

*Supporting Information*

**Highly Diastereo- and Branched-Selective Rearrangement of Substituted  
*N*-Alloc-*N*-Allyl Ynamides.**

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## 1. General Information

All reactions were carried out under an atmosphere of nitrogen in oven-dried glassware with a magnetic stirring bar. All reactions were monitored by thin layer chromatography (TLC) using Merck TLC silica gel 60 sheets, which were visualized with ultraviolet light and then developed with basic potassium permanganate solution. Flash chromatography was performed on Silacyle silica gel 60 as the stationary phase and the solvents employed were of analytical grade.

<sup>1</sup>H NMR spectra were recorded at 400 MHz or 500 MHz at ambient temperature. Data are reported as follows: chemical shift in parts per million (ppm) from deuterated chloroform (CDCl<sub>3</sub>) taken as 7.27 ppm, integration, multiplicity (s = singlet, d = doublet; t = triplet; dd = double doublets, dt = double triplets, dq = double quartets, qt = quartet triplets, ddd = double double doublets, ddt = double double triplets, dddd = double double double doublets, tq = triplet quartets, dtq = double triplet quartets, dqt = double quartet triplets, m = multiplet, br = broad), and coupling constant (Hz). <sup>13</sup>C NMR spectra were recorded at 100 MHz or 125 MHz. Chemical shifts are reported in ppm from CDCl<sub>3</sub> taken as 77.0 ppm. Infrared spectra were recorded on a Perkin Elmer RX I FT-IR spectrometer as liquid films or as dilute solutions between two KBr discs. Mass spectra were recorded on either a Micromass GCT Premier or a Waters Micromass LCT Premier spectrometer using electron ionisation (EI) at 70 eV or electrospray (ES) techniques, respectively.

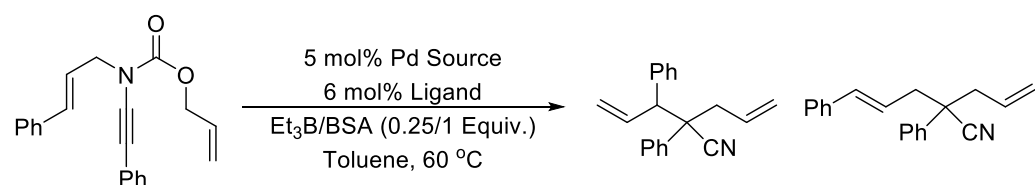
Unless stated otherwise, all commercially available reagents were used as received. When necessary, commonly used organic solvents were dried prior to use according to standard laboratory practices.<sup>1</sup>

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<sup>1</sup> Armarego, W. L. F.; Chai, C., *Purification of Laboratory Chemicals (Seventh Edition)*, Armarego, W. L. F.; Chai, C., Eds. Butterworth-Heinemann: Boston, 2013.

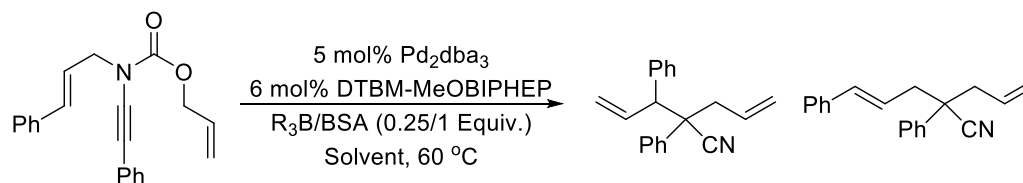
## 2. Selected Optimization Studies

**Table S1.** Palladium and Ligand Screen



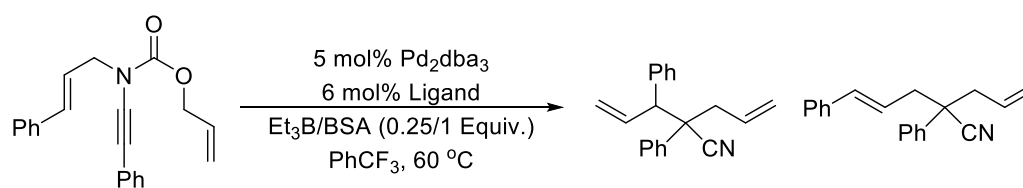
Entry	Pd Source	Ligand	Yield	b/l	d.r
1	$\text{Pd}(\text{OAc})_2$	BINAP	43%	1.5:1	1:1
2	$\text{Pd}(\text{OAc})_2$	SEGPHOS	61%	1.5:1	1.2:1
3	$\text{Pd}(\text{OAc})_2$	DM-SEGPHOS	93%	1.5:1	1.6:1
4	$\text{Pd}(\text{OAc})_2$	PHANEPHOS	45%	11.6:1	1:1
5	$\text{Pd}(\text{OAc})_2$	DIOP	24%	>20:1	1.4:1
6	$\text{Pd}(\text{OAc})_2$	DIPAMP	27%	1.5:1	4.8:1
7	$\text{Pd}(\text{OAc})_2$	JOSIPHOS	42%	2.4:1	1:1
8	$\text{Pd}(\text{OAc})_2$	MANDYPHOS	37%	10.4:1	1.1:1
9	$\text{Pd}(\text{OAc})_2$	Fur-MeOBIPHEP	37%	>20:1	1:1
10	$\text{Pd}(\text{OAc})_2$	DTBM-MeOBIPHEP	46%	17.3:1	4.3:1
<b>11</b>	<b><math>\text{Pd}_2\text{dba}_3</math></b>	<b>DTBM-MeOBIPHEP</b>	<b>62%</b>	<b>&gt;20:1</b>	<b>4.5:1</b>
12	$[\text{Pd}(\text{allylCl})_2]$	DTBM-MeOBIPHEP	n.r.	-	-
13	Buchwald G3	DTBM-MeOBIPHEP	35%	2.8:1	1.3:1
14	Buchwald G4	DTBM-MeOBIPHEP	n.r.	-	-

**Table S2.** Borane and Solvent Screen



Entry	Borane (Equiv.)	Solvent	Yield	b/l	d.r
1	$\text{Et}_3\text{B}$ (0.25)	Toluene	62%	>20:1	4.5:1
2	$\text{Et}_3\text{B}$ (0.05)	Toluene	13%	>20:1	4.5:1
3	$\text{Et}_3\text{B}$ (0.5)	Toluene	48%	13:1	4.5:1
4	$\text{Et}_3\text{B}$ (1)	Toluene	37%	10:1	3.1:1
5	$\text{Et}_2\text{B}(\text{OMe})$ (0.25)	Toluene	52%	>20:1	1.7:1
6	9-BBN-Hex (0.25)	Toluene	39%	>20:1	1.4:1
7	$\text{Ph}_3\text{B}$ (0.25)	Toluene	n.r.	-	-
8	$\text{Et}_3\text{B}$ (0.25)	<i>o</i> -Xylene	10%	>20:1	2.7:1
9	$\text{Et}_3\text{B}$ (0.25)	<i>m</i> -Xylene	24%	>20:1	1.9:1
10	$\text{Et}_3\text{B}$ (0.25)	<i>p</i> -Xylene	14%	>20:1	1.9:1
11	$\text{Et}_3\text{B}$ (0.25)	Benzene	32%	3.4:1	2.9:1
12	$\text{Et}_3\text{B}$ (0.25)	Chlorobenzene	38%	>20:1	5.8:1
<b>13</b>	<b><math>\text{Et}_3\text{B}</math> (0.25)</b>	<b>Trifluorotoluene</b>	<b>70%</b>	<b>&gt;20:1</b>	<b>13:1</b>



**Table S3.** Ligand Reoptimization

Entry	Ligand	Yield	b/l	d.r
1	MeOBIPHEP ( <b>L1a</b> )	11%	>20:1	1.8:1
2	i-Pr-MeOBIPHEP ( <b>L1b</b> )	5%	>20:1	1:1.2
3	Fur-MeOBIPHEP ( <b>L1c</b> )	35%	>20:1	1:1.1
4	DM-MeOBIPHEP ( <b>L1d</b> )	8%	>20:1	3.6:1
5	DTB-MeOBIPHEP ( <b>L1e</b> )	20%	>20:1	5.4:1
6	DMM-MeOBIPHEP ( <b>L1f</b> )	40%	>20:1	9:1
7	DTBM-MeOBIPHEP ( <b>L1g</b> )	70% (63%)	>20:1	13:1
8	i-Pr-Me <sub>2</sub> N-MeOBIPHEP ( <b>L1h</b> )	57%	>20:1	13:1
9	DTBM-SEGPHOS ( <b>L2g</b> )	15%	>20:1	13:1
10	DTBM-GARPHOS ( <b>L3g</b> )	25%	>20:1	5:1

### 3. General Procedures

#### General Procedure A for the Synthesis of *N*-Alloc-*N*-Allyl Ynamides<sup>2</sup>

To an oven dried round bottom flask equipped with reflux condenser and magnetic stirrer bar and purged with nitrogen was added alkynyl bromide (1.20 equiv.) in anhydrous toluene (0.5 M). Carbamate (1.00 equiv.), CuSO<sub>4</sub>·5H<sub>2</sub>O (0.10 equiv.), 1,10-phenanthroline (0.20 equiv.) and K<sub>3</sub>PO<sub>4</sub> (2.00 equiv.) were added in sequentially and the mixture stirred at 80 °C on a heating mantle for 3 days. The mixture filtered through a plug of Celite™, washed with CH<sub>2</sub>Cl<sub>2</sub> and concentrated *in vacuo*. The crude product was purified by flash column chromatography.

#### General Procedure B for the regio and stereoselective synthesis of complex nitriles

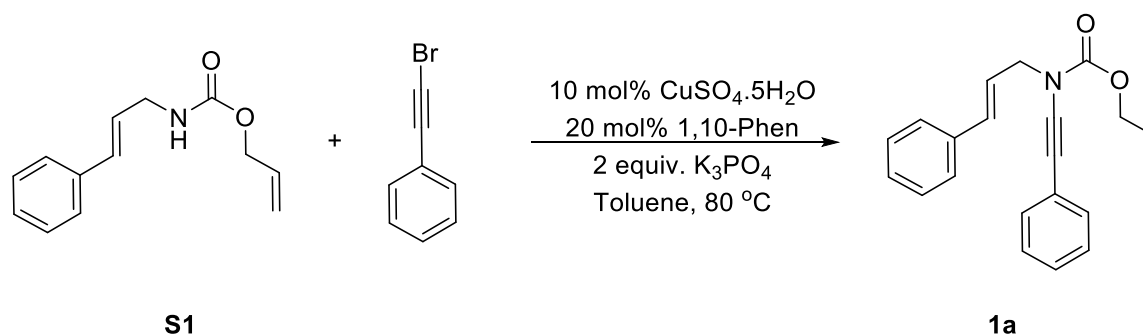
To an oven dried 5 mL reaction vial, equipped with a magnetic stirrer bar, was added Pd<sub>2</sub>dba<sub>3</sub> (2.5 mol%) and (R)-DTBM-MeOBIPHEP (6.0 mol%) under a nitrogen atmosphere. A solution of yne-carbamate (1.00 equiv.), BEt<sub>3</sub> (0.25 equiv.) and *N,O*-BSA (1.00 equiv.) in trifluorotoluene (0.044 M) was subsequently added to the mixture and was stirred at 25 °C for 15 minutes to allow for catalyst complex formation *in-situ*. The reaction was then heated to 60 °C using a heating mantle and stirred for 18 hours. The crude reaction mixture was concentrated *in vacuo* and then purified by flash column chromatography.

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<sup>2</sup> (a) De Korver, K. A.; Hsung, R. P.; Lohse, A. G.; Zhang, Y., *Org. Lett.* **2010**, *12*, 1840–1843; (b) DeKorver, K. A.; Wang, X.-N.; Walton, M. C.; Hsung, R. P., *Org. Lett.* **2012**, *14*, 1768–1771; (c) Alexander, J. A., Shchetepkina, V. I.; Stankevich, K. S.; Benedict, R. J.; Bernhard, S. P.; Dreiling, R. J.; Cook, M. J., *Org. Lett.* **2021**, *23* (2), 559-564.

#### 4. Synthesis of Substituted *N*-Allyl-*N*-Alloc Ynamides (**1**)

##### Allyl cinnamyl(phenylethynyl)carbamate (**1a**)

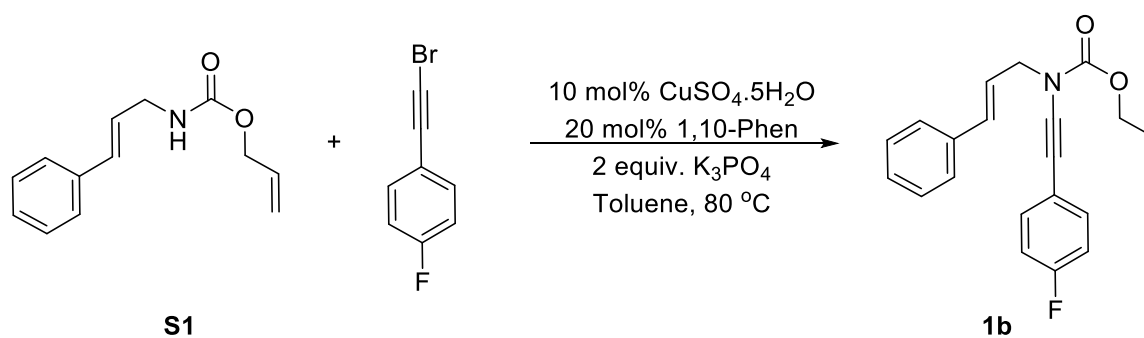


The title compound was prepared by General Procedure A from allyl cinnamyl carbamate<sup>3</sup> (700 mg, 3.23 mmol) and (bromoethynyl)benzene (701 mg, 3.87 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 20:1) to afford **1a** (541 mg, 53%) as an orange oil.

R<sub>f</sub> (Hexanes/EtOAc 5:1) = 0.59. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.44-7.40 (4H, m), 7.38-7.33 (3H, m), 7.31-7.27 (3H, m), 6.69 (1H, d, *J* = 15.8 Hz), 6.36 (1H, dt, *J* = 15.8, 6.7 Hz), 6.00 (1H, ddt, *J* = 17.1, 10.6, 5.1 Hz), 5.45 (1H, d, *J* = 17.5, 1.8 Hz), 5.30 (1H, ddt, *J* = 10.5, 1.3, 1.3 Hz), 4.76 (2H, ddd, *J* = 5.4, 1.3, 1.3 Hz), 4.35 (2H, d, *J* = 6.7 Hz); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 154.6, 136.3, 134.2, 131.7, 131.0, 128.5, 128.1, 127.9, 127.4, 126.5, 123.1, 122.6, 118.1, 82.7, 71.0, 67.5, 52.3. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>21</sub>H<sub>20</sub>NO<sub>2</sub> 318.1489 found 318.1474.

<sup>3</sup> Martínez, R.; Ramón, D. J.; Yus, M. *Adv. Synth. Catal.* **2008**, 350, 1235-1240.

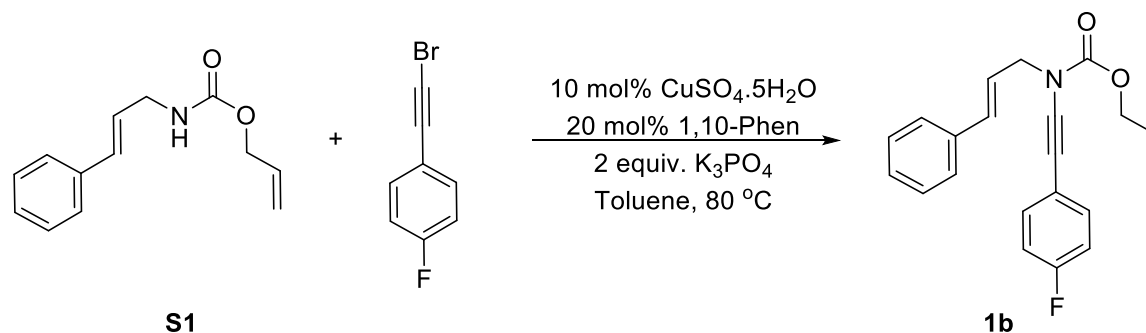
### Allyl cinnamyl(4-fluorophenyl)ethynyl)carbamate (**1b**)



The title compound was prepared by General Procedure A from allyl cinnamyl carbamate (500 mg, 2.30 mmol) and 4-(bromoethynyl)-1-fluorobenzene (546 mg, 2.76 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 20:1) to afford **1b** (509 mg, 66%) as an orange oil.

$R_f$  (Hexanes/EtOAc 5:1) = 0.54. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.42-7.40 (2H, m), 7.37-7.31 (4H, m), 7.28-7.25 (1H, m), 7.00-6.96 (2H, m), 6.68 (1H, d,  $J$  = 16.0, 1.3 Hz), 6.31 (1H, dt,  $J$  = 16.0, 6.9 Hz), 5.99 (1H, ddt,  $J$  = 17.2, 10.7, 5.3 Hz), 5.42 (1H, ddt,  $J$  = 17.2, 1.3, 1.3 Hz), 5.29 (1H, ddt,  $J$  = 10.7, 1.3, 1.3 Hz), 4.75 (2H, ddd,  $J$  = 5.3, 1.3, 1.3 Hz), 4.33 (2H, dd,  $J$  = 6.9, 1.3 Hz), <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 162.1 (d,  $^1J_{CF}$  = 248.5 Hz), 154.7, 136.4, 134.4, 133 (d,  $^3J_{CF}$  = 8.2 Hz), 131.9, 128.7, 128.0, 126.7, 122.7, 119.3 (d,  $^4J_{CF}$  = 3.7 Hz), 118.3, 115.6 (d,  $^2J_{CF}$  = 22.0 Hz), 82.4, 70.1, 67.7, 52.4. HRMS (ESI-TOF)  $m/z$ : [M + H]<sup>+</sup> Calcd. for C<sub>21</sub>H<sub>19</sub>FNO<sub>2</sub> 336.1394 found 336.1379.

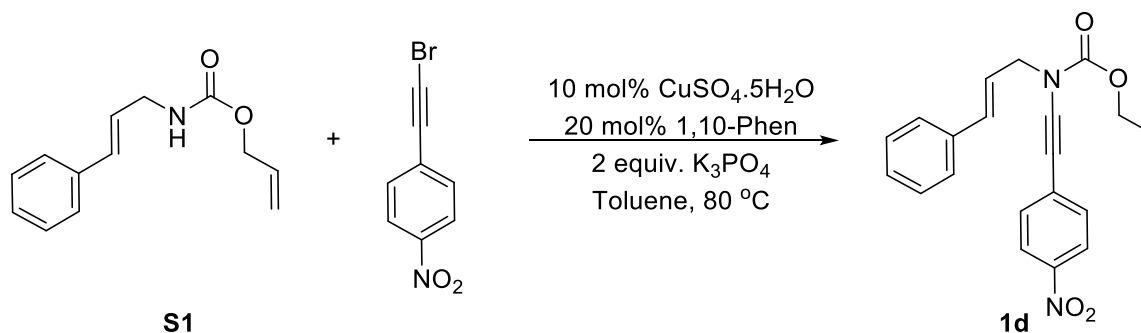
### Allyl cinnamyl(4-(trifluoromethyl)phenyl)ethynyl)carbamate (**1c**)



The title compound was prepared by General Procedure A from allyl cinnamyl carbamate (137 mg, 0.63 mmol) and 4-(bromoethynyl)-1-trifluoromethylbenzene (188 mg, 0.76 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 20:1) to afford **1c** (78 mg, 32%) as a yellow oil.

$R_f$  (Hexanes/ $\text{CH}_2\text{Cl}_2$  1:1) = 0.35.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.55-7.53 (2H, m), 7.48-7.45 (4H, m), 7.39-7.34 (2H, m), 7.32-7.27 (1H, m), 6.71 (1H, d,  $J = 15.8$  Hz), 6.33 (1H, ddd,  $J = 15.8, 6.7, 6.7$  Hz), 6.03 (1H, ddt,  $J = 17.0, 10.1, 6.0$  Hz), 5.46 (1H, ddt,  $J = 17.1, 1.3, 1.3$  Hz), 5.33 (1H, ddt,  $J = 10.6, 1.3, 1.3$  Hz), 4.79 (2H, ddt,  $J = 14.4, 13.1, 11.8$  Hz), 4.38 (2H, ddd,  $J = 6.7, 1.2, 1.2$  Hz),  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.5, 136.2, 134.7, 131.7, 130.9, 129.0 (q,  $^2J_{\text{CF}} = 32.5$  Hz), 128.1, 127.2, 127.2, 125.2 (q,  $^3J_{\text{CF}} = 3.9$  Hz), 124.1 (q,  $^1J_{\text{CF}} = 272.2$  Hz), 122.4, 118.4, 85.4, 70.5, 67.8, 52.4, HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{Na}]^+$  Calcd. for  $\text{C}_{22}\text{H}_{18}\text{F}_3\text{NO}_2\text{Na}$  386.1362 found 386.1364.

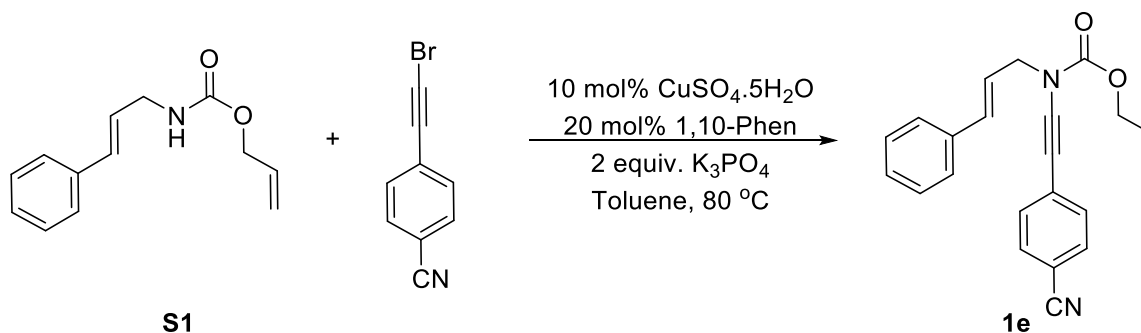
### Allyl cinnamyl((4-nitrophenyl)ethynyl)carbamate (**1d**)



The title compound was prepared by General Procedure A from allyl cinnamyl carbamate (795 mg, 3.66 mmol) and 4-(bromoethynyl)-1-nitrobenzene (985 mg, 4.40 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 3:1) to afford **1d** (924 mg, 70%) as an orange oil.

$R_f$  (Hexanes/EtOAc 3:1) = 0.47. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 8.16 (2H, dd,  $J$  = 8.7, 1.8 Hz), 7.49-7.41 (4H, m), 7.34-7.27 (2H, m), 7.28-7.23 (1H, m), 6.68 (1H, d,  $J$  = 15.8 Hz), 6.26 (1H, dt,  $J$  = 16.0, 6.9 Hz), 6.98 (1H, ddt,  $J$  = 17.2, 10.7, 5.3 Hz), 5.42 (1H, ddt,  $J$  = 18.3, 1.1, 1.1 Hz), 5.29 (1H, ddt,  $J$  = 10.5, 1.1, 1.1 Hz), 4.74 (2H, ddd,  $J$  = 6.8, 1.3, 1.3 Hz), 4.35 (2H, dd,  $J$  = 6.6, 1.1 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 154.2, 146.1, 136.1, 134.9, 131.6, 130.9, 130.7, 128.5, 128.2, 126.6, 123.6, 122.1, 118.6, 88.8, 71.0, 67.9, 52.4. HRMS (ESI-TOF)  $m/z$ : [M + Na]<sup>+</sup> Calcd. for C<sub>21</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>Na 385.1159 found 385.1153.

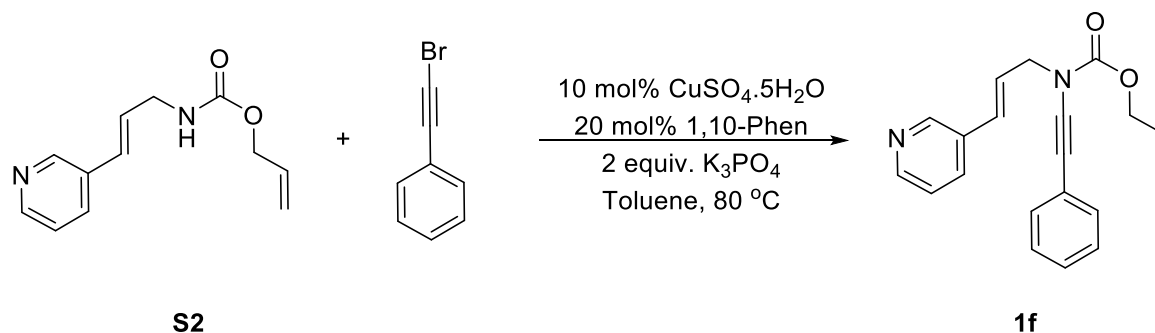
### Allyl cinnamyl(4-cyanophenyl)ethynyl)carbamate (**1e**)



The title compound was prepared by General Procedure A from allyl cinnamyl carbamate (1.05 g, 5.07 mmol) and 4-(bromoethynyl)benzonitrile (1.32 g, 6.08 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 20:1) to afford **1e** (347 mg, 33%) as a yellow oil.

$R_f$  (Hexanes/EtOAc 5:1) = 0.38.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60-7.53 (2H, m), 7.45-7.38 (3H, m), 7.36-7.32 (2H, m), 7.30-7.26 (2H, m), 6.68 (1H, d,  $J = 15.5$  Hz), 6.29 (1H, dt,  $J = 15.5, 6.8$  Hz), 5.99 (1H, ddt,  $J = 17.0, 10.7, 5.3$  Hz), 5.43 (1H, ddt,  $J = 17.2, 1.0$  Hz), 5.31 (1H, ddt,  $J = 10.4, 1.6, 1.6$  Hz), 4.76 (2H, ddd,  $J = 5.5, 1.1, 1.1$  Hz), 4.36 (2H, ddd,  $J = 6.6, 1.1, 1.1$  Hz).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.2, 136.0, 134.7, 131.9, 131.5, 130.0, 128.6, 128.4, 128.1, 126.5, 122.1, 118.7, 118.6, 110.2, 87.7, 70.6, 67.9, 52.2. HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd. for  $\text{C}_{23}\text{H}_{18}\text{N}_2\text{O}_2$  343.1441 found 343.1447.

**Allyl (E)-(phenylethynyl)(3-(pyridin-3-yl)allyl)carbamate (1f)**

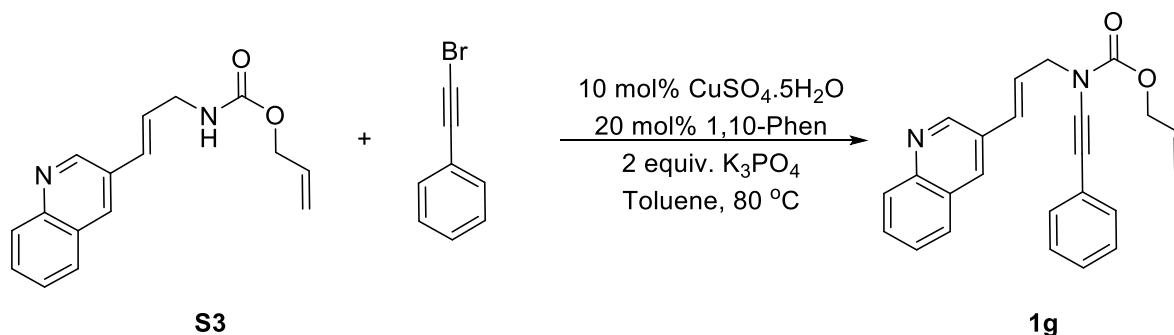


The title compound was prepared by General Procedure A from pyridyl carbamate **S2** (860 mg, 3.94 mmol) and (bromoethynyl)benzene (856 mg, 4.73 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 1:1) to afford **1f** (601 mg, 48%) as a yellow oil.

R<sub>f</sub> (Hexanes/EtOAc 2:1) = 0.59. <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) δ 8.64 (1H, d, *J* = 1.9 Hz), 8.51-8.48 (1H, m), 7.73 (1H, dd, *J* = 7.9, 1.7 Hz), 7.40-7.36 (2H, m), 7.31-7.22 (4H, m), 6.66 (1H, dd, *J* = 15.9, 2.8 Hz), 6.39 (1H, dt, *J* = 15.8, 6.7 Hz), 5.98 (1H, ddt, *J* = 17.1, 10.6, 5.1 Hz), 5.43 (1H, ddt, *J* = 17.2, 1.2, 1.2 Hz), 5.28 (1H, ddt, *J* = 10.4, 1.4, 1.4 Hz), 4.74 (2H, ddd, *J* = 5.5, 1.5, 1.5 Hz), 4.36 (2H, dd, *J* = 6.3, 1.2 Hz). <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) δ 154.7, 149.0, 148.4, 133.1, 132.0, 131.7, 131.3, 131.1, 130.5, 127.7, 125.3, 123.5, 123.0, 118.3, 82.6, 71.1, 67.7, 52.2. HRMS (ESI-TOF) *m/z*: [M + Na]<sup>+</sup> Calcd. for C<sub>20</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>Na 341.1260 found 341.1259.



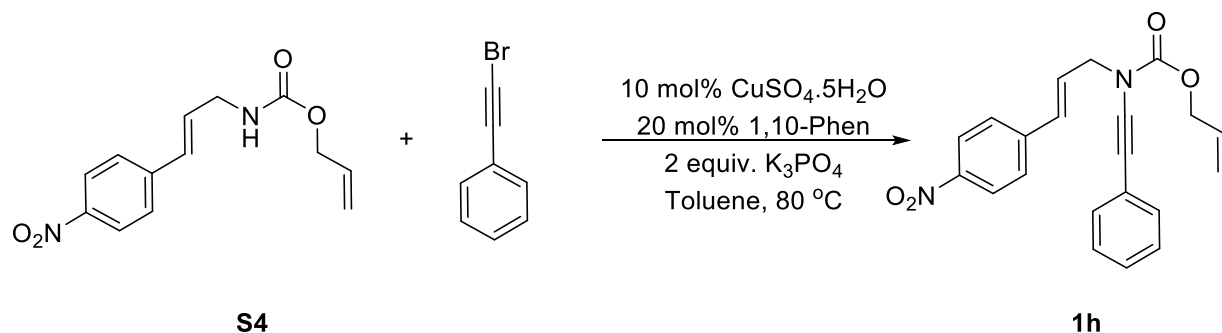
**Allyl (*E*)-(phenylethynyl)(3-(quinolin-3-yl)allyl)carbamate (**1g**)**



The title compound was prepared by General Procedure A from quinolyl carbamate **S3** (940 mg, 3.5 mmol) and (bromoethynyl)benzene (760 mg, 4.2 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 10:1) to afford **1g** (581 mg, 45%) as a yellow oil.

R<sub>f</sub> (Hexanes/EtOAc 2:1) = 0.41. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 9.03 (1H, d, *J* = 2.5 Hz), 8.12-8.10 (2H, m), 7.81 (1H, ddd, *J* = 9.5, 8.1, 1.3 Hz), 7.73-7.68 (1H, m), 7.58-7.55 (1H, m), 7.42-7.38 (2H, m), 7.33-7.26 (3H, m), 6.84, (1H, dd *J* = 15.8, 1.5 Hz) 6.56, (1H, dt, *J* = 15.6, 6.2 Hz), 6.02 (1H, ddt, *J* = 17.2, 10.5, 5.1 Hz), 5.45 (1H, ddt, *J* = 17.2, 1.2, 1.2 Hz), 5.31 (1H, ddt, *J* = 10.5, 1.2, 1.2 Hz), 4.78 (2H, ddd, *J* = 5.6, 1.2, 1.2 Hz), 4.43 (2H, dd, *J* = 6.4, 1.2 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 154.8, 149.0, 147.3, 133.2, 131.7, 131.2, 130.7, 129.6, 129.3, 129.2, 128.9, 128.3, 127.9, 127.7, 127.2, 125.5, 123.0, 118.4, 67.7, 59.5, 55.9, 52.3. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>24</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub> 369.1598 found 369.1603.

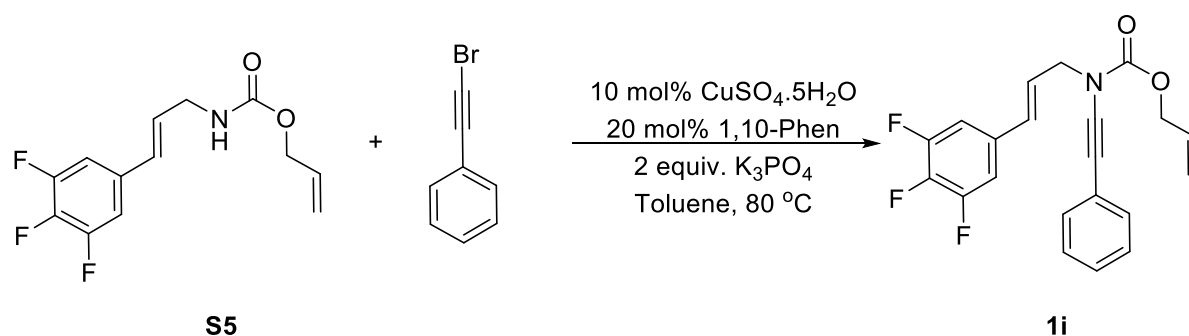
**Allyl (*E*)-(3-(4-nitrophenyl)allyl)(phenylethynyl)carbamate (**1h**)**



The title compound was prepared by General Procedure A from 4-nitrophenyl carbamate **S4** (1.93 g, 7.4 mmol) and 1-(2-bromoethynyl)benzene (1.47 g, 8.2 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 5:1) to afford **1h** (904 mg 34%) as a yellow oil.

$R_f$  (Hexanes/EtOAc 5:1) = 0.47. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.14 (2H, dd  $J$  = 8.9, 1.9 Hz), 7.49, (2H, dd  $J$  = 8.8 1.9 Hz, 7.37-7.20 (5H, m), 6.84 (1H, dd,  $J$  = 15.9, 1.6 Hz), 6.46 (1H, dt,  $J$  = 15.9, 6.5 Hz), 5.95 (1H, ddt,  $J$  = 17.1, 10.6, 5.2 Hz), 5.39 (1H, dd,  $J$  = 16.8, 1.3 Hz), 5.26 (1H, dd,  $J$  = 10.7, 1.3 Hz), 4.71 (2H, ddd,  $J$  = 5.4, 1.4, 1.4 Hz), 4.36 (2H, dd,  $J$  = 6.4, 1.2 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  155.0, 154.7, 147.2, 142.7, 131.7, 131.1, 128.9, 128.3, 127.8, 124.0, 122.9, 119.3, 118.4, 82.5 67.8, 52.1, 48.0. HRMS (ESI-TOF)  $m/z$ : [M + Na]<sup>+</sup> Calcd. for C<sub>21</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>Na 385.1159 found 385.1153.

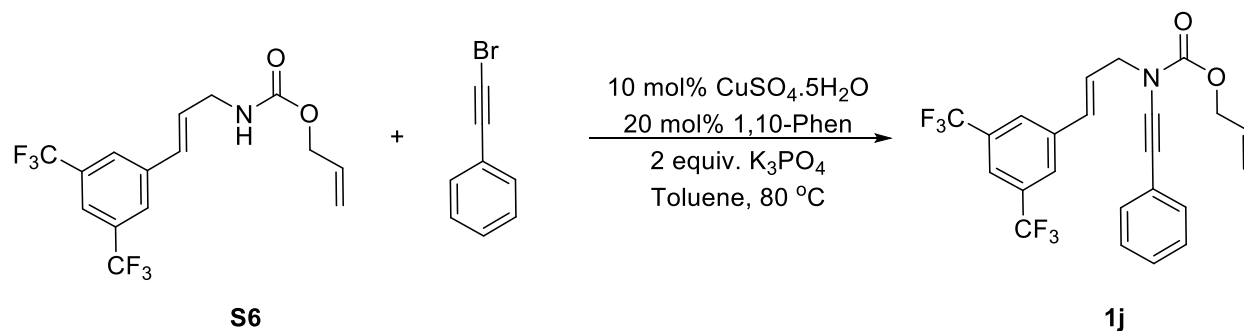
**Allyl (*E*)-(phenylethynyl)(3-(3,4,5-trifluorophenyl)allyl)carbamate (**1i**)**



The title compound was prepared by General Procedure A from 3,4,5-trifluorophenyl carbamate **S5** (900 mg, 3.32 mmol) and (bromoethynyl)benzene (722 mg, 3.99 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 10:1) to afford **1i**, (457 mg 37%) as a yellow oil.

$R_f$  (Hexanes/EtOAc 2:1) = 0.78.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40-7.35 (2H, m), 7.32-7.24 (3H, m), 6.98 (2H, dd,  $J_{\text{HF}} = 14.7, 7.3$  Hz) 6.51 (1H, d,  $J = 15.8$  Hz), 6.24 (1H, dt,  $J = 15.6, 6.2$  Hz), 5.98 (1H, ddt,  $J = 16.2, 10.5, 5.1$  Hz), 5.43 (1H, ddt,  $J = 17.1, 1.3, 1.3$  Hz), 5.29 (1H, ddt,  $J = 10.8, 1.3, 1.3$  Hz), 4.74 (2H, ddd,  $J = 5.4, 1.3, 1.3$  Hz), 4.31 (2H, dd,  $J = 6.3, 1.3$  Hz).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.7, 151.4 (ddd,  $^1J_{\text{CF}} = 249.5$  Hz,  $^3J_{\text{CF}} = 10.2$  Hz,  $^4J_{\text{CF}} = 4.0$  Hz), 139.3 (dt,  $^1J_{\text{CF}} = 252.3$  Hz,  $^2J_{\text{CF}} = 17.5$  Hz), 132.5 (td,  $^3J_{\text{CF}} = 7.8$  Hz,  $^4J_{\text{CF}} = 4.7$  Hz), 131.7, 131.1, 128.4, 128.3, 127.7, 125.5, 125.5, 123.0, 110.4 (m, second order C-F coupling), 82.5, 71.1, 67.7, 51.9. HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{Na}]^+$  Calcd. for  $\text{C}_{21}\text{H}_{16}\text{F}_3\text{NO}_2\text{Na}$  394.1025 found 394.1022.

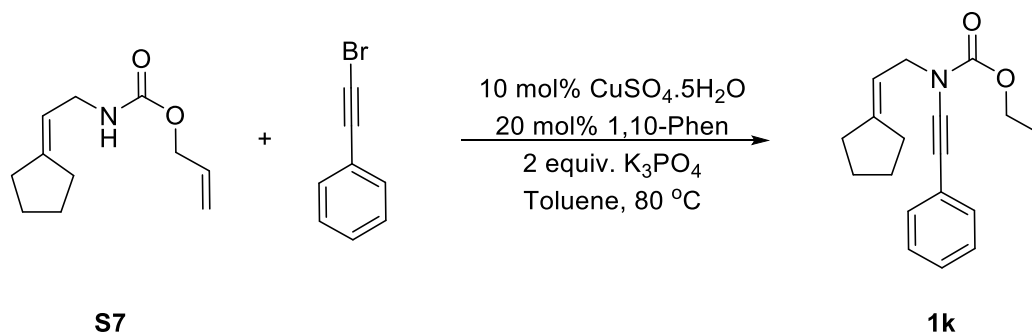
**Allyl (*E*)-3-(3,5-bis(trifluoromethyl)phenyl)allyl(phenylethynyl)carbamate (**1j**)**



The title compound was prepared by General Procedure A from 3,5-bis(trifluoromethyl)phenyl carbamate **S6** (675 mg, 1.91 mmol) and 1-(2-bromoethynyl)-benzene (380 mg, 2.10). The crude product was purified by silica chromatography (Hexanes/EtOAc 10:1) to afford **1j** (160 mg, 18%), as a yellow oil.

$R_f$  (Hexanes/EtOAc 2:1) = 0.78. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.84-7.82 (2H, m), 7.78-7.76 (1H, m), 7.41-7.37 (2H, m), 7.33-7.27 (3H, m), 6.75 (1H, d,  $J$  = 15.8, 2 Hz), 6.66 (1H, dt,  $J$  = 15.9, 6.2 Hz), 6.02 (1H, ddt,  $J$  = 16.2, 10.5, 5.1 Hz), 5.46 (1H, ddt,  $J$  = 17.2, 1.3 Hz), 5.31 (1H, ddt,  $J$  = 10.5, 1.2, 1.2 Hz), 4.77 (2H, ddd,  $J$  = 5.3, 1.4, 1.4 Hz), 4.40 (2H, dd,  $J$  = 6.2, 1.3 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 154.7, 138.4, 132.0 (q,  $^2J_{CF}$  = 33.4 Hz), 131.7, 131.2, 128.3, 127.8, 127.2, 126.4 (q,  $^3J_{CF}$  = 3.4 Hz), 124.6, 123.3 (q,  $^1J_{CF}$  = 272.2 Hz), 121.3 (sept.,  $^3J_{CF}$  = 3.7 Hz), 118.4, 82.5, 71.1, 67.8, 52.0. HRMS (ESI-TOF)  $m/z$ : [M + Na]<sup>+</sup> Calcd. for C<sub>23</sub>H<sub>17</sub>F<sub>6</sub>NO<sub>2</sub>Na 454.1236 found 454.1239.

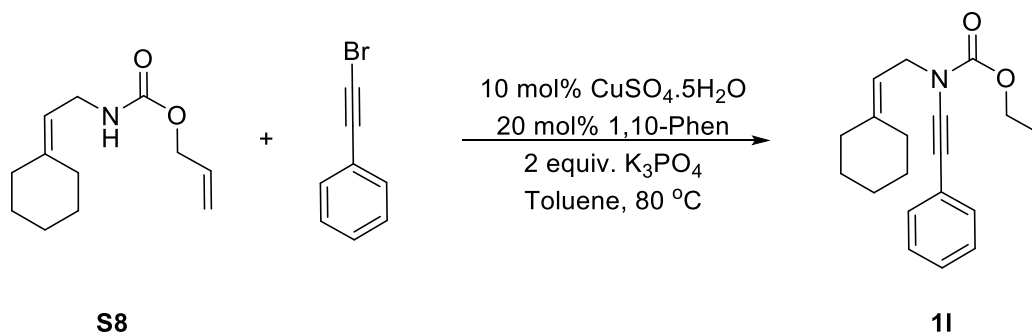
### Allyl (2-cyclopentylideneethyl)(phenylethynyl)carbamate (**1k**)



The title compound was prepared by general procedure A from cyclopentyl carbamate **S7** (291 mg, 1.49 mmol) and (bromoethynyl)benzene (322 mg, 1.79 mmol). The crude product was purified by flash column chromatography (Hexanes/Et<sub>2</sub>O 30:1) to afford **1k** (211 mg, 48%) as a yellow oil.

$R_f$  (Hexanes/Et<sub>2</sub>O 20:1) = 0.35. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.40-7.23 (5H, m), 6.04 (1H, ddt,  $J$  = 17.2, 10.6, 5.4 Hz), 5.50 (1H, tdd,  $J$  = 7.3, 2.5, 2.5 Hz), 5.41 (1H, ddt,  $J$  = 17.2, 1.1, 1.1 Hz), 5.24 (1H, ddt,  $J$  = 10.5, 1.1, 1.1 Hz), 4.71 (2H, ddd,  $J$  = 5.4, 1.2, 1.2 Hz), 4.16 (2H, d,  $J$  = 7.3 Hz), 2.41-2.29 (4H, m), 1.74-1.59 (4H, m). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  154.8, 149.9, 131.9, 130.9, 128.2, 127.3, 123.8, 123.5, 118.0, 113.6, 83.4, 67.4, 49.4, 33.8, 28.9, 26.3, 26.1. HRMS (ESI-TOF)  $m/z$ : [M + H]<sup>+</sup> Calcd. for C<sub>20</sub>H<sub>21</sub>NO<sub>2</sub> 296.1645 found 296.1647.

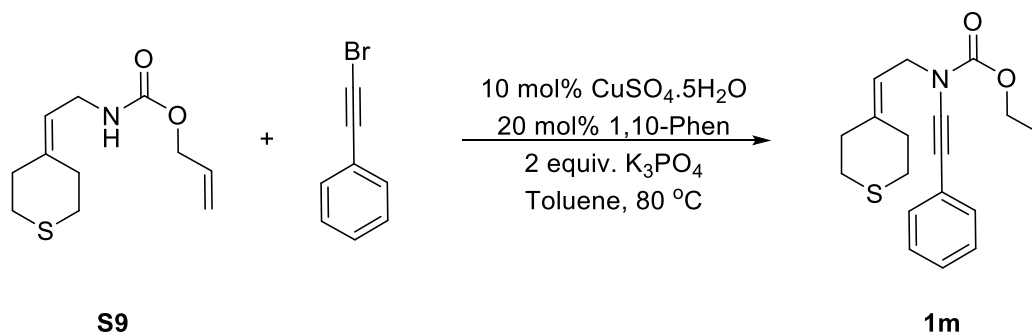
### Allyl (2-cyclohexylideneethyl)(phenylethynyl)carbamate (**11**)



The title compound was prepared by General Procedure A from cyclohexyl carbamate **S8** (692 mg, 3.31) and (bromoethynyl)benzene (715 mg, 3.97 mmol). The crude product was purified by flash column chromatography (Hexanes/Et<sub>2</sub>O 30:1) to afford **11** (237 mg, 23%) as a colorless oil.

R<sub>f</sub> (Hexanes/EtOAc 10:1) = 0.54. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.40-7.35 (2H, m), 7.32-7.24 (3H, m), 5.97 (1H, ddt, *J* = 17.6, 10.6, 5.5 Hz), 5.43 (1H, ddd, *J* = 17.6, 2.3, 2.3 Hz), 5.33 (1H, ddt, *J* = 10.6, 1.4, 1.4 Hz), 5.27 (1H, ddt, *J* = 10.4, 1.1, 1.1 Hz), 4.71 (2H, ddd, *J* = 5.3, 1.2, 1.2 Hz), 4.18 (2H, d, *J* = 7.5 Hz), 2.26-2.24 (2H, m), 2.19-2.12 (2H, m), 1.59-1.52 (6H, m). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 154.9, 146.4, 132.0, 131.0, 128.2, 127.3, 123.5, 118.0, 114.6, 83.2, 70.8, 67.4, 46.9 37.1, 29.1, 28.4, 28.0, 26.7, HRMS (ESI-TOF) *m/z*: [M + Na]<sup>+</sup> Calcd. for C<sub>20</sub>H<sub>23</sub>NO<sub>2</sub>Na 332.1621 found 332.1618.

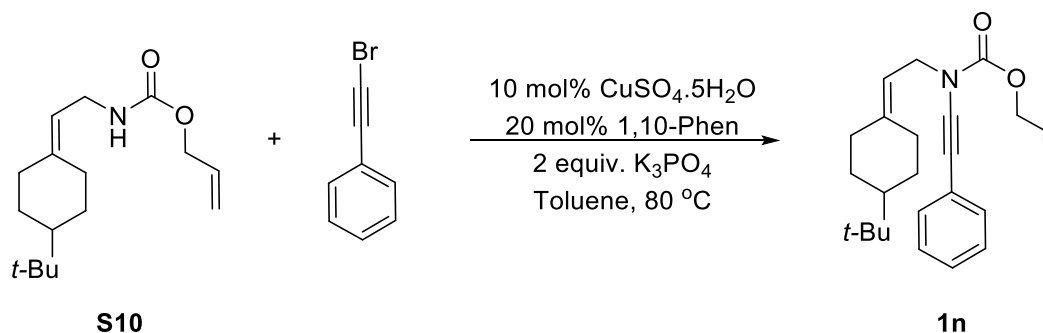
**Allyl (phenylethynyl)(2-(tetrahydro-4H-thiopyran-4-ylidene)ethyl)carbamate (1m)**



The title compound was prepared by General Procedure A from thiopyranyl carbamate **S9** (342 mg, 1.51 mmol) and 1-(2-bromoethynyl)-4-benzene (327 mg, 1.81 mmol). The crude product was purified by silica chromatography (Hexanes/Et<sub>2</sub>O 10:1) to afford **1m** (167 mg 34%) as a colorless oil.

R<sub>f</sub> (Hexanes/EtOAc 10:1) = 0.42. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.42-7.36 (2H, m), 7.34-7.25 (3H, m), 5.99 (1H, ddt, *J* = 16.3, 10.4, 5.4 Hz), 5.45 (1H, d, *J* = 7.5 Hz), 5.42 (1H, ddt, *J* = 16.3, 1.2, 1.2 Hz), 5.29 (1H, ddt, *J* = 10.6, 1.2, 1.2 Hz), 4.72 (2H, ddd, *J* = 5.4, 1.2, 1.2 Hz), 4.19 (2H, d, *J* = 7.6 Hz), 2.72-2.62 (6H, m) 2.53-2.48 (2H, m). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 154.7, 143.0, 131.9, 131.0, 128.3, 127.5, 123.2, 118.1, 117.9, 82.9, 70.8, 67.5, 46.5, 38.8, 31.0, 31.0, 30.4. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>19</sub>H<sub>22</sub>NO<sub>2</sub>S 328.1366 found 328.1369.

### Allyl (2-(4-(tert-butyl)cyclohexylidene)ethyl)(phenylethynyl)carbamate (**1n**)

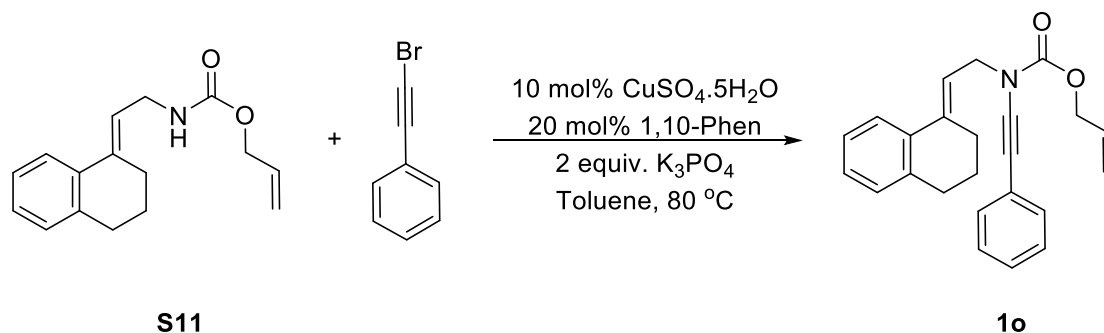


The title compound was prepared by General Procedure A from 4-*tert*-butylcyclohexyl carbamate **S10** (1.03 g, 3.89 mmol and 1-(2-bromoethynyl)-4-benzene (845 mg, 4.67 mmol) The crude product was purified by flash column chromatography (Hexanes/EtOAc 20:1) to afford **1n** (511 mg, 36%) as an amber oil.

$R_f$  (Hexanes/EtOAc 19:1) = 0.35.  $^1\text{H-NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.43-7.38 (2H, m), 7.33-7.26 (3H, m), 5.99 (1H, ddt,  $J = 17.2, 10.6, 5.6$  Hz), 5.43 (1H, ddt,  $J = 17.2, 1.4, 1.4$  Hz), 5.34 (1H, tdd,  $J = 7.5, 1.3, 1.3$  Hz), 5.29 (1H, ddt,  $J = 10.6, 1.4, 1.4$  Hz), 4.73 (2H, ddd,  $J = 5.5, 1.4, 1.4$  Hz), 4.41 (2H, ddd,  $J = 8.0, 2.2, 2.2$  Hz), 2.83 (1H, dddd,  $J = 13.6, 2.0, 2.0, 2.0$  Hz), 2.33 (1H, dddd,  $J = 13.5, 3.0, 3.0, 3.0$  Hz), 2.08 (1H, ddd,  $J = 12.9, 12.9, 3.0$  Hz), 1.93-1.84 (2H, m), 1.81 (1H, ddd,  $J = 13.1, 13.1, 3.5$  Hz), 1.21 (1H, dddd,  $J = 11.9, 11.9, 2.8, 2.8$  Hz), 1.09 (1H, ddd,  $J = 12.5, 3.7$  Hz), 1.04 (1H, dddd,  $J = 13.0, 13.0, 13.0, 3.3$  Hz) 0.83 (9H, s).  $^{13}\text{C-NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  154.9, 146.4, 132.0, 131.1, 128.2, 127.4, 127.3, 123.5, 118.0, 114.3, 77.2, 67.4, 48.3, 47.0, 37.0, 32.4, 29.1, 28.8, 28.7, 27.6. HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd. for  $\text{C}_{24}\text{H}_{32}\text{NO}_2$  366.2428 found 366.2448.



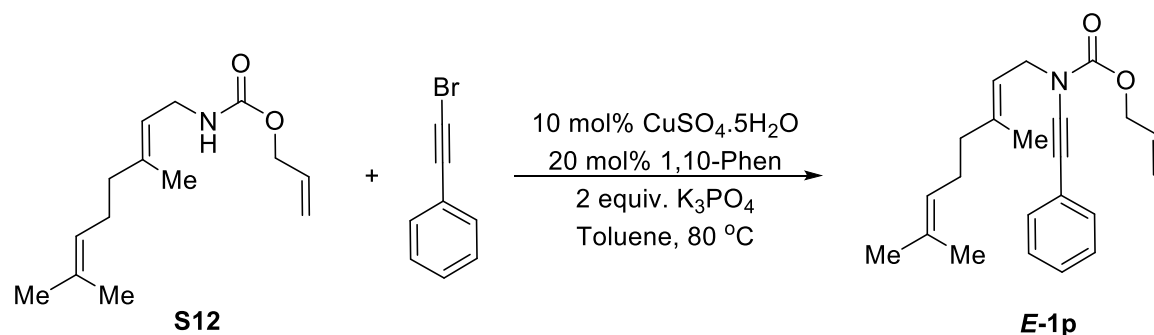
**Allyl (E)-2-(3,4-dihydronaphthalen-1(2H)-ylidene)ethyl(phenylethynyl)carbamate (1o)**



The title compound was prepared by General Procedure A from tetralone derived carbamate **S11** (216 mg, 0.84 mmol) and (bromoethynyl)benzene (227 mg, 1.26 mmol). The crude product was purified by silica chromatography (Hexanes/Et<sub>2</sub>O 10:1) to afford **1o** (169 mg, 56%) as a colorless oil.

$R_f$  (Hexanes/EtOAc 10:1) = 0.57. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.63-7.60 (1H, m), 7.40-7.35 (2H, m), 7.31-7.24 (3H, m), 7.19-7.14 (2H, m), 7.12-7.08 (1H, m), 6.17 (1H, dt,  $J = 7.3, 1.2, 1.2$  Hz), 5.99 (1H, ddt,  $J = 17.2, 10.5, 5.2$  Hz), 5.45 (1H, ddt,  $J = 17.2, 1.2, 1.2$  Hz), 5.28 (1H, ddt,  $J = 10.5, 1.2, 1.2$  Hz), 4.74 (2H, ddd,  $J = 8.5, 6.8, 5$  Hz), 4.42 (2H, dd,  $J = 7.18, 1.2$  Hz), 2.80 (2H, t,  $J = 6.2$  Hz), 2.65 (2H, dd,  $J = 5.9, 1.2$  Hz), 1.87 (2H, tt,  $J = 6.2, 5.9$  Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  154.9, 139.3, 137.9, 135.2, 131.9, 131.1, 129.0, 128.3, 127.6, 127.5, 126.2, 124.2, 123.4, 118.2, 116.9, 83.2, 70.9, 67.6, 48.0, 30.3, 26.7, 23.3, HRMS (ESI-TOF)  $m/z$ : [M + Na]<sup>+</sup> Calcd. for C<sub>24</sub>H<sub>23</sub>NO<sub>2</sub>Na 380.1621 found 380.1622.

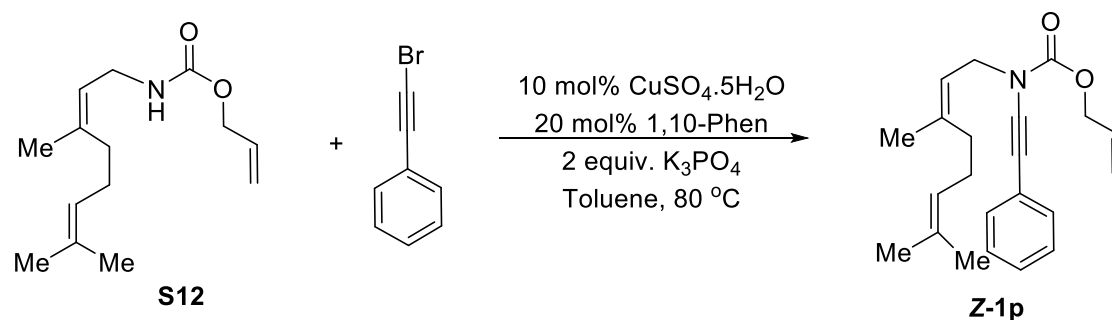
**Allyl (*E*)-(3,7-dimethylocta-2,6-dien-1-yl)(phenylethynyl)carbamate (*E*-1p)**



The title compound was prepared by General Procedure A from geranyl carbamate **S12** (280 mg, 1.94 mmol) and (bromoethynyl)benzene (428 mg, 2.38 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 30:1) to afford **1p** (280 mg, 43%) as a yellow oil.

$R_f$  (Hexanes/Et<sub>2</sub>O 20:1) = 0.36. <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) δ 7.42-7.36 (2H, m), 7.34-7.25 (3H, m), 5.99 (1H, ddt,  $J$  = 17.1, 10.6, 5.4 Hz), 5.42 (1H, ddt,  $J$  = 17.1, 1.4, 1.4 Hz), 5.41 (1H, tq,  $J$  = 7.8, 1.2 Hz), 5.29 (1H, ddt,  $J$  = 10.6, 1.2, 1.2 Hz), 5.12 (1H, tt,  $J$  = 6.8, 1.3 Hz), 4.74 (2H, ddd,  $J$  = 5.4, 1.4, 1.4 Hz), 4.22 (2H, d,  $J$  = 7.3 Hz), 2.18-2.07 (4H, m), 1.79 (3H, s), 1.69 (3H, s), 1.62 (3H, s). <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) δ 154.9, 141.7, 132.0, 131.8, 130.9, 128.2, 127.3, 123.8, 123.5, 118.0, 117.9, 83.2, 70.8, 67.4, 47.7, 39.6, 26.4, 25.7, 17.7, 16.5. HRMS (ESI-TOF)  $m/z$ : [M + H]<sup>+</sup> Calcd. for C<sub>22</sub>H<sub>28</sub>NO<sub>2</sub> 338.2115 found 338.2106.

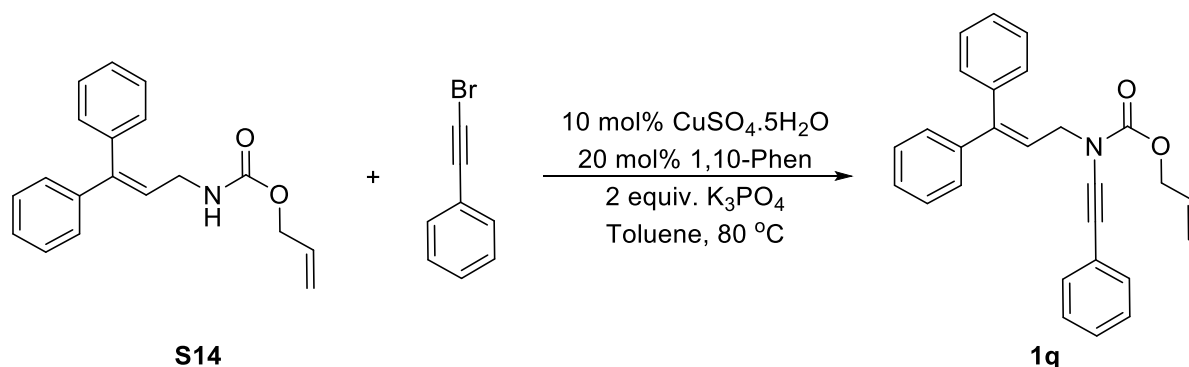
**Allyl (Z)-(3,7-dimethylocta-2,6-dien-1-yl)(phenylethynyl)carbamate (Z-1p)**



The title compound was prepared by General Procedure A from neryl carbamate **S13** (540 mg, 2.28 mmol) and (bromoethynyl)benzene (492 mg, 2.74 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 20:1) to afford **1p'** (499 mg, 65%) as a yellow oil.

$R_f$  (Hexanes/Et<sub>2</sub>O 30:1) = 0.36. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.38-736 (2H, m), 7.31-7.26 (3H, m), 5.98 (1H, ddt,  $J = 17.0, 10.5, 5.3$  Hz), 5.42 (1H, ddt,  $J = 17.0, 1.2, 1.2$  Hz), 5.38 (1H, t,  $J = 7.0$  Hz), 5.27 (1H, ddd,  $J = 10.5, 1.2, 1.2$  Hz), 5.12 (1H, tt,  $J = 7.0, 1.2, 1.2$  Hz), 4.72 (2H, ddd,  $J = 5.3, 1.2, 1.2$  Hz), 4.17 (2H, d,  $J = 7.3$  Hz), 2.20-2.10 (4H, m), 1.79 (3H, s), 1.69 (3H, s), 1.62 (3H, s). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 154.9, 141.6, 132.1, 131.9, 130.9, 128.2, 127.3, 123.7, 123.5, 118, 67.4, 47.6, 32.2, 29.7, 26.7, 25.7, 23.5, 17.7. HRMS (ESI-TOF)  $m/z$ :  $[\text{M} + \text{H}]^+$  Calcd. for C<sub>22</sub>H<sub>28</sub>NO<sub>2</sub> 338.2115 found 338.2106.

### Allyl (3,3-diphenylallyl)(phenylethynyl)carbamate (**1q**)

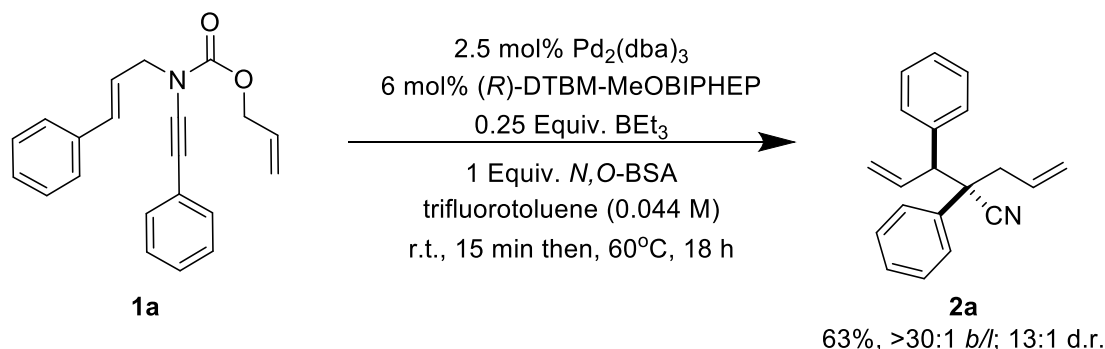


The title compound was prepared by General Procedure A from diphenyl carbamate **S14** (468 mg, 1.61 mmol) and 1-(2-bromoethynyl)-4-benzene (349 mg, 1.93 mmol). The crude product was purified by flash column chromatography (Hexanes/EtOAc 20:1) to afford **1q** (95 mg, 15%) as an amber oil.

$R_f$  (Hexanes/EtOAc 19:1) = 0.25. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.39-7.32 (5H, m), 7.32-7.22 (10H, m), 6.23 (1H, t,  $J$  = 7.1 Hz), 5.97 (1H, ddt,  $J$  = 16.5, 10.7, 5.7 Hz), 5.40 (1H, ddt,  $J$  = 17.1, 1.2, 1.2, Hz), 5.27 (1H, ddt,  $J$  = 10.5, 1.4, 1.4 Hz), 4.71 (2H, ddd,  $J$  = 5.1, 1.2, 1.2 Hz), 4.26 (2H, d,  $J$  = 7.1 Hz). <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  154.8, 146.1, 141.5, 138.7, 131.8, 131.0, 129.8, 128.4, 128.3, 128.2, 127.8, 127.6, 127.5, 127.4, 123.3, 122.2, 118.2, 82.9, 71.2, 67.6, 49.2, HRMS (ESI-TOF)  $m/z$ : [M + H]<sup>+</sup> Calcd. for C<sub>27</sub>H<sub>24</sub>NO<sub>2</sub>H 394.1802 found 394.1821.

## 5. Formation of Nitriles (**2**) via Auto-Tandem Catalysis

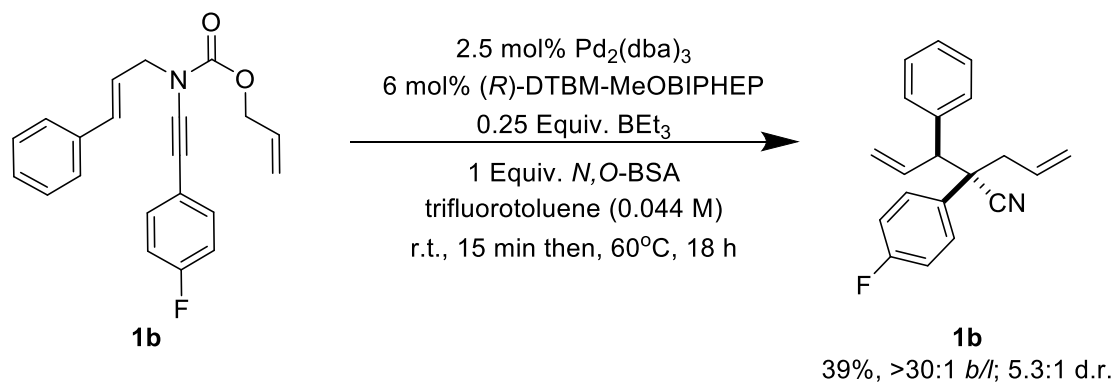
### (2*S*\*,3*S*\*)-2-allyl-2,3-diphenylpent-4-enitrile (**2a**)



The title compound was prepared by general procedure B from carbamate **1a** (58 mg, 0.18 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.1 mg, 4.5 μmol), (*R*)-DTBM-MeOBIPHEP (12.4 mg, 10.8 μmol), BEt<sub>3</sub> (1 M in THF, 45 μl, 45 μmol) and *N,O*-BSA (44 μl, 18 μmol) in trifluorotoluene (4.0 mL). The crude product was purified by flash column chromatography (Hexanes/CH<sub>2</sub>Cl<sub>2</sub> 4:1) to afford the requisite nitrile product **2a** (32 mg, 65%, 13:1 *d.r.*) as a colorless oil.

R<sub>f</sub> (Hexanes/CH<sub>2</sub>Cl<sub>2</sub> 1:1) = 0.40. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.30-7.01 (8H, m), 6.98-6.96 (2H, m), 6.34 (0.93H, ddd, *J* = 16.8, 10.0, 10.0 Hz, major), 5.99 (0.07H, ddt, *J* = 17.1, 10.2, 9.1 Hz, minor) 5.46 (0.93H, ddt, *J* = 16.9, 10.1, 6.7 Hz, major), 5.41-5.32 (0.07H, m, minor), 5.27 (0.93H, dd, *J* = 9.9, 1.1 Hz, major), 5.24 (0.93H, d, *J* = 16.3 Hz, major), 5.10 (0.93H, ddt, *J* = 17.0, 1.4, 1.4 Hz), 4.99 (0.93H, ddt, *J* = 10.2, 1.3, 1.3 Hz, major), 4.97-4.89 (0.28H, m, minor), 4.76 (0.07H, ddt, *J* = 17.1, 1.3, 1.3 Hz, minor), 3.62 (0.07H, d, *J* = 8.5 Hz, minor), 3.54 (0.93H, d, *J* = 9.8 Hz, major), 2.91 (0.93H, dd, *J* = 14.3, 7.6 Hz, major), 2.71 (0.93H, dd, *J* = 14.3, 6.5 Hz, major), 2.62 (0.07H, dd, *J* = 14.2, 6.4 Hz, minor), 2.38 (0.07H, dd, *J* = 14.0, 7.8 Hz, minor). <sup>13</sup>C-NMR (major isomer only) (100 MHz, CDCl<sub>3</sub>) δ 138.6, 136.4, 135.8 131.8, 128.7, 128.3, 128.0, 127.6, 127.2, 127.1, 119.9, 119.3, 60.0, 52.6, 42.8, HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. For C<sub>20</sub>H<sub>20</sub>N 274.1590 found 274.1579.

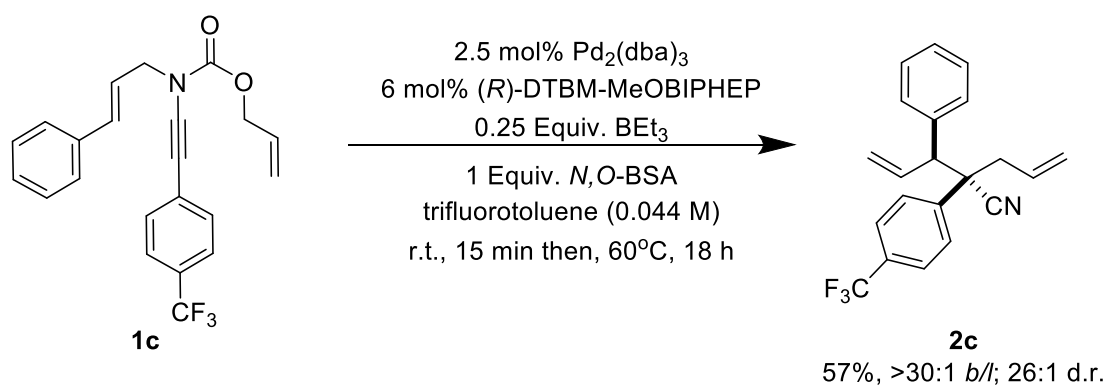
**(2*S*\*,3*S*\*)-2-Allyl-2-(4-fluorophenyl)-3-phenylpent-4-enenitrile (**1b**)**



The title compound was prepared by general procedure B from carbamate **1b** (67 mg, 0.2 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.6 mg, 5.0 μmol) and (*R*)-DTBM-MeOBIPHEP (13.8 mg, 12.0 μmol), BEt<sub>3</sub> (1 M in THF, 50 μl, 50 μmol) and *N,O*-BSA (49 μl, 20 μmol) in trifluorotoluene (4.5 mL). The crude product was purified by flash column chromatography (Hexanes/EtOAc 10:1) to afford the requisite nitrile product **2b** (21 mg, 39%, 5.3:1 d.r.) as a colorless oil.

R<sub>f</sub> (Hexanes/EtOAc 10:1) = 0.55. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.30-7.19 (2H, m), 7.08-6.98 (2H, m), 6.89-6.80 (4H, m), 6.32 (0.84H, ddd, *J* = 16.7, 10.0, 10.0 Hz, major), 5.97 (0.16H, ddd, *J* = 16.9, 10.1, 9.0 Hz, minor), 5.46 (0.84H, ddt, *J* = 17.1, 10.1, 7.1 Hz, major), 5.41-5.34 (0.16H, m, minor), 5.27 (0.84H, dd, *J* = 10.3, 1.1 Hz, major), 5.23 (0.84H, dd, *J* = 17.3, 1.1 Hz, major), 5.07 (0.84H, dd, *J* = 17.1, 1.3 Hz, major), 5.01 (0.84H, dd, *J* = 10.1, 1.2 Hz, major), 4.99 (0.16H, d, *J* = 9.9 Hz, minor), 4.94 (0.16H, ddd, *J* = 10.5, 1.2, 1.2 Hz, minor), 4.93 (0.16H, ddt, *J* = 17.1, 1.3, 1.3 Hz, minor), 4.78 (0.16H, ddt, *J* = 17.1, 1.2, 1.2 Hz, minor), 3.57 (0.16H, d, *J* = 8.9 Hz, minor), 3.48 (0.84H, d, *J* = 9.8 Hz, major), 2.91 (0.84H, dd, *J* = 14.4, 7.4 Hz, major), 2.65 (0.84H, dd, *J* = 14.4, 6.7 Hz, major), 2.57 (0.16H, dddd, *J* = 14.2, 6.8, 1.2, 1.2 Hz, minor), 2.40 (0.16H, dddd, *J* = 14.4, 7.4, 1.2, 1.2 Hz, minor). <sup>13</sup>CNMR [Major isomer only] (100 MHz, CDCl<sub>3</sub>) δ 161.6 (d, <sup>1</sup>*J*<sub>CF</sub> = 253.3 Hz), 137.3, 135.1, 134.0, 130.5, 127.6 (d, <sup>3</sup>*J*<sub>CF</sub> = 8.2 Hz), 127.6 (d, <sup>4</sup>*J*<sub>CF</sub> = 3.3 Hz), 127.6, 127.1, 126.2, 119.1, 118.4, 114.2 (d, <sup>2</sup>*J*<sub>CF</sub> = 21.6 Hz), 59.1, 51.0, 41.8. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>21</sub>H<sub>19</sub>FNO<sub>2</sub> 292.1496 found 292.1509.

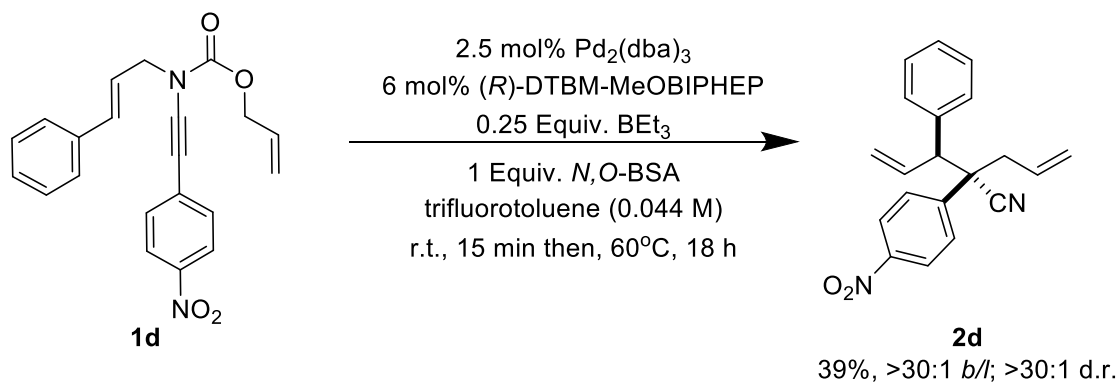
**(2*S*\*,3*S*\*)-2-Allyl-3-phenyl-2-(4-(trifluoromethyl)phenyl)pent-4-enitrile (**2c**)**



The title compound was prepared by general procedure B from carbamate **1c** (53 mg, 0.14 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (3.2 mg, 3.5 μmol), (*R*)-DTBM-MeOBIPHEP (9.7 mg, 4.0 μmol), BEt<sub>3</sub> (1 M in THF, 35 μl, 35 μmol) and *N,O*-BSA (34 μl, 14 μmol) in trifluorotoluene (3.2 mL). The crude product was purified by flash column chromatography (Hexanes:EtOAc 10:1) to afford the respective nitrile **2c** (25 mg, 57%, 26:1 d.r.) as a colorless oil.

R<sub>f</sub> (Hexanes/Ethyl Acetate 10:1) = 0.55. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.58-7.51 (1H, m), 7.24-7.14 (6H, m), 7.07-7.01 (2H, m), 6.37 (1H, ddd, *J* = 16.8, 9.9, 9.9 Hz), 5.48 (1H, ddt, *J* = 16.9, 7.4, 6.6, Hz), 5.41 (1H, d, *J* = 10.2 Hz), 5.32 (1H, d, *J* = 16.4 Hz), 5.11 (1H, ddt, *J* = 17.0, 1.3, 1.3 Hz), 5.03 (1H, ddt, *J* = 10.1, 1.3, 1.3, Hz), 3.67 (1H, d, *J* = 9.8 Hz), 2.91, (1H, dddd, *J* = 14.4, 7.6, 1.3, 1.3 Hz), 2.75, (1H, dddd, *J* = 14.4, 6.6, 1.3, 1.3 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 141.1, 134.9, 134.3, 131.2, 131.1 (q, <sup>2</sup>*J*<sub>CF</sub> = 23.4 Hz), 128.9, 128.8 (q, <sup>4</sup>*J*<sub>CF</sub> = 3.7 Hz), 128.3, 126.8, 122.9 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.7 Hz), 121.3, 121.1 (q, <sup>3</sup>*J*<sub>CF</sub> = 7.5 Hz), 121.0, 120.5, 59.5, 52.7, 42.2. HRMS (ESI-TOF) *m/z*: [M + Cl]<sup>-</sup> Calcd. for C<sub>21</sub>H<sub>18</sub>F<sub>3</sub>NCl 376.1085 found 376.1099.

**(2*S*\*,3*S*\*)-2-Allyl-2-(4-nitrophenyl)-3-phenylpent-4-enitrile (**2d**)**

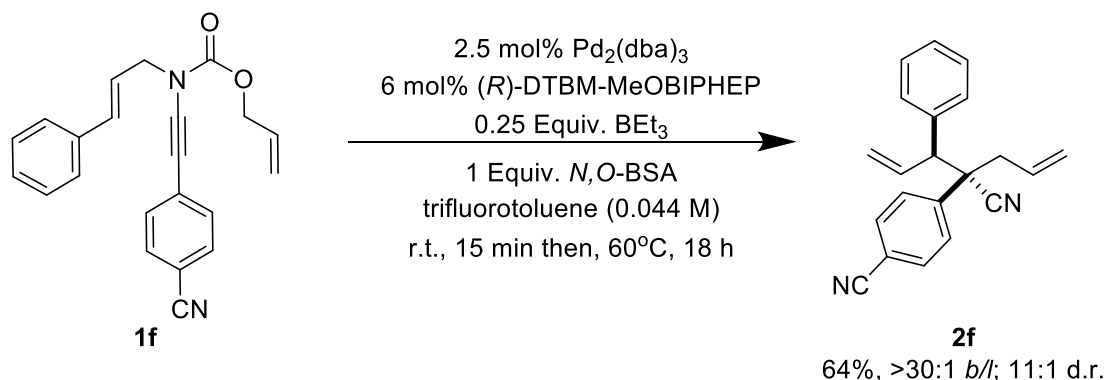


The title compound was prepared by general procedure B from carbamate **1d** (72.4 mg, 0.2 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.6 mg, 5.0 μmol), (*R*)-DTBM-MeOBIPHEP (13.8 mg, 12.0 μmol), BEt<sub>3</sub> (1 M in THF 50 μl, 50 μmol) and *N,O*-BSA (49 μl, 20 μmol) in trifluorotoluene (4.5 mL). The crude product was purified by flash column chromatography (Hexanes/EtOAc 10:1) to afford the requisite nitrile product **2d** (24.8 mg, 39%, >30:1 d.r.) as a colorless oil.

R<sub>f</sub> (Hexanes/EtOAc 5:1) = 0.17. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.99 (2H, d, *J* = 8.8 Hz), 7.26 (2H, d, *J* = 8.8 Hz), 7.06-7.01 (3H, m), 6.90-6.86 (2H, m), 6.33 (1H, ddd, *J* = 16.8, 9.9 Hz), 5.47 (1H, ddt, *J* = 17.1, 10.1, 7.1 Hz), 5.31 (1H, d, *J* = 10.1 Hz), 5.27 (1H, d, *J* = 16.9 Hz), 5.05 (1H, ddt, *J* = 18.1, 17.1, 1.2, 1.2 Hz) 5.00, (1H, ddt, *J* = 10.0, 1.2, 1.2 Hz) 3.53 (1H, d, *J* = 9.8 Hz), 3.00 (1H, dddd, *J* = 14.5, 7.2, 1.2, 1.2 Hz), 2.70 (1H, dddd, *J* = 14.4, 7.1, 1.2, 1.2 Hz), <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 147.2, 143.5, 137.8, 135.5, 130.7, 128.5, 128.4, 128.3, 127.8, 127.7, 123.5, 120.9, 120.1, 59.9, 52.8, 42.9. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. For C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub> 319.1441 Found 319.1440.



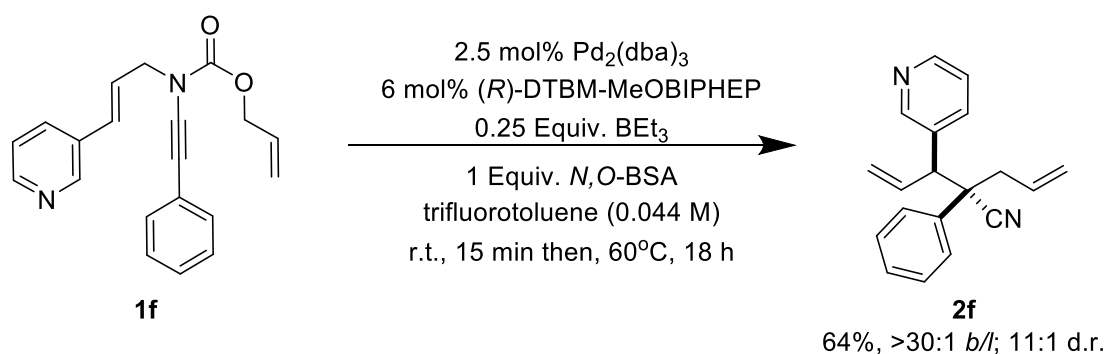
**(2*S*\*,3*S*\*)-2-Allyl-2-(4-cyanophenyl)-3-phenylpent-4-enitrile (2d)**



The title compound was prepared by general procedure B from carbamate **1e** (57 mg, 0.17 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (3.9 mg, 4.3 μmol), (*R*)-DTBM-MeOBIPHEP (11.7 mg, 10.0 μmol), BEt<sub>3</sub> (1 M in THF, 43 μl, 43 μmol) and *N,O*-BSA (42 μl, 0.17 μmol) in trifluorotoluene (3.9 mL). The crude product was purified by flash column chromatography (Hexanes/EtOAc 10:1) to afford the requisite nitrile product **2e** (43 mg, 85%, >30:1 d.r.) as a colorless oil

R<sub>f</sub> (Hexanes/CH<sub>2</sub>Cl<sub>2</sub> 1:1) = 0.63. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.52 (2H, d, *J* = 8.6 Hz), 7.28 (2H, d, *J* = 8.6 Hz), 7.15-7.08 (3H, m), 6.98-6.92 (2H, m), 6.32 (1H, ddd, *J* = 16.8, 9.9, 9.9 Hz), 5.41 (1H, ddt, *J* = 17.1, 10.1, 7.1 Hz), 5.31 (1H, dd, 10.1, 1.0 Hz) 5.26 (1H, d, *J* = 16.8 Hz), 5.14 (1H, ddt, *J* = 17.0, 1.4, 1.4 Hz), 5.09 (1H, ddt, *J* = 10.2, 1.3, 1.3 Hz), 3.50 (1H, d, *J* = 9.8 Hz), 2.98 (1H, dddd, *J* = 14.4, 7.2, 1.4, 1.4 Hz), 2.67 (1H, dddd, *J* = 14.4, 7.0, 1.3, 1.3 Hz). <sup>13</sup>CNMR (100 MHz, CDCl<sub>3</sub>) δ 141.5, 137.8, 135.5, 132.1, 130.9, 128.4, 128.4, 128.0, 127.6, 120.8, 120.1, 120.1, 118.2, 111.8, 59.9, 52.9, 42.7. HRMS (ESI-TOF) *m/z*: [M + Cl]<sup>-</sup> Calcd. for C<sub>21</sub>H<sub>18</sub>N<sub>2</sub>Cl 337.1164 found 333.1178.

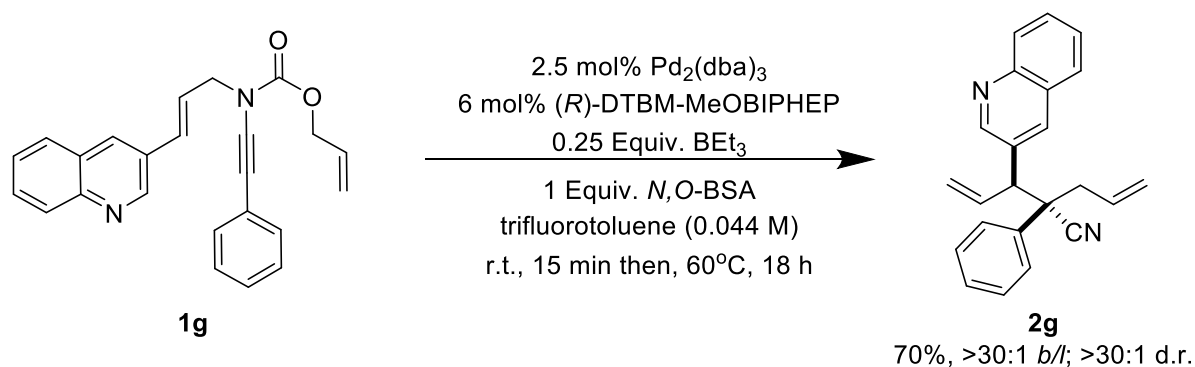
**(2*S*\*,3*S*\*)-2-Allyl-2-phenyl-3-(pyridin-3-yl)pent-4-enitrile (2f)**



The title compound was prepared by general procedure B from carbamate **1f** (63.6 mg, 0.20 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.6 mg, 5.0 μmol), (*R*)-DTBM-MeOBIPHEP (13.8 mg, 12.0 μmol), BEt<sub>3</sub> (1M in THF, 50 μl, 50 μmol) and *N,O*-BSA (49 μl, 0.2 mmol) in trifluorotoluene (4.5 mL). The crude product was purified by flash column chromatography (Hexanes/Ethyl Acetate 19:1) to afford the requisite nitrile product **2f** (35 mg, 64%, 11:1 d.r.) as a colorless oil.

R<sub>f</sub> (Hexanes/Ethyl Acetate 2:1) = 0.27. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 8.38 (1H, d, *J* = 2.8 Hz), 7.98 (1H, s), 7.69 (1H, d, *J* = 8.0 Hz), 7.21-7.13 (5H, m), 7.16 (2H, dd, *J* = 8.6, 1.3 Hz), 6.42 (1H, ddt, *J* = 26.8, 20, 16.7), 5.51 (1H, ddt, *J* = 17.0, 10.1, 6.9 Hz), 5.46 (1H, d, *J* = 10.2 Hz), 5.39 (1H, d, *J* = 16.8 Hz), 5.16 (1H, ddt, *J* = 17.0, 1.3, 1.3 Hz), 5.09 (1H, ddt, *J* = 10.1, 1.3, 1.3 Hz), 3.72 (1H, d, *J* = 9.7 Hz), 3.00 (1H, dddd, *J* = 14.2, 7.6, 1.3, 1.3 Hz), 2.81 (1H, dddd, *J* = 14.3, 6.5, 1.3, 1.3 Hz), <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 147.9, 146.3, 137.4, 135.0, 134.6, 131.2, 129.0, 128.4, 128.1, 126.8, 123.8, 121.1, 120.5, 120.3, 57.2, 52.6, 42.7, HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>19</sub>H<sub>19</sub>N<sub>2</sub> 275.1543 found 275.1548.

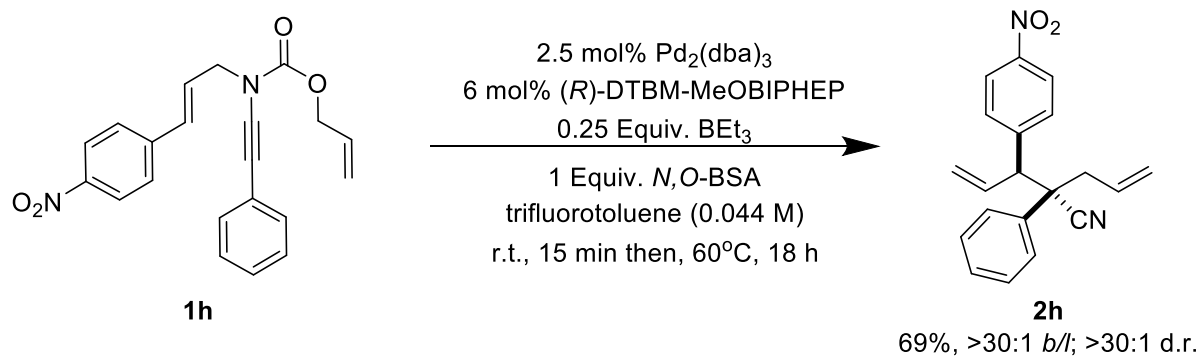
**(2*S*\*,3*S*\*)-2-Allyl-2-phenyl-3-(quinolin-3-yl)pent-4-enitrile (2g)**



The title compound was prepared by general procedure B from carbamate **1g** (43 mg, 0.12 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (2.8 mg, 3.0 μmol), (*R*)-DTBM-MeOBIPHEP (8.3 mg, 7.2 μmol), BEt<sub>3</sub> (1M in THF, 30 μl, 30 μmol) and *N,O*-BSA (29 μl, 12 μmol) in trifluorotoluene (2.7 mL). The crude product was purified by flash column chromatography (Hexanes/Ethyl Acetate 19:1) to afford the requisite nitrile product **2g** (28 mg, 70%, >30:1 d.r.) as a colorless solid.

R<sub>f</sub> (Hexanes/Ethyl Acetate 2:1) = 0.28. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 8.17 (1H, d, *J* = 1.8 Hz), 8.05 (1H, d, *J* = 1.8 Hz), 8.01 (1H, d, *J* = 8.5 Hz), 7.75 (1H, dd, *J* = 8.1, 1.2 Hz), 7.68 (1H, ddd, *J* = 8.2, 7.8, 1.2 Hz), 7.53 (1H, dd, *J* = 8.1, 7.8 Hz), 7.23-7.16 (5H, m), 6.53 (1H, ddd, *J* = 16.8, 10.0, 10.0 Hz), 5.56 (1H, ddt, *J* = 17.0, 10.1, 7.4 Hz), 5.46 (1H, d, *J* = 10.3 Hz), 5.42 (1H, d, *J* = 17.1 Hz), 5.19 (1H, ddt, *J* = 17.0, 1.3, 1.3 Hz), 5.11 (1H, dd, *J* = 10.1, 1.3, 1.3 Hz), 3.88 (1H, d, *J* = 9.8 Hz), 3.05 (1H, dddd, *J* = 14.3, 7.6, 1.3, 1.3 Hz), 2.85 (1H, dddd, *J* = 14.3, 6.5, 1.3, 1.3 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 150.6, 150.6, 135.6, 135.2, 135.1, 131.9, 131.4, 129.8, 128.8, 128.5, 128.4, 128.0, 127.5, 126.9, 120.5, 120.5, 120.4, 57.1, 52.8, 42.8. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>23</sub>H<sub>21</sub>N<sub>2</sub> 325.1699 found 325.1710.

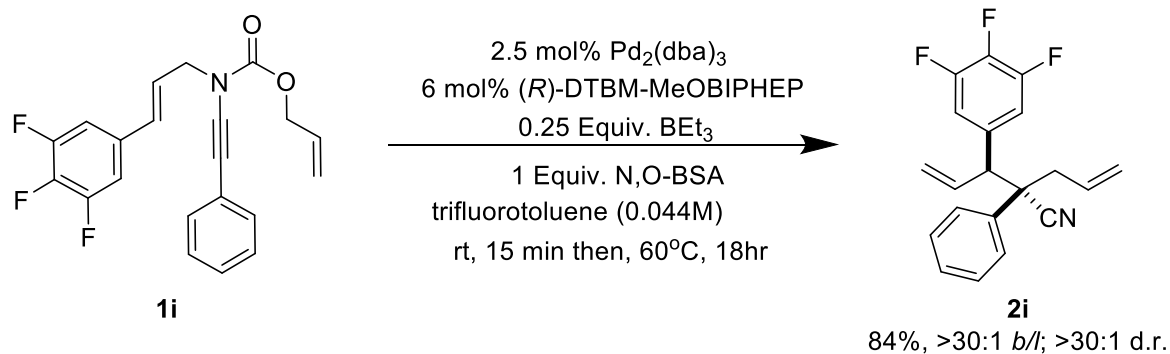
**(2*S*\*,3*S*\*)-2-Allyl-3-(4-nitrophenyl)-2-phenylpent-4-enitrile (2h)**



The title compound was prepared by general procedure B from carbamate **1h** (54.3 mg, 0.15 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (3.43 mg, 7.5 μmol), (*R*)-DTBM-MeOBIPHEP (10.4 mg, 12.0 μmol), BEt<sub>3</sub> (1M in THF, 38 μl, 38 μmol) and *N,O*-BSA (37 μl, 15 μmol) in trifluorotoluene (3.4 mL). The crude product was purified by flash column chromatography (Hexanes/Ethyl Acetate 19:1) to afford requisite nitrile product **2h** (33 mg 69%, >30:1 d.r.) as a colorless oil

R<sub>f</sub> (Hexanes/Ether 10:1) = 0.32. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.95 (2H, d, *J* = 8.8 Hz), 7.27-7.21 (3H, m), 7.16 (2H, dd, *J* = 8.1, 1.8 Hz), 7.13 (2H, d, *J* = 8.8 Hz), 6.44 (1H, ddd, *J* = 16.8, 10.0, 10.0 Hz), 5.32 (1H, ddt, *J* = 17.0, 10.1, 7.2 Hz), 5.44 (1H, d, *J* = 10.3 Hz), 5.37 (1H, d, *J* = 16.8 Hz), 5.16 (1H, ddt, *J* = 17.0, 1.2, 1.2 Hz), 5.09 (1H, ddt, *J* = 10.7, 1.2, 1.2 Hz), 3.73 (1H, d, *J* = 9.8 Hz), 3.01 (1H, dddd, *J* = 14.2, 7.6, 1.2, 1.2 Hz), 2.80 (1H, dddd, *J* = 14.2, 6.7, 1.2, 1.2 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 146.2, 135.2, 134.9, 133.4, 131.2, 129.4, 128.8, 128.2, 126.8, 123.2, 120.8, 120.4, 120.3, 59.7, 53.4, 42.9, HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. For C<sub>20</sub>H<sub>19</sub>N<sub>2</sub>O<sub>2</sub> 319.1441 Found 319.1440.

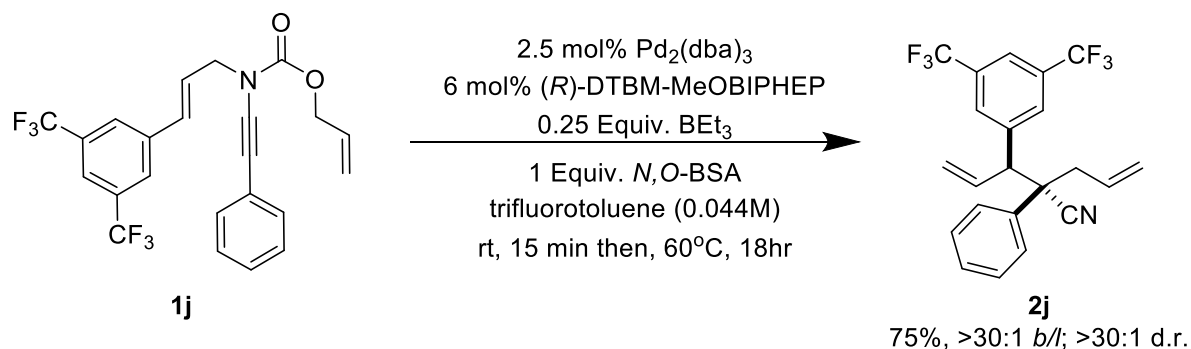
**(2*S*\*,3*S*\*)-2-Allyl-2-phenyl-3-(3,4,5-trifluorophenyl)pent-4-enenitrile (2i)**



The title compound was prepared by general procedure B from carbamate **1i** (74.2 mg, 0.2 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.6 mg, 10.0 μmol), (*R*)-DTBM-MeOBIPHEP (13.8 mg, 12.0 μmol), BEt<sub>3</sub> (1 M in THF, 50 μl, 50 μmol), *N,O*-BSA (49 μl, 0.2 μmol) in trifluorotoluene (4.5 mL). The crude product was purified by flash column chromatography (Hexanes/Ethyl Acetate 19:1) to afford the requisite nitrile product **2i** (55 mg, 84%, >30:1 d.r.) as a yellow oil.

R<sub>f</sub> (Hexanes/Ethyl Acetate 10:1) = 0.29. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.33-7.24 (3H, m), 7.18 (2H, dd, *J* = 6.8, 1.6 Hz), 6.63-6.53 (2H, m), 6.31 (1H, ddd, *J* = 16.8, 9.9, 9.9 Hz), 5.50 (1H, ddt, *J* = 17.0, 10.2, 6.8 Hz), 5.42 (1H, d, *J* = 10.1 Hz), 5.34 (1H, d, *J* = 16.8 Hz), 5.07 (1H, ddt, *J* = 17.0, 1.3, 1.3 Hz), 5.08 (1H, ddt, *J* = 10.2, 1.3, 1.3 Hz), 3.52 (1H, d, *J* = 9.7 Hz), 2.97 (1H, dddd, *J* = 14.2, 7.5, 1.3, 1.3 Hz), 2.76 (1H, dddd, *J* = 14.2, 6.5 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 152.6-149.6 (m, second order (*J*<sub>CF</sub>) coupling), 135.2 and 134.9 (rotamers), 134.9 and 134.8 (rotamers), 132.5 and 132.4 (rotamers), 129.1, 128.8, 126.8, 126.6, 125.1 and 125.1 (rotamers), 120.8 and 120.3 (rotamers), 120.4 and 120.0 (rotamers), 112.9-112.4 (m, second order (*J*<sub>CF</sub>) coupling), 112.8-112.4 (m, second order (*J*<sub>CF</sub>) coupling) and 110.3-109.9 (m, second order (*J*<sub>CF</sub>) coupling) (rotamers), 59.1 and 59.0 (rotamers), 52.7 and 51.5 (rotamers), 42.7 and 41.9 (rotamers). HRMS (ESI-TOF) *m/z*: [M + CH<sub>3</sub>CN + H<sub>2</sub>O]<sup>+</sup> Calcd. for C<sub>22</sub>H<sub>21</sub>F<sub>3</sub>N<sub>2</sub>O 386.1600 found 386.1584.

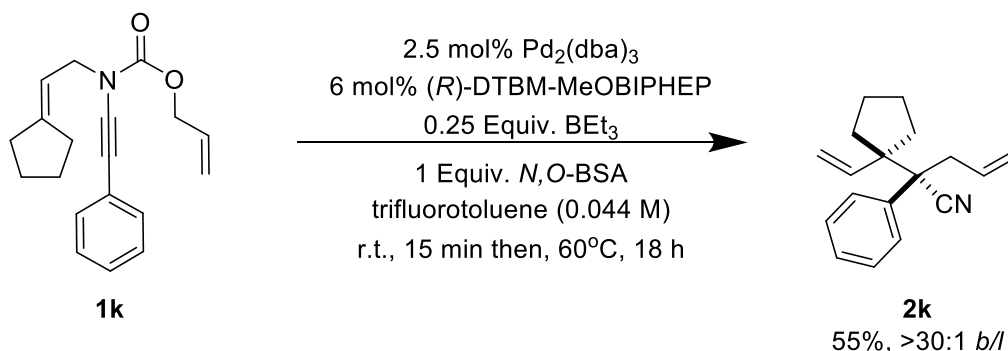
**(2*S*\*,3*S*\*)-2-Allyl-3-(3,5-bis(trifluoromethyl)phenyl)-2-phenylpent-4-enenitrile (2j)**



The title compound was prepared by general procedure B from carbamate **1j** (90.6 mg, 0.2 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.6 mg, 10.0 μmol), (*R*)-DTBM-MeOBIPHEP (13.8 mg, 12.0 μmol), BEt<sub>3</sub> (1M in THF, 50 μL, 50 μmol) and *N,O*-BSA (49 μL, 0.2 μmol) in trifluorotoluene (4.5 mL). The crude product was purified by flash column chromatography (Hexanes/Ethyl Acetate 19:1) to afford the requisite nitrile product **2j** (62 mg, 75%, >30:1 *d.r.*) as a colorless oil.

R<sub>f</sub> (Hexanes/Ethyl Acetate 10:1) = 0.63. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.63 (1H, br s), 7.30 (1H, br s), 7.29-7.23 (3H, m), 7.14-7.10 (2H, m), 6.46 (1H, ddd, *J* = 16.8, 10.0, 10.0 Hz), 5.57 (1H, dddd, *J* = 16.9, 10.1, 7.5, 6.6 Hz), 5.48 (1H, dd, *J* = 10.2, 0.7 Hz), 5.41 (1H, d, *J* = 16.8, 0.7 Hz), 5.18 (1H, ddt, *J* = 17.0, 1.4, 1.4 Hz), 5.11 (1H, ddt, *J* = 10.2, 1.4, 1.4 Hz), 3.74 (1H, d, *J* = 9.8 Hz), 2.99 (1H, dddd, *J* = 14.3, 7.6, 1.4, 1.4 Hz), 2.82 (1H, dddd, *J* = 14.4, 6.5, 1.4, 1.4 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 141.1, 134.9, 134.3, 131.2, 131.1 (q, <sup>2</sup>*J*<sub>CF</sub> = 33.5 Hz), 128.9, 128.8 1 (q, <sup>3</sup>*J*<sub>CF</sub> = 3.8 Hz), 126.8, 122.9 1 (q, <sup>1</sup>*J*<sub>CF</sub> = 272.7 Hz), 121.3, 121.1 (sept., <sup>3</sup>*J*<sub>CF</sub> = 3.8 Hz), 120.5, 119.9, 59.5, 52.7, 42.2. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>22</sub>H<sub>17</sub>F<sub>6</sub>N 410.1338 Found 410.1331.

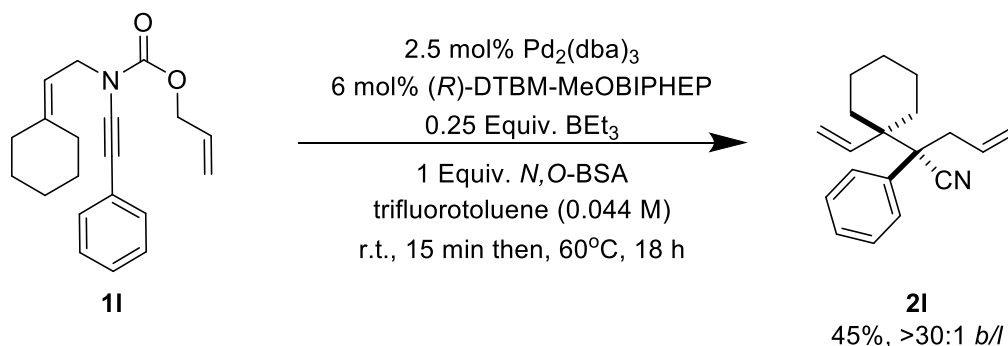
## 2-Phenyl-2-(1-vinylcyclopentyl)pent-4-enitrile (**2k**)



The title compound was prepared by general procedure B using carbamate **1k** (48 mg, 0.16 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (3.7 mg, 3.9 μmol), (*R*)-DTBM-MeOBIPHEP (11 mg, 9.1 μmol), BEt<sub>3</sub> (1M in THF, 40 μl, 40 μmol), *N,O*-BSA (39 μl, 16 μmol) in trifluorotoluene (3.6 mL). The crude product was purified by flash column chromatography (Hexanes/Et<sub>2</sub>O 30:1) to afford requisite nitrile product **2k** (22 mg, 55%) as a yellow oil.

R<sub>f</sub> (Hexanes/Ether 30:1) = 0.30. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.44-7.38 (2H, m), 7.37-7.27 (3H, m), 5.59 (1H, ddt, *J* = 17.0, 10.2, 6.9 Hz), 5.50 (1H, dd, *J* = 17.7, 10.9 Hz), 5.27 (1H, dd, *J* = 10.8, 0.6 Hz), 5.17 (1H, ddt, *J* = 17.0, 1.4, 1.4 Hz), 5.06 (1H, dd, *J* = 17.1, 0.6 Hz), 5.06 (1H, ddt, *J* = 10.1, 1.4, 1.4 Hz), 2.99 (1H, dddd, *J* = 14.6, 6.5, 1.4, 1.4 Hz), 2.69 (1H, dddd, *J* = 14.5, 7.4, 1.4, 1.4 Hz), 2.01-1.82 (3H, m), 1.76-1.53 (3H, m), 1.49-1.36 (1H, m), 1.34-1.25 (1H, m). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 139.3, 134.8, 132.6, 128.6, 127.8, 127.7, 122.3, 119.5, 117.1, 55.6, 55.3, 38.3, 34.4, 32.6, 23.1, 22.6, HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>18</sub>H<sub>22</sub>N 252.1747 found 252.1758.

## 2-Phenyl-2-(1-vinylcyclohexyl)pent-4-enitrile (**21**)

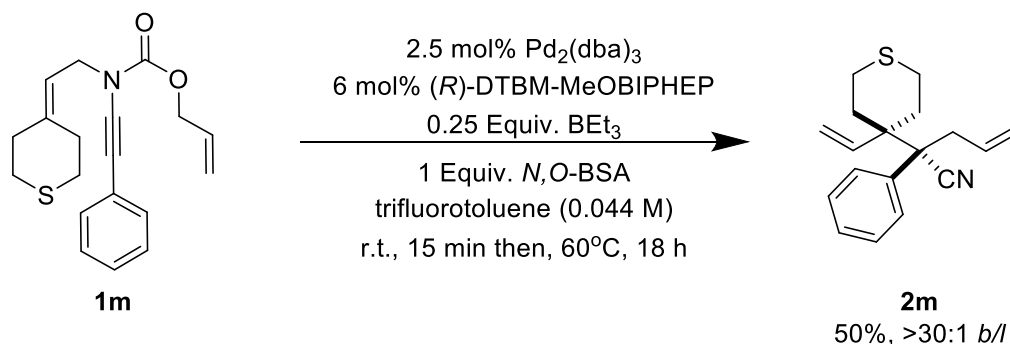


The title compound was prepared by general procedure B using carbamate **11** (58.5 mg, 0.19 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.6 mg, 4.8 μmol), (*R*)-DTBM-MeOBIPHEP (13.1 mg, 11.4 μmol), BEt<sub>3</sub> (1M in THF, 48 μl, 48 μmol) and *N,O*-BSA (46 μl, 19 μmol) in trifluorotoluene (4.3 mL). The crude product was purified by flash column chromatography (Hexanes/Et<sub>2</sub>O 30:1) to afford the requisite nitrile product **21** (21.5 mg, 45%) as a yellow oil.

R<sub>f</sub> (Hexanes/EtOAc 20:1) = 0.64. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.41-7.27 (5H, m), 5.51(1H, ddt, *J* = 17.0, 10.1, 6.9 Hz), 5.51 (1H, dd, *J* = 11.0, 0.8 Hz), 5.33 (1H, dd, *J* = 17.8, 10.9 Hz), 5.14 (1H, ddt, *J* = 17.0, 1.3, 1.3 Hz), 5.08 (1H, dd, *J* = 17.9, 0.8 Hz), 5.02 (1H, ddt, *J* = 10.2, 1.3, 1.3 Hz), 2.92 (1H, dddd, *J* = 14.4, 6.5, 1.3, 1.3 Hz), 2.78 (1H, dddd, *J* = 14.4, 7.3, 1.3, 1.3 Hz), 2.08 (1H, d, *J* = 12.8 Hz), 1.72-1.34 (8H, m), 1.23 (1H, dtt, *J* = 12.4, 12.4, 2.5 Hz), 1.10 (1H, dtt, *J* = 12.4, 12.4, 2.6 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 138.9, 133.8, 132.8, 128.4, 127.7, 127.6, 122.2, 119.9, 119.4, 57.3, 46.4, 36.3, 32.3, 31.1, 25.7, 22.3, 22.2, HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>19</sub>H<sub>24</sub>N 266.1903 found 266.1913.



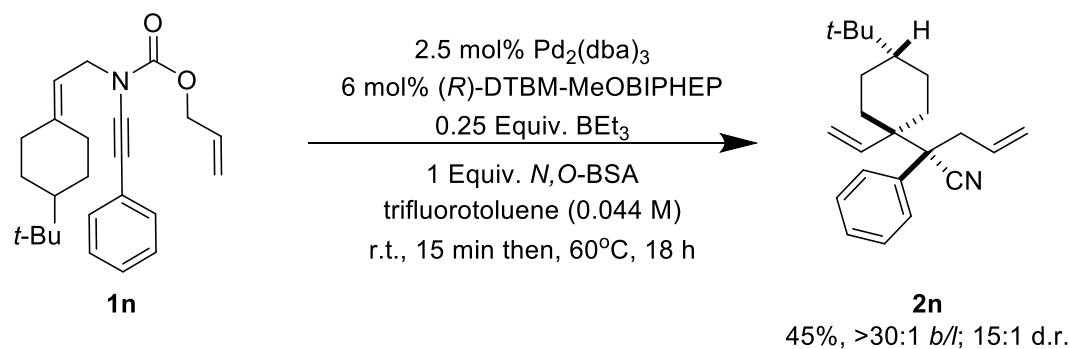
## 2-Phenyl-2-(4-vinyltetrahydro-2H-thiopyran-4-yl)pent-4-enitrile (**2m**)



The title compound was prepared by general procedure B using carbamate **1m** (65.4 mg, 0.2 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.6 mg, 5.0 μmol), (*R*)-DTBM-MeOBIPHEP (13.9 mg, 12.0 μmol), BEt<sub>3</sub> (1M in THF, 50 μl, 50 μmol) and *N,O*-BSA (49 μl, 20 μmol) in trifluorotoluene (4.5 mL). The crude product was purified by flash column chromatography (Hexanes/Et<sub>2</sub>O 30:1) to afford the requisite nitrile product **2m** (28.2 mg, 50%) as a yellow oil.

R<sub>f</sub> (Hexanes/EtOAc 20:1) = 0.17. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.44-7.27 (5H, m), 5.63 (1H, d, *J* = 11.1 Hz), 5.49 (1H, ddt, *J* = 16.9, 10.1, 6.8 Hz), 5.35 (1H, dd, *J* = 18.1, 10.1 Hz), 5.15 (1H, dd, *J* = 16.8, 1.2 Hz), 5.10 (1H, d, *J* = 17.9 Hz), 5.03 (1H, dd, *J* = 10.1, 1.2 Hz), 2.94 (1H, dd, *J* = 14.3, 6.4 Hz), 2.90 (1H, dd, *J* = 14.7, 3.4 Hz), 2.78 (1H, ddd, *J* = 14.5, 14.5, 2.4 Hz), 2.77 (1H, dd, *J* = 14.3, 6.9 Hz), 2.44-2.28 (3H, m), 2.01 (2H, dddd, *J* = 13.9, 13.9, 13.9, 3.4 Hz), 1.85 (1H, d, *J* = 13.6 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 138.1, 133.0, 132.3, 129.4, 128.0, 127.9, 121.4, 121.4, 119.8, 57.3, 45.8, 36.0, 33.1, 32.5, 24.3, 24.3. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. For C<sub>18</sub>H<sub>21</sub>NS 284.1467 found 284.1463.

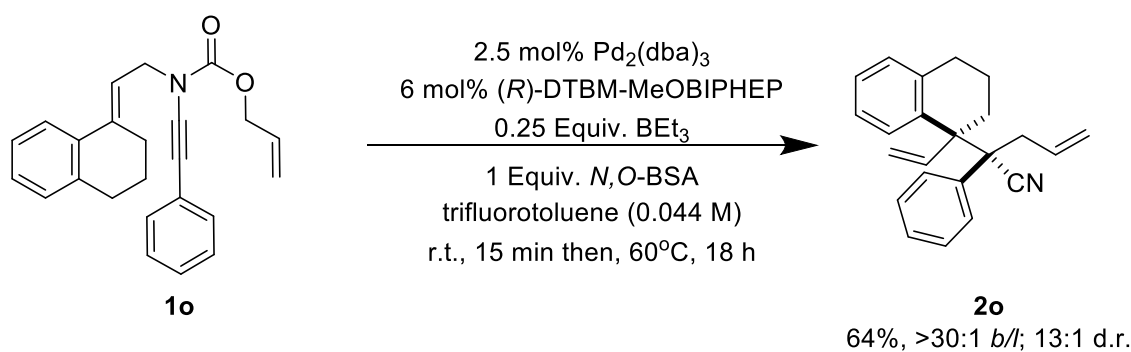
***anti*-4-(*tert*-Butyl)-1-vinylcyclohexyl)-2-phenylpent-4-enenitrile (**2n**)**



The title compound was prepared by general procedure B using carbamate **1n** (26 mg, 0.071 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (1.7 mg, 3.6 μmol), (*R*)-DTBM-MeOBIPHEP (5.0 mg, 4.3 μmol), BEt<sub>3</sub> (1M in THF, 18 μl, 18 μmol) and *N,O*-BSA (17 μl, 71 μmol) in trifluorotoluene (1.6 mL). The crude product was purified by flash column chromatography (Hexanes/Et<sub>2</sub>O 30:1) to afford the requisite nitrile product **2n** (10.2 mg, 45%, 15:1 d.r.) as a colorless oil.

R<sub>f</sub> (Hexanes/EtOAc 20:1) = 0.53. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.45-7.28 (5H, m), 5.52 (1H, ddt, *J* = 17.0, 10.1, 7.1 Hz), 5.49 (1H, dd, *J* = 18.0, 1.2 Hz), 5.32 (1H, dd, *J* = 17.7, 11.1 Hz), 5.14 (1H, ddt, *J* = 17.0, 1.3, 1.3 Hz), 5.08 (1H, dd, *J* = 18.1, 1.2 Hz), 5.02 (1H, ddt, *J* = 10.3, 1.3, 1.3 Hz), 2.93 (1H, dddd, *J* = 14.4, 6.5, 1.3, 1.3 Hz), 2.78 (1H, dddd, *J* = 14.4, 7.3, 1.2, 1.2 Hz), 2.14 (1H, dddd, *J* = 13.0, 3.2, 3.2, 3.2, Hz), 1.75-1.43 (6H, m), 1.15 (1H, dddd, *J* = 12.0, 12.0, 12.0, 3.8 Hz), 0.98 (1H, dddd, *J* = 12.3, 12.3, 12.3, 3.2 Hz), 0.78 (9H, s). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 138.0, 132.8, 131.8, 128.2, 126.6, 126.5, 121.2, 118.8, 118.4, 56.0, 46.5, 45.1, 35.5, 31.6, 31.2, 30.5, 26.4, 22.1, 22.0. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>23</sub>H<sub>32</sub>N 322.2529 found 322.2544.

**(*R*\*)-2-Phenyl-2-((*S*\*)-1-vinyl-1,2,3,4-tetrahydronaphthalen-1-yl)pent-4-enitrile (**2o**)**

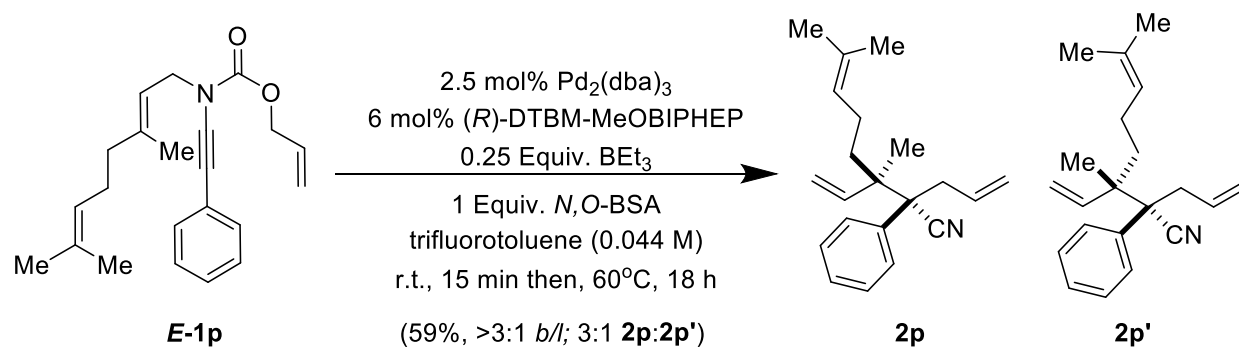


The title compound was prepared by general procedure B using carbamate **1o** (35.7 mg, 0.10 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.6 mg, 2.5 μmol), (*R*)-DTBM-MeOBIPHEP (6.9 mg, 6.0 μmol), BEt<sub>3</sub> (1M in THF, 25 μl, 25 μmol) and *N,O*-BSA (24 μl, 10 μmol) in trifluorotoluene (4.5 mL). The crude product was purified by flash column chromatography (Hexanes/Et<sub>2</sub>O 30:1) to afford the requisite nitrile product **2o** (19.7 mg, 63%, 13:1 d.r.) as a yellow oil.

R<sub>f</sub> (Hexanes/EtOAc 20:1) = 0.45. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) 7.58-7.50 (1H, m), 7.27-7.03 (9H, m), 6.42 (1H, dd, *J* = 17.1, 10.7 Hz), 5.49 (1H, ddt, *J* = 17.0, 10.2, 7.0 Hz), 5.32 (1H, dd, *J* = 10.7, 1.0 Hz), 5.08 (1H, ddt, *J* = 17.0, 1.5 Hz), 5.01 (1H, ddt, *J* = 10.1, 1.5, 1.5 Hz), 4.82 (1H, dd, *J* = 17.1, 1.0 Hz), 2.99 (1H, dddd, *J* = 14.1, 6.4, 1.5, 1.5 Hz), 2.78 (1H, dddd, *J* = 14.1, 7.4, 1.5, 1.5 Hz), 2.52 (1H, dddd, *J* = 15.9, 2.1, 2.1, 2.1 Hz), 2.30-2.12 (1H, m), 1.95 (1H, ddd, *J* = 13.1, 13.1, 2.9 Hz), 1.82-1.49 (4H, m), 1.37 (1H, ddd, *J* = 12.7, 3.0, 3.0 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 142.7, 142.7, 135.3, 134.7, 132.6, 130.8, 129.5, 129.4, 129.3, 127.9, 127.6, 126.8, 125.1, 119.6, 117.5, 52.1, 38.9, 34.1, 31.3, 29.7, 19.6. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. For C<sub>23</sub>H<sub>24</sub>N 314.1903 found 314.1918.

(2*S*\*,3*S*\*)-2-Allyl-3,7-dimethyl-2-phenyl-3-vinyloct-6-enenitrile (**2p**) and

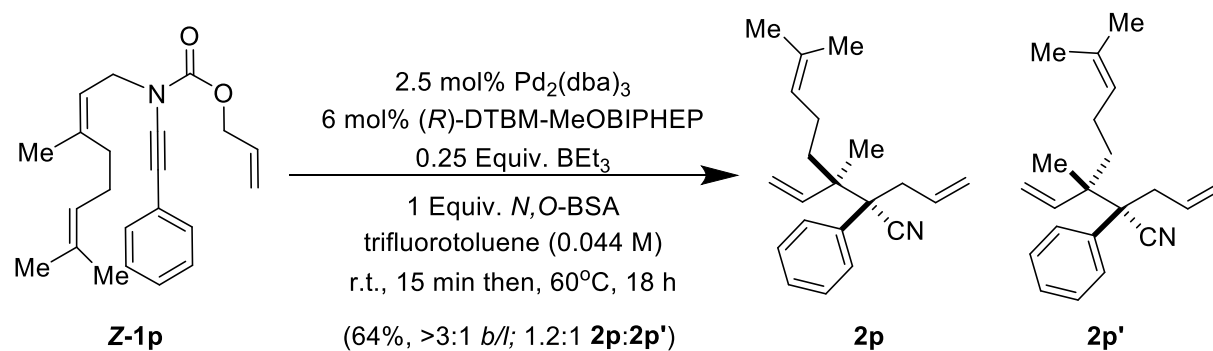
(2*S*\*,3*R*\*)-2-Allyl-3,7-dimethyl-2-phenyl-3-vinyloct-6-enenitrile (**2p'**)



The title compound was prepared by general procedure B from carbamate **2p** (67.4 mg, 0.20 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (4.6 mg, 5.0 μmol), (*R*)-DTBM-MeOBIPHEP (13.8 mg, 12.0 μmol), BEt<sub>3</sub> (1M in THF, 50 μl, 50 μmol) and *N,O*-BSA (49 μl, 0.2 μmol) in trifluorotoluene (4.5 mL). The crude product was purified by flash column chromatography (Hexanes/Ethyl Acetate 19:1) to afford the requisite nitrile products **2p/2p'** (35 mg, 59%, 3:1 d.r. [**2p:2p'**]) as a colorless oil.

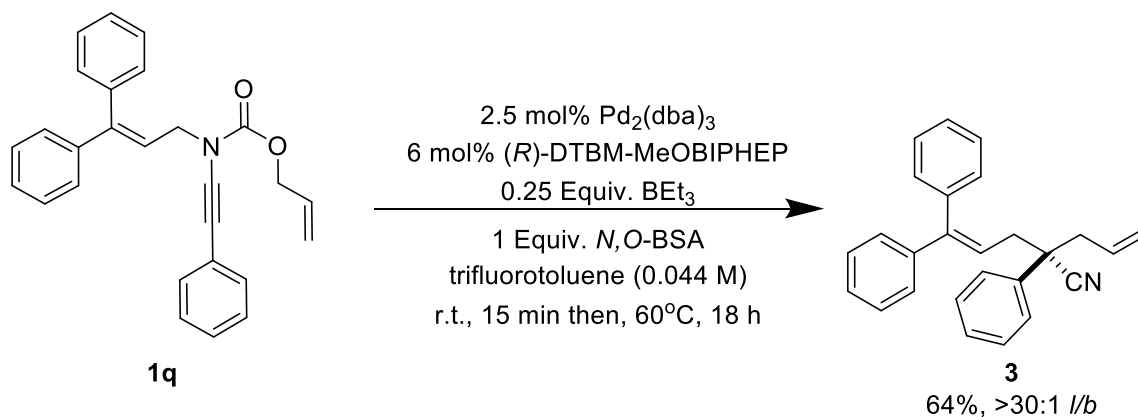
R<sub>f</sub> (Hexanes/Ethyl acetate 10:1) = 0.33, <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.42-7.29 (5H, m, **2p** and **2p'**), 5.86 (0.25H, dd, *J* = 17.5, 10.9 Hz, **2p'**), 5.64 (0.75H, dd, *J* = 17.6, 10.8 Hz, **2p**), 5.51 (0.25H, ddt, *J* = 16.6, 10.2, 7.0 Hz, **2p'**), 5.50 (0.75H, ddt, *J* = 17.0, 10.2, 7.1 Hz, **2p**), 5.35 (0.25H, d, *J* = 10.3 Hz, **2p'**), 5.32 (0.75H, dd, *J* = 10.9, 0.6 Hz, **2p'**), 5.15 (0.75H, ddt, *J* = 17.0, 1.4, 1.4 Hz, **2p**), 5.13 (0.25H, dd, *J* = 17.0, 1.4 Hz, **2p'**), 5.08 (0.75H, dd, *J* = 17.5, 0.6 Hz, **2p**), 5.05 (0.25H, d, *J* = 17.1 Hz, **2p'**), 5.03 (0.75H, ddt, *J* = 10.1, 1.4, 1.4 Hz, **2p**), 4.97 (1H, tt, *J* = 7.1, 1.3 Hz, **2p** and **2p'**), 2.94 (1H, dddd, *J* = 14.4, 6.5 Hz, **2p** and **2p'**), 2.77 (1H, dddd, *J* = 14.4, 7.2 Hz, **2p** and **2p'**), 1.90-1.49 (9H, m, **2p** and **2p'**), 1.67 (0.75H, s, **2p'**), 1.64 (2.25H, s, **2p**), 1.54 (0.75H, s, **2p'**), 1.52 (2.25H, s, **2p**), 1.38 (0.5H, td, *J* = 11.0, 4.9 Hz, **2p'**), 1.27 (2.25H, s, **2p**), 1.26 (1.5H, td, *J* = 12.9, 4.3 Hz, **2p**), 1.03 (0.75H, s, **2p'**). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 141.1 (**2p'**), 140.2 (**2p**), 134.0 (**2p'**), 134.0 (**2p**), 132.7 (**2p** and **2p'**), 131.7 (**2p'**), 131.7 (**2p**), 129.3 (**2p** and **2p'**), 127.8 (**2p**), 127.7 (**2p'**), 124.1 (**2p** and **2p'**), 122.1 (**2p**), 122.0 (**2p'**), 119.5 (**2p'**), 119.4 (**2p**), 117.4 (**2p**), 117.3 (**2p'**), 56.5 (**2p'**), 56.4 (**2p**), 46.5 (**2p'**), 46.2 (**2p**), 37.0 (**2p**), 37.0 (**2p'**), 36.5 (**2p**), 36.4 (**2p'**), 25.6 (**2p** and **2p'**), 23.1 (**2p'**), 23.1 (**2p**), 18.4 (**2p**),

17.6 (**2p** and **2p'**), 17.1 (**2p'**). HRMS (ESI-TOF)  $m/z$ :  $[M + H]^+$  Calcd. for  $C_{21}H_{28}N$  294.2216 found 294.2227.



Carbamate **1p'** (49 mg, 0.14 mmol),  $Pd_2(dba)_3$  (3.2 mg, 3.5  $\mu$ mol), (*R*)-DTBM-MeOBIPHEP (9.7 mg, 8.4  $\mu$ mol),  $BEt_3$  (1 M in THF, 35  $\mu$ l, 35  $\mu$ mol) and *N,O*-BSA (34  $\mu$ l, 0.14  $\mu$ mol) in trifluorotoluene (3.2 mL). The crude product was purified by flash column chromatography (Hexanes/Ethyl Acetate 19:1) to afford the requisite nitrile products **2p/2p'** (26.2 mg, 64%, 1.2:1 d.r. [**2p:2p'**]) as a colorless oil.

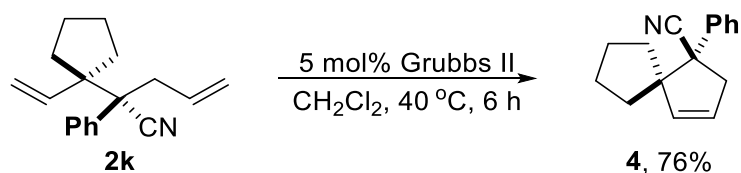
### 2-Allyl-2,5,5-triphenylpent-4-enenitrile (**3**)



The title compound was prepared by general procedure B using carbamate **1q** (22 mg, 0.056 mmol), Pd<sub>2</sub>(dba)<sub>3</sub> (1.3 mg, 2.8 μmol), (*R*)-DTBM-MeOBIPHEP (3.9 mg, 3.4 μmol) BEt<sub>3</sub> (1 M in THF, 14 μl, 14 μmol) and *N,O*-BSA (14 μl, 5.6 μmol) in trifluorotoluene (1.3 mL). The crude product was purified by flash column chromatography (Hexanes/Et<sub>2</sub>O 30:1) to afford the linear nitrile product **3** (8.2 mg, 42%) as a colorless solid.

R<sub>f</sub> (Hexanes/EtOAc 20:1) = 0.44. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ 7.40-7.29 (8H, m), 7.24-7.19 (3H, m), 7.11-7.07 (2H, m), 7.03-6.99 (2H, m), 6.00 (1H, t, *J* = 7.3 Hz), 5.60 (1H, ddt, *J* = 17.2, 9.7, 7.1 Hz), 5.11 (1H, d, *J* = 9.9 Hz), 5.09 (1H, d, *J* = 16.8 Hz), 2.85 (1H, dd, *J* = 14.7, 7.1 Hz), 2.73 (1H, dd, *J* = 14.7, 7.4 Hz), 2.68 (1H, dd, *J* = 14.2, 7.6 Hz), 2.62 (1H, dd, *J* = 14.1, 6.7 Hz). <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) δ 145.7, 141.9, 137.6, 131.6, 129.8, 128.8, 128.3, 128.1, 127.9, 127.4, 127.3, 127.3, 126.3, 122.3, 120.1, 115.8, 114.6, 48.0, 44.3, 40.0. HRMS (ESI-TOF) *m/z*: [M + H]<sup>+</sup> Calcd. for C<sub>26</sub>H<sub>24</sub>N 350.1903 found 350.1914.

### 1-Cyano-1-Phenyl Spiro[3,3]non-3-ene (**4a**)



The title compound (**4a**) was prepared by general procedure C using nitrile **2k** (15.0 mg, 0.060 mmol), Grubb's 2<sup>nd</sup> generation catalyst (2.6 mg, 3.1  $\mu\text{mol}$ ) in dichloromethane (4.5 mL). The crude product was purified by flash column chromatography (Hexanes/Et<sub>2</sub>O 30:1) to afford spirocycle **4a** (10.2 mg, 76%) as a colorless oil.

$R_f$  (Hexanes/EtOAc 19:1) = 0.54. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.53 (2H, dd,  $J$  = 8.0, 1.2 Hz), 7.39-7.30 (3H, m), 5.84 (1H, ddd,  $J$  = 5.9, 2.0, 2.0 Hz), 5.78 (1H, ddd,  $J$  = 5.9, 2.0, 2.0 Hz), 3.20 (2H, dd,  $J$  = 2.0, 2.0 Hz), 2.14 (1H, ddd,  $J$  = 13.1, 8.5, 8.5 Hz), 1.86 (1H, ddd,  $J$  = 12.8, 8.2, 4.5 Hz), 1.80-1.63 (2H, m), 1.55-1.35 (2H, m), 1.14 (1H, ddd,  $J$  = 13.4, 7.8, 6.2 Hz), 1.10 (1H, ddd,  $J$  = 13.0, 8.0, 8.0 Hz). <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  139.1, 137.7, 128.4, 127.9, 127.0, 125.7, 124.0, 63.9, 54.1, 45.0, 36.8, 34.7, 29.7, 24.0, 23.7. HRMS (ESI-TOF)  $m/z$ : [M + Na]<sup>+</sup> Calcd. for C<sub>16</sub>H<sub>18</sub>N 246.1263 found 246.1253.

## 6. Computational Methods Used

### General Comments

To explore the possible mechanistic pathways, we applied the two-layered QM/SE ONIOM method to palladium complexes.<sup>4,5,6</sup> In this model, the substrate as well as palladium and phosphorous atoms of the catalyst were included in the high layer, whereas the rest was placed in the low layer. The high level was treated with DFT using local meta-generalized gradient approximation functional M06L recommended for transition-metal chemistry calculations.<sup>7</sup> The 6-31G+(d) basis set was used for C, H, P, and O atoms in conjunction with the LANL2DZ relativistic pseudopotential for Pd (BSI). The low level was handled with semi-empirical method PM6. Given the bulky nature of the ligand, this two-layered ONIOM model allowed us to perform geometry optimization of palladium complexes within the reasonable timescale. The nature of stationary points in each case was confirmed by harmonic frequency calculations. The nature of located TSs was confirmed by unique imaginary vibrational mode and IRC calculations.

To get refined energies, we further performed single point (SP) energy calculations using the ONIOM geometries. The palladium complexes were fully treated by DFT. The larger basis set

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<sup>4</sup> Ananikov, V. P.; Musaev, D. G.; Morokuma, K., Real size of ligands, reactants and catalysts: Studies of structure, reactivity and selectivity by ONIOM and other hybrid computational approaches. *Journal of Molecular Catalysis A: Chemical* **2010**, *324* (1), 104-119.

<sup>5</sup> Li, Z.; Liu, L.; Fu, Y.; Guo, Q.-X., Assessing performance of diverse ONIOM methods in calculation of structures of organonickel and organopalladium compounds. *Journal of Molecular Structure: THEOCHEM* **2005**, *757* (1), 69-76.

<sup>6</sup> Karami, K.; Abedanzadeh, S.; Farrokhpour, H.; Lipkowski, J., Synthesis and characterization of the P,C-palladacycles with bridging and chelating dinitrogen ligands and ONIOM calculations on the pyrazine-bridged organometallic polymers (n = 1 to n = 10). *Journal of Organometallic Chemistry* **2016**, *805*, 68-76.

<sup>7</sup> Zhao, Y.; Truhlar, D. G., The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theoretical Chemistry Accounts* **2008**, *120* (1), 215-241.



6-311++G(2d,2p) for C, H, P and O atoms and LANL2DZ ECP for Pd (BSII) and M06L functional were employed. The single point solvation by trifluorotoluene was accounted by using conductor-like polarizable continuum model (C-PCM)<sup>8,9</sup> specifying the following parameters: static dielectric constant  $\epsilon = 9.4$ , dynamic dielectric constant  $n^2 = 1.414$ . The calculations were performed with the Gaussian 16.0 software.<sup>10</sup> The corrected single point energy was calculated as follows:

$$G_{\text{SP Corrected}} = E_{\text{elec}}[\text{CPCM}(\text{PhCF}_3)\text{M06L/BSII}] + G_{\text{Corr ONIOM}}[\text{ONIOM}(\text{M06L/BSI:PM6})]$$

where  $G_{\text{Corr ONIOM}}$  is the thermal correction to Gibbs free energy obtained in the gas phase at ONIOM(M06L/BSI:PM6) or M06L/BSI.

The obtained Gibbs Free energies were temperature-corrected and reported at 333.15 K. At the same temperature all energies were corrected to 1 mol/L standard state. The Grimme's quasi-rigid-rotor harmonic oscillator (quasi-RRHO) approximation was used to account for entropic

<sup>8</sup> Barone, V.; Cossi, M., Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model. *The Journal of Physical Chemistry A* **1998**, *102* (11), 1995-2001.

<sup>9</sup> Klamt, A.; Schüürmann, G., COSMO: a new approach to dielectric screening in solvents with explicit expressions for the screening energy and its gradient. *Journal of the Chemical Society, Perkin Transactions 2* **1993**, (5), 799-805.

<sup>10</sup> Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian 16 Rev. A.03, Wallingford, CT, 2016.

contributions of low frequency modes below 100 cm<sup>-1</sup>.<sup>11,12</sup> All corrections were obtained using the GoodVibes 3.0.1 program by Prof. Robert Paton.<sup>13</sup> Trifluorotoluene parameters (molecular weight and density) were manually added to media.py.

The optimized structures were visualized using CYLview 1.0b.<sup>14</sup> The potential energy surfaces were generated using GoodVibes 3.0.1.<sup>13</sup>

Conformational studies were done in CREST.<sup>15</sup> Each experiment was repeated twice to ensure reproducibility, the typical run was as follows. The conformational search for **6** was performed using default iMTD-GC algorithm at the GFN2-xTB level,<sup>16</sup> which resulted in 781 conformers within an energy window of 4.2 kcal/mol. The generated conformational ensemble was reduced to 25 lowest energy structures that were optimized using DFT at M06L/BSI level. The redundant conformers were eliminated. The structures in reactive conformation were considered for further analysis. The conformational search for **6** bound to **Pd-L1g** was performed using special NCI mode for non-covalently bound complexes at GFN-FF level.<sup>17</sup> The allyl group and allene system atoms were constrained in reactive conformation during meta-dynamic simulations. The search resulted in 1784 conformers within an energy window

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<sup>11</sup> Grimme, S., Supramolecular Binding Thermodynamics by Dispersion-Corrected Density Functional Theory. *Chemistry – A European Journal* **2012**, *18* (32), 9955-9964.

<sup>12</sup> Li, Y.-P.; Gomes, J.; Mallikarjun Sharada, S.; Bell, A. T.; Head-Gordon, M., Improved Force-Field Parameters for QM/MM Simulations of the Energies of Adsorption for Molecules in Zeolites and a Free Rotor Correction to the Rigid Rotor Harmonic Oscillator Model for Adsorption Enthalpies. *The Journal of Physical Chemistry C* **2015**, *119* (4), 1840-1850.

<sup>13</sup> Luchini, G.; Alegre-Requena, J.; IFunes; Rodríguez-Guerra, J.; Chen, J.; Paton, R. bobbypaton/GoodVibes: GoodVibes v3.0.0. <https://doi.org/10.5281/zenodo.3346166>.

<sup>14</sup> Legault, C. Y. CYLview 1.0b. Université de Sherbrooke (2009) (<http://www.cylview.org>) Dennington, R., Keith, T.A. & Millam J.M. GaussView 6.0.16. Semichem Inc., Shawnee Mission, KS (2016).

<sup>15</sup> Pracht, P.; Bohle, F.; Grimme, S., Automated exploration of the low-energy chemical space with fast quantum chemical methods. *Physical Chemistry Chemical Physics* **2020**, *22* (14), 7169-7192.

<sup>16</sup> Bannwarth, C.; Ehlert, S.; Grimme, S., GFN2-xTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. *Journal of Chemical Theory and Computation* **2019**, *15* (3), 1652-1671.

<sup>17</sup> Spicher, S.; Grimme, S., Robust Atomistic Modeling of Materials, Organometallic, and Biochemical Systems. *Angewandte Chemie International Edition* **2020**, *59* (36), 15665-15673.

of 5.8 kcal/mol. From generated conformational ensemble 3 conformers reflecting *exo*- and 3 conformers reflecting *endo*- binding mode of **6** to **Pd-L1g** were selected and reoptimized using ONIOM(M06L|BSI:PM6). The conformational changes occurring between C-N bond cleavage and C-C bond formation were found during potential energy surface scans.

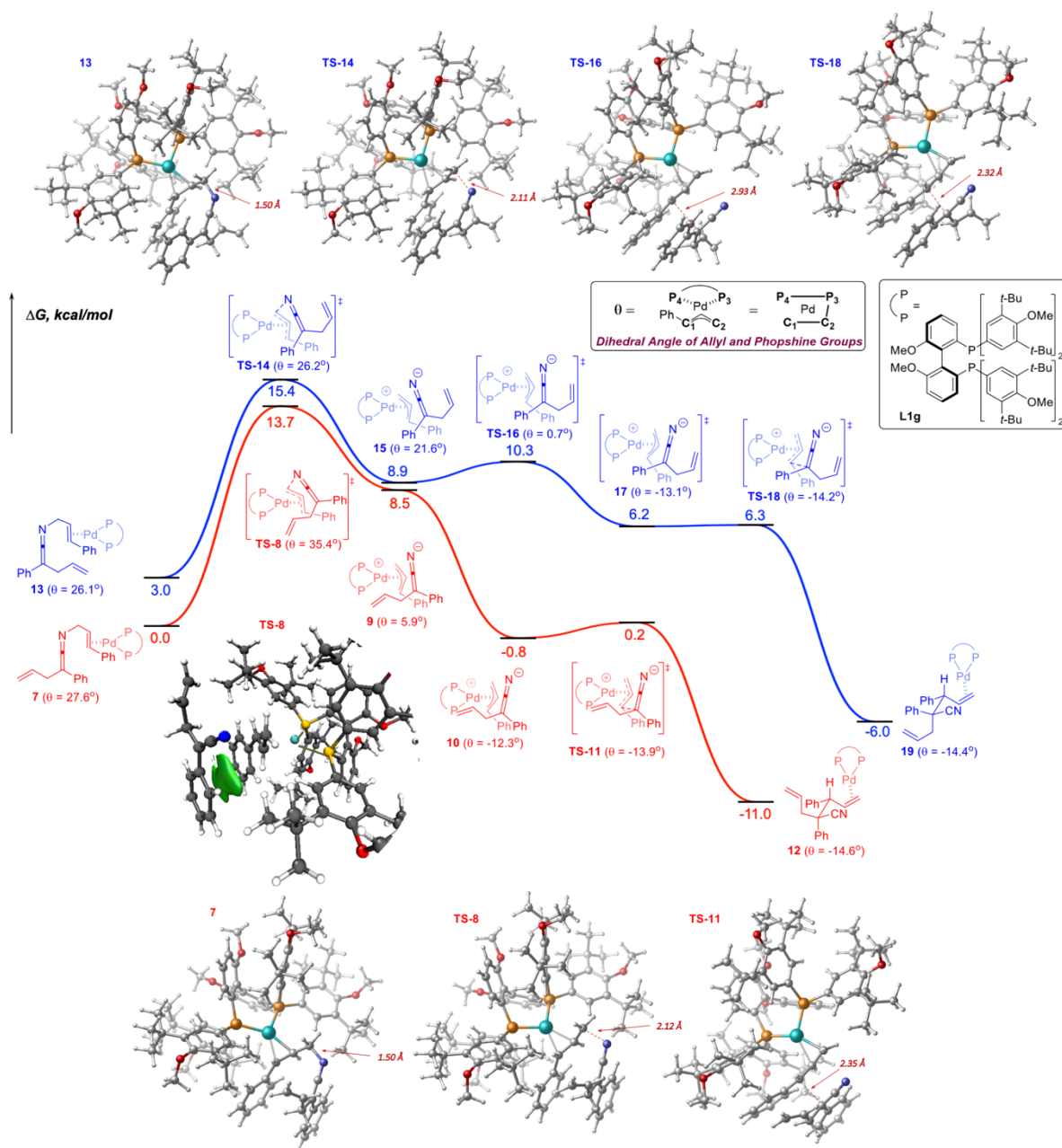
To evaluate noncovalent interactions between phenyl groups in transition states **TS-8** and **TS-14**, we utilized independent gradient model approach (IGM- $\delta g$ ).<sup>18</sup> Three-dimensional (3D) IGM isosurfaces representing non-covalent interactions were visualized in VMD.<sup>19</sup> These isosurfaces were color-coded with green and blue demonstrating van der Waals and strong attraction, respectively and yellow and red – weak and strong repulsion, respectively.

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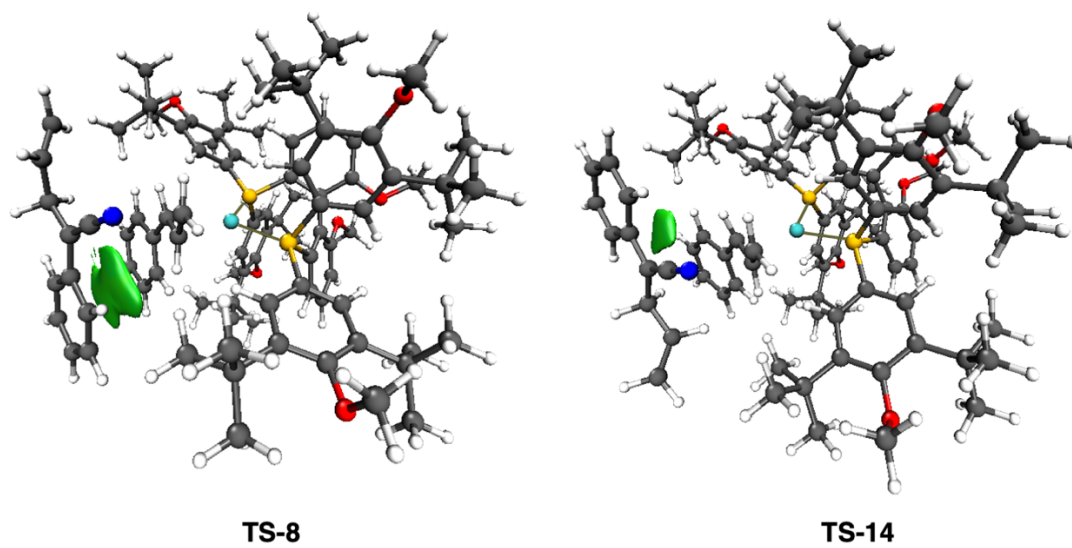
<sup>18</sup> Calculated using IGMPlot. <http://igmpplot.univ-reims.fr>. See: C. Levfevre, H. Khartabil, J.-C. Boisson, J. Contreras-Garcia, J.-P. Piquemal, E. Hénon, *ChemPhysChem* 2018, **19**, 724.

<sup>19</sup> Humphrey, W.; Dalke, A.; Schulten, K. *J. Mol. Graph.* 1996, **14**, 33-38.

## 7. Ground and Transition State Structures



**Scheme S1.** Summary of DFT Analysis Examining the Diastereoselectivity in the Formation of **2a**.



**Figure S1.** Three-dimensional IGM isosurfaces (IGM-  $\delta g^{\text{inter}}$ , isovalue 0.004).

**Table S4.** Energies and Lowest Frequencies of Minimum Energy Structures

Structure	E <sup>a</sup> , Ha	E_SPC <sup>b</sup> , Ha	G(T)_SPC <sup>c</sup>	qh-G(T)_SPC <sup>d</sup>	Lowest freq. <sup>e</sup>
<b>Pd-L1g</b>	-813.501332	-4143.787235	-4142.463347	-4142.439363	7.63
<b>2a</b>	-828.153777	-828.374439	-828.095958	-828.092312	29.89
<b>2a'</b>	-828.154072	-828.374968	-828.097850	-828.093492	33.42
<b>6</b>	-828.133083	-828.352815	-828.080602	-828.073598	3.01
<b>7</b>	-1641.674213	-4972.203260	-4970.576857	-4970.544879	7.31
<b>9</b>	-1641.660257	-4972.184384	-4970.563143	-4970.531380	5.93
<b>10</b>	-1641.663736	-4972.201144	-4970.576452	-4970.546098	10.87
<b>12</b>	-1641.686505	-4972.222121	-4970.591749	-4970.562400	10.42
<b>13</b>	-1641.674562	-4972.196636	-4970.572826	-4970.540080	6.18
<b>15</b>	-1641.659140	-4972.181976	-4970.563541	-4970.530636	8.04
<b>17</b>	-1641.662663	-4972.189895	-4970.565076	-4970.535013	9.22
<b>19</b>	-1641.680854	-4972.212984	-4970.585144	-4970.554390	3.23
<b>PhCF<sub>3</sub></b>	-569.237725	-569.391876	-569.319973	-569.318936	30.35
<b>TS-8</b>	-1641.650520	-4972.178215	-4970.553822	-4970.523034	-311.03
<b>TS-11</b>	-1641.661300	-4972.201236	-4970.573806	-4970.544546	-296.81
<b>TS-14</b>	-1641.652256	-4972.174166	-4970.552030	-4970.520387	-311.12
<b>TS-16</b>	-1641.661361	-4972.184066	-4970.557784	-4970.528542	-11.10
<b>TS-18</b>	-1641.658554	-4972.191876	-4970.563820	-4970.534853	-321.39

<sup>a</sup> Electronic energies calculated at ONIOM(M06L/BSI:PM6), where BSI = 6-31+G(d) (C, H, P, O)/LANL2DZ (ECP Pd).

<sup>b</sup> Single point energies calculated at at CPCM(Trifluorotoluene) M06L/BSII/[ONIOM(M06L/BSI:PM6)], where BSI = 6-31+G(d) (C, H, P, O)/LANL2DZ (ECP Pd) and BSII = 6-311++G(2d,2p) (C, H, P, O) /LANL2DZ (ECP Pd).

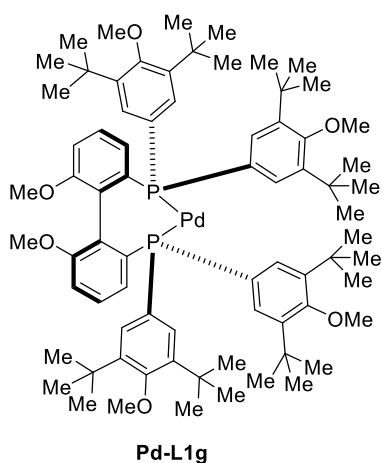
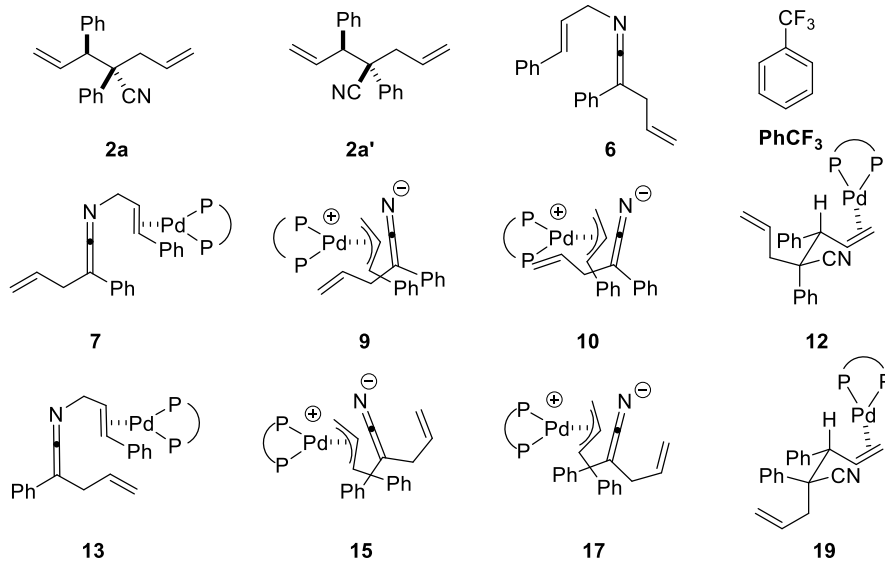
<sup>c</sup> Harmonic solvent and temperature (333.15 K) corrected Gibbs free energies.

<sup>d</sup> Quasi-harmonic solvent and temperature (333.15 K) corrected Gibbs free energies at 1 mol/L standard state.

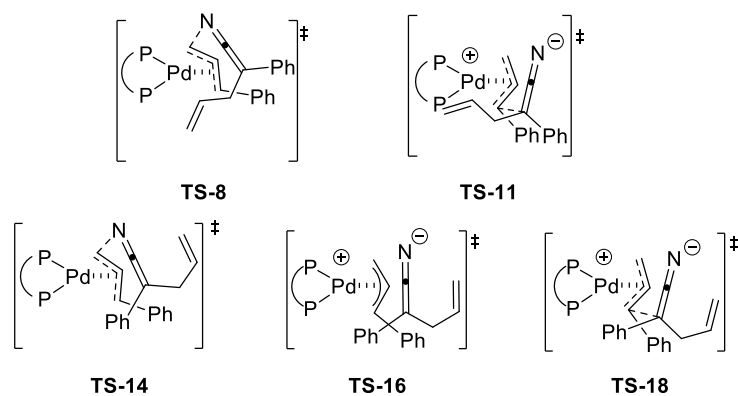
<sup>e</sup> Unscaled; calculated at ONIOM(M06L/BSI:PM6), where BSI = 6-31+G(d) (C, H, P, O)/LANL2DZ (ECP Pd).

## Graphical Guide to Numbered Compounds

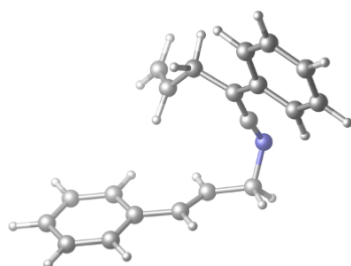
### Ground States



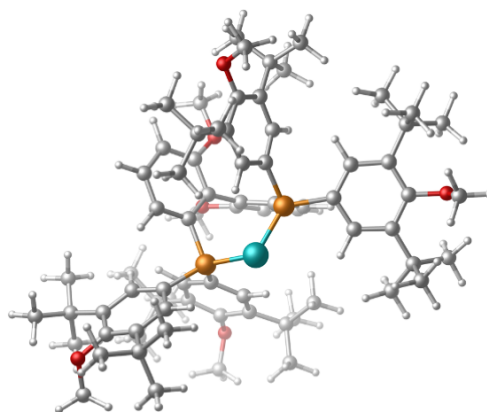
### Transition States



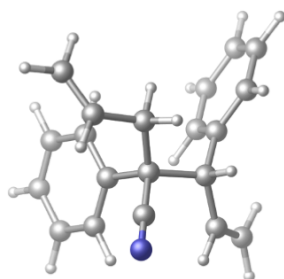
## CYLview Structures



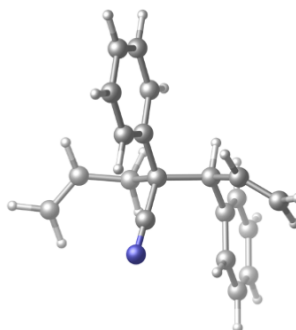
**6**



**Pd-L1g**

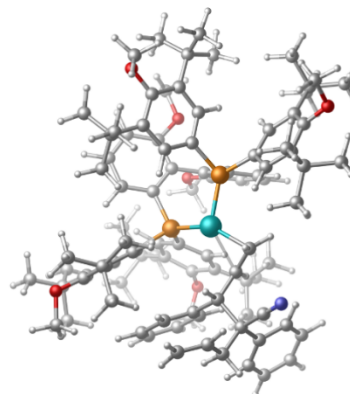
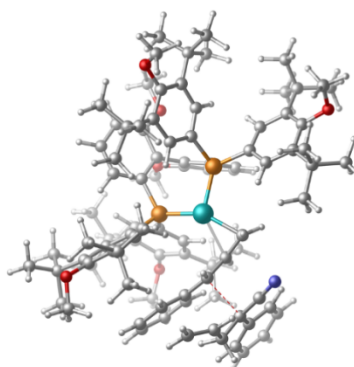
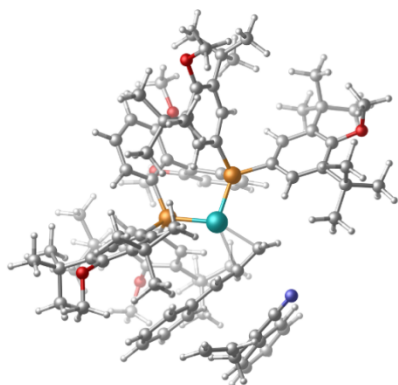
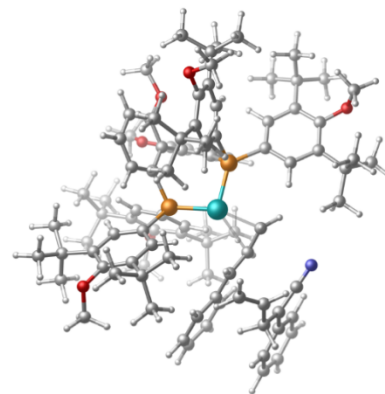
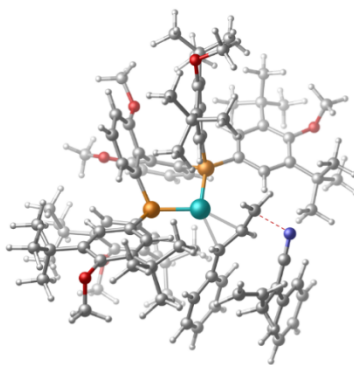
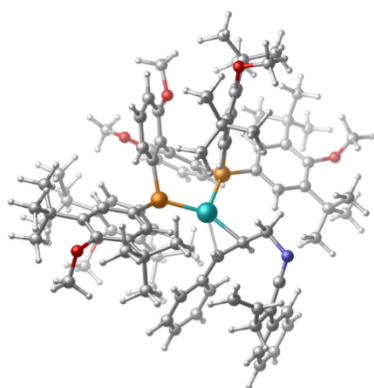


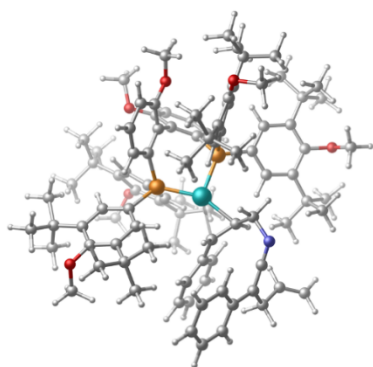
**2a**



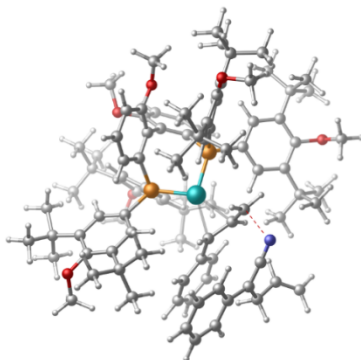
**2a'**



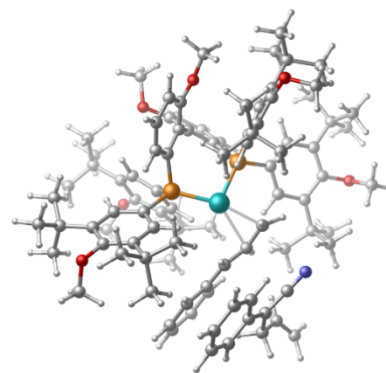




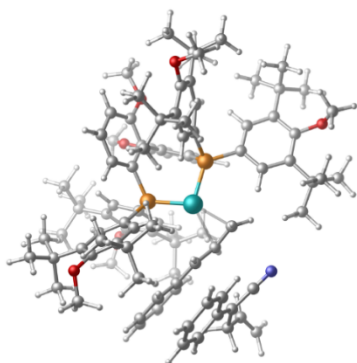
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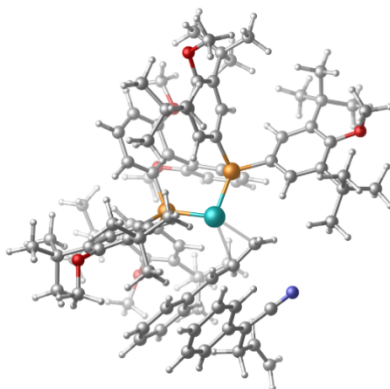
TS-14



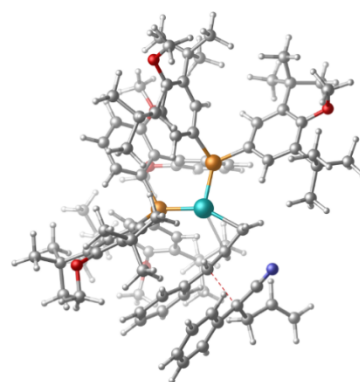
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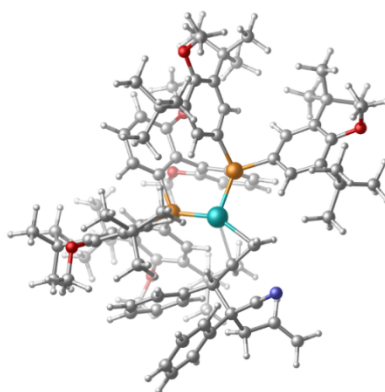
TS-16



17



TS-18



19

## 8. Cartesian Coordinates of Minimum Energy Structures

Pd-L1g				H	-2.78272200	0.61393800	4.87110200
				H	-1.23470400	1.23832300	5.59314400
Pd	0.09654800	0.20627200	-1.69014300	O	-7.00600600	-2.15935300	-2.75376600
P	-1.73781300	-0.17348400	-0.56038700	O	-4.09517000	4.65344000	2.14234000
P	1.91417900	0.18682900	-0.46855900	O	6.78399400	3.32378900	-2.16571800
C	-0.21997500	-1.01454800	1.69276700	O	4.00438900	-5.25900100	0.98287000
C	-1.18624700	-1.36709300	0.74608100	C	-7.84086400	-1.03431000	-3.12332000
C	-1.66401200	-2.68694600	0.66619300	H	-8.73092800	-1.52346900	-3.53152100
C	-1.19476000	-3.66703600	1.53746100	H	-8.08482000	-0.44113400	-2.22854100
C	-0.23686900	-3.35471200	2.50657400	H	-7.33429800	-0.42273700	-3.88596600
C	0.23279700	-2.04088700	2.57822400	C	5.13062600	-5.67710100	0.17525400
C	0.34558900	0.34163600	1.90149800	H	5.99109500	-5.01976600	0.37286900
C	1.38071000	0.91923900	1.15709700	H	5.31631000	-6.69373100	0.53648700
C	1.94498500	2.14354400	1.55281700	H	4.86163700	-5.67435600	-0.89229900
C	1.46723800	2.82010600	2.67343300	C	7.26121000	2.84555300	-3.44789100
C	0.39583400	2.30653000	3.40919100	H	8.10692600	3.51037800	-3.64955000
C	-0.15530800	1.08502500	3.01278300	H	7.58688200	1.79760400	-3.36051600
C	-2.40568500	1.24591800	0.42400500	H	6.47192400	2.96038400	-4.20687100
C	-1.88771400	2.50045200	0.11554700	C	-5.14133100	5.22763200	1.32124300
C	-2.39199500	3.66299300	0.72650700	H	-5.95667000	4.49936500	1.19123100
C	-3.49997300	3.50622600	1.58702100	H	-5.46523400	6.08751900	1.91582800
C	-3.99393500	2.24131700	1.98316200	H	-4.72860000	5.54445400	0.35066400
C	-3.39919500	1.11692800	1.39172000	C	-4.70606000	-1.86454200	-4.58114900
C	-3.36364200	-0.93170300	-1.12341200	C	-5.21110200	-0.59086200	-5.28899300
C	-4.42601000	-1.25618200	-0.28531800	H	-5.26116900	-0.73147500	-6.37248400
C	-5.65800400	-1.68784100	-0.79774000	H	-6.21858500	-0.31577800	-4.94279500
C	-5.76663400	-1.78553300	-2.20442600	H	-4.55196000	0.26055800	-5.09181600
C	-4.66903600	-1.59777500	-3.07101100	C	-5.60307400	-3.06698200	-4.92332400
C	-3.47500600	-1.12392200	-2.49626700	H	-6.65717300	-2.87565400	-4.68470600
C	2.54260300	-1.46180000	0.06599900	H	-5.54614800	-3.32248900	-5.98437100
C	2.09936600	-2.55926800	-0.66448000	H	-5.31240400	-3.95095100	-4.34545900
C	2.53241000	-3.86099700	-0.35075500	C	-3.29238000	-2.19739400	-5.11515200
C	3.50042700	-3.98430900	0.66882200	H	-2.58706200	-1.37187500	-4.96328000
C	3.91965600	-2.89458600	1.46998600	H	-2.87953700	-3.08047800	-4.61581300
C	3.39379200	-1.63329700	1.15589500	H	-3.31771400	-2.40756100	-6.18859100
C	3.49589000	1.12984400	-0.80691900	C	-6.80190200	-1.99634800	0.17650700
C	4.78123700	0.74183500	-0.45169400	C	-7.62582900	-3.20796400	-0.29254100
C	5.90631300	1.48735900	-0.84954700	H	-8.39589500	-3.47893100	0.43378800
C	5.67742900	2.60605300	-1.67746000	H	-8.12774900	-3.01538300	-1.25065900
C	4.38054100	3.07703600	-1.98580400	H	-6.98474200	-4.08183600	-0.44961800
C	3.30050700	2.28826300	-1.56277700	C	-7.69080700	-0.74092700	0.29004000
H	-2.40633400	-2.97957300	-0.07904100	H	-8.53629000	-0.91252100	0.96183800
H	-1.57104700	-4.68672600	1.46645100	H	-7.12158300	0.11955500	0.67982900
H	0.13471200	-4.12833400	3.16835800	H	-8.09822600	-0.44981600	-0.68913400
H	2.77580600	2.59261800	1.00511600	C	-6.26700000	-2.33796500	1.58772900
H	1.92491100	3.76009700	2.97895700	H	-5.54594800	-3.16120600	1.55209800
H	0.01414400	2.85262100	4.26369700	H	-5.77655900	-1.47532500	2.06751400
H	-1.06565900	2.58982000	-0.61598100	H	-7.08222300	-2.64710100	2.24946400
H	-3.73662600	0.11700900	1.69302400	C	1.91822900	-5.03751400	-1.12129300
H	-4.30634900	-1.15930000	0.80162000	C	1.73608600	-6.26986700	-0.21770100
H	-2.62466000	-0.90186100	-3.15617700	H	1.16335700	-6.01057100	0.68009700
H	1.38459900	-2.41430200	-1.49252800	H	1.20757200	-7.07354700	-0.73639700
H	3.65460000	-0.77067500	1.77809000	H	2.69349200	-6.67354600	0.13190900
H	4.94863900	-0.16483100	0.13554800	C	0.51442100	-4.66972100	-1.65752100
H	2.28317600	2.59046400	-1.85061000	H	-0.15634800	-4.37958400	-0.83873600
O	1.17210400	-1.61462700	3.49760900	H	0.54476900	-3.82863900	-2.36083300
O	-1.22358500	0.48246300	3.64663400	H	0.05614400	-5.51435600	-2.17876900
C	1.54074000	-2.53618100	4.55169200	C	2.82396700	-5.36850700	-2.32507500
H	2.17296500	-3.33984400	4.13627200	H	2.92466600	-4.50674800	-2.99256600
H	2.12036500	-1.88912400	5.22221900	H	3.83488800	-5.65550000	-2.00096800
H	0.65644200	-2.92816300	5.05968900	H	2.41755500	-6.19846500	-2.91028000
C	-1.87393000	1.22009600	4.70806200	C	4.91050000	-3.02251500	2.63409000
H	-2.15112600	2.22681200	4.37246800	C	4.56619800	-4.24616100	3.50178800
				H	4.64187500	-5.18196100	2.92898500

H	5.23001800	-4.33241900	4.36459500
H	3.52980400	-4.18198200	3.86647700
C	6.33640000	-3.13280600	2.05648100
H	7.08356900	-3.19877700	2.85219000
H	6.45051900	-4.02416200	1.42404000
H	6.57922000	-2.25429500	1.43846400
C	4.88312800	-1.78242900	3.55919800
H	5.27112900	-0.88783600	3.06051300
H	3.86605500	-1.55132600	3.89681400
H	5.49847800	-1.94431400	4.44908000
C	-5.15259800	2.03935900	2.96826500
C	-5.14175400	0.62503000	3.59632500
H	-5.32443200	-0.16628100	2.85079400
H	-4.18021400	0.40686500	4.08435900
H	-5.92506400	0.52952600	4.35444600
C	-5.08207200	3.04543400	4.13130300
H	-5.21491000	4.07902000	3.78198600
H	-5.85254300	2.85166600	4.88153800
H	-4.10665400	3.01174000	4.62592600
C	-6.47788100	2.19749900	2.19351500
H	-7.33989400	2.13290000	2.86312300
H	-6.52908400	3.16762800	1.67828600
H	-6.58911500	1.41095700	1.42825500
C	-1.71741000	5.00506100	0.41409100
C	-2.46040600	5.66756700	-0.76426200
H	-3.51584800	5.85456400	-0.51756000
H	-2.00829000	6.62767600	-1.02876500
H	-2.43816500	5.03053500	-1.65414000
C	-0.24096500	4.79369900	0.00382600
H	0.31790400	4.27956500	0.79652000
H	-0.14552200	4.18516800	-0.90371900
H	0.25614900	5.74830200	-0.18821900
C	-1.70913100	5.93246100	1.64212000
H	-1.15245900	6.85236600	1.44685200
H	-2.72281700	6.21661000	1.95118200
H	-1.24964100	5.43446700	2.50291800
C	7.29457300	1.04096900	-0.37253400
C	7.20297100	0.25595500	0.95793100
H	6.68254800	0.83991900	1.72438700
H	6.67538100	-0.70486600	0.84870800
H	8.20135900	0.02680700	1.34406400
C	7.90330900	0.11873600	-1.44809800
H	8.89875000	-0.22850300	-1.15769200
H	7.27546500	-0.76157100	-1.61795800
H	8.00203800	0.64342600	-2.41045900
C	8.21540400	2.24533500	-0.10653900
H	9.16961800	1.93592200	0.32683400
H	8.43620600	2.80555900	-1.02453500
H	7.74400400	2.95553900	0.58125400
C	4.09966600	4.37290800	-2.75730100
C	2.69296600	4.92286800	-2.42062800
H	1.89804800	4.22227300	-2.70216700
H	2.59316300	5.12574200	-1.34891600
H	2.50111700	5.85964900	-2.95244800
C	4.15566200	4.06224800	-4.26671100
H	3.96909100	4.95866300	-4.86471400
H	5.14160500	3.66902900	-4.55612900
H	3.40841500	3.31190500	-4.54490000
C	5.10788100	5.47644000	-2.39228700
H	6.12931000	5.21631600	-2.70102900
H	4.85253800	6.42780400	-2.86535300
H	5.14370300	5.63435700	-1.30924300

**2a**

C	1.29197600	1.81846900	-2.14650800
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C	1.98204900	2.81421600	-1.45931000
C	2.32020300	2.61608200	-0.12241600
C	1.96525900	1.43309000	0.51981500
C	1.26078200	0.43129700	-0.15693800
C	0.93476000	0.63754900	-1.50102100
C	0.78953000	-0.81303400	0.59111500
C	1.80587100	-1.20698000	1.57668500
C	-0.55549300	-0.53664100	1.40294900
C	-0.34959300	0.45725100	2.51457300
C	-1.19454000	1.41143000	2.90552800
C	0.56780700	-2.04237600	-0.32902400
C	1.78723400	-2.49287800	-1.06566100
C	1.83959500	-2.70694500	-2.38014000
N	2.59132100	-1.55468500	2.36623200
H	1.02701800	1.95800800	-3.19333800
H	2.26222400	3.73657600	-1.96526200
H	2.86758100	3.38176100	0.42448800
H	2.24592100	1.28367800	1.56218800
H	0.38394800	-0.11932600	-2.05498100
H	-0.76193900	-1.50695000	1.88842700
H	0.57107900	0.31393900	3.08649500
H	-0.96454900	2.03910800	3.76362900
H	-2.14070000	1.60133600	2.40118800
H	0.20220200	-2.85797600	0.31527700
H	-0.24849000	-1.82326200	-1.02883300
H	2.67911500	-2.66798100	-0.45759900
H	2.74627500	-3.05669900	-2.86848000
H	0.97287800	-2.54213700	-3.02208600
C	-1.71702100	-0.24202000	0.48585600
C	-2.65826300	-1.24176900	0.21819000
C	-1.87830300	1.00520700	-0.13238000
C	-3.72590100	-1.01457000	-0.64731800
H	-2.54836800	-2.21585500	0.69813600
C	-2.94259700	1.23571400	-1.00034200
H	-1.16470700	1.80257600	0.07219900
C	-3.86859800	0.22715300	-1.26275700
H	-4.44703100	-1.80763700	-0.83841100
H	-3.04877100	2.21129500	-1.47254000
H	-4.70148700	0.41086100	-1.93950100

**2a'**

C	0.43926400	0.25095100	0.17515100
C	-0.51545100	-0.92753800	-0.28005400
C	-0.22580300	-2.17863100	0.50564800
C	-1.11992400	-3.05296200	0.96645700
C	0.07550300	1.55451300	-0.59625700
C	1.01392200	2.68643000	-0.33267000
C	0.67868400	3.79226600	0.33209000
H	-0.19857800	-1.11633900	-1.31994600
H	0.83689900	-2.37552400	0.67122800
H	-0.80302700	-3.94442400	1.50295400
H	-2.19210800	-2.91844500	0.83051900
H	0.06506100	1.29826100	-1.66752400
H	-0.95042400	1.84180400	-0.33466600
H	2.03731400	2.56617100	-0.69731800
H	1.39486500	4.58995600	0.51672600
H	-0.32762500	3.93720800	0.72617600
C	-1.97103800	-0.52944200	-0.33392900
C	-2.59253000	-0.35456300	-1.57397600
C	-2.72027800	-0.29707100	0.82693100
C	-3.92303800	0.04934200	-1.66273500
H	-2.01986800	-0.53648400	-2.48545100
C	-4.04837900	0.11255000	0.74169600
H	-2.26005100	-0.43762200	1.80376100
C	-4.65446000	0.28834700	-0.50185300

H	-4.38668100	0.17806000	-2.63954600
H	-4.61367100	0.29331400	1.65458400
H	-5.69374200	0.60661200	-0.56464600
C	1.89574000	-0.13608000	-0.09282700
C	2.30596700	-0.35726000	-1.41317600
C	2.83859500	-0.26667900	0.92905300
C	3.62166700	-0.70282800	-1.70403700
H	1.59171000	-0.25398100	-2.23105200
C	4.15777600	-0.61382300	0.63916200
H	2.54145000	-0.09280300	1.96259400
C	4.55485100	-0.83366200	-0.67632400
H	3.91868800	-0.86890500	-2.73825800
H	4.87621900	-0.71049000	1.45135300
H	5.58469200	-1.10400200	-0.90238600
C	0.23312400	0.50982200	1.60434300
N	0.04767500	0.72650800	2.73496500

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N	0.79588300	-0.75610300	-2.33018000
C	1.82698100	0.61608600	-0.44494200
C	3.06863400	0.17765000	0.20495000
C	1.18831800	1.94195900	-0.07590700
C	-0.27330800	-1.77693100	-2.16593200
C	-1.50708500	-1.15907000	-1.60989600
C	-2.00370600	-1.44065300	-0.39483400
C	3.75882300	1.02655800	1.08575200
C	4.94181300	0.61667700	1.69723200
C	5.46758100	-0.64729600	1.44702600
C	4.79461100	-1.50087400	0.56999200
C	3.61585000	-1.09619400	-0.03936700
C	-0.23740200	2.07261000	-0.50648800
C	-0.69969700	2.99055700	-1.35518500
C	1.25145200	-0.13311700	-1.38003600
H	1.23470700	2.03860500	1.02081400
H	1.78417400	2.77605600	-0.48029800
H	-0.44420000	-2.20293400	-3.16077400
H	0.09179100	-2.58077600	-1.51187400
H	-1.96805600	-0.38970100	-2.23349300
H	-1.50434400	-2.21509800	0.19595000
H	3.37746200	2.02544400	1.28976800
H	5.45621900	1.29788500	2.37375500
H	6.39115300	-0.96612600	1.92656900
H	5.19242200	-2.49310800	0.36137400
H	3.10154900	-1.77503700	-0.72113100
H	-0.92878800	1.34194800	-0.07564900
H	-1.75380200	3.04497700	-1.62139700
H	-0.04217200	3.72893200	-1.81497500
C	-3.15681400	-0.81554000	0.24817100
C	-3.61219900	-1.31839500	1.47717500
C	-3.82979400	0.28995700	-0.30133800
C	-4.70175900	-0.74976800	2.12998000
H	-3.09732000	-2.17128700	1.92078300
C	-4.91629000	0.85918400	0.34941000
H	-3.49245300	0.71273400	-1.24720400
C	-5.35967000	0.34190300	1.56823500
H	-5.03626300	-1.15969700	3.08154700
H	-5.42050100	1.71685800	-0.09320900
H	-6.21079100	0.79122100	2.07672500

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Pd	-0.04930400	0.90533500	-0.33444800
P	1.82413900	-0.19772200	0.23539600
P	-1.45793700	-0.86195200	-0.18122600
C	0.76455400	-2.57478700	1.40341600

C	1.48491700	-1.39611900	1.60479400
C	1.83795500	-0.98518000	2.90207300
C	1.49595300	-1.76052300	4.00768700
C	0.79066600	-2.95714700	3.84580000
C	0.43140600	-3.35117800	2.55448600
C	0.33315700	-3.08276100	0.07697200
C	-0.69779400	-2.49003500	-0.67098600
C	-1.08752400	-3.05481800	-1.89559500
C	-0.44905500	-4.19109100	-2.39088000
C	0.59806500	-4.78457800	-1.68107200
C	0.98036700	-4.21809300	-0.46183700
C	2.48220900	-1.20731700	-1.16297700
C	1.91203600	-0.98278000	-2.41179100
C	2.37104100	-1.66278600	-3.55560100
C	3.49790700	-2.49756900	-3.39511900
C	4.08552900	-2.76353200	-2.13266600
C	3.53088500	-2.11439000	-1.02137900
C	3.44858600	0.52223000	0.79128400
C	4.44150700	-0.27191900	1.36337600
C	5.70145900	0.25286600	1.68286000
C	5.93467200	1.60616300	1.34916000
C	4.91550400	2.46503900	0.88429900
C	3.67092200	1.88052800	0.58710100
C	-2.06252700	-1.17714200	1.52861700
C	-1.82308100	-0.18033300	2.46884300
C	-2.25629300	-0.32295600	3.80140700
C	-3.03311400	-1.46050400	4.10668100
C	-3.26910400	-2.50468600	3.17765100
C	-2.74040200	-2.34010800	1.89135400
C	-3.05561400	-0.94231500	-1.12591800
C	-4.00133400	-1.95138100	-0.95166100
C	-5.21658100	-1.94098500	-1.64987700
C	-5.44395800	-0.85293200	-2.52444700
C	-4.45580600	0.10978800	-2.81881100
C	-3.27279900	0.06716300	-2.05879200
H	2.38152300	-0.05388900	3.07725100
H	1.77158100	-1.43379100	5.01006700
H	0.51424100	-3.54171300	4.71640500
H	-1.89713600	-2.62695100	-2.49155700
H	-0.76118600	-4.61977300	-3.34276300
H	1.10422000	-5.65197200	-2.08958300
H	1.07953300	-0.26469000	-2.52151500
H	3.92813100	-2.32637100	-0.02300700
H	4.25268300	-1.33533400	1.56318500
H	2.87399000	2.51570600	0.17931100
H	-1.28584200	0.74110000	2.17708600
H	-2.86884700	-3.13838200	1.15007400
H	-3.80386000	-2.77280100	-0.25098000
H	-2.51917900	0.85592200	-2.20544300
O	-0.28412500	-4.49867800	2.27418900
O	2.02328300	-4.69419000	0.31043700
C	-0.48058300	-5.44133300	3.35623600
H	-1.20431000	-5.02660600	4.08071100
H	-0.90510100	-6.30442400	2.82895000
H	0.47011300	-5.70154100	3.82738600
C	2.57952100	-5.98241200	-0.04793900
H	3.13420500	-5.89554000	-0.99912800
H	3.26100900	-6.17557400	0.78926400
H	1.79738000	-6.74395700	-0.09728100
O	7.22217700	2.13251200	1.54758500
O	4.00284800	-3.19831100	-4.50263800
O	-6.68440500	-0.77192700	-3.17939400
O	-3.50981900	-1.63796000	5.41653700
C	8.08304000	1.98470700	0.38992400
H	9.02561500	2.41852300	0.73890000
H	8.19922400	0.91917800	0.13995800
H	7.66875000	2.55691000	-0.45500300

C	-4.76442300	-0.97631700	5.70674400	H	4.62774700	-4.30650800	0.09287300
H	-5.56930500	-1.43644700	5.11391100	H	6.26479100	-4.82321300	-0.32199700
H	-4.89408200	-1.17448100	6.77551400	C	4.98971100	-5.05859300	-2.62752500
H	-4.68941200	0.10382000	5.50537200	H	4.79630700	-4.91945200	-3.70218700
C	-7.65387600	0.04596400	-2.47672100	H	5.82947100	-5.75029300	-2.53162900
H	-8.52543500	3.00002000	-3.13741000	H	4.09579800	-5.53814900	-2.20027400
H	-7.87198700	-0.39880800	-1.49358200	C	6.55321400	-3.06228500	-2.49167300
H	-7.27803300	1.07643500	-2.37976600	H	7.43626000	-3.67114900	-2.27616400
C	4.91983200	-2.45548800	-5.34107100	H	6.50319200	-2.94212800	-3.58275800
H	5.85836700	-2.28445700	-4.79295000	H	6.71323300	-2.07041200	-2.05717500
H	5.07225300	-3.13665500	-6.18488700	C	1.60824500	-1.45212700	-4.87175200
H	4.47180900	-1.50525100	-5.66904600	C	2.29034700	-0.32023900	-5.66611700
C	5.10492700	3.97370800	0.67464000	H	3.33532800	-0.674697500	-5.90572400
C	5.69982800	4.19584700	-0.73009900	H	1.77340700	-0.13164500	-6.61191900
H	5.87267900	5.25953200	-0.92253700	H	2.29589400	0.61565200	-5.09787300
H	6.66207000	3.67666400	-0.84588100	C	0.14337600	-1.02947400	-4.60198500
H	5.02638100	3.82749500	-1.51116000	H	-0.39145500	-1.80257400	-4.03784600
C	6.02051500	4.57803000	1.75392300	H	0.07676100	-0.09967900	-4.02273800
H	7.04483300	4.18714800	1.68998400	H	-0.39882900	-0.86917200	-5.53831800
H	6.07929700	5.66625200	1.66629100	C	1.54331300	-2.74761400	-5.69924600
H	5.65720900	4.33933700	2.75879600	H	0.90343800	-2.63109600	-6.57795500
C	3.75526600	4.72169100	0.76161100	H	2.52954900	-3.07020500	-6.04995500
H	3.06796900	4.43359400	-0.04318300	H	1.14648500	-3.57304800	-5.09687400
H	3.25525100	4.53641200	1.71753400	C	-6.22080800	-3.07721600	-1.41622100
H	3.90353600	5.80364800	0.67288200	C	-5.51596700	-4.35761300	-0.90874800
C	6.73685000	-0.66900400	2.33979700	H	-4.72733600	-4.67658700	-1.59814100
C	7.65646200	0.09842300	3.30436200	H	-5.06266300	-4.22413900	0.08737000
H	8.30578400	-0.57767600	3.86656900	H	-6.22799800	-5.18475000	-0.82250300
H	8.30139200	0.81403700	2.77879900	C	-7.22733000	-2.61562400	-0.34309000
H	7.07249600	0.68324100	4.02368200	H	-7.97263200	-3.38911700	-0.13740200
C	7.55856500	-1.33758800	1.21938900	H	-6.72213100	-2.37550400	0.59852100
H	8.35883700	-1.95984300	1.62952600	H	-7.76716300	-1.71258000	-0.66576000
H	6.92411700	-1.98197100	0.58790600	C	-6.94859700	-3.45821100	-2.71722200
H	8.02343600	-0.58561000	0.56474400	H	-7.60591400	-4.31957700	-2.57449900
C	6.03947300	-1.77157200	3.17173400	H	-7.56564100	-2.63270600	-3.09817900
H	5.41235600	-1.33535700	3.95699800	H	-6.23535400	-3.70359100	-3.51090800
H	5.39963600	-2.41657300	2.55937000	C	-4.60006800	1.19011500	-3.89845200
H	6.77538400	-2.41762000	3.66039500	C	-3.21131100	1.61136500	-4.43405300
C	-1.84797200	0.75815900	4.81276400	H	-2.59083400	2.07979600	-3.65957000
C	-1.54372800	0.15057800	6.19393900	H	-2.66066500	0.75176000	-4.82965200
H	-0.79621600	-0.64595800	6.11222400	H	-3.30932300	2.34027800	-5.24519600
H	-1.16253400	0.90503900	6.88688600	C	-5.28374800	2.41577500	-3.26358200
H	-2.42995800	-0.30195700	6.65316200	H	-5.40318500	3.22789400	-3.98604000
C	-0.55880700	1.48076800	4.35321800	H	-6.28289600	2.16255800	-2.87971000
H	0.26888400	0.77428000	4.22793400	H	-4.69454600	2.80117100	-2.41298900
H	-0.69865200	1.99812900	3.39314500	C	-5.40578500	0.68366100	-5.10744800
H	-0.24815900	2.23420600	5.08211200	H	-6.44901500	0.46492900	-4.84559200
C	-2.97678300	1.80251500	4.90287300	H	-5.41841100	1.41818800	-5.91703000
H	-3.18862300	2.23923900	3.91727800	H	-4.98411900	-0.24725900	-5.50074500
H	-3.91301600	1.36100600	5.27174600	N	1.17858400	4.79877100	-2.23106200
H	-2.71019000	2.62136100	5.57668800	C	-0.73319000	6.26310000	-1.38375200
C	-4.06612700	-3.77519200	3.50225100	C	-0.68115000	6.81250800	-0.02426700
C	-3.60365200	-4.36800800	4.84544500	C	-1.96884600	6.45199100	-2.23632500
H	-3.74483700	-3.65320100	5.67014100	C	1.18996400	3.33408300	-1.92472600
H	-4.15381700	-5.27660500	5.09911700	C	0.35070100	3.01144800	-0.72952500
H	-2.53017800	-4.60930600	4.81551500	C	-1.04344200	2.85779400	-0.86676000
C	-5.56891200	-3.42977000	3.54100700	C	-1.81355900	7.41559900	0.54640900
H	-6.17707400	-4.32203200	3.71556300	C	-1.78876100	7.88983500	1.85569100
H	-5.79992200	-2.71558900	4.34423500	C	-0.63638400	7.77770300	2.62862200
H	-5.89559800	-2.97931200	2.59771200	C	0.49930200	7.18446100	2.07210100
C	-3.87953300	-4.87070000	2.42486700	C	0.47791200	6.71117100	0.76762500
H	-4.37190700	-4.60179200	1.47591800	C	-1.81329100	5.96091600	-3.63850400
H	-2.82005600	-5.05167300	2.20856800	C	-2.59017300	5.04327900	-4.21453600
H	-4.31768500	-5.81841100	2.75063000	C	0.25430200	5.49801000	-1.83502200
C	5.27313600	-3.71507200	-1.93128000	H	-2.21574100	7.52760600	-2.25323000
C	5.54100400	-4.01092400	-0.43590000	H	-2.82618100	5.95143400	-1.75638900
H	5.96215200	-3.13325300	0.08382600	H	2.24515000	3.06085700	-1.80130700

H	0.83014500	2.82740300	-2.83049400	H	2.07365300	-0.31059300	5.08070400
H	0.71878700	3.47109300	0.19325800	H	1.32854400	-2.66876500	5.04189800
H	-1.43052800	2.75493700	-1.88599800	H	-1.02036500	-3.13665600	-2.22686800
H	-2.73523900	7.49518600	-0.02761800	H	0.54143100	-4.91459000	-2.84211200
H	-2.68557000	8.34494500	2.27497000	H	2.54878400	-5.37770600	-1.47090600
H	-0.61882400	8.14987600	3.65177000	H	1.35220900	-0.19782200	-2.55264400
H	1.41226600	7.09476900	2.66031400	H	4.48096600	-1.33950300	0.19747400
H	1.37452600	6.25671300	0.34320400	H	4.55346100	-0.16512600	1.62522600
H	-0.99030600	6.39993300	-4.20955400	H	2.50162900	3.23010200	-0.12366400
H	-2.43999300	4.72976600	-5.24571300	H	-1.32669900	0.65704300	2.15894000
H	-3.41716500	4.57774400	-3.67527300	H	-2.00517700	-3.53088500	1.35663400
C	-2.03670800	3.28950500	0.12163200	H	-3.06435000	-3.30428200	-0.03074600
C	-3.40024700	3.30356000	-0.22046400	H	-2.12607100	0.16503300	-2.44016300
C	-1.68469400	3.75819300	1.40051000	O	0.83536800	-4.05823300	2.72406900
C	-4.36652300	3.76663400	0.66711300	O	3.17709800	-3.98122600	0.80427300
H	-3.70513300	2.94011800	-1.21096800	C	0.74590900	-4.87773900	3.91613800
C	-2.64776000	4.22786200	2.28479200	H	-0.11497400	-4.55007400	4.52648800
H	-0.63698400	3.78837300	1.69766700	H	0.56459200	-5.87250800	3.48918000
C	-3.99640200	4.23494100	1.92750200	H	1.68219600	-4.86081400	4.47863500
H	-5.41518800	3.76539200	0.37084800	C	3.97772000	-5.17708900	0.62806900
H	-2.33765900	4.61098900	3.25700300	H	4.53446100	-5.11264500	-0.32360200
H	-4.74874000	4.60877500	2.62027100	H	4.65770200	-5.12219300	1.48729400
				H	3.35521700	-6.07373800	0.68138900
				O	6.80114100	3.78738200	1.32918200
				O	4.87938800	-2.65429900	-4.14990300
				O	-5.73920600	-2.37574800	-3.60927900
				O	-3.15819700	-1.92734500	5.47283000
				C	7.68056100	3.76209900	0.17552800
				H	8.50113500	4.41486700	0.49252800
				H	8.03021500	2.73464600	-0.00346200
				H	7.15913600	4.17719000	-0.70212300
				C	-4.54033100	-1.53806600	5.66956400
				H	-5.19613900	-2.19809600	5.08193100
				H	-4.67672300	-1.69475800	6.74491500
				H	-4.68918200	-0.48122200	5.39705100
				C	-6.96253100	-1.73597600	-3.16258900
				H	-7.69221400	-2.08546200	-3.90062200
				H	-7.21996000	-2.07628800	-2.14814200
				H	-6.84516200	-0.64142600	-3.20479900
				C	5.64010200	-1.83197600	-5.06931200
				H	6.50914000	-1.40889600	-4.54364000
				H	5.95121800	-2.55759300	-5.82909500
				H	5.01168000	-1.04030200	-5.50487400
				C	4.37605300	5.11814000	0.27544500
				C	4.91537200	5.32670300	-1.15348000
				H	4.86369400	6.38472500	-1.43644300
				H	5.96177100	5.00688000	-1.24664400
				H	4.32176500	4.77249400	-1.88810500
				C	5.16393700	5.97411400	1.28335700
				H	6.24508200	5.80526300	1.22309700
				H	4.98991800	7.04174700	1.11319900
				H	4.86258900	5.75090000	2.31198700
				C	2.91257700	5.59130300	0.33201700
				H	2.26967900	5.15622400	-0.44949100
				H	2.44594100	5.39111600	1.30001400
				H	2.83234800	6.67406400	0.16327100
				C	6.83813000	1.04442700	2.36552000
				C	7.52854600	2.05901400	3.29134600
				H	8.28529100	1.58317400	3.92072600
				H	8.02724500	2.85923100	2.72729100
				H	6.80486600	2.55338000	3.94881500
				C	7.83072200	0.49549500	1.32176400
				H	8.73216800	0.10059800	1.79967000
				H	7.38167200	-0.31859100	0.72989900
				H	8.14685300	1.28281500	0.62101900
				C	6.35836400	-0.12302700	3.26032600
				H	5.62737400	0.22188000	3.99986400

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Pd	-0.05987900	0.92299100	-0.29402300
P	2.03275200	0.32447600	0.20054600
P	-1.04300900	-1.09736800	-0.08012200
C	1.45572300	-2.06601700	1.63727300
C	1.87964300	-0.73801300	1.69685700
C	2.09012900	-0.10571800	2.93253800
C	1.90350300	-0.80692800	4.12410700
C	1.48961800	-2.14100800	4.10632800
C	1.26579700	-2.75857000	2.87186500
C	1.18738800	-2.79327800	0.37813100
C	0.07468800	-2.54102300	-0.43176700
C	-0.15334700	-3.30605000	-1.58221700
C	0.72998100	-4.32648800	-1.94322100
C	1.85782600	-4.59720900	-1.16798900
C	2.07898100	-3.83022800	-0.01817400
C	2.87146700	-0.67167100	-1.07810600
C	2.30555300	-0.71133700	-2.34952100
C	2.93094200	-1.40545100	-3.40119100
C	4.20284800	-1.96112800	-3.13788600
C	4.78967000	-1.96046600	-1.84676200
C	4.07864100	-1.32278100	-0.82273400
C	3.42425900	1.42664000	0.67108100
C	4.53665000	0.89259600	1.32812000
C	5.66002900	1.67703800	1.61213700
C	5.64170200	3.01829200	1.15892800
C	4.48997700	3.62064900	0.61029400
C	3.39370000	2.77996400	0.34835600
C	-1.64854600	-1.42081500	1.61609500
C	-1.67162100	-0.33706200	2.49091500
C	-2.13175000	-0.48000200	3.81268400
C	-2.66454400	-1.73680900	4.17476300
C	-2.62132100	-2.86580200	3.31844200
C	-2.08008000	-2.67669100	2.04070800
C	-2.48888200	-1.52936100	-1.13289800
C	-3.27703200	-2.65232000	-0.88744400
C	-4.35585200	-2.98498400	-1.71847700
C	-4.63082100	-2.10932200	-2.79335100
C	-3.78503000	-1.02869700	-3.13551900
C	-2.73992300	-0.72604400	-2.24638700
H	2.40196400	0.94082000	2.99800800

H	5.89543800	-0.93161500	2.68548400	C	-3.94715000	-0.21066900	-4.42665300
H	7.19738000	-0.55994500	3.81212300	C	-2.62884400	0.50324500	-4.80062200
C	-2.02010800	0.72935500	4.75492600	H	-2.31394000	1.22628000	-4.03728900
C	-1.66045100	0.29275600	6.18572200	H	-1.81512200	-0.20893100	-4.96011400
H	-0.74882200	-0.31309700	6.19537700	H	-2.74784800	1.07594400	-5.72868400
H	-1.49963700	1.15751100	6.83655400	C	-5.03468600	0.85575000	-4.22069000
H	-2.44669600	-0.31785300	6.64515400	H	-5.19111700	1.44761900	-5.12875600
C	-0.89865800	1.68943200	4.29003000	H	-6.00161000	0.41013300	-3.94925800
H	0.07173500	1.18533800	4.25377200	H	-4.76069100	1.55999100	-3.41490300
H	-1.09712000	2.11045400	3.29620900	C	-4.31062200	-1.13276600	-5.60555500
H	-0.80463700	2.53950500	4.97516000	H	-5.29743900	-1.59768400	-5.46948600
C	-3.35083200	1.50153900	4.72778500	H	-4.34077600	-0.57960900	-6.54880300
H	-3.61097800	1.81538600	3.70877700	H	-3.58846800	-1.94677900	-5.71492900
H	-4.18681900	0.89654300	5.10630100	N	-0.16204100	5.94694900	-1.30605700
H	-3.30052700	2.40709200	5.34217900	C	-2.72325200	5.68286000	-1.34559400
C	-3.14434500	-4.25463600	3.71217500	C	-3.48318400	5.96218200	-0.16091100
C	-2.64963400	-4.63352200	5.11906200	C	-3.41361900	5.44205900	-2.66318900
H	-3.02580100	-3.93409300	5.88105900	C	0.16549100	3.09795800	-0.63627900
H	-2.97551400	-5.63589100	5.40727800	C	-1.12464200	3.05961300	-0.07797600
H	-1.55149600	-4.59803800	5.17216600	C	-2.30282200	2.86541700	-0.79747700
C	-4.68458200	-4.24244300	3.65465800	C	-4.89888900	5.97138400	-0.17989100
H	-5.09863900	-5.22920100	3.88412600	C	-5.63151900	6.22717100	0.97147000
H	-5.11349300	-3.53530400	4.37979900	C	-4.99194500	6.48458400	2.18438800
H	-5.04512000	-3.95089400	2.66276400	C	-3.59424100	6.46962600	2.22760800
C	-2.65776000	-5.35361500	2.73753800	C	-2.85290400	6.21192100	1.08508500
H	-3.12065100	-5.25347200	1.74323500	C	-2.49933800	5.06698600	-3.78473400
H	-1.57051800	-5.33118600	2.60625300	C	-2.68454100	4.02876200	-4.60212900
H	-2.92369800	-6.34862600	3.10843400	C	-1.33887100	5.83265500	-1.32741100
C	6.14245200	-2.61627600	-1.53069000	H	-3.97787900	6.35126000	-2.94821300
C	6.42291800	-2.67653400	-0.01067600	H	-4.18357300	4.65986900	-2.53699200
H	6.65653500	-1.67906600	0.40061700	H	0.96652600	3.57644400	-0.07593200
H	5.57411700	-3.08253700	0.55041500	H	0.26149500	3.17871800	-1.71945400
H	7.28904300	-3.31171600	0.20074800	H	-1.20761700	3.24400900	0.99539800
C	6.15955000	-4.05897200	-2.06649800	H	-2.22067900	5.75782300	-1.88030400
H	5.96562200	-4.08837900	-3.14976300	H	-5.42803800	2.76738300	-1.10900900
H	7.12567200	-4.54123500	-1.89692400	H	-6.72025400	6.22180300	0.92122700
H	5.38167100	-4.66787600	-1.58206300	H	-5.57104200	6.69037900	3.08265900
C	7.27329500	-1.77966700	-2.16084000	H	-3.07715300	6.66662800	3.16642000
H	8.25771600	-2.15823400	-1.86741800	H	-1.76316800	6.20844700	1.13067100
H	7.23631600	-1.80460000	-3.25889600	H	-1.62465400	5.70663600	-3.92792200
H	7.21232100	-0.73110800	-1.85199300	H	-1.99814200	3.80875400	-5.41675300
C	2.18563800	-1.51331100	-4.74068900	H	-3.54312800	3.36312100	-4.49252900
C	2.63382000	-0.35576500	-5.65259300	C	-3.62332300	2.77863000	-0.23743000
H	3.71362200	-0.39007800	-5.85811700	C	-4.72360400	2.52033600	-1.08106600
H	2.11858000	-0.38855500	-6.61849800	C	-3.89102900	2.95626400	1.13908300
H	2.41869500	0.61819500	-5.19952900	C	-6.01836400	2.43301500	-0.58326700
C	0.65716600	-1.39313100	-4.53090900	H	-4.53725000	2.35921400	-2.14907400
H	0.28246400	-2.18262800	-3.87049100	C	-5.18428600	2.87395400	1.63187200
H	0.37050000	-0.42779200	-4.09617900	H	-3.07741500	3.18605300	1.82363700
H	0.12533400	-1.48560800	-5.48449900	C	-6.25697300	2.60371600	0.77934500
C	2.42777700	-2.87592600	-5.41185500	H	-6.84394700	2.22540500	-1.26148700
H	1.80150300	-3.00108200	-6.30030500	H	-5.36381400	3.03694800	2.69333800
H	3.46806100	-3.01123800	-5.72698600	H	-7.26894300	2.54131200	1.17335100
H	2.20449000	-3.69774900	-4.72244000				
C	-5.16053100	-4.25569400	-1.40970900				
C	-4.29980200	-5.29091700	-0.64533800	<b>10</b>			
H	-3.40074700	-5.55354000	-1.21231300	Pd	-0.06184000	0.96117600	0.20228100
H	-3.98443500	-4.93523800	0.34754700	P	-2.13245800	0.32313100	-0.28163700
H	-4.86355900	-6.21605200	-0.48273900	P	1.01932200	-0.98798600	-0.11923100
C	-6.35893100	-3.86080100	-0.52568700	C	-1.26959200	-1.57909100	-2.18309600
H	-6.97147000	-4.73082600	-0.27119300	C	-1.86027600	-0.33088800	-1.97665100
H	-6.03140100	-3.39477900	0.40923300	C	-2.07092900	0.55089800	-3.04782400
H	-7.01187300	-3.13742400	-1.03879900	C	-1.70648600	0.18427700	-4.34445100
C	-5.63714700	-4.94954200	-2.69709900	C	-1.08284800	-1.04150800	-4.58777500
H	-6.12512400	-5.90440900	-2.48331000	C	-0.85141000	-1.90174900	-3.50903500
H	-6.35492700	-4.33523000	-3.25681700	C	-1.04281900	-2.59611800	-1.13139100
H	-4.80083300	-5.14160900	-3.37737100				



C	0.00537800	-2.53555200	-0.20777000	H	6.46602400	-1.30327400	3.78620600
C	0.24186100	-3.59137400	0.67883400	H	5.49162400	-0.22718300	4.88289500
C	-0.59207700	-4.71285900	0.67639000	C	-6.05819000	-3.15530900	3.90999700
C	-1.67313400	-4.79391300	-0.20259500	H	-6.86935800	-2.57585800	3.44478500
C	-1.88962900	-3.74077600	-1.09935300	H	-6.44729600	-4.04606200	4.41580700
C	-2.99161100	-1.00313600	0.64124700	H	-5.46269400	-2.53364700	4.59569100
C	-2.51784100	-1.41425100	1.88417600	C	-4.58518400	4.78390900	1.18014400
C	-3.21651400	-2.37187700	2.64355900	C	-5.23793000	4.47859600	2.54352200
C	-4.46305000	-2.80752500	2.14056200	H	-5.22482100	5.36543900	3.18732800
C	-4.94357500	-2.44552500	0.85730200	H	-6.28557100	4.16687800	2.43103100
C	-4.16435800	-1.54930100	0.11645300	H	-4.70324700	3.68491500	3.07382200
C	-3.53634400	1.48315000	-0.45528600	C	-5.30429700	5.95165900	0.48353300
C	-4.59751400	1.21405000	-1.32048400	H	-6.38236300	5.77864100	0.38178900
C	-5.72133300	2.04834600	-1.36996400	H	-5.17242900	6.88577700	1.03921000
C	-5.75315600	3.14111600	-0.47162900	H	-4.91095500	6.11225200	-0.52616000
C	-4.64725500	3.50600000	0.32688500	C	-3.12731000	5.22434200	1.41212800
C	-3.54949900	2.62816300	0.33840500	H	-2.53487200	4.50148800	1.98551200
C	1.98462000	-1.09220700	-1.66558600	H	-2.59431000	5.41042900	0.47267400
C	2.07252100	0.06993700	-2.43166100	H	-3.07441300	6.16109600	1.98266800
C	2.84633600	0.10586900	-3.60369700	C	-6.84412300	1.71212700	-2.36104500
C	3.59842200	-1.05020000	-3.90752000	C	-7.54007200	2.97720500	-2.88732100
C	3.43693400	-2.27375800	-3.21746900	H	-8.24404200	2.74690500	-3.69172100
C	2.60632700	-2.26611500	-2.08710200	H	-8.10051200	3.50024100	-2.10153900
C	2.21159700	-1.36384400	1.22069900	H	-6.81131800	3.69893300	-3.27386600
C	3.32519500	-2.18441600	1.07778200	C	-7.85054700	0.79383900	-1.63922400
C	4.16391500	-2.47076100	2.16755000	H	-8.71262000	0.57198200	-2.27546200
C	3.86758300	-1.83583800	3.39572400	H	-7.38815500	-0.16579600	-1.35692200
C	2.72739100	-1.01512100	3.58084200	H	-8.23066900	1.26558600	-0.72078100
C	1.92765200	-0.77176300	2.45445400	C	-6.28256200	0.96584500	-3.59452600
H	-2.50816600	1.54207000	-2.89988100	H	-5.53703000	1.57473000	-4.11775500
H	-1.89563300	0.86564500	-5.17526100	H	-5.81167800	0.01283300	-3.33237200
H	-0.78252500	-1.30865500	-5.59672300	H	-7.08032900	0.74330200	-4.31124000
H	1.07408200	-3.57134600	1.38725000	C	2.83589100	1.38326800	-4.45764100
H	-0.40251300	-5.53187500	1.37101100	C	2.98886100	1.05750500	-5.95422600
H	-2.32861200	-5.65877000	-0.17630500	H	2.23460000	0.33847300	-6.28527400
H	-1.58875100	-0.99741200	2.29060300	H	2.88870500	1.95869600	-6.56703800
H	-4.48818700	-1.27535200	-0.89441200	H	3.96915700	0.61907500	-6.18133000
H	-4.57604100	0.33003700	-1.97155700	C	1.49132500	2.12952100	-4.29457000
H	-2.70225900	2.86714500	0.99736200	H	0.64192900	1.49263200	-4.55779400
H	1.53728400	0.98440100	-2.12743700	H	1.34037100	2.49426900	-3.27052500
H	2.46069300	-3.19995000	-1.53154600	H	1.45986000	3.01570100	-4.93915700
H	3.57502500	-2.61489600	0.10289400	C	3.97119800	2.30347200	-3.98221800
H	1.07636400	-0.08064200	2.54957400	H	3.81935200	2.63633200	-2.94028500
O	-0.21189500	-3.11543600	-3.60967800	H	4.95108900	1.81123900	-4.03826400
O	-2.92822500	-3.69613000	-2.00482000	H	4.02477400	3.22016800	-4.58165700
C	0.53931900	-3.38132200	-4.82095400	C	4.15769500	-3.57403200	-3.59587800
H	1.18943100	-2.53606500	-5.07446700	C	4.34587300	-3.71118800	-5.11627700
H	1.15264100	-4.24779900	-4.50842000	H	5.03646300	-2.95359200	-5.51281400
H	-0.14580300	-3.63973100	-5.63066200	H	4.75226500	-4.69036600	-5.38476500
C	-3.72242000	-4.89674500	-2.17273000	H	3.40290500	-3.57528000	-5.65276600
H	-4.34853500	-5.05419300	-1.27689800	C	5.52406100	-3.57043400	-2.88164100
H	-4.33810600	-4.63825100	-3.04373200	H	6.11385300	-4.45429700	-3.14112200
H	-3.08746500	-5.75926200	-2.39050200	H	6.11452900	-2.68412900	-3.16053800
O	-6.91271800	3.92745000	-0.42390900	H	5.40700400	-3.55675500	-1.78605200
O	-5.22421500	-3.72889000	2.87249000	C	3.35191600	-4.81009000	-3.13160500
O	4.66542800	-2.11640800	4.51237500	H	3.23003200	-4.84479900	-2.04367700
O	4.50445600	-1.01026300	-4.97739200	H	2.34552600	-4.81823600	-3.57862800
C	-7.87109500	3.47617000	0.56730500	H	3.85258900	-5.73766600	-3.42698600
H	-8.69108800	4.19189500	0.44262800	C	-6.25137400	-2.98499600	0.25887100
H	-8.19460900	2.45020900	0.33730400	C	-6.39421500	-2.63875100	-1.24198900
H	-7.42847200	3.55098700	1.57336300	H	-6.59909500	-1.56552600	-1.39591700
C	5.82330000	-0.54548700	-4.58411300	H	-5.49606400	-2.89903400	-1.81263400
H	6.25525500	-1.23879500	-3.84719600	H	-7.23258400	-3.18332100	-1.68873300
H	6.37402900	-0.56927500	-5.52997700	C	-6.28747100	-4.51797800	0.39035500
H	5.75566600	0.48098000	-4.18756500	H	-6.21711800	-4.83342200	1.44266500
C	5.82165000	-1.25767100	4.67724700	H	-7.21288400	-4.93697500	-0.01296300
H	6.31451500	-1.69687400	5.55130500	H	-5.44124200	-4.97839900	-0.14164200

C	-7.44803800	-2.33972000	0.98481800
H	-8.39656000	-2.63435800	0.52431700
H	-7.49689000	-2.64348300	2.03972100
H	-7.38783400	-1.24695700	0.95799900
C	-2.58173300	-2.88330600	3.94655600
C	-3.08708700	-2.01828100	5.11694400
H	-4.17901400	-2.08391300	5.23126500
H	-2.64158400	-2.33689400	6.06544400
H	-2.83618600	-0.96218700	4.97374400
C	-1.04147500	-2.77330500	3.89465000
H	-0.63464300	-3.25790600	3.00142300
H	-0.68642800	-1.72980800	3.90705800
H	-0.58420900	-3.26222200	4.76272900
C	-2.89846600	-4.37111200	4.18089300
H	-2.34651900	-4.76738700	5.03852600
H	-3.96182700	-4.55265300	4.37039200
H	-2.63318800	-4.97036000	3.30270800
C	5.33739500	-3.43677000	1.94274600
C	5.07828600	-4.36821300	0.73194200
H	4.13532800	-4.91210300	0.83959900
H	5.05579000	-3.81982100	-0.22425100
H	5.87444200	-5.11571400	0.64385600
C	6.59810800	-2.60366600	1.64443200
H	7.45414500	-3.24204900	1.40797600
H	6.43769900	-1.92519000	0.79831600
H	6.88264300	-1.97919300	2.50521200
C	5.55240700	-4.35456100	3.15791700
H	6.34952800	-5.08092900	2.97662500
H	5.82329600	-3.79356400	4.06130400
H	4.63947900	-4.90752600	3.40240100
C	2.32919700	-0.39932900	4.93295400
C	0.87379600	0.12575600	4.91535900
H	0.74653100	0.95807600	4.21263200
H	0.15426600	-0.66415400	4.65399600
H	0.58993000	0.50706100	5.90289500
C	3.24325000	0.79735000	5.24180100
H	2.89538700	1.35839100	6.11561400
H	4.27648400	0.48872100	5.45051000
H	3.27902100	1.51153500	4.39848700
C	2.41852200	-1.46190300	6.04304700
H	3.44300500	-1.84716300	6.15261100
H	2.12134000	-1.05165200	7.01229900
H	1.77712900	-2.32084500	5.82699900
N	0.62470400	5.60263300	2.42008200
C	2.99156300	5.22407600	1.46431900
C	3.20288800	5.41500000	0.05987600
C	4.15476800	5.05620100	2.40559400
C	-0.16275300	3.15593000	0.44091100
C	1.19147000	2.88506000	0.15247900
C	2.15179700	2.55815700	1.12187100
C	4.49083000	5.27549400	-0.51807800
C	4.68675300	5.42701700	-1.88474000
C	3.61653000	5.71277400	-2.73290300
C	2.33690700	5.85626200	-2.18382400
C	2.13016300	5.71661800	-0.82142100
C	3.78852000	4.87873300	3.84516000
C	4.39386600	4.03343400	4.68220400
C	1.71136200	5.43248100	1.99154500
H	4.81119600	5.94267700	2.31105700
H	4.78352700	4.20629800	2.08555800
H	-0.76625600	3.65511200	-0.31422500
H	-0.44552600	3.36571700	1.47077800
H	1.52156400	2.98017100	-0.88331700
H	1.83020600	2.56502900	2.16448800
H	5.34189500	5.03369800	0.11636600
H	5.69054400	5.31352500	-2.29369000
H	3.77543500	5.83621400	-3.80222300

H	1.49201900	6.09150200	-2.83058500
H	1.13079400	5.84130600	-0.40397000
H	2.98031900	5.51144500	4.22119000
H	4.11504600	3.96852900	5.73159400
H	5.20603500	3.38592900	4.34774800
C	3.49909100	2.13167400	0.87129600
C	4.29722000	1.69873600	1.95358400
C	4.08727900	2.11966400	-0.41373000
C	5.60229700	1.26711600	1.76731000
H	3.85736200	1.70664300	2.95636300
C	5.39451600	1.68550900	-0.59525600
H	3.52023800	2.46093300	-1.28330300
C	6.16097100	1.25242400	0.48728000
H	6.18825800	0.93736000	2.62285800
H	5.82239800	1.69009900	-1.59630900
H	7.18339400	0.91454900	0.33653200

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Pd	0.06245800	1.07478500	-0.40175500
P	2.13219100	0.41528900	0.17976000
P	-1.11024000	-0.75861900	0.19659800
C	1.11857900	-1.02180400	2.40666000
C	1.78210900	0.12928100	1.97615400
C	1.98777600	1.20300900	2.86225000
C	1.54577400	1.12801700	4.18110900
C	0.85336200	0.00182300	4.64037400
C	0.63497900	-1.05060500	3.74818300
C	0.88095300	-2.21765400	1.56804100
C	-0.12680100	-2.30051300	0.60430700
C	-0.34567700	-3.49907400	-0.08974700
C	0.45070500	-4.61770500	0.15615800
C	1.48406800	-4.56529100	1.09545600
C	1.68918000	-3.37080300	1.79167700
C	3.02981100	-1.11731100	-0.37500700
C	2.59273100	-1.75877800	-1.52880400
C	3.28382000	-2.87161000	-2.04818700
C	4.48340000	-3.24045700	-1.40205200
C	4.92536400	-2.64056200	-0.19751100
C	4.15502800	-1.58328300	0.30399300
C	3.63279700	1.52186900	0.22664400
C	4.63621500	1.40167500	1.18539400
C	5.79775800	2.18580100	1.12708300
C	5.92655700	3.05927200	0.02406500
C	4.88102700	3.28770700	-0.89630800
C	3.73823400	2.47600800	-0.78127800
C	-2.16115300	-0.66958700	1.71338400
C	-2.25263000	0.58614900	2.31019800
C	-3.08229300	0.79851900	3.42464500
C	-3.85420000	-0.29765200	3.86441800
C	-3.67516100	-1.60818000	3.37081100
C	-2.81075500	-1.76503200	2.27506100
C	-2.24826200	-1.44460000	-1.10147100
C	-3.33970100	-2.27598100	-0.87676600
C	-4.06248600	-2.83597100	-1.94390000
C	-3.68291600	-2.45265400	-3.25058300
C	-2.57519600	-1.61380500	-3.51388600
C	-1.88423900	-1.10100500	-2.40348400
H	2.48099500	2.12054200	2.53563400
H	1.72883000	1.95680600	4.86400100
H	0.49884500	-0.04036300	5.66339300
H	-1.13572700	-3.59323100	-0.83697900
H	0.27287800	-5.54284700	-0.39102800
H	2.11162600	-5.43396600	1.25872800
H	1.69407900	-1.40619600	-2.04779400
H	4.44489500	-1.11625400	1.25092100

H	4.53701800	0.67355700	2.00075700	C	-1.76975500	2.92100500	3.84928400
H	2.92653800	2.60315000	-1.50920600	H	-0.93054400	2.33716400	4.24739700
H	-1.66956900	1.43147500	1.90500200	H	-1.56340600	3.09986600	2.78650600
H	-2.65603200	-2.76911600	1.86240600	H	-1.76408800	3.89486000	4.34658500
H	-3.65369200	-2.50665000	0.14540700	C	-4.24080600	3.00440100	3.40804300
H	-1.05059000	-0.35682300	-2.56636100	H	-4.06105900	3.12940300	2.32905100
O	-0.05316100	-2.20359500	4.06391700	H	-5.21552000	2.51151600	3.53025400
O	2.68239300	-3.18742100	2.73379600	H	-4.31697700	4.00602800	3.84106900
C	-0.86919700	-2.19377100	5.25959900	C	-4.38845500	-2.84598600	3.92640600
H	-1.51668300	-1.30981800	5.28388400	C	-4.67134100	-2.73066000	5.43472400
H	-1.47743800	-3.10537800	5.11337000	H	-5.42072500	-1.95952800	5.65424100
H	-0.23316000	-2.26800500	6.14357000	H	-5.04175800	-3.67271300	5.84774000
C	3.42475800	-4.35682500	3.15527500	H	-3.77131300	-2.44636500	5.98831400
H	4.08104100	-4.69603300	2.33455300	C	-5.70824800	-3.01505300	3.14578600
H	4.01305800	-3.96031600	3.99192400	H	-6.28916600	-3.86142500	3.52243300
H	2.74997400	-5.14617300	3.49548100	H	-6.33358400	-2.11420100	3.23136600
O	7.12646100	3.77593600	-0.12832000	H	-5.52077700	-3.18922100	2.07404300
O	5.23038400	-4.32485500	-1.89455800	C	-3.51673200	-4.10849900	3.73231000
O	-4.36452400	-3.01415600	-4.34364200	H	-3.32625200	-4.32619900	2.67549300
O	-4.80868600	-0.08866200	4.87641100	H	-2.53664700	-3.98634200	4.22149000
C	8.11631400	3.06744600	-0.91590700	H	-3.99682200	-4.99198500	4.16242300
H	8.97030000	3.75181400	-0.89536300	C	6.17581800	-3.09255900	0.56897100
H	8.36038000	2.10574100	-0.43942400	C	6.25886000	-2.46153300	1.97971800
H	7.74123600	2.92741300	-1.94172200	H	6.49775800	-1.38542500	1.93058100
C	-6.11744200	0.24592800	4.34770000	H	5.31920600	-2.57114800	2.53286400
H	-6.48188000	-0.57026300	3.70596200	H	7.04677100	-2.93385300	2.57359700
H	-6.72361500	0.34258400	5.25394600	C	6.15339100	-4.62207100	0.74531000
H	-6.06202300	1.20063900	3.80161800	H	6.12225500	-5.13628500	-0.22730300
C	-5.52778400	-2.27718300	-4.78761400	H	7.03449600	-4.98226500	1.28045000
H	-5.90283200	-2.90173200	-5.60567000	H	5.25732400	-4.93595100	1.30234400
H	-6.26585300	-2.20093900	-3.97463000	C	7.43739400	-2.64350300	-0.19622200
H	-5.22500900	-1.28433200	-5.15415300	H	8.34609200	-2.87222300	0.36818400
C	6.15037700	-4.00055000	-2.96410600	H	7.52363800	-3.14976800	-1.16744700
H	6.95890300	-3.36622600	-2.57152000	H	7.41986200	-1.56551700	-0.38632500
H	6.52688200	-4.98569200	-3.25845300	C	2.68872800	-3.60597400	-3.25824100
H	5.62544100	-3.50730100	-3.79612700	C	3.30268300	-3.02104200	-4.54660800
C	4.93541400	4.34574900	-2.00653600	H	4.39296700	-3.16187300	-4.57478700
C	5.65514600	3.73020300	-3.22437400	H	2.88652400	-3.50180000	-5.43689500
H	5.72737300	4.44967900	-4.04535500	H	3.10972000	-1.94651300	-4.62506600
H	6.67726400	3.41618800	-2.96688800	C	1.15615700	-3.41784000	-3.33065500
H	5.12231000	2.85011200	-3.59711200	H	0.67721400	-3.69623500	-2.38504700
C	5.66223400	5.61694700	-1.53382200	H	0.86472500	-3.37939300	-3.55705200
H	6.72001400	5.42619800	-1.30922100	H	0.71835300	-4.04509500	-4.11371900
H	5.62169700	6.40637500	-2.28896100	C	2.93127600	-5.12404000	-3.17174000
H	5.21311000	6.00782600	-0.61460900	H	2.41317900	-5.66002200	-3.97116200
C	3.51472400	4.77343600	-2.43722300	H	3.99345200	-5.38367600	-3.23711100
H	2.93500200	3.94369900	-2.85572300	H	2.57613800	-5.51774300	-2.21237000
H	2.94382300	5.18069900	-1.59443100	C	-5.19355900	-3.82166000	-1.61796300
H	3.55153000	5.55487600	-3.20360400	C	-5.00631500	-4.45505600	-0.21678300
C	6.84729800	2.02389400	2.23381500	H	-4.02796200	-4.93818500	-0.12653000
C	7.58920400	3.34048200	2.51934100	H	-5.09814100	-3.71656400	0.59651100
H	8.23953300	3.25582400	3.39365200	H	-5.76496900	-5.22277400	-0.03308500
H	8.21242400	3.65541500	1.67311000	C	-6.53096500	-3.05414800	-1.61996800
H	6.88275400	4.15839800	2.69973200	H	-7.36275800	-3.70268300	-1.33068800
C	7.83597800	0.92496000	1.79448600	H	-6.50231500	-2.20801300	-0.92315600
H	8.64379400	0.80176200	2.52086900	H	-6.75988800	-2.65078400	-2.61749000
H	7.32887400	-0.04885300	1.68888500	C	-5.22811000	-4.98828300	-2.62066300
H	8.29326000	1.16776100	0.82397100	H	-5.98911300	-5.72625200	-2.35447700
C	6.18104100	1.59188900	3.56204600	H	-5.43967500	-4.65094200	-3.64313100
H	5.44072100	2.32997700	3.88919200	H	-4.25996000	-5.49913600	-2.66140900
H	5.66920000	0.62665500	3.47838900	C	-2.09595800	-1.23668900	-4.92320200
H	6.92387000	1.49511500	4.35970900	C	-0.64926900	-0.68864200	-4.90397700
C	-3.11318600	2.18901400	4.07065500	H	-0.56289200	0.22901600	-4.30970000
C	-3.33113100	2.10292800	5.59190800	H	0.05501700	-1.42522000	-4.48249800
H	-2.58408700	1.45450900	6.06023600	H	-0.30540300	-0.45371100	-5.91553900
H	-3.26540100	3.08764000	6.06188200	C	-3.00918900	-0.12441700	-5.47602200
H	-4.31404900	1.68225000	5.84191600	H	-2.64107100	0.25650600	-6.43268900

H	-4.03422000	-0.48536600	-5.63944200	C	-2.74156800	0.05415600	3.77890600
H	-3.06492000	0.72461700	-4.77499500	C	-4.00635700	-0.56653100	3.86355100
C	-2.09991600	-2.46341400	-5.85174400	C	-4.59069700	-1.27267000	2.78375400
H	-3.10886200	-2.88159100	-5.97235700	C	-3.89481800	-1.26268600	1.56801600
H	-1.72424700	-2.21526400	-6.84751800	C	-3.27579200	0.39762600	-1.18125400
H	-1.47706000	-3.26677300	-5.44472900	C	-4.55174300	-0.15967200	-1.23849300
N	-0.64914500	5.90857000	-2.69147600	C	-5.61192400	0.51158000	-1.86254300
C	-2.73723000	4.48548400	-1.94697300	C	-5.32754700	1.77661800	-2.43096800
C	-3.36166900	5.09665600	-0.69496000	C	-4.01999200	2.30115700	-2.51014200
C	-3.70992300	4.52645500	-3.15714800	C	-3.00858200	1.59487200	-1.83630200
C	0.18392900	3.20721800	-0.90868300	C	1.65552700	-2.02560800	-1.21882400
C	-1.15782200	2.95186600	-0.62505200	C	1.48507200	-1.31303900	-2.40370400
C	-2.24234900	2.98195200	-1.67277800	C	1.76823800	-1.90152800	-3.64878000
C	-4.73976500	5.02897400	-0.46412100	C	2.33557300	-3.19283300	-3.63082300
C	-5.29063600	5.52555900	0.71517400	C	2.43945900	-3.97047700	-2.45302800
C	-4.47302200	6.09693400	1.68693200	C	2.06072900	-3.35963600	-1.24799300
C	-3.09937500	6.17582400	1.46579700	C	3.09827700	-0.94457900	0.99155800
C	-2.55094600	5.68347200	0.28461900	C	4.06217500	-1.93799200	0.84610200
C	-3.10439000	4.14639600	-4.47043000	C	5.35873900	-1.77334900	1.35944100
C	-3.67464500	3.32540900	-5.35392500	C	5.64505400	-0.54988300	2.00639600
C	-1.56306200	5.27928100	-2.33062200	C	4.66017900	0.42965600	2.26286400
H	-4.10268500	5.55337900	-3.22100900	C	3.39421400	0.22574500	1.68978700
H	-4.56708800	3.87456400	-2.94831800	H	-2.74697100	-1.51644100	-2.75348100
H	0.83622800	3.65435300	-0.15808400	H	-2.46998600	-3.73269900	-3.76279200
H	0.51521500	3.33481300	-1.94008000	H	-1.32537500	-5.56356600	-2.50172300
H	-1.50063000	3.15472600	0.39269700	H	2.02135300	-1.68015400	3.08673100
H	-1.81879700	2.65648000	-2.63613900	H	0.82616600	-2.85425300	4.87246400
H	-5.39791000	4.56662900	-1.19729000	H	-1.31040300	-4.01520700	4.41965200
H	-6.36611100	5.46029500	0.87302500	H	-1.17937200	0.63973500	2.39380300
H	-4.90443400	6.48637200	2.60777400	H	-4.29927900	-1.82068100	0.71427400
H	-2.44914400	6.62933200	2.21242800	H	-4.74248300	-1.13526600	-0.77306900
H	-1.47708800	5.76044600	0.11452100	H	-1.98865100	2.01751200	-1.82369300
H	-2.15075200	4.61949500	-4.72049600	H	1.12920400	-0.26622900	-2.38243500
H	-3.21810200	3.11683000	-6.31931500	H	2.08596000	-3.94428900	-0.32063400
H	-4.63198700	2.84266600	-5.15079700	H	3.82765200	-2.86386700	0.31306900
C	-3.41945800	2.08918400	-1.35477500	H	2.63680900	1.01709100	1.78895500
C	-4.00425500	1.32249300	-2.36767100	O	-0.25222400	-5.29326000	-0.09223900
C	-3.96599100	2.00601200	-0.06810900	O	-2.43368900	-4.19290600	1.92405400
C	-5.10190400	0.50325600	-2.11252300	C	-1.01797000	-6.46598800	0.28567500
H	-3.57092500	1.35170000	-3.37344900	H	-1.36043600	-7.00093600	-0.60264700
C	-5.05652900	1.18006800	0.19498300	H	-0.28199500	-7.05232300	0.84690500
H	-3.54410100	2.59212500	0.75297700	H	-1.85539700	-6.16247900	0.92583700
C	-5.63300700	0.42808100	-0.82677700	C	-3.24874300	-4.76867900	2.97348800
H	-5.52376100	-0.09985400	-2.91505000	H	-3.66544900	-3.96925000	3.60787000
H	-5.44592800	1.11599800	1.21067000	H	-4.04562500	-5.25577500	2.39656800
H	-6.47456700	-0.23211900	-0.61846800	H	-2.68021200	-5.49819300	3.55511700
				O	-6.38454500	2.50353400	-3.00142800
				O	-4.68448400	-0.57193400	5.09365000
				O	6.95032400	-0.33568800	2.47939000
				O	2.75133000	-3.76658300	-4.84475100
				C	-6.99923800	3.44683000	-2.08771400
				H	-7.77192200	3.90925400	-2.71040200
				H	-7.43984400	2.90713900	-1.23562200
				H	-6.25589500	4.18911000	-1.75578900
				C	4.10960800	-3.42275100	-5.21547800
				H	4.80983200	-3.81847800	-4.46370500
				H	4.22867300	-3.93146100	-6.17726900
				H	4.20920400	-2.33129400	-5.32394200
				C	7.79674700	0.38330700	1.54742900
				H	8.73565400	0.47402600	2.10260900
				H	7.92823400	-0.21193200	0.63077600
				H	7.36339100	1.37174400	1.32711800
				C	-5.50324900	0.59944900	5.33098900
				H	-6.31066900	0.64509100	4.58411600
				H	-5.89881600	0.41168800	6.33447100
				H	-4.88476400	1.51036000	5.30820000
				C	-3.63888200	3.58852200	-3.25470100
Pd	0.08400000	0.76380300	-0.06106400				
P	-1.87229200	-0.32353400	-0.20925000				
P	1.38025100	-1.05007200	0.30988000				
C	-1.13519200	-3.05592000	-0.14351300				
C	-1.78405300	-2.04719300	-0.86984500				
C	-2.25488500	-2.29578300	-2.16538400				
C	-2.10358700	-3.55545900	-2.75264900				
C	-1.47224800	-4.58479800	-2.05315500				
C	-0.99279100	-4.32008700	-0.76687600				
C	-0.59260000	-2.89583500	1.22526900				
C	0.58226200	-2.19849700	1.52652600				
C	1.08911100	-2.19282400	2.83682600				
C	0.41830100	-2.85745600	3.86184200				
C	-0.78245500	-3.52689000	3.60820500				
C	-1.27011700	-3.54372900	2.29929400				
C	-2.71185500	-0.54186200	1.41786100				
C	-2.13233500	0.09410500	2.51099500				

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C	-3.83884100	4.78050400	-2.29963800	H	-1.94458900	2.64260300	5.94475100
H	-3.59243300	5.72890100	-2.78802600	H	-2.26345900	2.72649500	4.20914200
H	-4.87916000	4.84925800	-1.95040200	C	-0.46814800	0.68429700	4.70947800
H	-3.19790800	4.69916400	-1.41325300	H	-0.09464600	-0.33478300	4.55144900
C	-4.47445400	3.76665000	-4.53359800	H	-0.19242500	1.27265400	3.82558100
H	-5.54094200	3.90351600	-4.31281300	H	0.07206500	1.10709800	5.56154500
H	-4.14456200	4.63517400	-5.11008800	C	-2.22803900	-0.10397700	6.26258000
H	-4.40168300	2.88531800	-5.17943100	H	-1.62518700	0.29108800	7.08467700
C	-2.15368800	3.55040400	-3.68703400	H	-3.27710700	-0.07830500	6.58117300
H	-1.47187100	3.48758200	-2.82281200	H	-1.96952500	-1.16022200	6.13038200
H	-1.94872400	2.69560000	-4.33908100	C	6.38038800	-2.90480600	1.18085700
H	-1.88360400	4.45665200	-4.23934900	C	5.68390400	-4.26700600	0.95107500
C	-7.00244800	-0.13735900	-1.86039200	H	4.96568800	-4.48835000	1.74688600
C	-7.75165200	0.13733700	-3.17510100	H	5.15073600	-4.30752200	-0.01376600
H	-8.70671800	-0.39256800	-3.21523400	H	6.41599900	-5.08107700	0.93960500
H	-7.96276100	1.20690100	-3.31155700	C	7.24254000	-2.58866500	-0.05784400
H	-7.15604300	-0.17221400	-4.04054400	H	7.98423500	-3.37224200	-0.23663600
C	-7.78918300	0.41731200	-0.65526800	H	6.62590800	-2.49615200	-0.95773100
H	-8.81215500	0.03046600	-0.63793000	H	7.78687800	-1.64036200	0.06551800
H	-7.31171700	0.14245000	0.29960100	C	7.26083100	-3.06135700	2.43314500
H	-7.85096200	1.51525000	-0.69000900	H	7.94445600	-3.90909800	2.34212600
C	-6.90810400	-1.67481600	-1.71191600	H	7.86995000	-2.16584600	2.61967600
H	-6.27132100	-2.11159300	-2.48799300	H	6.64919000	-3.21338000	3.32838300
H	-6.50915100	-1.97752700	-0.73007400	C	4.89137500	1.68619700	3.11331300
H	-7.89711100	-2.13534300	-1.80582600	C	3.56069300	2.17909100	3.73275000
C	1.45492400	-1.10255100	-4.92043100	H	2.84206600	2.49381200	2.96648300
C	1.02445100	-2.02103700	-6.07733600	H	3.09070800	1.39981700	4.34003400
H	0.19723400	-2.67184200	-5.77471600	H	3.73186000	3.04529600	4.38012600
H	0.70220300	-1.44484200	-6.94832800	C	5.45040100	2.79576100	2.20602400
H	1.83650000	-2.68408200	-6.40099500	H	5.63975400	3.71672900	2.76649700
C	0.28361600	-0.12270500	-4.66664600	H	6.39334200	2.49353100	1.72926900
H	-0.61522500	-0.65754200	-4.34156300	H	4.74060300	3.05019800	1.39853800
H	0.52702900	0.61597900	-3.88973500	C	5.84773500	1.40519200	4.28590900
H	0.03170000	0.43235400	-5.57456000	H	6.85912400	1.15488100	3.94054000
C	2.70546300	-0.28885200	-5.30551200	H	5.93316300	2.26975100	4.94926900
H	2.99687600	0.39572800	-4.49861500	H	5.50396500	0.55296000	4.88095200
H	3.56520600	-0.94541800	-5.50398000	N	-0.82900100	5.06143600	0.77218000
H	2.53184600	0.31004500	-6.20358900	C	1.34653600	6.07431000	-0.09784800
C	2.97740200	-5.40764600	-2.42847400	C	2.49993600	6.15862800	0.80455100
C	2.48516800	-6.21108200	-3.64508000	C	1.48622100	6.49126800	-1.54614900
H	2.87241400	-5.80377600	-4.58884600	C	-1.06225100	3.58422800	0.72280900
H	2.79237700	-7.25802400	-3.58766500	C	-0.23449600	2.90205400	-0.31860000
H	1.39302300	-6.17966600	-3.71676700	C	1.15407000	2.72707100	-0.11649000
C	4.51899000	-5.33755900	-2.40410600	C	3.73696600	6.64300700	0.34669000
H	4.96081900	-6.33767900	-2.40630100	C	4.84337400	6.69693000	1.19105900
H	4.91167600	-4.79950600	-3.27870400	C	4.74755000	6.27327500	2.51391700
H	4.87827100	-4.81402100	-1.50326600	C	3.52285700	5.79389600	2.98509900
C	2.51021300	-6.16778700	-1.16815100	C	2.41914400	5.73642000	2.14568900
H	2.90741200	-5.73341200	-0.24557400	C	0.29713600	6.17548300	-2.39152000
H	1.41217700	-6.15234900	-1.08482800	C	-0.42071200	7.06921300	-3.07133100
H	2.82631800	-7.21358800	-1.19730600	C	0.20671300	5.54637500	0.33712000
C	-5.93606800	-2.00580500	2.86583500	H	2.36184100	5.95696600	-1.95678800
C	-6.11693400	-3.02295900	1.71337400	H	1.72169200	7.56578900	-1.61229900
H	-6.23009200	-2.52667500	0.73502600	H	-2.13878000	3.44702500	0.56429200
H	-5.26875800	-3.71150700	1.64034200	H	-0.83973300	3.21948500	1.73516800
H	-7.01882500	-3.62467400	1.86415400	H	-0.57274400	3.11017800	-1.34445300
C	-6.04196600	-2.79047300	4.18565100	H	1.53248100	2.92589500	0.89181700
H	-6.05172900	-2.11788000	5.05583400	H	3.84139700	6.97756400	-0.68389000
H	-6.95084700	-3.39500100	4.22878900	H	5.78898800	7.07870000	0.80731000
H	-5.17740700	-3.45460700	4.31483500	H	5.61175500	6.32335100	3.17421900
C	-7.06962800	-0.96738700	2.74496600	H	3.42758900	5.46450600	4.01933500
H	-8.05198000	-1.44032500	2.83326500	H	1.46767400	5.36684800	2.53124200
H	-7.00213800	-0.19996200	3.52944200	H	0.02409600	5.11614300	-2.44010000
H	-7.03461000	-0.44821600	1.77250200	H	-1.27357000	6.77756200	-3.68111600
C	-1.99485600	0.68503800	4.96257300	H	-0.18087000	8.13264100	-3.04383800
C	-2.46031700	2.14636500	5.11688800	C	2.16177400	2.86082200	-1.17254300
H	-3.54001400	2.20707100	5.31825000	C	3.48098900	3.20617500	-0.83353700

C	1.85440200	2.72725800	-2.53921200
C	4.44497400	3.42738700	-1.81237700
H	3.74858800	3.31956200	0.22467600
C	2.81634400	2.95038600	-3.51764800
H	0.84397000	2.44621400	-2.83996400
C	4.11902900	3.30507200	-3.16253900
H	5.45517200	3.70839500	-1.51547100
H	2.54595900	2.84920800	-4.56881700
H	4.87022300	3.48279600	-3.93040400

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Pd	-0.01463800	0.65813000	0.06263600
P	-2.00617500	-0.30133100	-0.15948000
P	1.24930200	-1.17853200	0.31516700
C	-1.35341600	-3.03262100	-0.16039900
C	-1.94566500	-1.98498400	-0.87719100
C	-2.42460000	-2.19094000	-2.17541400
C	-2.33295500	-3.45181200	-2.77609600
C	-1.75620000	-4.51794600	-2.08660600
C	-1.27035300	-4.29642400	-0.79306800
C	-0.81970900	-2.90360100	1.21389600
C	0.39551900	-2.28394000	1.52794400
C	0.89734800	-2.33395200	2.83462300
C	0.18006800	-2.97664900	3.84795700
C	-1.06516700	-3.54823000	3.58434200
C	-1.55446100	-3.50148700	2.27431500
C	-2.93181800	-0.47311300	1.39601500
C	-2.37153900	0.10984100	2.53146400
C	-3.06299000	0.12057600	3.75487100
C	-4.38652100	-0.37366500	3.74881400
C	-4.95482000	-1.03178200	2.63054300
C	-4.17903500	-1.09224300	1.46508100
C	-3.18234800	0.55701600	-1.25614800
C	-4.54023800	0.24371800	-1.30497600
C	-5.44014500	1.03120700	-2.03336500
C	-4.92135400	2.18437000	-2.67202900
C	-3.53545100	2.44460000	-2.76317300
C	-2.68274300	1.60094600	-2.03426100
C	1.48565500	-2.12739300	-1.21913100
C	1.36924500	-1.38816400	-2.39570000
C	1.64666600	-1.96788600	-3.64439400
C	2.15054200	-3.28711800	-3.63893500
C	2.19397900	-4.08728900	-2.47173600
C	1.82987700	-3.47823200	-1.26168400
C	2.93060800	-1.08629700	1.02674600
C	3.89335600	-2.07360100	0.83792000
C	5.15497800	-1.97937900	1.44628400
C	5.41645400	-0.82490000	2.21940100
C	4.43038100	0.15186000	2.49810500
C	3.20132500	0.02174000	1.83498200
H	-2.87803800	-1.38256300	-2.75842900
H	-2.70481600	-3.59861700	-3.79043400
H	-1.65779600	-5.50042400	-2.54515600
H	1.86029700	-1.88709300	3.10126700
H	0.59282400	-3.02548500	4.85690100
H	-1.62802800	-4.02332900	4.38225800
H	-1.37537900	0.58372300	2.48744000
H	-4.57735000	-1.61286000	0.58432800
H	-4.93070700	-0.62657100	-0.76253800
H	-1.60034800	1.79886000	-2.07392700
H	1.06672300	-0.32849900	-2.36852800
H	1.81934700	-4.07766000	-0.34289200
H	3.69046400	-2.93818200	0.19903500
H	2.45417700	0.81886100	1.95807100
O	-0.58523800	-5.31322900	-0.13036600

O	-2.76865300	-4.03503200	1.88681500
C	-1.43113700	-6.41094500	0.30472300
H	-1.85424200	-6.93012600	-0.55782300
H	-0.72136800	-7.04717300	0.84600900
H	-2.21238700	-6.02789500	0.97370000
C	-3.74270900	-4.30013100	2.92711700
H	-3.81234200	-3.45915300	3.62760600
H	-4.67673300	-4.37872600	2.34180000
H	-3.49587100	-5.23759200	3.42986100
O	-5.82069500	3.05865500	-3.29177900
O	-5.15106200	-0.29071700	4.91896600
O	6.68070500	-0.69432400	2.80772600
O	2.55517800	-3.86259200	-4.85159700
C	-6.25860900	4.14221800	-2.42827500
H	-6.91737600	4.71568600	-3.08885900
H	-6.80600800	3.73207300	-1.56707500
H	-5.38999200	4.74483700	-2.11108700
C	3.93049400	-3.57082000	-5.20978100
H	4.60752800	-4.02266100	-4.46855400
H	4.02706900	-4.05810100	-6.18587700
H	4.08338800	-2.48293600	-5.28796700
C	7.63025300	0.06229700	2.01341100
H	8.52315400	0.05371300	2.64741700
H	7.80920200	-0.44962900	1.05622300
H	7.25971600	1.08973300	1.86181300
C	-5.86023900	0.96558300	5.07957400
H	-6.60047300	1.07782500	4.27276500
H	-6.34559800	0.83726400	6.05315200
H	-5.14915600	1.80726000	5.09520900
C	-2.91626500	3.61157100	-3.55173300
C	-2.90734000	4.85138000	-2.64479300
H	-2.48816300	5.72519100	-3.15853700
H	-3.91336500	5.12714500	-2.30130900
H	-2.28574900	4.71513200	-1.74398800
C	-3.69626700	3.88019500	-4.84972500
H	-4.72108600	4.21975400	-4.65172100
H	-3.21105500	4.65781600	-5.44845300
H	-3.77361900	2.97965000	-5.46571500
C	-1.45873300	3.29008200	-3.95823200
H	-0.80066300	3.16571800	-3.08152400
H	-1.39661900	2.39162700	-4.57652300
H	-1.03164800	4.11999500	-4.53630000
C	-6.92042000	0.62557100	-2.05953000
C	-7.57481600	0.97419300	-3.40595900
H	-8.59937000	0.59748600	-3.46831100
H	-7.61603600	2.05997700	-3.57376000
H	-7.00926400	0.55485200	-4.24476000
C	-7.63369800	1.35000300	-0.90151700
H	-8.71406300	1.17839900	-0.93019900
H	-7.26672600	1.00512200	0.07807200
H	-7.47263900	2.43818000	-0.95273800
C	-7.08320900	-0.90154400	-1.86386300
H	-6.53044800	-1.45941100	-2.62642100
H	-6.74407600	-1.24323600	-0.87438100
H	-8.13672200	-1.19010000	-1.95160800
C	1.40249700	-1.12923700	-4.90707100
C	0.96458300	-2.00262300	-6.09442200
H	0.10595100	-2.62880300	-5.83095500
H	0.68563200	-1.39258500	-6.95861300
H	1.75768800	-2.68652400	-6.42140100
C	0.26678300	-0.10544800	-4.66296900
H	-0.66432100	-0.60433900	-4.37667300
H	0.52153400	0.61560000	-3.87662500
H	0.06488500	0.47340700	-5.57121400
C	2.69596300	-0.36222600	-5.23715000
H	2.99042900	0.30429000	-4.41635700
H	3.53674700	-1.04803100	-5.41903700

H	2.57689900	0.25507300	-6.13327000	C	1.91964800	5.90326400	-0.08586500
C	2.65945600	-5.55086800	-2.46427300	C	2.81381600	5.85782400	1.03191800
C	2.12977000	-6.31014500	-3.69255200	C	2.43177300	6.16437500	-1.47858900
H	2.53187800	-5.90442000	-4.63142600	C	-0.70956800	2.82705700	0.18736200
H	2.39655500	-7.36980700	-3.65556600	C	0.38853400	2.89928000	-0.67750400
H	1.03983800	-6.23740400	-3.76059400	C	1.72143100	2.92748600	-0.27452500
C	4.20145000	-5.55551700	-2.43700300	C	4.20905300	6.05891900	0.87053900
H	4.59393000	-6.57669400	-2.42131500	C	5.07319000	6.01500900	1.95725300
H	4.62385900	-5.05544600	-3.32053300	C	4.59380200	5.76627500	3.24372100
H	4.58792000	-5.03588300	-1.54539800	C	3.21991000	5.55902900	3.42444600
C	2.15172900	-6.30130400	-1.21414500	C	2.34929200	5.60395200	2.35032000
H	2.57515100	-5.90433600	-0.28628800	C	1.41642700	5.95472000	-2.55321900
H	1.05635400	-6.23576300	-1.12843600	C	1.13775600	6.81527500	-3.53258000
H	2.41458600	-7.36225300	-1.25893200	C	0.54167400	5.85138400	0.12070000
C	-6.37849400	-1.60696900	2.60691300	H	3.28221700	5.48063000	-1.66406300
C	-6.55576000	-2.64944700	1.47734200	H	2.85543500	7.18127600	-1.55833200
H	-6.48777100	-2.19461900	0.47683300	H	-1.70443700	3.07233800	-0.16970000
H	-5.80693000	-3.45148400	1.54489400	H	-0.55367000	3.00670300	1.25085600
H	-7.54318300	-3.12091600	1.53629000	H	0.17144800	2.93315600	-1.75318600
C	-6.72759600	-2.31141300	3.92871400	H	1.91527600	3.01835300	0.79402200
H	-6.71543800	-1.61359000	4.77909800	H	4.61218000	6.25756400	-0.12101900
H	-7.72625900	-2.75704700	3.89467600	H	6.13784100	6.18480400	1.79759300
H	-6.01300800	-3.10258500	4.16814600	H	5.27226000	5.74949300	4.09420900
C	-7.35389500	-0.44320500	2.34021700	H	2.82731600	5.36809800	4.42272600
H	-8.38975600	-0.79396300	2.29737900	H	1.28068500	5.44921800	2.50569800
H	-7.29960400	0.31773900	3.13357500	H	0.87255600	5.00579600	-2.50533200
H	-7.13621400	0.06479100	1.38609200	H	0.39475000	6.59623700	-4.29581900
C	-2.34359500	0.68231700	4.99136100	H	1.64334900	7.77841600	-3.60453200
C	-2.66239100	2.18363300	5.10238700	C	2.87478500	2.91261200	-1.13016700
H	-3.74020500	2.36627700	5.22265100	C	4.15689100	3.05543100	-0.55626800
H	-2.15800300	2.63635600	5.96330600	C	2.80347100	2.78309600	-2.53598000
H	-2.33545800	2.73521900	4.21247600	C	5.30160100	3.08710800	-1.34088600
C	-0.81221900	0.51355500	4.84959400	H	4.23575400	3.15192800	0.53177300
H	-0.53554000	-0.53612700	4.70579900	C	3.95057800	2.81370500	-3.31593200
H	-0.40608900	1.08866500	4.00817600	H	1.83693300	2.66520600	-3.02239700
H	-0.29656300	0.87069500	5.74829500	C	5.20863100	2.96511300	-2.72790000
C	-2.75693600	-0.06374000	6.27107500	H	6.27354700	3.21011200	-0.86640500
H	-2.18180300	0.28218000	7.13580500	H	3.86445300	2.72219500	-4.39742900
H	-3.81788900	0.07751400	6.51134300	H	6.10365900	2.99083800	-3.34475100
H	-2.59788400	-1.14189200	6.17157300				
C	6.16634400	-3.11566200	1.23417400				
C	5.45812300	-4.43965900	0.85904700	<b>17</b>			
H	4.70732000	-4.71595300	1.60595100	Pd	-0.03195800	0.86205800	-0.51138200
H	4.96406700	-4.39266500	-0.12509700	P	-2.15712300	0.21377900	-0.44779000
H	6.18018900	-5.26208100	0.80776800	P	0.95960300	-1.04528100	0.14474000
C	7.10233000	-2.71789200	0.07670000	C	-1.52841400	-2.45088500	-1.16626600
H	7.84505600	-3.49650400	-0.12083200	C	-2.07820200	-1.23372500	-1.57919800
H	6.54401800	-2.54249700	-0.84817300	C	-2.40869600	-1.00971100	-2.92374500
H	7.65163400	-1.79164000	0.30714000	C	-2.18615600	-2.00371300	-3.87846200
C	6.96948800	-3.39495100	2.51604500	C	-1.59388000	-3.21549100	-3.51668300
H	7.63159900	-4.25681800	2.39761100	C	-1.25587800	-3.42366200	-2.17472700
H	7.59666000	-2.53959300	2.80390100	C	-1.21630100	-2.81593700	0.23569800
H	6.30653000	-3.59121600	3.36495600	C	-0.10531300	-2.33379900	0.93602800
C	4.62887600	1.31573200	3.48449700	C	0.17711800	-2.77141900	2.23418500
C	3.26839100	1.84706100	3.99376900	C	-0.66303200	-3.69240800	2.86487000
H	2.67174300	2.29467500	3.18850400	C	-1.78670500	-4.19161800	2.20606800
H	2.67946700	1.06911300	4.48287400	C	-2.05086500	-3.76026600	0.89999200
H	3.42378900	2.65500700	4.72162000	C	-2.95443200	-0.44117300	1.06254900
C	5.35467500	2.46374600	2.77173400	C	-2.43749500	-0.17203400	2.32595500
H	5.49787800	3.32597700	3.43924500	C	-3.10758500	-0.60885900	3.48467200
H	6.34178100	2.17070000	2.39475900	C	-4.36620200	-1.22625400	3.30881900
H	4.76998400	2.85552000	1.91843800	C	-4.88189600	-1.57313100	2.03531900
C	5.42043400	0.84850900	4.71970900	C	-4.13163300	-1.17943800	0.92275000
H	6.44306100	0.54408500	4.45972000	C	-3.54670100	1.23158400	-1.07243100
H	5.50188900	1.64983400	5.46092300	C	-4.75544500	0.64688000	-1.45969600
H	4.94416600	-0.00977400	5.20108900	C	-5.86766700	1.42904400	-1.78865100
N	-0.62874200	5.79284700	0.28057200				

C	-5.70830100	2.83704700	-1.73323600	H	-4.91446400	5.05326300	-3.67608200
C	-4.46439600	3.45432500	-1.48548800	C	-2.72309800	5.23160500	-1.97142700
C	-3.40297100	2.61612000	-1.09683300	H	-2.01333300	4.94172000	-1.18631600
C	1.76251900	-2.00814800	-1.18496100	H	-2.41712400	4.72580300	-2.89279300
C	1.82312700	-1.40869100	-2.44223600	H	-2.52984900	6.30121600	-2.13486700
C	2.48156700	-2.03874400	-3.51111700	C	-7.19133600	0.74414700	-2.15760100
C	3.15219500	-3.24826300	-3.22608700	C	-7.87029300	1.45996800	-3.33693400
C	3.00751900	-3.93326000	-1.99812800	H	-8.77998400	0.94376000	-3.65480500
C	2.29123200	-3.28166300	-0.98250700	H	-8.15276700	2.49220100	-3.08209500
C	2.26694900	-0.77936600	1.39743300	H	-7.20032200	1.52618000	-4.20058800
C	3.33729800	-1.64047300	1.61564000	C	-8.10118300	0.75185700	-0.91269400
C	4.26985400	-1.39690000	2.63692300	H	-9.06136800	0.27070700	-1.12213400
C	4.11327300	-0.20798100	3.38647900	H	-7.63774100	0.22102400	-0.06568900
C	3.01287300	0.66814400	3.21524800	H	-8.31604500	1.77833600	-0.58039700
C	2.11729700	0.37064600	2.17797700	C	-6.97443600	-0.72597700	-2.58556800
H	-2.83703000	-0.06124600	-3.25916400	H	-6.25741000	-0.80374200	-3.40895500
H	-2.46421200	-1.83014400	-4.91889400	H	-6.61844700	-1.35298800	-1.75276700
H	-1.40268300	-3.97376100	-4.27025400	H	-7.91309800	-1.16995500	-2.93518400
H	1.05092200	-2.41328000	2.78560300	C	2.44876800	-1.36992800	-4.89263600
H	-0.44250000	-0.02396500	3.88009900	C	2.46487200	-2.40817000	-6.02751900
H	-2.44215200	-4.89344300	2.71290900	H	1.65905000	-3.13870700	-5.91036500
H	-1.49900900	0.38286700	2.43743800	H	2.34786800	-1.93095400	-7.00526300
H	-4.48506300	-1.45733400	-0.07921000	H	3.40409100	-2.97597000	-6.05399500
H	-4.84985600	-0.44616400	-1.48706700	C	1.15279300	-0.54248000	-5.05955300
H	-2.45447900	3.09240500	-0.80989100	H	0.26152700	-1.16511500	-4.92642700
H	1.35636200	-0.42592200	-2.61711900	H	1.09089600	0.28607500	-4.34398500
H	2.16122600	-3.78830100	-0.01866000	H	1.10007700	-0.09749500	-6.05935200
H	3.47868900	-2.52260700	0.98415400	C	3.66071900	-0.42765500	-5.00019900
H	1.29733500	1.07485300	1.97106500	H	3.62876200	0.36024800	-4.23086300
O	-0.63648900	-4.55527300	-1.69838000	H	4.60803000	-0.97221200	-4.87535000
O	-3.13416800	-4.18906100	0.16083300	H	3.69515700	0.07297100	-5.97347400
C	-0.05745300	-5.46699600	-2.66504000	C	3.63280000	-5.30239000	-1.70052200
H	0.57959800	-4.93056000	-3.37715300	C	3.67109100	-6.20522500	-2.94532200
H	0.56332100	-6.10688200	-2.00913600	H	4.35622000	-5.81722800	-3.71185900
H	-0.84772700	-6.03708200	-3.15739700	H	4.00456000	-7.21710200	-2.69762200
C	-3.86185900	-5.34041900	0.66165600	H	2.68953600	-6.27783000	-3.42137000
H	-4.44908300	-5.04602400	1.54828000	C	5.05930600	-5.05521100	-1.17112500
H	-4.51730600	-5.57860900	-0.18581900	H	5.57999200	-5.99597800	-0.96952400
H	-3.18356300	-6.17157600	0.87060200	H	5.66213700	-4.49272700	-1.90037100
O	-6.82744300	3.62854800	-2.02186500	H	5.04819100	-4.47359900	-0.23486100
O	-5.10781300	-1.61450400	4.43321400	C	2.82088500	-6.05869800	-0.62332200
O	5.02165000	0.06169100	4.41709900	H	2.79971900	-5.52689100	0.33415100
O	3.95214600	-3.82957700	-4.22083800	H	1.77774200	-6.20638100	-0.94386500
C	-7.52703700	4.11760500	-0.84968600	H	3.25078500	-7.04678600	-0.42999100
H	-8.30070400	4.75651800	-1.28994100	C	-6.19723500	-2.33692300	1.82101400
H	-7.96939200	3.26879300	-0.30744800	C	-6.32788600	-2.88106700	0.37896400
H	-6.84628700	4.70089800	-0.20939700	H	-6.50463400	-2.08013500	-0.35809100
C	5.32386000	-3.35235800	-4.19320100	H	-5.42907000	-3.42357600	0.06364900
H	5.78951500	-3.61784700	-3.23201700	H	-7.17522000	-3.56936200	0.29865400
H	5.78096000	-3.89868300	-5.02473900	C	-6.26518800	-3.54492900	2.77228200
H	5.34571900	-2.26499000	-4.36905300	H	-6.19406800	-3.23543600	3.82604900
C	6.19246300	0.81939200	4.01759300	H	-7.20246000	-4.09601200	2.65960400
H	6.77414100	0.85400800	4.94482400	H	-5.43419800	-4.24011400	2.58241600
H	6.73568200	0.29427500	3.21800800	C	-7.37846000	-1.37545000	2.05309600
H	5.88834200	1.83121500	3.70187200	H	-8.33657300	-1.89656200	1.96017600
C	-5.93339400	-0.56875800	5.00446400	H	-7.35011600	-0.92369200	3.05414800
H	-6.72052800	-0.28992800	4.28739300	H	-7.37498500	-0.55484800	1.31632400
H	-6.35672000	-1.06117400	5.88686700	C	-2.43356100	-0.39698700	4.84928500
H	-5.31881500	0.30013300	5.28637100	C	-2.90183100	0.95251500	5.42562500
C	-4.19665600	4.96457900	-1.61292400	H	-3.99086300	0.97230600	5.57961400
C	-4.50634700	5.62572300	-0.25527100	H	-2.43227000	1.15330700	6.39463800
H	-4.32113700	6.70563800	-0.29936200	H	-2.64919100	1.78409400	4.75981100
H	-5.55428800	5.48116600	0.04088600	C	-0.89554900	-0.36260200	4.70674800
H	-3.87081300	5.22384000	0.53986000	H	-0.52250600	-1.24380200	4.17471600
C	-5.04715900	5.59170500	-2.73131300	H	-0.53212300	0.53293900	4.17666300
H	-6.11854500	5.58019300	-2.50757800	H	-0.41180500	-0.35074900	5.69061600
H	-4.76060000	6.63457800	-2.90521600	C	-2.75173400	-1.54889400	5.81933200



H	-2.17340600	-1.46419100	6.74431200
H	-3.80993100	-1.58070700	6.10249600
H	-2.52213000	-2.51898800	5.36513500
C	5.38830900	-2.42595300	2.86087900
C	4.98176800	-3.82421300	2.33165200
H	4.04223900	-4.16247300	2.77838000
H	4.87173600	-3.84450600	1.23508900
H	5.74606000	-4.56782200	2.58308000
C	6.63511000	-1.96077000	2.08542100
H	7.45593300	-2.67748600	2.17880600
H	6.41834400	-1.83073700	1.01943600
H	7.00168200	-0.99136700	2.45811300
C	5.70099100	-2.60184300	4.35642500
H	6.44426700	-3.38633200	4.52280500
H	6.09276900	-1.68181700	4.80967000
H	4.80021000	-2.86246900	4.92162800
C	2.75404400	1.89637900	4.10482100
C	1.30867400	2.42466800	3.93844700
H	1.13098000	2.81232600	2.92801300
H	0.55695700	1.65388800	4.15833800
H	1.12761800	3.26115600	4.62383500
C	3.70636300	3.03067600	3.70719300
H	3.46758800	3.96954800	4.22309000
H	4.75542700	2.80566500	3.93859900
H	3.65417900	3.26520500	2.62699400
C	2.93468900	1.51686400	5.58621600
H	3.96160300	1.18195000	5.79400000
H	2.73657000	2.37085000	6.24056300
H	2.26602000	0.70275400	5.87710300
N	0.80764700	5.78312900	-1.82929600
C	3.25210000	5.25343900	-1.19786500
C	3.70552600	5.53228700	0.13140400
C	4.22967100	4.88755300	-2.28341200
C	-0.06137000	2.88179900	-1.42607500
C	1.26167500	2.43602700	-1.62179200
C	2.28581100	2.58625400	-0.67909700
C	5.07686600	5.42757900	0.48060700
C	5.51366900	5.69667900	1.77140200
C	4.61295000	6.07579400	2.76638000
C	3.25362000	6.18386300	2.44369900
C	2.80686100	5.91810500	1.16198600
C	3.59374100	4.43766800	-3.55773500
C	3.91986600	4.87140300	-4.77540700
C	1.92863400	5.54221500	-1.54737500
H	4.87015200	4.06881700	-1.90392500
H	4.92138700	5.72461500	-2.48534800
H	-0.71239500	2.97803700	-2.29067000
H	-0.25169200	3.59526100	-0.62696400
H	1.50806500	1.97707800	-2.58194700
H	2.03137500	3.10062400	0.24803100
H	5.80351500	5.13757700	-0.27583700
H	6.57566400	5.61495300	2.00162700
H	4.96146400	6.29771000	3.77275500
H	2.53749000	6.48608600	3.20696000
H	1.74761300	6.01445300	0.92188400
H	2.79970700	3.69216500	-3.44958400
H	3.42747000	4.49566500	-5.66936600
H	4.68859600	5.63011000	-4.92301200
C	3.62287700	2.07068500	-0.76340600
C	4.49962600	2.26492600	0.32720600
C	4.13014300	1.38509000	-1.89128300
C	5.81040600	1.80977600	0.29246700
H	4.12344700	2.78577300	1.21361300
C	5.43996800	0.92550700	-1.91723400
H	3.49354800	1.20783600	-2.76225400
C	6.29070400	1.13264400	-0.82904600
H	6.46133300	1.98578400	1.14621500

H	5.80404200	0.40014000	-2.79810800
H	7.31629600	0.77304100	-0.85831300

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Pd	-0.06140800	1.11689400	-0.34887100
P	-2.17452000	0.33447200	-0.35315800
P	1.04784300	-0.82172400	-0.04521100
C	-1.38513300	-2.08695300	-1.60932300
C	-2.03002600	-0.85613700	-1.76613900
C	-2.38052000	-0.39367900	-3.04685100
C	-2.07777000	-1.14773000	-4.17894000
C	-1.39036300	-2.36122300	-4.06615800
C	-1.04397700	-2.81140200	-2.78945800
C	-1.04537900	-2.70147700	-0.30532800
C	0.03064900	-2.29823200	0.48961500
C	0.30670800	-2.95123900	1.69961600
C	-0.48825100	-4.01206500	2.13207700
C	-1.56858800	-4.44927000	1.36194300
C	-1.83320600	-3.79855500	0.15325400
C	-2.99667600	-0.68712400	0.96406900
C	-2.50601400	-0.64271300	2.26341700
C	-3.14853600	-1.34399100	3.30338700
C	-4.35598500	-2.00234400	2.98549100
C	-4.84614800	-2.11616000	1.66159700
C	-4.11983900	-1.45711300	0.66294800
C	-3.67595300	1.34896900	-0.80421100
C	-4.85525600	0.78954900	-1.29460200
C	-6.00849800	1.56358400	-1.48158300
C	-5.91636800	2.94011800	-1.16502300
C	-4.70397900	3.56013000	-0.79763100
C	-3.59702900	2.71875400	-0.57731600
C	1.94594400	-1.58036600	-1.47037900
C	1.97405700	-0.82420000	-2.64074400
C	2.67516900	-1.27179300	-3.77333500
C	3.39820000	-2.47703200	-3.64292700
C	3.27706800	-3.32539900	-2.52188900
C	2.53463900	-2.84079900	-1.43224100
C	2.30351800	-0.79778400	1.32272700
C	3.36600100	-1.68184100	1.47463100
C	4.17803500	-1.65527800	2.62110800
C	3.92616900	-0.63393400	3.56560100
C	2.84919600	0.27446000	3.44581300
C	2.05861000	0.17830100	2.28873200
H	-2.88522800	0.56465200	-3.18347100
H	-2.36775900	-0.78815300	-5.16552000
H	-1.14024900	-2.93026600	-4.95372700
H	1.14124500	-2.65272400	2.33687700
H	-0.27037800	-4.50626100	3.07813600
H	-2.18989700	-5.26411400	1.71642600
H	-1.60468900	-0.06362800	2.49281000
H	-4.44589500	-1.54830800	-0.38062300
H	-4.89287800	-0.28390300	-1.51893800
H	-2.66207300	3.16833500	-0.21631300
H	1.44013700	0.13998300	-2.68474900
H	2.42686200	-3.47398300	-0.54326200
H	3.58494600	-2.41825200	0.69590200
H	1.23992500	0.90283400	2.13389500
O	-0.35291200	-3.97856000	-2.54010600
O	-2.87771300	-4.14517500	-0.68359100
C	0.31810800	-4.61705600	-3.65229100
H	0.94344900	-3.89874700	-4.19452200
H	0.95329400	-5.35260400	-3.12521900
H	-0.41360300	-5.10364400	-4.29981000
C	-3.53373000	-5.41180600	-0.42584700
H	-4.14618500	-5.32998300	0.48845000

H	-4.16481400	-5.52479100	-1.31595100	H	5.84695700	-5.47427600	-1.68017400
H	-2.80472500	-6.22345600	-0.36269100	H	5.93029900	-3.83001900	-2.33593900
O	-7.07080500	3.72951800	-1.30377800	H	5.21950600	-4.11475500	-0.73311700
O	-5.06455200	-2.66945200	4.00046700	C	3.05984600	-5.63903500	-1.52509500
O	4.71217600	-0.58122500	4.72914900	H	2.96357400	-5.26939800	-0.49803700
O	4.23462000	-2.87798600	-4.70050200	H	2.04093100	-5.72880000	-1.93542000
C	-7.81593300	3.90161200	-0.07323600	H	3.48746300	-6.64389600	-1.46756900
H	-8.63336500	4.56091900	-0.38235600	C	-6.10369400	-2.90539900	1.27279000
H	-8.19556500	2.92694900	0.26946600	C	-6.19333400	-3.15011600	-0.25283100
H	-7.18369900	4.37910500	0.69150800	H	-6.42051400	-2.22725100	-0.81163500
C	5.59860100	-2.41089300	-4.53994000	H	-5.25438400	-3.54909400	-0.65549600
H	6.01765700	-2.78852300	-3.59527800	H	-6.98722700	-3.86441600	-0.48797200
H	6.10491500	-2.84943100	-5.40571900	C	-6.09246000	-4.28572500	1.95502500
H	5.61688100	-1.31092900	-4.58317100	H	-6.04147700	-4.19275000	3.05021200
C	5.91145900	0.22147500	4.61964800	H	-6.98735300	-4.86409300	1.71546400
H	6.36182400	0.10651900	5.61144400	H	-5.21197700	-4.86583000	1.64028900
H	6.56948500	-0.18128400	3.83468300	C	-7.35274600	-2.09511600	1.67332200
H	5.64405900	1.27116100	4.42427700	H	-8.27077700	-2.64379900	1.44457700
C	-5.97769400	-1.83185000	4.74912200	H	-7.36484600	-1.86795300	2.74786400
H	-6.77842500	-1.47266700	4.08476200	H	-7.39169000	-1.13638900	1.12970900
H	-6.36786400	-2.52279300	5.50334000	C	-2.49620400	-1.35392300	4.69295100
H	-5.43841600	-0.99244000	5.21429300	C	-3.08229600	-0.19450700	5.52381100
C	-4.52379600	5.07432900	-0.61899400	H	-4.16800400	-0.30669900	5.66032300
C	-4.88853500	5.44049000	0.83399500	H	-2.62857200	-0.15068400	6.51827500
H	-4.77130500	6.51404000	1.01158800	H	-2.91176000	0.76985500	5.03503500
H	-5.93068900	5.17663000	1.06522000	C	-0.96618300	-1.15396400	4.59310800
H	-4.24712200	4.91493400	1.54854300	H	-0.51689500	-1.87725400	3.90245300
C	-5.38894600	5.86899000	-1.61324000	H	-0.68846100	-0.14637500	4.24436100
H	-6.46167900	5.73842500	-1.42769500	H	-0.48691200	-1.29247200	5.56747300
H	-5.17380800	6.93989000	-1.56304100	C	-2.70968800	-2.70186600	5.40590600
H	-5.20965900	5.53704000	-2.64158100	H	-2.15403500	-2.75230800	6.34572300
C	-3.05763400	5.48842100	-0.87726500	H	-3.76458100	-2.88927100	5.63700100
H	-2.35941800	5.03765000	-0.16159200	H	-2.38086100	-3.53218800	4.77063000
H	-2.73108800	5.20319900	-1.88253600	C	5.25692400	-2.73673400	2.77481000
H	-2.93028600	6.57312700	-0.79018600	C	4.92441700	-3.99005000	1.92722600
C	-7.29182600	0.88725900	-1.98154300	H	3.93391300	-4.38563900	2.17457500
C	-8.03375000	1.78225700	-2.98938600	H	4.94936300	-3.78649700	0.84422400
H	-8.91511400	1.28399600	-3.40026900	H	5.64886800	-4.78913900	2.11508000
H	-8.36969300	2.72270600	-2.53009000	C	6.60215300	-2.16911100	2.28007800
H	-7.38110600	2.06025300	-3.82347500	H	7.39370100	-2.92251900	2.32816500
C	-8.18515300	0.57837700	-0.76257600	H	6.52693200	-1.82343200	1.24357700
H	-9.11492900	0.08962600	-1.06666300	H	6.92548500	-1.31372900	2.89155100
H	-7.67512600	-0.08664800	-0.04604000	C	5.36682300	-3.21342300	4.23376300
H	-8.45588400	1.49688700	-0.22188500	H	6.08377300	-4.03176600	4.33774400
C	-6.98849800	-0.44706400	-2.70297000	H	5.68464400	-2.40890200	4.90934500
H	-6.26873200	-0.30860400	-3.51612100	H	4.39790900	-3.56217700	4.60705100
H	-6.58570800	-1.20730800	-2.01374700	C	2.50360400	1.34351500	4.49255000
H	-7.89805200	-0.86840800	-3.14266400	C	1.06109100	1.87144800	4.30848100
C	2.62382600	-0.43897900	-5.05966300	H	0.91747700	2.35278400	3.33357200
C	2.63767500	-1.33571700	-6.31072700	H	0.32047000	1.05844600	4.38967000
H	1.82922500	-2.07248900	-6.27615800	H	0.81359100	2.61182800	5.07507400
H	2.51971000	-0.74894100	-7.22550400	C	3.46780000	2.53459800	4.32115300
H	3.57618700	-1.89999200	-6.39859400	H	3.16887100	3.38458200	4.94061700
C	1.32442500	0.39597200	-5.11729600	H	4.49513800	2.26680300	4.60677200
H	0.43735600	-0.24776600	-5.05800000	H	3.49847800	2.87544800	3.27324500
H	1.25435000	1.11641800	-4.29345000	C	2.59266400	0.76723700	5.91638700
H	1.26018800	0.96344800	-6.05008900	H	3.60705500	0.41664300	6.15261300
C	3.83288700	0.51819000	-5.07065400	H	2.31678900	1.51048800	6.66861500
H	3.80160900	1.20680100	-4.21805600	H	1.92979400	-0.09632100	6.03372900
H	4.78020900	-0.03804300	-5.01954200	N	0.93886300	6.31580100	0.12558500
H	3.85311000	1.12121800	-5.98336500	C	2.91097300	4.69192700	-0.51453600
C	3.92523200	-4.70978900	-2.40768400	C	4.08906600	4.99082300	0.41382900
C	4.07104100	-5.40583300	-3.77255400	C	3.29500300	4.90190300	-2.00793700
H	4.82224400	-4.91803400	-4.40557200	C	-0.08469600	3.25322900	-0.84671500
H	4.36899500	-6.45189200	-3.66084700	C	1.22037500	2.81030200	-1.06907000
H	3.13381000	-5.37663300	-4.33691900	C	2.39463100	3.19296600	-0.20558800
C	5.30917900	-4.52483100	-1.75188100	C	5.40655500	4.77484000	-0.00355500

C	6.47077800	4.95600200	0.87577400
C	6.23676800	5.35090300	2.19095500
C	4.92808200	5.56590600	2.61818500
C	3.86489600	5.38633900	1.73687300
C	2.17867300	5.26581100	-2.93685200
C	2.21884600	6.31729200	-3.75553300
C	1.81275500	5.60329300	-0.17423700
H	3.79277100	3.98135700	-2.35054800
H	4.05481400	5.69281700	-2.05825900
H	-0.77350500	3.37513800	-1.68321000
H	-0.32687600	3.83558900	0.04234800
H	1.47870300	2.53285000	-2.09445900
H	2.06617200	3.24357500	0.84416600
H	5.61014100	4.43026200	-1.01675100
H	7.48797700	4.77764300	0.53009400
H	7.06962500	5.49561100	2.87709000
H	4.73035100	5.88240800	3.64118800
H	2.84592100	5.56830200	2.07910000
H	1.29142600	4.63170300	-2.93223000
H	1.39610200	6.55018700	-4.42809400
H	3.07571700	6.99164500	-3.78079700
C	3.54400300	2.21171600	-0.27777400
C	4.28878200	1.93618900	0.87423600
C	3.92469600	1.58067800	-1.46803200
C	5.38064300	1.07464100	0.84359900
H	4.00196000	2.41312200	1.81870100
C	5.01672500	0.71448000	-1.50539400
H	3.35848800	1.74250800	-2.38640800
C	5.75400700	0.46244800	-0.35121700
H	5.93323500	0.87290400	1.75976500
H	5.27799300	0.22154500	-2.44111400
H	6.60199800	-0.21957200	-0.37953700

### PhCF<sub>3</sub>

C	-2.11953100	1.18619600	0.23657100
C	-0.72965500	1.17154300	0.22824700
C	-0.05059100	-0.02493100	-0.01386200
C	-0.75807900	-1.20268000	-0.24579000
C	-2.15131300	-1.18159500	-0.23622600
C	-2.83181800	0.00926500	0.00422600
H	-2.64929700	2.11808300	0.42401500
H	-0.16604100	2.08555500	0.40747200
H	-0.22149100	-2.12907500	-0.43415300
H	-2.70480500	-2.10065100	-0.41845800
H	-3.92022200	0.02253000	0.01041600
C	1.44664500	-0.01132100	-0.00654600
F	1.98127100	-1.20614100	-0.33220600
F	1.94080500	0.32437100	1.21117200
F	1.94616700	0.89885300	-0.87795900

### TS-8

Pd	-0.05755000	0.90910100	-0.21436100
P	1.85493000	-0.17861100	0.25605600
P	-1.41526800	-0.88098600	-0.18619600
C	0.87573700	-2.67655800	1.18338700
C	1.56372000	-1.50485300	1.50551400
C	1.91945800	-1.22426500	2.83412800
C	1.61113700	-2.12592200	3.85268600
C	0.93905700	-3.31732000	3.56822300
C	0.57736100	-3.58306900	2.24385100
C	0.45097100	-3.03136700	-0.18816800
C	-0.59761200	-2.40136300	-0.86521100
C	-0.98038500	-2.83432100	-2.14292000
C	-0.31521800	-3.89332200	-2.76261500

C	0.75207300	-4.53164000	-2.12769000
C	1.12899600	-4.09486900	-0.85367400
C	2.55432900	-1.00916000	-1.22765000
C	1.98541300	-0.68855900	-2.45655600
C	2.49146900	-1.22282500	-3.65591900
C	3.65935500	-2.01143000	-3.56363300
C	4.24730800	-2.37325000	-2.32481000
C	3.64921300	-1.86986500	-1.16221000
C	3.41112300	0.59780600	0.87642600
C	4.46142400	-0.17697800	1.36714200
C	5.68564900	0.40298600	1.72586800
C	5.82450100	1.79379700	1.51270600
C	4.74399400	2.62069900	1.13339900
C	3.53767700	1.98233300	0.79606900
C	-1.98162500	-1.39232300	1.47627300
C	-1.75787700	-0.51106500	2.53005000
C	-2.17031300	-0.82858200	3.83809500
C	-2.91186000	-2.01789000	4.00884100
C	-3.13529100	-2.94406500	2.95887800
C	-2.62924400	-2.60746900	1.69761600
C	-2.98908300	-0.87685200	-1.13912100
C	-3.91869300	-1.91531200	-1.08863700
C	-5.11306000	-1.85693600	-1.81820700
C	-5.34129800	-0.69223300	-2.59076300
C	-4.37012100	0.31811100	-2.75164600
C	-3.20848800	0.22067700	-1.96587600
H	2.43949800	-0.30215000	3.10606800
H	1.88947400	-1.90031800	4.88256400
H	0.68934300	-4.00161800	4.37276200
H	-1.80296800	-2.36403400	-2.68840200
H	-0.62321000	-4.22219500	-3.75547800
H	1.27861700	-5.33550000	-2.63187700
H	1.12003800	-0.00633400	-2.51058200
H	4.05125800	-2.15770200	-0.18475000
H	4.34942500	-1.26463300	1.46955700
H	2.69603100	2.59925500	0.45610100
H	-1.25381500	0.45497300	2.35113400
H	-2.75279500	-3.31050300	0.86410000
H	-3.72450000	-2.79778500	-0.46567900
H	-2.47368000	1.04193400	-2.00765100
O	-0.10695300	-4.71229000	1.84510100
O	2.18748600	-4.61983800	-0.14126900
C	-0.26025200	-5.77753700	2.81553400
H	-0.99489700	-5.47416900	3.58302400
H	-0.65571100	-6.59148000	2.19508400
H	0.70250200	-6.05344700	3.25207600
C	2.81933400	-5.81353100	-0.66543400
H	3.37583800	-5.56592400	-1.58718000
H	3.50568300	-6.07975600	0.14801500
H	2.08388000	-6.60500300	-0.82873600
O	7.07527100	2.38344400	1.75019100
O	4.20971600	-2.57225000	-4.72533000
O	-6.55564400	-0.58626600	-3.28423500
O	-3.35509100	-2.37319600	5.29165600
C	7.93307200	2.39587100	0.58014900
H	8.84844800	2.85802200	0.96447400
H	8.11544600	1.36744300	0.23454200
H	7.47503300	3.01563600	-0.20731400
C	-4.62888000	-1.80748200	5.68525500
H	-5.42750000	-2.21234300	5.04548900
H	-4.73069700	-2.15618200	6.71837000
H	-4.59663300	-0.70772400	5.63538700
C	-7.57448700	0.15760400	-2.56804200
H	-8.41723300	0.13288400	-3.26701700
H	-7.81846000	-0.35892400	-1.62749400
H	-7.23427200	1.18951100	-2.38952800
C	5.09350800	-1.70624900	-5.47840400

H	6.02004200	-1.54574700	-4.90715700	H	6.82934200	-1.54408300	-2.14422400
H	5.28227200	-2.29348200	-6.38357300	C	1.73665600	-0.91105200	-4.95761000
H	4.60163300	-0.75061100	-5.71613900	C	2.37363400	0.32745600	-5.61611100
C	4.82865400	4.15283900	1.05280600	H	3.43237600	0.16210900	-5.86257900
C	5.40296900	4.53203900	-0.32585800	H	1.86056700	0.59172400	-6.54664600
H	5.49982400	5.61909900	-0.42536100	H	2.32528500	1.20126700	-4.95670300
H	6.39774400	4.09466000	-0.48749600	C	0.24960100	-0.58608000	-4.67305700
H	4.75021300	4.19468900	-1.13866500	H	-0.25694300	-1.43273700	-4.19761700
C	5.70550800	4.71864100	2.18344700	H	0.13078300	0.28475600	-4.01645600
H	6.75212700	4.39963100	2.09368200	H	-0.28561400	-0.36110200	-5.60145800
H	5.69688000	5.81281800	2.18394600	C	1.74412000	-2.11568100	-5.91431100
H	5.35438800	4.38144500	3.16392300	H	1.11612200	-1.93407700	-6.79126600
C	3.43332300	4.79738000	1.19653700	H	2.74921300	-2.35702000	-6.27696100
H	2.76886600	4.55785800	0.35639500	H	1.37310500	-3.01591900	-5.41195000
H	2.93651900	4.49637400	2.12368600	C	-6.10134600	-3.02793400	-1.72807100
H	3.50765900	5.89218300	1.21373400	C	-5.39312400	-4.33522600	-1.29972500
C	6.78795400	-0.50287100	2.29068900	H	-4.58246400	-4.59201400	-1.98946100
C	7.67618600	0.23738600	3.30371400	H	-4.97118700	-4.27742200	-0.28357500
H	8.36933700	-0.44257100	3.80618700	H	-6.09742000	-5.17409200	-1.30023200
H	8.27505500	1.02631300	2.83113900	C	-7.16404300	-2.67675300	-0.66813500
H	7.07154700	0.73237200	4.07201900	H	-7.90222100	-3.47740800	-0.56403300
C	7.62696700	-1.02318100	1.10638100	H	-6.70915300	-2.50861900	0.31317500
H	8.47751000	-1.61775700	1.45222800	H	-7.70914700	-1.75956200	-0.93874500
H	7.02536700	-1.65912400	0.43645900	C	-6.76063100	-3.30724200	-3.08957300
H	8.02584000	-0.19107100	0.50701300	H	-7.40310400	-4.19090600	-3.05337300
C	6.17358900	-1.71146300	3.03671900	H	-7.38173200	-2.46454400	-3.42485000
H	5.53832000	-1.38089300	3.86567200	H	-6.00866500	-3.46701900	-3.86912000
H	5.56345600	-2.34292800	2.38216100	C	-4.50117100	1.51138200	-3.70954700
H	6.95737000	-2.34839000	3.45938100	C	-3.10314500	2.02629100	-4.12296300
C	-1.78221600	0.13026700	4.97452100	H	-2.55426900	2.47194600	-3.28016100
C	-1.41972100	-0.64083400	6.25610500	H	-2.48896100	1.23043700	-4.55302300
H	-0.63549700	-1.37949800	6.06001000	H	-3.18390700	2.81791700	-4.87862500
H	-1.06239500	0.03380000	7.03914900	C	-5.24875000	2.63461200	-2.96958800
H	-2.27380100	-1.19366900	6.66465800	H	-5.20892000	3.58062400	-3.53305800
C	-0.53655900	0.96424700	4.59111500	H	-6.30423900	2.38344100	-2.80272800
H	0.31793100	0.32190200	4.35543100	H	-4.79170800	2.83722100	-1.98412800
H	-0.72398800	1.60733200	3.71996200	C	-5.23446800	1.12303800	-5.00422200
H	-0.23861000	1.62404500	5.41210600	H	-6.26678400	0.80135000	-4.81783900
C	-2.94998500	1.10235800	5.22241800	H	-5.27642500	1.96412900	-5.70295600
H	-3.22091200	1.63906900	4.30301300	H	-4.73409800	0.29044000	-5.50887700
H	-3.85141000	0.58164000	5.57402600	N	0.83293000	5.25127600	-2.25828400
H	-2.69144600	1.85273600	5.97580800	C	-1.27572900	6.11999100	-1.09973600
C	-3.89968300	-4.26467400	3.12904100	C	-1.18723000	6.46694800	0.30500200
C	-3.41973800	-5.00537600	4.38955600	C	-2.58688000	6.24103300	-1.83316200
H	-3.58325100	-4.40596500	5.29769100	C	0.95335300	3.21877100	-1.67645100
H	-3.94274100	-5.95491500	4.52542500	C	0.16101000	3.11980600	-0.52242900
H	-2.33969000	-5.20997300	4.33608200	C	-1.23440000	2.84857800	-0.57624000
C	-5.40926100	-3.96113900	3.21010700	C	-2.34117500	6.80928400	1.04085100
H	-5.99661300	-4.88221700	3.27376200	C	-2.26598900	7.11811700	2.39449200
H	-5.65592800	-3.35767400	4.09566500	C	-1.04431000	7.09789400	3.06392200
H	-5.75106700	-3.40598200	2.33045800	C	0.10985000	6.75548200	2.35292900
C	-3.68937100	-5.21561100	1.92622900	C	0.04211600	6.44542100	1.00338500
H	-4.19201000	-4.84681400	1.01746300	C	-2.48154300	6.11095300	-3.31805000
H	-2.62674700	-5.34625400	1.69105500	C	-3.30571600	5.40517900	-4.09311600
H	-4.10502700	-6.20622200	2.13453400	C	-0.16559700	5.69021100	-1.75770500
C	5.48563500	-3.27312900	-2.20343000	H	-3.01625200	7.23216800	-1.60083700
C	5.75685800	-3.70356700	-0.74176400	H	-3.31740500	5.51226600	-1.43703900
H	6.11773700	-2.85944300	-0.12951700	H	2.03157200	3.30830600	-1.60418900
H	4.86212700	-4.11226800	-0.26029600	H	0.57647300	2.84731100	-2.62581700
H	6.53213400	-4.47507700	-0.70072700	H	0.57422100	3.53114800	0.40029800
C	5.28429100	-4.55153300	-3.03662000	H	-1.68186700	2.77290400	-1.57380300
H	5.10952500	-4.31497200	-4.09755100	H	-3.31458400	6.80822800	0.55354300
H	6.15562900	-5.20883200	-2.98762100	H	-3.17927100	7.36711000	2.93453900
H	4.40664000	-5.11445300	-2.68478500	H	-0.98908100	7.34305500	4.12304800
C	6.73015700	-2.49569600	-2.67630700	H	1.07545500	6.73761800	2.85794700
H	7.64562500	-3.07148400	-2.50878700	H	0.95220800	6.19375600	0.45780400
H	6.68558500	-2.27044800	-3.75114500	H	-1.66641900	6.67146400	-3.78424400

H	-3.19337500	5.38354400	-5.17482900
H	-4.13485600	4.82410800	-3.67493800
C	-2.16031300	3.13837000	0.50704800
C	-3.54636400	3.14991500	0.25924100
C	-1.73368200	3.42865400	1.81925700
C	-4.46108800	3.43342200	1.26761400
H	-3.90461000	2.92428900	-0.75391700
C	-2.64723400	3.72222900	2.82134900
H	-0.66979200	3.45228900	2.05048200
C	-4.01823700	3.71962100	2.55823800
H	-5.52701600	3.43286100	1.04343600
H	-2.28338200	3.97107600	3.81780800
H	-4.73112800	3.95290000	3.34673400

### TS-11

Pd	-0.07805700	1.02888000	0.25168500
P	-2.14911500	0.36371300	-0.25130200
P	1.05347600	-0.89120900	-0.15264800
C	-1.22528400	-1.40842900	-2.25570000
C	-1.84879300	-0.18912500	-1.98413400
C	-2.06232300	0.74925200	-3.00782400
C	-1.66822500	0.46957300	-4.31591200
C	-1.01588400	-0.72810100	-4.62266500
C	-0.78556500	-1.64491600	-3.59280900
C	-0.98509200	-2.47862900	-1.26138500
C	0.05571700	-2.45240500	-0.32866700
C	0.29466300	-3.55167000	0.50531800
C	-0.52370300	-4.68104100	0.43705000
C	-1.59491500	-4.73170000	-0.45749400
C	-1.81562000	-3.63593300	-1.29877000
C	-3.02130100	-1.03773700	0.56594100
C	-2.55494500	-1.51816600	1.78587400
C	-3.24740400	-2.53040100	2.47830100
C	-4.47897900	-2.95530600	1.93296500
C	-4.95042400	-2.52374700	0.66849000
C	-4.17795700	-1.56972300	-0.00518800
C	-3.59433600	1.49871100	-0.39714700
C	-4.63527100	1.26027200	-1.29354000
C	-5.77307300	2.07813500	-1.31973800
C	-5.83974900	3.11778600	-0.36370200
C	-4.75515100	3.45564100	0.47472800
C	-3.64038500	2.59916800	0.45518700
C	2.04818800	-0.95072100	-1.69363000
C	2.14130400	0.23900900	-2.41377500
C	2.93225900	0.32224900	-3.57226800
C	3.68371000	-0.82205600	-3.91637600
C	3.51245100	-2.07207900	-3.27969400
C	2.67217000	-2.10722100	-2.15622200
C	2.23936200	-1.36006700	1.17975500
C	3.34780200	-2.18229400	1.01186800
C	4.14587800	-2.56247900	2.10400700
C	3.82052900	-2.01056300	3.36390000
C	2.68988300	-1.18384800	3.57165300
C	1.92651600	-0.85104500	2.44206000
H	-2.52420600	1.71903400	-2.80751800
H	-1.85710700	1.19499900	-5.10759700
H	-0.69567100	-0.92843800	-5.63980500
H	1.11786000	-3.55873600	1.22338200
H	-0.33133200	-5.53183000	1.09078700
H	-2.23873000	-5.60449100	-0.48213600
H	-1.63468500	-1.11498500	2.22443500
H	-4.49337100	-1.23840300	-1.00091900
H	-4.58588900	0.41255600	-1.98968100
H	-2.80507900	2.81496000	1.13538500
H	1.59254900	1.13581400	-2.08027600

H	2.51818500	-3.06213900	-1.64009100
H	3.62209700	-2.54466400	0.01638700
H	1.07761000	-0.15897300	2.55713400
O	-0.12612100	-2.84282200	-3.75584300
O	-2.84438500	-3.55919400	-2.21487600
C	0.64009200	-3.02833500	-4.97153400
H	1.29119000	-2.16699800	-5.15995100
H	1.25025400	-3.91294500	-4.70893200
H	-0.03330900	-3.23310000	-5.80594700
C	-3.61913500	-4.76002700	-2.45216500
H	-4.25258400	-4.97183100	-1.57287000
H	-4.22905100	-4.46670200	-3.31587300
H	-2.96943100	-5.60158700	-2.70519700
O	-7.01362100	3.88375300	-0.29168300
O	-5.23260400	-3.93327500	2.59998400
O	4.57869400	-2.38372500	4.48358800
O	4.60225100	-0.73732600	-4.97524900
C	-7.98782100	3.35055800	0.64111900
H	-8.82078800	4.05420200	0.53923100
H	-8.28132100	2.33387600	0.33962100
H	-7.57312400	3.36994500	1.66133500
C	5.92199300	-0.31424000	-4.54334000
H	6.33235100	-1.04639000	-3.83187900
H	6.48713300	-0.30576200	-5.48084000
H	5.86478400	0.69434600	-4.10307700
C	5.74596300	-1.56450100	4.73735900
H	6.20417000	-2.07000300	5.59431600
H	6.41632700	-1.56753600	3.86445800
H	5.43124900	-0.54281800	5.00097800
C	-6.09609000	-3.43380300	3.65053700
H	-6.90716100	-2.83978800	3.20384000
H	-6.48076400	-4.35728200	4.09680500
H	-5.52374900	-2.84365300	4.38221400
C	-4.73574900	4.68123800	1.40121500
C	-5.41973900	4.28982200	2.72719400
H	-5.43773100	5.13616300	3.42197200
H	-6.45943400	3.97166100	2.56571300
H	-4.89056900	3.46974100	3.22160400
C	-5.45258100	5.87897300	0.75447200
H	-6.52392600	5.69273900	0.60828400
H	-5.35527800	6.77960300	1.36819400
H	-5.03306100	6.10375600	-0.23207400
C	-3.29054800	5.12769400	1.70092900
H	-2.70721600	4.37220200	2.23877700
H	-2.73755900	5.37641100	0.78738900
C	-3.26989300	6.02835500	2.32674500
C	-6.86878800	1.77858800	-2.35137600
C	-7.58223400	3.05796800	-2.81758600
H	-8.26558500	2.86008200	-3.64769700
H	-8.16738500	3.52267300	-2.01380900
H	-6.86107900	3.81476600	-3.14670100
C	-7.86974200	0.79835400	-1.70734200
H	-8.71195900	0.59427800	-2.37478800
H	-7.39024200	-0.16544700	-1.46980900
H	-8.27926800	1.20697400	-0.77158300
C	-6.26688700	1.11859300	-3.61482300
H	-5.52199300	1.77125300	-4.08317700
H	-5.78057900	0.16155100	-3.39789300
H	-7.04403400	0.92271700	-4.36074200
C	2.94166100	1.63596100	-4.36656600
C	3.11581200	1.38221700	-5.87467400
H	2.36142900	0.68411600	-6.24903900
H	3.02986300	2.31092100	-6.44621400
H	4.09539100	0.94515200	-6.10744800
C	1.60029900	2.38441000	-4.18876000
H	0.75157100	1.76261700	-4.49290800
H	1.43166700	2.69396300	-3.14947300



C	-3.99327900	-1.08187900	1.65818100	H	-2.98644200	4.62770900	-1.74092000
C	-3.21636200	0.35992900	-1.18624300	C	-4.16927300	3.49439400	-4.83681400
C	-4.50854800	-0.15981200	-1.24772200	H	-5.23833100	3.68169400	-4.67601800
C	-5.51752700	0.48499000	-1.97410600	H	-3.78704400	4.30882300	-5.45969000
C	-5.17110500	1.69190500	-2.63025900	H	-4.09737900	2.56700300	-5.41399500
C	-3.84491200	2.17198200	-2.69325800	C	-1.89362500	3.27962700	-3.87829900
C	-2.88425500	1.49047800	-1.92668300	H	-1.24738200	3.28337200	-2.98420600
C	1.55062300	-2.05927700	-1.12035400	H	-1.68250800	2.37292700	-4.45218100
C	1.33497600	-1.40419400	-2.33147200	H	-1.57746600	4.13530100	-4.48735300
C	1.52658600	-2.06640200	-3.55615900	C	-6.92582700	-0.12570400	-1.98947500
C	2.06003000	-3.37181000	-3.50094700	C	-7.58551800	0.03362600	-3.36907400
C	2.21548600	-4.08742300	-2.28907100	H	-8.55735100	-0.46497400	-3.41337000
C	1.92130300	-3.40429100	-1.10006300	H	-7.74755100	1.09036900	-3.62595600
C	3.12197700	-0.90941100	0.96729700	H	-6.95507400	-0.38377000	-4.16115400
C	4.04120400	-1.94633500	0.82794500	C	-7.76265200	0.56907900	-0.89740100
C	5.35701900	-1.81873800	1.29862500	H	-8.79523500	0.20757800	-0.89809600
C	5.71323000	-0.58628200	1.89321000	H	-7.34470300	0.38720800	0.10635300
C	4.77702900	0.44409800	2.13856500	H	-7.79575100	1.65848200	-1.04943900
C	3.48726700	0.27363900	1.61090800	C	-6.88945100	-1.64197900	-1.68006000
H	-2.79692000	-1.71597100	-2.57466600	H	-6.23882400	-2.17596000	-2.37996900
H	-2.55903500	-4.01532100	-3.38994400	H	-6.54420800	-1.85568200	-0.65646800
H	-1.42234300	-5.74635200	-1.98594400	H	-7.89009600	-2.07839900	-1.77190300
H	2.10610600	-1.45187200	3.16030800	C	1.15685000	-1.32728600	-4.84980000
H	0.96076000	-2.49483400	5.05497200	C	0.62376300	-2.29338100	-5.92140900
H	-1.21983600	-3.63491200	4.75115600	H	-0.20581500	-2.89390800	-5.53398100
H	-1.22364300	0.76032000	2.44462900	H	0.26848100	-1.75511900	-6.80448400
H	-4.39909800	-1.68545200	0.83598300	H	1.39037300	-3.00345200	-6.25630200
H	-4.75369000	-1.08347500	-0.70759800	C	0.03551700	-0.29461600	-4.57979500
H	-1.85299900	1.88201400	-1.91432700	H	-0.85792800	-0.77597700	-4.16892600
H	1.01671700	-0.34608700	-2.35222600	H	0.35301000	0.48253000	-3.87125000
H	1.98717400	-3.94163200	-0.14552500	H	-0.25803900	0.21402900	-5.50356800
H	3.75705000	-2.88062900	0.33501900	C	2.40367400	-0.57949700	-5.35750500
H	2.76900000	1.10046100	1.70620900	H	2.77418900	0.13244800	-4.60880400
O	-0.30209200	-5.27983600	0.36846700	H	3.22611700	-1.27383600	-5.58386200
O	-2.44355800	-3.91963700	2.31605200	H	2.18793600	-0.01675400	-6.27055800
C	-1.09154900	-6.36829100	0.91578900	C	2.72451600	-5.53452900	-2.21803000
H	-1.50783200	-6.97883900	0.11181500	C	2.13123900	-6.39076600	-3.35011700
H	-0.34681000	-6.92414700	1.49641500	H	2.46254800	-6.04926000	-4.34029100
H	-1.87689100	-5.95870500	1.56419700	H	2.41874300	-7.44089000	-3.25335900
C	-3.36343300	-4.13296900	3.41509100	H	1.03780900	-6.33662100	-3.35036500
H	-3.45527300	-3.23159200	4.03351300	C	4.26464100	-5.49913500	-2.30307600
H	-4.31156800	-4.31633900	2.87770500	H	4.68518500	-6.50870100	-2.28170800
H	-3.04788300	-5.00230700	3.99532300	H	4.60873200	-5.01864900	-3.23007900
O	-6.18089000	2.38924700	-3.30730800	H	4.69703000	-4.93936000	-1.45787300
O	-4.88832000	-0.03738600	5.06993800	C	2.33394800	-6.21290300	-0.88752600
O	7.03431300	-0.42149900	2.33301100	H	2.79265000	-5.73081400	-0.01872600
O	2.37839900	-4.02490100	-4.70152000	H	1.24396800	-6.18727500	-0.73355500
C	-6.79732700	3.43976300	-2.51907900	H	2.64286800	-7.26185900	-0.87478100
H	-7.51344400	3.87310200	-3.22528600	C	-6.12000300	-1.61455000	2.92326900
H	-7.30701800	2.99938100	-1.64898200	C	-6.27004300	-2.77048800	1.90534500
H	-6.03989000	4.18006900	-2.21382100	H	-6.24340100	-2.41504000	0.86281800
C	3.71512200	-3.74332100	-5.18752300	H	-5.47816800	-3.52331900	2.03004000
H	4.45774100	-4.11535200	-4.46490100	H	-7.23028400	-3.28082000	2.03565800
H	3.75000100	-4.31197800	-6.12262300	C	-6.39207700	-2.20523600	4.31763000
H	3.83482900	-2.66384300	-5.37019700	H	-6.41175200	-1.42570500	5.09315400
C	7.90101200	0.22986800	1.36976200	H	-7.35547900	-2.72157700	4.35490100
H	8.84884600	0.29493700	1.91418600	H	-5.61582700	-2.91472800	4.61477800
H	7.99525700	-0.39857500	0.47134900	C	-7.17017800	-0.53873000	2.58046700
H	7.51157400	1.23134000	1.12464300	H	-8.18635500	-0.93838800	2.64971300
C	-5.66398800	1.18701000	5.13110500	H	-7.10658900	0.31891400	3.26692200
H	-6.42184400	1.18717000	4.33282900	H	-7.03485800	-0.15022100	1.55698700
H	-6.12629800	1.12351900	6.12171600	C	-2.13260700	1.05425300	4.96072800
H	-4.99925700	2.06240800	5.05536900	C	-2.52413000	2.54346800	4.95850200
C	-3.39281900	3.39060400	-3.51352300	H	-3.60712000	2.67985300	5.09407800
C	-3.59180500	4.65342600	-2.65704000	H	-2.02352300	3.08877800	5.76562500
H	-3.29182800	5.55648100	-3.20118600	H	-2.24870000	3.03334500	4.01739900
H	-4.64039700	4.78507700	-2.35560800	C	-0.59908200	0.94915200	4.78419300

H	-0.27534500	-0.09596300	4.72606100
H	-0.24898200	1.45783000	3.87778900
H	-0.07634100	1.41120500	5.62835300
C	-2.46985600	0.40166300	6.31228400
H	-1.88669200	0.84433600	7.12523400
H	-3.52965700	0.51311900	6.57351800
H	-2.26271300	-0.67294600	6.29516200
C	6.32575100	-2.99903800	1.13588700
C	5.56766000	-4.33636700	0.96126300
H	4.85854300	-4.50494100	1.77772400
H	5.01605600	-4.38478300	0.00769200
H	6.26597700	-5.18031300	0.96175700
C	7.17534400	-2.75798900	-0.12750300
H	7.87854700	-3.57885200	-0.29624400
H	6.54731500	-2.66367100	-1.01897700
H	7.76540700	-1.83268100	-0.04274900
C	7.22193000	-3.15519800	2.37647200
H	7.86684900	-4.03447600	2.30029800
H	7.87433500	-2.28276500	2.52382400
H	6.62302700	-3.25247500	3.28777300
C	5.08831300	1.71996600	2.93642200
C	3.79845500	2.31239100	3.55116200
H	3.08962100	2.64958300	2.78456100
H	3.29375300	1.59728800	4.20461600
H	4.03259100	3.20255400	4.14906400
C	5.69337900	2.75958400	1.98078600
H	5.94547400	3.68861800	2.50812300
H	6.60617600	2.39521100	1.49262800
H	4.97855600	3.04499300	1.18797000
C	6.04398300	1.42545700	4.10631800
H	7.03567100	1.10878900	3.75944600
H	6.18751800	2.31093200	4.73286200
H	5.66072500	0.62086900	4.74102800
N	-0.75113900	5.49711200	0.63191400
C	1.60902300	5.93896700	-0.25740600
C	2.72997200	5.97578100	0.65546700
C	1.82760500	6.14237200	-1.73725100
C	-0.99274300	3.40094700	0.58140400
C	-0.14738800	2.94466800	-0.44072600
C	1.24105600	2.69785000	-0.23618400
C	4.04499800	6.19388200	0.18743900
C	5.12279100	6.23989500	1.06472200
C	4.93429800	6.06850800	2.43527200
C	3.64098000	5.83944700	2.91635600
C	2.56222800	5.79062700	2.04819700
C	0.61182000	5.93817600	-2.57804100
C	0.12736300	6.81311800	-3.45943300
C	0.34839000	5.73934100	0.21782000
H	2.60119800	5.42066900	-2.06218100
H	2.25293400	7.14124400	-1.93168500
H	-2.06103200	3.49093900	0.41409700
H	-0.68539900	3.30682400	1.61953400
H	-0.51872500	3.05241300	-1.46811100
H	1.62403900	2.92688700	0.76097200
H	4.22238800	6.33274900	-0.87744500
H	6.12277300	6.42003900	0.67106100
H	5.77735600	6.12340000	3.12129700
H	3.47390000	5.70804600	3.98494500
H	1.55719000	5.62776500	2.43937100
H	0.10181100	4.97943100	-2.44066900
H	-0.75781400	6.59931200	-4.05431300
H	0.59889200	7.78359500	-3.61606600
C	2.23938300	2.71768300	-1.29476800
C	3.59311000	2.92566600	-0.96692500
C	1.91599600	2.57983200	-2.65987600
C	4.57115100	3.00678600	-1.95149300
H	3.87374800	3.04769900	0.08624400

C	2.89393400	2.66756200	-3.64254200
H	0.88082100	2.41231100	-2.95731100
C	4.22999600	2.87972000	-3.29801100
H	5.60683000	3.18282700	-1.66327800
H	2.60968000	2.57416100	-4.69014700
H	4.99328800	2.95052100	-4.07009300

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Pd	0.00325700	0.93484600	-0.28287200
P	-2.12896800	0.28546900	-0.30086300
P	0.94967200	-1.03760400	0.21348800
C	-1.69349000	-2.49264900	-0.73895700
C	-2.13446200	-1.27909900	-1.27315200
C	-2.49124600	-1.17143100	-2.62548600
C	-2.42258600	-2.28513000	-3.46339600
C	-1.98447300	-3.51590800	-2.97116600
C	-1.62418500	-3.61334600	-1.62258800
C	-1.29126000	-2.69403800	0.67233700
C	-0.10460200	-2.18556300	1.21502600
C	0.26462700	-2.46946900	2.53393900
C	-0.55908600	-3.25675900	3.34299700
C	-1.75815500	-3.76755900	2.84715400
C	-2.11263200	-3.49027000	1.52038100
C	-2.93315600	-0.15682500	1.27771400
C	-2.35708500	0.23997000	2.48150800
C	-3.00439200	-0.01074100	3.70590400
C	-4.29971200	-0.57041600	3.64788100
C	-4.87414900	-1.05457400	2.44664600
C	-4.14513200	-0.85012400	1.27050600
C	-3.47373800	1.25462800	-1.08966800
C	-4.74409000	0.70657400	-1.29141900
C	-5.80685400	1.48709100	-1.75948700
C	-5.54032200	2.85438200	-2.02091500
C	-4.23837200	3.39466200	-1.98457100
C	-3.22417400	2.57070200	-1.46628900
C	1.44698900	-2.10261800	-1.18279600
C	1.44868400	-1.53678900	-2.45506800
C	1.83892300	-2.28740600	-3.57815700
C	2.32708100	-3.59124000	-3.33986900
C	2.27722300	-4.21067500	-2.06718000
C	1.80673500	-3.43730600	-0.99790700
C	2.45943700	-0.89880200	1.23967900
C	3.48678500	-1.83605600	1.23902000
C	4.59619100	-1.70156100	2.09041400
C	4.66054700	-0.53762400	2.88882500
C	3.61042400	0.41342300	2.94559900
C	2.52857100	0.22128400	2.07529300
H	-2.82803300	-0.22528700	-3.05875900
H	-2.70666900	-2.19591200	-4.51287700
H	-1.91449800	-4.37035000	-3.63832800
H	1.19850600	-2.09644500	2.96468100
H	-0.26551400	-3.47278200	4.37102400
H	-2.40070400	-4.35921800	3.49218300
H	-1.38664700	0.75415100	2.49345600
H	-4.54408800	-1.23897300	0.32355800
H	-4.92748400	-0.35275100	-1.06791400
H	-2.21309000	3.00730900	-1.36566600
H	1.14120000	-0.48965700	-2.59867700
H	1.72630000	-3.89195900	-0.00399700
H	3.46113300	-2.69523700	0.56213400
H	1.73441800	0.98077700	2.04346800
O	-1.16808800	-4.76847900	-1.02975200
O	-3.27804700	-3.93971200	0.93468000
C	-1.14221100	-5.97641000	-1.83150300



H	-0.30365400	-5.92393500	-2.54702500	C	2.25140700	-6.59166700	-2.91658500
H	-0.95446700	-6.74416000	-1.06904500	H	2.70810200	-6.33979100	-3.88488800
H	-2.10087300	-6.14804800	-2.32602600	H	2.49692100	-7.63502200	-2.70298600
C	-4.03032500	-4.95452900	1.64859200	H	1.16354200	-6.51296900	-3.05204900
H	-4.54038300	-4.49184200	2.51134000	C	4.27043300	-5.65729900	-1.68764400
H	-4.75447700	-5.27480600	0.88864500	H	4.65187700	-6.66344600	-1.48942300
H	-3.38704800	-5.78682100	1.94445200	H	4.74690400	-5.30355800	-2.61363000
O	-6.61413000	3.67045400	-2.39986000	H	4.61308000	-5.00279400	-0.87042900
O	-5.02677000	-0.75243600	4.83223800	C	2.16444200	-6.19543600	-0.46643100
O	5.75634400	-0.36467600	3.74277700	H	2.58612500	-5.68067400	0.40377000
O	2.79399500	-4.35273700	-4.42081400	H	1.07520600	-6.08889500	-0.41580600
C	-7.18731400	4.42250700	-1.29915200	H	2.39892000	-7.25828500	-0.34785500
H	-7.95071000	5.02674400	-1.80140100	C	-6.23417800	-1.76444200	2.37889500
H	-7.63776700	3.72657100	-0.57611400	C	-6.44035300	-2.50165300	1.03544900
H	-6.41962100	5.05988000	-0.83127200	H	-6.60492600	-1.80430400	0.19696800
C	4.19331700	-4.14565700	-4.73963000	H	-5.58033900	-3.12949400	0.77662500
H	4.81825500	-4.47880000	-3.89687200	H	-7.32222000	-3.14879600	1.07799800
H	4.33147100	-4.78683000	-5.61671300	C	-6.33685100	-2.81674700	3.49736800
H	4.37810900	-3.08770300	-4.98408200	H	-6.23752500	-2.36024600	4.49393200
C	6.89105300	0.31501700	3.14583500	H	-7.29732000	-3.33812500	3.47534700
H	7.63762600	0.26695200	3.94551000	H	-5.53714000	-3.56631400	3.40475400
H	7.22820900	-0.21618800	2.24354600	C	-7.35143200	-0.71042200	2.50031200
H	6.61700200	1.35906300	2.92101600	H	-8.34016400	-1.17993500	2.49990100
C	-5.75990400	0.41901500	5.27211200	H	-7.26750000	-0.12975700	3.42944400
H	-6.55425600	0.64660100	4.54504300	H	-7.32224300	0.00180300	1.65874800
H	-6.17971100	0.08697200	6.22802200	C	-2.26817100	0.32934100	5.01042400
H	-5.07970700	1.27409000	5.40839100	C	-2.61695700	1.77513600	5.40954200
C	-3.86910100	4.81220000	-2.45522400	H	-3.69682300	1.89955400	5.57876300
C	-4.01640400	5.76712400	-1.25574700	H	-2.10621400	2.06574700	6.33394800
H	-3.77966800	6.79809400	-1.54639600	H	-2.32164400	2.49005900	4.63429700
H	-5.03619000	5.76065100	-0.84852300	C	-0.73875100	0.22348200	4.81468600
H	-3.32395900	5.50522900	-0.44767700	H	-0.45440100	-0.76069600	4.42648400
C	-4.76099800	5.26536100	-3.62470900	H	-0.34312900	0.98362700	4.12875700
H	-5.80534600	5.40784200	-3.32676800	H	-0.21451700	0.36081300	5.76799000
H	-4.40975800	6.21519200	-4.04184700	C	-2.62968400	-0.65282300	6.13873400
H	-4.75999300	4.52742700	-4.43345100	H	-2.00453600	-0.49358100	7.02266400
C	-2.41357400	4.86262900	-2.95945100	H	-3.67281500	-0.55812100	6.46073300
H	-1.66590000	4.65166800	-2.17332500	H	-2.49738200	-1.69072900	5.81453300
H	-2.24030200	4.17321900	-3.78873100	C	5.65272900	-2.81682500	2.08767900
H	-2.15040600	5.86920600	-3.31347200	C	5.04609600	-4.16432600	1.62136200
C	-7.19274800	0.85131200	-1.93659300	H	4.17679600	-4.43916500	2.22633000
C	-7.90206600	1.40263100	-3.18485000	H	4.74053700	-4.14761000	0.56359400
H	-8.85014100	0.89108200	-3.37099000	H	5.77984300	-4.97157700	1.72261200
H	-8.12399900	2.47572100	-3.09080000	C	6.77006000	-2.42237700	1.10393500
H	-7.27796600	1.29269000	-4.07787000	H	7.54028400	-3.19615500	1.04051000
C	-8.01767300	1.14157500	-0.66681000	H	6.37547900	-2.25368400	0.09601100
H	-9.03231500	0.74138800	-0.75430300	H	7.26622900	-1.48892600	1.41338300
H	-7.55805200	0.69499600	0.22949200	C	6.21865100	-3.06145000	3.49681300
H	-8.10585400	2.22388400	-0.48836900	H	6.91054200	-3.90793800	3.51158400
C	-7.09277500	-0.68069300	-2.11882500	H	6.76333900	-2.19017200	3.88296400
H	-6.42900300	-0.94273500	-2.94888200	H	5.41782600	-3.26492600	4.21533900
H	-6.72802400	-1.18624100	-1.21047300	C	3.60351900	1.60745400	3.91595500
H	-8.07550200	-1.10934400	-2.34421500	C	2.19980400	2.25031400	4.01700300
C	1.70576900	-1.64723800	-4.96812800	H	1.89593500	2.71282900	3.06989800
C	1.29842500	-2.68606500	-6.02729400	H	1.43499900	1.53043200	4.32156000
H	0.38699900	-3.21522600	-5.73172500	H	2.20393600	3.05721100	4.76014200
H	1.11649500	-2.21572100	-6.99816700	C	4.56944600	2.68865900	3.41788000
H	2.07065100	-3.45116500	-6.17614200	H	4.48801400	3.61495800	4.00249700
C	0.60529600	-0.55917300	-4.96536600	H	5.62010700	2.37750500	3.47145200
H	-0.36056900	-0.96864200	-4.65123600	H	4.36704900	2.98565600	2.37138900
H	0.84839100	0.27724200	-4.29954600	C	3.99301800	1.12969700	5.32769700
H	0.47409700	-0.13491000	-5.96693700	H	5.01034100	0.71148700	5.34395800
C	3.04471600	-0.98339700	-5.33705400	H	3.97477700	1.95687600	6.04346600
H	3.32637700	-0.21393200	-4.60834600	H	3.31764900	0.35112300	5.69031100
H	3.86507500	-1.71494400	-5.37572400	N	0.99333800	5.88171900	-1.41324300
H	2.99297900	-0.49938500	-6.31817300	C	3.47172000	5.24289800	-1.09765100
C	2.73332000	-5.65150700	-1.79837800	C	4.10188900	5.43072300	0.17419000

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C	1.25951600	2.62601900	-1.30079900
C	2.43614000	2.56237600	-0.55058300
C	5.49878500	5.24452800	0.34067700
C	6.10822100	5.43665600	1.57414300
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H	-0.72468000	3.45006300	-1.51809200
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H	1.29974300	2.32377100	-2.34994400
H	2.39872700	2.96791200	0.46113800
H	6.10816800	4.95520600	-0.51344300
H	7.18512400	5.29609600	1.66331200
H	5.84612700	5.98044800	3.64961500
H	3.38211900	6.30182800	3.40779400
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H	2.66411000	3.83784500	-3.36145100
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H	4.45024400	5.78881700	-4.94073900
C	3.68889100	1.99044000	-0.95389300
C	4.78952200	2.05833300	-0.07131100
C	3.89567300	1.37094600	-2.20749800
C	6.03200100	1.55111300	-0.42555100
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C	5.13881000	0.86022800	-2.55431900
H	3.07092400	1.29119800	-2.91440300
C	6.21623700	0.94501900	-1.66926800
H	6.86280200	1.63041800	0.27239700
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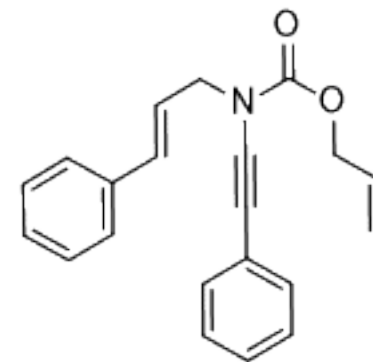
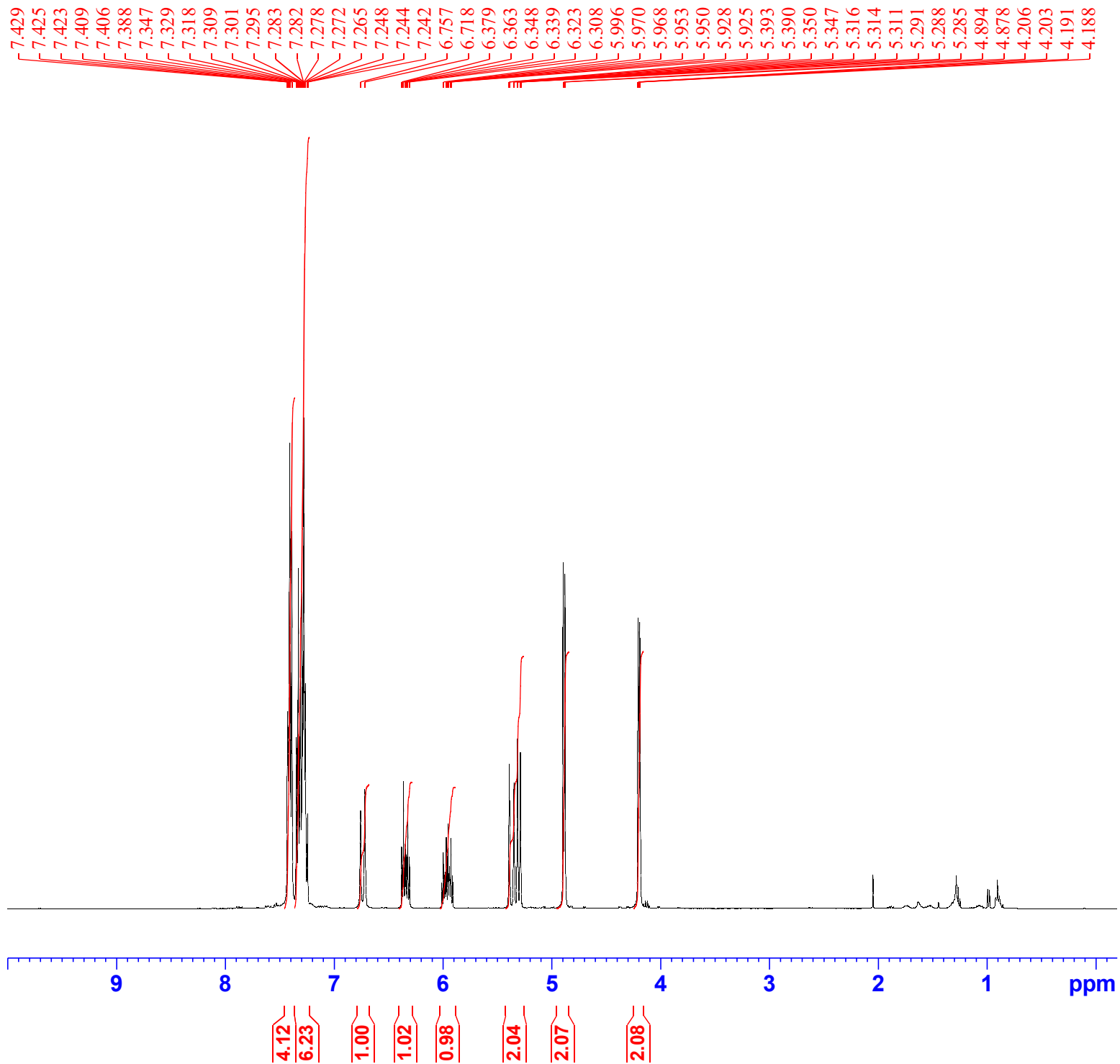
### TS-18

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C	-2.07821300	-1.00252100	-1.70181900
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C	-1.96068400	-3.80767700	0.43344500
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C	-5.81698600	2.97289900	-1.34406700
C	-4.58531300	3.57534300	-1.01202300

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H	5.90875400	-3.06185500	-3.52422400
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H	5.72310900	1.51001100	4.14750800
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C	-4.35199500	5.09247300	-0.92767500
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H	-4.53767800	6.63651500	0.60960100
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H	-6.27254700	5.77308800	-1.77023700
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C	-2.87675000	5.43963100	-1.21673700

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C	-7.25924300	0.92128300	-2.03736200	H	4.03589600	-4.31401500	2.34887800
C	-7.96185900	1.77188700	-3.10888600	H	4.94916000	-3.77925500	0.91876000
H	-8.86131300	1.28131800	-3.48950400	H	5.75565500	-4.67244600	2.20660800
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C	-8.16526800	0.73493500	-0.80337600	H	6.46795800	-1.72091800	1.08789400
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H	-8.40473900	1.69987100	-0.33288900	H	6.31285700	-3.75497000	4.33470200
C	-7.00697800	-0.47162200	-2.66076700	H	5.89524300	-2.11313200	4.82915000
H	-6.28699200	-0.41915800	-3.48364800	H	4.63232100	-3.32184800	4.68711100
H	-6.63334900	-1.19619900	-1.91933200	C	2.57814700	1.52485200	4.36717600
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C	2.51593300	-0.74941200	-5.00851800	H	0.96645900	2.50499200	3.22158500
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H	1.75439300	-2.43015300	-6.18281400	H	0.90504700	2.80933000	4.95273700
H	2.42096500	-1.11740300	-7.16437400	C	3.52729800	2.80865600	4.11395300
H	3.49676600	-2.22679300	-6.30970900	H	3.23508800	3.59234400	4.68989500
C	1.20459300	0.06511600	-5.09543900	H	4.56462900	2.47380100	4.39095700
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H	1.12565000	0.81529400	-4.29917900	C	2.71315400	1.00939600	5.81101800
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C	3.71069700	0.22258400	-5.03495600	H	2.46991500	1.78929400	6.53772200
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H	3.73078400	0.80553300	-5.96118700	C	3.10845800	4.99255000	-0.72336300
C	3.79948200	-4.93773500	-2.21070000	C	4.13750200	5.11664300	0.29962900
C	3.89276800	-5.70010600	-3.54384400	C	3.53776900	4.94552000	-2.17745500
H	4.60025100	-5.22792600	-4.23820400	C	-0.07846100	3.09092900	-1.04777500
H	4.22460800	-6.73142100	-3.39476200	C	1.24716800	2.65466800	-1.25869600
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C	5.20595800	-4.72194800	-1.61661000	C	5.48831500	4.83352400	0.01029500
H	5.74286300	-5.66839300	-1.50609900	C	6.46586800	4.91372600	0.99569400
H	5.81127200	-4.06837700	-2.26262000	C	6.12991200	5.26550300	2.30150600
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H	1.93872000	-5.93925500	-1.61418900	C	2.52882800	5.93446000	-4.24367000
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C	-6.29796900	-3.01041400	-0.01589200	H	4.32764900	5.69411500	-2.35427000
H	-6.49090200	-2.12335900	-0.64169700	H	-0.72398200	3.24862000	-1.91105600
H	-5.38122200	-3.48071200	-0.39086900	H	-0.29966000	3.71896800	-0.18601700
H	-7.12437100	-3.70484000	-0.19470900	H	1.50909500	2.31114000	-2.26195400
C	-6.22971000	-3.98325500	2.26940600	H	2.04655100	3.16719600	0.66543900
H	-6.17525600	-3.81304300	3.35521700	H	5.77332100	4.52967500	-0.99617100
H	-7.14751200	-4.54250800	2.07262000	H	7.50073400	4.68927900	0.73976500
H	-5.37428700	-4.62060400	1.99994000	H	6.89793600	5.33458000	3.06922300
C	-7.40045000	-1.76925600	1.83252300	H	4.51747900	5.82779300	3.62237000
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H	-7.39219400	-1.45725500	2.88581000	H	1.50214000	4.61575600	-2.97940800
H	-7.41127900	-0.85594800	1.21444000	H	1.70471400	6.04530300	-4.94470400
C	-2.49471900	-1.02681400	4.77227600	H	3.43326300	6.50453300	-4.45876600
C	-3.01759100	0.21349900	5.52285000	C	3.57710900	2.11956800	-0.43561400
H	-4.10644900	0.16631900	5.67196200	C	4.39623200	2.00491400	0.70236100
H	-2.55567900	0.30208500	6.51133600	C	4.03261600	1.52571300	-1.63017300
H	-2.80174700	1.13470300	4.97226300	C	5.60404100	1.31963800	0.65943300
C	-0.95852300	-0.91054700	4.64838000	H	4.06159000	2.46512500	1.63892500
H	-0.54981500	-1.69813900	4.00567300	C	5.24445900	0.84436500	-1.67319700
H	-0.63373600	0.05948000	4.23823000	H	3.42818100	1.57733600	-2.53893600
H	-0.47740200	-1.00887200	5.62768400	C	6.03635800	0.73536800	-0.52966200
C	-2.76732000	-2.31069000	5.57671900	H	6.21184400	1.24623300	1.55897000
H	-2.20162200	-2.32537900	6.51251000	H	5.56812000	0.38515000	-2.60573300
H	-3.82623100	-2.42692000	5.83455900	H	6.98118500	0.19685100	-0.56667100

## 9. Copies of NMR Spectra



**1a**

Current Data Parameters  
 NAME CS-1-19pure  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211005  
 Time\_ 14.43 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 52  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SF01 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300164 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

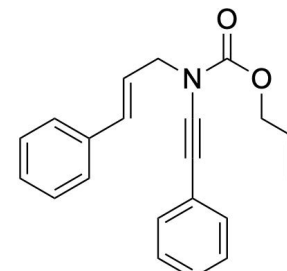
154.85  
136.19  
134.18  
131.58  
131.20  
128.78  
128.62  
128.42  
128.25  
128.12  
127.54  
126.70  
123.23  
122.82  
118.82

82.72

70.82

67.60

52.75

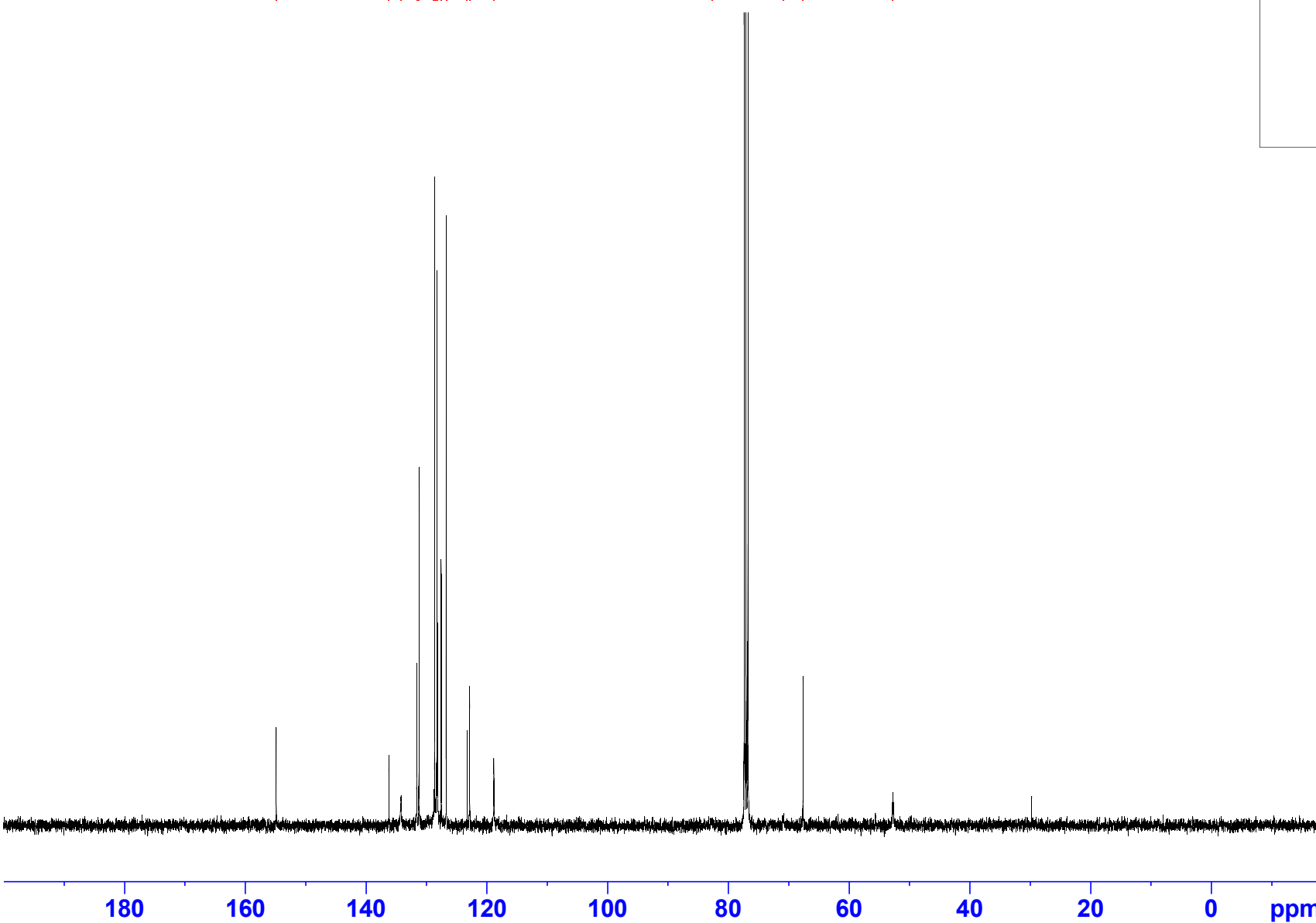


**1a**

Current Data Parameters  
NAME OJ-1-184-C  
EXPNO 19  
PROCNO 1

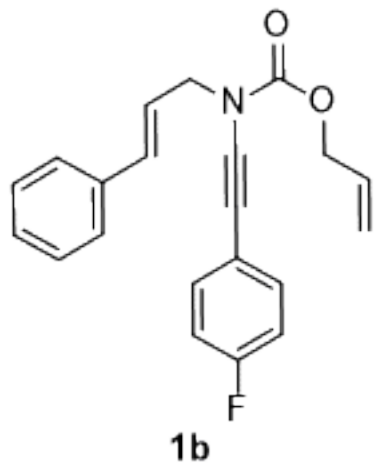
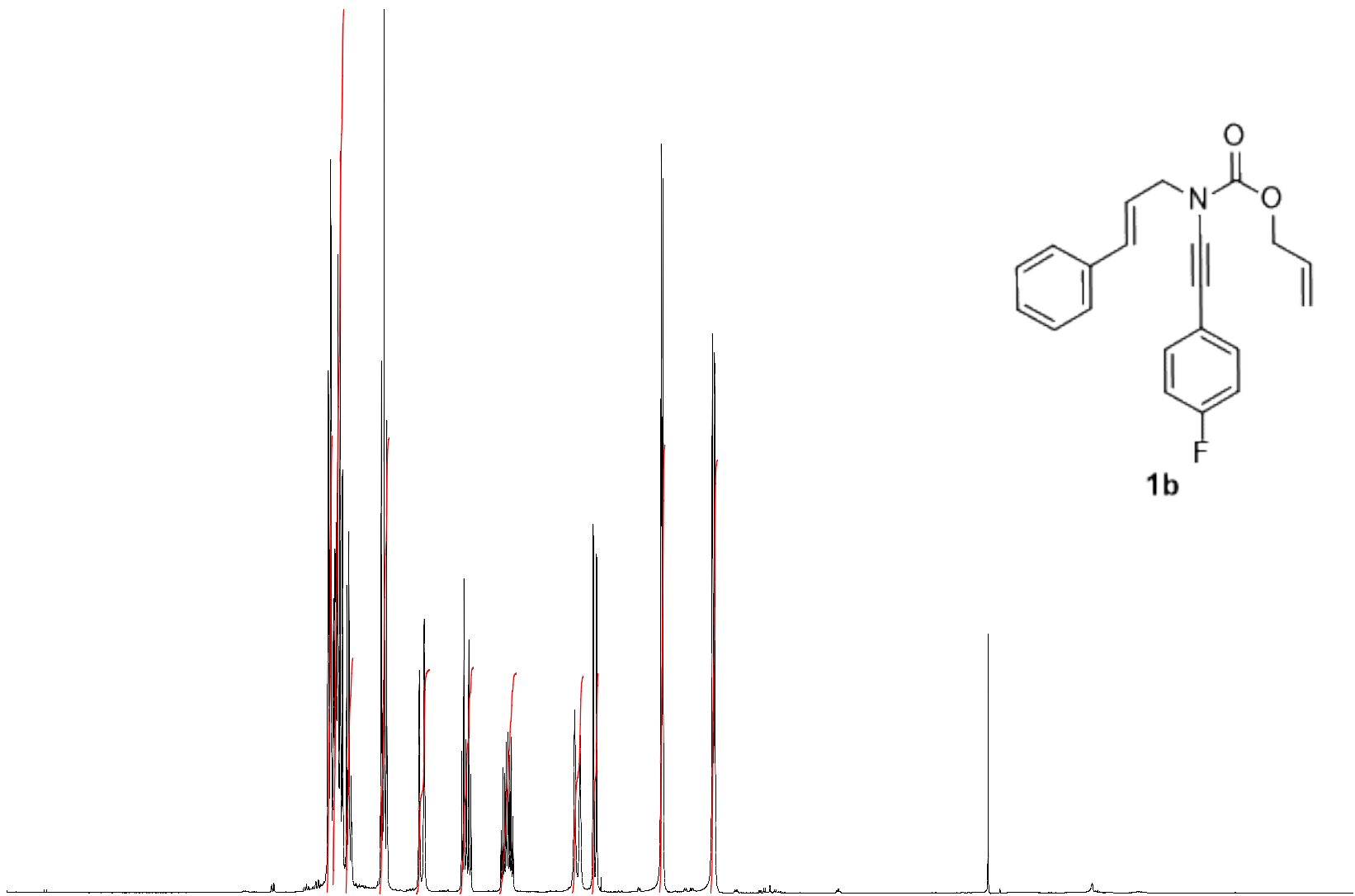
F2 - Acquisition Parameters  
Date\_ 20220904  
Time\_ 0.59 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



180 160 140 120 100 80 60 40 20 0 ppm

7.428  
7.424  
7.406  
7.385  
7.371  
7.363  
7.349  
7.331  
7.327  
7.311  
7.281  
7.278  
7.275  
7.266  
7.260  
7.000  
6.994  
6.983  
6.978  
6.973  
6.961  
6.956  
6.696  
6.657  
6.355  
6.339  
6.322  
6.316  
6.299  
6.026  
6.000  
5.984  
5.970  
5.957  
5.449  
5.406  
5.305  
5.302  
5.298  
5.295  
5.279  
5.276  
5.272  
5.269  
4.760  
4.756  
4.753  
4.747  
4.743  
4.739  
4.346  
4.344  
4.330  
4.327



Current Data Parameters  
 NAME Ph-F-Ynamide  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210327  
 Time\_ 13.43 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 32  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 293.2 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300194 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

9 8 7 6 5 4 3 2 1 0 ppm

2.03  
3.88  
1.04  
2.00  
0.98  
0.99  
0.97  
0.95  
0.97  
1.97  
1.90

163.39  
160.92  
154.73  
136.35  
134.41  
133.21  
131.88  
128.70  
128.09  
126.69  
122.71  
119.32  
118.30  
115.68  
115.46

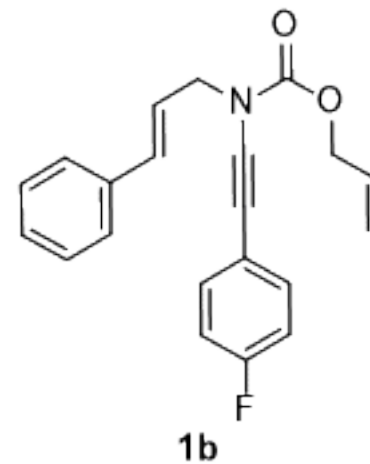
82.44

70.12  
67.67

52.39

Current Data Parameters  
NAME Ph-F-Yneamide-C  
EXPNO 14  
PROCNO 1

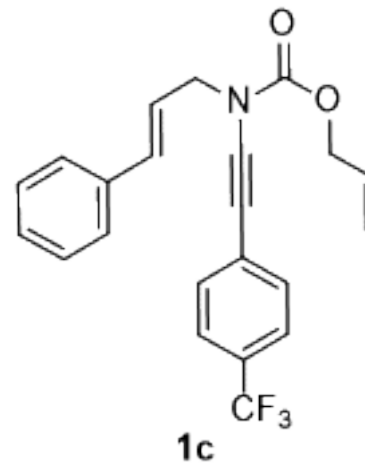
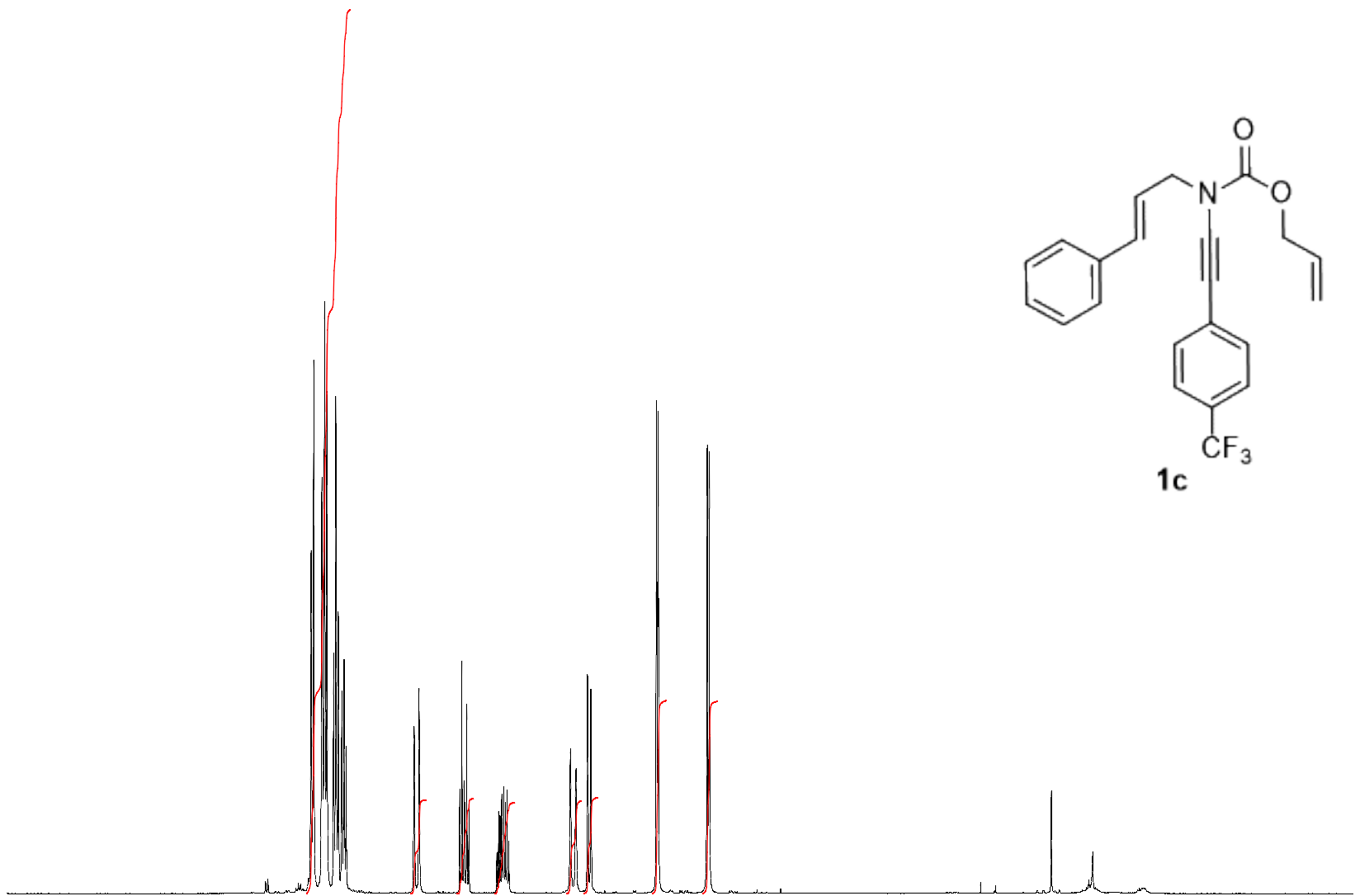
F2 - Acquisition Parameters  
Date\_ 20210327  
Time 17.03 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 11.0026  
DW 21.000 usec  
DE 6.50 usec  
TE 293.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W



F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

7.378  
7.365  
7.361  
7.346  
7.320  
7.317  
7.314  
7.305  
7.299  
7.284  
6.737  
6.697  
6.371  
6.354  
6.337  
6.332  
6.315  
6.298  
6.075  
6.061  
6.048  
6.035  
6.018  
6.005  
5.992  
5.978  
5.486  
5.483  
5.443  
5.440  
5.348  
5.344  
5.321  
5.318  
4.798  
4.794  
4.791  
4.784  
4.780  
4.777  
4.389  
4.386  
4.372  
4.370



Current Data Parameters  
NAME OJ-2-P-CF3-Ynamide-H  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210531  
Time 18.21 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 93.113  
DW 61.000 usec  
DE 13.89 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

9 8 7 6 5 4 3 2 1 0 ppm

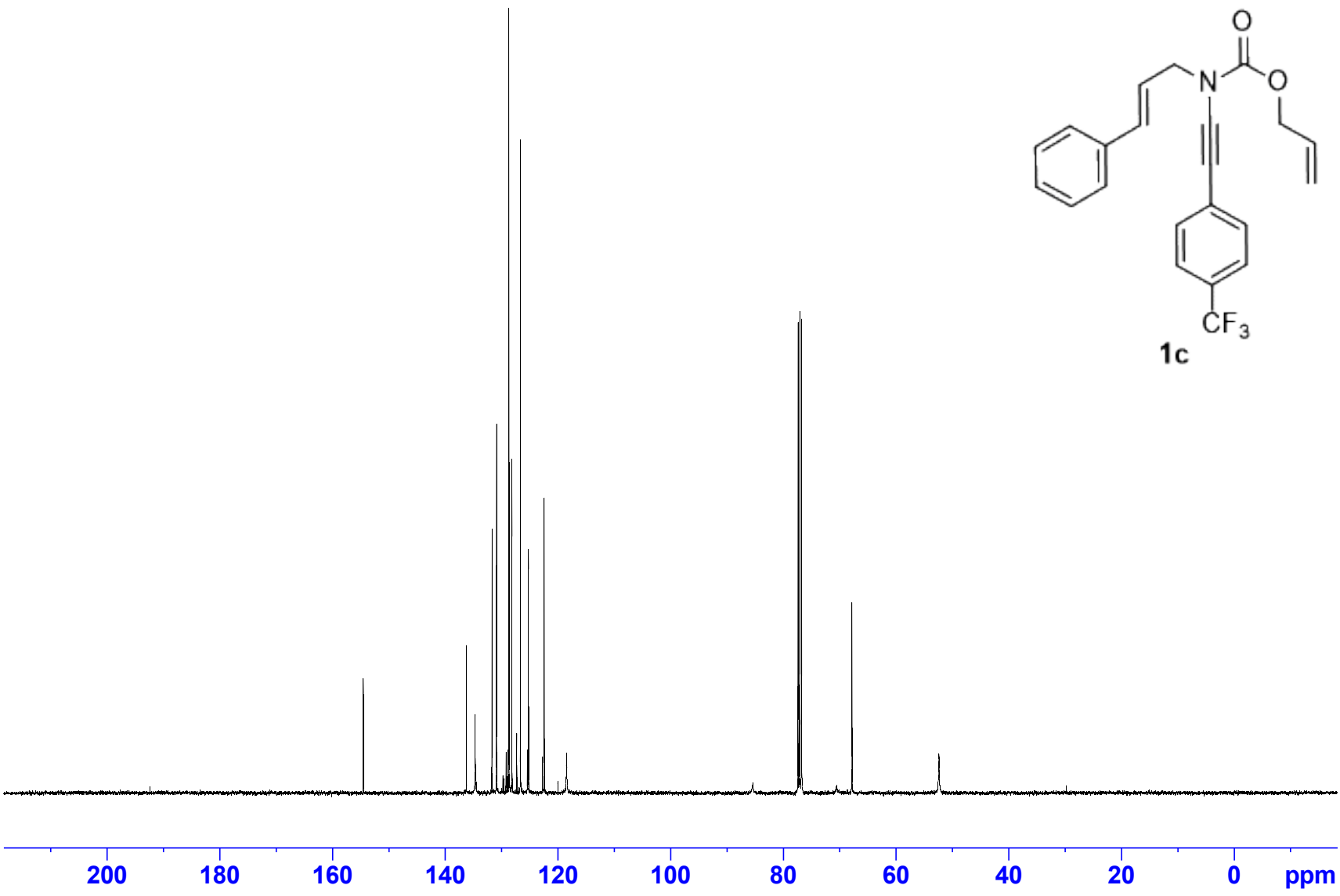
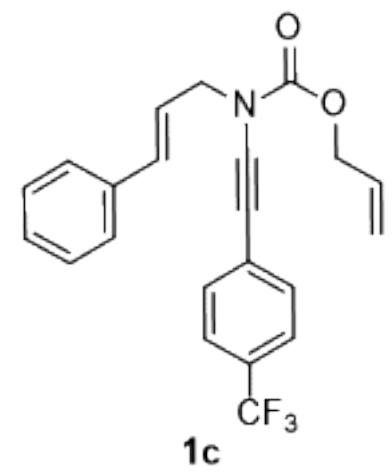
9.43  
1.00  
1.01  
0.97  
0.99  
1.02  
2.06  
2.05



154.50  
 136.21  
 134.66  
 134.46  
 131.67  
 130.88  
 129.92  
 129.76  
 129.51  
 129.18  
 129.01  
 128.86  
 128.67  
 128.53  
 128.27  
 128.13  
 127.28  
 127.26  
 126.90  
 126.64  
 126.32  
 125.40  
 125.24  
 125.21  
 125.17  
 125.13  
 122.69  
 122.41  
 119.99  
 118.44  
 85.41  
 70.49  
 67.79  
 52.36

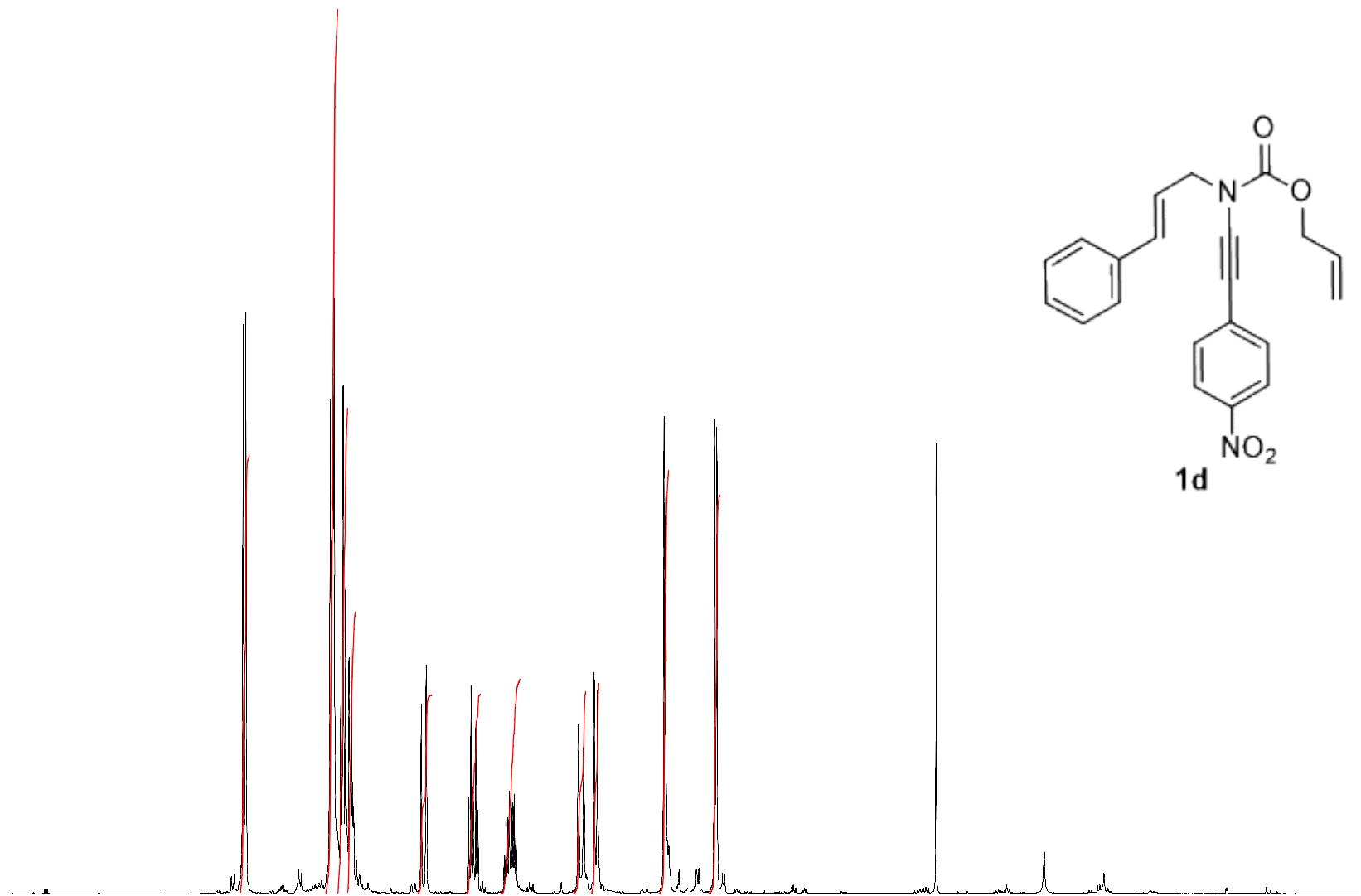
Current Data Parameters  
 NAME OJ-2-P-CF3-Ynamide-C  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210531  
 Time\_ 19.23 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (   
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W



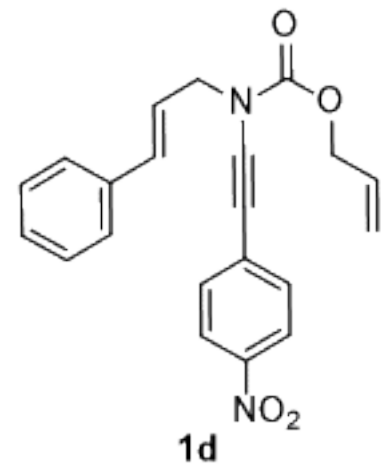
F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

7.408  
7.400  
7.390  
7.361  
7.336  
7.318  
7.299  
7.271  
7.259  
7.253  
7.246  
7.243  
7.235  
6.696  
6.656  
6.315  
6.299  
6.282  
6.276  
6.259  
6.243  
6.020  
6.007  
5.993  
5.977  
5.964  
5.951  
5.937  
5.442  
5.440  
5.400  
5.398  
5.316  
5.313  
5.289  
5.287  
4.758  
4.744  
4.354  
4.337



9 8 7 6 5 4 3 2 1 0 ppm

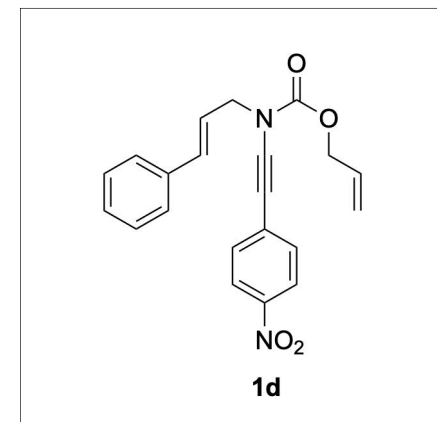
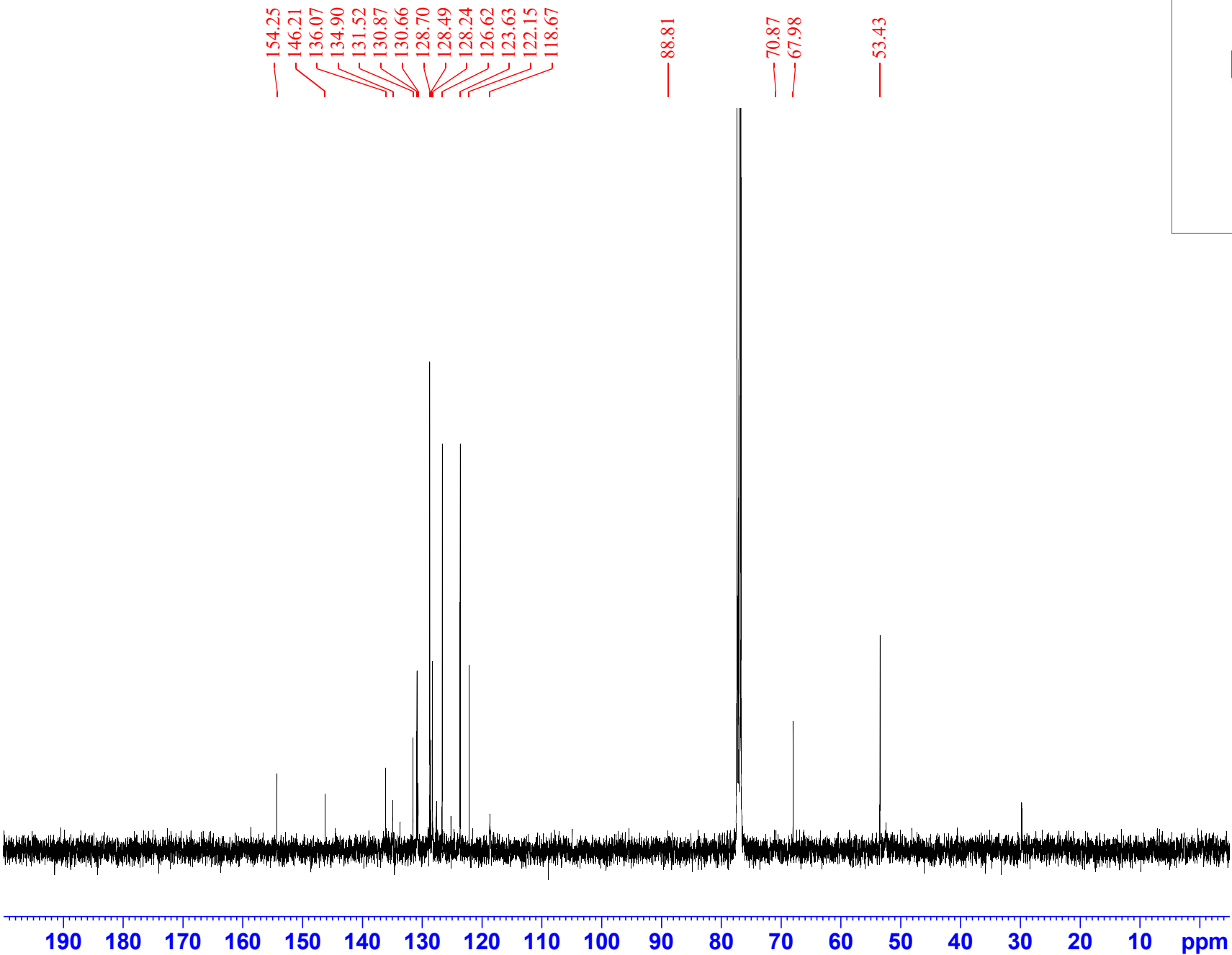
2.21  
4.47  
2.46  
1.42  
1.00  
1.00  
1.08  
1.02  
1.06  
2.14  
2.01



Current Data Parameters  
NAME OJ-2-257-H  
EXPNO 19  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210802  
Time\_ 22.01 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 (zg30)  
PULPROG 65536  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 50.7317  
DW 61.000 usec  
DE 13.89 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

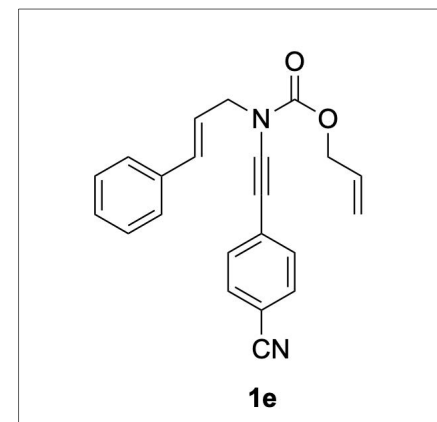
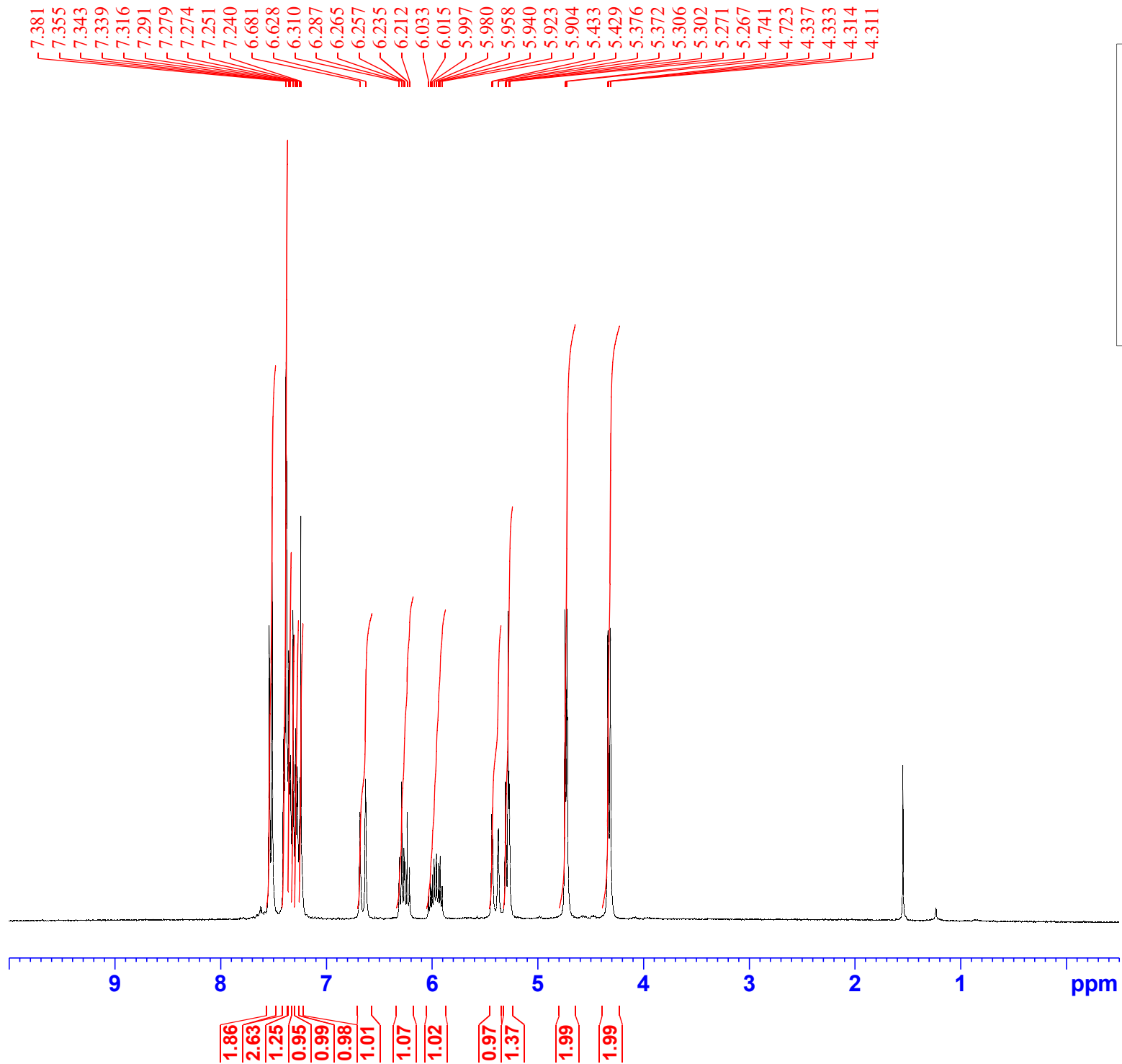
F2 - Processing parameters  
SI 65536  
SF 400.1300163 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
 NAME OJ-NO2-3-rev-C  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220902  
 Time\_ 3.48 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2048  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME OJ-1e-H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180205  
 Time\_ 10.02  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/13  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 3591.954 Hz  
 FIDRES 0.109618 Hz  
 AQ 4.5613055 sec  
 RG 322.5  
 DW 139.200 usec  
 DE 6.00 usec  
 TE 683.2 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 0 dB  
 SFO1 300.1715008 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1700170 MHz  
 WDW EM  
 SSB 0  
 LB 0.50 Hz  
 GB 0  
 PC 1.00

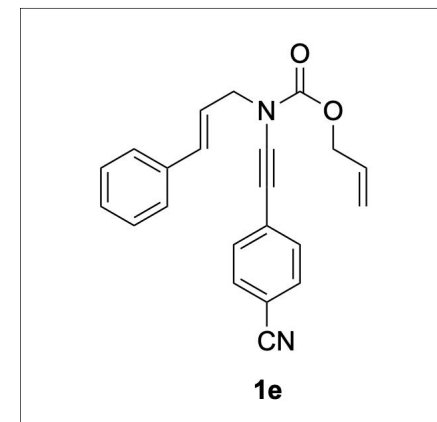
154.84  
 134.48  
 133.88  
 133.61  
 133.25  
 131.91  
 131.23  
 128.21  
 128.14  
 127.77  
 127.63  
 126.89  
 126.41  
 126.14  
 123.66  
 123.32  
 123.15  
 118.31

83.01

71.25

67.69

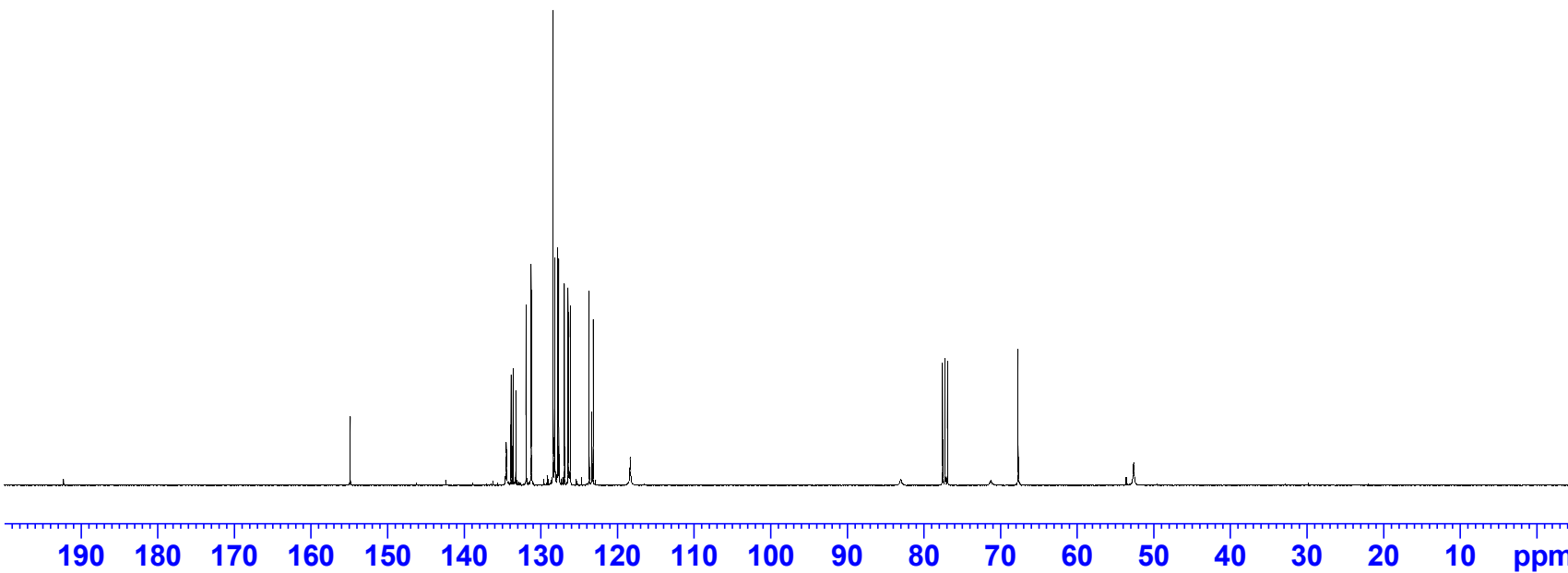
52.58

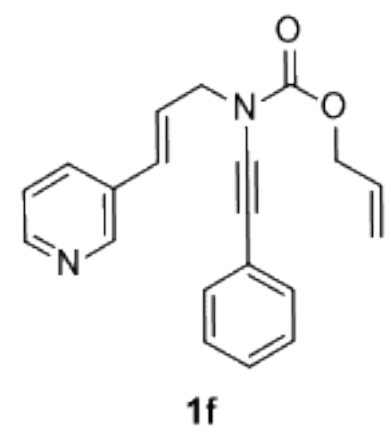
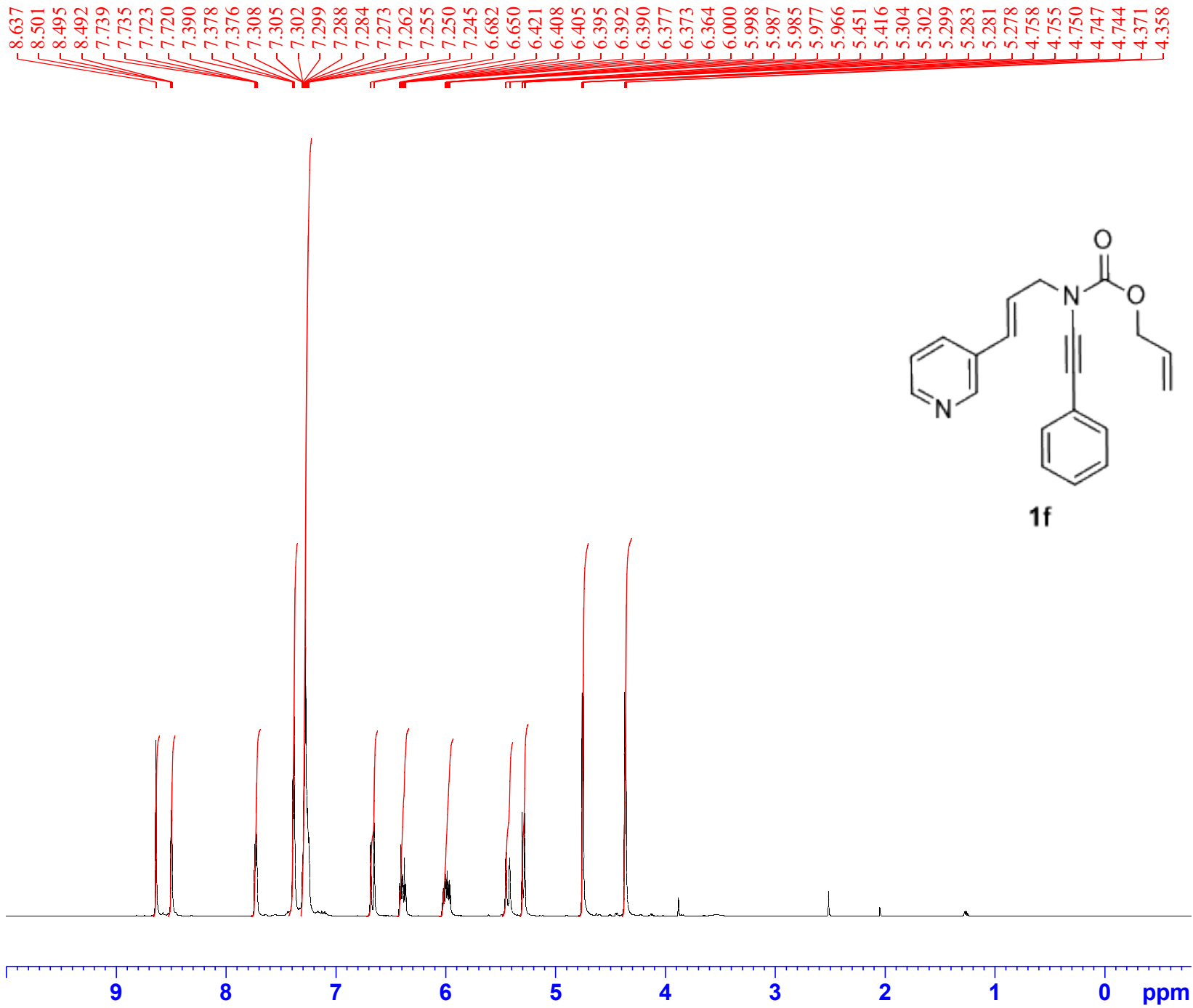


Current Data Parameters  
 NAME OJ-1-E-C  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210615  
 Time\_ 0.13 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
 NAME OJ-2-107A  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210622  
 Time\_ 12.24 h  
 INSTRUM spect  
 PROBHD z125869\_0055 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 64  
 DS 2  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 3.2767999 sec  
 RG 22.16  
 DW 50.000 usec  
 DE 16.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 TD0 1  
 SFO1 500.2330889 MHz  
 NUC1 1H  
 P0 4.00 usec  
 P1 12.00 usec  
 PLW1 11.44699955 W

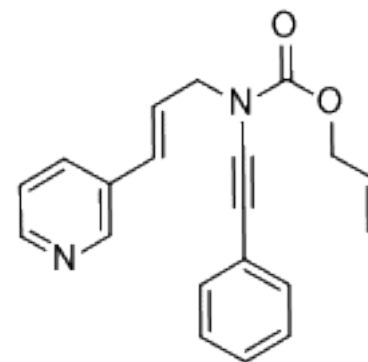
F2 - Processing parameters  
 SI 65536  
 SF 500.2330000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

154.68  
148.96  
148.43  
133.08  
131.99  
131.72  
131.13  
130.51  
128.29  
127.65  
125.28  
123.49  
123.03  
118.30

82.58

71.11  
67.68

52.19



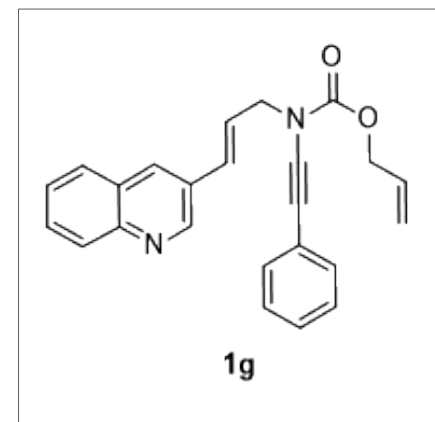
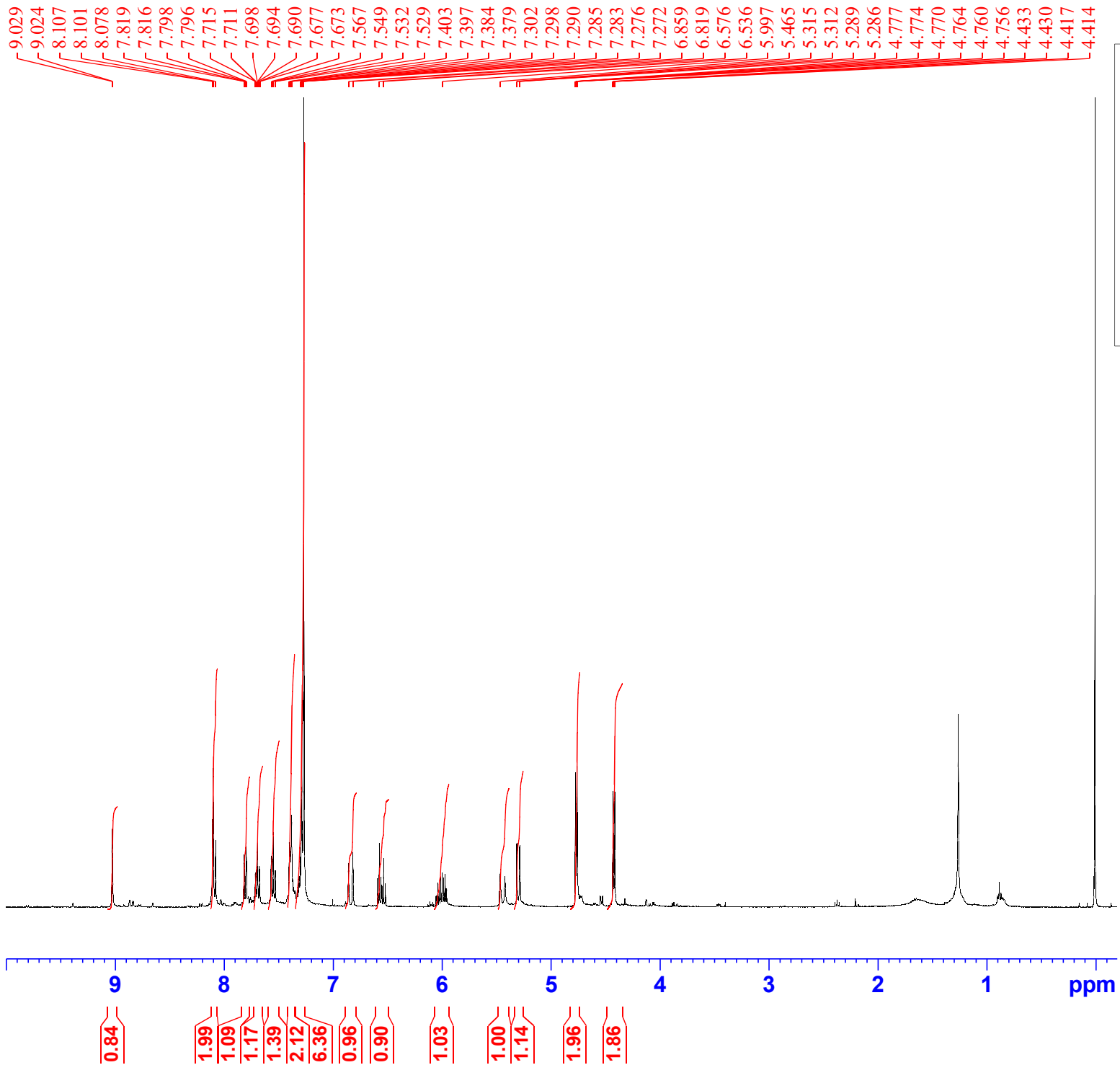
1f

Current Data Parameters  
NAME OJ-2-107-C  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210622  
Time\_ 13.20 h  
INSTRUM spect  
PROBHD Z125869\_0055 (   
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 190.44  
DW 16.800 usec  
DE 18.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 125.7955118 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 56.90299988 W  
SFO2 500.2320009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 11.44699955 W  
PLW12 0.25756001 W  
PLW13 0.12955000 W

F2 - Processing parameters  
SI 32768  
SF 125.7829335 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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



Current Data Parameters  
 NAME OJ-1g-vac-H  
 EXPNO 16  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20220312  
 Time 17.48 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SF01 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300067 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



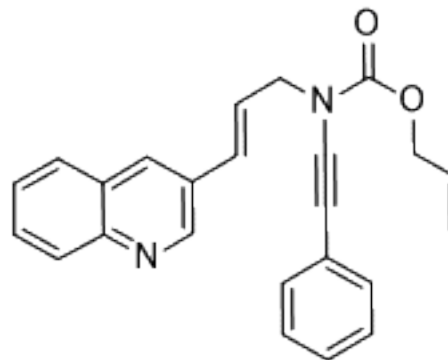
154.76  
149.02  
147.29  
133.17  
131.72  
131.17  
130.71  
129.62  
129.32  
128.96  
128.31  
127.97  
127.91  
127.68  
127.17  
125.50  
123.01  
118.38

82.46

71.06

67.75

52.34



1g

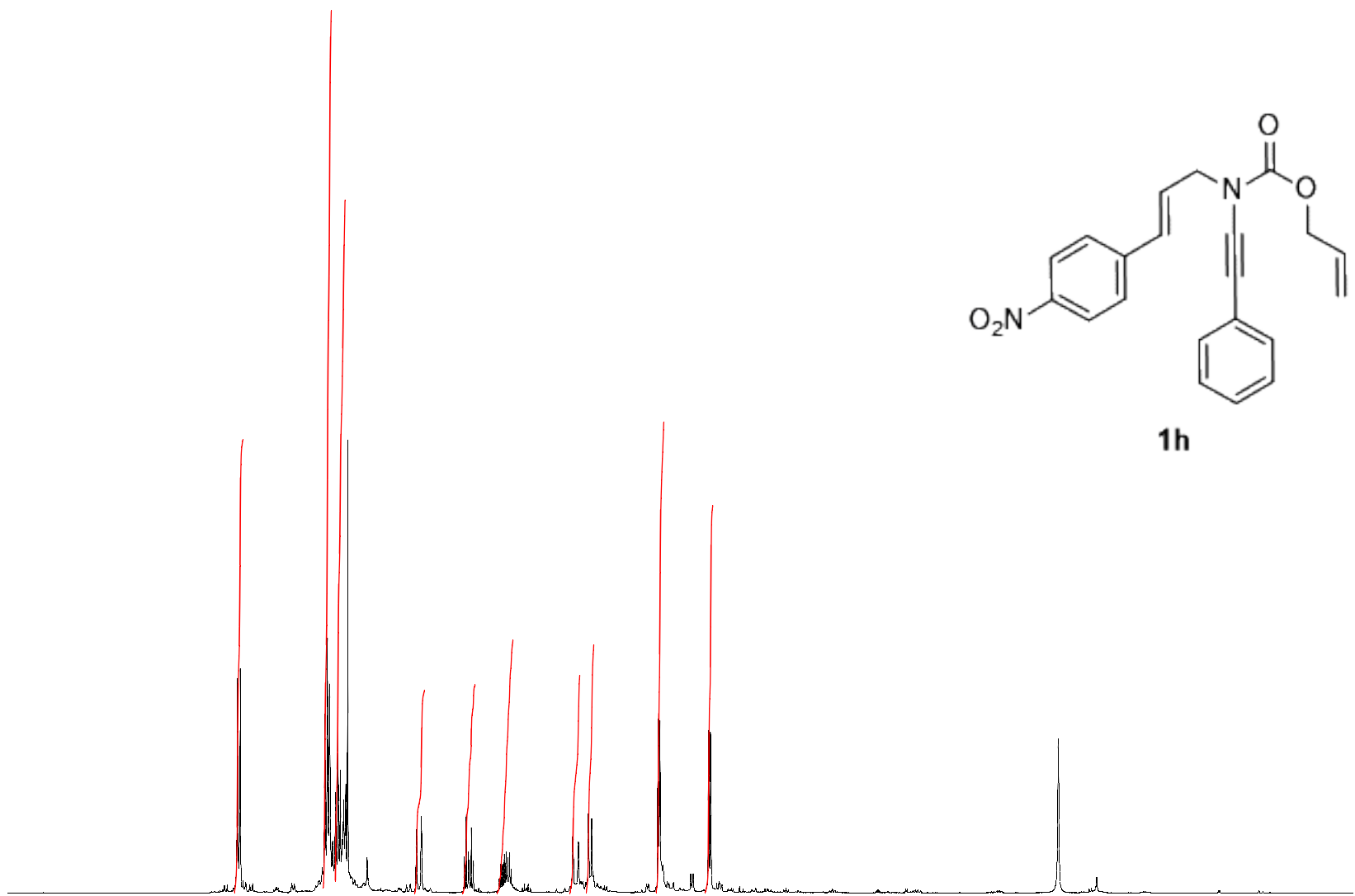
Current Data Parameters  
NAME OJ-2-Quinoline ynamide-C  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210911  
Time 2.42 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (zpgg30)  
PULPROG zpgg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

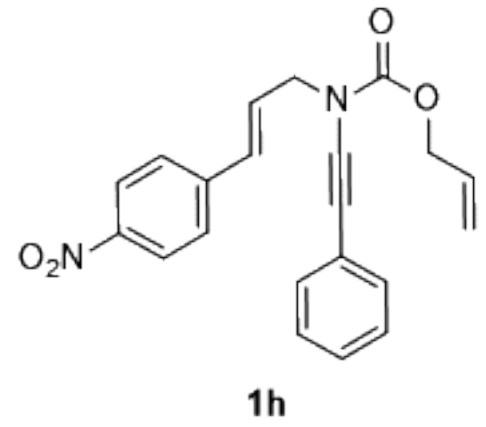
F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

7.432  
7.415  
7.368  
7.365  
7.348  
7.329  
7.307  
7.303  
7.286  
6.718  
6.679  
6.336  
6.319  
6.302  
6.296  
6.279  
6.263  
6.041  
6.028  
6.015  
5.999  
5.985  
5.972  
5.959  
5.465  
5.462  
5.423  
5.419  
5.341  
5.338  
5.315  
5.312  
4.783  
4.780  
4.777  
4.770  
4.766  
4.763  
4.378  
4.375  
4.361  
4.359



2.23  
4.35  
3.48  
1.00  
1.03  
1.25  
1.08  
1.23  
2.32  
1.91



Current Data Parameters  
NAME OJ-Para-Nitro(tert)-H-3  
EXPNO 18  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210808  
Time\_ 20.19 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.89 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300059 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

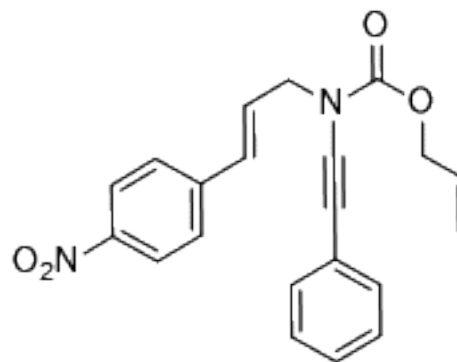
154.26  
146.21  
136.07  
134.91  
131.53  
130.87  
130.66  
128.70  
128.24  
126.63  
125.19  
123.63  
122.15  
118.67

82.38

71.05

67.98

52.43



1h

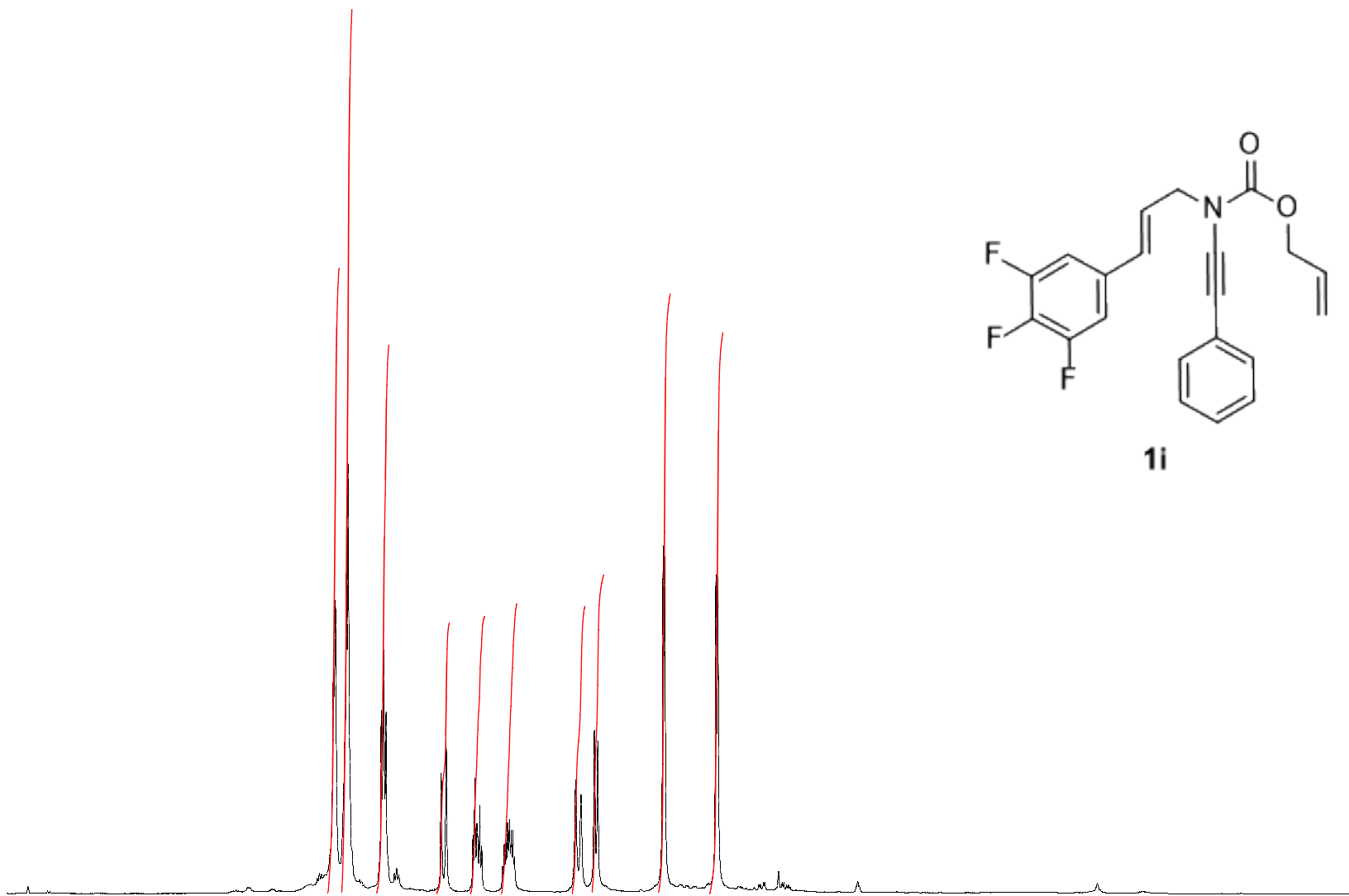
Current Data Parameters  
NAME OJ-Para-Nitro(tert)-C-3  
EXPNO 20  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210808  
Time\_ 21.20 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 (zpgp30)  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

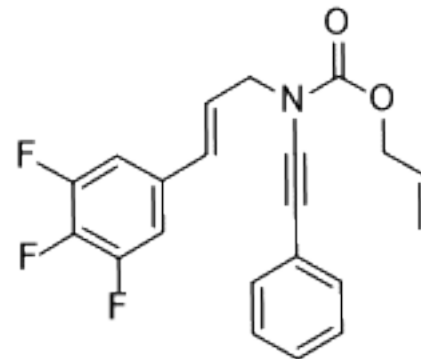
F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

7.387  
7.372  
7.299  
7.286  
7.271  
7.005  
6.988  
6.968  
6.526  
6.486  
6.273  
6.257  
6.241  
6.234  
6.218  
6.202  
6.035  
6.022  
6.009  
5.995  
5.979  
5.966  
5.953  
5.939  
5.450  
5.407  
5.300  
5.274  
4.750  
4.737  
4.328  
4.312



2.31  
3.26  
2.03  
1.00  
1.02  
1.07  
1.06  
1.18  
2.21  
2.07



1i

Current Data Parameters  
NAME OJ-2-116-H  
EXPNO 7  
PROCNO 1

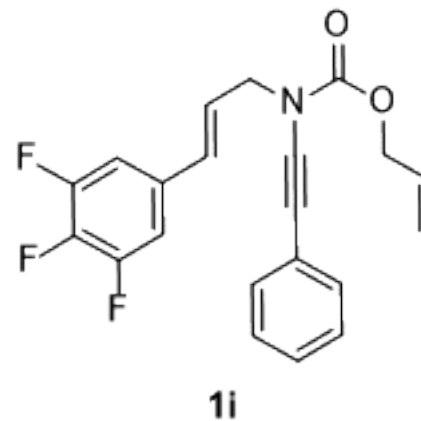
F2 - Acquisition Parameters  
Date\_ 20210705  
Time\_ 15.28 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 32  
DW 61.000 usec  
DE 13.89 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300115 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

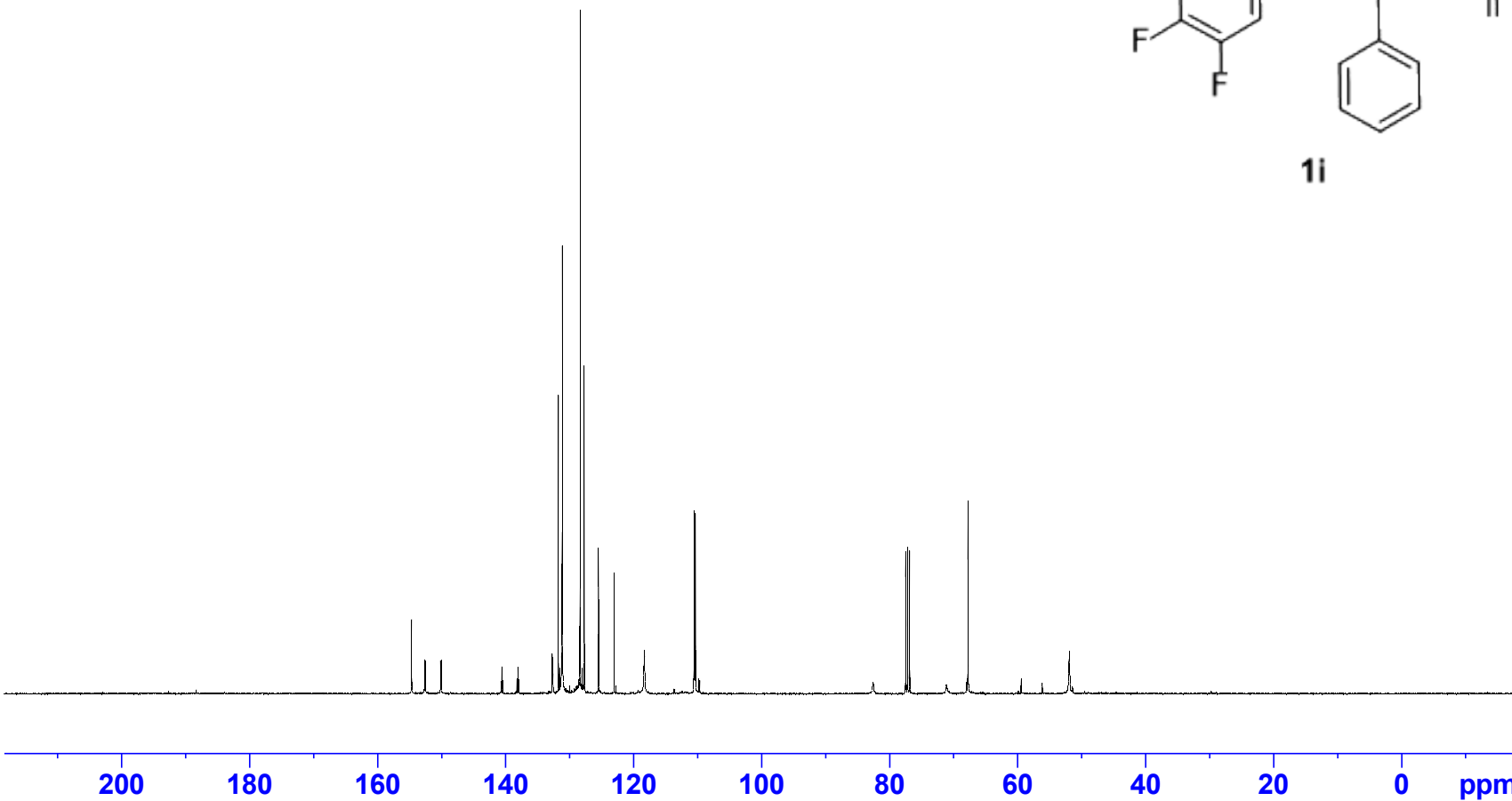
154.67  
 152.63  
 152.59  
 152.53  
 152.49  
 150.15  
 150.11  
 150.05  
 150.01  
 140.72  
 140.56  
 140.41  
 138.21  
 138.05  
 137.90  
 132.75  
 132.70  
 132.68  
 132.63  
 132.60  
 132.55  
 131.72  
 131.54  
 131.25  
 131.12  
 128.41  
 128.33  
 127.99  
 127.71  
 125.49  
 125.47  
 123.01  
 122.70  
 118.29  
 110.53  
 110.47  
 110.37  
 110.32  
 82.53  
 71.09  
 67.73  
 51.91

Current Data Parameters  
 NAME OJ-2-116-C  
 EXPNO 9  
 PROCNO 1

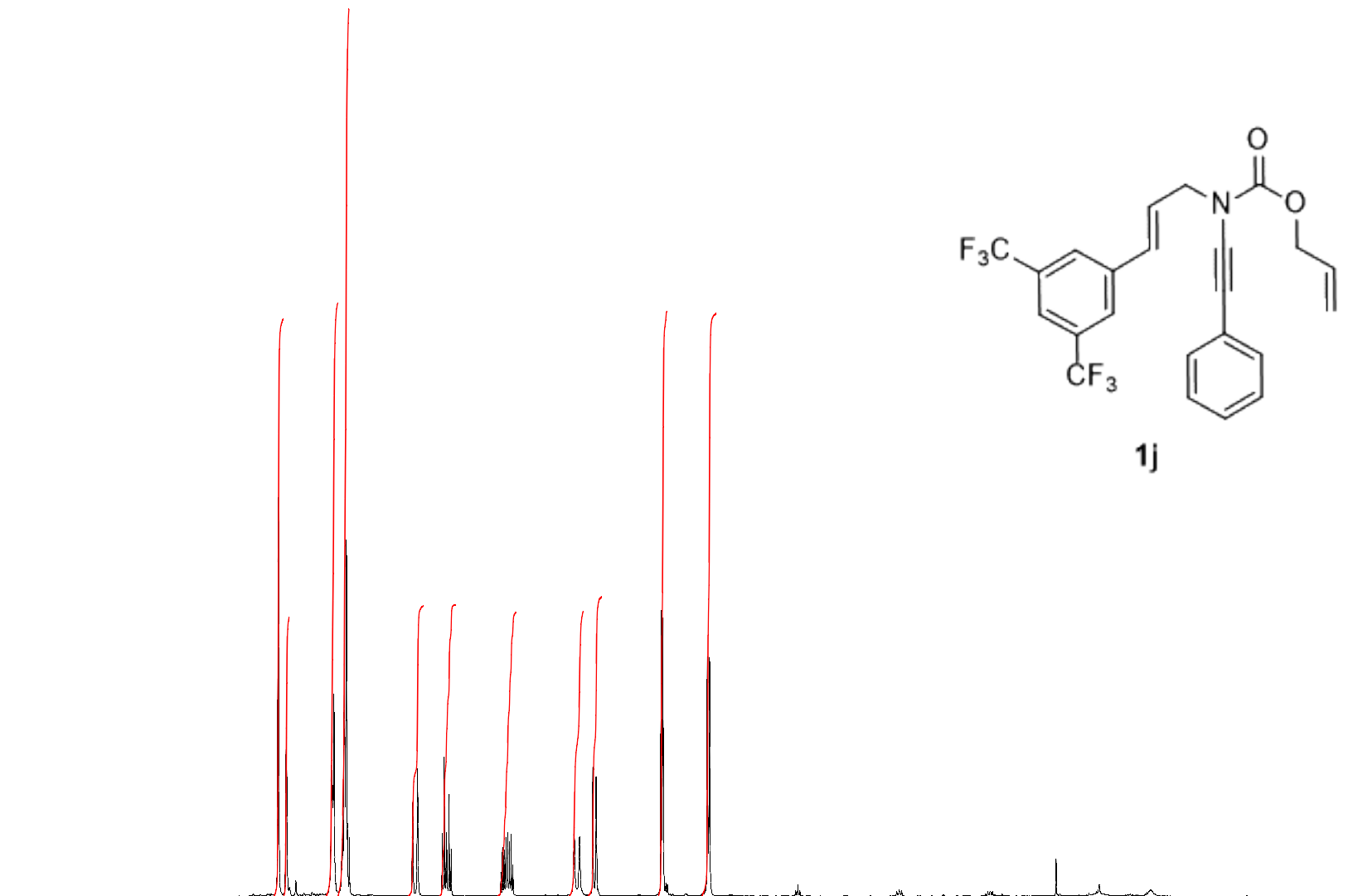
F2 - Acquisition Parameters  
 Date\_ 20210705  
 Time\_ 16.30 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 12.5744  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W



F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

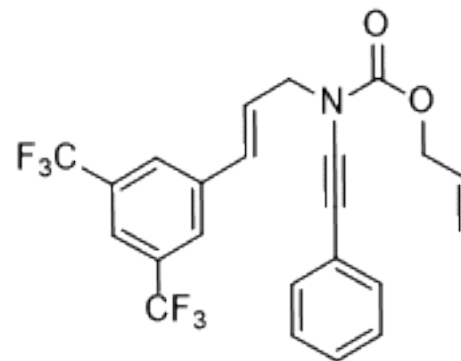


7.836  
7.772  
7.415  
7.407  
7.404  
7.395  
7.390  
7.333  
7.329  
7.322  
7.318  
7.310  
7.305  
7.303  
7.296  
7.292  
7.286  
7.280  
6.765  
6.725  
6.528  
6.512  
6.497  
6.488  
6.473  
6.457  
6.047  
6.034  
6.021  
6.019  
6.005  
5.991  
5.978  
5.965  
5.475  
5.432  
5.331  
5.328  
5.324  
5.321  
5.304  
5.301  
5.298  
5.295  
4.784  
4.780  
4.777  
4.770  
4.767  
4.763  
4.413  
4.410  
4.397  
4.394



9 8 7 6 5 4 3 2 1 0 ppm

1.99  
0.96  
2.05  
3.06  
1.00  
1.01  
0.98  
0.98  
1.03  
2.02  
2.01



1j

Current Data Parameters  
NAME OJ-2-bis-cf3 ynamide  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210530  
Time 16.16 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 78.2407  
DW 61.000 usec  
DE 13.89 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300056 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

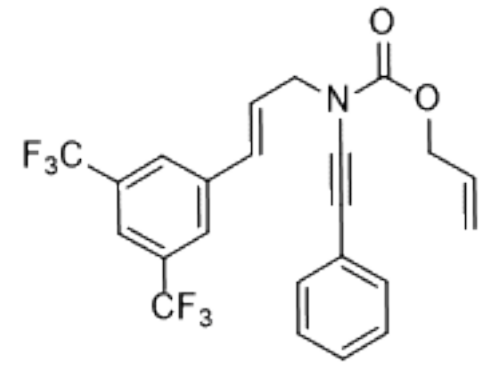
154.69  
138.40  
132.51  
132.18  
131.85  
131.52  
131.17  
131.03  
128.32  
127.76  
127.33  
127.24  
126.47  
126.44  
124.62  
122.92  
121.91  
121.37  
121.34  
121.30  
119.20  
118.40  
82.44

71.06  
67.80

52.02

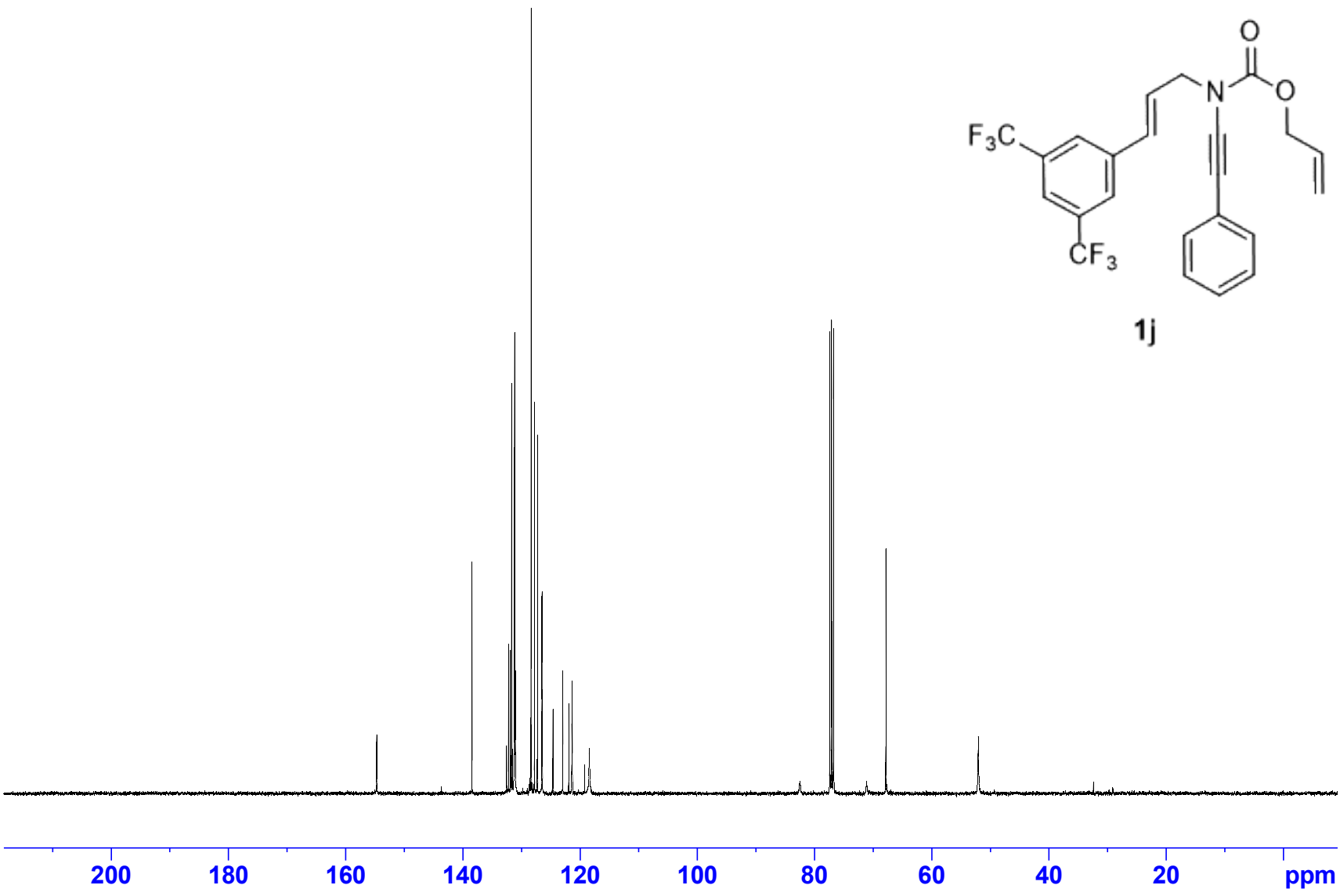
Current Data Parameters  
NAME OJ-2-bis-cf3 ynamide-C  
EXPNO 16  
PROCNO 1

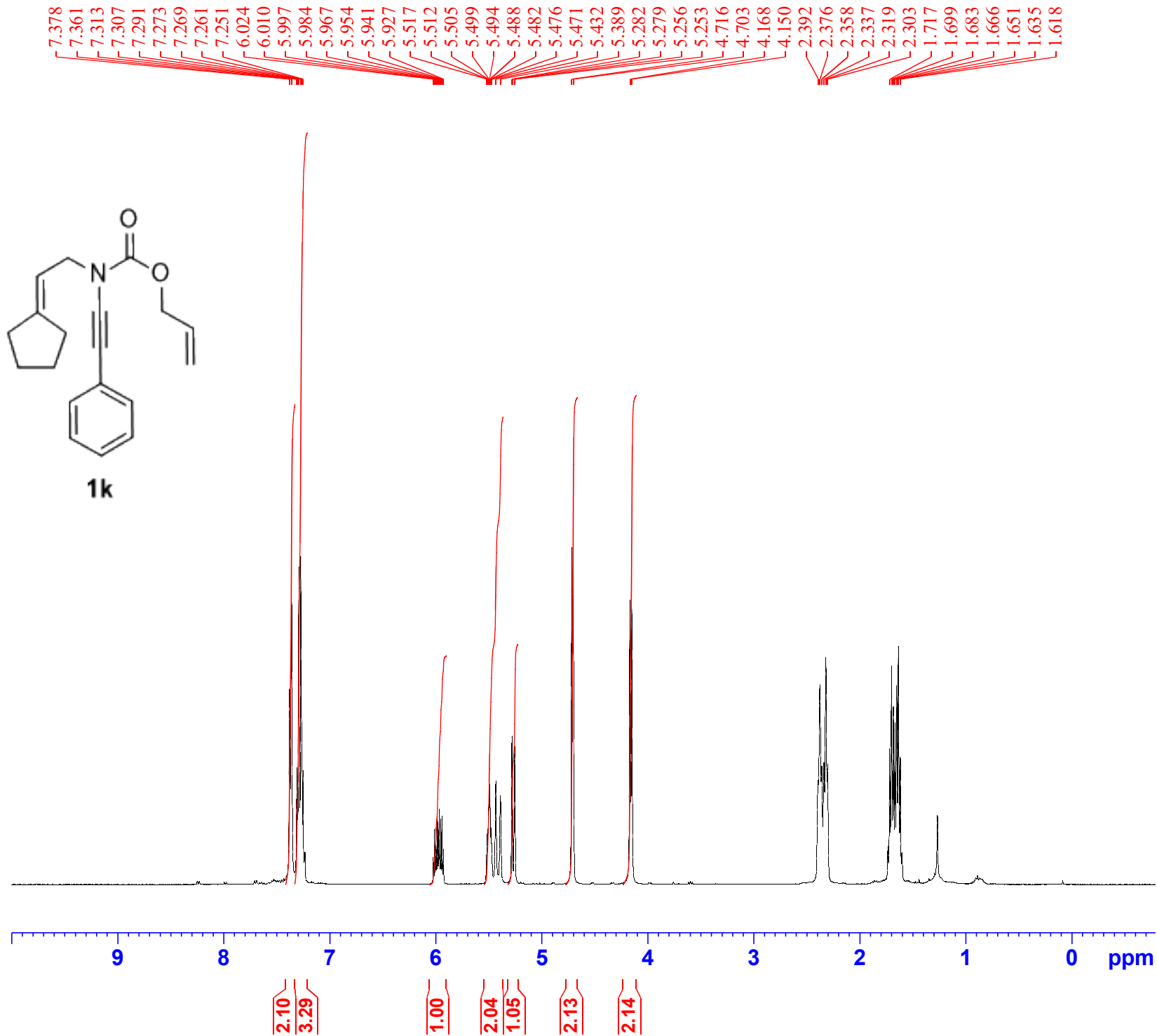
F2 - Acquisition Parameters  
Date\_ 20210530  
Time 17.29 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W



1j

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



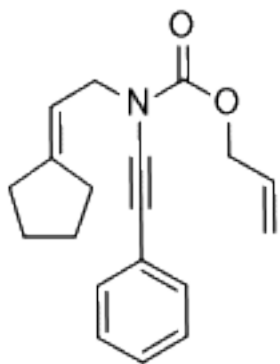


Current Data Parameters  
 NAME OJ-Cyclopentyl-ynamide-H  
 EXPNO 14  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210810  
 Time\_ 18.32 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (   
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 54.7368  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300092 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





**1k**

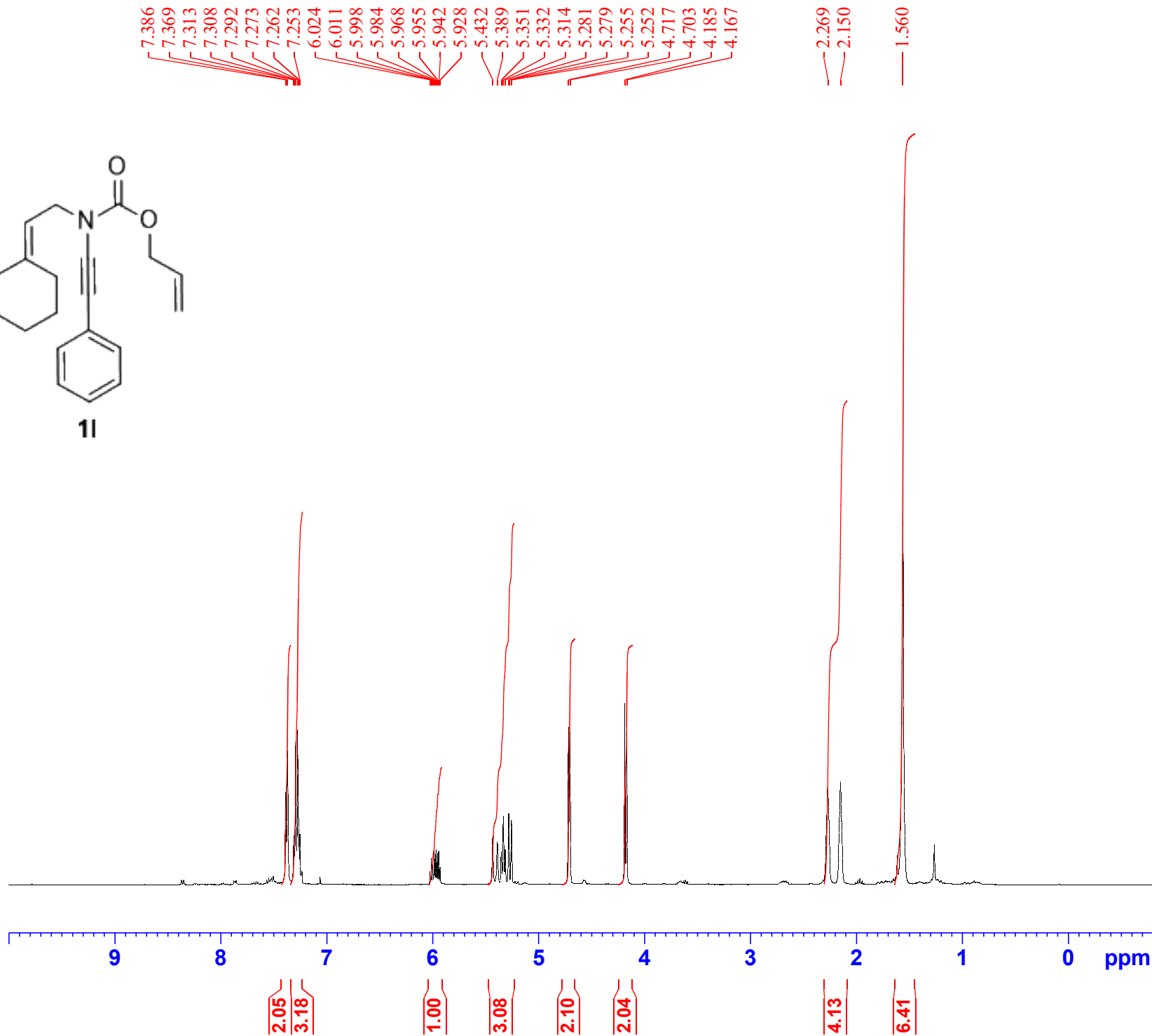
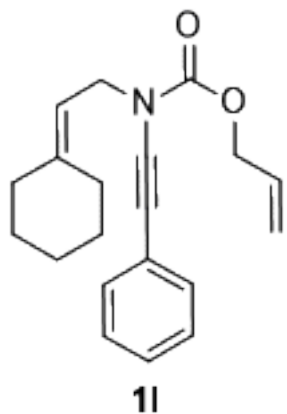
154.85  
149.99  
131.95  
130.92  
128.25  
127.31  
123.53  
118.00  
113.58  
83.40  
70.64  
67.38  
49.44  
33.79  
28.90  
26.31  
26.15

Current Data Parameters  
NAME OJ-Cyclopentyl-ynamide-C  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210810  
Time 19.15 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 538  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

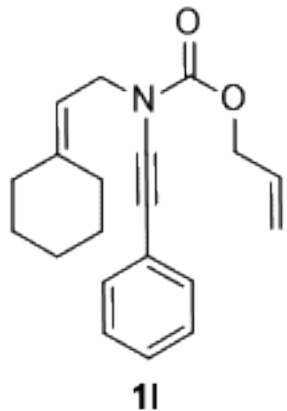
200 180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters  
 NAME OJ-2-270-H  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210820  
 Time\_ 22.34 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 63.0303  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.130088 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



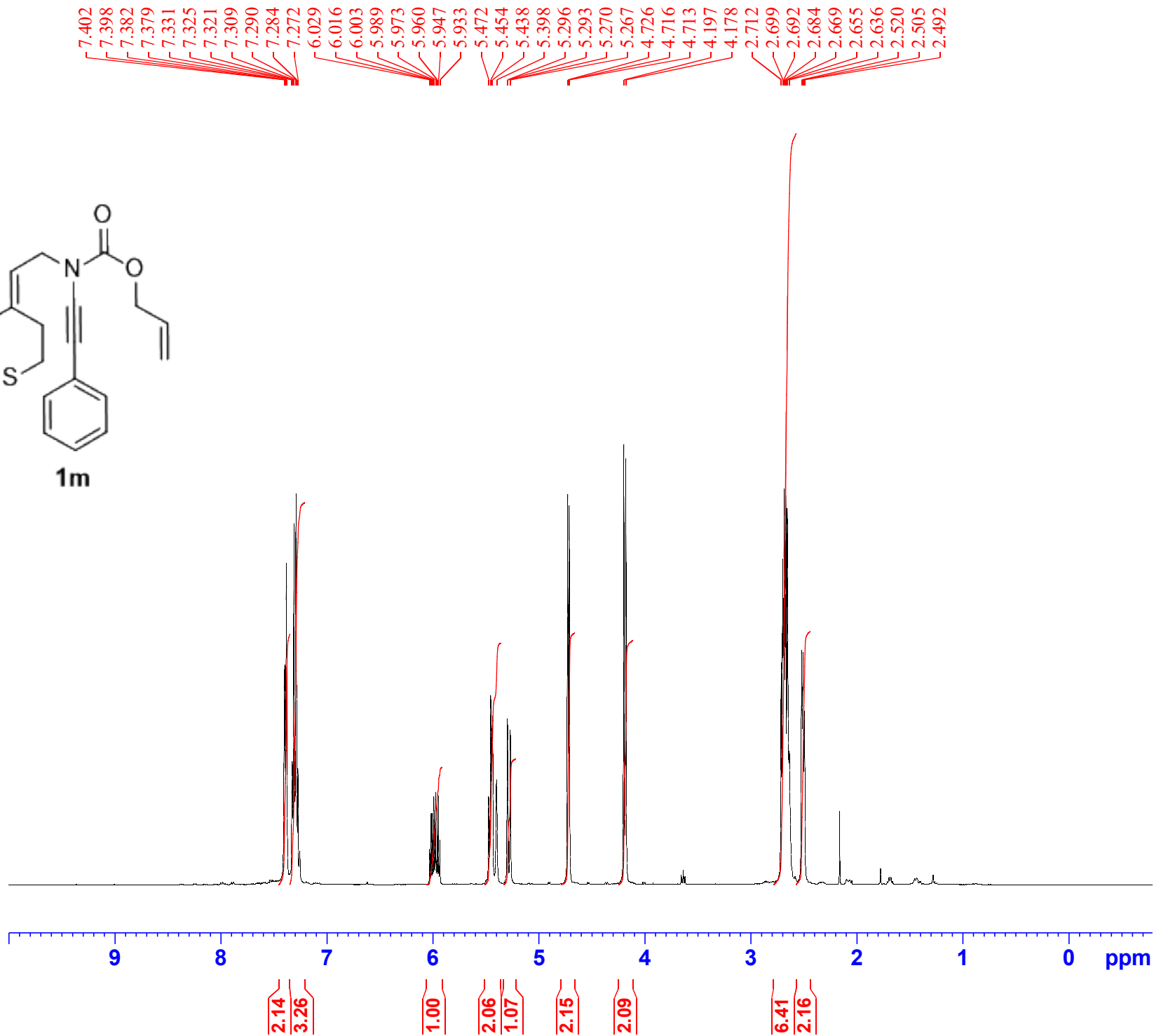
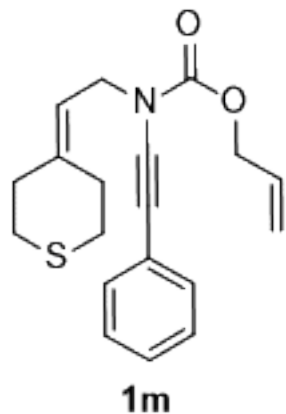
154.88  
 146.36  
 131.96  
 130.97  
 128.24  
 127.31  
 123.53  
 118.01  
 114.63  
 83.25  
 70.75  
 67.39  
 46.95  
 37.12  
 29.06  
 28.44  
 27.97  
 26.69

Current Data Parameters  
 NAME OJ-2-270-C  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210821  
 Time\_ 1.47 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

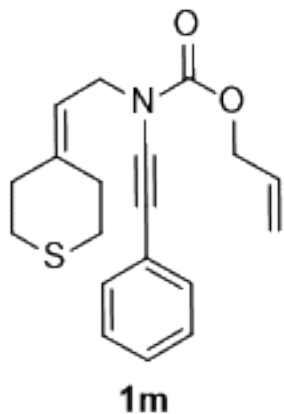
200 180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters  
 NAME OJ-2-288-H  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210902  
 Time\_ 20.31 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (z  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 32  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



154.88  
154.73  
143.03  
131.86  
131.02  
128.34  
127.55  
123.24  
118.12  
117.94  
82.99  
70.84  
67.49  
46.46  
38.83  
30.98  
30.96  
30.41

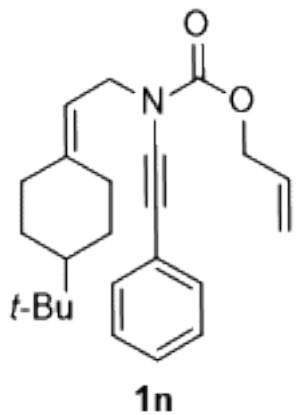
Current Data Parameters  
NAME OJ-2-288-C  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210902  
Time\_ 21.31 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

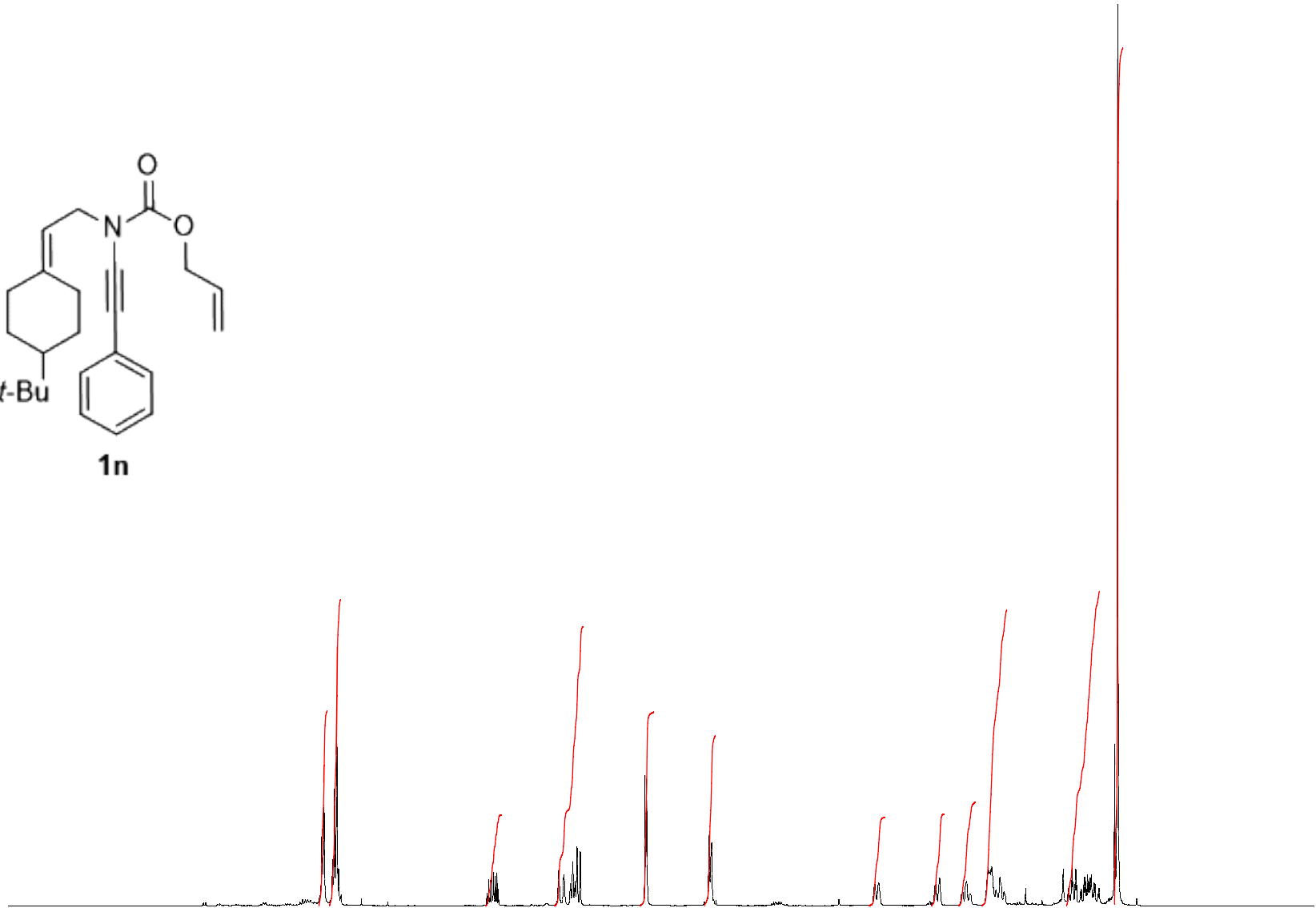
7.413  
7.409  
7.393  
7.389  
7.328  
7.321  
7.317  
7.306  
7.302  
7.298  
7.291  
7.286  
7.284  
7.278  
7.271  
7.269  
6.007  
5.990  
5.977  
5.964  
5.454  
5.452  
5.411  
5.409  
5.337  
5.306  
5.303  
5.299  
5.277  
5.273  
4.743  
4.739  
4.736  
4.729  
4.726  
4.722  
4.209  
4.189  
2.308  
1.905  
1.898  
1.889  
1.881  
1.874  
1.865  
1.807  
1.209  
1.179  
1.111  
1.102  
1.082  
1.061  
1.051  
0.834



Current Data Parameters  
NAME OJ-2-320-Pure-Tert-butyl-cyclohexyl  
EXPNO 5  
PROCNO 1

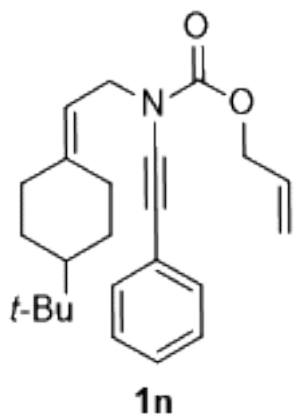
F2 - Acquisition Parameters  
Date\_ 20211118  
Time\_ 13:59 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 (4  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.89 usec  
TE 298.0 K  
D1 1.0000000 sec  
TDO 1  
SF01 400.1324708 MHz  
NUC1 1H  
PO 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



9 8 7 6 5 4 3 2 1 0 ppm

2.15  
3.37  
1.00  
3.07  
2.13  
1.87  
0.97  
1.01  
1.15  
3.26  
3.46  
9.45



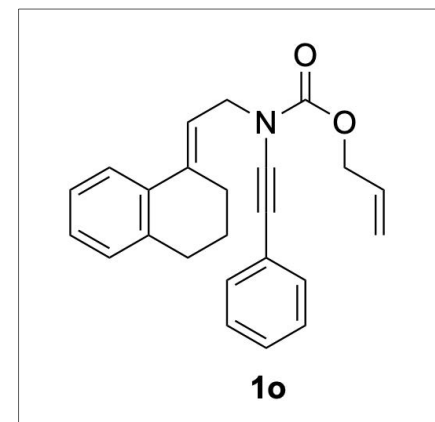
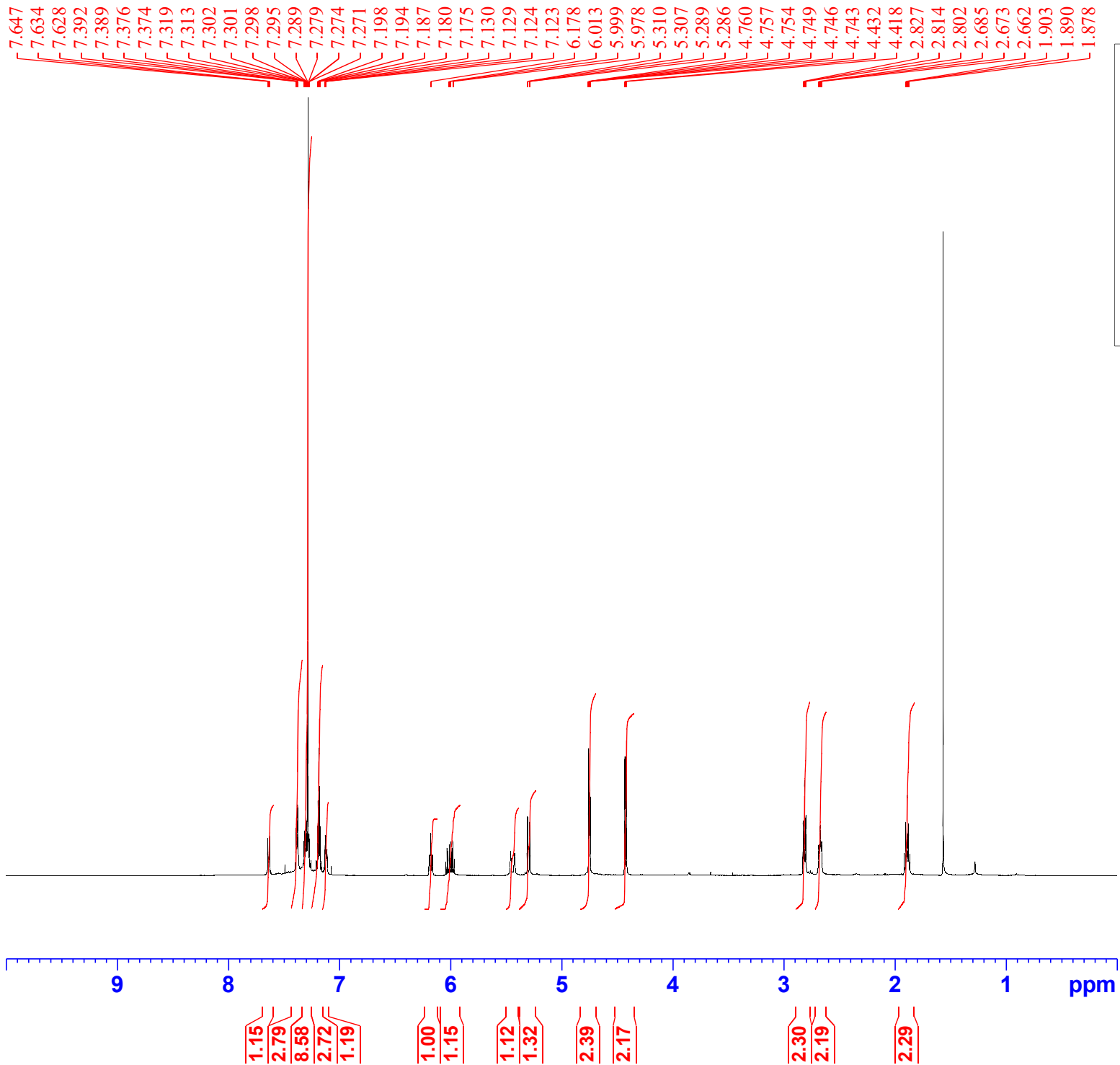
154.89  
 146.35  
 131.96  
 131.07  
 128.22  
 127.35  
 123.48  
 118.00  
 114.26  
 83.38  
 70.81  
 67.40  
 48.29  
 46.96  
 36.96  
 32.44  
 29.06  
 28.85  
 28.67  
 27.57

Current Data Parameters  
 NAME OJ-2-320-Pure-C-Tert-butyl-cyclohexyl  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20211118  
 Time 15.09 h  
 INSTRUM Avance Neo  
 PROBHD 2152088\_0031 (zggg30)  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TDO 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 PO 2.67 usec  
 PI 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPMPCPG2 waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18999999 W  
 PLW13 0.09552100 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

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

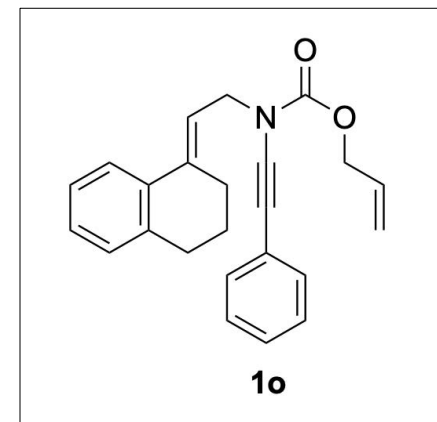


Current Data Parameters  
 NAME OJ-rev-tetra  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220825  
 Time\_ 23.21 h  
 INSTRUM spect  
 PROBHD Z125869\_0055 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 64  
 DS 2  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 3.2767999 sec  
 RG 151.18  
 DW 50.000 usec  
 DE 16.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 TD0 1  
 SF01 500.2330889 MHz  
 NUC1 1H  
 P0 4.00 usec  
 P1 12.00 usec  
 PLW1 11.44699955 W

F2 - Processing parameters  
 SI 65536  
 SF 500.2330000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



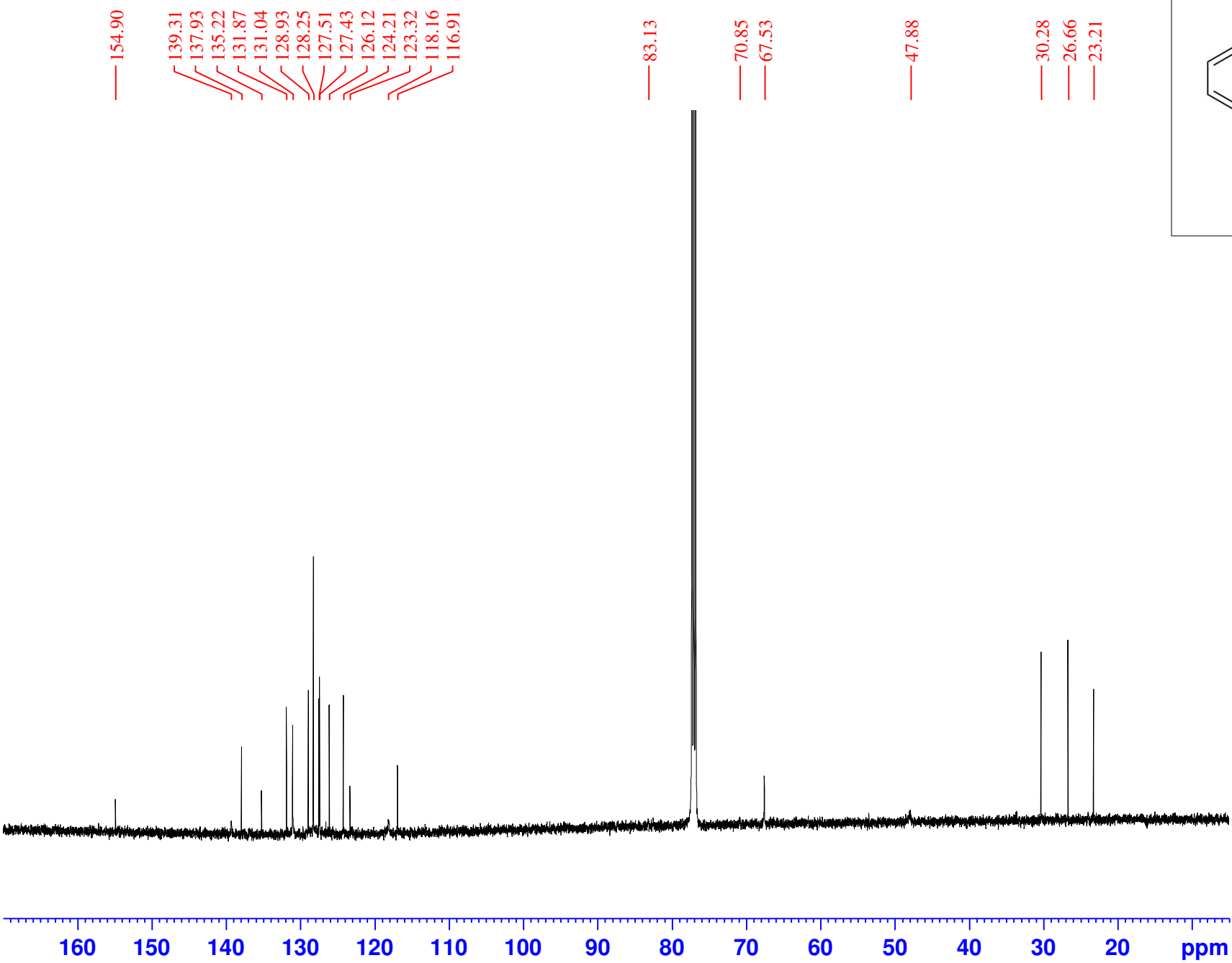


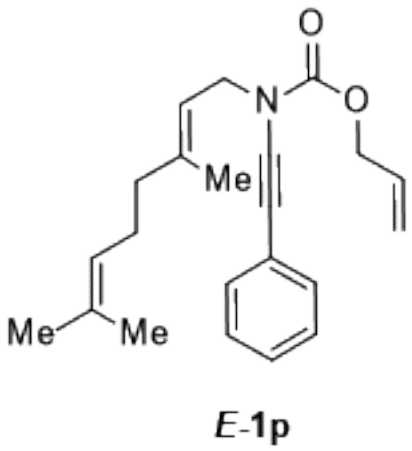
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Current Data Parameters
NAME      OJ-rev-tetra-C-2
EXPNO     14
PROCNO    1

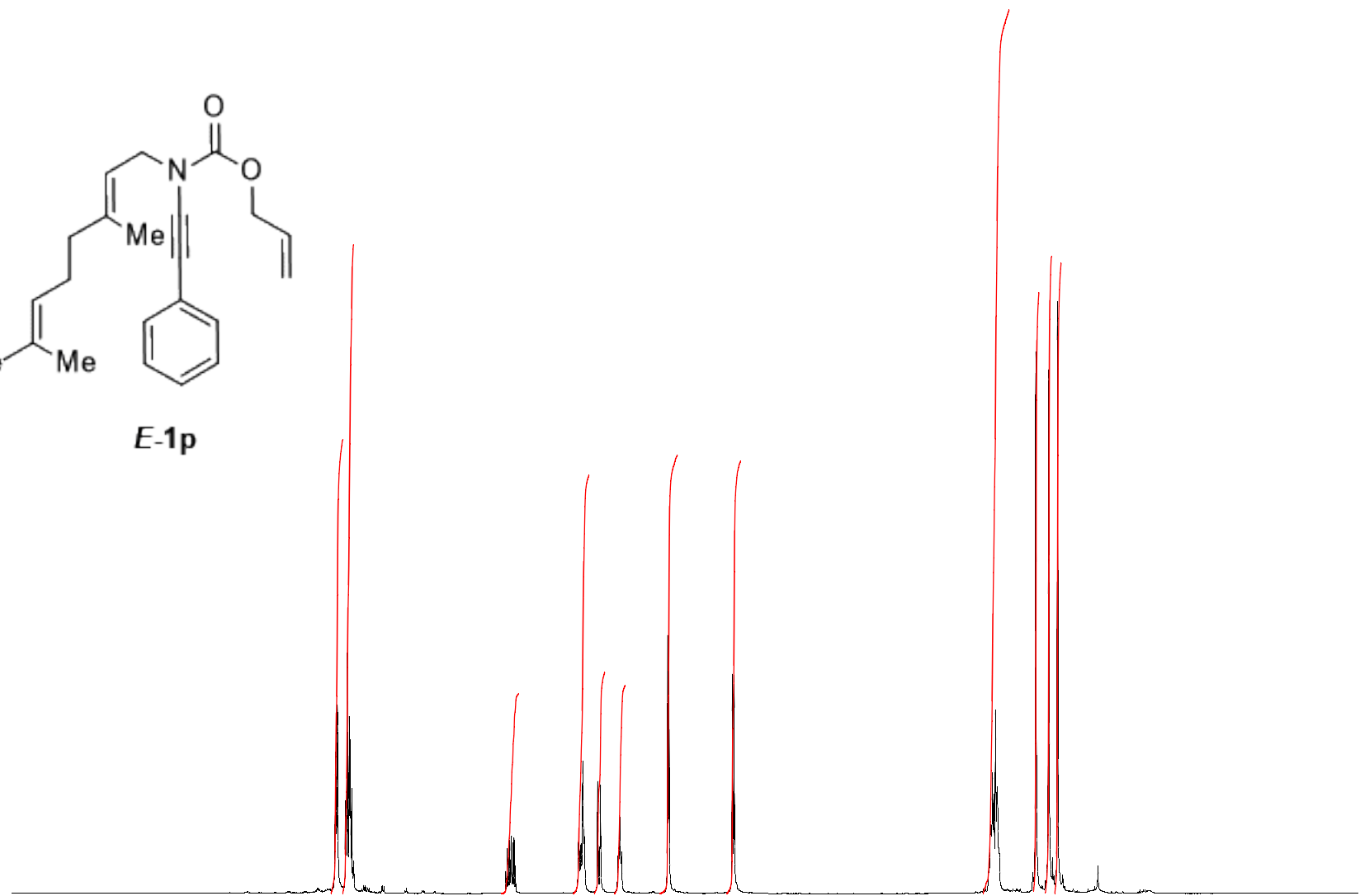
F2 - Acquisition Parameters
Date_     20220826
Time      18.58 h
INSTRUM   spect
PROBHD    Z125869_0055 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         3072
DS         4
SWH        29761.904 Hz
FIDRES     0.908261 Hz
AQ         1.1010048 sec
RG         190.44
DW         16.800 usec
DE         18.00 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1       125.7955118 MHz
NUC1       13C
P0         3.33 usec
P1         10.00 usec
PLW1       56.90299988 W
SFO2       500.2320009 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2      80.00 usec
PLW2       11.44699955 W
PLW12      0.25756001 W
PLW13      0.12955000 W

F2 - Processing parameters
SI         32768
SF         125.7829335 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```





7.409  
7.406  
7.393  
7.330  
7.326  
7.322  
7.312  
7.310  
7.300  
7.298  
7.293  
7.290  
7.287  
7.284  
7.282  
7.276  
6.010  
5.997  
5.986  
5.976  
5.457  
5.440  
5.427  
5.425  
5.416  
5.413  
5.410  
5.309  
5.306  
5.304  
5.301  
5.285  
5.283  
5.280  
5.131  
5.128  
5.126  
4.748  
4.745  
4.742  
4.737  
4.734  
4.731  
4.226  
4.212  
2.154  
2.141  
2.129  
2.116  
2.102  
1.794  
1.691  
1.689  
1.620

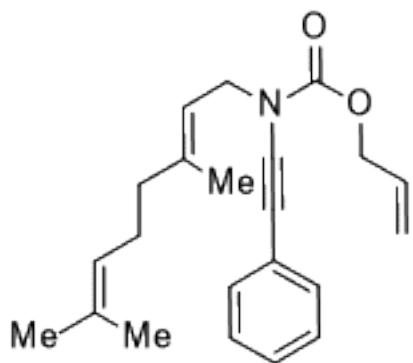


9 8 7 6 5 4 3 2 1 0 ppm

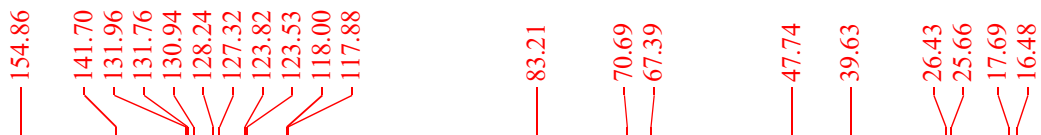
Current Data Parameters  
 NAME OJ-2-109  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210622  
 Time\_ 13.39 h  
 INSTRUM spect  
 PROBHD z125869\_0055 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 64  
 DS 2  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 3.2767999 sec  
 RG 19.46  
 DW 50.000 usec  
 DE 16.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 TD0 1  
 SFO1 500.2330889 MHz  
 NUC1 1H  
 P0 4.00 usec  
 P1 12.00 usec  
 PLW1 11.44699955 W

F2 - Processing parameters  
 SI 65536  
 SF 500.2330000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



**E-1p**

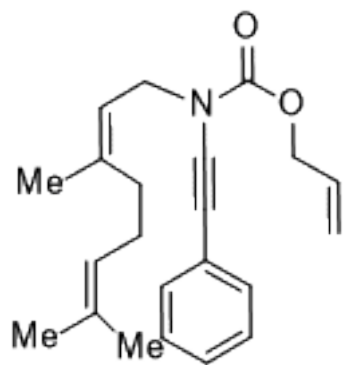


Current Data Parameters  
 NAME OJ-2-109-C  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210622  
 Time\_ 14.35 h  
 INSTRUM spect  
 PROBHD Z125869\_0055 ( )  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 1024  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 1.1010048 sec  
 RG 190.44  
 DW 16.800 usec  
 DE 18.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 125.7955118 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 56.90299988 W  
 SFO2 500.2320009 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 80.00 usec  
 PLW2 11.44699955 W  
 PLW12 0.25756001 W  
 PLW13 0.12955000 W

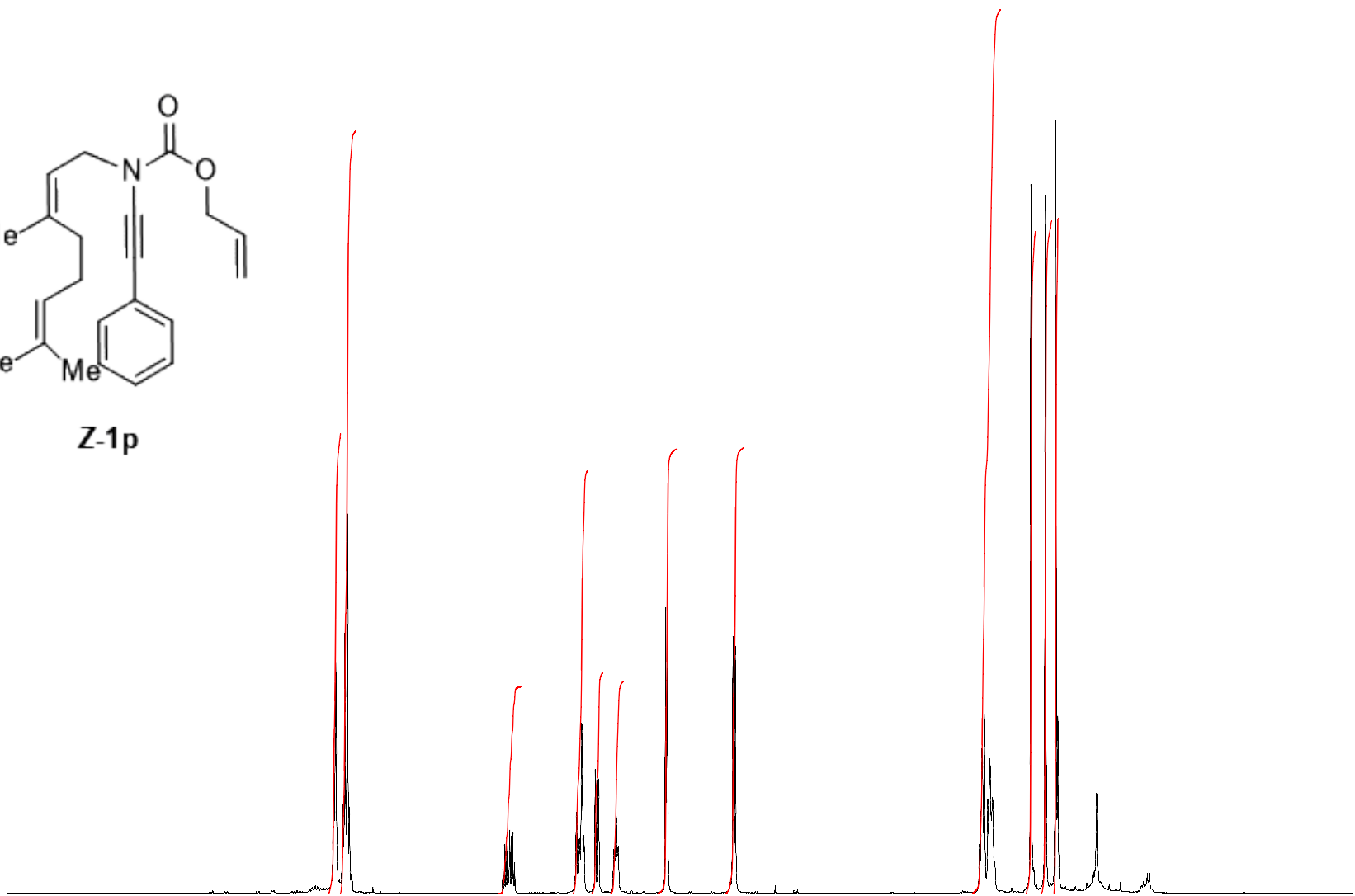
F2 - Processing parameters  
 SI 32768  
 SF 125.7829335 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

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



**Z-1p**

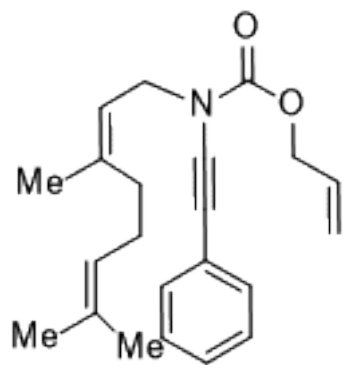
7.385  
7.381  
7.365  
7.363  
7.314  
7.308  
7.304  
7.293  
7.273  
7.268  
7.256  
6.027  
6.014  
6.000  
5.987  
5.971  
5.958  
5.944  
5.931  
5.436  
5.412  
5.394  
5.376  
5.286  
5.283  
5.260  
5.257  
5.136  
5.133  
5.118  
5.102  
4.723  
4.720  
4.717  
4.710  
4.707  
4.703  
4.181  
4.163  
2.206  
2.201  
2.185  
2.179  
2.166  
2.137  
2.121  
2.101  
2.083  
1.793  
1.677  
1.594



9 8 7 6 5 4 3 2 1 0 ppm

2.09  
3.45  
0.94  
1.91  
1.00  
0.96  
2.01  
2.02  
4.00  
3.00  
3.04  
3.18

Current Data Parameters  
 NAME OJ-Nerol ynamide  
 EXPNO 10  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20210730  
 Time\_ 17.48 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W  
 F2 - Processing parameters  
 SI 65536  
 SF 400.1300062 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



**Z-1p**

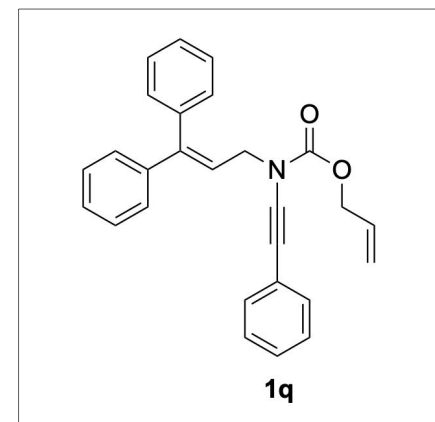
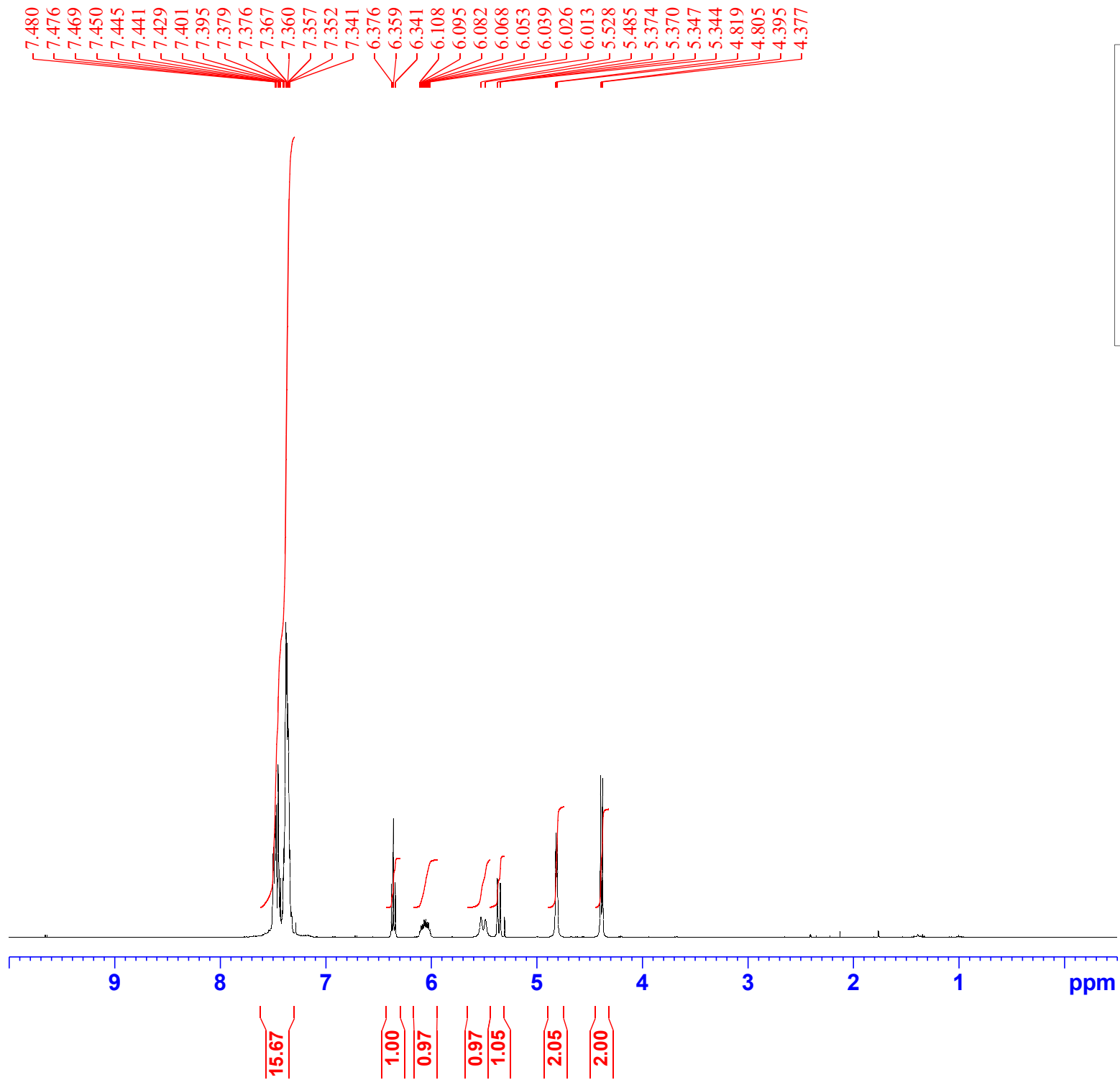


Current Data Parameters  
 NAME OJ-Nerol ynamide-C  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210730  
 Time\_ 18.54 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

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



Current Data Parameters  
 NAME OJ-1-183-H  
 EXPNO 17  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220903  
 Time\_ 21.41 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 32  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SF01 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

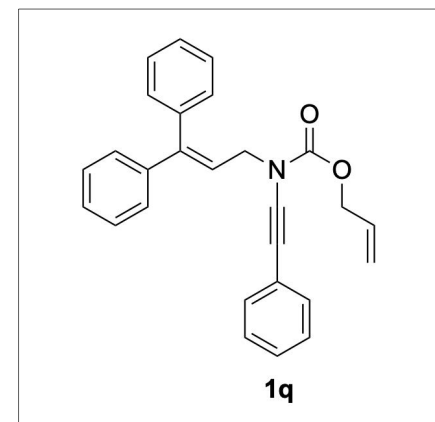
154.855  
146.251  
141.608  
138.822  
131.938  
131.088  
129.938  
128.732  
128.463  
128.387  
128.334  
127.887  
127.799  
127.753  
127.636  
127.554  
123.427  
122.336  
118.228

83.156

71.293

67.611

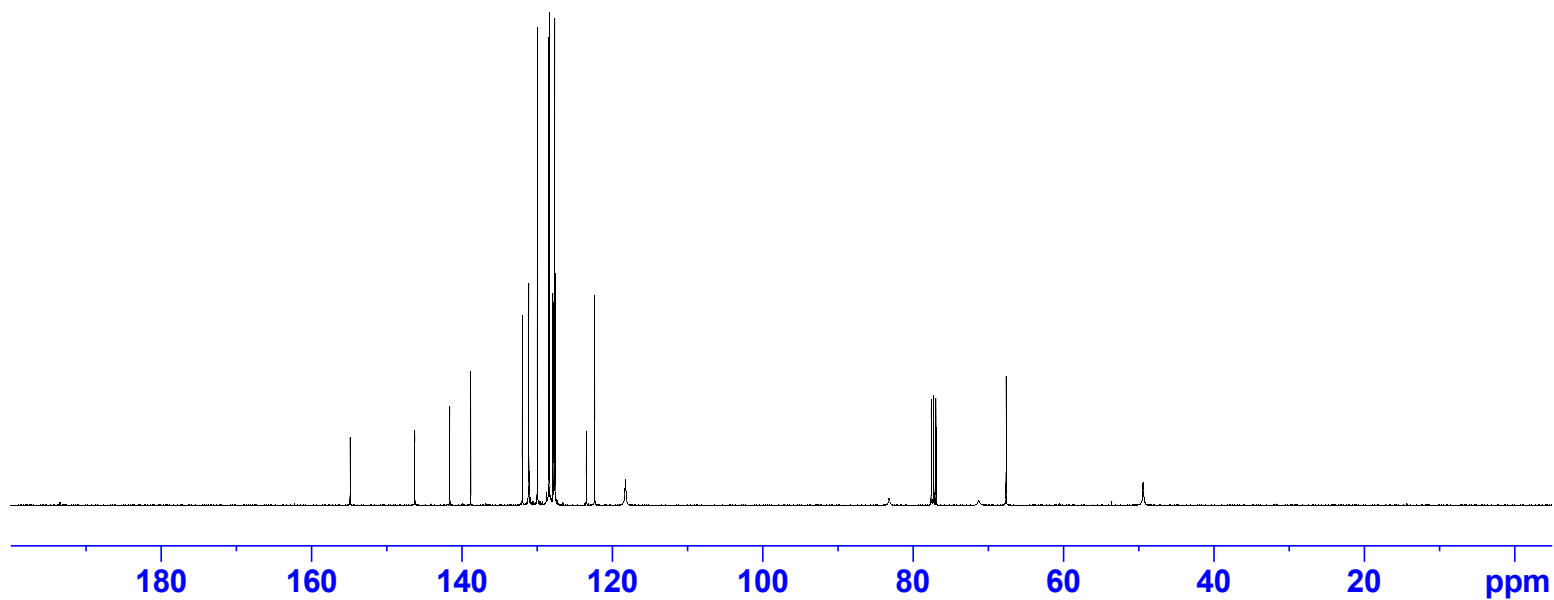
49.370



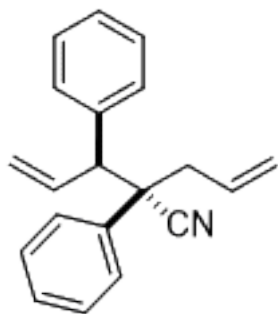
Current Data Parameters  
NAME OJ-1-183-C  
EXPNO 19  
PROCNO 1

F2 - Acquisition Parameters  
Date 20220903  
Time 22.41 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 10.7781  
DW 21.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

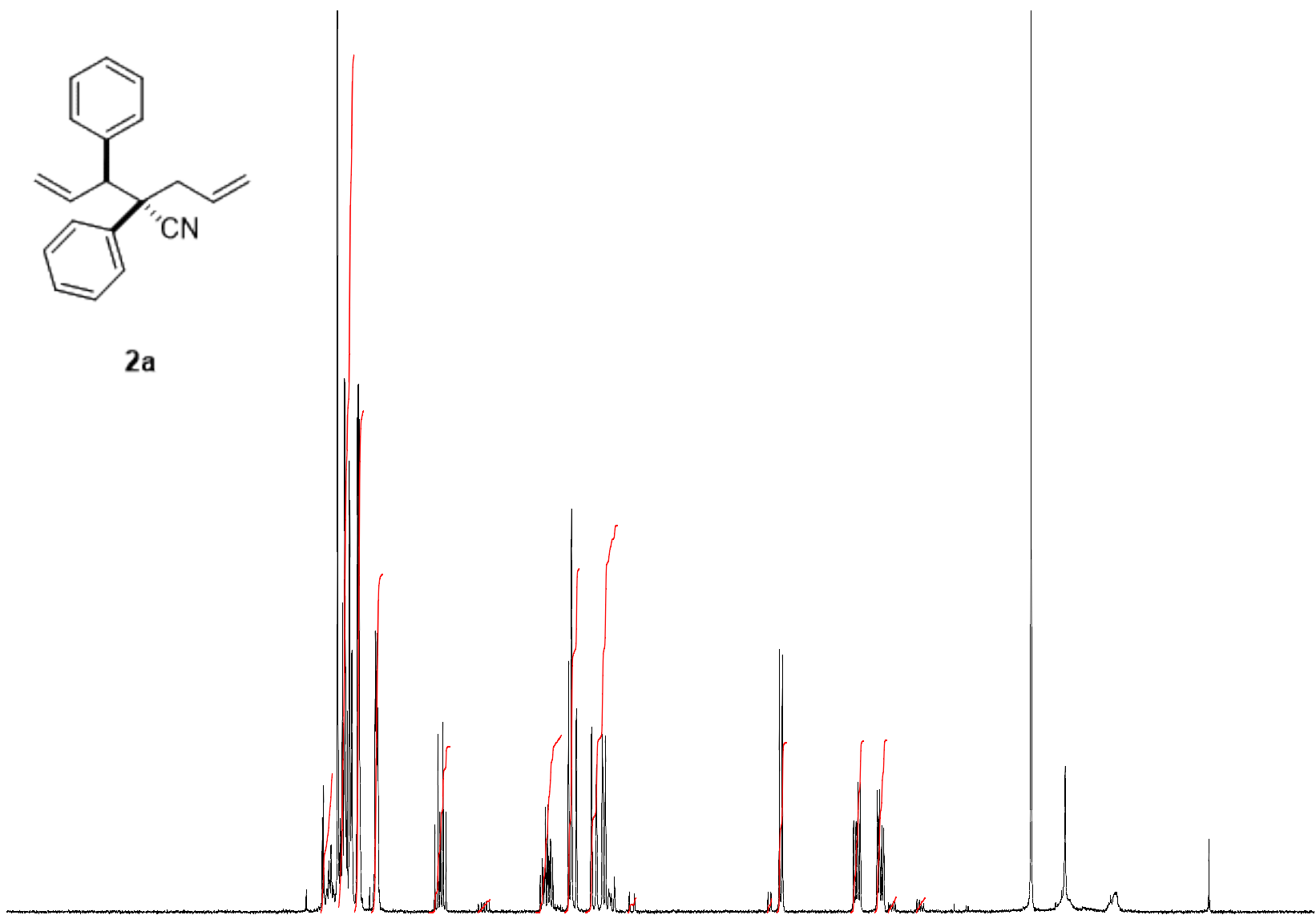
F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
FC 1.40



7.397  
7.387  
7.270  
7.247  
7.231  
7.212  
7.207  
7.202  
7.198  
7.191  
7.173  
7.168  
7.163  
7.157  
7.153  
7.149  
7.107  
7.100  
7.091  
6.961  
6.955  
6.949  
6.946  
6.937  
6.467  
6.443  
6.426  
6.418  
6.401  
6.376  
5.556  
5.537  
5.513  
5.365  
5.362  
5.340  
5.299  
5.177  
5.174  
5.135  
5.131  
5.086  
5.061  
3.011  
2.992  
2.975  
2.957  
2.815  
2.798  
2.779  
2.763  
1.546  
1.264  
0.079



2a



9 8 7 6 5 4 3 2 1 0 ppm

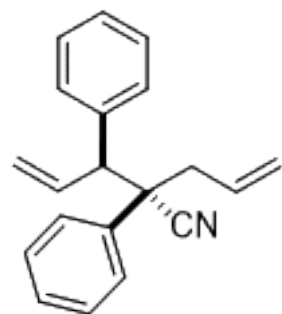
0.79  
4.82  
2.81  
1.90  
0.93  
0.07  
0.99  
1.93  
2.17  
0.08  
0.08  
0.95  
0.96  
0.97  
0.08  
0.08

Current Data Parameters  
 NAME OJ-2-48-pure  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210516  
 Time\_ 23.32 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (zg30)  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300057 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





2a

138.58  
136.34  
131.84  
128.65  
128.33  
128.03  
127.64  
127.19  
127.10  
119.92  
119.26

60.01  
52.63  
42.78

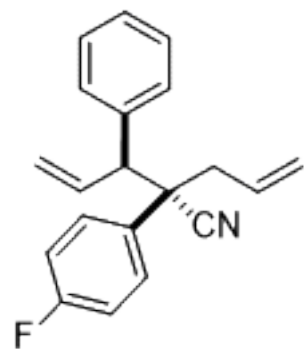
Current Data Parameters  
NAME OJ-2-48-pure  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210517  
Time\_ 1.55 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

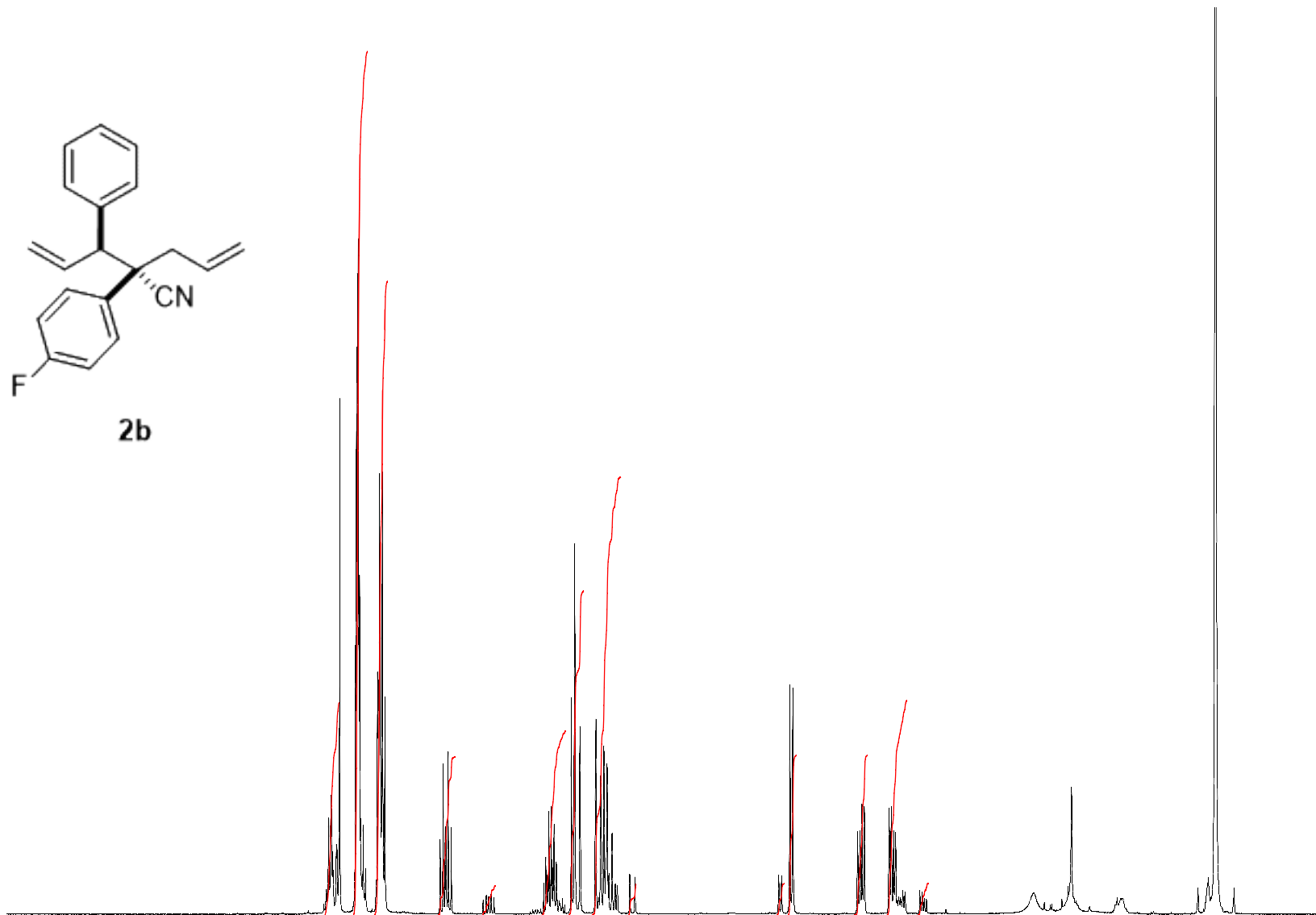
F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

7.362  
7.348  
7.344  
7.339  
7.333  
7.326  
7.322  
7.298  
7.293  
7.141  
7.133  
7.128  
7.125  
7.118  
7.107  
7.099  
7.078  
7.056  
6.961  
6.954  
6.951  
6.942  
6.937  
6.921  
6.899  
6.447  
6.422  
6.405  
6.397  
6.380  
6.355  
5.536  
5.529  
5.519  
5.511  
5.493  
5.299  
5.172  
5.168  
5.126  
5.103  
5.086  
5.078  
5.036  
3.577  
3.553  
3.021  
3.002  
2.985  
2.966  
2.762  
2.745  
2.726  
2.709



2b



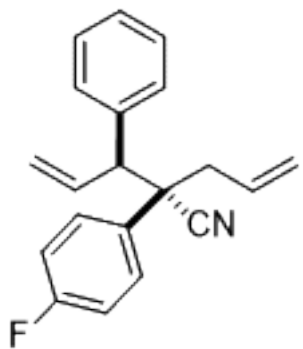
9 8 7 6 5 4 3 2 1 0 ppm

1.13  
4.58  
3.36  
0.84  
0.16  
0.98  
1.72  
2.32  
0.17  
0.17  
0.85  
0.85  
1.14  
0.17

Current Data Parameters  
NAME OJ-2-50-1-Pure  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210519  
Time\_ 0.02 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.89 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300059 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



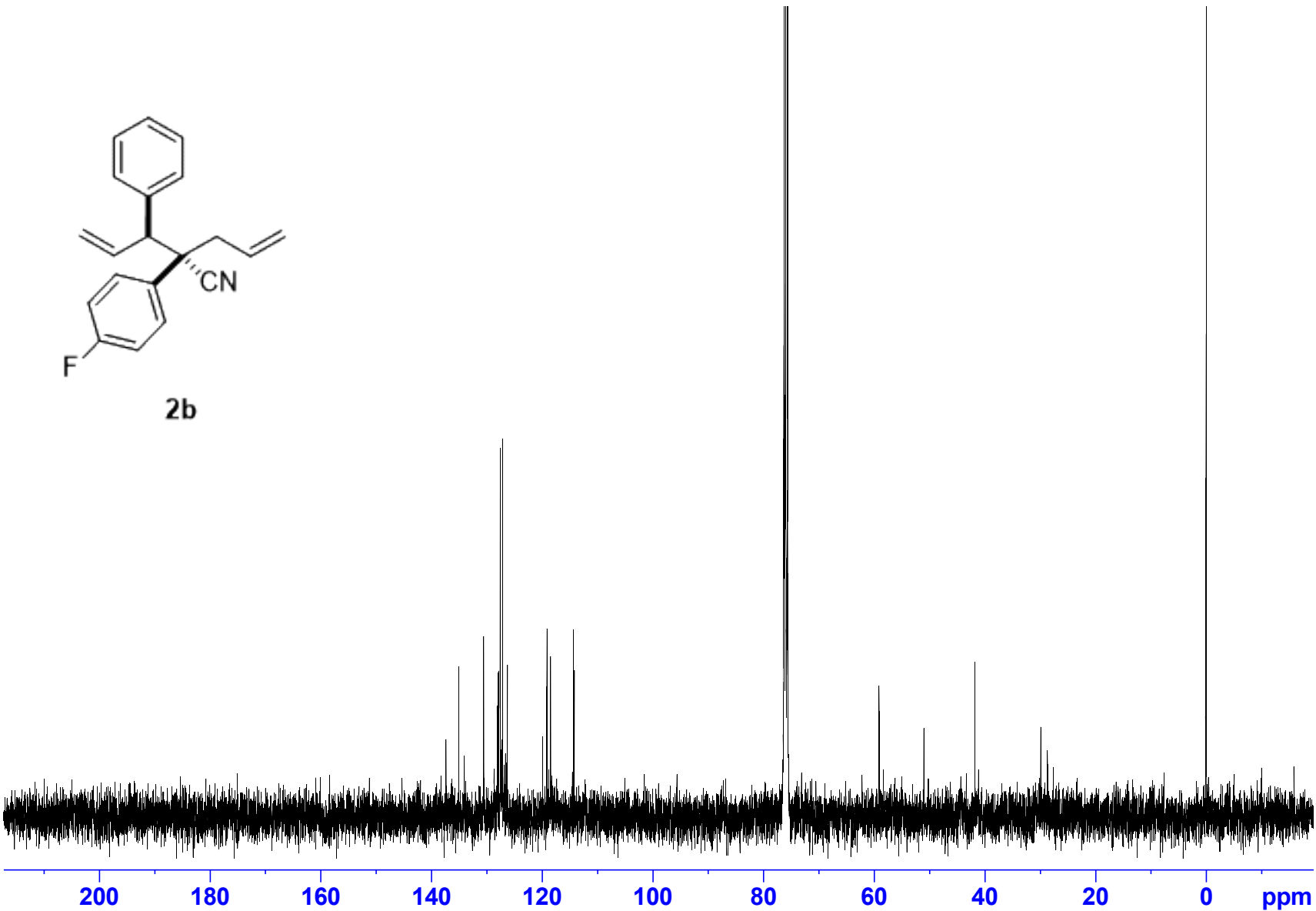
2b

162.61  
160.10  
137.33  
135.07  
134.04  
130.53  
128.12  
127.92  
127.83  
127.60  
127.57  
127.45  
127.24  
127.14  
126.64  
126.23  
119.90  
119.13  
119.06  
118.44  
114.35  
114.14  
76.30  
76.18  
75.98  
75.66  
59.10  
51.03  
41.79  
29.91  
28.68  
-0.00

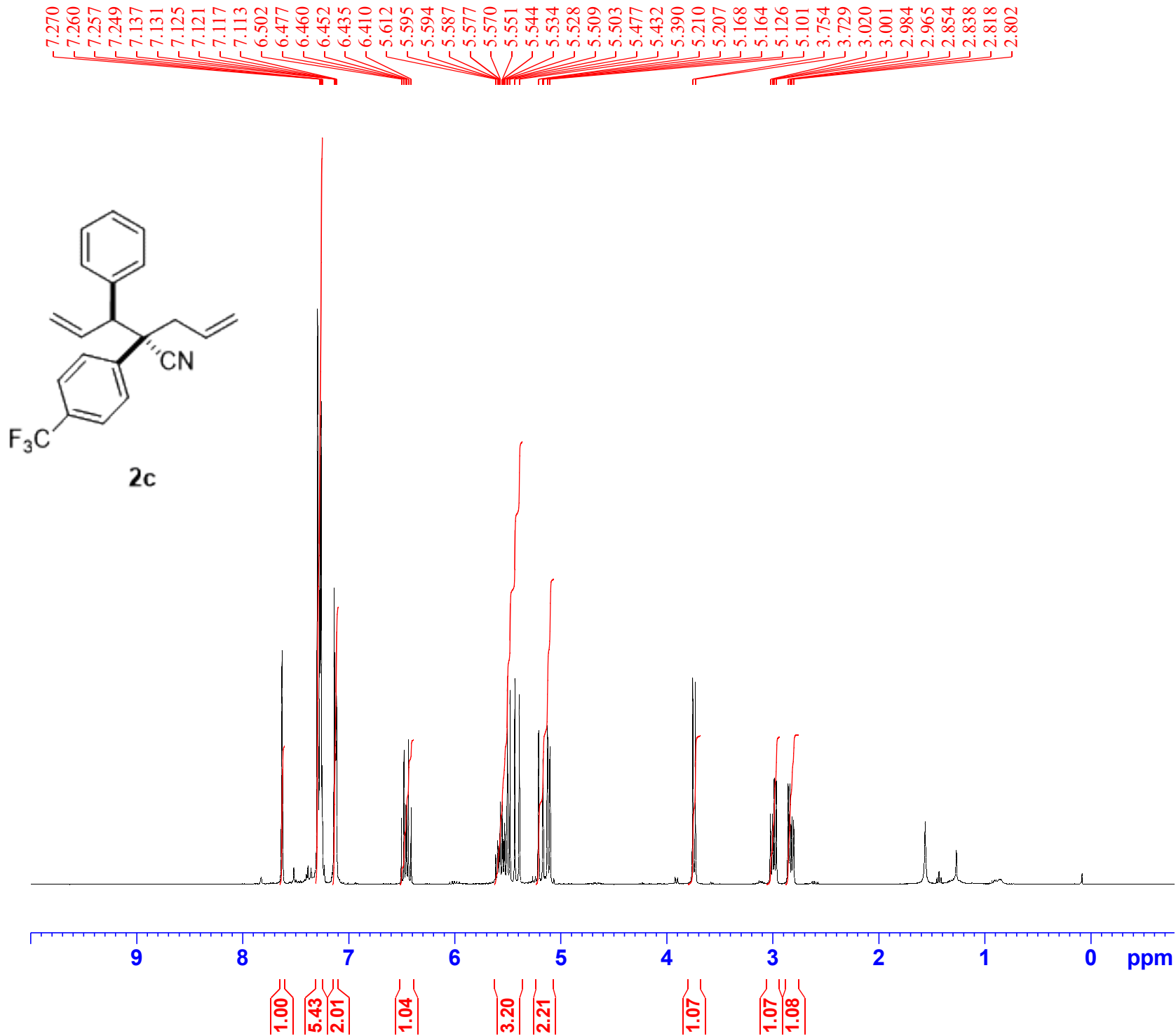
Current Data Parameters  
NAME OJ-2-Para-fluoro-nitrile-C  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210910  
Time 23.27 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (4  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2048  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6128727 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



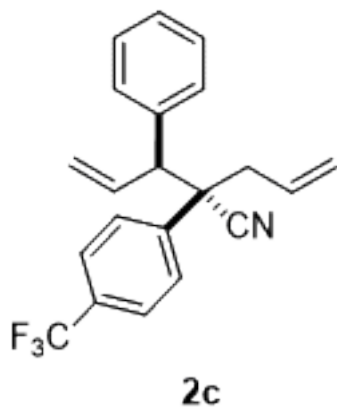
200 180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters  
 NAME OJ-2-82-1-Pure-H  
 EXPNO 16  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210601  
 Time\_ 17.47 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (   
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300057 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



141.07  
 134.86  
 134.32  
 131.58  
 131.25  
 131.21  
 130.92  
 130.59  
 128.86  
 128.37  
 127.52  
 127.08  
 126.84  
 124.37  
 121.65  
 121.29  
 121.10  
 121.06  
 121.03  
 120.49  
 119.94  
 118.94  
 77.33  
 77.22  
 77.02  
 76.70  
 59.50  
 52.72  
 42.24

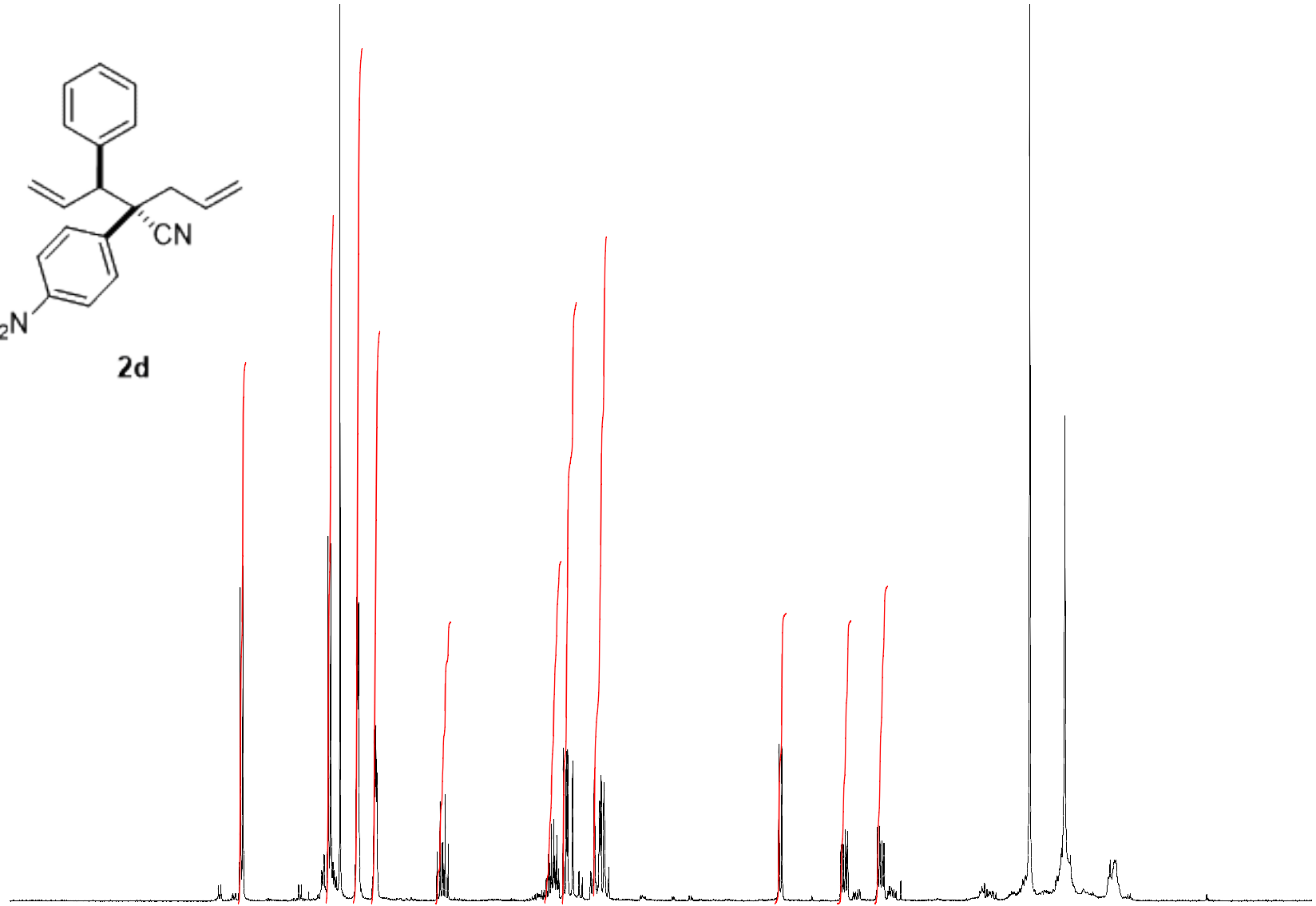
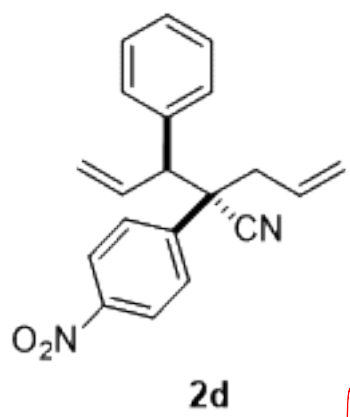
Current Data Parameters  
 NAME OJ-2-82-1-Pure-C  
 EXPNO 17  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210601  
 Time\_ 18.49 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

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

8.070  
7.364  
7.342  
7.128  
7.121  
7.112  
6.983  
6.977  
6.968  
6.959  
6.461  
6.436  
6.419  
6.411  
6.394  
6.370  
5.556  
5.538  
5.531  
5.520  
5.513  
5.496  
5.488  
5.478  
5.470  
5.461  
5.453  
5.414  
5.389  
5.379  
5.337  
5.160  
5.157  
5.117  
5.114  
5.104  
5.079  
3.629  
3.605  
3.115  
3.097  
3.079  
3.061  
2.812  
2.794  
2.776  
2.758



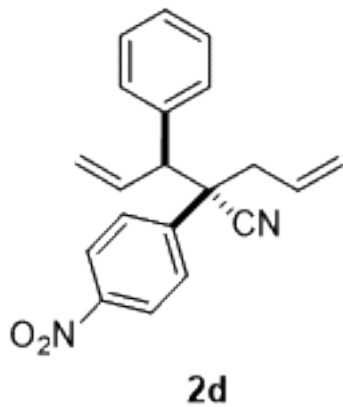
9 8 7 6 5 4 3 2 1 0 ppm

1.80  
2.30  
2.85  
1.90  
0.94  
1.14  
2.00  
2.22  
0.97  
0.94  
1.06

Current Data Parameters  
 NAME OJ-2-259-H  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210812  
 Time\_ 10.45 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (zg30)  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300074 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



147.17  
143.52  
137.78  
135.50  
130.75  
128.49  
128.36  
128.25  
127.82  
127.65  
123.50  
120.92  
120.15

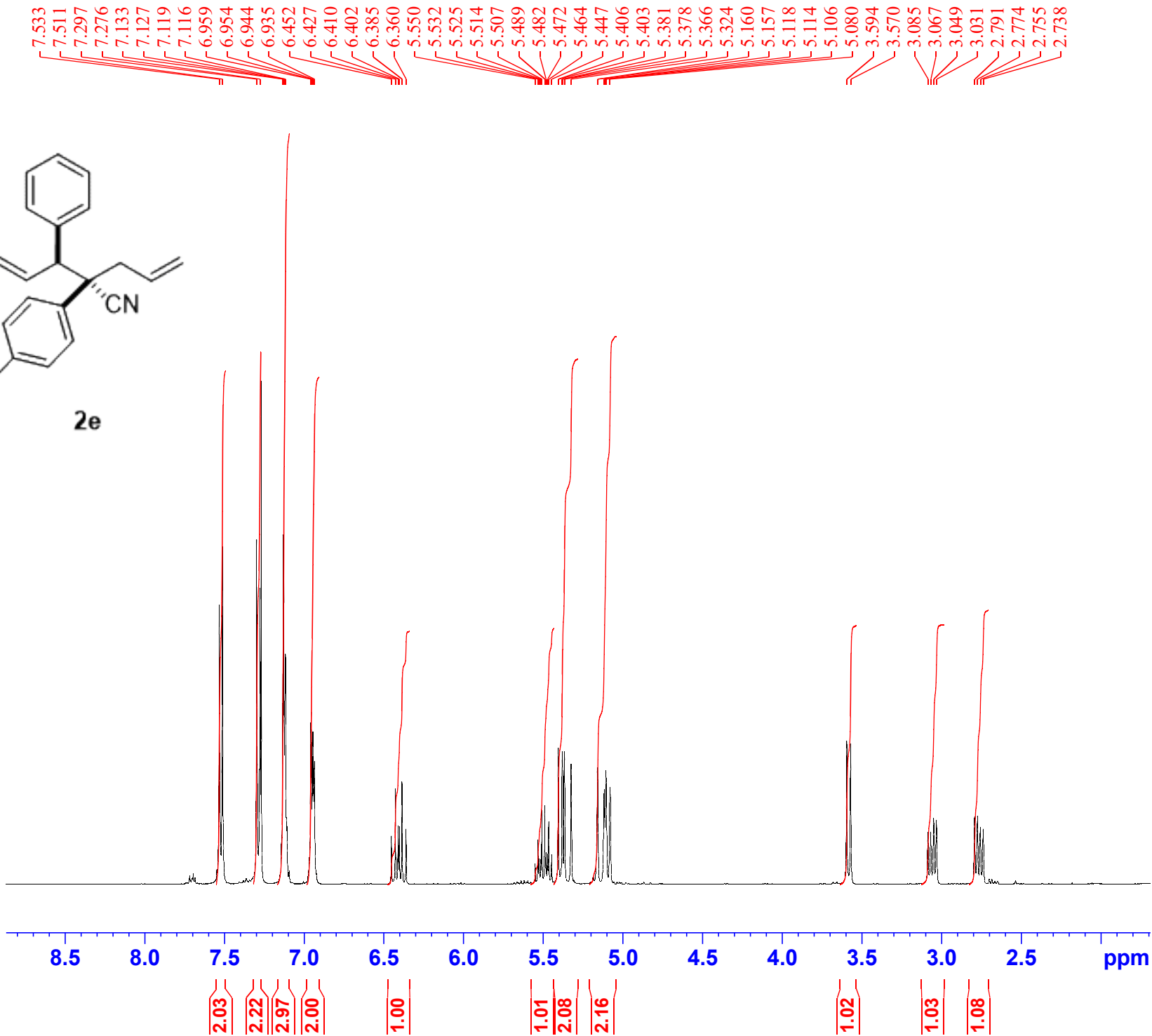
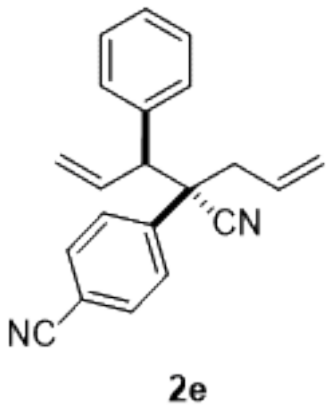
59.93  
52.84  
42.97

Current Data Parameters  
NAME OJ-2-259-C  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210812  
Time\_ 19.21 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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



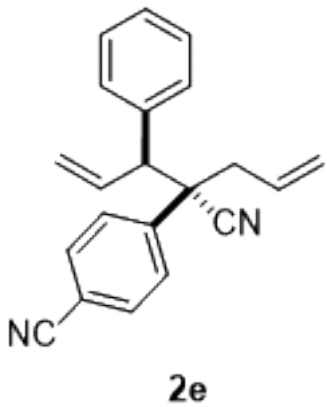
7.533  
7.511  
7.297  
7.276  
7.133  
7.127  
7.119  
7.116  
6.959  
6.954  
6.944  
6.935  
6.452  
6.427  
6.410  
6.402  
6.385  
6.360  
5.550  
5.532  
5.525  
5.514  
5.507  
5.489  
5.482  
5.472  
5.464  
5.447  
5.406  
5.403  
5.381  
5.378  
5.366  
5.324  
5.160  
5.157  
5.118  
5.114  
5.106  
5.080  
3.594  
3.570  
3.085  
3.067  
3.049  
3.031  
2.791  
2.774  
2.755  
2.738

Current Data Parameters  
NAME OJ-2-49-Pure  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210516  
Time\_ 23.38 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 (zg30)  
PULPROG 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.89 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300062 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





141.54  
137.84  
135.54  
132.12  
130.86  
128.41  
128.38  
128.04  
127.58  
120.80  
120.12  
120.05  
118.17  
111.78

77.34  
77.23  
77.02  
76.71

59.92

52.93

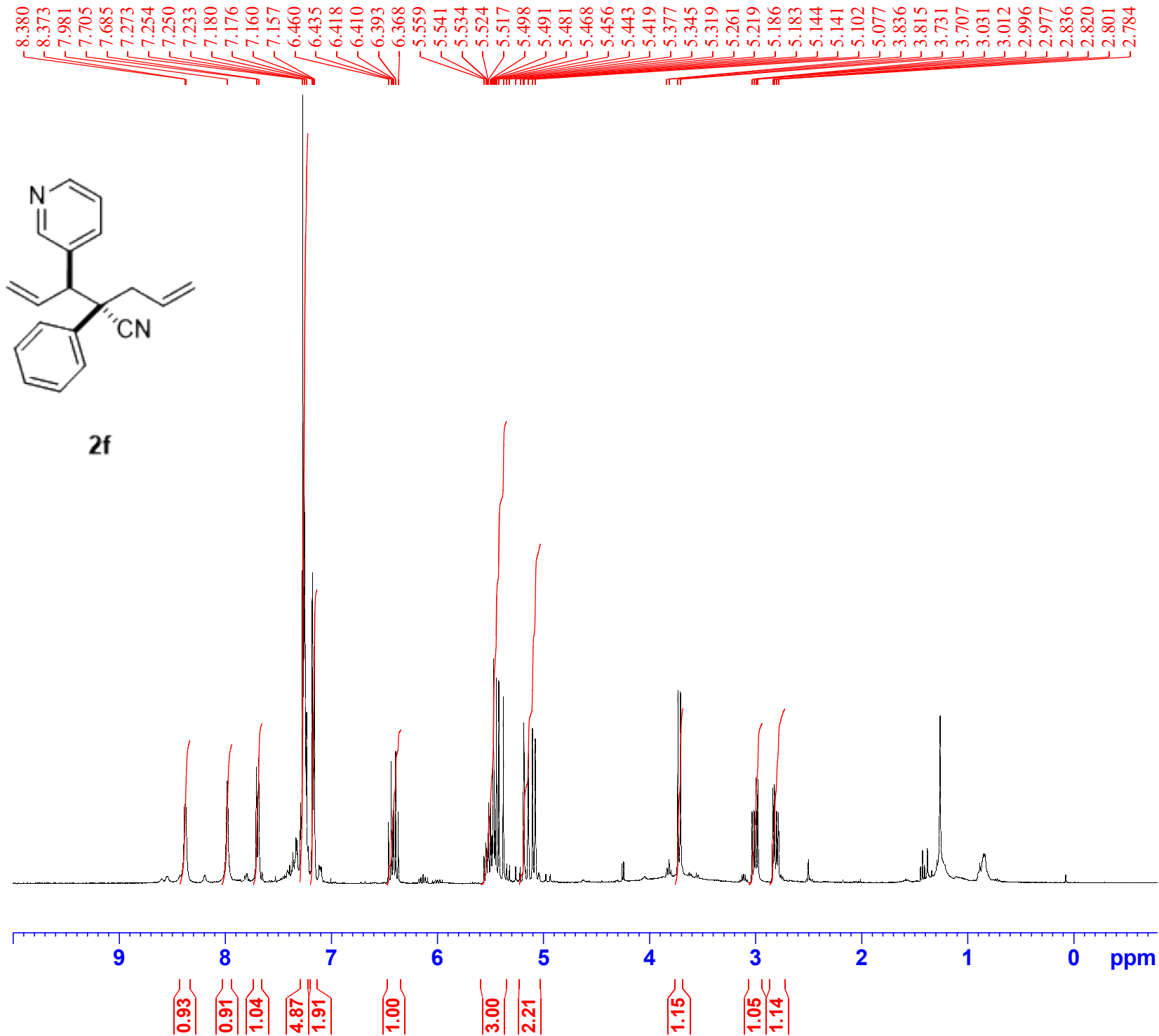
42.72

Current Data Parameters  
NAME OJ-2-49-Pure  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210517  
Time\_ 0.48 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

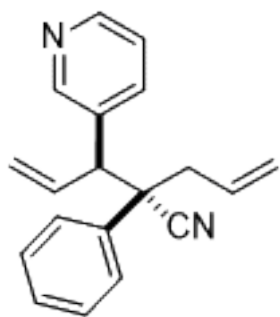
200 180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters  
 NAME OJ-2-110-Pure  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210625  
 Time\_ 22.14 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (z  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300067 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



2f

147.92  
146.33  
137.41  
134.99  
134.62  
131.17  
129.04  
128.96  
128.41  
128.10  
126.79  
123.77  
121.08  
120.46  
120.31

77.34  
77.23  
77.02  
76.71

57.16  
52.57

42.70

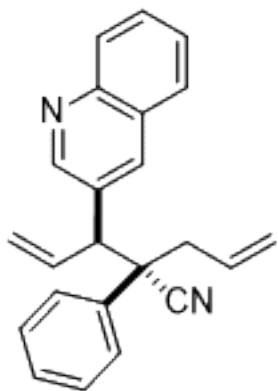
Current Data Parameters  
NAME OJ-2-110-Pure-C  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210625  
Time\_ 23.16 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

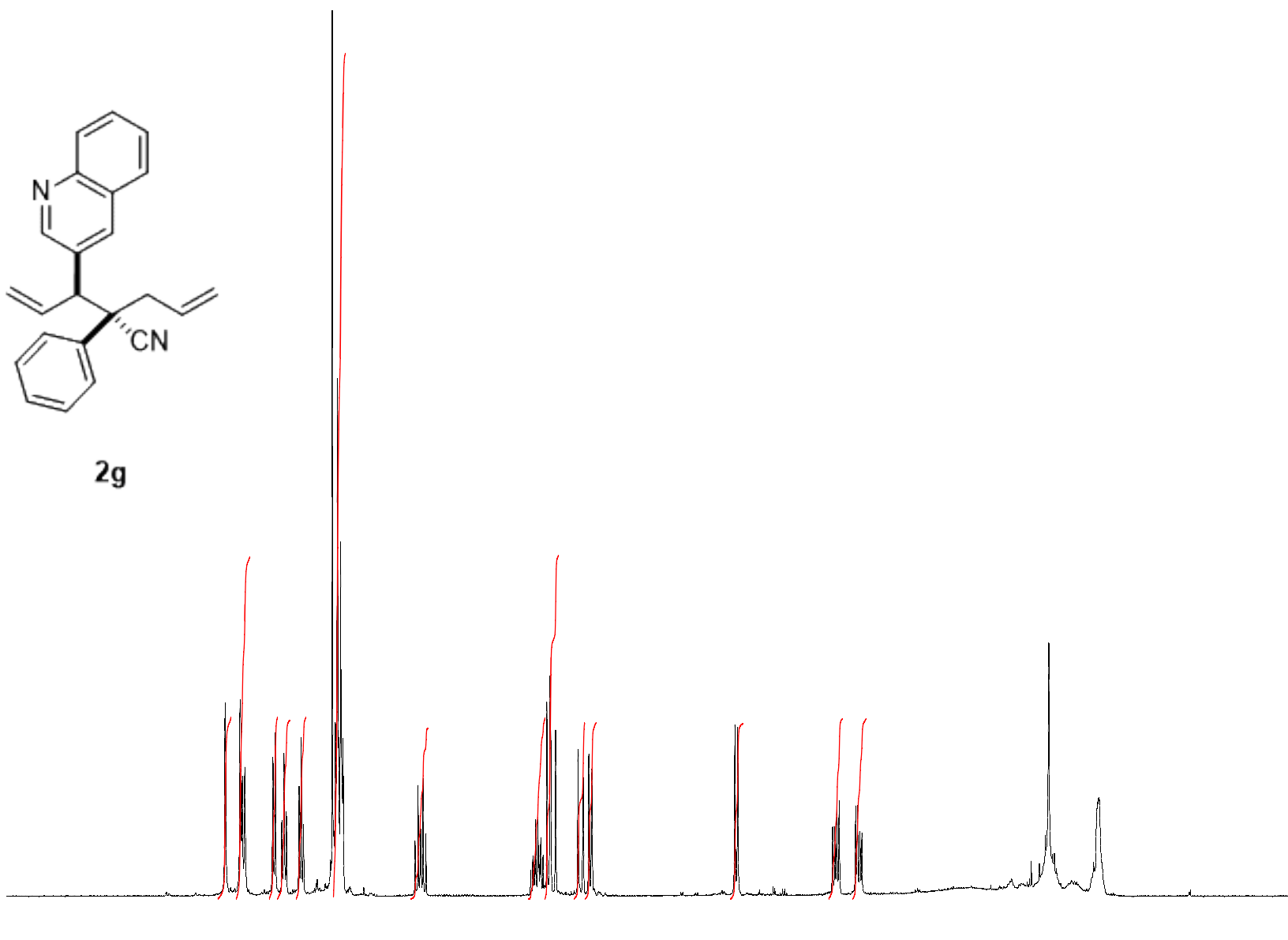
F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

8.172  
8.167  
8.045  
8.026  
8.005  
7.770  
7.750  
7.697  
7.694  
7.676  
7.659  
7.656  
7.551  
7.532  
7.513  
7.246  
7.228  
7.219  
7.203  
7.196  
7.191  
7.183  
7.179  
6.578  
6.553  
6.536  
6.528  
6.511  
6.486  
5.566  
5.548  
5.541  
5.531  
5.524  
5.473  
5.447  
5.443  
5.400  
5.213  
5.210  
5.171  
5.168  
5.121  
5.095  
3.898  
3.873  
3.078  
3.059  
3.042  
3.023  
2.885  
2.869  
2.850  
2.833



2g



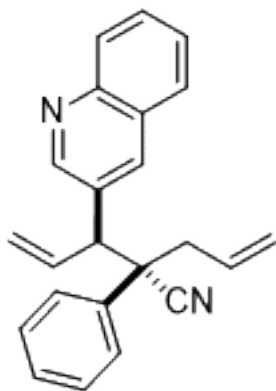
1.06  
2.00  
1.07  
1.05  
1.06  
4.95  
1.00  
1.06  
2.01  
1.03  
1.03  
1.03  
1.06  
1.05

Current Data Parameters  
NAME OJ-Quinoline Nitrile  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210704  
Time 20.40 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (zg30)  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.89 usec  
TE 298.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300052 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

9 8 7 6 5 4 3 2 1 0 ppm



2g

150.65  
150.59  
135.63  
135.19  
135.08  
131.87  
131.37  
129.81  
128.86  
128.50  
128.36  
127.99  
127.52  
126.97  
120.55  
120.51  
120.36

57.13  
52.85

42.77

Current Data Parameters  
NAME OJ-Quinoline Nitrile-C  
EXPNO 13  
PROCNO 1

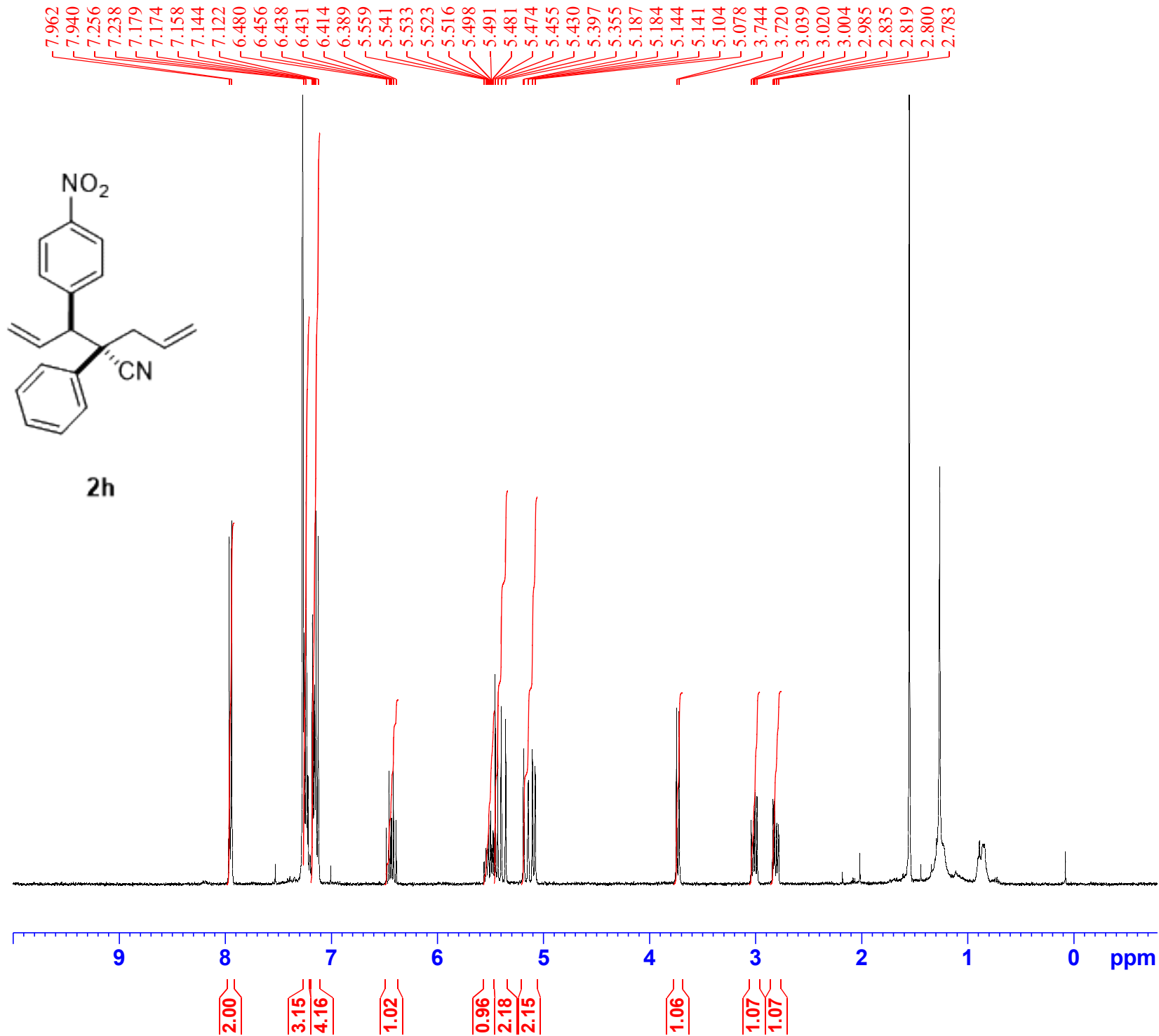
F2 - Acquisition Parameters

Date\_ 20210705  
Time 1.42 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters

SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

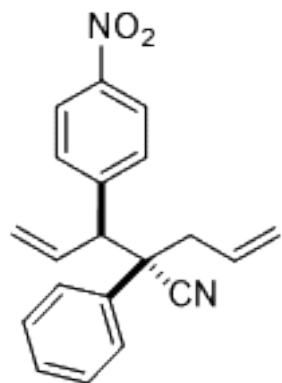
200 180 160 140 120 100 80 60 40 20 0 ppm



Current Data Parameters  
 NAME OJ-2-105-Pure  
 EXPNO 13  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210625  
 Time\_ 23.21 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300063 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



2h

146.22  
135.21  
134.94  
133.42  
131.17  
129.41  
128.80  
128.19  
126.81  
123.21  
120.80  
120.44

59.72  
53.44  
42.87

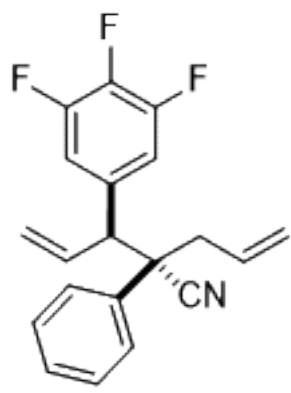
Current Data Parameters  
NAME OJ-2-105-Pure-C  
EXPNO 15  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210626  
Time\_ 0.22 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG2 waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

7.285  
7.257  
7.197  
7.193  
7.176  
6.620  
6.612  
6.601  
6.585  
6.580  
6.563  
6.552  
6.545  
6.361  
6.336  
6.319  
6.311  
6.294  
6.269  
5.554  
5.537  
5.528  
5.518  
5.511  
5.493  
5.486  
5.476  
5.469  
5.450  
5.432  
5.406  
5.362  
5.320  
5.176  
5.173  
5.134  
5.130  
5.099  
5.074  
5.074  
3.539  
3.515  
2.987  
2.968  
2.951  
2.932  
2.792  
2.775  
2.756  
2.740



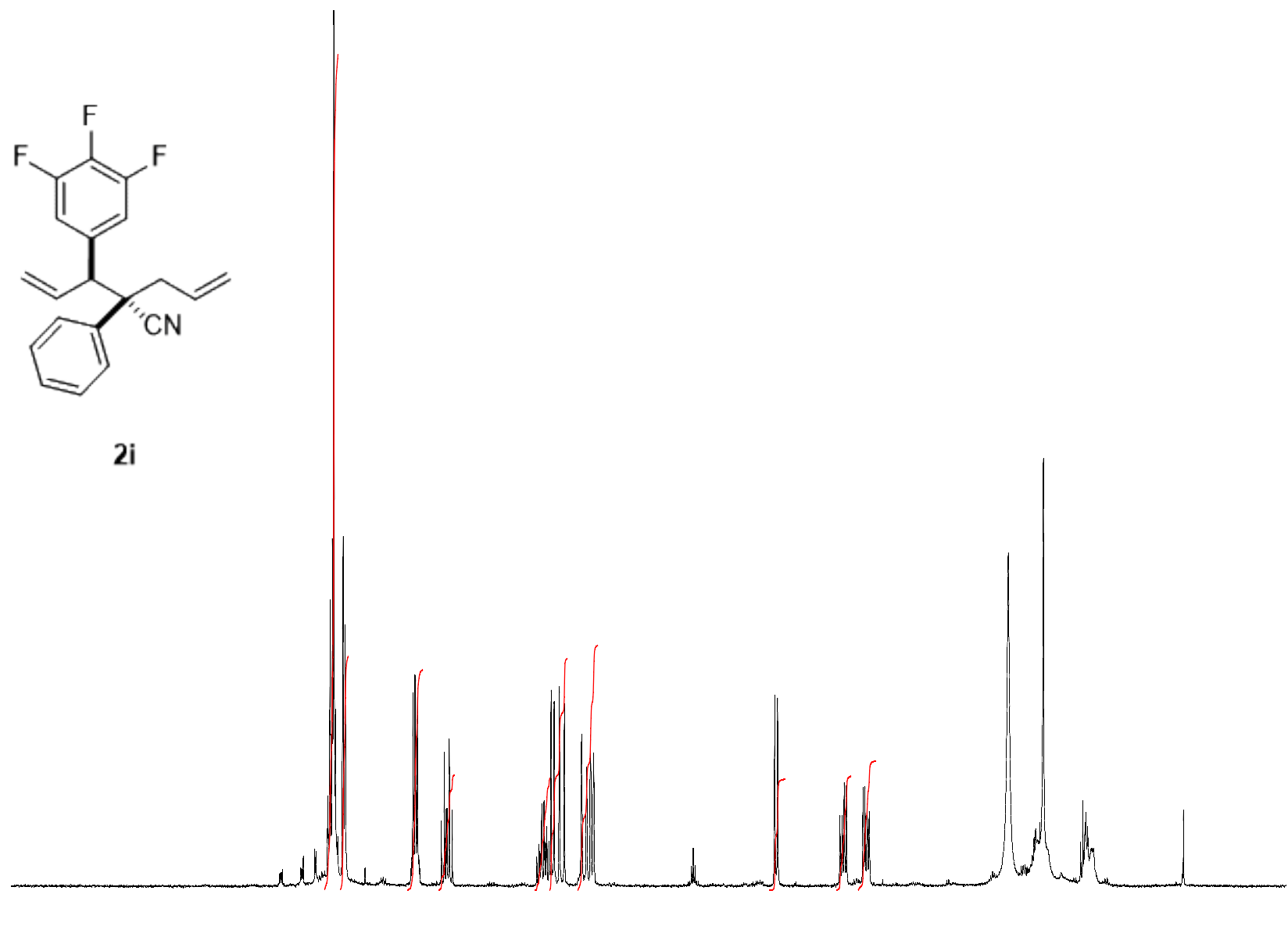
2i

```

Current Data Parameters
NAME      OJ-2-3,4,5-F-nitrile-pure
EXPNO    10
PROCNO    1

F2 - Acquisition Parameters
Date_    20210717
Time     11.20 h
INSTRUM  Avance Neo
PROBHD   z152088_0031 (
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8196.722 Hz
FIDRES   0.250144 Hz
AQ       3.9976959 sec
RG       101
DW       61.000 usec
DE       13.89 usec
TE       298.1 K
D1       1.00000000 sec
TDO      1
SFO1     400.1324708 MHz
NUC1     1H
P0       2.67 usec
P1       8.00 usec
PLW1     24.03499985 W

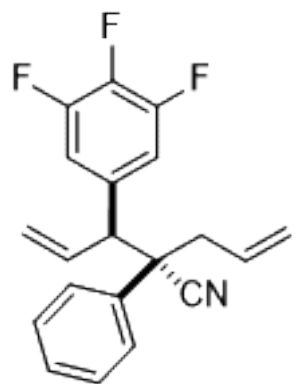
F2 - Processing parameters
SI       65536
SF       400.1300053 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



9 8 7 6 5 4 3 2 1 0 ppm

7.29  
2.04  
1.92  
1.00  
0.98  
2.02  
2.13  
0.96  
0.99  
1.13





2i

150.03  
135.20  
134.93  
134.90  
134.78  
134.63  
132.47  
132.45  
131.20  
129.07  
128.82  
128.54  
128.23  
126.79  
126.64  
125.14  
125.13  
120.81  
120.55  
120.38  
120.26  
120.05  
112.75  
112.53  
110.21  
110.00

59.09  
59.03  
52.71  
52.49  
42.74  
41.88

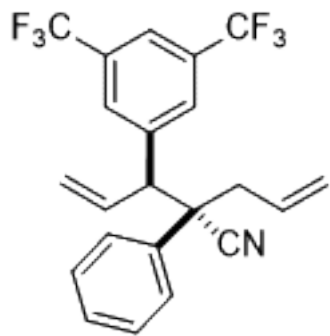
Current Data Parameters  
NAME OJ-2-3,4,5-F-nitrile-pure-2-C  
EXPNO 14  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210717  
Time\_ 13.03 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 |  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG2 waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

7.480  
7.303  
7.282  
7.128  
7.121  
7.113  
7.111  
6.964  
6.958  
6.949  
6.940  
6.461  
6.436  
6.419  
6.411  
6.394  
6.369  
5.567  
5.549  
5.542  
5.531  
5.524  
5.506  
5.499  
5.489  
5.481  
5.464  
5.398  
5.396  
5.370  
5.327  
5.179  
5.175  
5.136  
5.133  
5.108  
5.082  
3.627  
3.602  
3.069  
3.050  
3.033  
3.014  
2.818  
2.801  
2.782  
2.765

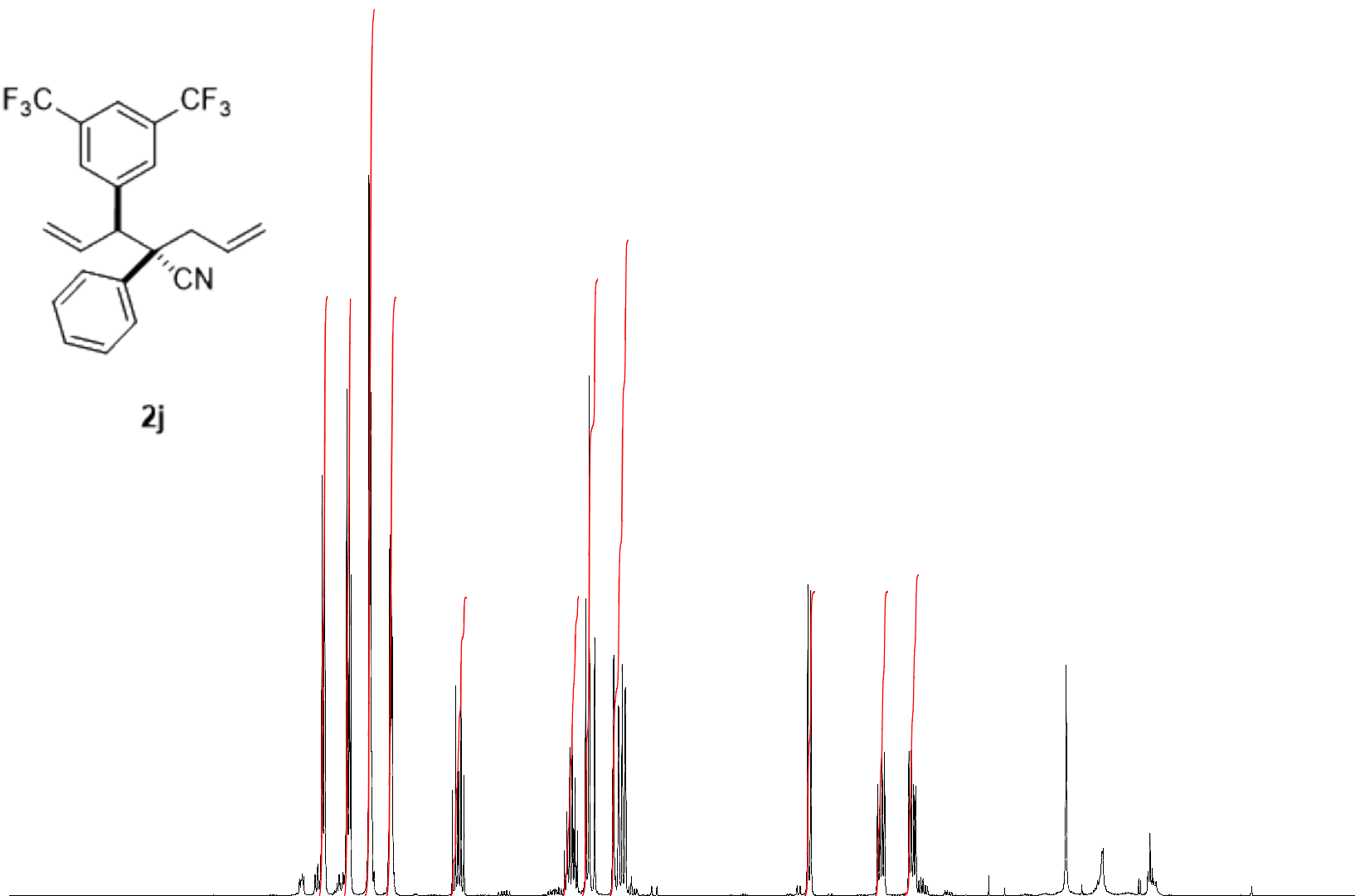


2j

Current Data Parameters  
NAME OJ-2-84-Pure  
EXPNO 17  
PROCNO 1

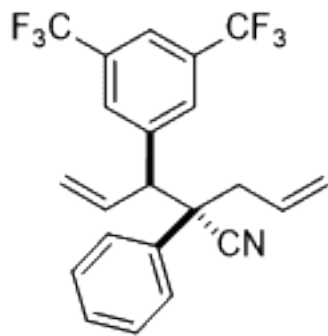
F2 - Acquisition Parameters  
Date\_ 20210602  
Time\_ 15.44 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 (zg30)  
PULPROG 65536  
TD CDC13  
SOLVENT 16  
NS 2  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.89 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300056 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



9 8 7 6 5 4 3 2 1 0 ppm

2.00  
1.99  
2.96  
2.00  
1.00  
1.00  
2.06  
2.19  
1.02  
1.02  
1.07



2j

141.07  
134.86  
134.31  
131.58  
131.25  
131.21  
130.92  
130.59  
128.86  
128.81  
128.77  
128.37  
126.84  
124.36  
121.65  
121.29  
121.10  
121.06  
121.03  
120.49  
119.94

59.50  
52.72  
42.23

Current Data Parameters  
NAME OJ-Bis-CF3-Nitrile-C-2  
EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters

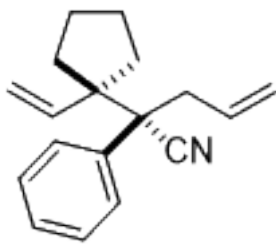
Date\_ 20210704  
Time 23.35 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters

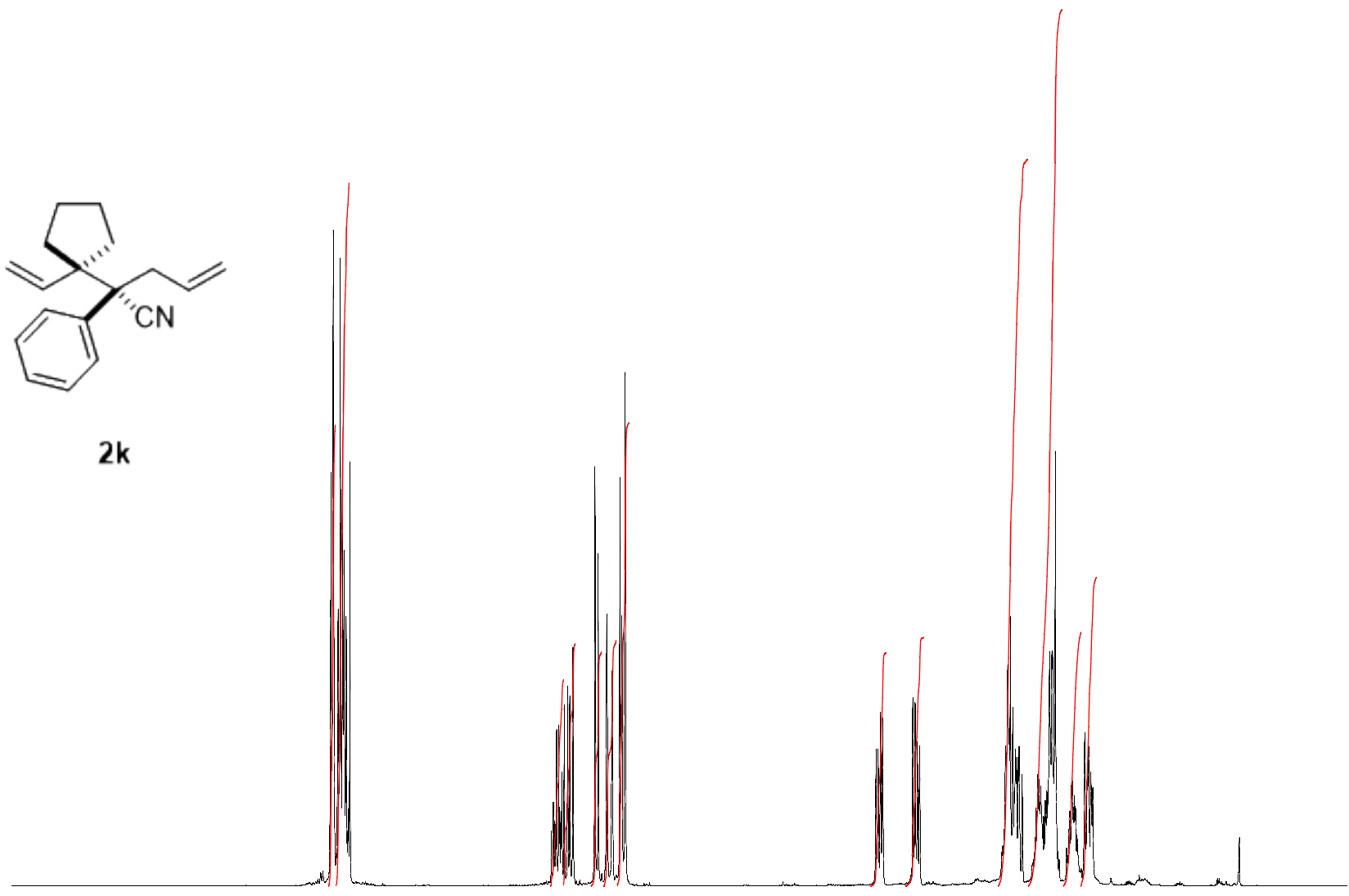
SI 32768  
SF 100.6127685 MHz  
WDB EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

7.425  
7.421  
7.404  
7.402  
7.368  
7.364  
7.359  
7.347  
7.328  
7.320  
7.317  
7.299  
5.599  
5.581  
5.537  
5.509  
5.493  
5.466  
5.290  
5.289  
5.263  
5.262  
5.194  
5.190  
5.151  
5.148  
5.087  
5.074  
5.072  
5.044  
3.017  
3.001  
2.980  
2.964  
2.719  
2.701  
2.683  
2.664  
1.971  
1.968  
1.963  
1.953  
1.943  
1.940  
1.932  
1.911  
1.892  
1.861  
1.615  
1.595  
1.590  
1.568  
1.330  
1.299



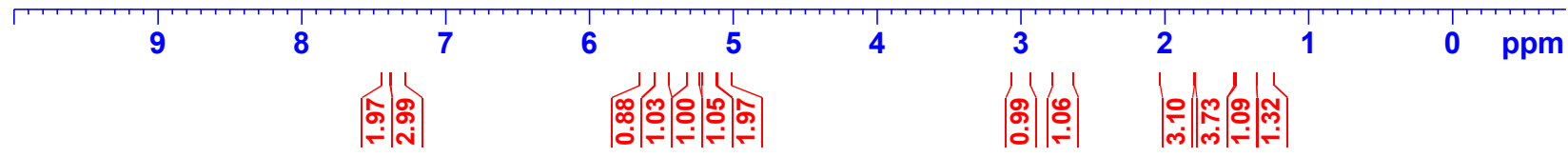
2k

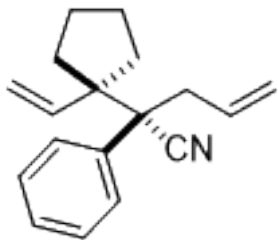


Current Data Parameters  
 NAME OJ-2-264-H  
 EXPNO 10  
 PROCNO 1

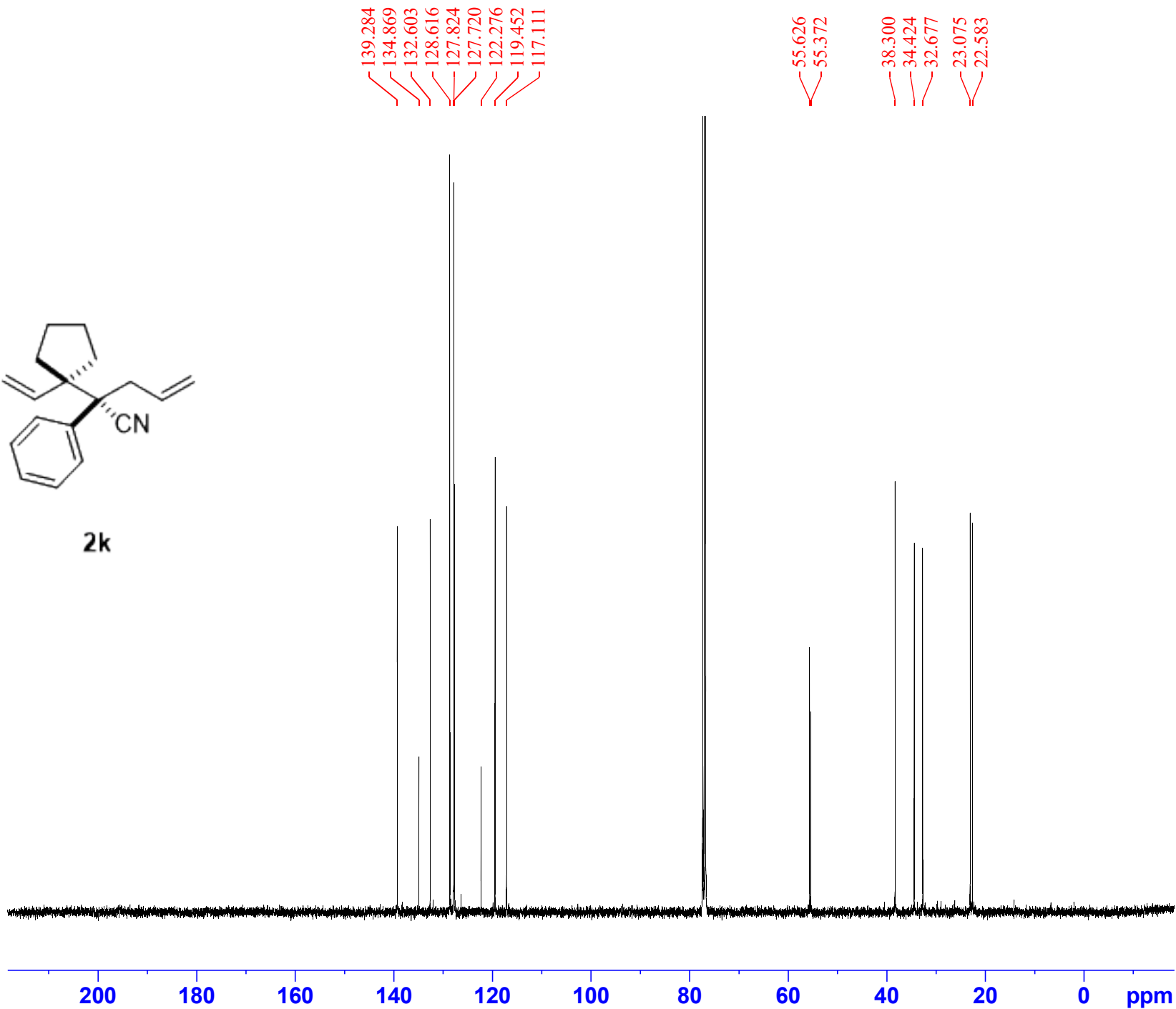
F2 - Acquisition Parameters  
 Date\_ 20210812  
 Time\_ 10.52 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (zg30)  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300060 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





2k

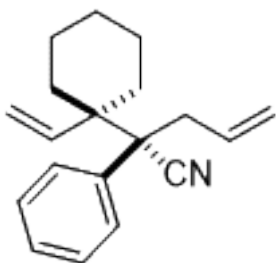


Current Data Parameters  
 NAME OJ-2-264-H-C  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210812  
 Time\_ 12.05 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

7.355  
7.337  
7.317  
7.296  
5.528  
5.526  
5.501  
5.498  
5.479  
5.373  
5.346  
5.328  
5.301  
5.169  
5.165  
5.126  
5.123  
5.109  
5.065  
5.037  
5.012  
2.954  
2.938  
2.918  
2.902  
2.809  
2.791  
2.773  
2.755  
2.099  
2.067  
1.666  
1.657  
1.625  
1.618  
1.605  
1.596  
1.585  
1.575  
1.563  
1.553  
1.514  
1.482  
1.476  
1.437  
1.428  
1.419  
1.403  
1.394  
1.251  
1.226  
1.218  
1.120  
1.087

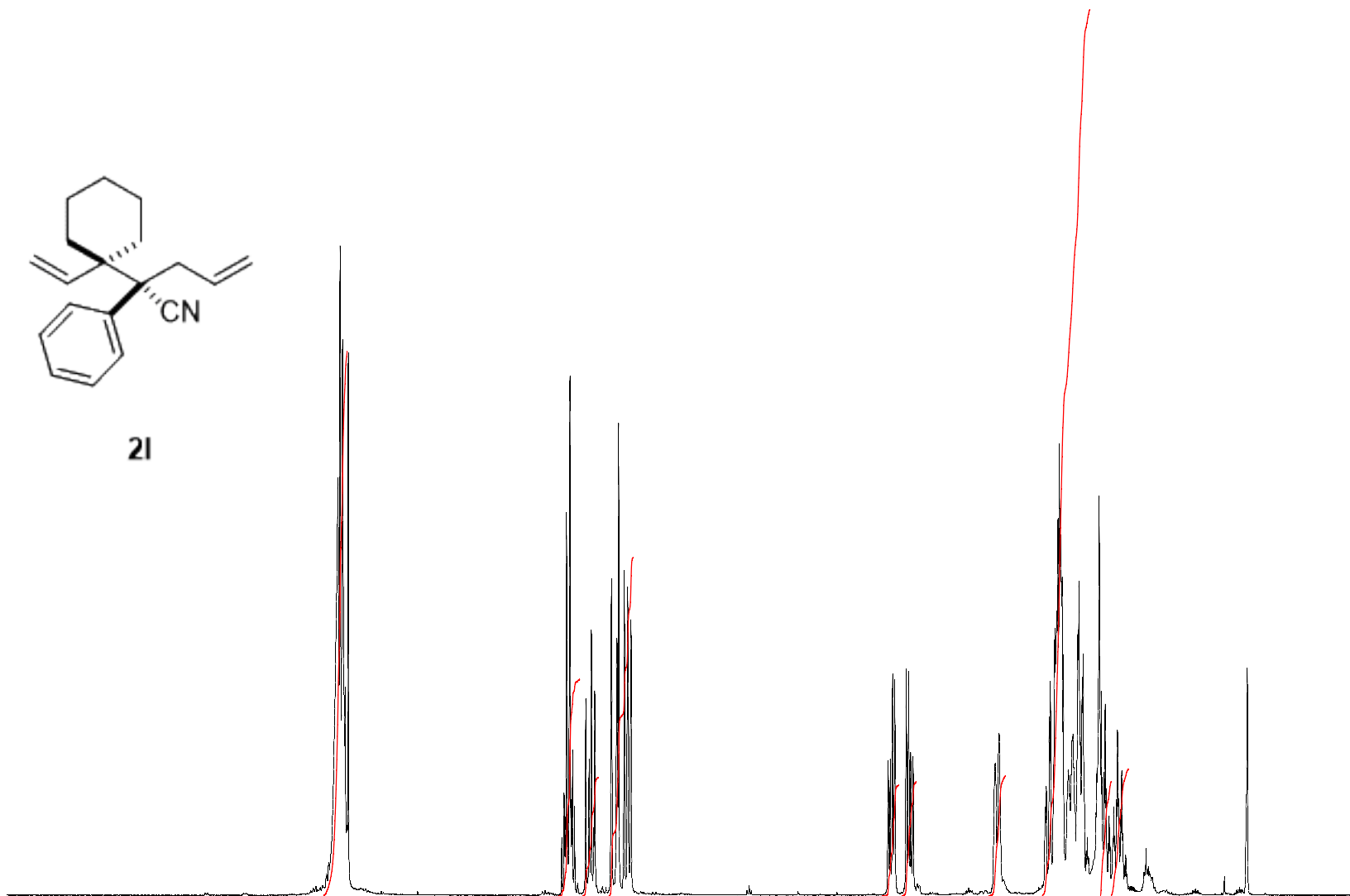


2I

Current Data Parameters  
NAME OJ-Cyclopentyl-Nitrile-H  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210826  
Time\_ 14.14 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.89 usec  
TE 298.1 K  
D1 1.0000000 sec  
TDO 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300051 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



9 8 7 6 5 4 3 2 1 0 ppm

4.92

1.96

1.07

3.06

1.00

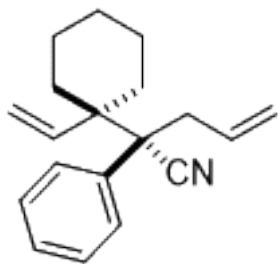
1.03

1.09

8.01

1.04

1.15



2I

138.95  
133.79  
132.79  
129.34  
127.66  
127.57  
122.16  
119.92  
119.41

57.28

46.36

36.31

32.32

31.07

25.74

22.26

22.20

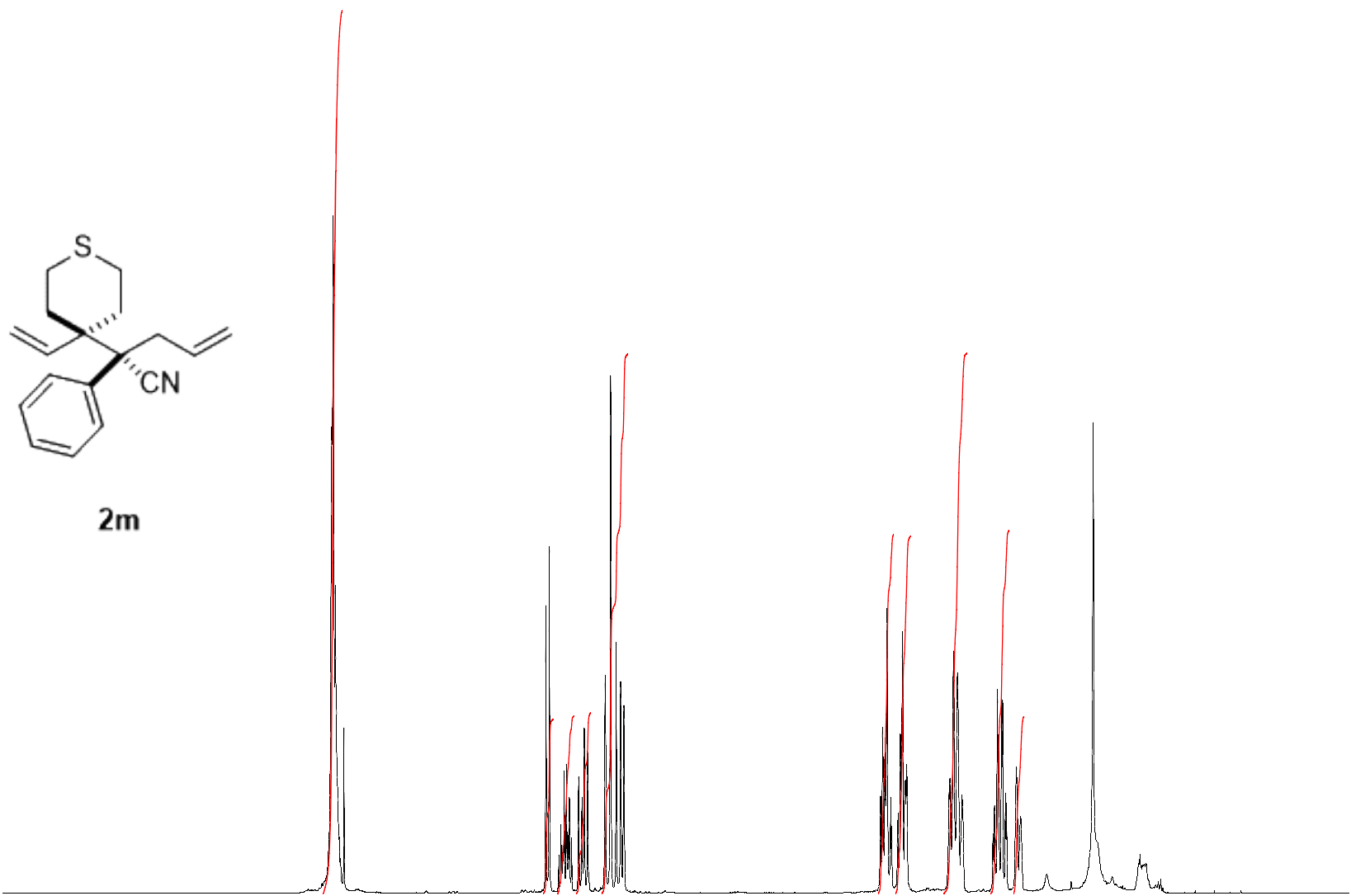
Current Data Parameters  
NAME OJ-Cyclohexyl-Nitrile-C  
EXPNO 13  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210826  
Time\_ 15.19 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 (zpgg30)  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

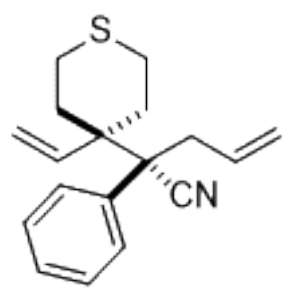
200 180 160 140 120 100 80 60 40 20 0 ppm

7.365  
7.354  
7.336  
5.648  
5.621  
5.527  
5.502  
5.485  
5.477  
5.468  
5.460  
5.386  
5.358  
5.341  
5.313  
5.174  
5.171  
5.129  
5.085  
5.050  
5.048  
5.023  
2.966  
2.950  
2.930  
2.913  
2.885  
2.876  
2.830  
2.824  
2.807  
2.789  
2.771  
2.764  
2.757  
2.754  
2.416  
2.410  
2.402  
2.381  
2.349  
2.344  
2.314  
2.309  
2.064  
2.052  
2.029  
2.021  
1.996  
1.988  
1.964  
1.956  
1.876  
1.843



9 8 7 6 5 4 3 2 1 0 ppm

5.07  
1.00  
1.02  
1.04  
3.09  
2.06  
2.05  
3.10  
2.08  
1.02



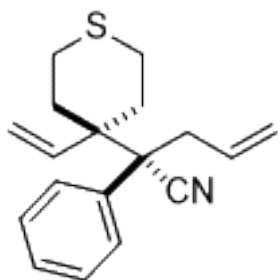
2m

Current Data Parameters  
NAME OJ-2-290-H  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210905  
Time\_ 18.28 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 ( )  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8196.722 Hz  
FIDRES 0.250144 Hz  
AQ 3.9976959 sec  
RG 101  
DW 61.000 usec  
DE 13.89 usec  
TE 298.1 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.1324708 MHz  
NUC1 1H  
P0 2.67 usec  
P1 8.00 usec  
PLW1 24.03499985 W

F2 - Processing parameters  
SI 65536  
SF 400.1300070 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





2m

138.12  
133.04  
132.27  
129.39  
128.05  
127.85  
121.42  
121.38  
119.83

57.32  
45.84  
36.04  
33.08  
32.54  
24.27  
24.26

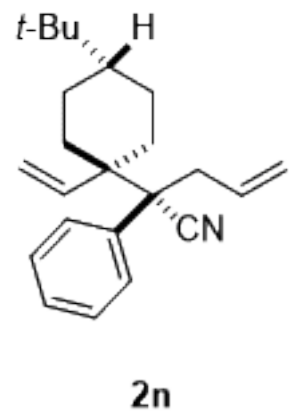
Current Data Parameters  
NAME OJ-2-290-C  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210905  
Time\_ 19.29 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

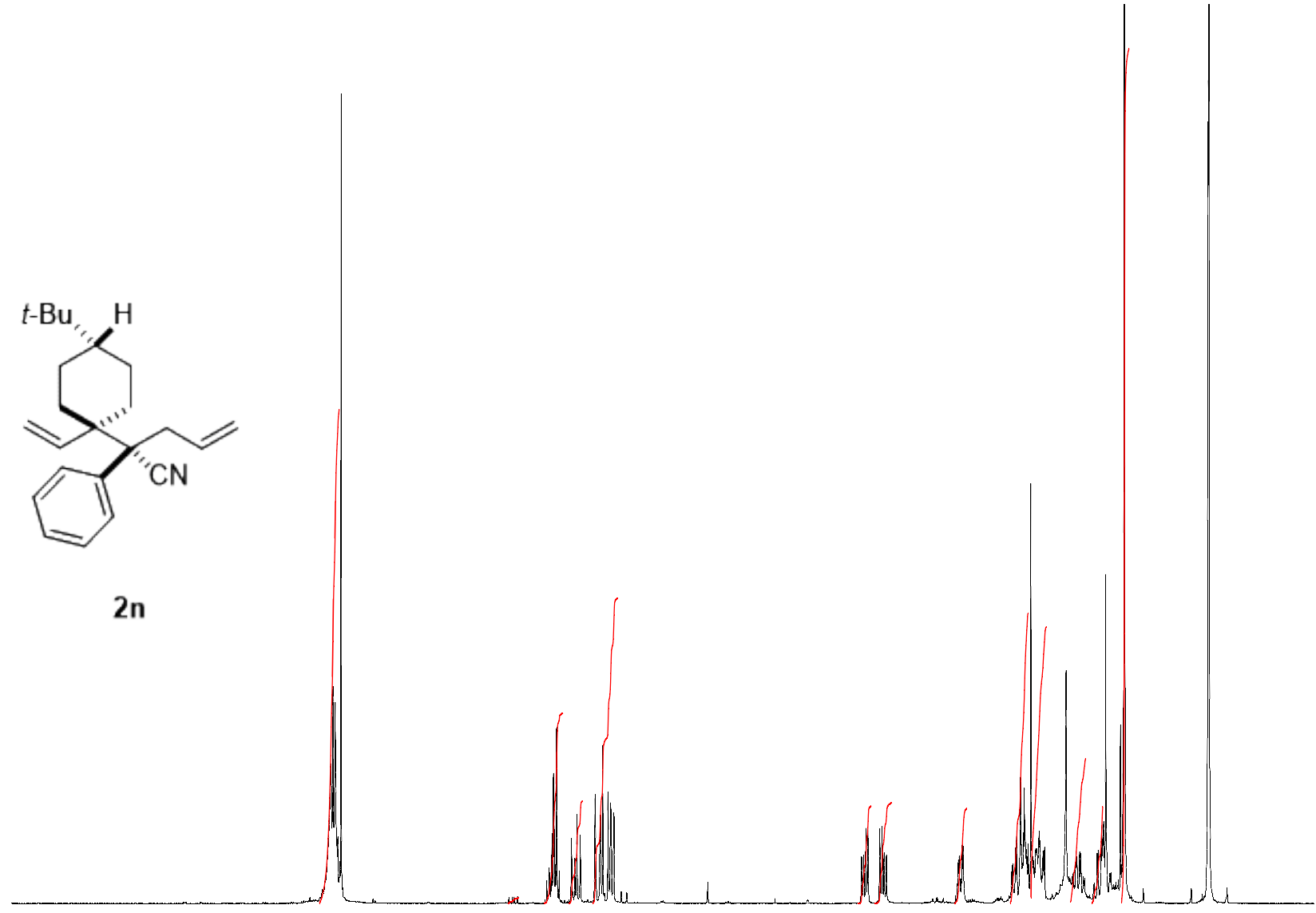
5.524  
5.515  
5.512  
5.507  
5.488  
5.485  
5.362  
5.318  
5.290  
5.168  
5.165  
5.126  
5.122  
5.106  
5.103  
5.061  
5.058  
5.040  
5.038  
5.036  
5.015  
5.013  
5.011  
2.923  
2.907  
2.808  
2.790  
2.772  
2.125  
2.118  
1.684  
1.675  
1.643  
1.637  
1.619  
1.611  
1.604  
1.596  
1.579  
1.517  
1.512  
1.505  
1.489  
1.482  
1.457  
1.443  
1.183  
1.153  
1.144  
1.007  
0.999  
0.977  
0.969  
0.783



Current Data Parameters  
 NAME OJ-2-334-Product-A  
 EXPNO 10  
 PROCNO 1

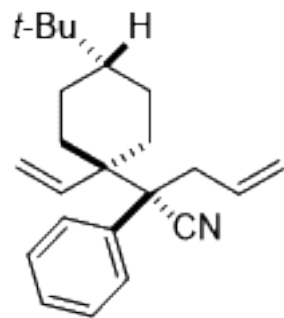
F2 - Acquisition Parameters  
 Date\_ 20211121  
 Time\_ 20.56 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300054 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



9  
8  
7  
6  
5  
4  
3  
2  
1  
0 ppm

5.10  
0.06  
1.96  
1.05  
3.14  
1.00  
1.03  
0.98  
2.98  
2.84  
1.50  
1.04  
8.79



2n

137.96  
132.84  
131.76  
128.25  
126.62  
126.54  
121.16  
118.82  
118.36

56.03  
46.53  
45.09  
35.46  
31.63  
31.19  
30.48  
26.36  
22.08  
21.95

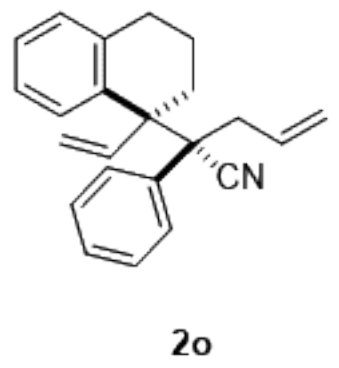
Current Data Parameters  
NAME OJ-2-334-Product-A-C  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211121  
Time\_ 22.13 h  
INSTRUM Avance Neo  
PROBHD z152088\_0031 (   
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2 waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6128730 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

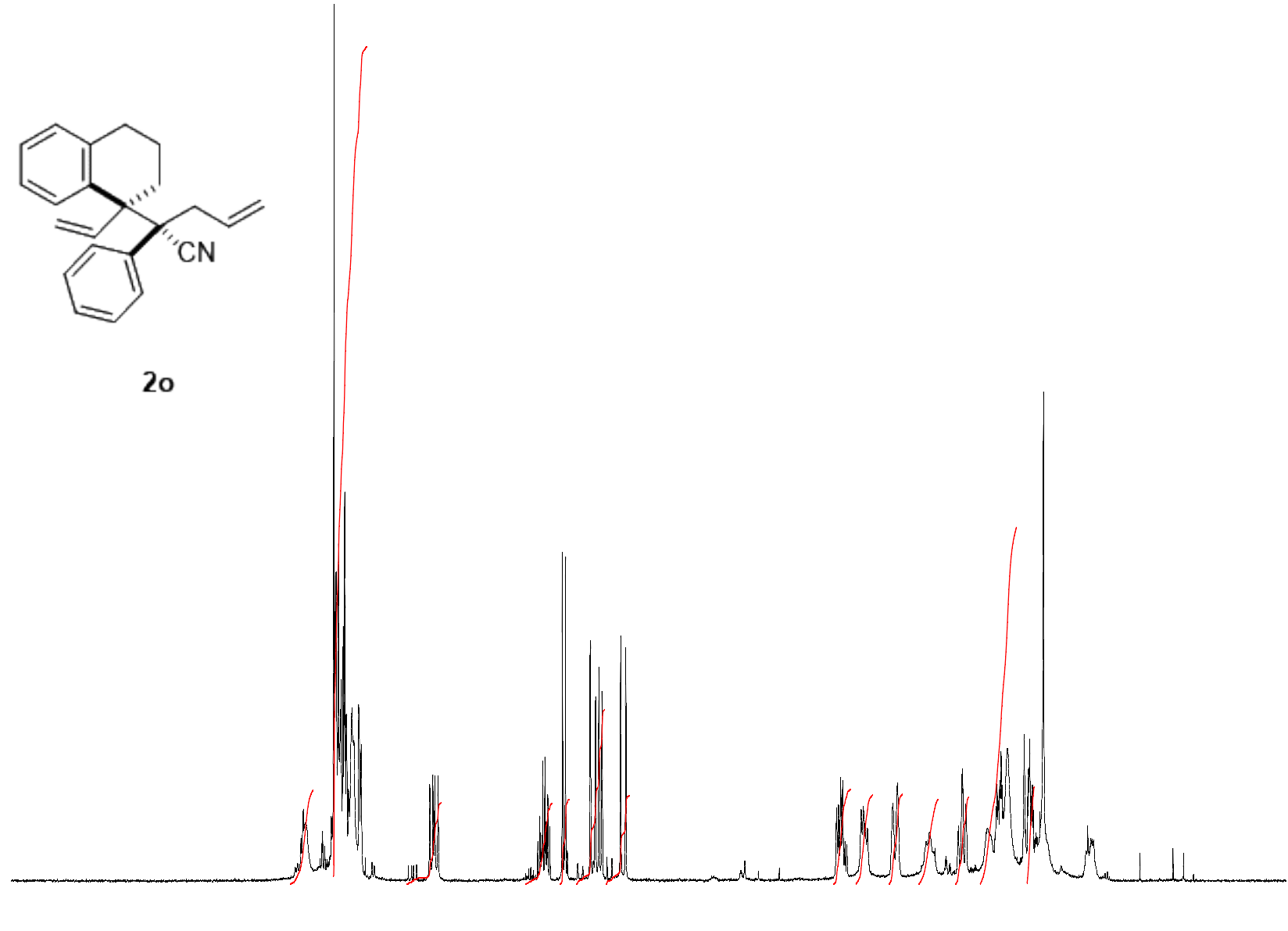
7.262  
7.258  
7.252  
7.232  
7.215  
7.211  
7.197  
7.192  
7.185  
7.180  
7.174  
7.166  
7.162  
7.119  
7.101  
7.061  
7.055  
7.039  
6.459  
6.432  
6.416  
6.389  
5.503  
5.485  
5.338  
5.336  
5.311  
5.309  
5.105  
5.101  
5.098  
5.094  
5.059  
5.055  
5.029  
5.027  
5.025  
5.003  
4.999  
4.844  
4.802  
2.981  
2.964  
2.498  
1.956  
1.949  
1.657  
1.635  
1.624  
1.569  
1.428  
1.390  
1.382  
1.358



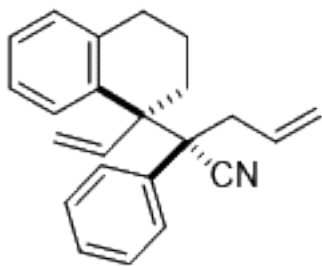
Current Data Parameters  
 NAME OJ-2-291-COL-1-H  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210910  
 Time\_ 0.22 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



1.07  
9.48  
0.92  
0.91  
0.96  
1.97  
1.00  
1.08  
1.01  
1.02  
0.96  
0.99  
4.04  
1.12



2o

142.70  
142.67  
135.27  
134.71  
132.56  
130.79  
129.46  
129.35  
129.33  
127.85  
127.64  
126.84  
125.12  
119.59  
117.45

52.07

38.91

34.11

31.26

29.71

19.61

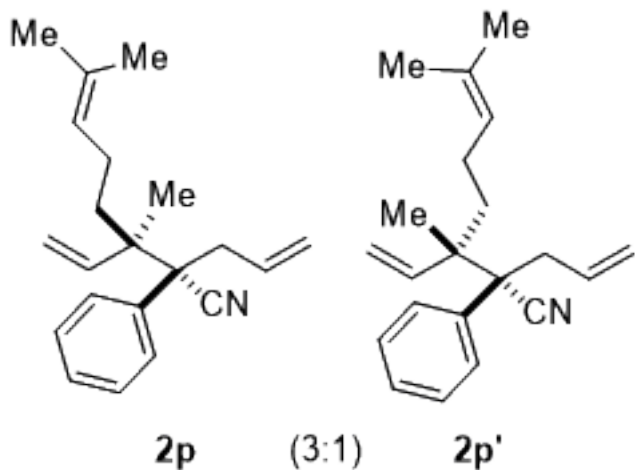
Current Data Parameters  
NAME OJ-2-Tetralone-nitrile-C  
EXPNO 12  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210911  
Time 1.36 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (   
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 2048  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

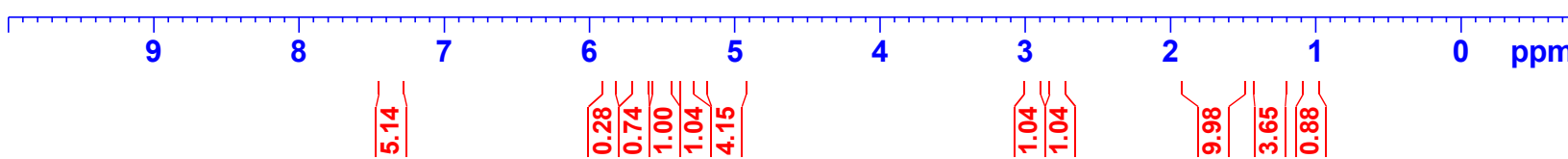
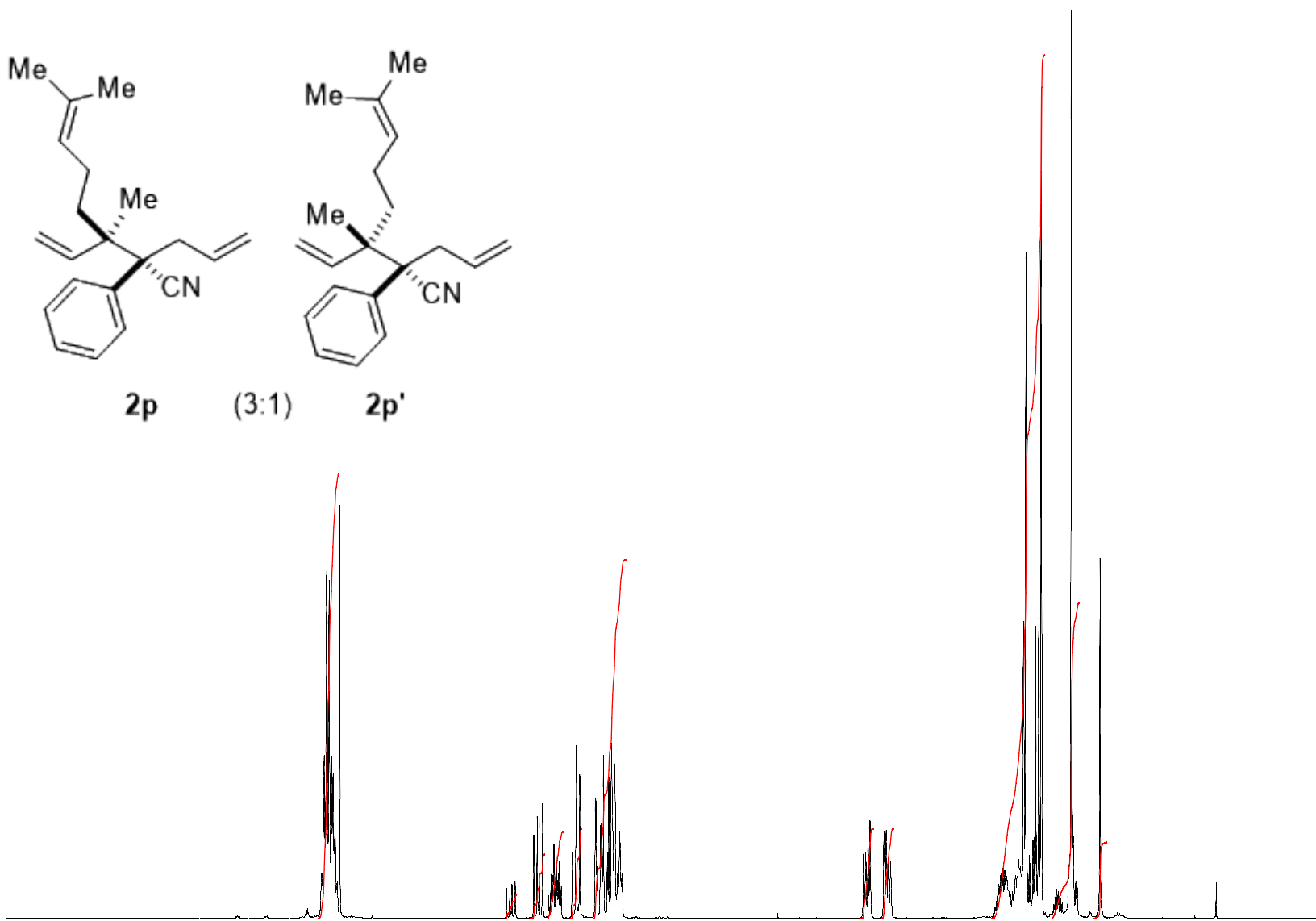
7.398  
7.376  
7.357  
7.338  
7.328  
7.324  
7.318  
7.315  
7.308  
5.677  
5.650  
5.633  
5.606  
5.512  
5.495  
5.470  
5.363  
5.333  
5.329  
5.327  
5.301  
5.300  
5.173  
5.169  
5.161  
5.130  
5.127  
5.107  
5.074  
5.063  
5.040  
5.032  
5.015  
4.972  
2.971  
2.955  
2.935  
2.919  
2.805  
2.787  
2.769  
2.751  
1.830  
1.699  
1.687  
1.640  
1.583  
1.570  
1.535  
1.516  
1.292  
1.268  
1.252  
1.033

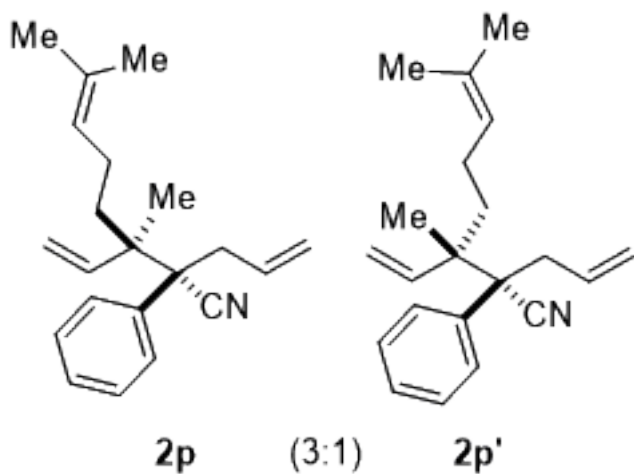


Current Data Parameters  
 NAME OJ-2-111-H  
 EXPNO 17  
 PROCNO 1

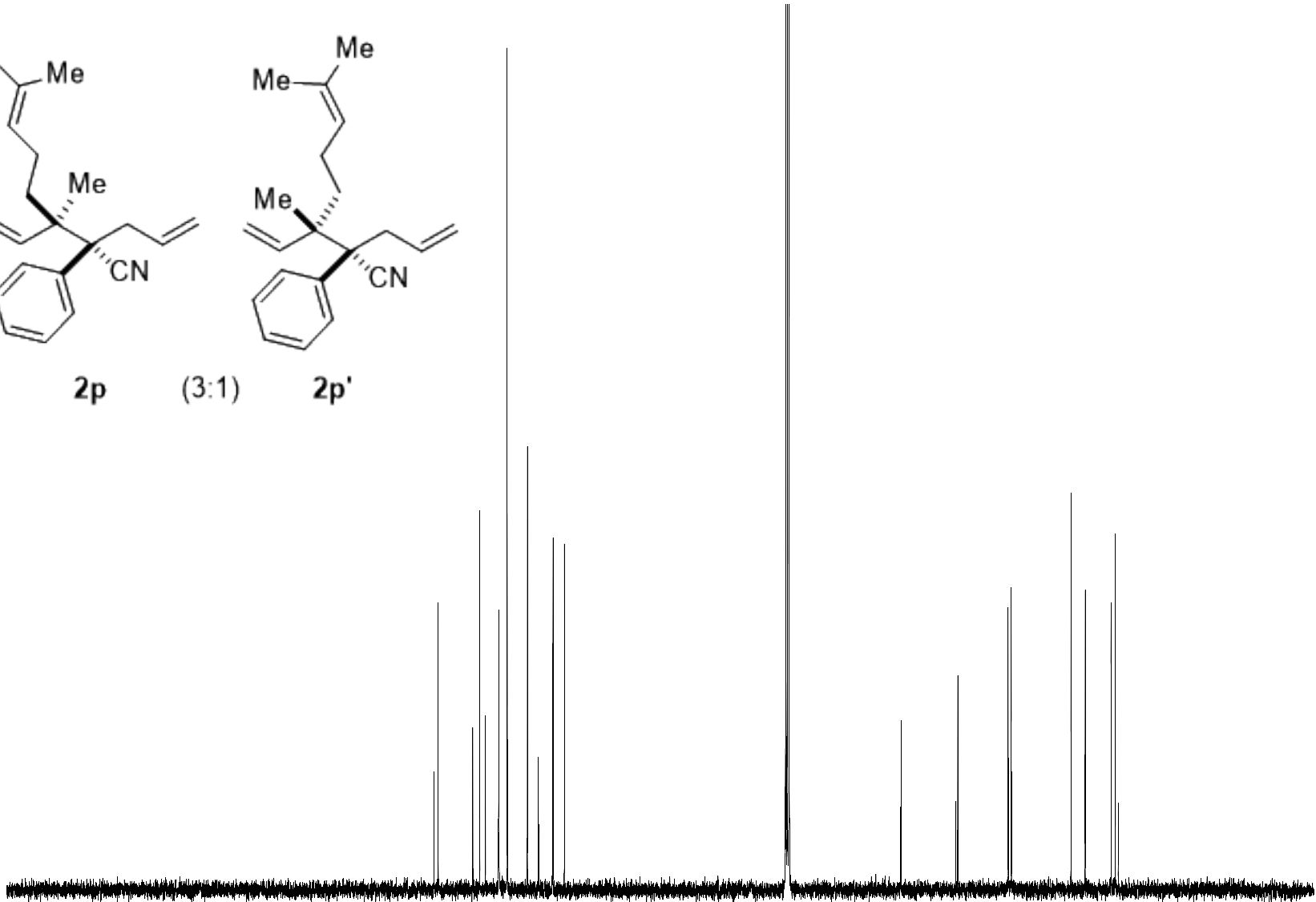
F2 - Acquisition Parameters  
 Date\_ 20210624  
 Time\_ 1.22 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (zg30)  
 PULPROG 65536  
 TD CDC13  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.0 K  
 D1 1.0000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



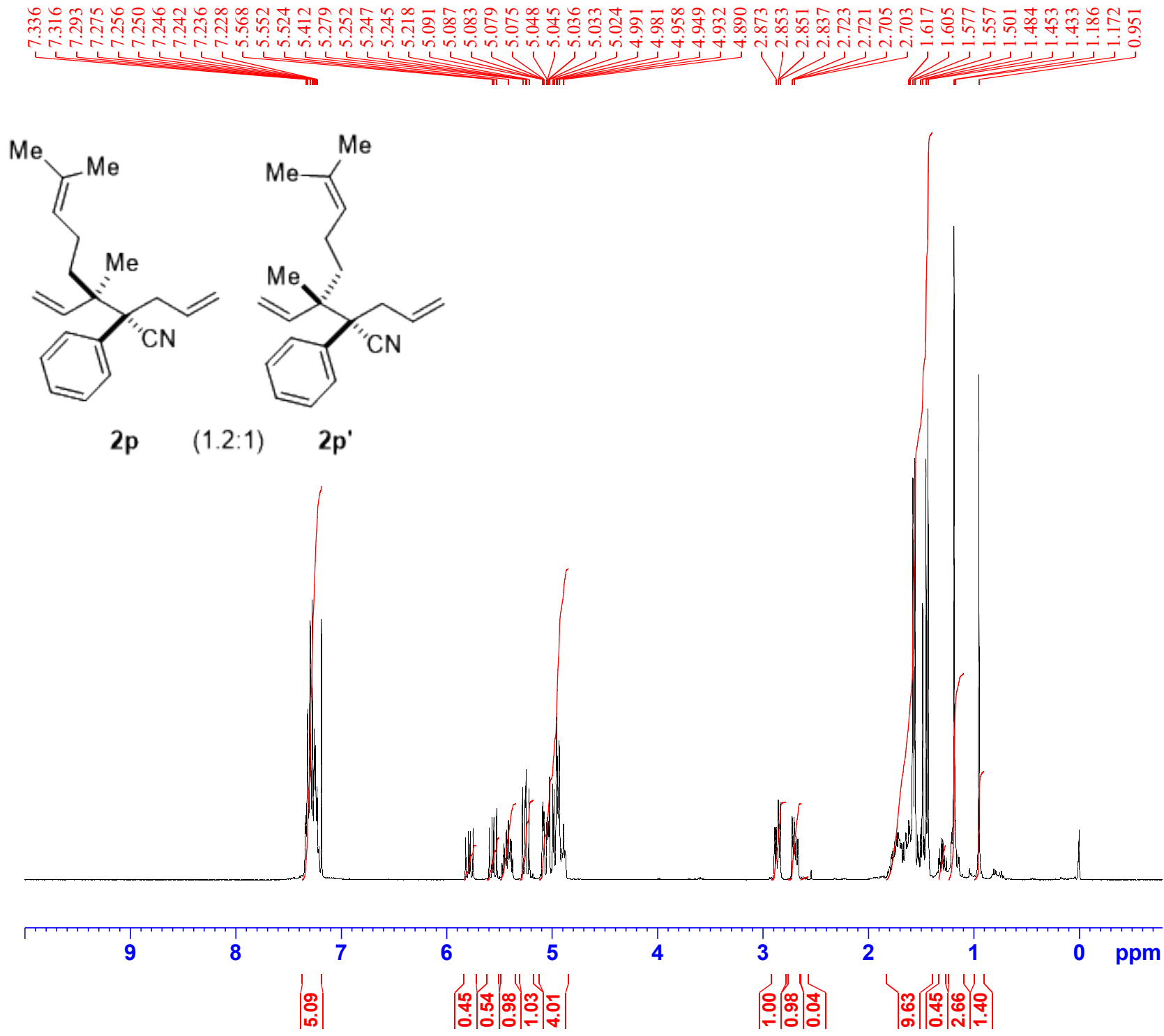


141.010  
 140.248  
 134.033  
 133.955  
 132.726  
 131.729  
 131.687  
 129.262  
 127.778  
 127.730  
 124.083  
 122.111  
 121.958  
 119.507  
 119.453  
 117.379  
 117.346  
 77.341  
 77.227  
 77.023  
 76.706  
 56.528  
 56.415  
 46.492  
 46.169  
 37.040  
 36.992  
 36.481  
 36.408  
 25.647  
 23.133  
 23.087  
 18.406  
 17.632  
 17.088



Current Data Parameters  
 NAME OJ-2-111-C  
 EXPNO 19  
 PROCNO 1  
  
 F2 - Acquisition Parameters  
 Date\_ 20210624  
 Time\_ 2.28 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (   
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W  
  
 F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

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

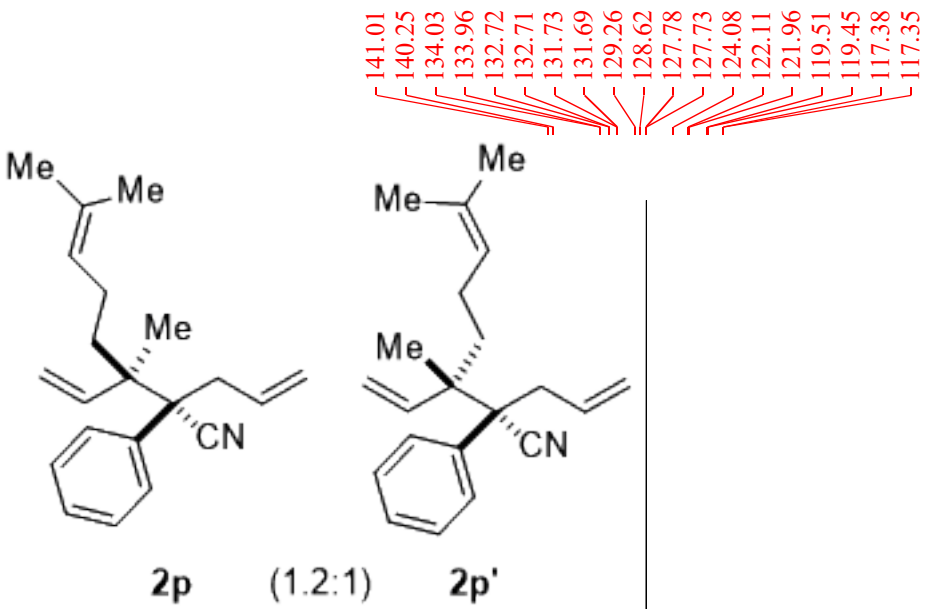


Current Data Parameters  
 NAME OJ-2-265-H  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210812  
 Time\_ 10.58 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (zg30)  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

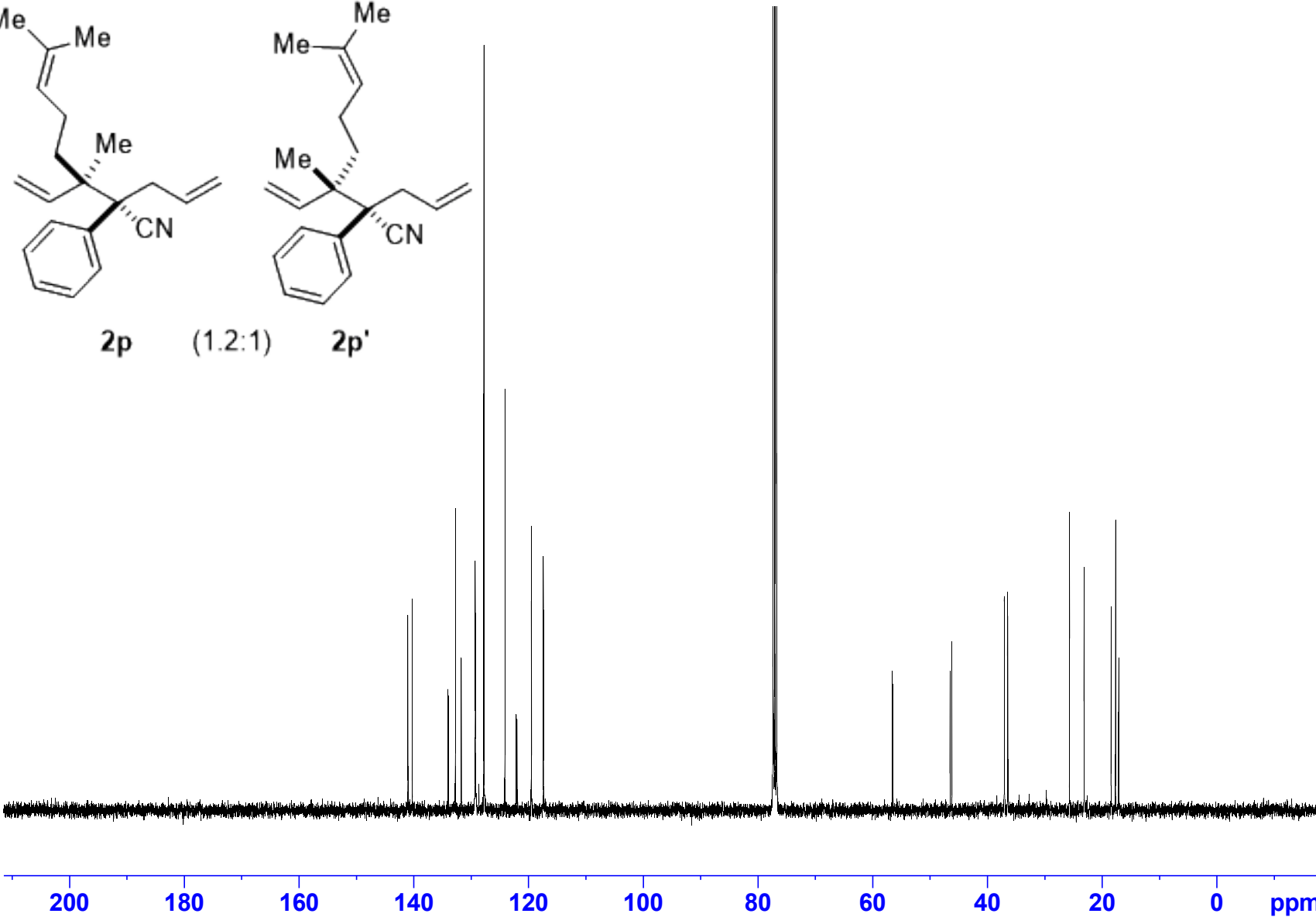
F2 - Processing parameters  
 SI 65536  
 SF 400.1300388 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





141.01  
 140.25  
 134.03  
 133.96  
 132.72  
 132.71  
 131.73  
 131.69  
 129.26  
 128.62  
 127.78  
 127.73  
 124.08  
 122.11  
 121.96  
 119.51  
 119.45  
 117.38  
 117.35

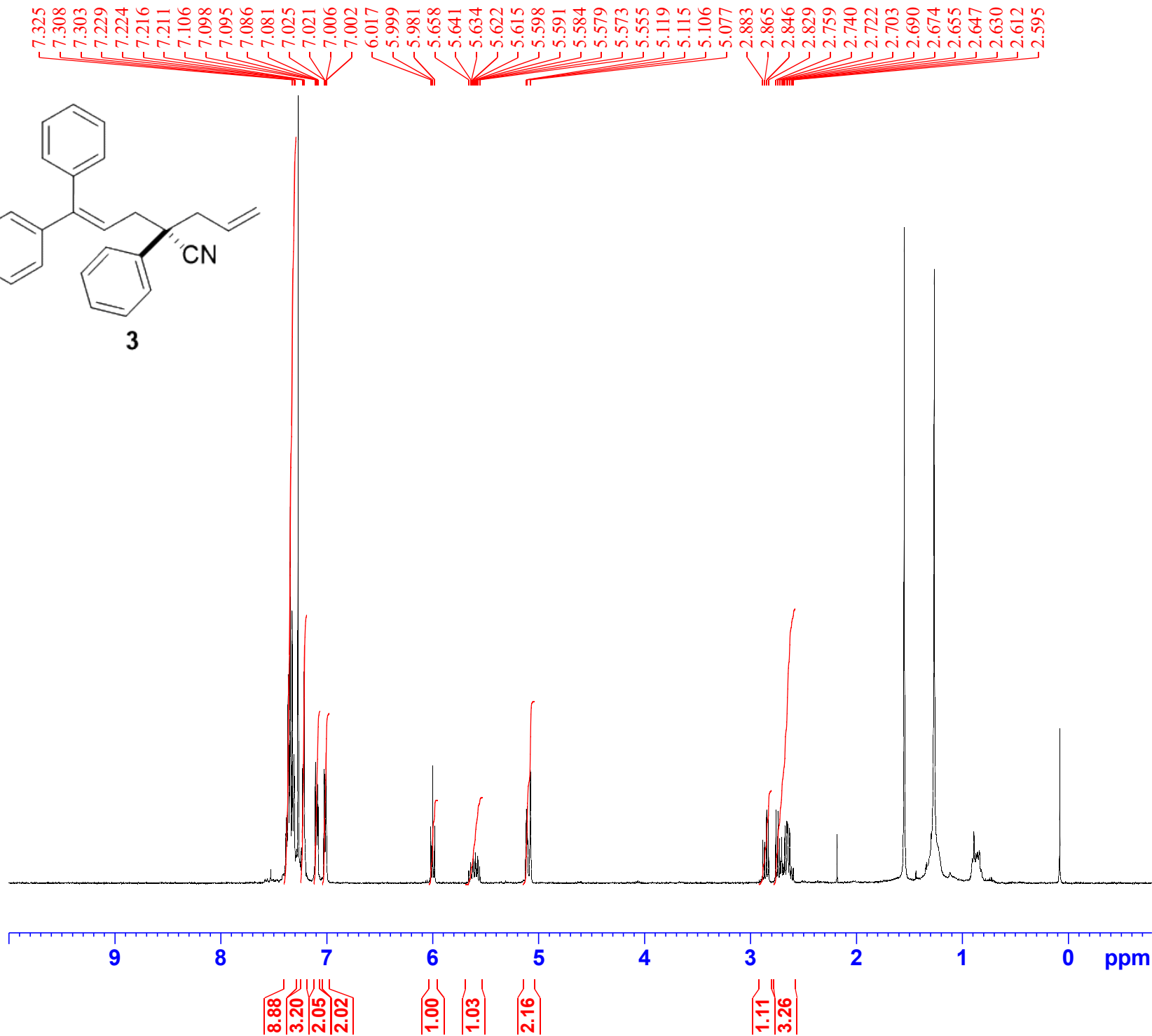
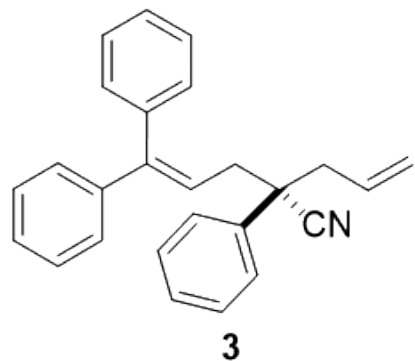
56.53  
 56.42  
 46.49  
 46.17  
 37.04  
 36.99  
 36.48  
 36.41  
 29.71  
 25.66  
 25.65  
 23.13  
 23.09  
 18.41  
 17.63  
 17.09



Current Data Parameters  
 NAME OJ-2-265-C  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210812  
 Time\_ 14.35 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 1024  
 DS 4  
 SWH 23809.523 Hz  
 FIDRES 0.726609 Hz  
 AQ 1.3762560 sec  
 RG 8.125  
 DW 21.000 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6228298 MHz  
 NUC1 13C  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 86.55400085 W  
 SFO2 400.1316005 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 24.03499985 W  
 PLW12 0.18990999 W  
 PLW13 0.09552100 W

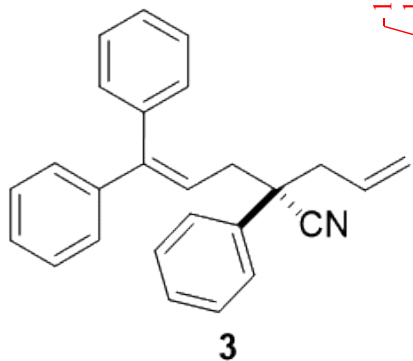
F2 - Processing parameters  
 SI 32768  
 SF 100.6127685 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Current Data Parameters  
 NAME OJ-2-333-H-2  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211121  
 Time\_ 18.54 h  
 INSTRUM Avance Neo  
 PROBHD Z152088\_0031 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300061 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



145.71  
141.89  
137.63  
131.64  
129.79  
128.82  
128.28  
128.11  
127.85  
127.44  
127.34  
127.32  
126.35  
122.28  
120.12  
115.82  
114.65

48.04  
44.28  
39.97

Current Data Parameters  
NAME OJ-2-333-C  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters

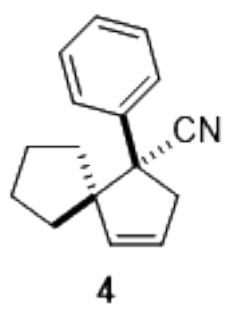
Date\_ 20211121  
Time\_ 20.11 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters

SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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

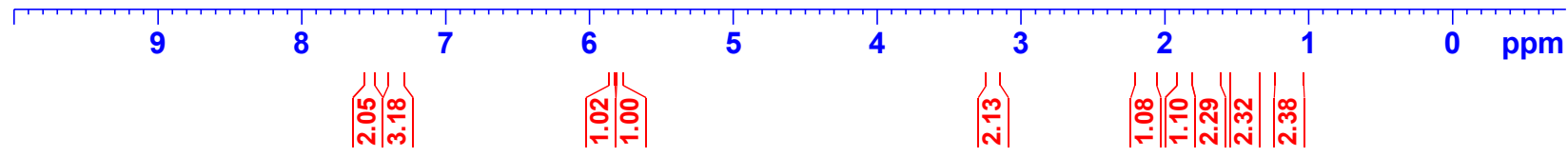
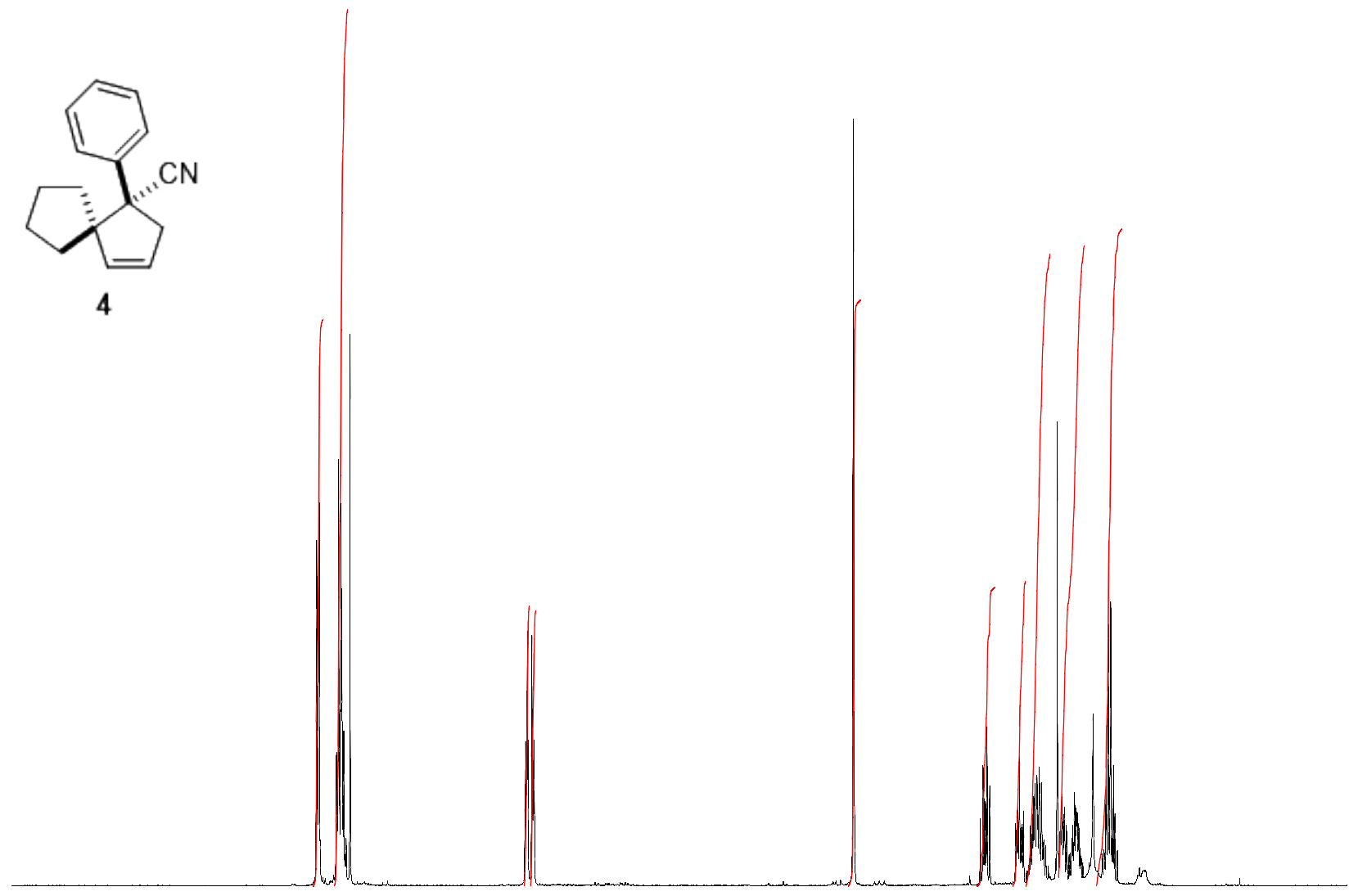
7.541  
7.537  
7.524  
7.520  
7.517  
7.382  
7.377  
7.372  
7.360  
7.345  
7.342  
7.335  
7.331  
7.325  
7.317  
5.855  
5.850  
5.841  
5.835  
5.830  
5.802  
5.797  
5.793  
5.787  
5.782  
5.778  
3.204  
3.199  
3.194  
2.153  
2.142  
2.132  
2.120  
2.099  
1.878  
1.869  
1.857  
1.825  
1.746  
1.735  
1.731  
1.720  
1.715  
1.700  
1.694  
1.679  
1.513  
1.495  
1.414  
1.399  
1.157  
1.140  
1.120  
1.099

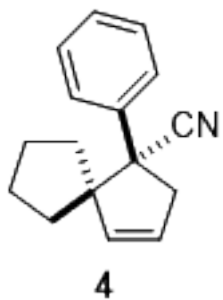


Current Data Parameters  
 NAME OJ-2-274-H  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210822  
 Time\_ 20.01 h  
 INSTRUM Avance Neo  
 PROBHD z152088\_0031 (z  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8196.722 Hz  
 FIDRES 0.250144 Hz  
 AQ 3.9976959 sec  
 RG 101  
 DW 61.000 usec  
 DE 13.89 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P0 2.67 usec  
 P1 8.00 usec  
 PLW1 24.03499985 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300066 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





139.05  
137.67  
128.40  
127.90  
127.01  
125.66  
124.01

63.93  
54.12  
45.04  
36.77  
34.68  
29.71  
24.01  
23.66

Current Data Parameters  
NAME OJ-2-274-C  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210822  
Time\_ 21.15 h  
INSTRUM Avance Neo  
PROBHD Z152088\_0031 (  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 1024  
DS 4  
SWH 23809.523 Hz  
FIDRES 0.726609 Hz  
AQ 1.3762560 sec  
RG 8.125  
DW 21.000 usec  
DE 6.50 usec  
TE 298.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6228298 MHz  
NUC1 13C  
P0 2.67 usec  
P1 8.00 usec  
PLW1 86.55400085 W  
SFO2 400.1316005 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 90.00 usec  
PLW2 24.03499985 W  
PLW12 0.18990999 W  
PLW13 0.09552100 W

F2 - Processing parameters  
SI 32768  
SF 100.6127685 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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