Electronic Supplementary Information

# Phosphine-catalyzed regioselective Michael addition to allenoates

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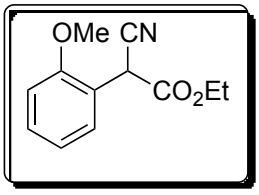
**General**

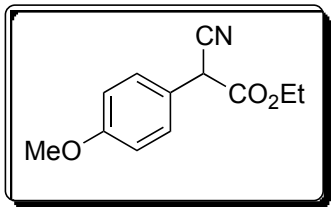
All anaerobic and moisture-sensitive manipulations were carried out with standard Schlenk techniques under inert gas. NMR spectra were recorded on a Bruker AMX 500 (500 MHz for $^{1}H$, 125 MHz for $^{13}C$). Chemical shifts are reported in δ (ppm) referenced to the residual peaks of $CDCl_3$ (δ 7.26) for $^{1}H$ NMR and $CDCl_3$ (δ 77.00) for $^{13}C$ NMR. The following abbreviations are used; s: singlet, d: doublet, t: triplet, q: quartet, sext: sextet, m: multiplet. High-resolution mass spectra (HRMS) were obtained on a Bruker micrOTOF-Q II spectrometer. For thin layer chromatography (TLC), Merck pre-coated TLC plates (Merck 60 F254) were used, and compounds were visualized with a UV light at 254 nm. Flash column chromatography was performed with Silicaflash 60 (Silicycle). Optical rotations were recorded on an Anton Paar MCP 200 machine. Enantiomeric excesses (ee) were determined by HPLC analysis on Shimadzu HPLC with Daicel chiral columns.

**Preparation of Aryl Cyano esters:**

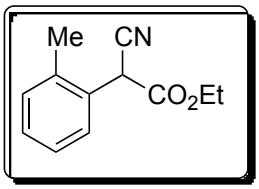
**General Procedure:** To 5.0 mL (10.0 mmol) of 2 M *n*-butyllithium in hexane at 0 ºC, was added rapidly 5.0 mL of anhydrous THF followed by a solution of 0.59 g (5.0 mmol) of the appropriate commercially available phenylacetonitrile in 5.0 mL of THF and the reaction mixture refluxed spontaneously. After 2 h, treatment of the brown solution with a solution of 0.60 mL (5.0 mmol) of diethyl carbonate in 5.0 mL THF afforded a yellow solution, which was refluxed for 5 h. Upon cooling, the resulting suspension was treated with 5 mL of 2 N hydrochloric acid and the aqueous solution vigorously extracted with EtOAc (3 x 20 mL). The organic layer was dried over anhydrous $Na_2SO_4$ and filtered. The solvent was evaporated under reduced pressure and the crude product was purified by silica gel column chromatography to give the desired α- cyano arylacetates in good yields. (isolated yields ranging from 76% to 92%).



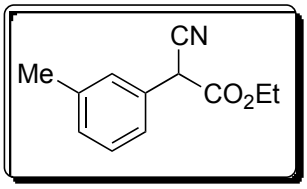

**Ethyl 2-cyano-2-(2-methoxyphenyl)acetate:** $^{1}H$ NMR (500 MHz, $CDCl_3$): δ 7.48-7.32 (m, 2H), 7.0 (t, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 8.2 Hz, 1H), 5.03 (s, 1H), 4.24 (q, *J* = 7.6 Hz, 2H), 3.85 (s, 3H), 1.28 (t, *J* = 7.6 Hz, 3H). $^{13}C$ NMR ($CDCl_3$): δ 165.1, 156.4, 130.6, 129.3, 121.0, 119.0, 115.8, 111.0, 62.8, 55.6, 38.1, 13.8.



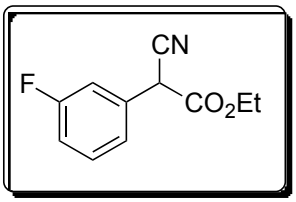

**Ethyl 2-cyano-2-(4-methoxyphenyl)acetate:** $^{1}H$ NMR (500 MHz, $CDCl_3$): δ 7.34 (d, *J* = 8.8 Hz, 2H), 6.90 (d, *J* = 8.8 Hz, 2H), 4.66 (s, 1H), 4.30-4.14 (m, 2H), 3.78 (s, 3H), 1.24 (t, *J* = 7.6 Hz, 3H). $^{13}C$ NMR ($CDCl_3$): δ 165.1, 160.0, 129.0, 121.8, 115.8, 114.5, 63.0, 55.2, 42.7, 13.7.



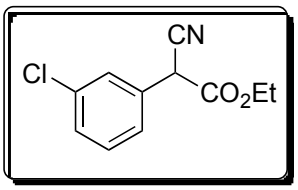

**Ethyl 2-cyano-2-(o-tolyl)acetate:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.48 (d, *J* = 7.0 Hz, 1H), 7.40-7.20 (m, 3H), 4.91 (s, 1H), 4.38-4.20 (m, 2H), 2.43 (s, 3H), 1.30 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 165.0, 136.2, 131.2, 129.3, 128.9, 128.6, 127.0, 115.8, 63.2, 41.0, 19.3, 13.8.



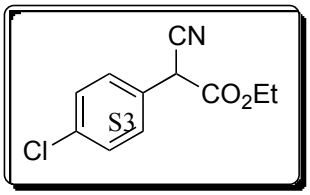

**Ethyl 2-cyano-2-(m-tolyl)acetate:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.40-7.20 (m, 4H), 4.71 (s, 1H), 4.38-4.20 (m, 2H), 2.40 (s, 3H), 1.30 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 165.0, 139.2, 129.9, 129.8, 129.1, 128.4, 124.9, 115.7, 63.1, 43.6, 21.2, 13.8.



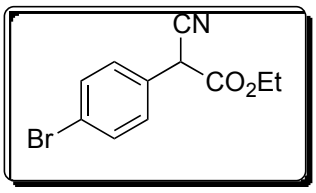

**Ethyl 2-cyano-2-(3-fluorophenyl)acetate:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.40 (q, *J* = 8.2 Hz, 1H), 7.28 (s, 1H), 7.22 (d, *J* = 8.8 Hz, 1H), 7.12 (t, *J* = 8.2 Hz, 1H), 4.76 (s, 1H), 4.27 (q, *J* = 7.0 Hz, 2H), 1.29 (t, *J* = 7.6 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 164.4, 163.7, 161.8, 132.0, 130.9, 123.6, 116.3, 116.1, 115.2, 115.1, 63.4, 43.2, 13.7.



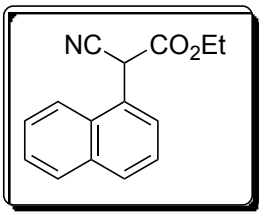

**Ethyl 2-cyano-2-(3-chlorophenyl)acetate:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.46 (s, 1H), 7.44-7.28 (m, 3H), 4.70 (s, 1H), 4.24 (q, *J* = 7.0 Hz, 2H), 1.28 (t, *J* = 7.6 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 164.3, 135.1, 131.6, 130.4, 129.4, 128.0, 126.1, 115.0, 63.5, 43.1, 13.7.



**Ethyl 2-cyano-2-(4-chlorophenyl)acetate:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.52-7.28 (m, 4H), 4.71 (s, 1H), 4.24 (q, *J* = 7.0 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 164.5, 135.3, 129.4, 129.2, 128.4, 115.2, 63.4, 43.0, 13.7.



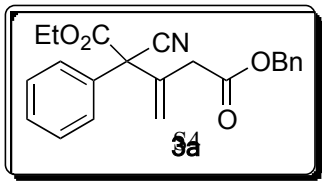

**Ethyl 2-cyano-2-(4-bromophenyl)acetate:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.56 (d, *J* = 6.3 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 4.71 (s, 1H), 4.26 (q, *J* = 7.0 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 164.5, 132.5, 132.3, 129.6, 129.0, 123.6, 115.2, 63.6, 43.2, 13.9.




**Ethyl 2-cyano-2-(naphthalen-1-yl)acetate:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 8.02 (d, *J* = 8.8 Hz, 1H), 7.92 (d, *J* = 7.6 Hz, 2H), 7.72 (d, *J* = 7.0 Hz, 1H), 7.62 (t, *J* = 7.0 Hz, 1H), 7.56 (t, *J* = 7.0 Hz, 1H), 7.51 (t, *J* = 7.0 Hz, 1H), 5.39 (s, 1H), 4.26 (q, *J* = 7.6 Hz, 2H), 1.26 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 165.0, 133.9, 130.3, 130.1, 129.1, 127.5, 127.3, 126.4, 126.2, 125.4, 122.5, 115.8, 63.3, 41.4, 13.8.

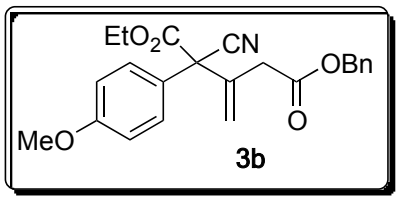
## General Procedure for Phosphine catalyzed *β*-additions:

To a solution of Ethyl 2-cyano-2-phenyl acetate (20 mg, 0.1 mmol) and benzyl buta-2,3-dienoate (25 mg, 0.15 mmol) in dichloromethane (0.5 mL) was added triphenyl phophine (1.3 mg, 0.005 mmol) at room temperature and the reaction mixture was stirred for 2 h at same temperature. Evaporation of the solvent under reduced pressure and the crude reaction mixture was subjected to the silica gel column chromatography to give the corresponding product as a colorless oil (36 mg, 99% yield).



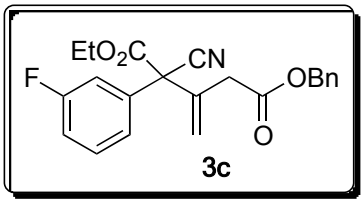

3a

**5-benzyl 1-ethyl 2-cyano-3-methylene-2-phenylpentanedioate 3a:** (colorless oil) $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.80-7.28 (m, 10H), 5.55 (s, 1H), 5.49 (s, 1H), 5.06 (s, 2H), 4.28 (q, *J* = 7.6 Hz, 2H), 3.22 (s, 2H), 1.30 (t, *J* = 7.6 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 169.8, 166.0, 136.3, 135.5, 133.1, 129.2, 129.0, 128.5, 128.3, 127.7, 121.9, 117.3, 66.8, 63.6, 59.8, 38.5, 13.7. HRMS (ESI-TOF) calcd for $C_{22}H_{22}NO_4$ $(M+H)^+$ 364.1543, found 364.1548.



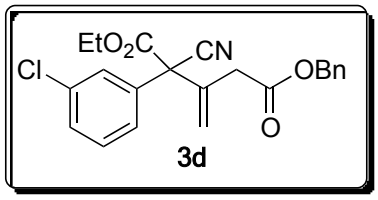
**3b**

**5-benzyl 1-ethyl 2-cyano-2-(4-methoxyphenyl)-3-methylenepentanedioate 3b:** (pale yellow oil) $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.48-7.28 (m, 7H), 7.0-6.80 (m, 2H), 5.53 (s, 1H), 5.49 (s, 1H), 5.07 (s, 2H), 4.26 (q, *J* = 7.6 Hz, 2H), 3.80 (s, 3H), 3.22 (s, 2H), 1.30 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 169.9, 166.2, 160.1, 136.5, 135.5, 129.0, 128.5, 128.2, 124.9, 121.5, 117.5, 114.3, 66.8, 63.5, 59.1, 55.3, 38.4, 13.8. HRMS (ESI-TOF) calcd for $C_{23}H_{23}NO_5$ (M+Na) 416.1468, found 416.1482.



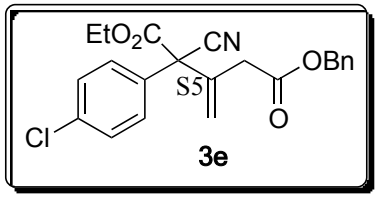
**3c**

**5-benzyl 1-ethyl 2-cyano-2-(3-fluorophenyl)-3-methylenepentanedioate 3c:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.42-7.28 (m, 6H), 7.24-7.22 (m, 1H), 7.22-7.18 (m, 1H), 7.16-7.04 (m, 1H), 5.57 (s, 1H), 5.50 (s, 1H), 5.08 (s, 2H), 4.28 (q, *J* = 7.6 Hz, 2H), 3.22 (s, 2H), 1.31 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 169.6, 165.5, 163.8, 161.8, 135.8, 135.4, 135.3, 130.6, 130.6, 128.5, 128.3, 123.5, 122.2, 116.9, 116.5, 116.3, 115.3, 115.1, 66.9, 63.9, 59.4, 38.5, 13.8. HRMS (ESI-TOF) calcd for $C_{22}H_{20}FNO_4$ (M+Na) 404.1269, found 404.1278.



**3d**

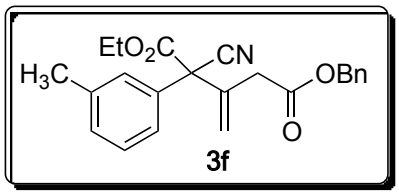
**5-benzyl 1-ethyl 2-(3-chlorophenyl)-2-cyano-3-**



**3e**

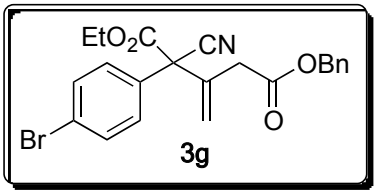
**methylenepentanedioate 3d:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.50-7.30 (m, 9H), 5.59 (s, 1H), 5.50 (s, 1H), 5.10 (s, 2H), 4.30 (q, *J* = 7.6 Hz, 2H), 3.24 (s, 2H), 1.32 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 169.6, 165.6, 135.9, 135.4, 135.3, 131.5, 129.2, 129.1, 128.5, 128.3, 122.1, 116.9, 66.9, 63.8, 59.1, 38.4, 13.7. HRMS (ESI-TOF) calcd for $C_{22}H_{20}ClNO_4$ (M+Na) 420.0973, found 420.0985.

**5-benzyl 1-ethyl 2-(4-chlorophenyl)-2-cyano-3-methylenepentanedioate 3e:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.48 (s, 1H), 7.46-7.28 (m, 8H), 5.58 (s, 1H), 5.50 (s, 1H), 5.08 (s, 2H), 4.30 (q, *J* = 7.0 Hz, 2H), 3.22 (s, 2H), 1.30 (t, *J* = 7.6 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 169.6, 165.5, 135.7, 135.4, 135.1, 135.0, 130.2, 129.5, 128.5, 128.3, 127.9, 126.0, 122.3, 116.8, 67.0, 63.9, 59.3, 38.5, 13.8. HRMS (ESI-TOF) calcd for $C_{22}H_{20}ClNO_4$ (M+Na) 420.0973, found 420.0982.



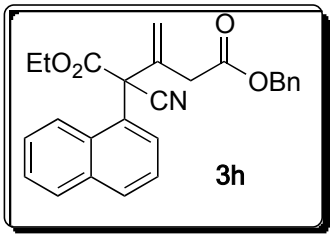
**3f**

**5-benzyl 1-ethyl 2-cyano-3-methylene-2-(*m*-tolyl)pentanedioate 3f:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.50-7.10 (m, 9H), 5.54 (s, 1H), 5.49 (s, 1H), 5.06 (s, 2H), 4.28 (q, *J* = 7.6 Hz, 2H), 3.22 (s, 2H), 2.34 (s, 3H), 1.30 (t, *J* = 7.6 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 169.9, 166.0, 139.0, 136.2, 135.5, 133.0, 129.9, 128.9, 128.5, 128.27, 128.25, 128.20, 124.7, 121.8, 117.5, 66.8, 63.6, 59.7, 38.5, 21.4, 13.8. HRMS (ESI-TOF) calcd for $C_{23}H_{23}NO_4$ (M+Na) 400.1519, found 400.1532.

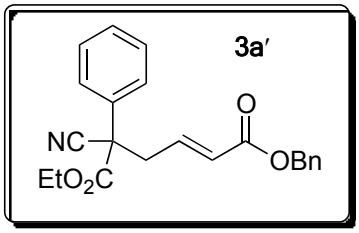


**3g**

**5-benzyl 1-ethyl 2-(4-bromophenyl)-2-cyano-3-methylenepentanedioate 3g:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.52 (d, *J* = 7.0 Hz, 2H), 7.42-7.26 (m, 7H), 5.56 (s, 1H), 5.47 (s, 1H), 5.06 (s, 2H), 4.28 (q, *J* = 7.0 Hz, 2H), 3.21 (s, 2H), 1.30 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 169.6, 165.5, 135.9, 135.4, 132.2, 132.1, 129.5, 129.0, 128.6, 128.5, 128.38, 128.35, 128.3, 127.7, 123.7, 122.2, 116.9, 67.0, 63.9, 59.3, 38.5, 13.8. HRMS (ESI-TOF) calcd for $C_{22}H_{20}BrNO_4$ (M+Na) 464.0468, found 464.0478.




**5-benzyl 1-ethyl 2-cyano-3-methylene-2-(naphthalen-1-yl)pentanedioate 3h:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 8.12-8.06 (m, 1H), 7.92-7.88 (m, 2H), 7.60-7.50 (m, 2H), 7.48-7.40 (m, 2H), 7.38-7.28 (m, 5H), 5.86 (s, 1H), 5.72 (s, 1H), 5.05 (ABq, *J* = 12.6 Hz, 2H), 4.31 (q, *J* = 7.0 Hz, 2H), 3.34 (s, 2H), 1.30 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 170.0, 166.7, 135.5, 135.1, 134.5, 130.8, 130.4, 129.4, 129.3, 128.5, 128.29, 128.25, 126.95, 126.88, 126.24, 124.84, 123.9, 123.0, 117.4, 66.8, 63.8, 59.1, 38.6, 13.7. HRMS (ESI-TOF) calcd for $C_{26}H_{23}NO_4$ $(M+H)^+$ 414.1700, found 414.1708.




**(*E*)-1-benzyl 6-ethyl 5-cyano-5-phenylhex-2-enedioate 3a′:** $^{1}$H NMR (500 MHz, $CDCl_3$): δ 7.80-7.20 (m, 10H), 6.84 (dt, *J* = 15.1 & 7.6 Hz, 1H), 6.06 (d, *J* = 15.1 Hz, 1H), 5.16 (s, 2H), 4.40-4.10 (m, 2H), 3.24 (dd, *J* = 14.6 & 7.6 Hz, 1H), 3.00 (dd, *J* = 14.6 & 7.6 Hz, 1H), 1.30 (t, *J* = 7.0 Hz, 3H). $^{13}$C NMR ($CDCl_3$): δ 166.6, 165.2, 140.4, 135.7, 133.4, 129.4, 129.2, 128.5, 128.2, 128.1, 126.6, 125.9, 117.4, 66.4, 63.6, 53.2, 40.5, 13.7. HRMS (ESI-TOF) calcd for $C_{22}H_{21}NO_4$ (M+Na) 386.1363, found 386.1367.

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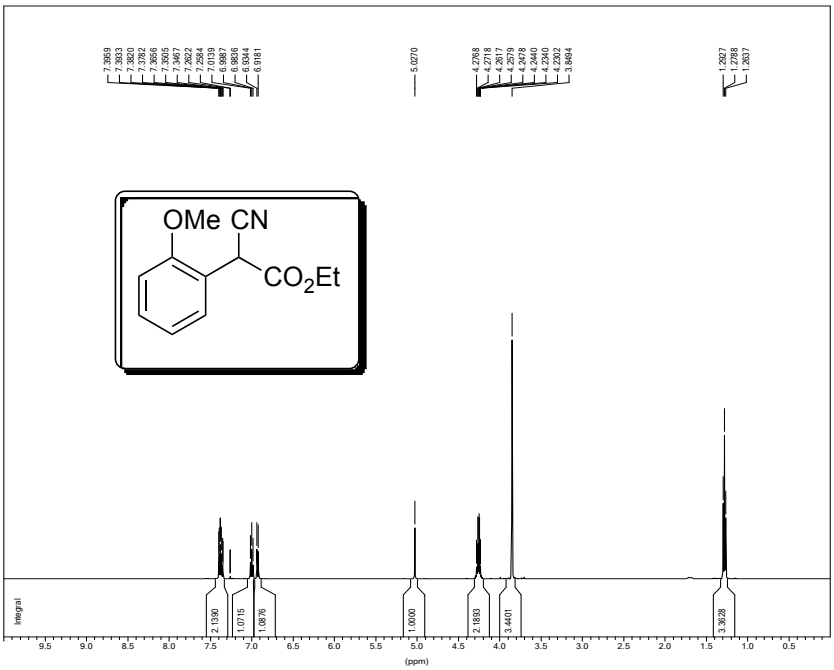


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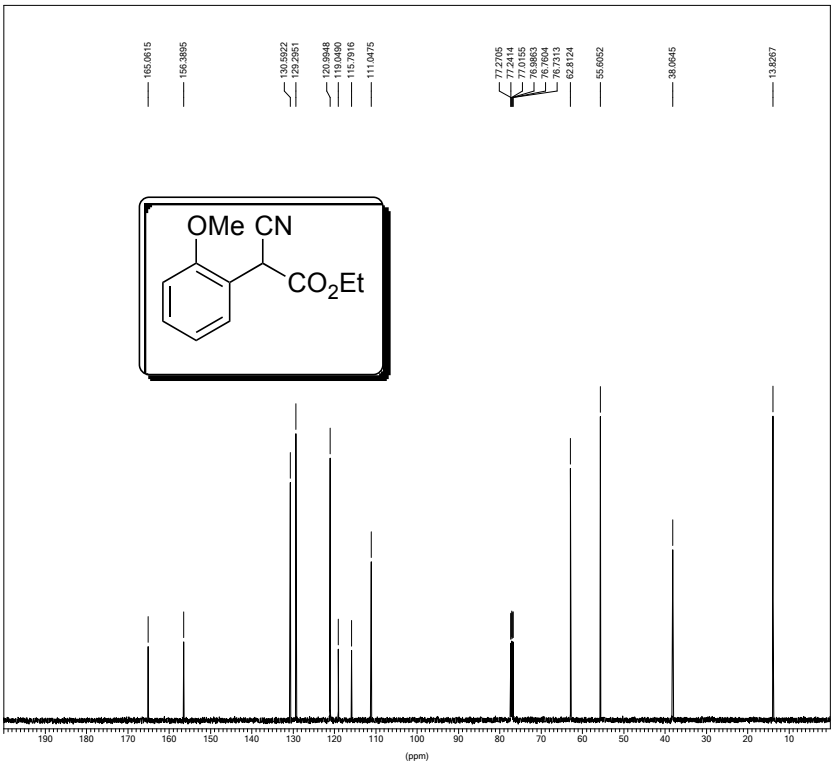


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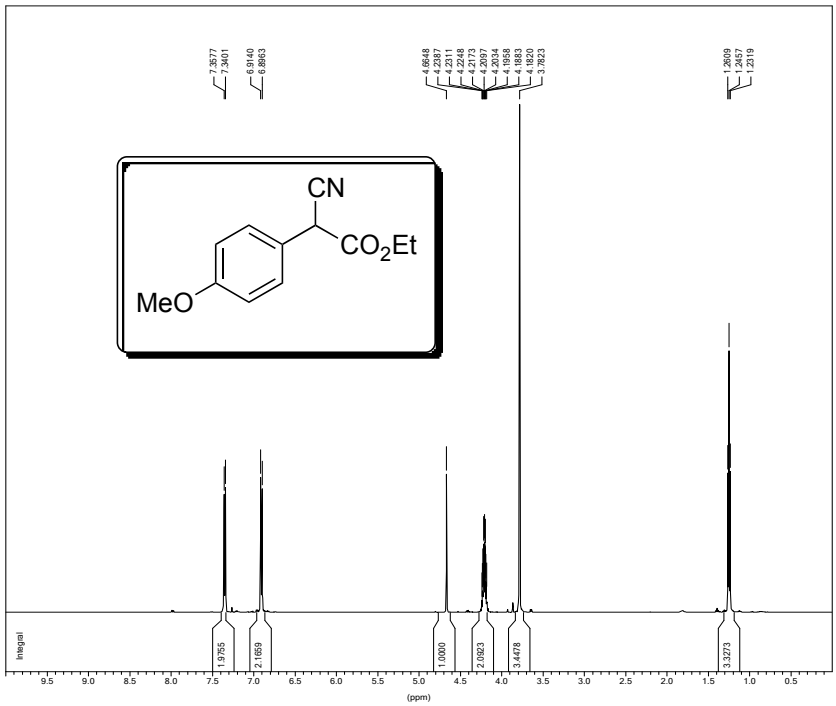
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.1 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.257 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

4_methoxy

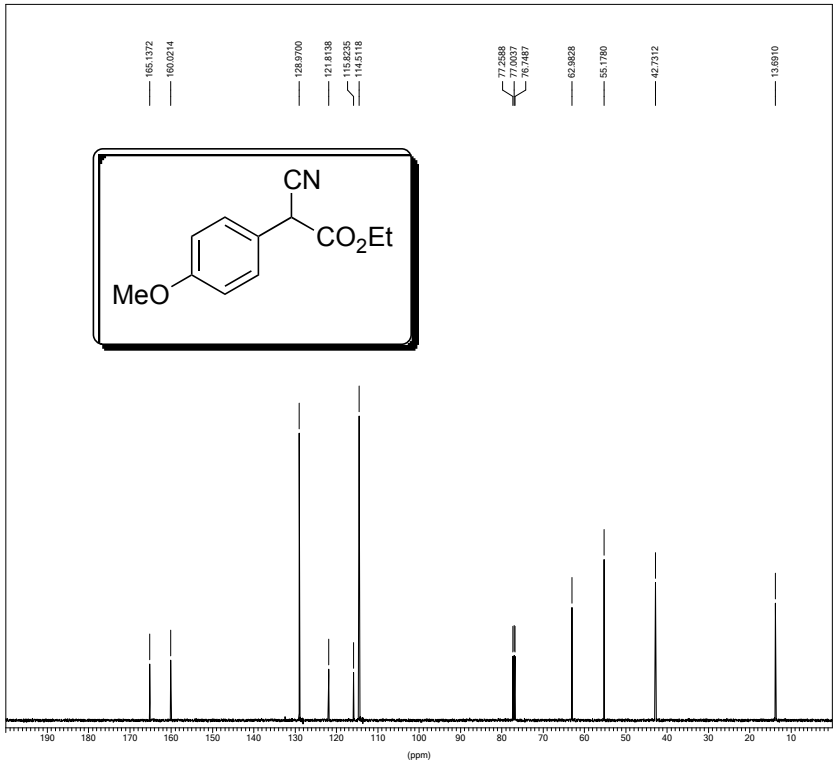



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0127 |
| EXPNO | : | 1 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 31 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 298.7 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.478 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

4-Methoxy

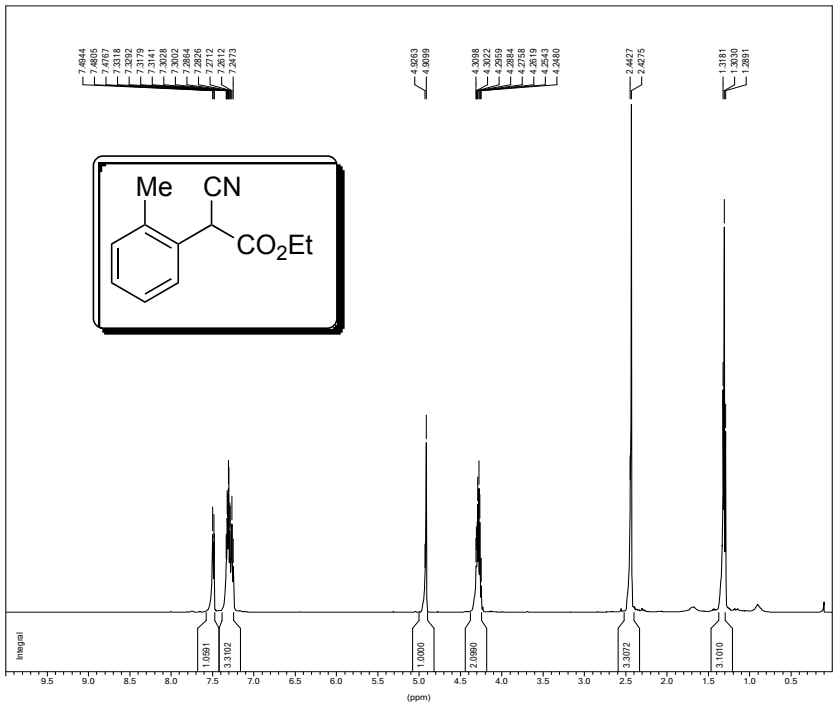



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0127 |
| EXPNO | : | 2 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 33 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.1 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.209 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

2-Methyl

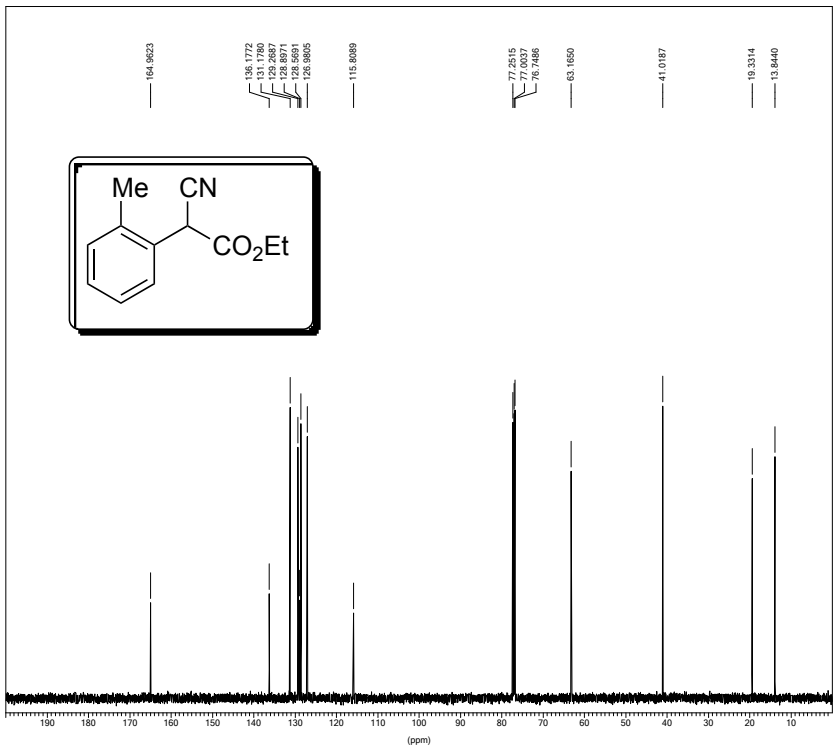



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0127 |
| EXPNO | : | 4 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 51 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 299.0 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.499 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

2-mETHYL

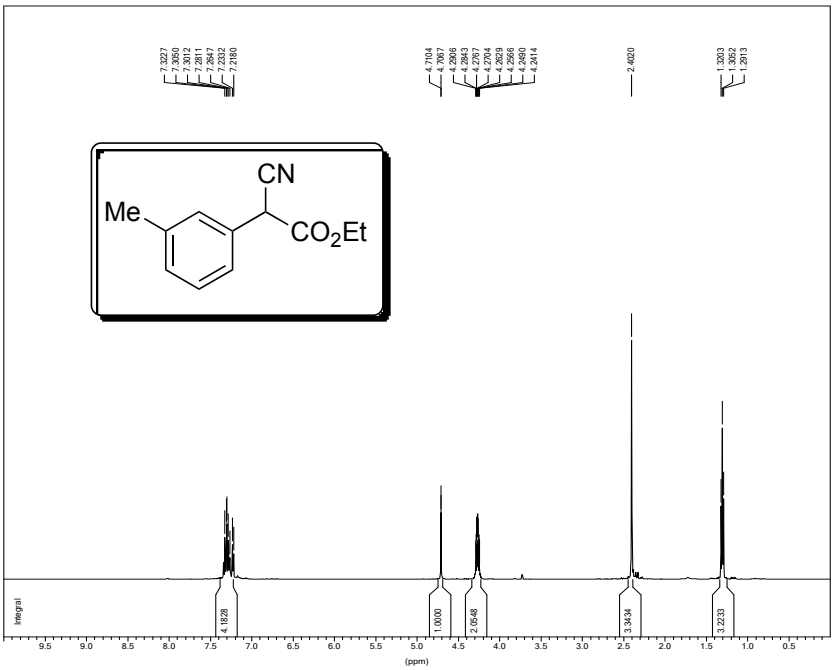



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0127 |
| EXPNO | : | 3 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 103 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.4 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.325 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

6.140



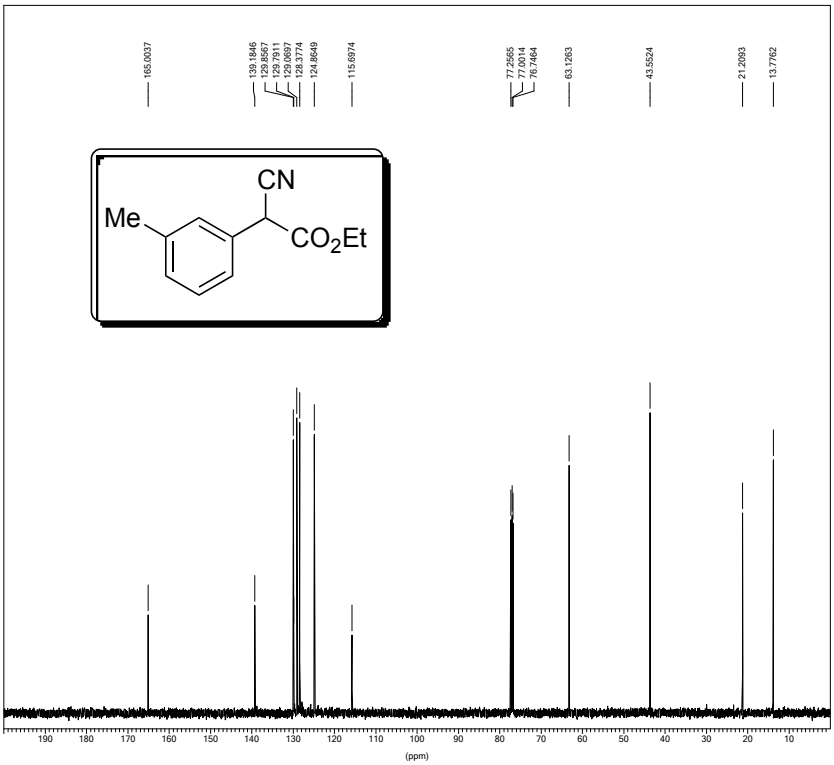

Bruker

*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0205 |
| EXPNO | : | 2 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 23 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 299.1 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.503 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

6.140



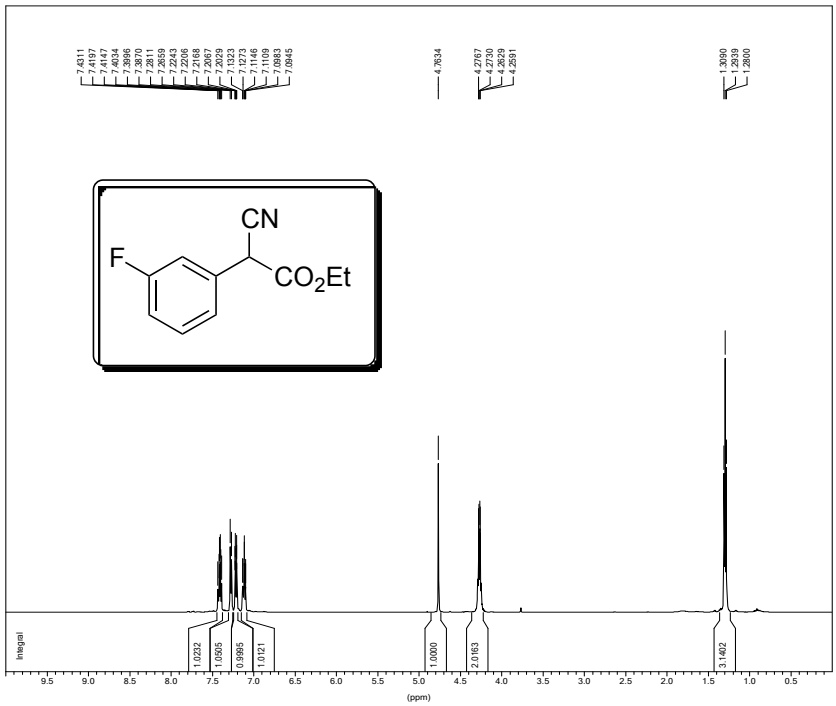

Bruker

*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0205 |
| EXPNO | : | 3 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 34 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.5 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.272 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

3-Fluoro

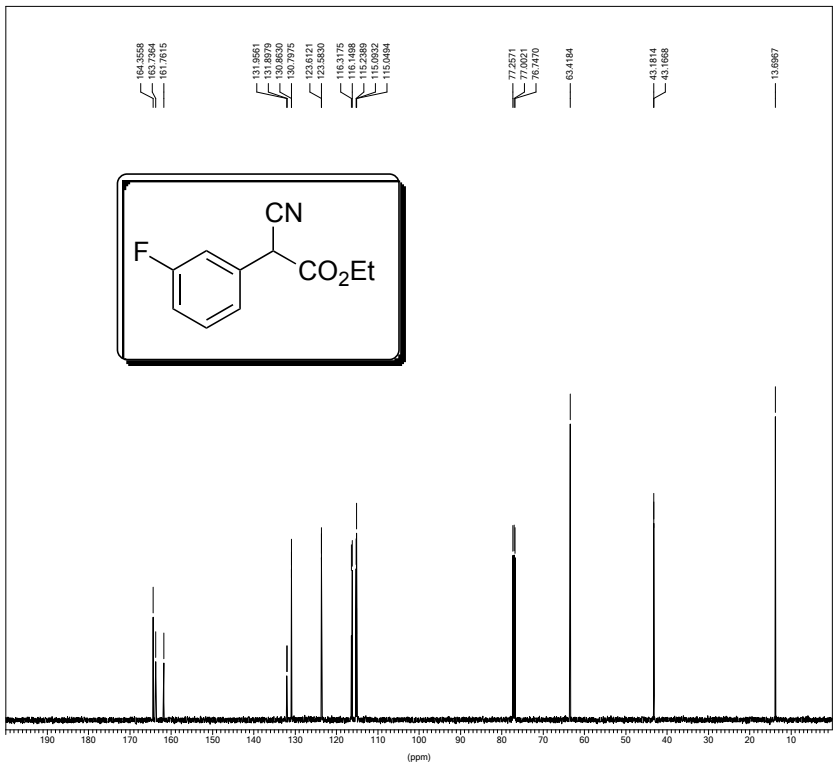



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0125 |
| EXPNO | : | 4 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 31 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 298.9 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.503 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

3-Fluoro

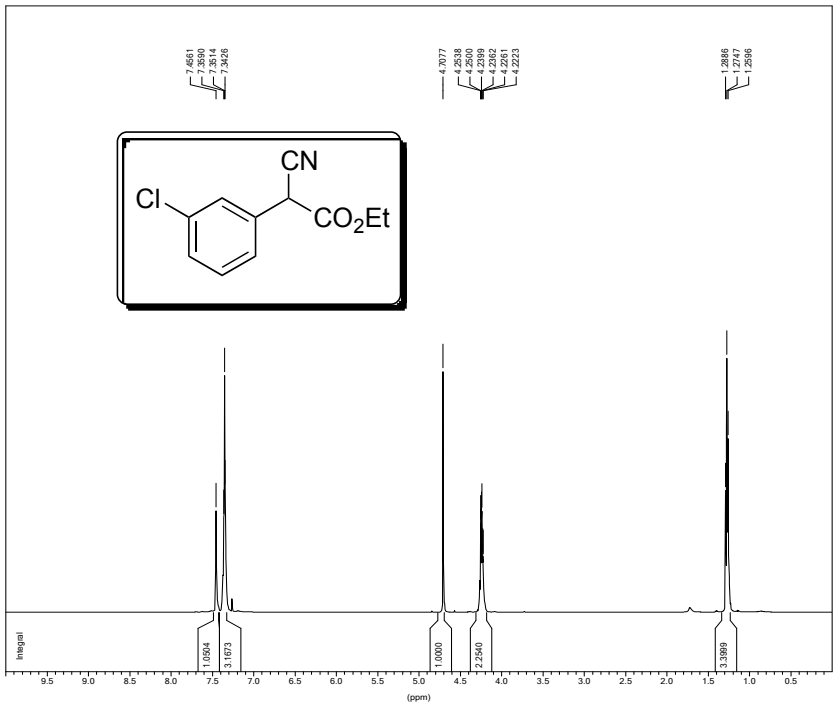



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0125 |
| EXPNO | : | 5 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 60 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.5 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.251 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

3-Chloro

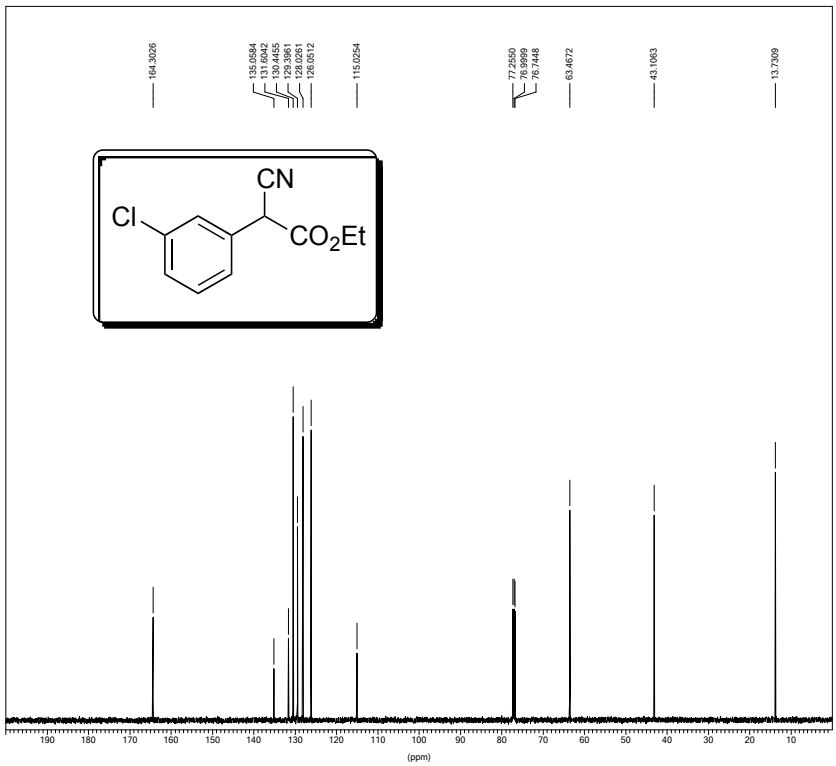



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0125 |
| EXPNO | : | 6 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 34 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 298.9 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.475 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

3-Chloro

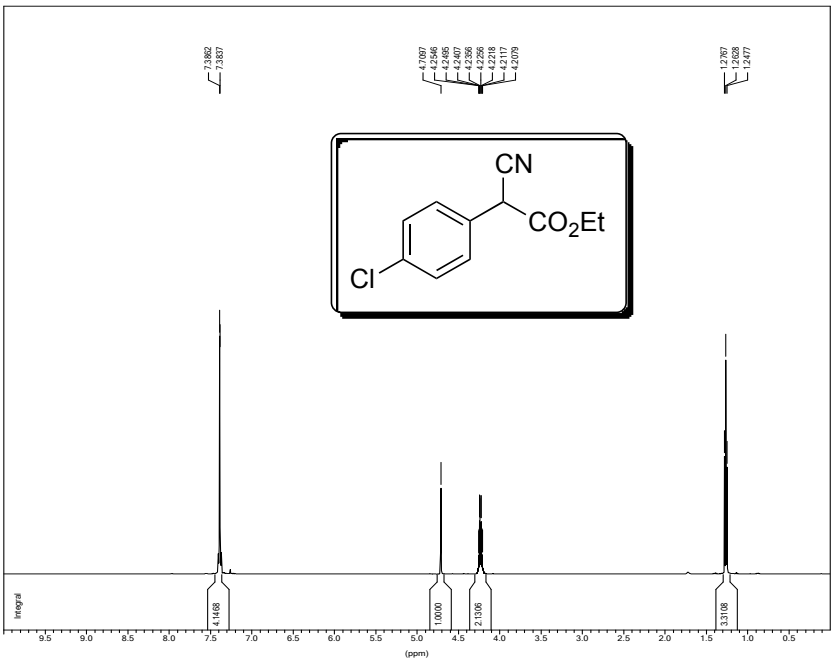



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0125 |
| EXPNO | : | 7 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 54 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.7 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.256 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

4-Chloro

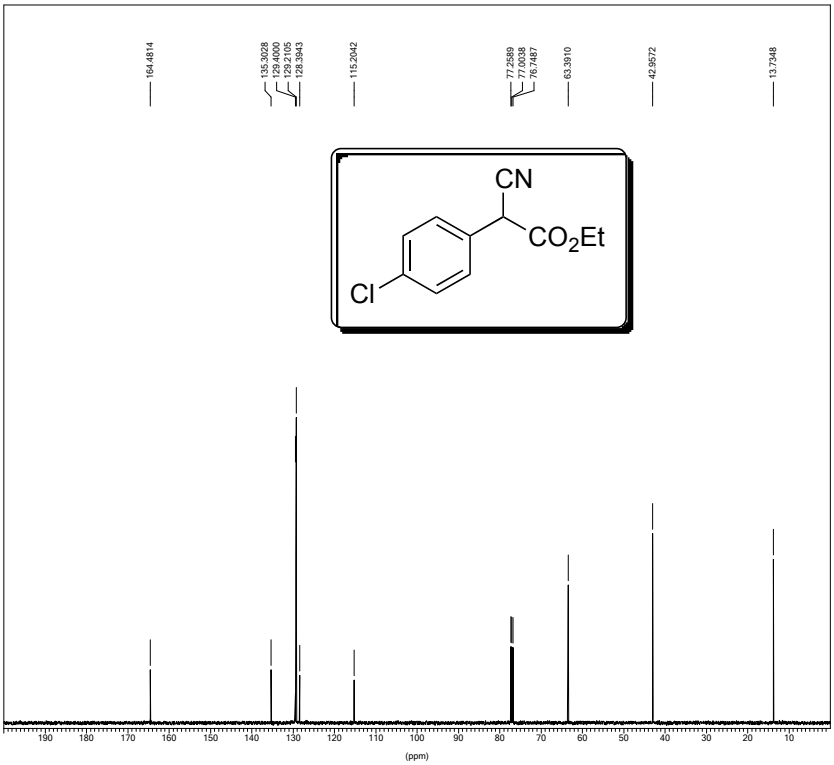



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0125 |
| EXPNO | : | 8 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 22 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 299.0 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.477 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

4-Chloro

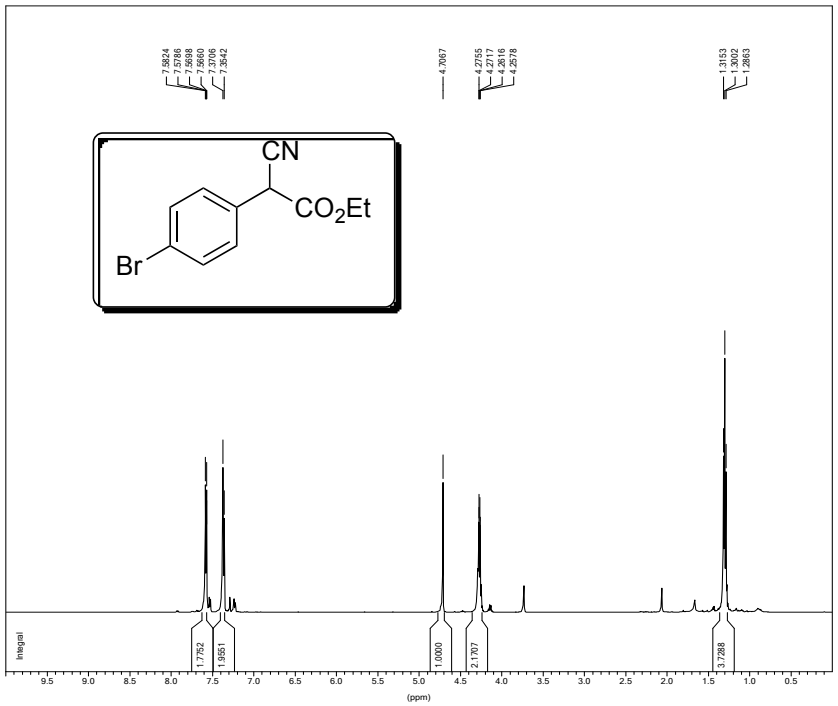



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0125 |
| EXPNO | : | 9 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 36 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.3 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.260 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

6.139A

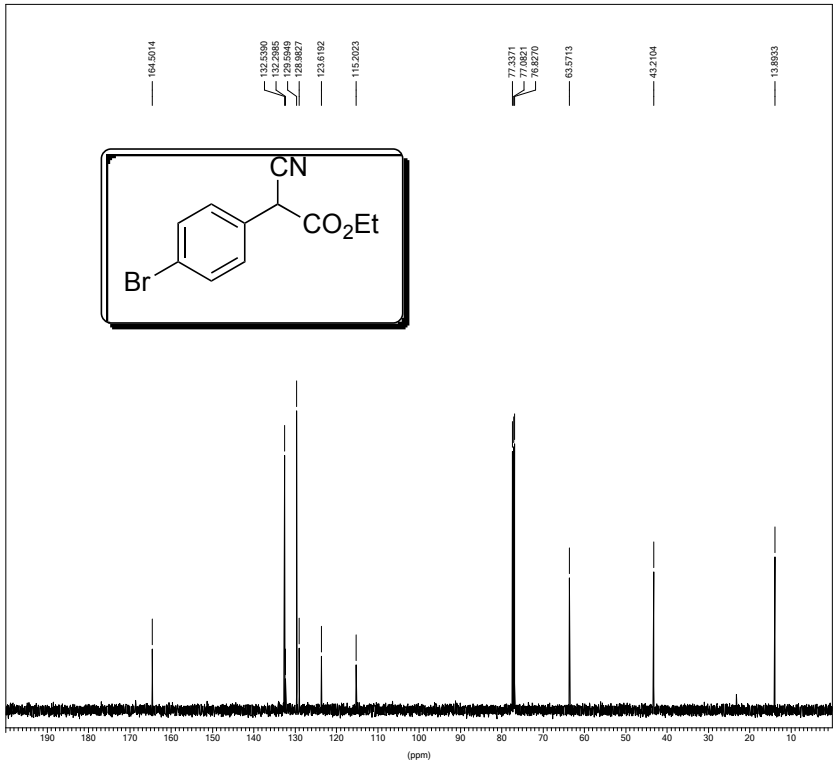



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0130 |
| EXPNO | : | 1 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 30 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 298.0 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.503 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

6.139A

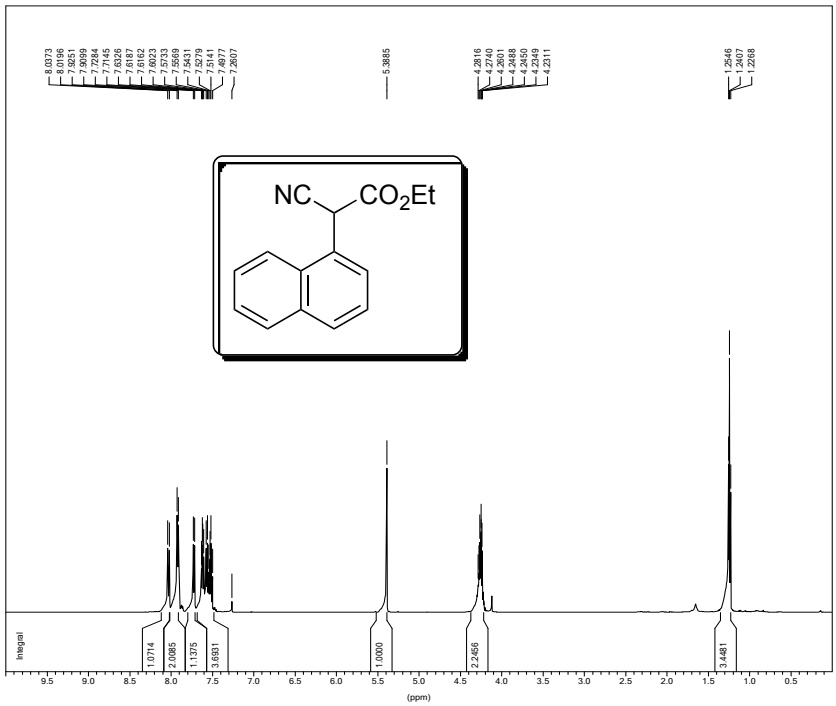



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0130 |
| EXPNO | : | 2 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 24 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 298.5 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.396 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

1-Naphthyl

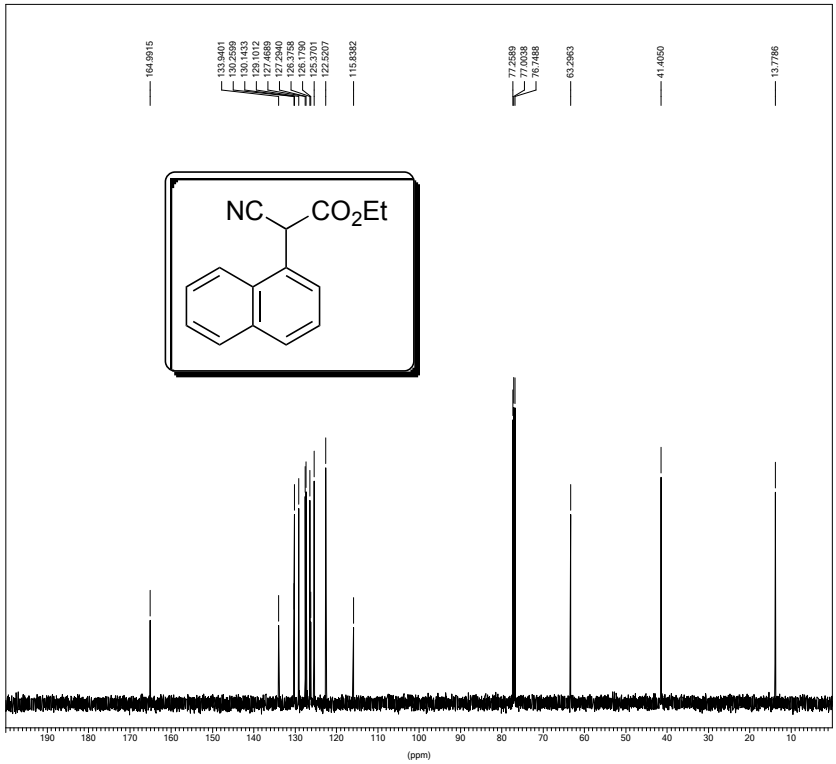



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0125 |
| EXPNO | : | 10 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 27 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 298.9 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.478 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

1-Naphthyl

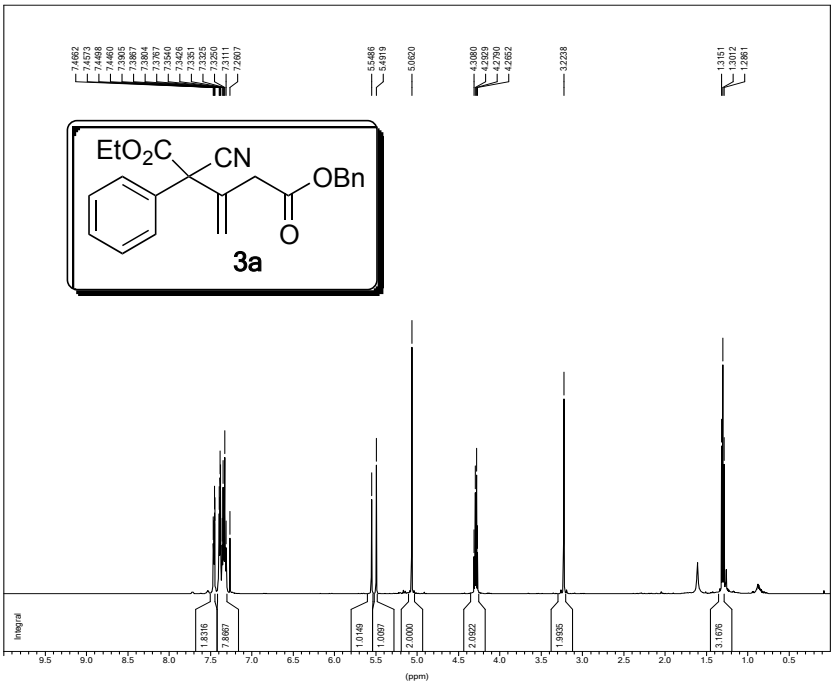



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0125 |
| EXPNO | : | 11 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 36 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.4 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.274 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

6.17D

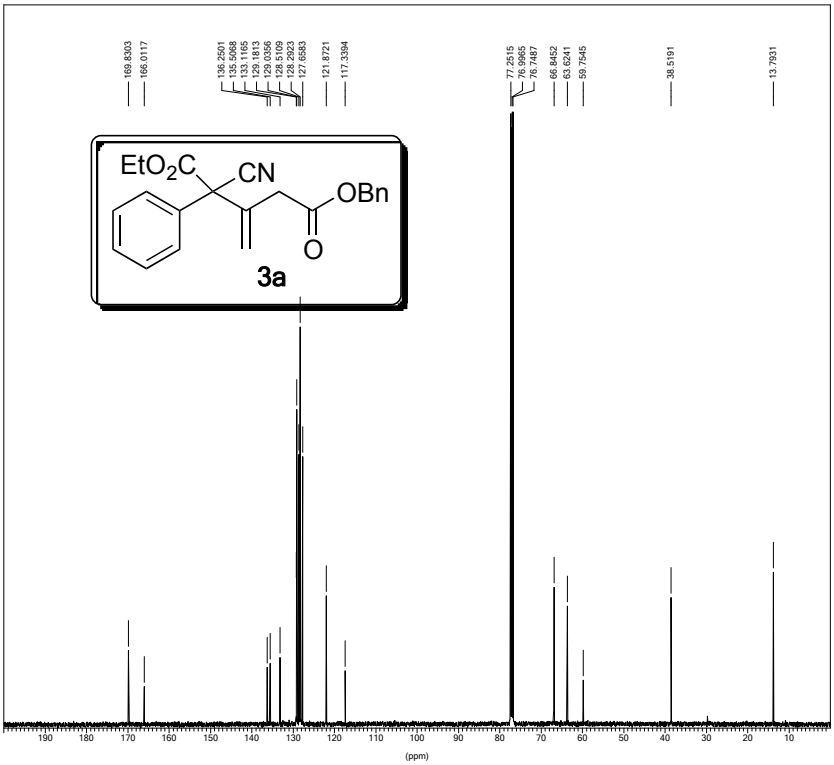



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg1203 |
| EXPNO | : | 2 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 51 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 298.8 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.477 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

6.17D

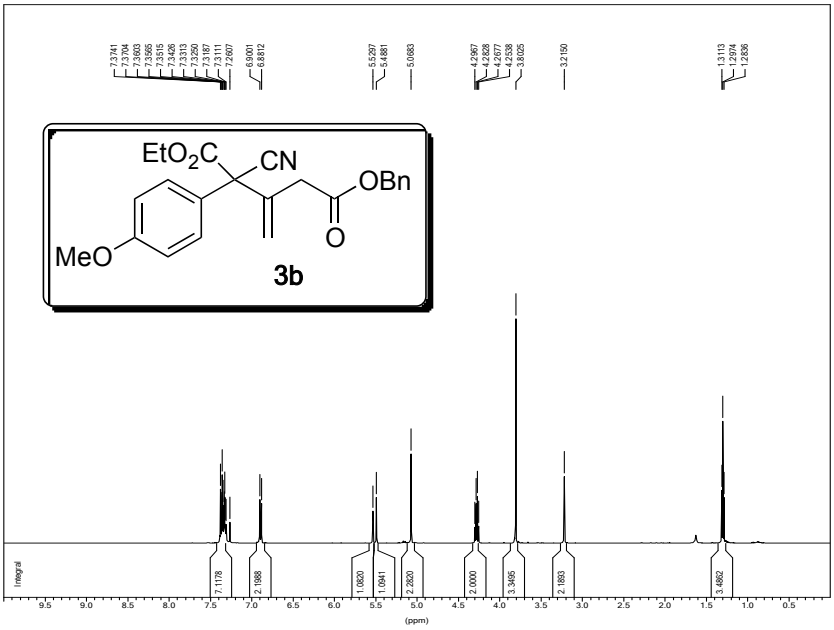



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg1203 |
| EXPNO | : | 4 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 1665 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.5 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.362 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

6.53



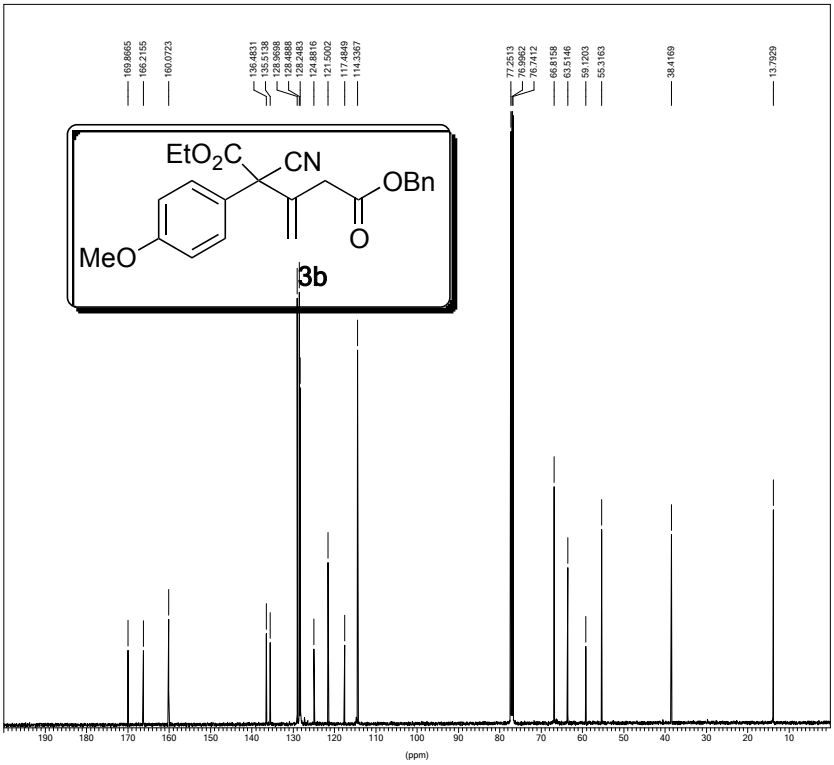

Bruker

*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg1125 |
| EXPNO | : | 2 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 100 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 298.9 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.477 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

6.53



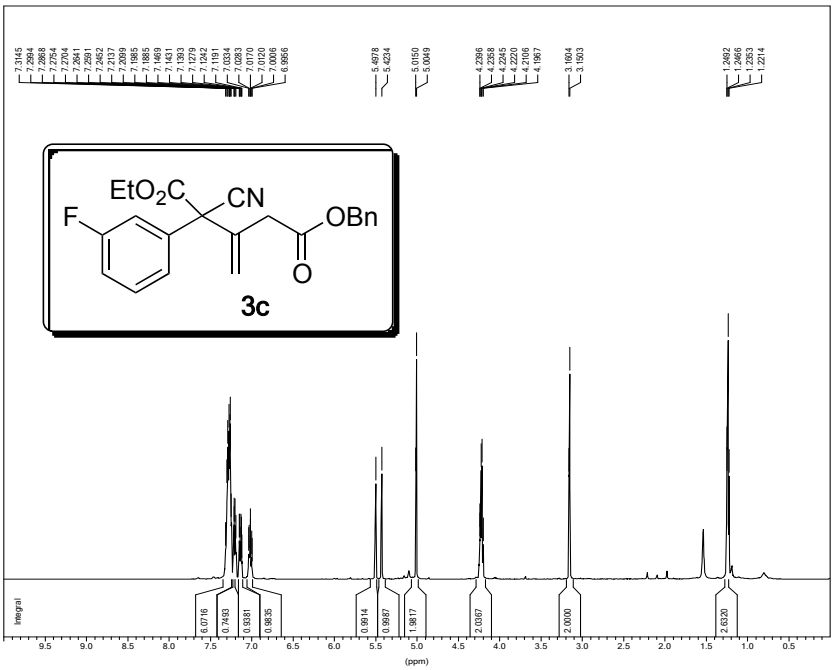

Bruker

*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg1125 |
| EXPNO | : | 3 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 3304 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.3 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.347 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

6.115A

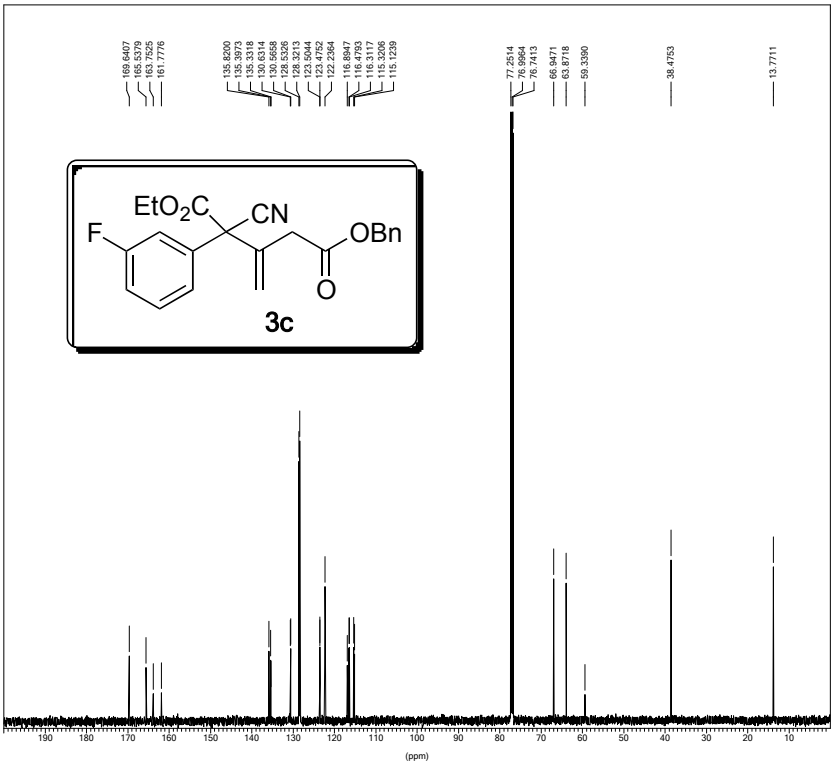



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0107 |
| EXPNO | : | 2 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 20 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 297.3 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.406 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

6.115




*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0107 |
| EXPNO | : | 3 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 510 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 298.2 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.354 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

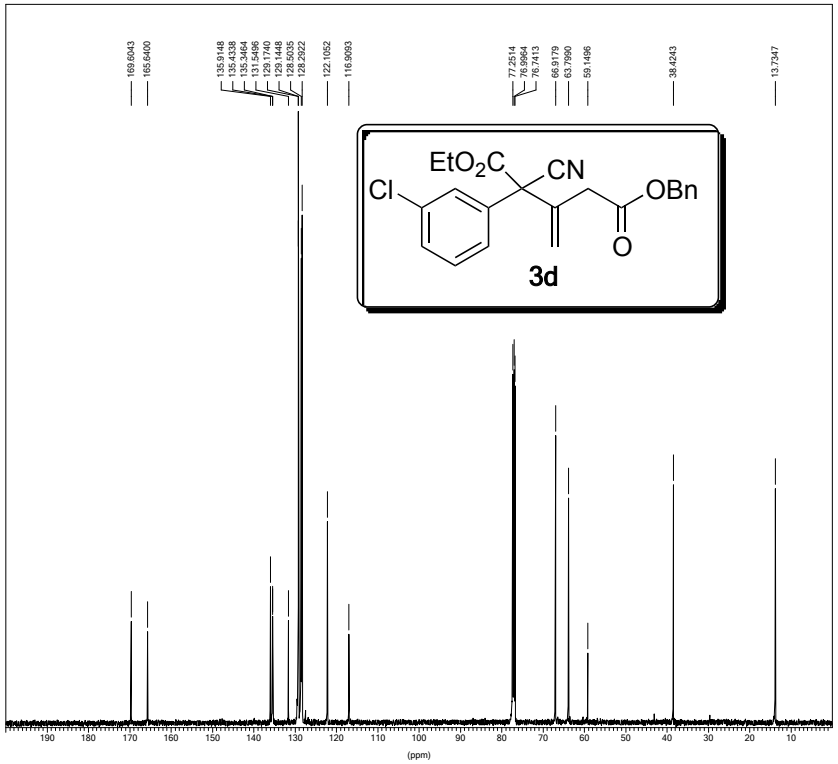
6.109


*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0301 |
| EXPNO | : | 1 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 12 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 298.6 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.503 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

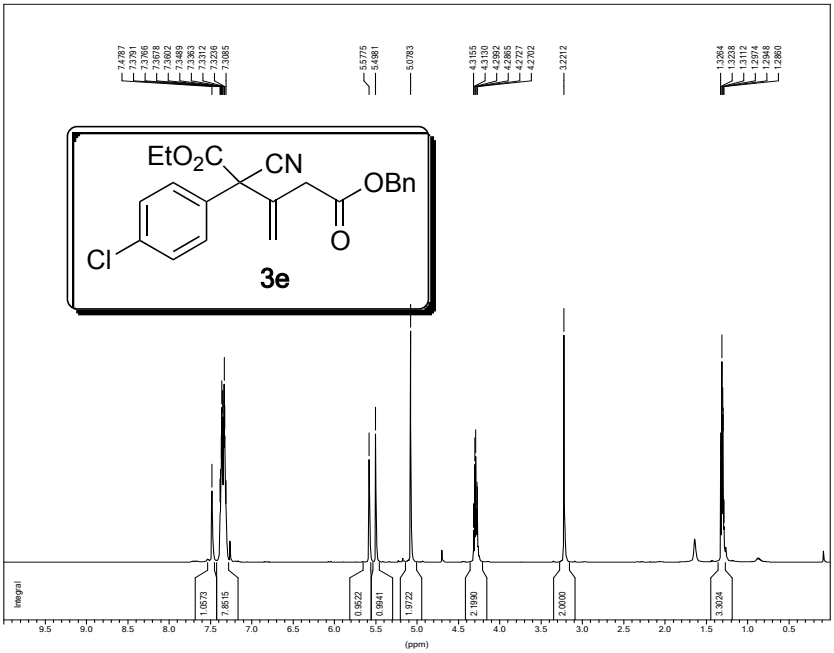
6.109




*** Current Data Parameters ***

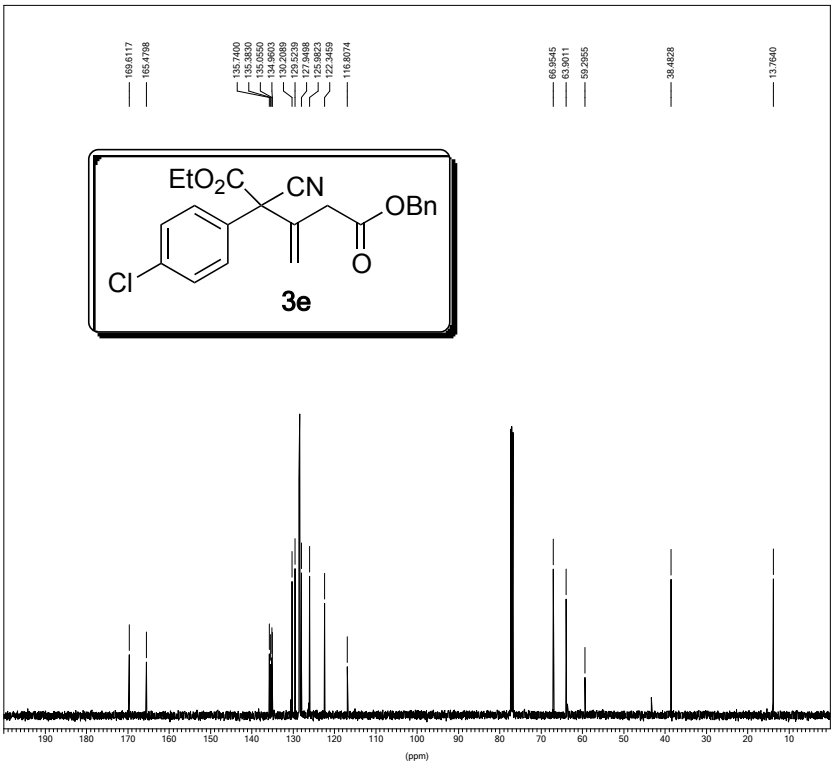
| | | |
|---|---|---|
| NAME | : | vrg0110 |
| EXPNO | : | 3 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 1381 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 298.1 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.311 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500
6.110




*** Current Data Parameters ***
NAME : vrg0110
EXPNO : 5
PROCNO : 1
*** Acquisition Parameters ***
DS : 0
INSTRUM : spect
LOCNUC : 2H
NS : 81
NUCLEUS : off
O1 : 3088.51 Hz
PULPROG : zg30
SFO1 : 500.1330885 MHz
SOLVENT : CDCl3
SW : 20.6557 ppm
TD : 32768
TE : 297.9 K
*** Processing Parameters ***
LB : 0.30 Hz
OFFSET : 16.477 ppm
SI : 16384
*** 1D NMR Plot Parameters ***
NUCLEUS : off

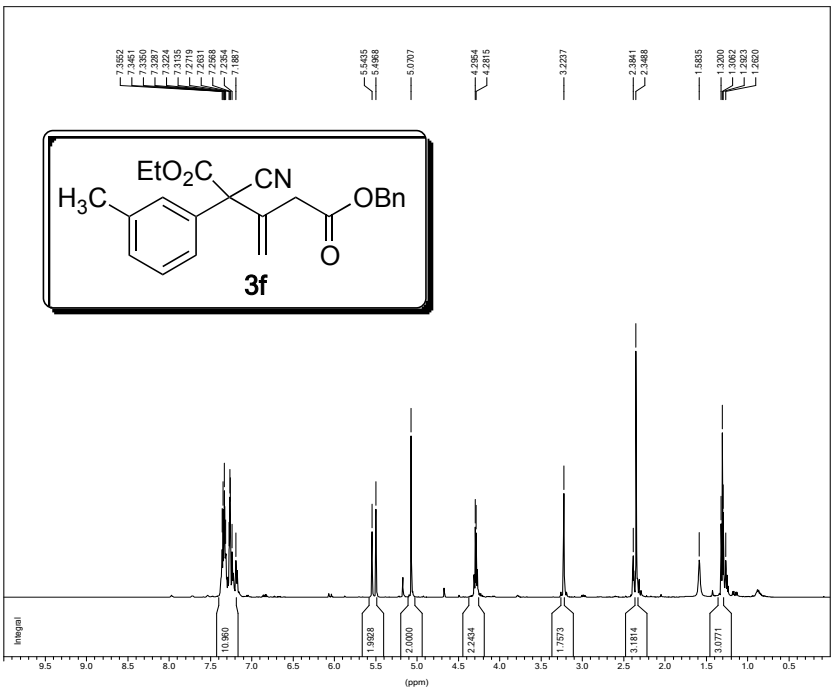
13C AMX500
6.110




*** Current Data Parameters ***
NAME : vrg0110
EXPNO : 6
PROCNO : 1
*** Acquisition Parameters ***
DS : 0
INSTRUM : spect
LOCNUC : 2H
NS : 148
NUCLEUS : off
O1 : 13204.57 Hz
PULPROG : zgpg30
SFO1 : 125.7709936 MHz
SOLVENT : CDCl3
SW : 238.7675 ppm
TD : 65536
TE : 298.8 K
*** Processing Parameters ***
LB : 1.00 Hz
OFFSET : 224.340 ppm
SI : 32768
*** 1D NMR Plot Parameters ***
NUCLEUS : off

1H AMX500

6.178A

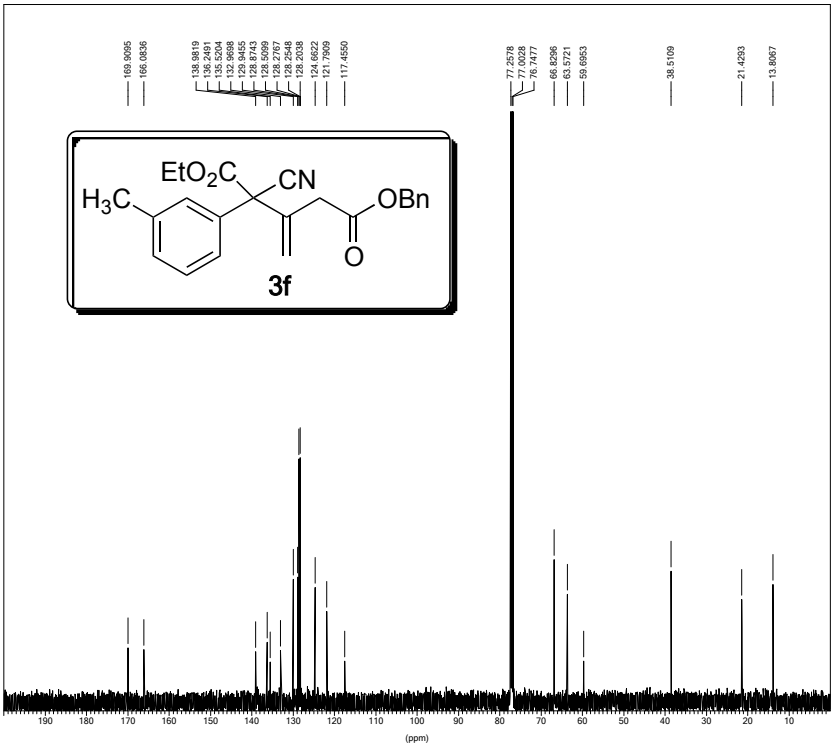



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0203 |
| EXPNO | : | 2 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 20 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 299.2 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.479 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

6.178A



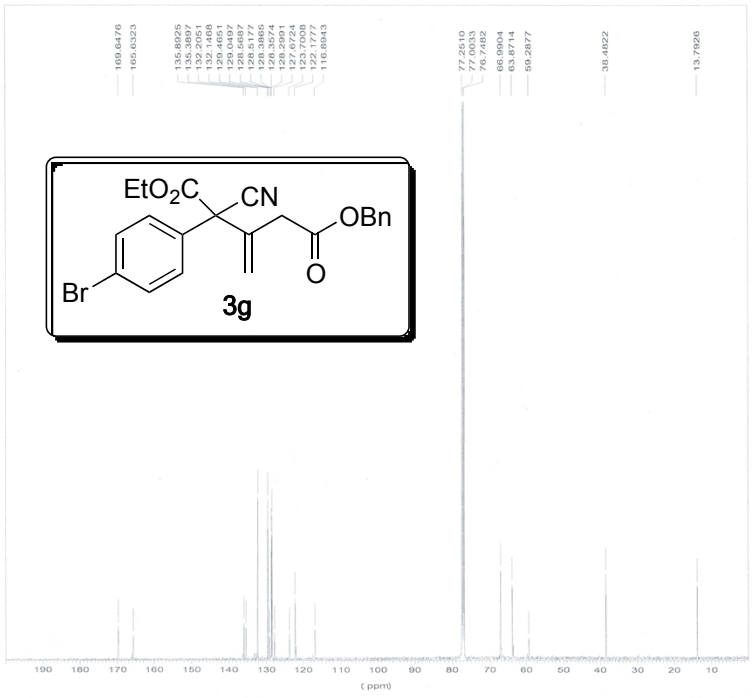

*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0320 |
| EXPNO | : | 2 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 255 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 296.8 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.361 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500
6.118A


*** Current Data Parameters ***
NAME : vrg0110
EXPNO : 4
PROCNO : 1
*** Acquisition Parameters ***
DS : 0
INSTRUM : spect
LOCNUC : 2H
NS : 100
NUCLEUS : off
O1 : 3088.51 Hz
PULPROG : zg30
SFO1 : 500.1330885 MHz
SOLVENT : CDCl3
SW : 20.6557 ppm
TD : 32768
TE : 298.1 K
*** Processing Parameters ***
LB : 0.30 Hz
OFFSET : 16.478 ppm
SI : 16384
*** 1D NMR Plot Parameters ***
NUCLEUS : off

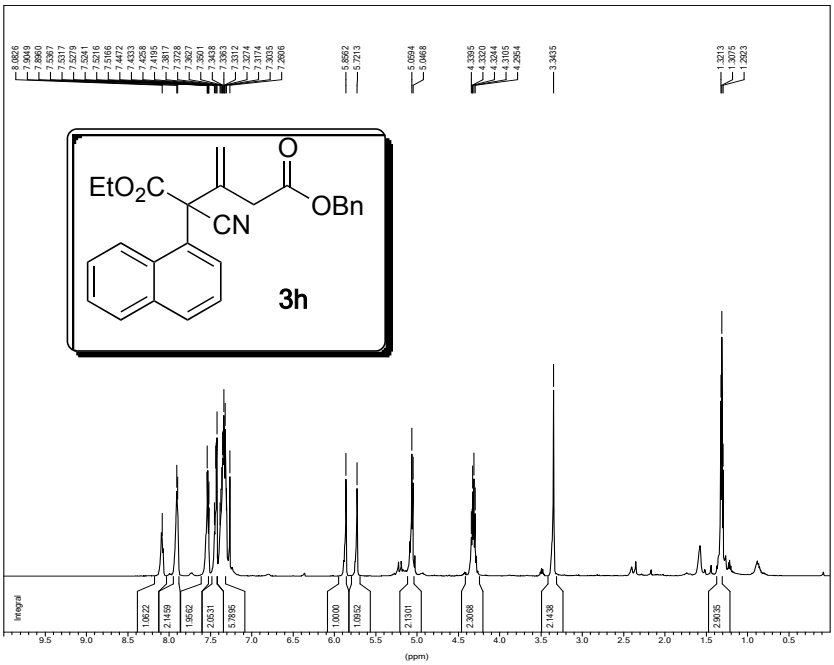
13C AMX500
6.118B




*** Current Data Parameters ***
NAME : vrg0214
EXPNO : 2
PROCNO : 1
*** Acquisition Parameters ***
DS : 0
INSTRUM : spect
LOCNUC : 2H
NS : 12416
NUCLEUS : off
O1 : 13204.57 Hz
PULPROG : zgpg30
SFO1 : 125.7709936 MHz
SOLVENT : CDCl3
SW : 238.7675 ppm
TD : 65536
TE : 298.4 K
*** Processing Parameters ***
LB : 1.00 Hz
OFFSET : 224.376 ppm
SI : 32768
*** 1D NMR Plot Parameters ***
NUCLEUS : off

1H AMX500

6.120

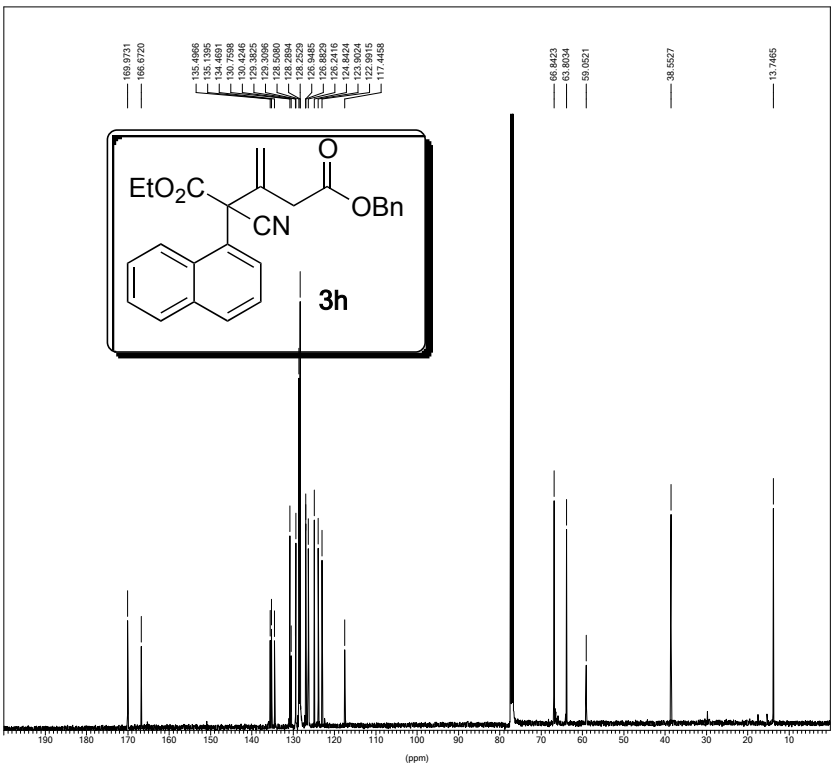



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0115 |
| EXPNO | : | 6 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 27 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 298.2 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.478 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

6.120

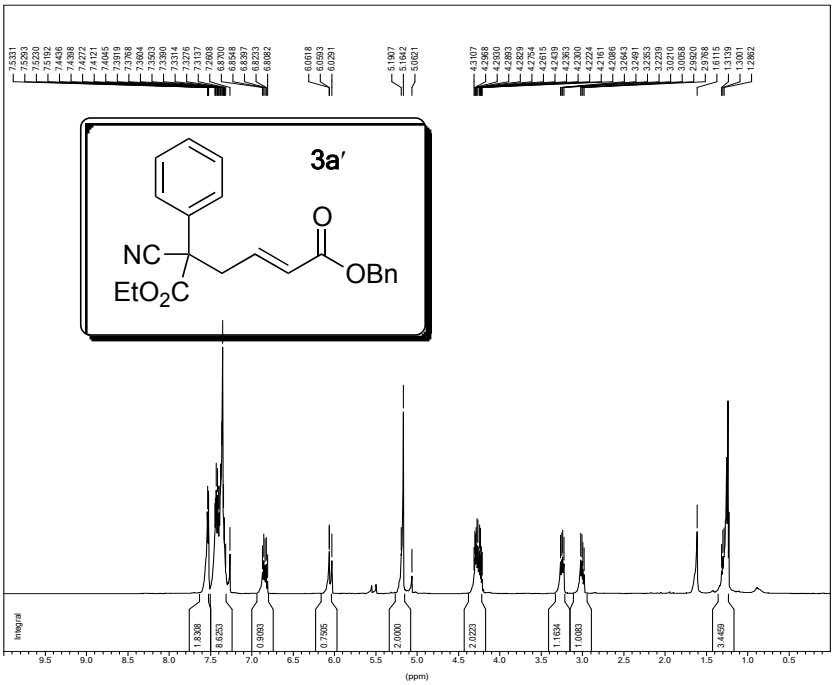



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0115 |
| EXPNO | : | 7 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 11105 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 298.4 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.359 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

1H AMX500

5.167C

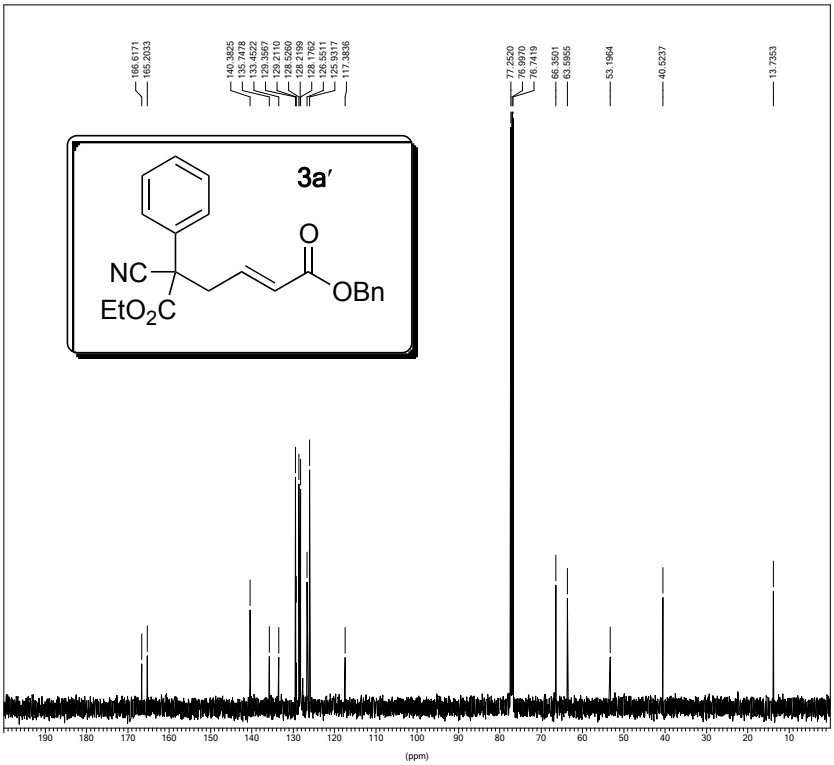



*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0203 |
| EXPNO | : | 4 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 28 |
| NUCLEUS | : | off |
| O1 | : | 3088.51 Hz |
| PULPROG | : | zg30 |
| SFO1 | : | 500.1330885 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 20.6557 ppm |
| TD | : | 32768 |
| TE | : | 299.1 K |
| *** Processing Parameters *** | | |
| LB | : | 0.30 Hz |
| OFFSET | : | 16.478 ppm |
| SI | : | 16384 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |

13C AMX500

5.167C




*** Current Data Parameters ***

| | | |
|---|---|---|
| NAME | : | vrg0203 |
| EXPNO | : | 5 |
| PROCNO | : | 1 |
| *** Acquisition Parameters *** | | |
| DS | : | 0 |
| INSTRUM | : | spect |
| LOCNUC | : | 2H |
| NS | : | 162 |
| NUCLEUS | : | off |
| O1 | : | 13204.57 Hz |
| PULPROG | : | zgpg30 |
| SFO1 | : | 125.7709936 MHz |
| SOLVENT | : | CDCl3 |
| SW | : | 238.7675 ppm |
| TD | : | 65536 |
| TE | : | 299.6 K |
| *** Processing Parameters *** | | |
| LB | : | 1.00 Hz |
| OFFSET | : | 224.355 ppm |
| SI | : | 32768 |
| *** 1D NMR Plot Parameters *** | | |
| NUCLEUS | : | off |