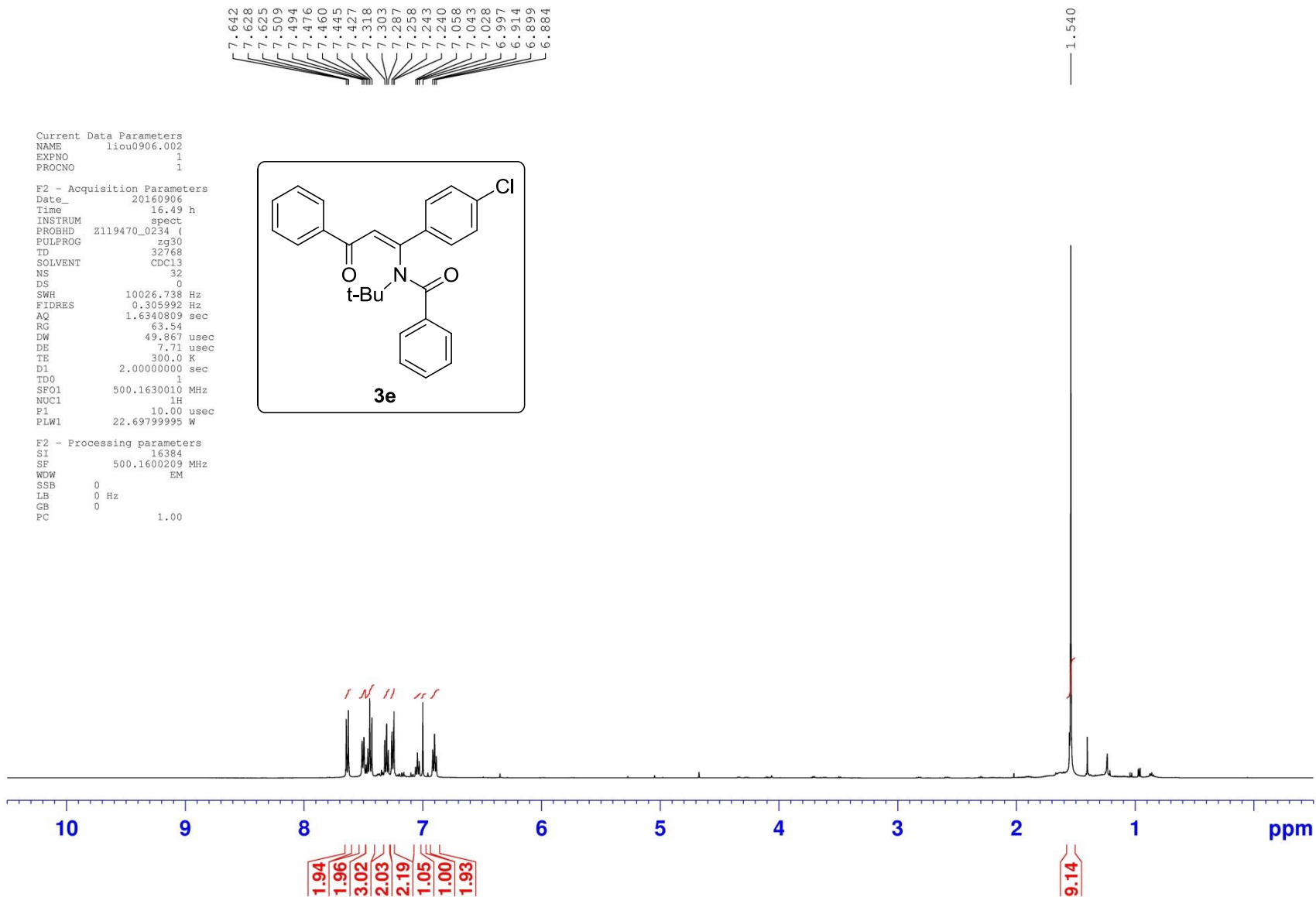
7.642  
7.628  
7.625  
7.509  
7.494  
7.476  
7.460  
7.445  
7.427  
7.318  
7.303  
7.287  
7.258  
7.243  
7.240  
7.058  
7.043  
7.028  
6.997  
6.914  
6.899  
6.884

Current Data Parameters  
NAME liou0906.002  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160906  
Time 16.49 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zg30  
TD 32768  
SOLVENT CDC13  
NS 32  
DS 0  
SWH 10026.738 Hz  
FIDRES 0.305992 Hz  
AQ 1.6340809 sec  
RG 63.54  
DW 49.867 usec  
DE 7.71 usec  
TE 300.0 K  
D1 2.00000000 sec  
TDO 1  
SFO1 500.1630010 MHz  
NUC1 1H  
F1 10.00 usec  
PLW1 22.69799995 W

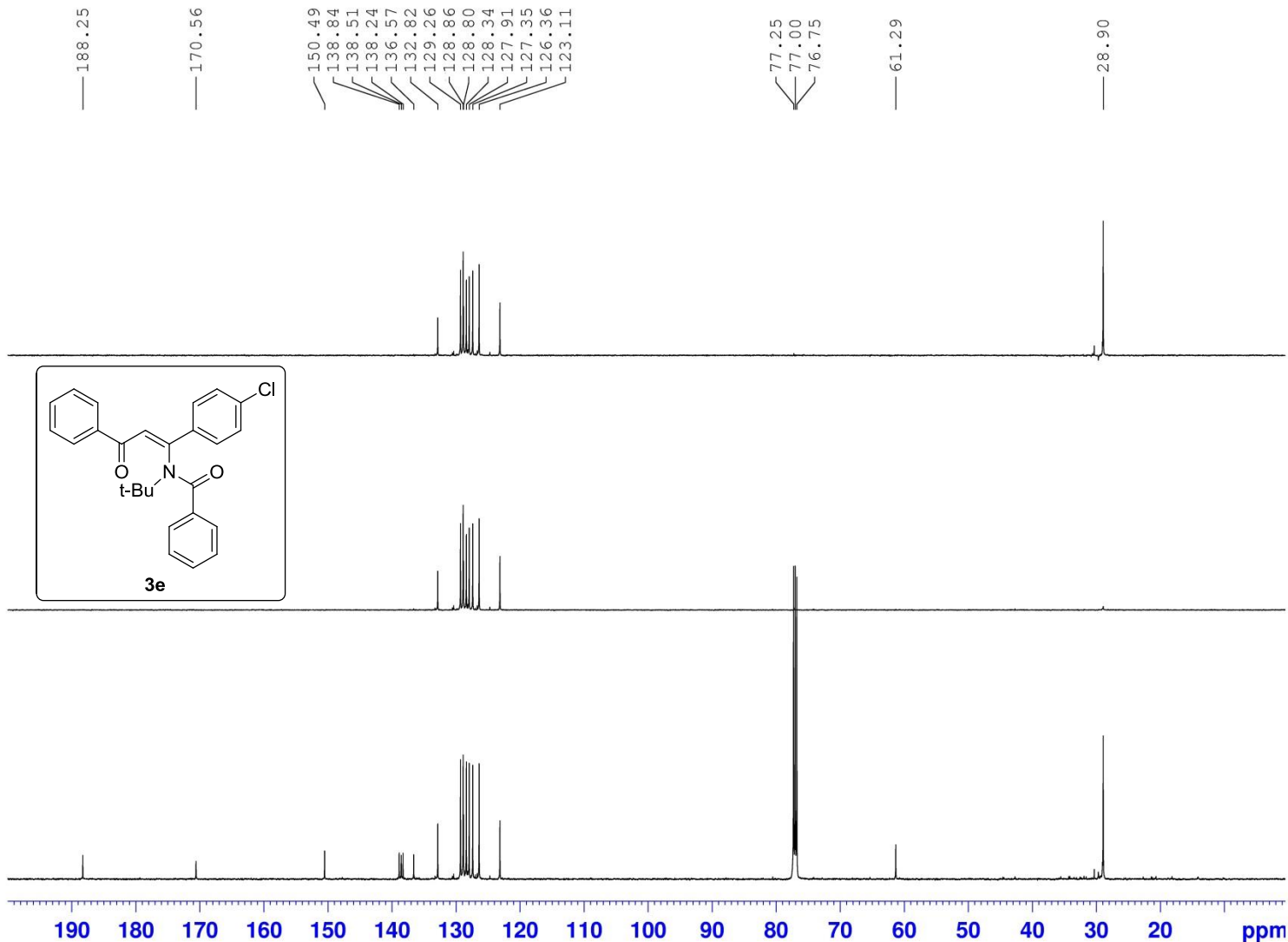
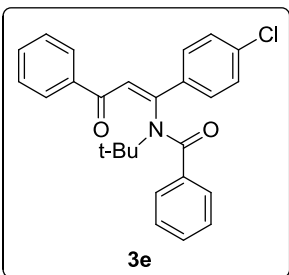


F2 - Processing parameters  
SI 16384  
SF 500.1600209 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME liou0906.002  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160906  
Time\_ 16.53 h  
INSTRUM spect  
PROBHD z119470\_0234 (  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 3000  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7785374 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 80.55799866 W  
SFO2 500.1620006 MHz  
NUC2 1H  
CPDPRG2 bi\_waltz65 256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W





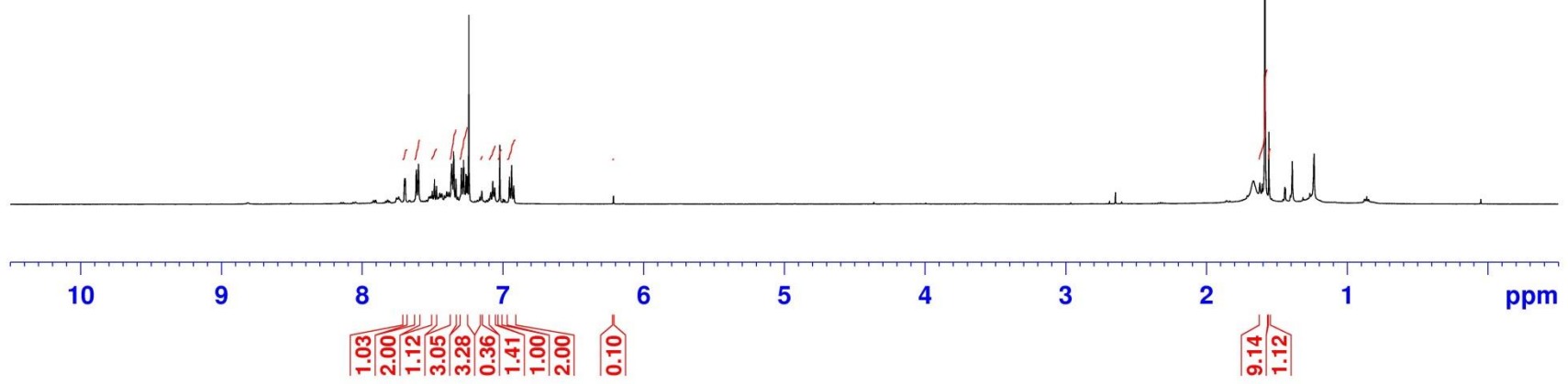
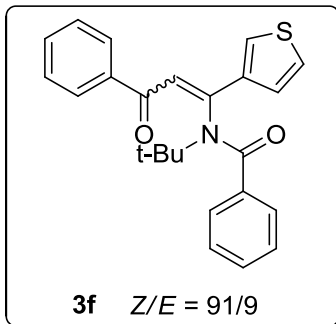
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7.693  
7.691  
7.614  
7.599  
7.597  
7.500  
7.485  
7.470  
7.363  
7.360  
7.355  
7.349  
7.332  
7.293  
7.292  
7.278  
7.261  
7.259  
7.251  
7.240  
7.162  
7.149  
7.146  
7.070  
7.058  
7.056  
7.020  
6.951  
6.936  
6.921  
6.213

1.584  
1.555

Current Data Parameters  
 NAME liou1021.001  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161021  
 Time 15.01 h  
 INSTRUM spect  
 PROBHD Z119470\_0234 ( )  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 0  
 SWH 10026.738 Hz  
 FIDRES 0.305992 Hz  
 AQ 1.6340809 sec  
 RG 154.01  
 DW 49.867 usec  
 DE 7.71 usec  
 TE 299.5 K  
 D1 2.0000000 sec  
 TDO 1  
 SF01 500.1630010 MHz  
 NUC1 1H  
 P1 10.00 usec  
 PLW1 22.69799995 W

F2 - Processing parameters  
 SI 16384  
 SF 500.1600214 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00



yu-6-73 / 13C

—188.45

—170.61

146.31  
143.52  
138.88  
138.64  
132.74  
130.13  
128.65  
128.42  
127.93  
127.24  
127.17  
126.41  
126.06  
121.31

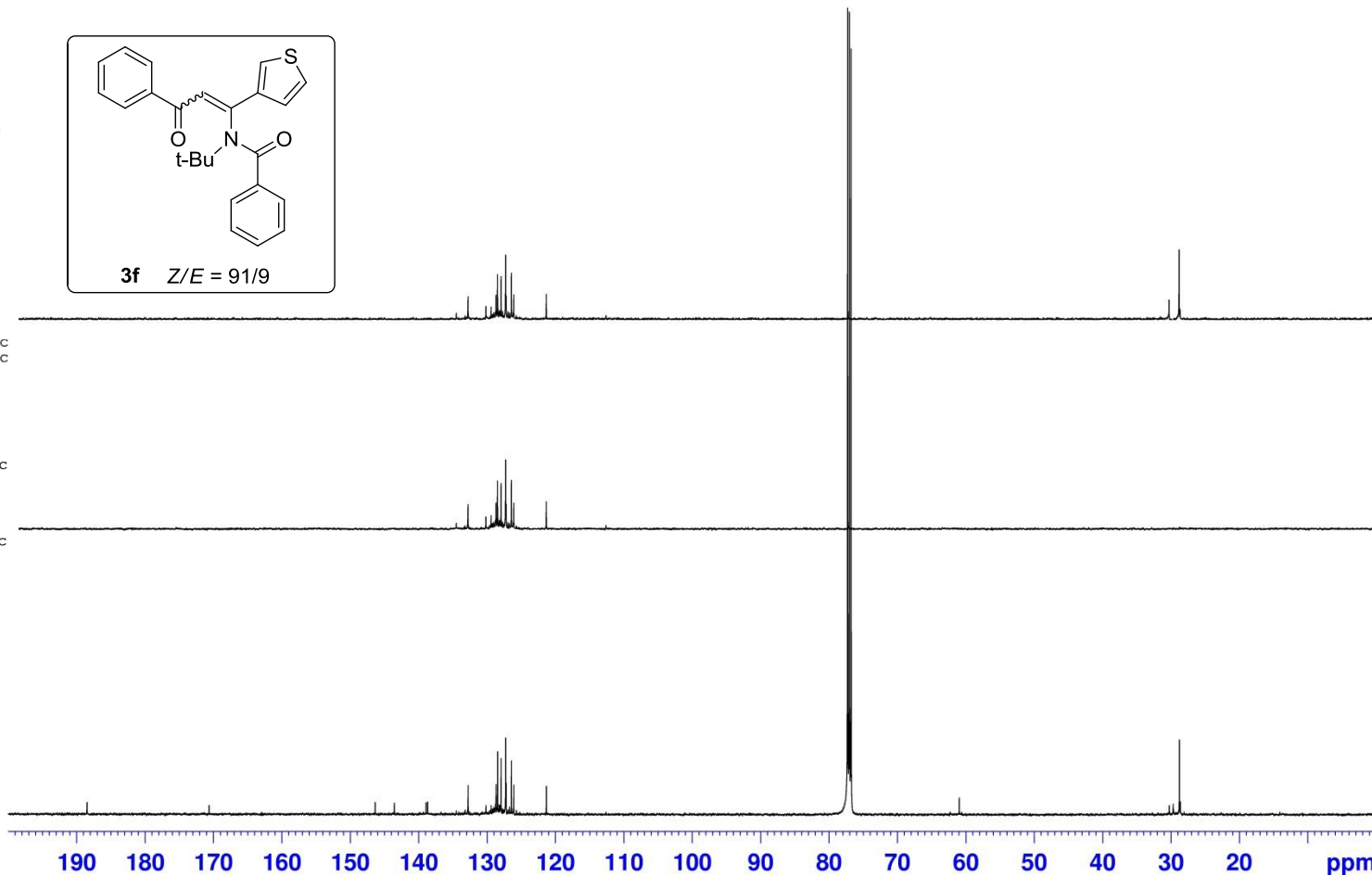
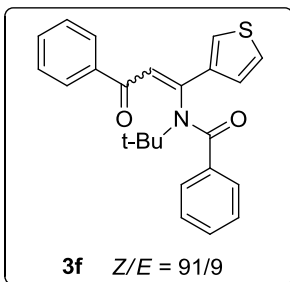
77.25  
77.00  
76.75

—60.92

—28.77

Current Data Parameters  
NAME liou1019.002  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161019  
Time\_ 1.11 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 10000  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.8 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 125.7785374 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 80.55799866 W  
SF02 500.1620006 MHz  
NUC2 1H  
CPDPRG[2 bi\_waltz65\_256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W



7.715  
7.713  
7.707  
7.700  
7.500  
7.481  
7.478  
7.472  
7.464  
7.281  
7.267  
7.241  
7.240  
7.046  
7.034  
7.023  
6.962  
6.958  
6.949  
6.933  
6.902  
6.889  
6.876

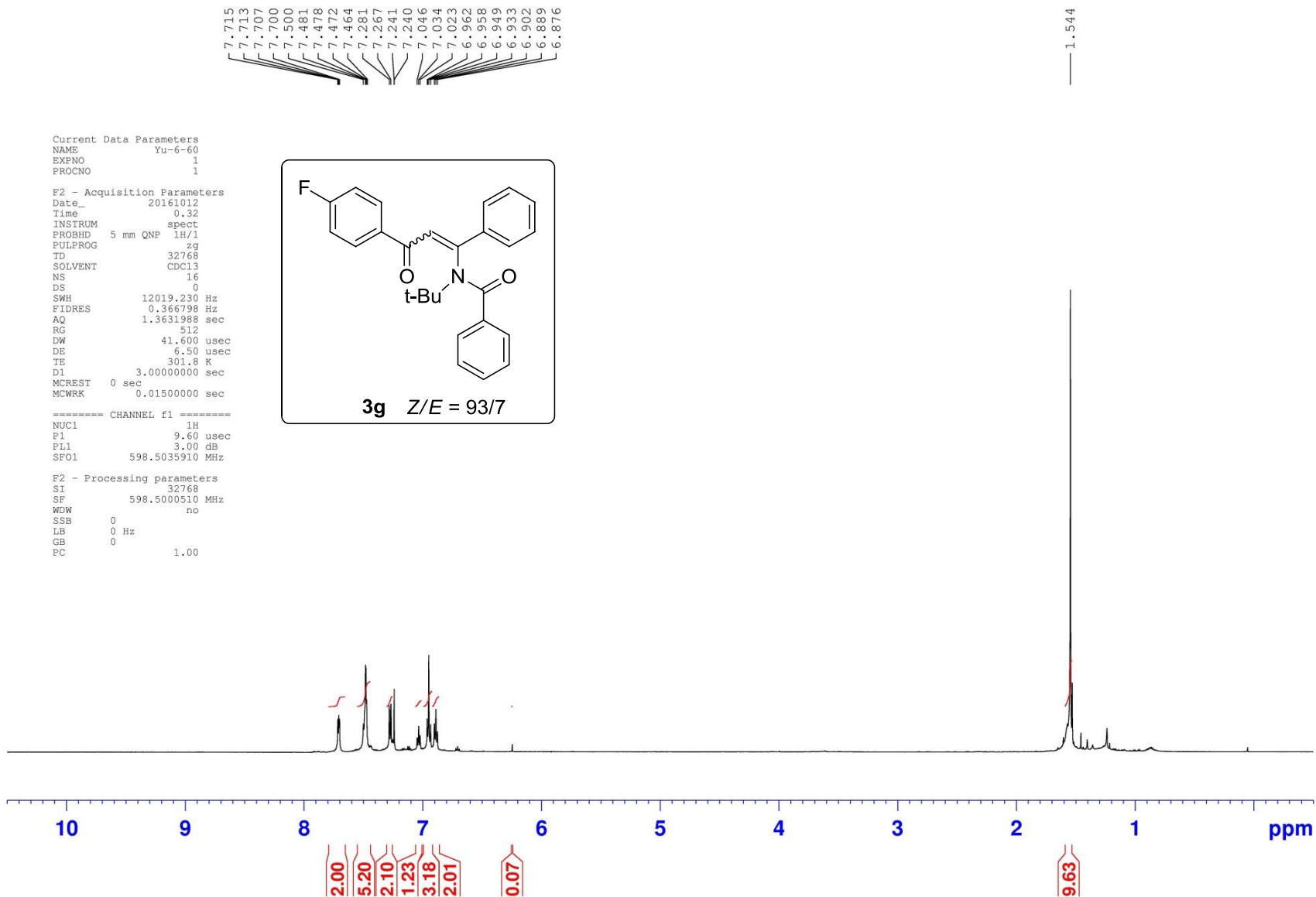
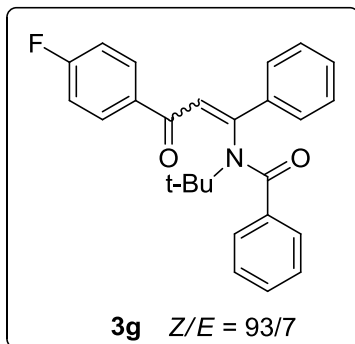
```

Current Data Parameters
NAME      Yu-6-60
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20161012
Time     0.32
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SWH      12019.230 Hz
FIDRES   0.366798 Hz
AQ        1.3631988 sec
RG        512
DW        41.600 usec
DE        6.50 usec
TE        301.8 K
D1        3.00000000 sec
MCREST   0 sec
MCWRK    0.01500000 sec

----- CHANNEL f1 -----
NUC1      1H
P1        9.60 usec
PL1       3.00 dB
SF01     598.5035910 MHz

F2 - Processing parameters
SI        32768
SF        598.5000510 MHz
WDW       no
SSB       0
LB        0 Hz
GB        0
PC        1.00
  
```



— 186.92  
 — 170.44  
 — 166.30  
 — 164.60  
 — 151.98  
 — 140.28  
 — 138.63  
 — 134.74  
 — 130.54  
 — 129.03  
 — 127.72  
 — 127.31  
 — 126.48  
 — 122.87  
 — 115.43  
 — 115.28

— 77.21  
 — 77.00  
 — 76.79

— 61.24

— 28.82

Current Data Parameters  
 NAME Yu-6-60  
 EXPNO 2  
 PROCNO 1

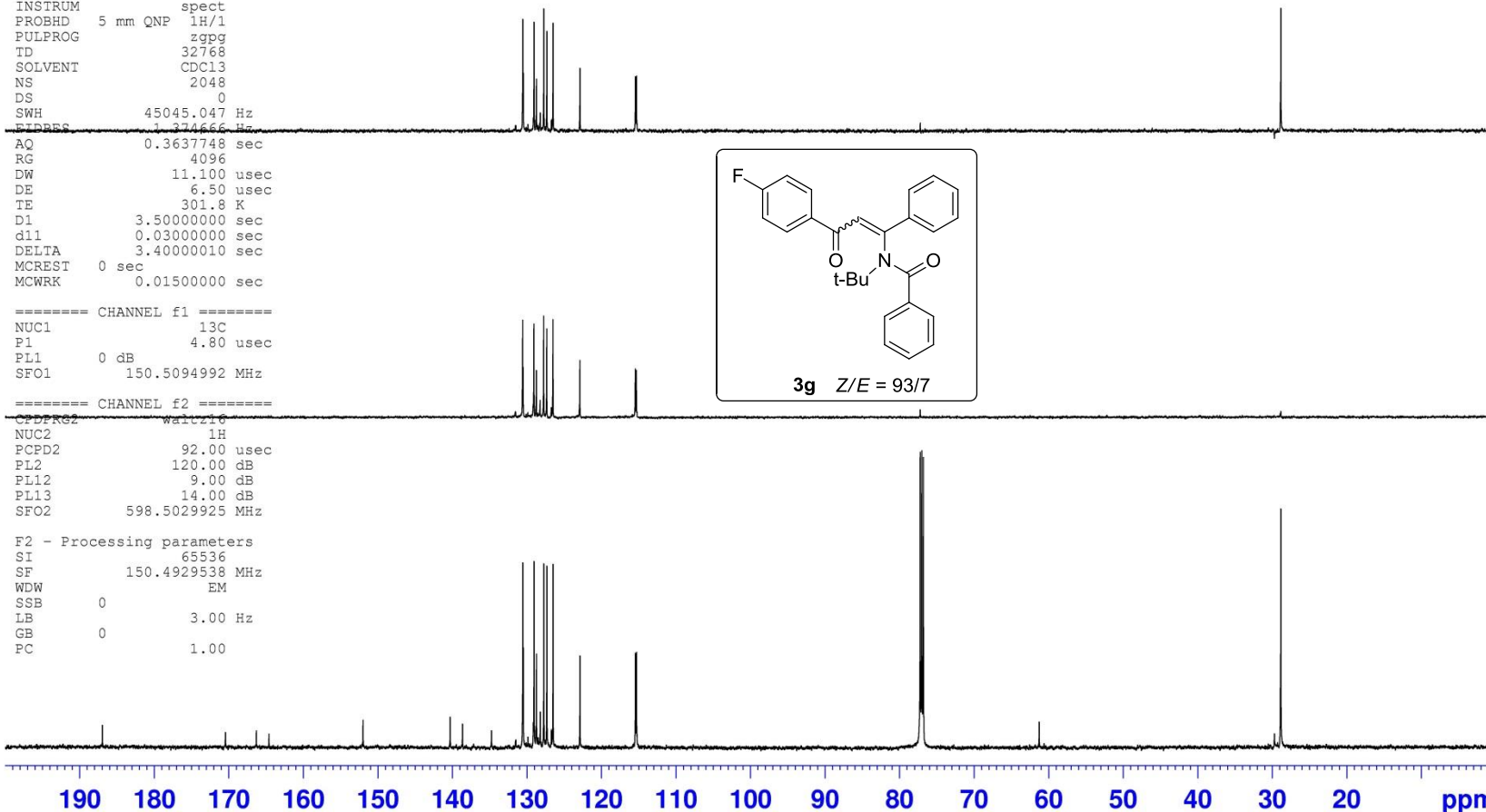
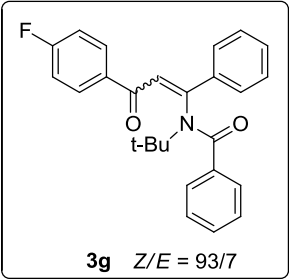
F2 - Acquisition Parameters

Date\_ 20161012  
 Time\_ 0.33  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpgg  
 TD 32768  
 SOLVENT CDCl3  
 NS 2048  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 0.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 301.8 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0 sec  
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0 dB  
 SFO1 150.5094992 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.5029925 MHz

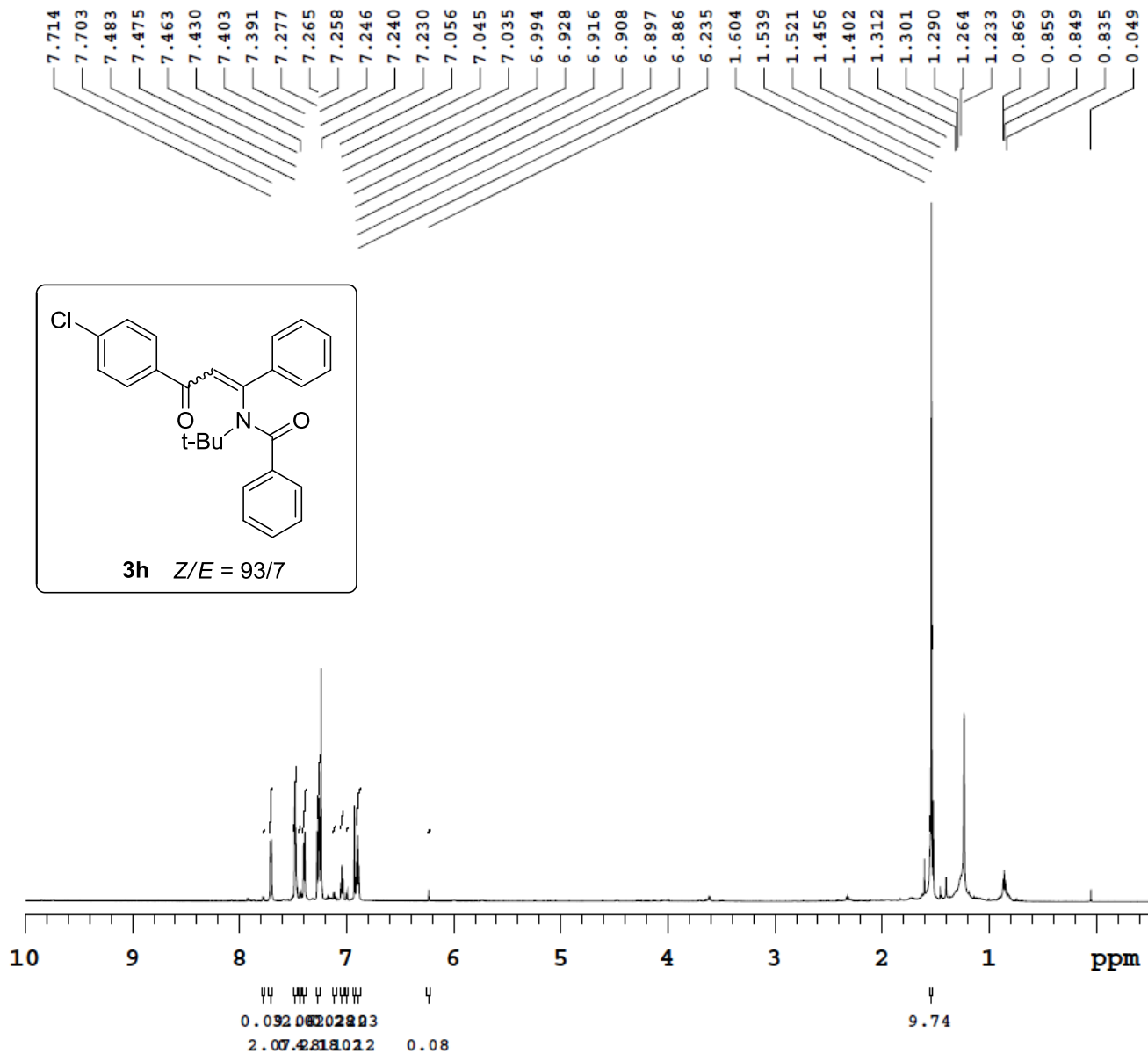
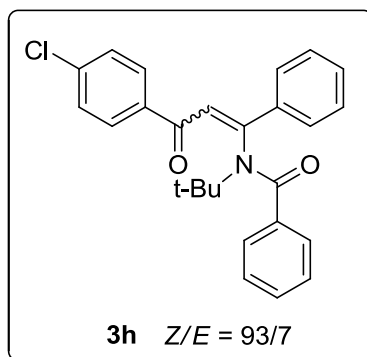
F2 - Processing parameters  
 SI 65536  
 SF 150.4929538 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00



Yu-6-59

exp1 PROTON

SAMPLE		PRESATURATION	
date	Oct 7 2016	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmr1/D- esktop/Yu-6-59-H.f-	SPECIAL	
	temp	25.0	
	id	gain	12
ACQUISITION		SPECIAL	
sw	11904.8	hst	0.008
at	2.753	pw90	6.500
np	65536	alfa	10.000
fb	4000	FLAGS	
bs	8	il	n
dl	2.000	in	n
nt	16	dp	y
ct	16	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	699.749	DISPLAY	
tof	349.9	sp	-350.0
tpwr	62	wp	7347.1
pw	3.250	rfl	7173.1
DECOUPLER		rfp	5066.2
dn	C13	rp	-64.1
dof	0	lp	0
dm	nnn	PLOT	
decwave	W40_Cold	wc	165
dpwr	40	sc	8
dmf	38462	vs	356
		th	1
		ai	ph



Yu-6-59

187.211

170.443

152.354

140.225

139.080

138.579

136.690

130.633

129.298

129.053

128.768

128.559

127.748

127.357

126.450

122.645

77.183

77.000

76.819

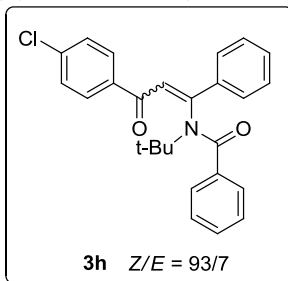
61.314

29.694

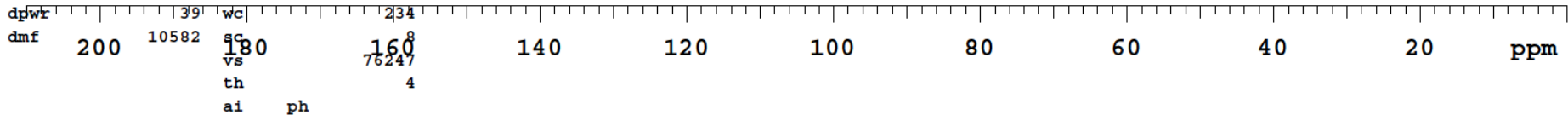
28.851

exp1 CARBON

SAMPLE		PRESATURATION	
date	Oct 7 2016	satmode	n
solvent	cdcl3	wet	n
file	/home/vnmr1/D-	SPECIAL	
esktop/Yu-6-59-C.f-		temp	25.0
		id	gain
			30
ACQUISITION		not used	
sw	46296.3	hst	0.008
at	1.468	pw90	14.000
np	135926	alfa	10.000
fb	17000	FLAGS	
bs	8	il	n
d1	3.500	in	n
nt	5000	dp	y
ct	2128	hs	nn



TRANSMITTER		PROCESSING	
tn	C13	lb	3.00
sfrq	175.972	fn	262144
tof	4438.8	DISPLAY	
tpwr	59	sp	-0.3
pw	7.000	wp	36949.6
DECOUPLER		rf1	
dn	H1	rfl	15579.5
dof	0	rpf	13548.2
dm	nyy	rp	-43.5
		lp	0



7.681  
7.678  
7.520  
7.505  
7.456  
7.452  
7.450  
7.447  
7.445  
7.430  
7.427  
7.422  
7.420  
7.418  
7.416  
7.414  
7.414  
7.295  
7.293  
7.281  
7.279  
7.275  
7.261  
7.259  
7.240  
7.238  
7.235  
7.231  
7.230  
7.228  
7.174  
7.172  
7.160  
7.156  
7.149  
7.147  
7.145  
7.128  
7.127  
7.124  
7.116  
7.114  
7.107  
7.105  
7.104  
7.102  
7.100  
7.092  
7.088  
7.030  
7.017  
7.001  
6.895  
6.883  
6.870  
6.780  
6.765  
6.566  
6.551  
6.258  
3.821  
3.739

1.547

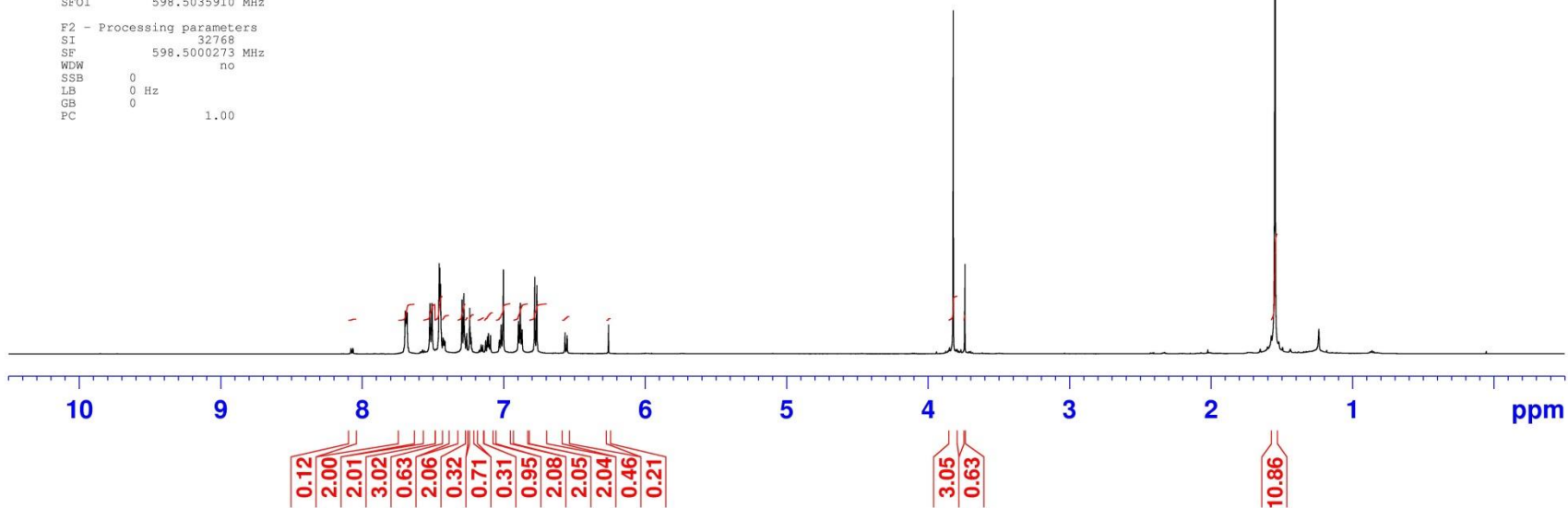
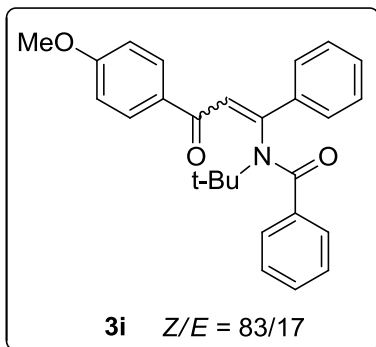
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Current Data Parameters
NAME Yu-6-82
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161103
Time 3.22
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 9541.984 Hz
FIDRES 0.291198 Hz
AQ 1.7170932 sec
RG 1024
DW 52.400 usec
DE 6.50 usec
TE 302.1 K
D1 2.0000000 sec
MCREST 0 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.60 usec
PL1 0 dB
SFO1 598.5035910 MHz

F2 - Processing parameters
SI 32768
SF 598.5000273 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
  
```



187.07

170.63  
163.26  
150.83  
140.43  
138.78  
133.45  
131.46  
131.26  
131.00  
130.25  
130.23  
130.11  
129.47  
129.01  
128.91  
128.67  
128.53  
128.40  
128.12  
128.09  
127.63  
127.19  
126.68  
126.45  
123.25  
113.49

77.21  
77.00  
76.79

61.05  
60.48  
55.43  
55.34

28.87  
28.79

Current Data Parameters  
NAME Yu-6-82  
EXPNO 2  
PROCNO 1

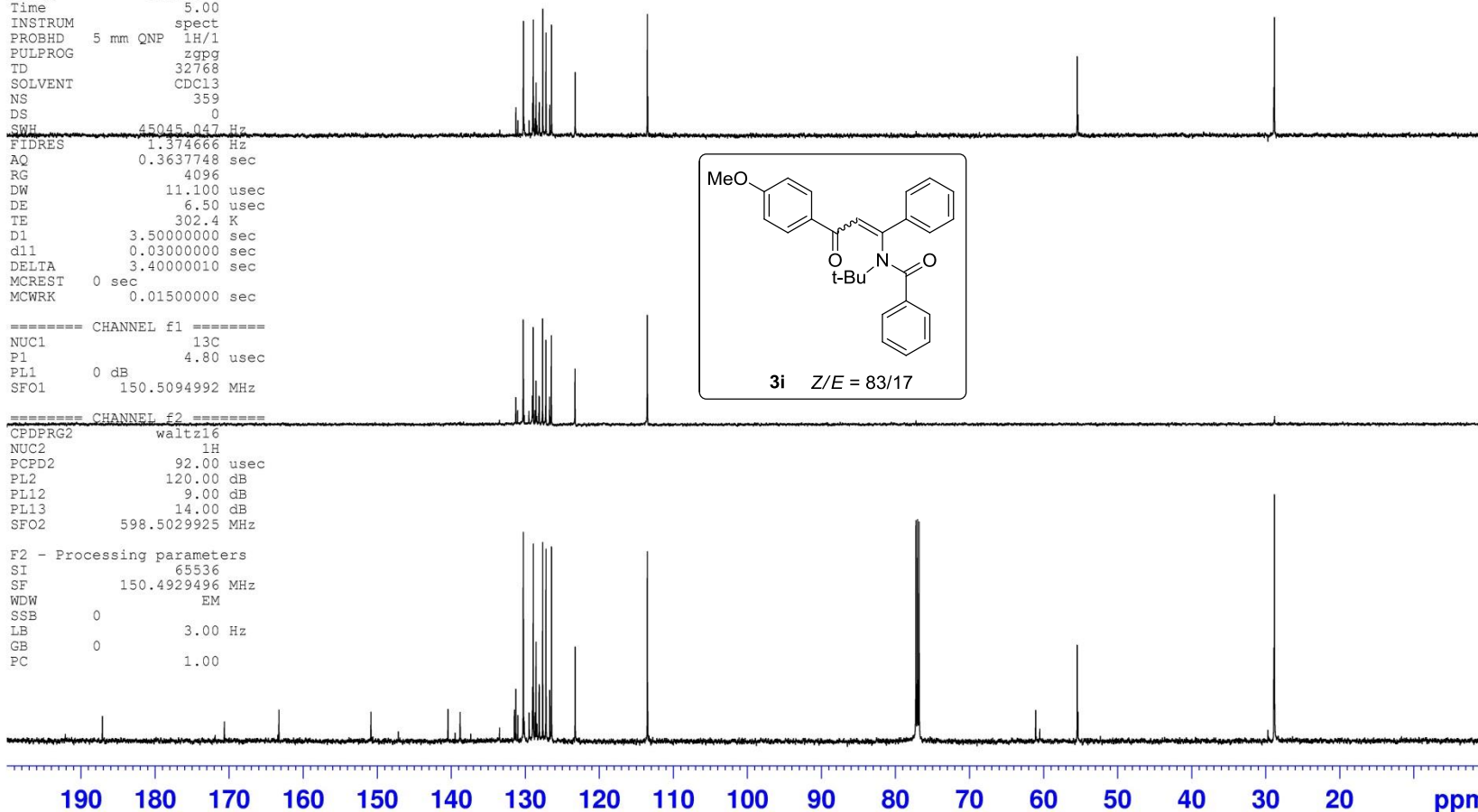
F2 - Acquisition Parameters

Date\_ 20161104  
Time 5.00  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 359  
DS 0  
SWH 45045.047 Hz  
FIDRES 1.374666 Hz  
AQ 0.3637748 sec  
RG 4096  
DW 11.100 usec  
DE 6.50 usec  
TE 302.4 K  
D1 3.50000000 sec  
d11 0.03000000 sec  
DELTA 3.40000010 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

=====  
CHANNEL f1  
NUC1 13C  
P1 4.80 usec  
PL1 0 dB  
SFO1 150.5094992 MHz

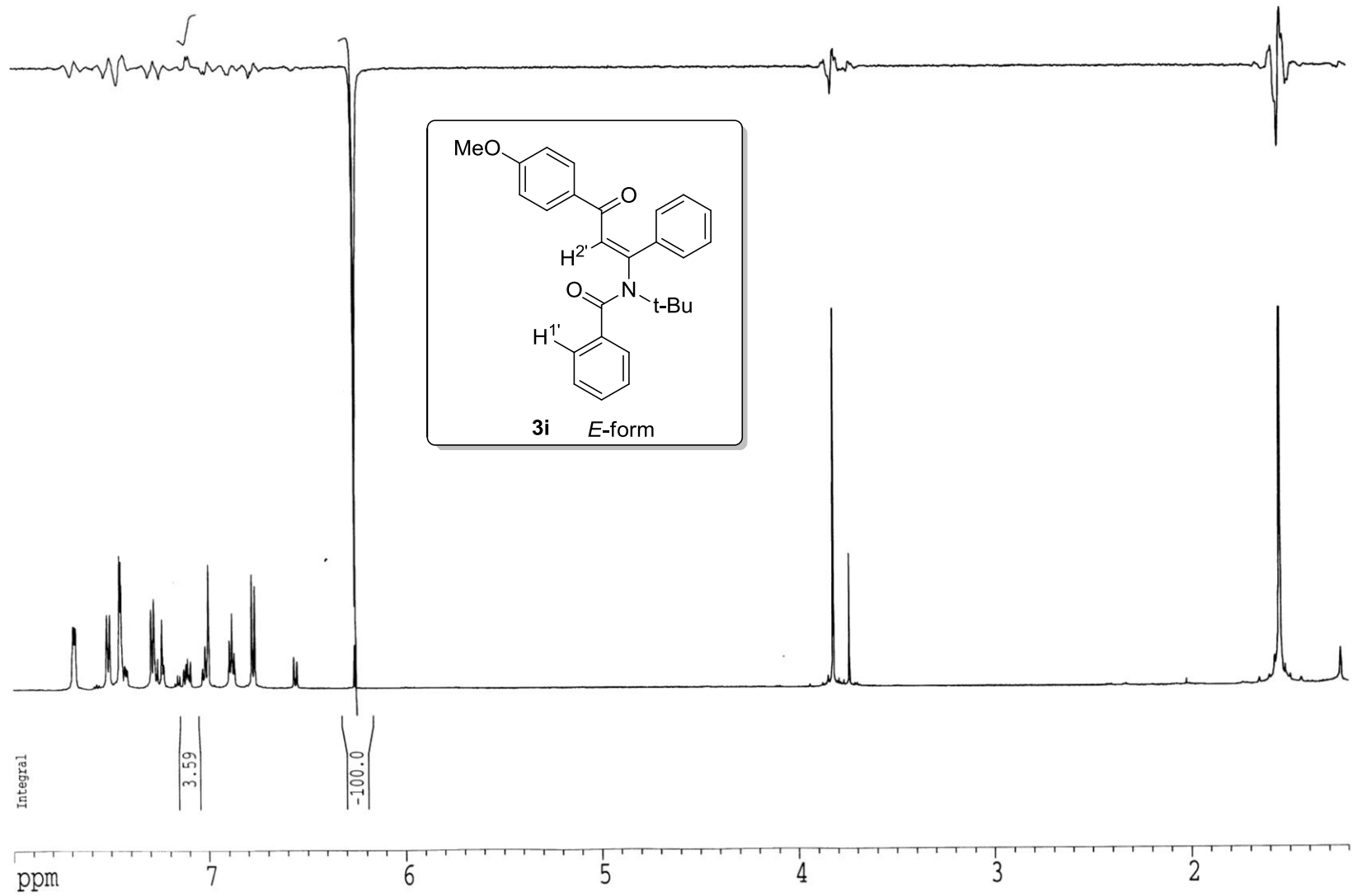
=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 92.00 usec  
PL2 120.00 dB  
PL12 9.00 dB  
PL13 14.00 dB  
SFO2 598.5029925 MHz

F2 - Processing parameters  
SI 65536  
SF 150.4929496 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

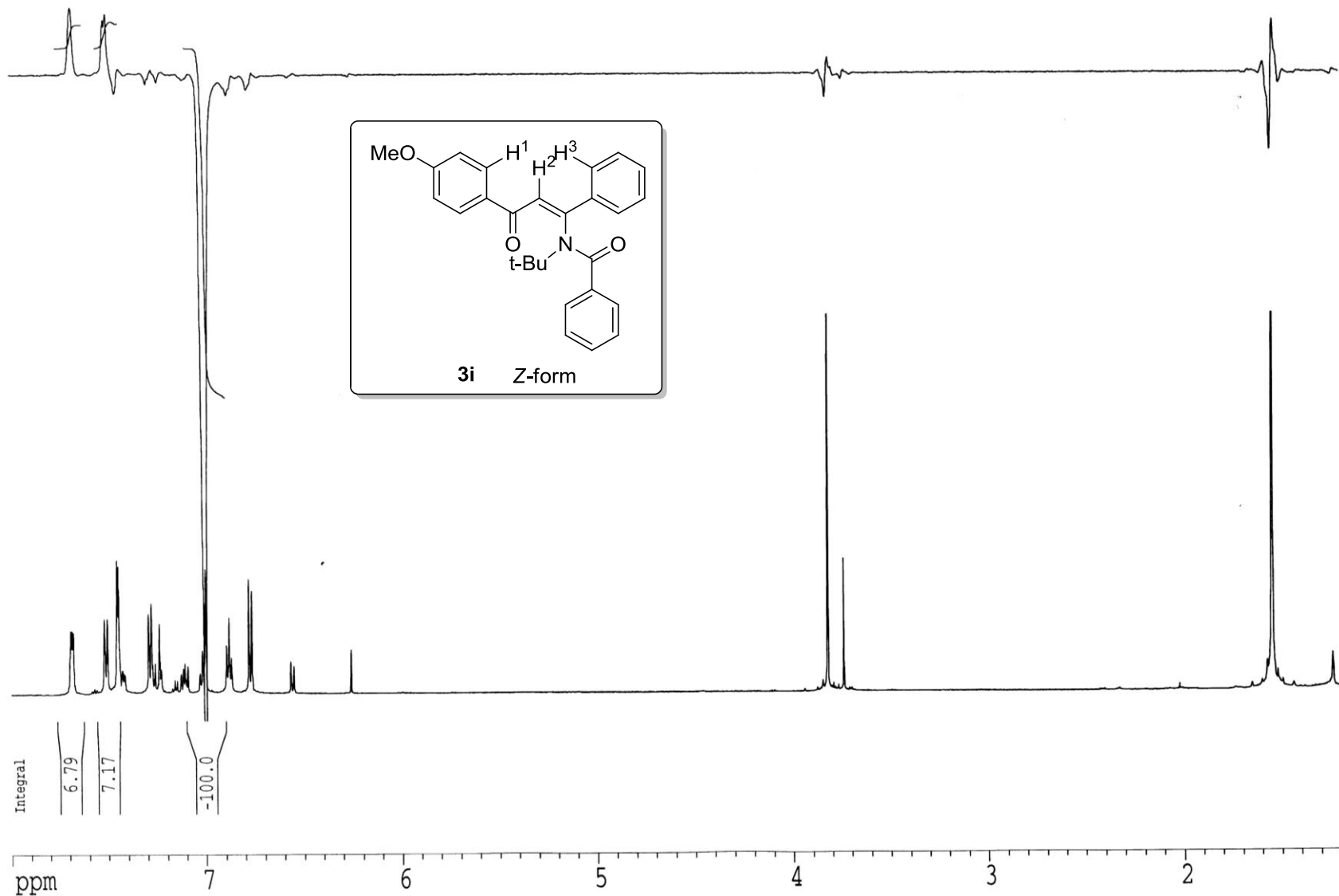




# NOE



# NOE



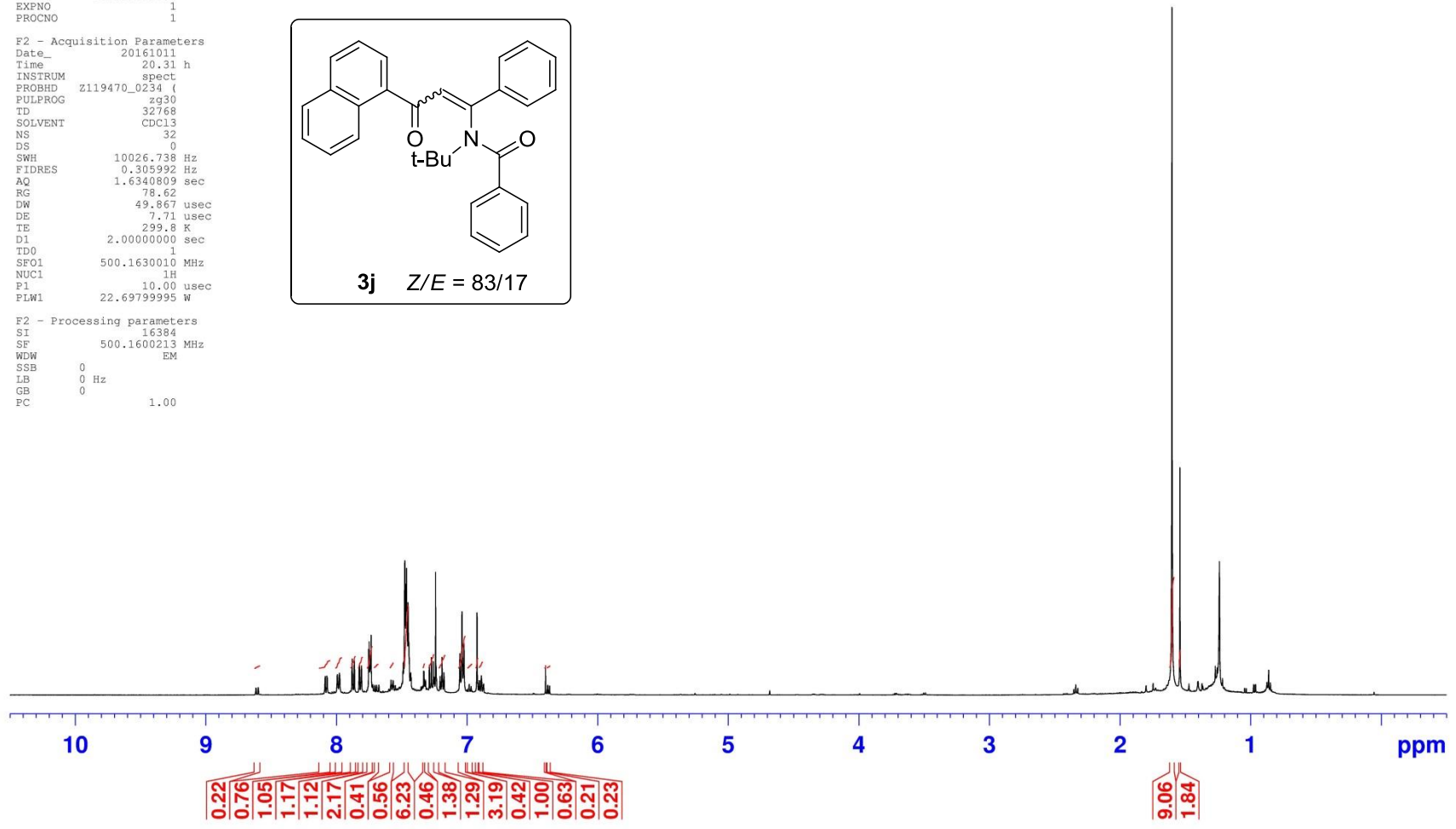
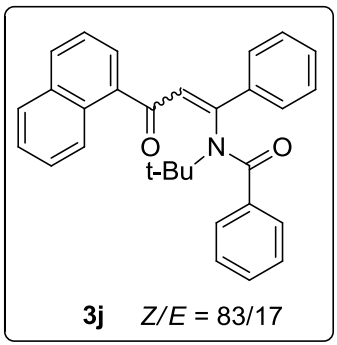
7.976  
7.879  
7.863  
7.826  
7.823  
7.808  
7.753  
7.750  
7.746  
7.738  
7.734  
7.706  
7.691  
7.675  
7.582  
7.578  
7.567  
7.565  
7.561  
7.478  
7.475  
7.469  
7.466  
7.463  
7.457  
7.452  
7.450  
7.445  
7.332  
7.329  
7.288  
7.273  
7.258  
7.206  
7.191  
7.176  
7.054  
7.039  
7.024  
6.998  
6.984  
6.969  
6.967  
6.923  
6.906  
6.903  
6.890  
6.888  
6.876  
6.872  
6.398  
6.384  
6.382  
6.369  
6.367

1.602  
1.541

Current Data Parameters  
 NAME liou1011.001  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161011  
 Time 20.31 h  
 INSTRUM spect  
 PROBHD Z119470\_0234 ( )  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 0  
 SWH 10026.738 Hz  
 FIDRES 0.305992 Hz  
 AQ 1.6340809 sec  
 RG 78.62  
 DW 49.867 usec  
 DE 7.71 usec  
 TE 299.8 K  
 D1 2.0000000 sec  
 TD0 1  
 SFO1 500.1630010 MHz  
 NUC1 1H  
 F1 10.00 usec  
 PLW1 22.69799995 W

F2 - Processing parameters  
 SI 16384  
 SF 500.1600213 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
NAME liou1011.001  
EXPNO 2  
PROCNO 1

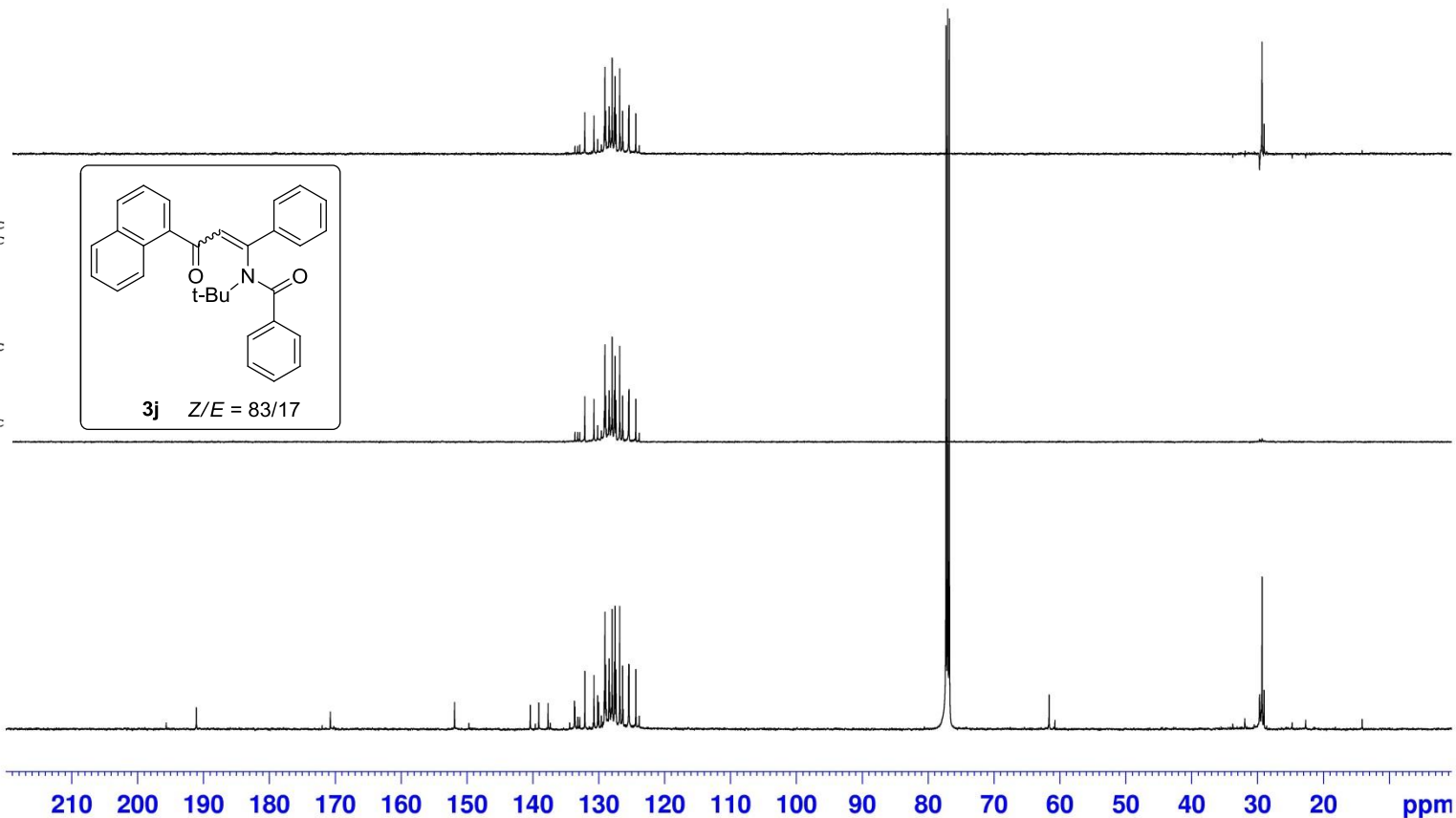
F2 - Acquisition Parameters

Date\_ 20161012  
Time\_ 7.25 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 15000  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7785374 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 80.55799866 W  
SFO2 500.1620006 MHz  
NUC2 1H  
CPDPRG2 bi\_waltz65 256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W

F2 - Processing parameters  
SI 32768  
SF 125.7653348 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

195.60  
191.04  
171.95  
170.69  
151.85  
149.66  
140.37  
139.59  
137.65  
137.33  
134.38  
133.65  
133.56  
133.17  
132.84  
132.07  
130.68  
130.13  
129.97  
129.56  
129.13  
129.02  
128.90  
128.81  
128.43  
128.40  
128.29  
128.07  
127.95  
127.85  
127.59  
127.48  
127.34  
126.79  
126.70  
126.34  
126.27  
125.42  
125.37  
124.34  
123.82  
77.25  
77.00  
76.75  
61.61  
60.72

29.29  
28.98



7.711  
7.708  
7.701  
7.699  
7.695  
7.540  
7.537  
7.474  
7.470  
7.466  
7.465  
7.463  
7.364  
7.362  
7.355  
7.353  
7.297  
7.285  
7.283  
7.240  
7.213  
7.208  
7.204  
7.200  
7.195  
7.195  
7.035  
7.023  
7.012  
7.011  
7.008  
6.904  
6.888  
6.878

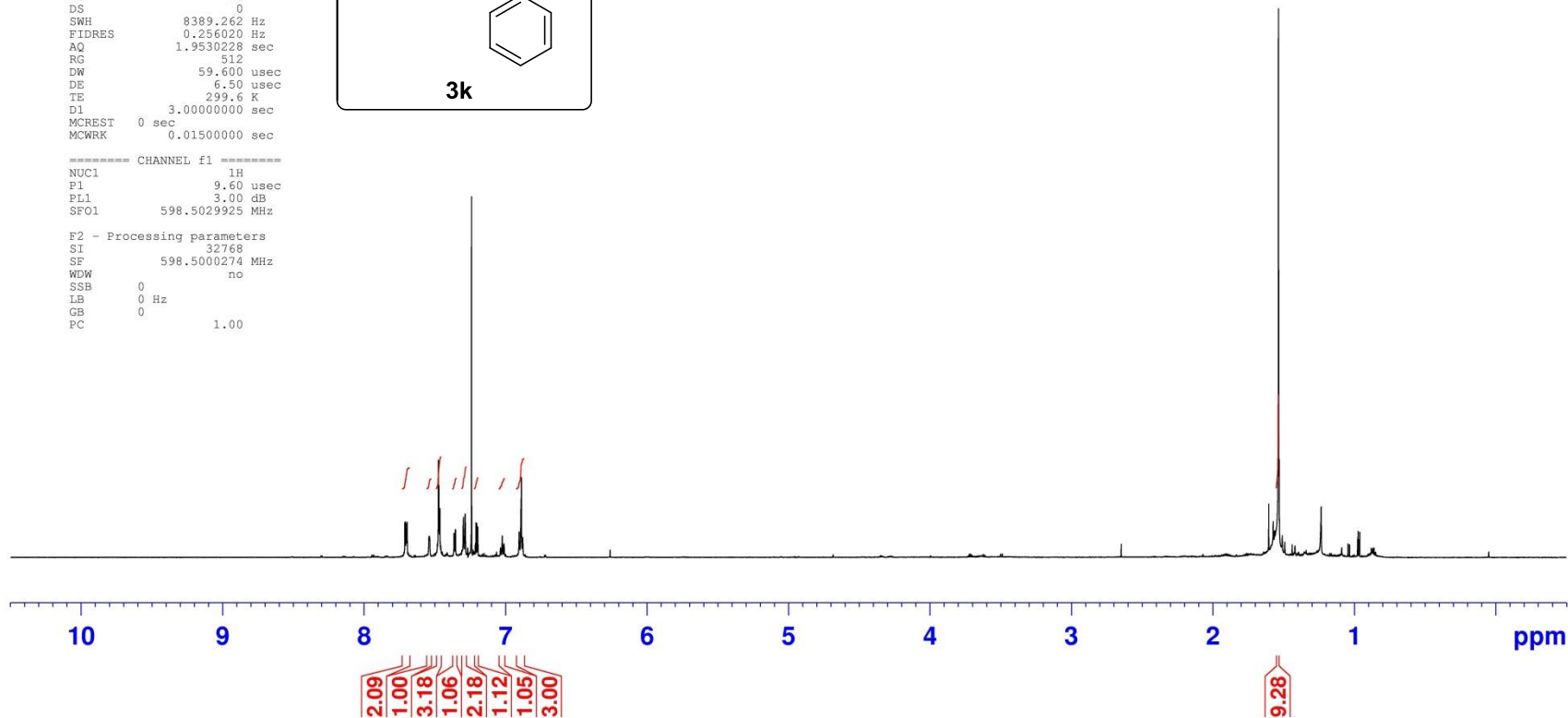
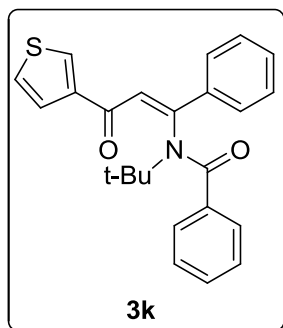
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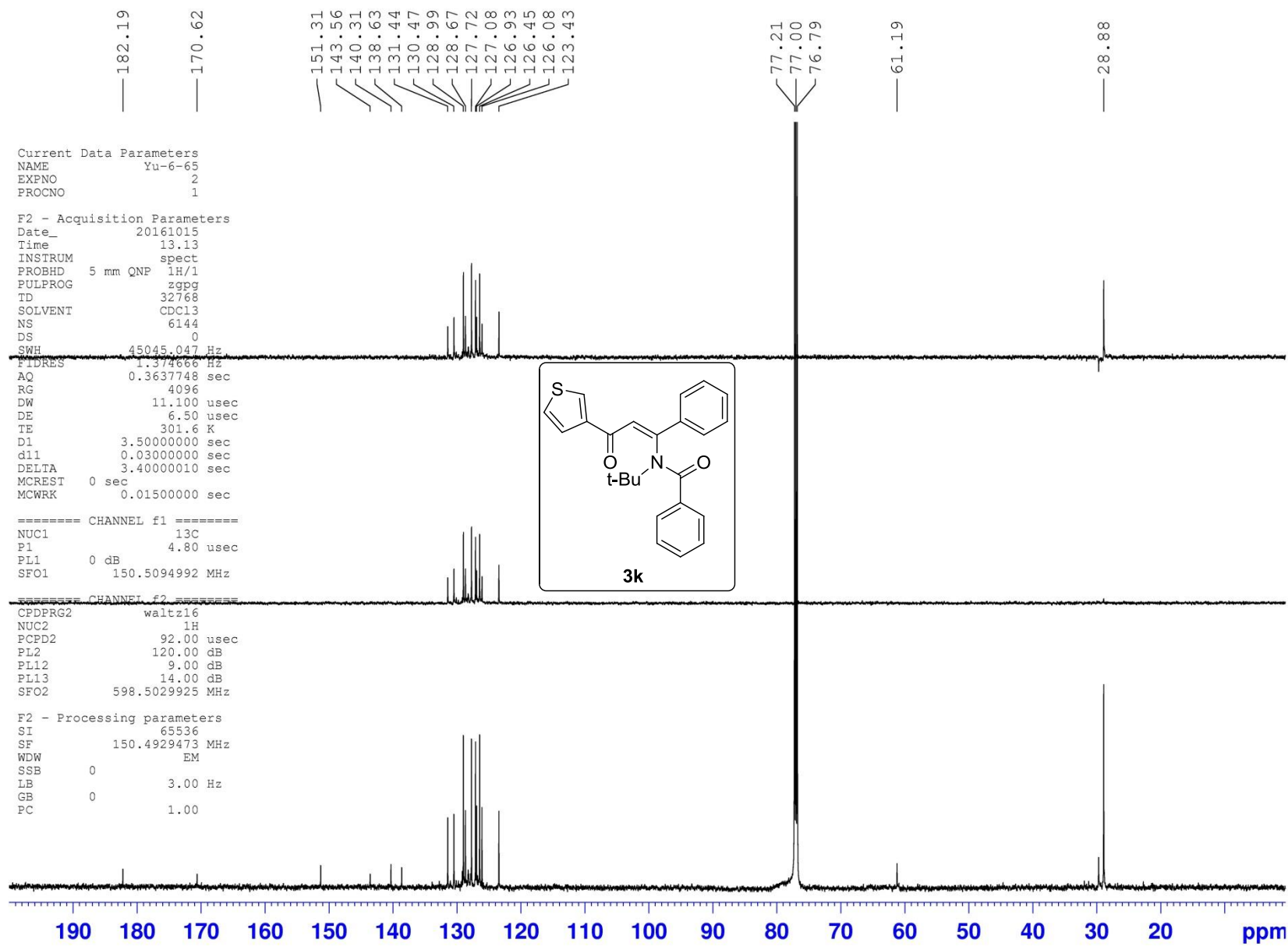
Current Data Parameters
NAME      Yu-6-65
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20161015
Time     6.31
INSTRUM spect
PROBHD   5 mm QNP 1H/1
PULPROG zg
TD       32768
SOLVENT  CDCl3
NS       16
DS       0
SWH      8389.262 Hz
FIDRES   0.256020 Hz
AQ       1.9530228 sec
RG       512
DW       59.600 usec
DE       6.50 usec
TE       299.6 K
D1       3.0000000 sec
MCREST   0 sec
MCWRK    0.0150000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       9.60 usec
PL1      3.00 dB
SFO1     598.5029925 MHz

F2 - Processing parameters
SI       32768
SF       598.5000274 MHz
WDW      no
SSB      0
LB       0 Hz
GB       0
PC       1.00
  
```





7.702  
7.690  
7.688  
7.681  
7.678  
7.672  
7.670  
7.665  
7.460  
7.457  
7.454  
7.450  
7.445  
7.442  
7.435  
7.401  
7.390  
7.388  
7.376  
7.375  
7.355  
7.343  
7.341  
7.335  
7.332  
7.329  
7.323  
7.320  
7.319  
7.240  
7.187  
7.175  
7.164  
7.162  
7.079  
7.066  
7.053  
6.330  
5.776

2.177  
2.167  
2.163  
2.152  
2.149  
2.139  
2.135  
2.124  
1.855  
1.845  
1.840  
1.830  
1.817  
1.812  
1.802  
1.466  
1.385  
1.381  
1.370  
1.356  
1.345  
1.332  
1.318  
1.187  
1.175  
1.163  
1.151  
0.833  
0.820  
0.808

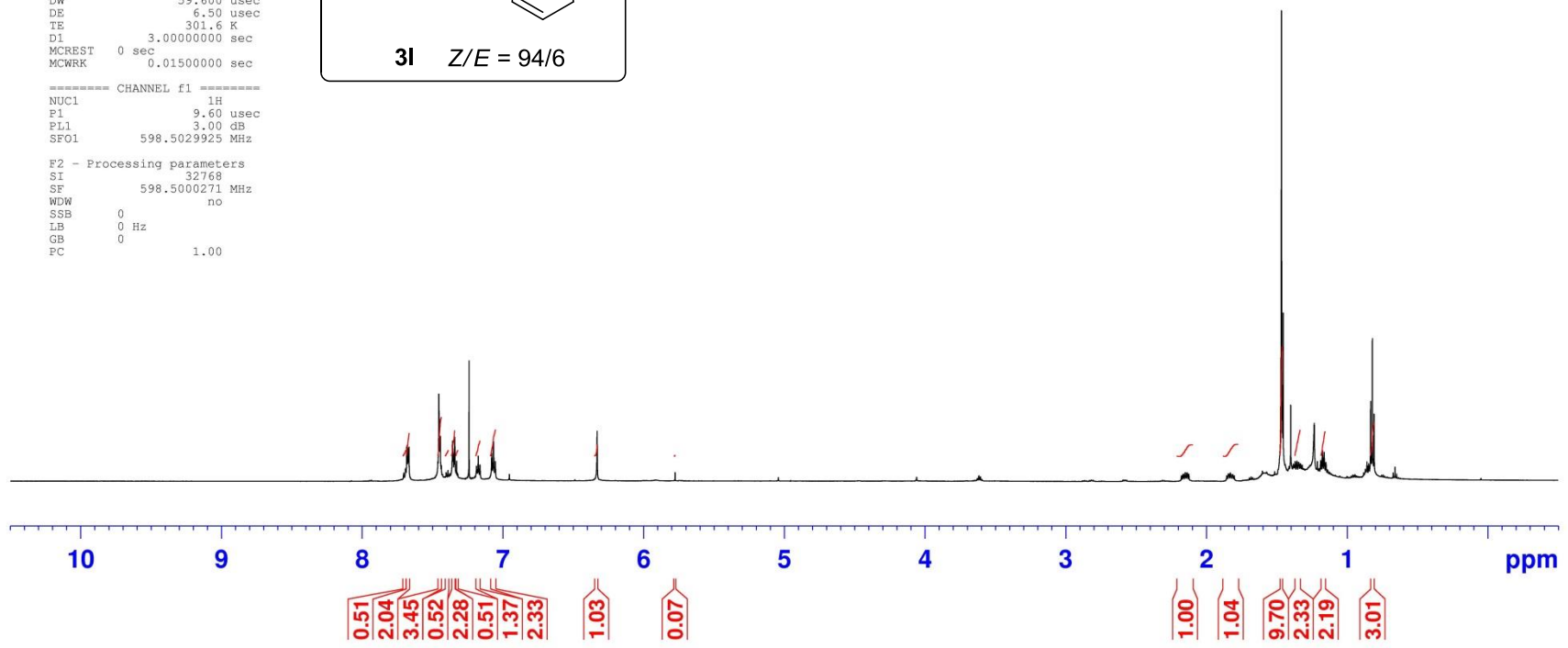
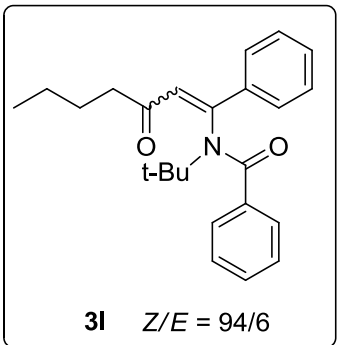
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Current Data Parameters
NAME Yu-6-39
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160930
Time 0.58
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 301.6 K
D1 3.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.60 usec
PL1 3.00 dB
SFO1 598.5029925 MHz

F2 - Processing parameters
SI 32768
SF 598.5000271 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
  
```



— 197.72

— 170.46

— 149.50

— 140.17

— 138.75

— 130.43

— 128.93

— 128.78

— 127.71

— 127.15

— 126.68

— 124.60

— 77.21

— 77.00

— 76.79

— 61.12

— 44.28

— 29.00

— 25.73

— 22.19

— 13.83

Current Data Parameters  
NAME Yu-6-39  
EXPNO 2  
PROCNO 1

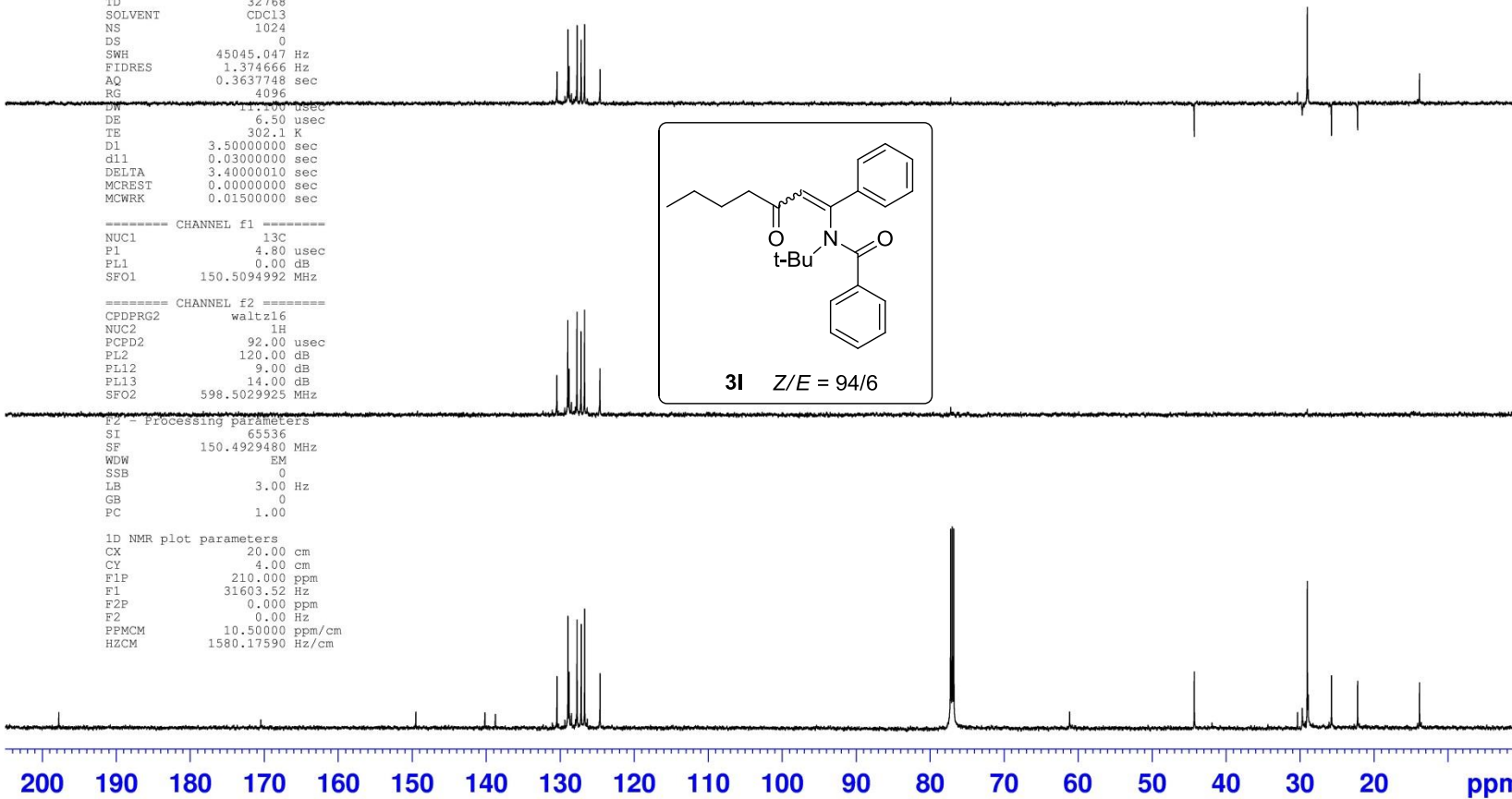
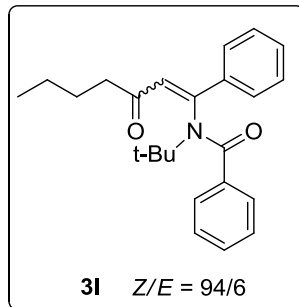
F2 - Acquisition Parameters  
Date\_ 20160929  
Time 10.28  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 1024  
DS 0  
SWH 45045.047 Hz  
FIDRES 1.374666 Hz  
AQ 0.3637748 sec  
RG 4096  
DM 11.100 usec  
DE 6.50 usec  
TE 302.1 K  
D1 3.50000000 sec  
d11 0.03000000 sec  
DELTA 3.40000010 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 4.80 usec  
PL1 0.00 dB  
SFO1 150.5094992 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 92.00 usec  
PL2 120.00 dB  
PL12 9.00 dB  
PL13 14.00 dB  
SFO2 598.5029925 MHz

F2 - Processing parameters  
SI 6536  
SF 150.4929480 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
CY 4.00 cm  
FLP 210.000 ppm  
F1 31603.52 Hz  
F2P 0.000 ppm  
F2 0.00 Hz  
PPMCM 10.50000 ppm/cm  
HZCM 1580.17590 Hz/cm





7.692 7.688 7.683 7.681 7.679 7.675 7.451 7.445 7.441 7.436 7.434 7.427 7.354 7.351 7.348 7.340 7.328 7.326 7.317 7.312 7.309 7.301 7.298 7.240 7.185 7.184 7.182 7.171 7.164 7.161 7.159 7.151 7.150 7.138 7.078 7.065 7.052 6.513 5.852 1.602 1.596 1.589 1.581 1.576 1.576 1.507 1.465 0.991 0.986 0.983 0.977 0.975 0.971 0.970 0.967 0.964 0.960 0.956 0.953 0.950 0.949 0.945 0.943 0.937 0.934 0.929 0.818 0.813 0.807 0.805 0.802 0.800 0.798 0.793 0.791 0.789 0.785 0.778 0.774 0.721 0.716 0.710 0.706 0.703 0.701 0.697 0.693 0.690

```

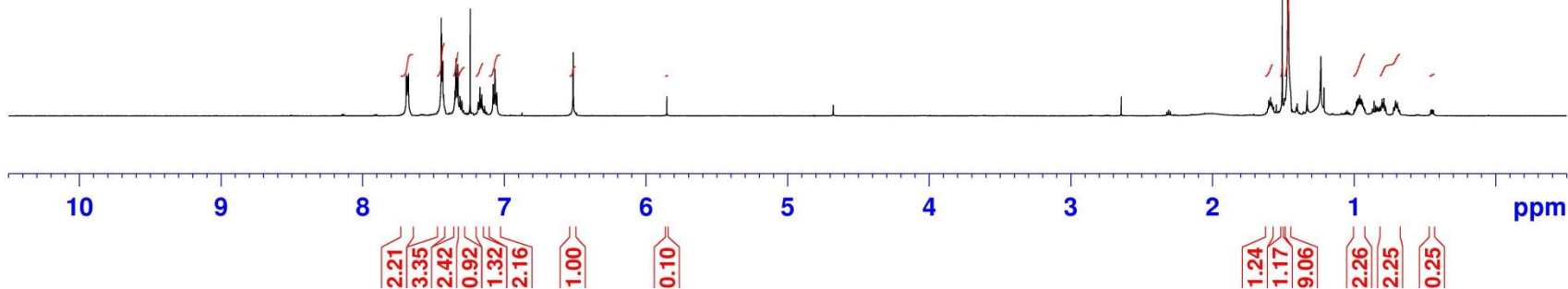
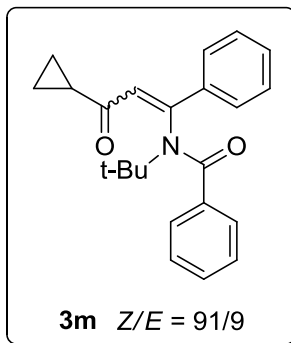
Current Data Parameters
NAME Yu-6-36
EXPNO 1
PROCNO 1

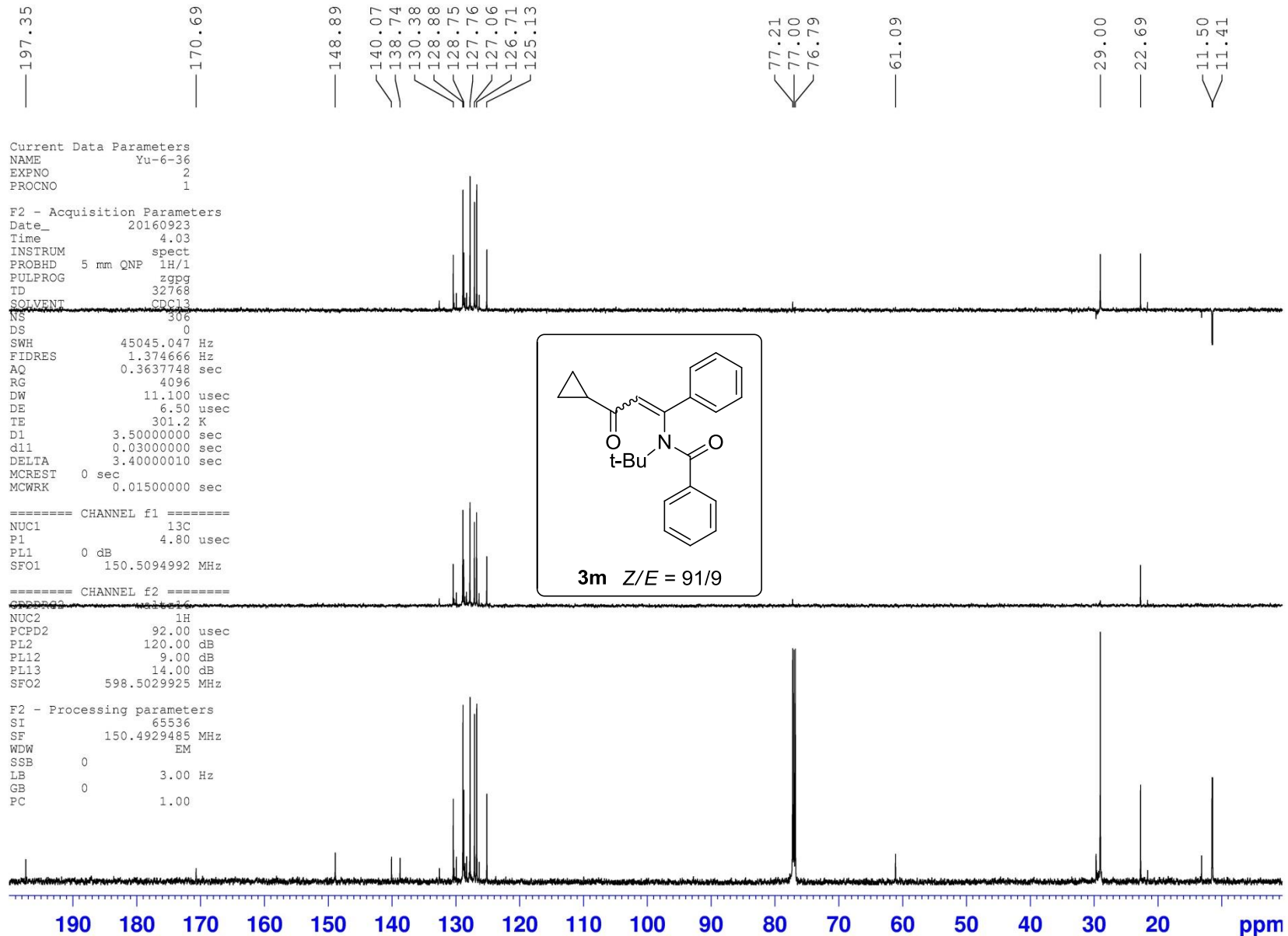
F2 - Acquisition Parameters
Date_ 20160923
Time 4.03
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT MeOD
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 301.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.60 usec
PL1 3.00 dB
SFO1 598.5029070 MHz

F2 - Processing parameters
SI 32768
SF 598.5000275 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

```





7.700  
7.697  
7.689  
7.681  
7.455  
7.451  
7.442  
7.405  
7.390  
7.369  
7.354  
7.240  
7.195  
7.180  
7.165  
7.151  
7.063  
7.048  
7.032  
6.448

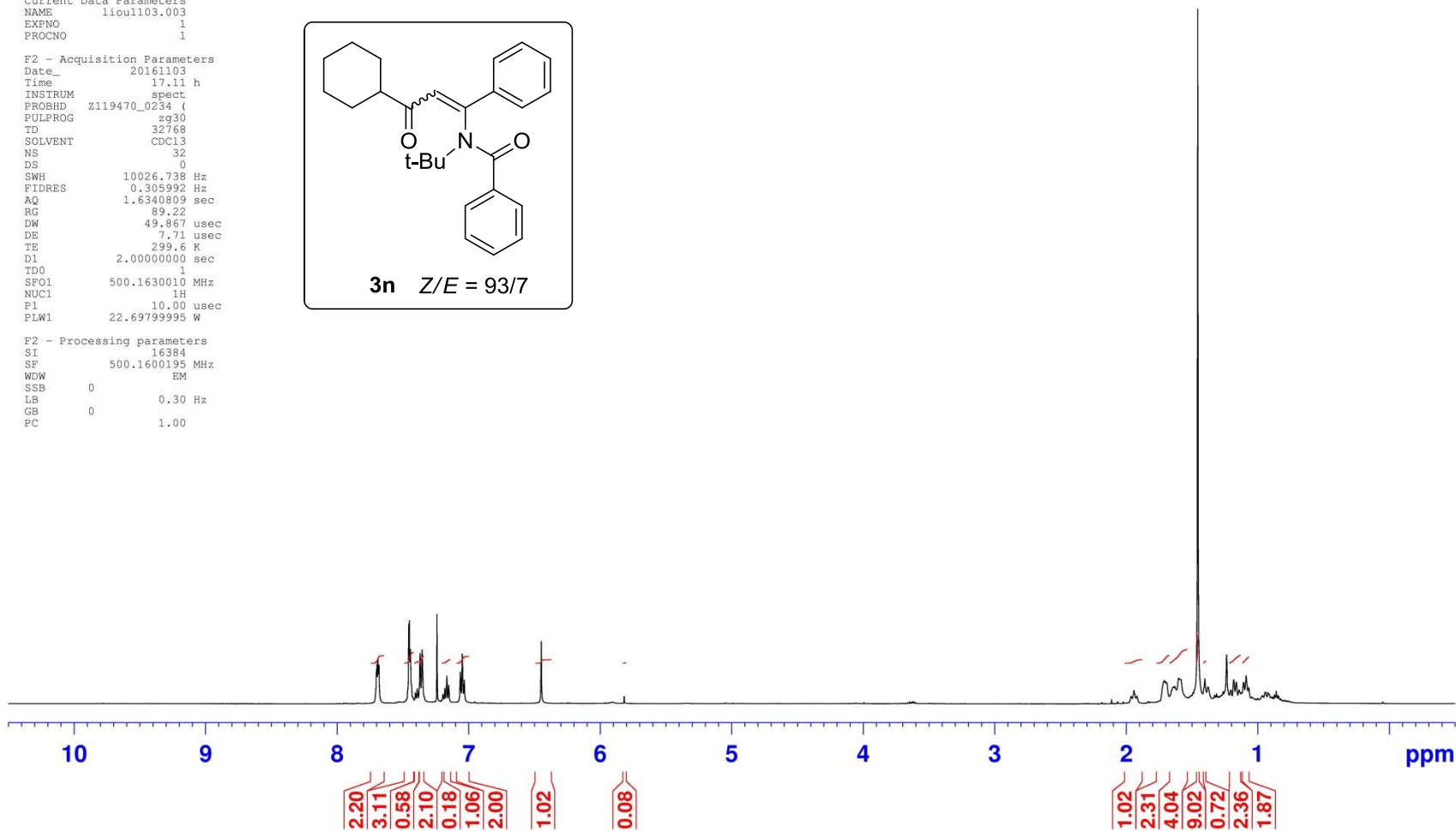
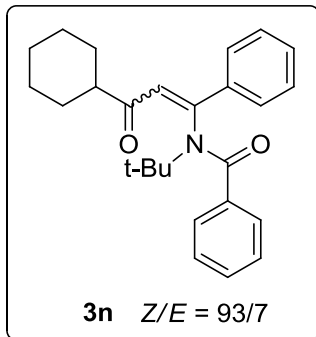
5.816

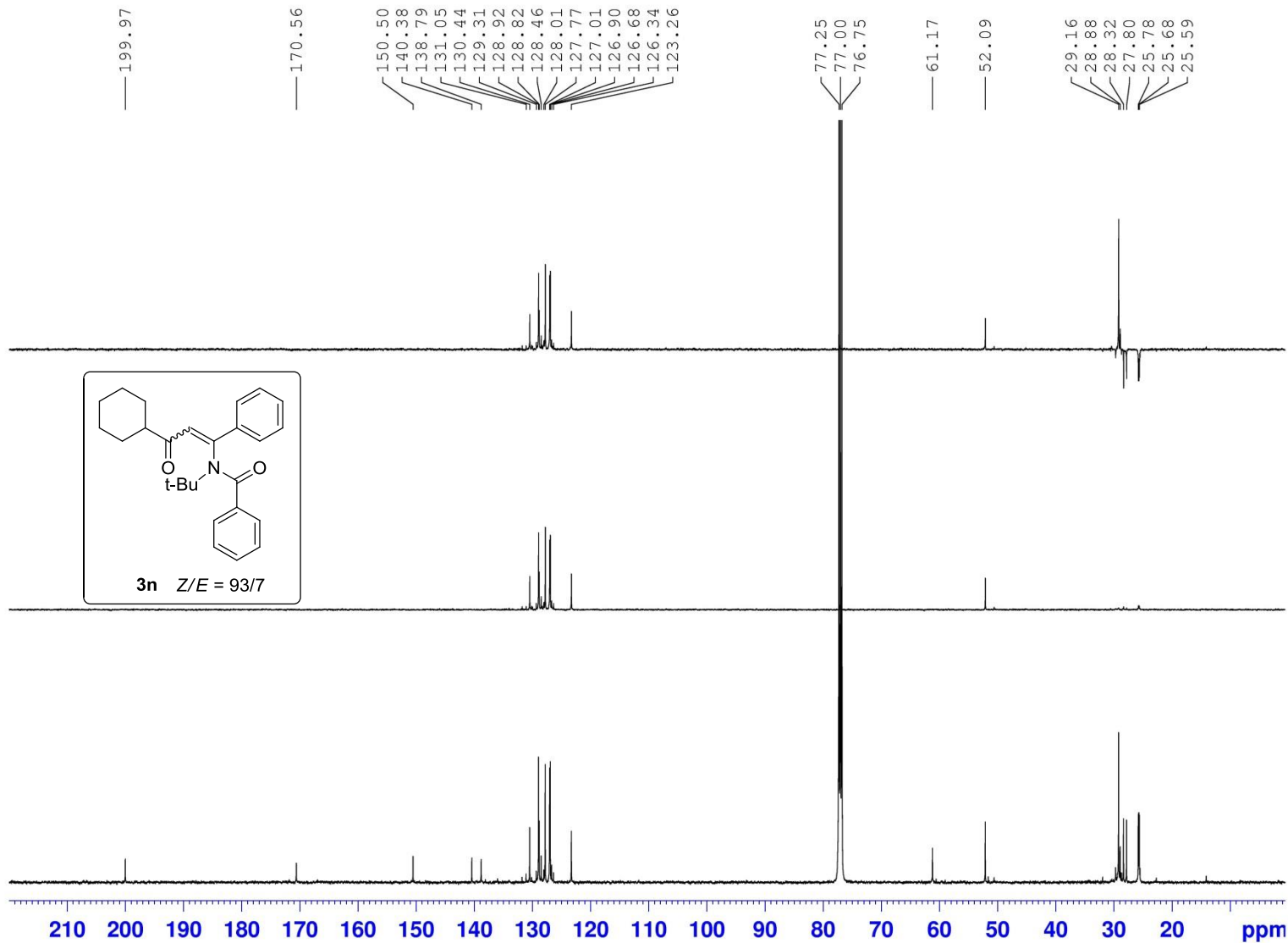
1.964  
1.957  
1.941  
1.935  
1.919  
1.715  
1.708  
1.701  
1.694  
1.655  
1.644  
1.636  
1.630  
1.603  
1.596  
1.583  
1.456  
1.401  
1.377  
1.206  
1.202  
1.183  
1.162  
1.141  
1.107  
1.088  
1.070  
0.963  
0.945  
0.939  
0.921  
0.914  
0.901

Current Data Parameters  
 NAME liou1103.003  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161103  
 Time 17.11 h  
 INSTRUM spect  
 PROBHD Z119470\_0234 (  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 32  
 DS 0  
 SWH 10026.738 Hz  
 FIDRES 0.305992 Hz  
 AQ 1.6340809 sec  
 RG 89.22  
 DW 49.867 usec  
 DE 7.71 usec  
 TE 299.6 K  
 D1 2.00000000 sec  
 TDO 1  
 SFO1 500.1630010 MHz  
 NUC1 1H  
 P1 10.00 usec  
 PLW1 22.69799995 W

F2 - Processing parameters  
 SI 16384  
 SF 500.1600195 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





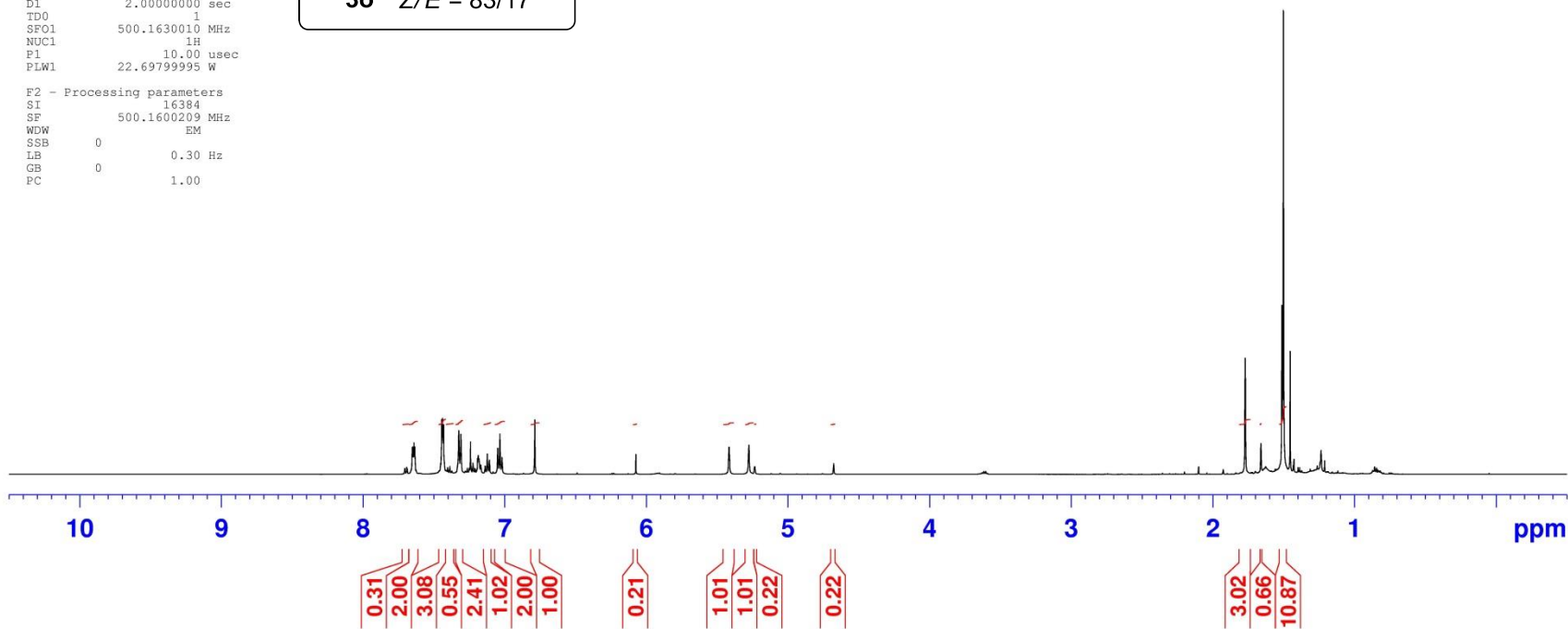
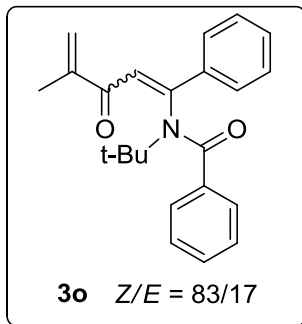
7.704  
7.690  
7.687  
7.657  
7.652  
7.648  
7.644  
7.640  
7.633  
7.451  
7.444  
7.438  
7.431  
7.402  
7.387  
7.372  
7.333  
7.329  
7.323  
7.313  
7.309  
7.306  
7.240  
7.223  
7.210  
7.207  
7.190  
7.186  
7.181  
7.177  
7.168  
7.165  
7.137  
7.122  
7.107  
7.048  
7.033  
7.018  
6.787  
6.073  
5.414  
5.276  
5.234  
4.676

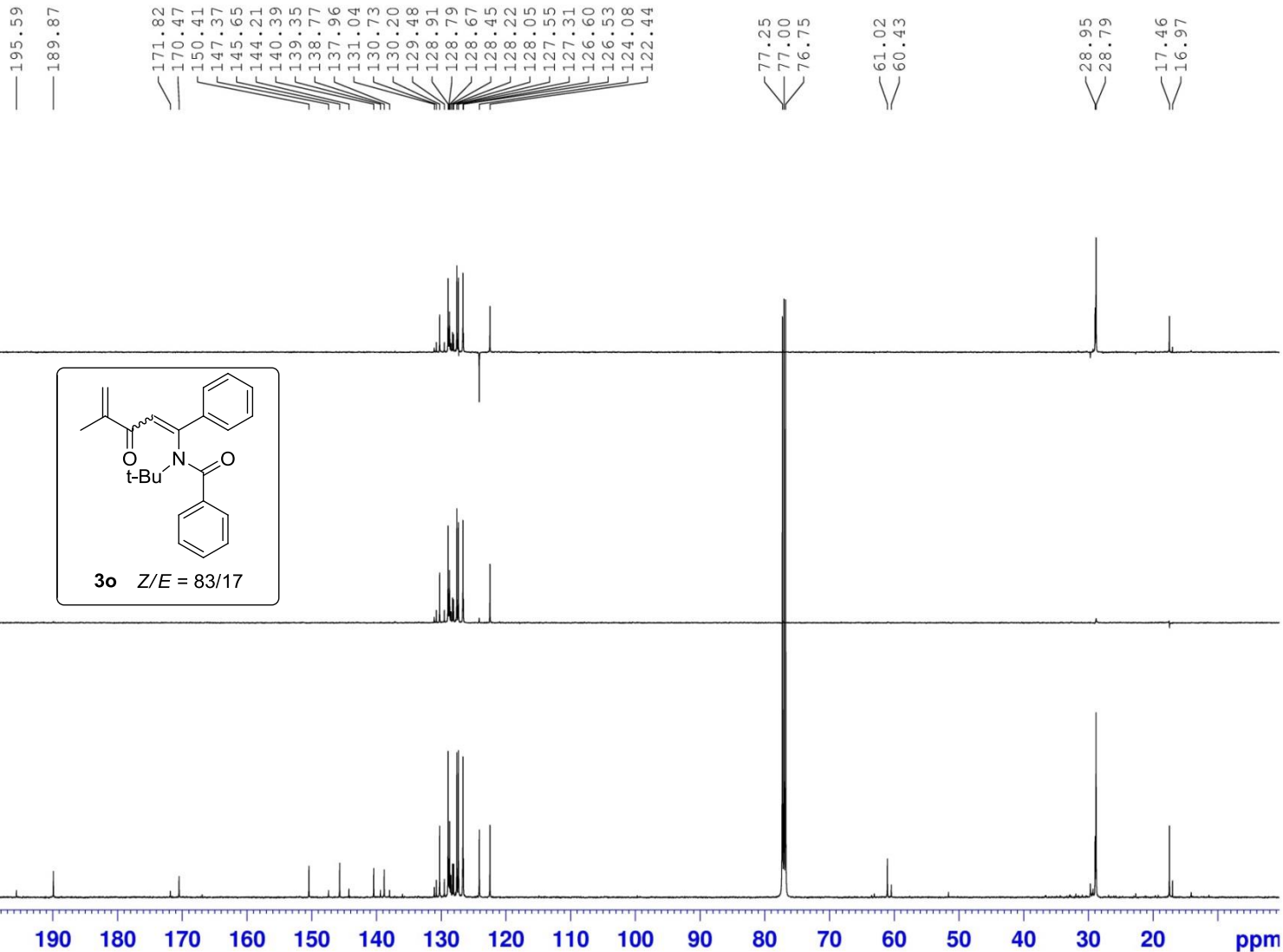
1.771  
1.660  
1.512  
1.502

Current Data Parameters  
NAME l1ou1201.001  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20161201  
Time 16.42 h  
INSTRUM spect  
PROBHD z119470\_0234 (  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 10026.738 Hz  
FIDRES 0.305992 Hz  
AQ 1.6340809 sec  
RG 71.36  
DW 49.867 usec  
DE 7.71 usec  
TE 299.6 K  
DI 2.00000000 sec  
TDO 1  
SFO1 500.1630010 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 22.69799995 W

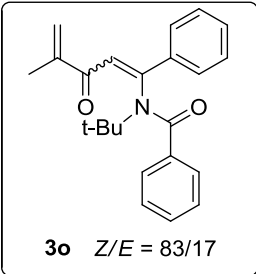
F2 - Processing parameters  
SI 16384  
SF 500.1600209 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





Current Data Parameters  
 NAME liou1201.001  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161201  
 Time\_ 16.50 h  
 INSTRUM spect  
 PROBHD Z119470\_0234 (  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDC13  
 NS 12800  
 DS 0  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 0.5505024 sec  
 RG 191.01  
 DW 16.800 usec  
 DE 6.50 usec  
 TE 300.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 125.7785374 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 80.55799866 W  
 SFO2 500.1620006 MHz  
 NUC2 1H  
 CPDPRG[2 bi\_waltz65 256  
 ECPD2 80.00 usec  
 PLW2 22.69799995 W  
 PLW12 0.36415839 W  
 PLW13 0.18251620 W



F2 - Processing parameters  
 SI 32768  
 SF 125.7653349 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

8.088  
8.075  
7.617  
7.603  
7.585  
7.572  
7.560  
7.515  
7.500  
7.452  
7.438  
7.427  
7.413  
7.388  
7.379  
7.375  
7.253  
7.240  
7.204  
7.189  
7.138  
7.123  
7.108  
7.094  
7.043  
7.030  
7.018  
6.974  
6.904  
6.891  
6.878  
6.784  
6.769  
6.609  
6.595  
6.299

3.817  
3.760

1.537

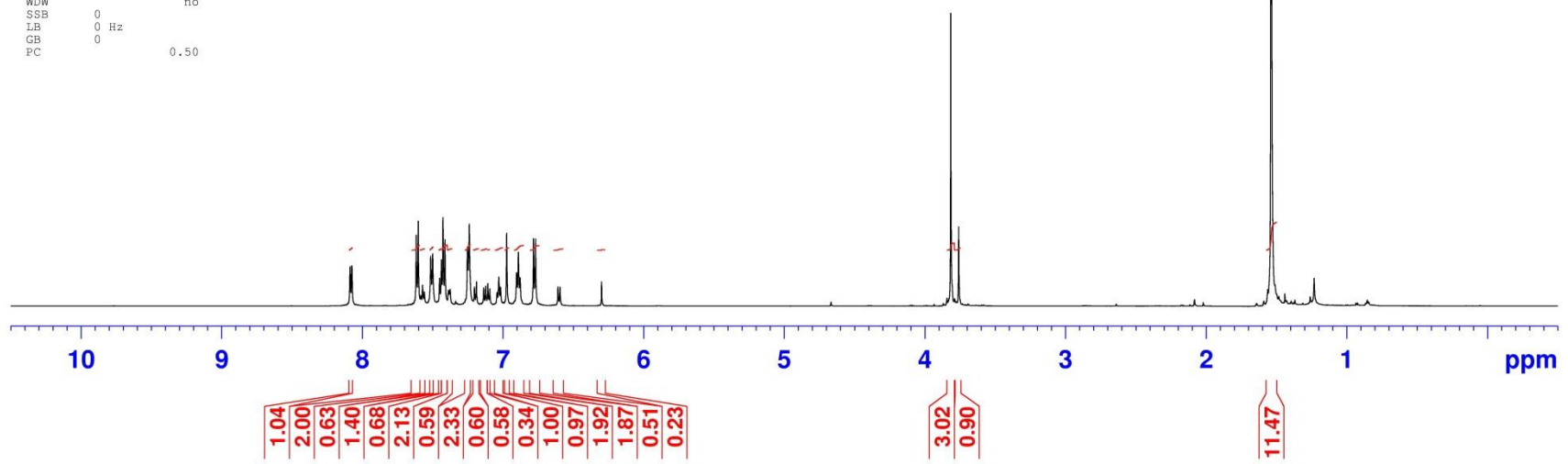
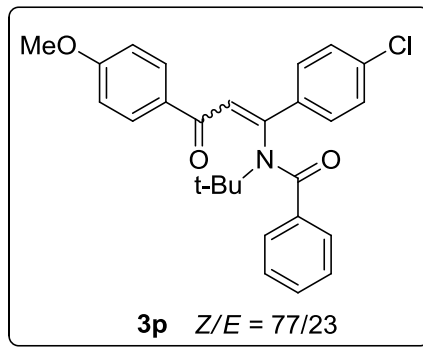
```

Current Data Parameters
NAME Yu-6-90
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161209
Time 4.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 16384
SOLVENT H2O
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.512040 Hz
AQ 0.9765364 sec
RG 128
DW 59.600 usec
DE 6.00 usec
TE 295.9 K
D1 2.0000000 sec
MCREST 0 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 0 dB
SF01 598.4029920 MHz

F2 - Processing parameters
SI 32768
SF 598.4000268 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.50
  
```



— 191.60  
 — 186.89  
 171.23  
 170.66  
 163.65  
 163.34  
 149.57  
 146.05  
 138.85  
 138.47  
 136.29  
 133.53  
 131.22  
 131.19  
 131.12  
 130.26  
 130.10  
 129.50  
 129.17  
 128.84  
 128.74  
 128.70  
 128.43  
 128.38  
 128.16  
 127.26  
 126.56  
 126.30  
 123.40  
 113.62  
 113.53

77.21  
 77.00  
 76.79

61.16  
 60.61  
 55.43  
 55.38

28.88  
 28.77

Current Data Parameters  
 NAME Yu-6-90  
 EXPNO 2  
 PROCNO 1

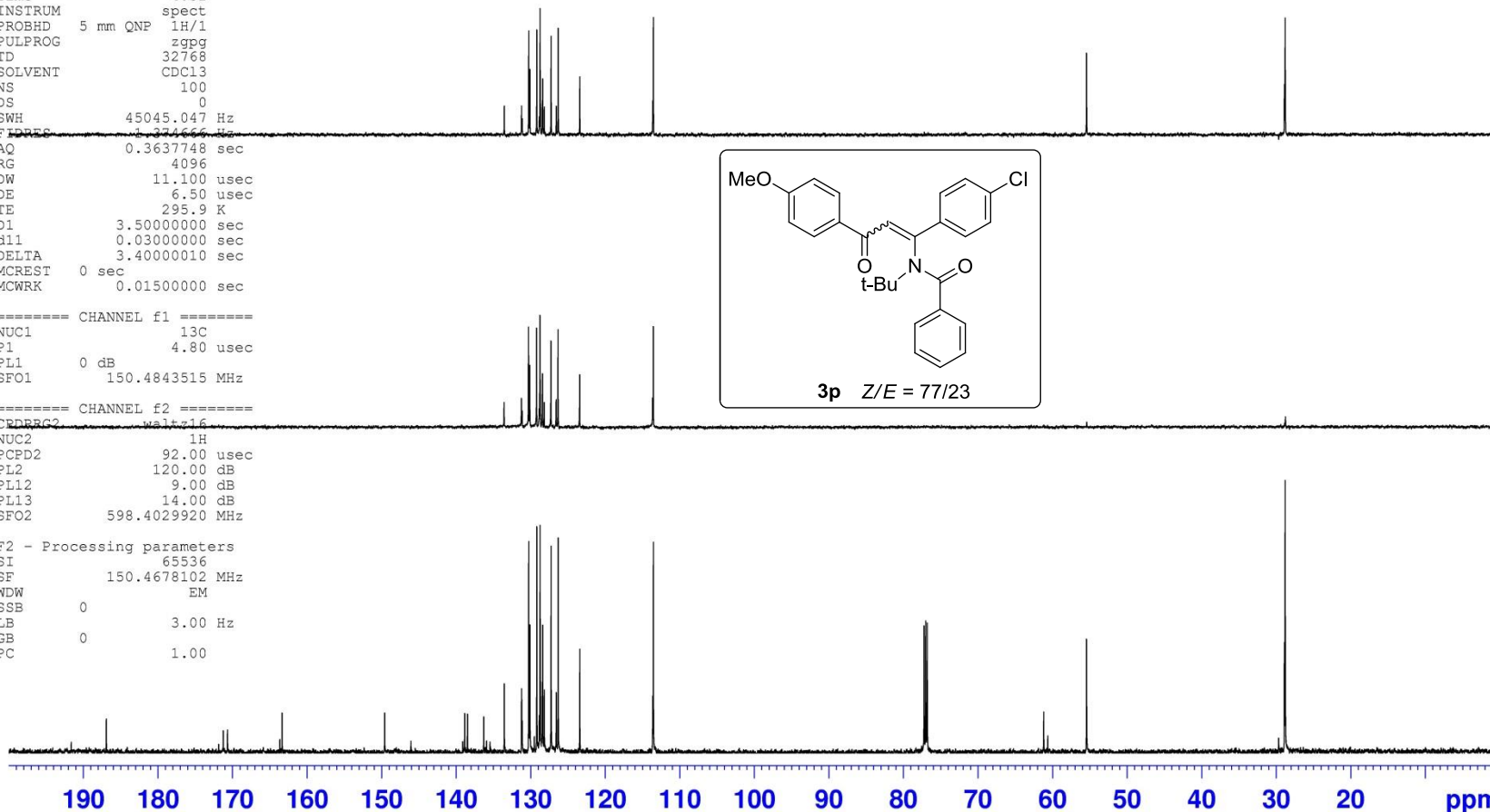
F2 - Acquisition Parameters

Date\_ 20161209  
 Time 4.52  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDC13  
 NS 100  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 295.9 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0 sec  
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0 dB  
 SFO1 150.4843515 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.4029920 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4678102 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00





7.723  
7.720  
7.718  
7.715  
7.713  
7.710  
7.708  
7.706  
7.491  
7.477  
7.475  
7.472  
7.470  
7.467  
7.465  
7.462  
7.460  
7.447  
7.295  
7.282  
7.271  
7.269  
7.240  
7.240  
7.186  
7.172  
7.012  
6.680  
6.667  
6.286

2.249  
2.095  
1.535  
1.526

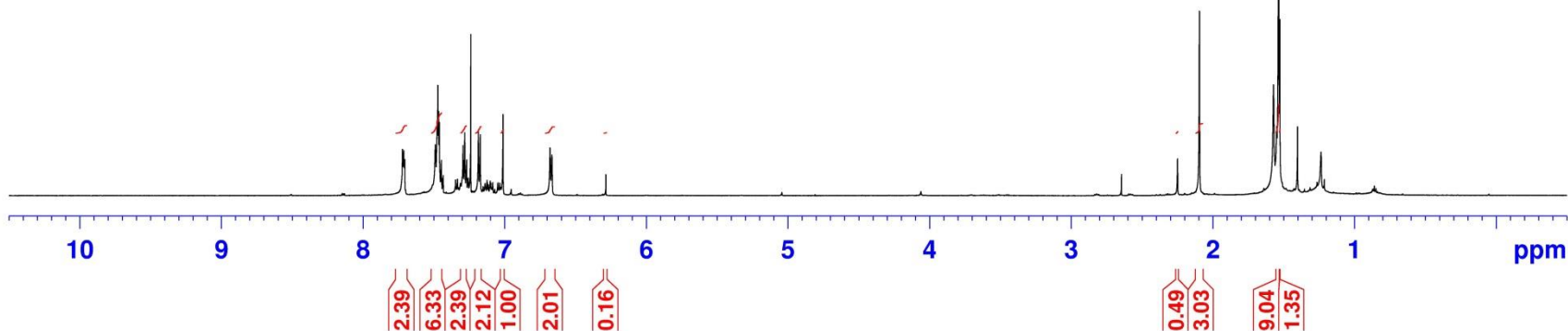
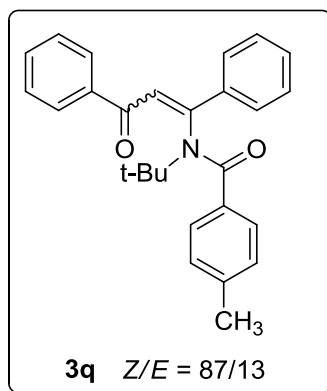
```

Current Data Parameters
NAME Yu-6-40
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161001
Time 0.05
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 301.6 K
D1 3.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.60 usec
PL1 3.00 dB
SFO1 598.5029049 MHz

F2 - Processing parameters
SI 32768
SF 598.5000269 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
  
```



188.38

170.73

151.66  
140.49  
138.57  
138.36  
135.78  
132.57  
130.37  
128.96  
128.13  
128.08  
127.92  
127.71  
126.58  
123.21

77.21  
77.00  
76.79

61.08

28.86

21.05

Current Data Parameters  
NAME Yu-6-40  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters

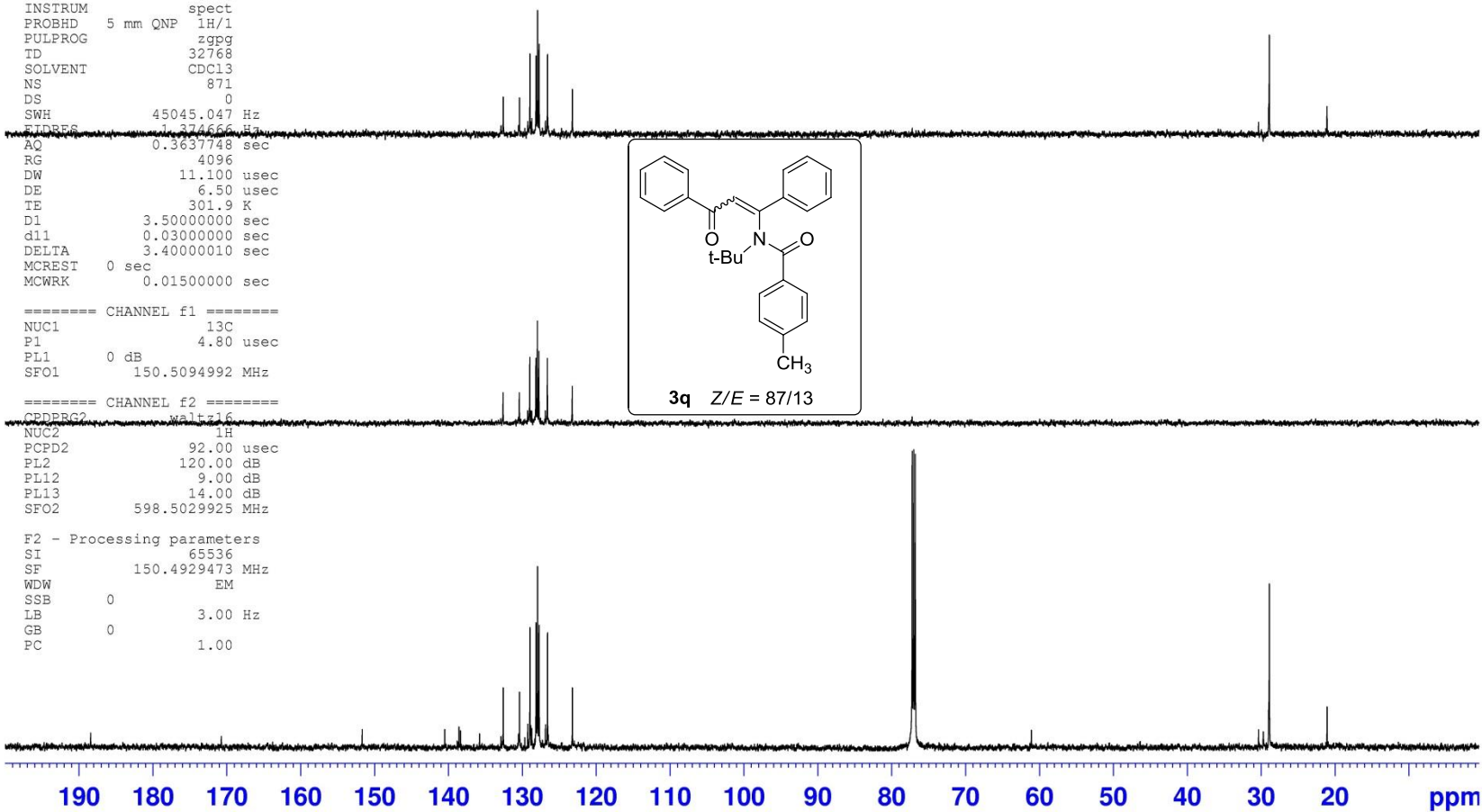
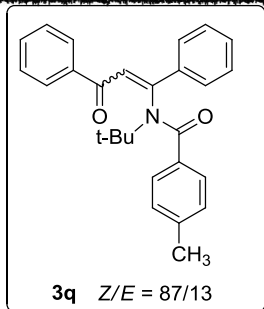
Date\_ 20161001  
Time 0.13  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 871  
DS 0  
SWH 45045.047 Hz  
FIDRES 0.374556 Hz  
AQ 0.3637748 sec  
RG 4096  
DW 11.100 usec  
DE 6.50 usec  
TE 301.9 K  
D1 3.50000000 sec  
d11 0.03000000 sec  
DELTA 3.40000010 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
NUC1 13C  
P1 4.80 usec  
PL1 0 dB  
SFO1 150.5094992 MHz

==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 92.00 usec  
PL2 120.00 dB  
PL12 9.00 dB  
PL13 14.00 dB  
SFO2 598.5029925 MHz

F2 - Processing parameters

SI 65536  
SF 150.4929473 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00



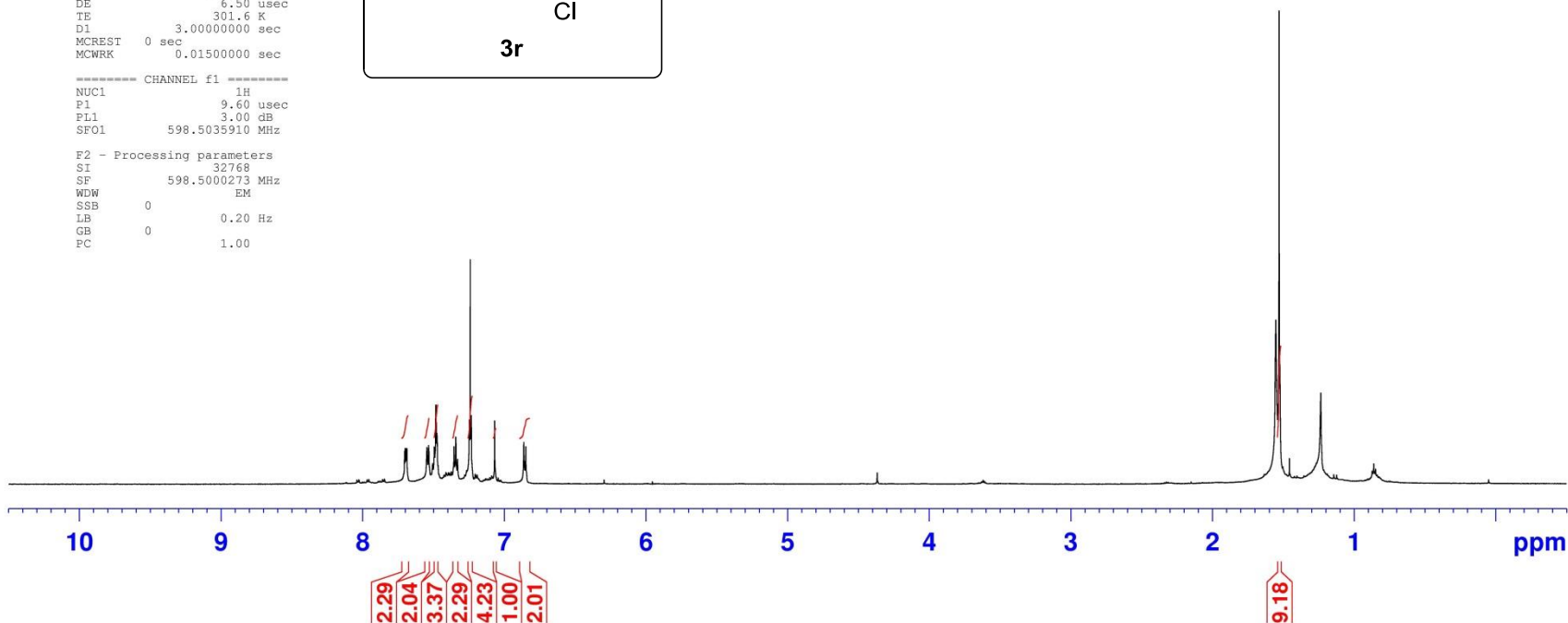
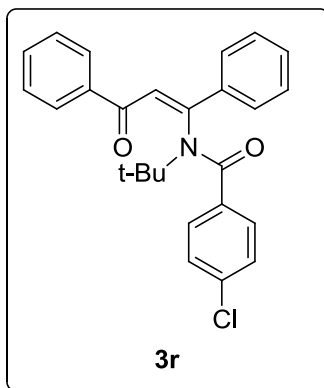
7.703  
7.700  
7.694  
7.691  
7.687  
7.546  
7.534  
7.532  
7.494  
7.491  
7.484  
7.481  
7.475  
7.473  
7.355  
7.342  
7.341  
7.328  
7.246  
7.240  
7.232  
7.067  
6.862  
6.848

Current Data Parameters  
NAME Yu-6-41  
EXPNO 1  
PROCNO 1

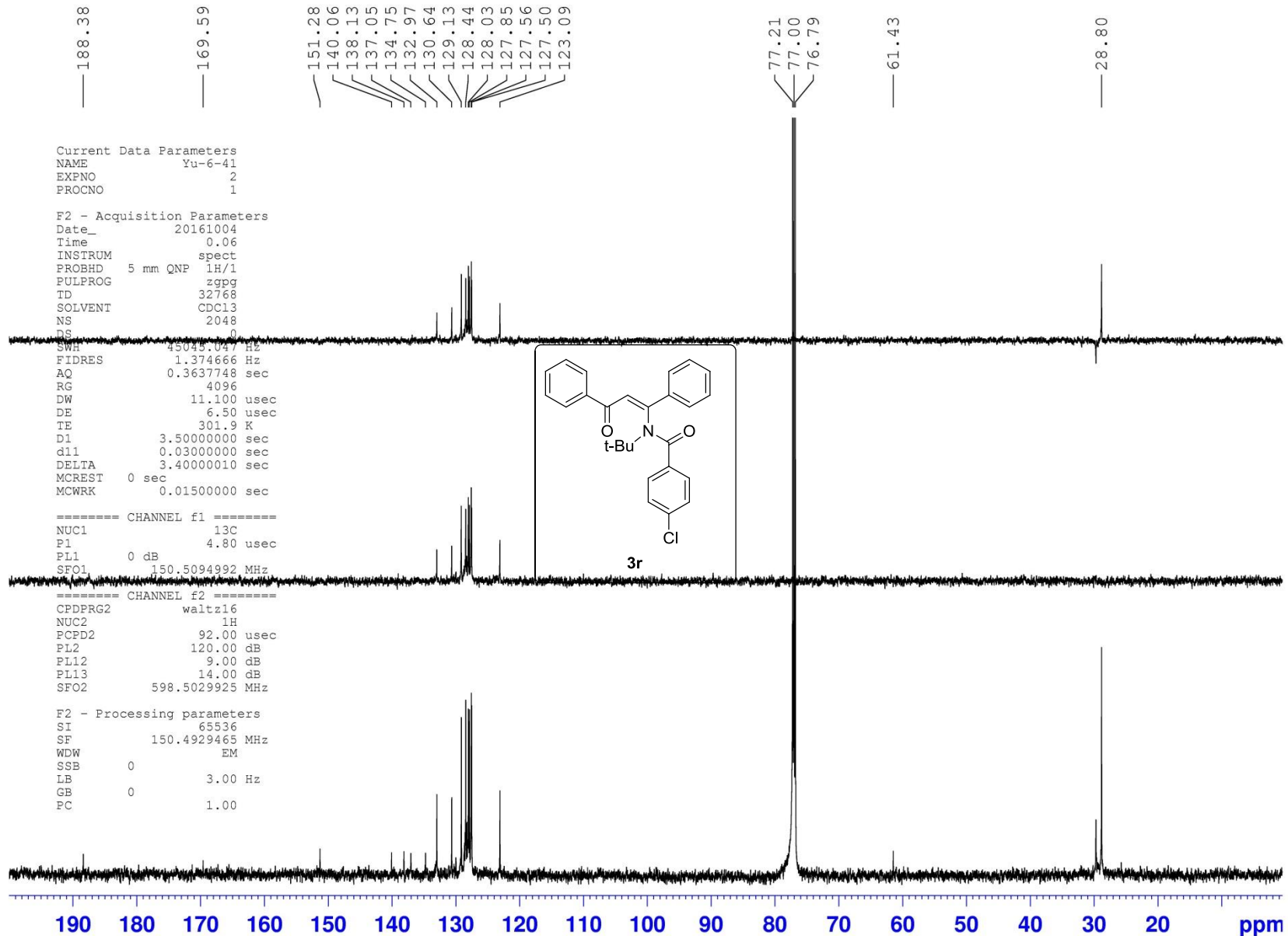
F2 - Acquisition Parameters  
Date\_ 20161003  
Time 23.47  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631988 sec  
RG 512  
DW 41.600 usec  
DE 6.50 usec  
TE 301.6 K  
D1 3.0000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

----- CHANNEL f1 -----  
NUC1 1H  
P1 9.60 usec  
PL1 3.00 dB  
SF01 598.5035910 MHz

F2 - Processing parameters  
SI 32768  
SF 598.5000273 MHz  
WDW EM  
SSB 0  
LB 0.20 Hz  
GB 0  
PC 1.00



— 1.529



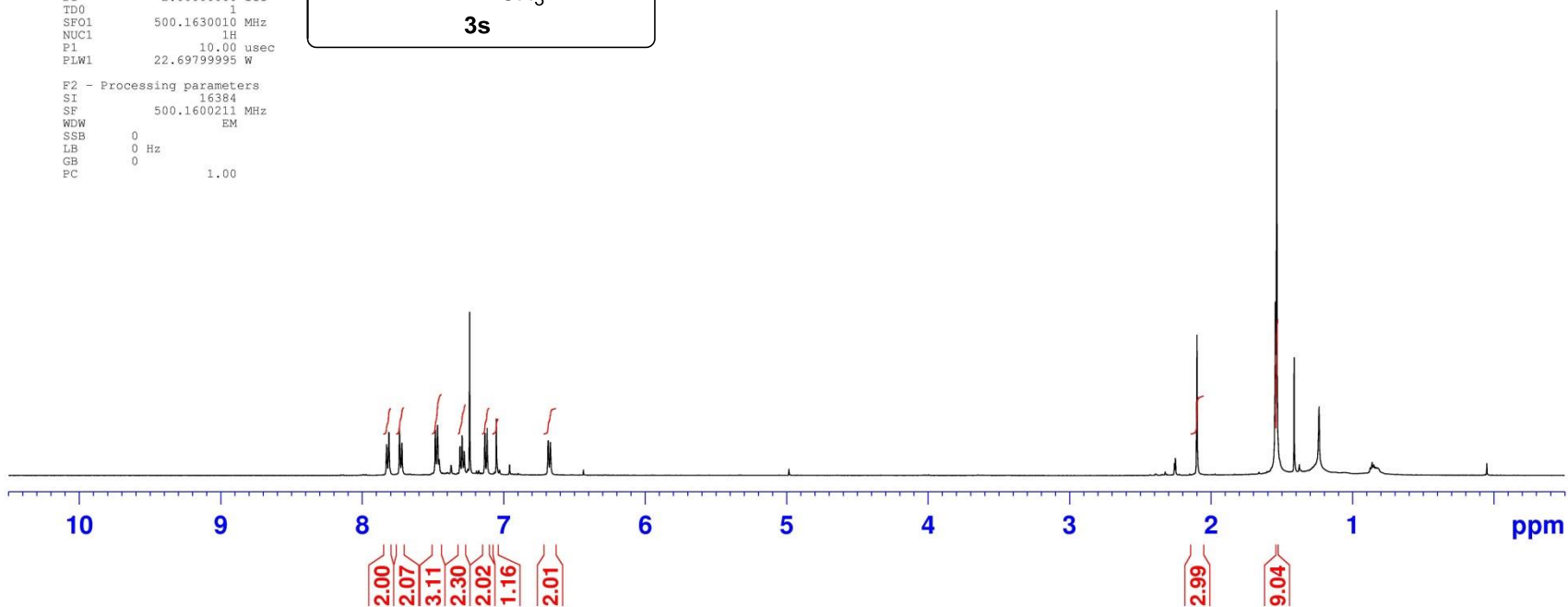
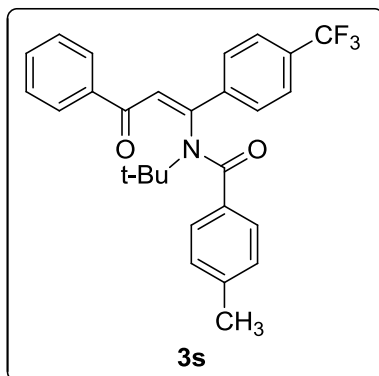
7.827  
7.811  
7.735  
7.718  
7.483  
7.467  
7.456  
7.309  
7.293  
7.277  
7.240  
7.132  
7.116  
7.051  
6.685  
6.669

```

Current Data Parameters
NAME      liou0817.002
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20160816
Time      16.55 h
INSTRUM   spect
PROBHD    Z119470_0234 (
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         32
DS         0
SWH        10026.738 Hz
FIDRES     0.305992 Hz
AQ         1.6340809 sec
RG         191.01
DW         49.867 usec
DE         7.71 usec
TE         300.0 K
D1         2.00000000 sec
TD0        1
SFO1      500.1630010 MHz
NUC1       1H
P1         10.00 usec
PLW1       22.69799995 W

F2 - Processing parameters
SI         16384
SF         500.1600211 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         1.00
  
```

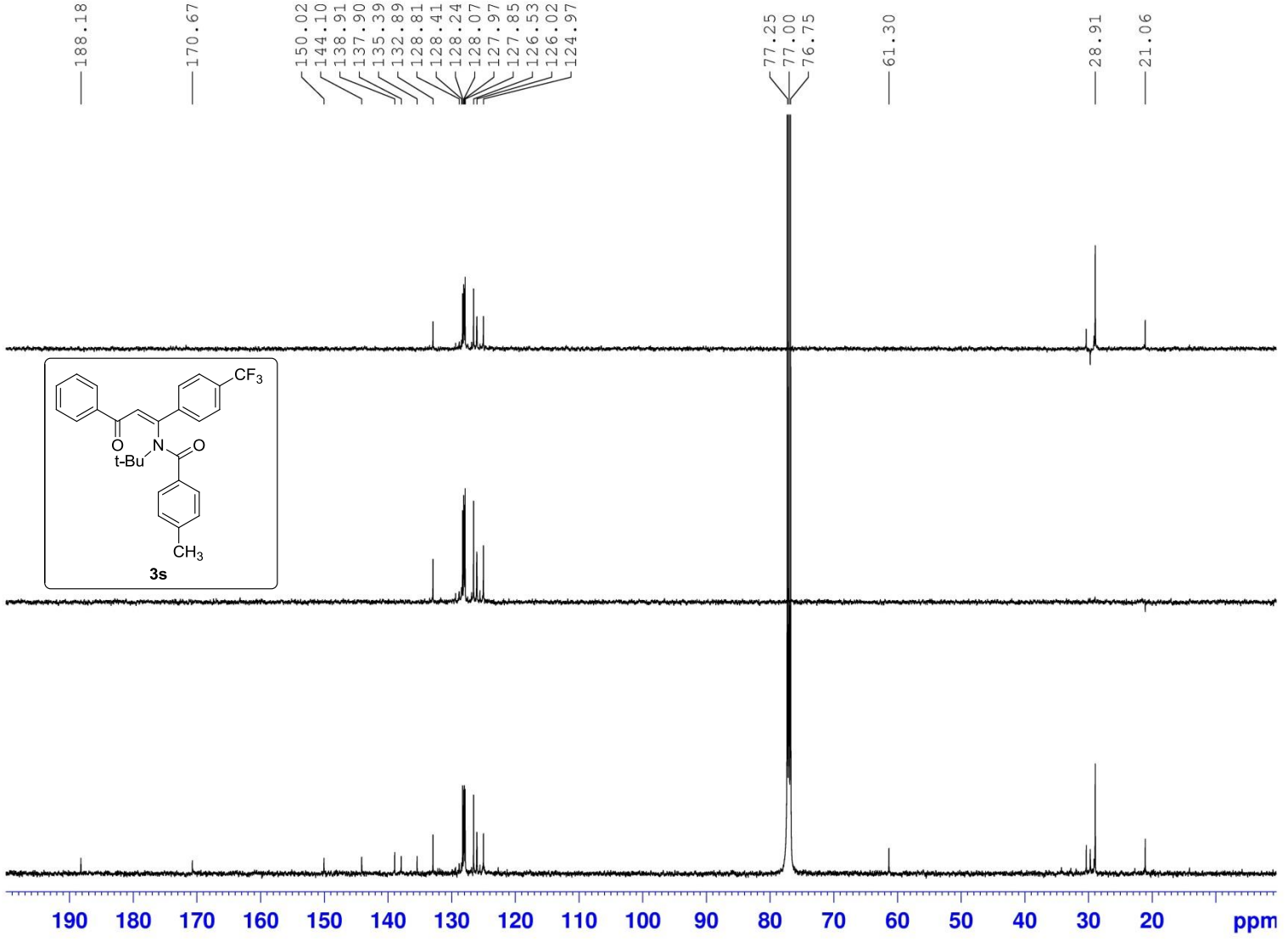
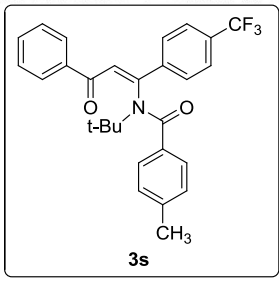


2.099  
1.535

Yu-6-1 / 13C

Current Data Parameters  
NAME liou0817.002  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160816  
Time\_ 17.15 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 6000  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7785374 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 80.55799866 W  
SFO2 500.1620006 MHz  
NUC2 1H  
CPDPRG2 bi\_waltz65\_256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W

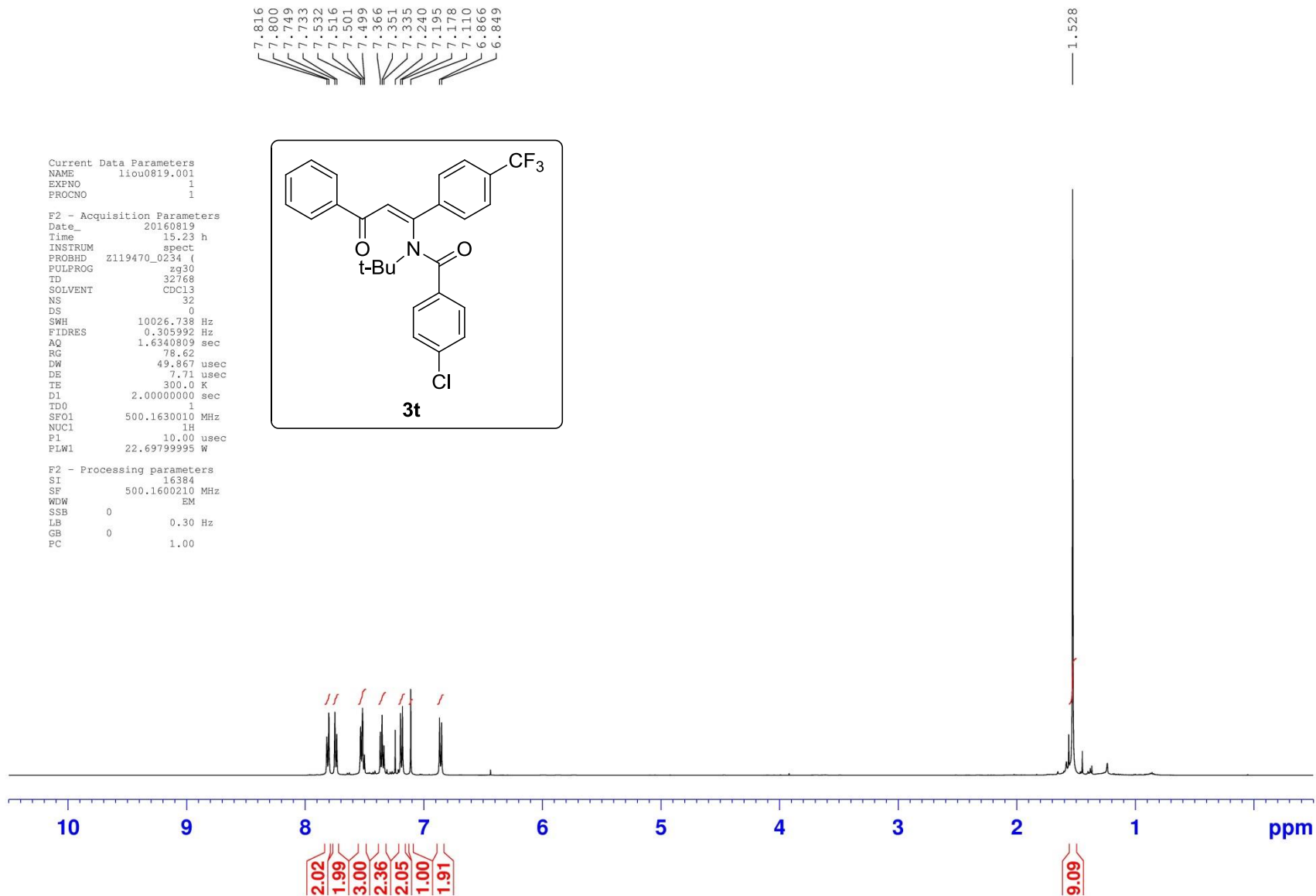
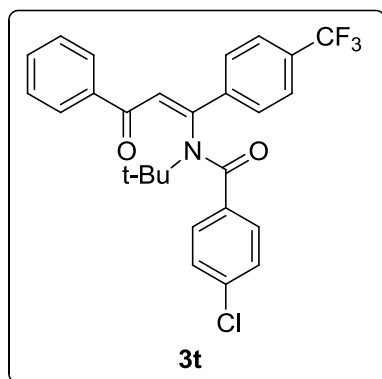


Current Data Parameters  
NAME liou0819.001  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160819  
Time 15.23 h  
INSTRUM spect  
PROBHD z119470\_0234 (  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 0  
SWH 10026.738 Hz  
FIDRES 0.305992 Hz  
AQ 1.6340809 sec  
RG 78.62  
DW 49.867 usec  
DE 7.71 usec  
TE 300.0 K  
D1 2.00000000 sec  
TD0 1  
SFO1 500.1630010 MHz  
NUC1 1H  
P1 10.00 usec  
PLW1 22.69799995 W

F2 - Processing parameters  
SI 16384  
SF 500.1600210 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.816  
7.800  
7.749  
7.733  
7.532  
7.516  
7.501  
7.499  
7.366  
7.351  
7.335  
7.240  
7.195  
7.178  
7.110  
6.866  
6.849



Yu-6-2 / 13C

Current Data Parameters  
NAME liou0819.001  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160819  
Time 15.37 h  
INSTRUM spect  
PROBHD Z119470\_0234 (  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 6000  
DS 0  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 0.5505024 sec  
RG 191.01  
DW 16.800 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7785374 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 80.55799866 W  
SFO2 500.1620006 MHz  
NUC2 1H  
CPDPRG[2 bi\_waltz65 256  
PCPD2 80.00 usec  
PLW2 22.69799995 W  
PLW12 0.36415839 W  
PLW13 0.18251620 W

F2 - Processing parameters  
SI 32768  
SF 125.7653349 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

