

Supplementary Information for

Nickel-catalyzed Regio- and Stereoselective Hydrocyanation of Alkynoates and Its Mechanistic Insights Proposed by DFT Calculations

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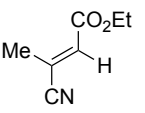
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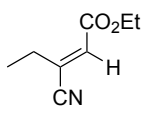
General remarks

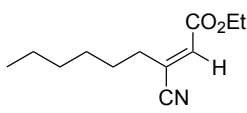
All reactions were performed with dry solvents and reagents that were purified by the usual methods. Reactions were monitored by thin-layer chromatography carried out on 0.25 mm Merck silica gel plates (60F-254). Column chromatography was performed with Wakogel® 60N from Wako Pure Chemical Industries. Infrared (IR) spectra were recorded on JUSCO FT/IR-4700 spectrophotometer. NMR spectra were recorded on JEOL-JMN-ECZ400 and -ECZ600 spectrometers operating at 400 and 600 MHz for ¹H NMR and at 100 and 150 MHz for ¹³C NMR, with calibration using residual undeuterated solvent as an internal reference. Mass spectra were measured by The AccuTOFLC-plus JMS-T100LP (TOF) for LRMS and HRMS. Microwave were operated on CEMDISCOVER SYSTEM at 908005 (model number). Melting points were collected by placing the sample on a glass coverslip on a heating block of a melting temperature measurement device ATM-02. X-ray crystallographic analysis was measured by Rigaku MicroMax-007HF. X-ray crystallographic data were collected at -180 ± 1 °C using filtered CuK α radiation. Ellipsoids are drawn at the 50% probability level.

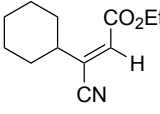
General procedure for Ni-catalyzed hydrocyanation of alkynoates, synthesis of (*E*)-2a:

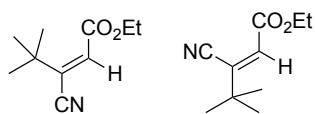
A mixture of TMSCN (0.19 mL, 1.5 mmol, 5.0 eq) and trifluoroethanol (0.11 mL, 1.5 mmol, 5.0 eq) was stirred for 10 min at room temperature and then toluene (0.6 mL) and ethyl 2-butynoate (**1a**) (85.5 mg, 0.3 mmol) and Ni[(P(OPh)₃]₄ (39.0 mg, 0.03 mmol, 10 mol%) were added. After being stirred for 2 h at 100 °C under argon atmosphere, the reaction mixture was charged on a silica gel pad. The following column chromatography (hexane:AcOEt = 9:1) gave (*E*)-**2a** (83.8 mg, 0.27 mmol, 71%, 10:1) as a colorless oil. Its stereoselectivity was also determined by ¹H NMR of the crude product to be 10:1.

 **(*E*)-Ethyl-3-cyanobut-2-enoate** ¹H NMR (CDCl₃, 400 MHz) δ: 1.30 (t, *J* = 7.2 Hz, 3H), 2.35 (d, *J* = 1.6 Hz, 3H), 4.24 (q, *J* = 7.2 Hz, 2H), 6.42 (t, *J* = 1.6 Hz, 1H); ¹³C NMR (CDCl₃, 100 MHz) δ: 14.0, 17.2, 61.2, 118.8, 125.9, 132.7, 163.8; IR (ATR) ν: 3736, 2927, 2208, 1724, 1623, 1372, 1066 cm⁻¹; HRMS (ESI) *m/z* calcd for C₇H₉NNaO₂ [M+Na]⁺ 162.0531 found 162.0529. Colorless oil.

 **(*E*)-Ethyl-3-cyanopent-2-enoate** ¹H NMR (CDCl₃, 400 MHz) δ: 1.21 (t, *J* = 7.6 Hz, 3H), 1.31 (t, *J* = 7.2 Hz, 3H), 2.81 (dq, *J* = 1.2, 7.6 Hz, 2H), 4.23 (q, *J* = 7.2 Hz, 2H), 6.38 (t, *J* = 1.2 Hz, 1H); ¹³C NMR (CDCl₃, 100 MHz) δ: 12.3, 14.0, 23.6, 61.2, 118.0, 131.8, 132.6, 163.7; IR (ATR) ν: 3677, 2207, 1723, 1624, 1327 cm⁻¹; HRMS (ESI) *m/z* calcd for C₈H₁₁NNaO₂ [M+Na]⁺ 176.0688 found 176.0692. Colorless oil.

 **(*E*)-Ethyl-3-cyanonon-2-enoate** ¹H NMR (CDCl₃, 400 MHz) δ: 0.89 (t, *J* = 6.8 Hz, 3H), 1.29-1.40 (m, 9H), 1.65 (quin, *J* = 7.6 Hz, 2H), 2.77 (t, *J* = 7.6 Hz, 2H), 4.23 (q, *J* = 6.8 Hz, 2H), 6.40 (s, 1H); ¹³C NMR (CDCl₃, 100 MHz) δ: 13.9, 14.0, 22.4, 27.9, 28.6, 30.0, 31.3, 61.2, 118.2, 131.5, 132.2, 163.7; IR (ATR) ν: 3676, 2240, 1713, 1515, 1498 cm⁻¹; HRMS (ESI) *m/z* calcd for C₁₂H₁₉NNaO₂ [M+Na]⁺ 232.1314 found 232.1319. Colorless oil.

 **(*E*)-Ethyl-3-cyano-3-cyclohexacrylate** ¹H NMR (CDCl₃, 400 MHz) δ: 1.20-1.29 (m, 1H), 1.30-1.33 (m, 4H), 1.36-1.48 (m, 3H), 1.70-1.83 (m, 5H), 3.47-3.53 (m, 1H), 4.23 (q, *J* = 6.8 Hz, 2H), 6.32 (s, 1H); ¹³C NMR (CDCl₃, 100 MHz) δ: 14.0, 25.3, 25.5, 31.0, 37.7, 61.2, 117.1, 130.8, 137.0, 163.7; IR (ATR) ν: 3751, 2221, 1720, 1623 cm⁻¹; HRMS (ESI) *m/z* calcd. for C₁₂H₁₇NNaO₂ [M+Na]⁺ 230.1157 found 230.1161. Colorless oil.

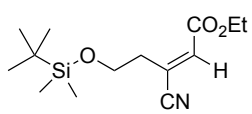


(*E*)-, and (*Z*)-**2e** (1.4:1)

(*E*)- and (*Z*)-Ethyl-2-cyano-4,4-dimethylpent-2-enoate ^1H

NMR (CDCl_3 , 400 MHz) δ : 1.30 (s, 0.58x 9H), 1.32 (s, 0.42 x 9H), 1.33 (t, $J = 7.2$ Hz, 0.58 x 3H), 1.36 (t, $J = 7.2$ Hz, 0.42 x 3H), 4.25 (q, $J = 7.2$ Hz, 0.58 x 2H), 4.32 (q, $J = 7.2$ Hz, 0.42 x 3H), 6.44 (s, 0.58 x 1H), 7.65 (s, 0.42 x 1H); ^{13}C NMR (CDCl_3 ,

100 MHz) δ : 13.9, 14.0, 28.7, 28.8, 35.0, 35.8, 61.7, 62.5, 105.7, 114.2, 118.1, 132.5, 132.9, 162.1, 164.6, 171.8; IR (ATR) ν : 1732, 1368, 1254 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{10}\text{H}_{15}\text{NNaO}_2$ $[\text{M}+\text{Na}]^+$ 204.1001 found 204.0994. Colorless oil.

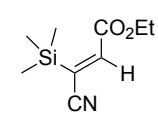


(*E*)-**2f**

(*E*)-Ethyl-5-((*tert*-butyldimethylsilyloxy)-3-cyanopent-2-enoate ^1H

NMR (CDCl_3 , 400 MHz) δ : 0.09 (s, 6H), 0.89 (s, 9H), 1.35 (t, $J = 7.2$ Hz, 3H), 3.03 (dt, $J = 1.2, 6.4$ Hz, 2H), 3.90 (t, $J = 6.4$ Hz, 2H), 4.25 (q, $J = 7.2$ Hz, 2H), 6.51 (d, $J = 1.2$ Hz, 1H); ^{13}C NMR (CDCl_3 ,

100 MHz) δ : 14.0, 18.2, 25.8, 33.4, 60.8, 61.2, 118.2, 128.9, 133.8, 163.7; IR (ATR) ν : 3648, 2955, 2222, 1720, 1380 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{25}\text{NNaO}_3\text{Si}$ $[\text{M}+\text{Na}]^+$ 306.1501 found 306.1500. Colorless oil.

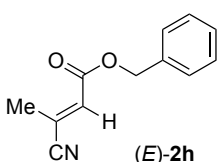


(*Z*)-**2g**

(*Z*)-Ethyl-3-cyano-3-(trimethylsilyl) acrylate ^1H NMR (CDCl_3 , 400 MHz)

δ : 0.35 (s, 6H), 1.33 (t, $J = 7.2$ Hz, 3H), 4.25 (q, $J = 7.2$ Hz, 2H), 7.04 (s, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : -1.1, 14.1, 61.7, 119.7, 129.7, 134.4, 147.0, 164.5; IR (ATR) ν : 3750, 2206, 1623, 1372 cm^{-1} ; HRMS (ESI) m/z calcd for

$\text{C}_9\text{H}_{15}\text{NNaO}_2\text{Si}$ $[\text{M}+\text{Na}]^+$ 220.0770 found 220.0769. Colorless oil.

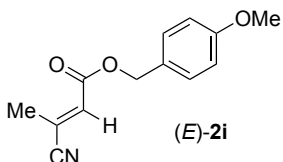


(*E*)-**2h**

(*E*)-Benzyl-3-cyanobut-2-enoate ^1H NMR (CDCl_3 , 400 MHz) δ : 2.36

(d, $J = 1.6$ Hz, 3H), 5.20 (s, 2H), 6.46 (q, $J = 1.6$ Hz, 1H), 7.35-7.37 (m, 5H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 17.5, 67.1, 118.9, 126.7, 128.6, 128.77, 128.83, 132.4, 135.1, 164.8; IR (ATR) ν : 3629, 2959, 2225, 1479,

1348 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{11}\text{NNaO}_2$ $[\text{M}+\text{Na}]^+$ 201.0790 found 201.0788. Colorless oil.

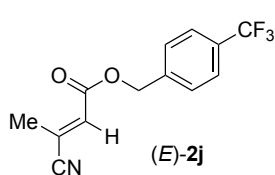


(*E*)-**2i**

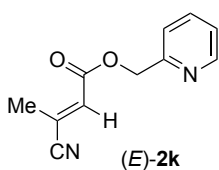
(*E*)-4-Methoxybenzyl-3-cyanobut-2-enoate ^1H NMR (CDCl_3 , 400

MHz) δ : 2.34 d, $J = 1.2$ Hz, 3H), 3.81 (s, 3H), 5.13 (s, 2H), 6.42 (t, $J = 1.2$ Hz, 1H), 6.90 (d, $J = 8.4$ Hz, 2H), 7.30 (d, $J = 8.4$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 17.3, 55.2, 66.8, 114.0, 118.7, 126.3,

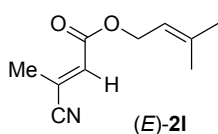
127.0, 130.3, 132.4, 159.9, 163.6; IR (ATR) ν : 3676, 2855, 2221, 1722, 1636, 1374 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{13}\text{NNaO}_3$ $[\text{M}+\text{Na}]^+$ 254.0793 found 254.0791. Colorless solid. mp. 54-55 $^{\circ}\text{C}$.



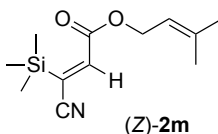
(E)-4-(Trifluoromethyl)benzyl-3-cyanobut-2-enoate ^1H NMR (CDCl_3 , 400 MHz) δ : 2.37 (d, $J = 1.2$ Hz, 3H), 5.26 (s, 2H), 6.47 (t, $J = 1.2$ Hz, 1H), 7.48 (d, $J = 6.4$ Hz, 2H), 7.64 (d, $J = 6.4$ Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 17.4, 65.9, 118.6, 125.6, 125.7, 127.2, 128.4, 131.7, 138.9, 163.4; IR (ATR) ν : 3676, 2855, 2207, 1623, 1449 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{10}\text{F}_3\text{NNaO}_2$ $[\text{M}+\text{Na}]^+$ 292.0561 found 292.0567. Colorless solid. mp. 40-41 $^\circ\text{C}$.



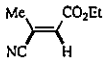
(E)-Pyridin-2-ylmethyl-3-cyanobut-2-enoate ^1H NMR (CDCl_3 , 400 MHz) δ : 2.38 (d, $J = 1.6$ Hz, 3H), 5.31 (s, 2H), 6.54 (d, $J = 1.6$ Hz, 1H), 7.26 (d, $J = 7.2$ Hz, 1H), 7.36 (d, $J = 8.0$ Hz, 1H), 7.74 (t, $J = 8.0$ Hz, 1H), 8.61 (d, $J = 4.0$ Hz, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 17.4, 67.3, 118.6, 121.9, 123.1, 126.9, 131.8, 136.8, 149.6, 154.7, 163.4; [IR (ATR) ν : 2940, 2224, 1714, 1379, 1164 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{11}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 203.0821 found 203.0825; Colorless solid. mp. 56-57 $^\circ\text{C}$.



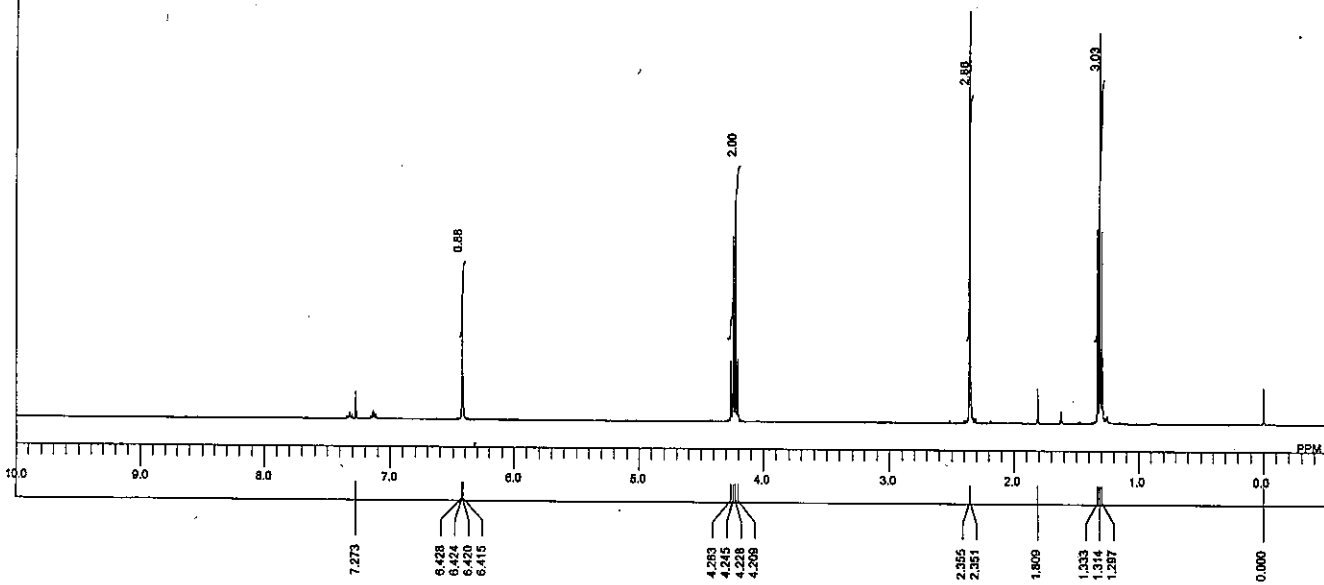
(E)-3-Methylbut-2-en-1-yl-3-cyanobut-2-enoate ^1H NMR (CDCl_3 , 400 MHz) δ : 1.73 (s, 3H), 1.78 (s, 3H), 2.35 (d, $J = 1.6$ Hz, 3H), 4.67 (d, $J = 7.2$ Hz, 2H), 5.33-5.38 (m, 1H), 6.42 (q, $J = 1.6$ Hz, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : 17.2, 18.0, 25.7, 62.0, 117.6, 118.8, 125.9, 132.7, 140.3, 163.8; IR (ATR) ν : 2225, 1719, 1216, 1144 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{13}\text{NNaO}_2$ $[\text{M}+\text{Na}]^+$ 202.0884, found 202.0881. Colorless oil.



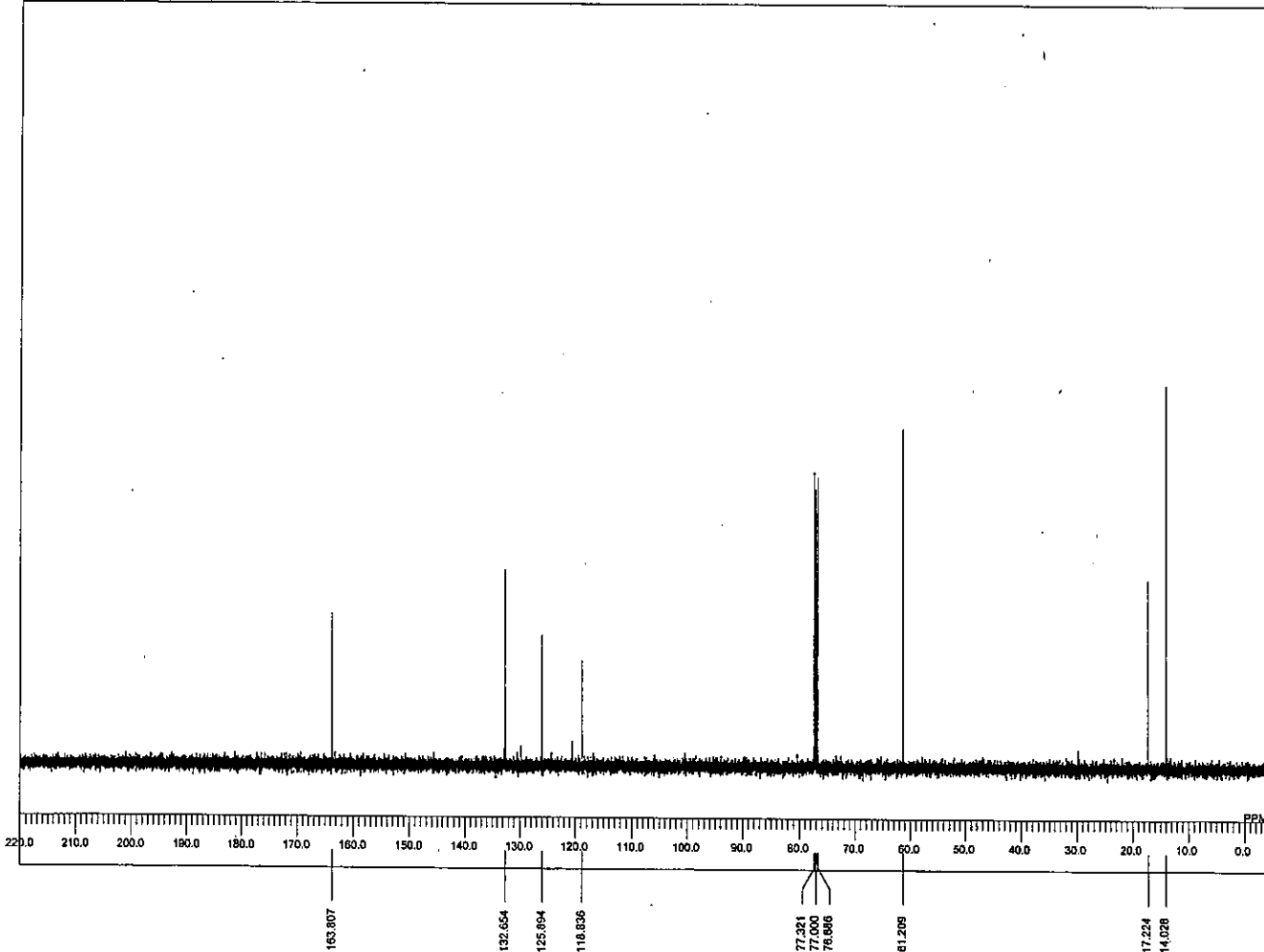
(Z)-3-Methylbut-2-en-1-yl-3-cyano-3-(trimethylsilyl)acrylate ^1H NMR (CDCl_3 , 400 MHz) δ : 0.34 (s, 9H), 1.73 (s, 3H), 1.78 (s, 3H), 4.69 (d, $J = 7.2$ Hz, 2H), 5.33-5.38 (m, 1H), 6.42 (s, 1H); ^{13}C NMR (CDCl_3 , 100 MHz) δ : -1.1, 18.1, 25.8, 62.4, 117.5, 119.8, 134.2, 140.6, 147.0, 164.5; IR (ATR) ν : 2207, 1723, 1251, 1197, 848 cm^{-1} ; HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{19}\text{NNaO}_2\text{Si}$ $[\text{M}+\text{Na}]^+$ 260.1083, found 260.1081. Colorless oil.



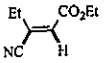
(E)-2a



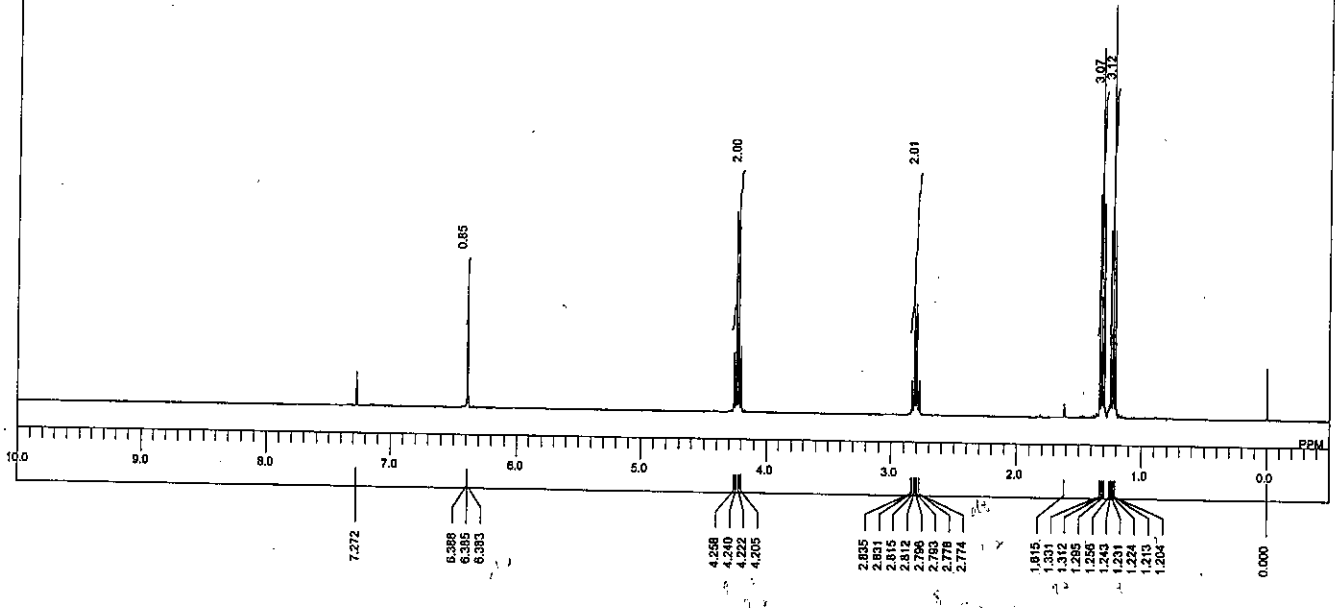
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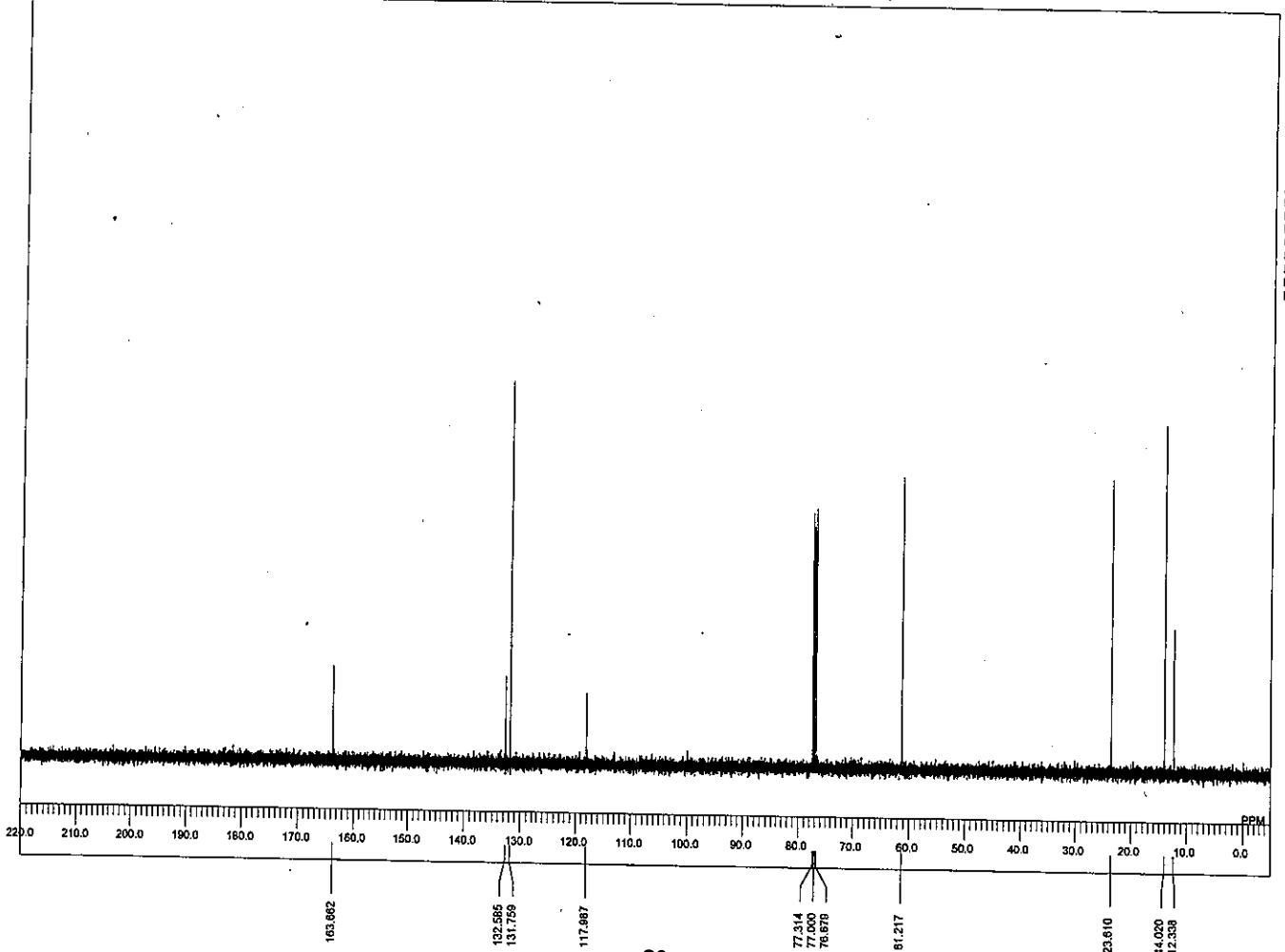
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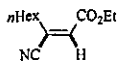
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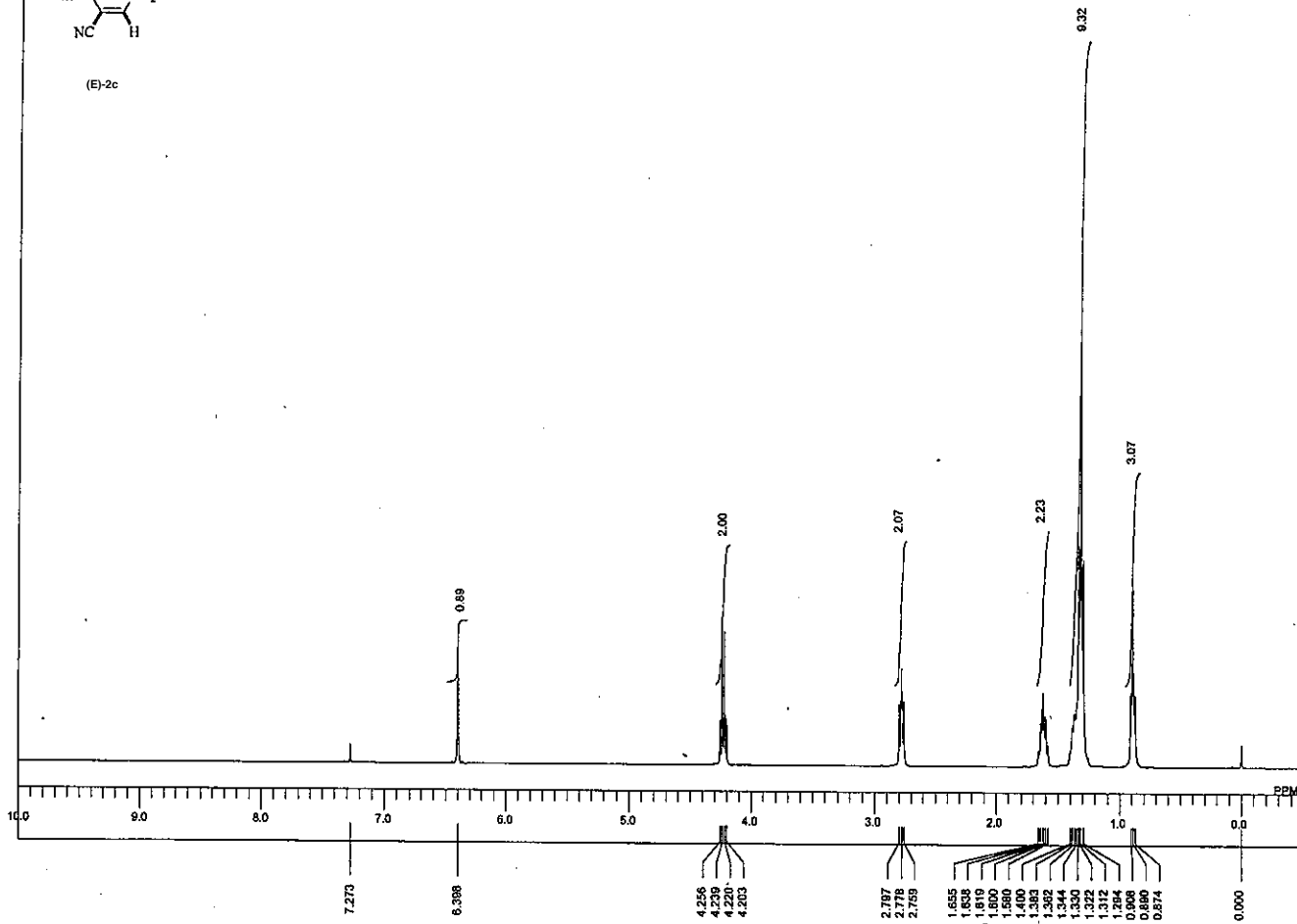
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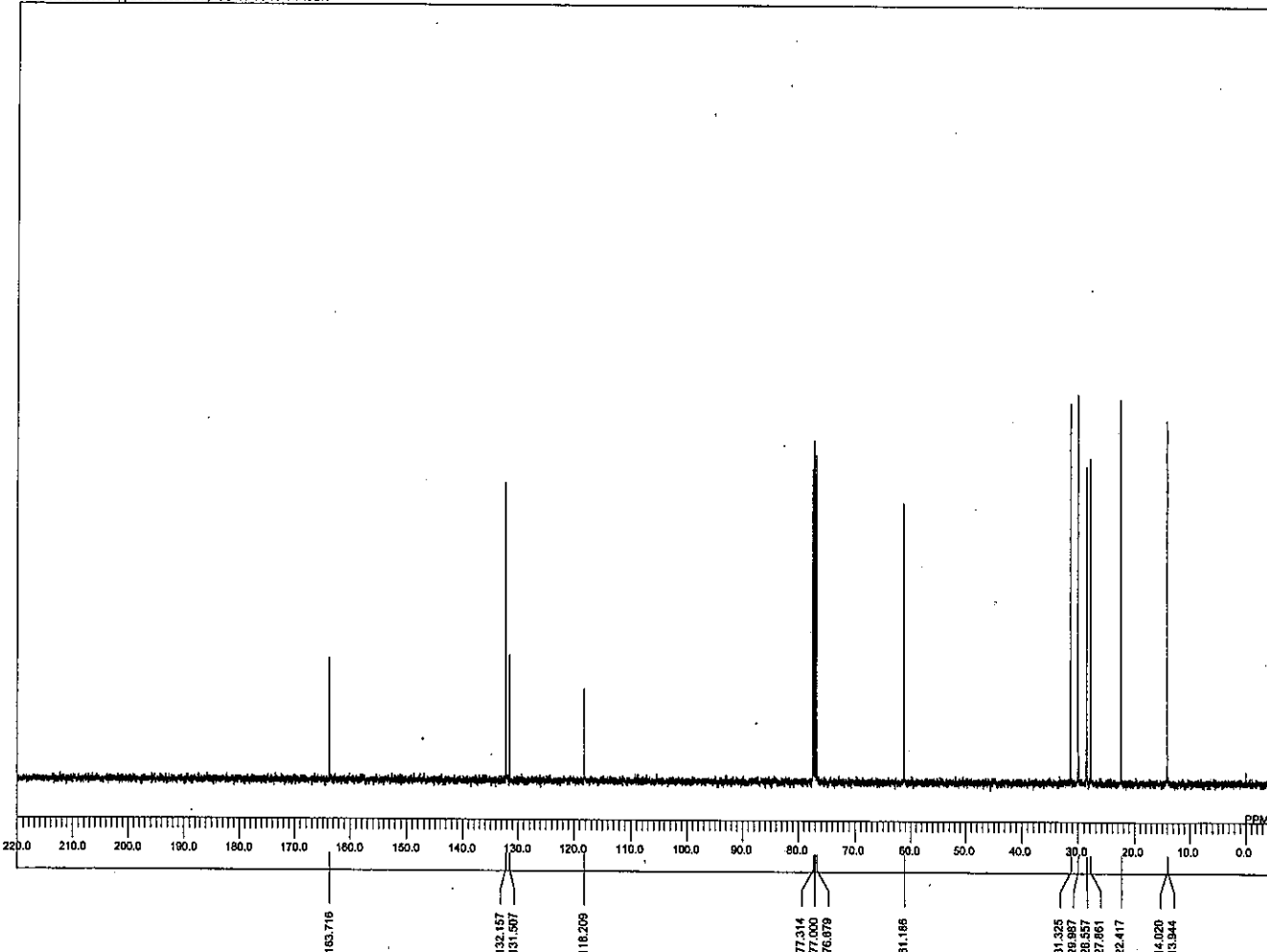
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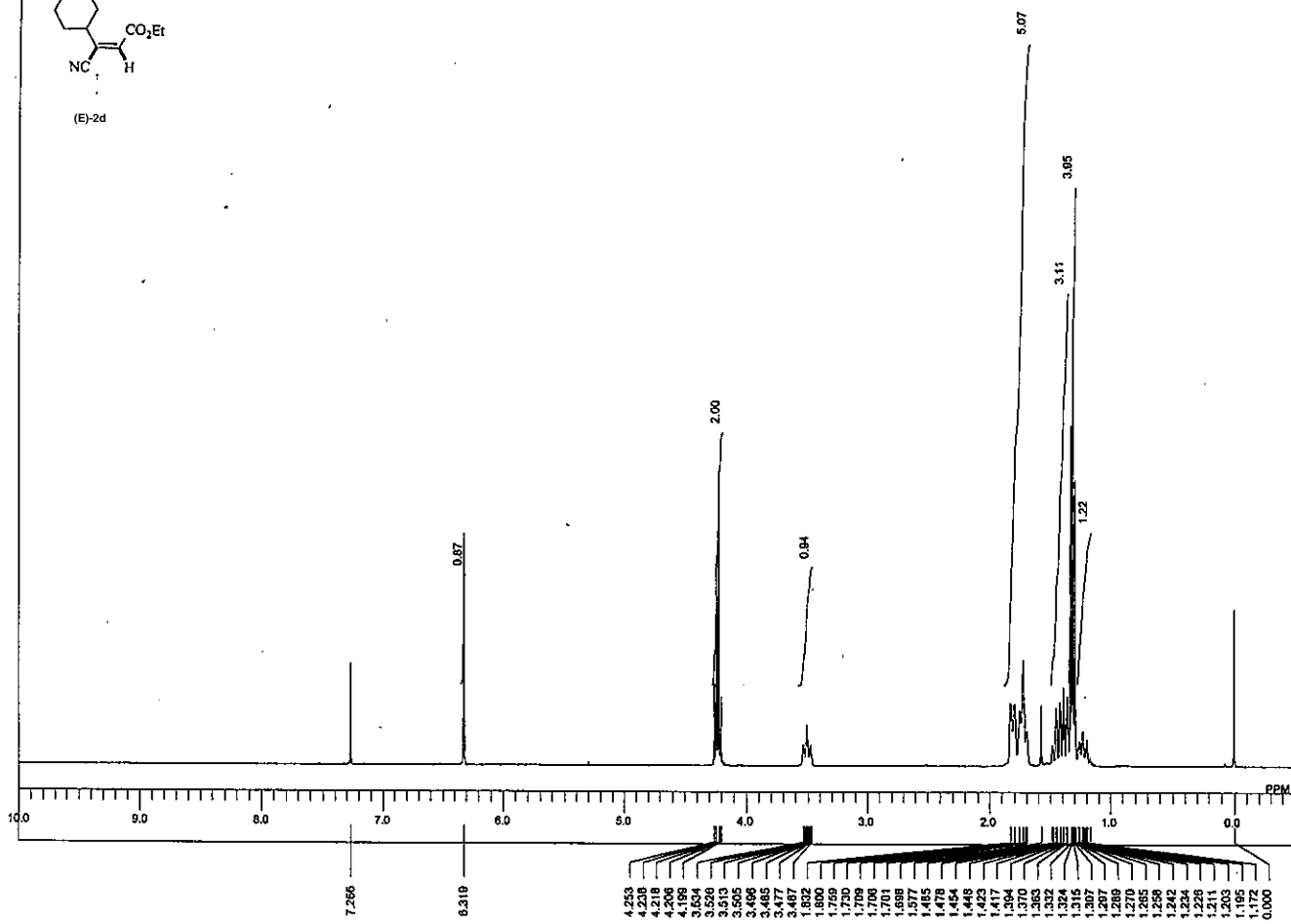
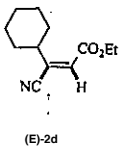
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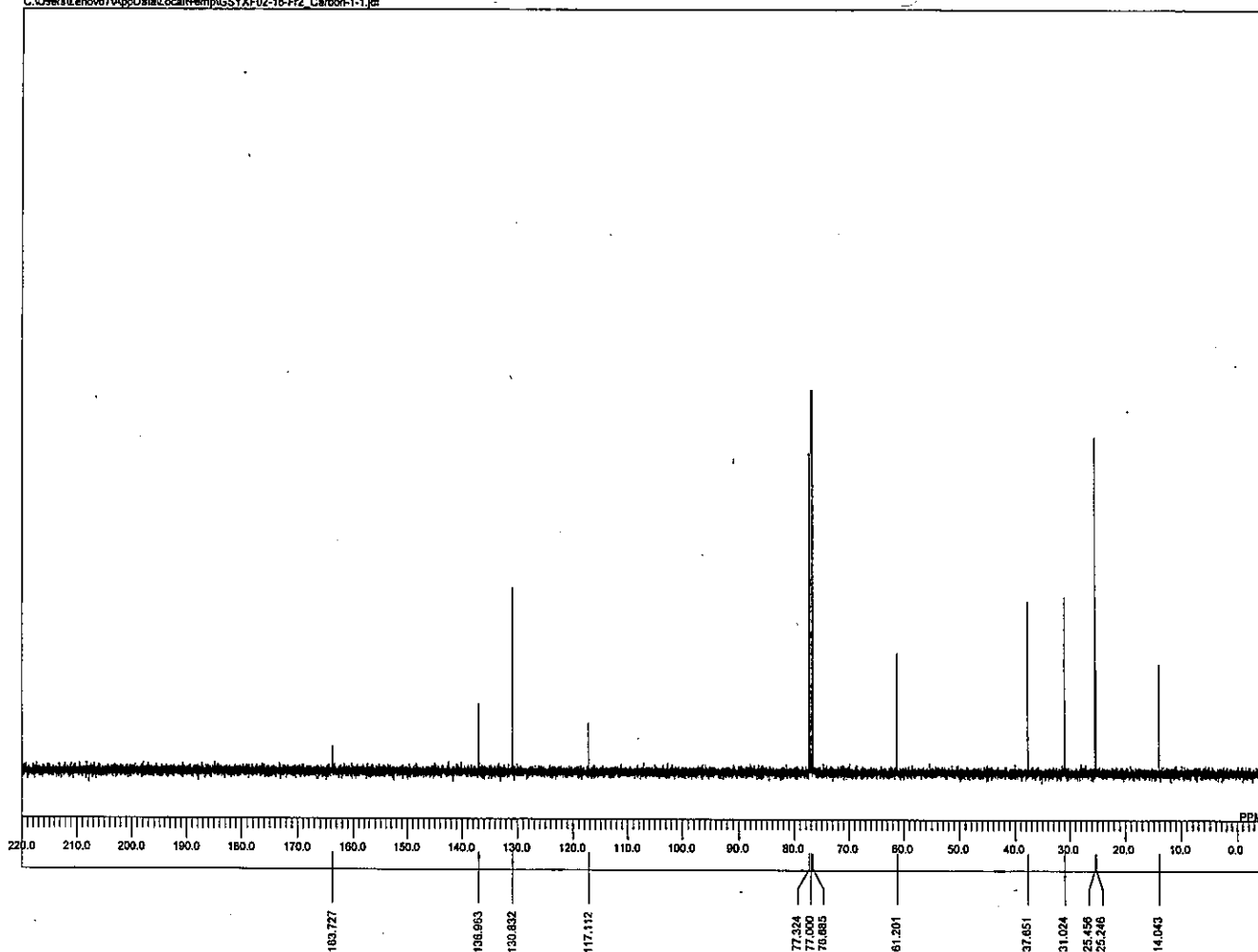
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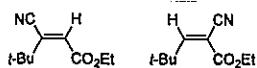
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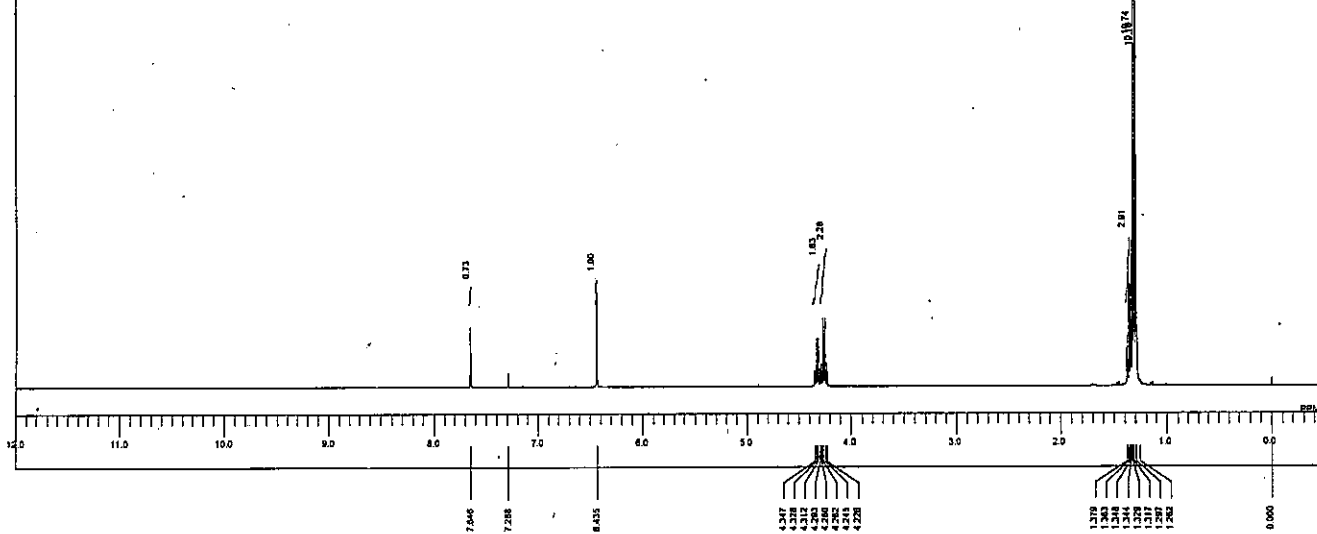


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 BF 0.12 Hz
 RGAIN 50

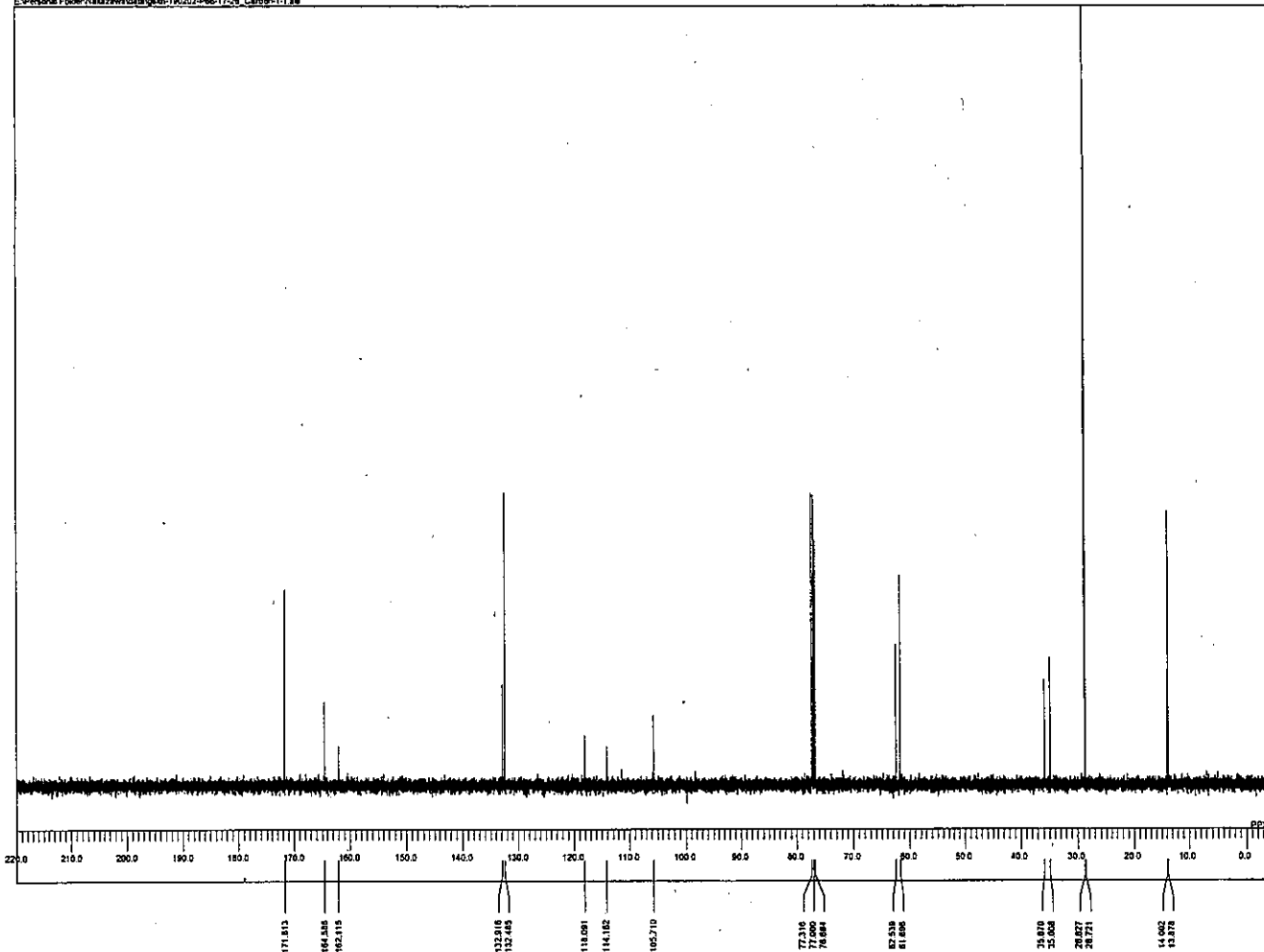


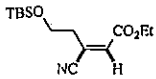
(E)-, and (Z)-2e (1.4:1)

DFILE gain-190202-P66-17-26_Proton
COMINT angle_pulse
DATEM 2019-02-02 11:06:36
1H
EXMOO proton_jsp
OBPRO 388.78 kHz
OBSET 4.16 kHz
OBPN 7.29 Hz
POINT 13127
FREQU 599.820 Hz
SCANS 8
ACQTM 2.1883 sec
PD 8.0000 sec
PWI 5.80 usec
IRNUC 1H
CTEMP 16.5 c
SOLVT CDCl3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 38

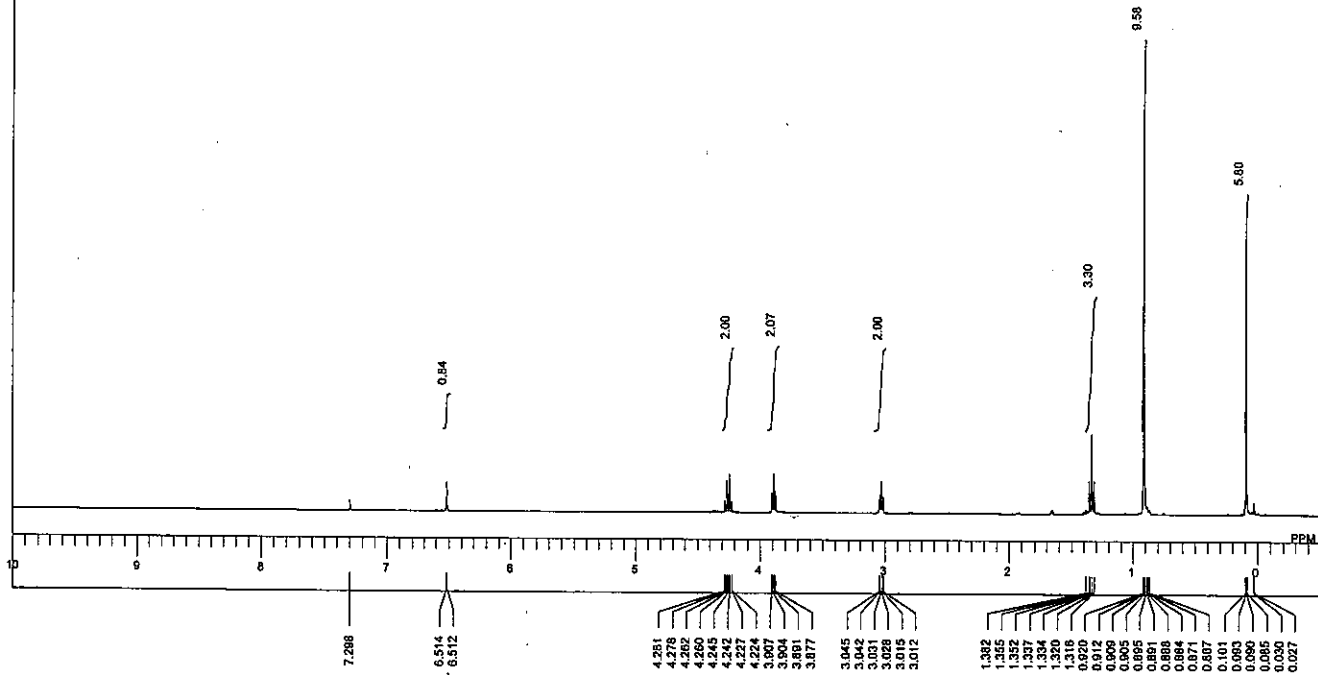


DFILE gain-190202-P66-17-26_Carb
COMINT single pulse decoupled gated
DATEM 2019-02-02 11:12:49
13C
EXMOO carbon_jsp
OBPRO 100.53 MHz
OBSET 5.35 kHz
OBPN 5.86 Hz
POINT 38214
FREQU 25292.53 Hz
SCANS 80
ACQTM 1.0381 sec
PD 2.0000 sec
PWI -3.02 usec
IRNUC 13C
CTEMP 16.7 c
SOLVT CDCl3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50

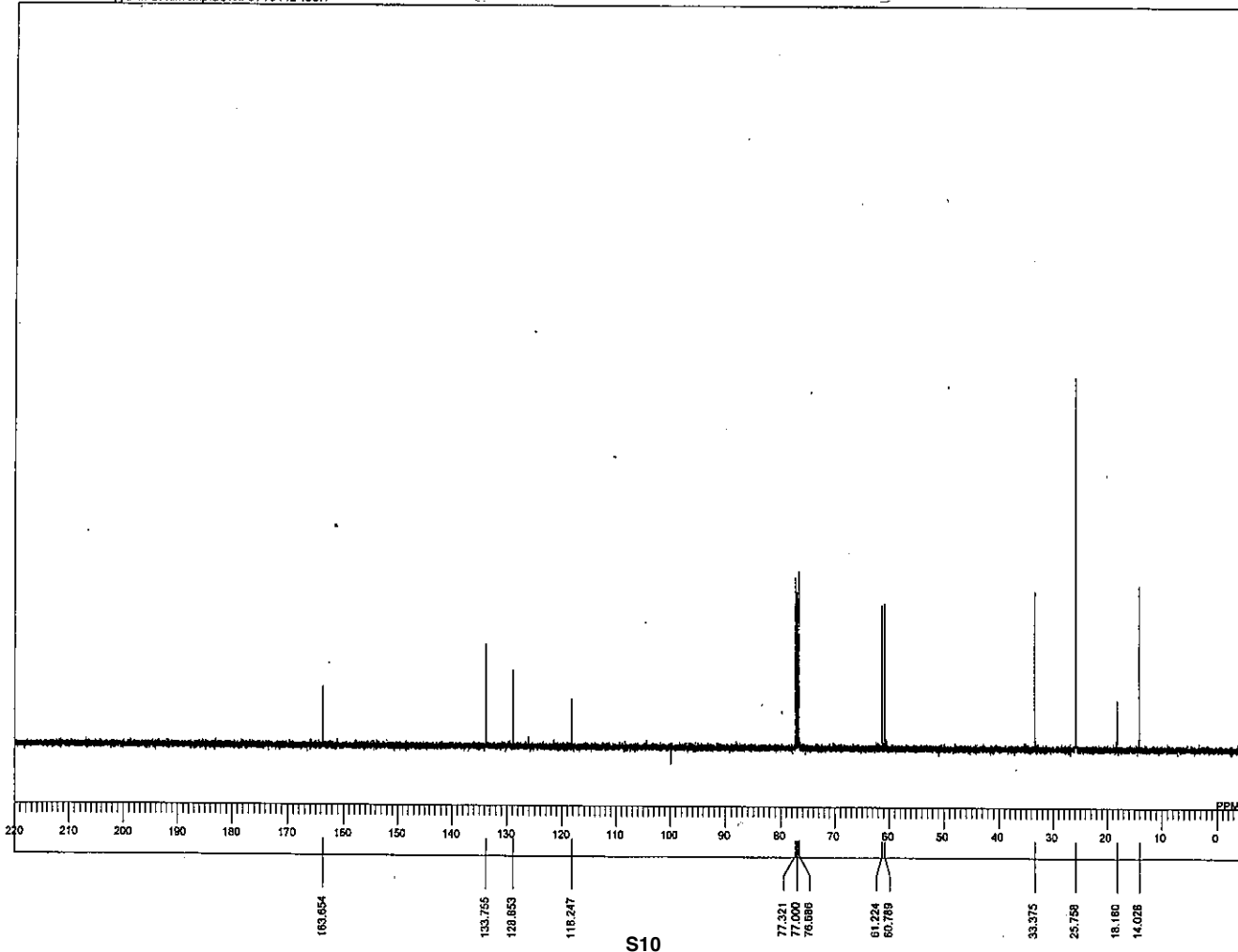




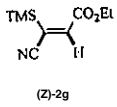
(E)-2f



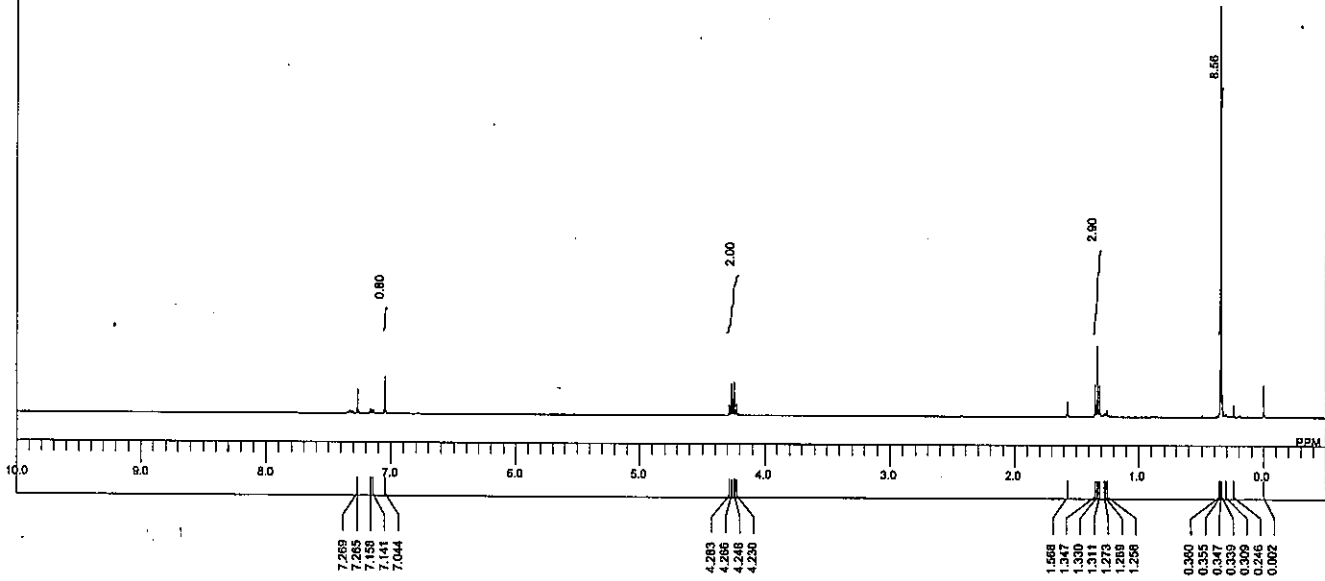
DFILE GSYXF01-73-Fr2
 COMNT
 DATIM 2013-06-03 10:43:
 OBNUC 1H
 EXMOD single_pulse_exp
 OBFRQ 399.78 MHz
 OBSFQ 4.18 KHz
 OBSFM 7.29 Hz
 POINT 16384
 FREQU 5998.80 Hz
 SCANS 8
 ACQTM 2.7312 sec
 PD 2.0000 sec
 PW1 6.00 usec
 IRNUC
 CTEMP 23.0 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 10



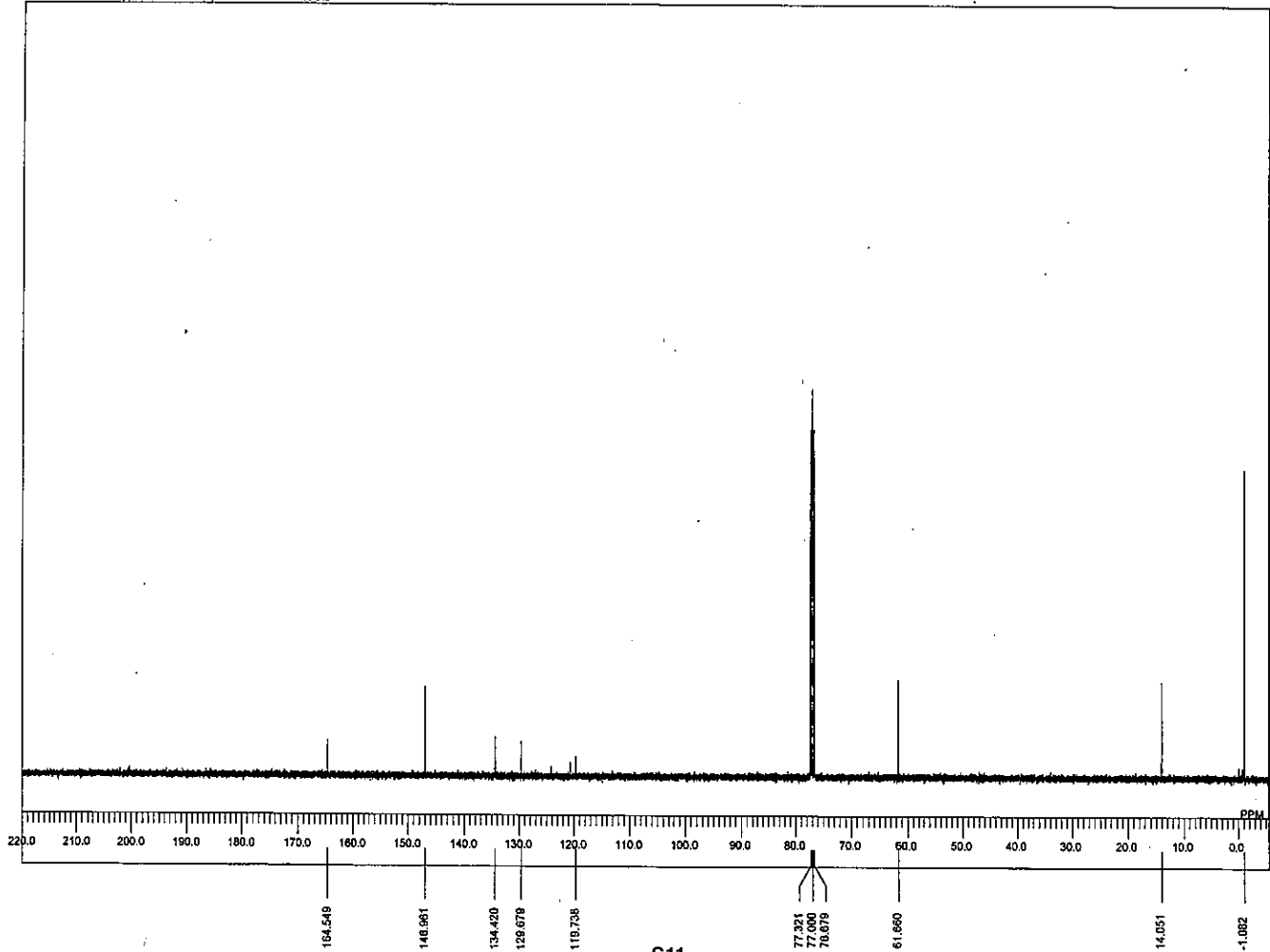
DFILE GSYXF01-73-Fr2
 COMNT
 DATIM 2013-06-03 11:01
 OBNUC 13C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSFQ 5.36 KHz
 OBSFM 5.85 Hz
 POINT 32768
 FREQU 25188.92 Hz
 SCANS 289
 ACQTM 1.3009 sec
 PD 1.0000 sec
 PW1 3.17 usec
 IRNUC 1H
 CTEMP 24.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 24

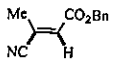


DFILE GSYXF02-05.1
 COMNT 2013-08-08 09:23
 DATIM 1H
 OBNUC single_pulse.exp
 EXMOD 399.78 MHz
 OFPRQ 4.19 KHz
 OBSET 7.28 Hz
 OFBIN 16384
 POINT 5998.80 Hz
 FREQU 8
 SCANS 2.7312 sec
 ACQTM 2.0000 sec
 PD 6.00 usec
 PWI 22.2 c
 IRNUC CDCL3
 CTEMP 0.00 ppm
 SLVNT 0.12 Hz
 EXREF 15
 BF
 RGAIN

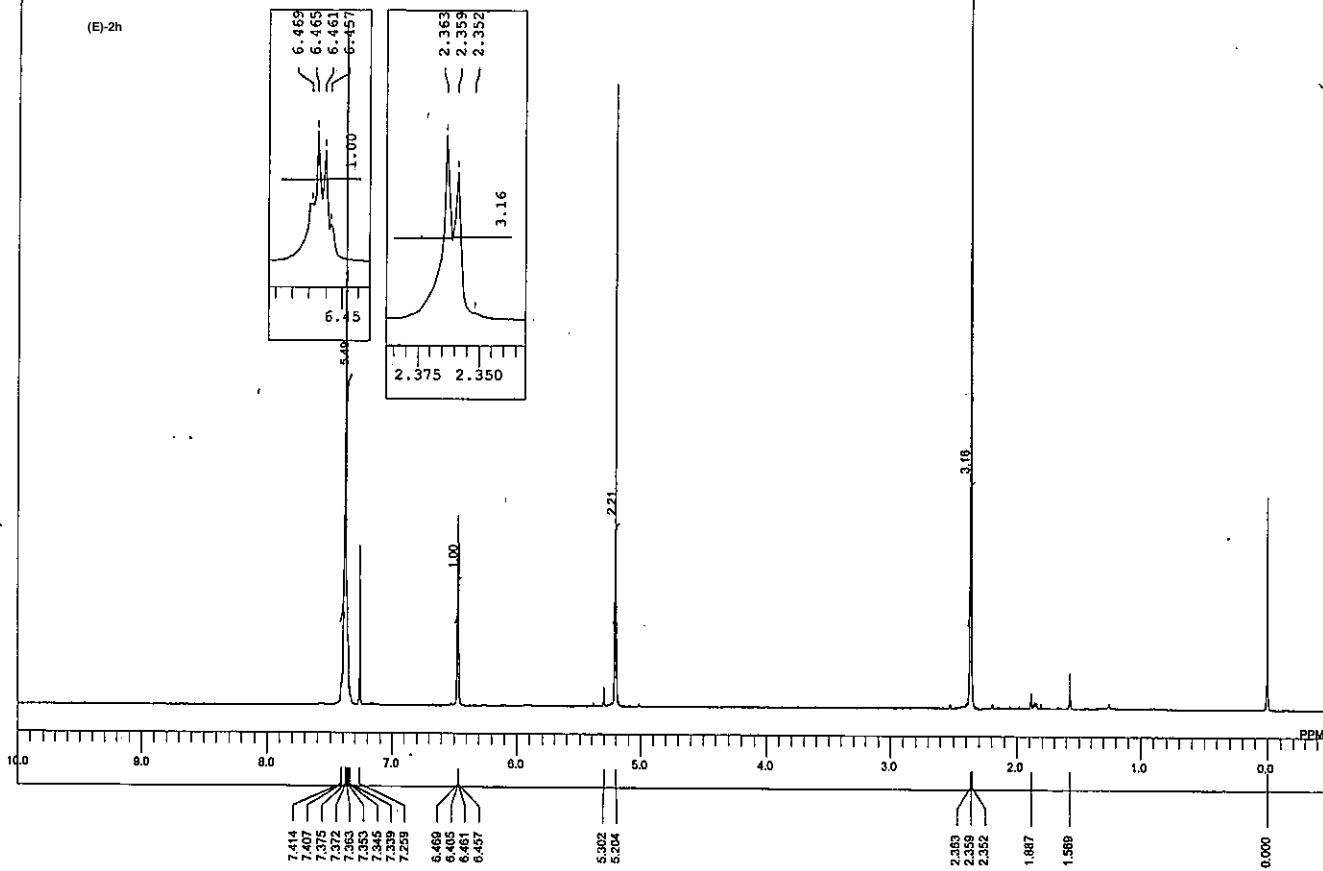


DFILE GSYXF02-05TM1
 COMNT 2013-06-08 15:05
 DATIM 13C
 OBNUC single_pulse_dec
 EXMOD 100.63 MHz
 OFPRQ 5.35 KHz
 OBSET 5.85 Hz
 OFBIN 32768
 POINT 25188.92 Hz
 FREQU 1535
 SCANS 1.3009 sec
 ACQTM 1.0000 sec
 PD 3.17 usec
 PWI 23.7 c
 IRNUC CDCL3
 CTEMP 77.00 ppm
 SLVNT 0.12 Hz
 EXREF 24
 BF
 RGAIN





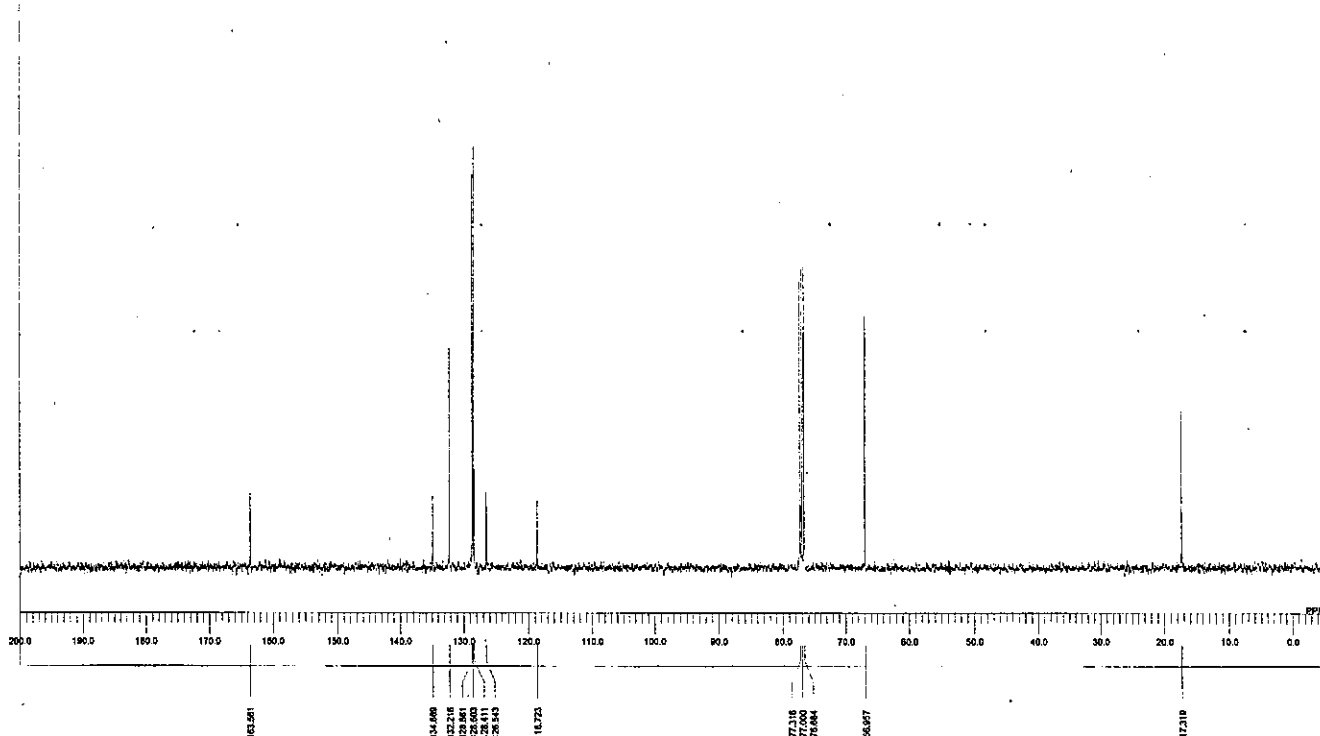
(E)-2h



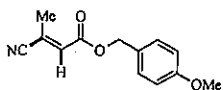
DFILE GSYXF01-04-Fr2
 COMNT single_pulse
 DATIM 2013-04-11 14:33
 OBNUC 1H
 EXMOD proton.jpg
 OBFREQ 399.76 MHz
 OBSSET 4.19 KHz
 OBFIN 7.29 Hz
 POINT 20480
 FREQU 8378.75 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PWT 5.00 usec
 IRNUC 1H
 CTEMP 18.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 44

single pulse decoupled gated NMR

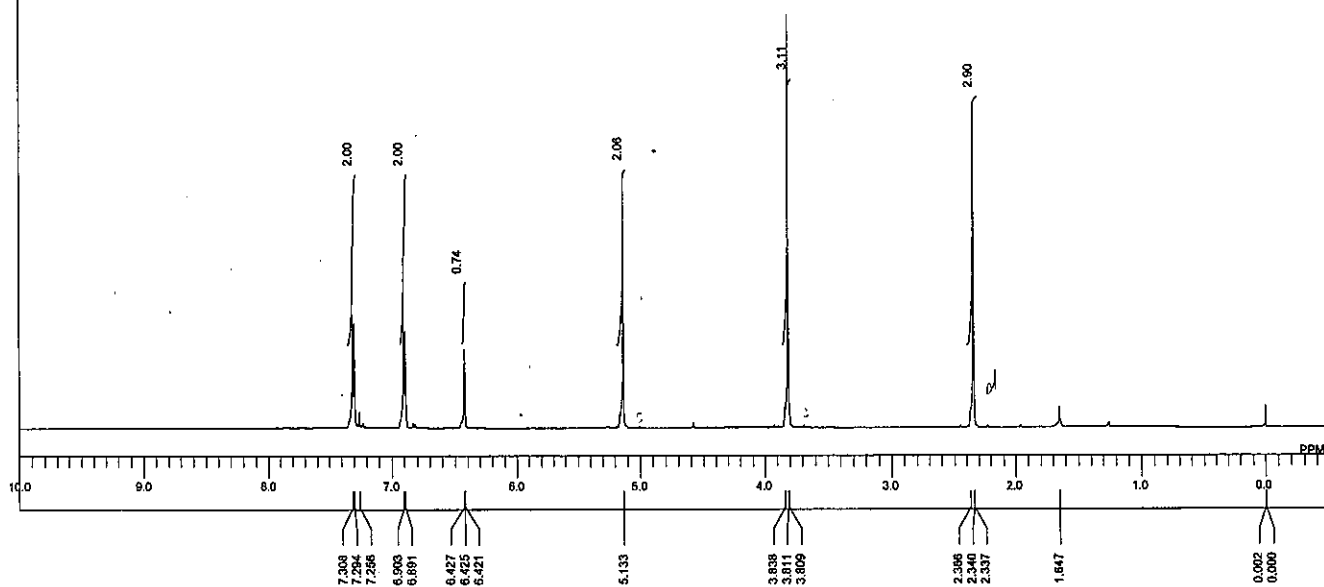
C:\Users\Lenovo\TVAppData\LocalTemp\GSYXF-Me,Bn,HCN_Carbon_8-1-11.d



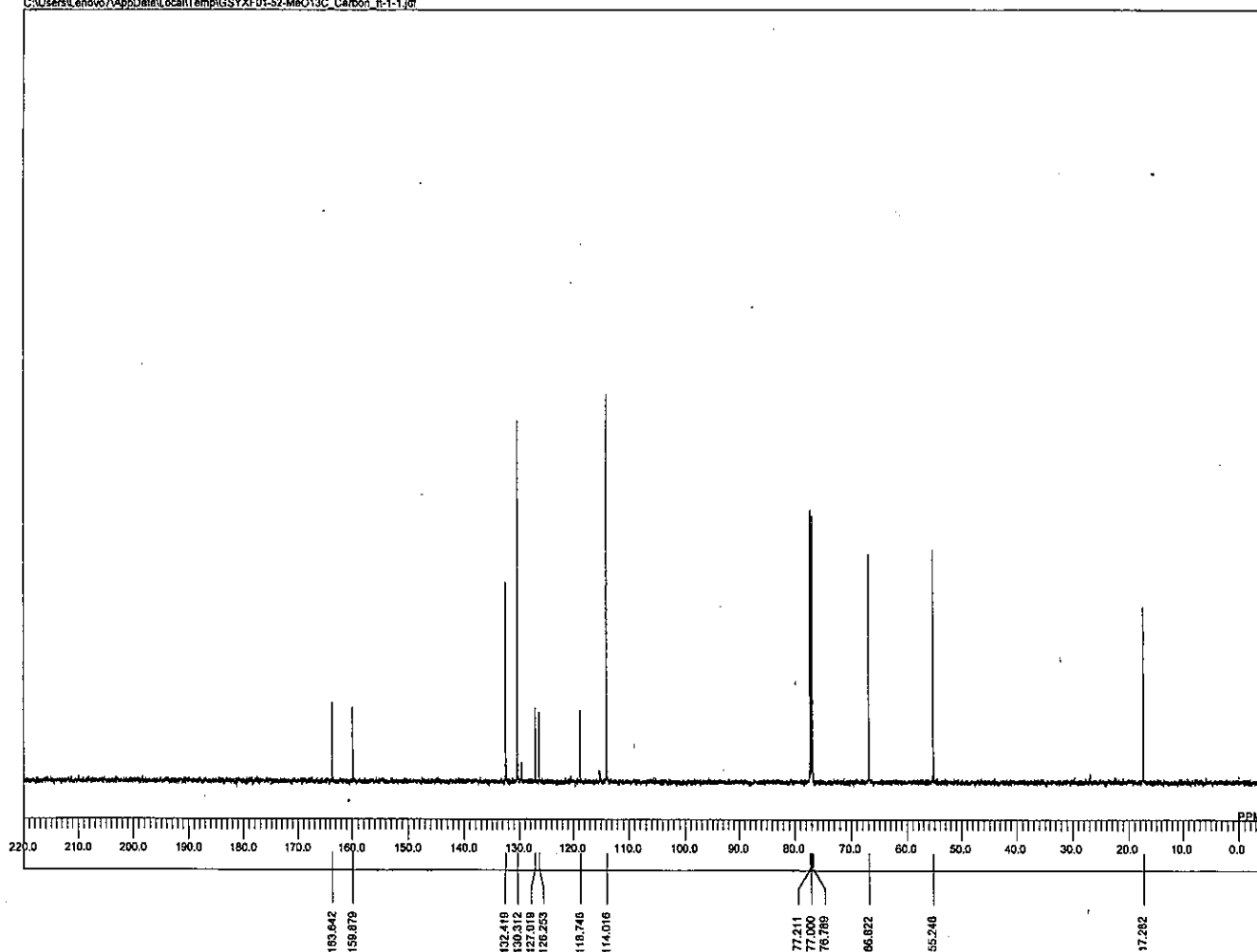
DFILE GSYXF-Me,Bn,HCN_C
 COMNT single pulse decoupled
 DATIM 2016-01-15 16:18:08
 OBNUC 13C
 EXMOD carbon.jpg
 OBFREQ 100.53 MHz
 OBSSET 5.35 KHz
 OBFIN 3.88 Hz
 POINT 40960
 FREQU 39457.07 Hz
 SCANS 87
 ACQTM 1.0381 sec
 PD 2.0000 sec
 PWT 3.52 usec
 IRNUC 13C
 CTEMP 18.4 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 50



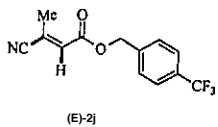
(E)-2i



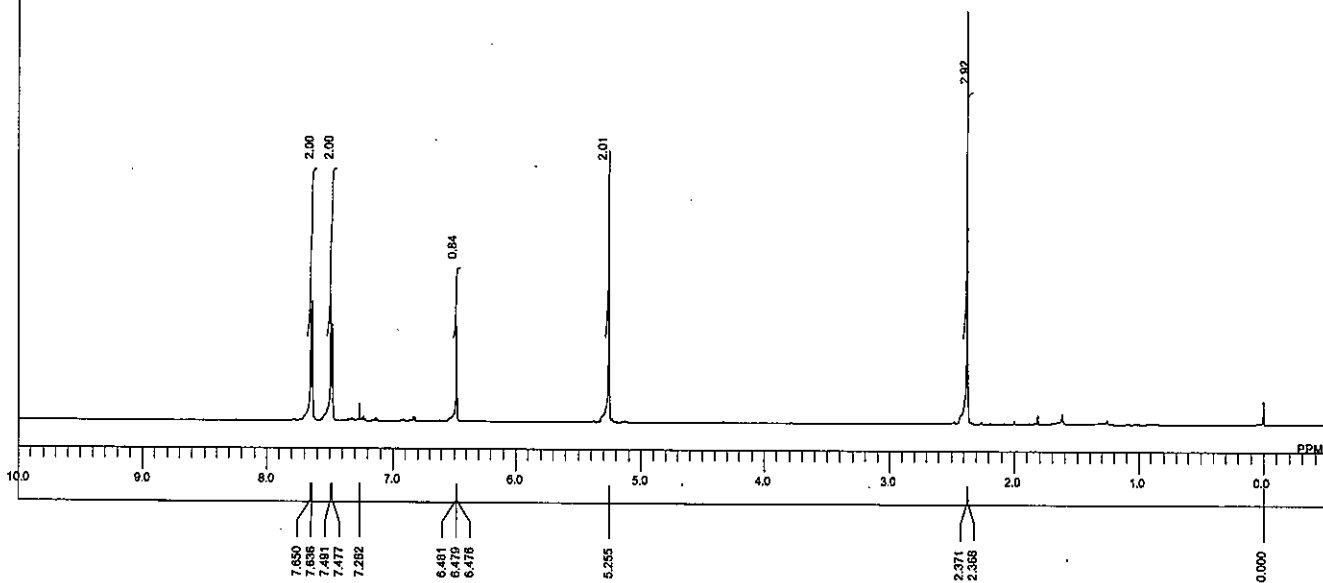
DFILE GSYXF01-52-MeC
 COMNT single_pulse
 DATIM 2013-05-29 19:02:
 OBNUC ¹H
 EXMOD proton.jcp
 OBFRQ 600.17 MHz
 OBSET 5.30 KHz
 OBFIN 5.47 Hz
 POINT 20480
 FREQU 14079.58 Hz
 SCANS 8
 ACQTM 1.4549 sec
 PD 5.0000 sec
 PW1 6.55 usec
 IRNUC ¹H
 CTEMP 22.9 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 34



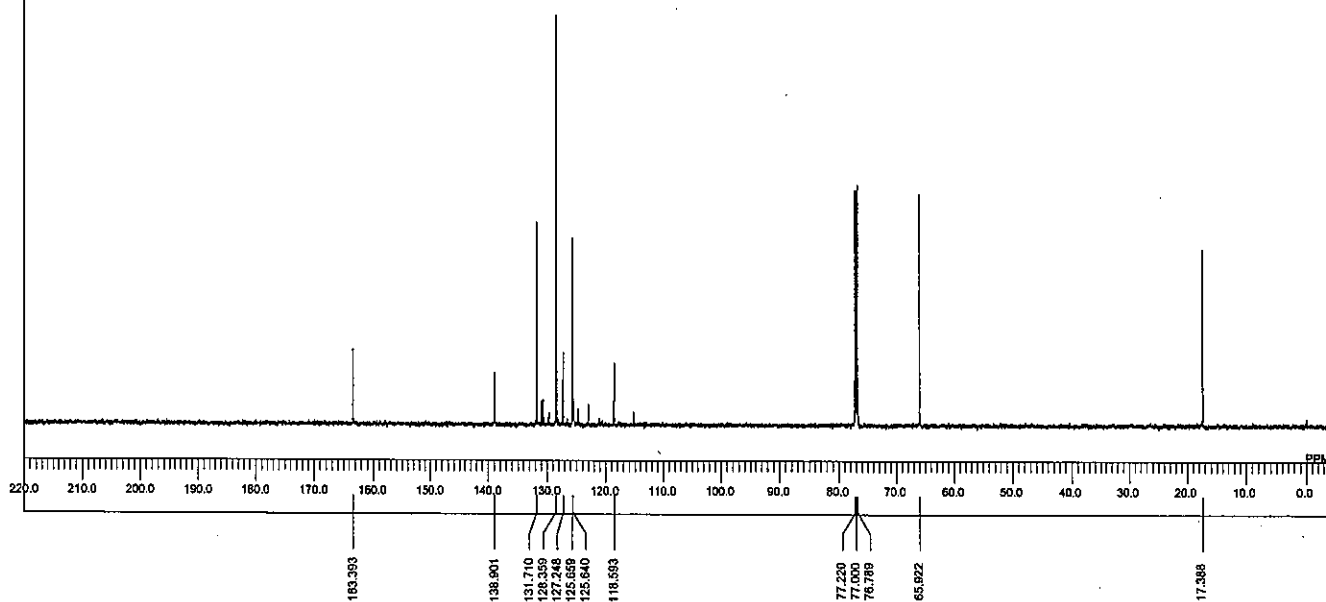
DFILE GSYXF01-52-MeC
 COMNT single_pulse deco
 DATIM 2013-05-29 19:04
 OBNUC ¹³C
 EXMOD carbon.jcp
 OBFRQ 150.92 MHz
 OBSET 6.52 KHz
 OBFIN 1.74 Hz
 POINT 40960
 FREQU 59185.50 Hz
 SCANS 132
 ACQTM 0.6921 sec
 PD 2.0000 sec
 PW1 3.27 usec
 IRNUC ¹H
 CTEMP 23.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 50

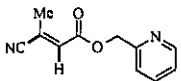


DFILE GSYXF01-59-CF31
COMNT single_pulse
DATIM 2013-05-29 19:11:3
OBNUC 1H
EXMOD proton.jxp
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 20480
FREQU 14078.58 Hz
SCANS 8
ACQTM 1.4349 sec
PD 5.0000 sec
PWI 6.55 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 36

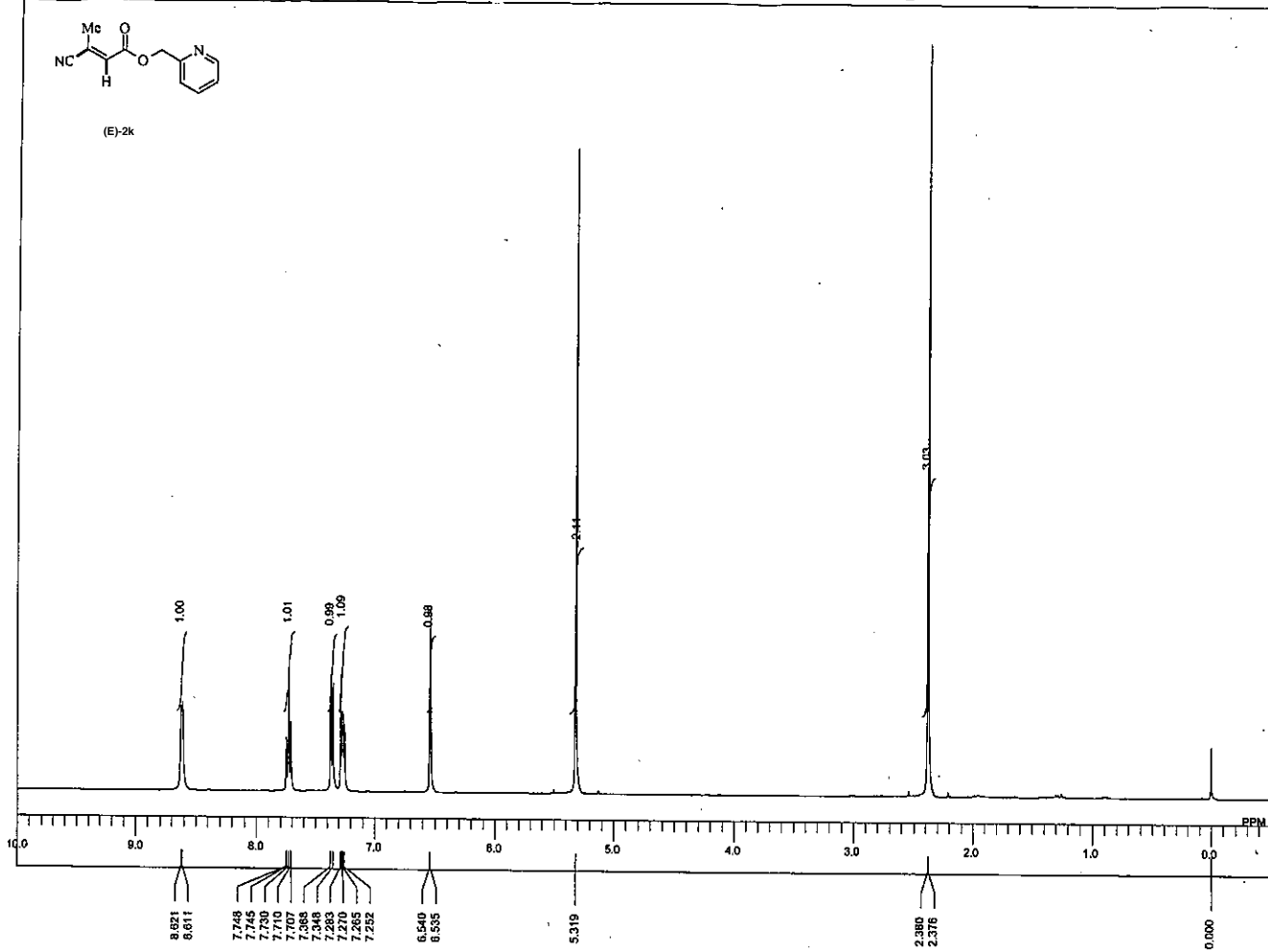


DFILE GSYXF01-59-CF
COMNT single_pulse_deca
DATIM 2013-05-29 19:12
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 40960
FREQU 59185.80 Hz
SCANS 161
ACQTM 0.6921 sec
PD 2.0000 sec
PWI 3.27 usec
IRNUC 1H
CTEMP 23.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50

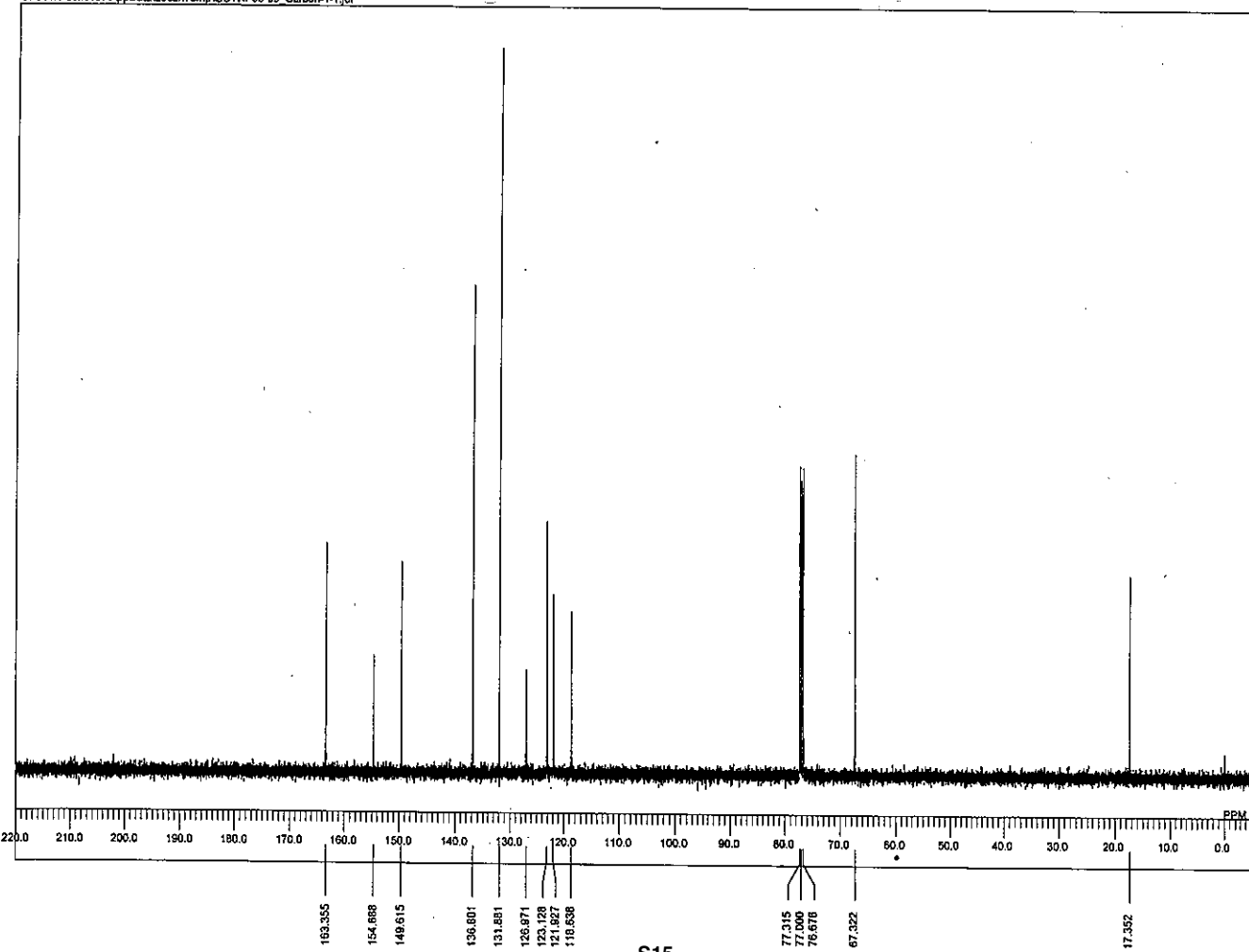




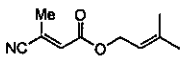
(E)-2k



DFILE GSYXF08-59_Pr
 COMNT single_pulse
 DATIM 2013-03-06 10:58
 OBNUC 1H
 EXMOD proton.jxp
 OBFRO 399.78 MHz
 OBSF7 4.19 KHz
 OBSF1 7.29 Hz
 POINT 20480
 FREQU 9378.75 Hz
 SCANS 16
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PWH 5.00 usec
 IRNUC 1H
 CTEMP 22.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 36

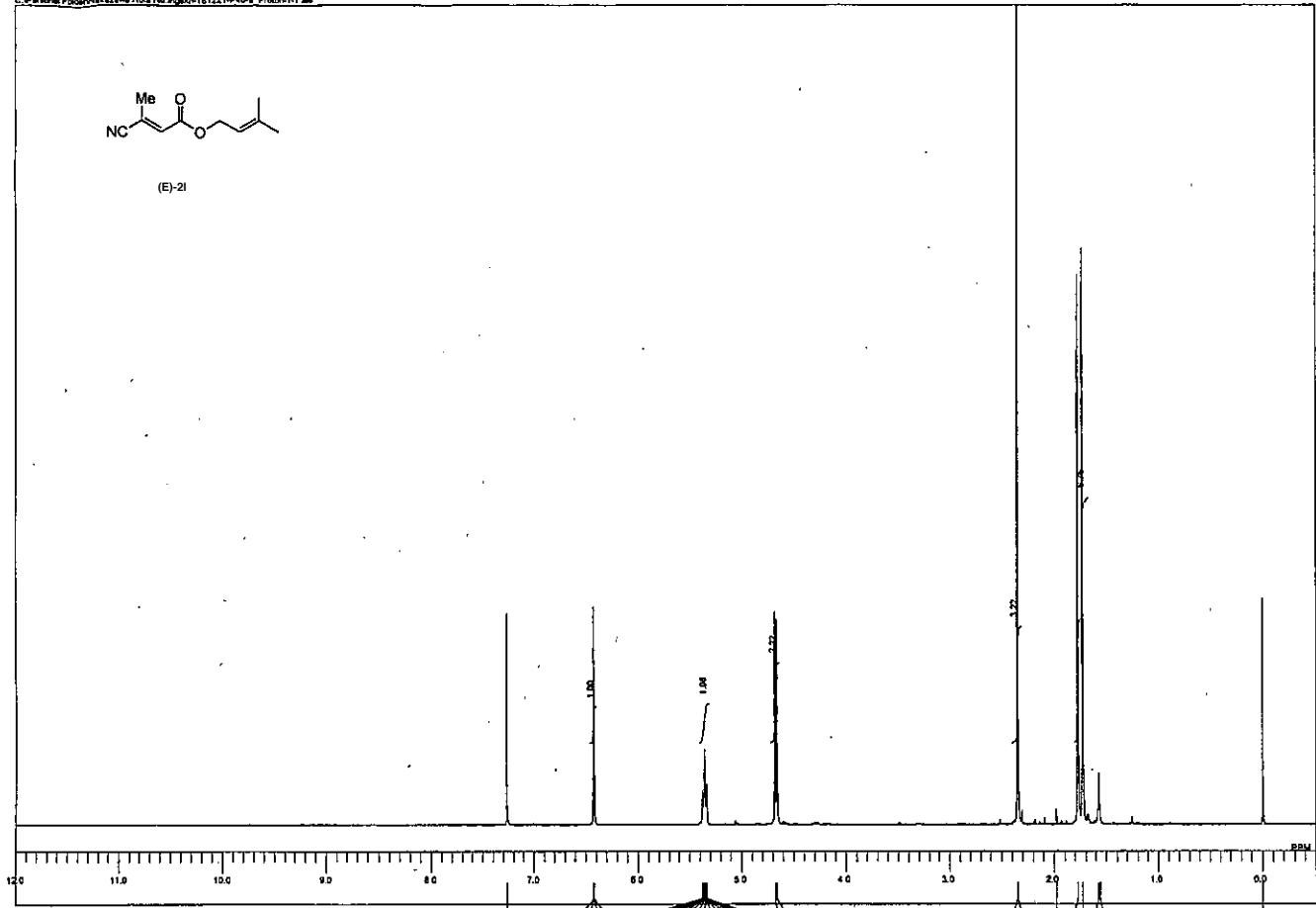


DFILE GSYXF08-59_Car
 COMNT single_pulse_decou
 DATIM 2013-03-06 11:01
 OBNUC 13C
 EXMOD carbon.jxp
 OBFRO 100.63 MHz
 OBSF7 5.35 KHz
 OBSF1 5.86 Hz
 POINT 32767
 FREQU 31407.04 Hz
 SCANS 181
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PWH 3.07 usec
 IRNUC 1H
 CTEMP 23.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 50



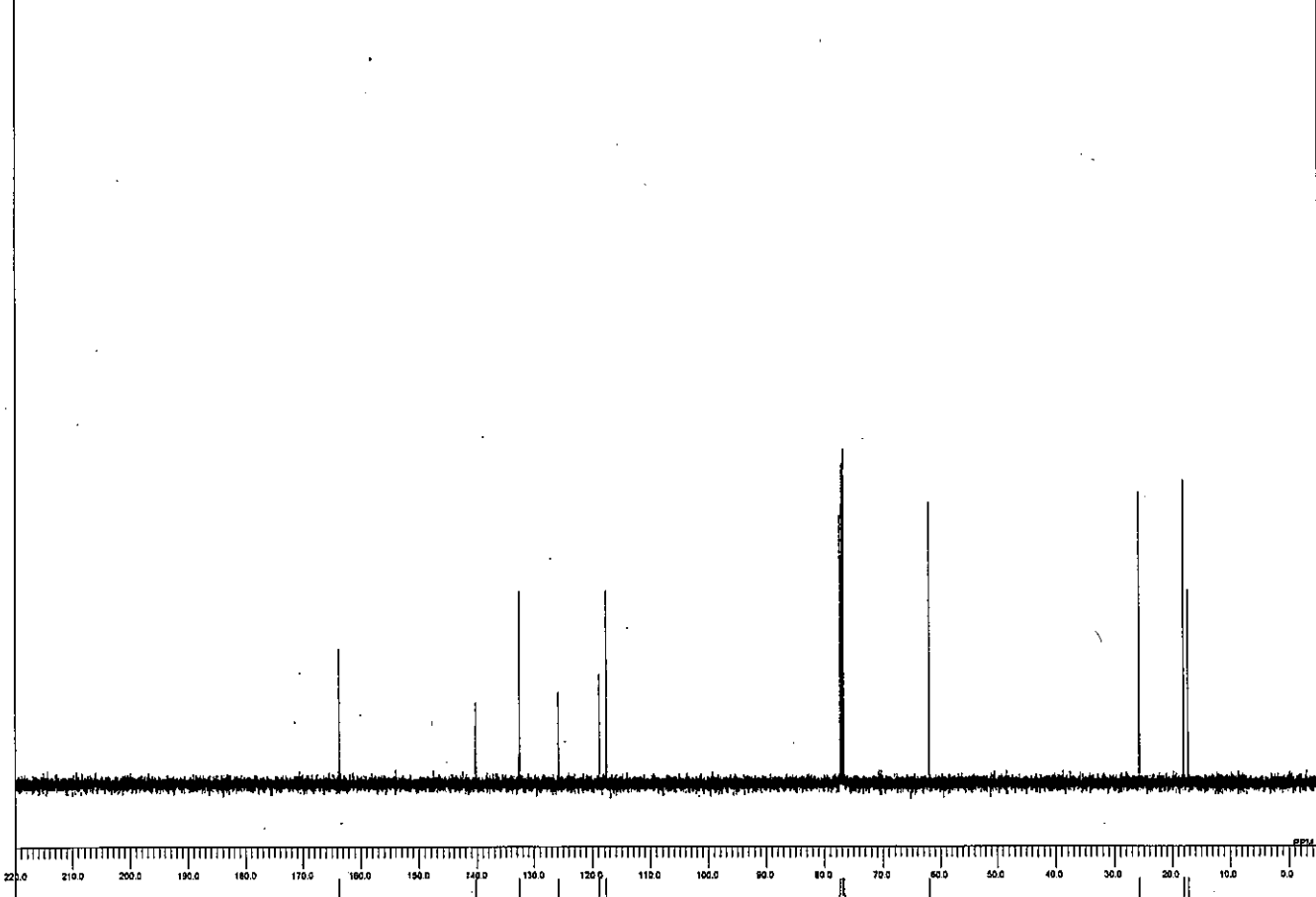
(E)-21

DFILE gdn-181221-P40-9_Proton-1-
 COUNT single_pulse
 DATUM 2016-12-21 17:04:28
 OBNUC 1H
 EXMODE proton3d
 OBPRO 399.76 MHz
 OBSET 4.18 KHz
 OBPN 7.28 Hz
 POINT 13157
 FREQU 6002.40 Hz
 SCANS 8
 ACQTM 2.1837 sec
 PD 5.0000 sec
 PWT 9.05 usec
 RVUC 1H
 CTEMP 18.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.12 Hz
 RGAIN 44

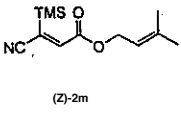


7.26
 6.427
 6.416
 6.415
 6.415
 5.378
 5.374
 5.370
 5.365
 5.365
 5.359
 5.359
 5.348
 5.348
 5.340
 5.337
 5.330
 5.330
 4.898
 4.898
 2.34
 2.35
 1.961
 1.777
 1.771
 1.577
 1.580
 0.000

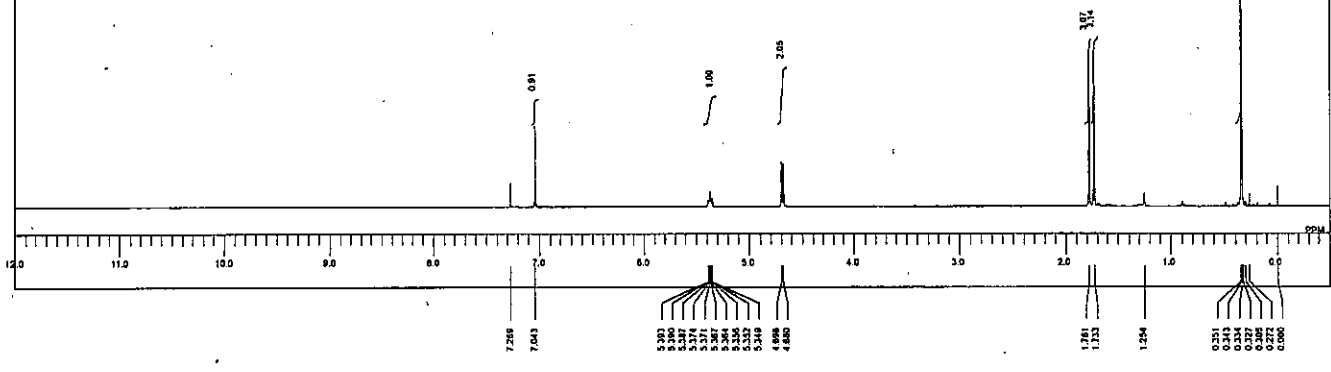
DFILE gdn-181227-gm1HCN_Car
 COMNT single pulse decoupled gated f
 DATUM 2016-12-27 15:00:07
 OBNUC 13C
 EXMODE carbon1p
 OBPRO 100.63 MHz
 OBSET 5.35 KHz
 OBPN 5.66 Hz
 POINT 2614
 FREQU 25252.53 Hz
 SCANS 108
 ACQTM 1.0281 sec
 PD 2.0000 sec
 PWT 3.33 usec
 RVUC 1H
 CTEMP 18.3 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.12 Hz
 RGAIN 80



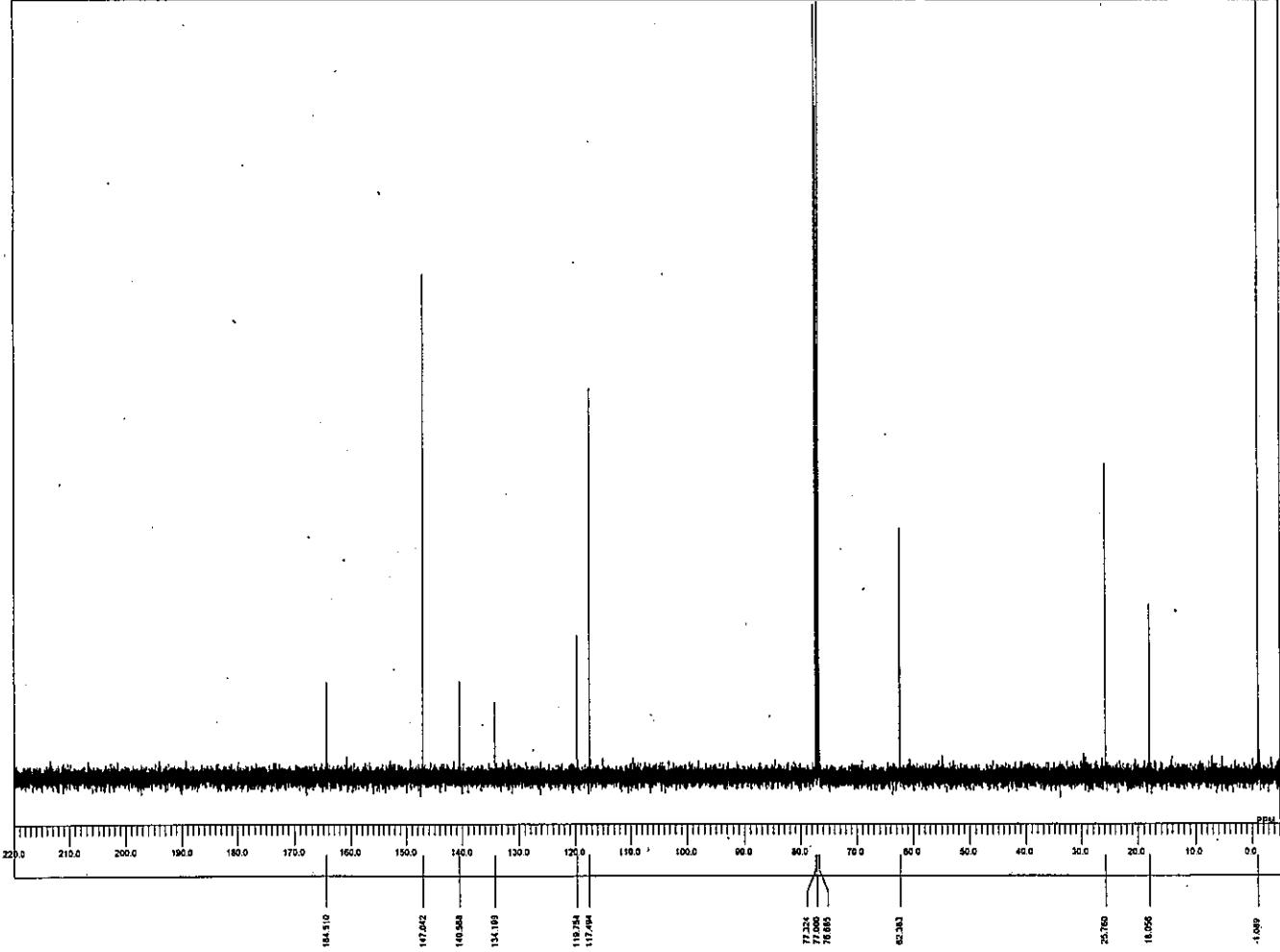
143.611
 140.335
 132.607
 122.463
 119.846
 117.031
 77.000
 76.004
 61.993
 25.741
 18.037
 17.232



OF1E gln-190214-TMSPre-CN_Pr
COMINT sample_1466
DATM 2018-02-14 19:55:07
OBNUC 1H
EZMOD proton [ppm]
OSPRQ 300.78 MHz
OBSET 4.19 KHz
OBPN 7.29 Hz
POINT 13107
FREQU 5992.20 Hz
SCANS 8
ACQTM 2.1863 sec
PD 5.0000 sec
PWI 5.60 usec
IRNUC 1H
CTEMP 16.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 45



OF1E gln-190214-TMSPre-CN_Ca
COMINT single pulse decoupled gated 1
DATM 2018-02-14 17:08:40
OBNUC 13C
EZMOD carbon [ppm]
OSPRQ 100.63 MHz
OBSET 5.35 KHz
OBPN 5.96 Hz
POINT 26214
FREQU 25125.83 Hz
SCANS 204
ACQTM 1.0433 sec
PD 3.0000 sec
PWI 3.10 usec
IRNUC 1H
CTEMP 20.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50



Calculation details

All calculations were performed with Gaussian 16 program. We used M06 as functionals and SDD (for Ni) and 6-31G** (for others) as basis sets. Single point energy was corrected using SDD (for Ni) and 6-311++G** (for others) basis sets in toluene (SMD). Structure optimizations were carried out at 298.15 K in gas phase. Harmonic vibrational frequencies were computed at the same level of theory to confirm no imaginary vibration was observed for the optimized structure, and only one imaginary vibration was observed for the transition state. The intrinsic reaction coordinate (IRC) method was used to track minimum energy paths from transition structures to the corresponding local minima.

Geometry of the calculation

```
SM_NiL2_HCN.log
Charge = 0, Spin = 1
Ni -0.223054 0.292569 -1.214397
H 1.283759 1.627018 -3.189715
P 1.396484 0.327975 0.120879
P -2.010133 -0.498727 -0.355099
O 1.312438 -0.415959 1.569528
O 2.829581 -0.266839 -0.462215
O 1.955222 1.782407 0.660193
O -3.398465 -0.079801 -1.088914
O -2.300624 -0.064973 1.221990
O -2.303128 -2.109938 -0.183047
C 0.402477 1.146360 -2.776426
N -0.755811 0.853613 -2.988703
C -1.942729 1.207539 1.614908
C -1.148523 1.336936 2.750262
C -2.380696 2.331466 0.916767
C -0.789219 2.605556 3.189264
H -0.814359 0.438179 3.263732
C -2.012357 3.596154 1.368540
H -3.013877 2.213735 0.039356
C -1.216353 3.738509 2.500725
H -0.171132 2.709302 4.078855
H -2.357514 4.475408 0.828991
H -0.932721 4.728556 2.848455
C -4.686418 -0.091986 -0.586047
C -5.534005 0.888222 -1.093150
C -5.142079 -1.025056 0.339859
C -6.854662 0.939184 -0.665346
H -5.138551 1.589321 -1.824378
C -6.465811 -0.955953 0.762706
H -4.474024 -1.792167 0.717468
C -7.325170 0.018784 0.266772
H -7.517947 1.703303 -1.063958
H -6.827017 -1.681225 1.488282
H -8.358081 0.059489 0.603329
C -1.277412 -2.983273 0.119762
C -0.594971 -2.893612 1.328001
C -0.987400 -3.986603 -0.799383
C 0.401135 -3.824018 1.611521
H -0.847174 -2.100616 2.027392
C 0.000560 -4.917490 -0.498191
H -1.543912 -4.019747 -1.732676
C 0.701272 -4.836053 0.703769
H 0.941726 -3.754028 2.553261
H 0.226395 -5.710015 -1.208671
H 1.475245 -5.564022 0.934129
C 2.386643 -0.546724 2.435538
C 2.588160 0.411846 3.420782
C 3.201195 -1.668982 2.337803
C 3.624240 0.234237 4.331290
H 1.935674 1.281524 3.447545
C 4.234342 -1.833612 3.253801
H 3.013249 -2.393382 1.547544
C 4.446862 -0.885999 4.251297
H 3.790683 0.978481 5.106600
H 4.878417 -2.707151 3.185086
H 5.255547 -1.019507 4.965657
C 2.194675 2.737254 -0.312629
C 1.169389 3.599656 -0.683374
C 3.451191 2.811835 -0.904221
C 1.407456 4.549380 -1.671338
H 0.200178 3.499733 -0.198149
C 3.677154 3.765989 -1.892105
H 4.226743 2.121855 -4.9581289
C 2.657338 4.631626 -2.280373
H 0.608758 5.223612 -1.971139
H 4.657188 3.833867 -2.359129
H 2.838262 5.373905 -3.053947
C 2.794461 -1.034193 -1.609199
C 2.067793 -2.219331 -1.649902
C 3.505844 -0.588916 -2.717649
C 2.038270 -2.953459 -2.831687
H 1.527325 -2.560941 -0.766956
C 3.477869 -1.338188 -3.888286
H 4.055073 0.347939 -2.648035
C 2.739628 -2.517803 -3.951101
H 1.459286 -3.873947 -2.867241
H 4.029740 -0.993531 -4.759746
H 2.712880 -3.095750 -4.871358
C -1.784700 0.808327 1.996146
C -0.970754 0.496613 3.079599
C -1.872155 2.114826 1.518629
C -0.222941 1.503391 3.679313
H -0.916748 -0.534513 3.421029
C -1.106528 3.110675 2.119811
H -2.533309 2.347788 0.685324
C -0.277627 2.808645 3.195367
H 0.414457 1.262593 4.527684
H -1.164517 4.127980 1.738613
H 0.320359 3.588582 3.659676
C -4.833718 0.391731 -0.259535
C -5.488497 1.615045 -0.346657
C -5.429353 -0.703393 0.356503
C -6.761377 1.746158 0.195429
H -4.986030 2.440894 -0.845580
C -6.700988 -0.554213 0.900367
H -4.901020 -1.651303 0.404783
C -7.370533 0.663145 0.822498
H -7.277490 2.701004 0.127933
H -7.172813 -1.404428 1.387648
H -8.365228 0.767019 1.248782
C -1.632489 -2.879353 -0.435638
C -0.741414 -2.980122 0.627542
C -1.554176 -3.746516 -1.521332
C 0.247526 -3.959053 0.592757
H -0.818791 -2.293526 1.466711
C -0.567632 -4.726247 -1.540459
H -2.270105 -3.636565 -2.332112
C 0.339590 -4.832465 -0.487222
H 0.950099 -4.032216 1.420694
H -0.505329 -5.408655 -2.385338
H 1.111193 -5.598238 -0.506571
C 2.701464 -1.327709 2.038234
C 3.128199 -0.707371 3.205534
C 3.380556 -2.418894 1.507761
C 4.254757 -1.197468 3.856683
H 2.571880 0.150936 3.574649
C 4.506497 -2.898770 2.168232
H 3.016716 -2.871779 0.587701
C 4.944590 -2.291988 3.341817
H 4.596620 -0.719021 4.771518
H 5.044712 -3.751515 1.760993
H 5.824662 -2.671378 3.855272
C 2.815750 2.389021 0.116023
C 1.896785 3.341659 -0.310331
C 4.148927 2.445188 -0.276246
C 2.321030 4.357205 -1.161966
TS1.log
Charge = 0, Spin = 1
Imaginary frequency: -136.894
Ni -0.355263 0.504684 -0.742935
H -0.001048 1.004720 -2.750001
P 1.502454 0.179649 0.198175
P -2.225100 -0.338582 -0.255748
O 1.536231 -0.891788 1.427855
O 2.673702 -0.444020 -0.808326
O 2.409804 1.349307 0.934329
O -3.586989 0.326369 -0.855695
O -2.481970 -0.217141 1.384243
O -2.633202 -1.929506 -0.443425
C -0.564182 1.809241 -2.261709
N -1.082051 2.829878 -2.002594
```

H 0.861615 3.269001 0.017838
C 4.565568 3.477567 -1.110198
H 4.830390 1.673274 0.072409
C 3.652377 4.428537 -1.561771
H 1.599973 5.092033 -1.512576
H 5.607569 3.532976 -1.417065
H 3.980299 5.226880 -2.223151
C 2.272945 -0.638027 -2.115015
C 1.474704 -1.732507 -2.438047
C 2.654177 0.287208 -3.082267
C 1.048253 -1.895765 -3.753150
H 1.191315 -2.440346 -1.658219
C 2.226709 0.108546 -4.395117
H 3.262873 1.140233 -2.784190
C 1.420119 -0.977650 -4.732090
H 0.417505 -2.745677 -4.004848
H 2.518308 0.827850 -5.156778
H 1.083919 -1.107978 -5.757708

CP_cis.log

Charge = 0, Spin = 1

Ni 0.206512 0.225819 1.332832
H -0.901496 0.763740 2.124237
P -1.340016 0.281740 -0.104930
P 2.010331 -0.466432 0.347887
O -1.103063 -0.365861 -1.573477
O -2.744133 -0.410487 0.363649
O -1.875968 1.748223 -0.573964
O 3.367359 0.005889 1.071899
O 2.212448 0.054176 -1.204105
O 2.348003 -2.044702 0.123248
C 0.977147 0.508107 2.990462
N 1.479251 0.705875 4.028737
C 1.773407 1.321131 -1.533054
C 1.195772 1.484556 -2.787587
C 1.909366 2.399721 -0.660312
C 0.742858 2.740678 -3.169399
H 1.097441 0.616968 -3.436430
C 1.434212 3.649732 -1.052489
H 2.391969 2.273926 0.308332
C 0.849783 3.825213 -2.300789
H 0.297545 2.871877 -4.153657
H 1.537309 4.492875 -0.372950
H 0.486886 4.804461 -2.601365
C 4.631245 0.148993 0.518737
C 5.369279 1.231026 0.983273
C 5.156520 -0.744839 -0.406686
C 6.659203 1.425842 0.505559
H 4.920716 1.890712 1.722044
C 6.447467 -0.531071 -0.879545
H 4.568555 -1.593349 -0.743020
C 7.200866 0.548030 -0.429177
H 7.243116 2.268129 0.868647
H 6.867490 -1.223594 -1.605192
H 8.210076 0.702332 -0.802574
C 1.352668 -2.961487 -0.176803
C 0.710451 -2.929064 -1.408635
C 1.073169 -3.944517 0.765356
C -0.233214 -3.910970 -1.698455
H 0.955079 -2.145607 -2.121872
C 0.134682 -4.923767 0.458676
H 1.597601 -3.926616 1.717400

C -0.522185 -4.907945 -0.770282
H -0.738080 -3.895957 -2.661992
H -0.083628 -5.704117 1.184399
H -1.253582 -5.676720 -1.006612
C -2.112985 -0.513059 -2.517793
C -2.303098 0.478484 -3.471416
C -2.868890 -1.679055 -2.517924
C -3.269081 0.287257 -4.453850
H -1.695566 1.379074 -3.422655
C -3.831200 -1.856422 -3.505784
H -2.693802 -2.426189 -1.746429
C -4.031631 -0.877108 -4.474687
H -3.427206 1.055939 -5.206593
H -4.429818 -2.764146 -3.515066
H -4.784863 -1.020562 -5.245382
C -2.413473 2.605962 0.378519
C -1.571409 3.427417 1.118105
C -3.792221 2.633628 0.547438
C -2.129542 4.293388 2.052526
H -0.496086 3.370828 0.957128
C -4.337307 3.509097 1.481268
H -4.411013 1.971223 -0.052588
C -3.508823 4.335934 2.235403
H -1.479569 4.932920 2.644224
H -5.415356 3.543049 1.620040
H -3.938723 5.014445 2.967957
C -2.746889 -1.161771 1.532436
C -2.086819 -2.382399 1.570706
C -3.407963 -0.651381 2.641110
C -2.080269 -3.102323 2.761619
H -1.580439 -2.758080 0.681368
C -3.401876 -1.386885 3.820564
H -3.889526 0.321795 2.567277
C -2.735931 -2.608568 3.884554
H -1.554373 -4.053628 2.804794
H -3.906015 -0.994549 4.700076
H -2.723382 -3.172172 4.813776

CP_trans.log

Charge = 0, Spin = 1

Ni -0.312665 0.711102 -0.671181
H -0.195801 -0.399789 0.312375
C -0.460870 2.068281 -1.962490
N -0.538159 2.886844 -2.795385
P 1.791648 0.708803 -0.491637
O 2.529372 -0.376585 -1.466320
O 2.465791 0.366986 0.956402
O 2.584040 2.074309 -0.809722
C 1.782248 -1.382189 -2.068532
C 2.773182 -0.924305 1.345287
C 3.965691 2.166548 -0.657031
C 2.042953 -2.697234 -1.703386
C 0.834184 -1.065734 -3.036659
C 4.059486 -1.393698 1.098172
C 1.826517 -1.702953 1.999818
C 4.479466 2.654001 0.537411
C 4.791167 1.802731 -1.712439
C 1.340917 -3.719880 -2.333539
H 2.788595 -2.897287 -0.935623
C 0.123059 -2.100082 -3.639926
H 0.662519 -0.027037 -3.313725
C 4.403321 -2.673956 1.515949

H 4.763295 -0.743720 0.580785
C 2.185433 -2.984522 2.409366
H 0.827833 -1.306382 2.178612
C 5.857426 2.773943 0.676362
H 3.794286 2.923440 1.336704
C 6.168514 1.926627 -1.558916
H 4.347268 1.433164 -2.632353
C 0.377033 -3.425341 -3.295694
H 1.547698 -4.754376 -2.067244
H -0.622566 -1.862257 -4.394382
C 3.466165 -3.472353 2.169608
H 5.407276 -3.048699 1.331164
H 1.449009 -3.601532 2.919229
C 6.703291 2.408327 -0.367726
H 6.271707 3.153772 1.607199
H 6.825568 1.646707 -2.378765
H -0.171850 -4.228768 -3.780655
H 3.737991 -4.472847 2.497371
H 7.780337 2.503711 -0.254042
P -2.352196 0.330545 -0.288228
O -2.714601 0.828167 1.233218
O -2.946978 -1.186719 -0.259472
O -3.479834 1.021335 -1.202023
C -1.744240 1.586783 1.877665
C -2.330302 -2.156708 0.516283
C -4.836135 1.017197 -0.884199
C -1.183703 1.080796 3.043639
C -1.345746 2.810546 1.349710
C -2.726973 -2.323505 1.837527
C -1.352742 -2.959239 -0.058916
C -5.648236 0.005206 -1.376409
C -5.349193 2.067172 -0.134990
C -0.199686 1.818180 3.692327
H -1.516698 0.112761 3.412469
C -0.345617 3.529610 1.999581
H -1.801078 3.185811 0.434572
C -2.134876 -3.330850 2.594389
H -3.496790 -1.673536 2.245632
C -0.767063 -3.958201 0.709389
H -1.057492 -2.790159 -1.093597
C -7.011549 0.050176 -1.105508
H -5.204505 -0.794970 -1.961930
C -6.713845 2.099128 0.128819
H -4.678222 2.844031 0.223010
C 0.224231 3.038352 3.169853
H 0.247181 1.430398 4.604639
H -0.017546 4.478576 1.583299
C -1.160287 -4.150609 2.031885
H -2.445487 -3.480020 3.625860
H 0.009145 -4.581277 0.268934
C -7.545709 1.093140 -0.354247
H -7.659574 -0.734988 -1.487478
H -7.127978 2.917742 0.712320
H 1.000230 3.606189 3.677045
H -0.709032 -4.943972 2.624249
H -8.612732 1.124086 -0.148217

SM_Alkyne.log

Charge = 0, Spin = 1

Imaginary frequency: -36.7185

C 1.997642 -0.064291 0.001671

C 0.800614 0.101211 0.000798
C 3.432563 -0.265184 0.000277
H 3.926520 0.425152 0.692476
H 3.693621 -1.287679 0.292807
H 3.846183 -0.085026 -0.998068
C -0.617682 0.365787 0.000128
O -1.116164 1.466056 -0.000273
O -1.318550 -0.780607 0.000043
C -2.732861 -0.606876 -0.000273
H -3.158463 -1.610701 -0.000824
H -3.056127 -0.055044 0.887664
H -3.055674 -0.054176 -0.887813

SM_TS2a.log

Charge = 0, Spin = 1

C 1.933607 -1.915922 0.127229
C 1.295639 -2.636413 -0.645252
Ni 0.400468 -0.596549 -0.560397
H 0.627494 -0.231702 0.837482
P -1.625813 -0.808858 0.252425
P 1.136374 1.365579 -0.868145
O -2.500665 0.514651 -0.104974
O -2.716640 -2.030545 0.012198
O -1.767988 -0.801061 1.888538
O -0.006428 2.291401 -1.536172
O 2.374934 1.591546 -1.901877
O 1.725666 2.290033 0.352890
C 0.140541 -0.735872 -2.438122
N 0.057347 -0.825154 -3.602987
C 0.719705 -3.645333 -1.516067
H -0.309353 -3.885514 -1.213435
H 0.668259 -3.266981 -2.544297
H 1.321755 -4.560286 -1.487211
C 2.936355 -1.548312 1.114651
O 3.732413 -2.602182 1.358022
O 3.058771 -0.473592 1.654817
C 4.758194 -2.354684 2.312284
H 5.423486 -1.556437 1.965810
H 4.327653 -2.056575 3.274340
H 5.308404 -3.290908 2.413176
C -0.831118 -1.523268 2.606388
C -0.708100 -2.900088 2.441562
C -0.008484 -0.825738 3.481898
C 0.269082 -3.580699 3.161396
H -1.373261 -3.420900 1.755679
C 0.961560 -1.518057 4.196822
H -0.128808 0.251516 3.573637
C 1.105911 -2.894315 4.037314
H 0.375255 -4.655673 3.035596
H 1.618248 -0.969477 4.869311
H 1.868011 -3.432949 4.596005
C -3.803217 0.717476 0.337326
C -4.015203 1.351683 1.554544
C -4.859980 0.337755 -0.479218
C -5.319889 1.613920 1.957528
H -3.155840 1.615652 2.166630
C -6.159806 0.605085 -0.063798
H -4.652087 -0.158843 -1.424328
C -6.392307 1.243288 1.151220
H -5.498610 2.109334 2.908971
H -6.994945 0.311870 -0.695307
H -7.410582 1.451070 1.470504

C -2.788628 -2.774593 -1.145758
C -3.011850 -4.142113 -0.997328
C -2.663218 -2.200877 -2.404929
C -3.083887 -4.945343 -2.129183
H -3.130025 -4.550438 0.003958
C -2.712059 -3.020839 -3.528316
H -2.481349 -1.134342 -2.514186
C -2.923249 -4.388878 -3.396846
H -3.259032 -6.013034 -2.018463
H -2.566136 -2.574312 -4.508538
H -2.963850 -5.022168 -4.279472
C -0.047284 3.670071 -1.650889
C 1.078180 4.442815 -1.909985
C -1.307915 4.243375 -1.521727
C 0.924590 5.820289 -2.032531
H 2.049866 3.971451 -2.022081
C -1.443848 5.619583 -1.653396
H -2.158061 3.592136 -1.326749
C -0.327923 6.412505 -1.906508
H 1.798859 6.434504 -2.235208
H -2.427652 6.072703 -1.557112
H -0.434843 7.489549 -2.008230
C 3.401008 0.649196 -1.915863
C 4.394774 0.708472 -0.947522
C 3.409108 -0.311269 -2.919559
C 5.420144 -0.231797 -0.981806
H 4.343072 1.474697 -0.177782
C 4.439716 -1.245030 -2.938556
H 2.596147 -0.329367 -3.641485
C 5.441851 -1.210784 -1.971509
H 6.208032 -0.192946 -0.232148
H 4.455760 -2.006476 -3.714696
H 6.244340 -1.944315 -1.993287
C 1.117326 2.405182 1.583450
C 1.940636 2.314273 2.701951
C -0.243354 2.672866 1.712524
C 1.400994 2.525299 3.963899
H 2.988808 2.069244 2.556833
C -0.769329 2.880559 2.985650
H -0.878965 2.737106 0.830737
C 0.045364 2.814959 4.111304
H 2.044188 2.462786 4.838804
H -1.826015 3.118107 3.091772
H -0.373472 2.987988 5.099433

SM_TS2b.log

Charge = 0, Spin = 1

C -0.352124 -1.964407 -2.063693
C -0.338011 -2.562815 -1.008192
Ni -0.372313 0.113435 0.116988
H -0.196506 0.831348 -1.174892
P 1.742568 0.113543 -0.111509
P -2.311463 0.907679 -0.170777
O 2.282903 1.559435 0.406716
O 2.810699 -0.947355 0.499943
O 2.265279 0.020462 -1.649623
O -3.376273 0.710712 1.032833
O -3.172392 0.552522 -1.503275
O -2.262907 2.523809 -0.415608
C -0.643026 -0.629915 1.824755
N -0.838996 -1.051471 2.899588
C -0.364796 -1.255247 -3.326849

H -1.248453 -0.608370 -3.388941
H 0.528823 -0.628608 -3.425871
H -0.397344 -1.959070 -4.165688
C -0.501954 -3.304136 0.227054
O -1.563985 -3.761990 0.585226
O 0.648090 -3.412499 0.891156
C 0.534814 -3.997948 2.196152
H 1.555033 -4.050033 2.580412
H -0.080418 -3.347222 2.826959
H 0.086983 -4.993519 2.128369
C -3.984995 -0.576070 -1.579573
C -3.649990 -1.771018 -0.956532
C -5.153082 -0.443894 -2.319125
C -4.510187 -2.856958 -1.080208
H -2.744949 -1.871696 -0.361552
C -6.001290 -1.538459 -2.436269
H -5.385024 0.516624 -2.772132
C -5.684348 -2.745790 -1.817609
H -4.237357 -3.787605 -0.588520
H -6.920507 -1.442688 -3.009441
H -6.353820 -3.597400 -1.910417
C -4.747678 0.927271 0.941265
C -5.563910 -0.092937 1.413609
C -5.275853 2.102163 0.420287
C -6.942422 0.061411 1.346413
H -5.100344 -0.992636 1.809949
C -6.659714 2.237808 0.354626
H -4.613938 2.886868 0.065319
C -7.493935 1.223012 0.811370
H -7.588276 -0.734777 1.708456
H -7.085465 3.150446 -0.056089
H -8.573556 1.338426 0.755094
C -1.202105 3.225699 0.141285
C -0.496033 4.085035 -0.690728
C -0.875620 3.084937 1.486671
C 0.561763 4.816453 -0.161826
H -0.789099 4.165704 -1.734330
C 0.200898 3.806300 1.994535
H -1.451226 2.418223 2.126384
C 0.919420 4.671351 1.176421
H 1.115558 5.499486 -0.802792
H 0.471656 3.689681 0.304095
H 1.758511 5.233140 1.579284
C 3.530022 2.062338 0.068944
C 3.589520 3.041470 -0.916083
C 4.671119 1.619498 0.725386
C 4.823899 3.585226 -1.254044
H 2.662615 3.354485 -1.392786
C 5.900693 2.167736 0.372578
H 4.587040 0.860926 1.500355
C 5.981132 3.145636 -0.614484
H 4.882118 4.353461 -2.021638
H 6.801589 1.826695 0.876743
H 6.945504 3.570524 -0.881813
C 3.340580 -0.720961 -2.130312
C 3.246109 -2.106254 -2.205363
C 4.455569 -0.041925 -2.599976
C 4.301110 -2.820839 -2.760748
H 2.356978 -2.603577 -1.820729
C 5.500842 -0.770910 -3.158899
H 4.492274 1.042222 -2.519589
C 5.428310 -2.157688 -3.239586

H 4.238305 -3.904847 -2.821421
H 6.378236 -0.246628 -3.530161
H 6.248893 -2.722471 -3.675164
C 2.969556 -1.376840 1.799710
C 2.425219 -0.718385 2.894611
C 3.766018 -2.507795 1.953019
C 2.661083 -1.234635 4.165933
H 1.796018 0.158608 2.764723
C 4.011457 -2.995094 3.230131
H 4.170080 -2.981435 1.061100
C 3.453396 -2.363578 4.340684
H 2.209441 -0.743575 5.023988
H 4.636010 -3.876418 3.357079
H 3.635731 -2.752365 5.339305

TS2a.log

Charge = 0, Spin = 1

Imaginary frequency: -406.7058
C 2.131808 1.562637 -0.068878
C 1.588602 2.264667 0.814942
Ni 0.563974 0.491280 0.655439
H 1.014185 0.306062 -0.731852
P -1.484795 0.991455 -0.238262
P 0.834028 -1.612940 0.840404
O -2.544354 -0.220175 0.006171
O -2.416505 2.328953 0.067450
O -1.575536 1.103058 -1.878959
O -0.441223 -2.394072 1.444193
O 2.010948 -2.067812 1.873107
O 1.309404 -2.543948 -0.424764
C 0.235801 0.538494 2.522194
N 0.114625 0.555110 3.686752
C 1.302810 3.348514 1.744728
H 0.305204 3.767349 1.548671
H 1.280547 2.959570 2.769909
H 2.050676 4.144593 1.660523
C 3.187162 1.272308 -1.030841
O 4.056776 2.294215 -1.069775
O 3.289302 0.270502 -1.701762
C 5.127065 2.121309 -1.990249
H 5.723971 1.241044 -1.729448
H 4.743421 1.993698 -3.008487
H 5.733135 3.025454 -1.921934
C -0.557087 1.807319 -2.500093
C -0.430463 3.182765 -2.324202
C 0.338741 1.096322 -3.287980
C 0.627170 3.845649 -2.939637
H -1.157596 3.712605 -1.713618
C 1.393079 1.769754 -3.893894
H 0.207667 0.022947 -3.399958
C 1.543051 3.143319 -3.719162
H 0.735375 4.919618 -2.806791
H 2.108461 1.205290 -4.489250
H 2.369925 3.668237 -4.192262
C -3.866529 -0.192744 -0.420031
C -4.181820 -0.630337 -1.699932
C -4.849754 0.213186 0.472659
C -5.516835 -0.665267 -2.088094
H -3.376762 -0.922387 -2.369912
C -6.180367 0.173855 0.071580
H -4.560696 0.552633 1.464843
C -6.516516 -0.266034 -1.205674

H -5.776039 -1.005536 -3.087938
H -6.958070 0.489468 0.762848
H -7.558612 -0.296452 -1.514095
C -2.358772 3.028540 1.253566
C -2.361550 4.419063 1.165282
C -2.324578 2.389989 2.487030
C -2.309789 5.174809 2.330653
H -2.414128 4.885262 0.183997
C -2.246765 3.158120 3.645002
H -2.314476 1.303953 2.548608
C -2.242743 4.546761 3.572909
H -2.315280 6.260489 2.266008
H -2.174321 2.652429 4.604456
H -2.187303 5.140306 4.481960
C -0.684560 -3.758060 1.444109
C 0.301214 -4.696835 1.723347
C -1.995764 -4.137576 1.179943
C -0.045238 -6.044236 1.724110
H 1.314525 -4.373685 1.942666
C -2.325675 -5.487360 1.191132
H -2.733612 -3.363224 0.978707
C -1.351232 -6.444413 1.459696
H 0.718569 -6.787565 1.940059
H -3.350067 -5.790405 0.988286
H -1.609997 -7.500247 1.466278
C 3.184000 -1.314143 1.866974
C 4.106646 -1.494935 0.844923
C 3.398623 -0.405732 2.896799
C 5.271920 -0.734222 0.849580
H 3.896375 -2.214462 0.057720
C 4.567637 0.347593 2.886415
H 2.635101 -0.283091 3.661229
C 5.502088 0.189699 1.864320
H 5.999978 -0.868528 0.052180
H 4.746056 1.066825 3.682326
H 6.412534 0.784646 1.863141
C 0.773911 -2.437759 -1.690766
C 1.671867 -2.327503 -2.748014
C -0.598208 -2.510639 -1.913275
C 1.189280 -2.323757 -4.050562
H 2.731168 -2.231644 -2.526963
C -1.066616 -2.497117 -3.224954
H -1.286860 -2.594363 -1.073584
C -0.180269 -2.413487 -4.294243
H 1.887815 -2.244268 -4.880441
H -2.136354 -2.573998 -3.408734
H -0.555197 -2.412827 -5.314574

TS2b.log

Charge = 0, Spin = 1

Imaginary frequency: -404.6588
C 0.238731 -1.275747 -2.786380
C -0.056463 -2.161312 -1.956904
Ni -0.591966 -0.467710 -1.007750
H -0.058276 0.368910 -2.099291
P 1.455300 0.070271 0.049178
P -2.051732 1.051587 -0.779072
O 1.515065 1.555577 0.744282
O 2.336867 -0.841304 1.092958
O 2.647126 0.211443 -1.083127
O -2.144300 1.504724 0.780173
O -3.575616 0.766781 -1.236183

O -1.974723 2.472513 -1.588189
C -1.499191 -1.442846 0.329839
N -2.073119 -2.008903 1.179085
C 0.795637 -0.712629 -4.021941
H 0.038599 -0.141864 -4.571635
H 1.631639 -0.039840 -3.793302
H 1.157067 -1.520782 -4.666585
C -0.319904 -3.448612 -1.322643
O -1.199510 -4.199561 -1.665465
O 0.525000 -3.642915 -0.307307
C 0.147781 -4.683709 0.599513
H 0.953646 -4.740564 1.333270
H -0.791090 -4.399469 1.089455
H 0.024451 -5.633765 0.072127
C -4.153404 -0.502114 -1.175083
C -3.731476 -1.500977 -2.041017
C -5.171627 -0.708265 -0.256856
C -4.319681 -2.757702 -1.951499
H -2.934899 -1.299414 -2.754399
C -5.764441 -1.963956 -0.192311
H -5.472641 0.105998 0.398555
C -5.334294 -2.989935 -1.028724
H -3.965391 -3.558418 -2.595011
H -6.559482 -2.143378 0.527386
H -5.788916 -3.974899 -0.958940
C -3.321567 1.793066 1.456728
C -3.687569 0.935099 2.485757
C -4.077972 2.909742 1.125283
C -4.841474 1.216651 3.209182
H -3.080392 0.050034 2.670424
C -5.234043 3.172702 1.853663
H -3.766842 3.546753 0.300225
C -5.614891 2.332427 2.896286
H -5.142457 0.552889 4.016141
H -5.839425 4.040428 1.602702
H -6.517806 2.545258 3.463378
C -0.803332 3.204844 -1.620734
C -0.016360 3.147727 -2.765511
C -0.467542 4.029196 -0.552317
C 1.118303 3.948878 -2.849692
H -0.323932 2.500348 -3.583785
C 0.663971 4.829912 -0.650982
H -1.095060 4.036106 0.335497
C 1.451952 4.798854 -1.799293
H 1.733201 3.918663 -3.746003
H 0.935438 5.479386 0.177796
H 2.332653 5.433342 -1.870509
C 2.702860 2.092647 1.217596
C 3.429116 2.945755 0.395111
C 3.133946 1.787204 2.502975
C 4.604019 3.513566 0.877066
H 3.059053 3.141535 -0.608184
C 4.314964 2.354003 2.970096
H 2.543571 1.110506 3.116932
C 5.050744 3.216947 2.162301
H 5.175990 4.185995 0.241418
H 4.661364 2.117931 3.973401
H 5.971243 3.659362 2.535338
C 3.772340 -0.597222 -1.139423
C 3.669123 -1.873792 -1.679623
C 4.986960 -0.103651 -0.680798
C 4.809158 -2.664665 -1.772109

H 2.694077 -2.234497 -2.003770
C 6.120630 -0.902643 -0.784595
H 5.026048 0.891316 -0.241442
C 6.037066 -2.180967 -1.329407
H 4.734533 -3.665745 -2.190560
H 7.075897 -0.523171 -0.429141
H 6.926808 -2.801402 -1.404399
C 1.838857 -1.628158 2.105557
C 0.660543 -1.332700 2.779345
C 2.619650 -2.725755 2.457526
C 0.243520 -2.181155 3.801462
H 0.053191 -0.475027 2.492305
C 2.205405 -3.544964 3.499614
H 3.536920 -2.909577 1.902068
C 1.011375 -3.279857 4.169581
H -0.699198 -1.975940 4.302670
H 2.814712 -4.399790 3.785043
H 0.681267 -3.930275 4.975652

INT1a.log

Charge = 0, Spin = 1

C 2.414156 2.061988 -0.273940
C 2.016739 1.222670 -1.246258
Ni 0.182664 0.721377 -1.018645
H 1.707028 2.363318 0.500779
P 0.847125 -0.996279 0.106814
P -1.967462 0.543749 -0.572344
O -0.368225 -1.807860 0.816628
O 1.576549 -2.151552 -0.795304
O 1.863523 -0.943891 1.363633
O -2.663478 -0.858596 -0.986121
O -3.080095 1.561091 -1.181328
O -2.290418 0.645942 1.029428
C -0.052927 2.039171 -2.303961
N -0.213688 2.835911 -3.146534
C 2.812594 0.727228 -2.406022
H 3.572794 0.009708 -2.061696
H 2.179928 0.232499 -3.150210
H 3.350556 1.549791 -2.889996
C 3.727787 2.673534 -0.051010
O 4.686494 2.238437 -0.898393
O 3.951094 3.479398 0.830645
C 5.961988 2.827364 -0.700478
H 5.913438 3.915939 -0.807600
H 6.345359 2.596786 0.299802
H 6.616940 2.399979 -1.462043
C 3.219625 -0.630524 1.368473
C 4.142209 -1.406547 0.676648
C 3.617879 0.432470 2.167798
C 5.492686 -1.081192 0.772998
H 3.803024 -2.254639 0.090174
C 4.969404 0.738913 2.260340
H 2.857550 1.024142 2.674297
C 5.909722 -0.014505 1.561643
H 6.223298 -1.679151 0.233201
H 5.281424 1.589800 2.860768
H 6.967104 0.229828 1.633794
C -0.255292 -3.093422 1.332906
C 0.246389 -3.290017 2.613221
C -0.726248 -4.148328 0.561329
C 0.279461 -4.583585 3.124653
H 0.605055 -2.436497 3.182584

C -0.688625 -5.434881 1.086863
H -1.118007 -3.942209 -0.433434
C -0.185465 -5.654132 2.366432
H 0.671499 -4.753560 4.124492
H -1.054254 -6.268571 0.492554
H -0.157039 -6.661603 2.773807
C 1.321974 -2.294577 -2.150124
C 2.398999 -2.653424 -2.951692
C 0.052841 -2.104093 -2.686069
C 2.208172 -2.788263 -4.320596
H 3.374187 -2.797136 -2.492388
C -0.117362 -2.221150 -4.063967
H -0.798029 -1.875145 -2.046436
C 0.954137 -2.558466 -4.882525
H 3.048680 -3.061200 -4.953854
H -1.102192 -2.051744 -4.491474
H 0.812598 -2.648113 -5.956247
C -3.909390 -1.241718 -0.490325
C -5.064773 -0.847439 -1.150975
C -3.947401 -2.050979 0.637715
C -6.292653 -1.284708 -0.663787
H -4.987628 -0.209382 -2.026680
C -5.181643 -2.482860 1.109796
H -3.012498 -2.326572 1.122383
C -6.353520 -2.100737 0.462049
H -7.206542 -0.985105 -1.170971
H -5.226470 -3.119358 1.990192
H -7.316446 -2.440036 0.835736
C -3.317780 2.814306 -0.618603
C -4.203287 2.906783 0.449446
C -2.692628 3.931710 -1.156265
C -4.445975 4.154684 1.011608
H -4.678604 2.003996 0.825828
C -2.948786 5.173617 -0.580244
H -2.011425 3.812637 -1.996780
C -3.815285 5.287379 0.502738
H -5.130795 4.240865 1.851853
H -2.461720 6.057067 -0.985726
H -4.004666 6.260903 0.948543
C -1.331869 1.091408 1.923253
C -0.725827 2.334738 1.767386
C -1.022169 0.264783 2.998021
C 0.232388 2.737728 2.695739
H -1.007667 2.984492 0.938011
C -0.078968 0.687963 3.925953
H -1.521045 -0.698702 3.077968
C 0.553939 1.920863 3.774880
H 0.731897 3.695306 2.565710
H 0.167905 0.047445 4.769941
H 1.296200 2.245964 4.500110

INT1b.log

Charge = 0, Spin = 1

C 1.014586 -3.307834 0.891958
C 0.652745 -2.169422 1.503233
Ni -0.603169 -0.960524 0.688427
H 0.613380 -3.470000 -0.115303
P 1.153307 -0.062028 -0.145655
P -2.296069 0.032999 -0.291765
O 0.846549 1.145261 -1.206635
O 2.282982 0.557631 0.847005
O 2.107064 -1.025359 -1.016259

O -3.591581 0.258246 0.636505
O -2.859690 -0.942832 -1.457660
O -2.242320 1.410221 -1.194535
C -1.897870 -2.102031 1.393336
N -2.762323 -2.813422 1.735640
C 1.868276 -4.416142 1.414474
H 1.327761 -5.368495 1.342910
H 2.770695 -4.522824 0.795855
H 2.179237 -4.249794 2.447278
C 1.097799 -1.799925 2.859594
O 2.136588 -2.133748 3.400021
O 0.210378 -0.972273 3.446806
C 0.488849 -0.621123 4.795625
H -0.261589 0.119975 5.075012
H 0.409862 -1.501336 5.442496
H 1.494090 -0.200643 4.890845
C -1.968390 -1.860799 -2.003994
C -0.920064 -1.412540 -2.799100
C -2.165210 -3.210239 -1.743643
C -0.034868 -2.343866 -3.334206
H -0.816964 -0.344031 -2.985175
C -1.281448 -4.129777 -2.297833
H -2.980281 -3.509105 -1.089823
C -0.215389 -3.701001 -3.087046
H 0.802867 -2.004309 -3.940428
H -1.420442 -5.189503 -2.098773
H 0.476414 -4.426671 -3.507164
C -4.906417 0.078362 0.203584
C -5.519530 -1.134875 0.482112
C -5.563695 1.116558 -0.439139
C -6.846300 -1.302120 0.101529
H -4.944128 -1.911311 0.986923
C -6.891045 0.930052 -0.813719
H -5.038655 2.048977 -0.634254
C -7.531916 -0.275249 -0.543903
H -7.347847 -2.243777 0.311791
H -7.424633 1.732567 -1.317436
H -8.569609 -0.415303 -0.837113
C -1.839681 2.626589 -0.683430
C -1.031102 3.409042 -1.503376
C -2.246616 3.086443 0.567462
C -0.606945 4.653856 -1.060734
H -0.733784 3.012716 -2.471513
C -1.821678 4.344582 0.992856
H -2.896903 2.478194 1.191201
C -0.998984 5.127034 0.190973
H 0.036630 5.256219 -1.697776
H -2.148767 4.712266 1.963451
H -0.669584 6.104490 0.534076
C 1.820605 1.703331 -2.019652
C 1.808062 1.378177 -3.371404
C 2.744216 2.601318 -1.498848
C 2.751914 1.952561 -4.216134
H 1.061120 0.677517 -3.739802
C 3.689638 3.160398 -2.352823
H 2.709341 2.856175 -0.442308
C 3.699479 2.836584 -3.706549
H 2.747543 1.705391 -5.275031
H 4.421933 3.858301 -1.954504
H 4.440405 3.280235 -4.366719
C 3.482064 -1.216903 -0.897808
C 4.036966 -1.751249 0.259780

C 4.258990 -0.916582 -2.008160
C 5.407152 -1.988479 0.289359
H 3.411595 -1.968544 1.123871
C 5.626759 -1.165781 -1.962416
H 3.782844 -0.487200 -2.887529
C 6.203772 -1.702129 -0.815955
H 5.851677 -2.404691 1.190295
H 6.241669 -0.935275 -2.829201
H 7.273228 -1.894938 -0.782086
C 2.037798 1.369157 1.938018
C 1.006865 2.301577 1.954665
C 2.927241 1.245204 2.999212
C 0.858244 3.108570 3.079752
H 0.334579 2.411238 1.104507
C 2.776748 2.074911 4.103348
H 3.708390 0.490771 2.941504
C 1.738925 3.003714 4.150723
H 0.049739 3.836229 3.098034
H 3.470377 1.986772 4.936355
H 1.621207 3.646856 5.019106

INT1a2.log

Charge = 0, Spin = 1

C -2.457442 2.021041 0.235586
C -2.062561 1.196099 1.221381
Ni -0.216516 0.730118 1.019695
H -1.744039 2.324417 -0.532442
P -0.826501 -1.021478 -0.083950
P 1.944215 0.609776 0.595571
O 0.419465 -1.794945 -0.781896
O -1.515026 -2.186503 0.838741
O -1.846776 -1.035476 -1.338253
O 2.675742 -0.757992 1.061621
O 3.008621 1.683763 1.193772
O 2.309513 0.682652 -0.998262
C -0.028280 2.051894 2.308811
N 0.097797 2.847403 3.158413
C -2.868501 0.692338 2.370109
H -3.607417 -0.042983 2.015859
H -2.238921 0.214997 3.128170
H -3.431819 1.506318 2.839307
C -3.775537 2.611105 -0.016604
O -4.738110 2.188338 0.832202
O -3.996978 3.393420 -0.919763
C -6.016264 2.762975 0.610936
H -5.976180 3.854081 0.692868
H -6.390755 2.506319 -0.386286
H -6.673759 2.348900 1.377672
C -3.202676 -0.724313 -1.351549
C -4.120115 -1.461551 -0.612481
C -3.606008 0.293832 -2.204812
C -5.471238 -1.141361 -0.716951
H -3.776235 -2.277465 0.015586
C -4.957882 0.596179 -2.303833
H -2.847495 0.851705 -2.750639
C -5.893326 -0.118384 -1.558914
H -6.198301 -1.708975 -0.140860
H -5.274981 1.412693 -2.947706
H -6.951177 0.121972 -1.637212
C 0.345702 -3.076379 -1.315634
C -0.061004 -3.254566 -2.631616
C 0.760751 -4.141405 -0.526119

C -0.057699 -4.540580 -3.161846
H -0.371521 -2.389530 -3.212114
C 0.760210 -5.420932 -1.070744
H 1.083690 -3.949332 0.495941
C 0.349975 -5.622015 -2.385796
H -0.375712 -4.696863 -4.189811
H 1.082340 -6.263098 -0.463398
H 0.350428 -6.623882 -2.807763
C -1.259687 -2.294234 2.196826
C -2.327346 -2.666233 3.005058
C 0.002990 -2.058351 2.729882
C -2.134560 -2.767232 4.376695
H -3.297669 -2.848046 2.549125
C 0.174607 -2.141641 4.110053
H 0.848477 -1.820394 2.086670
C -0.888244 -2.490976 4.934737
H -2.967969 -3.050546 5.014766
H 1.153932 -1.936183 4.534366
H -0.745807 -2.554297 6.010202
C 3.926036 -1.138155 0.574427
C 5.081216 -0.636829 1.158619
C 3.968371 -2.054952 -0.467932
C 6.312792 -1.072507 0.678545
H 5.002255 0.078798 1.971805
C 5.206261 -2.483681 -0.932968
H 3.034205 -2.420226 -0.891039
C 6.378190 -1.992771 -0.363346
H 7.226494 -0.689883 1.126844
H 5.253610 -3.203977 -1.746129
H 7.344201 -2.329739 -0.731105
C 3.184770 2.935718 0.603645
C 4.068816 3.050004 -0.463623
C 2.503273 4.031899 1.115712
C 4.251784 4.296461 -1.050967
H 4.590430 2.164598 -0.819059
C 2.699537 5.272650 0.514362
H 1.828963 3.898100 1.959274
C 3.563567 5.406792 -0.568062
H 4.935414 4.399032 -1.890347
H 2.168263 6.139117 0.900486
H 3.706402 6.379093 -1.033419
C 1.371820 1.029159 -1.952147
C 0.618803 2.194015 -1.840188
C 1.236435 0.181877 -3.046596
C -0.317307 2.488461 -2.830916
H 0.771024 2.869051 -0.996785
C 0.315767 0.499232 -4.036853
H 1.847902 -0.716796 -3.090492
C -0.468733 1.646741 -3.928033
H -0.933744 3.380304 -2.734031
H 0.206247 -0.157163 -4.897599
H -1.193820 1.887684 -4.701784

TS3.log

Charge = 0, Spin = 1

Imaginary frequency: -183.9952
C -2.527621 2.079926 0.320244
C -2.181480 1.137204 1.232991
Ni -0.370772 0.586568 0.837397
H -1.743566 2.646301 -0.184304
P -0.581802 -1.340610 -0.163567
P 1.757944 0.916263 0.545623

O 0.840919 -1.875671 -0.744866
O -1.054161 -2.592739 0.795359
O -1.507117 -1.679274 -1.463039
O 2.732931 -0.250745 1.107337
O 2.538146 2.203175 1.188676
O 2.229891 1.048076 -1.023176
C -0.736924 1.721251 2.231437
N -0.700467 2.306597 3.251982
C -3.099475 0.295226 2.057892
H -3.647065 -0.396006 1.398778
H -2.540234 -0.289930 2.793470
H -3.842384 0.906887 2.579011
C -3.860726 2.429221 -0.168522
O -4.866211 1.984838 0.616271
O -4.056660 3.069491 -1.184369
C -6.169612 2.348777 0.189051
H -6.248175 3.431093 0.046927
H -6.424716 1.856213 -0.756869
H -6.850332 2.017150 0.974984
C -2.873032 -1.422997 -1.422997
C -3.731728 -2.381429 -0.898668
C -3.348575 -0.238621 -1.972837
C -5.102203 -2.140710 -0.922470
H -3.315147 -3.299579 -0.492936
C -4.721025 -0.015529 -1.997412
H -2.642587 0.490629 -2.369433
C -5.597426 -0.961241 -1.471287
H -5.784701 -2.883033 -0.515409
H -5.093434 0.917361 -2.415789
H -6.669865 -0.779458 -1.491765
C 1.082260 -3.179620 -1.155845
C 0.744409 -3.577927 -2.443231
C 1.733585 -4.033831 -0.274513
C 1.067635 -4.868573 -2.849386
H 0.231425 -2.878047 -3.079459
C 2.052051 -5.320207 -0.695189
H 1.985023 -3.674004 0.721710
C 1.719661 -5.739019 -1.980651
H 0.807776 -5.194473 -3.853746
H 2.562322 -5.996902 -0.014218
H 1.970419 -6.745456 -2.306372
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C -0.949396 -2.320256 4.937451
H -2.859398 -3.316092 4.860053
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PD.log

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H 2.264379 0.493649 -2.050067
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H 0.056847 -2.616499 -5.237351
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4. X-ray Crystallographic Analysis

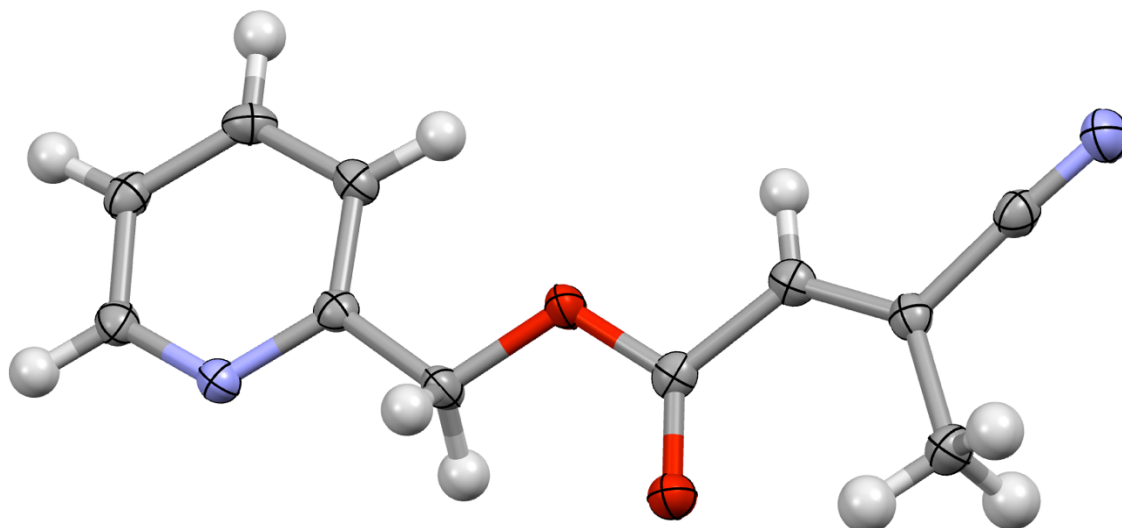


Figure S_{xray}-1. X-ray crystallographic analysis of (E)-**2k**. Ellipsoids are drawn at the 50% probability level.
CCDC 940594

Empirical Formula	C ₁₁ H ₁₀ N ₂ O ₂
Formula Weight	202.21
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.400 X 0.300 X 0.100 mm
Crystal System	monoclinic
Lattice Parameters	a = 25.8200(6) Å b = 6.09696(14) Å c = 12.7480(3) Å β = 94.7721(17) ° V = 1999.88(9) Å ³
Space Group	C2/c (#15)
Z value	8
D _{calc}	1.343 g/cm ³
F ₀₀₀	848.00
μ(CuKα)	7.81 cm ⁻¹