SUPPORTING INFORMATION

Cu-Based Carbene Involved in a Radical Process: A New Crossover Reaction to Construct γ-Peroxy Ester and 1,4-Dicarbonyl Compounds

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General Information

All manipulations were carried out under air atmosphere. Column chromatography was generally performed on silica gel (300-400 mesh) and reactions were monitored by thin layer chromatography (TLC) using UV light to visualize the course of the reactions. The ^{1}H (400MHz) and ^{13}C NMR (100MHz) data were recorded with $CDCl_3$ as solvent. The chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. ^{1}H NMR spectra was recorded with tetramethylsilane (δ= 0.00 ppm) as internal reference; ^{13}C NMR spectra was recorded with $CDCl_3$ (δ = 77.00 ppm) as internal reference.

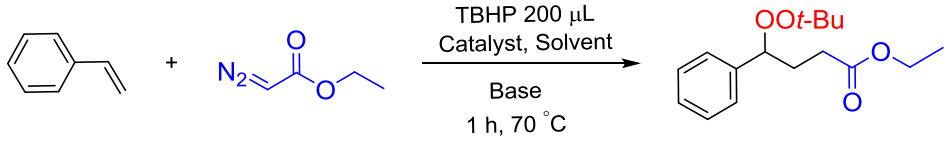
General procedures for reactions

The synthesis of γ-peroxy esters: Cupric nitrate trihydrate (0.05 mmol), DABCO (1.0 mmol) was added to test tube. Isopropanol (3.0 mL), alkenes (0.5 mmol), diazoacetic ester (1.0 mmol) and *tert*-butyl hydroperoxide (TBHP, 1.45 mmol, 0.20 mL, 70% solution in water) were added via syringe. The reaction mixture was stirred at 70 ^{o}C for 1 h. Removal of solvent followed by flash column chromatographic purification afforded products using petroleum and ethyl acetate.

The synthesis of 1,4-dicarbonyl compounds: Cupric acetylacetonate (0.05 mmol), DABCO (1.5 mmol) was added to test tube. Isopropanol (2.0 mL), alkenes (0.5 mmol), diazoacetic ester (1.0 mmol) and *tert*-butyl hydroperoxide (TBHP, 1.45 mmol, 0.20 mL, 70% solution in water) were added via syringe. The reaction mixture was stirred at 70 ^{o}C for 8 h. Removal of solvent followed by flash column chromatographic purification afforded products using petroleum and ethyl acetate.

Optimization of Reaction Conditions

Table S1. Optimization of Reaction Conditions of γ-peroxy ester[a]

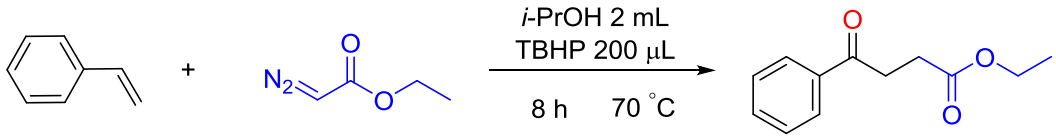


1a **2a** **3a**

Entry	Solvent (3 mL)	Catalyst (10 mol%)	Base (2 eq)	Yield[b]
1	*i*-PrOH	$Cu(NO_3)_2{\cdot}3H_2O$	DABCO	76%
2	*i*-PrOH	$Cu(acac)_2$	DABCO	61%
3	*i*-PrOH	CuI	DABCO	45%
4	*i*-PrOH	$Co(acac)_2$	DABCO	40%
5	*i*-PrOH	$Pd(OAc)_2$	DABCO	10%
6	EtOH	$Cu(NO_3)_2{\cdot}3H_2O$	DABCO	30%
7	*i*-PrOH	$Cu(NO_3)_2{\cdot}3H_2O$	DBU	<5%
8	*i*-PrOH	$Cu(NO_3)_2{\cdot}3H_2O$	DMAP	<5%
9	*i*-PrOH	$Cu(NO_3)_2{\cdot}3H_2O$	NaOAc	<5%
10	*i*-PrOH	$Cu(NO_3)_2{\cdot}3H_2O$	DABCO	60%[c]
11	*i*-PrOH	——	DABCO	< 5%
12	*i*-PrOH	Bu_4NI	DABCO	< 5%

[a] 0.5 mmol of **1a**, 1.0 mmol of **2a**, 0.05 mmol of catalyst, 1.46 mmol of TBHP, 1.0 mmol of base in 3.0 mL solvent was stirred at 70 °C for 1 h. [b] Isolated yield. [c] 15 mmol of **1a**, 30 mmol of **2a**, 1.5 mmol of catalyst, 43.86 mmol of TBHP, 30 mmol of base in 90 mL solvent was stirred at 70 °C for 1.5 h.

Table S2. Optimization of Reaction Conditions of 1,4-Dicarbonyl compound[a]



1a **2a** **8a**

Entry	Catalyst (10 mol%)	Base (3 eq)	Yield[b]
1	$Cu(acac)_2$	DABCO	72%
2	$Co(acac)_3$	DABCO	53%
3	$Pd(OAc)_2$	DABCO	<5%
4	$AgNO_3$	DABCO	12%
5	MnO_2	DABCO	30%
6	$Mn(acac)_2$	DABCO	56%
7	$Fe(acac)_2$	DABCO	41%
8	$Cu(NO_3)_2 \cdot 3H_2O$	DABCO	53%[c]
9	CuI	DABCO	38%
10	$Cu(acac)_2$	Cs_2CO_3	<5%
11	$Cu(acac)_2$	NaOAc	<5%
12	$Cu(acac)_2$	$NaHCO_3$	<5%

[a] 0.5 mmol of **1a**, 1.0 mmol of **2a**, 0.05 mmol of catalyst, 1.46 mmol of TBHP, 1.5 mmol of base in 2.0 mL *i*-PrOH was stirred at 70 °C for 8 h. [b] Isolated yield. [c] 0.5 mmol of **1a**, 1.0 mmol of **2a**, 0.05 mmol of catalyst, 1.46 mmol of oxidant, 1.0 mmol of base in 3.0 mL *i*-PrOH was stirred at 70 °C for 1 h.

Computational Methods

The geometries of all stationary points were optimized using the ωB97XD density functional method[1] with the 6-31G(d) basis set[2] for all the atoms. For open-shell models, unrestricted DFT calculations were performed. Vibrational frequency analyses at the same level of theory were performed on all optimized structures to characterize stationary points as local minima or transition states. Transition states were verified to have one imaginary vibrational frequency and were connected to appropriate reactant and product by optimizations along the reaction coordinate. The Gibbs free energies for all species were obtained at 343.15K (70 °C) and 1 atm at optimized structures. Unless otherwise specified, the Gibbs free energy was used in the present discussions. The Gaussian 09 suite of programs[3] was used for all the calculations.

Computational Results and Discussion

The activation of 2a by a Cu(II) species.

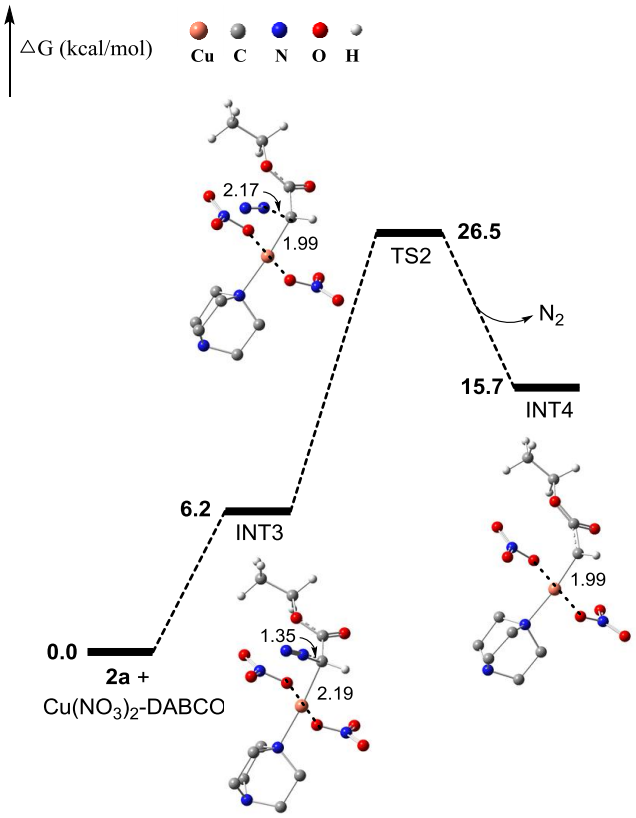


Figure S1. Free energy profile for the activation of **2a** by the Cu(II) species, $Cu(NO_3)_2$-DABCO complex. Bond lengths are shown in Å.

INT2 induced hydrogen abstraction reactions

The predicted energy barrier for the **INT2** induced hydrogen abstraction from the secondary carbon of *i*-PrOH is 6 kcal/mol relative to the separated **INT2** and *i*-PrOH (Figure S2). The corresponding energy barriers of the hydrogen abstractions from the hydroxyl group of *i*-PrOH and the hydroperoxyl group of TBHP, however, are 8.5 kcal/mol and 8.9 kcal/mol higher in energy (Figure S3 and S4), respectively, than that of the hydrogen abstraction from the secondary carbon of *i*-PrOH. Therefore, abstracting the hydrogen attached to the secondary carbon of *i*-PrOH is favorable induced by **INT2**.

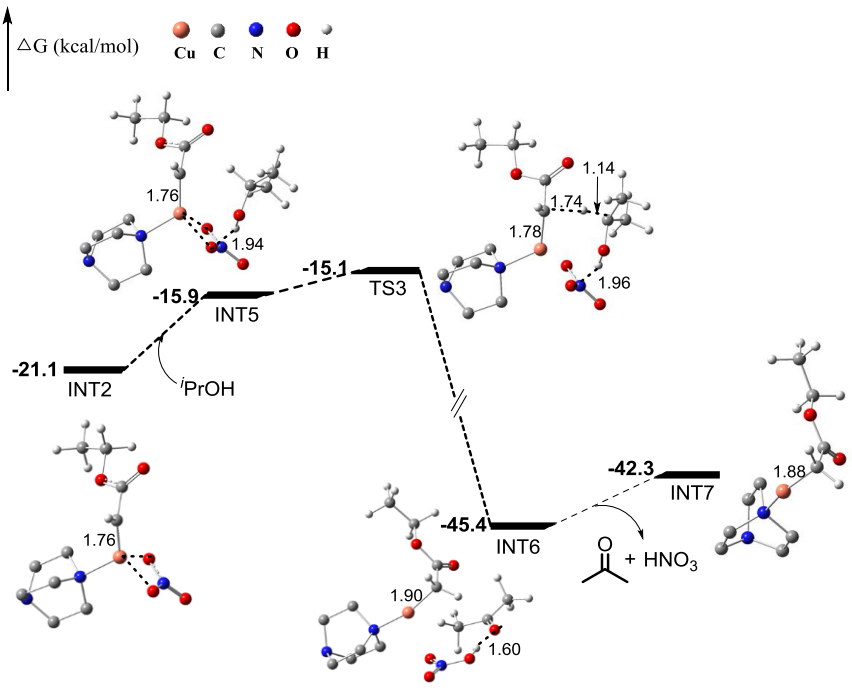


Figure S2. Free energy profile for the **INT2** induced hydrogen abstraction from the secondary carbon of *i*-PrOH and the subsequent conversion to afford **INT7**. Bond lengths are shown in Å.

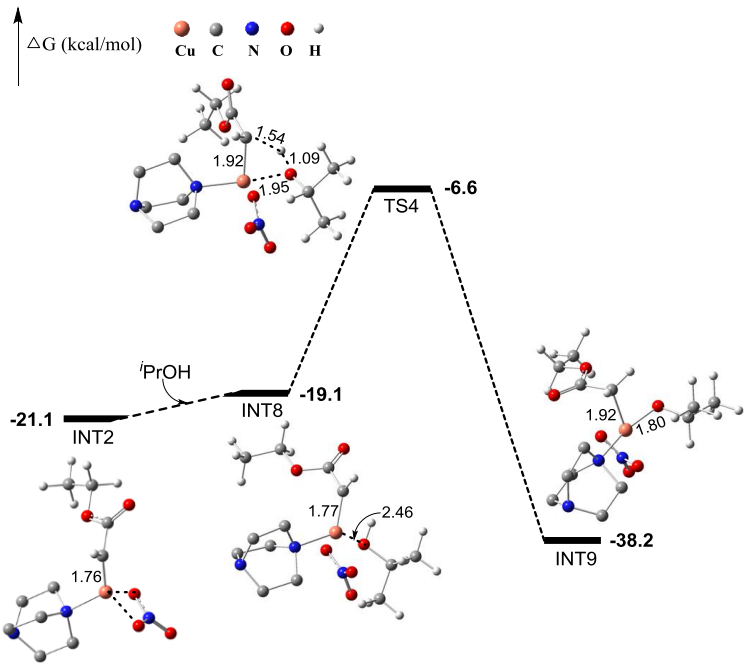


Figure S3. Free energy profile for the **INT2** induced hydrogen abstraction from the hydroxyl group of *i*-PrOH. Bond lengths are shown in Å.

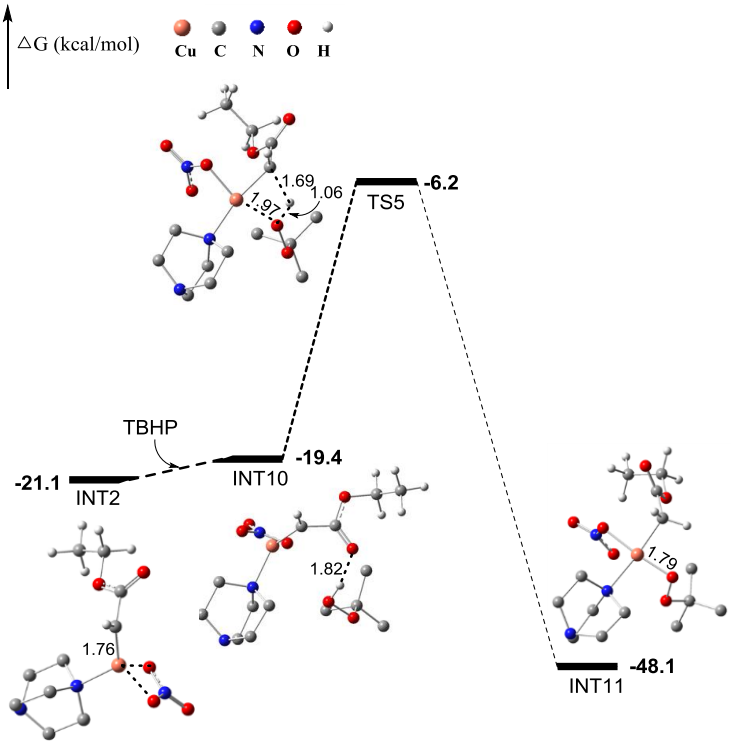


Figure S4. Free energy profile for the **INT2** induced hydrogen abstraction from the hydroperoxyl group of TBHP. Bond lengths are shown in Å.

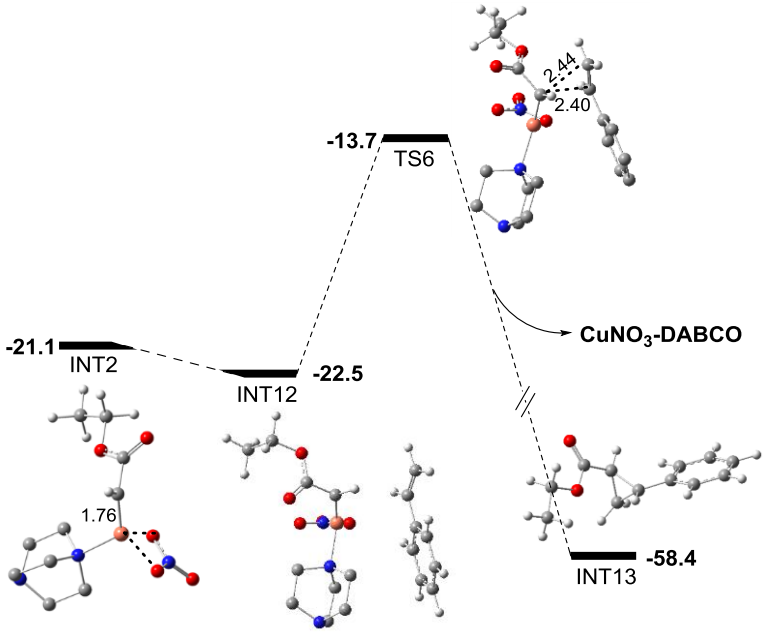


Figure S5. Free energy profile for the **INT2** induced cyclopropanation in the presence of styrene. Bond lengths are shown in Å.

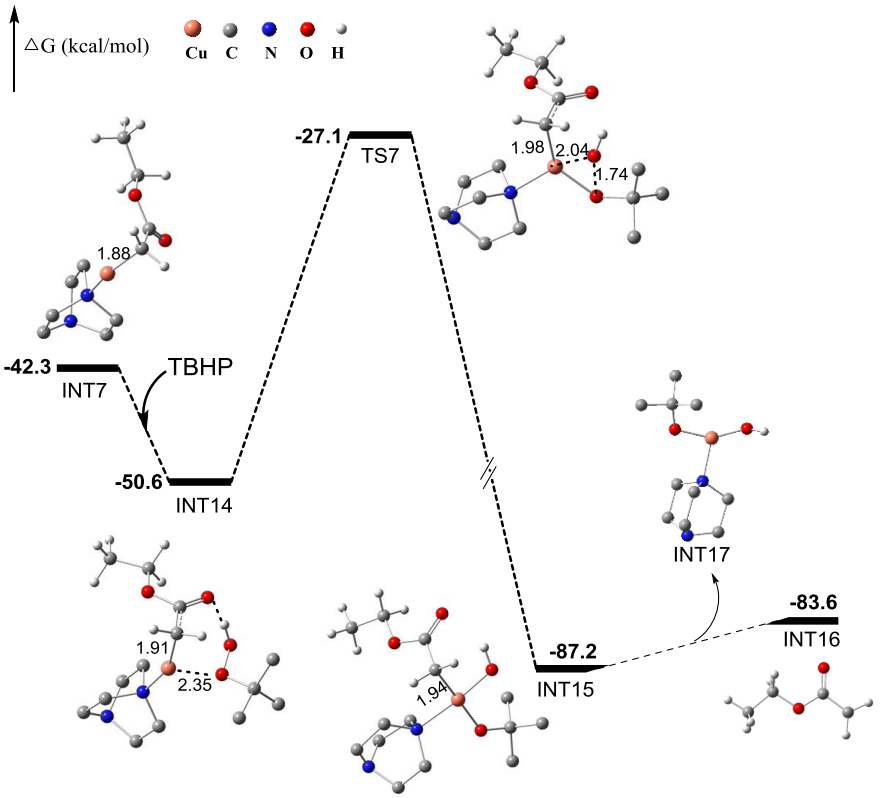


Figure S6. Free energy profile for the OA of ^{t}BuOOH onto **INT7**. Bond lengths are shown in Å.

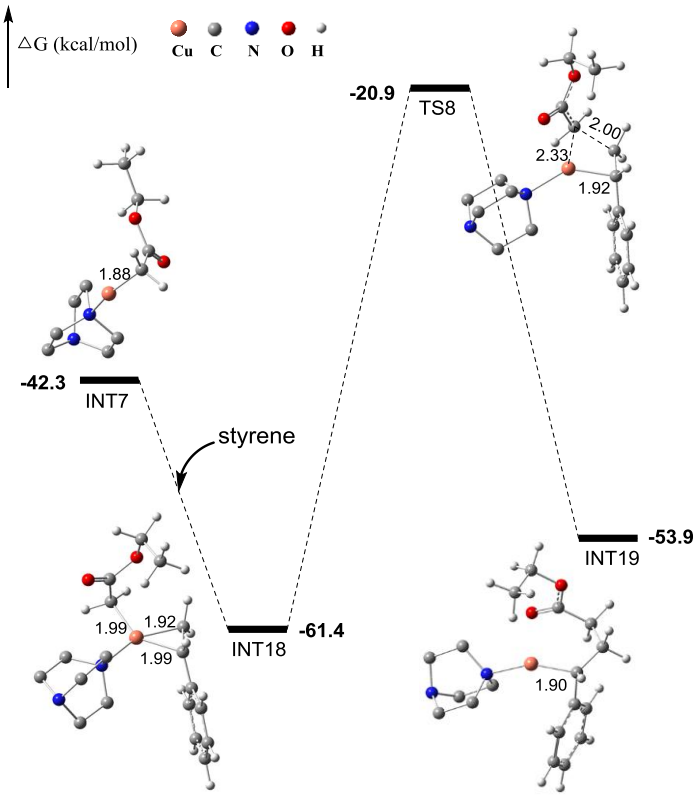


Figure S7. Free energy profile for the intermolecular carbocupration of the styrene to **INT7**. Bond lengths are shown in Å.

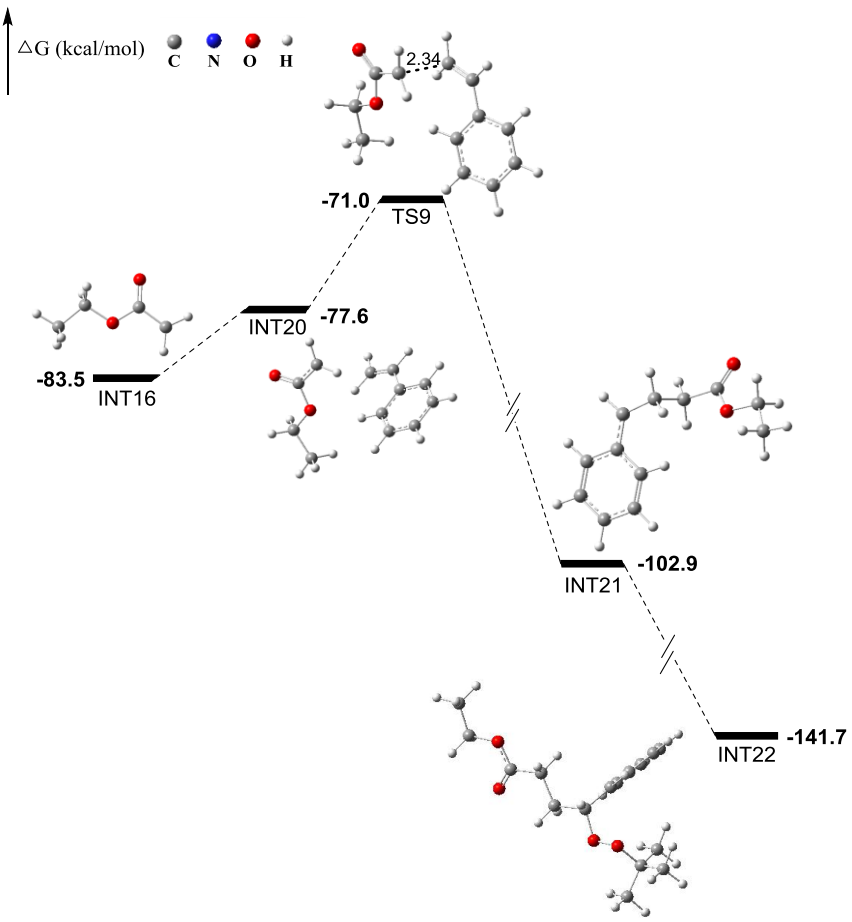


Figure S8. Energy profile for the radical addition to styrene and the formation of the final product. Bond lengths are shown in Å.

References:

1. J.-D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615.

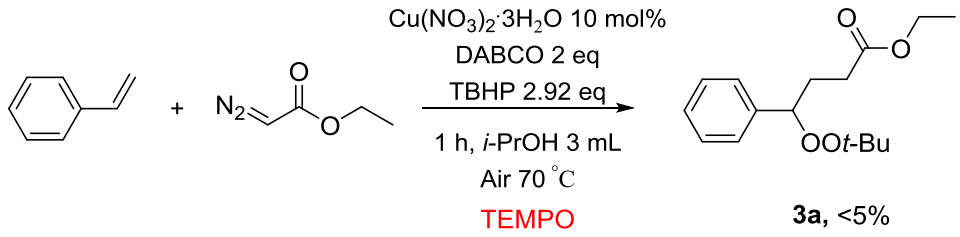
2. P. C. Hariharan, J. A. Pople, *Theor. Chim. Acta* **1973**, *28*, 213.

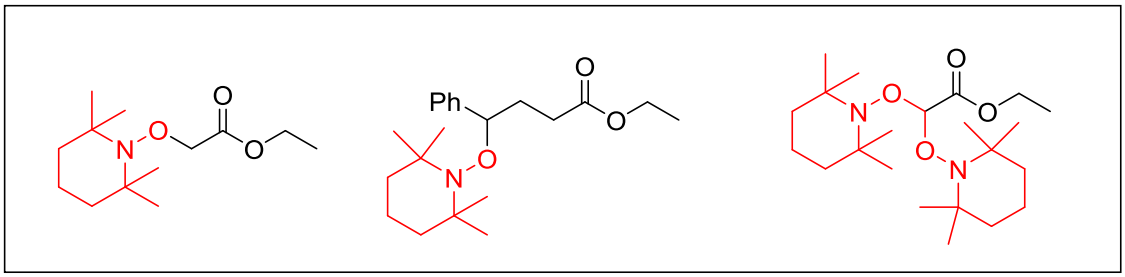
3. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell,

J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.

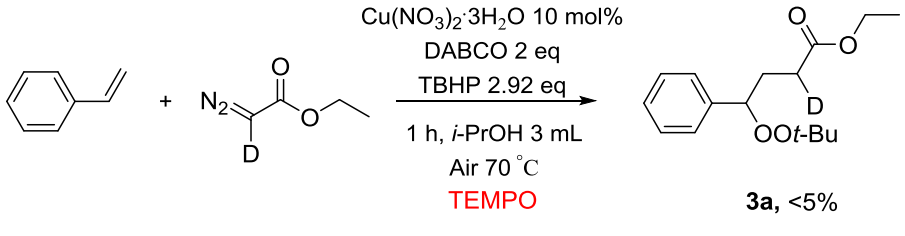
Trapping of Radicals

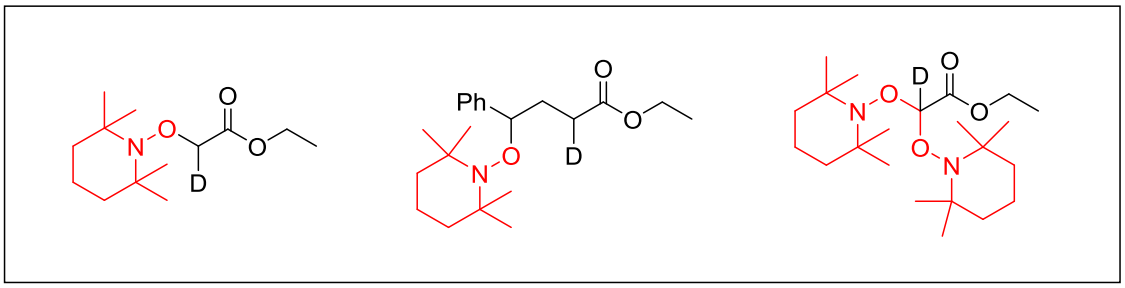
Scheme S1. Trapping of Radicals by **TEMPO**[a]





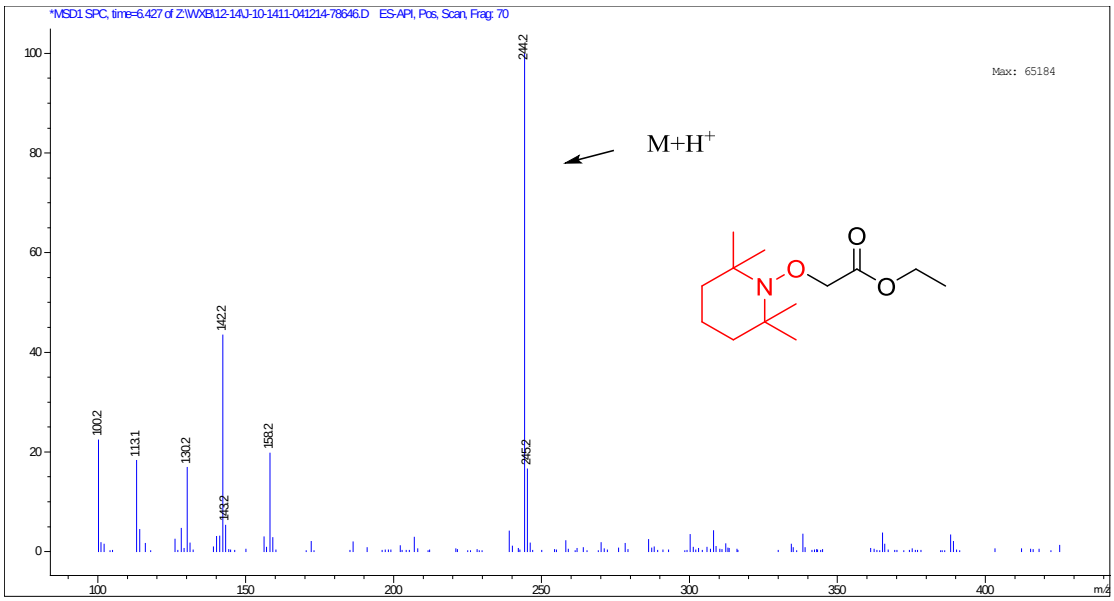
[a] TEMPO was added after the standard system being stirred for 5 minutes, the reaction was stopped after another 5 minutes.





[a] TEMPO was added after the standard system being stirred for 5 minutes, the reaction was stopped after another 5 minutes.

Adduct Detected by LC-MS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130.2
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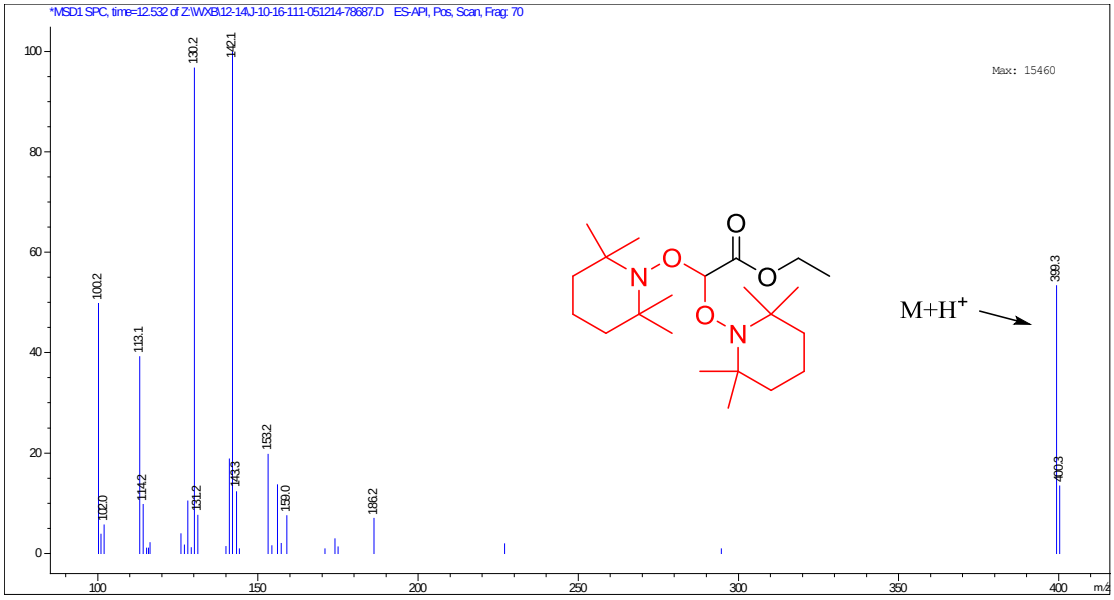
245.2
143.2
m/z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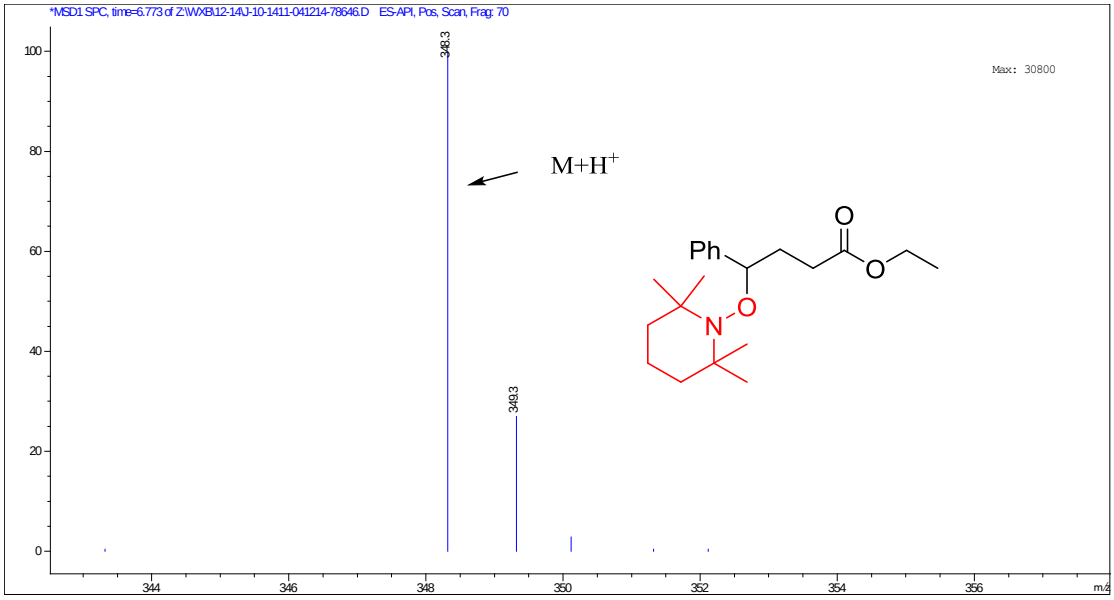
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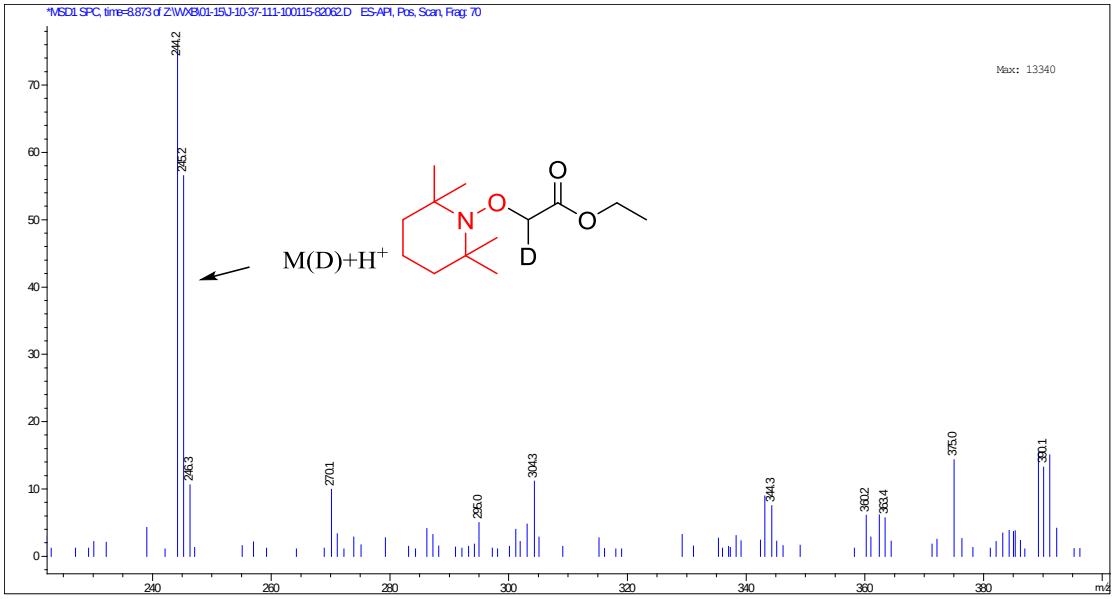
m/z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363.4
375.0
390.1
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N
O
O
O
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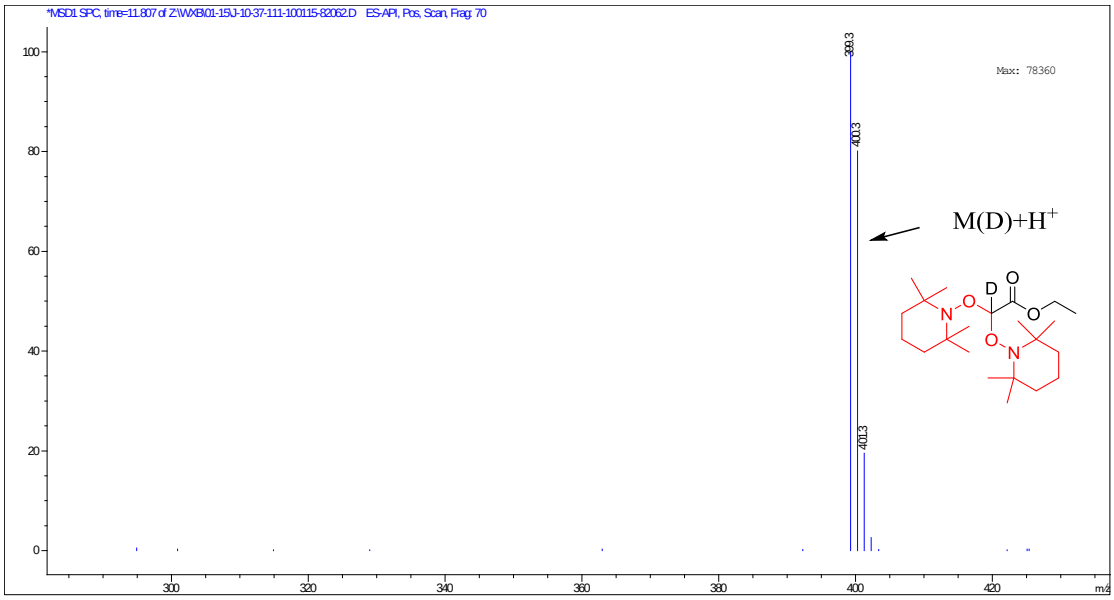
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D
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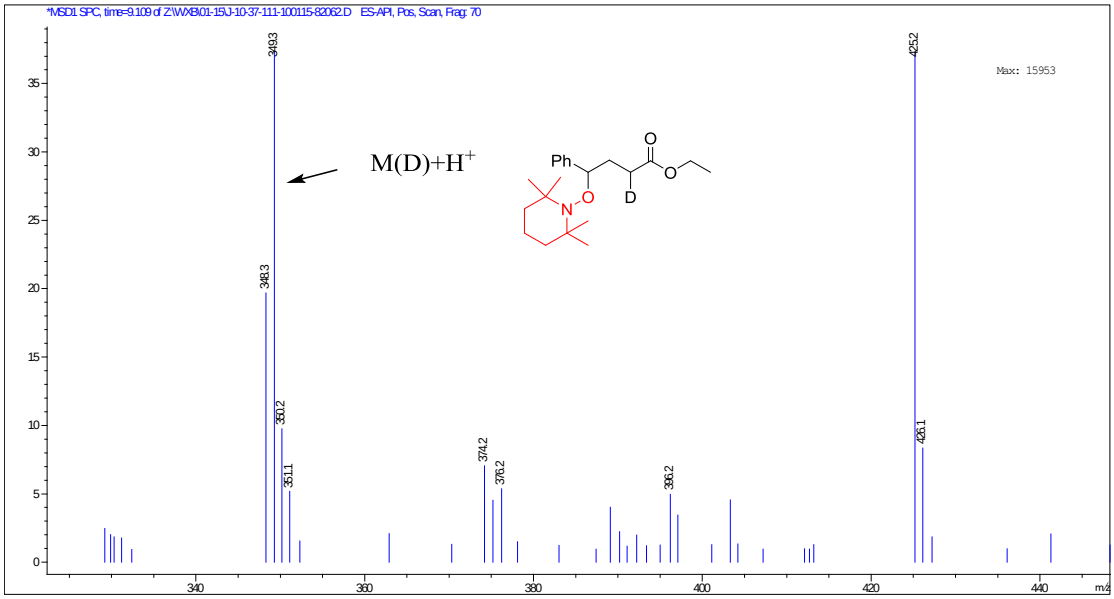
m/z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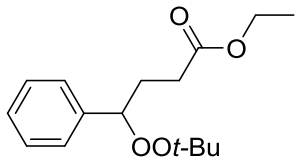
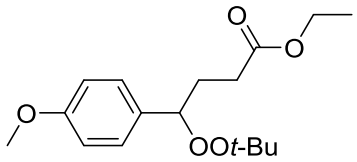
396.2
425.2
426.1
M(D)+H+
Ph
O
O
D
N
O
35
30
25
20
15
10
5
0
340
360
380
400
420
440
m/z

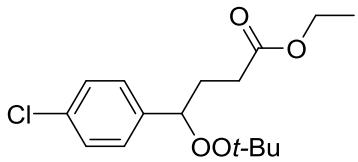
Compound characterizations



Ethyl 4-(*tert*-butylperoxy)-4-phenylbutanoate (3a). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 - 7.25 (m, 5H), 4.90 - 4.87 (m, 1H), 4.10 (q, *J* = 7.1 Hz, 2H), 2.39 - 2.35 (m, 2H), 2.24 - 2.14 (m, 1H), 2.08 - 2.00 (m, 1H), 1.23 (t, *J* = 7.1 Hz, 3H), 1.20 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 140.7, 128.2, 127.7, 126.7, 84.6, 80.2, 60.3, 30.6, 30.2, 26.4, 14.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{24}O_4$ +Na^+: 303.1567, Found: 303.1572; IR (neat, cm^{-1}): υ 2979, 2933, 1733, 1363, 1195.

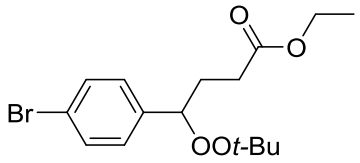


Ethyl 4-(*tert*-butylperoxy)-4-(4-methoxyphenyl)butanoate (3b). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 - 7.23 (m, 2H), 6.89 - 6.85 (m, 2H), 4.84 - 4.81 (m, 1H), 4.10 (q, *J* = 7.1 Hz, 2H), 3.80 (s, 3H), 2.36 - 2.32 (m, 2H), 2.27 - 2.18 (m, 1H), 2.06 - 1.99 (m, 1H), 1.23 (t, *J* = 7.1 Hz, 3H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 159.2, 132.6, 128.2, 113.6, 84.3, 80.1, 60.3, 55.2, 30.7, 30.0, 26.4, 14.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{17}H_{26}O_5$+Na^+: 333.1672, Found: 333.1683; IR (neat, cm^{-1}): υ 2978, 2934, 1732, 1512, 1246.

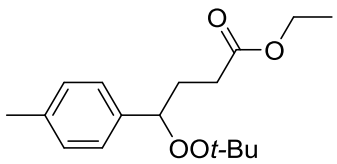


Ethyl 4-(*tert*-butylperoxy)-4-(4-chlorophenyl)butanoate (3c). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 - 7.25 (m, 4H), 4.88 - 4.85 (m, 1H), 4.11 (q, *J* = 7.1 Hz, 2H), 2.40 - 2.36 (m, 2H), 2.18 - 2.08 (m, 1H), 2.05 - 1.95 (m, 1H), 1.24 (t, *J* = 7.1 Hz, 2H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 139.5, 133.3, 128.3, 128.0, 83.8, 80.3, 60.4, 30.5,

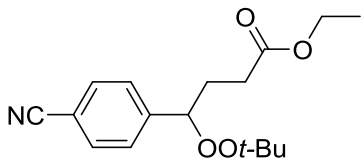
30.2, 26.3, 14.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{23}{}^{35}ClO_4$+Na^+: 337.1177, $C_{16}H_{23}{}^{37}ClO_4$+Na^+: 339.1148, Found: 337.1190, 339.1167; IR (neat, cm^{-1}): υ 2979, 2932, 1733, 1363, 1195.



Ethyl 4-(4-bromophenyl)-4-(*tert*-butylperoxy)butanoate (3d). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 - 7.45 (m, 2H), 7.22 - 7.20 (m, 2H), 4.87 - 4.83 (m, 1H), 4.11 (q, *J* = 7.2 Hz, 2H), 2.40 - 2.36 (m, 2H), 2.17 - 2.08 (m, 1H), 2.03 - 1.95 (m, 1H), 1.24 (t, *J* = 7.2 Hz, 2H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 140.1, 131.3, 128.4, 121.5, 83.9, 80.4, 60.4, 30.5, 30.2, 26.4, 14.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{23}{}^{79}BrO_4$+Na^+: 381.0672, $C_{16}H_{23}{}^{81}BrO_4$+Na^+: 383.0651, Found: 381.0696, 383.0680; IR (neat, cm^{-1}): υ 2979, 2932, 1733, 1363, 1011.

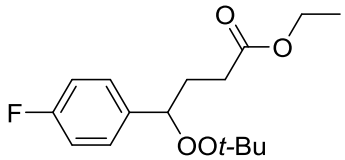


Ethyl 4-(*tert*-butylperoxy)-4-(*p*-tolyl)butanoate (3e). ^{1}H NMR (400 MHz, $CDCl_3$) δδ 7.22 - 7.20 (m, 2H), 7.15 - 7.13 (m, 2H), 4.85 (t, *J*= 6.8 Hz, 1H), 4.10 (q, *J* = 7.1 Hz, 2H), 2.38 - 2.33 (m, 5H), 2.25 - 2.16 (m, 1H), 2.07 - 1.98 (m, 1H), 1.25 - 1.20 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 137.6, 137.3, 128.9, 126.7, 84.5, 80.2, 60.3, 30.6, 30.1, 26.4, 21.1, 14.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{17}H_{26}O_4$+Na^+: 317.1723, Found: 317.1694; IR (neat, cm^{-1}): υ 2979, 2931, 1734, 1363, 1196.

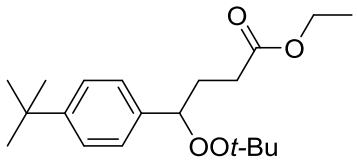


Ethyl 4-(*tert*-butylperoxy)-4-(4-cyanophenyl)butanoate (3f). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.45 (d, *J* = 8.2 Hz, 2H), 4.97 - 4.94 (m, 1H), 4.13 (q, *J* = 7.1 Hz, 2H), 2.47 - 2.38 (m, 2H), 2.07 - 2.00 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.20

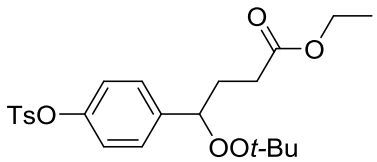
(s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 146.9, 132.1, 127.2, 118.8, 111.3, 83.7, 80.7, 60.5, 30.4, 30.3, 26.3, 14.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{17}H_{23}NO_4$+Na^+: 328.1519, Found: 328.1504; IR (neat, cm^{-1}): υ 2979, 2933, 2229, 1731, 1364, 1193.



Ethyl 4-(*tert*-butylperoxy)-4-(4-fluorophenyl)butanoate (3g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 - 7.27 (m, 2H), 7.04 - 7.00 (m, 2H), 4.88 - 4.85 (m, 1H), 4.11 (q, *J* = 7.1 Hz, 2H), 2.39 - 2.35 (m, 2H), 2.21 - 2.12 (m, 1H), 2.04 - 1.96 (m, 1H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 162.3 (d, *J* = 243.9 Hz), 136.6 (d, *J* = 3.1 Hz), 128.4 (d, *J* = 8.0 Hz), 115.0 (d, *J* = 21.2 Hz), 83.9, 80.3, 60.4, 30.5, 30.2, 26.4, 14.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{23}FO_4$+Na^+: 321.1473, Found: 321.1493; IR (neat, cm^{-1}): υ 2980, 2933, 1733, 1510, 1223.

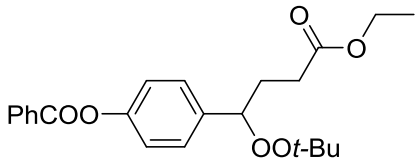


Ethyl 4-(4-(*tert*-butyl)phenyl)-4-(*tert*-butylperoxy)butanoate (3h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 - 7.34 (m, 2H), 7.25 - 7.23 (m, 2H), 4.87 (t, *J* = 6.8 Hz, 1H), 4.09 (q, *J* = 7.1 Hz, 2H), 2.38 - 2.36 (m, 2H), 2.26 - 2.17 (m, 1H), 2.09 - 2.01 (m, 1H), 1.31 (s, 9H), 1.24 - 1.21 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 150.5, 137.4, 126.4, 125.1, 84.5, 80.2, 60.3, 34.4, 31.3, 30.6, 30.1, 26.4, 14.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{20}H_{32}O_4$+Na^+: 359.2193, Found: 359.2176; IR (neat, cm^{-1}): υ 2966, 2905, 1735, 1363, 1195.

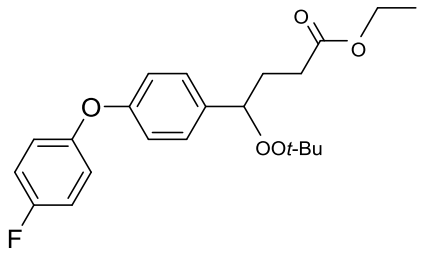


Ethyl 4-(*tert*-butylperoxy)-4-(4-(tosyloxy)phenyl)butanoate (3i). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.31 - 7.24 (m, 4H), 6.96 - 6.94 (m, 2H), 4.87 -

4.84 (m, 1H), 4.11 (q, *J* = 7.1 Hz, 2H), 2.44 (s, 3H), 2.39 - 2.35 (m, 2H), 2.14 - 2.05 (m, 1H), 2.03 - 1.93 (m, 1H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.17 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 148.9, 145.2, 140.0, 132.3, 129.6, 128.4, 127.8, 122.0, 83.6, 80.2, 60.3, 30.4, 30.1, 26.3, 21.6, 14.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{23}H_{30}O_7S+Na^+$: 473.1604, Found: 473.1600; IR (neat, cm^{-1}): υ 2980, 2933, 1732, 1373, 1196.

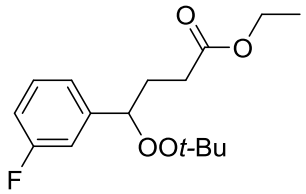


4-(1-(*Tert*-butylperoxy)-4-ethoxy-4-oxobutyl)phenyl benzoate (3j). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 - 8.18 (m, 2H), 7.64 - 7.60 (m, 1H), 7.52 - 7.48 (m, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.20 (d, *J* = 8.5 Hz, 2H), 4.95 - 4.91 (m, 1H), 4.12 (q, *J* = 7.1 Hz, 2H), 2.43 - 2.39 (m, 2H), 2.22 - 2.14 (m, 1H), 2.10 - 2.03 (m, 1H), 1.26 - 1.21 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 165.1, 150.4, 138.5, 133.5, 130.1, 129.5, 128.5, 127.8, 121.4, 84.0, 80.3, 60.4, 30.6, 30.3, 26.4, 14.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{23}H_{28}O_6+Na^+$: 423.1778, Found: 423.1807; IR (neat, cm^{-1}): υ 2966, 2905, 1735, 1508, 1262.

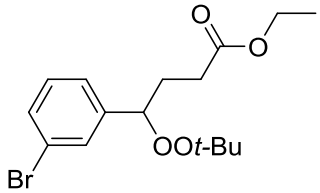


Ethyl 4-(*tert*-butylperoxy)-4-(4'-fluoro-[1,1'-biphenyl]-4-yl)butanoate (3k). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 - 7.26 (m, 2H), 7.05 - 6.91 (m, 6H), 4.88 - 4.85 (m, 1H), 4.11 (q, *J* = 7.1 Hz, 2H), 2.38 (t, *J* = 7.6 Hz, 2H), 2.25 - 2.15 (m, 1H), 2.07 - 1.98 (m, 1H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.21 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 158.8 (d, *J* = 240.3 Hz), 157.3, 152.7 (d, *J* = 2.6 Hz), 135.4, 128.3, 120.6 (d, *J* = 8.3 Hz), 117.8, 116.3 (d, *J* = 23.2 Hz), 84.2, 80.3, 60.4, 30.7, 30.2, 26.4, 14.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{22}H_{27}FO_5+Na^+$: 413.1735, Found: 413.1759; IR (neat,

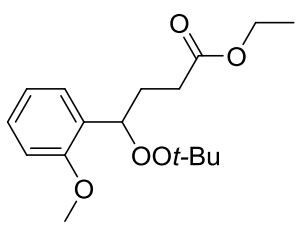
cm^{-1}): υ 2979, 2933, 1733, 1496, 1211.



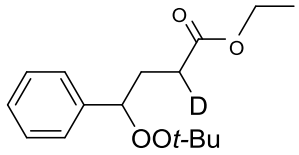
Ethyl 4-(*tert*-butylperoxy)-4-(3-fluorophenyl)butanoate (3l). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 - 7.27 (m, 1H), 7.10 - 7.04 (m, 2H), 6.98 - 6.94 (m, 1H), 4.91 - 4.87 (m, 1H), 4.12 (q, *J* = 7.1 Hz, 2H), 2.41 - 2.37 (m, 2H), 2.17 - 1.97 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.21 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 162.8 (d, *J* = 244.1 Hz), 143.8 (d, *J* = 6.7 Hz), 129.7 (d, *J* = 8.1 Hz), 122.2 (d, *J* = 2.9 Hz), 114.5 (d, *J* = 21.0 Hz), 113.5 (d, *J* = 21.6 Hz), 83.8 (d, *J* = 1.6 Hz), 80.4, 60.4, 30.4, 30.3, 26.3, 14.1; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{23}FO_4$+Na^+: 321.1473, Found: 321.1492; IR (neat, cm^{-1}): υ 2980, 2934, 1733, 1449, 1194.



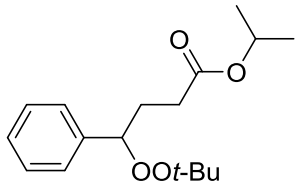
Ethyl 4-(3-bromophenyl)-4-(*tert*-butylperoxy)butanoate (3m). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 - 7.47 (m, 1H), 7.42 - 7.39 (m, 1H), 7.27 - 7.19 (m, 2H), 4.87 - 4.83 (m, 1H), 4.12 (q, *J* = 7.1 Hz, 2H), 2.41 - 2.37 (m, 2H), 2.16 - 2.07 (m, 1H), 2.05 - 1.96 (m, 1H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.20 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 143.5, 130.7, 129.8, 129.7, 125.3, 122.3, 83.8, 80.4, 60.4, 30.5, 30.4, 26.4, 14.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{23}{}^{79}BrO_4$+Na^+: 381.0672, $C_{16}H_{23}{}^{81}BrO_4$+Na^+: 383.0651, Found: 381.0692, 383.0673; IR (neat, cm^{-1}): υ 2979, 2933, 1732, 1363, 1193.



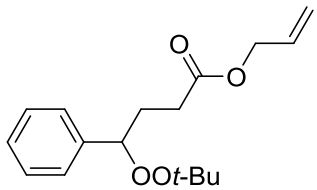
Ethyl 4-(*tert*-butylperoxy)-4-(2-methoxyphenyl)butanoate (3n). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 - 7.39 (m, 1H), 7.25 - 7.20 (m, 1H), 6.98 - 6.94 (m, 1H), 6.85 - 6.83 (m, 1H), 5.36 (t, *J* = 6.4 Hz, 1H), 4.09 (q, *J* = 7.1 Hz, 2H), 3.80 (s, 3H), 2.41 - 2.36 (m, 2H), 2.13 - 2.06 (m, 2H), 1.24 - 1.21 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3, 156.4, 129.2, 128.2, 127.0, 120.4, 110.2, 80.1, 78.5, 60.2, 55.2, 30.5, 29.2, 26.4, 14.2; HRMS (ESI-TOF): Anal. Calcd. For $C_{17}H_{26}O_5$+Na^+: 333.1672, Found: 333.1696; IR (neat, cm^{-1}): υ 2978, 2935, 1734, 1492, 1242.



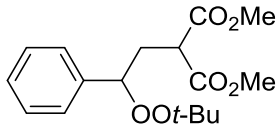
Ethyl 4-(*tert*-butylperoxy)-4-phenylbutanoate-2-d (*D*-3a). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 - 7.27 (m, 5H), 4.90 - 4.87 (m, 1H), 4.10 (q, *J* = 7.1 Hz, 2H), 2.39 - 2.34 (m, 1H), 2.22 - 2.13 (m, 1H), 2.07 - 2.00 (m, 1H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.20 (s, 9H); HRMS (ESI-TOF): Anal. Calcd. For $C_{16}H_{23}DO_4$ +Na^+: 304.1630, Found: 304.1641.



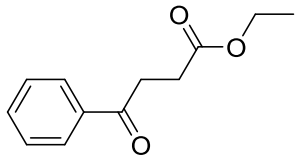
Isopropyl 4-(*tert*-butylperoxy)-4-phenylbutanoate (4b). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 - 7.25 (m, 5H), 5.04 - 4.94 (m, 1H), 4.90 - 4.87 (m, 1H), 2.36 - 2.32 (m, 2H), 2.20 - 2.13 (m, 1H), 2.07 - 1.98 (m, 1H), 1.22 - 1.20 (m, 15H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 140.8, 128.2, 127.7, 126.7, 84.7, 80.2, 67.6, 30.9, 30.3, 26.4, 21.8; MS (ESI-quadrupole): Anal. Calcd. For $C_{17}H_{26}O_4$ +Na^+: 317, Found: 317; IR (neat, cm^{-1}): υ 2981, 2935, 1729, 1219, 1109.



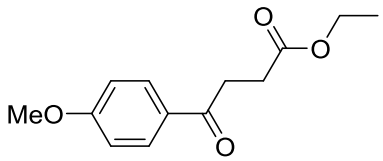
Allyl 4-(*tert*-butylperoxy)-4-phenylbutanoate (4c). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 - 7.25 (m, 5H), 5.94 - 5,85 (m, 1H), 5.33 - 5.21 (m, 2H), 4.94 - 4.88 (m, 1H), 4.56 - 4.54 (m, 2H), 2.44 -2.40 (m, 2H), 2,22 - 2.16 (m, 1H), 2.10 -2.01 (m, 1H), 1.20 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 140.7, 132.1, 128.2, 127.7, 126.7, 118.2, 84.6, 65.1, 30.5, 30.2, 26.4; HRMS (ESI-TOF): Anal. Calcd. For $C_{17}H_{24}O_4$ +Na^+: 315.1567, Found: 315.1579; IR (neat, cm^{-1}): υ 2979, 2932, 1737, 1363, 1197.



Dimethyl 2-(2-(*tert*-butylperoxy)-2-phenylethyl)malonate (4d). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 - 7.26 (m, 5H), 4.93 - 4.89 (m, 1H), 4.712 - 3.709 (m, 6H), 3.64 - 3.60 (m, 1H), 2.49 - 2.42 (m, 1H), 2.37 - 2.30 (m, 1H), 1.17 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 169.4, 140.2, 128.2, 127.9, 126.7, 83.1, 80.3, 52.49, 52.45, 48.6, 34.4, 26.3; MS (ESI-quadrupole): Anal. Calcd. For $C_{17}H_{24}O_6$ +Na^+: 347, Found: 347; IR (neat, cm^{-1}): υ 2979, 2955, 1754, 1737, 1197.

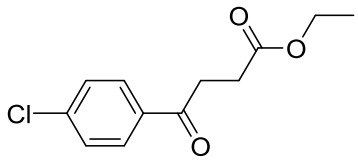


Ethyl 4-oxo-4-phenylbutanoate (9a).[5] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 - 7.98 (m, 2H), 7.58 - 7.55 (m, 1H), 7.48 - 7.44 (m, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.31 (t, *J* = 6.6 Hz, 2H), 2.76 (t, *J* = 6.6 Hz, 2H), 1.26 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.1, 172.8, 136.5, 133.1, 128.5, 127.9, 60.6, 33.3, 28.2, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{12}H_{14}O_3$+H^+: 207, Found: 207; IR (neat, cm^{-1}): υ 2981, 2932, 1730, 1686, 1216, 1159.

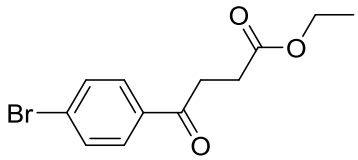


Ethyl 4-(4-methoxyphenyl)-4-oxobutanoate (9b).[6] ^{1}H NMR (400 MHz, $CDCl_3$) δ

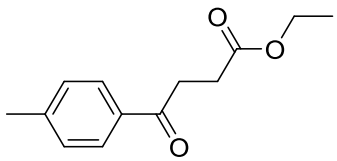
7.97 (d, *J* = 8.8 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.87 (s, 3 H), 3.27 (t, *J* = 6.6 Hz, 2H), 2.74 (t, *J* = 6.6 Hz, 2H), 1.27 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.6, 173.0, 163.5, 130.2, 129.7, 113.7, 60.5, 55.4, 33.0, 28.3, 14.2; MS (ESI-quadrupole): Anal. Calcd. For $C_{13}H_{16}O_4+H^+$: 237, Found: 237; IR (neat, cm^{-1}): υ 2921, 2851, 1731, 1718, 1676, 1027.



Ethyl 4-(4-chlorophenyl)-4-oxobutanoate (9c).[7] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.5 Hz, 2H), 7.44 (d, *J* = 8.5 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.27 (t, *J* = 6.6 Hz, 2H), 2.75 (t, *J* = 6.6 Hz, 2H), 1.26 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 172.7, 139.5, 134.8, 129.4, 128.8, 60.6, 33.2, 28.1, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{12}H_{13}{}^{35}ClO_3+H^+$: 241, $C_{12}H_{13}{}^{37}ClO_3+H^+$: 243, Found: 241, 243; IR (neat, cm^{-1}): υ 2957, 2927, 1731, 1689, 1671, 1161.

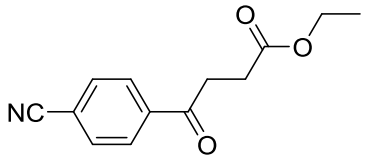


Ethyl 4-(4-bromophenyl)-4-oxobutanoate (9d).[7] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.4 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.27 (t, *J* = 6.6 Hz, 2H), 2.75 (t, *J* = 6.6 Hz, 2H), 1.26 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 172.6, 135.2, 131.8, 129.5, 128.2, 60.6, 33.2, 28.1, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{12}H_{13}{}^{79}BrO_3+H^+$: 285, $C_{12}H_{13}{}^{81}BrO_3+H^+$: 287, Found: 285, 287; IR (neat, cm^{-1}): υ 2979, 2927, 1728, 1689, 1669, 1068.

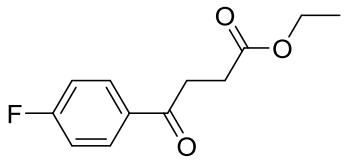


Ethyl 4-oxo-4-(p-tolyl)butanoate (9e).[8] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.26 (d, *J* = 7.8 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.29 (t, *J* = 6.6 Hz, 2H),

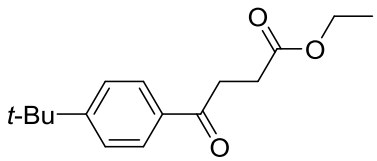
2.75 (t, *J* = 6.6 Hz, 2H), 2,41 (s, 3H), 1.27 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 172.9, 143.9, 134.1, 129.2, 128.1, 60.6, 33.2, 28.3, 21.6, 14.2; MS (ESI-quadrupole): Anal. Calcd. For $C_{13}H_{16}O_3$+H^+: 221, Found: 221; IR (neat, cm^{-1}): υ 2984, 2922, 1722, 1677, 1607, 1159.



Ethyl 4-(4-cyanophenyl)-4-oxobutanoate (9f). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.5 Hz, 2H), 7.79 (d, *J* = 8.5 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.31 (t, *J* = 6.4 Hz, 2H), 2.79 (t, *J* = 6.4 Hz, 2H), 1.27 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 172.4, 139.4, 132.4, 128.4, 117.8, 116.4, 60.7, 33.6, 28.0, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{13}H_{13}NO_3$+H^+: 232, Found: 232; IR (neat, cm^{-1}): υ 2986, 2923, 1724, 1683, 1172.

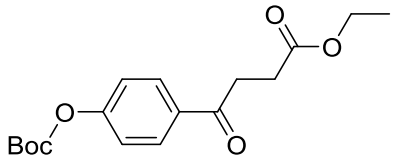


Ethyl 4-(4-fluorophenyl)-4-oxobutanoate (9g).[7] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 - 8.00 (m, 2H), 7.16 - 7.11 (m, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.28 (t, *J* = 6.6 Hz, 2H), 2.76 (t, *J* = 6.6 Hz, 2H), 1.27 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 172.8, 165.7 (d, *J*= 253.1 Hz), 133.0 (d, *J* = 3.3 Hz), 130.6 (d, *J* = 9.3 Hz), 115.6 (d, *J* = 21.7 Hz), 60.6, 33.2, 28.2, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{12}H_{13}FO_3$+H^+: 225, Found: 225; IR (neat, cm^{-1}): υ 3048, 2928, 1719, 1676, 1591, 1157.

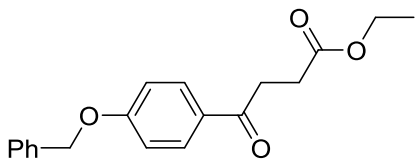


Ethyl 4-(4-(tert-butyl)phenyl)-4-oxobutanoate (9h).[9] ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.3 Hz, 2H), 7.48 (d, *J* = 8.3 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.29 (t, *J* =

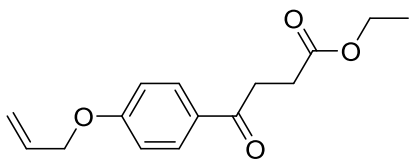
6.6 Hz, 2H), 2.75 (t, *J* = 6.6 Hz, 2H), 1.34 (s, 9H), 1.26 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 172.9, 156.8, 134.0, 127.9, 125.5, 60.5, 35.0, 33.2, 31.0, 28.3, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{16}H_{22}O_3+H^+$: 263, Found: 263; IR (neat, cm^{-1}): υ 2964, 2907, 1732, 1683, 1161.



Ethyl 4-(4-((tert-butoxycarbonyl)oxy)phenyl)-4-oxobutanoate (9i). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.7 Hz, 2H), 7.28 (d, *J* = 8.7 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.29 (t, *J* = 6.6 Hz, 2H), 2.75 (t, *J* = 6.6 Hz, 2H), 1.57 (s, 9H), 1.26 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 172.7, 154.6, 150.9, 133.9, 129.5, 121.2, 84.1, 60.5, 33.2, 28.1, 27.5, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{17}H_{22}O_6+H^+$: 323, Found: 323; IR (neat, cm^{-1}): υ 2982, 2935, 1757, 1732, 1600, 1138.

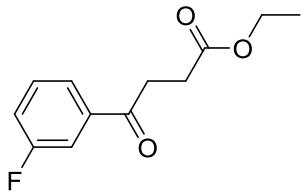


Ethyl 4-(4-(benzyloxy)phenyl)-4-oxobutanoate (9j). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.8 Hz, 2H), 7.43 - 7.31 (m, 5H), 7.00 (d, *J* = 8.8 Hz, 2H), 5.11 (s, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.24 (t, *J* = 6.8 Hz, 2H), 2.73 (t, *J* = 6.8 Hz, 2H), 1.25 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 172.9, 162.6, 136.1, 130.2, 129.8, 128.6, 128.1, 127.4, 114.5, 70.0, 60.5, 32.9, 28.3, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{19}H_{20}O_4+H^+$: 313, Found: 313; IR (neat, cm^{-1}): υ 3034, 2931, 1728, 1663, 1598, 1166.

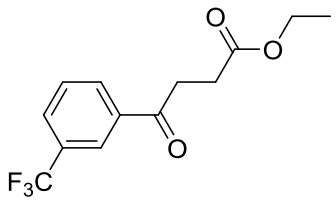


Ethyl 4-(4-(allyloxy)phenyl)-4-oxobutanoate (9k). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.9 Hz, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 6.09 - 6.00 (m, 1H), 5.44 - 5.30 (m,

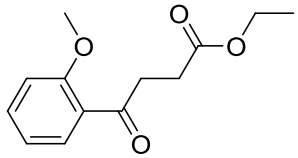
2H), 4.60 (d, *J* = 5.2 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.26 (t, *J* = 6.7 Hz, 2H), 2.73 (t, *J* = 6.7 Hz, 2H), 1.26 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 172.9, 162.4, 132.4, 130.1, 129.7, 118.0, 114.3, 68.7, 60.5, 32.9, 28.3, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{15}H_{18}O_4$+H^+: 263, Found: 263; IR (neat, cm^{-1}): υ 2982, 2917, 1730, 1677, 1599, 1165.



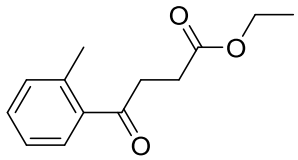
Ethyl 4-(3-fluorophenyl)-4-oxobutanoate (9l). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 - 7.76 (m, 1H), 7.67 - 7.65 (m, 1H), 7.48 - 7.43 (m, 1H), 7.29 - 7.25 (m, 1H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.29 (t, *J* = 6.6 Hz, 2H), 2.76 (t, *J* = 6.6 Hz, 2H), 1.27 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9 (d, *J* = 2.0 Hz), 172.6, 162.8 (d, *J* = 248.4 Hz), 138.6 (d, *J* = 6.0 Hz), 130.2 (d, *J* = 7.6 Hz), 123.7 (d, *J* = 3.0 Hz), 120.2 (d, *J* = 21.3 Hz), 114.7 (d, *J* = 22.2 Hz), 60.7, 33.5, 28.1, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{12}H_{13}FO_3$+H^+: 225, Found: 225; IR (neat, cm^{-1}): υ 2983, 2933, 1730, 1689, 1589, 1149.



Ethyl 4-oxo-4-(3-(trifluoromethyl)phenyl)butanoate (9m).[7] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 - 8.23 (m, 1H), 8.23 - 8.22 (m, 1H), 8.18 - 8.16 (m, 1H), 7.84 - 7.82 (m, 1H), 7.64 - 7.60 (m, 1H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.34 (t, *J* = 6.4 Hz, 2H), 2.79 (t, *J* = 6.4 Hz, 2H), 1.27 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 172.6, 137.0, 131.7, 131.4, 131.1, 131.0, 130.7, 129.59, 129.56, 129.52, 129.48, 129.3, 127.7, 124.97, 124.8 (q, 300Hz), 122.3, 60.7, 33.4, 28.1, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{13}H_{13}F_3O_3$+H^+: 275, Found: 275; IR (neat, cm^{-1}): υ 2984, 1731, 1694, 1328, 1123.

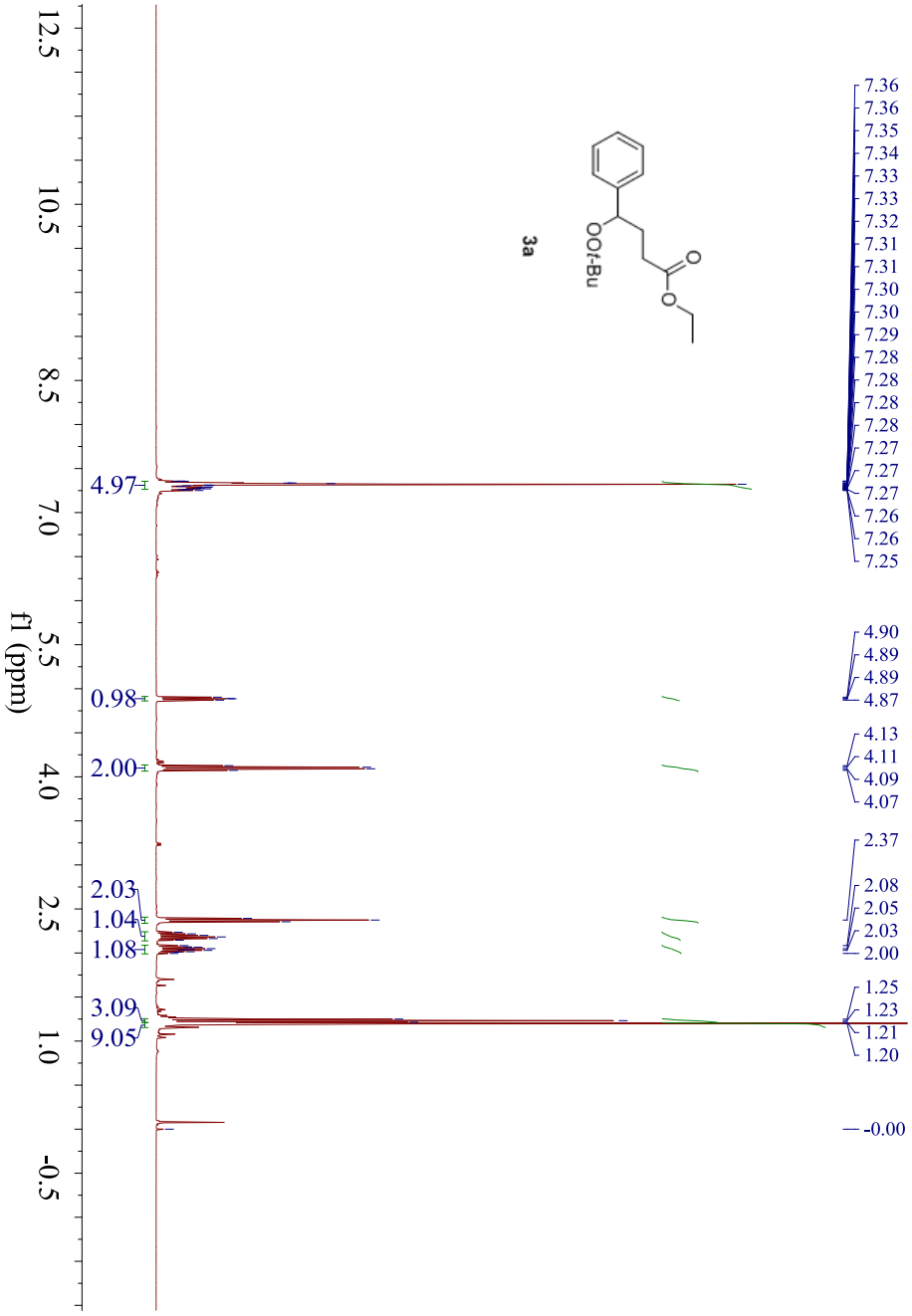


Ethyl 4-(2-methoxyphenyl)-4-oxobutanoate (9n). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 - 7.74 (m, 1H), 7.49 - 7.44 (m, 1H), 7.02 - 6.96 (m, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.92 (s, 3H), 3.32 (t, *J* = 6.7 Hz, 2H), 2.70 (t, *J* = 6.7 Hz, 2H), 1.26 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.9, 173.1, 158.8, 133.6, 130.4, 127.5, 120.6, 111.5, 60.4, 55.4, 38.7, 28.7, 14.1; MS (ESI-quadrupole): Anal. Calcd. For $C_{13}H_{16}O_4+H^+$: 237, Found: 237; IR (neat, cm^{-1}): υ 2980, 2941, 1730, 1672, 1597, 1159.



Ethyl 4-oxo-4-(o-tolyl)butanoate (9o). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 - 7.70 (m, 1H), 7.40 - 7.36 (m, 1H), 7.29 – 7.24 (m, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.22 (t, *J* = 6.6 Hz, 2H), 2.74 (t, *J* = 6.6 Hz, 2H), 2.49 (s, 3H), 1.27 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.1, 172.9, 138.1, 137.5, 131.9, 131.4, 128.5, 125.7, 60.6, 36.1, 28.5, 21.2, 14.2; MS (ESI-quadrupole): Anal. Calcd. For $C_{13}H_{16}O_4+H^+$: 221, Found: 221; IR (neat, cm^{-1}): υ 2980, 2929, 1731, 1686, 1162.

NMR Spectroscopic Data for Products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7.34
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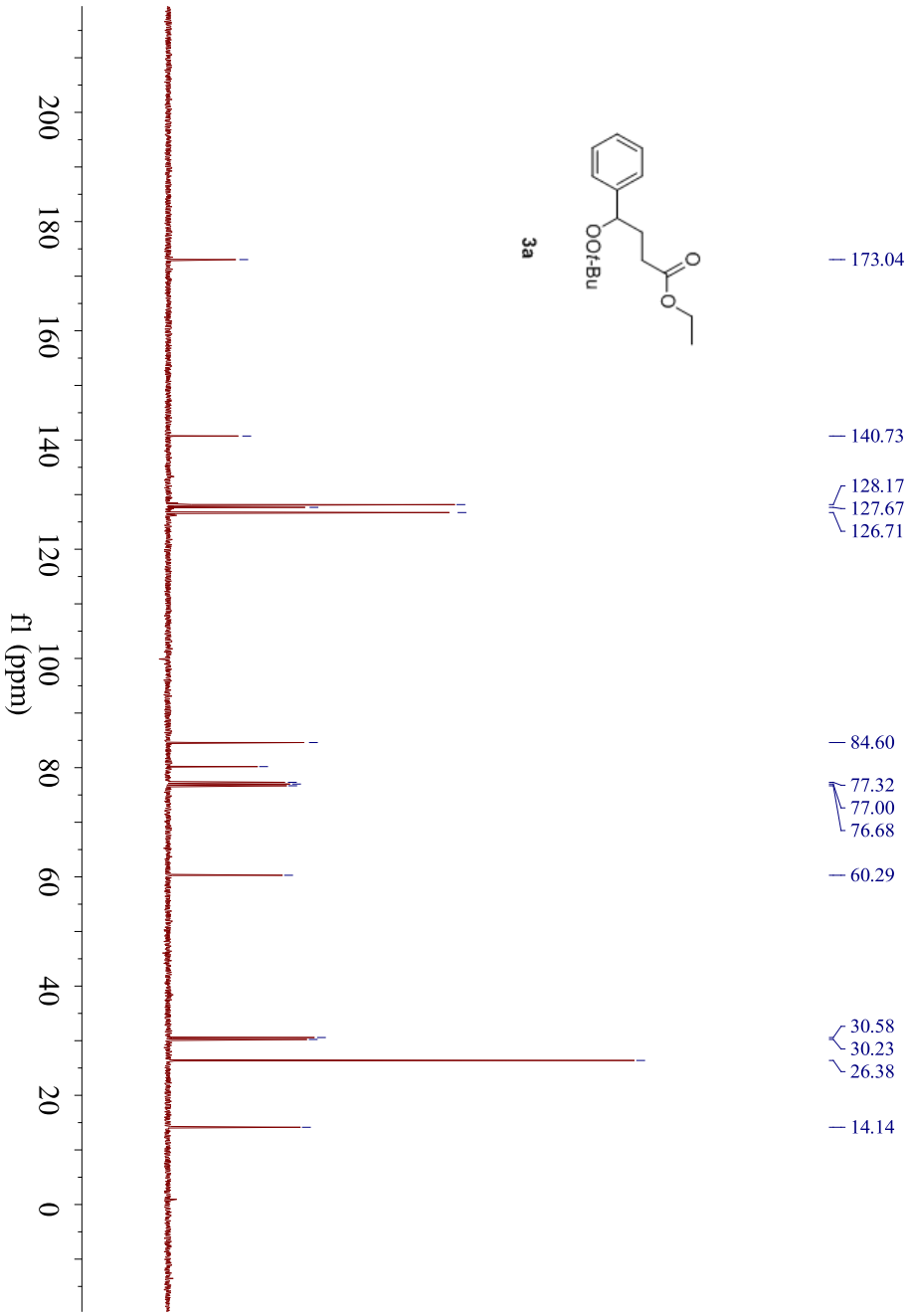
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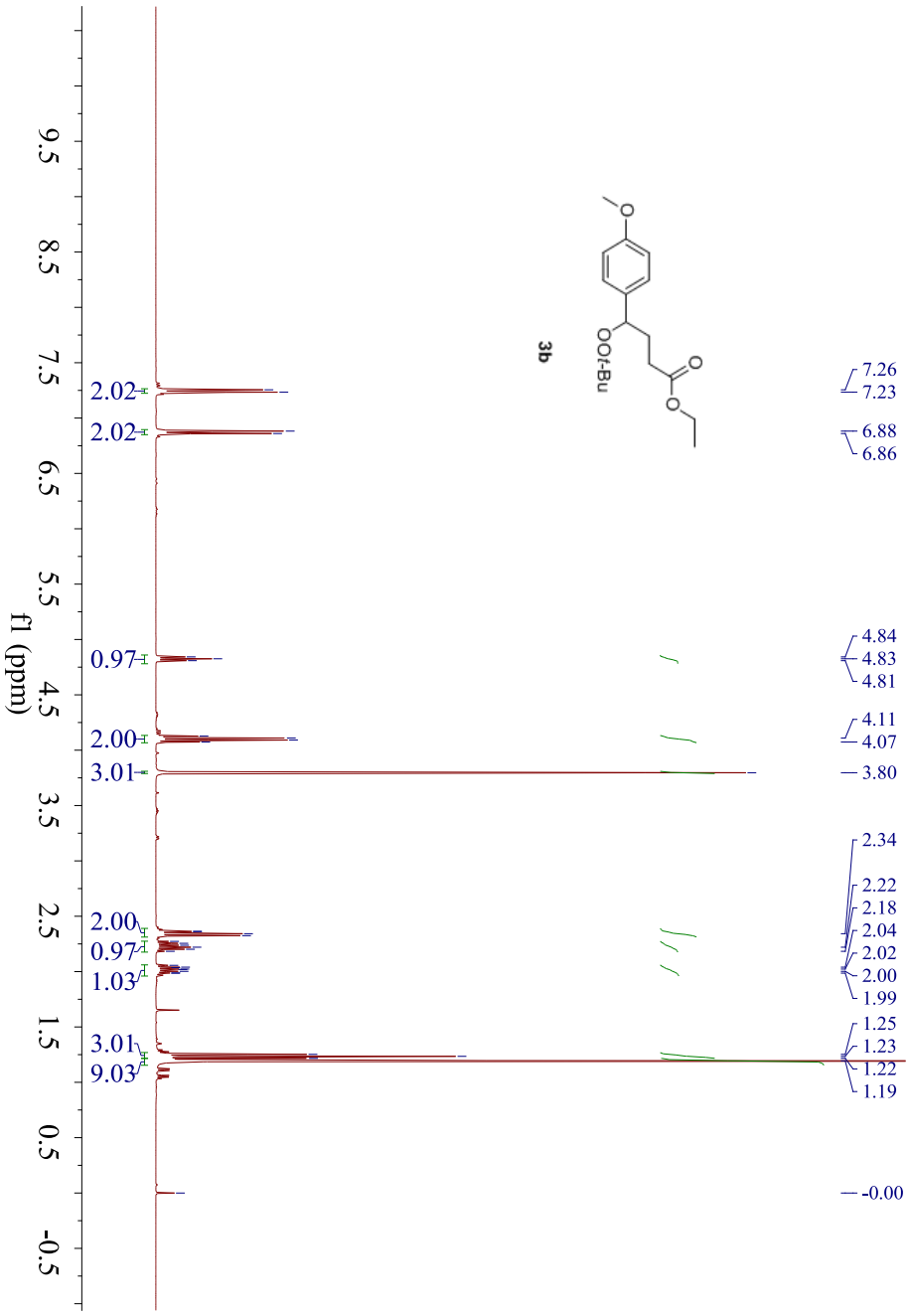
14.14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2.02
0.97
2.00
3.01
2.00
0.97
1.03
3.01
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4.81
4.11
4.07
3.80
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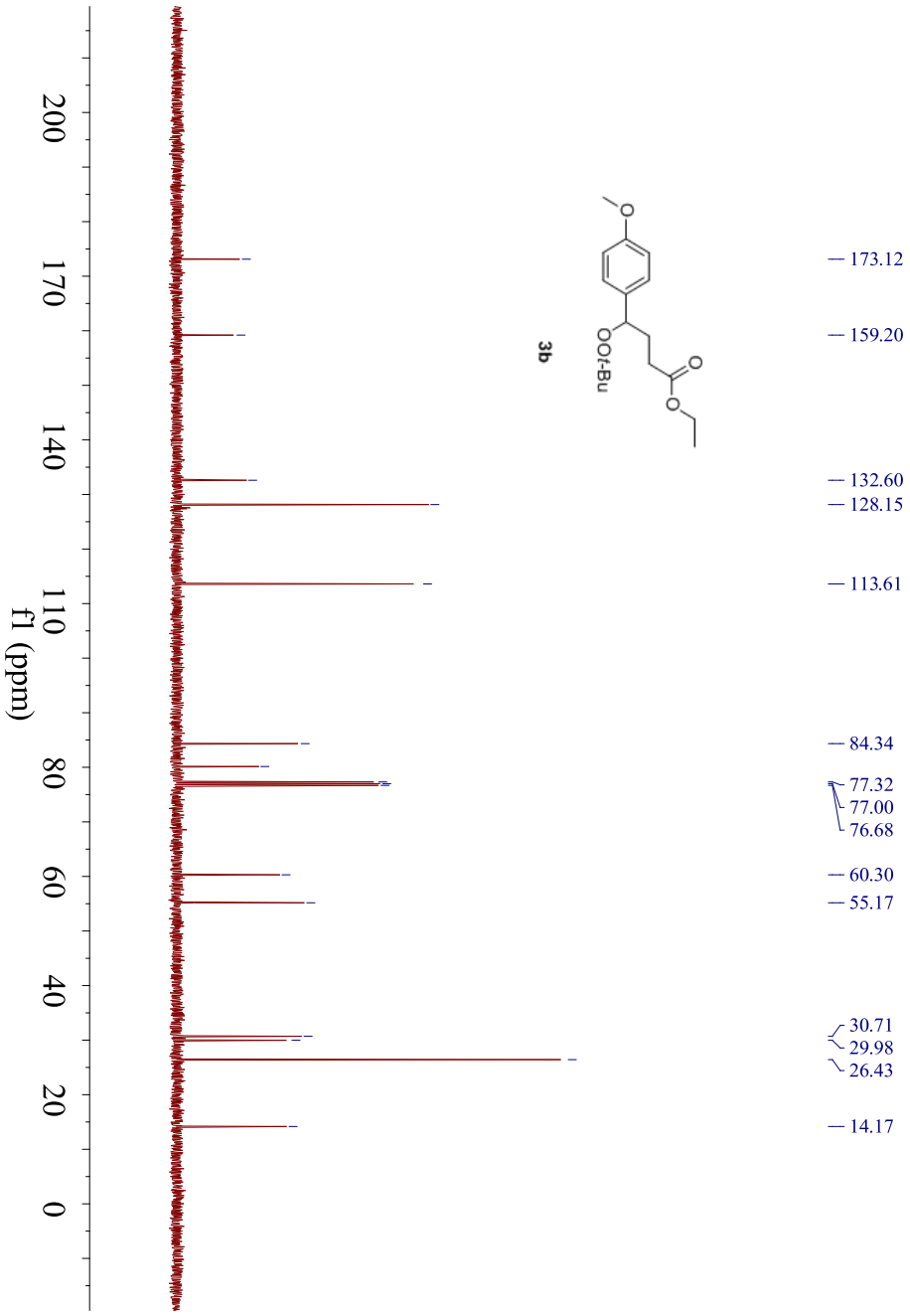
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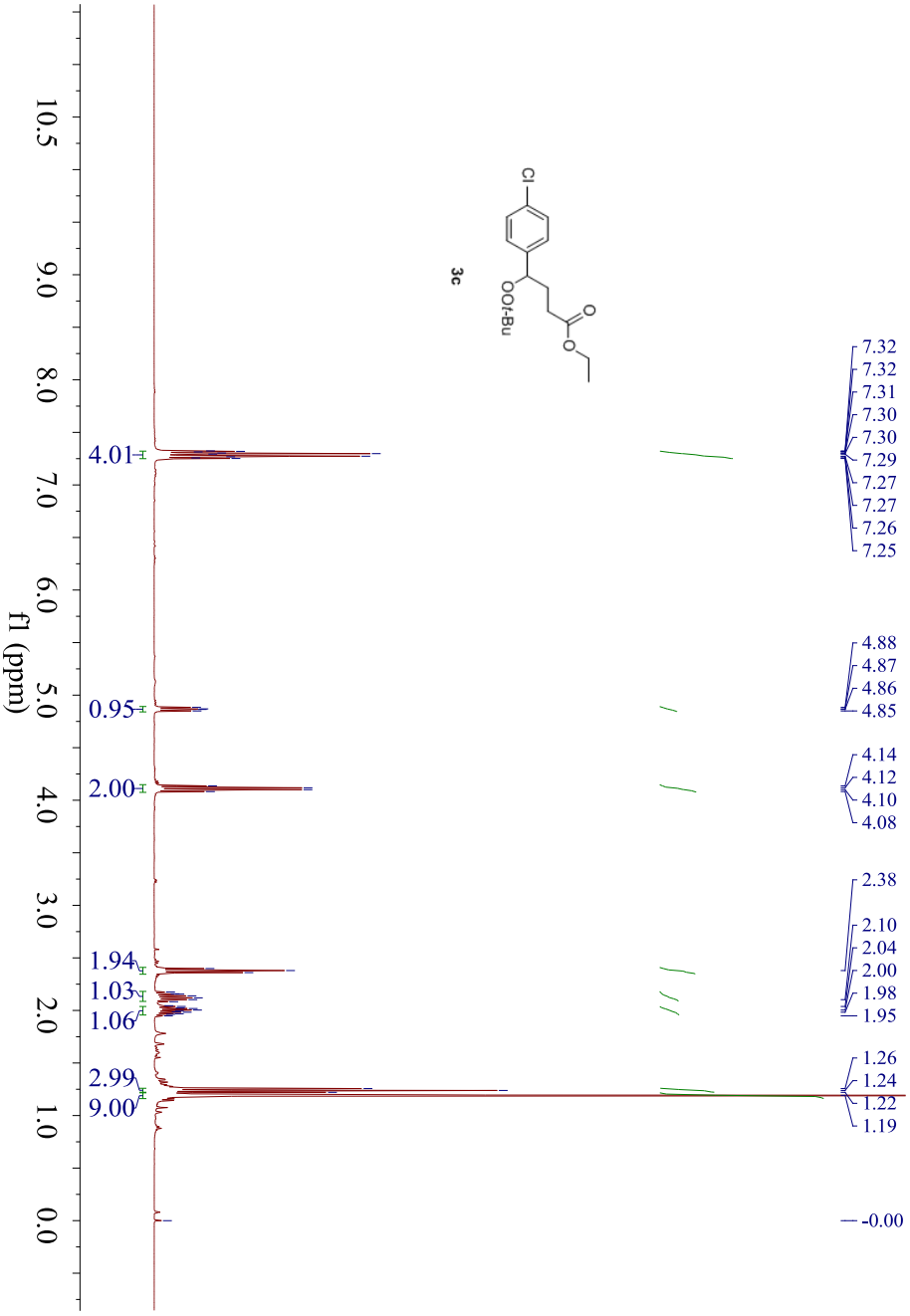
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O
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1.06
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9.00
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7.30
7.30
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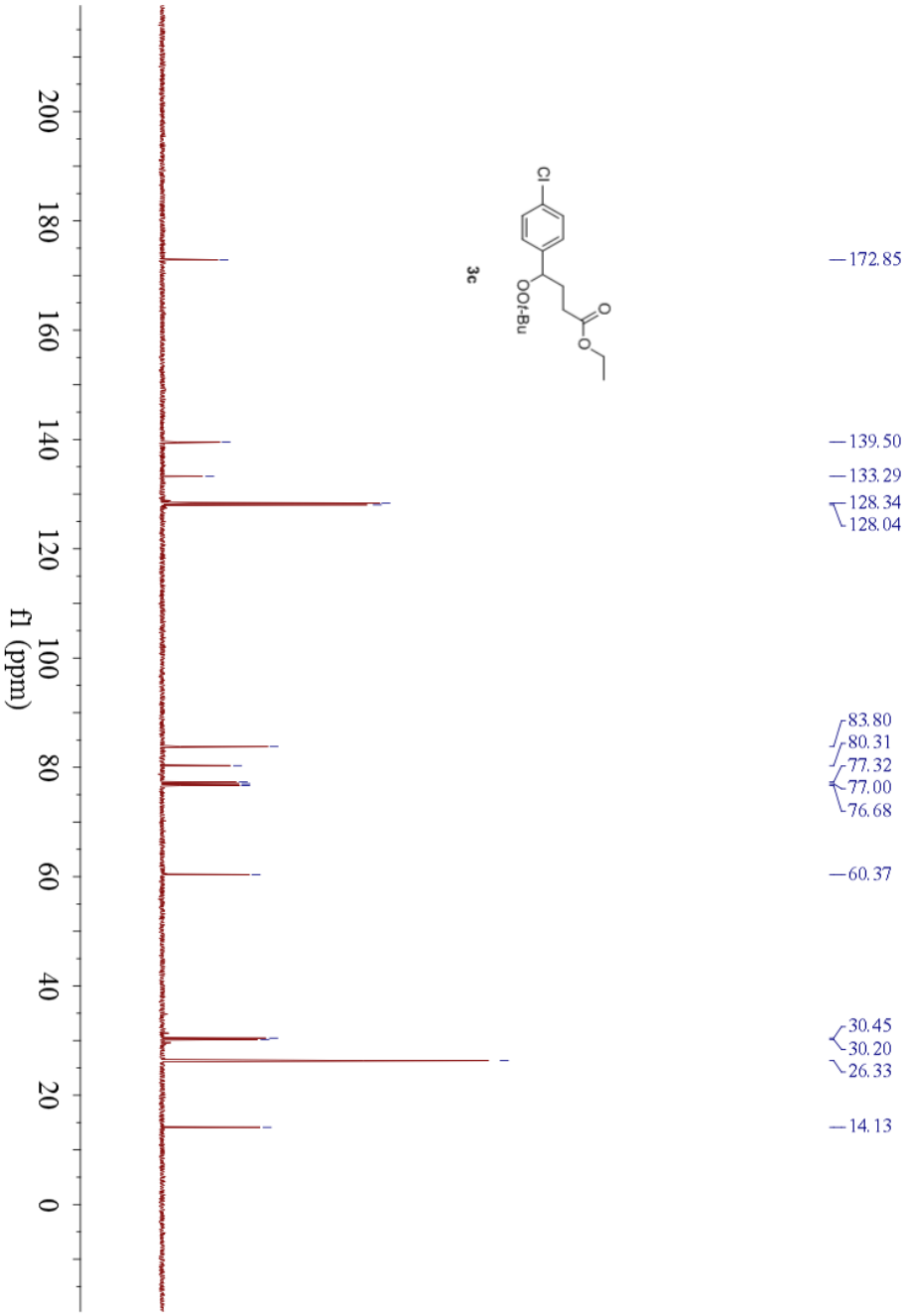
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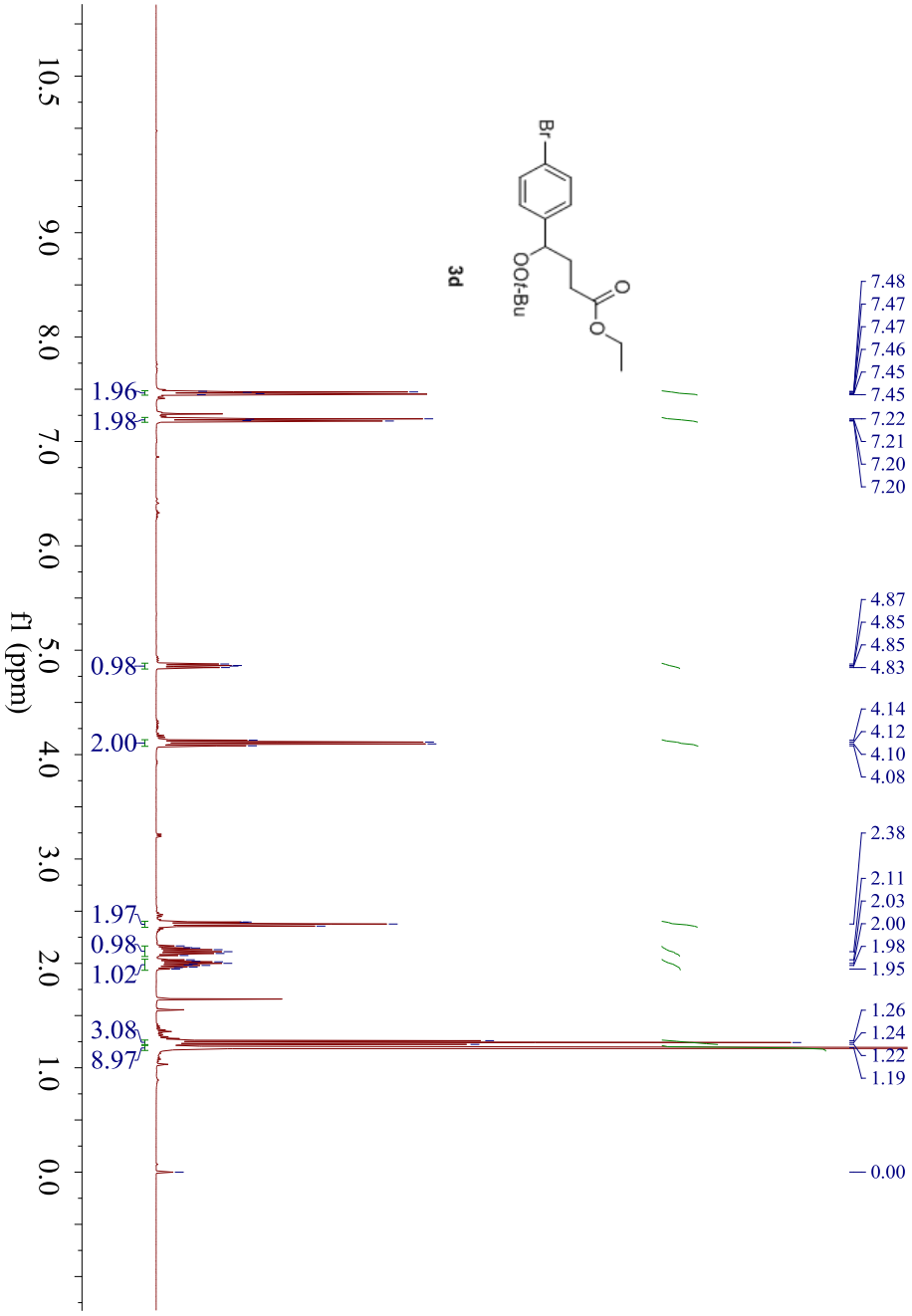
f1 (ppm)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1.98
0.98
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1.02
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7.22
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4.85
4.83
4.14
4.12
4.10
4.08
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2.11
2.03
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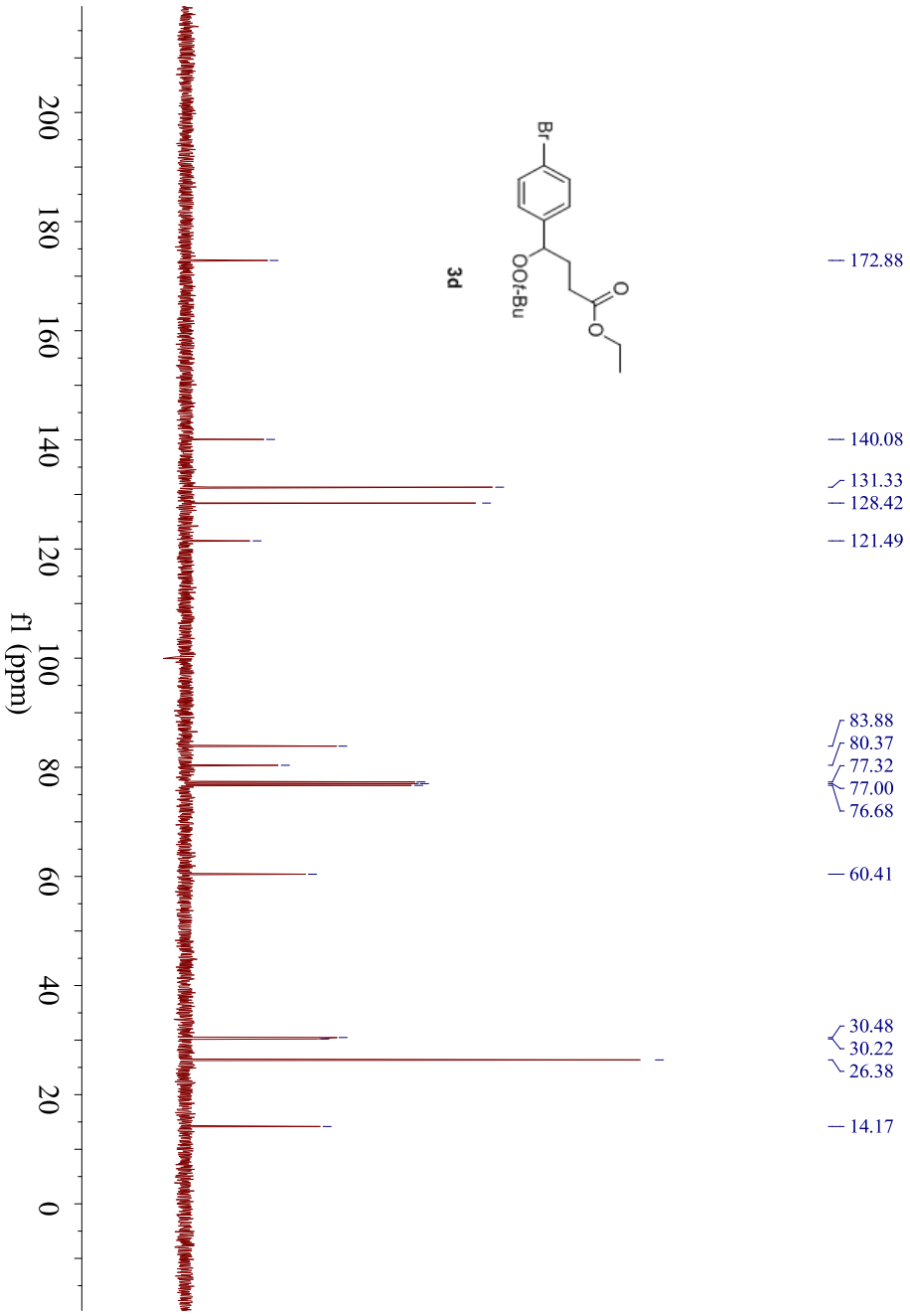
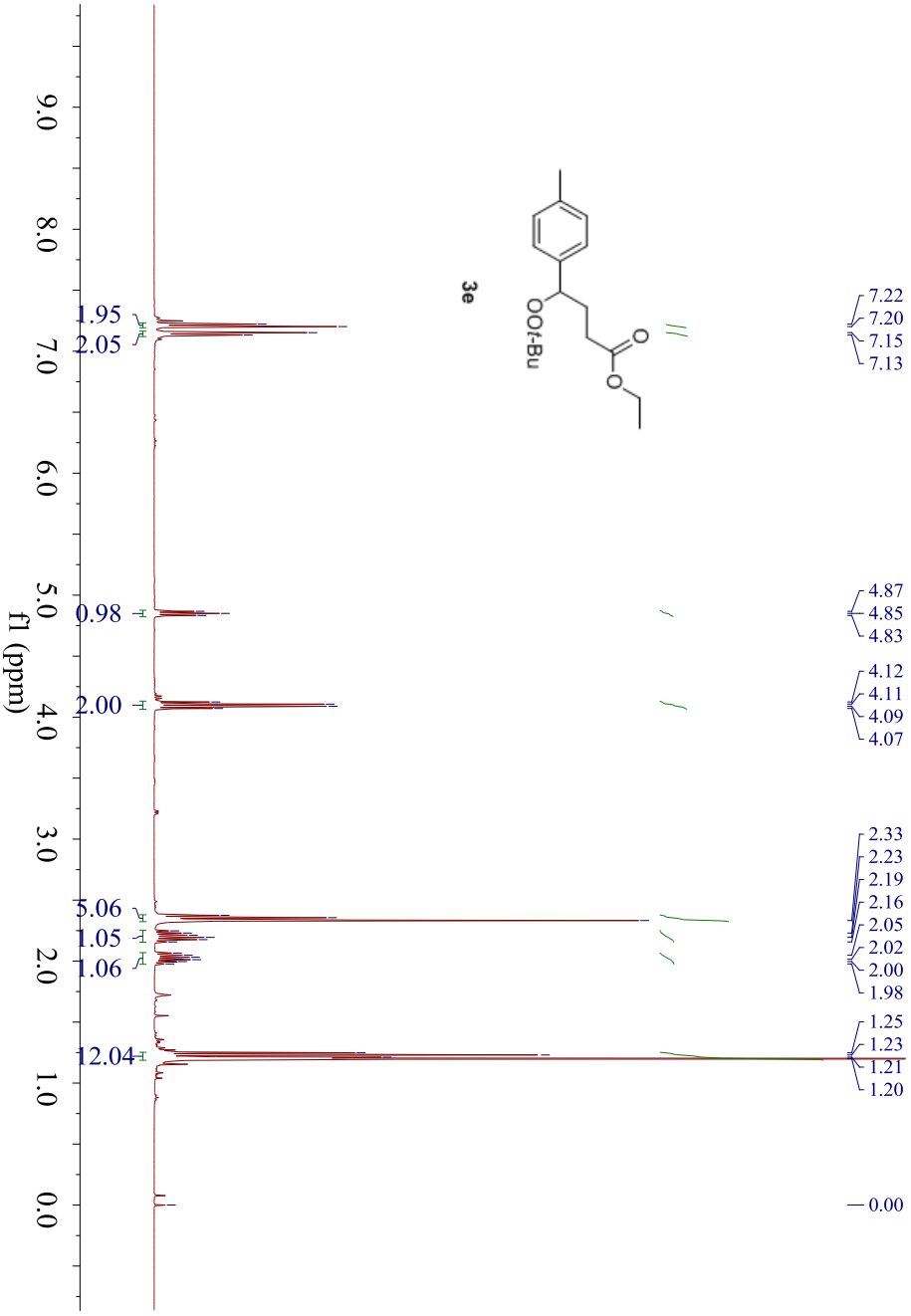
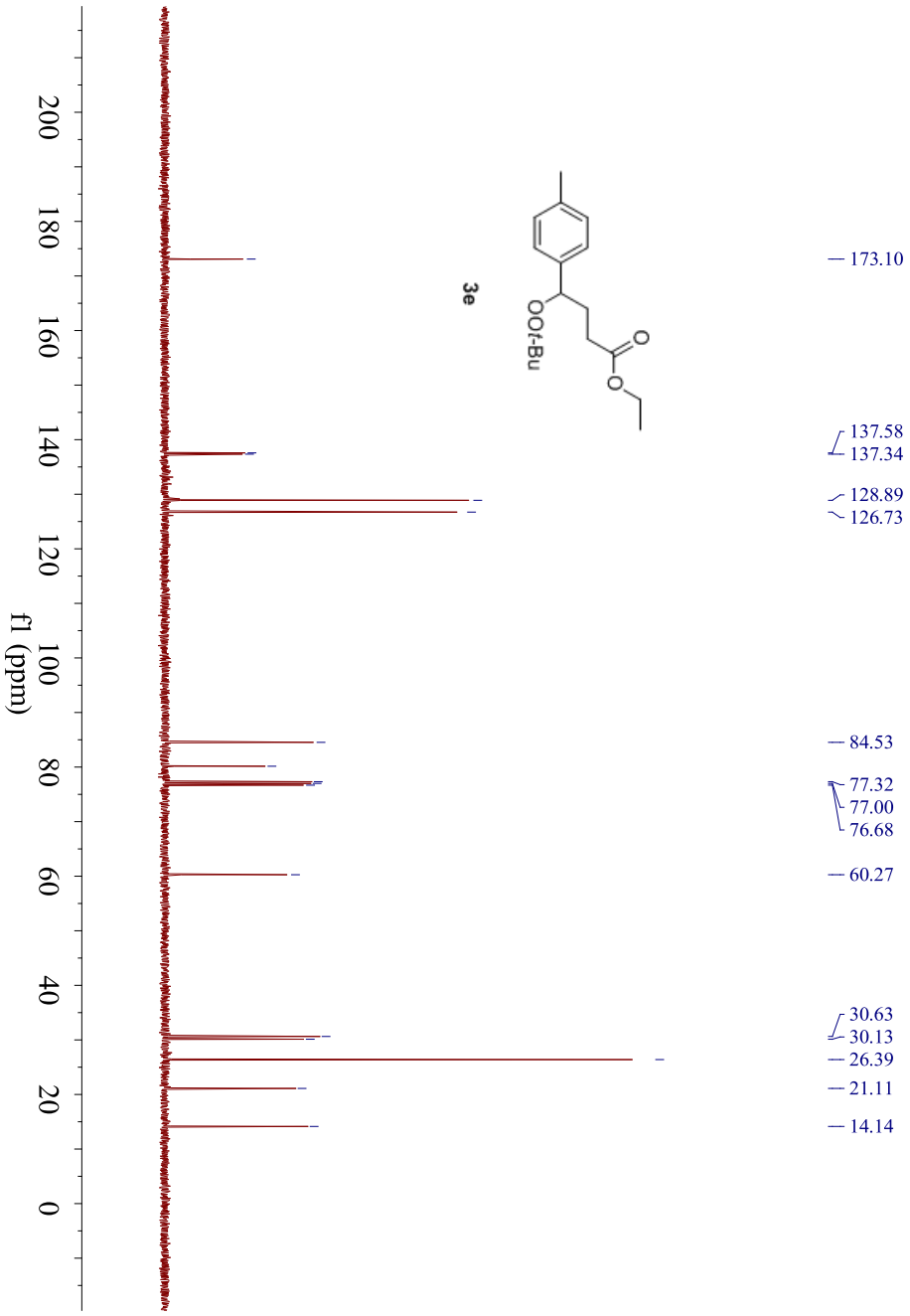
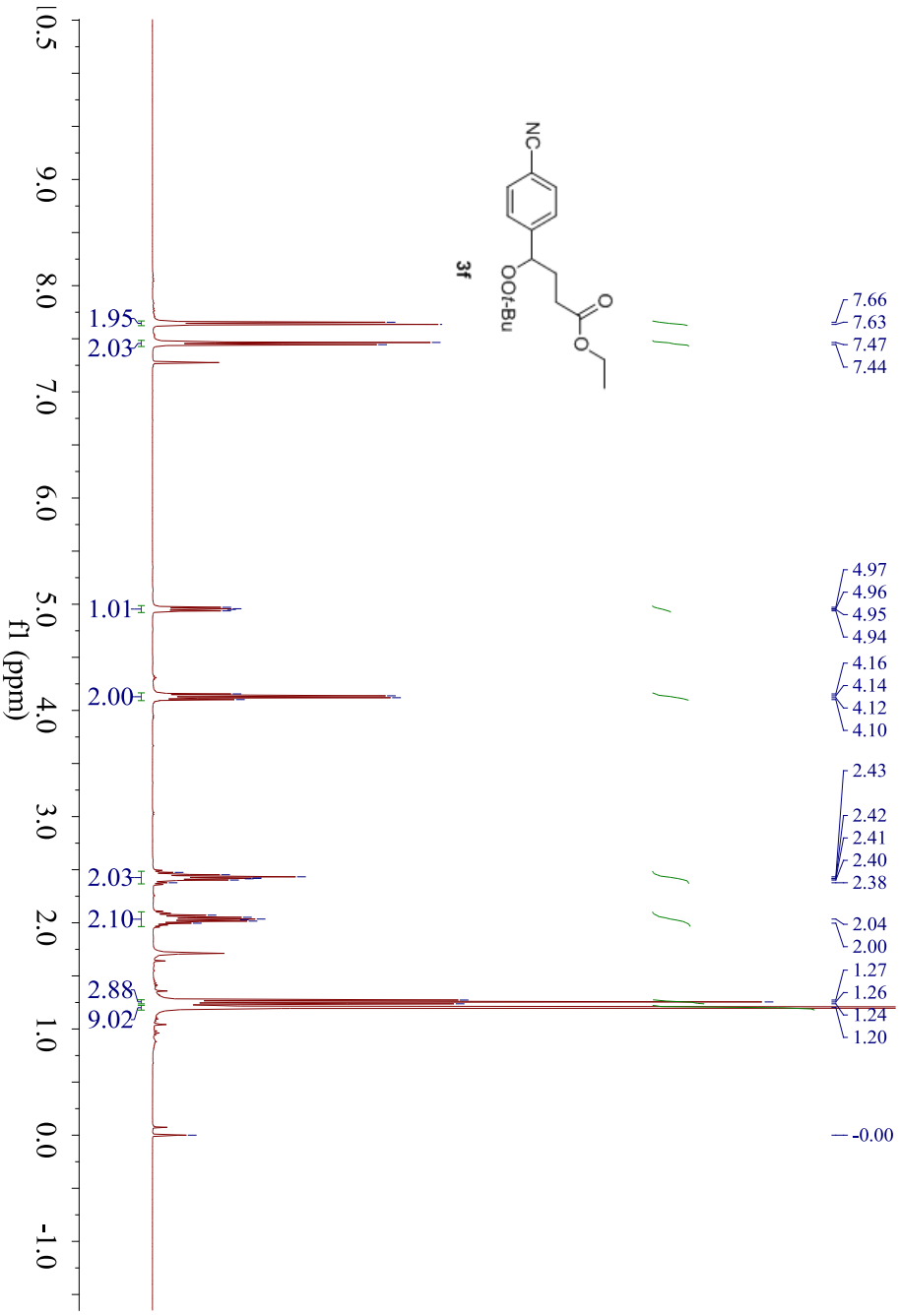
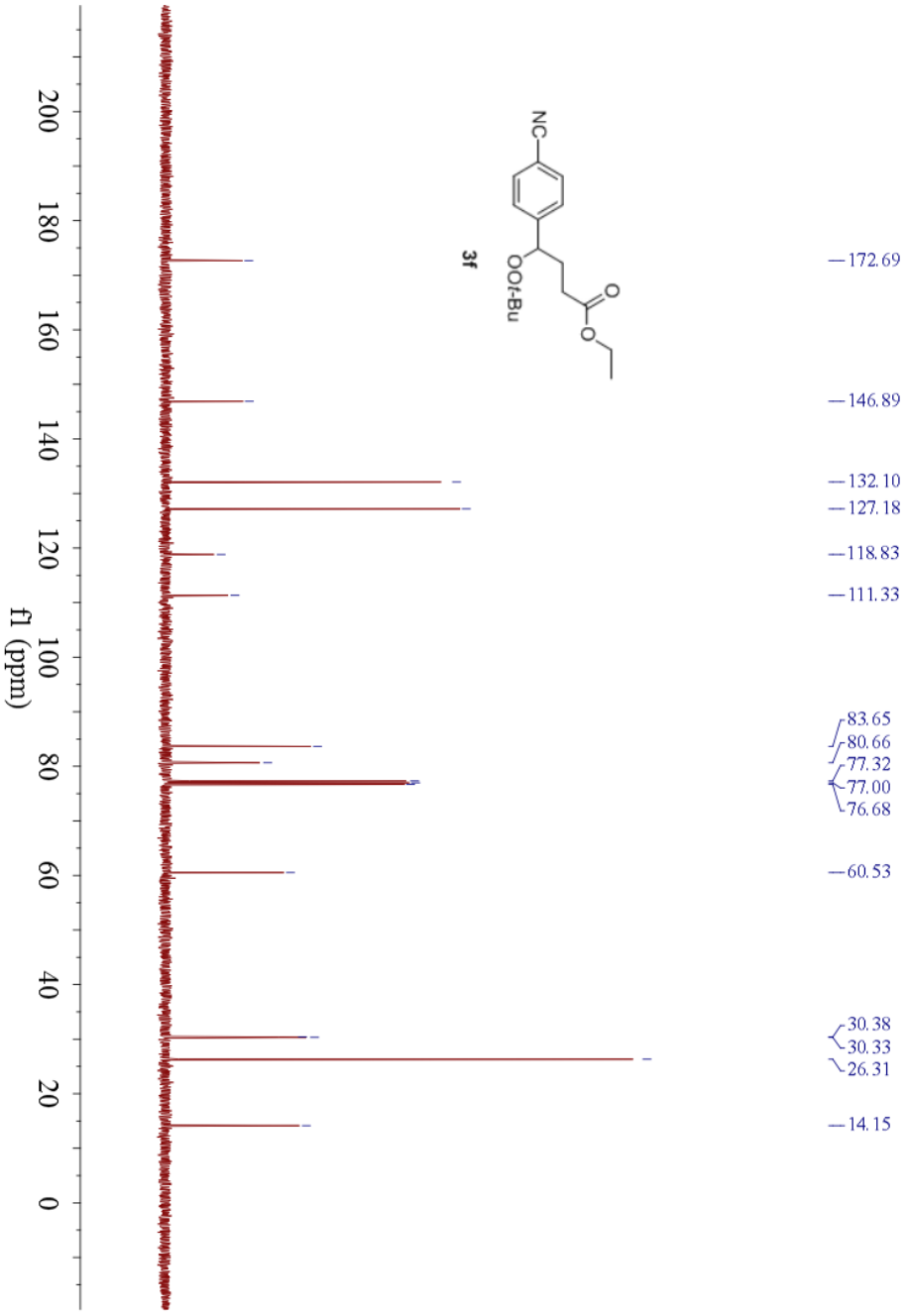
1.26
1.24
1.22
1.19
0.00

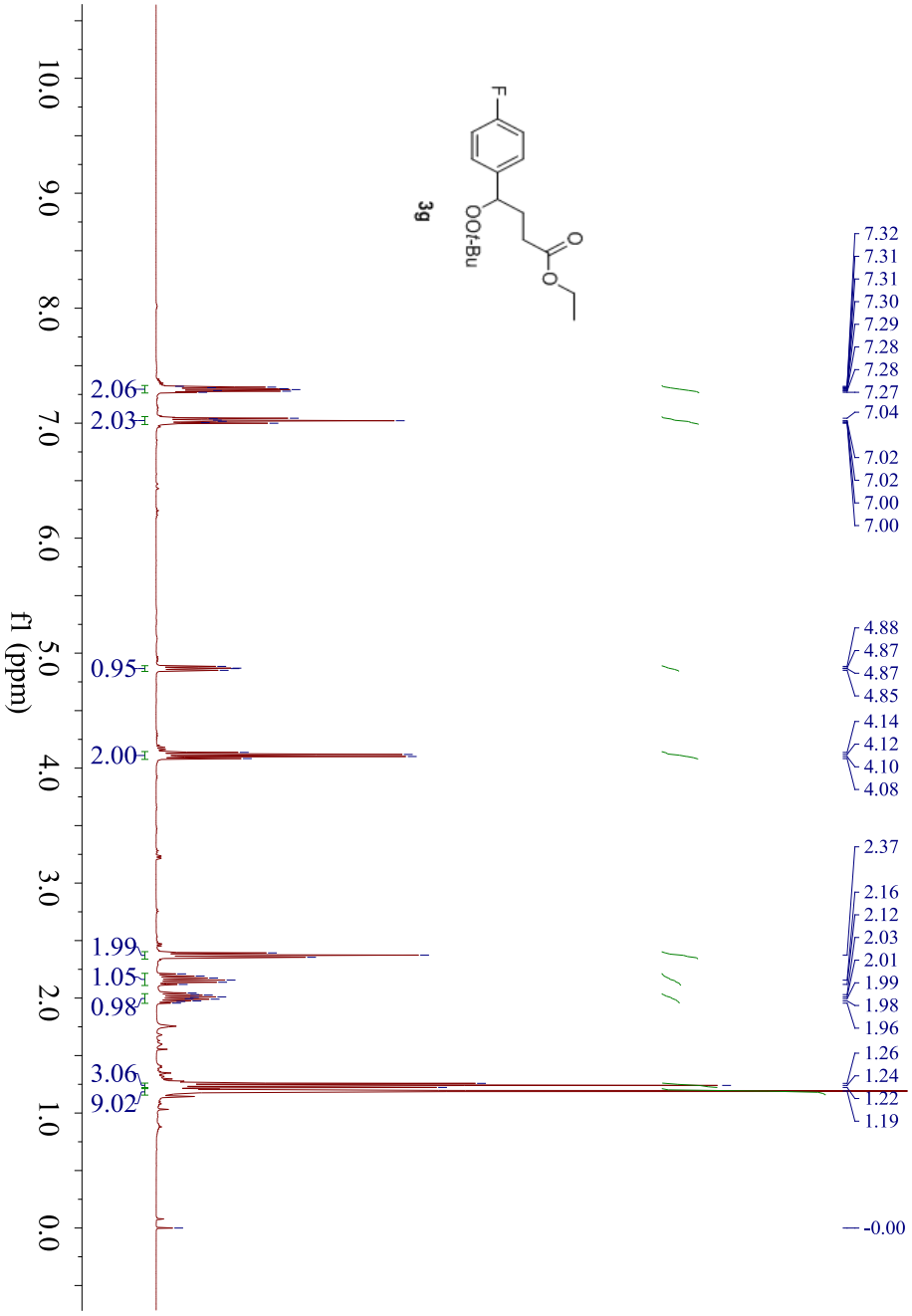

Br
OOt-Bu
O
O
3d
172.88
140.08
131.33
128.42
121.49
83.88
80.37
77.32
77.00
76.68
60.41
30.48
30.22
26.38
14.17
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

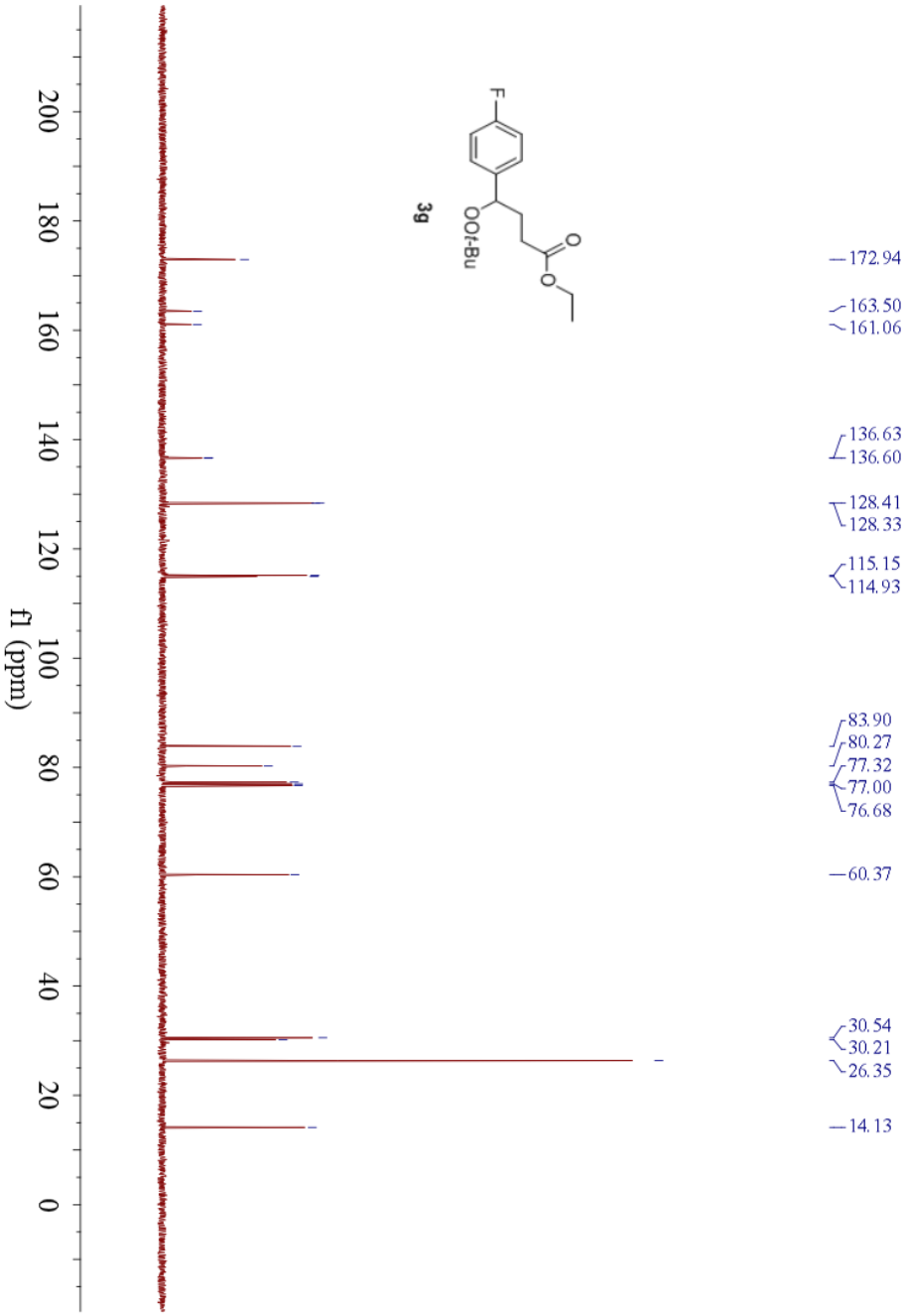

3e
OOt-Bu
O
O
f1 (ppm)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.95
2.05
0.98
2.00
5.06
1.05
1.06
12.04
7.22
7.20
7.15
7.13
4.87
4.85
4.83
4.12
4.11
4.09
4.07
2.33
2.23
2.19
2.16
2.05
2.02
2.00
1.98
1.25
1.23
1.21
1.20
0.00

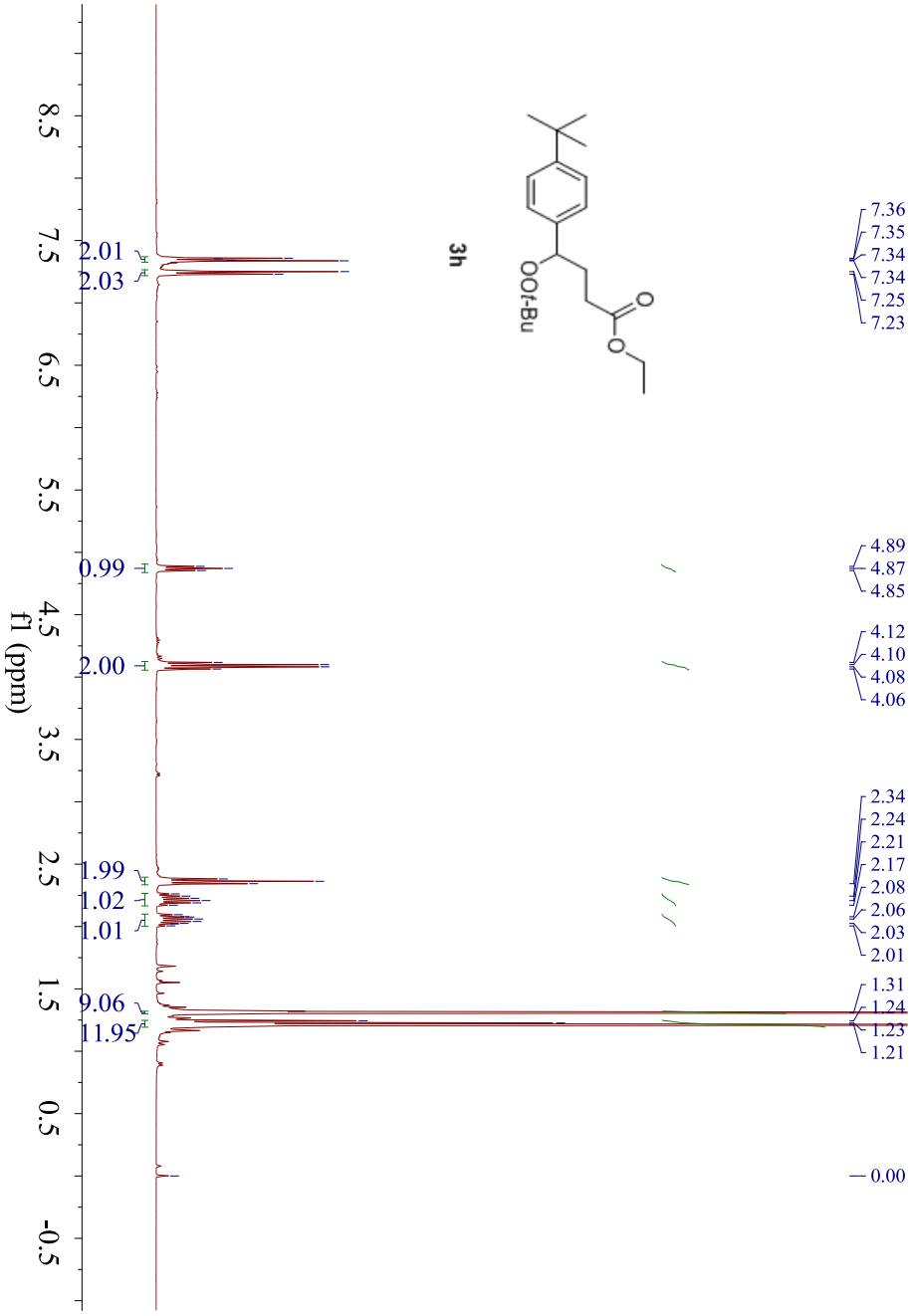

3e
OOt-Bu
O
O
173.10
137.58
137.34
128.89
126.73
84.53
77.32
77.00
76.68
60.27
30.63
30.13
26.39
21.11
14.14
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

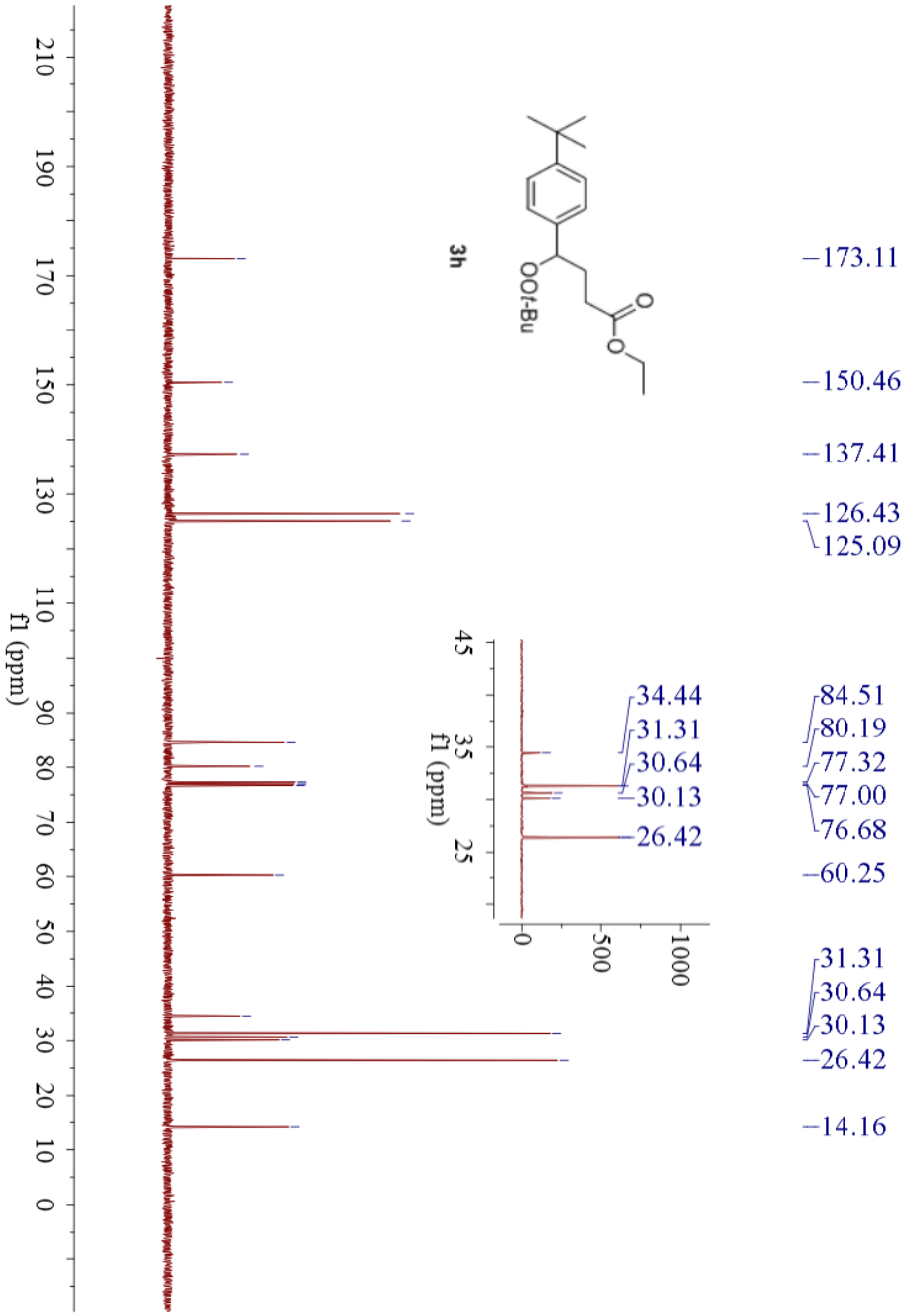

NC
OOt-Bu
O
O
3f
f1 (ppm)
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
1.95
2.03
1.01
2.00
2.03
2.10
2.88
9.02
7.66
7.63
7.47
7.44
4.97
4.96
4.95
4.94
4.16
4.14
4.12
4.10
2.43
2.42
2.41
2.40
2.38
2.04
2.00
1.27
1.26
1.24
1.20
-0.00

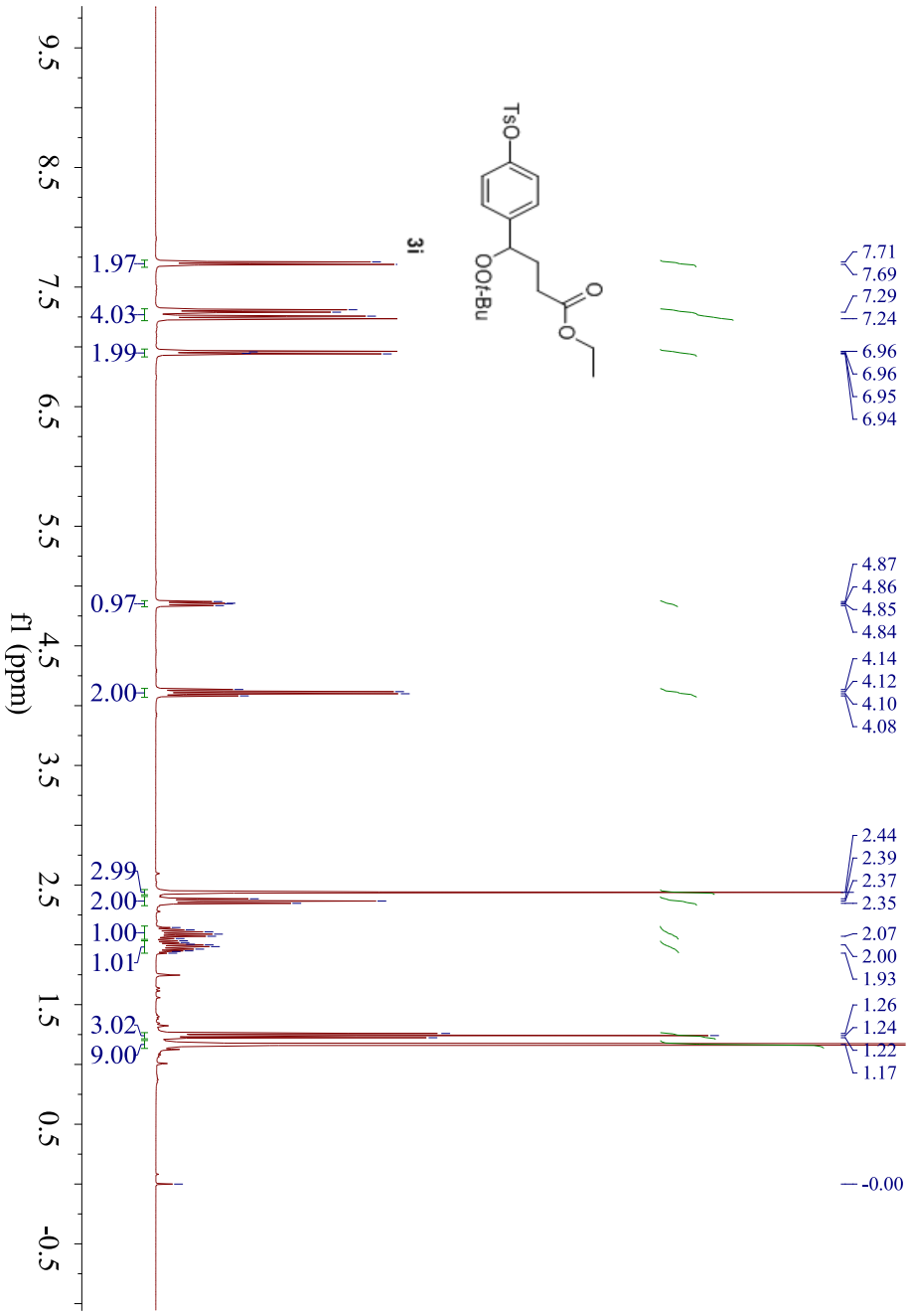

NC
OOt-Bu
O
O
3f
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0
172.69
146.89
132.10
127.18
118.83
111.33
83.65
80.66
77.32
77.00
76.68
60.53
30.38
30.33
26.31
14.15

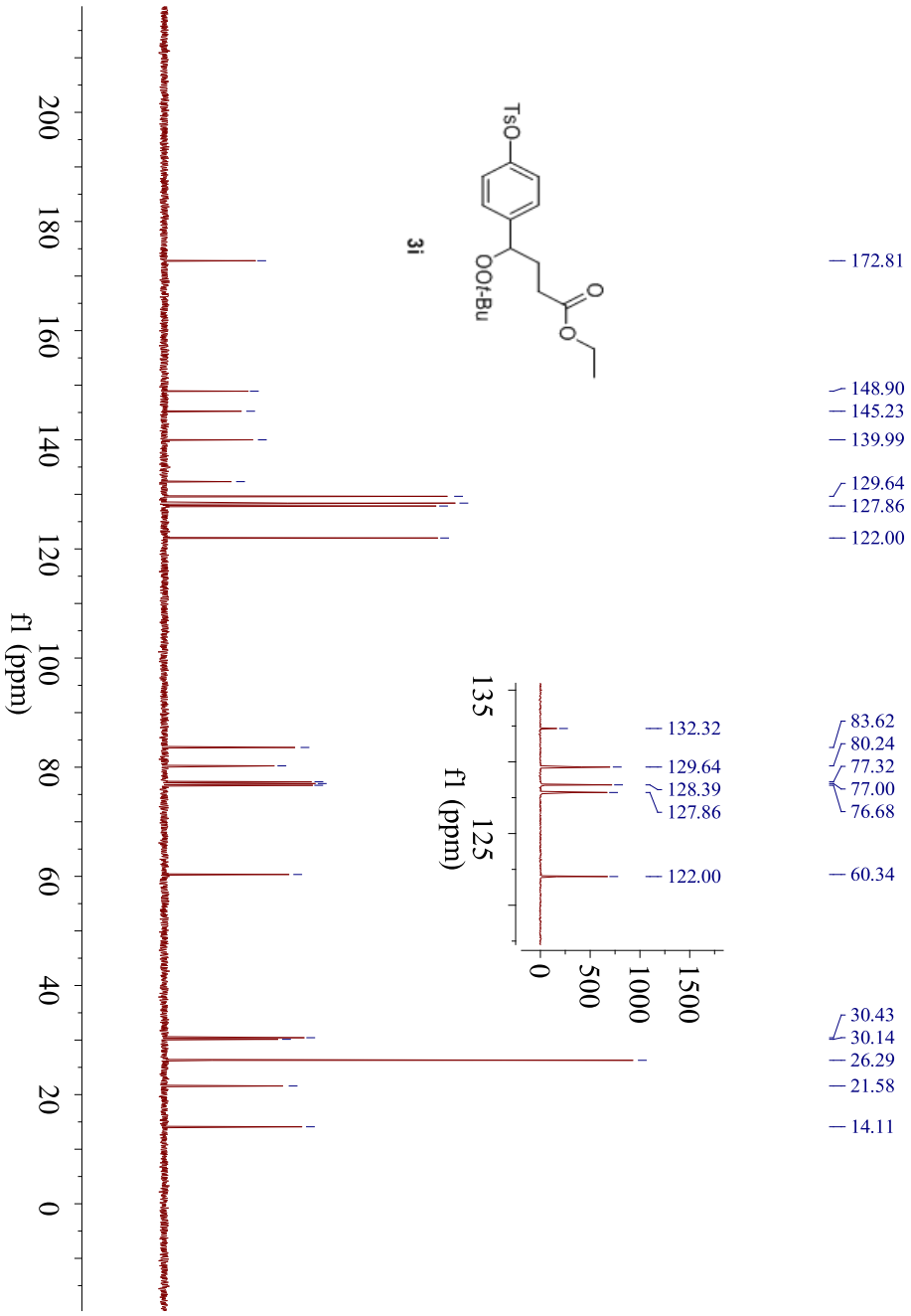

3g
F
OOt-Bu
O
O
f1 (ppm)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
2.06
2.03
0.95
2.00
1.99
1.05
0.98
3.06
9.02
7.32
7.31
7.31
7.30
7.29
7.28
7.28
7.27
7.04
7.02
7.02
7.00
7.00
4.88
4.87
4.87
4.85
4.14
4.12
4.10
4.08
2.37
2.16
2.12
2.03
2.01
1.99
1.98
1.96
1.26
1.24
1.22
1.19
-0.00

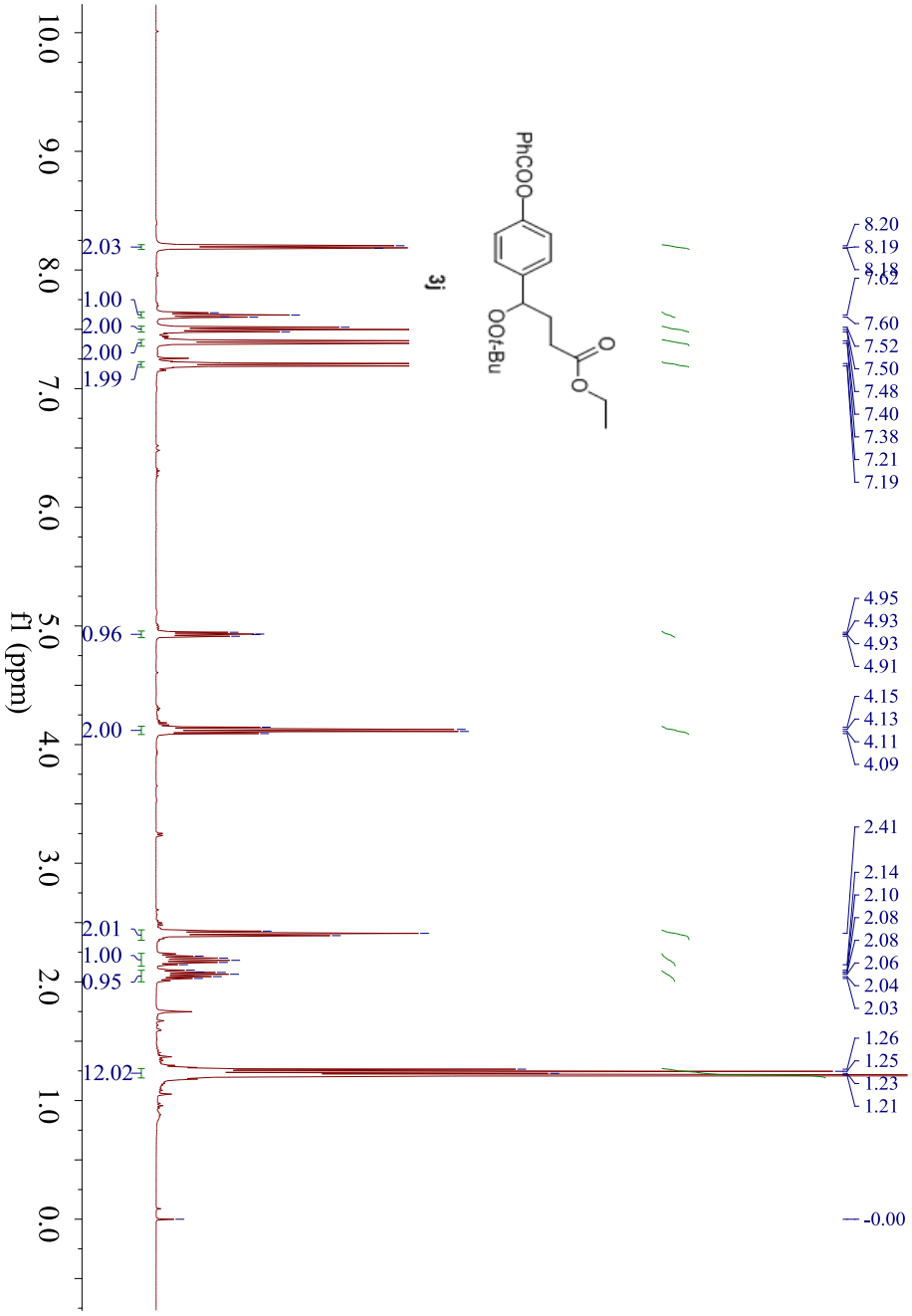

F
OOt-Bu
O
O
3g
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)
172.94
163.50
161.06
136.63
136.60
128.41
128.33
115.15
114.93
83.90
80.27
77.32
77.00
76.68
60.37
30.54
30.21
26.35
14.13

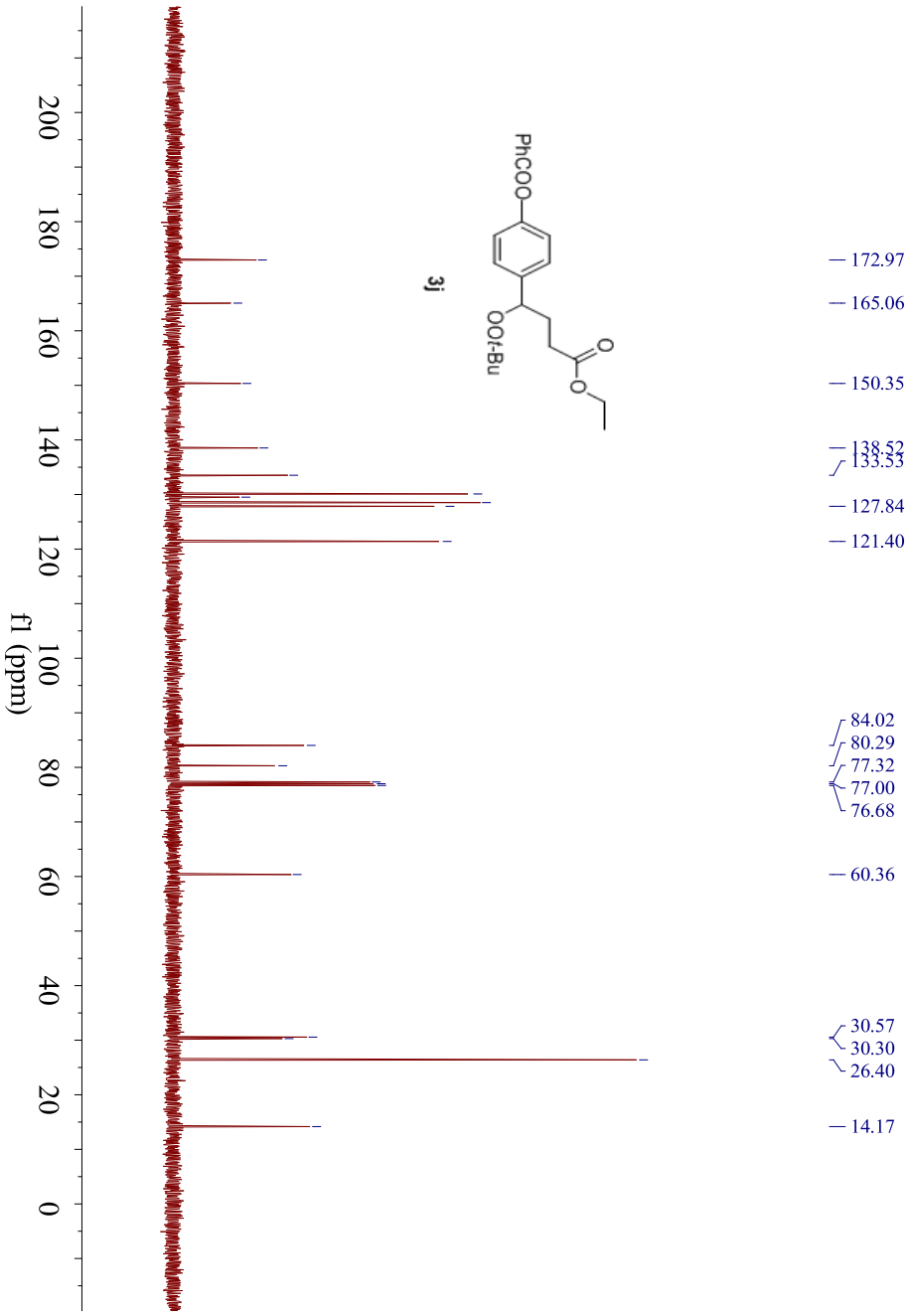

3h
OOt-Bu
O
O
f1 (ppm)
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
2.01
2.03
0.99
2.00
1.99
1.02
1.01
9.06
11.95
7.36
7.35
7.34
7.34
7.25
7.23
4.89
4.87
4.85
4.12
4.10
4.08
4.06
2.34
2.24
2.21
2.17
2.08
2.06
2.03
2.01
1.31
1.24
1.23
1.21
0.00

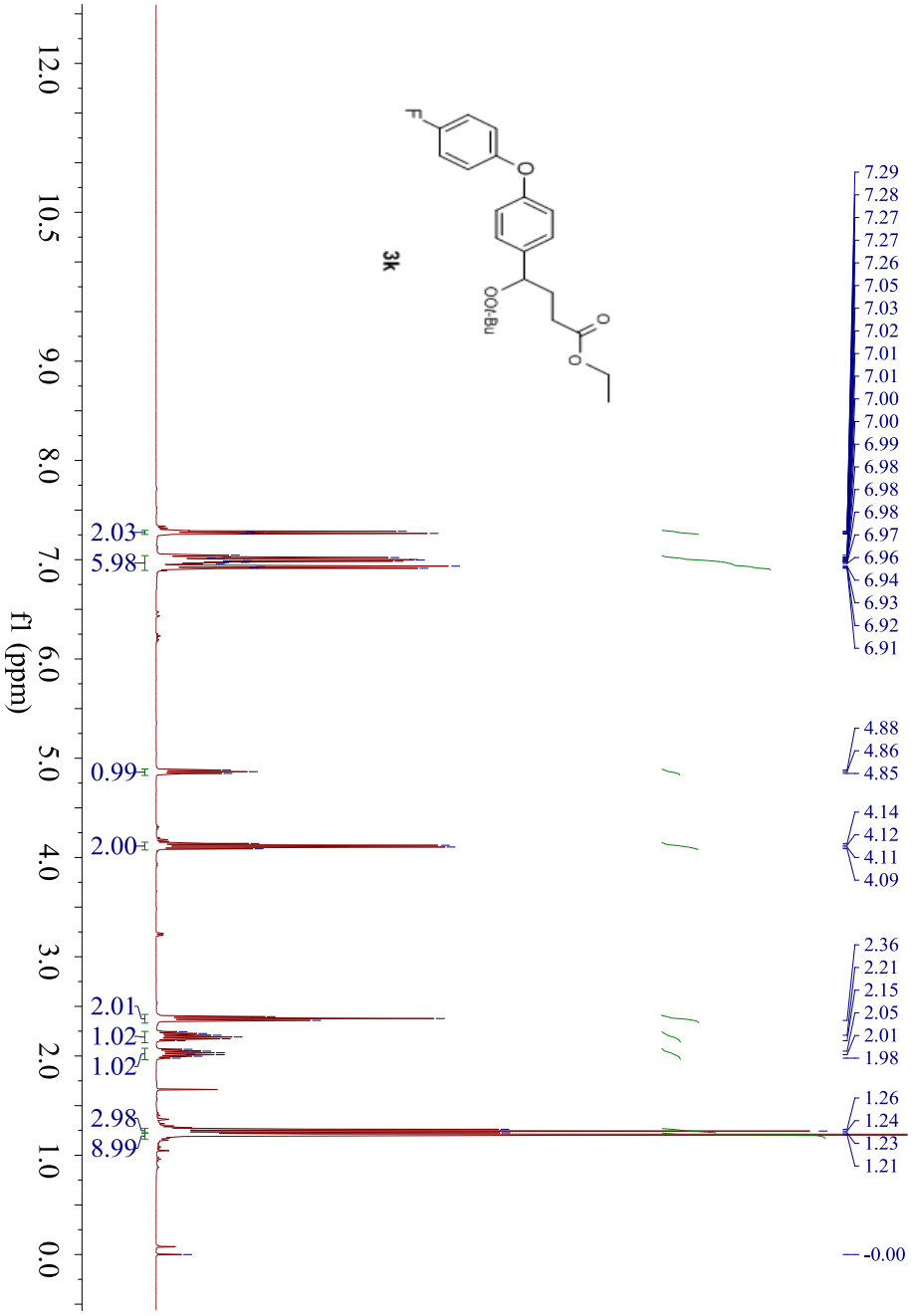

3h
OOt-Bu
O
O
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
45
35
25
f1 (ppm)
0
500
1000
173.11
150.46
137.41
126.43
125.09
84.51
80.19
77.32
77.00
76.68
60.25
34.44
31.31
30.64
30.13
26.42
31.31
30.64
30.13
26.42
14.16

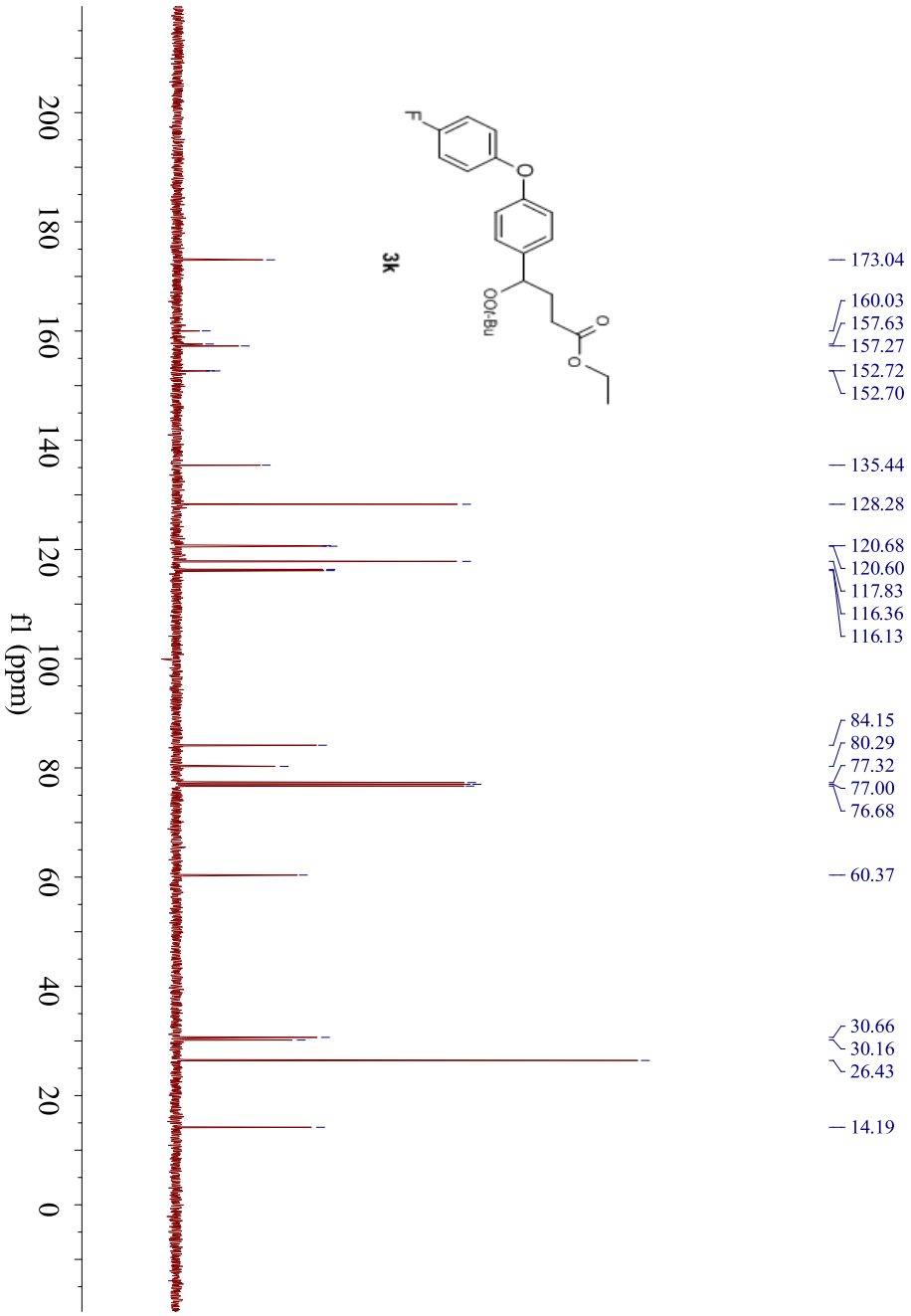

3i
TsO
OOt-Bu
O
O
f1 (ppm)
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
1.97
4.03
1.99
0.97
2.00
2.99
2.00
1.00
1.01
3.02
9.00
7.71
7.69
7.29
7.24
6.96
6.96
6.95
6.94
4.87
4.86
4.85
4.84
4.14
4.12
4.10
4.08
2.44
2.39
2.37
2.35
2.07
2.00
1.93
1.26
1.24
1.22
1.17
-0.00

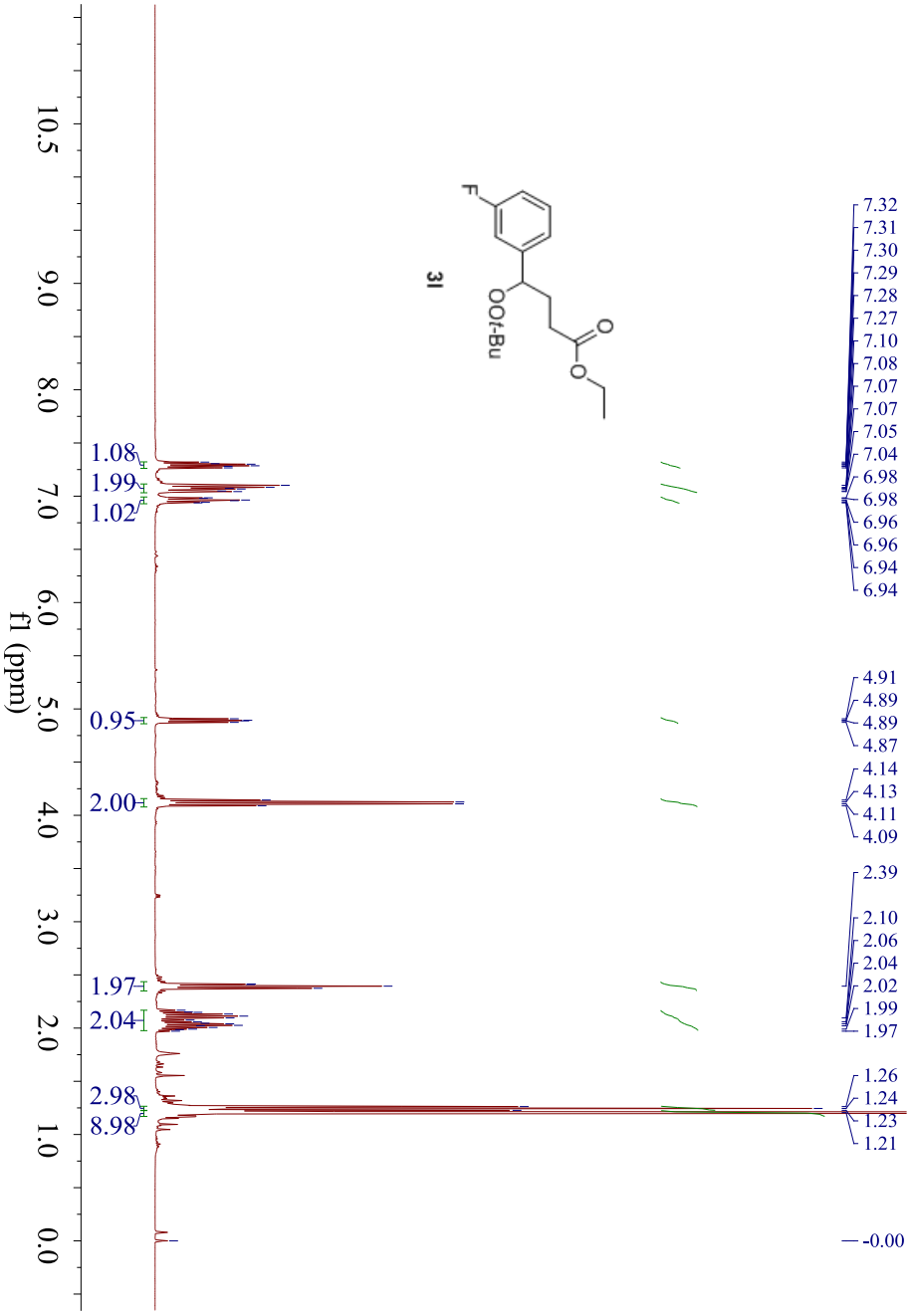

3i
TsO
OOt-Bu
O
O
172.81
148.90
145.23
139.99
129.64
127.86
122.00
83.62
80.24
77.32
77.00
76.68
60.34
30.43
30.14
26.29
21.58
14.11
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0
132.32
129.64
128.39
127.86
122.00
135
125
f1 (ppm)
0
500
1000
1500

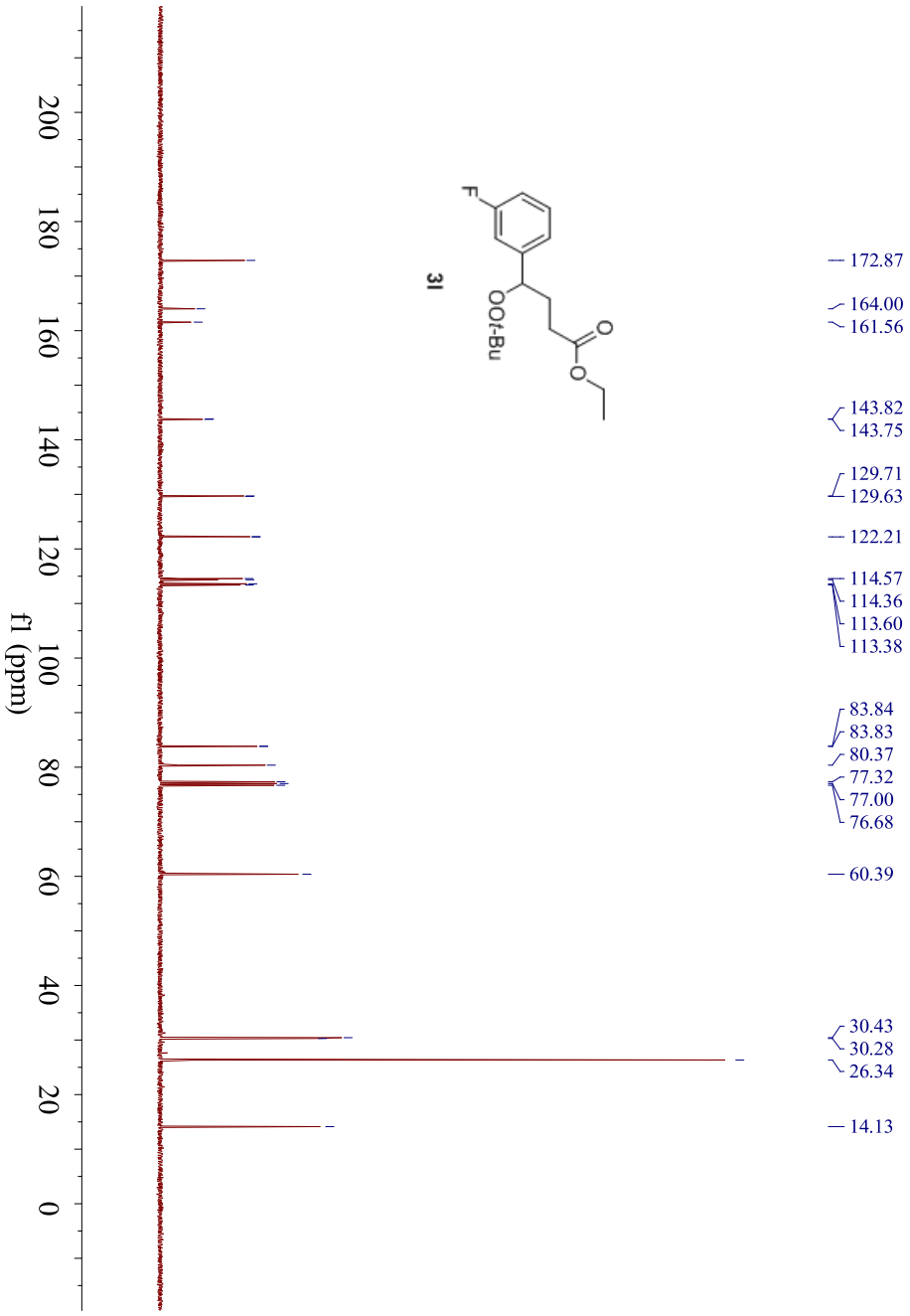

3j
PhCOO
OOt-Bu
f1 (ppm)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
2.03
1.00
2.00
2.00
1.99
0.96
2.00
2.01
1.00
0.95
12.02
8.20
8.19
8.18
7.62
7.60
7.52
7.50
7.48
7.40
7.38
7.21
7.19
4.95
4.93
4.93
4.91
4.15
4.13
4.11
4.09
2.41
2.14
2.10
2.08
2.08
2.06
2.04
2.03
1.26
1.25
1.23
1.21
-0.00

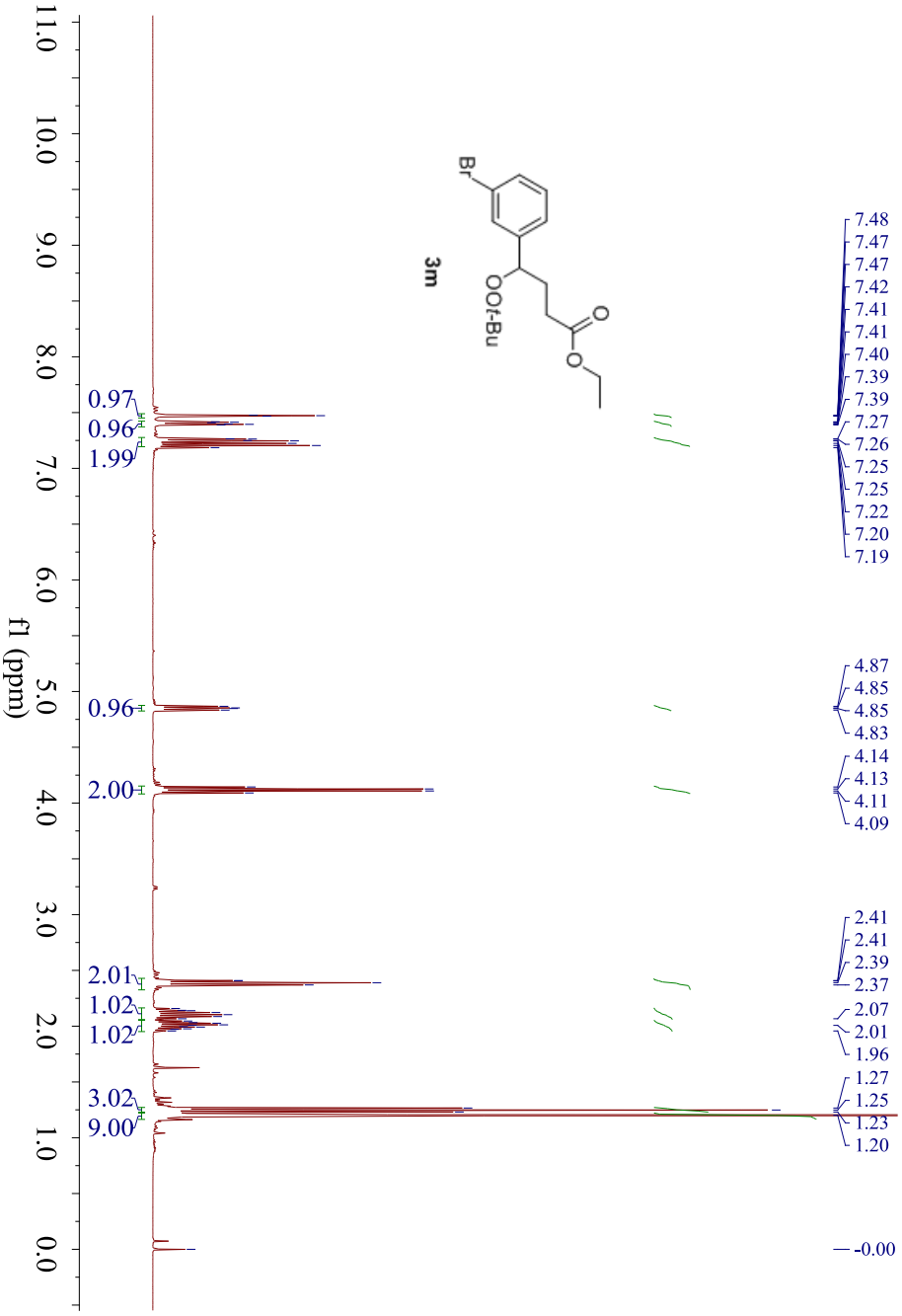

PhCOO
OOt-Bu
O
O
3j
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0
172.97
165.06
150.35
138.52
133.53
127.84
121.40
84.02
80.29
77.32
77.00
76.68
60.36
30.57
30.30
26.40
14.17

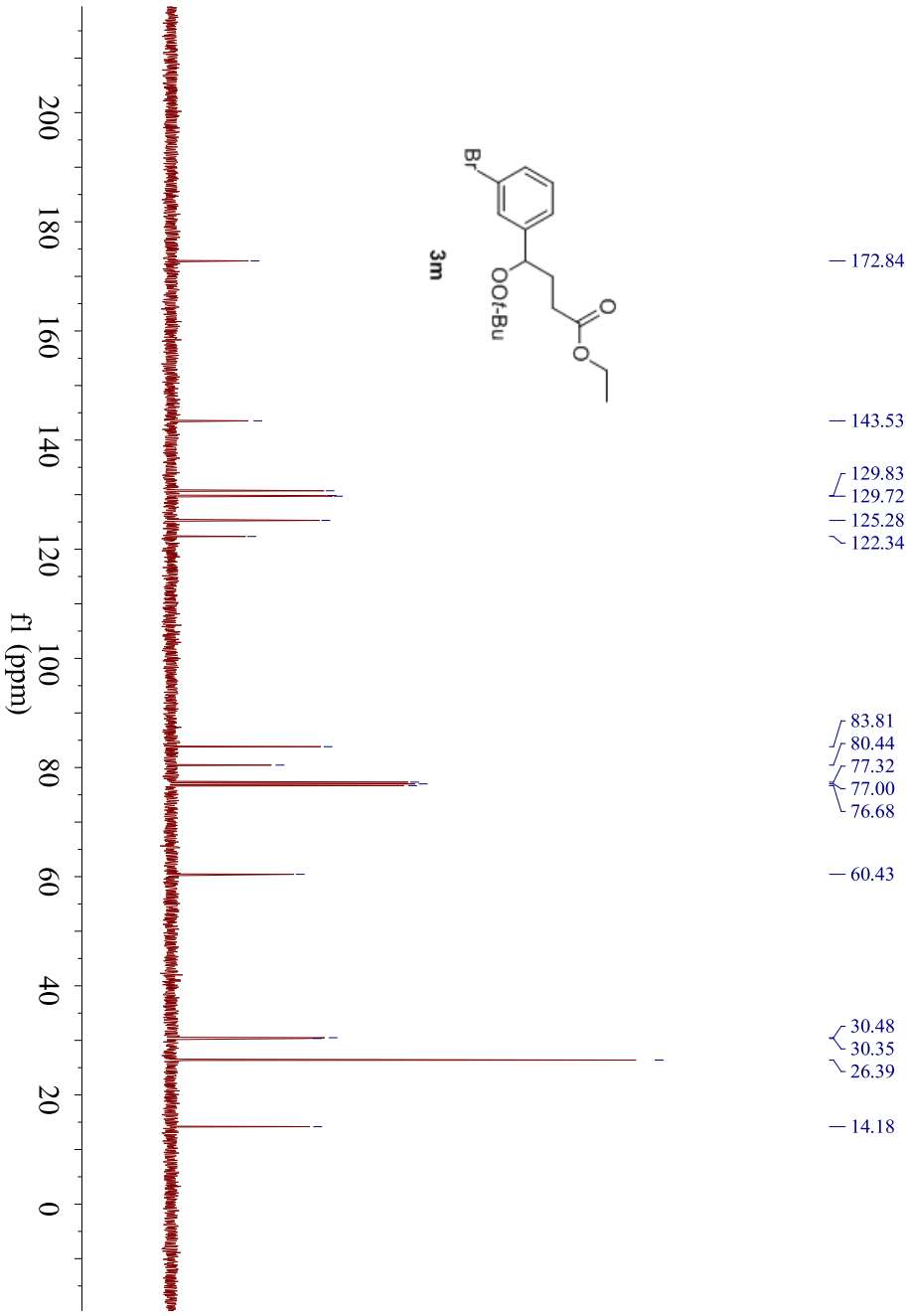

3k
F
O
OO-t-Bu
O
O
f1 (ppm)
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
2.03
5.98
0.99
2.00
2.01
1.02
1.02
2.98
8.99
7.29
7.28
7.27
7.27
7.26
7.05
7.03
7.02
7.01
7.01
7.00
7.00
6.99
6.98
6.98
6.98
6.97
6.96
6.94
6.93
6.92
6.91
4.88
4.86
4.85
4.14
4.12
4.11
4.09
2.36
2.21
2.15
2.05
2.01
1.98
1.26
1.24
1.23
1.21
-0.00

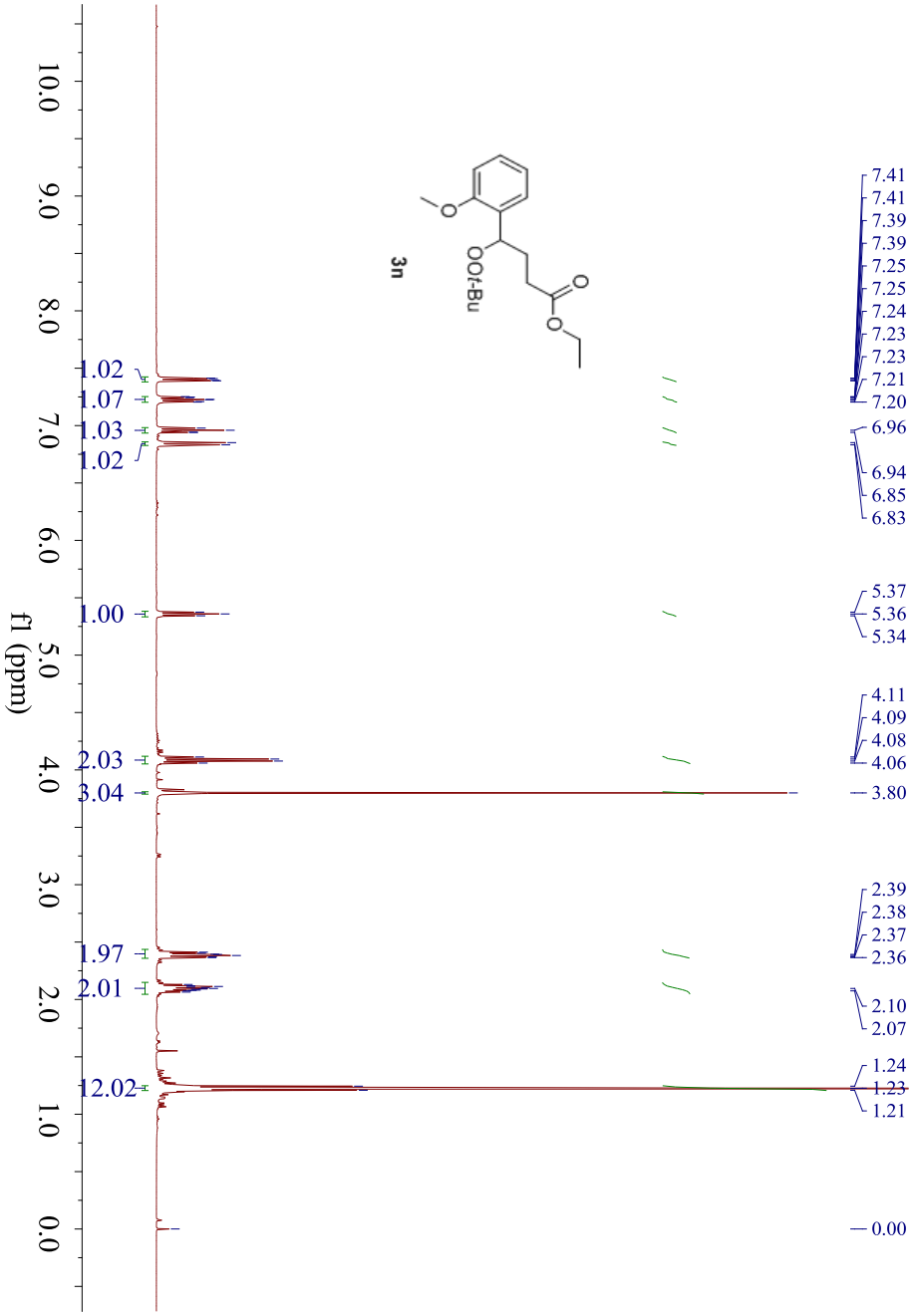

3k
F
O
OO-t-Bu
O
O
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0
173.04
160.03
157.63
157.27
152.72
152.70
135.44
128.28
120.68
120.60
117.83
116.36
116.13
84.15
80.29
77.32
77.00
76.68
60.37
30.66
30.16
26.43
14.19

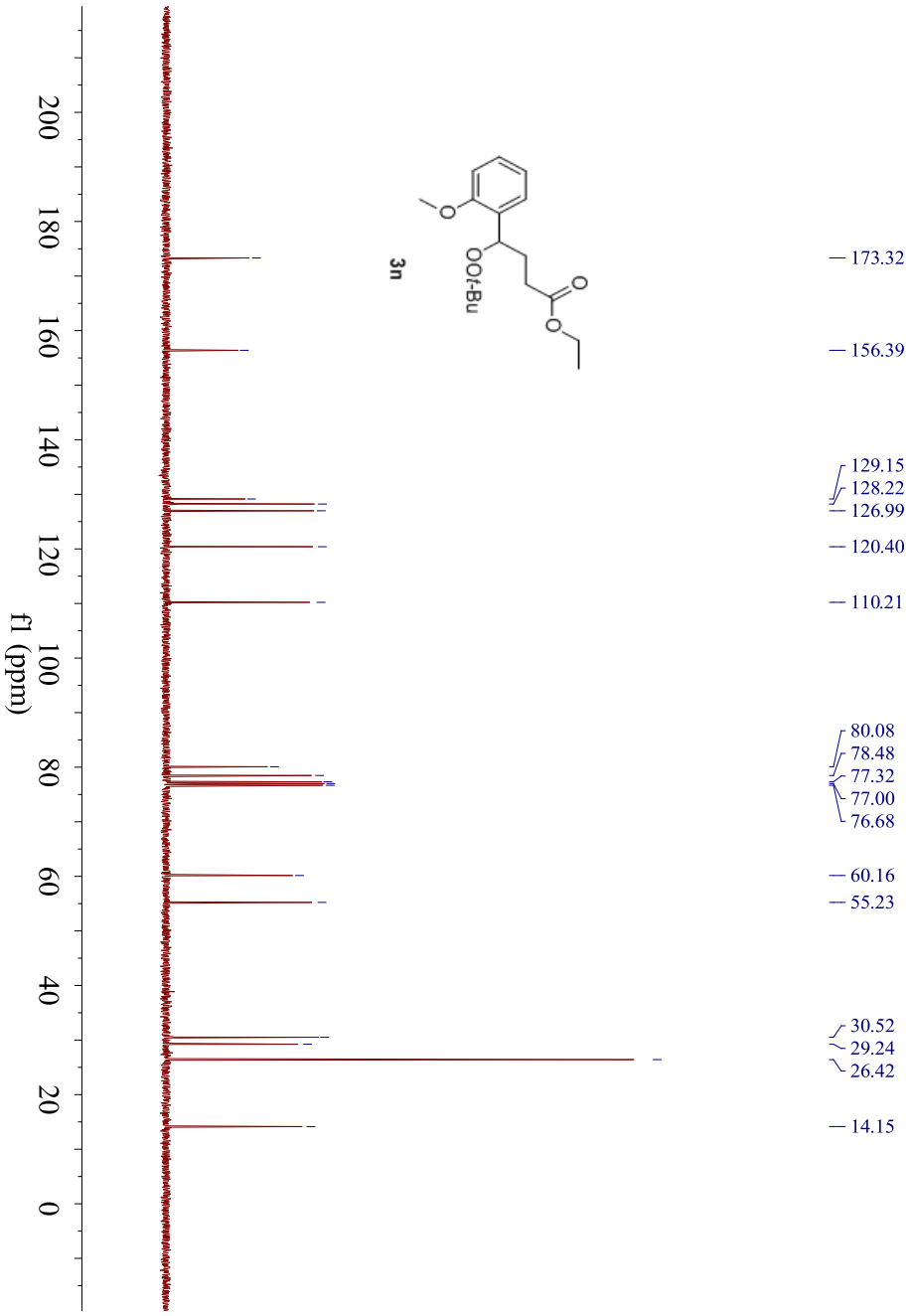

3l
F
OOt-Bu
O
O
f1 (ppm)
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.08
1.99
1.02
0.95
2.00
1.97
2.04
2.98
8.98
7.32
7.31
7.30
7.29
7.28
7.27
7.10
7.08
7.07
7.07
7.05
7.04
6.98
6.98
6.96
6.96
6.94
6.94
4.91
4.89
4.89
4.87
4.14
4.13
4.11
4.09
2.39
2.10
2.06
2.04
2.02
1.99
1.97
1.26
1.24
1.23
1.21
-0.00

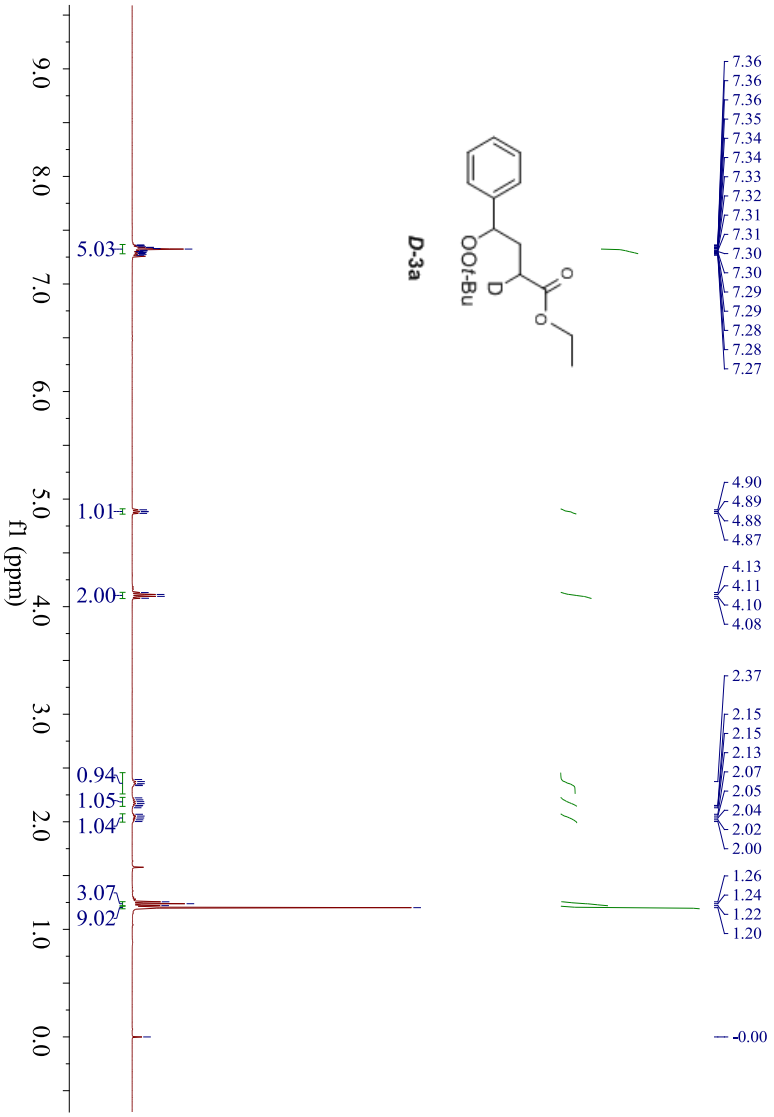

F
OOt-Bu
O
O
3l
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0
172.87
164.00
161.56
143.82
143.75
129.71
129.63
122.21
114.57
114.36
113.60
113.38
83.84
83.83
80.37
77.32
77.00
76.68
60.39
30.43
30.28
26.34
14.13

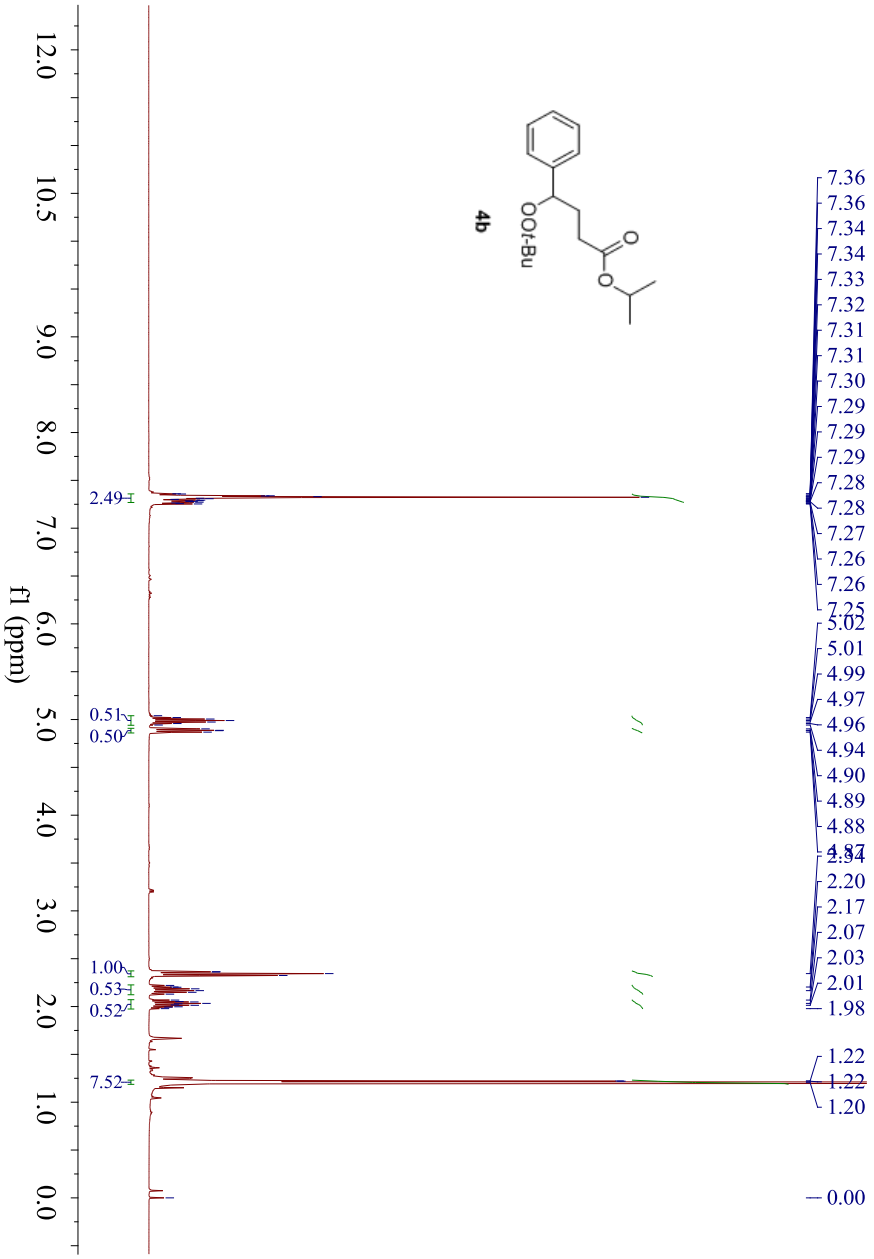

3m
Br
OOt-Bu
O
O
f1 (ppm)
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.97
0.96
1.99
0.96
2.00
2.01
1.02
1.02
3.02
9.00
7.48
7.47
7.47
7.42
7.41
7.41
7.40
7.39
7.39
7.27
7.26
7.25
7.25
7.22
7.20
7.19
4.87
4.85
4.85
4.83
4.14
4.13
4.11
4.09
2.41
2.41
2.39
2.37
2.07
2.01
1.96
1.27
1.25
1.23
1.20
-0.00

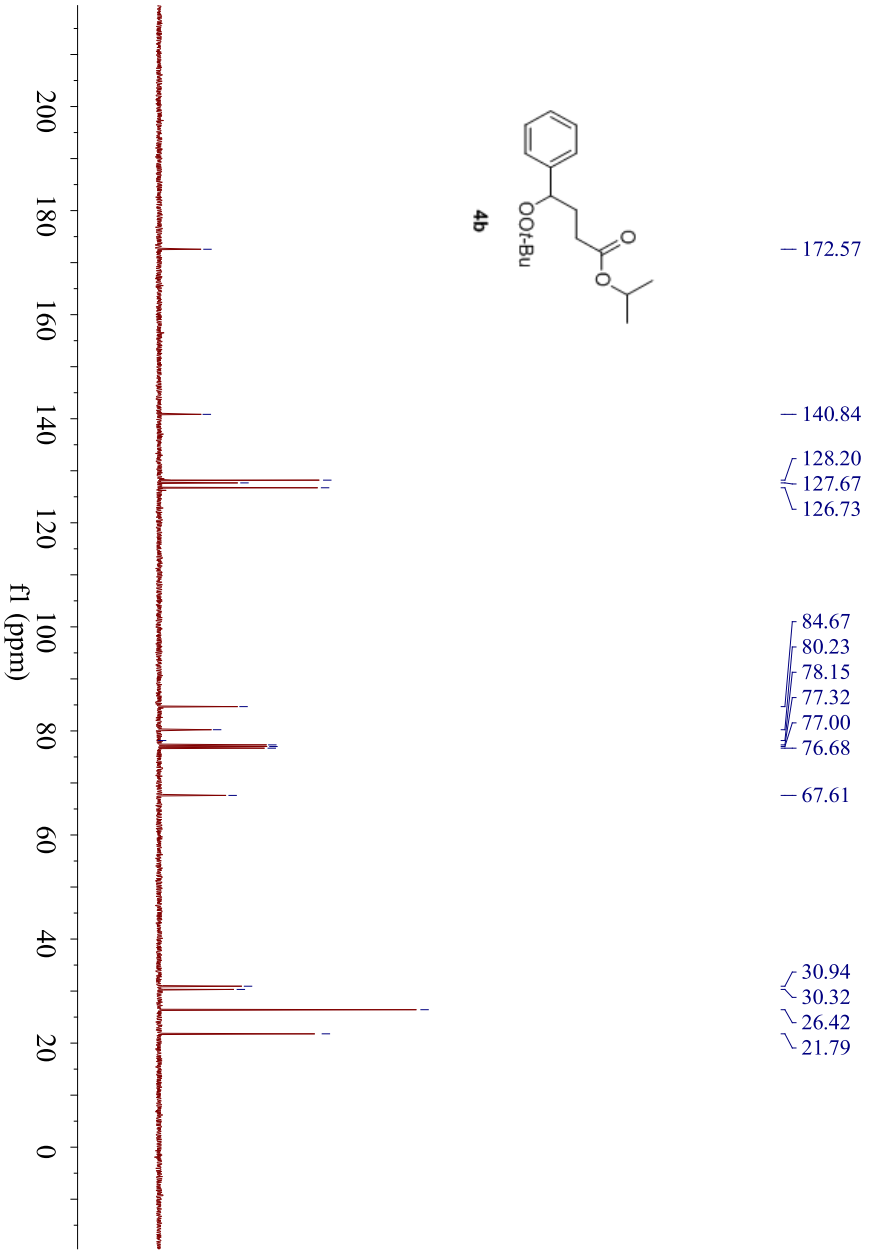

Br
OOt-Bu
O
O
3m
172.84
143.53
129.83
129.72
125.28
122.34
83.81
80.44
77.32
77.00
76.68
60.43
30.48
30.35
26.39
14.18
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

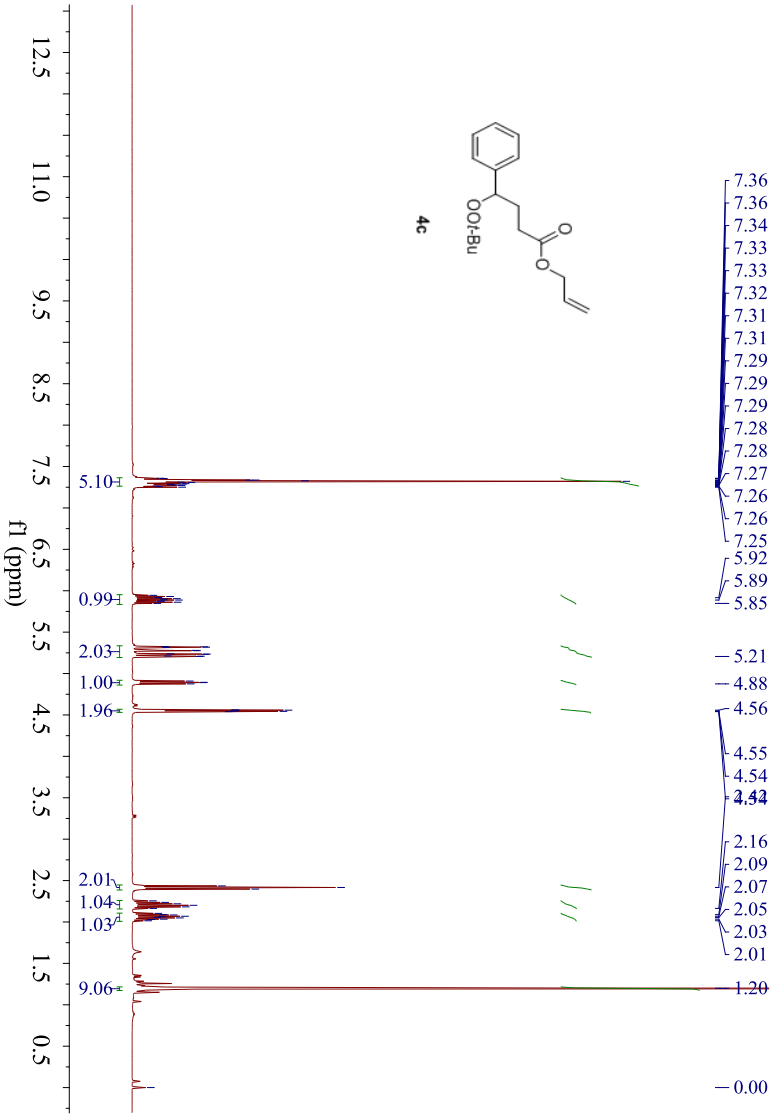

3n
OOt-Bu
O
O
O
f1 (ppm)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.02
1.07
1.03
1.02
1.00
2.03
3.04
1.97
2.01
12.02
7.41
7.41
7.39
7.39
7.25
7.25
7.24
7.23
7.23
7.21
7.20
6.96
6.94
6.85
6.83
5.37
5.36
5.34
4.11
4.09
4.08
4.06
3.80
2.39
2.38
2.37
2.36
2.10
2.07
1.24
1.23
1.21
0.00

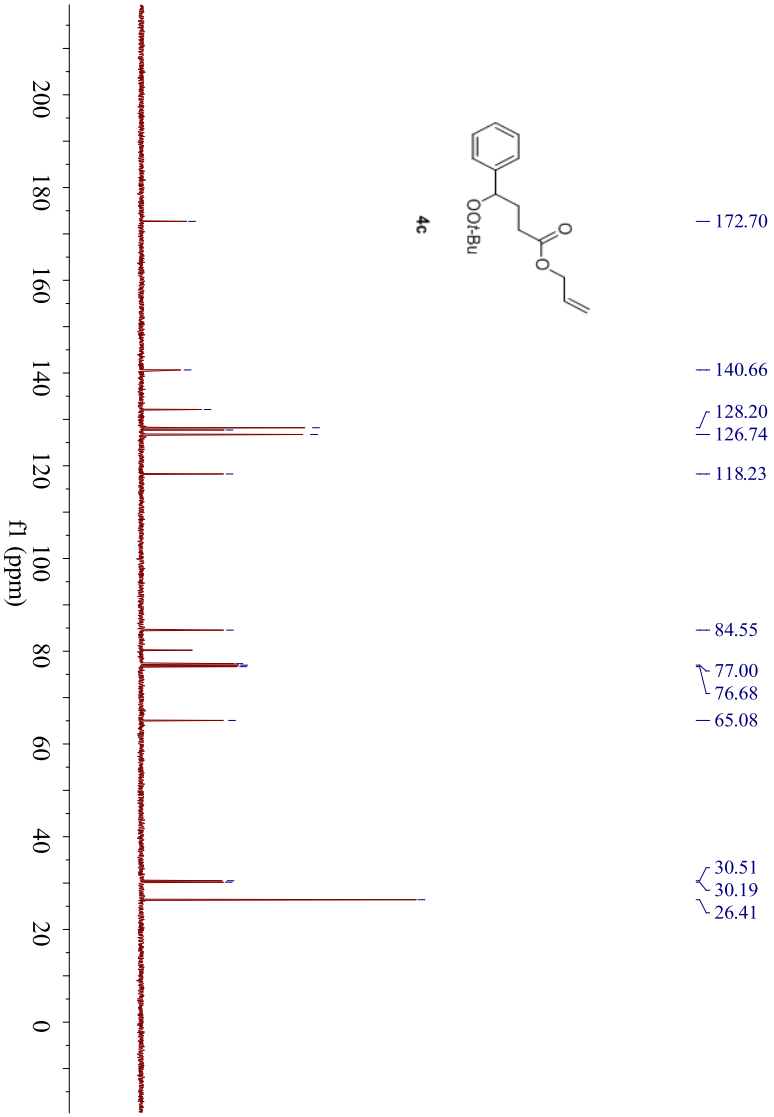

f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0
3n
OOt-Bu
O
O
O
173.32
156.39
129.15
128.22
126.99
120.40
110.21
80.08
78.48
77.32
77.00
76.68
60.16
55.23
30.52
29.24
26.42
14.15

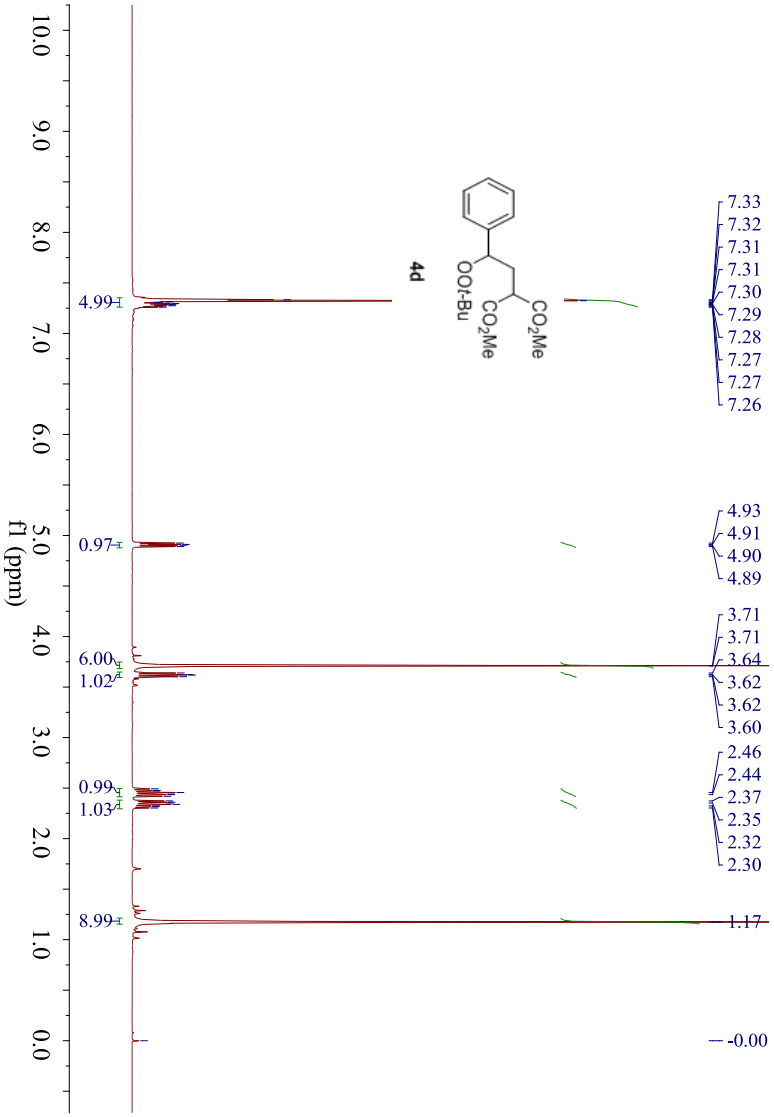

f1 (ppm)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
5.03
1.01
2.00
0.94
1.05
1.04
3.07
9.02
D-3a
OOt-Bu
D
O
O
7.36
7.36
7.36
7.35
7.34
7.34
7.33
7.32
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.27
4.90
4.89
4.88
4.87
4.13
4.11
4.10
4.08
2.37
2.15
2.15
2.13
2.07
2.05
2.04
2.02
2.00
1.26
1.24
1.22
1.20
-0.00

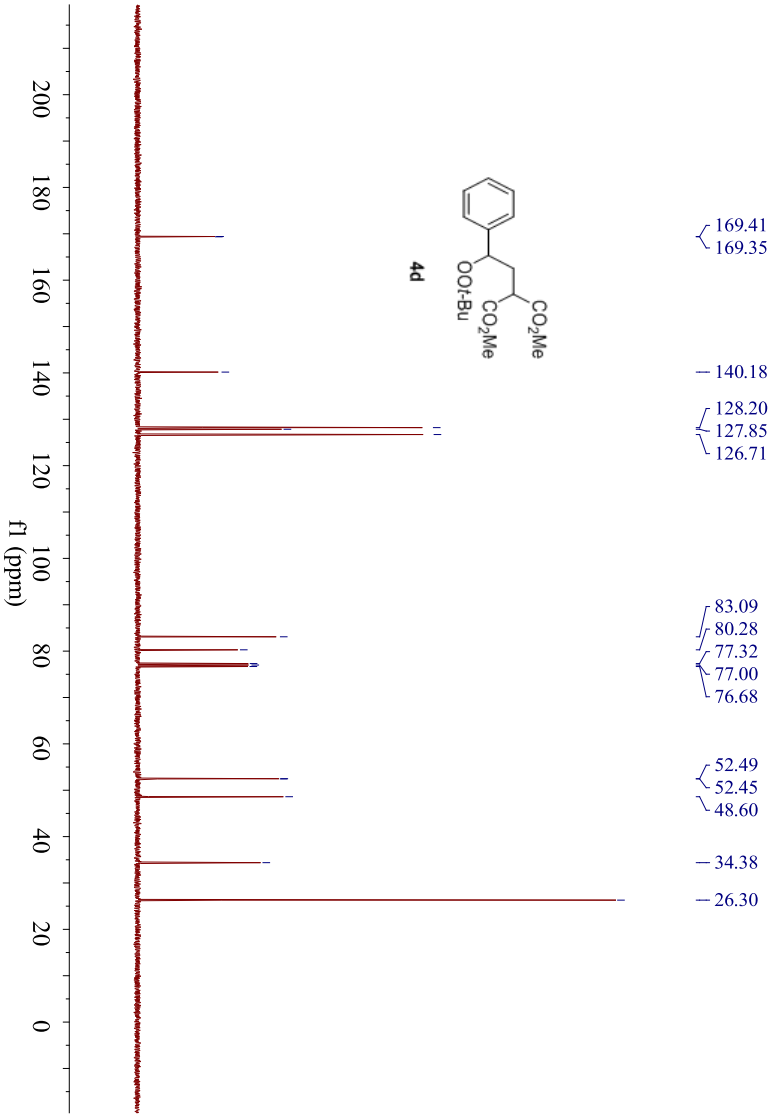

4b
OOt-Bu
O
O
f1 (ppm)
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
2.49
0.51
0.50
1.00
0.53
0.52
7.52
7.36
7.36
7.34
7.34
7.33
7.32
7.31
7.31
7.30
7.29
7.29
7.29
7.28
7.28
7.27
7.26
7.26
7.25
5.02
5.01
4.99
4.97
4.96
4.94
4.90
4.89
4.88
2.20
2.17
2.07
2.03
2.01
1.98
1.22
1.22
1.20
0.00

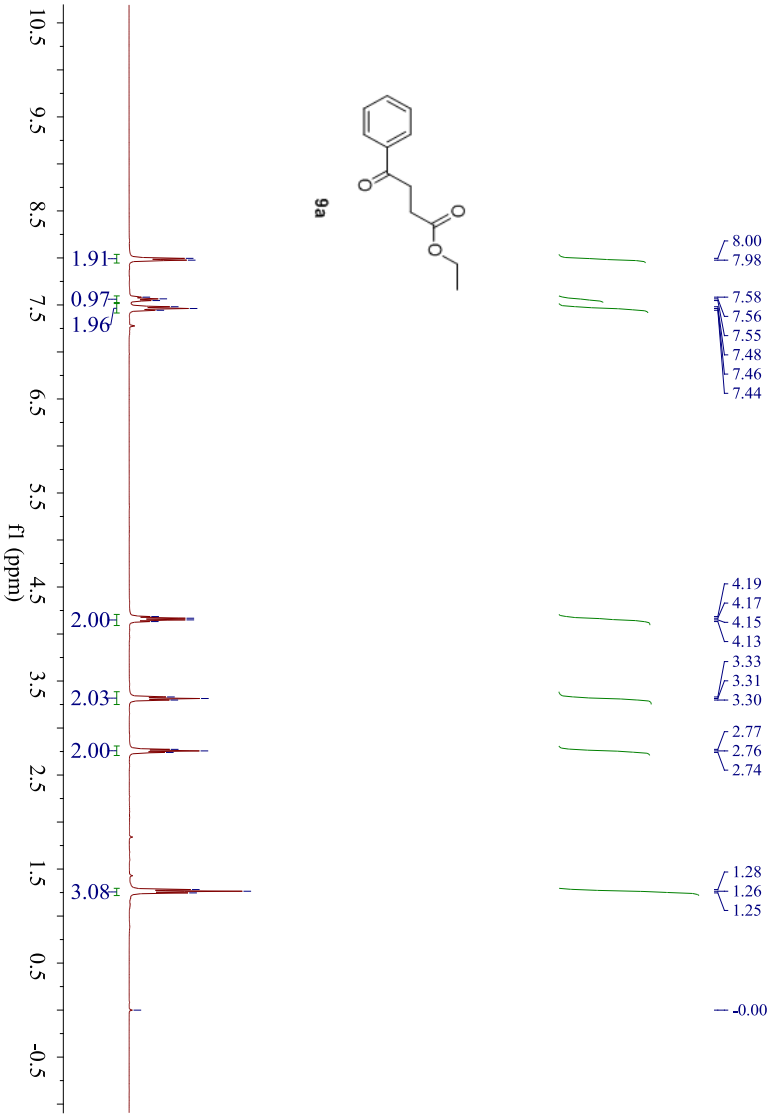

4b
OOt-Bu
O
O
172.57
140.84
128.20
127.67
126.73
84.67
80.23
78.15
77.32
77.00
76.68
67.61
30.94
30.32
26.42
21.79
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

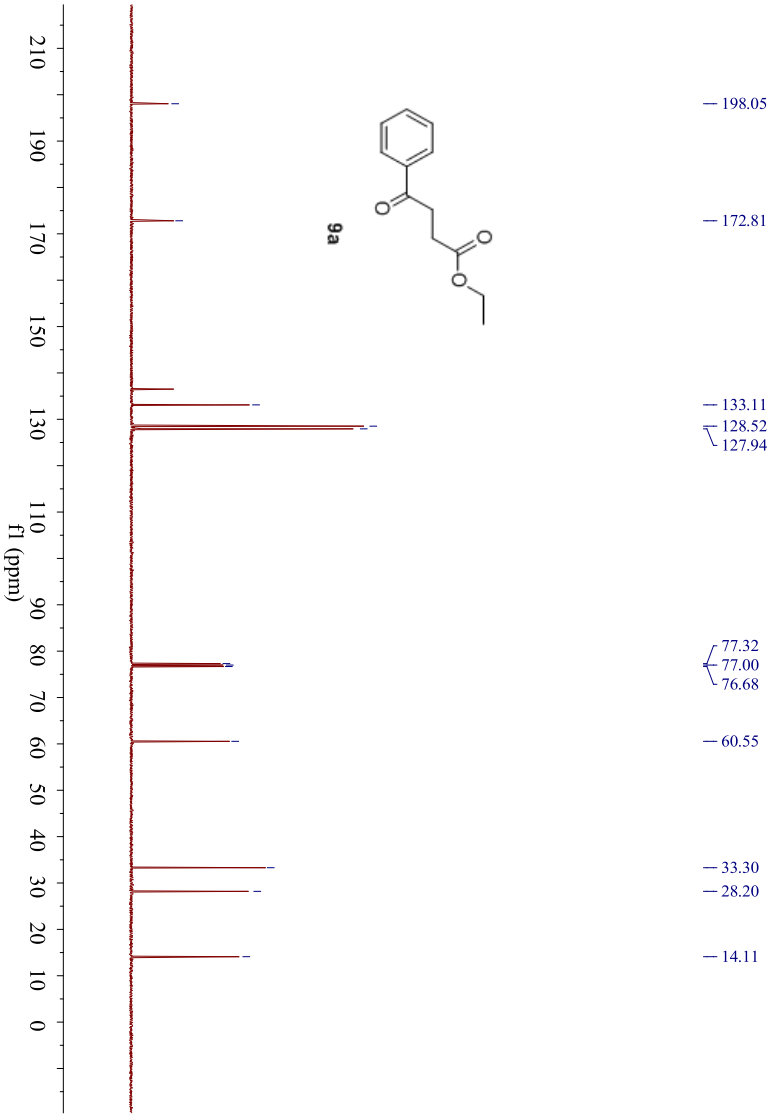

4c
OOt-Bu
O
O
f1 (ppm)
12.5
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
5.10
0.99
2.03
1.00
1.96
2.01
1.04
1.03
9.06
7.36
7.36
7.34
7.33
7.33
7.32
7.31
7.31
7.29
7.29
7.29
7.28
7.28
7.27
7.26
7.26
7.25
5.92
5.89
5.85
5.21
4.88
4.56
4.55
4.54
2.16
2.09
2.07
2.05
2.03
2.01
1.20
0.00

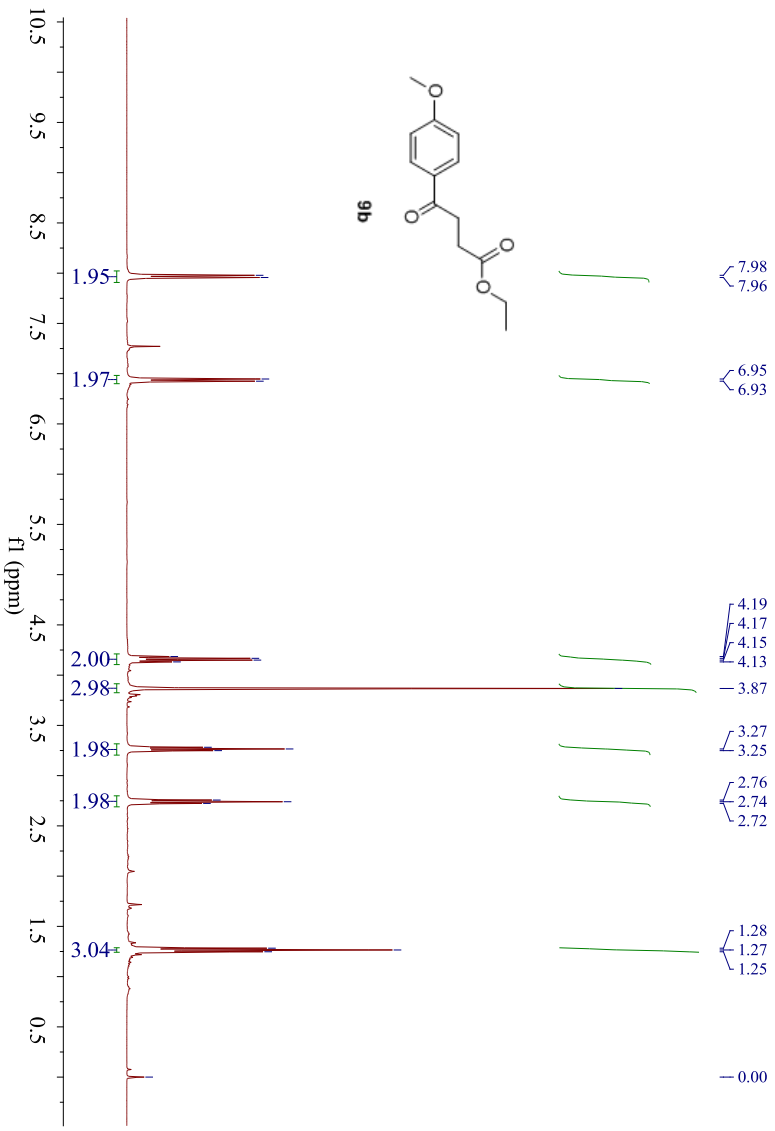

4c
OOt-Bu
O
O
172.70
140.66
128.20
126.74
118.23
84.55
77.00
76.68
65.08
30.51
30.19
26.41
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

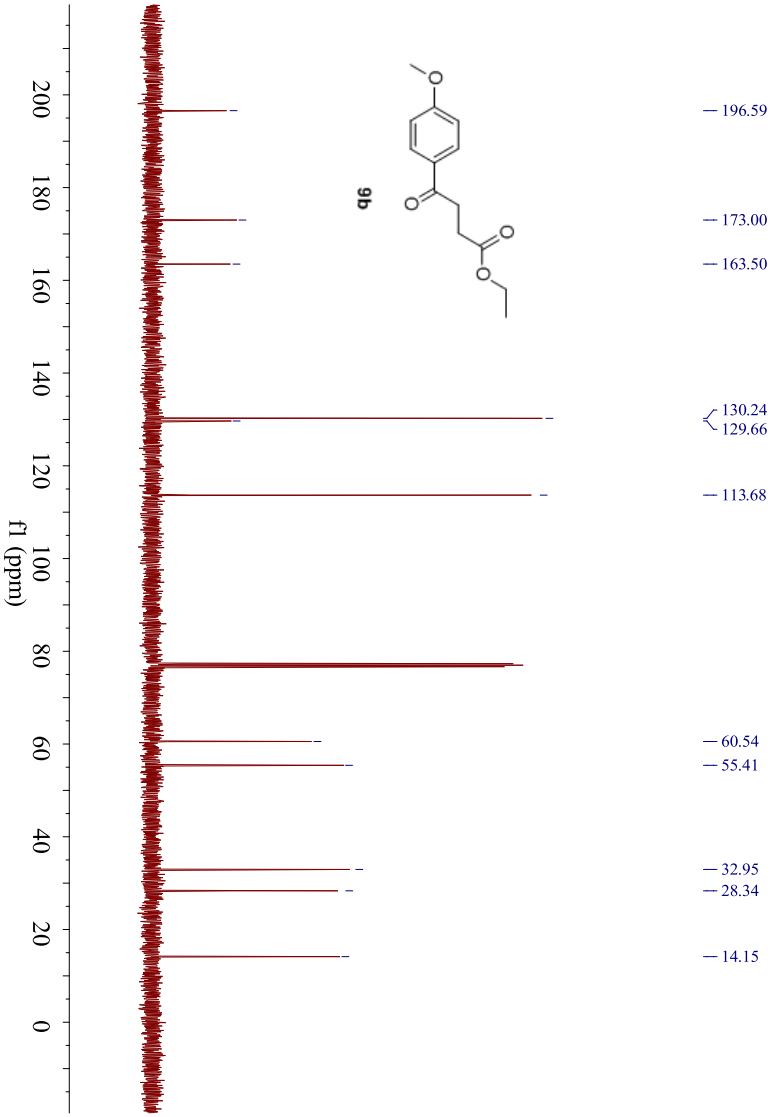

4d
OOt-Bu
CO2Me
CO2Me
f1 (ppm)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
4.99
0.97
6.00
1.02
0.99
1.03
8.99
7.33
7.32
7.31
7.31
7.30
7.29
7.28
7.27
7.27
7.26
4.93
4.91
4.90
4.89
3.71
3.71
3.64
3.62
3.62
3.60
2.46
2.44
2.37
2.35
2.32
2.30
1.17
-0.00

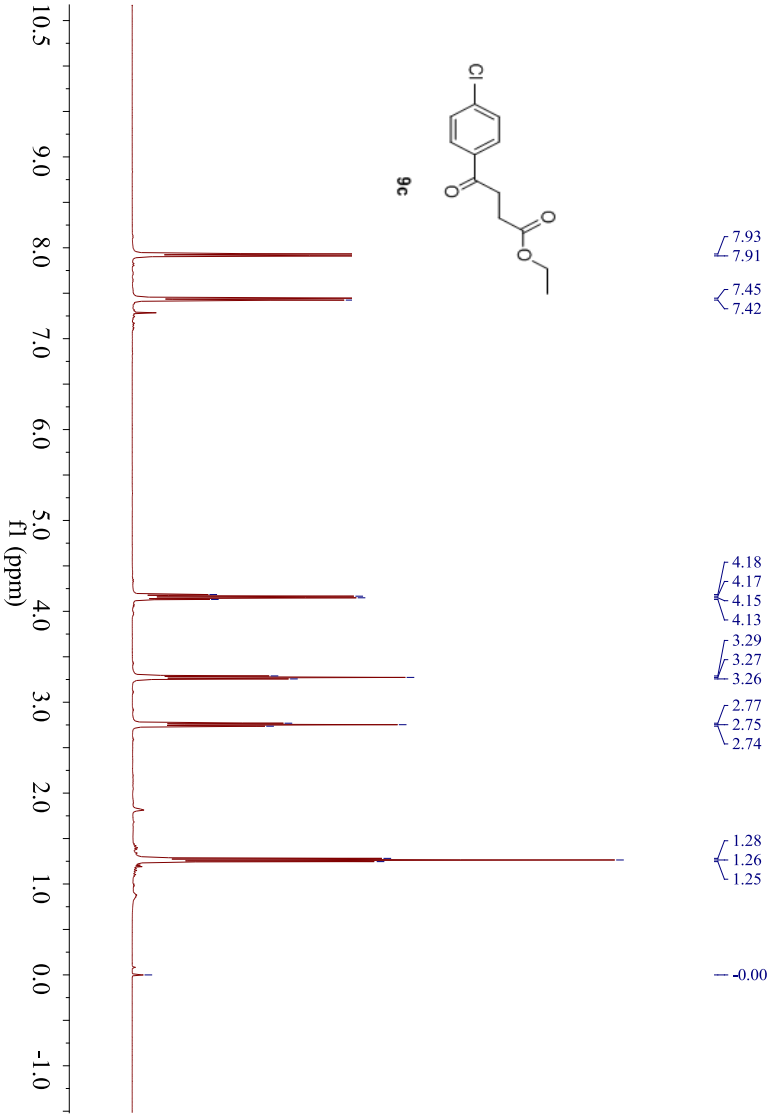

4d
OOt-Bu
CO2Me
CO2Me
169.41
169.35
140.18
128.20
127.85
126.71
83.09
80.28
77.32
77.00
76.68
52.49
52.45
48.60
34.38
26.30
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

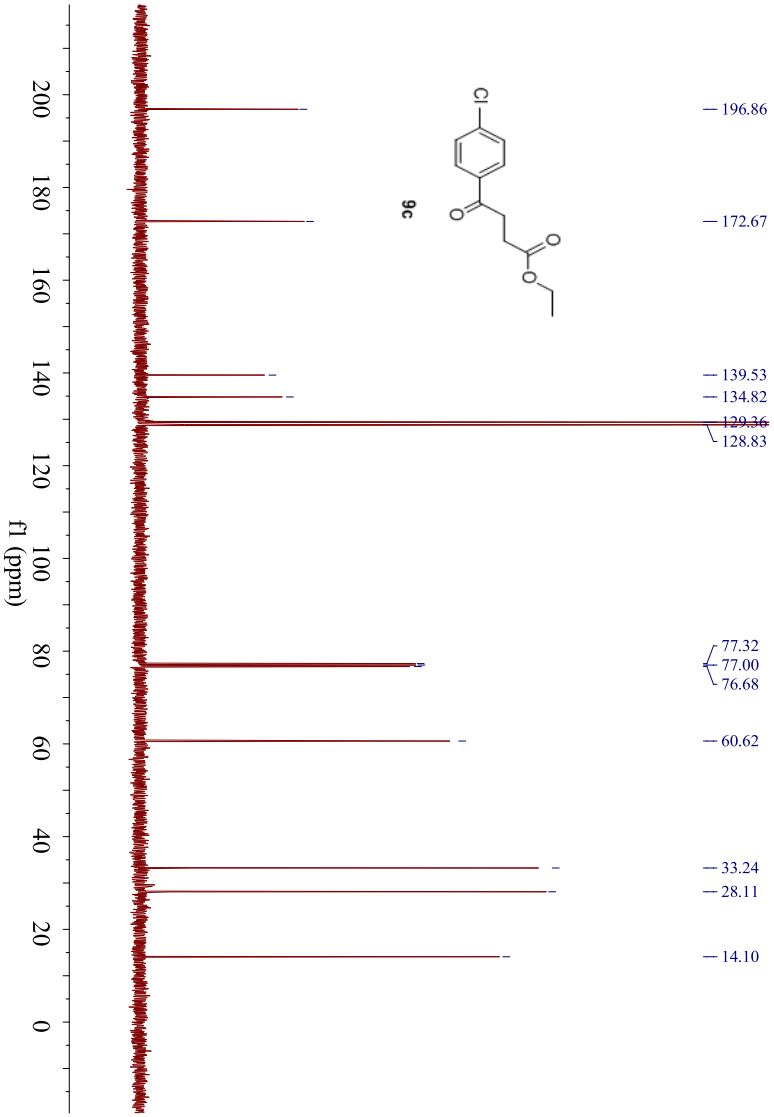

9a
f1 (ppm)
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
1.91
0.97
1.96
2.00
2.03
2.00
3.08
8.00
7.98
7.58
7.56
7.55
7.48
7.46
7.44
4.19
4.17
4.15
4.13
3.33
3.31
3.30
2.77
2.76
2.74
1.28
1.26
1.25
-0.00

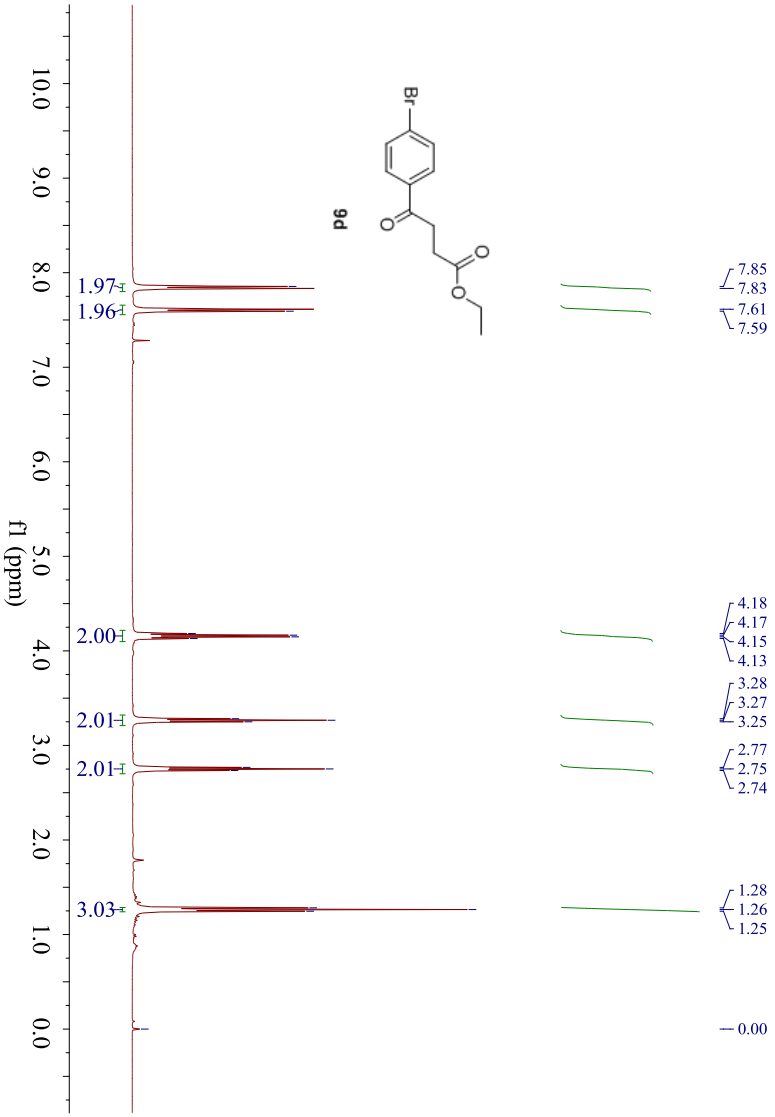

198.05
172.81
133.11
128.52
127.94
77.32
77.00
76.68
60.55
33.30
28.20
14.11
9a
f1 (ppm)

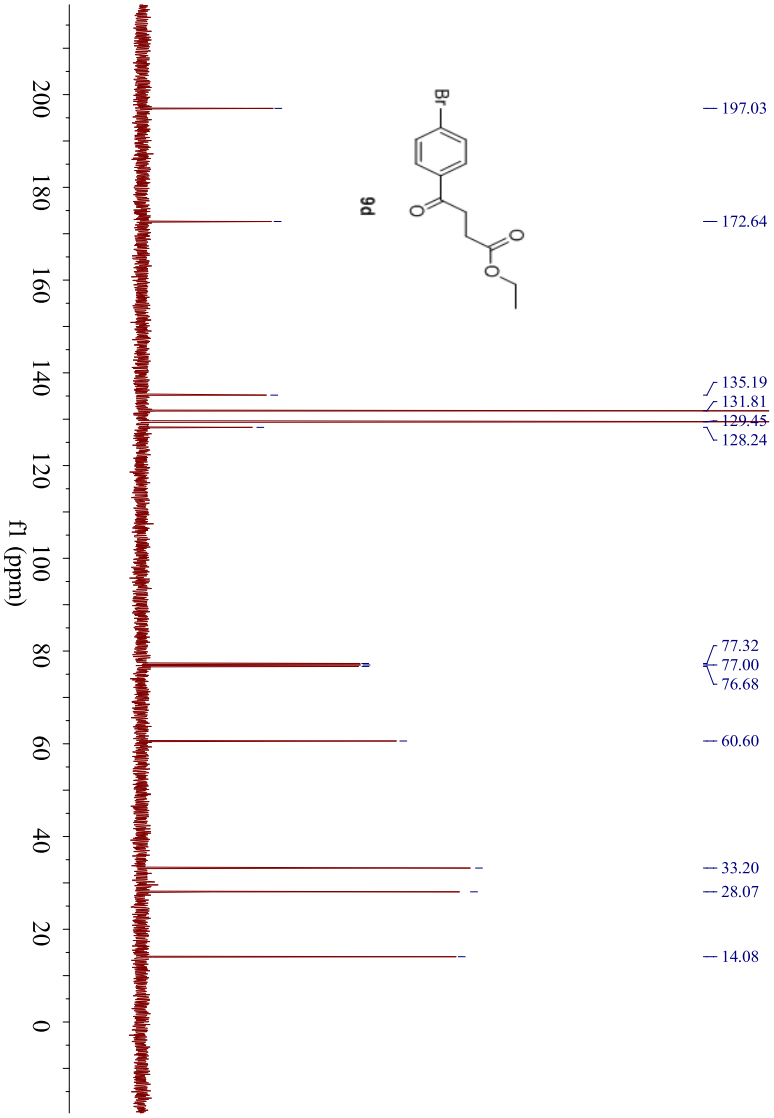

9b
f1 (ppm)
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
1.95
1.97
2.00
2.98
1.98
1.98
3.04
7.98
7.96
6.95
6.93
4.19
4.17
4.15
4.13
3.87
3.27
3.25
2.76
2.74
2.72
1.28
1.27
1.25
0.00

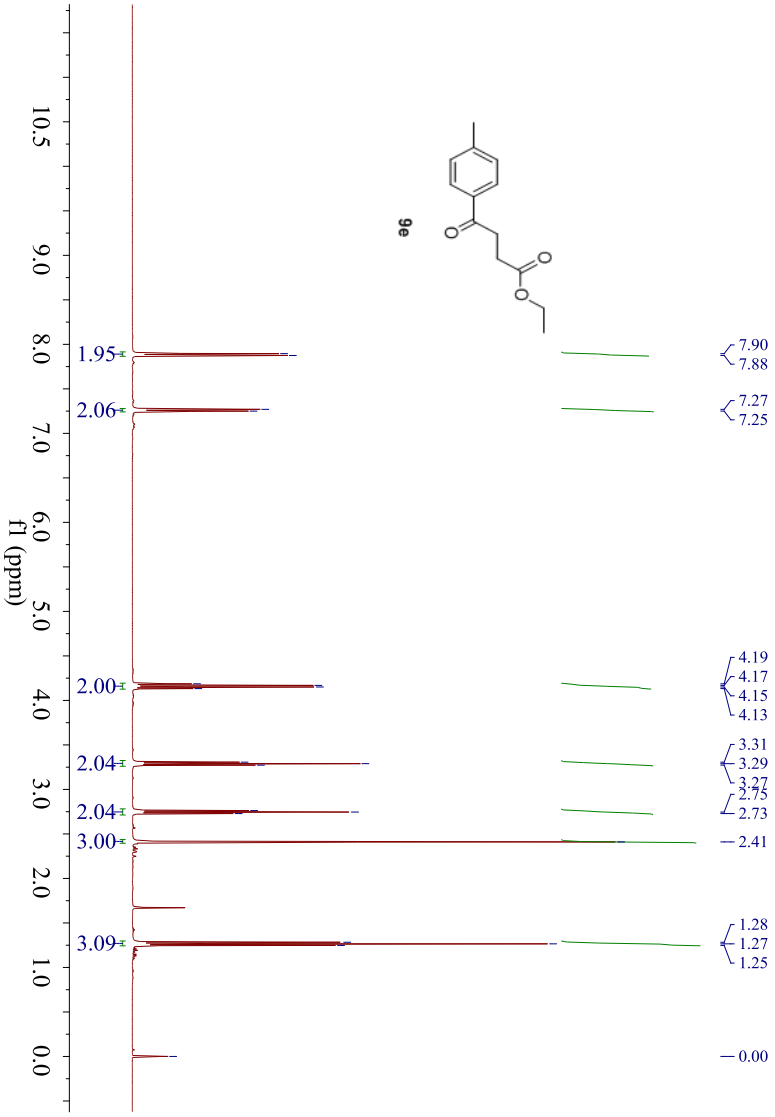

9b
196.59
173.00
163.50
130.24
129.66
113.68
60.54
55.41
32.95
28.34
14.15
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

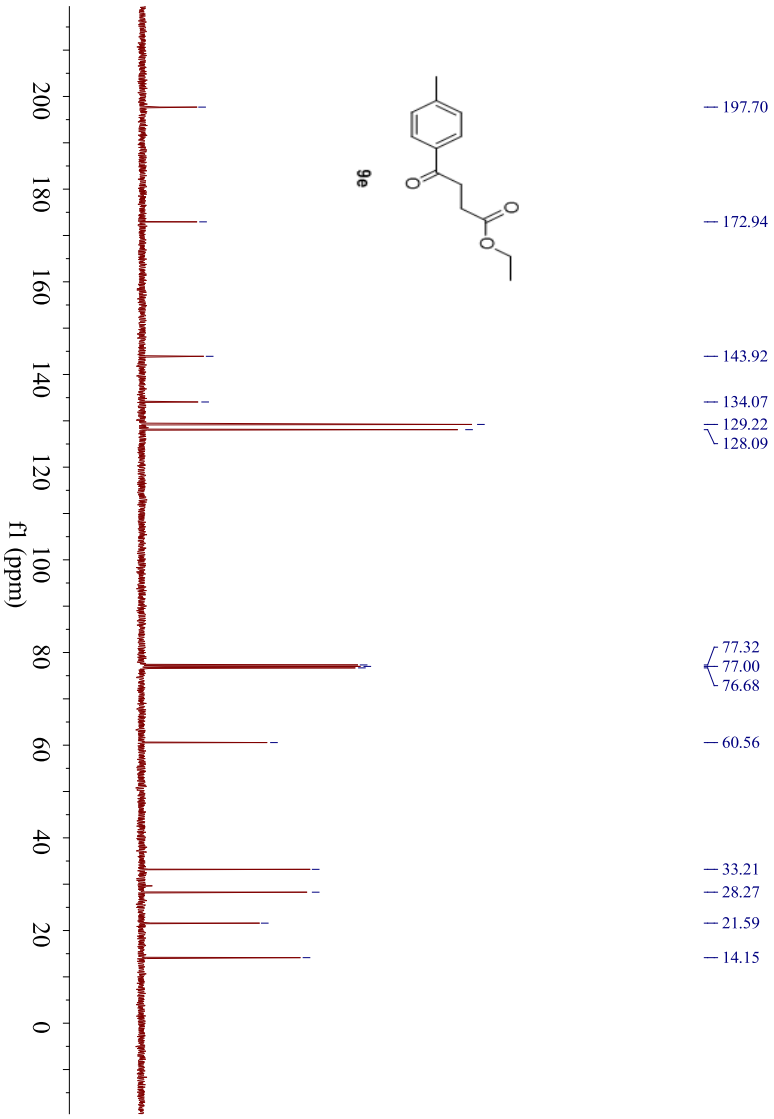

10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)
Cl
O
O
O
9c
7.93
7.91
7.45
7.42
4.18
4.17
4.15
4.13
3.29
3.27
3.26
2.77
2.75
2.74
1.28
1.26
1.25
-0.00

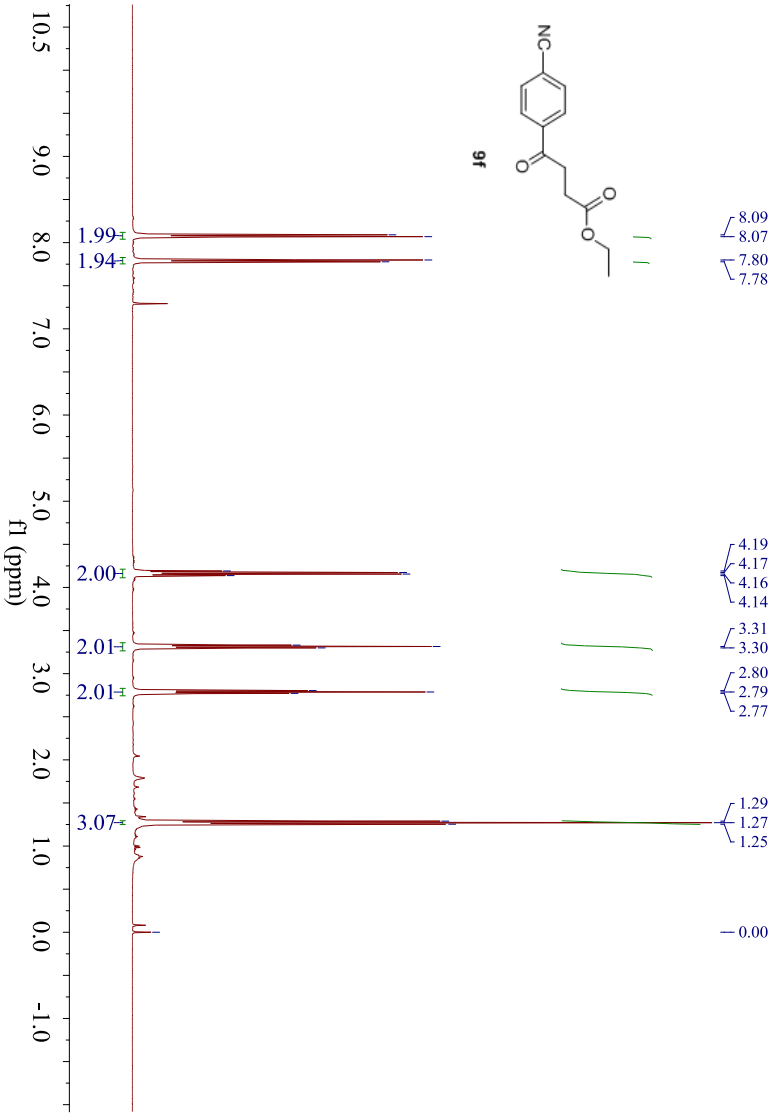

196.86
172.67
139.53
134.82
129.36
128.83
77.32
77.00
76.68
60.62
33.24
28.11
14.10
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0
9c
Cl
O
O
O

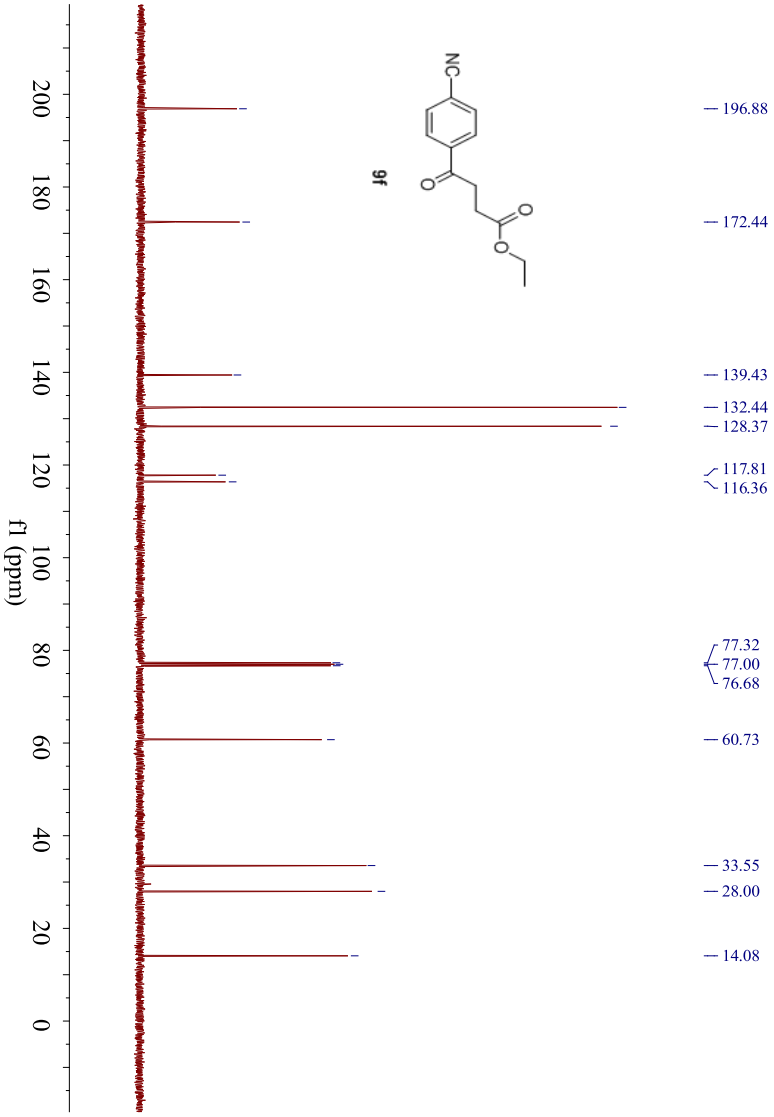

9d
Br
f1 (ppm)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.97
1.96
2.00
2.01
2.01
3.03
7.85
7.83
7.61
7.59
4.18
4.17
4.15
4.13
3.28
3.27
3.25
2.77
2.75
2.74
1.28
1.26
1.25
0.00

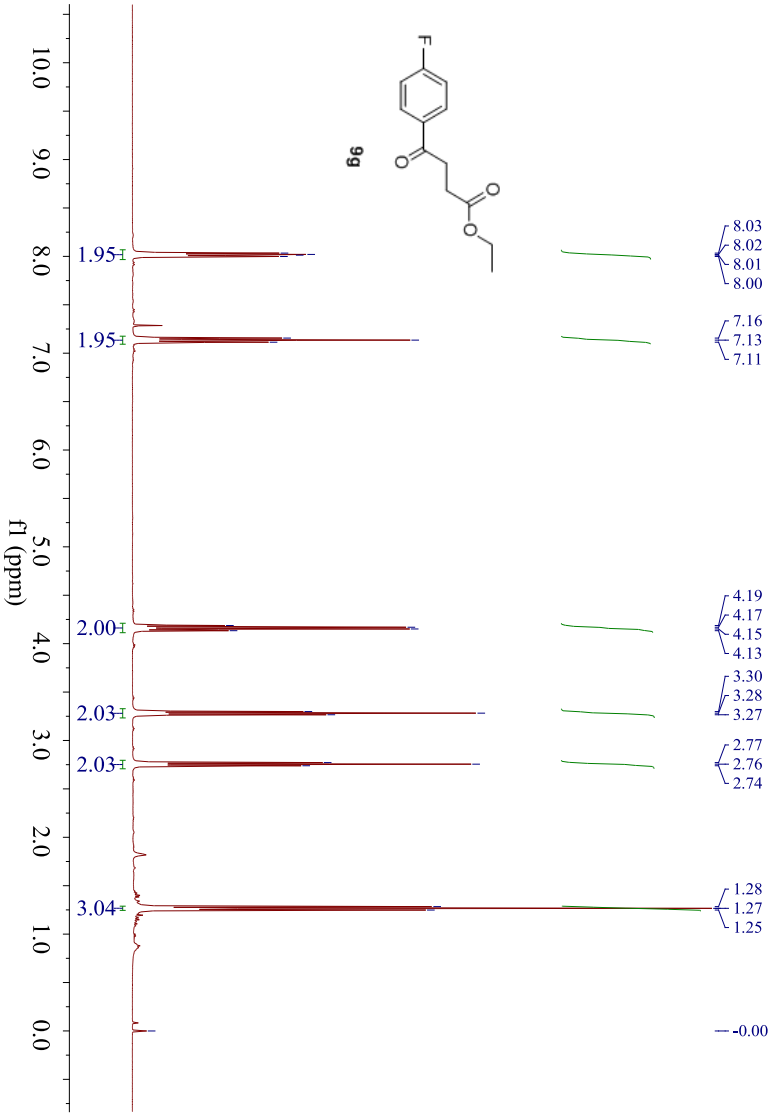

9d
Br
O
O
O
197.03
172.64
135.19
131.81
129.45
128.24
77.32
77.00
76.68
60.60
33.20
28.07
14.08
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

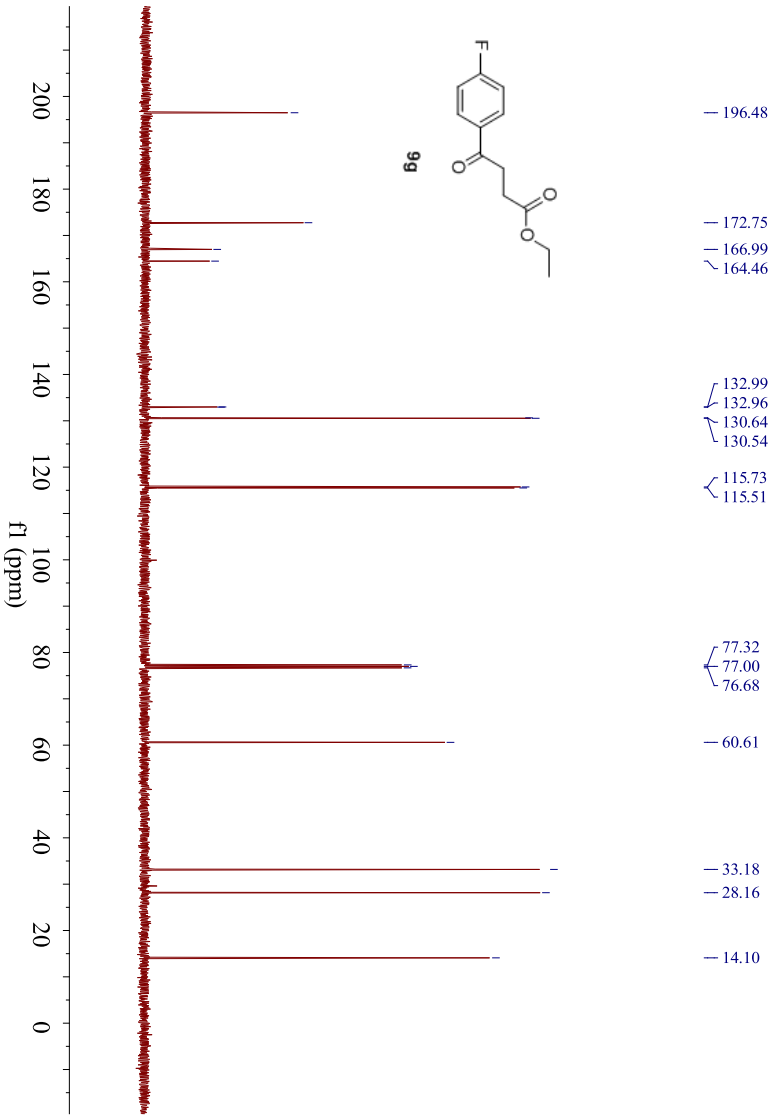

9e
f1 (ppm)
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.95
2.06
2.00
2.04
2.04
3.00
3.09
7.90
7.88
7.27
7.25
4.19
4.17
4.15
4.13
3.31
3.29
3.27
2.75
2.73
2.41
1.28
1.27
1.25
0.00

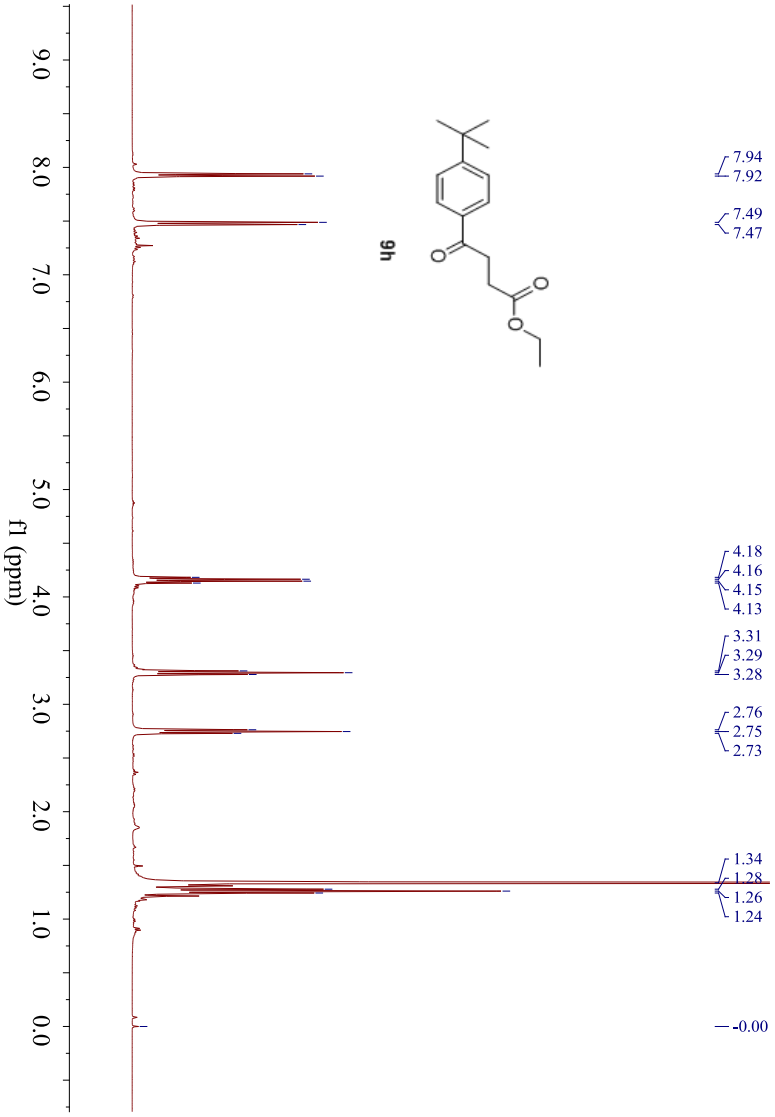

6e
197.70
172.94
143.92
134.07
129.22
128.09
77.32
77.00
76.68
60.56
33.21
28.27
21.59
14.15
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

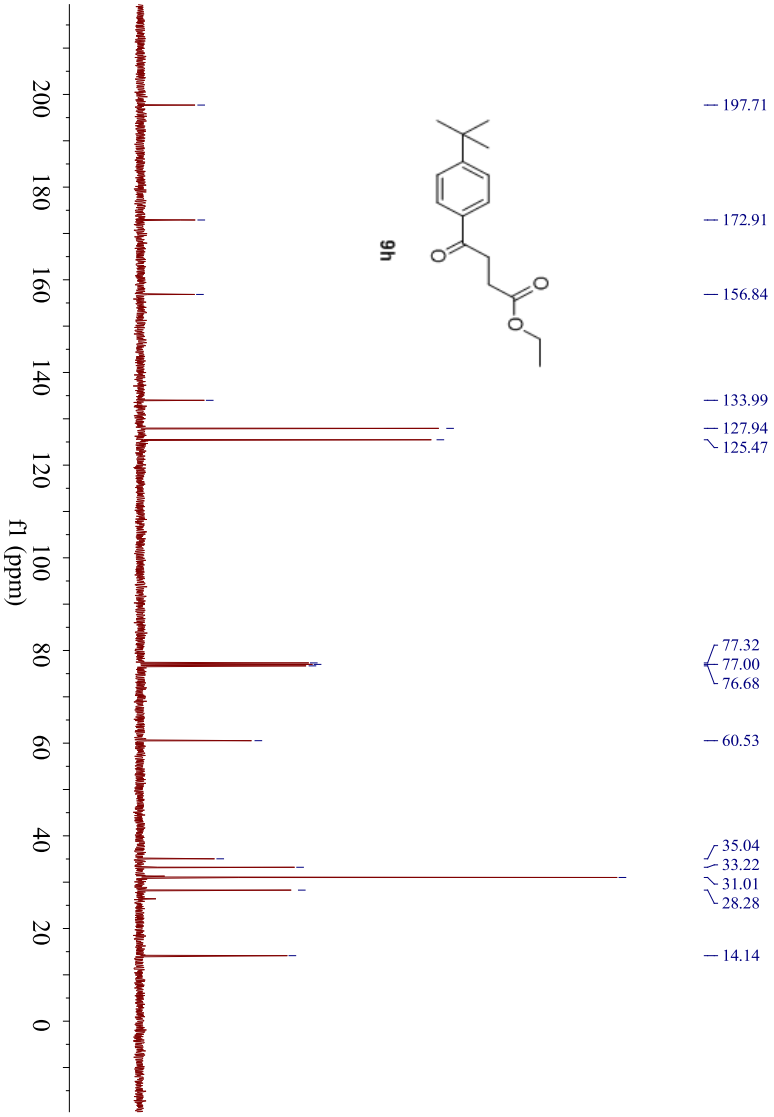

9f
NC
O
O
O
f1 (ppm)
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
1.99
1.94
2.00
2.01
2.01
3.07
8.09
8.07
7.80
7.78
4.19
4.17
4.16
4.14
3.31
3.30
2.80
2.79
2.77
1.29
1.27
1.25
0.00

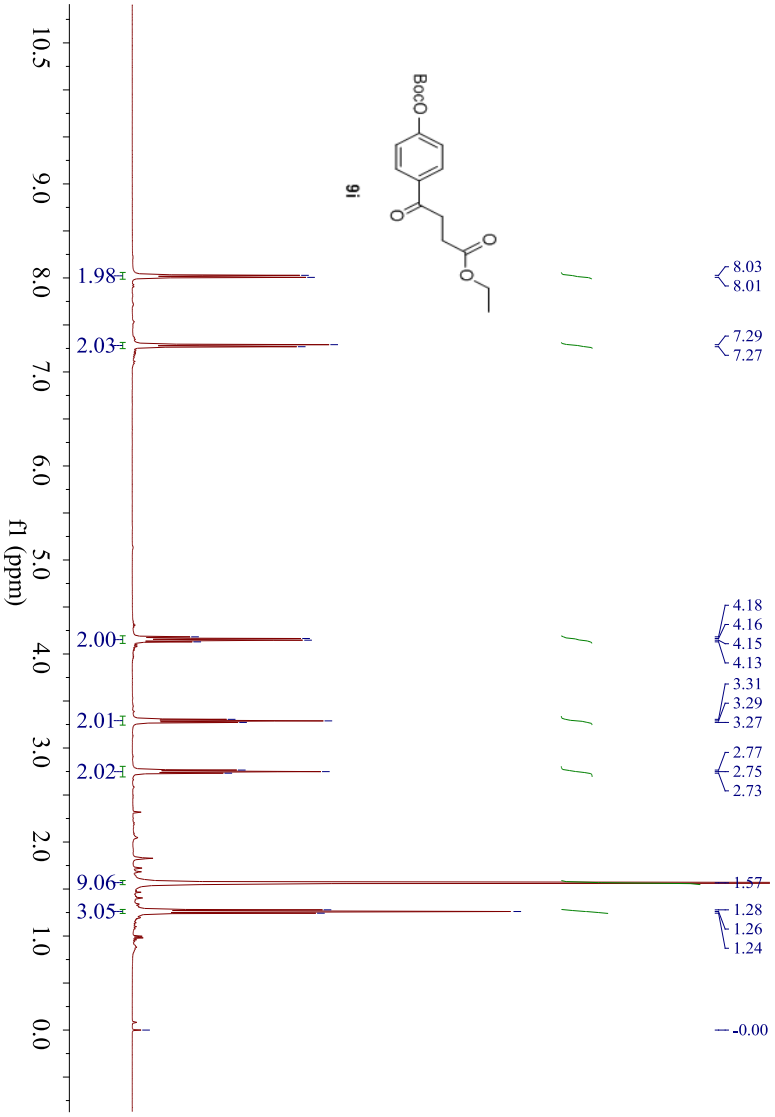

9f
NC
O
O
O
196.88
172.44
139.43
132.44
128.37
117.81
116.36
77.32
77.00
76.68
60.73
33.55
28.00
14.08
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

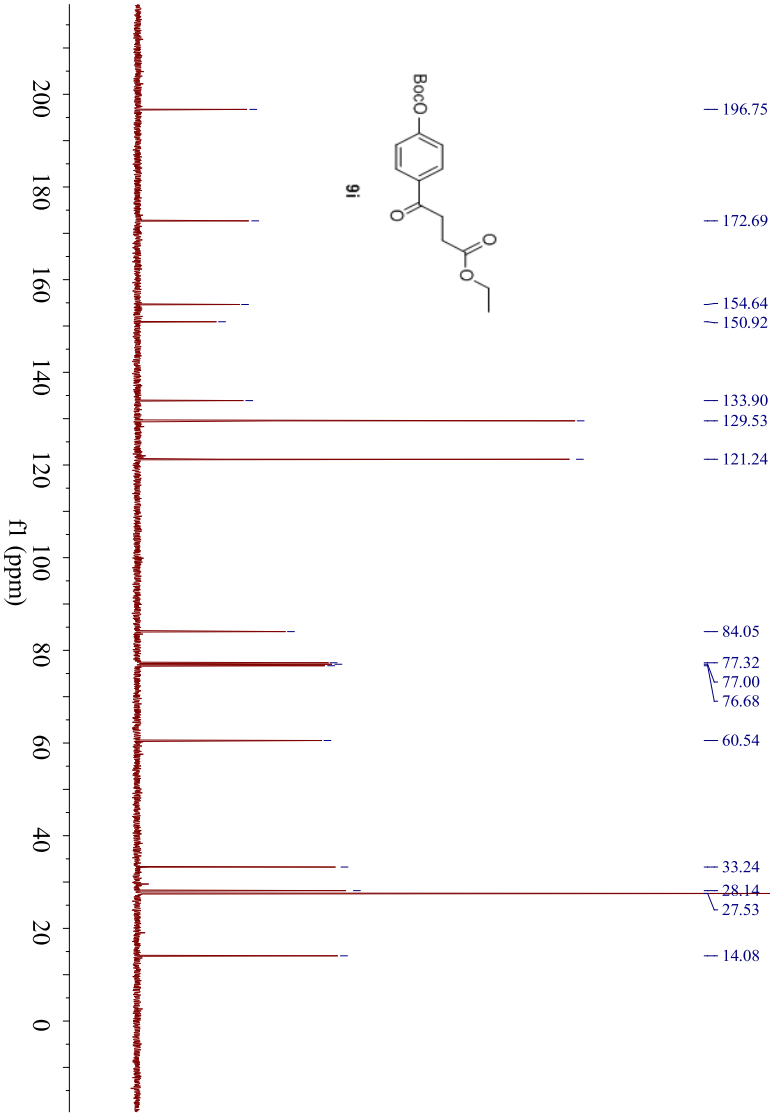

9g
F
O
O
O
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
1.95
1.95
2.00
2.03
2.03
3.04
8.03
8.02
8.01
8.00
7.16
7.13
7.11
4.19
4.17
4.15
4.13
3.30
3.28
3.27
2.77
2.76
2.74
1.28
1.27
1.25
-0.00

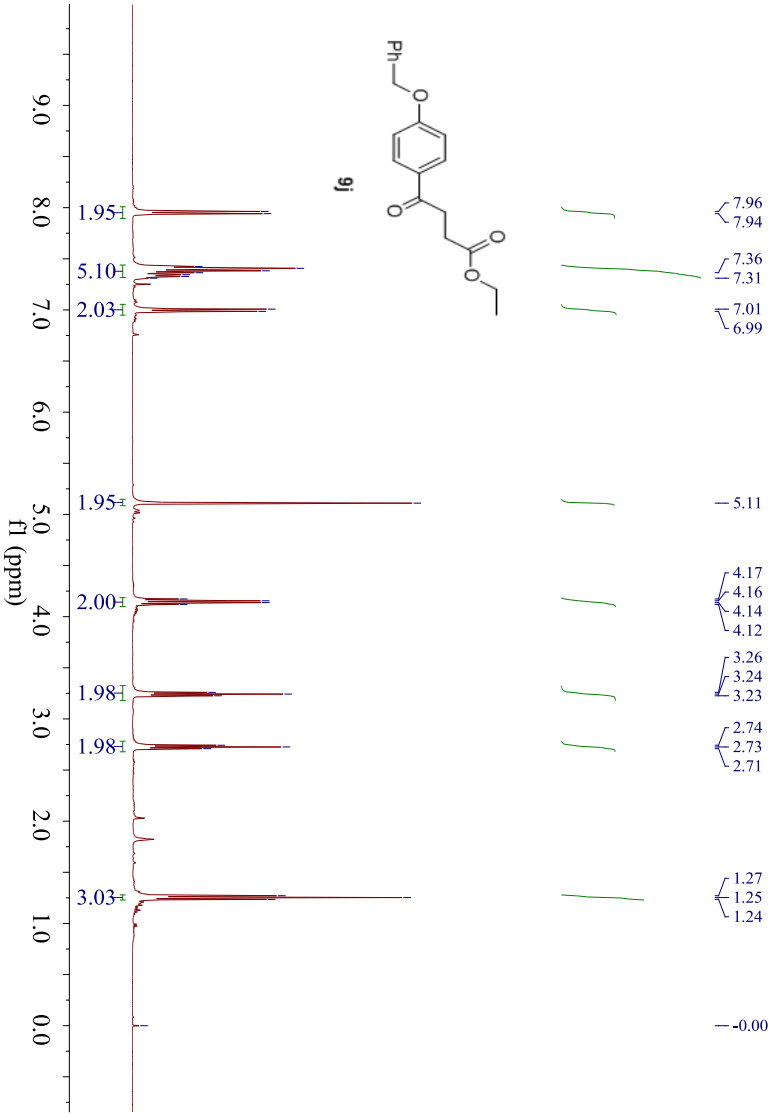

F
O
O
O
9g
196.48
172.75
166.99
164.46
132.99
132.96
130.64
130.54
115.73
115.51
77.32
77.00
76.68
60.61
33.18
28.16
14.10
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

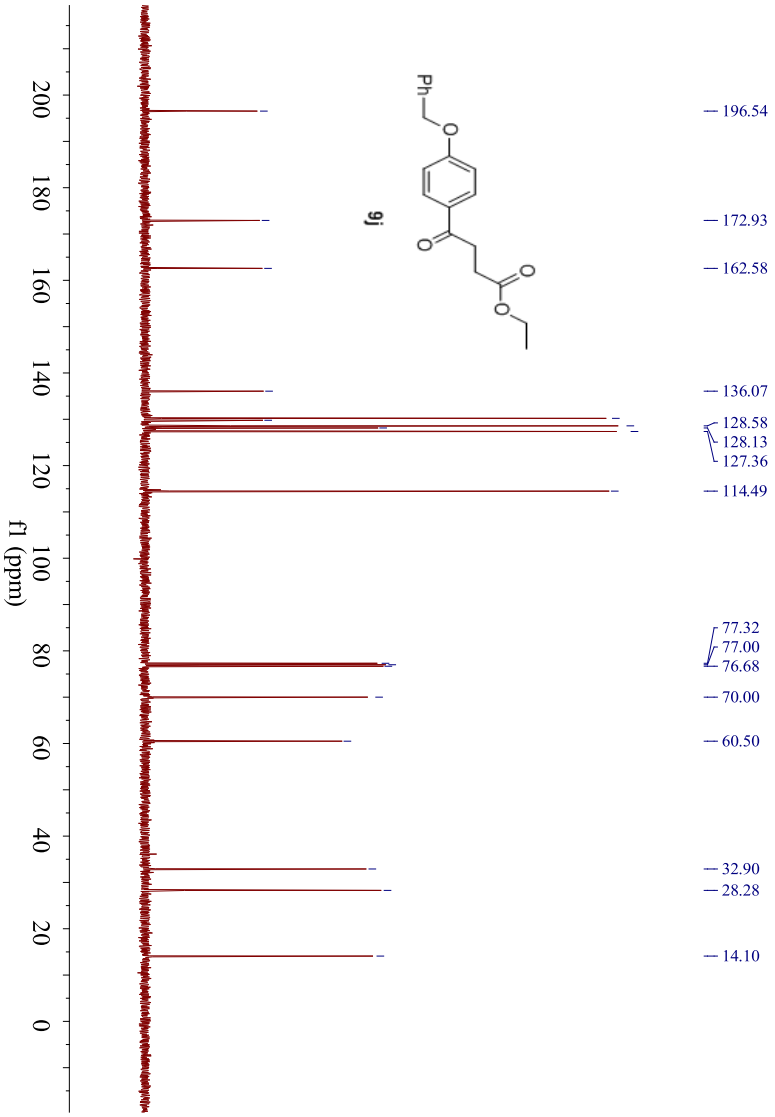

9h
7.94
7.92
7.49
7.47
4.18
4.16
4.15
4.13
3.31
3.29
3.28
2.76
2.75
2.73
1.34
1.28
1.26
1.24
-0.00
f1 (ppm)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

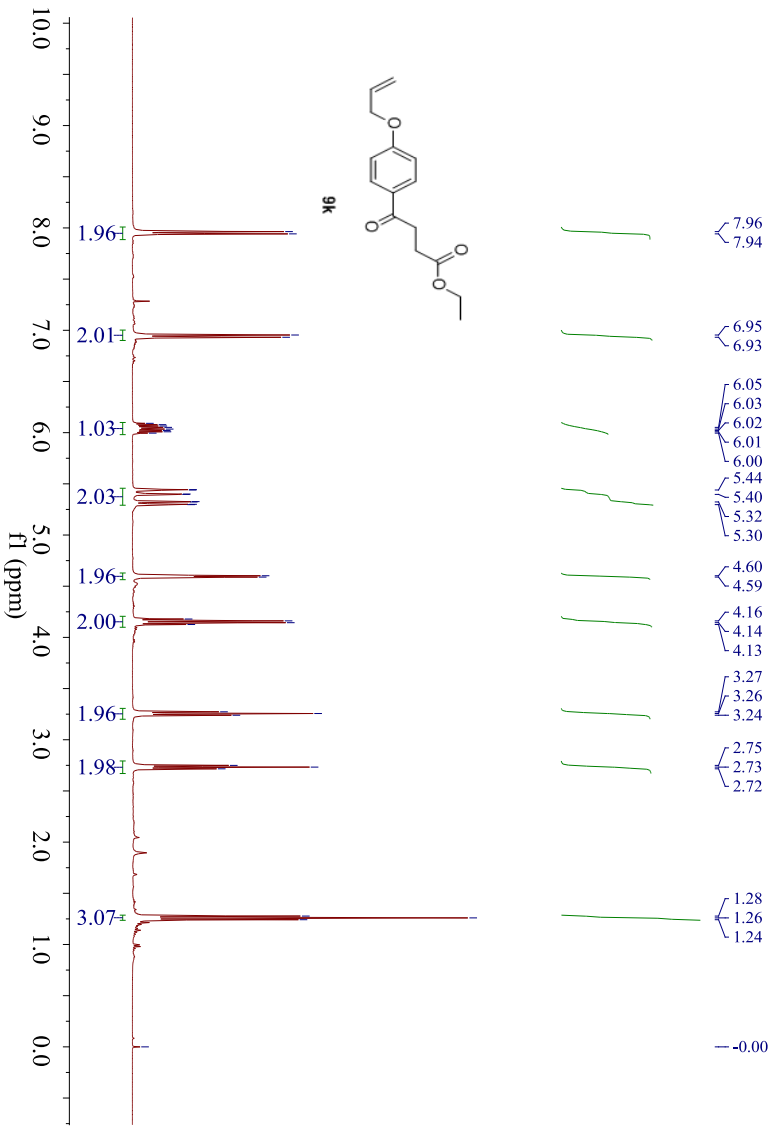

9h
197.71
172.91
156.84
133.99
127.94
125.47
77.32
77.00
76.68
60.53
35.04
33.22
31.01
28.28
14.14
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

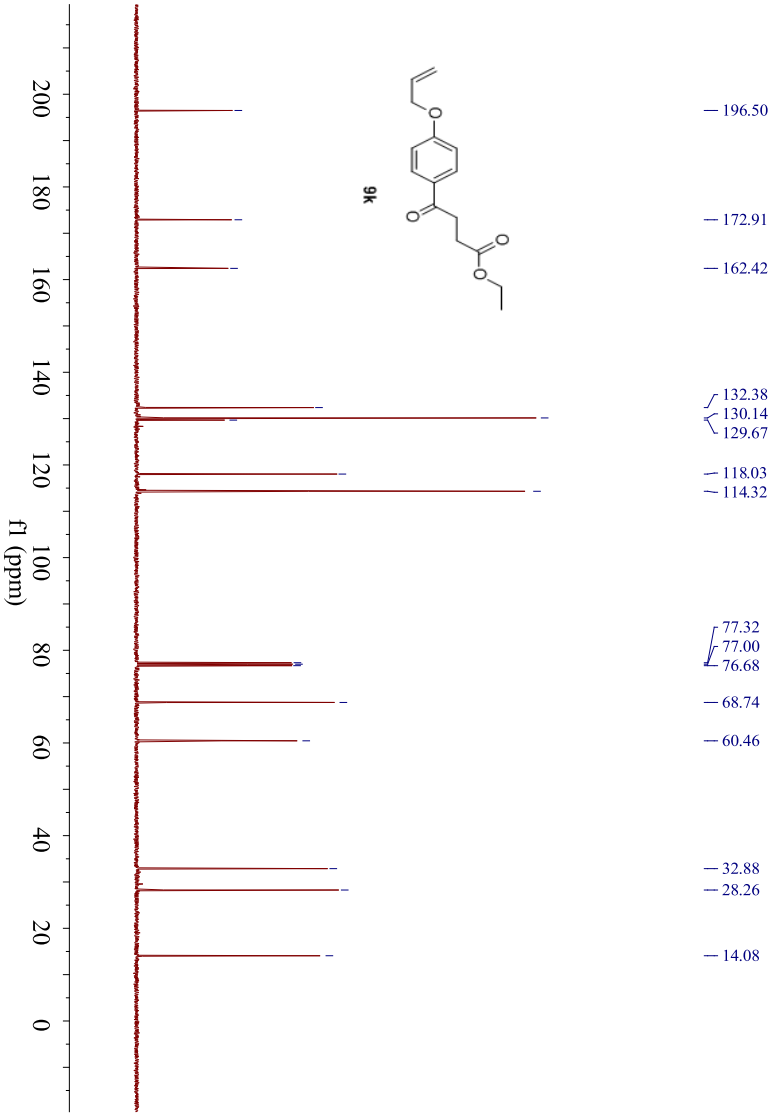

BocO
9i
f1 (ppm)
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.98
2.03
2.00
2.01
2.02
9.06
3.05
8.03
8.01
7.29
7.27
4.18
4.16
4.15
4.13
3.31
3.29
3.27
2.77
2.75
2.73
1.57
1.28
1.26
1.24
-0.00

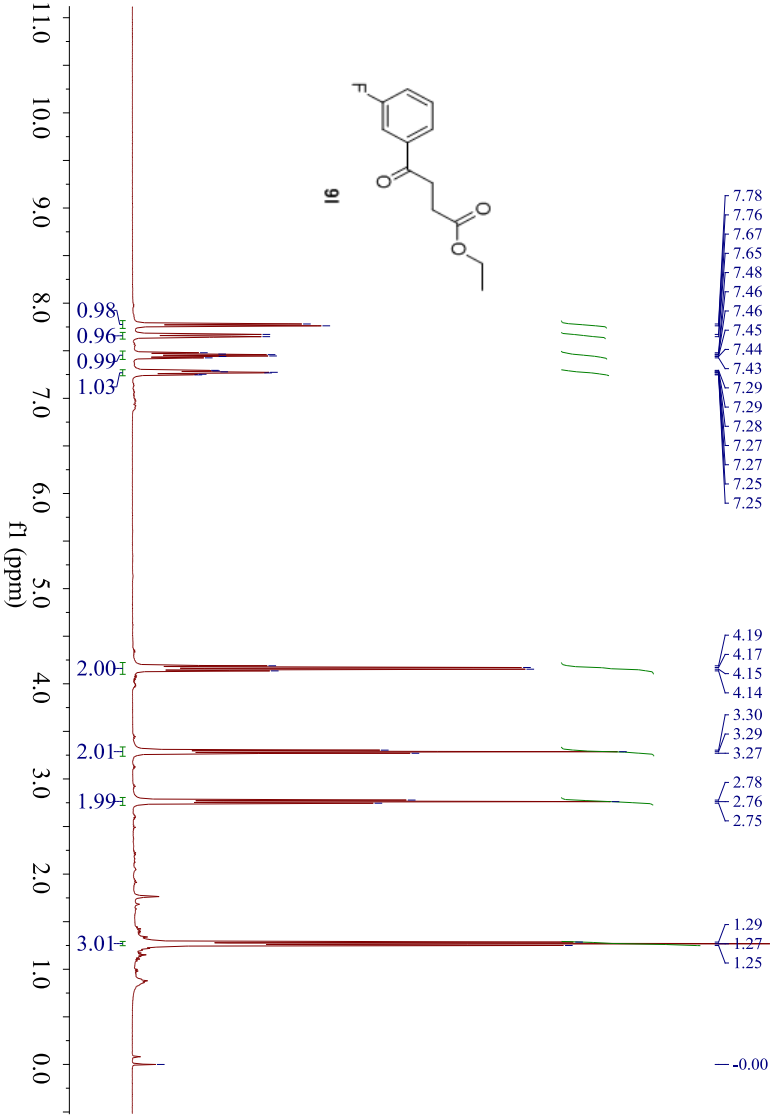

BocO
O
O
O
9i
196.75
172.69
154.64
150.92
133.90
129.53
121.24
84.05
77.32
77.00
76.68
60.54
33.24
28.14
27.53
14.08
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

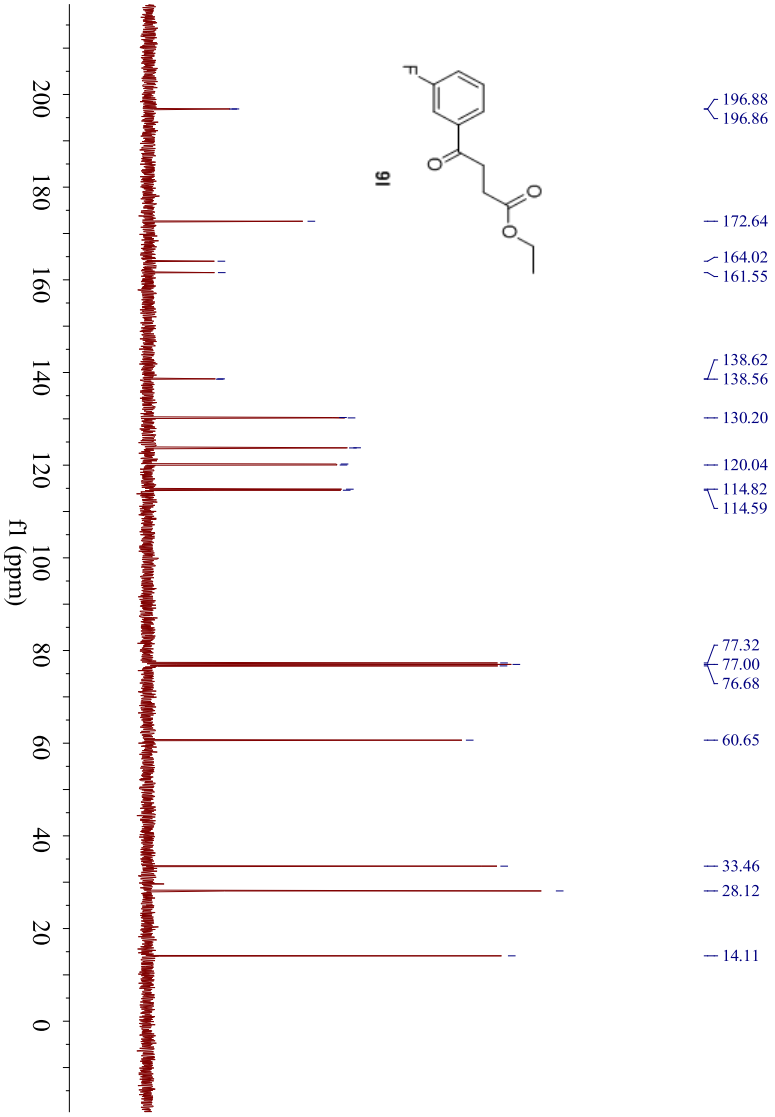

9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
1.95
5.10
2.03
1.95
2.00
1.98
1.98
3.03
Ph
O
O
O
O
9j
7.96
7.94
7.36
7.31
7.01
6.99
5.11
4.17
4.16
4.14
4.12
3.26
3.24
3.23
2.74
2.73
2.71
1.27
1.25
1.24
-0.00

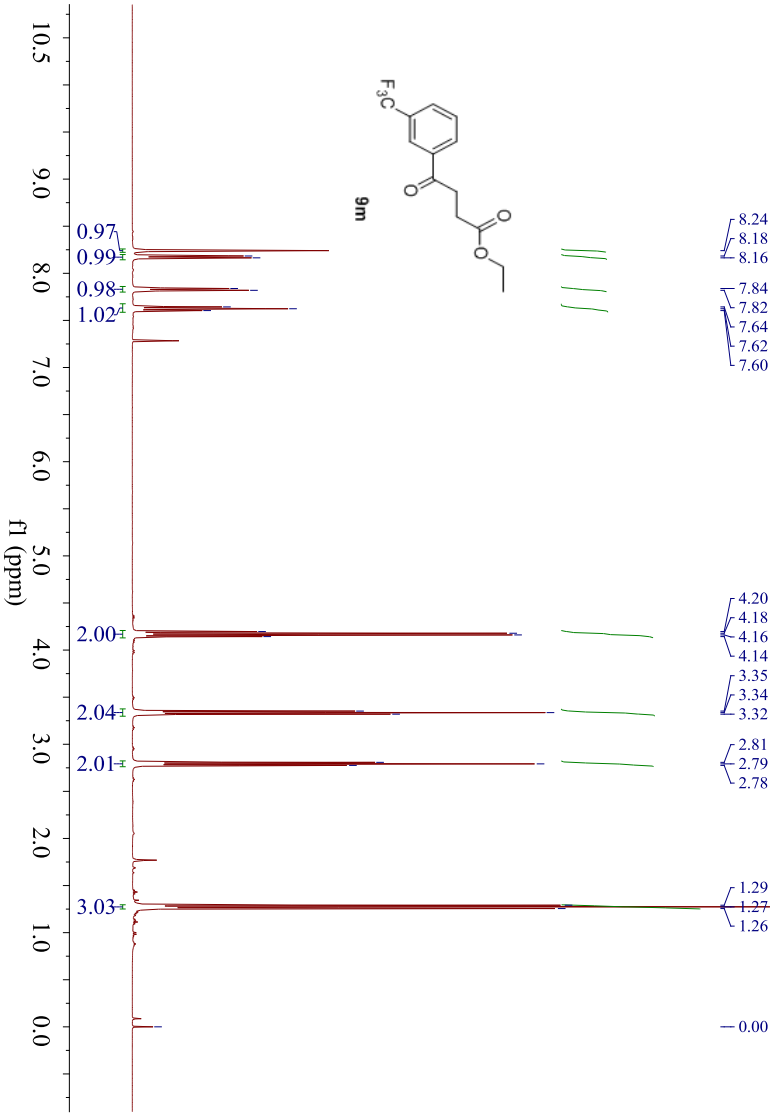

9g
196.54
172.93
162.58
136.07
128.58
128.13
127.36
114.49
77.32
77.00
76.68
70.00
60.50
32.90
28.28
14.10
f1 (ppm)

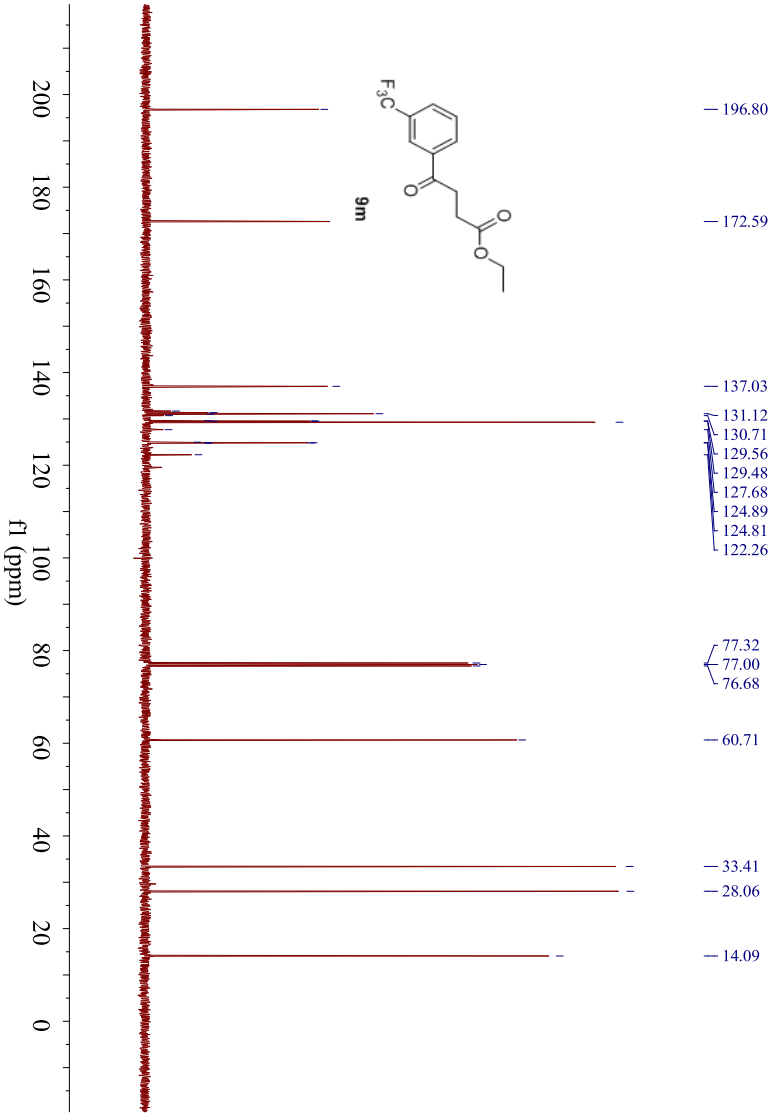

9k
f1 (ppm)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1.96
2.01
1.03
2.03
1.96
2.00
1.96
1.98
3.07
7.96
7.94
6.95
6.93
6.05
6.03
6.02
6.01
6.00
5.44
5.40
5.32
5.30
4.60
4.59
4.16
4.14
4.13
3.27
3.26
3.24
2.75
2.73
2.72
1.28
1.26
1.24
-0.00

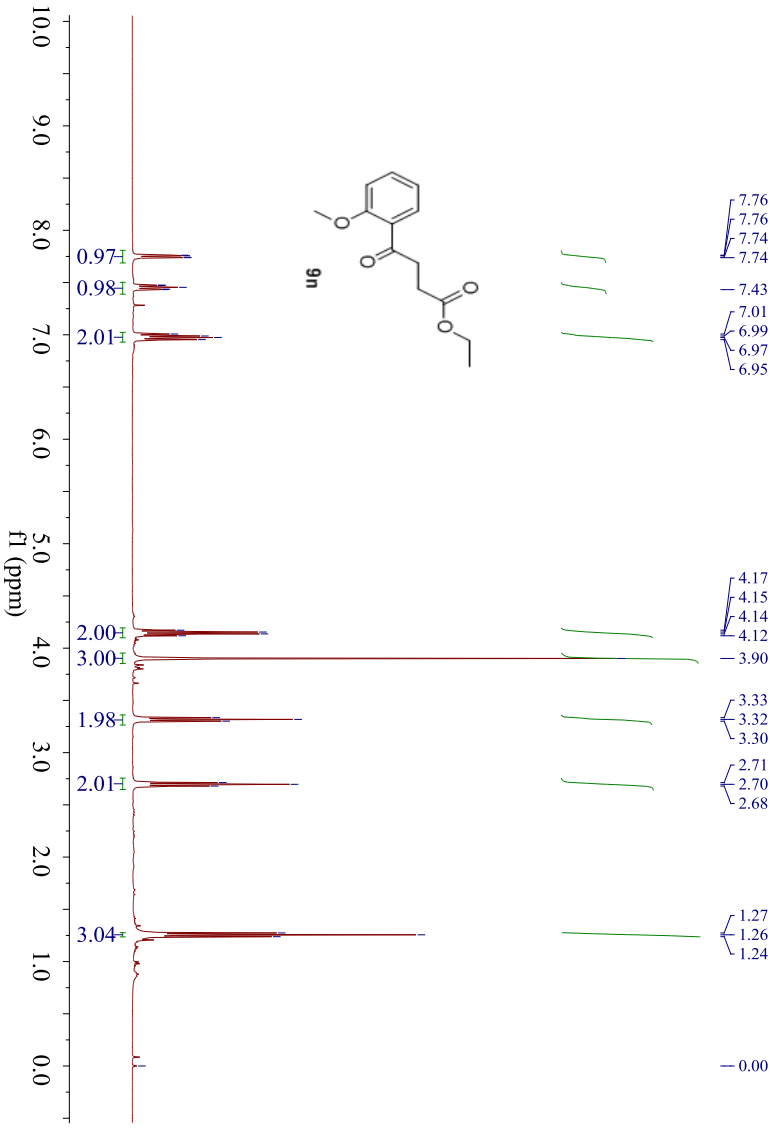

9k
196.50
172.91
162.42
132.38
130.14
129.67
118.03
114.32
77.32
77.00
76.68
68.74
60.46
32.88
28.26
14.08
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

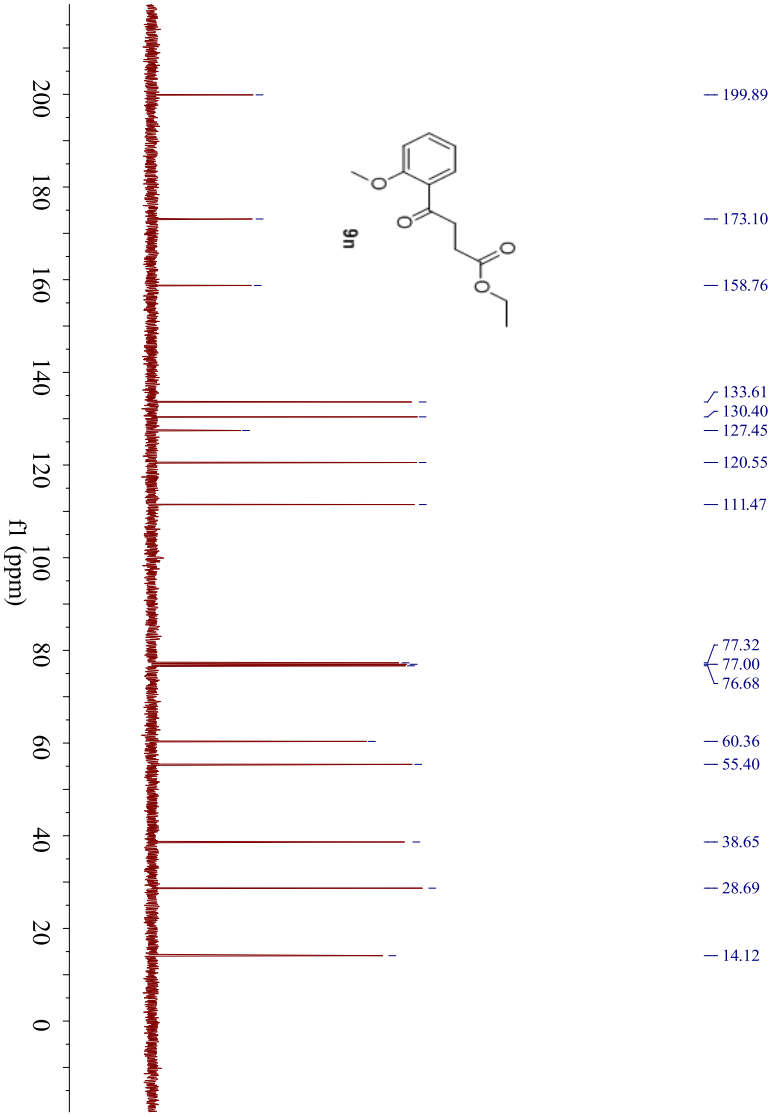

9l
F
O
O
O
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
0.98
0.96
0.99
1.03
2.00
2.01
1.99
3.01
7.78
7.76
7.67
7.65
7.48
7.46
7.46
7.45
7.44
7.43
7.29
7.29
7.28
7.27
7.27
7.25
7.25
4.19
4.17
4.15
4.14
3.30
3.29
3.27
2.78
2.76
2.75
1.29
1.27
1.25
-0.00

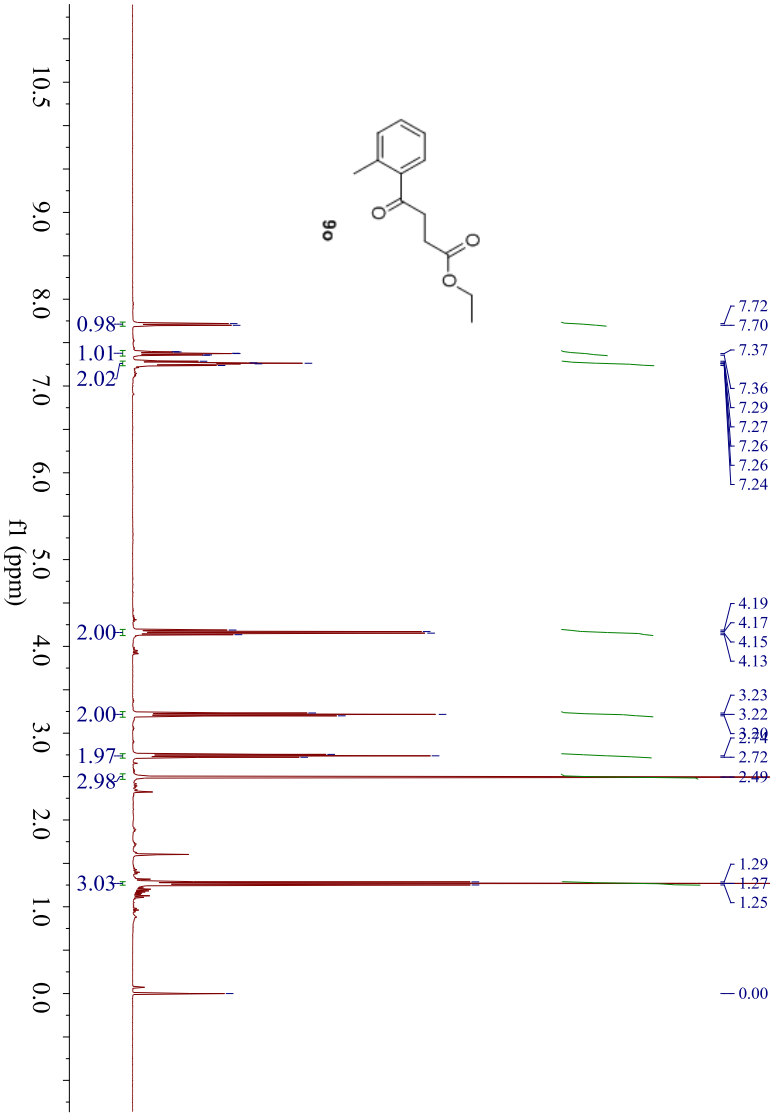

F
O
O
O
9l
196.88
196.86
172.64
164.02
161.55
138.62
138.56
130.20
120.04
114.82
114.59
77.32
77.00
76.68
60.65
33.46
28.12
14.11
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

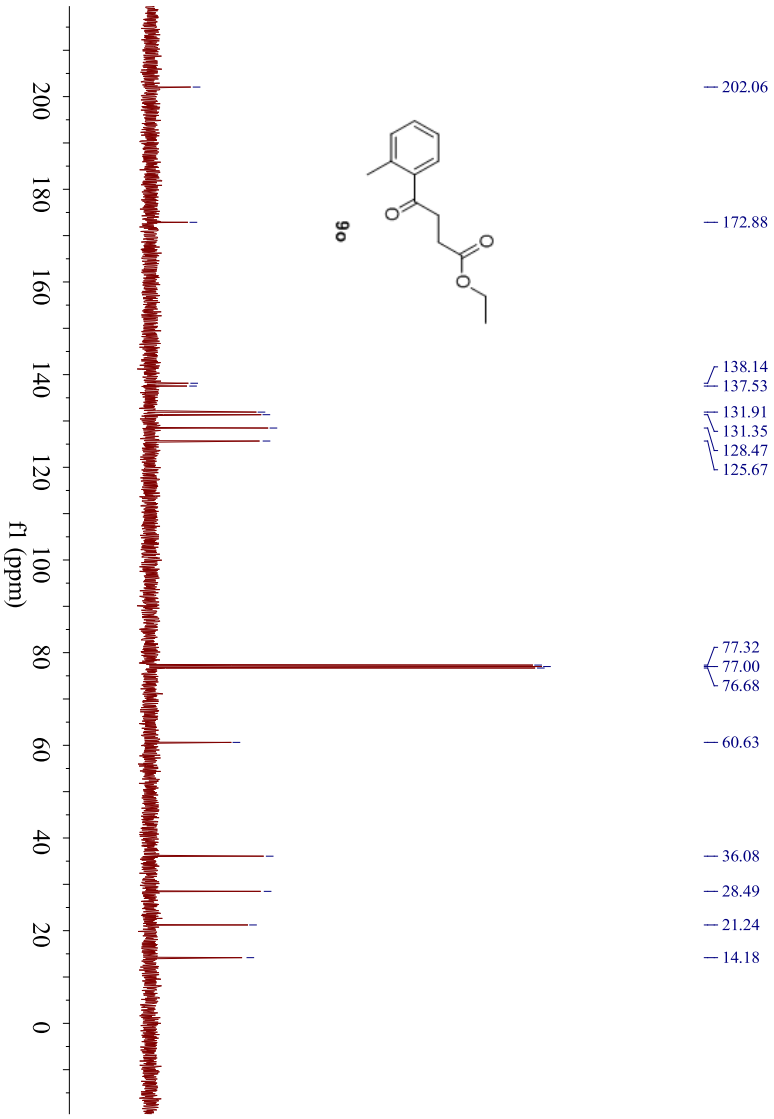

9m
F3C
O
O
O
f1 (ppm)
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.97
0.99
0.98
1.02
2.00
2.04
2.01
3.03
8.24
8.18
8.16
7.84
7.82
7.64
7.62
7.60
4.20
4.18
4.16
4.14
3.35
3.34
3.32
2.81
2.79
2.78
1.29
1.27
1.26
0.00


F3C
O
O
O
9m
196.80
172.59
137.03
131.12
130.71
129.56
129.48
127.68
124.89
124.81
122.26
77.32
77.00
76.68
60.71
33.41
28.06
14.09
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

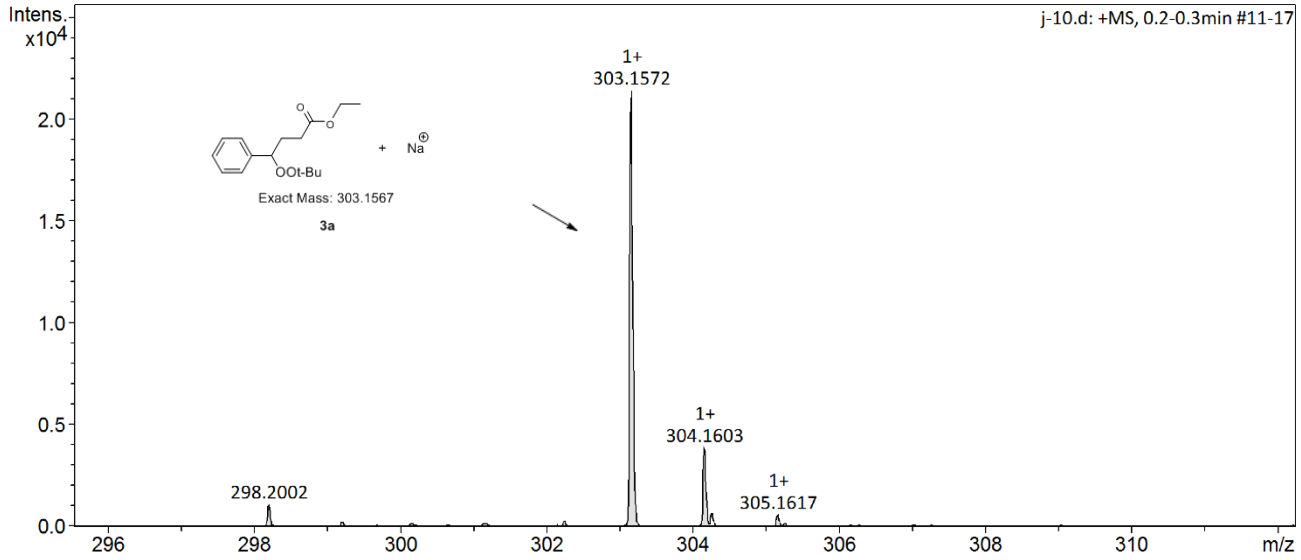

9n
f1 (ppm)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.97
0.98
2.01
2.00
3.00
1.98
2.01
3.04
7.76
7.76
7.74
7.74
7.43
7.01
6.99
6.97
6.95
4.17
4.15
4.14
4.12
3.90
3.33
3.32
3.30
2.71
2.70
2.68
1.27
1.26
1.24
0.00

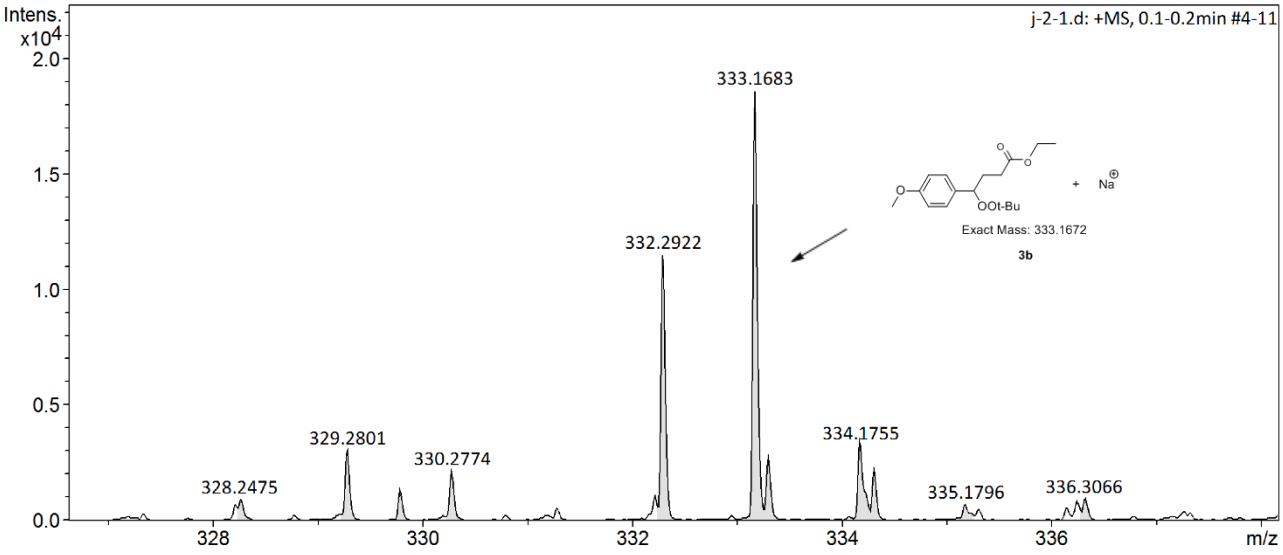

199.89
173.10
158.76
133.61
130.40
127.45
120.55
111.47
77.32
77.00
76.68
60.36
55.40
38.65
28.69
14.12
9n
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

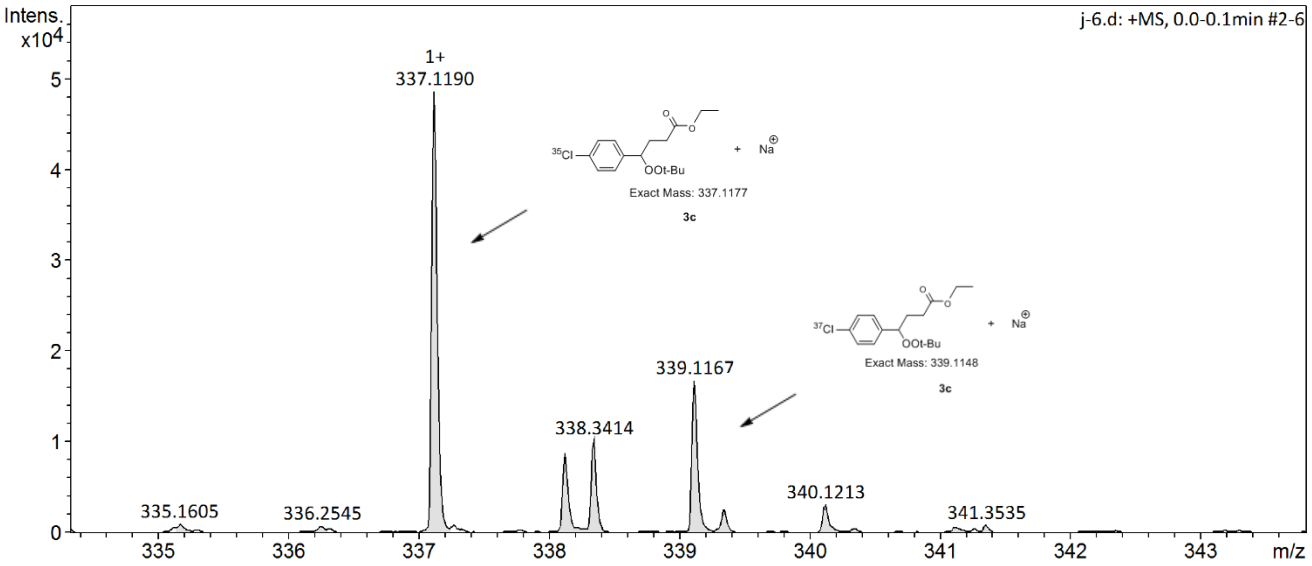

9o
f1 (ppm)
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.98
1.01
2.02
2.00
2.00
1.97
2.98
3.03
7.72
7.70
7.37
7.36
7.29
7.27
7.26
7.26
7.24
4.19
4.17
4.15
4.13
3.23
3.22
2.72
2.49
1.29
1.27
1.25
0.00

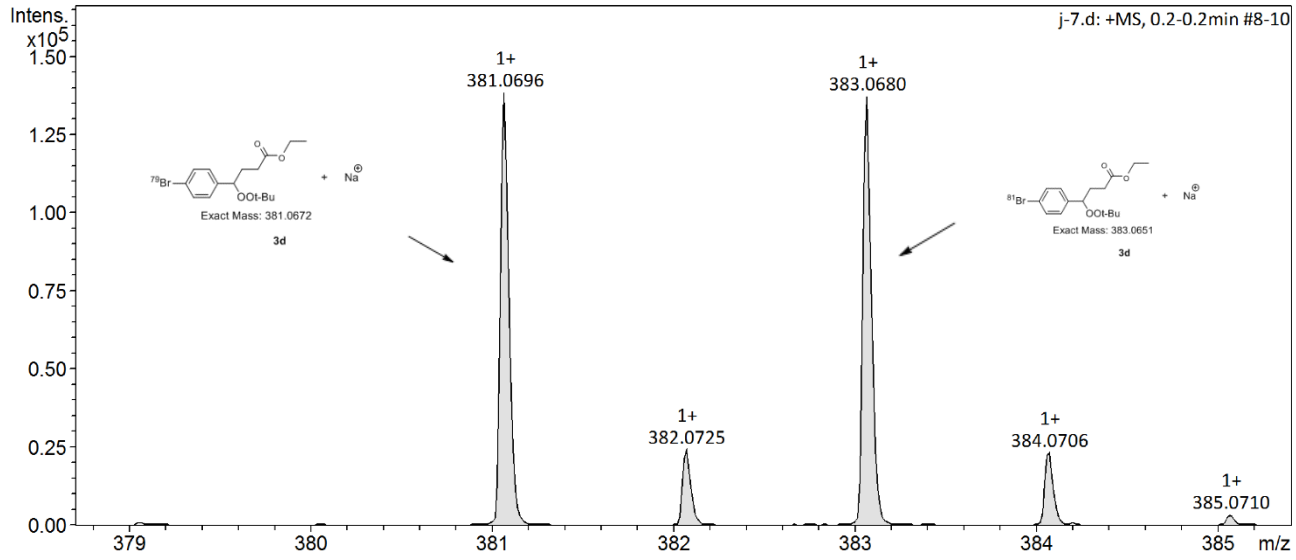

90
202.06
172.88
138.14
137.53
131.91
131.35
128.47
125.67
77.32
77.00
76.68
60.63
36.08
28.49
21.24
14.18
f1 (ppm)
200
180
160
140
120
100
80
60
40
20
0

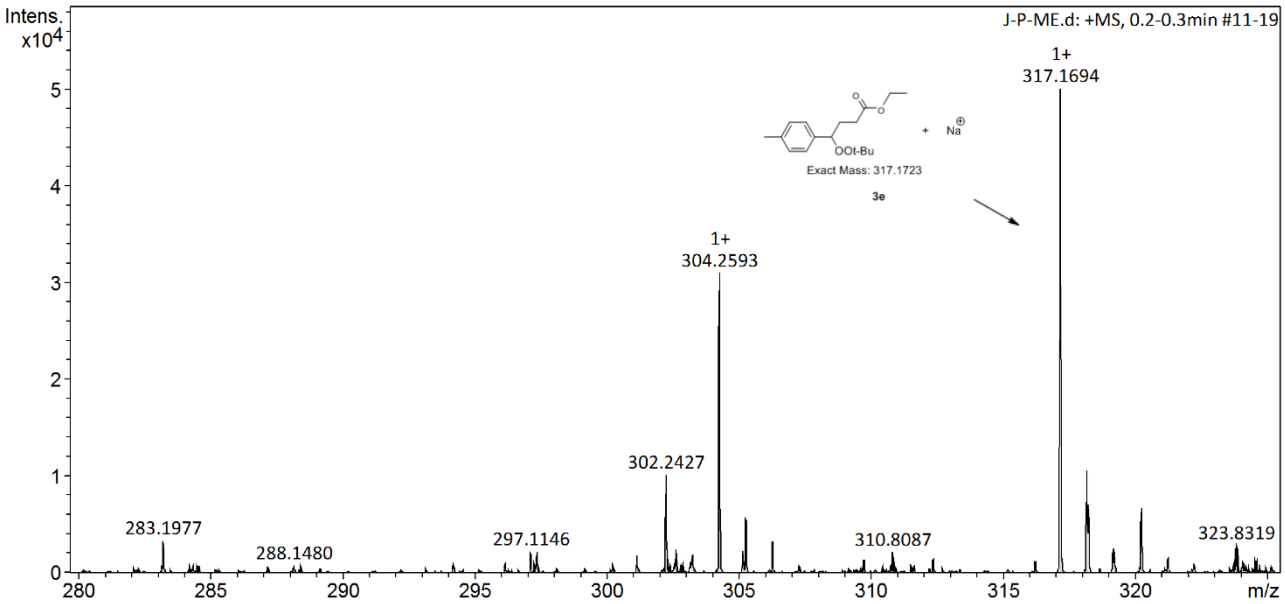
MS Spectroscopic Data for Products

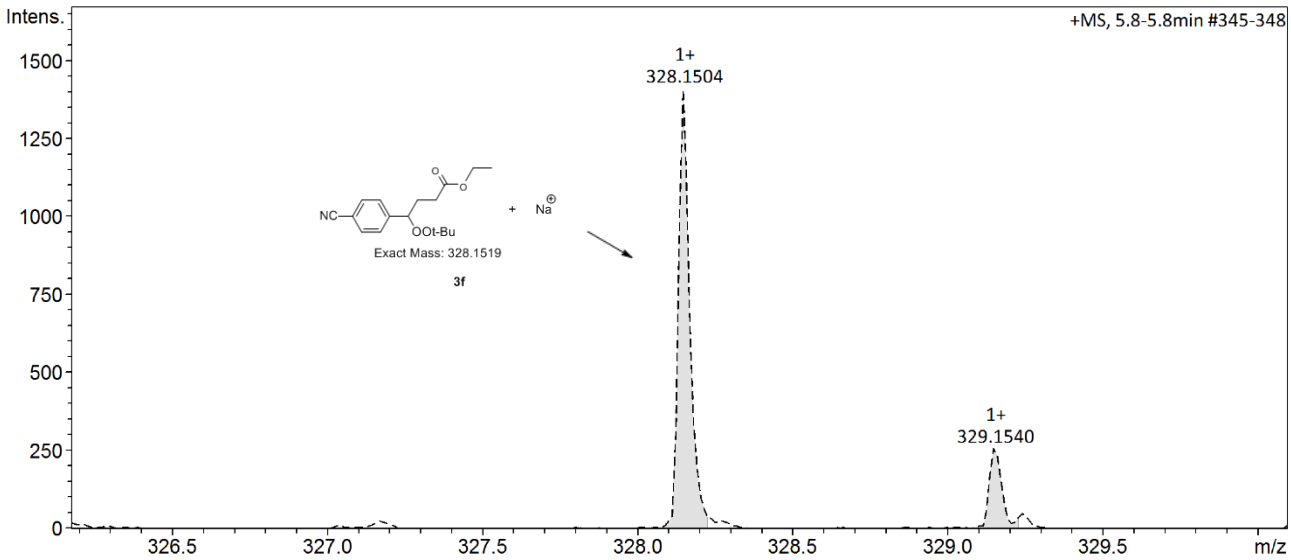


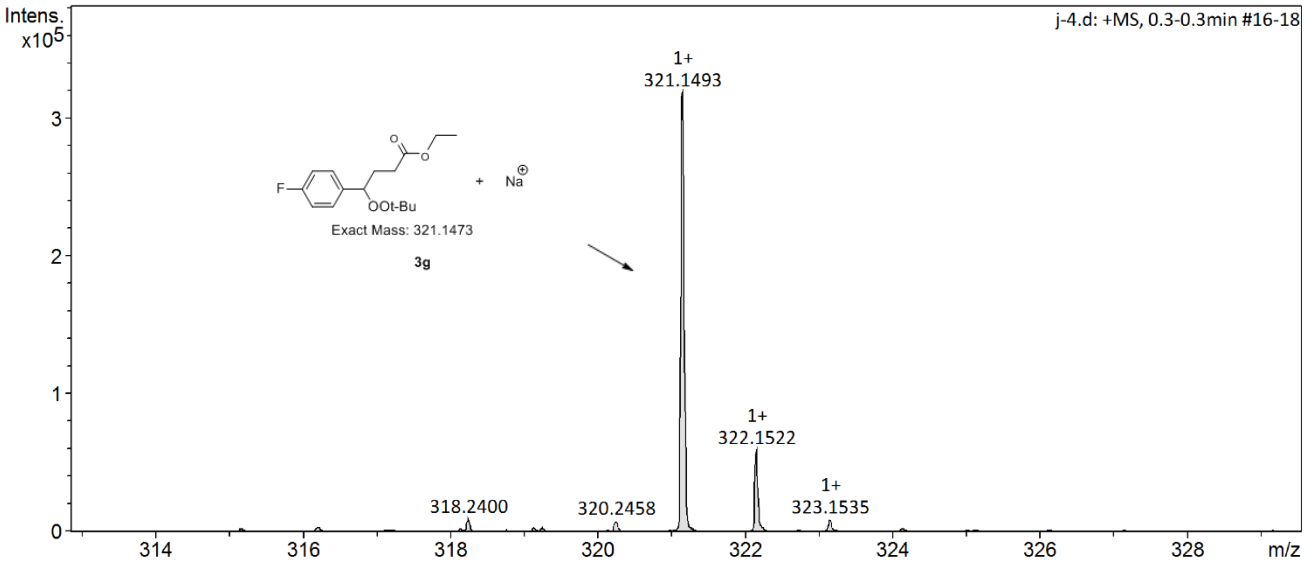


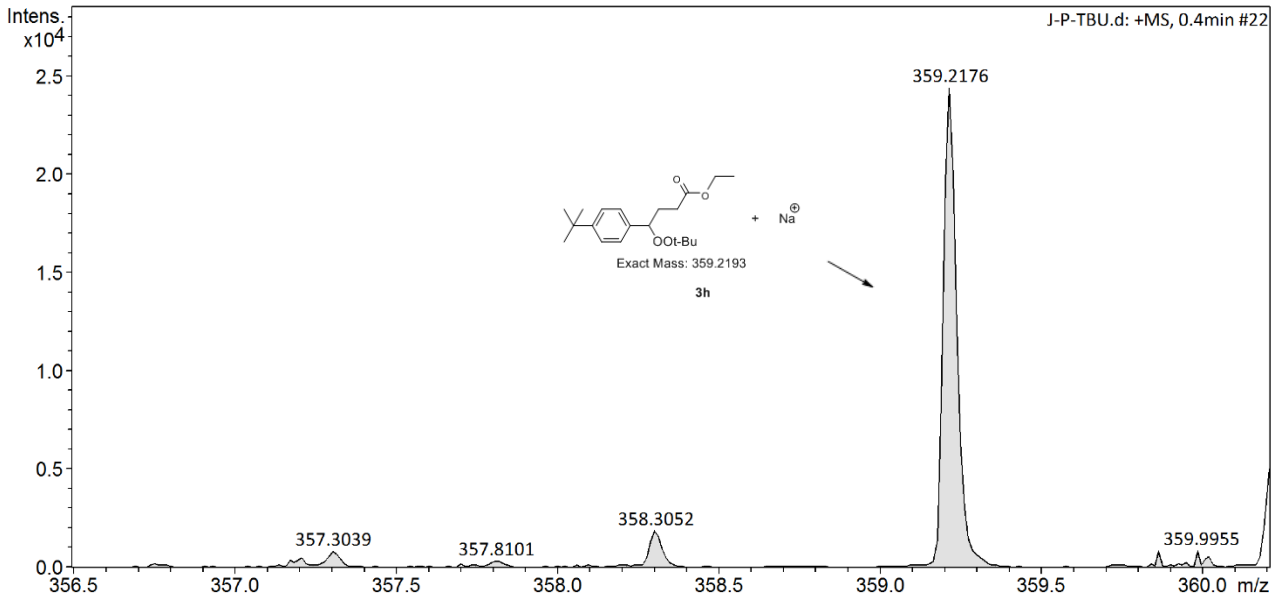

Intens.
x10^4
j-6.d: +MS, 0.0-0.1min #2-6
1+
337.1190
339.1167
338.3414
340.1213
335.1605
336.2545
341.3535
Exact Mass: 337.1177
3c
Exact Mass: 339.1148
3c
m/z

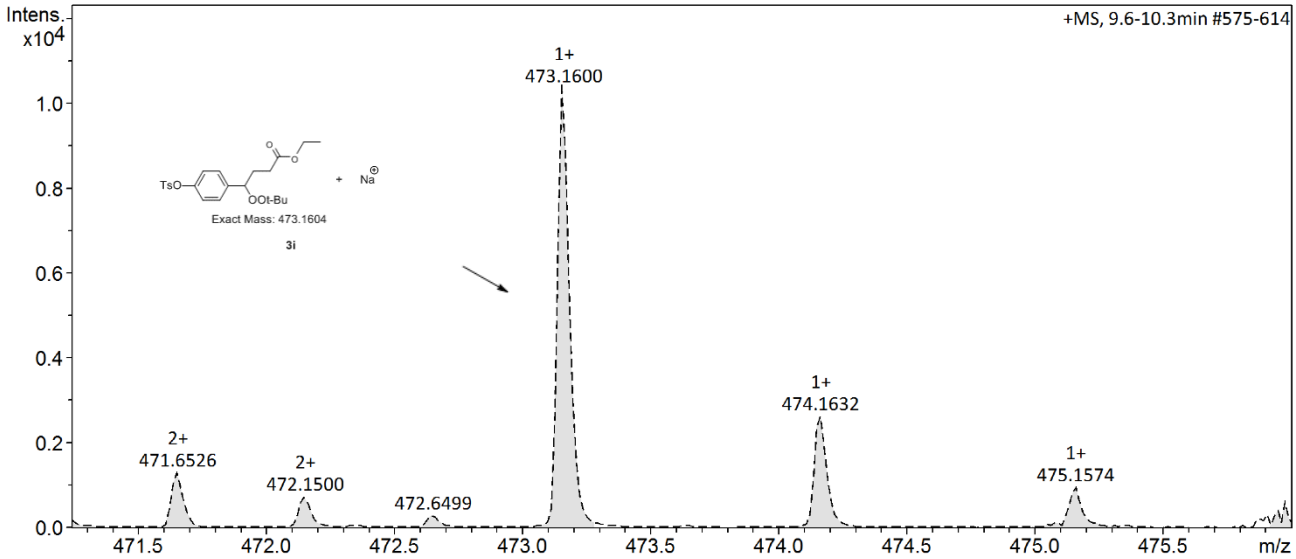

Intens.
x10^5
j-7.d: +MS, 0.2-0.2min #8-10
1+
381.0696
1+
383.0680
1+
382.0725
1+
384.0706
1+
385.0710
Exact Mass: 381.0672
3d
Exact Mass: 383.0651
3d
m/z

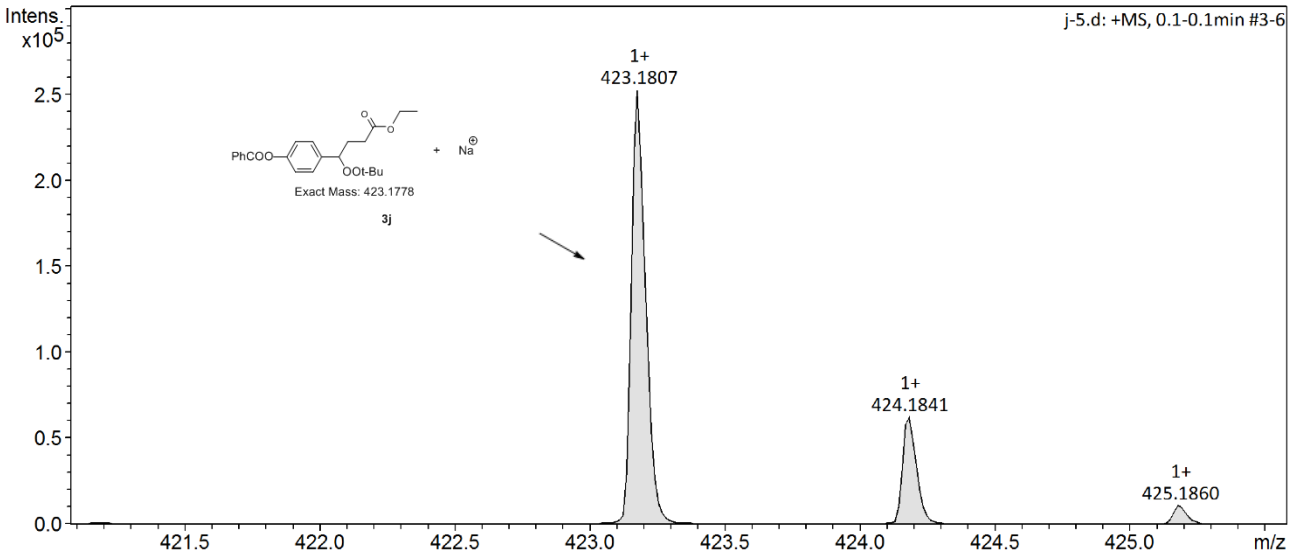

Intens.
x10^4
J-P-ME.d: +MS, 0.2-0.3min #11-19
1+
317.1694
1+
304.2593
302.2427
283.1977
288.1480
297.1146
310.8087
323.8319
OOt-Bu
Exact Mass: 317.1723
3e
m/z

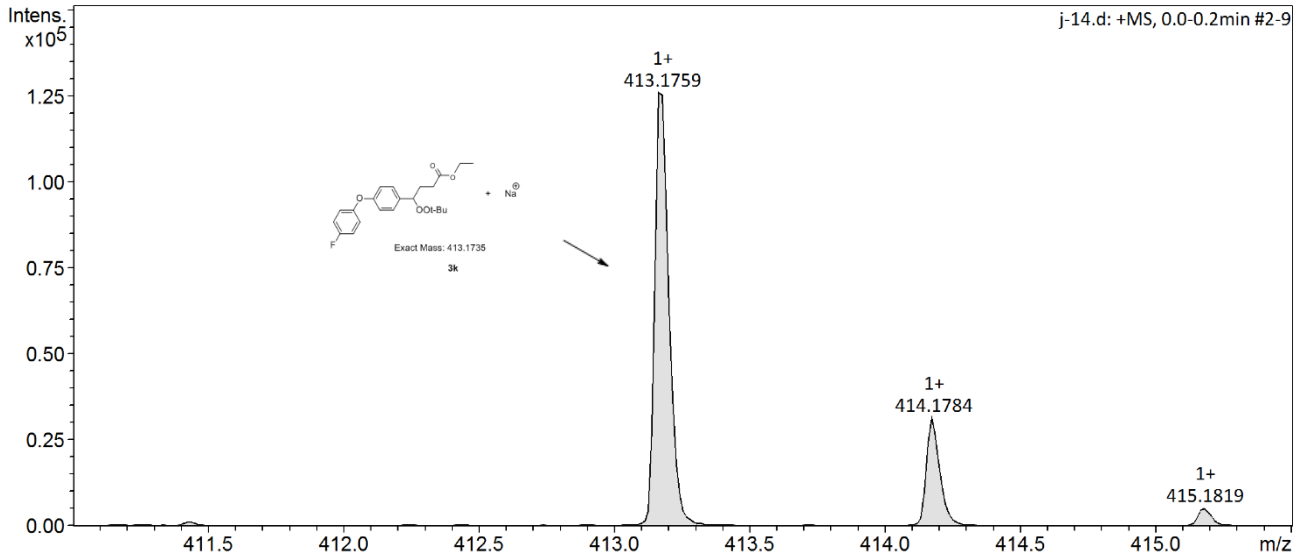

Intens.
+MS, 5.8-5.8min #345-348
1+
328.1504
1+
329.1540
NC
OOt-Bu
Exact Mass: 328.1519
3f
m/z

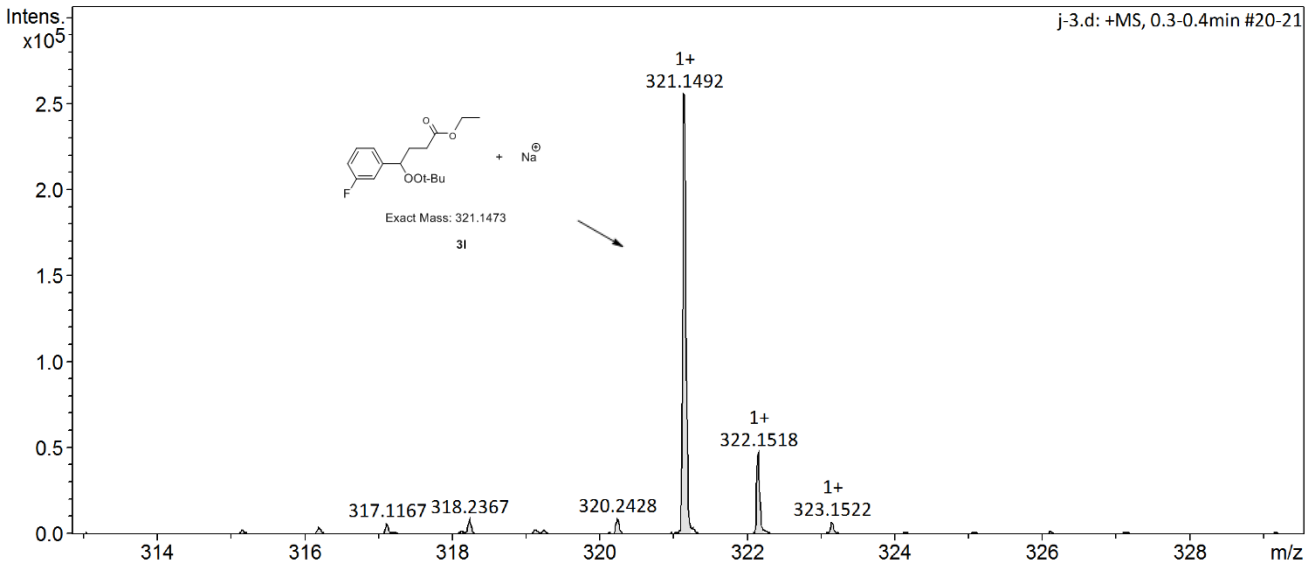

Intens.
x10^5
j-4.d: +MS, 0.3-0.3min #16-18
1+
321.1493
F
OOt-Bu
+ Na
Exact Mass: 321.1473
3g
1+
322.1522
1+
323.1535
318.2400
320.2458
m/z

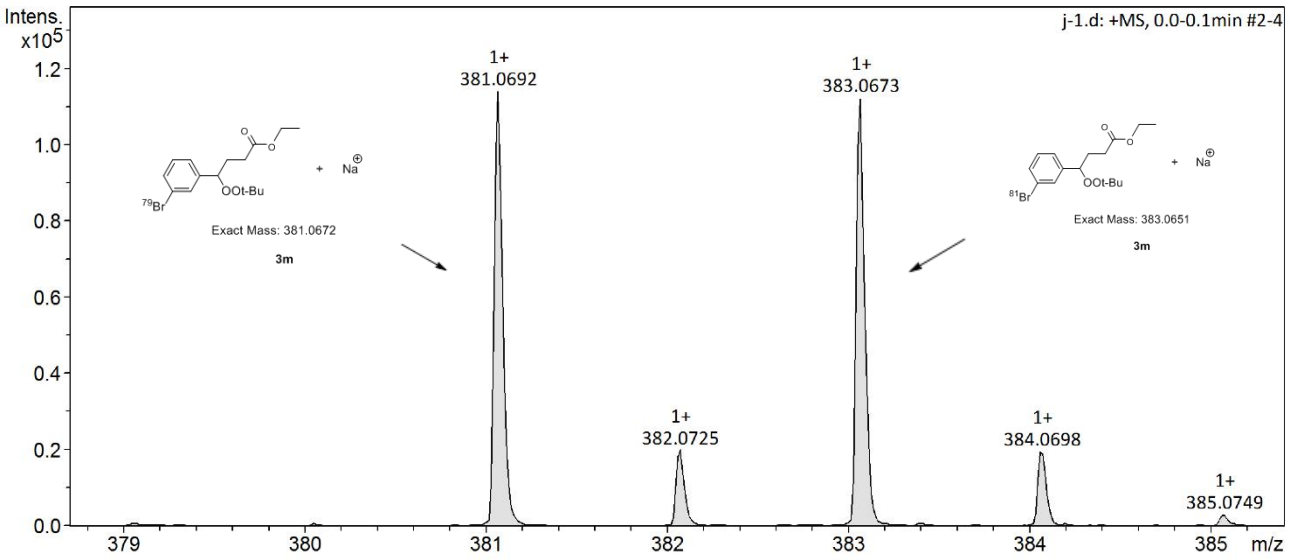

Intens.
x10^4
J-P-TBU.d: +MS, 0.4min #22
359.2176
OOt-Bu
+ Na
Exact Mass: 359.2193
3h
358.3052
357.3039
357.8101
359.9955
m/z

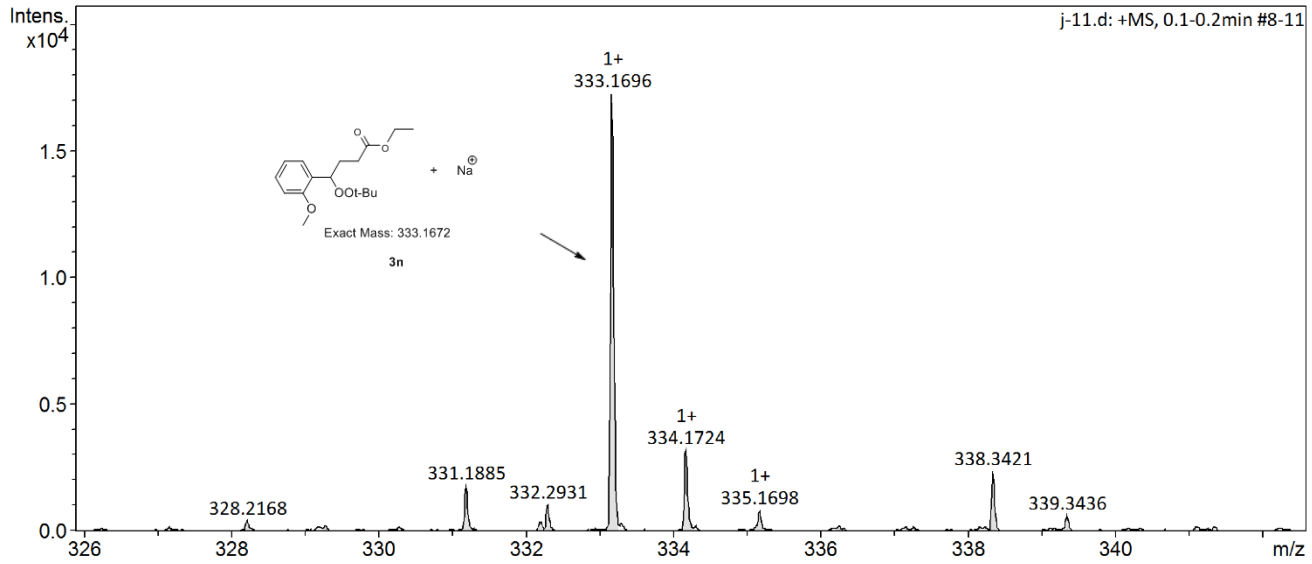

Intens.
x10^4
+MS, 9.6-10.3min #575-614
1+
473.1600
TsO
OOt-Bu
+ Na
Exact Mass: 473.1604
3i
1+
474.1632
2+
471.6526
2+
472.1500
472.6499
1+
475.1574
m/z

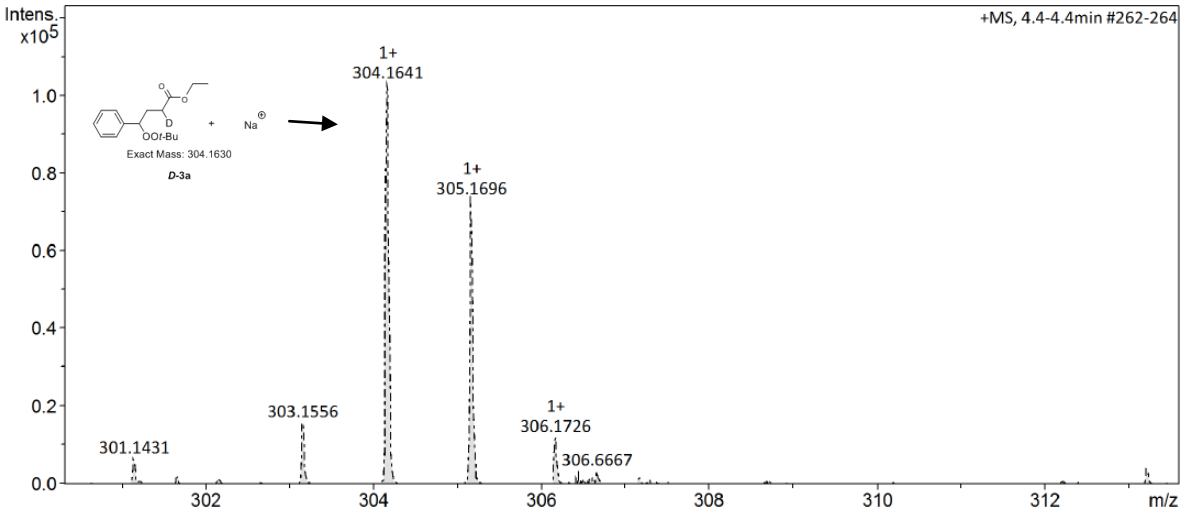

Intens.
x10^5
j-5.d: +MS, 0.1-0.1min #3-6
1+
423.1807
PhCOO
OOt-Bu
+ Na
Exact Mass: 423.1778
3j
1+
424.1841
1+
425.1860
m/z

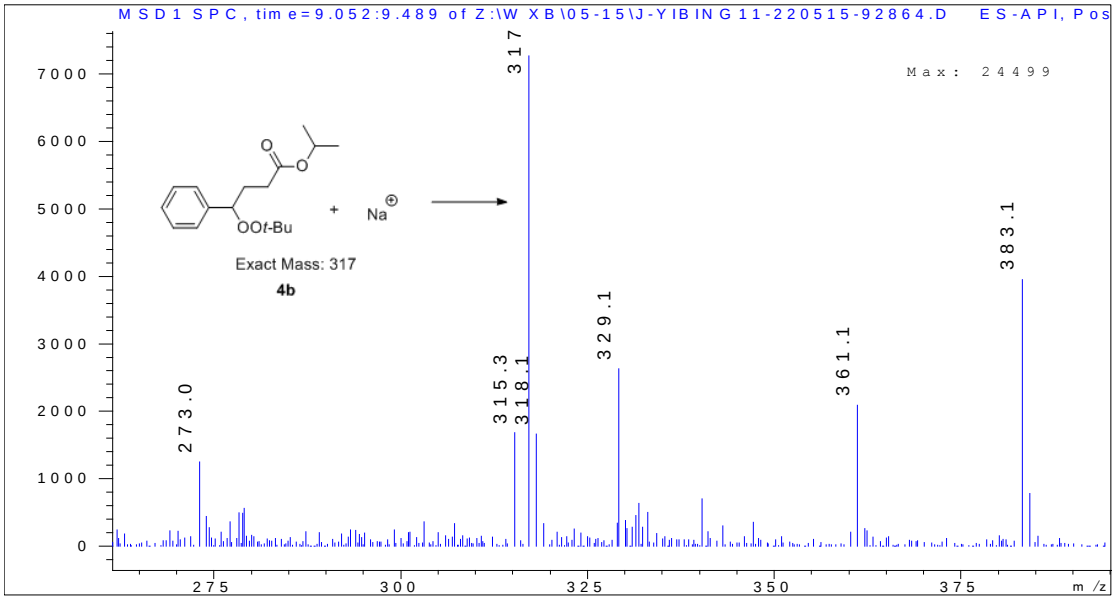

Intens.
x10^5
j-14.d: +MS, 0.0-0.2min #2-9
1+
413.1759
1+
414.1784
1+
415.1819
Exact Mass: 413.1735
3k
m/z

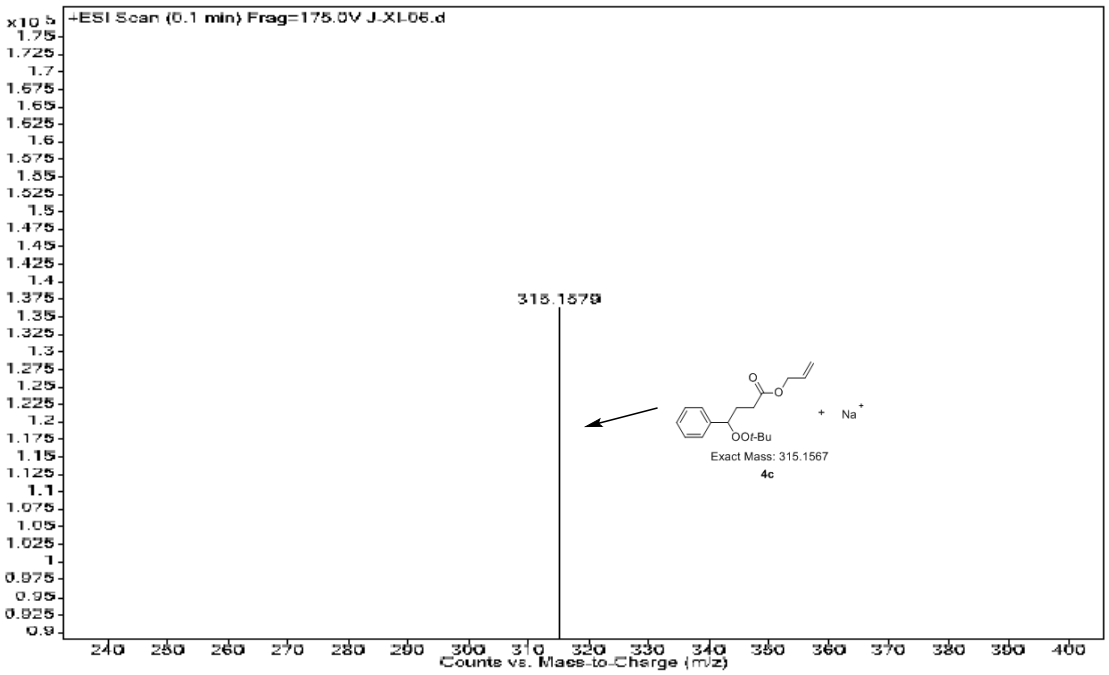

Intens.
x10^5
j-3.d: +MS, 0.3-0.4min #20-21
1+
321.1492
1+
322.1518
1+
323.1522
317.1167
318.2367
320.2428
Exact Mass: 321.1473
3l
m/z

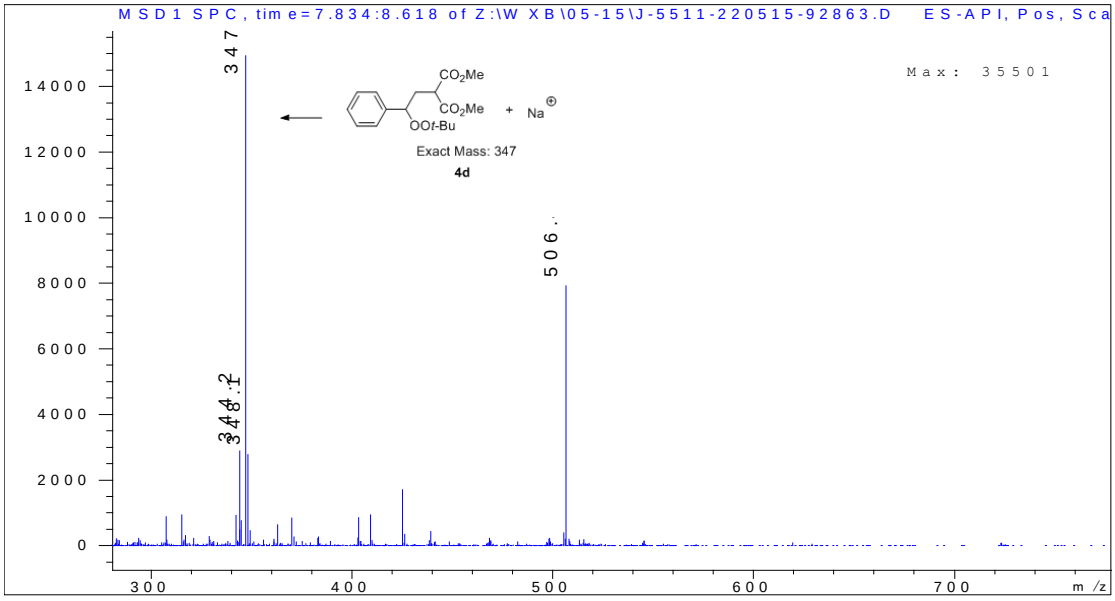

Intens.
x10^5
j-1.d: +MS, 0.0-0.1min #2-4
1+
381.0692
1+
383.0673
1+
382.0725
1+
384.0698
1+
385.0749
Exact Mass: 381.0672
3m
Exact Mass: 383.0651
3m
m/z

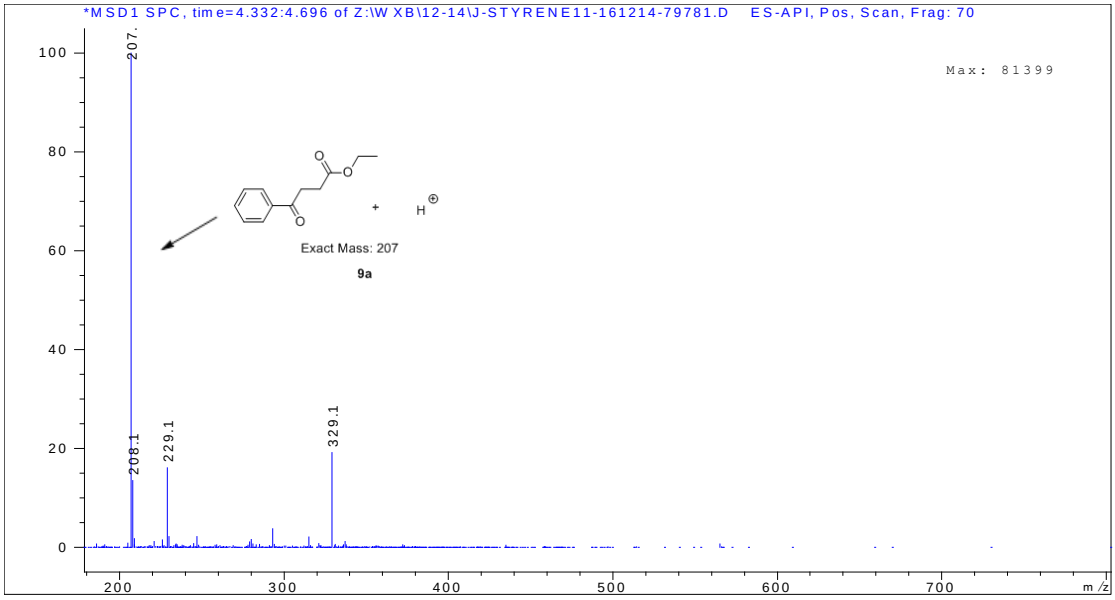

Intens.
x10^4
j-11.d: +MS, 0.1-0.2min #8-11
1+
333.1696
1+
334.1724
1+
335.1698
331.1885
332.2931
328.2168
338.3421
339.3436
Exact Mass: 333.1672
3n
m/z

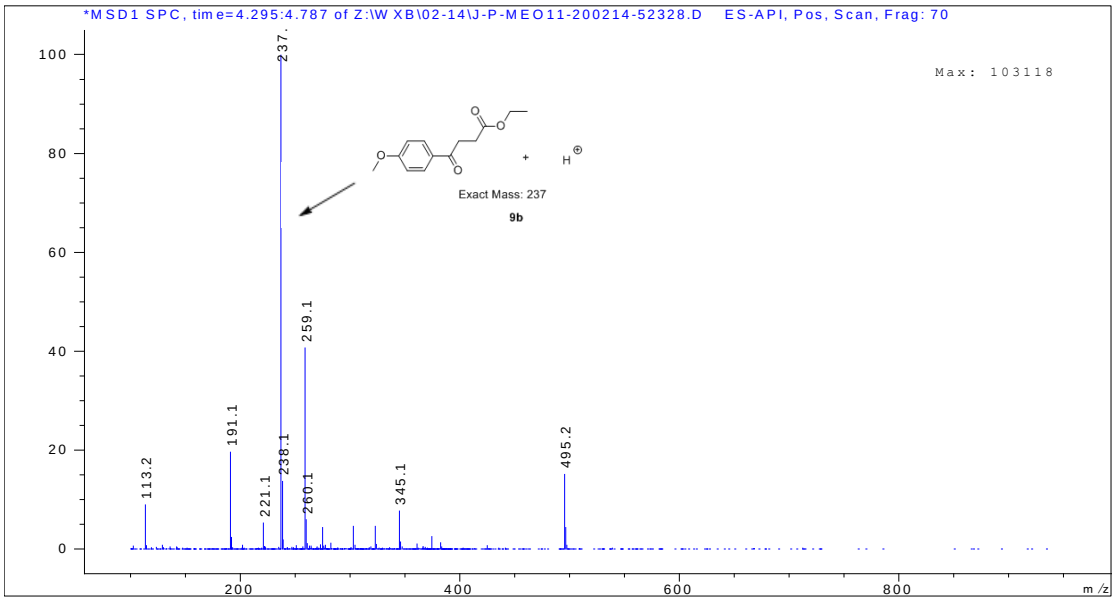

Intens.
x10^5
+MS, 4.4-4.4min #262-264
1+
304.1641
1+
305.1696
1+
306.1726
303.1556
301.1431
306.6667
Exact Mass: 304.1630
D-3a
1.0
0.8
0.6
0.4
0.2
0.0
302
304
306
308
310
312
m/z

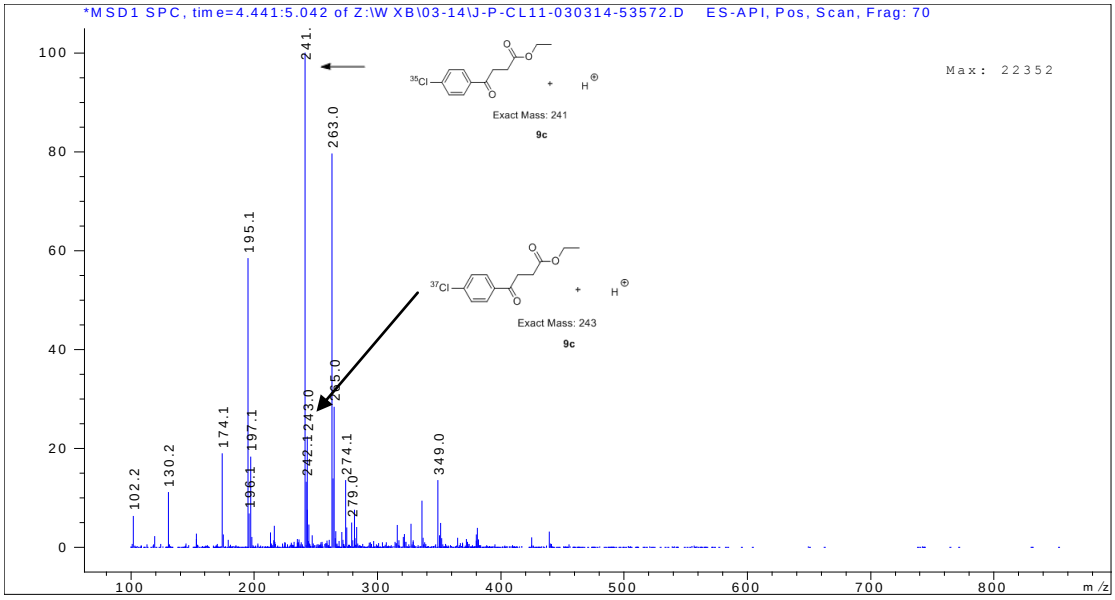

MSD1 SPC, time=9.052:9.489 of Z:\WXB\05-15\J-YIBING11-220515-92864.D ES-API, Pos
Max: 24499
317
383.1
329.1
361.1
315.3
318.1
273.0
Exact Mass: 317
4b
7000
6000
5000
4000
3000
2000
1000
0
275
300
325
350
375
m/z

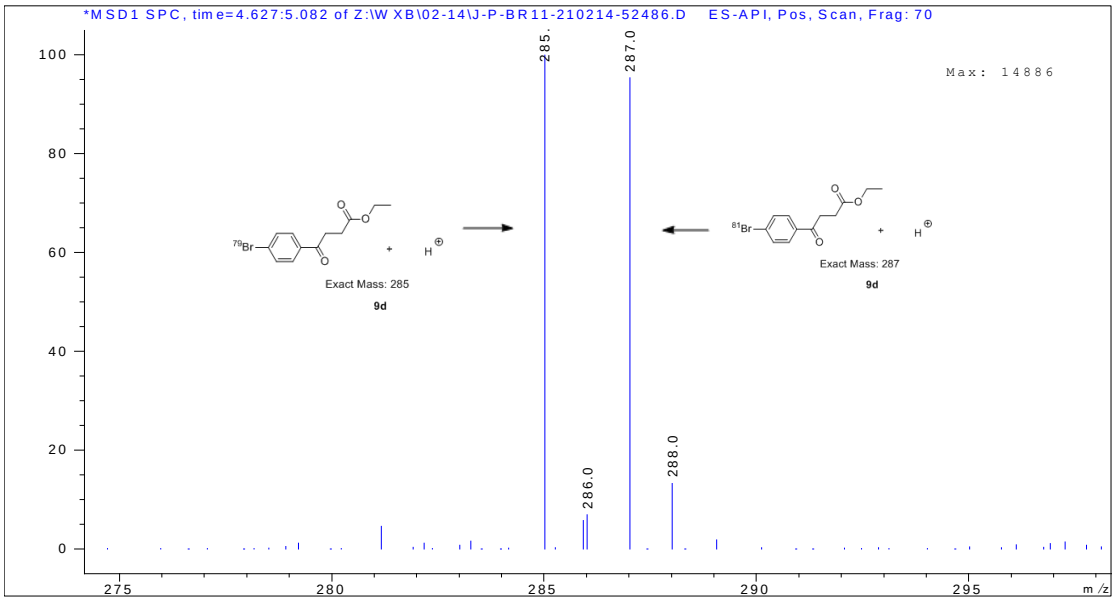

+ESI Scan (0.1 min) Frag=175.0V J-XI-06.d
x10 5
315.1579
OOt-Bu
+ Na+
Exact Mass: 315.1567
4c
Counts vs. Mass-to-Charge (m/z)

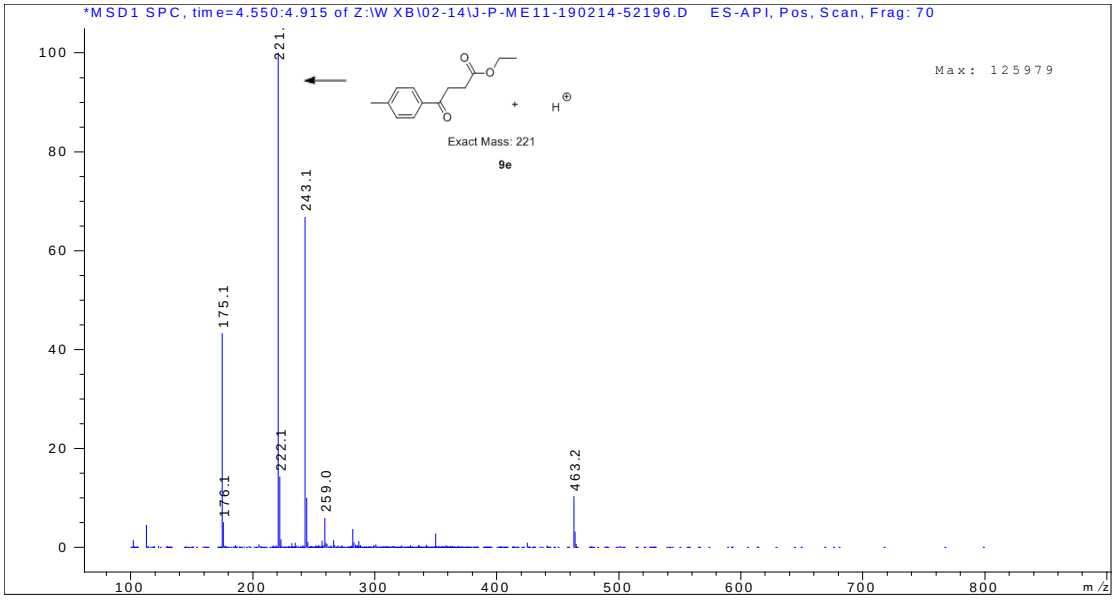

MSD1 SPC, time=7.834:8.618 of Z:\WXB\05-15\J-5511-220515-92863.D ES-API, Pos, Sca
Max: 35501
347
506
344
CO2Me
CO2Me
OOt-Bu
+ Na
Exact Mass: 347
4d
m/z

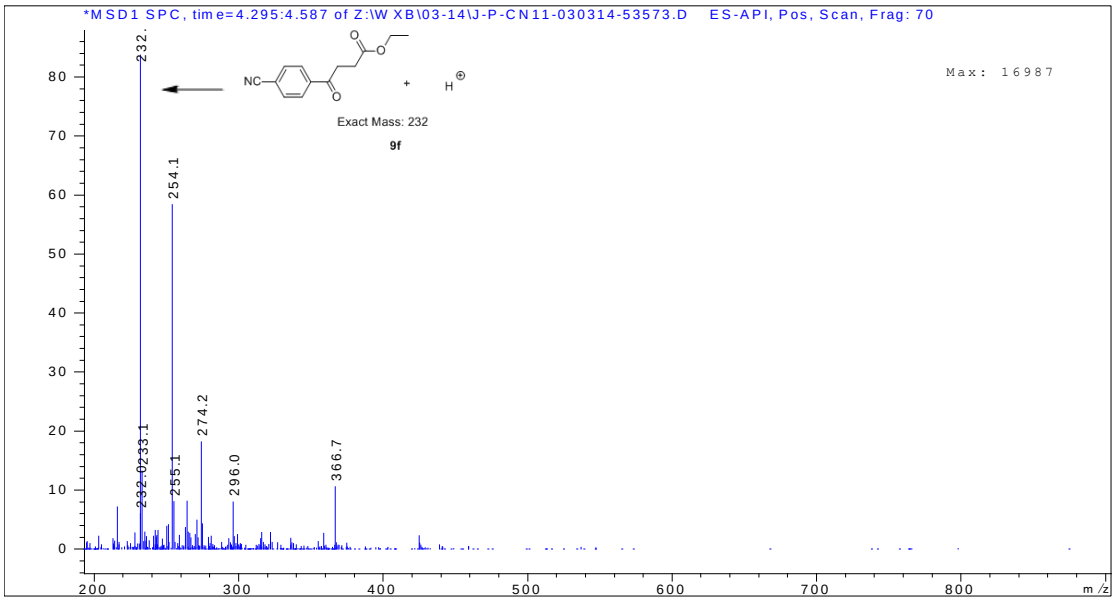

*MSD1 SPC, time=4.332:4.696 of Z:\W XB\12-14\J-STYRENE11-161214-79781.D ES-API, Pos, Scan, Frag: 70
Max: 81399
207.
208.1
229.1
329.1
Exact Mass: 207
9a
m/z

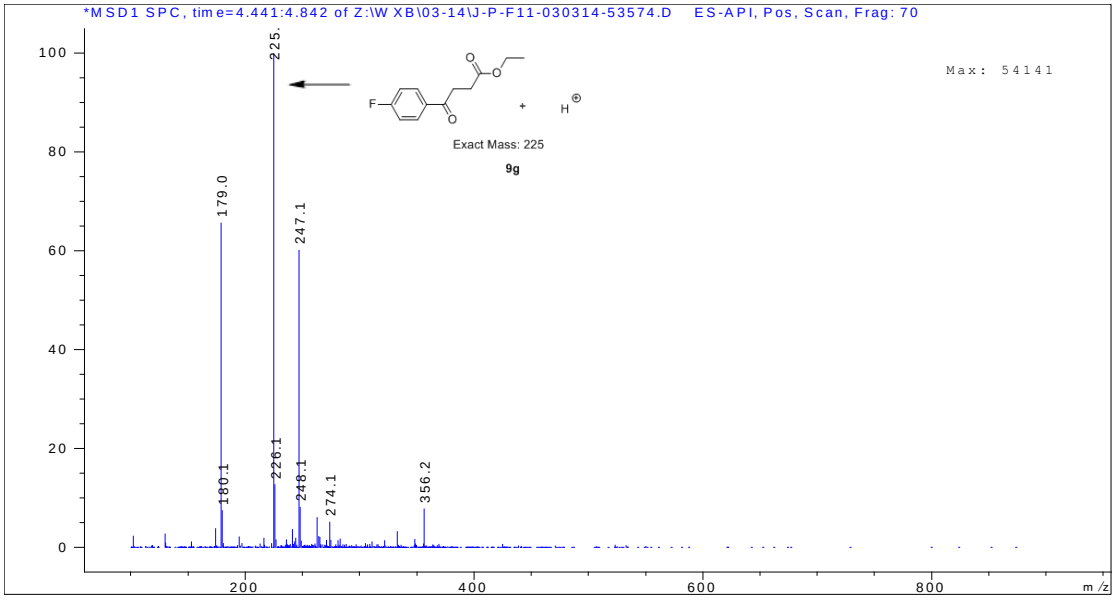

*MSD1 SPC, time=4.295:4.787 of Z:\W XB\02-14\J-P-MEO11-200214-52328.D ES-API, Pos, Scan, Frag: 70
Max: 103118
237.
113.2
191.1
221.1
238.1
259.1
260.1
345.1
495.2
Exact Mass: 237
9b
m/z

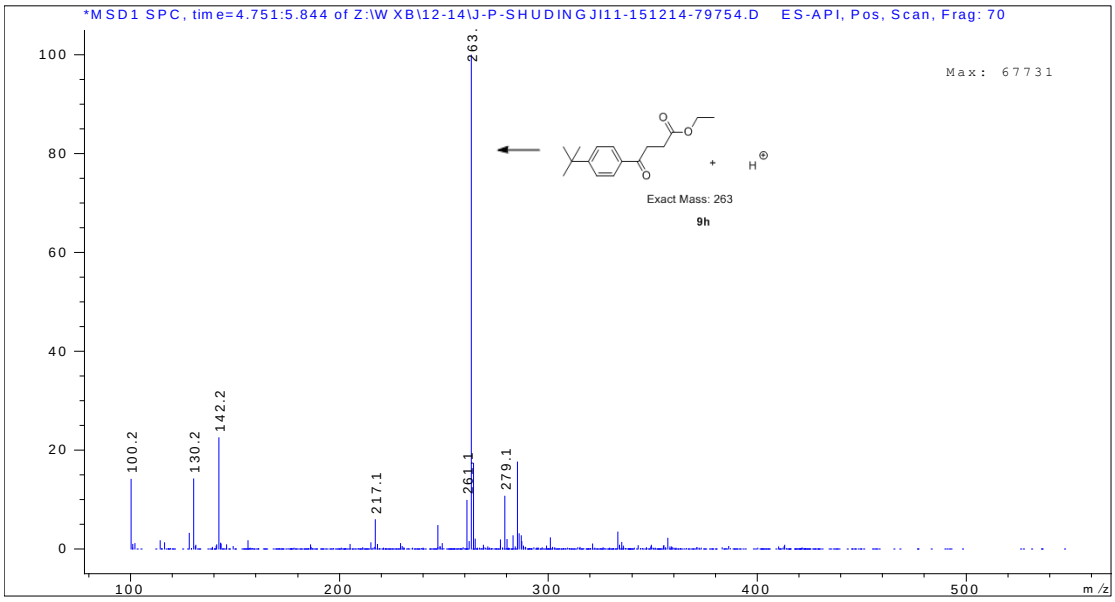

*MSD1 SPC, time=4.441:5.042 of Z:\WXB\03-14\J-P-CL11-030314-53572.D ES-API, Pos, Scan, Frag: 70
Max: 22352
241.
263.0
195.1
174.1
197.1
130.2
102.2
243.0
265.0
274.1
279.0
349.0
Exact Mass: 241
9c
Exact Mass: 243
9c
m/z

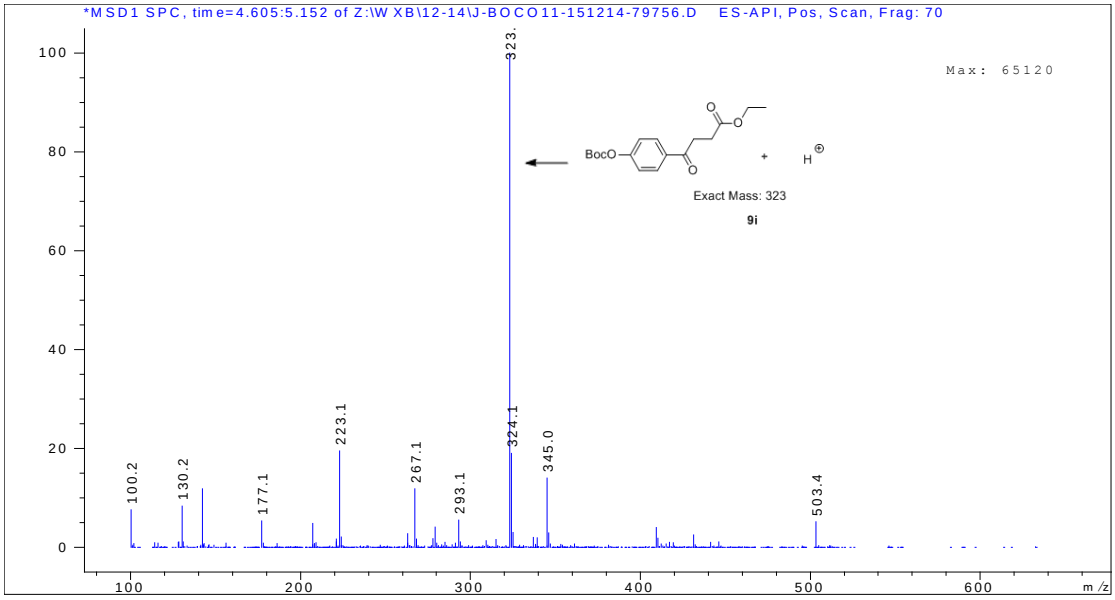

*MSD1 SPC, time=4.627:5.082 of Z:\WXB\02-14\J-P-BR11-210214-52486.D ES-API, Pos, Scan, Frag: 70
Max: 14886
285.
287.0
286.0
288.0
Exact Mass: 285
9d
Exact Mass: 287
9d
m/z


*MSD1 SPC, time=4.550:4.915 of Z:\WXB\02-14\J-P-ME11-190214-52196.D ES-API, Pos, Scan, Frag: 70
Max: 125979
Exact Mass: 221
9e
221.
243.1
175.1
222.1
259.0
176.1
463.2
m/z


*MSD1 SPC, time=4.295:4.587 of Z:\WXB\03-14\J-P-CN11-030314-53573.D ES-API, Pos, Scan, Frag: 70
Max: 16987
Exact Mass: 232
9f
232.
254.1
274.2
233.1
255.1
296.0
366.7
m/z


*MSD1 SPC, time=4.441:4.842 of Z:\WXB\03-14\J-P-F11-030314-53574.D ES-API, Pos, Scan, Frag: 70
Max: 54141
225.
179.0
247.1
226.1
180.1
248.1
274.1
356.2
Exact Mass: 225
9g
m/z


*MSD1 SPC, time=4.751:5.844 of Z:\WXB\12-14\J-P-SHUDINGJI11-151214-79754.D ES-API, Pos, Scan, Frag: 70
Max: 67731
263.
142.2
100.2
130.2
217.1
261.1
279.1
Exact Mass: 263
9h
m/z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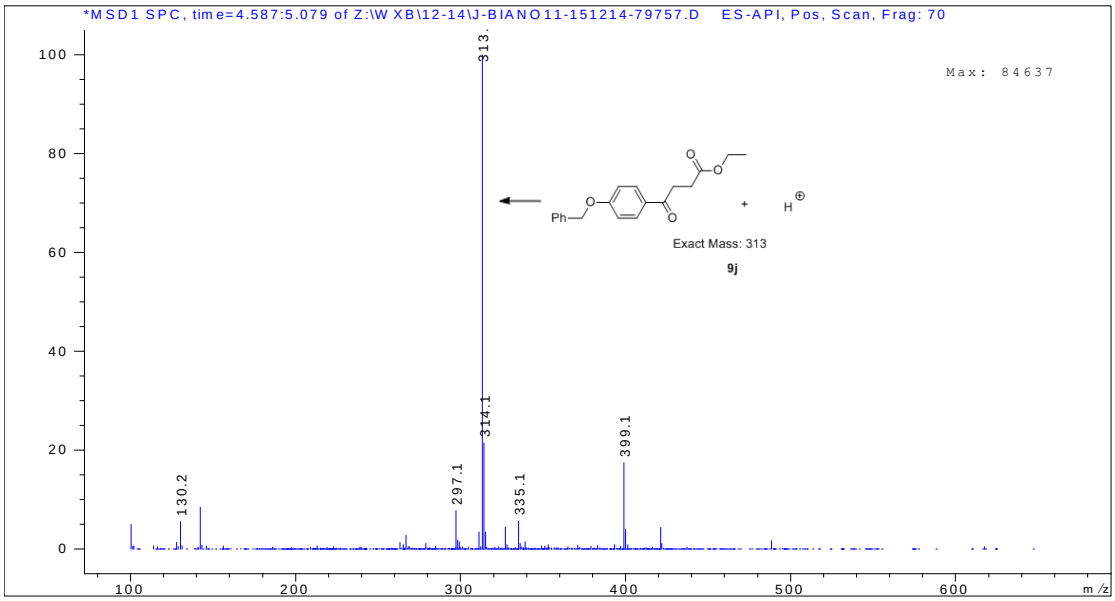
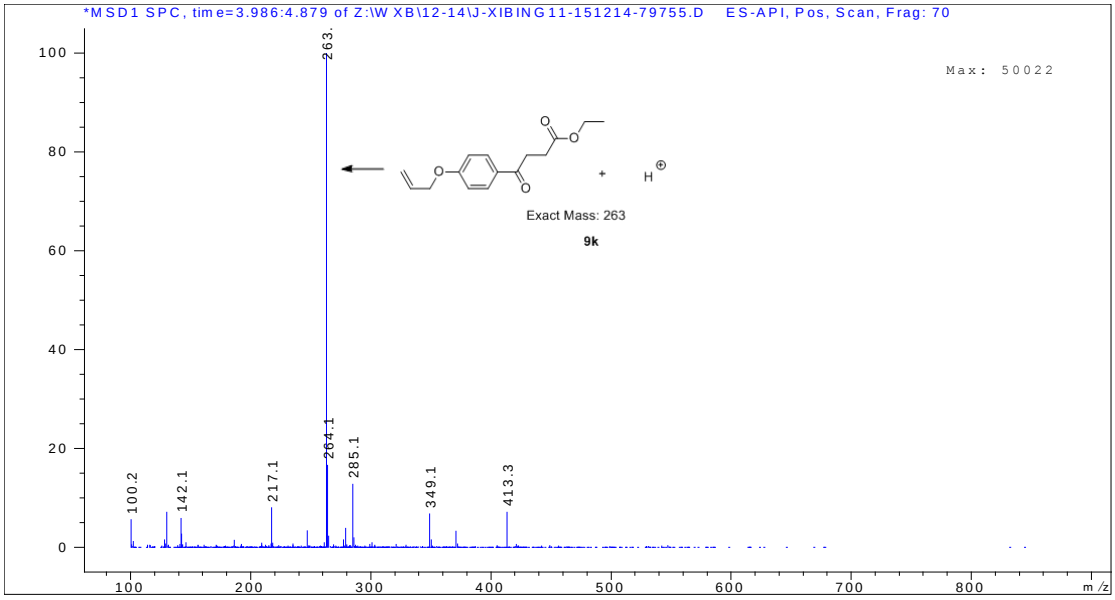
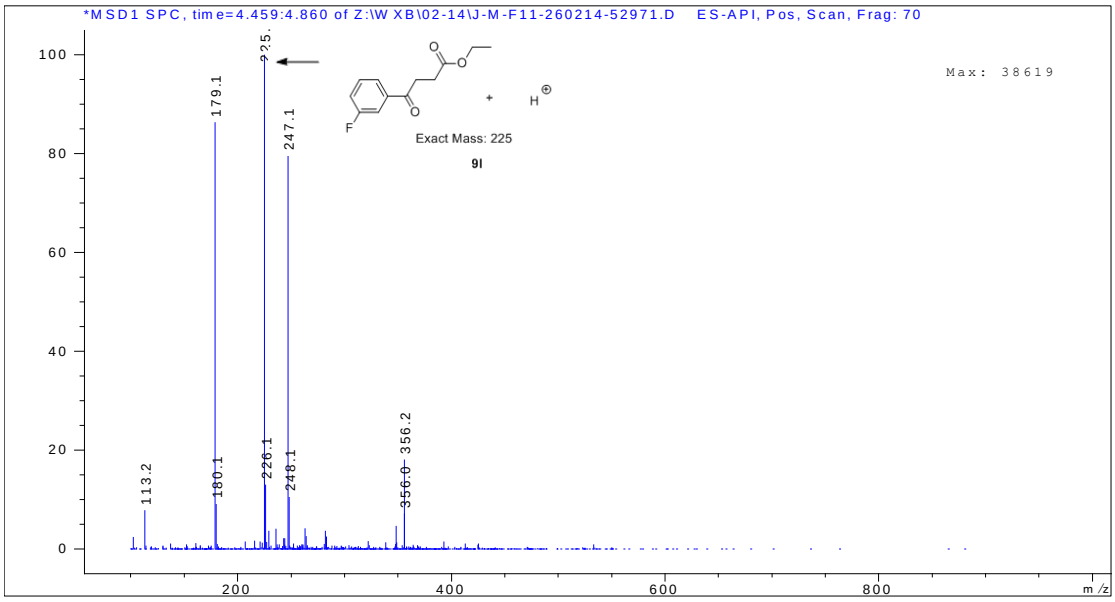
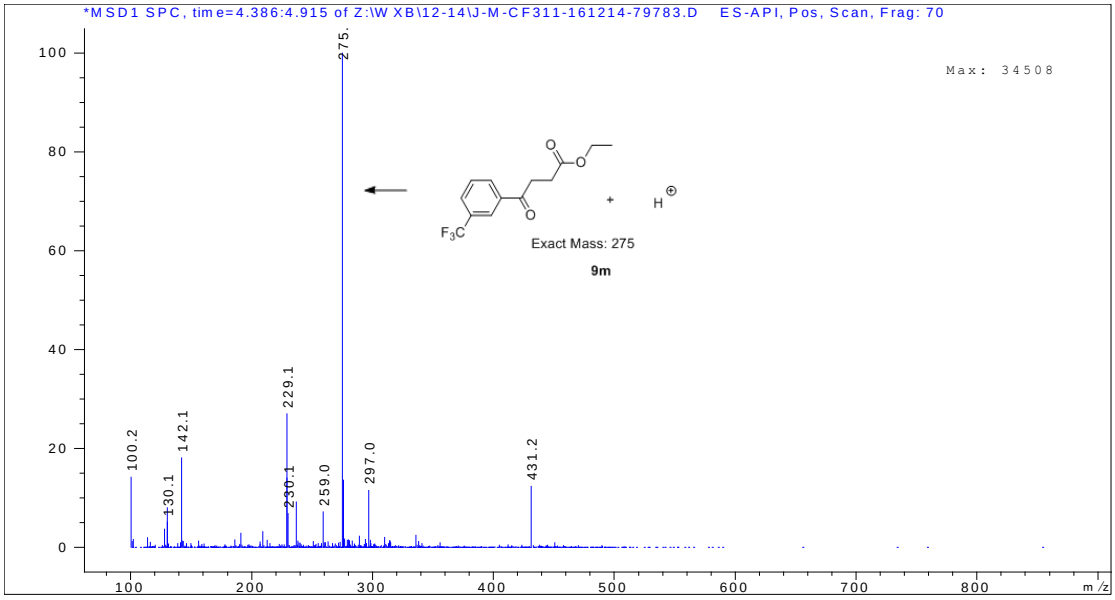
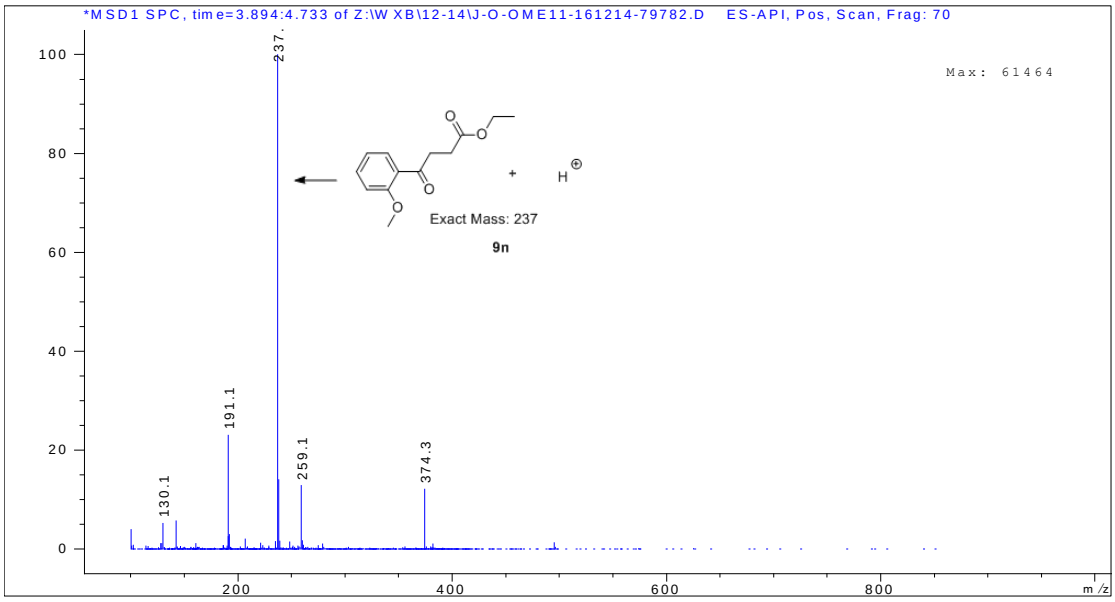
Max: 65120
323.
223.1
324.1
267.1
345.0
293.1
177.1
130.2
100.2
503.4
BocO
H
Exact Mass: 323
9i
m/z

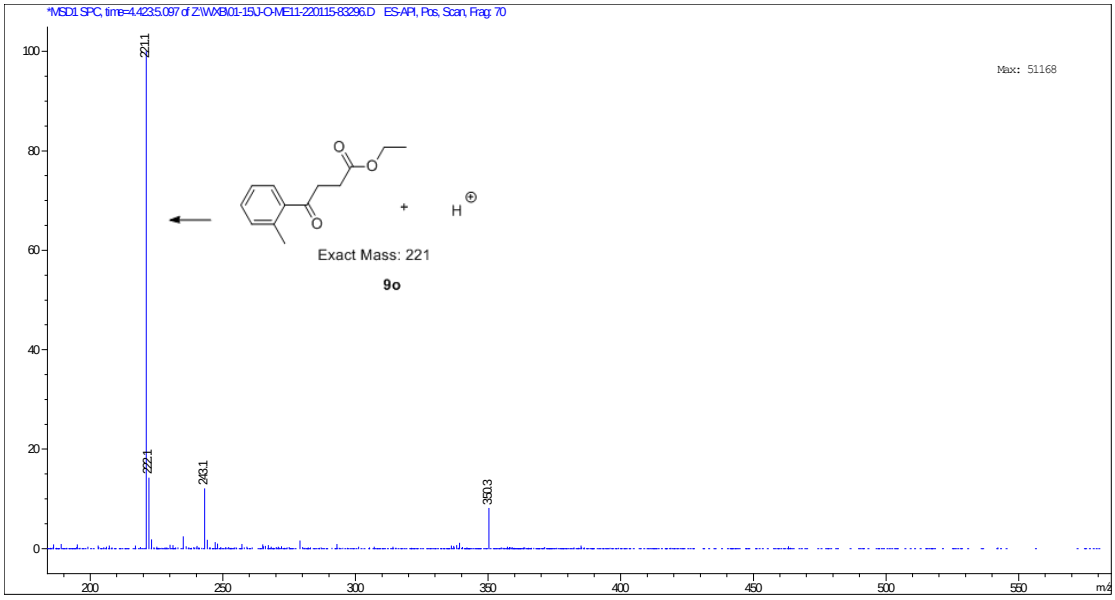

*MSD1 SPC, time=4.587:5.079 of Z:\WXB\12-14\J-BIANO11-151214-79757.D ES-API, Pos, Scan, Frag: 70
Max: 84637
313.
314.1
399.1
297.1
335.1
130.2
Ph
H
Exact Mass: 313
9j
m/z


*MSD1 SPC, time=3.986:4.879 of Z:\WXB\12-14\J-XIBING11-151214-79755.D ES-API, Pos, Scan, Frag: 70
Max: 50022
263.
264.1
285.1
100.2
142.1
217.1
349.1
413.3
Exact Mass: 263
9k
m/z


*MSD1 SPC, time=4.459:4.860 of Z:\WXB\02-14\J-M-F11-260214-52971.D ES-API, Pos, Scan, Frag: 70
Max: 38619
225.
179.1
247.1
113.2
180.1
226.1
248.1
356.0
356.2
Exact Mass: 225
9l
m/z


*MSD1 SPC, time=4.386:4.915 of Z:\WXB\12-14\J-M-CF311-161214-79783.D ES-API, Pos, Scan, Frag: 70
Max: 34508
275.
229.1
142.1
100.2
130.1
230.1
259.0
297.0
431.2
Exact Mass: 275
9m
m/z


*MSD1 SPC, time=3.894:4.733 of Z:\WXB\12-14\J-O-OME11-161214-79782.D ES-API, Pos, Scan, Frag: 70
Max: 61464
237.
191.1
259.1
374.3
130.1
Exact Mass: 237
9n
m/z


*MSD1 SPC, time=4.423:5.097 of Z:\WXB\01-15\J-O-ME11-220115-83296.D ES-API, Pos, Scan, Frag: 70
Max: 51168
221.1
222.1
243.1
350.3
Exact Mass: 221
9o

Cartesian Coordinates and Energies

2a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.263054	0.961231	-0.000009
2	8	0	0.156124	2.096547	-0.000035
3	8	0	0.510366	-0.140424	0.000143
4	6	0	-1.682232	0.628546	-0.000145
5	7	0	-2.066143	-0.617377	-0.000015
6	7	0	-2.386135	-1.702806	0.000083
7	6	0	1.926001	0.097211	0.000198
8	1	0	2.186490	0.687888	-0.883263
9	1	0	2.186473	0.687401	0.883993
10	1	0	-2.449699	1.387039	-0.000271
11	6	0	2.610347	-1.252977	-0.000187
12	1	0	2.334667	-1.829165	0.887772
13	1	0	2.333695	-1.829040	-0.887929
14	1	0	3.696028	-1.115898	-0.000797

Zero-point correction= 0.106721 (Hartree/Particle)
Thermal correction to Energy= 0.114353
Thermal correction to Enthalpy= 0.115297
Thermal correction to Gibbs Free Energy= 0.074073
Sum of electronic and zero-point Energies= -415.696135
Sum of electronic and thermal Energies= -415.688503
Sum of electronic and thermal Enthalpies= -415.687559
Sum of electronic and thermal Free Energies= -415.728783
Sum of electronic and thermal Free Energies(343K)= -415.735156

$CuNO_3$-DABCO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.992104	-0.710830	-0.000014
2	7	0	-0.823246	-0.321931	0.000019
3	6	0	-1.792978	-1.445457	0.000008
4	1	0	-1.586305	-2.057326	-0.881880
5	1	0	-1.586239	-2.057421	0.881815
6	6	0	-1.057481	0.519957	-1.208458
7	1	0	-0.308152	1.315376	-1.193745
8	1	0	-0.861526	-0.103508	-2.085383
9	6	0	-1.057493	0.519961	1.208480
10	1	0	-0.308089	1.315311	1.193844
11	1	0	-0.861668	-0.103537	2.085413
12	7	0	3.155716	0.424824	0.000004
13	8	0	2.190306	1.228789	-0.000084
14	8	0	2.837685	-0.841299	0.000007
15	8	0	4.315869	0.756416	0.000071
16	6	0	-3.239199	-0.876876	0.000090
17	1	0	-3.792761	-1.213218	-0.882116
18	1	0	-3.792613	-1.213096	0.882435
19	6	0	-2.512639	1.058082	-1.190901
20	1	0	-2.526217	2.152270	-1.188944
21	1	0	-3.064633	0.724064	-2.074947
22	6	0	-2.512595	1.058231	1.190819
23	1	0	-3.064620	0.724444	2.074932
24	1	0	-2.526057	2.152422	1.188650
25	7	0	-3.219429	0.586201	0.000000

Zero-point correction= 0.206087 (Hartree/Particle)
Thermal correction to Energy= 0.218441
Thermal correction to Enthalpy= 0.219386
Thermal correction to Gibbs Free Energy= 0.163946
Sum of electronic and zero-point Energies= -2265.580957
Sum of electronic and thermal Energies= -2265.568602
Sum of electronic and thermal Enthalpies= -2265.567658
Sum of electronic and thermal Free Energies= -2265.623097

Sum of electronic and thermal Free Energies(343K)= -2265.631714

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.401479	-0.771091	-0.520443
2	8	0	3.385115	-0.103835	-0.723732
3	8	0	2.069688	-1.343582	0.648848
4	6	0	1.424519	-1.128881	-1.596292
5	7	0	0.840089	-2.324546	-1.462244
6	7	0	0.323217	-3.314061	-1.316366
7	6	0	2.856876	-0.924536	1.783904
8	1	0	3.852329	-1.369536	1.695638
9	1	0	2.948401	0.162637	1.747510
10	1	0	1.740741	-0.933591	-2.617167
11	29	0	0.362902	0.334455	-0.826770
12	7	0	-1.526874	0.079582	-0.205049
13	6	0	-2.359359	-0.736071	-1.115433
14	1	0	-2.383060	-0.231454	-2.086229
15	1	0	-1.860691	-1.700376	-1.252789
16	6	0	-2.172535	1.403237	-0.018761
17	1	0	-1.527319	1.983188	0.645576
18	1	0	-2.183848	1.907066	-0.989453
19	6	0	-1.455271	-0.593453	1.115033
20	1	0	-0.818945	0.023755	1.754360
21	1	0	-0.949469	-1.554244	0.974986
22	7	0	1.252730	2.527166	-0.010291
23	8	0	1.061788	1.591360	0.831868
24	8	0	0.937201	2.251995	-1.217677
25	8	0	1.689860	3.610323	0.307484
26	6	0	-3.781918	-0.908276	-0.512833
27	1	0	-4.546148	-0.504013	-1.184389
28	1	0	-4.013913	-1.965621	-0.348921
29	6	0	-3.599326	1.210541	0.562910
30	1	0	-3.706427	1.723911	1.523545
31	1	0	-4.360360	1.614822	-0.112281
32	6	0	-2.887269	-0.765294	1.691972
33	1	0	-3.122237	-1.821875	1.857140
34	1	0	-2.988951	-0.251827	2.653200
35	7	0	-3.879800	-0.212076	0.769253
36	6	0	2.128692	-1.389905	3.024508
37	1	0	1.147347	-0.911605	3.091401
38	1	0	1.994054	-2.475885	3.021953
39	1	0	2.704256	-1.114739	3.913386

Zero-point correction= 0.314757 (Hartree/Particle)
Thermal correction to Energy= 0.336818
Thermal correction to Enthalpy= 0.337762
Thermal correction to Gibbs Free Energy= 0.260777
Sum of electronic and zero-point Energies= -2681.307481
Sum of electronic and thermal Energies= -2681.285421
Sum of electronic and thermal Enthalpies= -2681.284477
Sum of electronic and thermal Free Energies= -2681.361461
Sum of electronic and thermal Free Energies(343k)= -2681.373508

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.683421	-0.441738	-0.681818
2	8	0	3.554480	0.356327	-0.933520
3	8	0	2.566799	-1.120027	0.465360
4	6	0	1.530903	-0.637438	-1.604585
5	7	0	1.124346	-2.320076	-1.419225
6	7	0	0.494601	-3.199637	-1.176008
7	6	0	3.441665	-0.691255	1.526890
8	1	0	4.478813	-0.857076	1.221960
9	1	0	3.287194	0.380533	1.674576
10	1	0	1.846542	-0.697195	-2.646379
11	29	0	0.190834	0.396389	-0.933295
12	7	0	-1.619269	-0.006238	-0.165035

13	6	0	-2.415490	-0.809515	-1.118155
14	1	0	-2.605461	-0.185881	-1.997364
15	1	0	-1.802146	-1.657610	-1.440298
16	6	0	-2.388851	1.207098	0.206001
17	1	0	-1.796803	1.741703	0.952464
18	1	0	-2.458023	1.847006	-0.677338
19	6	0	-1.392081	-0.806103	1.063506
20	1	0	-0.733718	-0.223674	1.712474
21	1	0	-0.857057	-1.716683	0.773619
22	7	0	0.699737	2.609657	0.177571
23	8	0	0.851078	1.579212	0.897420
24	8	0	0.269824	2.400875	-1.014391
25	8	0	0.924572	3.731308	0.575685
26	6	0	-3.733824	-1.272850	-0.438417
27	1	0	-4.605713	-0.988711	-1.036380
28	1	0	-3.755897	-2.361220	-0.320473
29	6	0	-3.779712	0.788359	0.753728
30	1	0	-3.966725	1.238822	1.733472
31	1	0	-4.583072	1.113069	0.084639
32	6	0	-2.756766	-1.130224	1.730289
33	1	0	-2.871552	-2.206816	1.892960
34	1	0	-2.845403	-0.639342	2.704528
35	7	0	-3.860480	-0.668072	0.886720
36	6	0	3.073527	-1.491245	2.756938
37	1	0	2.030877	-1.309720	3.033479
38	1	0	3.211263	-2.563126	2.585639
39	1	0	3.709381	-1.190906	3.595145

Zero-point correction= 0.311942 (Hartree/Particle)
Thermal correction to Energy= 0.334241
Thermal correction to Enthalpy= 0.335185
Thermal correction to Gibbs Free Energy= 0.256754
Sum of electronic and zero-point Energies= -2681.289809
Sum of electronic and thermal Energies= -2681.267511
Sum of electronic and thermal Enthalpies= -2681.266566
Sum of electronic and thermal Free Energies= -2681.344998
Sum of electronic and thermal Free Energies(343k)= -2681.357262

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.846172	-0.113614	-0.891752
2	8	0	3.918896	0.421957	-1.057205
3	8	0	2.611700	-1.109866	-0.026157
4	6	0	1.626906	0.320260	-1.593234
5	6	0	3.735953	-1.542530	0.761724
6	1	0	4.495289	-1.960622	0.093713
7	1	0	4.167663	-0.671642	1.261423
8	1	0	1.722544	0.125528	-2.667970
9	29	0	0.190759	0.927269	-0.767289
10	7	0	-1.293669	-0.297529	-0.309984
11	6	0	-1.740414	-1.001791	-1.538437
12	1	0	-2.131972	-0.248778	-2.229356
13	1	0	-0.857474	-1.451162	-2.000083
14	6	0	-2.462028	0.374646	0.317802
15	1	0	-2.100620	0.847693	1.232544
16	1	0	-2.797879	1.165258	-0.356791
17	6	0	-0.756337	-1.300110	0.649243
18	1	0	-0.385446	-0.748865	1.516481
19	1	0	0.101567	-1.784492	0.176868
20	7	0	-0.308233	2.768393	0.913815
21	8	0	0.264807	1.770262	1.420391
22	8	0	-0.586369	2.674486	-0.347126
23	8	0	-0.609678	3.761289	1.535117
24	6	0	-2.808905	-2.067120	-1.165888
25	1	0	-3.740423	-1.899431	-1.715211
26	1	0	-2.457458	-3.074045	-1.412292
27	6	0	-3.566303	-0.676767	0.608370
28	1	0	-3.844088	-0.665428	1.666816
29	1	0	-4.471942	-0.468704	0.029926
30	6	0	-1.878961	-2.307974	1.016840
31	1	0	-1.571007	-3.334930	0.795709

32	1	0	-2.115584	-2.258831	2.084192
33	7	0	-3.101497	-2.020362	0.265084
34	6	0	3.220245	-2.566204	1.749591
35	1	0	2.460883	-2.123993	2.401173
36	1	0	2.781577	-3.424352	1.231506
37	1	0	4.043343	-2.925324	2.374612

Zero-point correction= 0.304342 (Hartree/Particle)
Thermal correction to Energy= 0.324370
Thermal correction to Enthalpy= 0.325314
Thermal correction to Gibbs Free Energy= 0.251723
Sum of electronic and zero-point Energies= -2571.835198
Sum of electronic and thermal Energies= -2571.815170
Sum of electronic and thermal Enthalpies= -2571.814226
Sum of electronic and thermal Free Energies= -2571.887817
Sum of electronic and thermal Free Energies(343k)= -2571.899314

N2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.550870
2	7	0	0.000000	0.000000	-0.550870

Zero-point correction= 0.005708 (Hartree/Particle)
Thermal correction to Energy= 0.008069
Thermal correction to Enthalpy= 0.009013
Thermal correction to Gibbs Free Energy= -0.012735
Sum of electronic and zero-point Energies= -109.479340
Sum of electronic and thermal Energies= -109.476980
Sum of electronic and thermal Enthalpies= -109.476036
Sum of electronic and thermal Free Energies= -109.497784
Sum of electronic and thermal Free Energies(343k)= -109.501102

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.894883	0.800397	-0.630632
2	8	0	-3.127214	1.087295	-1.775657
3	8	0	-3.514234	-0.132705	0.091108
4	6	0	-1.806425	1.462595	0.151878
5	7	0	-1.963207	1.414113	1.491840
6	7	0	-2.022526	1.317311	2.601925
7	6	0	-4.461040	-0.962374	-0.618266
8	1	0	-5.238101	-0.318957	-1.039614
9	1	0	-3.927429	-1.452254	-1.436804
10	1	0	-1.564886	2.466806	-0.184759
11	29	0	0.118684	0.471683	-0.144214
12	7	0	1.941417	-0.473300	-0.108697
13	6	0	2.998173	0.370536	-0.732434
14	1	0	2.733547	0.516714	-1.782561
15	1	0	2.981130	1.341982	-0.239245
16	6	0	1.945366	-1.804577	-0.774905
17	1	0	1.202011	-2.427265	-0.275796
18	1	0	1.622928	-1.666607	-1.809036
19	6	0	2.284988	-0.668499	1.327837
20	1	0	1.480023	-1.253491	1.778056
21	1	0	2.293471	0.318578	1.796175
22	7	0	-1.178771	-1.756824	0.003544
23	8	0	-0.864201	-1.355150	1.143417
24	8	0	-0.813090	-1.008740	-0.994150
25	7	0	1.054355	2.857089	-0.205268
26	8	0	0.696097	2.436293	-1.327271
27	8	0	0.886365	2.023864	0.785595
28	8	0	1.533480	3.946466	0.000753
29	8	0	-1.783021	-2.784289	-0.214631
30	6	0	-5.006252	-1.960454	0.377772
31	1	0	-5.725764	-2.616636	-0.121031
32	1	0	-4.195373	-2.574127	0.778148
33	1	0	-5.514256	-1.453894	1.203826

34	6	0	4.385114	-0.306740	-0.557365
35	1	0	4.864602	-0.472695	-1.526963
36	1	0	5.051943	0.326717	0.035644
37	6	0	3.661515	-1.379977	1.441126
38	1	0	4.358333	-0.784057	2.038482
39	1	0	3.557158	-2.353583	1.929857
40	6	0	3.358648	-2.439893	-0.668565
41	1	0	3.302751	-3.424726	-0.194669
42	1	0	3.803072	-2.576645	-1.659322
43	7	0	4.249918	-1.593395	0.119490

Zero-point correction= 0.333969 (Hartree/Particle)
Thermal correction to Energy= 0.359537
Thermal correction to Enthalpy= 0.360481
Thermal correction to Gibbs Free Energy= 0.275732
Sum of electronic and zero-point Energies= -2961.533778
Sum of electronic and thermal Energies= -2961.508211
Sum of electronic and thermal Enthalpies= -2961.507266
Sum of electronic and thermal Free Energies= -2961.592016
Sum of electron ic and thermal Free Energies(343k)= -2961.605304

$Cu(NO_3)_2$-DABCO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.962754	-0.002528	-0.156760
2	7	0	-1.013286	-0.148128	-0.085753
3	6	0	-1.436436	-1.198768	-1.051037
4	1	0	-1.198823	-0.832114	-2.054742
5	1	0	-0.833790	-2.090882	-0.862438
6	6	0	-1.734806	1.115004	-0.398484
7	1	0	-1.449427	1.842202	0.365431
8	1	0	-1.372254	1.483634	-1.360196
9	6	0	-1.388242	-0.575513	1.291313
10	1	0	-0.994213	0.173154	1.983822
11	1	0	-0.882173	-1.522696	1.492645
12	7	0	1.187697	2.460526	0.132394
13	8	0	1.095286	1.793198	1.197875
14	8	0	1.136784	1.758785	-0.960774
15	7	0	2.529783	-1.789180	0.055269
16	8	0	2.808834	-0.680806	-0.513454
17	8	0	1.310100	-1.836151	0.479838
18	8	0	3.298823	-2.694697	0.182077
19	8	0	1.298391	3.658263	0.088663
20	6	0	-2.956636	-1.469500	-0.877761
21	1	0	-3.478183	-1.381755	-1.835510
22	1	0	-3.131071	-2.480451	-0.497265
23	6	0	-2.932922	-0.709495	1.379728
24	1	0	-3.215588	-1.696996	1.756632
25	1	0	-3.351782	0.035877	2.062522
26	6	0	-3.262860	0.841219	-0.396846
27	1	0	-3.782534	1.546755	0.258148
28	1	0	-3.683265	0.955019	-1.400776
29	7	0	-3.541493	-0.518195	0.064160

Zero-point correction= 0.224635 (Hartree/Particle)
Thermal correction to Energy= 0.240643
Thermal correction to Enthalpy= 0.241587
Thermal correction to Gibbs Free Energy= 0.178307
Sum of electronic and zero-point Energies= -2545.823829
Sum of electronic and thermal Energies= -2545.807821
Sum of electronic and thermal Enthalpies= -2545.806877
Sum of electronic and thermal Free Energies= -2545.870157
Sum of electron ic and thermal Free Energies(343k)= -2545.880027

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.861821	0.891724	-0.497625
2	8	0	-2.996771	1.322630	-1.626141

3	8	0	-3.574433	-0.006224	0.130964
4	6	0	-1.624229	1.408322	0.073608
5	7	0	-1.853731	1.010533	2.197466
6	7	0	-1.729610	0.612033	3.215163
7	6	0	-4.582008	-0.700441	-0.656307
8	1	0	-5.325560	0.031123	-0.982865
9	1	0	-4.080754	-1.121391	-1.530626
10	1	0	-1.669459	2.476637	0.290940
11	29	0	0.133752	0.502829	-0.188193
12	7	0	1.928841	-0.477064	-0.125294
13	6	0	3.008964	0.337606	-0.747384
14	1	0	2.762485	0.465372	-1.804408
15	1	0	2.996130	1.318978	-0.274952
16	6	0	1.915408	-1.818097	-0.771588
17	1	0	1.161365	-2.415784	-0.258677
18	1	0	1.598366	-1.691012	-1.808453
19	6	0	2.251445	-0.660561	1.317533
20	1	0	1.426322	-1.218588	1.766374
21	1	0	2.283599	0.332733	1.771355
22	7	0	-1.247799	-1.748429	-0.257121
23	8	0	-0.882815	-1.519027	0.914305
24	8	0	-0.811431	-0.944166	-1.173633
25	7	0	1.087473	2.893709	-0.234382
26	8	0	0.731023	2.452473	-1.352265
27	8	0	0.980603	2.062841	0.759380
28	8	0	1.515384	4.009663	-0.047844
29	8	0	-1.975297	-2.670651	-0.571515
30	6	0	-5.163267	-1.773080	0.234082
31	1	0	-5.923018	-2.331328	-0.320900
32	1	0	-4.377578	-2.466489	0.543557
33	1	0	-5.632011	-1.336990	1.120857
34	6	0	4.381218	-0.357399	-0.536187
35	1	0	4.880897	-0.536175	-1.493300
36	1	0	5.043392	0.269960	0.068654
37	6	0	3.607005	-1.407161	1.456246
38	1	0	4.307980	-0.827737	2.065027
39	1	0	3.470093	-2.377272	1.944136
40	6	0	3.318029	-2.472596	-0.651905
41	1	0	3.244273	-3.457108	-0.179413
42	1	0	3.771436	-2.614686	-1.637938
43	7	0	4.213208	-1.638280	0.145507

Zero-point correction= 0.329951 (Hartree/Particle)
Thermal correction to Energy= 0.356360
Thermal correction to Enthalpy= 0.357305
Thermal correction to Gibbs Free Energy= 0.270508
Sum of electronic and zero-point Energies= -2961.499841
Sum of electronic and thermal Energies= -2961.473431
Sum of electronic and thermal Enthalpies= -2961.472487
Sum of electronic and thermal Free Energies= -2961.559284
Sum of electron ic and thermal Free Energies(343k)= -2961.572886

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.927518	0.947033	0.264752
2	8	0	-2.877939	1.717961	-0.708619
3	8	0	-3.740518	0.018043	0.591550
4	6	0	-1.670789	1.448298	0.661427
5	6	0	-4.702969	-0.413068	-0.433666
6	1	0	-5.357031	0.433427	-0.654930
7	1	0	-4.116594	-0.676601	-1.316415
8	1	0	-1.714001	2.373856	1.237557
9	29	0	0.031389	0.584749	0.088651
10	7	0	1.778668	-0.473281	-0.054334
11	6	0	2.832878	0.300931	-0.765667
12	1	0	2.499741	0.440904	-1.797100
13	1	0	2.901005	1.281296	-0.295714
14	6	0	1.637369	-1.797493	-0.718737
15	1	0	0.926090	-2.377006	-0.129280
16	1	0	1.207640	-1.636902	-1.709351
17	6	0	2.230432	-0.703564	1.346392

18	1	0	1.419137	-1.213594	1.871897
19	1	0	2.374860	0.277687	1.804481
20	7	0	-1.444847	-1.640965	-0.047489
21	8	0	-0.985893	-1.538207	1.105191
22	8	0	-1.067722	-0.754185	-0.914504
23	7	0	1.062622	2.927255	-0.049229
24	8	0	0.587124	2.500500	-1.127025
25	8	0	1.033204	2.095761	0.949259
26	8	0	1.540454	4.029615	0.094836
27	8	0	-2.222905	-2.512174	-0.395160
28	6	0	-5.435825	-1.599971	0.139222
29	1	0	-6.148335	-1.970135	-0.603750
30	1	0	-4.725351	-2.396382	0.371589
31	1	0	-5.986215	-1.325936	1.043285
32	6	0	4.188592	-0.449997	-0.673393
33	1	0	4.617993	-0.607905	-1.667721
34	1	0	4.912467	0.129304	-0.091632
35	6	0	3.537697	-1.542714	1.338624
36	1	0	4.324530	-1.040376	1.910049
37	1	0	3.375571	-2.524472	1.794676
38	6	0	3.016209	-2.506986	-0.774719
39	1	0	2.947939	-3.513162	-0.349291
40	1	0	3.366577	-2.609429	-1.806691
41	7	0	4.017960	-1.749526	-0.027830

Zero-point correction= 0.322091 (Hartree/Particle)
Thermal correction to Energy= 0.346116
Thermal correction to Enthalpy= 0.347060
Thermal correction to Gibbs Free Energy= 0.265342
Sum of electronic and zero-point Energies= -2852.017251
Sum of electronic and thermal Energies= -2851.993226
Sum of electronic and thermal Enthalpies= -2851.992282
Sum of electronic and thermal Free Energies= -2852.074000
Sum of electron ic and thermal Free Energies(343k)= -2852.089076

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.328493	2.227717	-0.379040
2	8	0	-2.464944	2.556503	-0.123110
3	8	0	-0.234654	2.927745	-0.046131
4	6	0	-0.990969	0.964137	-1.052588
5	6	0	-0.464982	4.162972	0.657698
6	1	0	-1.105954	4.804332	0.045732
7	1	0	-0.996303	3.941331	1.587192
8	1	0	-1.264552	1.002670	-2.113643
9	29	0	-0.145399	-0.384626	-0.291643
10	7	0	1.814418	-0.587862	-0.351790
11	6	0	2.264067	-0.547767	-1.767226
12	1	0	1.827153	-1.411364	-2.277816
13	1	0	1.845263	0.354444	-2.220221
14	6	0	2.318956	-1.833747	0.283512
15	1	0	1.993962	-1.812215	1.325710
16	1	0	1.827808	-2.681403	-0.200064
17	6	0	2.393182	0.577366	0.370553
18	1	0	2.004127	0.547948	1.391219
19	1	0	2.008551	1.484308	-0.102950
20	7	0	-0.667849	-1.803905	1.791616
21	8	0	-0.202028	-0.677736	2.077905
22	8	0	-0.719151	-2.081435	0.520110
23	8	0	-1.049610	-2.613314	2.602936
24	6	0	3.816618	-0.559966	-1.817400
25	1	0	4.183625	-1.403832	-2.409647
26	1	0	4.199906	0.356245	-2.277420
27	6	0	3.865546	-1.885114	0.157490
28	1	0	4.333748	-1.990935	1.140857
29	1	0	4.182798	-2.738594	-0.449913
30	6	0	3.942677	0.491259	0.319749
31	1	0	4.369960	1.393675	-0.128742
32	1	0	4.364676	0.392245	1.324651
33	7	0	4.371227	-0.664340	-0.469485
34	6	0	0.888084	4.790915	0.912153

35	1	0	1.510511	4.136326	1.529530
36	1	0	1.409440	4.984777	-0.029900
37	1	0	0.761425	5.741968	1.437903
38	6	0	-3.781339	-0.779141	-0.817168
39	1	0	-3.308678	0.130375	-1.229296
40	6	0	-5.153684	-0.931994	-1.457036
41	1	0	-5.757107	-0.031591	-1.301055
42	1	0	-5.049791	-1.102369	-2.532921
43	1	0	-5.677685	-1.790946	-1.023909
44	6	0	-3.861965	-0.603661	0.694864
45	1	0	-4.246629	-1.515707	1.165375
46	1	0	-2.876868	-0.377767	1.118016
47	1	0	-4.520451	0.231652	0.951004
48	8	0	-3.014815	-1.914523	-1.183995
49	1	0	-2.391502	-2.114476	-0.469534

Zero-point correction= 0.416301 (Hartree/Particle)
Thermal correction to Energy= 0.443131
Thermal correction to Enthalpy= 0.444075
Thermal correction to Gibbs Free Energy= 0.354834
Sum of electronic and zero-point Energies= -2766.034258
Sum of electronic and thermal Energies= -2766.007428
Sum of electronic and thermal Enthalpies= -2766.006484
Sum of electronic and thermal Free Energies= -2766.095725
Sum of electronic and thermal Free Energies(343k)= -2766.107516

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.465788	2.132654	-0.047610
2	8	0	-2.521975	2.445232	0.451285
3	8	0	-0.340675	2.869380	0.047731
4	6	0	-1.170775	0.904769	-0.823577
5	6	0	-0.457930	4.104916	0.774921
6	1	0	-1.124151	4.774745	0.222592
7	1	0	-0.915442	3.902052	1.746638
8	1	0	-1.368153	1.075653	-1.891143
9	29	0	-0.178692	-0.472662	-0.286536
10	7	0	1.797567	-0.491895	-0.332726
11	6	0	2.251780	0.009511	-1.653921
12	1	0	1.890012	-0.687616	-2.416088
13	1	0	1.763533	0.972966	-1.822195
14	6	0	2.409043	-1.820146	-0.078238
15	1	0	2.062680	-2.149328	0.903826
16	1	0	2.014113	-2.519066	-0.820247
17	6	0	2.257693	0.452470	0.718775
18	1	0	1.876438	0.082109	1.673627
19	1	0	1.783841	1.417917	0.520218
20	7	0	-0.630396	-2.444488	1.315001
21	8	0	-0.215108	-1.405684	1.881997
22	8	0	-0.716088	-2.377434	0.021185
23	8	0	-0.938743	-3.458778	1.897014
24	6	0	3.800564	0.129398	-1.658906
25	1	0	4.241347	-0.484114	-2.450948
26	1	0	4.111278	1.164492	-1.832892
27	6	0	3.956037	-1.695395	-0.138257
28	1	0	4.411808	-2.028424	0.799279
29	1	0	4.370598	-2.312429	-0.941701
30	6	0	3.808054	0.535253	0.690456
31	1	0	4.143385	1.563686	0.521555
32	1	0	4.237516	0.201332	1.640171
33	7	0	4.350986	-0.306912	-0.376843
34	6	0	0.934727	4.681649	0.911724
35	1	0	1.579039	4.010039	1.487447
36	1	0	1.388168	4.845326	-0.070320
37	1	0	0.887636	5.641906	1.434094
38	6	0	-3.601595	-0.519565	-0.683767
39	1	0	-2.789030	0.271896	-0.772949
40	6	0	-4.813795	0.016595	-1.419539
41	1	0	-5.098702	0.991652	-1.014507
42	1	0	-4.595159	0.122119	-2.486085
43	1	0	-5.654903	-0.676670	-1.309045

44	6	0	-3.817425	-0.703345	0.810204
45	1	0	-4.552103	-1.496435	0.986896
46	1	0	-2.882254	-0.975441	1.311179
47	1	0	-4.172448	0.227542	1.259576
48	8	0	-3.156822	-1.671884	-1.329585
49	1	0	-2.482305	-2.104901	-0.778053

Zero-point correction= 0.415193 (Hartree/Particle)
Thermal correction to Energy= 0.440959
Thermal correction to Enthalpy= 0.441903
Thermal correction to Gibbs Free Energy= 0.356038
Sum of electronic and zero-point Energies= -2766.033865
Sum of electronic and thermal Energies= -2766.008099
Sum of electronic and thermal Enthalpies= -2766.007154
Sum of electronic and thermal Free Energies= -2766.093019
Sum of electronic and thermal Free Energies(343k)= -2766.106220

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.951913	1.522051	0.608066
2	8	0	2.606489	1.471409	-0.428885
3	8	0	1.453796	2.715960	1.043868
4	6	0	1.567258	0.403476	1.457422
5	6	0	1.687789	3.834661	0.196664
6	1	0	2.764238	3.972293	0.051683
7	1	0	1.249907	3.647034	-0.791349
8	1	0	1.418963	0.712584	2.495253
9	29	0	-0.095117	0.017801	0.629653
10	7	0	-1.872229	0.077296	-0.087742
11	6	0	-2.352500	1.483130	-0.060229
12	1	0	-2.233040	1.857427	0.959915
13	1	0	-1.689800	2.071416	-0.701829
14	6	0	-2.771742	-0.748109	0.763028
15	1	0	-2.361559	-1.759387	0.793843
16	1	0	-2.722831	-0.340683	1.777169
17	6	0	-1.943115	-0.423550	-1.483266
18	1	0	-1.593107	-1.458248	-1.474822
19	1	0	-1.239356	0.161454	-2.083429
20	7	0	0.389481	-2.986833	1.115984
21	8	0	-0.294122	-3.461378	1.987318
22	8	0	1.699276	-3.234212	1.184725
23	8	0	0.001340	-2.273232	0.192176
24	6	0	-3.828902	1.534519	-0.540107
25	1	0	-4.490771	1.885042	0.258263
26	1	0	-3.943407	2.221080	-1.385163
27	6	0	-4.213025	-0.702176	0.189325
28	1	0	-4.535900	-1.693938	-0.142949
29	1	0	-4.927656	-0.361113	0.945012
30	6	0	-3.397336	-0.291628	-2.009876
31	1	0	-3.448424	0.403010	-2.854631
32	1	0	-3.780596	-1.257112	-2.355316
33	7	0	-4.281243	0.206730	-0.956227
34	6	0	1.056606	5.042879	0.859854
35	1	0	-0.019268	4.893432	0.994852
36	1	0	1.502949	5.218485	1.843008
37	1	0	1.209164	5.935845	0.245073
38	6	0	3.058531	-1.233838	-1.467060
39	1	0	2.308665	-0.395076	1.387891
40	6	0	4.246587	-0.592540	-2.116309
41	1	0	4.199630	0.475455	-1.878412
42	1	0	5.172377	-1.024858	-1.734494
43	1	0	4.191510	-0.700780	-3.205266
44	6	0	1.688401	-0.885422	-1.979974
45	1	0	1.240257	-1.773702	-2.439025
46	1	0	1.068079	-0.611081	-1.121535
47	1	0	1.713523	-0.061765	-2.694326
48	8	0	3.209078	-2.037713	-0.552436
49	1	0	2.143151	-2.720799	0.427178

Zero-point correction= 0.416229 (Hartree/Particle)
Thermal correction to Energy= 0.442817

Thermal correction to Enthalpy= 0.443761
Thermal correction to Gibbs Free Energy= 0.355785
Sum of electronic and zero-point Energies= -2766.080307
Sum of electronic and thermal Energies= -2766.053719
Sum of electronic and thermal Enthalpies= -2766.052775
Sum of electronic and thermal Free Energies= -2766.140752
Sum of electronic and thermal Free Energies(343k)= -2766.154544

INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.203791	-0.644498	0.608927
2	8	0	-1.688946	-0.164534	1.621593
3	8	0	-3.028388	0.110362	-0.169049
4	6	0	-2.004944	-1.989244	0.075385
5	6	0	-3.176514	1.475813	0.205219
6	1	0	-3.458295	1.542334	1.260221
7	1	0	-2.216132	1.995036	0.090997
8	1	0	-2.748773	-2.282077	-0.662955
9	29	0	-0.310298	-1.339883	-0.423814
10	7	0	1.280304	-0.313816	-0.285851
11	6	0	0.839497	1.108892	-0.294290
12	1	0	0.389542	1.316374	-1.269801
13	1	0	0.057899	1.197669	0.464769
14	6	0	2.375140	-0.490904	-1.267931
15	1	0	2.637639	-1.552372	-1.287756
16	1	0	1.976934	-0.231685	-2.253193
17	6	0	1.789737	-0.626459	1.079820
18	1	0	2.121018	-1.669311	1.075709
19	1	0	0.939194	-0.544893	1.762381
20	6	0	2.055895	2.027218	-0.005596
21	1	0	2.287689	2.662515	-0.866702
22	1	0	1.853345	2.686229	0.844350
23	6	0	3.578173	0.406415	-0.864460
24	1	0	4.454738	-0.199644	-0.613606
25	1	0	3.863852	1.072658	-1.684755
26	6	0	2.943767	0.348349	1.434097
27	1	0	2.676937	0.975543	2.290350
28	1	0	3.854897	-0.198268	1.697613
29	7	0	3.241496	1.224975	0.300253
30	6	0	-4.232010	2.079291	-0.699698
31	1	0	-3.937935	1.992809	-1.750098
32	1	0	-5.188825	1.565409	-0.569391
33	1	0	-4.372675	3.139084	-0.463603
34	1	0	-1.896039	-2.724788	0.876085

Zero-point correction= 0.299546 (Hartree/Particle)
Thermal correction to Energy= 0.315151
Thermal correction to Enthalpy= 0.316096
Thermal correction to Gibbs Free Energy= 0.254508
Sum of electronic and zero-point Energies= -2292.258400
Sum of electronic and thermal Energies= -2292.242794
Sum of electronic and thermal Enthalpies= -2292.241850
Sum of electronic and thermal Free Energies= -2292.303438
Sum of electron ic and thermal Free Energies(343k)= -2292.313055

HNO3+acetone

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.018122	0.043028	-0.159515
2	8	0	-3.189139	0.228597	0.040293
3	8	0	-1.449405	-0.915251	0.619504
4	8	0	-1.294529	0.607818	-0.959743
5	6	0	1.840604	-0.099305	0.089157
6	6	0	3.251047	-0.081685	-0.436248
7	1	0	3.952984	-0.028989	0.404419
8	1	0	3.449297	-0.980135	-1.021722
9	1	0	3.415551	0.813145	-1.046579
10	6	0	1.335614	1.149680	0.765528

11	1	0	0.910488	1.805957	-0.002799
12	1	0	0.543252	0.909083	1.477271
13	1	0	2.142365	1.690031	1.268001
14	8	0	1.138488	-1.089548	-0.049281
15	1	0	-0.493987	-0.975361	0.321207

Zero-point correction= 0.114326 (Hartree/Particle)
Thermal correction to Energy= 0.124321
Thermal correction to Enthalpy= 0.125265
Thermal correction to Gibbs Free Energy= 0.076828
Sum of electronic and zero-point Energies= -473.791502
Sum of electronic and thermal Energies= -473.781507
Sum of electronic and thermal Enthalpies= -473.780563
Sum of electronic and thermal Free Energies= -473.829001
Sum of electron ic and thermal Free Energies(343k)= -473.836489

INT8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.873176	2.236551	-0.884715
2	8	0	2.168381	3.410102	-0.904527
3	8	0	2.727686	1.244697	-0.569657
4	6	0	0.519261	1.738244	-1.166217
5	6	0	4.066538	1.646557	-0.233984
6	1	0	4.514869	2.142303	-1.100493
7	1	0	4.022266	2.370560	0.583509
8	1	0	0.290126	1.933047	-2.223255
9	29	0	-0.405131	0.671863	-0.096705
10	7	0	0.115478	-1.233025	-0.097179
11	6	0	0.629786	-1.630472	-1.434521
12	1	0	-0.142495	-1.387381	-2.168480
13	1	0	1.506966	-1.009786	-1.636218
14	6	0	-1.018444	-2.126510	0.252971
15	1	0	-1.468508	-1.748749	1.173060
16	1	0	-1.758986	-2.023070	-0.542861
17	6	0	1.200762	-1.417475	0.904025
18	1	0	0.782570	-1.182027	1.884296
19	1	0	1.971603	-0.674494	0.691941
20	7	0	-1.071904	1.017845	2.429034
21	8	0	0.157125	1.175735	2.325374
22	8	0	-1.710900	0.681110	1.342939
23	8	0	-1.695900	1.144580	3.461691
24	6	0	0.977218	-3.143279	-1.424102
25	1	0	0.290029	-3.711938	-2.059025
26	1	0	1.990150	-3.311599	-1.803907
27	6	0	-0.498069	-3.581927	0.389614
28	1	0	-0.538148	-3.918285	1.430494
29	1	0	-1.110378	-4.270282	-0.201736
30	6	0	1.733458	-2.870919	0.816103
31	1	0	2.754420	-2.891596	0.420284
32	1	0	1.755088	-3.339238	1.805007
33	7	0	0.889570	-3.679500	-0.066196
34	6	0	4.825569	0.396066	0.156057
35	1	0	4.386644	-0.064060	1.046563
36	1	0	4.815481	-0.335514	-0.657922
37	1	0	5.866836	0.647042	0.379412
38	6	0	-4.165269	-0.417177	-0.511117
39	1	0	-5.228994	-0.220800	-0.345131
40	1	0	-4.063812	-1.430952	-0.911668
41	1	0	-3.644725	-0.349088	0.448444
42	6	0	-3.598721	0.600527	-1.483982
43	1	0	-4.126534	0.513383	-2.444999
44	6	0	-3.707997	2.028486	-0.965662
45	1	0	-3.258511	2.740543	-1.668557
46	1	0	-4.758745	2.307113	-0.834750
47	1	0	-3.197977	2.116124	-0.001964
48	8	0	-2.218840	0.250752	-1.710398
49	1	0	-1.876486	0.869637	-2.367427

Zero-point correction= 0.416571 (Hartree/Particle)

Thermal correction to Energy= 0.443195
Thermal correction to Enthalpy= 0.444139
Thermal correction to Gibbs Free Energy= 0.356739
Sum of electronic and zero-point Energies= -2766.039039
Sum of electronic and thermal Energies= -2766.012415
Sum of electronic and thermal Enthalpies= -2766.011471
Sum of electronic and thermal Free Energies= -2766.098871
Sum of electronic and thermal Free Energies(343k)= -2766.11258

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.218416	2.455285	-0.959212
2	8	0	0.495132	3.450501	-1.599257
3	8	0	0.529810	2.314955	0.358971
4	6	0	-0.545006	1.329379	-1.457955
5	6	0	1.091208	3.456143	1.016395
6	1	0	1.933124	3.835032	0.428946
7	1	0	0.332258	4.243455	1.057476
8	1	0	-0.225804	0.990914	-2.446299
9	29	0	-0.605305	-0.113322	-0.190499
10	7	0	1.241580	-0.686427	-0.461890
11	6	0	2.207279	0.104793	-1.283286
12	1	0	1.753330	0.311552	-2.251302
13	1	0	2.357796	1.054681	-0.769707
14	6	0	1.131702	-2.049171	-1.069484
15	1	0	0.350434	-2.598635	-0.542432
16	1	0	0.821273	-1.909278	-2.109770
17	6	0	1.825575	-0.825711	0.911255
18	1	0	1.181592	-1.510795	1.460062
19	1	0	1.768552	0.153745	1.388758
20	7	0	-1.272518	-1.073190	2.107404
21	8	0	-0.889444	0.111285	2.172614
22	8	0	-1.066218	-1.667345	0.965205
23	8	0	-1.791645	-1.682899	3.015229
24	6	0	3.531261	-0.688011	-1.440624
25	1	0	3.651218	-1.047086	-2.467658
26	1	0	4.389103	-0.047273	-1.214942
27	6	0	2.503119	-2.770766	-0.961325
28	1	0	2.453932	-3.578920	-0.225534
29	1	0	2.780483	-3.214551	-1.922274
30	6	0	3.270313	-1.373700	0.808529
31	1	0	4.005505	-0.603251	1.060774
32	1	0	3.410807	-2.202566	1.508728
33	7	0	3.551739	-1.841463	-0.547674
34	6	0	1.512042	3.014565	2.402641
35	1	0	0.669936	2.562458	2.933487
36	1	0	2.322231	2.279154	2.350334
37	1	0	1.872552	3.874190	2.975944
38	6	0	-4.089231	-1.399921	-0.082386
39	1	0	-4.761057	-2.091747	-0.602052
40	1	0	-3.386008	-1.978409	0.520008
41	1	0	-4.686554	-0.770130	0.584810
42	6	0	-3.357778	-0.530668	-1.090833
43	1	0	-2.753385	-1.170199	-1.753624
44	6	0	-4.307518	0.303320	-1.940629
45	1	0	-3.755102	0.920349	-2.656759
46	1	0	-4.989863	-0.346572	-2.498246
47	1	0	-4.900586	0.963439	-1.299526
48	8	0	-2.481316	0.364362	-0.381143
49	1	0	-2.006387	1.094241	-1.041056

Zero-point correction= 0.414229 (Hartree/Particle)
Thermal correction to Energy= 0.439321
Thermal correction to Enthalpy= 0.440265
Thermal correction to Gibbs Free Energy= 0.357202
Sum of electronic and zero-point Energies= -2766.022606
Sum of electronic and thermal Energies= -2765.997514
Sum of electronic and thermal Enthalpies= -2765.996570
Sum of electronic and thermal Free Energies= -2766.079633
Sum of electronic and thermal Free Energies(343k)= -2766.092672

INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.926332	1.739383	-1.366062
2	8	0	-0.042887	2.576835	-1.282822
3	8	0	-2.178755	1.947626	-0.975368
4	6	0	-0.729359	0.342573	-1.852065
5	6	0	-2.441516	3.168316	-0.263129
6	1	0	-1.637751	3.329213	0.459328
7	1	0	-2.434128	3.996683	-0.978966
8	1	0	0.090298	0.265417	-2.560976
9	29	0	-0.290257	-0.504319	-0.191336
10	7	0	1.655639	-0.029244	-0.150904
11	6	0	2.295188	0.434566	-1.417265
12	1	0	2.078951	-0.309373	-2.188995
13	1	0	1.817955	1.376792	-1.689750
14	6	0	2.338625	-1.295516	0.257428
15	1	0	1.831625	-1.687381	1.138728
16	1	0	2.211763	-2.011387	-0.561803
17	6	0	1.892474	1.004930	0.900818
18	1	0	1.490938	0.609987	1.832683
19	1	0	1.317857	1.889490	0.620739
20	7	0	-0.895902	-0.263947	2.287652
21	8	0	-1.135448	0.783634	1.655352
22	8	0	-0.183048	-1.158500	1.658848
23	8	0	-1.251347	-0.478736	3.422521
24	6	0	3.825964	0.592162	-1.208019
25	1	0	4.381713	-0.120516	-1.825797
26	1	0	4.147529	1.597697	-1.495334
27	6	0	3.838655	-1.004797	0.544029
28	1	0	4.059453	-1.150345	1.605682
29	1	0	4.479786	-1.686226	-0.023647
30	6	0	3.412333	1.289953	1.018599
31	1	0	3.643999	2.310768	0.700242
32	1	0	3.742077	1.184993	2.056668
33	7	0	4.184312	0.367577	0.187694
34	6	0	-3.781670	3.003892	0.418619
35	1	0	-4.570132	2.801278	-0.311894
36	1	0	-3.737190	2.176537	1.131380
37	1	0	-4.035244	3.921327	0.959102
38	6	0	-3.015083	-3.386867	-0.249669
39	1	0	-2.927636	-4.477104	-0.312331
40	1	0	-3.390499	-3.117255	0.740559
41	1	0	-3.735822	-3.044953	-0.999708
42	6	0	-1.659336	-2.725669	-0.489711
43	1	0	-0.966219	-3.090418	0.288068
44	6	0	-1.094214	-3.098181	-1.863997
45	1	0	-0.115242	-2.629152	-2.035264
46	1	0	-0.964403	-4.181777	-1.957889
47	1	0	-1.771151	-2.757705	-2.655403
48	8	0	-1.869518	-1.341759	-0.356987
49	1	0	-1.645772	-0.113294	-2.207590

Zero-point correction= 0.419813 (Hartree/Particle)
Thermal correction to Energy= 0.444699
Thermal correction to Enthalpy= 0.445643
Thermal correction to Gibbs Free Energy= 0.364093
Sum of electronic and zero-point Energies= -2766.074522
Sum of electronic and thermal Energies= -2766.049636
Sum of electronic and thermal Enthalpies= -2766.048692
Sum of electronic and thermal Free Energies= -2766.130242
Sum of electronic and thermal Free Energies(343k)= -2766.143053

INT10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.048622	-1.615287	0.942137
2	8	0	-2.242417	-0.597265	1.590089
3	8	0	-2.996503	-2.293569	0.309774

4	6	0	-0.716913	-2.206775	0.758344
5	6	0	-4.318808	-1.709855	0.288281
6	1	0	-4.220502	-0.630456	0.154840
7	1	0	-4.781085	-2.142564	-0.599724
8	1	0	-0.619813	-3.129919	1.343215
9	29	0	0.561759	-1.453663	-0.197001
10	7	0	2.122400	-0.425131	0.408323
11	6	0	2.033556	-0.093659	1.857265
12	1	0	1.163359	0.553127	1.986657
13	1	0	1.855404	-1.027512	2.397679
14	6	0	2.260826	0.837923	-0.369786
15	1	0	2.384913	0.555556	-1.417956
16	1	0	1.325002	1.386850	-0.263400
17	6	0	3.333373	-1.256355	0.180014
18	1	0	3.335320	-1.559400	-0.869883
19	1	0	3.234685	-2.158335	0.793282
20	7	0	0.383315	-0.911543	-2.668758
21	8	0	1.188034	-1.710780	-2.038176
22	8	0	-0.411596	-0.265544	-1.944718
23	8	0	0.438101	-0.816593	-3.873004
24	6	0	3.347691	0.600371	2.305323
25	1	0	3.133824	1.557234	2.790909
26	1	0	3.898198	-0.018037	3.021933
27	6	0	3.480399	1.633245	0.164736
28	1	0	4.163535	1.897638	-0.648568
29	1	0	3.157523	2.563828	0.641132
30	6	0	4.595583	-0.433635	0.560808
31	1	0	5.217499	-0.982449	1.275115
32	1	0	5.208841	-0.231833	-0.322998
33	7	0	4.217557	0.846855	1.155620
34	6	0	-5.092542	-2.048719	1.547659
35	1	0	-5.150253	-3.131853	1.689046
36	1	0	-4.620386	-1.596862	2.423269
37	1	0	-6.111539	-1.657211	1.464692
38	6	0	-2.896942	1.927428	-0.667915
39	1	0	-2.386811	0.976726	-0.843588
40	1	0	-3.635453	1.801460	0.131790
41	1	0	-3.421324	2.198277	-1.590096
42	6	0	-1.895307	3.018661	-0.290429
43	6	0	-0.801064	3.155809	-1.347694
44	1	0	-0.031103	3.853733	-1.001934
45	1	0	-0.346738	2.186809	-1.566764
46	1	0	-1.226770	3.542880	-2.279603
47	6	0	-2.597613	4.354026	-0.047936
48	1	0	-3.351680	4.257624	0.739382
49	1	0	-1.874401	5.117410	0.254484
50	1	0	-3.092084	4.686360	-0.965691
51	8	0	-1.324845	2.752382	1.004666
52	8	0	-0.580604	1.538059	0.966482
53	1	0	-1.225135	0.883278	1.303757

Zero-point correction= 0.449173 (Hartree/Particle)
Thermal correction to Energy= 0.477769
Thermal correction to Enthalpy= 0.478713
Thermal correction to Gibbs Free Energy= 0.387896
Sum of electronic and zero-point Energies= -2880.425251
Sum of electronic and thermal Energies= -2880.396656
Sum of electronic and thermal Enthalpies= -2880.395712
Sum of electronic and thermal Free Energies= -2880.486529
Sum of electronic and thermal Free Energies(343k)= -2880.500800

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.837006	-0.383455	-1.178957
2	8	0	3.855791	-0.455918	-1.835926
3	8	0	2.820095	-0.348542	0.174023
4	6	0	1.507915	-0.192693	-1.757717
5	6	0	4.065402	-0.567215	0.851960
6	1	0	4.859841	-0.049664	0.308876
7	1	0	3.926644	-0.098593	1.828697
8	1	0	1.384586	-0.886401	-2.595814

9	29	0	-0.036678	-0.379345	-0.662913
10	7	0	-2.032700	-0.419516	-0.188203
11	6	0	-2.757513	0.039806	-1.402312
12	1	0	-2.327364	0.995699	-1.707668
13	1	0	-2.557569	-0.688144	-2.196333
14	6	0	-2.343836	0.505011	0.930978
15	1	0	-1.742841	0.188880	1.787809
16	1	0	-2.011770	1.502630	0.632515
17	6	0	-2.521750	-1.773350	0.174480
18	1	0	-2.022788	-2.053956	1.104545
19	1	0	-2.199552	-2.472498	-0.601458
20	7	0	0.626674	-2.373098	0.752498
21	8	0	0.436378	-2.191620	-0.534547
22	8	0	0.369577	-1.407046	1.489265
23	8	0	1.017564	-3.452441	1.129101
24	6	0	-4.275373	0.148139	-1.092336
25	1	0	-4.609324	1.189648	-1.136245
26	1	0	-4.866500	-0.418161	-1.818968
27	6	0	-3.866476	0.457373	1.232938
28	1	0	-4.058148	0.033887	2.224054
29	1	0	-4.301358	1.461675	1.214011
30	6	0	-4.064833	-1.740626	0.337280
31	1	0	-4.557026	-2.333205	-0.440558
32	1	0	-4.363391	-2.156969	1.304433
33	7	0	-4.562564	-0.368144	0.245070
34	6	0	4.356480	-2.050743	0.983673
35	1	0	3.532526	-2.562596	1.489320
36	1	0	4.497276	-2.499639	-0.003194
37	1	0	5.272522	-2.201461	1.564258
38	6	0	2.112530	3.255074	-0.198586
39	1	0	2.503651	2.293867	-0.544964
40	1	0	2.004253	3.927734	-1.054847
41	1	0	2.856300	3.678271	0.483713
42	6	0	0.779211	3.090594	0.527350
43	6	0	0.875177	2.045964	1.634561
44	1	0	-0.085084	1.928567	2.144692
45	1	0	1.201202	1.076529	1.250725
46	1	0	1.616003	2.366127	2.374448
47	6	0	0.282137	4.429469	1.072476
48	1	0	0.197048	5.168738	0.270799
49	1	0	-0.696493	4.311810	1.547663
50	1	0	0.987088	4.804361	1.820317
51	8	0	-0.271924	2.773502	-0.415572
52	8	0	-0.027830	1.541051	-1.104687
53	1	0	0.890397	1.367181	-1.599872

Zero-point correction= 0.445759 (Hartree/Particle)
Thermal correction to Energy= 0.473110
Thermal correction to Enthalpy= 0.474054
Thermal correction to Gibbs Free Energy= 0.387542
Sum of electronic and zero-point Energies= -2880.407929
Sum of electronic and thermal Energies= -2880.380579
Sum of electronic and thermal Enthalpies= -2880.379635
Sum of electronic and thermal Free Energies= -2880.466146
Sum of electronic and thermal Free Energies(343k)= -2880.479758

INT11

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.800619	-0.815870	1.349239
2	8	0	-3.295757	-1.850500	1.729612
3	8	0	-3.328233	-0.032156	0.394563
4	6	0	-1.553533	-0.216965	1.911701
5	6	0	-4.532072	-0.498768	-0.235556
6	1	0	-5.184991	-0.932008	0.526246
7	1	0	-4.993033	0.406618	-0.635593
8	1	0	-1.150191	-0.869984	2.689751
9	29	0	-0.109264	-0.147951	0.652377
10	7	0	1.934603	-0.518413	0.213285
11	6	0	2.794605	0.359182	1.052619
12	1	0	2.608298	1.386991	0.744819
13	1	0	2.462932	0.263074	2.089957

14	6	0	2.289326	-0.303717	-1.213121
15	1	0	1.709948	-1.011081	-1.810658
16	1	0	1.962922	0.701490	-1.483421
17	6	0	2.240848	-1.930482	0.565640
18	1	0	1.543415	-2.576735	0.031881
19	1	0	2.043310	-2.050485	1.636423
20	7	0	-0.873772	-1.628331	-1.269230
21	8	0	-0.612849	-1.846503	-0.003447
22	8	0	-0.788901	-0.445194	-1.641838
23	8	0	-1.159833	-2.564664	-1.975733
24	6	0	4.283315	-0.042883	0.876201
25	1	0	4.891743	0.831479	0.622852
26	1	0	4.692051	-0.469792	1.798080
27	6	0	3.816428	-0.510941	-1.407163
28	1	0	4.013199	-1.211103	-2.225271
29	1	0	4.312559	0.432910	-1.655055
30	6	0	3.719845	-2.249727	0.213582
31	1	0	4.237514	-2.692870	1.070326
32	1	0	3.776381	-2.967472	-0.611029
33	7	0	4.428820	-1.036279	-0.186401
34	6	0	-4.225153	-1.498387	-1.334340
35	1	0	-3.544231	-1.065077	-2.072752
36	1	0	-3.766578	-2.398620	-0.918088
37	1	0	-5.151175	-1.786637	-1.842422
38	6	0	-0.196125	4.282206	0.566689
39	1	0	-0.540547	3.957638	1.552125
40	1	0	0.837935	4.630260	0.655160
41	1	0	-0.819985	5.119846	0.238039
42	6	0	-0.291134	3.128776	-0.428233
43	6	0	-1.722448	2.627642	-0.575220
44	1	0	-1.765634	1.750275	-1.225623
45	1	0	-2.150285	2.357523	0.391901
46	1	0	-2.341462	3.418211	-1.012611
47	6	0	0.306820	3.498355	-1.783125
48	1	0	1.361056	3.773797	-1.676632
49	1	0	0.228512	2.657166	-2.479109
50	1	0	-0.230801	4.351436	-2.207826
51	8	0	0.595517	2.069395	0.006399
52	8	0	0.168356	1.518929	1.236047
53	1	0	-1.708767	0.799890	2.267695

Zero-point correction= 0.451202 (Hartree/Particle)
Thermal correction to Energy= 0.478606
Thermal correction to Enthalpy= 0.479550
Thermal correction to Gibbs Free Energy= 0.392641
Sum of electronic and zero-point Energies= -2880.474355
Sum of electronic and thermal Energies= -2880.446952
Sum of electronic and thermal Enthalpies= -2880.446007
Sum of electronic and thermal Free Energies= -2880.532917
Sum of electronic and thermal Free Energies(343k)= -2880.546589

INT12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.829789	-0.507828	-1.347164
2	8	0	-2.921282	0.524073	-1.986967
3	8	0	-3.850415	-1.268799	-0.959525
4	6	0	-1.520683	-1.003182	-0.907081
5	6	0	-5.174722	-0.757951	-1.217272
6	1	0	-5.194026	-0.304432	-2.210724
7	1	0	-5.808379	-1.646522	-1.212691
8	1	0	-1.130770	-1.771056	-1.587014
9	29	0	-0.549194	-0.204426	0.327095
10	7	0	0.532587	1.375410	-0.128905
11	6	0	1.368917	1.047565	-1.312766
12	1	0	1.989969	0.186357	-1.062391
13	1	0	0.685648	0.749844	-2.112492
14	6	0	1.403414	1.852861	0.974231
15	1	0	0.760345	2.045946	1.835093
16	1	0	2.081650	1.037846	1.233185
17	6	0	-0.404107	2.471596	-0.497042
18	1	0	-0.983635	2.709106	0.398519

19	1	0	-1.097111	2.085581	-1.249494
20	7	0	-0.823581	0.159485	2.852993
21	8	0	-1.568752	0.902558	2.172649
22	8	0	-0.022745	-0.603977	2.177935
23	8	0	-0.810418	0.134207	4.063696
24	6	0	2.219667	2.283650	-1.701933
25	1	0	3.285827	2.081990	-1.555574
26	1	0	2.072621	2.543404	-2.755152
27	6	0	2.157490	3.130655	0.517694
28	1	0	1.870879	3.993438	1.127455
29	1	0	3.239902	3.001121	0.618416
30	6	0	0.417465	3.685268	-1.012152
31	1	0	0.202922	3.882514	-2.067274
32	1	0	0.169919	4.592108	-0.451415
33	7	0	1.855109	3.437408	-0.879938
34	6	0	-5.588341	0.231344	-0.144088
35	1	0	-5.518201	-0.224882	0.847186
36	1	0	-4.947925	1.116896	-0.169487
37	1	0	-6.623089	0.547523	-0.310858
38	6	0	2.683868	-1.706548	0.926490
39	6	0	2.037025	-2.469844	-0.054996
40	6	0	2.582179	-2.490007	-1.346650
41	6	0	3.750603	-1.795959	-1.638626
42	6	0	4.396382	-1.057603	-0.647309
43	6	0	3.855251	-1.012070	0.634518
44	1	0	2.254301	-1.653708	1.922889
45	1	0	2.083147	-3.046770	-2.134613
46	1	0	4.158527	-1.827912	-2.644697
47	1	0	5.311887	-0.519945	-0.875615
48	1	0	4.346952	-0.437426	1.414518
49	6	0	0.821891	-3.223704	0.312415
50	1	0	0.363692	-2.926878	1.254347
51	6	0	0.275507	-4.224382	-0.381108
52	1	0	0.700382	-4.599153	-1.308921
53	1	0	-0.620850	-4.720429	-0.023260

Zero-point correction= 0.441394 (Hartree/Particle)
Thermal correction to Energy= 0.469804
Thermal correction to Enthalpy= 0.470748
Thermal correction to Gibbs Free Energy= 0.376871
Sum of electronic and zero-point Energies= -2881.259277
Sum of electronic and thermal Energies= -2881.230867
Sum of electronic and thermal Enthalpies= -2881.229923
Sum of electronic and thermal Free Energies= -2881.323800
Sum of electron ic and thermal Free Energies(343k)= -2881.338528

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.500591	-0.035644	-1.653702
2	8	0	-2.642800	0.622901	-2.664357
3	8	0	-3.378477	-0.095189	-0.649846
4	6	0	-1.207400	-0.693284	-1.378512
5	6	0	-4.459427	0.855350	-0.687980
6	1	0	-4.058341	1.819762	-1.007473
7	1	0	-5.192484	0.523282	-1.430210
8	1	0	-0.868706	-1.357605	-2.173009
9	29	0	-0.258082	0.193198	-0.136883
10	7	0	1.482427	1.168708	-0.222745
11	6	0	2.382155	0.347858	-1.067018
12	1	0	2.484340	-0.632027	-0.591044
13	1	0	1.882451	0.196561	-2.028034
14	6	0	2.110554	1.353412	1.106278
15	1	0	1.419795	1.939129	1.717527
16	1	0	2.199026	0.366425	1.569037
17	6	0	1.301744	2.496318	-0.855085
18	1	0	0.605822	3.062082	-0.230453
19	1	0	0.819396	2.338128	-1.824374
20	7	0	-1.456212	1.148986	1.908705
21	8	0	-1.492045	1.866783	0.878352
22	8	0	-0.674030	0.128086	1.862874
23	8	0	-2.113425	1.379847	2.905350

24	6	0	3.749824	1.067823	-1.219959
25	1	0	4.566520	0.445679	-0.839182
26	1	0	3.965247	1.286676	-2.270971
27	6	0	3.487548	2.050203	0.934221
28	1	0	3.521595	2.997030	1.482634
29	1	0	4.298591	1.420685	1.314927
30	6	0	2.684233	3.190791	-0.997414
31	1	0	2.905363	3.416209	-2.045740
32	1	0	2.709932	4.136145	-0.446028
33	7	0	3.749145	2.329359	-0.478540
34	6	0	-5.043975	0.927473	0.705731
35	1	0	-5.416089	-0.050001	1.027786
36	1	0	-4.290745	1.272279	1.419633
37	1	0	-5.880101	1.633944	0.714985
38	6	0	0.935408	-2.451888	1.487092
39	6	0	0.239489	-2.755286	0.309822
40	6	0	0.947065	-3.309657	-0.764089
41	6	0	2.311277	-3.553332	-0.664134
42	6	0	2.994003	-3.249502	0.512684
43	6	0	2.301145	-2.698154	1.587284
44	1	0	0.401809	-1.998112	2.316781
45	1	0	0.434719	-3.544664	-1.692733
46	1	0	2.843795	-3.981806	-1.507854
47	1	0	4.059807	-3.442037	0.590648
48	1	0	2.822631	-2.460125	2.509652
49	6	0	-1.206063	-2.456353	0.245031
50	1	0	-1.603903	-1.911213	1.096871
51	6	0	-2.072021	-2.868780	-0.708440
52	1	0	-1.769640	-3.488998	-1.547117
53	1	0	-3.127560	-2.643049	-0.618435

Zero-point correction= 0.442141 (Hartree/Particle)
Thermal correction to Energy= 0.469226
Thermal correction to Enthalpy= 0.470170
Thermal correction to Gibbs Free Energy= 0.382111
Sum of electronic and zero-point Energies= -2881.250762
Sum of electronic and thermal Energies= -2881.223677
Sum of electronic and thermal Enthalpies= -2881.222733
Sum of electronic and thermal Free Energies= -2881.310792
Sum of electron ic and thermal Free Energies(343k)= -2881.324628

INT13

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.931158	-0.885878	-0.448577
2	8	0	-2.391739	-1.578712	-1.325998
3	8	0	-2.596645	0.142461	0.110877
4	6	0	-0.576188	-1.063524	0.132900
5	6	0	-3.911847	0.387501	-0.405708
6	1	0	-3.839214	0.582803	-1.479843
7	1	0	-4.517601	-0.513952	-0.273458
8	1	0	-0.044420	-1.898214	-0.310722
9	6	0	-4.484187	1.569400	0.347289
10	1	0	-4.546367	1.356476	1.418470
11	1	0	-3.863832	2.459222	0.205978
12	1	0	-5.491404	1.788629	-0.020072
13	6	0	2.282156	1.406688	-0.217407
14	6	0	1.711923	0.202300	0.201301
15	6	0	2.538080	-0.921187	0.308748
16	6	0	3.892676	-0.840680	0.006959
17	6	0	4.449744	0.366313	-0.407782
18	6	0	3.638191	1.490787	-0.518013
19	1	0	1.655260	2.290358	-0.307261
20	1	0	2.124974	-1.874352	0.630184
21	1	0	4.515430	-1.726104	0.095478
22	1	0	5.508150	0.429445	-0.641530
23	1	0	4.059926	2.438029	-0.841208
24	6	0	0.255507	0.156854	0.515980
25	1	0	-0.259798	1.104853	0.392142
26	6	0	-0.304740	-0.735744	1.579708
27	1	0	0.379981	-1.387122	2.114537
28	1	0	-1.134951	-0.357038	2.165888

Zero-point correction= 0.237898 (Hartree/Particle)
Thermal correction to Energy= 0.251020
Thermal correction to Enthalpy= 0.251964
Thermal correction to Gibbs Free Energy= 0.196044
Sum of electronic and zero-point Energies= -615.713439
Sum of electronic and thermal Energies= -615.700317
Sum of electronic and thermal Enthalpies= -615.699372
Sum of electronic and thermal Free Energies= -615.755293
Sum of electron ic and thermal Free Energies(343k)= -615.764006

INT14

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.070460	2.277271	0.467042
2	8	0	1.832166	2.190595	-0.508980
3	8	0	-0.068158	3.024374	0.357744
4	6	0	1.231946	1.651359	1.757228
5	6	0	-0.349560	3.548846	-0.936472
6	1	0	0.421116	4.273989	-1.216841
7	1	0	-0.320022	2.741637	-1.677593
8	1	0	0.716029	2.173141	2.563738
9	29	0	0.218652	0.185604	1.070233
10	7	0	-1.329727	-0.752169	0.410425
11	6	0	-2.490178	-0.513528	1.303095
12	1	0	-2.272126	-0.988004	2.264337
13	1	0	-2.560289	0.563526	1.476662
14	6	0	-1.169553	-2.212766	0.209422
15	1	0	-0.317062	-2.347362	-0.458691
16	1	0	-0.912353	-2.655390	1.177064
17	6	0	-1.611934	-0.117880	-0.906771
18	1	0	-0.720980	-0.228713	-1.529832
19	1	0	-1.759014	0.950584	-0.721311
20	6	0	-3.776763	-1.086097	0.646664
21	1	0	-4.264540	-1.813750	1.303548
22	1	0	-4.501926	-0.291378	0.443221
23	6	0	-2.481274	-2.807147	-0.369857
24	1	0	-2.291888	-3.329855	-1.312910
25	1	0	-2.928706	-3.528827	0.321731
26	6	0	-2.870920	-0.769032	-1.537218
27	1	0	-3.629488	-0.014818	-1.770609
28	1	0	-2.622550	-1.284172	-2.470586
29	7	0	-3.458574	-1.747336	-0.619291
30	6	0	-1.721493	4.189790	-0.872534
31	1	0	-2.485554	3.449266	-0.612556
32	1	0	-1.743990	4.980253	-0.116991
33	1	0	-1.979377	4.627550	-1.842094
34	1	0	2.279571	1.457255	1.984984
35	6	0	2.785500	-1.506882	-0.250905
36	6	0	3.096916	-2.550524	-1.318396
37	1	0	2.280901	-3.276912	-1.394339
38	1	0	3.228294	-2.069879	-2.290798
39	1	0	4.017406	-3.087922	-1.066923
40	6	0	2.469130	-2.152308	1.096717
41	1	0	3.369550	-2.606816	1.519677
42	1	0	2.097637	-1.393786	1.794211
43	1	0	1.707091	-2.931382	0.989875
44	6	0	3.901629	-0.475092	-0.121639
45	1	0	4.083424	0.018652	-1.078910
46	1	0	3.636444	0.290167	0.611083
47	1	0	4.826969	-0.967212	0.195073
48	8	0	1.534636	-0.855946	-0.572928
49	8	0	1.642644	-0.137691	-1.802171
50	1	0	1.788884	0.777465	-1.446495

Zero-point correction= 0.443444 (Hartree/Particle)
Thermal correction to Energy= 0.467928
Thermal correction to Enthalpy= 0.468872
Thermal correction to Gibbs Free Energy= 0.387598
Sum of electronic and zero-point Energies= -2600.861883

Sum of electronic and thermal Energies= -2600.837399
Sum of electronic and thermal Enthalpies= -2600.836454
Sum of electronic and thermal Free Energies= -2600.917729
Sum of electron ic and thermal Free Energies(343k)= -2600.930492

TS7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.855888	2.312154	0.800331
2	8	0	1.893380	2.471841	0.130781
3	8	0	-0.268748	3.000001	0.458037
4	6	0	0.649287	1.374048	1.864997
5	6	0	-0.207012	3.739584	-0.760352
6	1	0	0.567164	4.509212	-0.685328
7	1	0	0.074278	3.068414	-1.579388
8	1	0	-0.224186	1.593691	2.478681
9	29	0	0.468913	-0.113630	0.569023
10	7	0	-1.401195	-0.891298	0.205534
11	6	0	-2.182197	-1.049819	1.449120
12	1	0	-1.672569	-1.793703	2.070068
13	1	0	-2.145286	-0.096406	1.983649
14	6	0	-1.392280	-2.173004	-0.527734
15	1	0	-0.786117	-2.032503	-1.426725
16	1	0	-0.877656	-2.909757	0.097457
17	6	0	-2.054656	0.136843	-0.638707
18	1	0	-1.443665	0.255092	-1.538453
19	1	0	-2.018670	1.084691	-0.092615
20	6	0	-3.635746	-1.477708	1.101720
21	1	0	-3.884586	-2.441914	1.557347
22	1	0	-4.362151	-0.744603	1.467634
23	6	0	-2.852463	-2.595670	-0.852632
24	1	0	-3.004101	-2.696776	-1.932317
25	1	0	-3.096312	-3.560585	-0.395660
26	6	0	-3.506532	-0.305485	-0.969066
27	1	0	-4.236393	0.423820	-0.602252
28	1	0	-3.655187	-0.404282	-2.049425
29	7	0	-3.799581	-1.599396	-0.347879
30	6	0	-1.576750	4.347023	-0.987000
31	1	0	-2.340041	3.566588	-1.072355
32	1	0	-1.851125	5.005688	-0.157743
33	1	0	-1.579868	4.933219	-1.911577
34	1	0	1.551983	1.203358	2.452884
35	6	0	3.057809	-1.429792	-0.289500
36	6	0	3.713303	-1.299994	-1.662726
37	1	0	3.189722	-1.929382	-2.387981
38	1	0	3.681178	-0.268803	-2.017956
39	1	0	4.759214	-1.618926	-1.606723
40	6	0	3.152214	-2.877815	0.214270
41	1	0	4.205936	-3.141394	0.352433
42	1	0	2.637997	-2.988457	1.173710
43	1	0	2.708998	-3.568403	-0.508846
44	6	0	3.664866	-0.472056	0.733935
45	1	0	3.491320	0.576599	0.474200
46	1	0	3.233193	-0.646172	1.725091
47	1	0	4.746050	-0.633722	0.796364
48	8	0	1.640223	-1.264072	-0.392940
49	8	0	1.376416	0.246572	-1.224935
50	1	0	1.893283	0.980967	-0.796902

Zero-point correction= 0.440167 (Hartree/Particle)
Thermal correction to Energy= 0.464384
Thermal correction to Enthalpy= 0.465329
Thermal correction to Gibbs Free Energy= 0.384616
Sum of electronic and zero-point Energies= -2600.824913
Sum of electronic and thermal Energies= -2600.800696
Sum of electronic and thermal Enthalpies= -2600.799752
Sum of electronic and thermal Free Energies= -2600.880464
Sum of electron ic and thermal Free Energies(343k)= -2600.893139

NT15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.742569	2.177673	0.617750
2	8	0	-1.587348	3.345022	0.319810
3	8	0	-2.620701	1.378759	-0.030144
4	6	0	-0.961369	1.443415	1.637308
5	6	0	-3.334774	1.969629	-1.124058
6	1	0	-4.005279	2.742552	-0.736269
7	1	0	-2.620455	2.453778	-1.795811
8	1	0	-1.543735	0.664743	2.121356
9	29	0	0.561168	0.672710	0.723535
10	7	0	-0.271707	-1.168826	0.524598
11	6	0	0.662977	-2.244359	0.975293
12	1	0	1.669194	-1.931620	0.699143
13	1	0	0.589745	-2.279159	2.067021
14	6	0	-0.406566	-1.219391	-0.964326
15	1	0	-1.026571	-0.367049	-1.259881
16	1	0	0.597365	-1.075589	-1.362444
17	6	0	-1.604608	-1.488400	1.107062
18	1	0	-2.323407	-0.768094	0.715114
19	1	0	-1.540599	-1.364131	2.191208
20	6	0	0.247172	-3.588444	0.328286
21	1	0	0.949499	-3.871522	-0.462204
22	1	0	0.249013	-4.391475	1.072272
23	6	0	-1.034428	-2.568736	-1.393795
24	1	0	-2.053671	-2.430732	-1.770424
25	1	0	-0.446356	-3.024363	-2.196434
26	6	0	-1.997316	-2.946355	0.737089
27	1	0	-1.967212	-3.595905	1.617890
28	1	0	-3.017980	-2.975176	0.342401
29	7	0	-1.088187	-3.494584	-0.263777
30	6	0	-4.096508	0.855737	-1.811859
31	1	0	-3.409386	0.095435	-2.197884
32	1	0	-4.793923	0.374561	-1.119627
33	1	0	-4.667811	1.258232	-2.653544
34	1	0	-0.566240	2.138222	2.376701
35	6	0	3.154868	0.435628	-0.647821
36	6	0	2.681761	1.228817	-1.875000
37	1	0	2.058119	0.591751	-2.515518
38	1	0	2.095497	2.092627	-1.556118
39	1	0	3.533318	1.576218	-2.471815
40	6	0	3.962630	-0.785946	-1.117309
41	1	0	4.850376	-0.481747	-1.684092
42	1	0	4.288821	-1.376150	-0.253641
43	1	0	3.344675	-1.426028	-1.758641
44	6	0	4.033553	1.307559	0.258247
45	1	0	3.465812	2.169434	0.612035
46	1	0	4.359563	0.721866	1.125572
47	1	0	4.925661	1.658064	-0.275220
48	8	0	2.065473	-0.102239	0.061601
49	8	0	1.190219	2.318679	0.563308
50	1	0	0.481279	2.973815	0.642786

Zero-point correction= 0.445414 (Hartree/Particle)
Thermal correction to Energy= 0.468895
Thermal correction to Enthalpy= 0.469839
Thermal correction to Gibbs Free Energy= 0.392185
Sum of electronic and zero-point Energies= -2600.923384
Sum of electronic and thermal Energies= -2600.899903
Sum of electronic and thermal Enthalpies= -2600.898959
Sum of electronic and thermal Free Energies= -2600.976613
Sum of electron ic and thermal Free Energies(343k)= -2600.988827

INT16

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.084434	0.077343	-0.000047
2	8	0	1.287161	1.278604	-0.000197
3	8	0	-0.148259	-0.471401	0.000206
4	6	0	2.125892	-0.928637	-0.000045
5	6	0	-1.238081	0.458135	0.000445

6	1	0	-1.160250	1.100550	0.883568
7	1	0	-1.159784	1.101671	-0.881814
8	1	0	3.156579	-0.598524	-0.000625
9	6	0	-2.520807	-0.346687	-0.000362
10	1	0	-2.579357	-0.982867	-0.888253
11	1	0	-2.580096	-0.983617	0.886938
12	1	0	-3.381798	0.328852	-0.000447
13	1	0	1.884861	-1.984617	0.000614

Zero-point correction= 0.105978 (Hartree/Particle)
Thermal correction to Energy= 0.113095
Thermal correction to Enthalpy= 0.114039
Thermal correction to Gibbs Free Energy= 0.074076
Sum of electronic and zero-point Energies= -306.836411
Sum of electronic and thermal Energies= -306.829293
Sum of electronic and thermal Enthalpies= -306.828349
Sum of electronic and thermal Free Energies= -306.868312
Sum of electron ic and thermal Free Energies(343k)= -306.874483

INT17

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.663902	-1.006492	-0.085668
2	7	0	-1.147919	-0.212838	-0.001526
3	6	0	-1.392316	0.427736	-1.319626
4	1	0	-0.558429	1.110175	-1.496762
5	1	0	-1.352531	-0.361185	-2.077591
6	6	0	-1.173780	0.830565	1.053609
7	1	0	-0.965026	0.337101	2.009047
8	1	0	-0.344548	1.506632	0.837551
9	6	0	-2.212912	-1.206297	0.262302
10	1	0	-1.996797	-1.676157	1.225882
11	1	0	-2.139305	-1.983488	-0.501826
12	6	0	-2.772904	1.136880	-1.290955
13	1	0	-2.663216	2.211224	-1.468524
14	1	0	-3.437859	0.741438	-2.065430
15	6	0	-2.563646	1.521056	1.050335
16	1	0	-3.068176	1.399077	2.014277
17	1	0	-2.465031	2.595074	0.864383
18	6	0	-3.588436	-0.480988	0.257451
19	1	0	-4.243829	-0.888694	-0.518716
20	1	0	-4.099927	-0.605567	1.217277
21	7	0	-3.419223	0.950580	0.008967
22	6	0	2.764340	0.754545	0.005524
23	6	0	2.903005	0.295013	1.467893
24	1	0	2.179598	0.831727	2.093196
25	1	0	2.699895	-0.781958	1.551745
26	1	0	3.907418	0.470724	1.869363
27	6	0	3.100981	2.245196	-0.101623
28	1	0	4.135117	2.452717	0.196896
29	1	0	2.961523	2.580794	-1.134456
30	1	0	2.428966	2.827869	0.538391
31	6	0	3.711093	-0.063403	-0.885804
32	1	0	3.477297	-1.133319	-0.812220
33	1	0	3.584876	0.238532	-1.930701
34	1	0	4.762443	0.073170	-0.605989
35	8	0	1.437148	0.594143	-0.417017
36	8	0	0.649286	-2.781231	0.010938
37	1	0	0.570374	-3.186915	0.880497

Zero-point correction= 0.330535 (Hartree/Particle)
Thermal correction to Energy= 0.347923
Thermal correction to Enthalpy= 0.348867
Thermal correction to Gibbs Free Energy= 0.283195
Sum of electronic and zero-point Energies= -2294.050985
Sum of electronic and thermal Energies= -2294.033598
Sum of electronic and thermal Enthalpies= -2294.032654
Sum of electronic and thermal Free Energies= -2294.098326
Sum of electron ic and thermal Free Energies(343k)= -2294.108598

INT18

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.003384	-0.463503	-0.731509
2	8	0	3.328119	0.574985	-0.158742
3	8	0	3.436873	-1.674761	-0.267820
4	6	0	2.084370	-0.593596	-1.848608
5	6	0	4.107554	-1.668877	0.989387
6	1	0	4.702572	-2.585636	0.996330
7	1	0	4.775715	-0.806508	1.045645
8	1	0	2.125866	0.273109	-2.508771
9	7	0	0.009143	1.289698	-0.229189
10	6	0	-1.439165	1.556657	-0.418982
11	1	0	-1.689289	1.326445	-1.459490
12	1	0	-1.995966	0.862277	0.211452
13	6	0	0.778936	2.267401	-1.046642
14	1	0	1.836035	2.018427	-0.936442
15	1	0	0.495031	2.108454	-2.091220
16	6	0	0.350229	1.513393	1.200027
17	1	0	1.426656	1.346352	1.296475
18	1	0	-0.173384	0.754761	1.789343
19	1	0	2.211679	-1.528814	-2.392493
20	29	0	0.489363	-0.620056	-0.666049
21	6	0	3.113723	-1.658754	2.141274
22	1	0	2.431979	-2.513551	2.074710
23	1	0	3.638063	-1.711928	3.101302
24	1	0	2.524769	-0.736485	2.125144
25	6	0	-1.753435	3.032817	-0.055604
26	1	0	-2.099497	3.592116	-0.930922
27	1	0	-2.543620	3.084279	0.700595
28	6	0	-0.061102	2.950698	1.619353
29	1	0	-0.846925	2.928644	2.381697
30	1	0	0.791802	3.491873	2.040778
31	6	0	0.464612	3.710422	-0.572494
32	1	0	1.360300	4.187761	-0.162438
33	1	0	0.111217	4.332899	-1.401185
34	7	0	-0.563652	3.701522	0.468858
35	6	0	-4.258226	-1.123576	1.284269
36	6	0	-2.888183	-1.328417	1.412614
37	6	0	-2.095664	-1.658178	0.305702
38	6	0	-2.728105	-1.776080	-0.940413
39	6	0	-4.096463	-1.574432	-1.069978
40	6	0	-4.870392	-1.243014	0.040465
41	1	0	-4.848256	-0.870892	2.160764
42	1	0	-2.418293	-1.231732	2.388833
43	1	0	-2.142750	-2.019377	-1.823672
44	1	0	-4.562015	-1.672146	-2.046524
45	1	0	-5.938714	-1.081401	-0.064690
46	6	0	-0.635220	-1.795062	0.475784
47	6	0	0.212177	-2.499433	-0.393479
48	1	0	-0.292994	-1.679992	1.505877
49	1	0	1.143386	-2.920255	-0.023287
50	1	0	-0.187443	-2.998184	-1.274576

Zero-point correction= 0.438801 (Hartree/Particle)
Thermal correction to Energy= 0.461243
Thermal correction to Enthalpy= 0.462187
Thermal correction to Gibbs Free Energy= 0.385927
Sum of electronic and zero-point Energies= -2601.715692
Sum of electronic and thermal Energies= -2601.693250
Sum of electronic and thermal Enthalpies= -2601.692306
Sum of electronic and thermal Free Energies= -2601.768566
Sum of electronic and thermal Free Energies(343k)= -2601.780556

TS8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.839937	-0.099701	-0.718470
2	8	0	-2.412385	-0.841956	0.179517
3	8	0	-4.110256	0.331504	-0.741162
4	6	0	-1.980992	0.511542	-1.706955

5	6	0	-4.921414	0.006812	0.396710
6	1	0	-5.947225	0.102852	0.034918
7	1	0	-4.736989	-1.029705	0.687492
8	1	0	-1.259192	-0.181530	-2.142535
9	7	0	0.656911	-1.378242	0.015749
10	6	0	2.095374	-1.051206	-0.139074
11	1	0	2.218586	-0.525308	-1.088924
12	1	0	2.365844	-0.341527	0.647800
13	6	0	0.262602	-2.321276	-1.056237
14	1	0	-0.809594	-2.504663	-0.949207
15	1	0	0.423766	-1.815061	-2.013995
16	6	0	0.460442	-2.046251	1.326697
17	1	0	-0.606738	-2.259510	1.427637
18	1	0	0.731823	-1.327534	2.105359
19	1	0	-2.511306	1.056683	-2.482978
20	29	0	-0.459808	0.255703	0.036945
21	6	0	-4.646544	0.959516	1.547325
22	1	0	-4.815185	1.995328	1.237655
23	1	0	-5.313094	0.736017	2.386909
24	1	0	-3.612970	0.855286	1.888793
25	6	0	2.932500	-2.358142	-0.080921
26	1	0	3.479118	-2.518072	-1.016122
27	1	0	3.670607	-2.318274	0.726526
28	6	0	1.333598	-3.328881	1.396307
29	1	0	2.061635	-3.266962	2.211739
30	1	0	0.717994	-4.217130	1.572601
31	6	0	1.106974	-3.620266	-0.953842
32	1	0	0.469653	-4.491803	-0.771663
33	1	0	1.659627	-3.805595	-1.880739
34	7	0	2.067338	-3.518773	0.144545
35	6	0	3.326319	2.803360	1.219193
36	6	0	1.952029	2.640720	1.316269
37	6	0	1.156630	2.349553	0.189493
38	6	0	1.827443	2.256257	-1.046766
39	6	0	3.204951	2.422942	-1.142173
40	6	0	3.972186	2.690823	-0.012417
41	1	0	3.900823	3.023218	2.115733
42	1	0	1.467643	2.726432	2.286657
43	1	0	1.267565	2.032819	-1.952341
44	1	0	3.683185	2.339290	-2.115138
45	1	0	5.047531	2.818189	-0.089522
46	6	0	-0.287275	2.141639	0.345076
47	6	0	-1.188433	2.103462	-0.795025
48	1	0	-0.722771	2.494304	1.277537
49	1	0	-2.177130	2.505930	-0.579234
50	1	0	-0.806103	2.498249	-1.736403

Zero-point correction= 0.436608 (Hartree/Particle)
Thermal correction to Energy= 0.459149
Thermal correction to Enthalpy= 0.460093
Thermal correction to Gibbs Free Energy= 0.382410
Sum of electronic and zero-point Energies= -2601.649713
Sum of electronic and thermal Energies= -2601.627173
Sum of electronic and thermal Enthalpies= -2601.626228
Sum of electronic and thermal Free Energies= -2601.703912
Sum of electronic and thermal Free Energies(343k)= -2601.716112

INT19

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.642587	0.148890	-0.976144
2	8	0	1.765458	0.879284	-1.409576
3	8	0	3.674585	0.603752	-0.259755
4	6	0	2.727391	-1.334770	-1.210416
5	6	0	3.640562	1.987739	0.119574
6	1	0	4.687432	2.266982	0.252035
7	1	0	3.211024	2.569945	-0.698482
8	1	0	1.964588	-1.575796	-1.953489
9	7	0	-0.967523	1.184376	0.165586
10	6	0	-2.006944	1.137957	1.224273
11	1	0	-2.267044	0.087062	1.375800
12	1	0	-1.555092	1.508360	2.149579

13	6	0	-1.554467	0.630675	-1.087718
14	1	0	-0.771360	0.655035	-1.849235
15	1	0	-1.806305	-0.417010	-0.897552
16	6	0	-0.580334	2.595822	-0.069309
17	1	0	0.213950	2.593154	-0.818590
18	1	0	-0.155516	2.978437	0.864254
19	1	0	3.710382	-1.566607	-1.636515
20	29	0	0.463262	-0.047129	0.553049
21	6	0	2.840324	2.152183	1.398632
22	1	0	3.345738	1.677713	2.244144
23	1	0	2.680258	3.211143	1.624987
24	1	0	1.870961	1.655772	1.273544
25	6	0	-3.230089	1.991475	0.790766
26	1	0	-4.140965	1.384639	0.763184
27	1	0	-3.405273	2.814829	1.491272
28	6	0	-1.826299	3.410661	-0.510809
29	1	0	-2.017079	4.242282	0.175708
30	1	0	-1.684629	3.835908	-1.509789
31	6	0	-2.796087	1.468074	-1.492409
32	1	0	-2.670047	1.903850	-2.488910
33	1	0	-3.697643	0.847449	-1.515786
34	7	0	-3.015999	2.559300	-0.540596
35	6	0	-2.359134	-2.930502	1.004595
36	6	0	-1.121010	-2.421030	1.359614
37	6	0	-0.024595	-2.408796	0.465493
38	6	0	-0.247923	-3.002651	-0.790294
39	6	0	-1.495734	-3.509030	-1.151900
40	6	0	-2.567700	-3.468375	-0.268763
41	1	0	-3.170319	-2.916576	1.728824
42	1	0	-0.979474	-2.001493	2.354732
43	1	0	0.564110	-3.069083	-1.507559
44	1	0	-1.623197	-3.949041	-2.138053
45	1	0	-3.538206	-3.863900	-0.552421
46	6	0	1.249196	-1.748312	0.871912
47	6	0	2.513643	-2.121546	0.102100
48	1	0	1.412422	-1.931411	1.939629
49	1	0	3.379292	-1.921561	0.742611
50	1	0	2.551380	-3.194138	-0.147789

Zero-point correction= 0.440468 (Hartree/Particle)
Thermal correction to Energy= 0.462792
Thermal correction to Enthalpy= 0.463737
Thermal correction to Gibbs Free Energy= 0.387530
Sum of electronic and zero-point Energies= -2601.703696
Sum of electronic and thermal Energies= -2601.681372
Sum of electronic and thermal Enthalpies= -2601.680427
Sum of electronic and thermal Free Energies= -2601.756634
Sum of electronic and thermal Free Energies(343k)= -2601.768609

Styrene

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.776931	-1.042290	0.000118
2	6	0	-0.406244	-1.278264	0.000010
3	6	0	0.511408	-0.221432	-0.000103
4	6	0	0.010517	1.087375	-0.000153
5	6	0	-1.357198	1.326150	-0.000060
6	6	0	-2.258245	0.262705	0.000088
7	1	0	-2.469280	-1.879067	0.000224
8	1	0	-0.036590	-2.301072	0.000038
9	1	0	0.695495	1.930008	-0.000290
10	1	0	-1.724220	2.348508	-0.000104
11	1	0	-3.327490	0.452211	0.000158
12	6	0	1.953589	-0.531004	-0.000192
13	1	0	2.188317	-1.595125	-0.000654
14	6	0	2.966204	0.336896	0.000248
15	1	0	2.820643	1.413554	0.000776
16	1	0	3.994526	-0.009827	0.000123

Zero-point correction= 0.134978 (Hartree/Particle)
Thermal correction to Energy= 0.140876
Thermal correction to Enthalpy= 0.141820

Thermal correction to Gibbs Free Energy= 0.105074
Sum of electronic and zero-point Energies= -309.401448
Sum of electronic and thermal Energies= -309.395551
Sum of electronic and thermal Enthalpies= -309.394606
Sum of electronic and thermal Free Energies= -309.431353
Sum of electron ic and thermal Free Energies(343k)= -309.437040

INT20

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.466731	-0.727450	-0.897208
2	8	0	-3.621238	-1.111472	-0.942014
3	8	0	-2.087085	0.391879	-0.233250
4	6	0	-1.346755	-1.391600	-1.525113
5	6	0	-3.129843	1.107752	0.437755
6	1	0	-3.859553	1.451470	-0.302340
7	1	0	-3.648373	0.428992	1.122022
8	1	0	-1.536586	-2.315413	-2.055609
9	6	0	-2.478995	2.262585	1.169845
10	1	0	-1.757142	1.898817	1.907767
11	1	0	-1.955653	2.920530	0.469743
12	1	0	-3.239926	2.849490	1.693200
13	1	0	-0.343790	-0.987082	-1.460079
14	6	0	4.016919	0.272070	-0.449220
15	6	0	3.314405	-0.747650	0.184243
16	6	0	1.951447	-0.615621	0.475478
17	6	0	1.306359	0.573834	0.105969
18	6	0	2.006926	1.591020	-0.530270
19	6	0	3.364838	1.447174	-0.808643
20	1	0	5.074540	0.146509	-0.661704
21	1	0	3.830103	-1.664140	0.461097
22	1	0	0.246087	0.703492	0.299984
23	1	0	1.487869	2.502893	-0.811332
24	1	0	3.908481	2.245612	-1.304888
25	6	0	1.256623	-1.728708	1.148750
26	1	0	1.870051	-2.613860	1.314970
27	6	0	-0.012193	-1.753796	1.562627
28	1	0	-0.687390	-0.912162	1.438698
29	1	0	-0.420141	-2.636069	2.045315

Zero-point correction= 0.243311 (Hartree/Particle)
Thermal correction to Energy= 0.258777
Thermal correction to Enthalpy= 0.259721
Thermal correction to Gibbs Free Energy= 0.196597
Sum of electronic and zero-point Energies= -616.245405
Sum of electronic and thermal Energies= -616.229938
Sum of electronic and thermal Enthalpies= -616.228994
Sum of electronic and thermal Free Energies= -616.292119
Sum of electron ic and thermal Free Energies(343k)= -616.301952

TS9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.478084	-0.847244	0.488936
2	8	0	3.553435	-1.308846	0.158590
3	8	0	2.160699	0.464221	0.335878
4	6	0	1.360974	-1.601423	1.028778
5	6	0	3.177139	1.293835	-0.234424
6	1	0	4.026486	1.341232	0.455034
7	1	0	3.533507	0.842109	-1.165260
8	1	0	1.540825	-2.641743	1.267194
9	6	0	2.563826	2.659287	-0.465893
10	1	0	1.731407	2.595464	-1.173725
11	1	0	2.189714	3.080725	0.471797
12	1	0	3.313681	3.342099	-0.877234
13	1	0	0.572310	-1.074566	1.551380
14	6	0	-4.119658	0.283895	0.199271
15	6	0	-3.330931	-0.823236	-0.086598
16	6	0	-1.943068	-0.698466	-0.252149

17	6	0	-1.364420	0.572678	-0.095622
18	6	0	-2.155046	1.677142	0.194243
19	6	0	-3.534417	1.540140	0.338597
20	1	0	-5.192514	0.165648	0.318586
21	1	0	-3.792438	-1.801942	-0.193503
22	1	0	-0.287404	0.693813	-0.170905
23	1	0	-1.689283	2.650458	0.318562
24	1	0	-4.148083	2.406137	0.568192
25	6	0	-1.144937	-1.884496	-0.554756
26	1	0	-1.630852	-2.843520	-0.382137
27	6	0	0.153847	-1.877038	-0.960308
28	1	0	0.617211	-0.965592	-1.323818
29	1	0	0.654004	-2.803755	-1.220361

Zero-point correction= 0.244080 (Hartree/Particle)
Thermal correction to Energy= 0.258162
Thermal correction to Enthalpy= 0.259107
Thermal correction to Gibbs Free Energy= 0.200294
Sum of electronic and zero-point Energies= -616.238586
Sum of electronic and thermal Energies= -616.224504
Sum of electronic and thermal Enthalpies= -616.223559
Sum of electronic and thermal Free Energies= -616.282372
Sum of electron ic and thermal Free Energies(343k)= -616.291539

INT21

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.409594	-0.912142	-0.490414
2	8	0	-3.362882	-1.605313	-0.753643
3	8	0	-2.512698	0.365183	-0.078425
4	6	0	-0.960839	-1.333302	-0.560874
5	6	0	-3.844702	0.883141	0.044017
6	1	0	-4.331139	0.844419	-0.935523
7	1	0	-4.416162	0.242120	0.722082
8	1	0	-0.920006	-2.333990	-0.995344
9	6	0	-3.731626	2.300277	0.564682
10	1	0	-3.241966	2.316096	1.542726
11	1	0	-3.150531	2.921756	-0.122817
12	1	0	-4.728346	2.739534	0.670061
13	1	0	-0.433455	-0.645858	-1.231062
14	6	0	4.428618	0.106599	-0.176123
15	6	0	3.504291	-0.846862	0.209257
16	6	0	2.125139	-0.530922	0.333668
17	6	0	1.735491	0.804726	0.044911
18	6	0	2.669927	1.751179	-0.341082
19	6	0	4.020405	1.414288	-0.455205
20	1	0	5.477084	-0.163340	-0.263889
21	1	0	3.828600	-1.862335	0.422878
22	1	0	0.690570	1.090759	0.125404
23	1	0	2.346361	2.765661	-0.556089
24	1	0	4.747080	2.161214	-0.759041
25	6	0	1.200112	-1.527904	0.727762
26	1	0	1.582640	-2.530429	0.904111
27	6	0	-0.275356	-1.308678	0.827720
28	1	0	-0.490406	-0.345448	1.304496
29	1	0	-0.726885	-2.081513	1.458632

Zero-point correction= 0.247993 (Hartree/Particle)
Thermal correction to Energy= 0.261738
Thermal correction to Enthalpy= 0.262682
Thermal correction to Gibbs Free Energy= 0.204439
Sum of electronic and zero-point Energies= -616.289599
Sum of electronic and thermal Energies= -616.275854
Sum of electronic and thermal Enthalpies= -616.274910
Sum of electronic and thermal Free Energies= -616.333153
Sum of electron ic and thermal Free Energies(343k)= -616.342228

INT22

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.390729	-0.769072	0.208082
2	8	0	3.489209	-1.609272	1.070992
3	8	0	4.442675	-0.152061	-0.352761
4	6	0	2.094038	-0.258425	-0.376643
5	6	0	5.733523	-0.539702	0.139690
6	1	0	5.772651	-0.359137	1.218296
7	1	0	5.867751	-1.613762	-0.021177
8	1	0	2.177125	-0.283775	-1.469671
9	1	0	2.001313	0.801421	-0.110021
10	6	0	-1.546663	3.083480	-0.900880
11	6	0	-1.200151	1.764507	-1.182533
12	6	0	-0.724347	0.921615	-0.179837
13	6	0	-0.600513	1.423551	1.117681
14	6	0	-0.942779	2.739951	1.404530
15	6	0	-1.418224	3.574277	0.394754
16	1	0	-1.918900	3.726919	-1.692780
17	1	0	-1.316485	1.375403	-2.190667
18	1	0	-0.247397	0.776094	1.915807
19	1	0	-0.840719	3.116655	2.418101
20	1	0	-1.685303	4.603034	0.617743
21	6	0	-0.414696	-0.528582	-0.495125
22	1	0	-0.371402	-0.650117	-1.586650
23	6	0	0.886725	-1.052398	0.108258
24	1	0	0.839634	-1.024812	1.201326
25	1	0	0.993748	-2.105786	-0.165922
26	6	0	-3.756269	-1.179991	-0.027770
27	8	0	-2.571708	-1.166242	-0.838195
28	8	0	-1.426385	-1.399808	-0.003758
29	6	0	6.766739	0.276405	-0.608094
30	1	0	6.614163	1.345911	-0.437075
31	1	0	7.770819	0.010215	-0.263783
32	1	0	6.707144	0.086279	-1.683580
33	6	0	-4.847273	-0.944405	-1.071801
34	1	0	-4.828548	-1.729427	-1.833526
35	1	0	-5.829035	-0.949664	-0.588628
36	1	0	-4.704689	0.023786	-1.561599
37	6	0	-3.738034	-0.053972	1.004275
38	1	0	-4.690605	-0.030217	1.544710
39	1	0	-2.934670	-0.204608	1.729045
40	1	0	-3.586002	0.914197	0.517607
41	6	0	-3.915054	-2.547711	0.636638
42	1	0	-3.102650	-2.728433	1.345316
43	1	0	-4.865443	-2.599234	1.178543
44	1	0	-3.899346	-3.339045	-0.118984

Zero-point correction= 0.383894 (Hartree/Particle)
Thermal correction to Energy= 0.405213
Thermal correction to Enthalpy= 0.406158
Thermal correction to Gibbs Free Energy= 0.331811
Sum of electronic and zero-point Energies= -924.325273
Sum of electronic and thermal Energies= -924.303954
Sum of electronic and thermal Enthalpies= -924.303010
Sum of electronic and thermal Free Energies= -924.377357
Sum of electron ic and thermal Free Energies(343k)= -924.389015