

Supporting Information

**Trisubstituted Alkenes Having Single Activator as Dipolarophile in
Highly Diastereo- and Enantioselective [3+2]-Cycloaddition with
Vinyl Epoxides under Pd-Catalysis**

Juan Du,^{a,d} Yang-Jie Jiang,^{a,d} Jia-Jia Suo,^{a,d} Wen-Qiong Wu,^a Xiu-Yan Liu,^a Di Chen,^a
Chang-Hua Ding,^{*a,b} Yin Wei,^{*a} and Xue-Long Hou^{*a,c}

^a State Key Laboratory of Organometallic Chemistry, Center for Excellence in Molecular Synthesis, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, China. ^b Department of Chemistry, Innovative Drug Research Center, Shanghai University, Shanghai 200444, China. ^c Shanghai–Hong Kong Joint Laboratory in Chemical Synthesis, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences. ^d University of Chinese Academy of Sciences, Beijing 100049, China.

*dingchanghua@shu.edu.cn; weiyin@sioc.ac.cn; xlhou@sioc.ac.cn

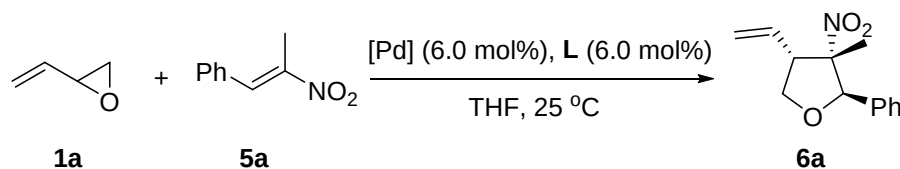
Table of Contents

1. General Methods.....	S2
2. Optimization of reaction conditions for Pd-catalyzed [3+2] cycloaddition reaction of vinyl epoxide 1a and tri-substituted nitroalkene 5a.....	S2
3. General experimental procedure for Table 2 and characterization of products.....	S3
4. Pd-catalyzed [3+2] cycloaddition reaction of vinyl epoxide 1a and nitroalkene 5a on 6 mmol scale.....	S15
5. The preparation of compound 8 and its ORTEP diagram of X-ray diffraction structure.....	S15
6. The preparation of compound 9.....	S19
7. The preparation of compound 10.....	S21
8. The preparation of compound 11.....	S21
9. The study of whether the vinyl epoxide ring-opening was kinetic resolution.....	S24
10. Computational Details.....	S25
11. References	S33
12. Spectra.....	S35

1. General Methods

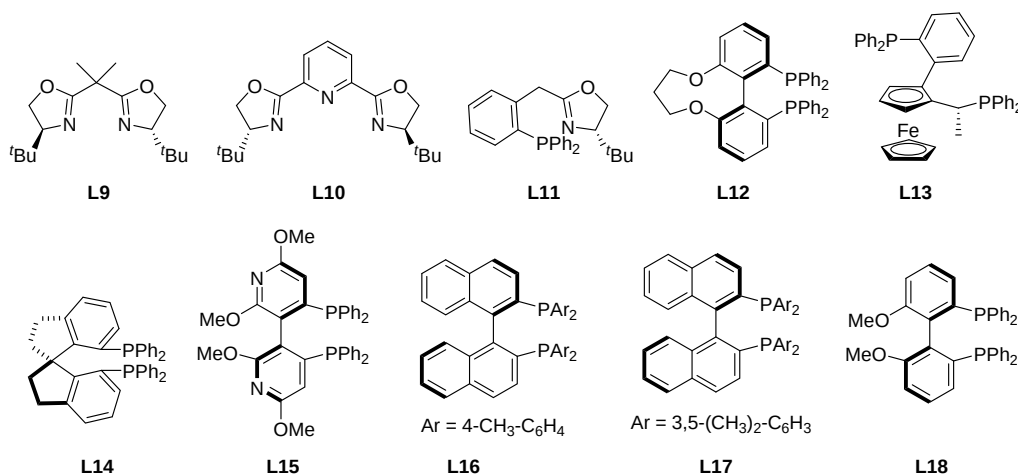
The reactions were carried out in flame-dried glassware under a dry argon atmosphere with standard vacuum-line techniques. All solvents were purified and dried by using standard methods prior to use. Commercially available reagents were used without further purification. NMR spectra were recorded on 400 MHz Varian-400, 400M Agilent-400 or 300 MHz Bruker AM-300 NMR spectrometers. Chemical shifts of ^1H NMR are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (CDCl_3 : δ 7.26 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet or unresolved), coupling constants (Hz), and integration. Chemical shifts of ^{13}C NMR are reported in ppm from tetramethylsilane with the solvent resonance as the internal standard (CDCl_3 : δ 77.1 ppm). Infrared spectra were recorded from thin films of pure samples. Mass and HRMS spectra were measured in EI or ESI mode and the mass analyzer type used for the HRMS was TOF. Thin layer chromatography was performed on pre-coated glassback plates and visualized with UV light at 254 nm. Flash column chromatography was performed on silica gel. Enantiomer ratios were determined by chiral HPLC analysis in comparison with authentic racemic materials. The nitroalkenes were prepared according to literature procedures.¹

2. Optimization of reaction conditions for Pd-catalyzed [3+2] cycloaddition reaction of vinyl epoxide **1a** and tri-substituted nitroalkene **5a**^a



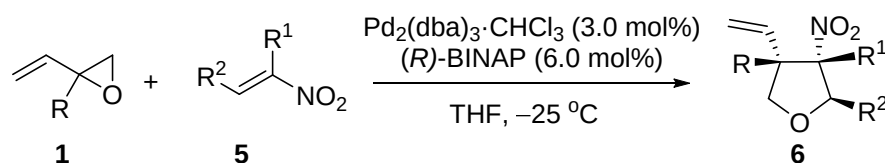
entry	L	[Pd]	Yield% ^b	dr ^c	ee ^d
1	L9	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	nr	--	--
2	L10	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	nr	--	--
3	L11	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	13	9/1	14
4	L12	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	94	1/1	68

5	L13	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	28	2/1	8
6	L14	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	24	1/1	62
7	L15	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	82	2/1	80
8	L16	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	90	5/1	96
9	L17	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	79	0.7/1	68
10	L18	$\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3$	90	4/1	94
11	(<i>R</i>)-BINAP	$\text{Pd}(\text{dba})_2$	88	6/1	94
12	(<i>R</i>)-BINAP	$[\text{Pd}(\text{C}_3\text{H}_5)\text{Cl}]_2$	43	5/1	94
13	(<i>R</i>)-BINAP	$\text{Pd}(\text{OAc})_2$	15	4/1	96



^aMolar ratio of $\text{Pd}_2\text{dba}_3 \cdot \text{CHCl}_3/\text{L}/\mathbf{1a}/\mathbf{5a} = 3.0/6.0/200/100$. ^bIsolated yield. ^cdr determined by ^1H NMR. ^dee of **6** determined by chiral HPLC.

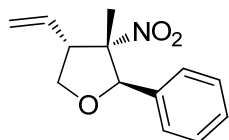
3. General experimental procedure for Table 2 and characterization of products



To a flame dried sealing tube was added $\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$ (0.006 mmol, 6.2 mg), (*R*)-BINAP (0.012 mmol, 7.5 mg), freshly distilled anhydrous THF (1.5 mL). The resulting mixture was allowed to stir for 30 mins. The vinyl epoxide **1** (0.4 mmol) and nitroalkene **5** (0.2 mmol) were added subsequently. The resulting reaction mixture

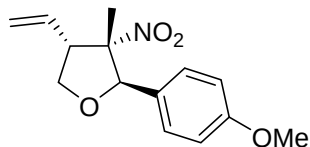
was stirred at -25 for 80 h (monitored by TLC). After the volatiles were removed in vacuo, the ratio of two diastereoisomers was determined by ^1H NMR. Then the resulting residue was purified by flash chromatography (FC) on silica gel with petroleum ether and ethyl acetate as eluent to give product **6**.

(2R,3S,4R)-3-methyl-3-nitro-2-phenyl-4-vinyltetrahydrofuran (6a)



Colorless oil; yield: 94%; 43 mg; dr: 12/1; ee (major isomer): 98%; HPLC (Chiralcel OJ-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 90/10, 0.7 ml/min, 214nm), t_{major} = 23.3 min, t_{minor} = 12.1 min; $[\alpha]_{\text{D}}^{25}$ = 36.51 (*c* 1.15, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.42 – 7.29 (m, 3H), 7.25 (dd, J = 4.3, 3.8 Hz, 2H), 5.65 (s, 1H), 5.63 – 5.53 (m, 1H), 5.26 (ddd, J = 10.7, 6.7, 1.8 Hz, 1H), 4.47 – 4.31 (m, 1H), 4.15 (dd, J = 10.1, 8.9 Hz, 1H), 2.93 (dd, J = 18.1, 8.0 Hz, 1H), 1.17 (s, 3H).; ^{13}C NMR (101 MHz, CDCl_3) δ 137.71, 130.24, 128.50, 128.46, 126.32, 121.74, 98.52, 87.53, , 71.14, 55.38, 20.88; IR (film) 3084, 3032, 2963, 2886, 1641, 1538, 1454, 1388, 1059, 932, 800, 700, 652 cm^{-1} ; MS (ESI) m/z : 256.0 ($\text{M}+\text{Na}^+$); HRMS (ESI) calc for $\text{C}_{13}\text{H}_{19}\text{N}_2\text{O}_3$ ($\text{M}+\text{NH}_4^+$): 251.1390, found: 251.1392.

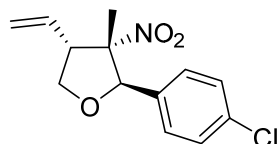
(2R,3S,4R)-2-(4-methoxyphenyl)-3-methyl-3-nitro-4-vinyltetrahydrofuran (6b)



Colorless oil; yield: 86%; 45 mg; dr: 16/1; ee (major isomer): 99%; HPLC (Chiralcel AD-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 95/5, 0.7 ml/min, 214nm), t_{major} = 12.3 min, t_{minor} = 14.8 min; $[\alpha]_{\text{D}}^{25}$ = 53.03 (*c* 1.06, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.16 (t, J = 5.7 Hz, 2H), 6.95 – 6.80 (m, 2H), 5.71 – 5.47 (m, 2H), 5.34 – 5.16 (m, 2H), 4.42 – 4.26 (m, 1H), 4.12 (dd, J = 10.0, 8.9 Hz, 1H), 3.80 (s, 3H), 2.91 (dd, J = 18.0, 8.0 Hz, 1H), 1.17 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 159.60,

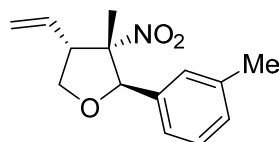
130.33, 129.73, 127.56, 121.62, 113.84, 98.61, 87.37, 71.00, 55.33, 55.21, 20.84; IR (film) 3082, 2993, 2938, 2888, 1612, 1536, 1512, 1387, 1247, 1174, 1059, 1031, 831, 533 cm^{-1} ; MS (ESI) m/z : 286.1 ($\text{M}+\text{Na}$)⁺; HRMS (ESI) calc for $\text{C}_{14}\text{H}_{18}\text{NO}_4$ ($\text{M}+\text{H}$)⁺: 264.1230, found: 264.1232.

(2R,3S,4R)-2-(4-chlorophenyl)-3-methyl-3-nitro-4-vinyltetrahydrofuran (6c)



Colorless oil; yield: 96%; 51 mg; dr: 10/1; ee (major isomer): 99%; HPLC (Chiralcel OJ-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 90/10, 0.7 ml/min, 214nm), t_{major} = 15.5 min, t_{minor} = 12.0 min; $[\alpha]_{\text{D}}^{25}$ = 49.37 (c 1.03, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.39 – 7.32 (m, 2H), 7.21 (t, J = 5.4 Hz, 2H), 5.70 – 5.49 (m, 2H), 5.27 (dd, J = 13.5, 8.0 Hz, 2H), 4.48 – 4.21 (m, 1H), 4.21 – 4.02 (m, 1H), 2.91 (dd, J = 17.9, 8.0 Hz, 1H), 1.18 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 136.15, 134.33, 130.14, 128.78, 127.75, 121.93, 98.23, 86.66, 71.17, 55.48, 20.99; IR (film) 3087, 2989, 2943, 2886, 1538, 1492, 1388, 1349, 1289, 1088, 993, 828, 800, 746 cm^{-1} ; MS (EI) m/z : 220 ($\text{M}-\text{HNO}_2$)⁺; HRMS (EI) calc for $\text{C}_{13}\text{H}_{13}\text{ClO}$ ($\text{M}-\text{HNO}_2$)⁺: 220.0655, found: 220.0662.

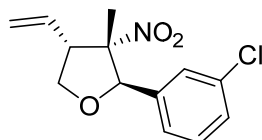
(2R,3S,4R)-3-methyl-3-nitro-2-(*m*-tolyl)-4-vinyltetrahydrofuran (6d)



Colorless oil; yield: 85%; 42 mg; dr: 8/1; ee (major isomer): 97%; HPLC (Chiralcel OJ-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 99.5/0.5, 0.7 ml/min, 214nm), t_{major} = 36.3 min, t_{minor} = 20.5 min; $[\alpha]_{\text{D}}^{25}$ = 37.02 (c 1.05, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.25 (dd, J = 9.8, 5.3 Hz, 1H), 7.13 (d, J = 7.6 Hz, 1H), 7.08 – 7.00 (m, 2H), 5.68 – 5.52 (m, 2H), 5.31 – 5.21 (m, 2H), 4.37 (dd, J = 8.7, 7.6 Hz, 1H), 4.15 (dd, J = 10.2, 8.8 Hz, 1H), 2.99 – 2.83 (m, 1H), 2.35 (s, 3H), 1.18 (s, 3H); ^{13}C NMR (101

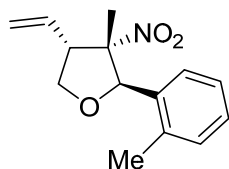
MHz, CDCl₃) δ 138.25, 137.67, 130.26, 129.22, 128.41, 126.88, 123.46, 121.76, 98.58, 87.68, 71.13, 55.44, 21.45, 20.89; IR (film) 3084, 2986, 2921, 2885, 1642, 1609, 1450, 1387, 1290, 1165, 1060, 994, 868, 736 cm⁻¹; MS (ESI) m/z : 270.1 (M+Na)⁺; HRMS (ESI) calc for C₁₄H₁₈NO₃ (M+H)⁺: 248.1281, found: 248.1283.

(2R,3S,4R)-2-(3-chlorophenyl)-3-methyl-3-nitro-4-vinyltetrahydrofuran (6e)



Colorless oil; yield: 85%; 45 mg; dr:9/1; ee (major isomer): 98%; HPLC (Chiralcel OJ-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 92/8, 0.7 ml/min, 214nm), t_{major} = 13.2 min, t_{minor} = 11.9 min; $[\alpha]_{\text{D}}^{25}$ = 54.40 (*c* 0.97, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.34 – 7.27 (m, 3H), 7.14 – 7.06 (m, 1H), 5.67 – 5.50 (m, 2H), 5.37 – 5.18 (m, 2H), 4.37 (dd, *J* = 8.8, 7.6 Hz, 1H), 4.13 (dd, *J* = 10.0, 8.9 Hz, 1H), 2.91 (d, *J* = 9.6 Hz, 1H), 1.20 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 139.74, 134.67, 129.99, 129.81, 128.68, 126.41, 124.64, 122.01, 98.22, 86.55, 71.17, 55.41, 20.94; IR (film) 3082, 2988, 2943, 2885, 1538, 1475, 1387, 1348, 1208, 1060, 932, 791, 687 cm⁻¹; MS (ESI) m/z : 290.0 (M+Na)⁺; HRMS (ESI) calc for C₁₃H₁₈N₂O₃Cl (M+NH₄)⁺: 285.1000, found: 285.1003.

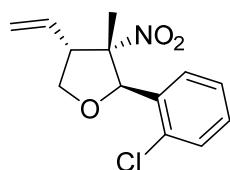
(2R,3S,4R)-3-methyl-3-nitro-2-(*o*-tolyl)-4-vinyltetrahydrofuran (6f)



Colorless oil; yield: 65%; 32 mg; dr:1/1; ee: 86%/76; HPLC (Chiralcel OJ-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 99.5/0.5, 0.7 ml/min, 214nm), Major diastereomer: t_{major} = 23.6 min, t_{minor} = 13.8 min; Minor diastereomer: t_{major} = 15.2 min, t_{minor} = 26.6 min; $[\alpha]_{\text{D}}^{25}$ = -9.58 (*c* 1.00, CHCl₃); ¹H NMR (400 MHz, CDCl₃) (taken as a mixture of diastereomers) δ (diastereomer 1) 7.43 (t, *J* = 7.1 Hz, 1H), 7.29 – 7.18 (m, 2H),

7.14 (dd, $J = 11.0, 5.8$ Hz, 1H), 5.90 (s, 1H), 5.60 – 5.46 (m, 1H), 5.34 – 5.15 (m, 2H), 4.34 (t, $J = 8.0$ Hz, 1H), 4.22 (dd, $J = 10.7, 9.2$ Hz, 1H), 2.90 (dd, $J = 18.8, 7.8$ Hz, 1H), 2.13 (s, 3H), 1.14 (s, 3H); (diastereomer 2) 7.43 (t, $J = 7.1$ Hz, 1H), 7.29 – 7.18 (m, 2H), 7.14 (dd, $J = 11.0, 5.8$ Hz, 1H), 5.79 (s, 1H), 5.75 – 5.63 (m, 1H), 5.34 – 5.15 (m, 2H), 4.44 (t, $J = 8.1$ Hz, 1H), 4.06 – 3.99 (m, 1H), 3.99 – 3.90 (m, 1H), 2.11 (s, 3H), 1.16 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) (taken as a mixture of diastereomers) δ 136.37, 135.54, 134.69, 134.33, 132.11, 130.68, 130.48, 129.46, 128.24, 128.09, 126.91, 126.29, 125.92, 125.75, 122.24, 120.42, 98.73, 96.39, 85.50, 84.82, 70.95, 70.74, 56.76, 54.77, 20.42, 19.34, 19.01, 16.34; IR (film) 3080, 2986, 2944, 2881, 1641, 1537, 1487, 1444, 1389, 1058, 994, 931, 737, 703 cm^{-1} ; MS (ESI) m/z : 270.1 ($\text{M}+\text{Na}$) $^{+}$; HRMS (ESI) calc for $\text{C}_{14}\text{H}_{18}\text{NO}_3$ ($\text{M}+\text{H}$) $^{+}$: 248.1281, found: 248.1284.

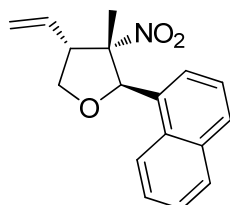
(2R,3S,4R)-2-(2-chlorophenyl)-3-methyl-3-nitro-4-vinyltetrahydrofuran (6g)



Colorless oil; yield: 89%; 47 mg; dr: 2/1; ee (major isomer): 89%; HPLC (Chiralcel OJ-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 99.5/0.5, 0.7 ml/min, 214nm), Major diastereomer: $t_{\text{major}} = 24.8$ min, $t_{\text{minor}} = 15.2$ min; Minor diastereomer: $t_{\text{major}} = 18.2$ min, $t_{\text{minor}} = 31.9$ min; $[\alpha]_{\text{D}}^{25} = -30.09$ (c 1.05, CHCl_3); ^1H NMR (400 MHz, CDCl_3) (taken as a mixture of diastereomers) δ (diastereomer 1) 7.53 (t, $J = 8.3$ Hz, 1H), 7.39 – 7.22 (m, 3H), 6.09 (s, 1H), 5.55 – 5.42 (m, 1H), 5.34 – 5.09 (m, 2H), 4.32 (t, $J = 8.0$ Hz, 1H), 4.25 – 4.17 (m, 1H), 2.85 (dt, $J = 11.0, 7.7$ Hz, 1H), 1.22 (s, 3H); (diastereomer 2) 7.53 (t, $J = 8.3$ Hz, 1H), 7.39 – 7.22 (m, 3H), 6.00 (s, 1H), 5.64 (dd, $J = 17.9, 8.9$ Hz, 1H), 5.34 – 5.09 (m, 2H), 4.50 – 4.41 (m, 1H), 4.07 – 3.99 (m, 1H), 3.81 (d, $J = 8.2$ Hz, 1H), 1.15 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) (taken as a mixture of diastereomers) δ 136.04, 134.71, 132.44, 132.18, 131.87, 129.48, 129.45, 129.37, 129.31, 129.05, 128.12, 127.51, 127.13, 126.76, 122.39, 120.45, 98.08, 96.08, 85.06,

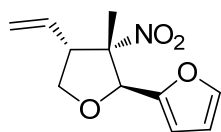
84.56, 71.29, 70.64, 56.63, 55.44, 19.91, 16.57; IR (film) 3080, 2986, 2944, 2882, 1641, 1540, 1473, 1272, 1205, 1080, 884, 746, 720 cm^{-1} ; MS (ESI) m/z : 290.0 ($\text{M}+\text{Na}$)⁺; HRMS (ESI) calc for $\text{C}_{13}\text{H}_{15}\text{NO}_3\text{Cl}$ ($\text{M}+\text{H}$)⁺: 268.0735, found: 268.0739.

(2*R*,3*S*,4*R*)-3-methyl-2-(naphthalen-1-yl)-3-nitro-4-vinyltetrahydrofuran (6h)



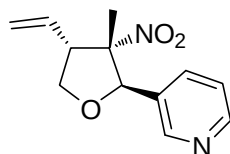
Pale yellow solid; yield: 95%; 54 mg; dr: 3/1; ee (major isomer): 93%; HPLC (Chiralcel OJ-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 95/5, 0.7 ml/min, 214nm), $t_{\text{major}} = 16.3$ min, $t_{\text{minor}} = 14.2$ min; $[\alpha]_{\text{D}}^{25} = -61.90$ (c 0.99, CHCl_3); ^1H NMR (400 MHz, CDCl_3) (taken as a mixture of diastereomers) δ (diastereomers 1) 7.93 – 7.80 (m, 2H), 7.69 (t, $J = 5.4$ Hz, 1H), 7.61 – 7.54 (m, 1H), 7.54 – 7.45 (m, 3H), 6.53 (s, 1H), 5.57 (m, 1H), 5.35 – 5.24 (m, 2H), 4.49 – 4.40 (m, 1H), 4.32 (dd, $J = 11.2, 8.8$ Hz, 1H), 2.96 (dt, $J = 11.2, 7.8$ Hz, 1H), 1.06 (s, 3H); (diastereomers 2) 7.93 – 7.80 (m, 2H), 7.69 (t, $J = 5.4$ Hz, 1H), 7.61 – 7.54 (m, 1H), 7.54 – 7.45 (m, 3H), 6.43 (s, 1H), 5.79 – 5.67 (m, 1H), 5.35 – 5.24 (m, 1H), 5.22 (d, $J = 6.4$ Hz, 1H), 4.55 – 4.49 (m, 1H), 4.12 (dd, $J = 8.7, 6.9$ Hz, 1H), 4.02 (d, $J = 8.4$ Hz, 1H), 1.09 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) (taken as a mixture of diastereomers) δ 134.10, 133.51, 133.45, 132.30, 132.05, 130.80, 130.46, 129.40, 129.04, 128.86, 128.81, 126.82, 126.73, 125.80, 125.76, 125.33, 124.96, 124.78, 123.91, 122.25, 122.18, 120.49, 99.20, 97.14, 84.82, 84.23, 71.03, 70.75, 56.33, 55.08, 20.00, 16.39; IR (film) 3070, 2984, 2904, 1641, 1536, 1350, 1237, 1078, 883, 780, 752 cm^{-1} ; MS (ESI) m/z : 306.0 ($\text{M}+\text{Na}$)⁺; HRMS (ESI) calc for $\text{C}_{17}\text{H}_{18}\text{NO}_3$ ($\text{M}+\text{H}$)⁺: 284.1281, found: 284.1283.

2-((2S,3S,4R)-3-methyl-3-nitro-4-vinyltetrahydrofuran-2-yl)furan (6i)



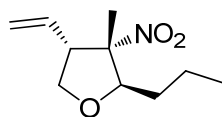
Yellow oil; yield: 83%; 37 mg; dr:20/1; ee: 98% (major isomer); HPLC (Chiralcel AD-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 95/5, 0.7 ml/min, 214nm), t_{major} = 11.3 min, t_{minor} = 12.7 min; $[\alpha]_{\text{D}}^{25}$ = 81.02 (*c* 1.25, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.42 (s, 1H), 6.44 – 6.29 (m, 2H), 5.64 – 5.44 (m, 2H), 5.35 – 5.24 (m, 2H), 4.34 (t, *J* = 8.2 Hz, 1H), 4.08 (dd, *J* = 10.4, 8.6 Hz, 1H), 3.18 – 2.98 (m, 1H), 1.34 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 150.83, 143.15, 129.60, 122.04, 110.39, 109.47, 98.33, 81.70, 71.03, 54.37, 18.85; IR (film) 3151, 3125, 3087, 2989, 2917, 2893, 2850, 1642, 1540, 1503, 1477, 1389, 1350, 1055, 873, 743 cm⁻¹; MS (ESI) *m/z*: 246.0 (M+Na)⁺; HRMS (ESI) calc for C₁₁H₁₄NO₄ (M + H)⁺: 224.0917, found: 224.0918.

3-((2R,3S,4R)-3-methyl-3-nitro-4-vinyltetrahydrofuran-2-yl)pyridine (6j)



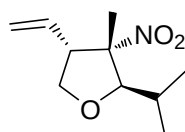
Brown oil; yield: 89%; 42 mg; dr:10/1; ee (major isomer): 94%; HPLC (Chiralcel OJ-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 85/15, 0.7 ml/min, 214nm), t_{major} = 17.2 min, t_{minor} = 15.6 min; $[\alpha]_{\text{D}}^{25}$ = 32.02 (*c* 1.10, CHCl₃); ¹H NMR (400 MHz, CHCl₃) δ 8.62 – 8.42 (m, 2H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.30 (dd, *J* = 7.8, 4.9 Hz, 1H), 5.68 (s, 1H), 5.63 – 5.52 (m, 1H), 5.26 (dd, *J* = 13.5, 7.7 Hz, 2H), 4.37 (t, *J* = 8.2 Hz, 1H), 4.12 (t, *J* = 9.3 Hz, 1H), 2.93 (d, *J* = 8.7 Hz, 1H), 1.20 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 149.84, 148.02, 134.20, 133.20, 129.93, 123.34, 122.04, 97.96, 84.98, 71.17, 55.36, 21.12; IR (film) 3085, 2989, 2943, 2886, 1641, 1579, 1537, 1478, 1426, 1388, 1348, 1059, 993, 880, 802, 713, 649 cm⁻¹; MS (ESI) *m/z*: 235.1 (M+H)⁺; HRMS (ESI) calc for C₁₂H₁₅N₂O₃ (M+H)⁺: 235.1077, found: 235.1073.

(2R,3S,4R)-3-methyl-3-nitro-2-propyl-4-vinyltetrahydrofuran (6k)



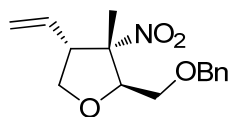
Colorless oil; yield: 70%; 28 mg; dr: 20/1; ee (major isomer): 99%; HPLC (Chiralcel OJ-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 99/1, 0.7 ml/min, 214nm), t_{major} = 9.4 min, t_{minor} = 8.5 min; $[\alpha]_{\text{D}}^{25}$ = -4.23 (*c* 0.90, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 5.64 – 5.47 (m, 1H), 5.24 (s, 1H), 5.20 (dd, *J* = 4.9, 0.9 Hz, 1H), 4.56 – 4.41 (m, 1H), 4.10 (dd, *J* = 8.6, 7.8 Hz, 1H), 3.88 (t, *J* = 9.2 Hz, 1H), 2.80 (dd, *J* = 17.1, 8.5 Hz, 1H), 1.62 – 1.34 (m, 7H), 0.96 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 130.99, 121.28, 97.12, 84.87, 70.40, 55.89, 33.67, 19.59, 19.28, 13.94; IR (film) 2959, 2935, 2874, 1641, 1538, 1458, 1387, 1349, 1047, 995, 930, 697 cm⁻¹; MS (ESI) *m/z*: 222.1 (M+Na)⁺; HRMS (ESI) calc for C₁₀H₁₈NO₃ (M+H)⁺: 200.1281, found: 200.1283.

(2R,3S,4R)-2-isopropyl-3-methyl-3-nitro-4-vinyltetrahydrofuran (6l)



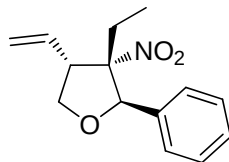
Colorless oil; yield: 70%; 28 mg; dr:14/1; ee (major isomer): 99%; HPLC (Chiralcel OJ-H, 4.6 mm $\times$ 250 mm, Hexane/*i*-Propanol = 99.9/0.1, 0.5 ml/min, 214nm), t_{major} = 14.0 min, t_{minor} = 12.8 min; $[\alpha]_{\text{D}}^{25}$ = -34.44 (*c* 1.19, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 5.53 (dd, *J* = 17.8, 9.0 Hz, 1H), 5.23 – 5.05 (m, 2H), 4.24 – 4.01 (m, 2H), 3.74 (t, *J* = 9.2 Hz, 1H), 2.80 – 2.60 (m, 1H), 1.87 – 1.70 (m, 1H), 1.61 (s, 3H), 1.01 (d, *J* = 6.5 Hz, 3H), 0.81 (d, *J* = 6.7 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 131.56, 120.95, 96.23, 90.42, 70.77, 57.27, 29.02, 19.71, 19.54, 18.92; IR (film) 3086, 2972, 2943, 2876, 1640, 1538, 1471, 1388, 1348, 1186, 1056, 929, 806, 714 cm⁻¹; MS (EI) *m/z*: 152 (M-HNO₂)⁺; HRMS (EI) calc for C₁₀H₁₆O (M-HNO₂)⁺:152.1201, found: 152.1206.

(2S,3S,4R)-2-((benzyloxy)methyl)-3-methyl-3-nitro-4-vinyltetrahydrofuran (6m)



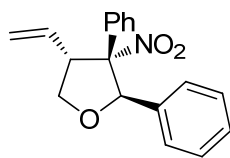
Pale yellow oil; yield: 45%; 25 mg; dr: 20/1; ee (major isomer): 99%; HPLC (Chiralcel AD-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 98/2, 0.5 ml/min, 214nm), $t_{\text{major}} = 18.0$ min, $t_{\text{minor}} = 21.2$ min; $[\alpha]_{\text{D}}^{25} = 15.43$ (c 1.06, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.42 – 7.27 (m, 5H), 5.44 (d, $J = 8.3$ Hz, 1H), 5.28 – 5.16 (m, 2H), 4.65 (t, $J = 4.3$ Hz, 1H), 4.55 (q, $J = 12.0$ Hz, 2H), 4.19 (t, $J = 8.2$ Hz, 1H), 3.96 (dd, $J = 10.1$, 8.5 Hz, 1H), 3.59 (dd, $J = 4.3$, 1.8 Hz, 2H), 2.97 (d, $J = 10.0$ Hz, 1H), 1.66 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 137.46, 130.24, 128.44, 127.83, 127.62, 121.69, 97.17, 83.77, 73.71, 70.92, 69.64, 55.15, 17.92; IR (film) 3085, 3030, 2872, 1641, 1538, 1451, 1349, 1093, 931, 737, 697, 466 cm^{-1} ; MS (ESI) m/z : 300.1 ($\text{M} + \text{Na}$) $^{+}$; HRMS (ESI) calc for $\text{C}_{15}\text{H}_{23}\text{N}_2\text{O}_4$ ($\text{M} + \text{NH}_4$) $^{+}$: 295.1652, found: 295.1654.

(2R,3S,4R)-3-ethyl-3-nitro-2-phenyl-4-vinyltetrahydrofuran (6n)



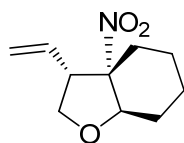
Colorless oil; yield: 95%; 47 mg; dr: 9/1; ee (major isomer): 97%; HPLC (Chiralcel OJ-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 98/2, 0.7 ml/min, 214nm), $t_{\text{major}} = 38.6$ min, $t_{\text{minor}} = 14.7$ min; $[\alpha]_{\text{D}}^{25} = 43.34$ (c 0.93, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.44 – 7.24 (m, 5H), 5.83 – 5.56 (m, 2H), 5.41 – 5.16 (m, 2H), 4.35 (t, $J = 8.1$ Hz, 1H), 4.01 (t, $J = 9.5$ Hz, 1H), 3.12 (dd, $J = 17.5$, 8.4 Hz, 1H), 1.72 – 1.51 (m, 2H), 0.73 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 137.38, 131.42, 128.53, 128.39, 126.91, 121.01, 101.58, 87.87, 71.21, 53.21, 27.89, 8.22; IR (film) 3088, 3033, 2983, 2942, 2883, 1641, 1536, 1454, 1351, 1068, 994, 821, 702, 652 cm^{-1} ; MS (ESI) m/z : 270.1 ($\text{M} + \text{Na}$) $^{+}$; HRMS (ESI) calc for $\text{C}_{14}\text{H}_{18}\text{NO}_3$ ($\text{M} + \text{H}$) $^{+}$: 248.1281, found: 248.1284.

(2R,3R,4R)-3-nitro-2,3-diphenyl-4-vinyltetrahydrofuran (6o)



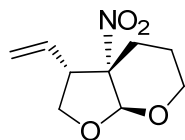
Colorless oil; yield: 90%; 53 mg; dr: 5/1; ee (major isomer): 97%; HPLC (Chiralcel OJ-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 85/15, 0.7 ml/min, 214nm), $t_{\text{major}} = 21.3$ min, $t_{\text{minor}} = 19.7$ min; $[\alpha]_{\text{D}}^{25} = 126.53$ (*c* 1.00, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.16 (dt, *J* = 14.7, 7.3 Hz, 3H), 7.10 – 6.99 (m, 3H), 6.89 (dd, *J* = 16.8, 7.6 Hz, 4H), 6.09 (s, 1H), 5.83 (dd, *J* = 17.4, 9.4 Hz, 1H), 5.40 – 5.20 (m, 2H), 4.62 (t, *J* = 8.2 Hz, 1H), 4.08 (t, *J* = 9.0 Hz, 1H), 4.03 – 3.93 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 137.21, 133.90, 131.38, 128.72, 128.04, 127.94, 127.61, 127.24, 127.18, 120.71, 105.02, 86.23, 70.49, 48.87; IR (film) 3088, 3064, 3033, 2929, 2879, 1641, 1537, 1495, 1344, 1205, 991, 738, 693, 612 cm⁻¹; MS (ESI) *m/z*: 318.0 (M+Na)⁺; HRMS (ESI) calc for C₁₈H₂₁N₂O₃ (M+NH₄)⁺: 313.1547, found: 313.1549.

(3R,3aS,7aR)-3a-nitro-3-vinyloctahydrobenzofuran (6p)



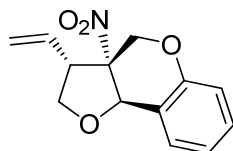
Colorless oil; yield: 69%; 27 mg; dr: 12/1; ee (major isomer): 98%; HPLC (Chiralcel AD-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 99/1, 0.7 ml/min, 214nm), $t_{\text{major}} = 17.1$ min, $t_{\text{minor}} = 13.3$ min; $[\alpha]_{\text{D}}^{25} = 29.88$ (*c* 1.00, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 5.66 (dt, *J* = 17.5, 9.3 Hz, 1H), 5.19 – 5.08 (m, 2H), 4.52 (t, *J* = 3.9 Hz, 1H), 4.22 (dd, *J* = 9.1, 7.8 Hz, 1H), 3.80 (dt, *J* = 15.7, 7.8 Hz, 1H), 2.93 (dd, *J* = 14.0, 8.4 Hz, 1H), 2.52 (dd, *J* = 14.6, 3.9 Hz, 1H), 1.96 – 1.72 (m, 3H), 1.65 – 1.39 (m, 3H), 1.35 – 1.13 (m, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 132.94, 120.10, 94.29, 76.32, 70.51, 52.47, 31.91, 26.12, 21.37, 19.38; IR (film) 3084, 2940, 2866, 1641, 1535, 1434, 1344, 1127, 1091, 1028, 991, 807, 696, 661 cm⁻¹; MS (ESI) *m/z*: 220.0 (M+Na)⁺; HRMS (ESI) calc for C₁₀H₁₆NO₃ (M+H)⁺: 198.1125, found: 198.1127.

(3*R*,3*aS*,7*aS*)-3*a*-nitro-3-vinylhexahydro-4*H*-furo[2,3-*b*]pyran (6q)



Colorless oil; yield: 65%; 26 mg; dr: 2/1; ee (major isomer): 90%; HPLC (Chiralcel AD-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 95/5, 0.7 ml/min, 214nm), $t_{\text{major}} = 30.1$ min, $t_{\text{minor}} = 14.2$ min; $[\alpha]_{\text{D}}^{25} = -35.5$ (c 0.5, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 5.70 – 5.57 (m, 1H), 5.40 (s, 1H), 5.29 (dd, $J = 15.0, 14.1$ Hz, 2H), 4.38 (t, $J = 8.5$ Hz, 1H), 4.05 (t, $J = 8.6$ Hz, 1H), 3.96 (m, 1H), 3.62 – 3.51 (m, 1H), 3.35 (q, $J = 8.6$ Hz, 1H), 2.48 (m, 1H), 2.35 (dt, $J = 14.4, 4.3$ Hz, 1H), 1.77 (m, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 130.41, 121.90, 102.21, 94.22, 70.93, 62.97, 46.91, 26.87, 21.32; IR (film) 3084, 2961, 2897, 2869, 1640, 1536, 1478, 1358, 1278, 1156, 1107, 1067, 1034, 960, 929, 870, 815, 75 cm⁻¹; MS (EI) m/z : 152 (M–HNO₂)⁺; HRMS (EI) calc for C₉H₁₃NO₄ (M)⁺: 199.0845, found: 199.0853.

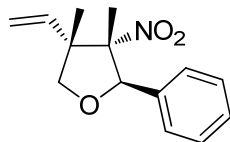
(3*R*,3*aR*,9*bR*)-3*a*-nitro-3-vinyl-2,3,3*a*,9*b*-tetrahydro-4*H*-furo[3,2-*c*]chromene (6r)



White solid, yield: 90%; 44 mg; dr: 20/1; ee (major isomer): 99%; mp: 81.2–82 °C, HPLC (Chiralcel OJ-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 90/10, 1.0 ml/min, 214nm), $t_{\text{major}} = 22.6$ min, $t_{\text{minor}} = 43.6$ min; $[\alpha]_{\text{D}}^{25} = 8.46$ (c 1.1, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.41 (m, 1H), 7.31 – 7.20 (m, 1H), 7.05 (m, 1H), 6.94 (dd, $J = 8.3, 1.1$ Hz, 1H), 5.61 (ddd, $J = 17.0, 10.0, 8.8$ Hz, 1H), 5.50 (s, 1H), 5.37 – 5.27 (m, 2H), 4.75 (td, $J = 12.1, 1.4$ Hz, 1H), 4.22 (dd, $J = 9.0, 7.8$ Hz, 1H), 4.07 (dd, $J = 12.2, 1.6$ Hz, 1H), 3.98 (t, $J = 9.0$ Hz, 1H), 3.09 (dd, $J = 16.8, 8.5$ Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 153.68, 153.57, 130.48, 130.42, 130.26, 130.22, 130.07, 129.88, 122.61, 122.45, 122.36, 121.89, 119.83, 118.85, 117.22, 117.06, 92.70, 90.85, 76.28, 75.79, 70.89, 70.00, 66.41, 65.12, 52.31, 50.20; IR (film) 2919, 2897, 2871, 2849, 1642, 1612, 1587, 1490, 1320, 1182, 1121, 1051, 988, 848, 761, 664 cm⁻¹; MS (EI)

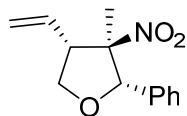
m/z : 247.0 (M)⁺; HRMS (EI) calc for C₁₃H₁₃NO₄ (M)⁺: 247.0845, found: 247.0840.

(2R,3S,4R)-3,4-dimethyl-3-nitro-2-phenyl-4-vinyltetrahydrofuran (6s)



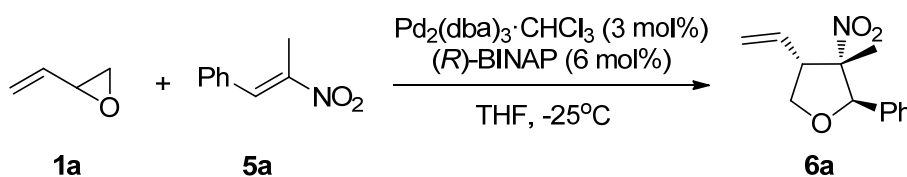
Colorless oil; yield: 59%; 29 mg; dr: 7/1; ee (major isomer): 92%; HPLC (Chiralcel OJ-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 92/8, 0.7 ml/min, 214nm), t_{major} = 15.9 min, t_{minor} = 9.4 min; $[\alpha]_D^{25}$ = 41.03 (c 1.18, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.41 – 7.27 (m, 5H), 6.02 – 5.80 (m, 2H), 5.39 – 5.17 (m, 2H), 4.32 (d, J = 8.8 Hz, 1H), 3.96 (d, J = 8.8 Hz, 1H), 1.30 (s, 3H), 1.21 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 137.82, 137.37, 128.27, 128.21, 126.70, 117.02, 99.30, 84.24, 76.32, 51.89, 18.89, 18.15; IR (film) 3089, 2984, 2926, 2881, 1536, 1450, 1388, 1345, 1212, 1058, 929, 773, 719, 699, 551 cm⁻¹; MS (ESI) m/z : 248.0 ($M + H$)⁺, 270.0 ($M + Na$)⁺; HRMS (ESI) calc for C₁₄H₁₈NO₃ ($M + H$)⁺: 248.1281, found: 248.1283.

(2R,3S,4S)-3-methyl-3-nitro-2-phenyl-4-vinyltetrahydrofuran (6a')



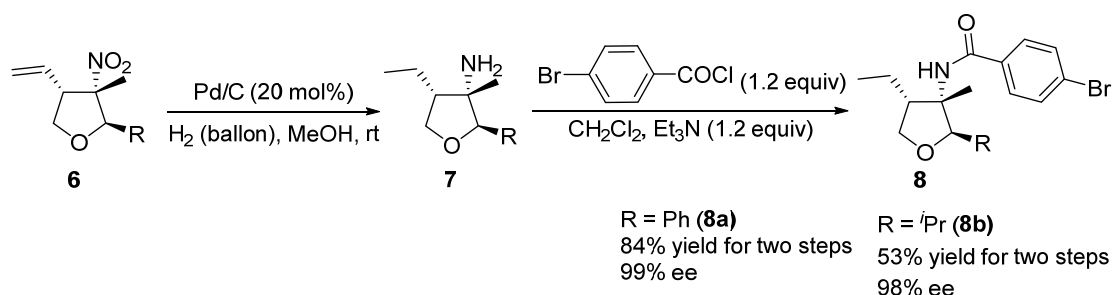
Colorless oil; yield: 45%; 21 mg; ee: 99%; HPLC (Chiralcel OJ-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 90/10, 0.7 ml/min, 214nm), t_{major} = 10.2 min, t_{minor} = 21.1 min; $[\alpha]_D^{25}$ = -21.24 (c 1.0, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.29 (m, 3H), 7.24 (t, J = 8.7 Hz, 2H), 5.78 – 5.60 (m, 1H), 5.56 (s, 1H), 5.23 (t, J = 12.8 Hz, 2H), 4.50 – 4.33 (m, 1H), 4.06 – 3.89 (m, 2H), 1.14 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 135.57, 131.54, 128.57, 128.37, 126.14, 120.81, 95.99, 86.84, 70.35, 53.44, 14.91; IR (film) 3084, 3032, 2963, 2886, 1641, 1538, 1454, 1388, 1059, 932, 800, 700, 652 cm⁻¹; MS (ESI) m/z : 256.0 ($M + Na$)⁺; HRMS (ESI) calc for C₁₃H₁₉N₂O₃ ($M + NH_4$)⁺: 251.1390, found: 251.1392.

4. Pd-catalyzed [3+2] cycloaddition reaction of vinyl epoxide **1a** and nitroalkene **5a** on 6 mmol scale



To a flame dried sealing tube was added $\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$ (0.18 mmol, 186 mg), (*R*)-BINAP (0.36 mmol, 224 mg), freshly distilled anhydrous THF (45 mL). The resulting mixture was allowed to stir for 30 mins. The vinyl epoxide **1a** (12 mmol, 840 mg) and nitroalkene **5a** (6 mmol, 978 mg) were added subsequently. The resulting reaction mixture was stirred at -25 °C for 44 h (monitored by TLC). After the volatiles were removed in vacuo, the ratio of two diastereoisomers was determined by ^1H NMR. Then the resulting residue was purified by flash chromatography on silica gel with petroleum ether and ethyl acetate as eluent to give product **6a** (1.33 g, yield: 95%, dr = 9/1, ee: 98%).

5. The preparation of compound **8** and its ORTEP diagram of X-ray diffraction structure

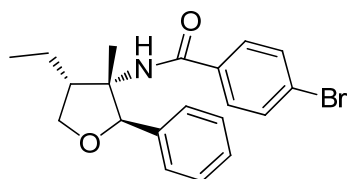


The optically active **6a** (ee: 98%, 0.5 mmol) was dissolved in MeOH (8.0 mL). Then 10 wt% Pd/C (20 mol%) was added subsequently. The resulting solution was allowed to stir for 4.0 hours at room temperature under H_2 balloon. The reaction mixture was filtered through celite and washed with methanol. After concentrated in vacuo, the resulting crude product was used for the next step without further purification.

The 8.0 mL of dry CH_2Cl_2 was added to above crude product. The resulting mixture was then put under a positive pressure of N_2 and chilled to 0 °C. Once chilled, dry

triethylamine (1.2 equiv) and benzoyl chloride (1.2 equiv) were added, and the reaction mixture was stirred at 0 °C for 30 minutes. The ice bath was then removed and the reaction mixture was stirred at room temperature for over night (monitored by TLC). The solvent was removed under reduced pressure. The crude product was purified by preparative TLC to give product **8** (yield for two steps).

4-bromo-*N*-((2*R*,3*S*,4*R*)-4-ethyl-3-methyl-2-phenyltetrahydrofuran-3-yl)benzamide (8a)



White solid; yield: 84%; 162 mg; ee: 99%; mp: 169-170.7 °C, HPLC (Chiralcel OJ-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 85/15, 0.7 ml/min, 214nm), $t_{\text{major}} = 27.9$ min, $t_{\text{minor}} = 24.8$ min; $[\alpha]_{\text{D}}^{25} = 169.8$ (c 1.0, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.63 – 7.55 (m, 4H), 7.45 – 7.32 (m, 4H), 7.32 – 7.25 (m, 1H), 6.17 (s, 1H), 5.49 (s, 1H), 4.55 – 4.34 (m, 1H), 3.85 (t, $J = 9.1$ Hz, 1H), 2.30 – 2.14 (m, 1H), 1.68 (ddd, $J = 13.1$, 7.7, 3.5 Hz, 1H), 1.37 (ddd, $J = 13.1$, 11.2, 7.1 Hz, 1H), 1.15 (s, 3H), 1.02 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.41, 139.97, 134.17, 131.84, 128.27, 128.06, 127.55, 126.55, 126.14, 86.97, 71.97, 64.82, 49.65, 20.94, 19.87, 13.11; IR (film) 3322, 3025, 2968, 2882, 1663, 1586, 1530, 1385, 1067, 1044, 842, 702, 642 cm^{-1} ; MS (ESI) m/z : 388.0 ($\text{M} + \text{H}^+$); HRMS (ESI) calc for $\text{C}_{20}\text{H}_{23}\text{NO}_2\text{Br}$ ($\text{M} + \text{H}^+$): 388.0907, found: 388.0909.

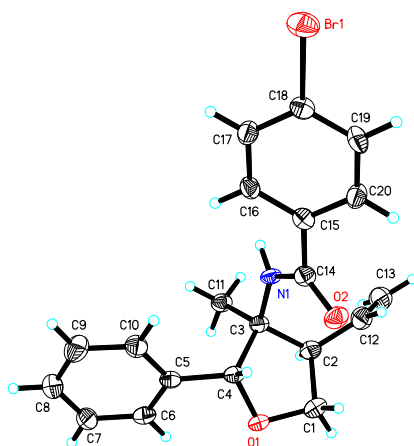
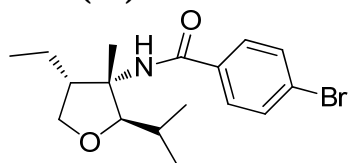


Table 1. Crystal data and structure refinement for cd17020.

Identification code	cd17020	
Empirical formula	C ₂₀ H ₂₀ Br N O ₂	
Formula weight	386.28	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.901(2) Å	$\alpha = 90^\circ$.
	b = 6.2481(11) Å	$\beta = 98.052(4)^\circ$.
	c = 13.318(2) Å	$\gamma = 90^\circ$.
Volume	898.1(3) Å ³	
Z	2	
Density (calculated)	1.428 Mg/m ³	
Absorption coefficient	2.300 mm ⁻¹	
F(000)	396	
Crystal size	0.200 x 0.100 x 0.050 mm ³	
Theta range for data collection	1.887 to 25.496°.	
Index ranges	-8 ≤ h ≤ 13, -7 ≤ k ≤ 7, -16 ≤ l ≤ 16	
Reflections collected	5164	
Independent reflections	3261 [R(int) = 0.0344]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6170	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3261 / 1 / 222	
Goodness-of-fit on F ²	0.976	
Final R indices [I > 2σ(I)]	R1 = 0.0436, wR2 = 0.0895	
R indices (all data)	R1 = 0.0562, wR2 = 0.0945	
Absolute structure parameter	0.031(10)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.641 and -0.237 e.Å ⁻³	

CCDC 1870646 (**8a**) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

4-bromo-*N*-((2*R*,3*S*,4*R*)-4-ethyl-2-isopropyl-3-methyltetrahydrofuran-3-yl)benzamide (8b)



White solid; yield: 53%; 94 mg; ee: 98%; mp: 150.0-151.5 °C, HPLC (Chiralcel IA, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 95/5, 0.7 ml/min, 214nm), $t_{\text{major}} = 14.5$ min, $t_{\text{minor}} = 12.9$ min; $[\alpha]_{\text{D}}^{25} = 37.5$ (c 1.1, CHCl_3); ^1H NMR (400 MHz, CDCl_3) δ 7.55 (d, $J = 1.5$ Hz, 4H), 5.97 (s, 1H), 4.13 – 3.98 (m, 1H), 3.66 (dd, $J = 8.8, 5.2$ Hz, 1H), 3.45 (d, $J = 8.6$ Hz, 1H), 2.31 (d, $J = 4.4$ Hz, 1H), 1.90 (d, $J = 7.3$ Hz, 1H), 1.56 (s, 3H), 1.20 (d, $J = 7.2$ Hz, 1H), 1.04 (dd, $J = 6.6, 2.4$ Hz, 6H), 0.89 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.78, 134.10, 131.86, 128.21, 126.06, 88.84, 70.64, 63.67, 50.74, 29.18, 21.81, 20.54, 19.82, 19.46, 12.38; IR (film) 3285, 3067, 2958, 2928, 1636, 1588, 1543, 1477, 1312, 1105, 841, 723, 658, 530 cm^{-1} ; MS (ESI) m/z : 353.1 ($\text{M}+\text{H}^+$); HRMS (ESI) calc for $\text{C}_{17}\text{H}_{25}\text{NO}_2\text{Br}$ ($\text{M}+\text{H}^+$): 354.1063, found: 354.1060.

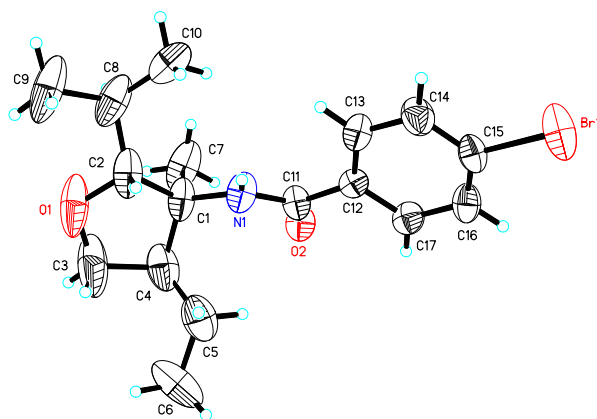


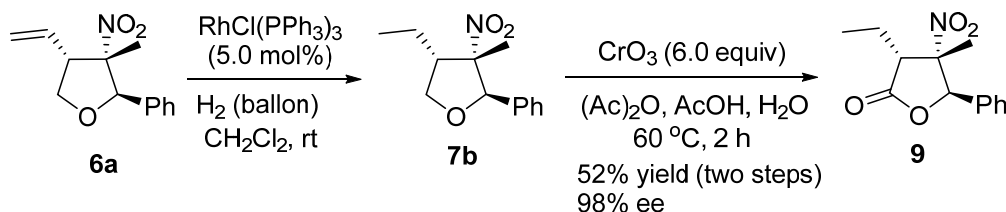
Table 1. Crystal data and structure refinement for cd17129.

Identification code	cd17129
Empirical formula	$\text{C}_{17}\text{H}_{23.40}\text{Br}\text{N}\text{O}_2$
Formula weight	353.68
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P 21 21 21
Unit cell dimensions	$a = 10.2614(10)$ Å $\alpha = 90^\circ$.

	$b = 21.747(2) \text{ \AA}$	$\beta = 90^\circ$.
	$c = 40.341(4) \text{ \AA}$	$\gamma = 90^\circ$.
Volume	$9002.2(15) \text{ \AA}^3$	
Z	20	
Density (calculated)	1.305 Mg/m^3	
Absorption coefficient	2.287 mm^{-1}	
F(000)	3668	
Crystal size	$0.180 \times 0.150 \times 0.080 \text{ mm}^3$	
Theta range for data collection	1.781 to 24.999° .	
Index ranges	$-12 \leq h \leq 9$, $-23 \leq k \leq 25$, $-47 \leq l \leq 46$	
Reflections collected	50143	
Independent reflections	15865 [$R(\text{int}) = 0.1163$]	
Completeness to $\theta = 25.242^\circ$	97.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5713	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15865 / 0 / 964	
Goodness-of-fit on F^2	0.939	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0558$, $wR2 = 0.1170$	
R indices (all data)	$R1 = 0.1936$, $wR2 = 0.1641$	
Absolute structure parameter	0.010(7)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.360 and $-0.404 \text{ e.\AA}^{-3}$	

CCDC 1870648 (**8b**) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

6. The preparation of compound 9

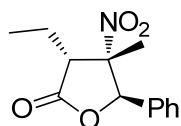


The optically active **6a** (ee: 98%, 0.2 mmol) was dissolved in CH_2Cl_2 (2.0 mL). Then 9.2 mg (0.01 mmol) of Wilkinson's catalyst was added subsequently. The resulting solution was allowed to stir for 12.0 hours at room temperature under H_2 balloon. The

reaction mixture was filtered through celite and washed with CH₂Cl₂. After concentrated in vacuo, the crude product was purified by preparative TLC to give product **7b** (43.7 mg, 93% yield).

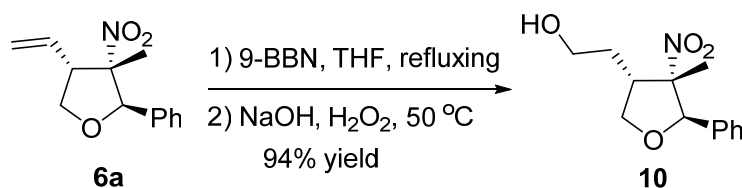
CrO₃ (60 mg, 0.6 mmol, 6 eq) was dissolved in a mixture of AcOH (720 μL) and H₂O (72 μL), which was then added to a solution of **7a** (23 mg, 0.1 mmol) in Ac₂O (216 μL) at 60 °C. After 2 hours, the solution was cooled to 0 °C, excess oxidant was quenched with ethanol (15.0 μL, 0.25 mmol, 10.0 eq) and the mixture was poured onto crushed ice. The aq. phase was extracted with Et₂O (5 x 10 mL), and the combined organics were dried over Na₂SO₄, filtered and concentrated. Product **9** (14 mg, 56% yield) was obtained by preparative TLC.

(3R,4S,5R)-3-ethyl-4-methyl-4-nitro-5-phenyldihydrofuran-2(3H)-one (9)



White solid; dr: 8/1; ee (major isomer): 98%; mp: 98.5-102.6 °C; HPLC (Chiralcel IC, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 97/3, 1.0 ml/min, 214nm), *t*_{major} = 32.9 min, *t*_{minor} = 28.9 min; [α]_D²⁵ = 49.30 (*c* 1.20, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.44 (m, 3H), 7.26 (m, 2H), 5.82 (s, 1H), 2.64 (dd, *J* = 7.8, 5.7 Hz, 1H), 1.88 (m, 1H), 1.56 – 1.45 (m, 1H), 1.36 (s, 3H), 1.18 (t, *J* = 7.5 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 173.90, 133.99, 129.68, 129.10, 126.07, 94.55, 83.83, 49.61, 20.27, 18.98, 12.14; IR (film) 2973, 2940, 2886, 1785, 1546, 1498, 1454, 1390, 1351, 1208, 1190, 1076, 1016, 936, 905, 847, 774, 752, 702, 604, 556, 491 cm⁻¹; MS (ESI) *m/z*: 250.1 (M+H)⁺; HRMS (ESI) calc for C₁₃H₁₉N₂O₄ (M+NH₄)⁺: 267.1339, found: 267.1340.

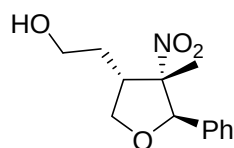
7. The preparation of compound 10



A sample of the alkene **6a** (0.5 mmol, 116 mg, ee: 98%) in dry THF (2.5 mL) was added via a syringe to a solution of 9-BBN (3.0 mL of a 0.5 N THF solution). The

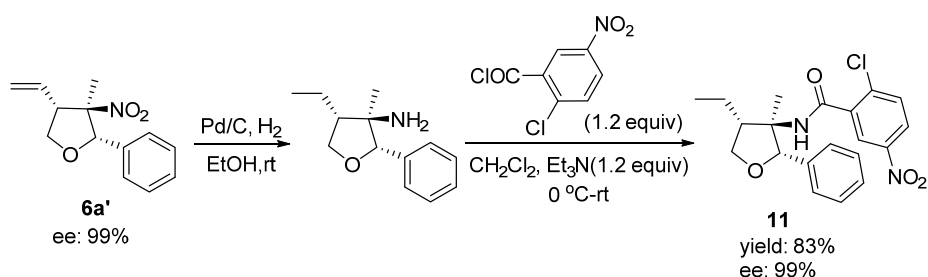
reaction was refluxed for 1.0 h. The reaction mixture was cooled to 0 °C, and EtOH (5.0 mL) with NaOH (2.0 N, 2.0 mL) and H₂O₂ (30%, 2.0 mL) were added. The reaction mixture was stirred at 50 °C for 1 h. The reaction mixture was diluted with water (10.0 mL) and then was extracted with EtOAc (3 × 15.0 mL). The organic layer was dried over Na₂SO₄. After the volatiles were removed under reduced pressure, the residue was purified by column chromatography on silica gel to give **10** (118.0 mg, 94%).

2-((3*R*,4*S*,5*R*)-4-methyl-4-nitro-5-phenyltetrahydrofuran-3-yl)ethanol (**10**)



Colorless oil; ee: 98%; HPLC (Chiralcel OJ-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 85/15, 0.7 ml/min, 214nm), $t_{\text{major}} = 44.2$ min, $t_{\text{minor}} = 20.8$ min; $[\alpha]_{\text{D}}^{25} = 55.6$ (c 1.01, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.31 (m, 3H), 7.24 – 7.22 (m, 2H), 5.60 (s, 1H), 4.48 (t, $J = 8.0$ Hz, 1H), 3.96 (t, $J = 8.0$ Hz, 1H), 3.66 – 3.62 (m, 2H), 2.52 – 2.49 (m, 1H), 2.13 (s, 1H), 1.75 – 1.65 (m, 1H), 1.48 – 1.44 (m, 1H), 1.16 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 138.00, 128.45, 128.41, 126.37, 98.62, 87.72, 72.15, 60.47, 47.82, 29.59, 21.05; IR (film) 3397, 2928, 2881, 1535, 1477, 1453, 1389, 1350, 1210, 1053, 700, 646, 571, 495 cm⁻¹; MS (ESI) m/z : 274.0 (M+Na)⁺; HRMS (ESI) calc for C₁₃H₂₁N₂O₄ (M+NH₄)⁺: 269.1496, found: 269.1499.

8. The preparation of compound **11**

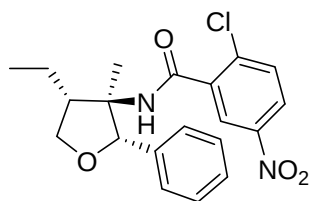


The optically active **6a'** (ee: 99%, 0.06 mmol) was dissolved in EtOH (2.0 mL). Then, 10 wt% Pd/C (20 mol%, 13 mg) was added subsequently. The resulting solution was allowed to stir for 4.0 hours at room temperature under H₂ balloon. The reaction

mixture was filtered through celite and washed with ethanol. After concentrated in vacuo, the resulting crude product was used for the next step without purification.

A 1.5 mL of dry CH₂Cl₂ was added to above crude product. The resulting mixture was then put under a positive pressure of N₂ and chilled to 0 °C. Once chilled, dry triethylamine (1.2 equiv, 6 mg) and benzoyl chloride (1.2 equiv, 13 mg) were added, and the reaction mixture was stirred at 0 °C for 30 minutes. The ice bath was then removed and the reaction mixture was stirred at room temperature for over night (monitored by TLC). The solvent was removed under reduced pressure. The crude product was purified by preparative TLC to give product **11** (19 mg; yield: 83% for two steps).

2-chloro-*N*-((2*R*,3*S*,4*S*)-4-ethyl-3-methyl-2-phenyltetrahydrofuran-3-yl)-5-nitrobenzamide (11)



White solid; ee: 99%; mp: 139.0–142.7 °C, HPLC (Chiralcel ID, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 80/20, 1.0 ml/min, 214 nm), $t_{\text{major}} = 23.0$ min, $t_{\text{minor}} = 17.4$ min; $[\alpha]_{\text{D}}^{25} = -37.19$ (c 1.1, CHCl₃); ¹H NMR (400 MHz, CDCl₃) δ 8.45 (d, $J = 2.4$ Hz, 1H), 8.22 (dd, $J = 8.8, 2.4$ Hz, 1H), 7.61 (d, $J = 8.8$ Hz, 1H), 7.40 – 7.25 (m, 5H), 5.81 (s, 1H), 5.67 (s, 1H), 4.36 (t, $J = 8.0$ Hz, 1H), 3.74 (t, $J = 8.0$ Hz, 1H), 3.63 (dd, $J = 9.3, 4.6$ Hz, 1H), 1.72 – 1.58 (m, 1H), 1.45 – 1.34 (m, 1H), 1.01 (t, $J = 8.0$ Hz, 3H), 0.86 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 163.55, 146.54, 137.77, 137.36, 137.12, 131.52, 127.98, 127.69, 126.54, 125.63, 124.71, 81.25, 70.98, 65.28, 43.84, 21.02, 16.70, 12.74; IR (film) 3259, 3081, 2961, 2921, 2872, 1643, 1609, 1556, 1524, 1455, 1378, 1343, 1306, 1080, 1050, 953, 906, 849, 798, 739, 635, 563, 534 cm⁻¹; MS (ESI) m/z : 411.0 (M+Na)⁺; HRMS (ESI) calc for C₂₀H₂₂N₂O₄Cl (M+H)⁺: 389.1263, found: 389.1261.

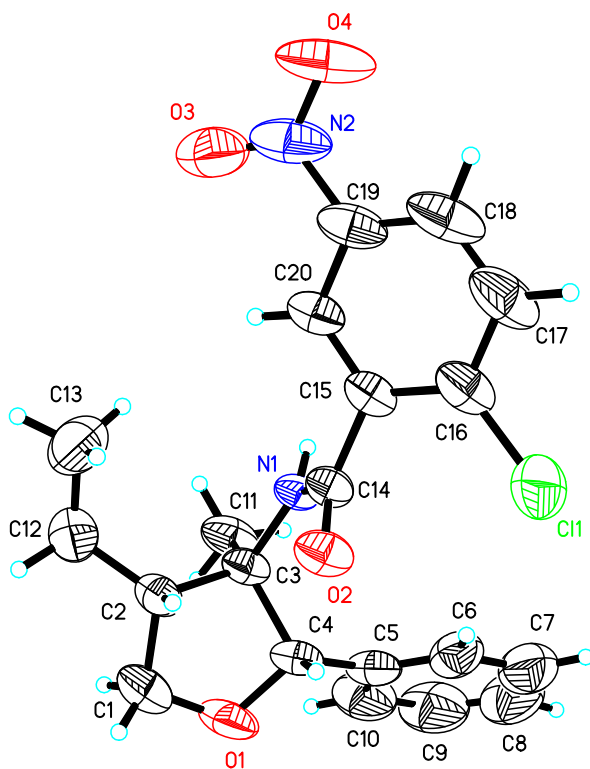
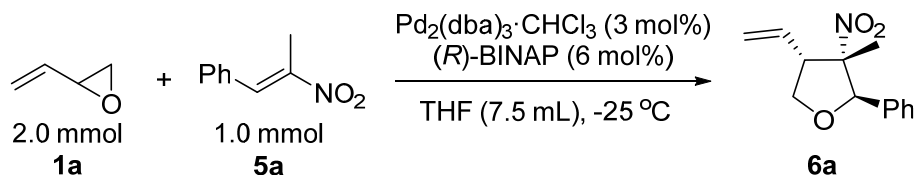


Table 1. Crystal data and structure refinement for mo_d8v18616_0m.

Identification code	mo_d8v18616_0m	
Empirical formula	C ₂₀ H ₂₁ Cl N ₂ O ₄	
Formula weight	388.84	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 10.4038(4) Å	α = 90°.
	b = 20.5233(6) Å	β = 90°.
	c = 37.6117(11) Å	γ = 90°.
Volume	8030.9(5) Å ³	
Z	16	
Density (calculated)	1.286 Mg/m ³	
Absorption coefficient	0.217 mm ⁻¹	
F(000)	3264	
Crystal size	0.180 x 0.150 x 0.120 mm ³	
Theta range for data collection	2.383 to 25.500°.	

Index ranges	-8<=h<=12, -22<=k<=24, -45<=l<=41
Reflections collected	43420
Independent reflections	14873 [R(int) = 0.0546]
Completeness to theta = 25.242°	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6473
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	14873 / 0 / 982
Goodness-of-fit on F ²	1.009
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.1215
R indices (all data)	R1 = 0.0995, wR2 = 0.1509
Absolute structure parameter	-0.01(3)
Largest diff. peak and hole	0.195 and -0.190 e.Å ⁻³
CCDC 1870647 (11) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif .	

9. The study of whether the vinyl epoxide ring-opening was kinetic resolution

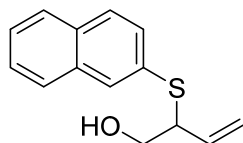


Whether the vinyl epoxide ring-opening was kinetic resolution was studied by stopping the reaction of vinyl epoxide **1a** with nitroalkene (*E*)-**5a** in 12 hours. Enantiomeric excess of unreacted vinyl oxirane **1a** was determined according to the reported procedure.²

Following the general procedure for Table 2 (vide supra), the reaction of vinyl epoxide **1a** (2.0 mmol, 140 mg), nitroalkene **5a** (1.0 mmol, 163 mg), $\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$ (0.03 mmol, 31.0 mg) and (*R*)-BINAP (0.06 mmol, 37.3 mg) in THF (7.5 mL) was stopped in 12 hours. Then, the reaction mixture (0.5 mL) was added to a solution of 2-naphthalenethiol (16.0 mg, 0.1 mmol) and triethylamine (10.0 mg, 0.1 mmol) in methanol (5.0 mL) at 0 °C. The resulting mixture was stirred at 0 °C for 1.0 h. The mixture was filtered through a cotton wool plug (dichloromethane wash) and the filtrate was concentrated under reduced pressure. The crude product was subjected to preparative TLC to give 2-(naphthalen-2-ylsulfanyl)-but-3-en-1-ol (5.0 mg). The chiral HPLC analysis of 2-(naphthalen-2-ylsulfanyl)-but-3-en-1-ol showed it is racemic. This result indicates the epoxide ring-opening was not a kinetic resolution in

this case.

2-(naphthalen-2-ylsulfanyl)-but-3-en-1-ol³

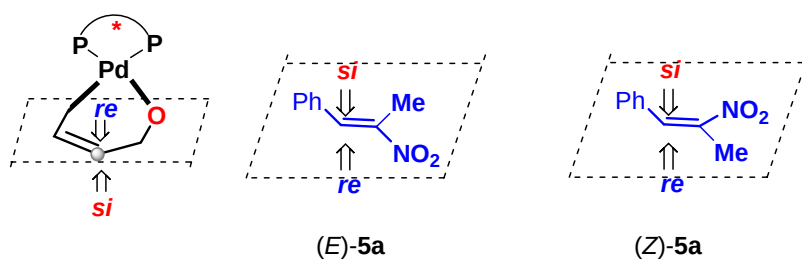


HPLC (Chiralcel OD-H, 4.6 mm × 250 mm, Hexane/*i*-Propanol = 92/8, 0.7 ml/min, 215 nm), $t_{\text{major}} = 24.4$ min, $t_{\text{minor}} = 17.9$ min; ^1H NMR (400 MHz, CDCl_3) δ 7.03 (m, 1H), 7.82 – 7.76 (m, 3H), 7.49 – 7.46 (m, 3H), 5.86 – 5.79 (m, 1H), 5.22 – 5.17 (m, 2H), 3.89 – 3.85 (m, 1H), 3.75 (m, 2H), 2.11 (brs, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 135.11, 133.53, 132.49, 132.06, 132.20, 128.48, 127.67, 127.43, 126.56, 126.39, 118.34, 63.70, 54.59.

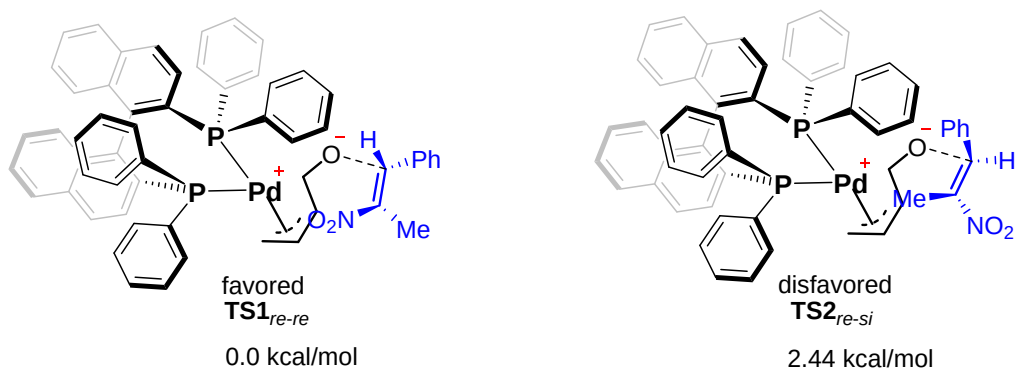
10. Computational Details

All calculations were performed with Gaussian 16, A03 program package.⁴ Geometry optimizations were performed at the (dispersion-corrected) ωB97XD ⁵ functional without any symmetry constraints. The effective core potentials (ECPs) of Hay and Wadt with a double- ζ basis set (LanL2DZ)⁶ were used for Pd, and the 6-31G(d) basis set was used for H, C, N, O and P (BS1). The energies were further estimated using a larger basis set def2-TZVP (BS2)⁷ for all atoms in implicit solvent treated with the SMD universal solvation mode⁸. Tetrahydrofuran (THF) was used as solvent with a dielectric constant value of 7.4257, using UAHF (United Atom Hartree-Fock) radii for the respective atoms (Pd, H, C, N, O and P) in the SMD calculations. All transition structures by the presence of a single imaginary vibrational frequency. Free energies were evaluated at 298K using harmonic vibrational frequencies. The energies given throughout the paper are relative energy values computed with Gaussian 09 at 288 K and P=1 atm.

Reference



(a) (E)-5a



(b) (Z)-5a

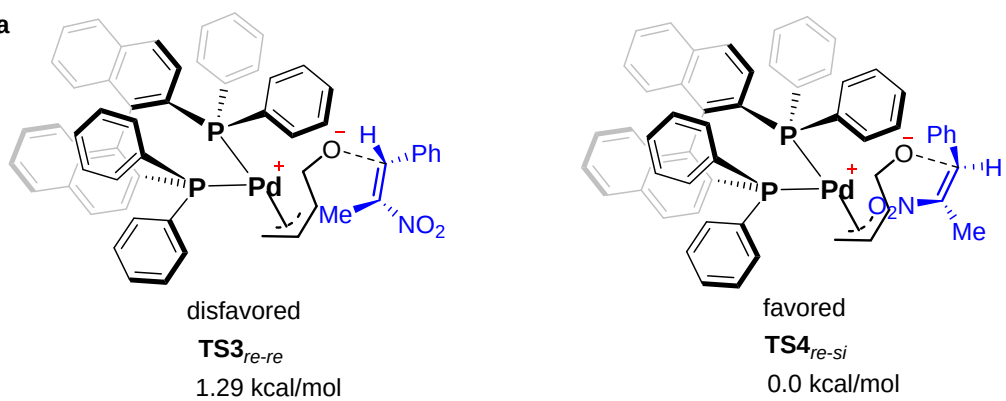
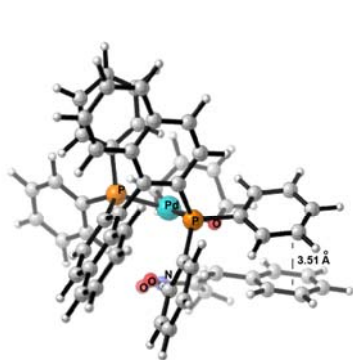
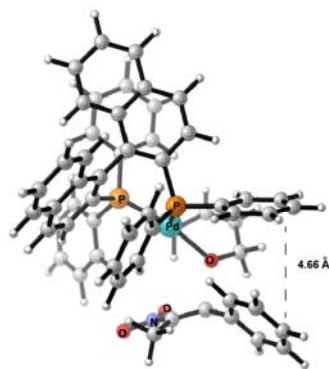


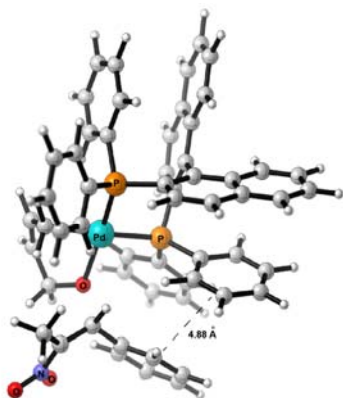
Figure S1. The relative free energies of key transition states (Calculated at SMD- ω B97XD/def2-TZVP// ω B97XD/6-31G*/lanl2dz level of theory).



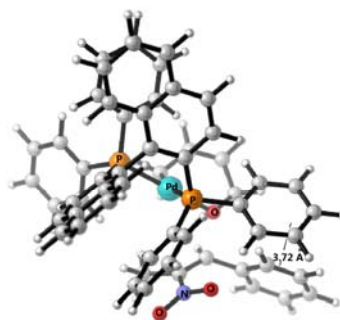
TS1_{re-re}



TS2_{re-si}



TS3_{re-re}



TS4_{re-si}

Figure S2. The optimized structures of key transition states.

Other possible transition states **TS5_{si-re}** [for (*E*)-**5a**], **TS6_{si-si}** [for (*E*)-**5a**], **TS7_{si-re}** [for (*Z*)-**5a**], **TS8_{si-si}** [for (*Z*)-**5a**] were also investigated. They were not considered to affect the selectivities since they have relatively higher energies (**TS5_{si-re}** (4.74 kcal/mol), **TS6_{si-si}** (6.63 kcal/mol), **TS7_{si-re}** (2.37 kcal/mol), **TS8_{si-si}** (7.40 kcal/mol)).

Table S1. The total energies, enthalpies and free energies of the lowest conformers of all species shown in Figure S1.

	E _{tot} (E _h)	H _{298,THF}	G _{298,THF}
TS1_{re-re}	-3291.531272	-3290.578864	-3290.721537
TS2_{re-si}	-3291.527796	-3290.574894	-3290.717645

TS3_{re-re}	-3291.522631	-3290.570451	-3290.714719
TS4_{re-si}	-3291.525354	-3290.573445	-3290.716780

Cartesian Coordinates for Transition States

TS1_{re-re}	TS2_{re-si}
Pd,-0.0000831866,0.0019446037,0.0002384456	Pd,-0.8224763707,0.9587153063,-0.7588473134
P,-0.0006720167,0.0008929532,2.2782070761	P,1.209223631,1.7196463372,-0.051585463
P,2.4131607374,0.0003411936,-0.1967577567	P,-0.3053191851,-1.371919151,-0.3483292592
C,1.4386077363,-0.9473303017,2.9459149973	C,1.8707076404,0.6841710988,1.3284406368
C,1.2064885194,-2.2835445382,3.3672526877	C,1.7067744028,1.1675243397,2.6542713865
H,0.1949406031,-2.6710136592,3.3826321362	H,1.3066331079,2.1616244739,2.8152315189
C,2.2387938095,-3.0979156576,3.7384232091	C,2.0310463891,0.3953891351,3.7338514653
H,2.041277237,-4.1226946308,4.0410422644	H,1.8828459758,0.7780444505,4.7400773629
C,3.5711897553,-2.6224689208,3.7446170005	C,2.5704920616,-0.9012807999,3.5620694937
C,4.6516636246,-3.4514971046,4.143125565	C,2.9207631559,-1.7103891469,4.6738812974
H,4.4388050831,-4.4757978883,4.437611051	H,2.7567575883,-1.317349021,5.673788525
C,5.9344922939,-2.9716630015,4.1631140425	C,3.459767561,-2.9564957368,4.4928141661
H,6.7542269109,-3.6118094045,4.4752886522	H,3.7305323766,-3.5666963734,5.3492570921
C,6.1915166393,-1.6366697909,3.7767533863	C,3.6670383173,-3.4490170661,3.1842550108
H,7.2091636723,-1.2578582187,3.7943918827	H,4.0982411007,-4.435719516,3.0436911114
C,5.169020016,-0.8197121267,3.3700239204	C,3.3221519625,-2.6955410911,2.0924384616
H,5.3856443651,0.1963204524,3.0602362559	H,3.4733834968,-3.0957316801,1.0962367254
C,3.8247967329,-1.2843316123,3.3417935105	C,2.762601336,-1.3966266604,2.2445075321
C,2.7373853488,-0.4568825595,2.9054651134	C,2.3728317078,-0.5936189846,1.1214853122
C,3.0572870722,0.9188827263,2.4024517259	C,2.516604492,-1.1828917281,-0.2498180618
C,3.4094792783,1.9327126212,3.3524139359	C,3.8289786454,-1.282974824,-0.8177225648
C,3.5013636267,1.6673840606,4.7465685686	C,4.9940818146,-0.8699920795,-0.1141241167
H,3.3078275748,0.6633122193,5.1074067434	H,4.892234283,-0.4680688008,0.8878408297
C,3.8266359824,2.6589646877,5.6351271306	C,6.2363300595,-0.9689178057,-0.6845230068
H,3.8964180974,2.431599332,6.6947789012	H,7.1125933527,-0.6521288237,-0.1266565054
C,4.062290149,3.9779187075,5.1849982262	C,6.3866307152,-1.471449091,-1.9971413105
H,4.3109103662,4.7568420638,5.8995943313	H,7.3754280995,-1.5394427527,-2.4406106057
C,3.9806363566,4.2667381916,3.8482110422	C,5.2841441698,-1.8758205236,-2.7027795447
H,4.1637707775,5.2757967854,3.4879459146	H,5.3864189135,-2.2689342818,-3.7109974156
C,3.6663727955,3.2556590701,2.9034763989	C,3.9876511336,-1.8020709847,-2.1306425132
C,3.6103584608,3.5298972097,1.5159754494	C,2.8419747607,-2.2458159681,-2.8335958574
H,3.8140842728,4.5395873084,1.1688853936	H,2.9620317781,-2.6536417954,-3.833950795
C,3.3218477771,2.5406263247,0.6176789542	C,1.6020057719,-2.1852793979,-2.2612272284
H,3.3036580619,2.772287129,-0.441531049	H,0.7434719216,-2.5509372317,-2.8133620277
C,3.037428391,1.2174365977,1.0469271078	C,1.4177379501,-1.6492742824,-0.959125435
C,2.9749465071,0.6564912401,-1.816215574	C,-1.3460821721,-2.4908080326,-1.3599124347

C,4.1545248718,0.2473035562,-2.4448508842	C,-1.7620550775,-3.7566128423,-0.9386828415
H,4.7983772565,-0.4894173437,-1.97775259	H,-1.4603775778,-4.1398045323,0.0298579866
C,4.5034901138,0.7556198629,-3.6927589459	C,-2.5925917048,-4.5299632545,-1.7450773877
H,5.4197711697,0.4211395666,-4.1706067356	H,-2.9137178631,-5.5088218955,-1.4008610029
C,3.6770441248,1.6746508554,-4.3305277907	C,-3.0174124978,-4.049618581,-2.9797677728
H,3.9422886927,2.0580908114,-5.3112957499	H,-3.6724167598,-4.6512239505,-3.6026443088
C,2.5013312387,2.0904069703,-3.7120099159	C,-2.6079324216,-2.7895613972,-3.4074710009
H,1.8437292564,2.7986309805,-4.2068308841	H,-2.9454710036,-2.3985355768,-4.3626424266
C,2.1492361653,1.5820764808,-2.4672357179	C,-1.7857466563,-2.0127484747,-2.599391944
H,1.2158585044,1.8866711282,-2.0067738235	H,-1.4934933165,-1.0176722476,-2.9258126019
C,3.3940792308,-1.5139882787,0.0700253054	C,-0.3476812347,-2.0670798995,1.3317991474
C,4.7782318997,-1.485205832,0.2771388801	C,0.2154656366,-3.3003073779,1.6756836723
H,5.3016211201,-0.5331938982,0.3148395165	H,0.7409351872,-3.8855197764,0.9254632069
C,5.4822151182,-2.6657143504,0.4768517378	C,0.137816353,-3.7605019166,2.9842733343
H,6.5525031779,-2.632150866,0.6549085012	H,0.5932648529,-4.7093697302,3.2496127975
C,4.8080413477,-3.8854991128,0.4832910767	C,-0.4961656535,-2.9914194396,3.9590790151
H,5.3580217978,-4.8064435297,0.6531904172	H,-0.5480289215,-3.3524595096,4.9818771985
C,3.4315042747,-3.9198046659,0.2879289442	C,-1.0504068055,-1.7597553277,3.62503774
H,2.8979742413,-4.8651592116,0.3055429389	H,-1.5391618892,-1.1512030947,4.3797834438
C,2.7212241864,-2.7387132046,0.0834270991	C,-0.9699688544,-1.2980519575,2.3148120984
H,1.6418880687,-2.7728785592,-0.043583861	H,-1.3783545298,-0.3294370216,2.0453872753
C,0.1089043219,1.6611496741,3.0245576555	C,2.5231280041,1.7563861041,-1.3120100243
C,-0.0181620903,2.7772356021,2.1934075168	C,2.1842066356,1.4890728346,-2.6410702075
H,-0.1768656014,2.6331792293,1.1282013958	H,1.1494617124,1.2783621471,-2.8966925376
C,0.0849093822,4.0600866329,2.7222158506	C,3.1689339271,1.4680626682,-3.6234701815
H,-0.0010427959,4.9205364792,2.0656590995	H,2.8996475514,1.2455937417,-4.6514503482
C,0.3108787104,4.2374549885,4.0838754793	C,4.4960554334,1.718420391,-3.2868219264
H,0.4013703535,5.2382165471,4.4953052232	H,5.2661816734,1.6914821696,-4.0515360612
C,0.4361726169,3.1297526236,4.9185054482	C,4.8397524819,1.9900149267,-1.9648508633
H,0.6368777783,3.263782513,5.9766361312	H,5.8768125863,2.1645164107,-1.6966456318
C,0.3438037067,1.8475978529,4.390721607	C,3.859363714,2.0018864089,-0.9801365386
H,0.4883044079,0.9873422444,5.0390258966	H,4.138636853,2.168594374,0.0568774786
C,-1.4770022872,-0.7963374422,3.0181438698	C,1.0899085065,3.407228308,0.6421950207
C,-2.1383536205,-0.302587849,4.1457613815	C,2.0571059616,4.4006144814,0.4725514473
H,-1.7880440823,0.5931894323,4.6461283495	H,2.9655946173,4.2006052619,-0.0851659938
C,-3.2789138722,-0.9432928283,4.6240998608	C,1.8447477557,5.6732878746,0.9978005759
H,-3.7880806871,-0.5471229192,5.4978629957	H,2.598679967,6.4422443859,0.8562128209
C,-3.7701595698,-2.0755669471,3.9809117372	C,0.6696024947,5.9646925748,1.6861657917
H,-4.6642576064,-2.567211223,4.353445167	H,0.5064156386,6.9632115844,2.081050364
C,-3.1225561304,-2.5636539476,2.8485702747	C,-0.3026995061,4.9813062427,1.8526105809
H,-3.5036335959,-3.4292939164,2.3161914068	H,-1.2462174296,5.1787933456,2.3503128922
C,-1.9866326269,-1.9260904217,2.3633457983	C,-0.0902088093,3.7128696274,1.3293732917
H,-1.5061894173,-2.3084166466,1.4643582382	H,-0.8631614625,2.9605370119,1.4499806893
C,-1.2127365632,0.5788010353,-2.7972132636	C,-3.4141294262,0.857981183,-2.4447097126

C,-1.7292323112,1.7769894525,-2.0476919594 O,-0.1930472276,-0.1082141099,-2.1157970601 H,-2.0584553192,-0.1125899169,-2.9725639219 H,-0.844716544,0.8957376338,-3.7847925603 H,-1.7990010737,2.725705042,-2.5750446626 C,-2.1010524573,1.684015228,-0.7615706662 C,-2.0367333738,0.4321715966,0.0197711121 H,-2.4207981435,2.5844977403,-0.2371505886 H,-2.5006887773,0.5210493242,1.0015500815 H,-2.4475620088,-0.4420691354,-0.4987414332 C,-1.1850859818,-2.6501067181,-2.431350615 C,-0.0097741912,-1.9501293006,-2.6938310501 H,0.7479917044,-2.0629345666,-1.9305460955 C,0.5644972904,-1.7077416624,-4.0367922412 C,-0.1767194776,-1.313991059,-5.1580115715 C,1.9493003488,-1.8553672106,-4.1759861778 C,0.4505630924,-1.0860462607,-6.3785033938 H,-1.245851309,-1.1561888265,-5.0751366166 C,2.5757912678,-1.6367527115,-5.3965665723 H,2.5411053545,-2.1383373591,-3.3094833482 C,1.8272319309,-1.250830784,-6.5047189447 H,-0.1413077447,-0.7747687687,-7.2345087077 H,3.6521029518,-1.755659875,-5.4769629647 H,2.3135722309,-1.0732051242,-7.4595853225 C,-2.3055167038,-2.9887104398,-3.3677159824 H,-3.1158839596,-2.2474705854,-3.3617317285 H,-1.930857798,-3.0812832161,-4.3898528868 H,-2.7510287769,-3.9439222176,-3.0796403291 N,-1.3891961142,-3.0124687563,-1.0965233658 O,-0.4626802258,-2.8986297041,-0.251959573 O,-2.4977170598,-3.4481745164,-0.7533840798	C,-2.4426340589,1.5044180365,-3.3916193353 O,-2.9253687649,0.7062337546,-1.149011117 H,-4.3226899383,1.4901956635,-2.4199009469 H,-3.7432698302,-0.1082289288,-2.8658478586 H,-2.5650432461,1.2664530464,-4.4476920148 C,-1.4682272179,2.3548337515,-3.017931935 C,-1.1932924571,2.8015434796,-1.6391877673 H,-0.7904355162,2.7148832396,-3.7928005773 H,-0.3875765074,3.5341390473,-1.5840023308 H,-2.0617381932,3.1350981161,-1.0644681719 C,-3.7405760234,1.5339728986,1.3561263105 C,-4.2719890717,1.099930719,0.1473851782 H,-4.640690995,1.9067320958,-0.4795218113 C,-5.0125725205,-0.1826398286,0.0319506728 C,-4.3932401355,-1.4196833022,0.2364732072 C,-6.3638638311,-0.1567799637,-0.3171683831 C,-5.1144643205,-2.5996267305,0.1146763438 H,-3.3340163396,-1.4497354712,0.4675479579 C,-7.090611377,-1.3395834779,-0.4353866165 H,-6.8506223706,0.7990521232,-0.4937151994 C,-6.4681272502,-2.5643583902,-0.2189897069 H,-4.6138051324,-3.5509652286,0.2672307757 H,-8.1428316905,-1.3005358073,-0.7025690604 H,-7.0296944494,-3.488941936,-0.3178444796 C,-3.6572294331,0.7891357803,2.655194465 H,-2.6794417368,0.9101213711,3.1328447961 H,-4.3935782733,1.1734665652,3.3721153767 H,-3.8508399844,-0.2746900539,2.5052463735 N,-3.4111213615,2.8960534088,1.4340370468 O,-3.0092257458,3.3316279247,2.5315822113 O,-3.5130423151,3.6372833323,0.4400255725
TS3_{re-re} Pd,-0.7652035392,1.181847146,-0.4579386916 P,1.3027532256,1.7303455662,0.3085408054 P,-0.3558637948,-1.1923497857,-0.530020126 C,2.0551381216,0.4182163333,1.3678596789 C,2.0727897824,0.6165364985,2.77417211 H,1.7453953232,1.563178734,3.1872607818 C,2.4900701021,-0.3700709481,3.6230478984 H,2.4866581894,-0.2017770169,4.6966528066 C,2.9368706674,-1.6152811915,3.1223796132 C,3.3726895314,-2.649433735,3.9908957036 H,3.3476767438,-2.4729680216,5.0629434439 C,3.8186564374,-3.8434833556,3.4896380958	TS4_{re-si} Pd,-0.7814708351,1.2600036146,-0.2745556917 P,1.3593533589,1.6778378945,0.4062627982 P,-0.4336960448,-1.124546737,-0.4894545036 C,2.0968963572,0.3025964816,1.3931995959 C,2.1678298658,0.4503025628,2.804161208 H,1.8958879055,1.3943863389,3.2608134717 C,2.5751577734,-0.5799658994,3.6040290312 H,2.6181422059,-0.4474302931,4.6816793901 C,2.9563280831,-1.8230898542,3.0470161581 C,3.3927884494,-2.8974184807,3.8647012803 H,3.4208935123,-2.7526554904,4.9413892895 C,3.7755438744,-4.0892684048,3.3093853124

H,4.1541816197,-4.6276398924,4.161559601	H,4.112031982,-4.905276507,3.9417774104
C,3.843491701,-4.0552535797,2.0921962274	C,3.7293406603,-4.2592719041,1.9071860599
H,4.1993753879,-5.0023974231,1.6980648634	H,4.0271948249,-5.20774399,1.4705142042
C,3.414670227,-3.0791723331,1.2311636776	C,3.2985199681,-3.2430266232,1.0953531562
H,3.4259431144,-3.2622593599,0.1626647035	H,3.2484217028,-3.3972483899,0.0236579593
C,2.9477391543,-1.8267028636,1.7177162521	C,2.9021073077,-1.989352961,1.6374906801
C,2.4766826803,-0.7950911407,0.8402787231	C,2.4460239779,-0.9085286934,0.8114610381
C,2.4751504837,-1.0706354796,-0.6334473423	C,2.3947818755,-1.1305905672,-0.6707672585
C,3.7336092127,-1.0542983295,-1.3212123573	C,3.6400824277,-1.1568692047,-1.3835110032
C,4.9658739831,-0.8231065448,-0.6492202226	C,4.8945540366,-0.9944740614,-0.7325301064
H,4.9629956585,-0.6566307626,0.422205718	H,4.921926768,-0.8549873261,0.3421767245
C,6.1526120416,-0.8045513265,-1.3343446899	C,6.0673828571,-1.0049145544,-1.4420864271
H,7.0817143232,-0.6317843906,-0.7993219902	H,7.0125830642,-0.8829132967,-0.9213951261
C,6.1780838092,-0.9999912524,-2.7338924147	C,6.0573688054,-1.1641571479,-2.8464270806
H,7.1243477948,-0.9756944372,-3.2657766583	H,6.9931921233,-1.1648510888,-3.3973081478
C,5.0088686358,-1.2250067949,-3.4114156773	C,4.8663932208,-1.3236049742,-3.5039894182
H,5.0143303875,-1.3837208015,-4.486690446	H,4.8419051597,-1.4543732276,-4.5827677038
C,3.7675937457,-1.2689450855,-2.7251205437	C,3.6386146144,-1.334409113,-2.7925561605
C,2.5548388457,-1.5358332704,-3.4043875517	C,2.4033406947,-1.5339945561,-3.4521588419
H,2.5788089191,-1.7127731661,-4.4765255357	H,2.3978033072,-1.6949176719,-4.5271612563
C,1.3688684115,-1.5933463197,-2.7268379066	C,1.2293334204,-1.5474791801,-2.7524411823
H,0.457837459,-1.8212676686,-3.2685607395	H,0.3032580792,-1.731206638,-3.283295195
C,1.3072660003,-1.356708637,-1.3276015329	C,1.1995608688,-1.3310474086,-1.3492088264
C,-1.5071471114,-2.0529120246,-1.6581468769	C,-1.6625878776,-1.8567709545,-1.6262709629
C,-1.9368671116,-3.3672532683,-1.4719683419	C,-2.3501333598,-3.0390199729,-1.3461142647
H,-1.6377625861,-3.9263251135,-0.5933737021	H,-2.1689057394,-3.5700490077,-0.4189657344
C,-2.796273962,-3.9611379739,-2.3921767375	C,-3.3083357884,-3.5202704313,-2.2363296032
H,-3.1323595986,-4.9800871615,-2.2267124874	H,-3.842115634,-4.4359463013,-2.0014700605
C,-3.2408306558,-3.2487437114,-3.4995342808	C,-3.591369763,-2.8266910281,-3.4081471623
H,-3.9176829992,-3.7130302436,-4.2106724125	H,-4.3393381596,-3.2037913601,-4.0994465748
C,-2.8376405643,-1.9273299317,-3.6791480918	C,-2.9306558833,-1.6302004694,-3.6798620353
H,-3.200936916,-1.3541253196,-4.5267118409	H,-3.1680608062,-1.0646728369,-4.5759900405
C,-1.9840719773,-1.3305412949,-2.7604061245	C,-1.9851885246,-1.1422208888,-2.7870983036
H,-1.6971102422,-0.2914361206,-2.8924600736	H,-1.5029717692,-0.1882105211,-2.9857525448
C,-0.2614392666,-2.1845295073,0.9927188169	C,-0.3194198201,-2.246292311,0.9327640624
C,0.2322972545,-3.4926664643,1.0117228625	C,0.0864635707,-3.5781627282,0.7910703977
H,0.5974630605,-3.9488935645,0.0955256896	H,0.3405206609,-3.9677587551,-0.1916044227
C,0.2951248406,-4.2010285564,2.2057181	C,0.1867508517,-4.3959695534,1.9084368738
H,0.6935531076,-5.210523004,2.2130177179	H,0.5160334114,-5.4245728092,1.797520245
C,-0.1200250335,-3.6036480641,3.393458193	C,-0.1165722734,-3.8897450998,3.1719979506
H,-0.0580592888,-4.1537346839,4.3275042999	H,-0.0357688571,-4.5323671268,4.04366849
C,-0.5975478787,-2.2966869698,3.3853876344	C,-0.5244815373,-2.5688005197,3.3160498305
H,-0.912141396,-1.8222415921,4.3098076812	H,-0.7871313101,-2.1705829266,4.2896886982
C,-0.6673911447,-1.5913102575,2.1889644437	C,-0.6183323786,-1.7472905623,2.1981685733

H,-1.0268400352,-0.5662852662,2.1807729061	H,-0.9229038084,-0.7131337703,2.3139172208
C,2.5287056592,2.0577134669,-0.9961698524	C,2.515194446,1.961813187,-0.9748736944
C,2.0996996461,2.0984459503,-2.3257794274	C,2.0035426558,2.0760499884,-2.2701924465
H,1.0472933131,1.9572733291,-2.5542890406	H,0.9324684711,2.0004594278,-2.4339330226
C,3.0204972295,2.2855132519,-3.3513427288	C,2.8637568234,2.2599886112,-3.3482569466
H,2.6809155331,2.3004623014,-4.3823813783	H,2.457468046,2.3348894058,-4.352216768
C,4.3723148086,2.4369667852,-3.0567344477	C,4.2377071636,2.3353644601,-3.1404776678
H,5.0926157052,2.5707976249,-3.8578924885	H,4.9091491214,2.4703173144,-3.9830005456
C,4.8055866986,2.3998391184,-1.7337564015	C,4.7541429238,2.2222997772,-1.8522927724
H,5.8619483981,2.4941693194,-1.5038379914	H,5.8264278781,2.2557731593,-1.6887312017
C,3.8896279676,2.2019810081,-0.7078092684	C,3.8981830355,2.0269264706,-0.7751903589
H,4.2405833026,2.1171366976,0.317423185	H,4.3103804527,1.8878590327,0.2207775379
C,1.2524920442,3.2040356324,1.3950055542	C,1.5056855357,3.1441850676,1.4990705532
C,2.2531583467,4.1758049241,1.4464131978	C,2.5510299181,4.0668186609,1.4332311949
H,3.1236697923,4.1043810442,0.8032507788	H,3.3387605094,3.9559787513,0.6967567701
C,2.1285126701,5.2630904125,2.3091491831	C,2.5805228507,5.1571840798,2.3004631115
H,2.9094063545,6.0169151183,2.3355325512	H,3.3951151754,5.8720824623,2.2343452523
C,1.0093266377,5.3876235922,3.1262797658	C,1.571731872,5.3344504629,3.2414291642
H,0.9156126642,6.2378315483,3.7950129134	H,1.5985829406,6.1844375657,3.9166046624
C,0.0009224653,4.4272777523,3.0729672668	C,0.5177226949,4.4250236043,3.3051158359
H,-0.8871428948,4.5261725432,3.6893962196	H,-0.2841307199,4.5616328862,4.0241827405
C,0.1199700575,3.3485468342,2.2065645832	C,0.4801096211,3.345915872,2.4312057465
H,-0.681579953,2.6168135192,2.141132532	H,-0.3595820806,2.6576964965,2.4568920892
C,-3.5104146934,1.6974571353,-1.8606873329	C,-3.2984827292,1.7937495932,-2.0173677949
C,-2.553578643,2.4364741768,-2.7511551649	C,-2.3254953238,2.7473934364,-2.6487778129
O,-2.8500770192,0.8974703827,-0.9006064312	O,-2.8353643076,1.1627873027,-0.8587527509
H,-4.1414718047,2.4238344575,-1.3249611423	H,-4.2168685683,2.3593026252,-1.7715867781
H,-4.1823749557,1.0715951849,-2.461658145	H,-3.6162489465,1.0488765675,-2.7660402622
H,-2.7524130066,2.4279825202,-3.820586495	H,-2.4398932884,2.9146018051,-3.7188406052
C,-1.4942330923,3.11298558,-2.2751668576	C,-1.3633835698,3.4013771564,-1.9783698143
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H,-1.9979385863,3.3984405455,-0.1860621328	H,-1.9963809717,3.4540682937,0.095701249
C,-4.5256770506,1.824572045,0.9417649502	C,-3.5112750536,0.8065981685,1.7556219247
C,-3.7065929051,0.7222115695,0.6110770059	C,-4.100048424,1.1899314333,0.5560192636
H,-2.8015436453,0.7628240372,1.2195120393	H,-4.1958632177,2.2741784898,0.5030982699
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C,-4.8125371784,-1.2888154045,-0.5560443628	C,-5.1531028322,-0.6413624116,-0.8881697797
C,-3.8996899488,-1.50807485,1.6507138173	C,-6.4998648045,1.1418740098,-0.0007578091
C,-5.1809937301,-2.6274706754,-0.5252867981	C,-6.2798598252,-1.1754758751,-1.501235691
H,-5.0395193067,-0.6850432041,-1.4230113301	H,-4.1864618717,-1.1082572945,-1.0018497209
C,-4.2560699746,-2.8538944353,1.680707412	C,-7.6313662574,0.6004281248,-0.6040935152
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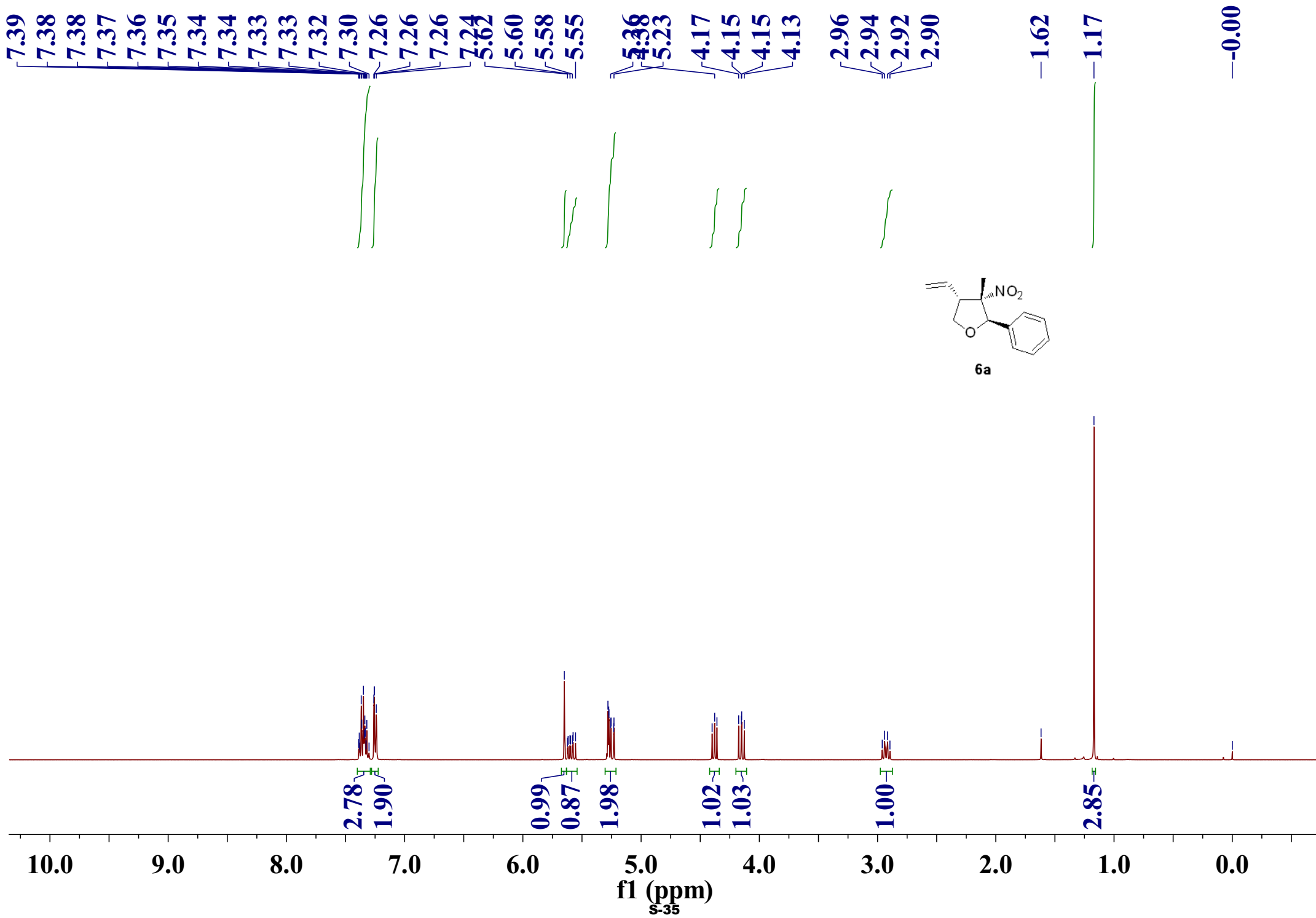
C,-4.9018941833,-3.4191049863,0.5877752428	C,-7.5234904113,-0.5634260914,-1.3590220859
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H,-4.0242366885,-3.4527122159,2.5572276871	H,-8.5922501458,1.0944346536,-0.4912422014
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C,-4.0252565517,2.9856457448,1.7519098409	C,-2.9620094125,1.7968023307,2.7421537046
H,-4.6075978247,3.129500872,2.6697609168	H,-3.6162695715,1.9274346472,3.6132997011
H,-2.978484104,2.8161532621,2.0328759883	H,-1.9909516799,1.4732656408,3.1368900849
H,-4.0748428638,3.9360701384,1.2020563761	H,-2.8308069517,2.7704595374,2.2576837121
N,-5.8355219686,1.9239410257,0.4916560822	N,-3.4772842557,-0.5278794506,2.1747405617
O,-6.2724291419,1.1086404703,-0.3466486988	O,-3.2221014027,-0.7458133812,3.3733552565
O,-6.5349633964,2.8553171755,0.9288230845	O,-3.659440047,-1.4481472247,1.3632590206

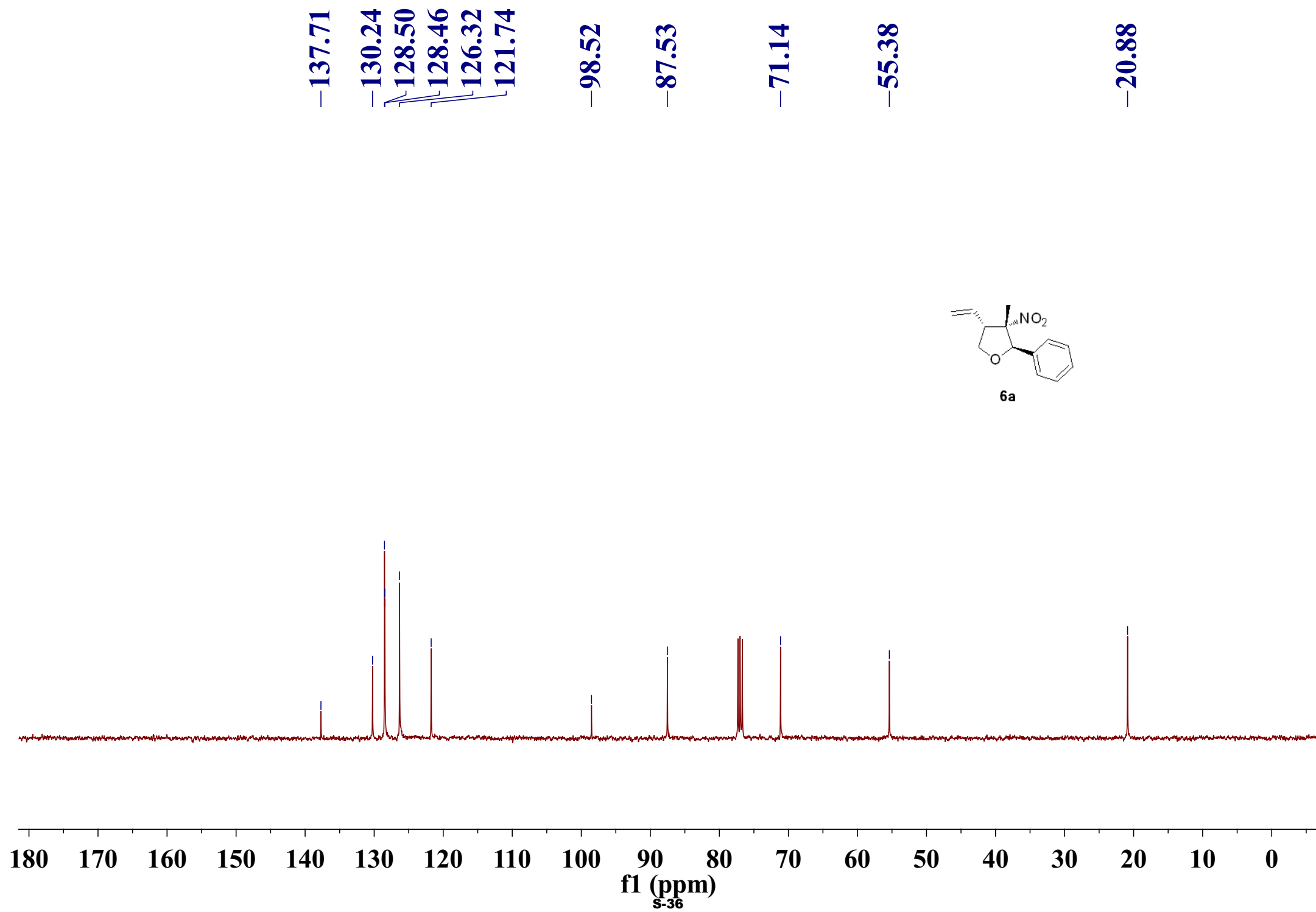
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Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

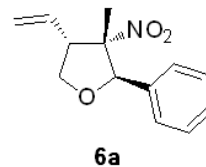
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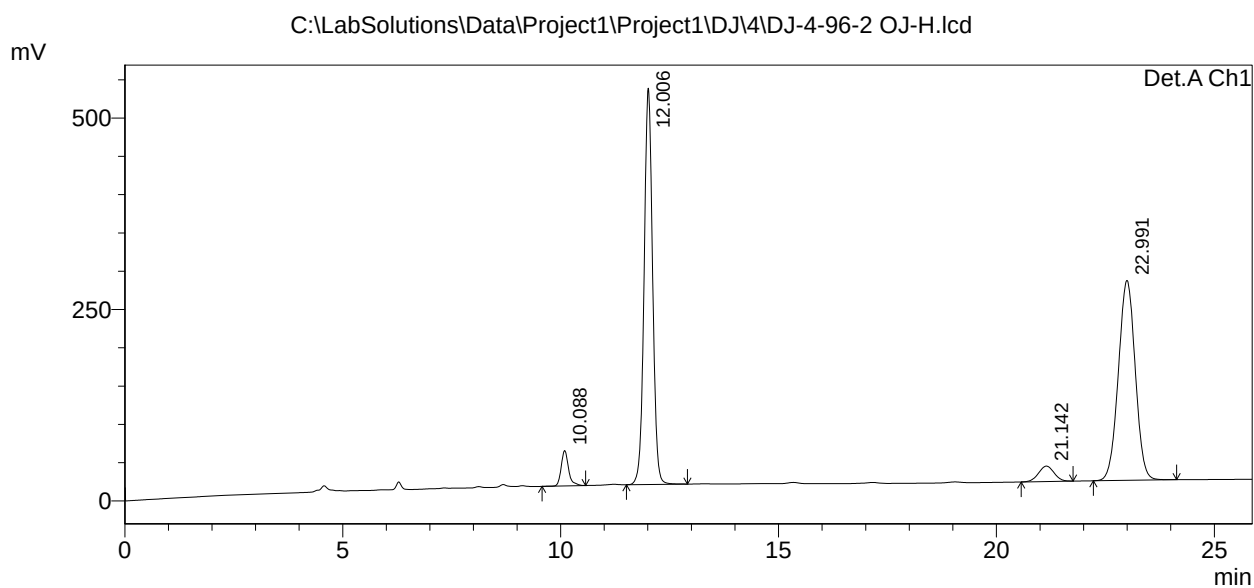


==== Shimadzu LCsolution Analysis Report =====

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 Sample ID : OJ-H,90/10,0.7,214
 Vail # :
 Injection Volume : 2 uL
 Data File Name : DJ-4-96-2 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-9-3 21:41:54
 Data Processed : 2016-9-3 22:07:46



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1 Det.A Ch1/214nm

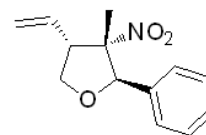
PeakTable

Detector A Ch1 214nm

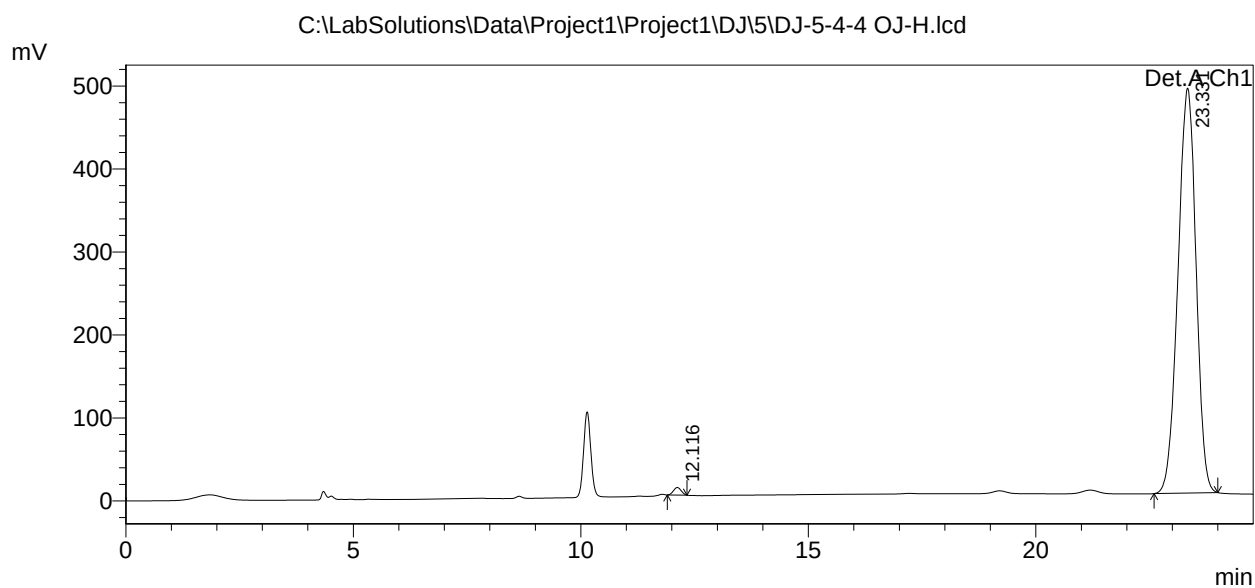
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.088	542166	46174	3.591	5.465
2	12.006	7014615	517538	46.464	61.254
3	21.142	500166	20165	3.313	2.387
4	22.991	7040067	261026	46.632	30.894
Total		15097014	844904	100.000	100.000

==== Shimadzu LcSolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\5\DJ-5-4-4 OJ-H.lcd
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 Sample ID : OJ-H,90/10,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-5-4-4 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-9-11 19:19:44
 Data Processed : 2016-9-11 21:49:47

**6a**

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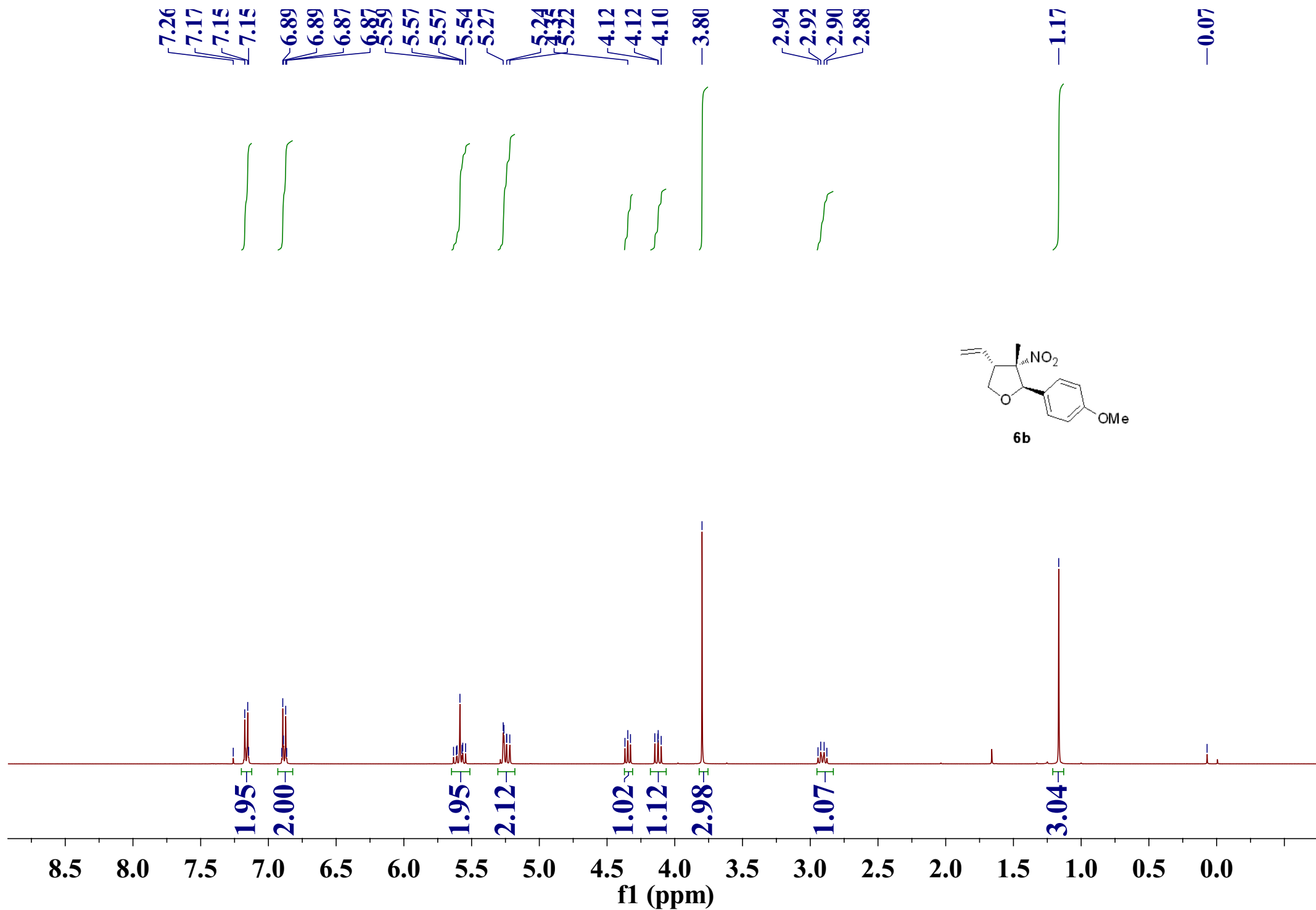


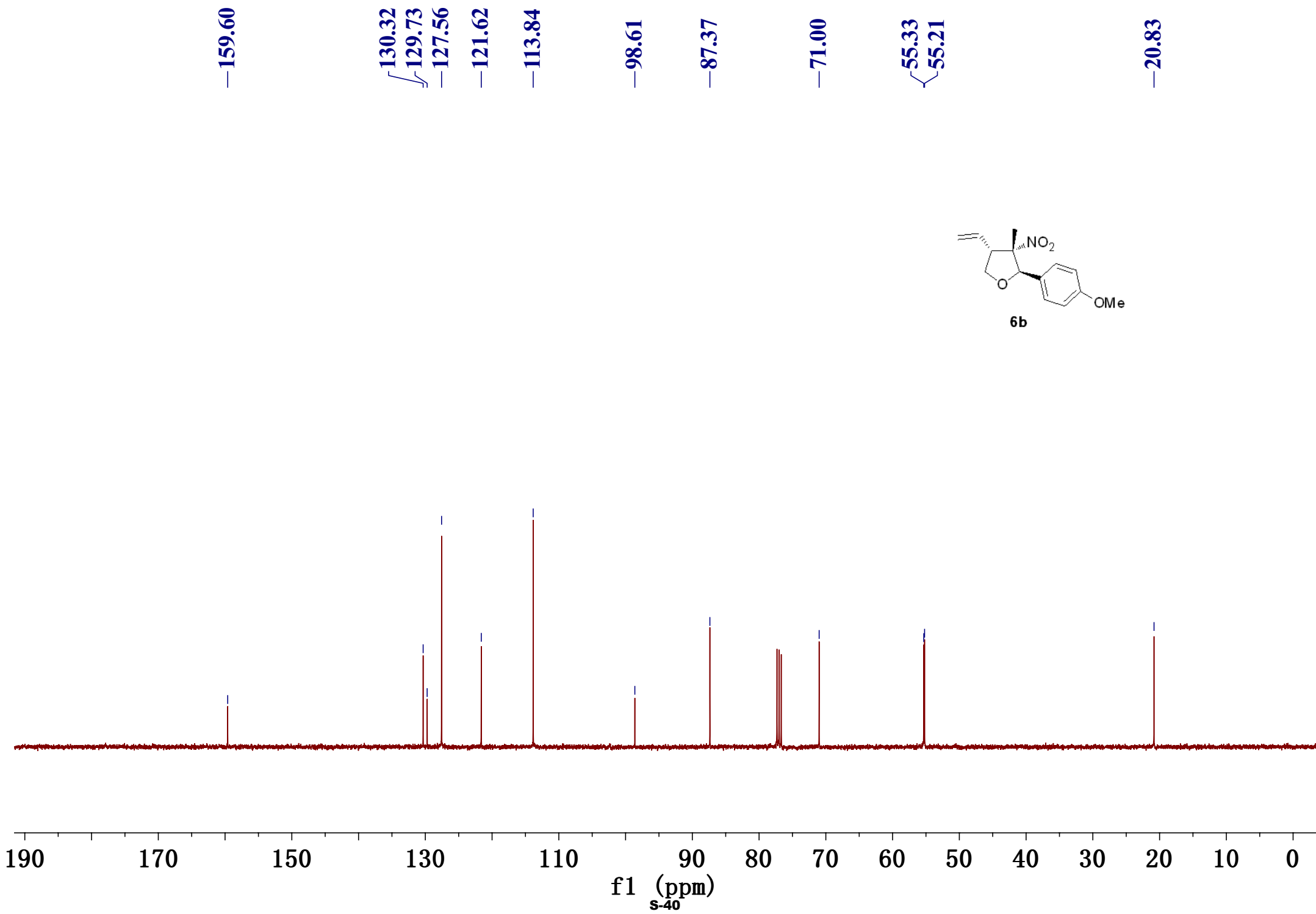
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.116	108080	9129	0.796	1.836
2	23.331	13471524	487987	99.204	98.164
Total		13579604	497116	100.000	100.000

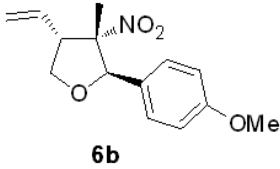




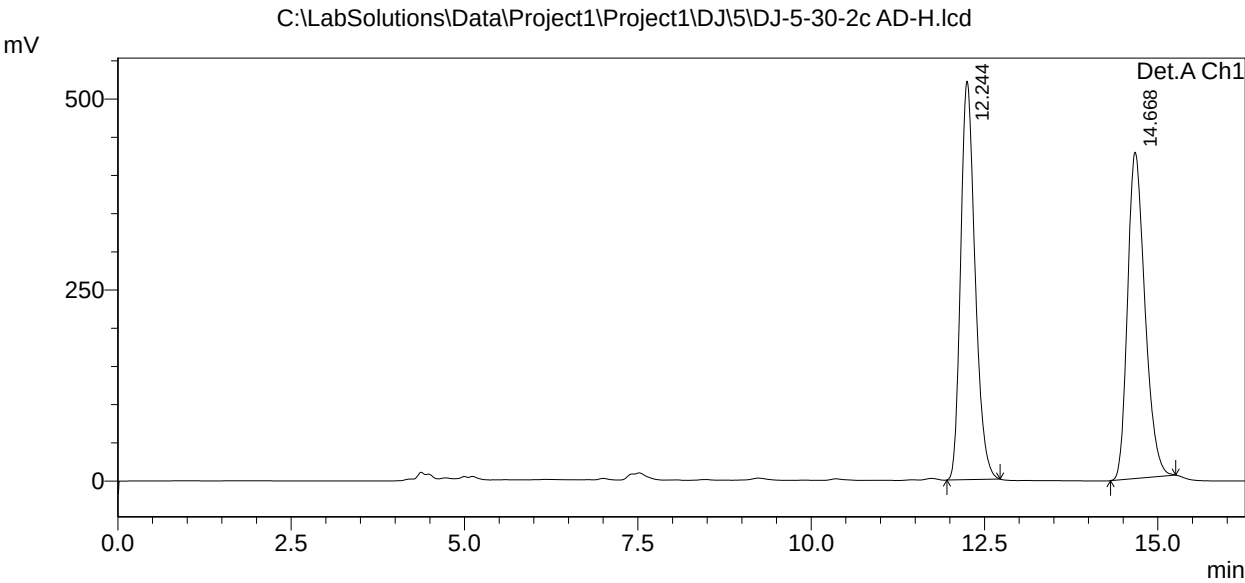
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\5\DJ-5-30-2c AD-H.lcd

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Sample Name : DJ-5-30-2c AD-H
Sample ID : AD-H,95/5,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : DJ-5-30-2c AD-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
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1 Det.A Ch1/214nm

PeakTable

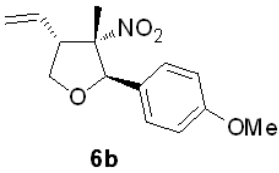
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.244	7551254	521569	50.353	54.981
2	14.668	7445416	427060	49.647	45.019
Total		14996669	948629	100.000	100.000

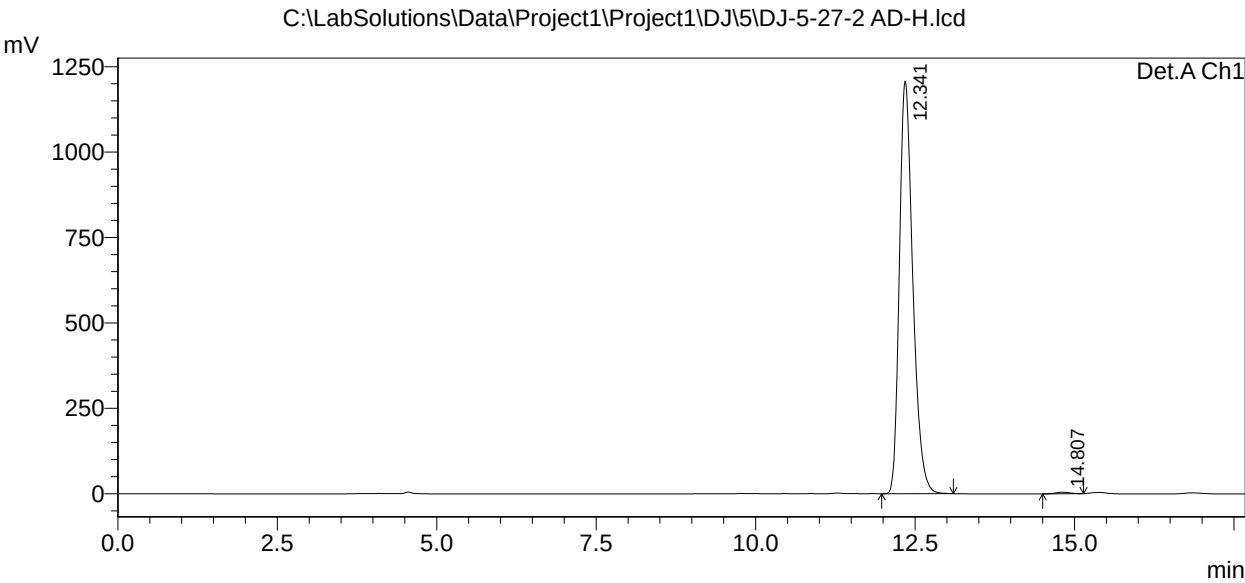
==== Shimadzu LCsolution Analysis Report ====

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Sample ID : AD-H,95/5,0.7,214
Vail # :
Injection Volume : 2 uL
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Method File Name : 123.lcm
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Report File Name : Default.lcr
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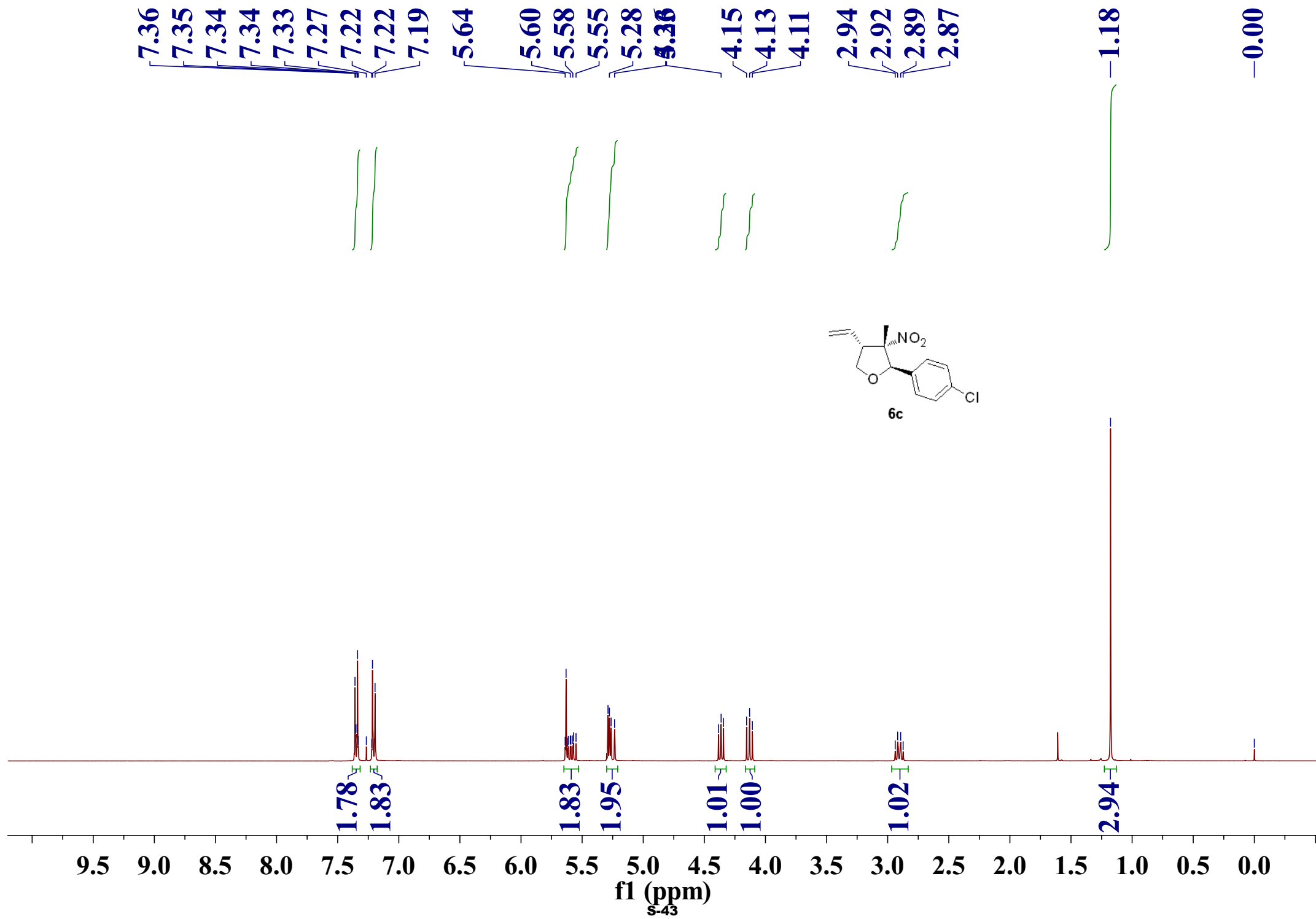
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1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm					
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2	14.807	73828	4764	0.415	0.393
Total		17793557	1212552	100.000	100.000



136.15
134.33
130.14
128.78
127.75
121.93

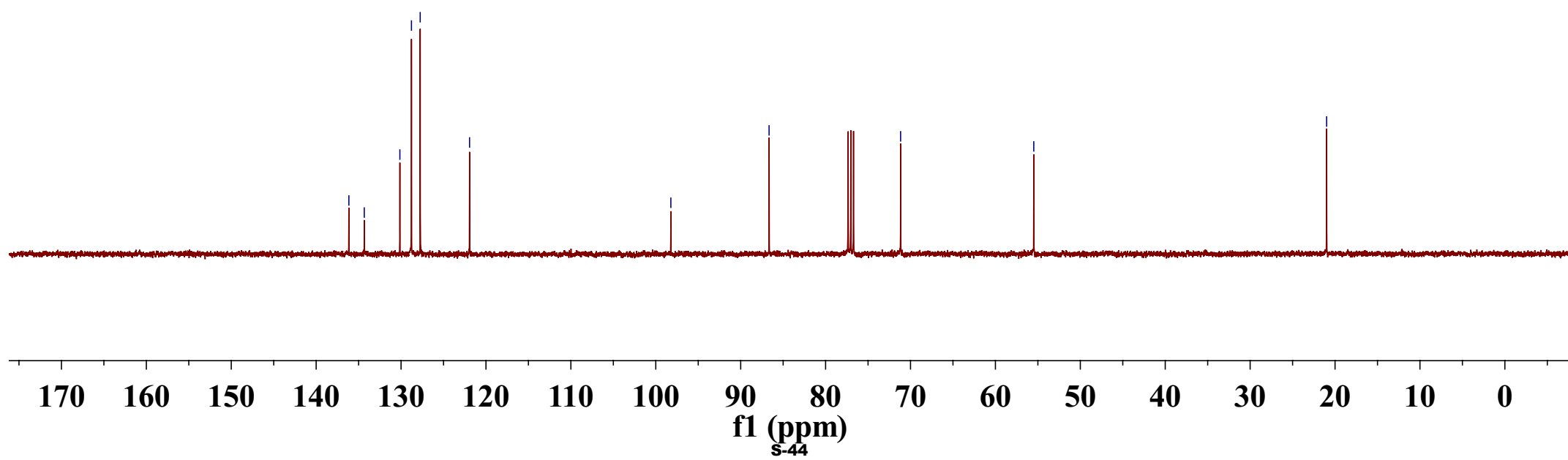
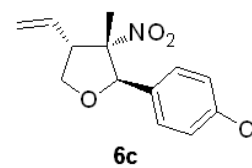
98.23

86.66

71.17

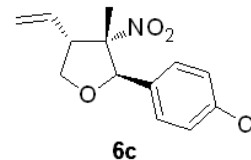
55.48

20.99

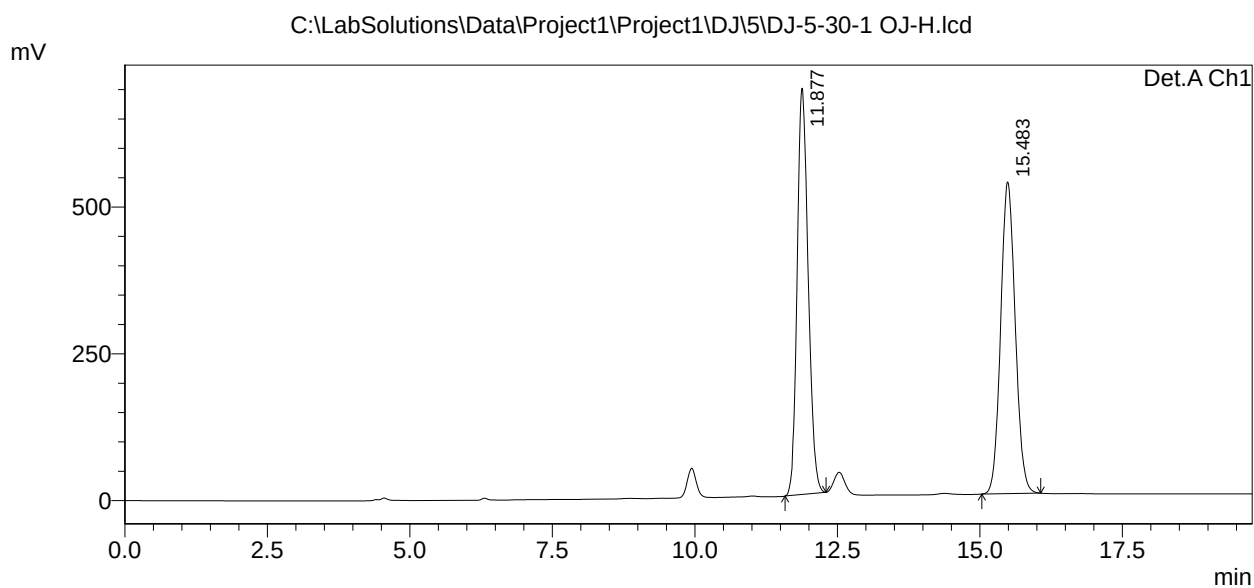


==== Shimadzu LCsolution Analysis Report =====

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 Sample ID : OJ-H,90/10,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-5-30-1 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
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1 Det.A Ch1/214nm

PeakTable

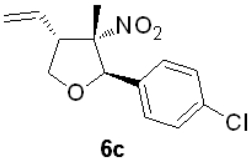
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.877	9332643	692195	49.686	56.587
2	15.483	9450515	531037	50.314	43.413
Total		18783158	1223232	100.000	100.000

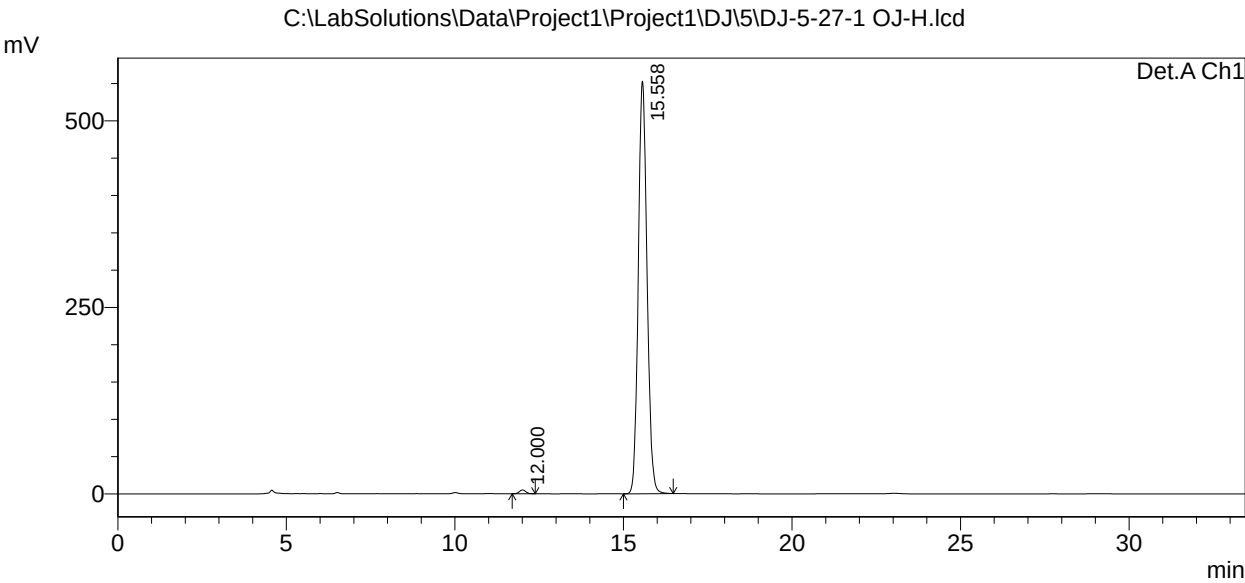
==== Shimadzu LCsolution Analysis Report ====

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Acquired by : Admin
Sample Name : DJ-5-27-1 OJ-H
Sample ID : OJ-H,90/10,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : DJ-5-27-1 OJ-H.lcd
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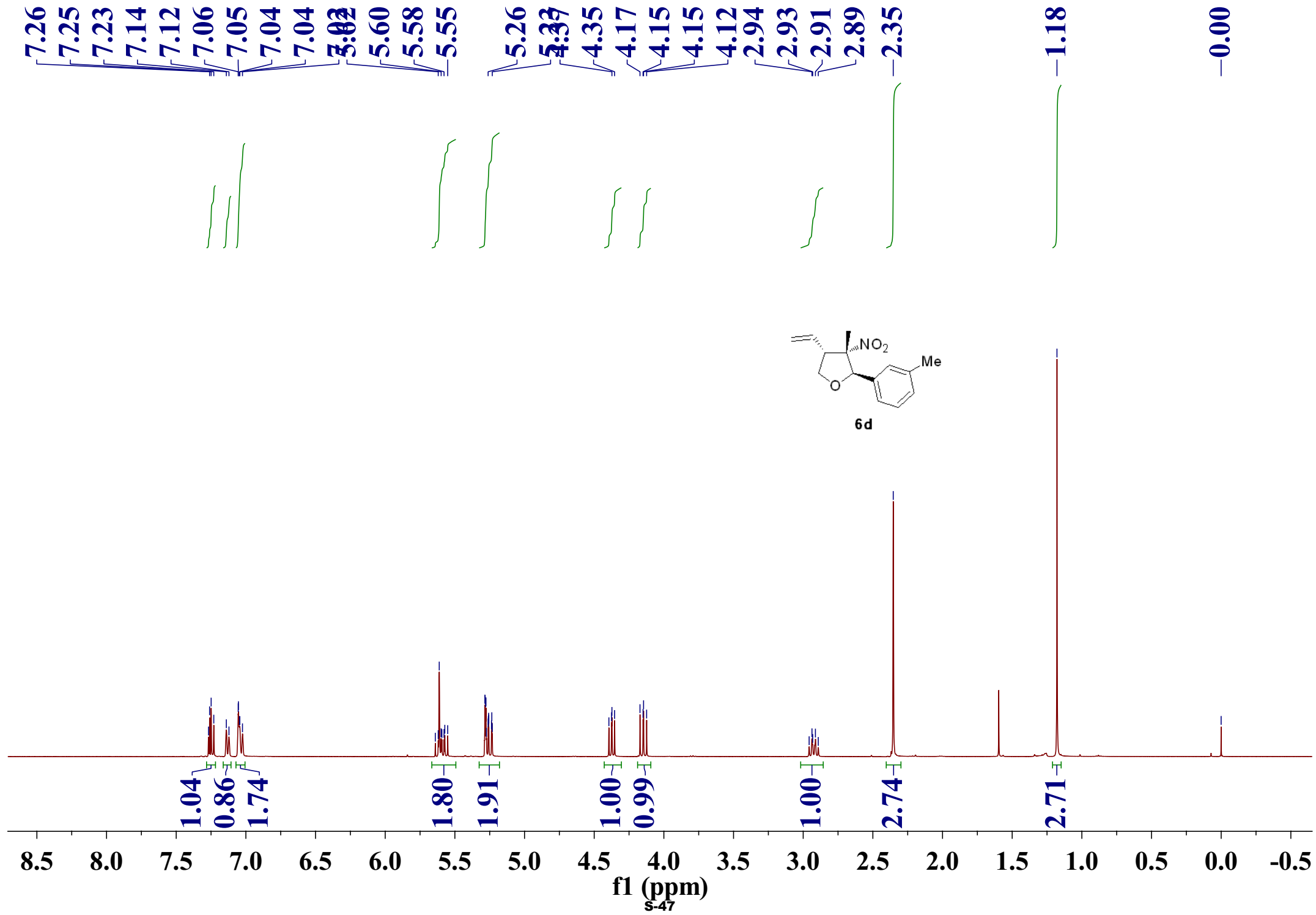
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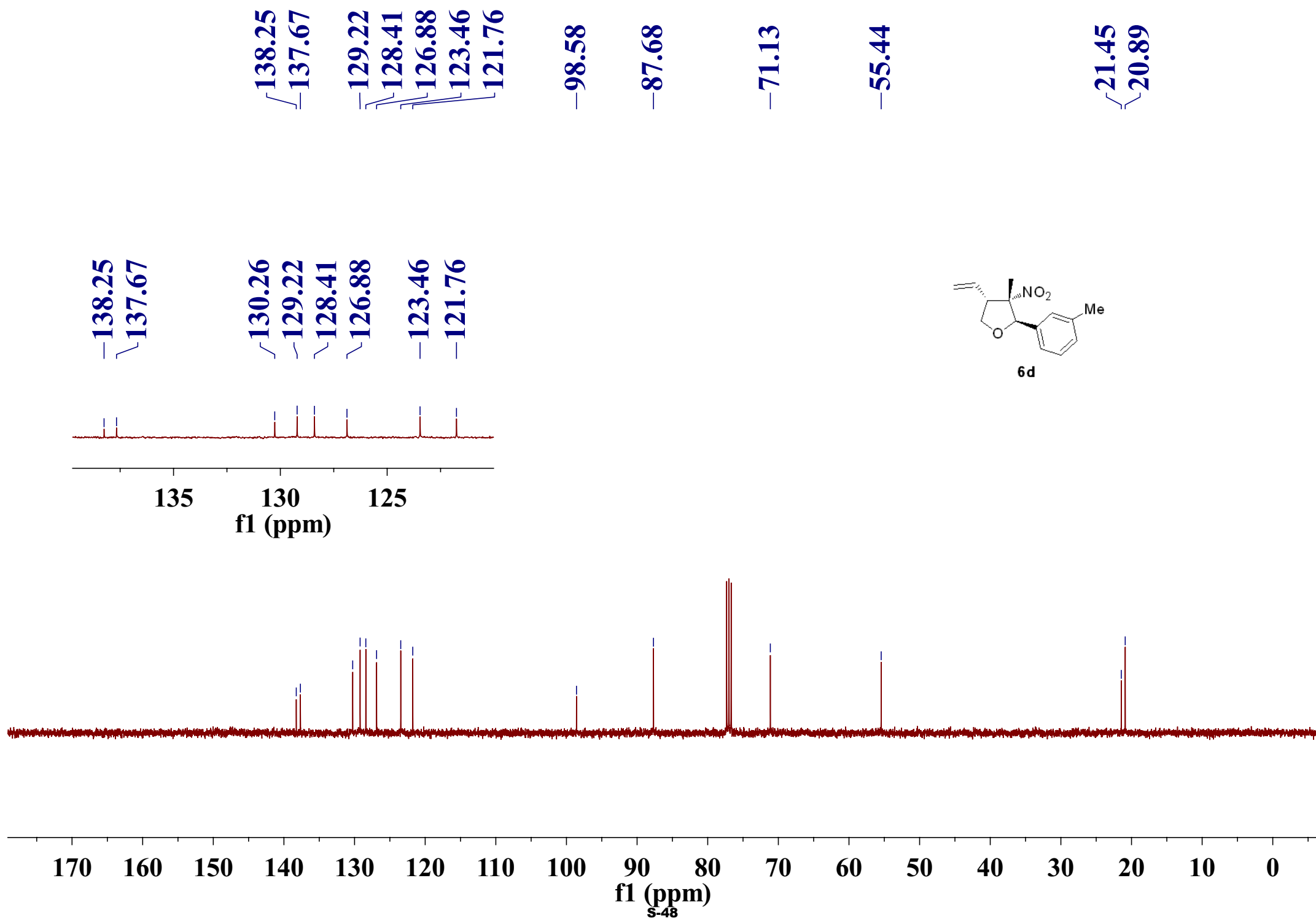


1 Det.A Ch1/214nm

PeakTable

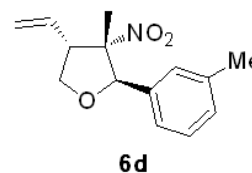
Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
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2	15.558	9957512	552967	99.300	99.075
Total		10027666	558128	100.000	100.000



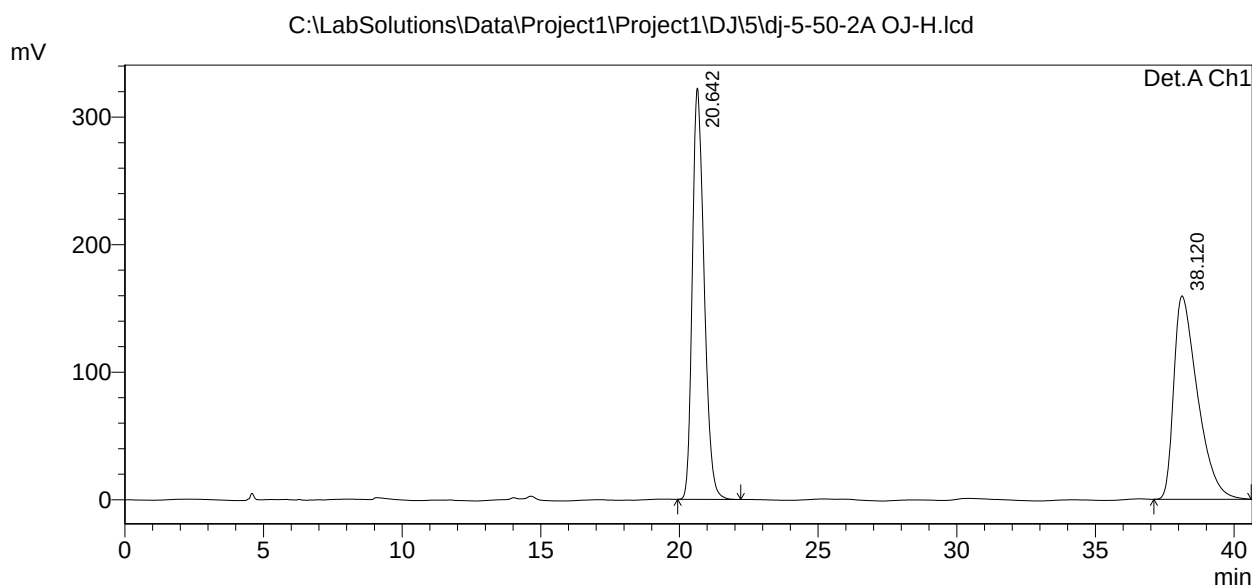


==== Shimadzu LCsolution Analysis Report =====

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 Sample ID : OJ-H,99.5/0.5,0.7,214
 Vial # :
 Injection Volume : 2 uL
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 Method File Name : 123.lcm
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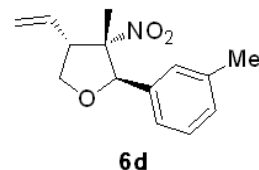
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Detector A Ch1 214nm

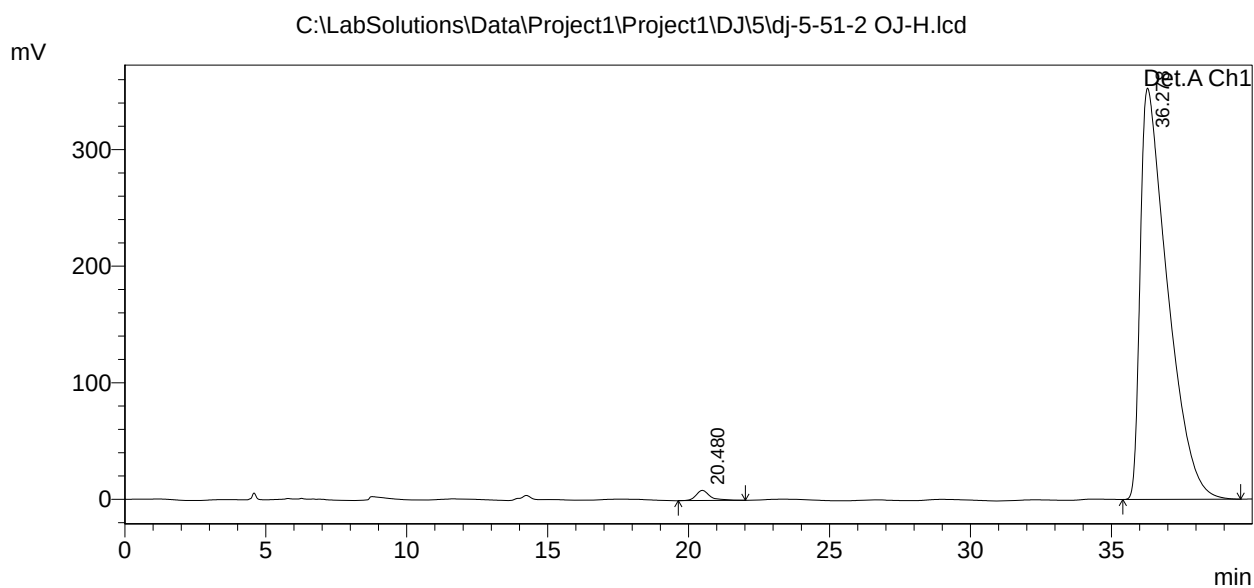
Peak#	Ret. Time	Area	Height	Area %	Height %
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2	38.120	9493625	159525	49.766	33.094
Total		19076582	482037	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

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 Sample ID : OJ-H,99.5/0.5,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-5-51-2 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-10-29 13:44:57
 Data Processed : 2016-10-29 14:24:57



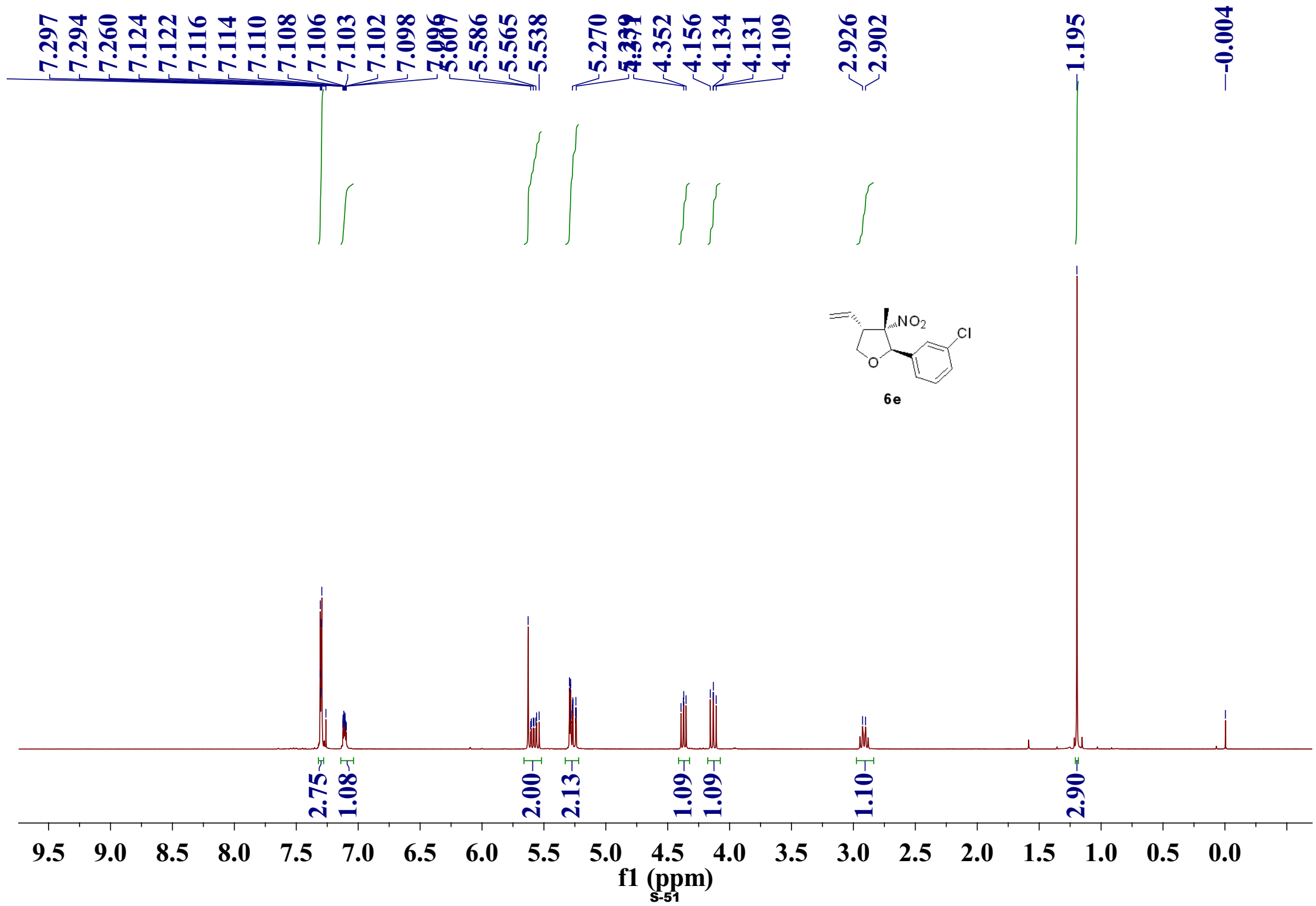
<Chromatogram>

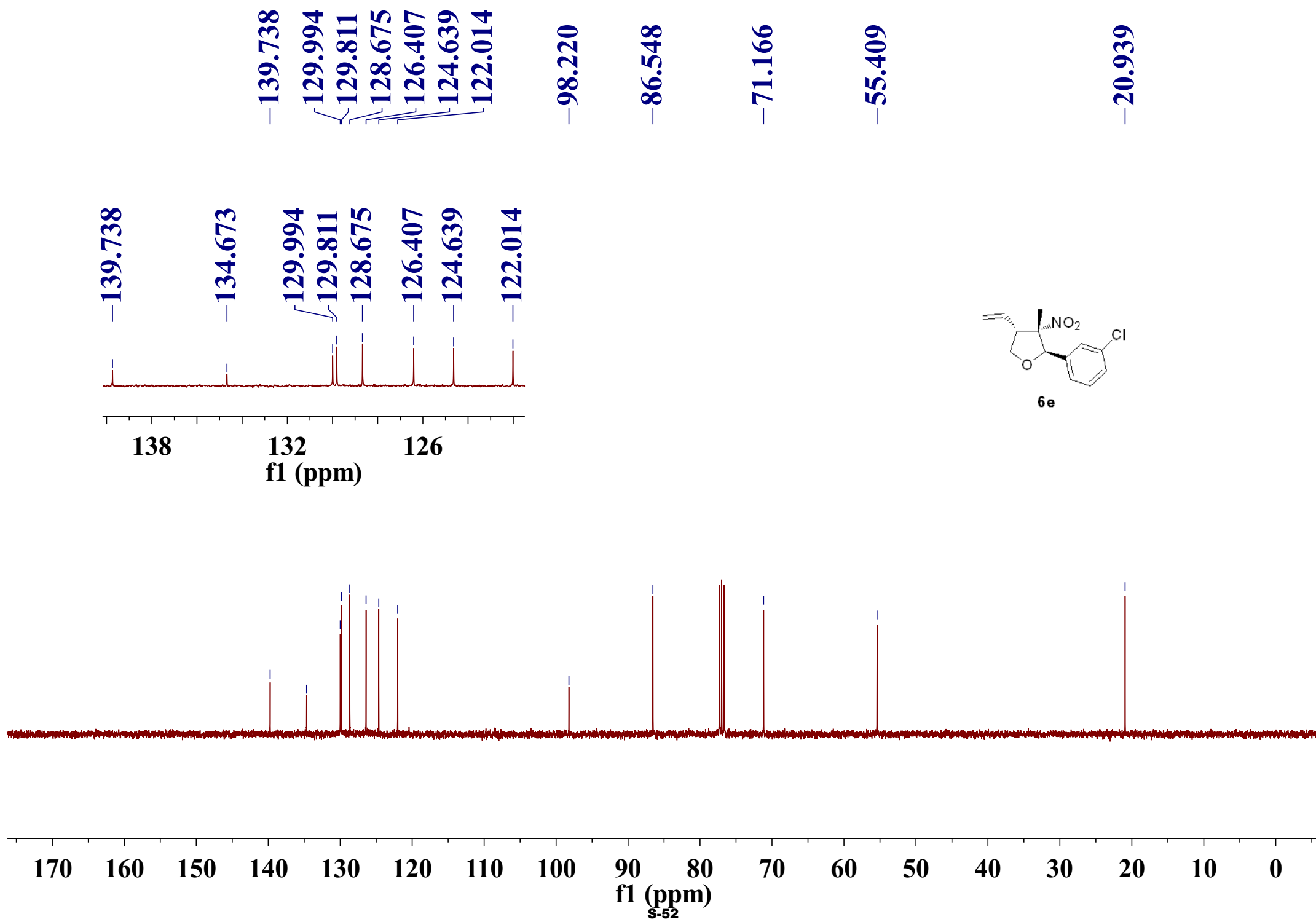


PeakTable

Detector A Ch1 214nm

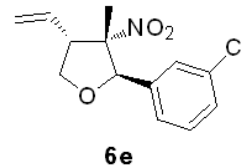
Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.480	303874	8700	1.264	2.406
2	36.278	23735988	352855	98.736	97.594
Total		24039863	361555	100.000	100.000



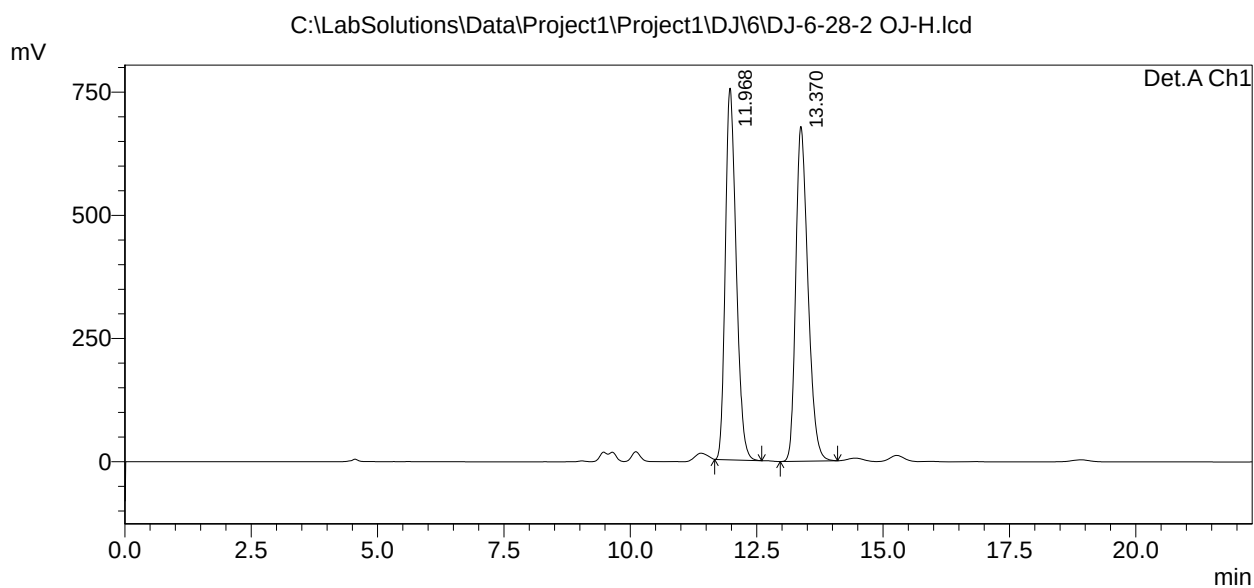


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\DJ-6-28-2 OJ-H.lcd
 Acquired by : Admin
 Sample Name : DJ-6-28-2 OJ-H
 Sample ID : OJ-H,92/8,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-6-28-2 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-12-19 9:19:21
 Data Processed : 2016-12-19 9:41:39



<Chromatogram>



1 Det.A Ch1/214nm

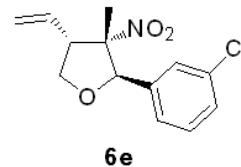
PeakTable

Detector A Ch1 214nm

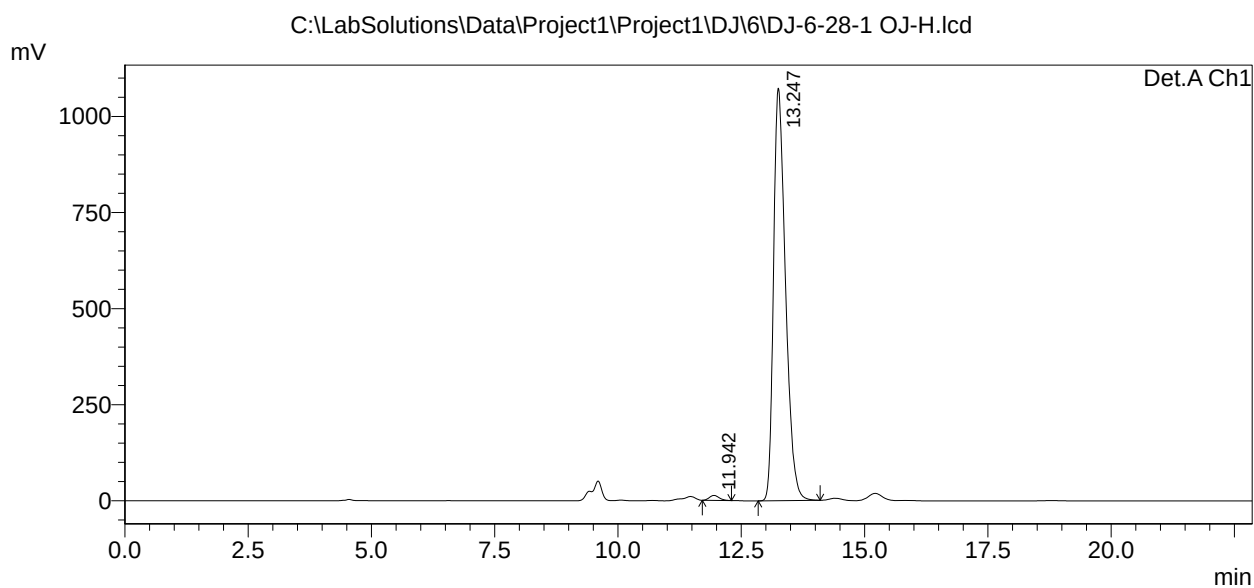
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.968	11272620	754175	49.671	52.608
2	13.370	11422148	679389	50.329	47.392
Total		22694768	1433564	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\DJ-6-28-1 OJ-H.lcd
 Acquired by : Admin
 Sample Name : DJ-6-28-1 OJ-H
 Sample ID : OJ-H,92/8,0.7,214
 Vail # :
 Injection Volume : 2 uL
 Data File Name : DJ-6-28-1 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-12-19 9:45:33
 Data Processed : 2016-12-19 10:08:25



<Chromatogram>

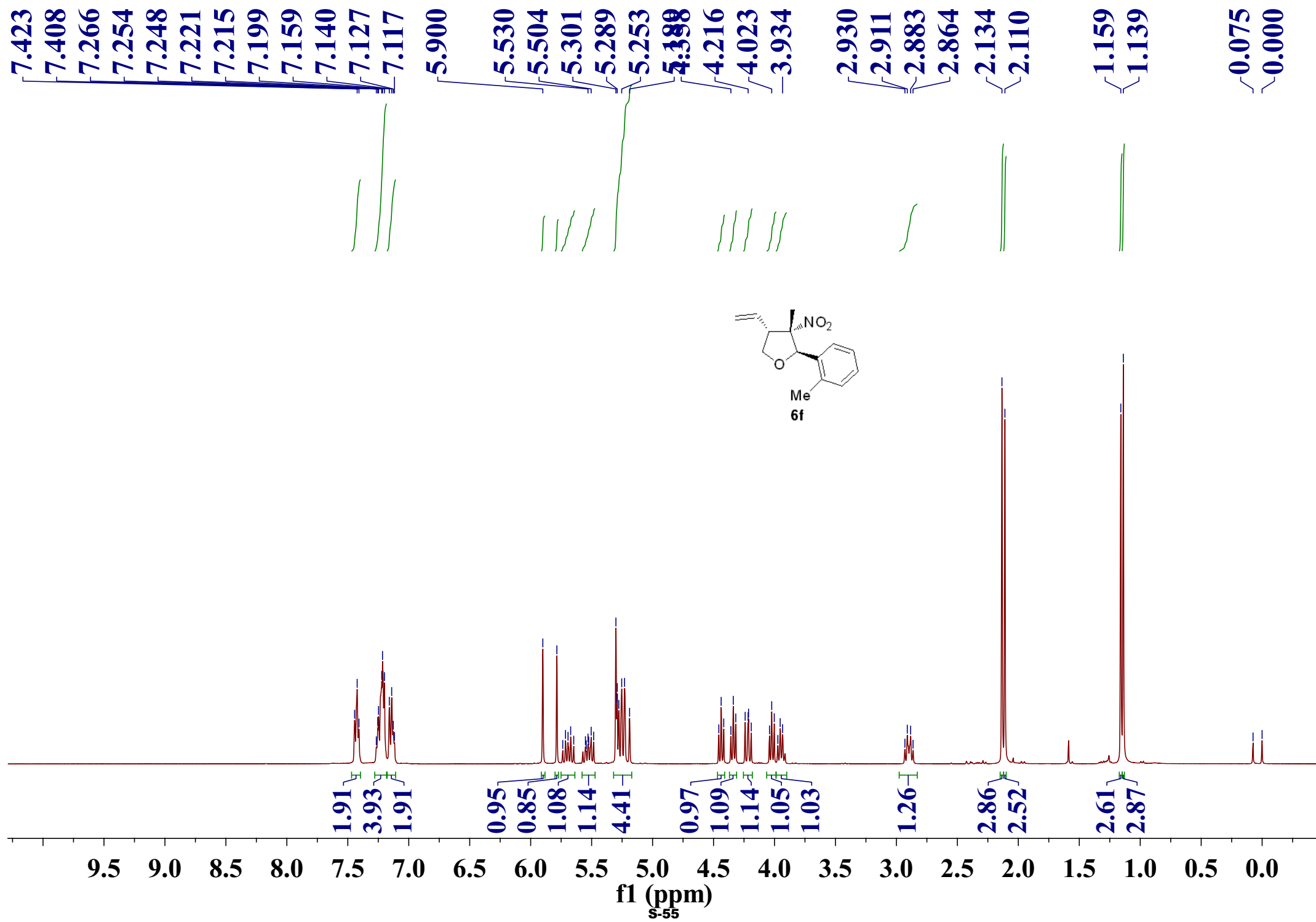


1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.942	179484	12922	0.979	1.189
2	13.247	18153640	1073762	99.021	98.811
Total		18333124	1086683	100.000	100.000



136.369
135.542
134.694
134.326
132.111
130.678
130.480
129.456
128.240
128.092
126.908
126.294
125.923
125.748
122.238
120.418

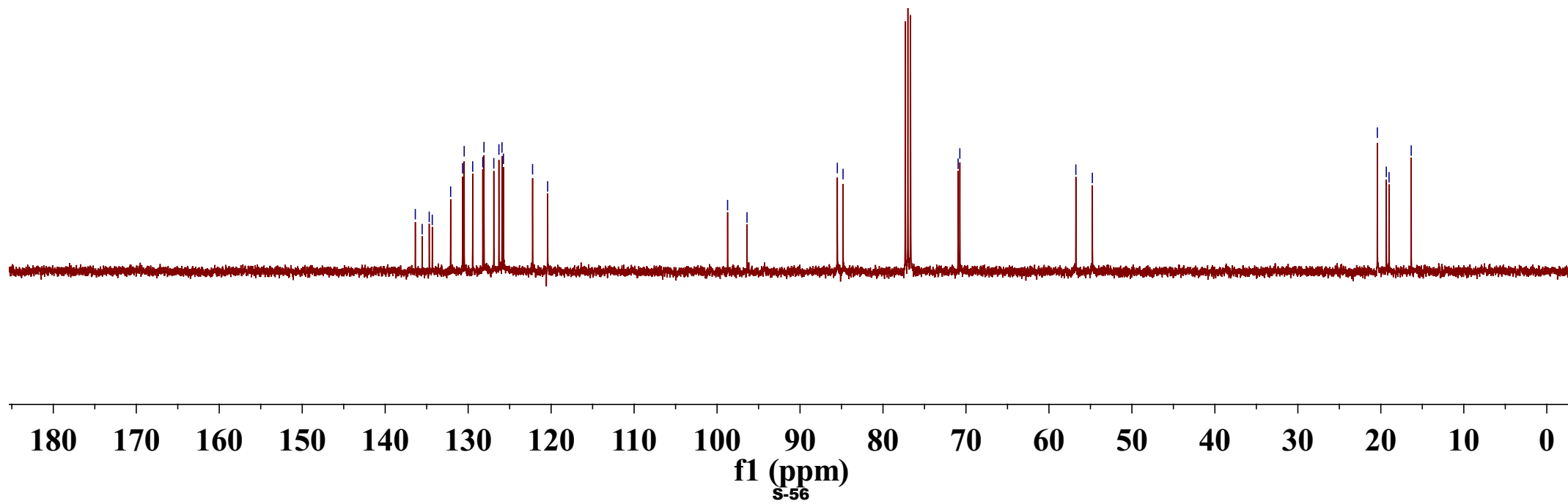
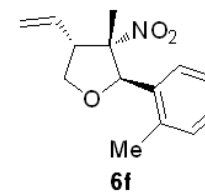
98.732
96.391

85.504
84.816

70.947
70.740

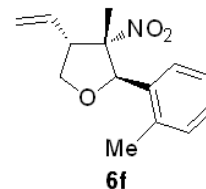
56.756
54.768

20.418
19.339
19.007
16.338

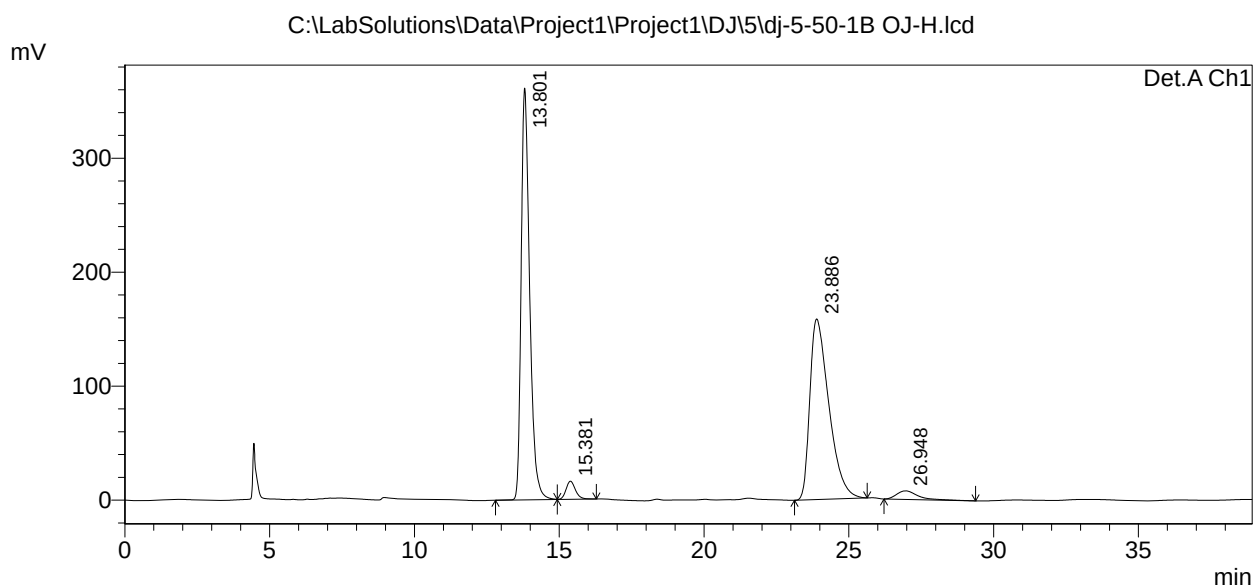


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\5\dj-5-50-1B OJ-H.lcd
 Acquired by : Admin
 Sample Name : dj-5-50-1B OJ-H
 Sample ID : OJ-H,99.5/0.5,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-5-50-1B OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-10-29 15:12:29
 Data Processed : 2016-10-29 15:51:26



<Chromatogram>



1 Det.A Ch1/214nm

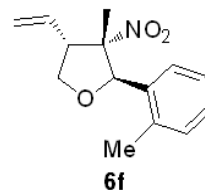
PeakTable

Detector A Ch1 214nm

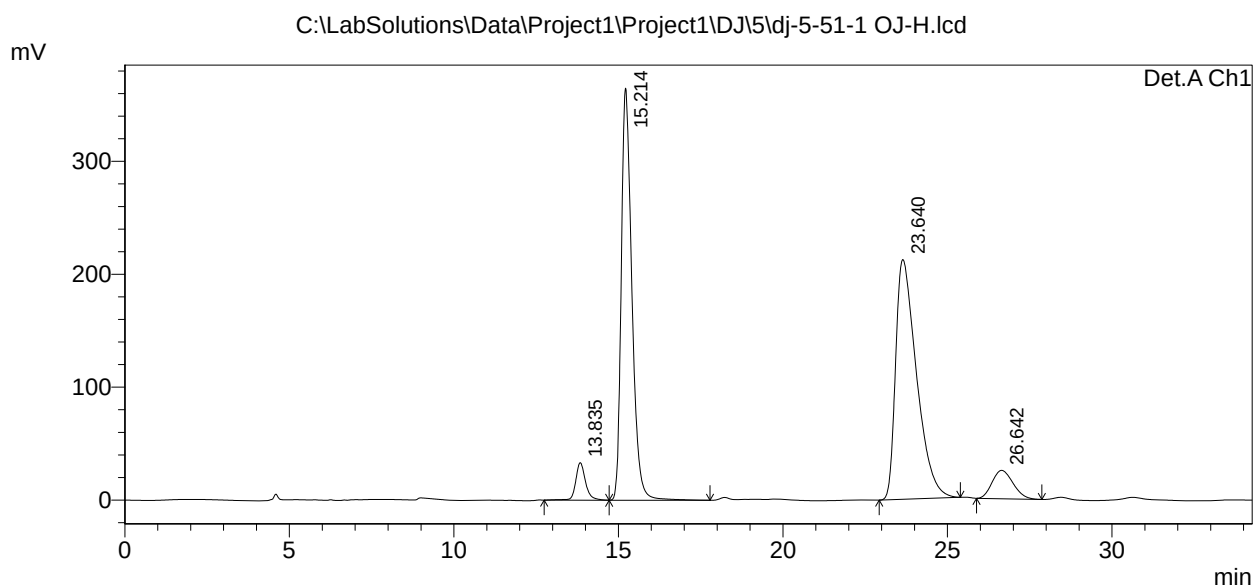
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.801	7379752	361268	48.008	66.501
2	15.381	360810	15951	2.347	2.936
3	23.886	7241497	158487	47.108	29.174
4	26.948	389983	7543	2.537	1.389
Total		15372042	543250	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\5\dj-5-51-1 OJ-H.lcd
 Acquired by : Admin
 Sample Name : dj-5-51-1 OJ-H
 Sample ID : OJ-H,99.5/0.5,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-5-51-1 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-10-29 13:08:55
 Data Processed : 2016-10-29 13:43:11



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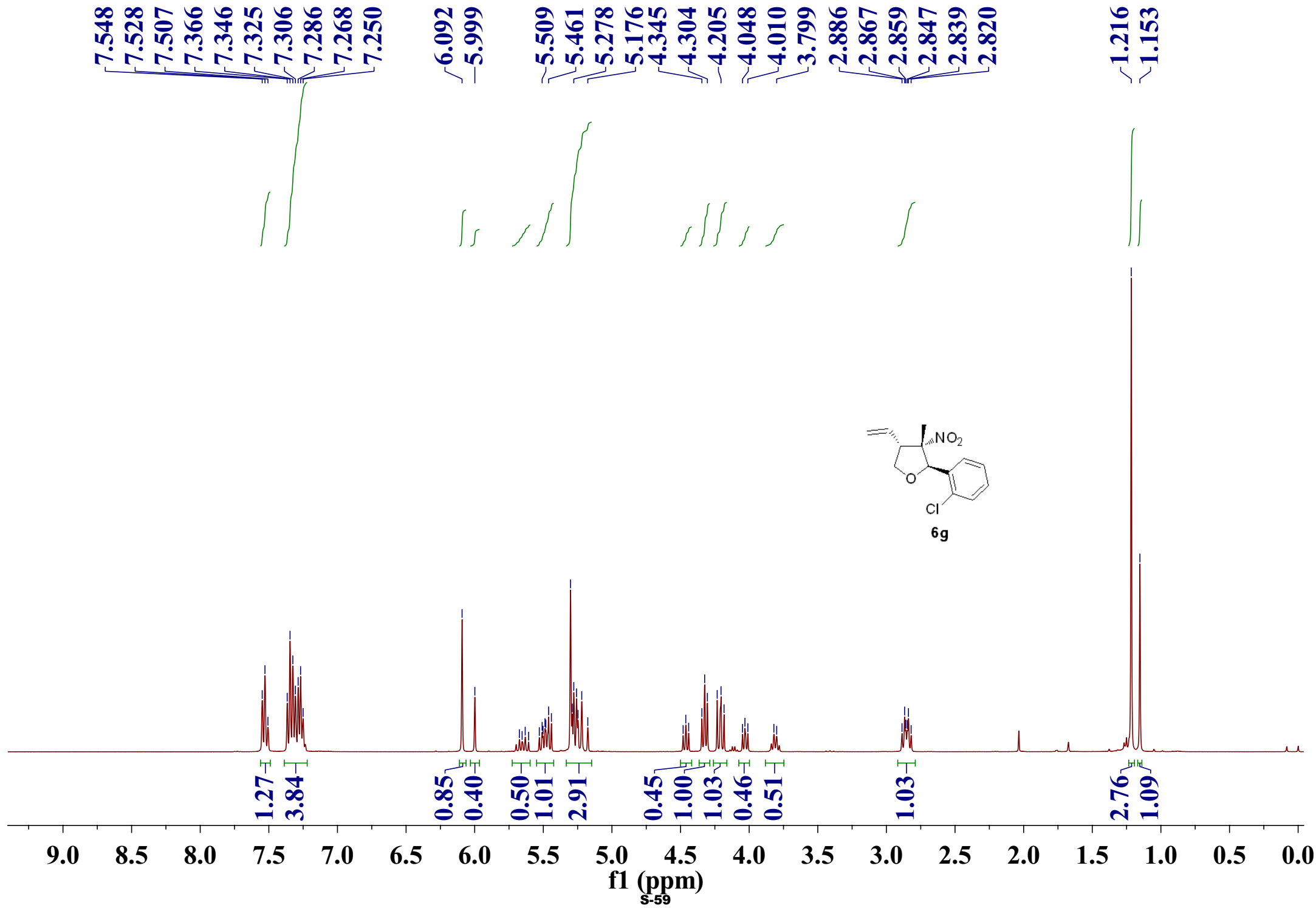


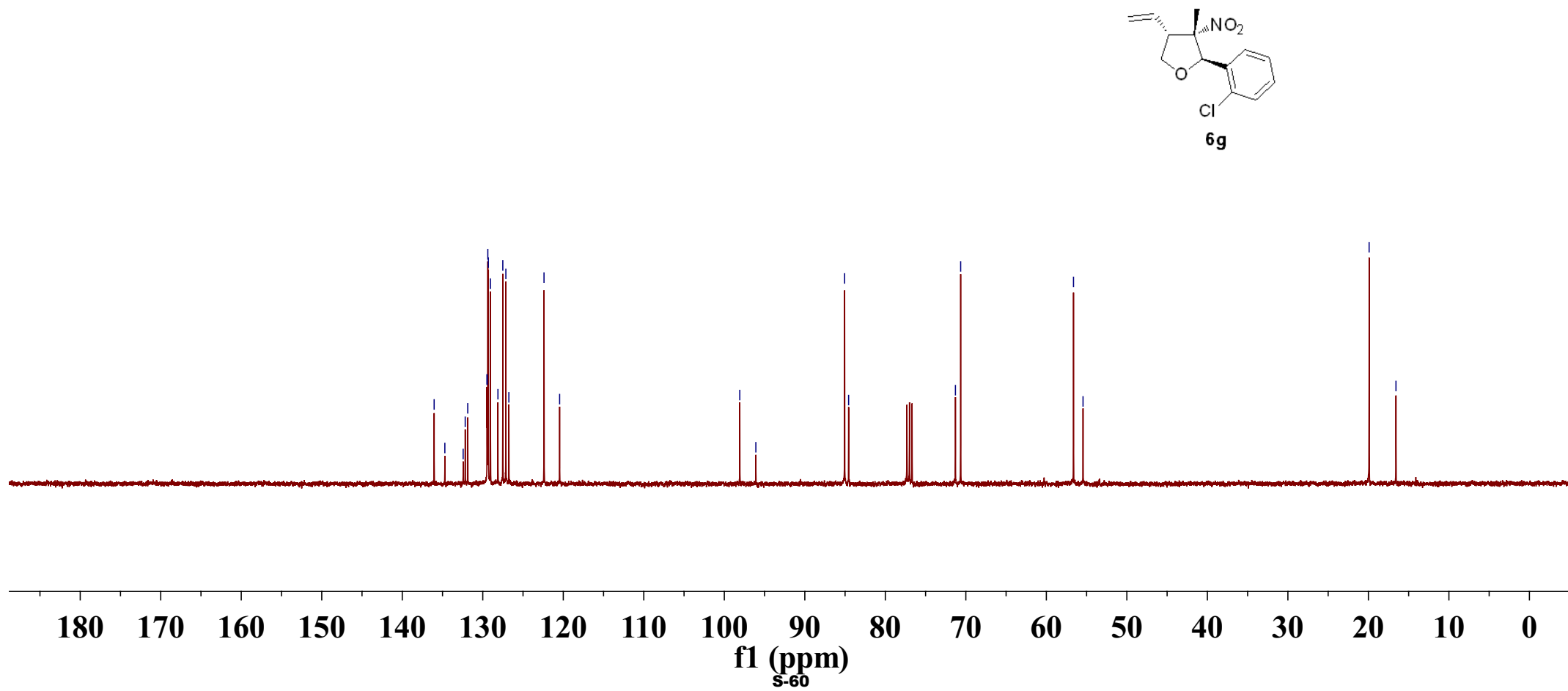
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

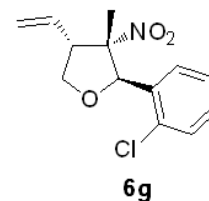
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.835	690039	33217	3.562	5.226
2	15.214	8212859	364950	42.396	57.414
3	23.640	9356027	212351	48.297	33.407
4	26.642	1112793	25125	5.744	3.953
Total		19371718	635643	100.000	100.000



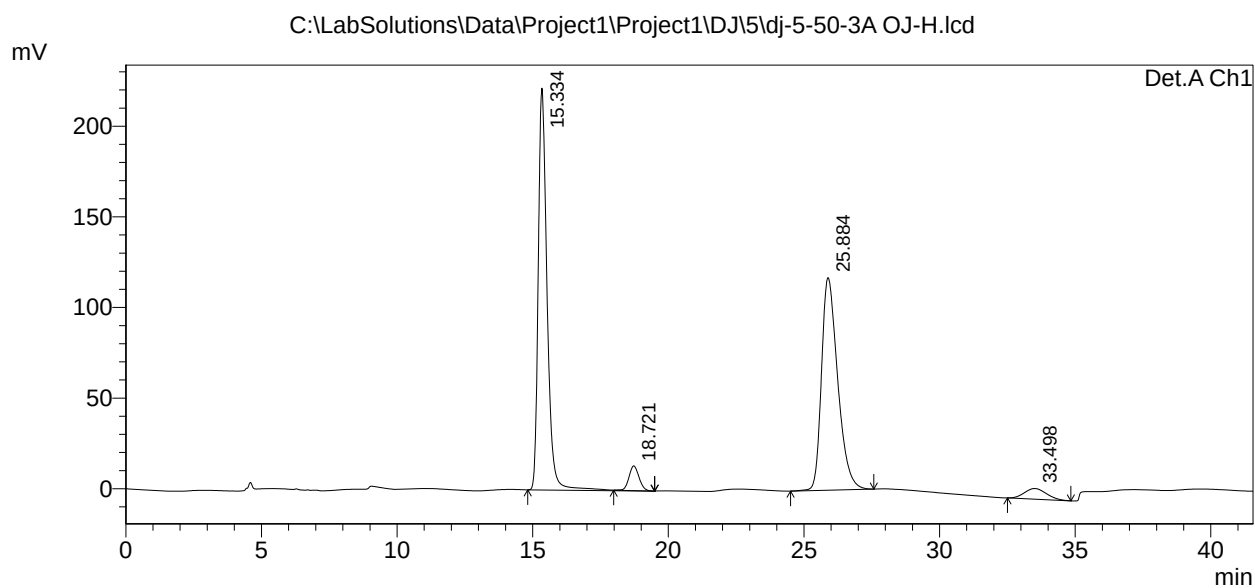


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\5\dj-5-50-3A OJ-H.lcd
 Acquired by : Admin
 Sample Name : dj-5-50-3A OJ-H
 Sample ID : OJ-H,99.5/0.5,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-5-50-3A OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-10-29 12:25:37
 Data Processed : 2016-10-29 13:07:11



<Chromatogram>



1 Det.A Ch1/214nm

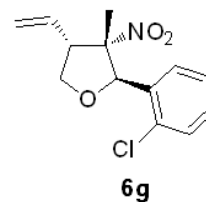
PeakTable

Detector A Ch1 214nm

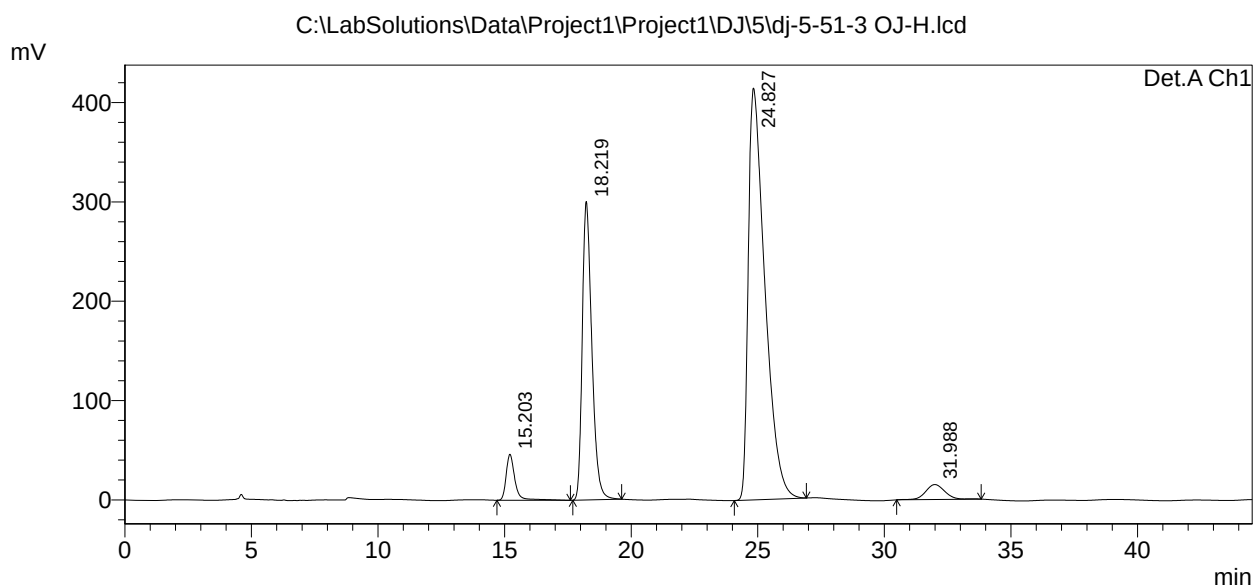
Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.334	5029203	221710	47.523	61.845
2	18.721	349989	13634	3.307	3.803
3	25.884	4868531	117259	46.004	32.709
4	33.498	335024	5892	3.166	1.643
Total		10582746	358494	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\5\dj-5-51-3 OJ-H.lcd
 Acquired by : Admin
 Sample Name : dj-5-51-3 OJ-H
 Sample ID : OJ-H,99.5/0.5,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-5-51-3 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-10-29 14:26:28
 Data Processed : 2016-10-30 20:14:08



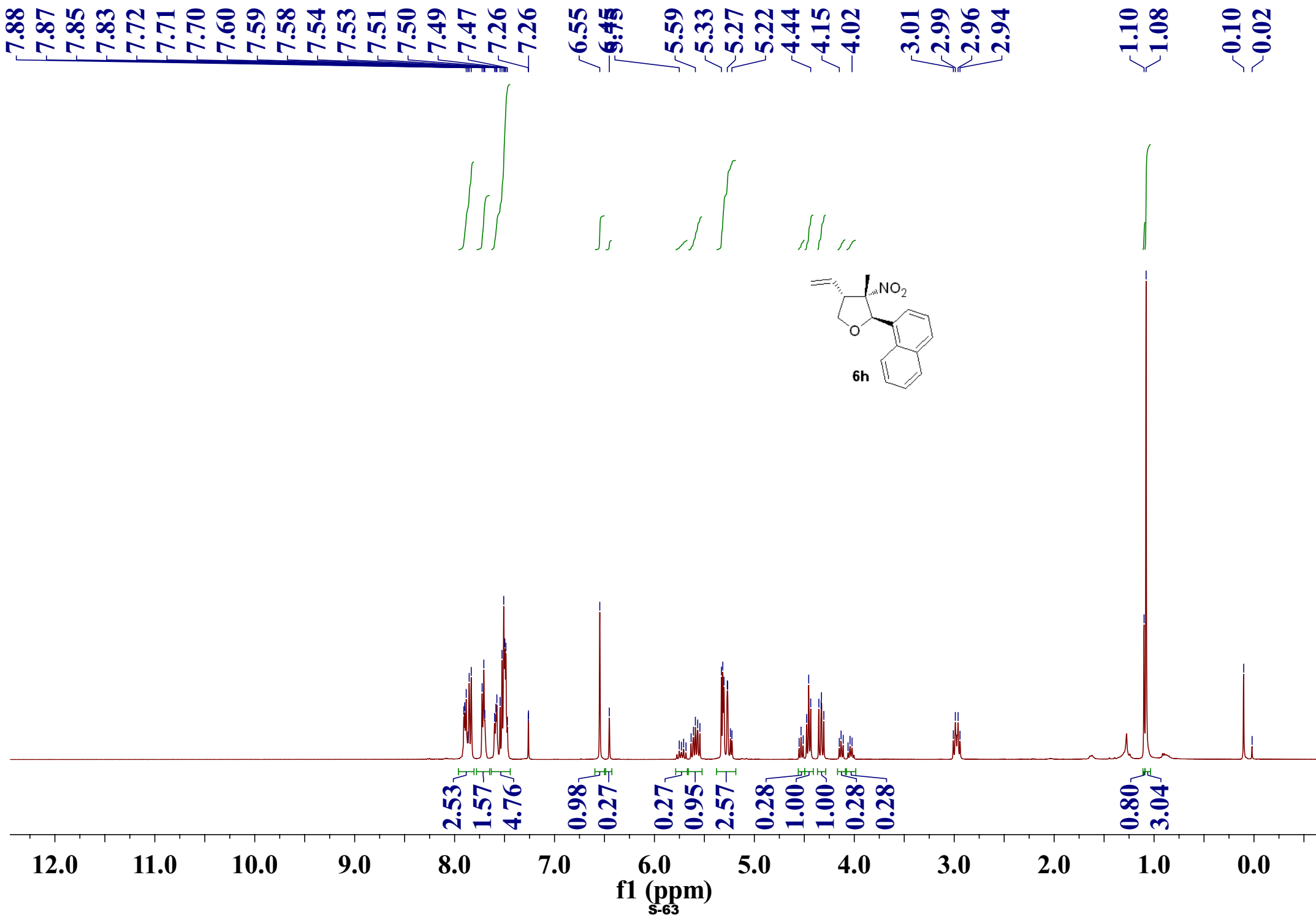
<Chromatogram>



PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.203	1128730	46340	3.926	5.969
2	18.219	7890306	300466	27.444	38.702
3	24.827	18936457	414505	65.866	53.391
4	31.988	794557	15044	2.764	1.938
Total		28750050	776355	100.000	100.000



134.10
129.39
129.05
128.88
128.82
126.84
126.76
125.82
125.78
125.35
124.98
124.78
123.91
122.31
122.19
120.54

99.21
97.13

84.82
84.22

71.04
70.75

56.35
55.10

20.01
16.40

134.10
133.50
133.45

132.29
132.04

130.79
130.46

129.39
129.05
128.88
128.82

126.84
126.76

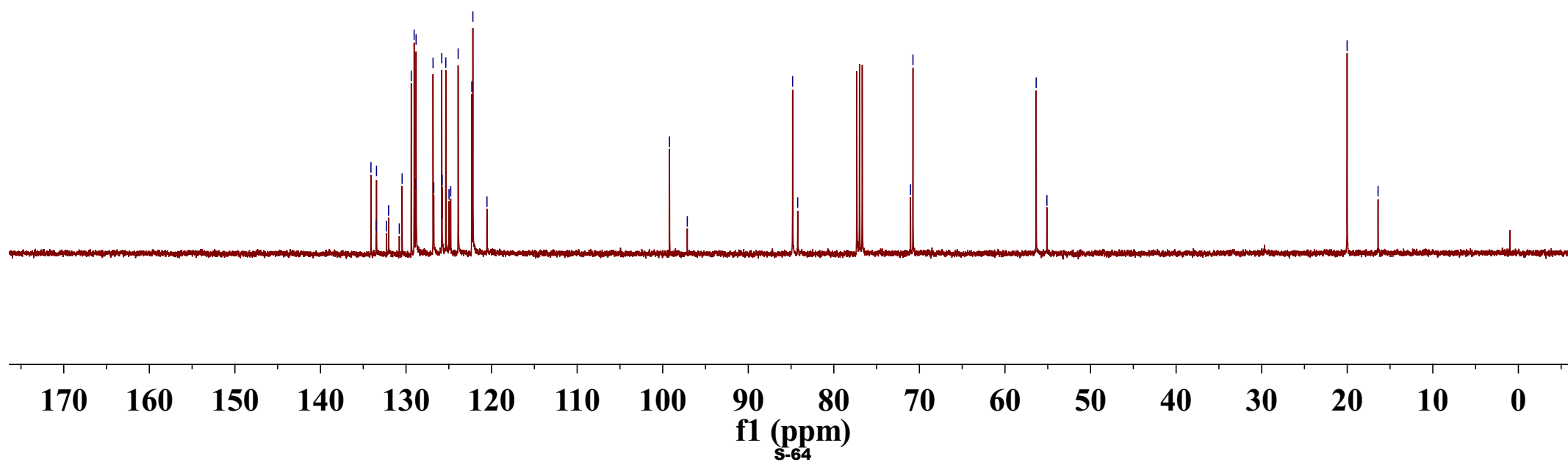
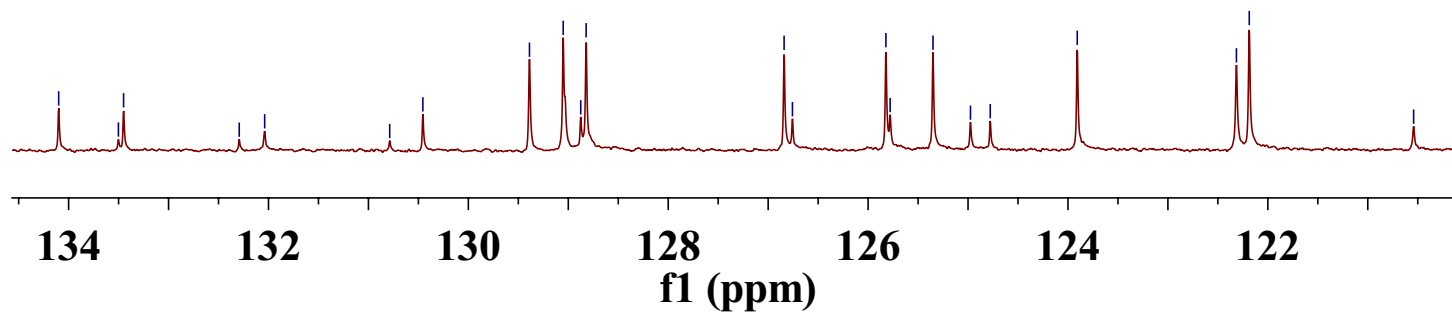
125.82
125.78

125.35
124.98
124.78

123.91

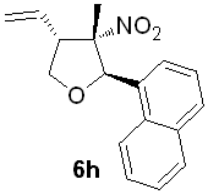
122.31
122.19

120.54

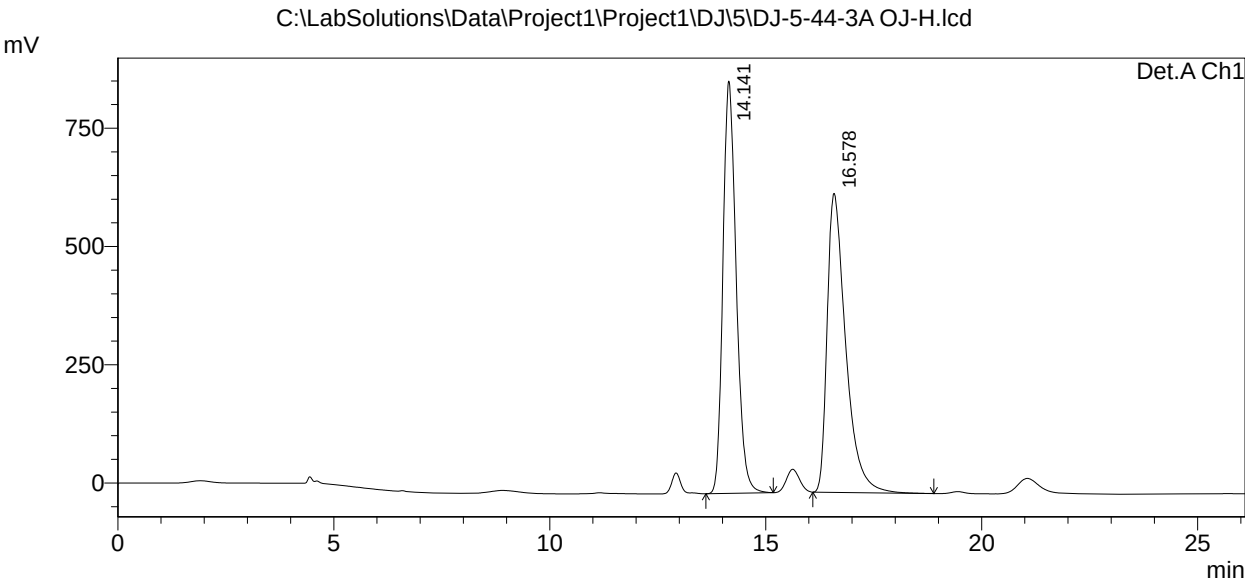


==== Shimadzu LCsolution Analysis Report ====

Acquired by : Admin
Sample Name : DJ-5-44-3A OJ-H
Sample ID : OJ-H,95/5,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : DJ-5-44-3A OJ-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2016-10-19 14:57:06
Data Processed : 2016-10-21 8:42:52



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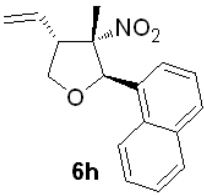
1 Det.A Ch1/214nm

PeakTable

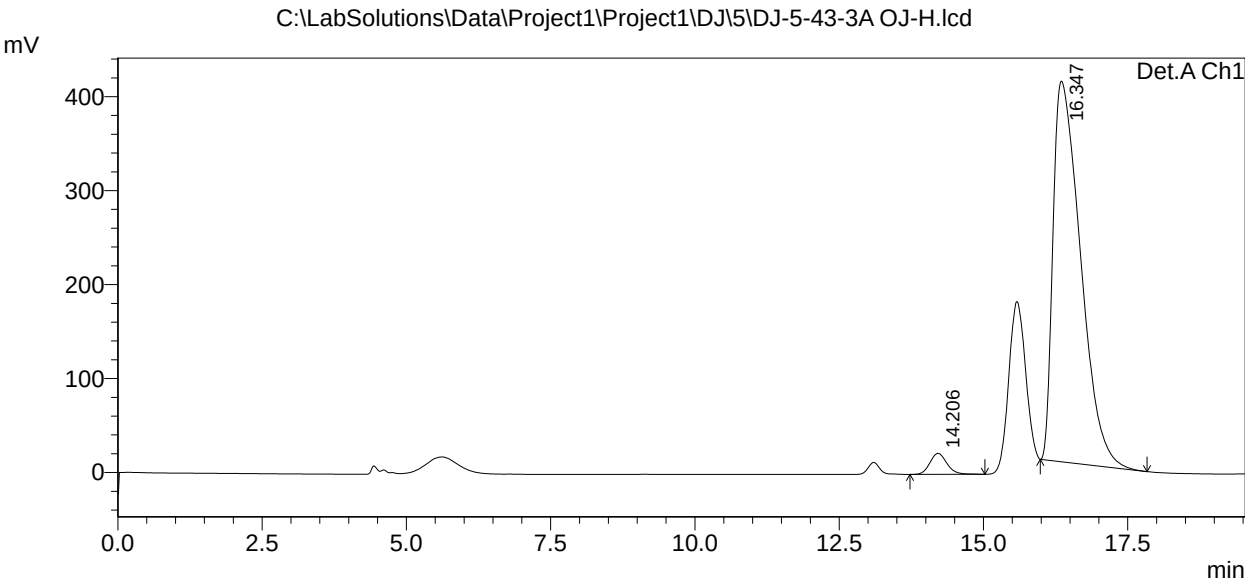
Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.141	18667004	871544	49.713	57.956
2	16.578	18882235	632251	50.287	42.044
Total		37549240	1503795	100.000	100.000

==== Shimadzu LCsolution Analysis Report ====

Acquired by : Admin
Sample Name : DJ-5-43-3A OJ-H
Sample ID : OJ-H,95/5,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : DJ-5-43-3A OJ-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2016-10-19 15:25:49
Data Processed : 2016-10-19 15:45:22

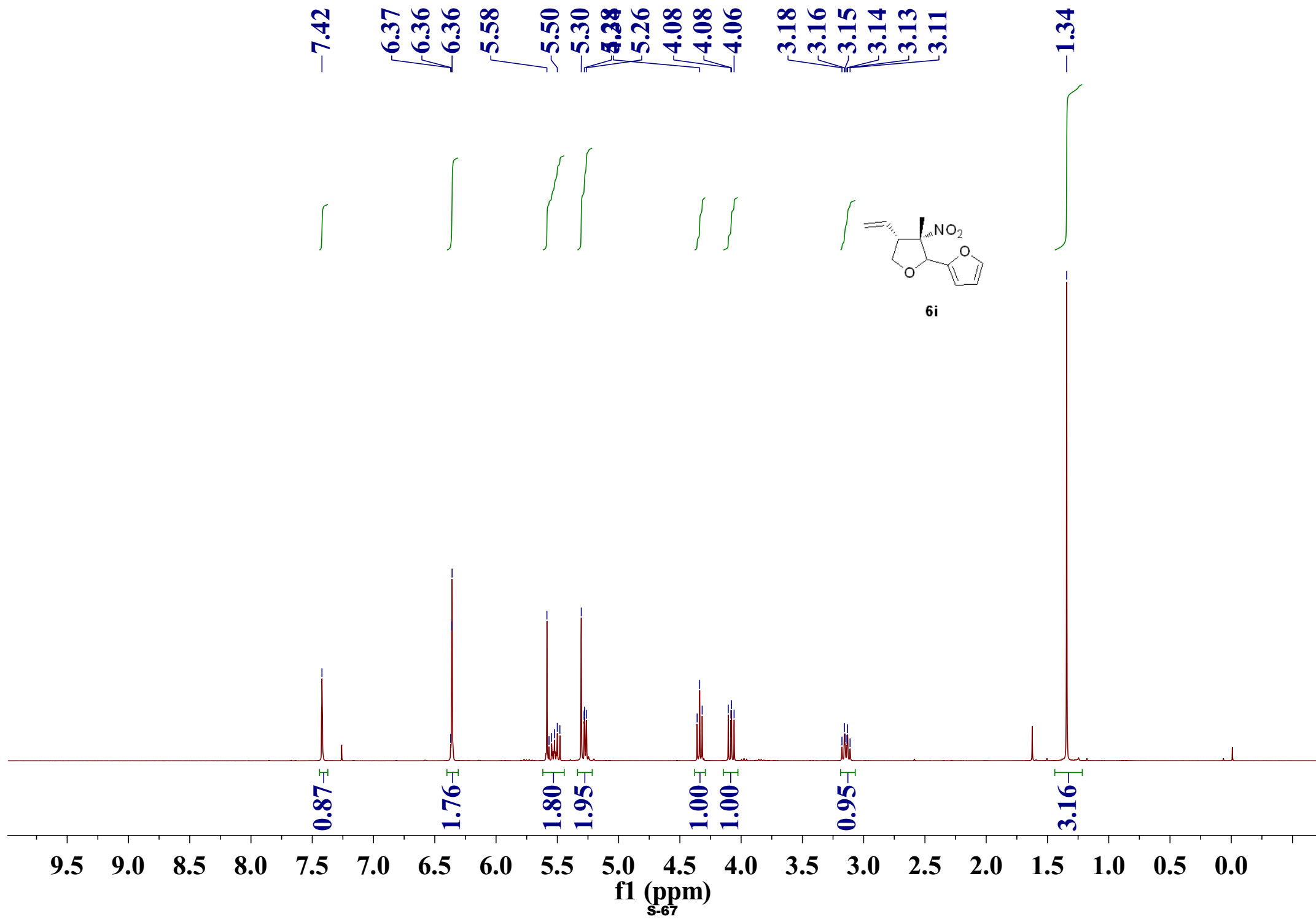


<Chromatogram>



PeakTable

Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.206	459224	22409	3.303	5.241
2	16.347	13443874	405176	96.697	94.759
Total		13903098	427585	100.000	100.000



—150.83

—143.15

—129.60

—122.04

—110.39

—109.47

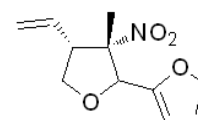
—98.33

—81.70

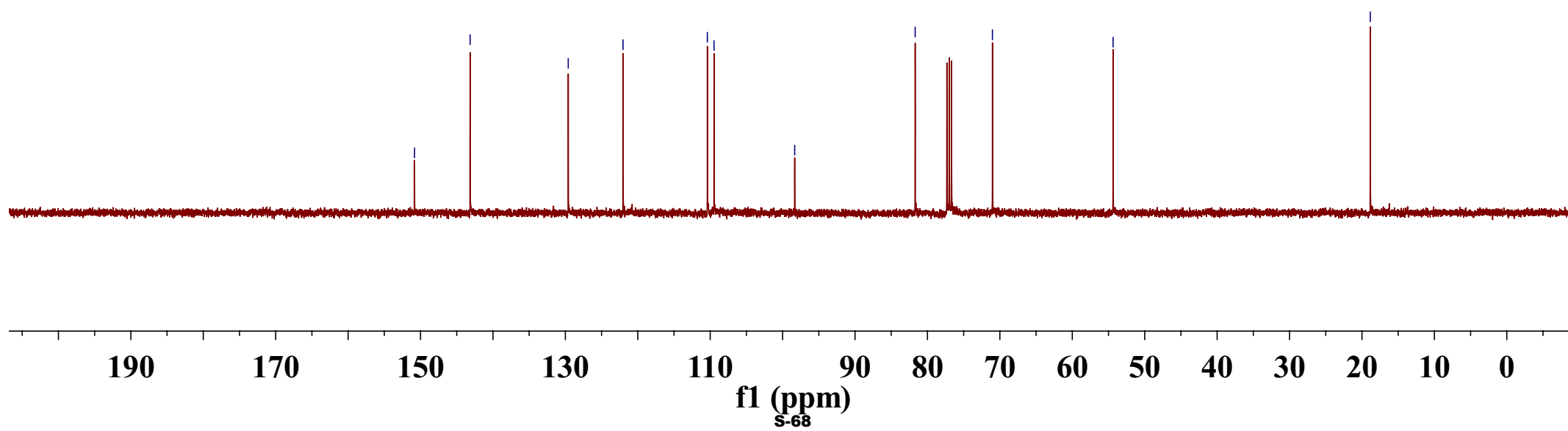
—71.03

—54.37

—18.85



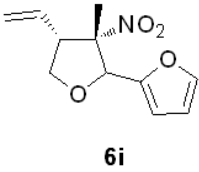
6i



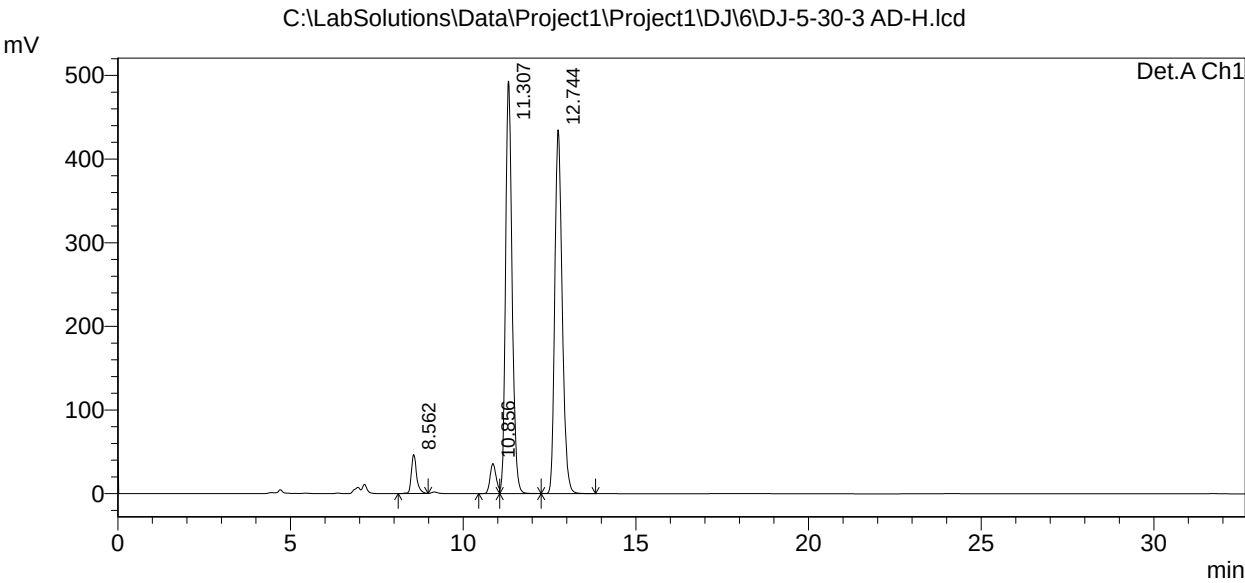
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\6\DJ-5-30-3 AD-H.lcd

Acquired by : Admin
Sample Name : DJ-5-30-3 AD-H
Sample ID : AD-H,95/5,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : DJ-5-30-3 AD-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2016-12-6 13:14:13
Data Processed : 2016-12-6 13:46:53



<Chromatogram>



1 Det.A Ch1/214nm

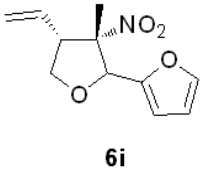
PeakTable

Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.562	492953	46542	3.533	4.606
2	10.856	439539	35866	3.150	3.549
3	11.307	6510199	493161	46.655	48.802
4	12.744	6511171	434970	46.662	43.043
Total		13953862	1010539	100.000	100.000

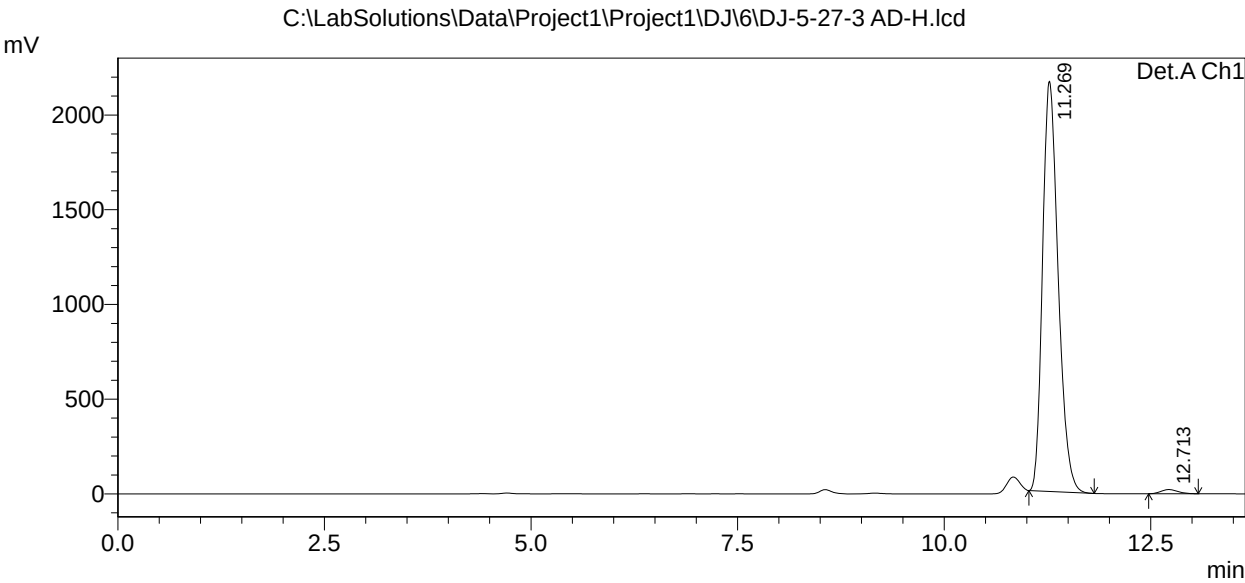
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\6\DJ-5-27-3 AD-H.lcd

Acquired by : Admin
Sample Name : DJ-5-27-3 AD-H
Sample ID : AD-H,95/5,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : DJ-5-27-3 AD-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2016-12-6 13:48:58
Data Processed : 2016-12-6 14:02:37



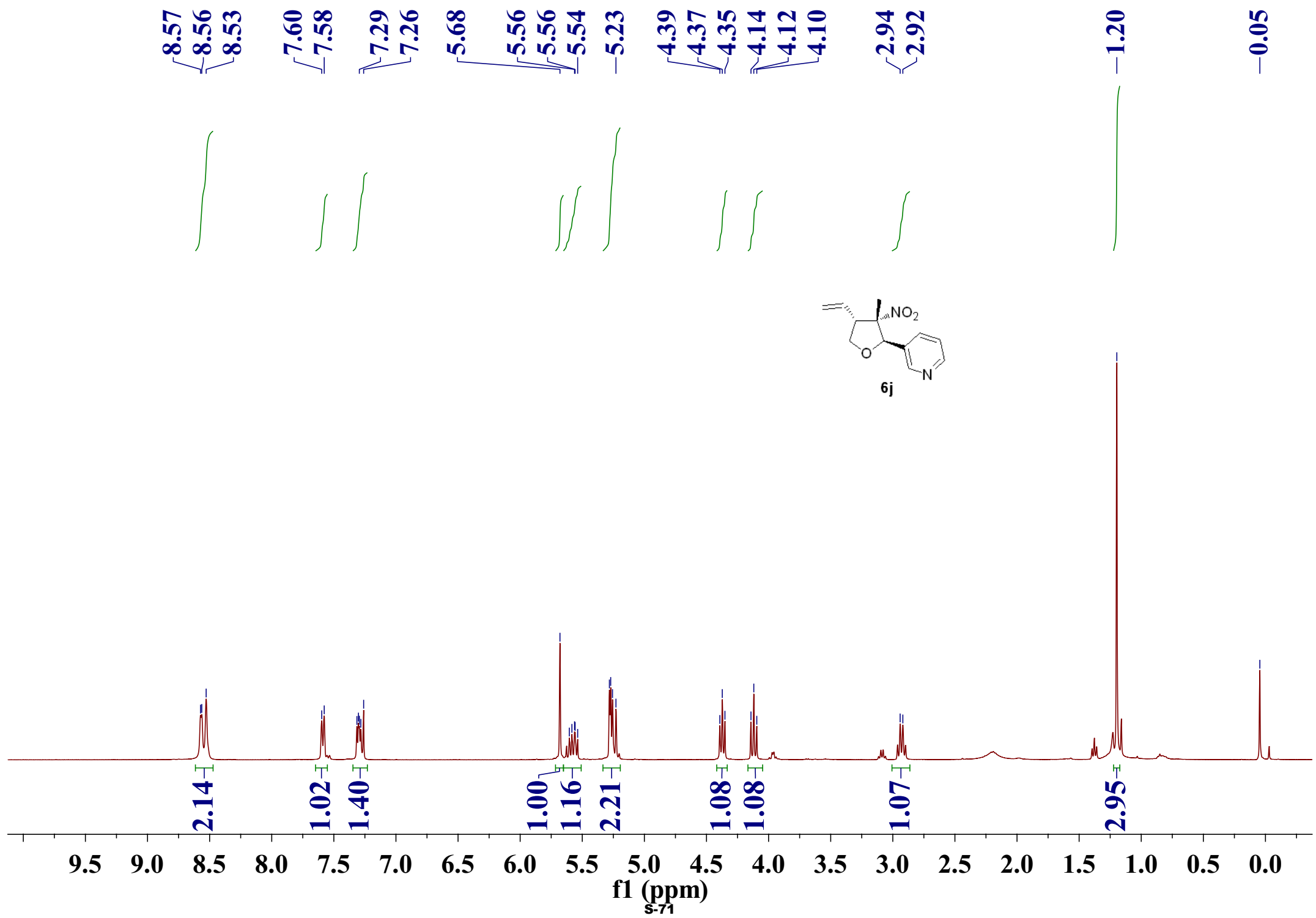
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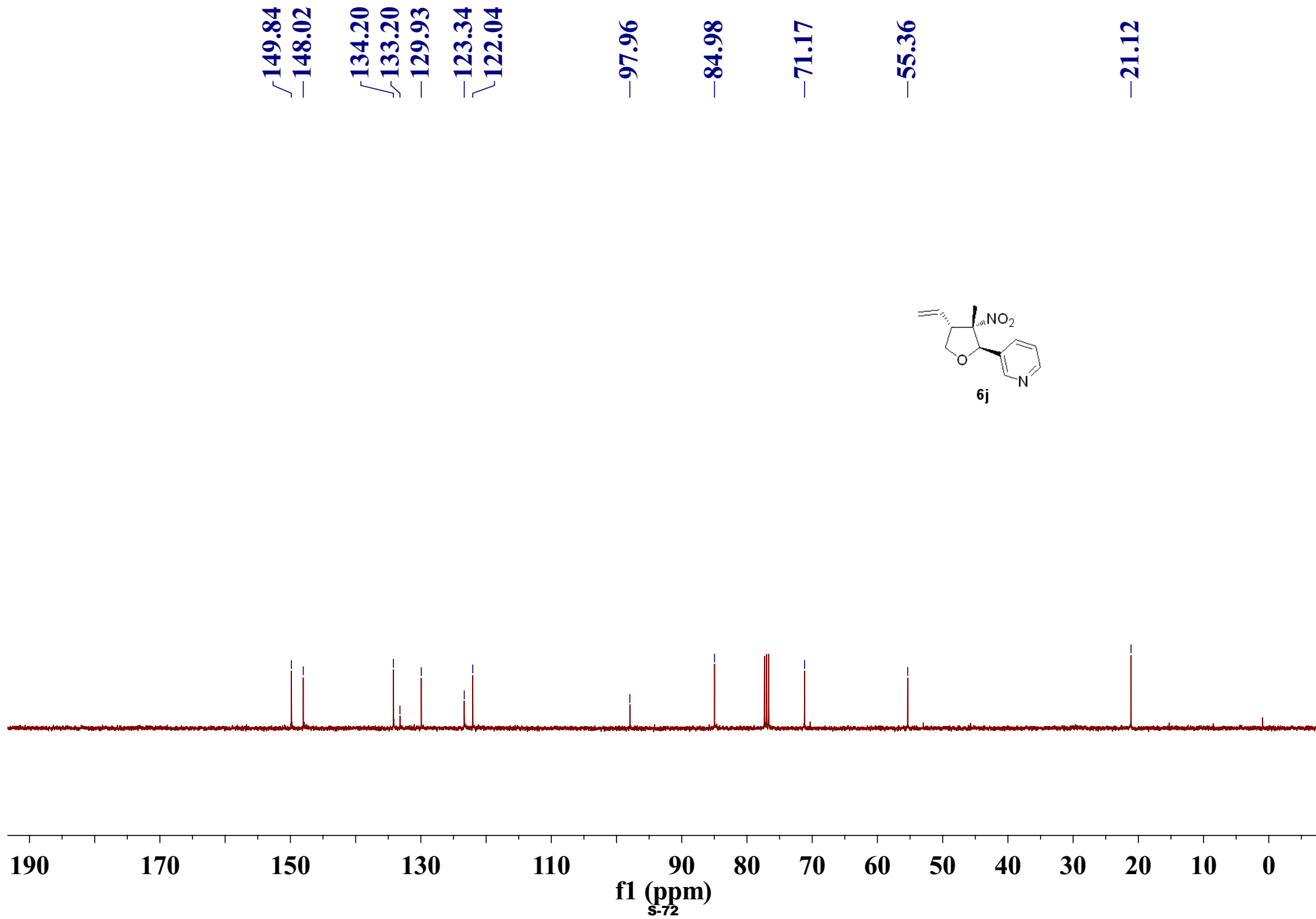
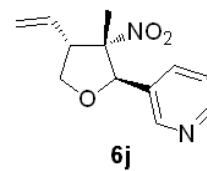


1 Det.A Ch1/214nm

PeakTable

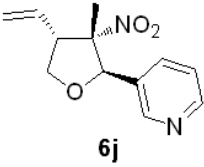
Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.269	28466786	2165869	98.897	98.985
2	12.713	317528	22212	1.103	1.015
Total		28784315	2188081	100.000	100.000



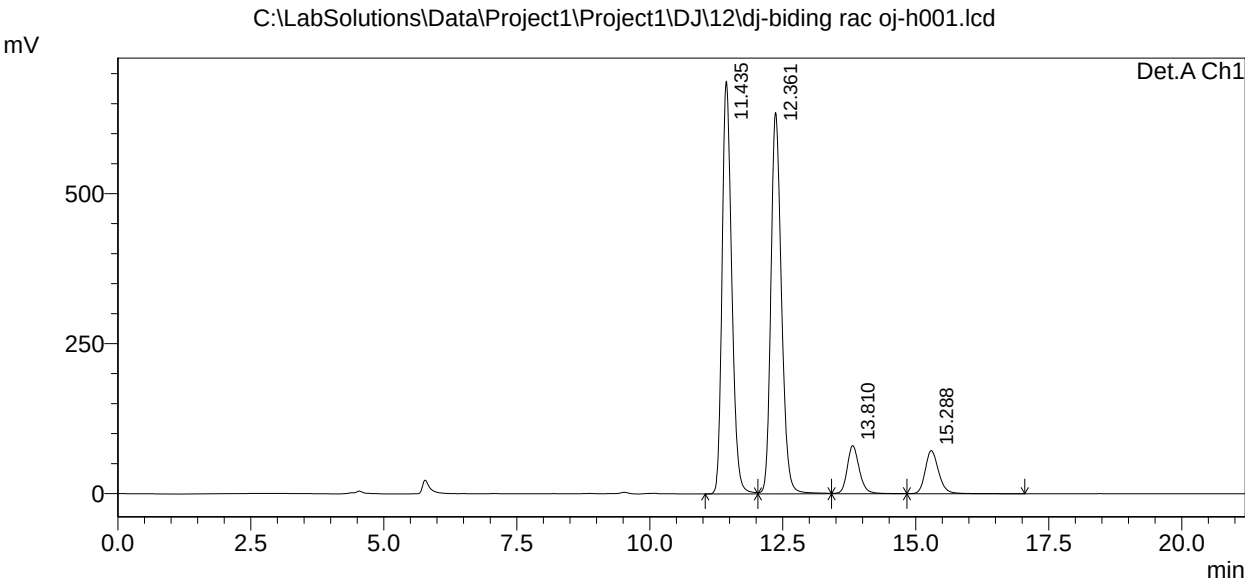


==== Shimadzu LCsolution Analysis Report ====

Acquired by : Admin
Sample Name : dj-biding RAC oj-h
Sample ID : OJ-H,85/15,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : dj-biding rac oj-h001.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2018-7-17 19:20:17
Data Processed : 2018-7-17 19:41:29



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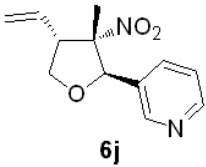
1 Det.A Ch1/214nm

PeakTable

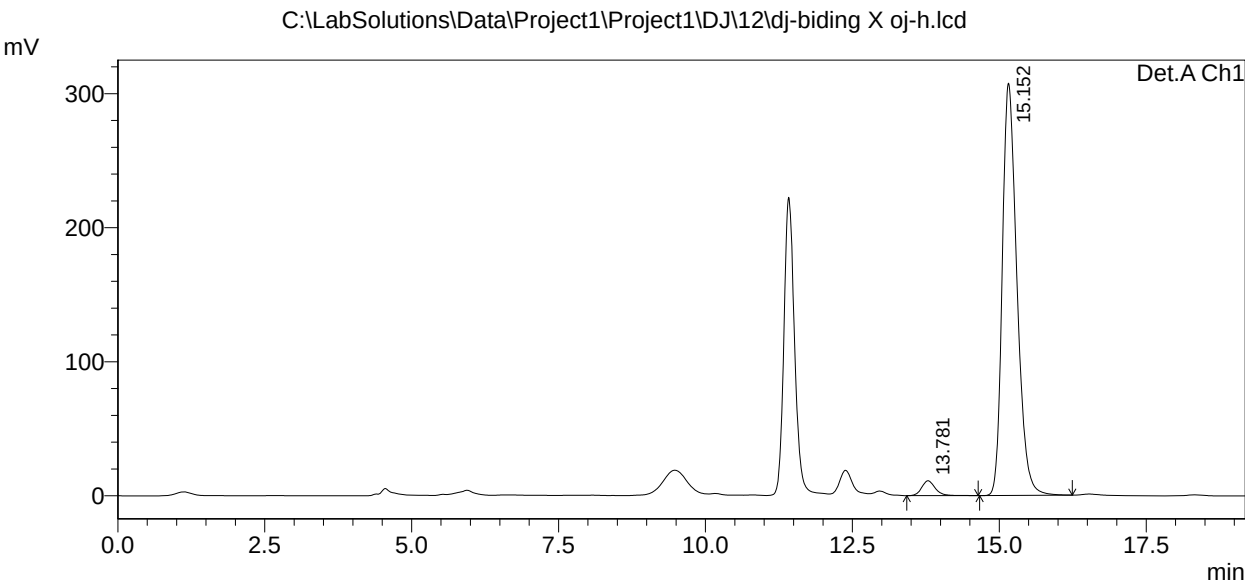
Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	11.435	8675079	688047	43.325	46.612
2	12.361	8791146	635649	43.905	43.062
3	13.810	1284109	80332	6.413	5.442
4	15.288	1272841	72082	6.357	4.883
Total		20023174	1476110	100.000	100.000

==== Shimadzu LCsolution Analysis Report ====

Acquired by : Admin
Sample Name : dj-biding X oj-h
Sample ID : OJ-H,85/15,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : dj-biding X oj-h.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2018-7-17 17:19:30
Data Processed : 2018-7-17 17:38:42



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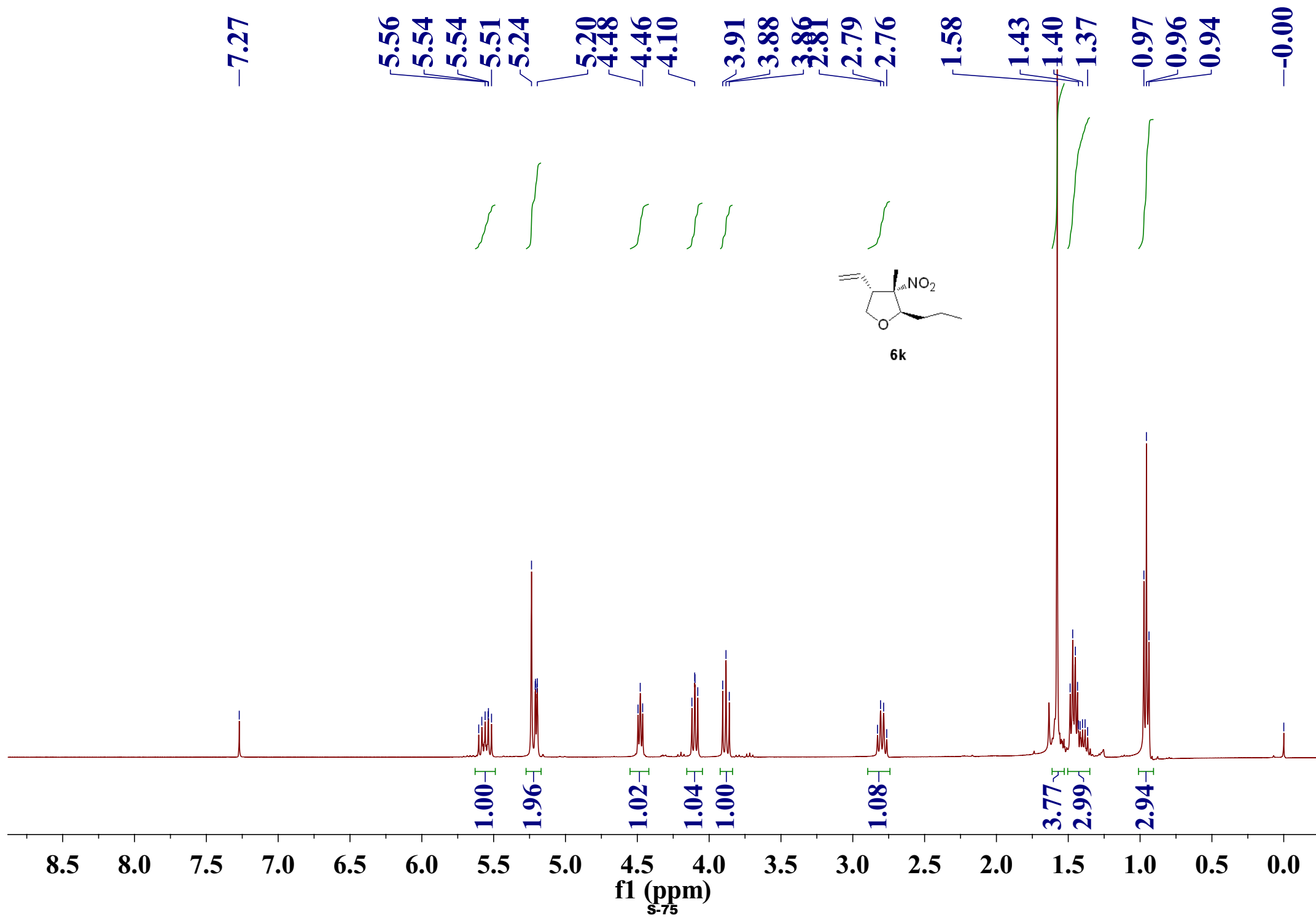


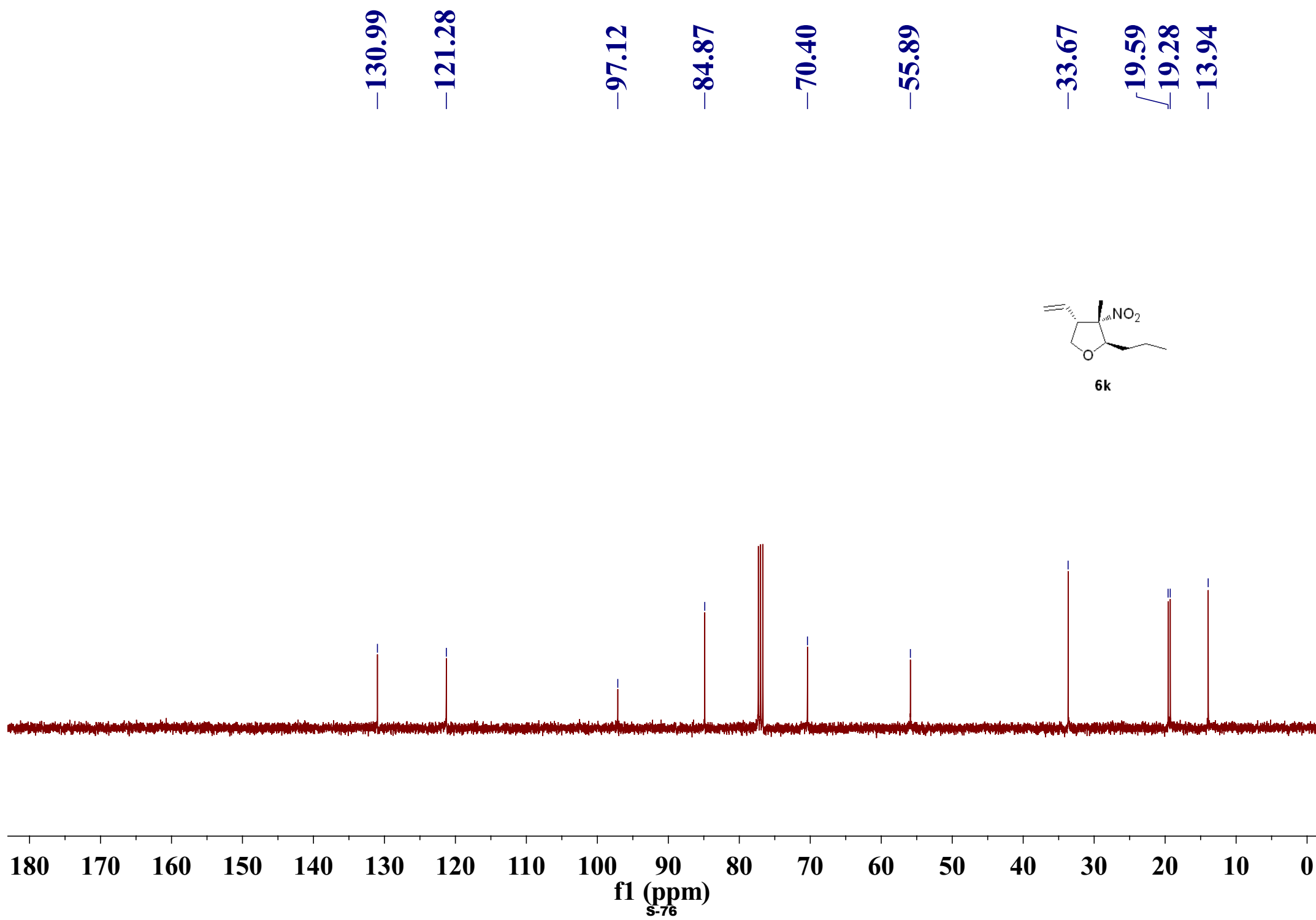
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

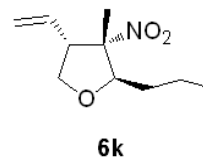
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.781	176828	11085	3.204	3.478
2	15.152	5342521	307619	96.796	96.522
Total		5519349	318704	100.000	100.000



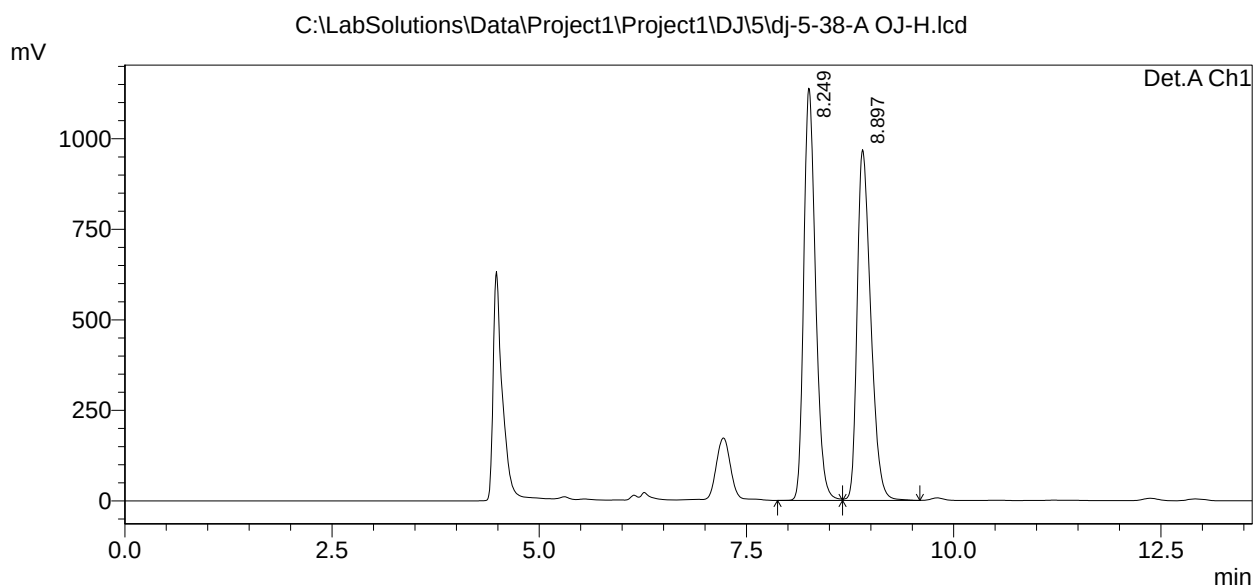


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\5\dj-5-38-A OJ-H.lcd
 Acquired by : Admin
 Sample Name : dj-5-38-A OJ-H
 Sample ID : OJ-H,99/1,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-5-38-A OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-10-21 10:46:31
 Data Processed : 2016-11-1 18:17:29



<Chromatogram>



1 Det.A Ch1/214nm

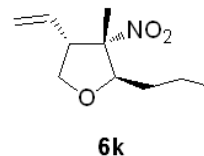
PeakTable

Detector A Ch1 214nm

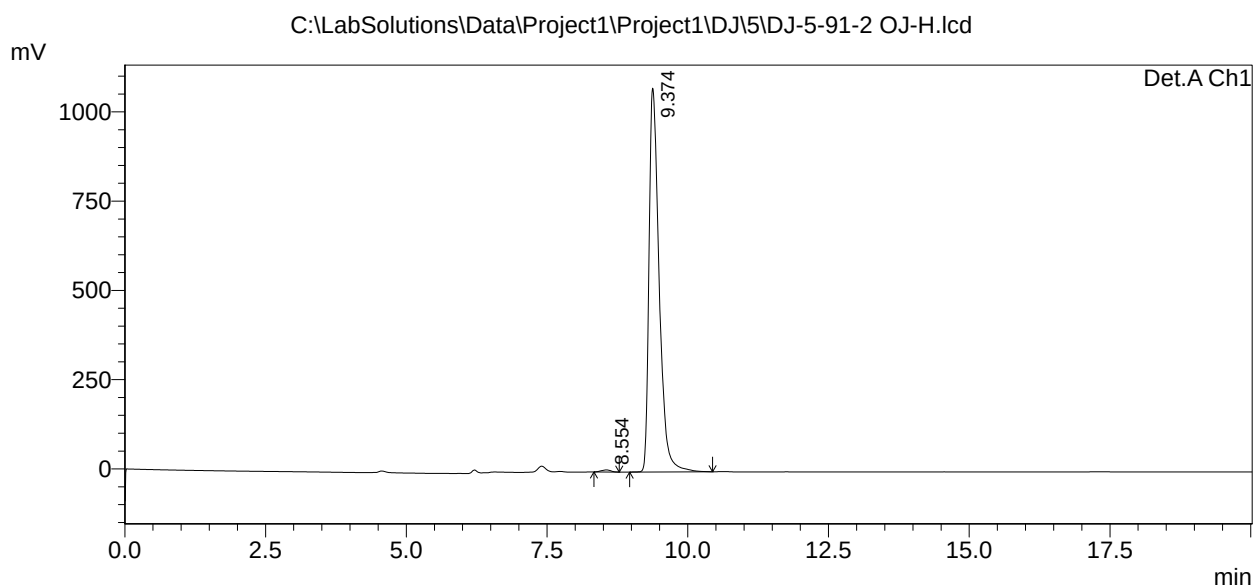
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.249	11284060	1138576	50.535	54.024
2	8.897	11045016	968962	49.465	45.976
Total		22329075	2107537	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\5\DJ-5-91-2 OJ-H.lcd
 Acquired by : Admin
 Sample Name : DJ-5-91-2 OJ-H
 Sample ID : OJ-H,99/1,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-5-91-2 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-11-22 13:37:08
 Data Processed : 2016-11-22 13:57:11



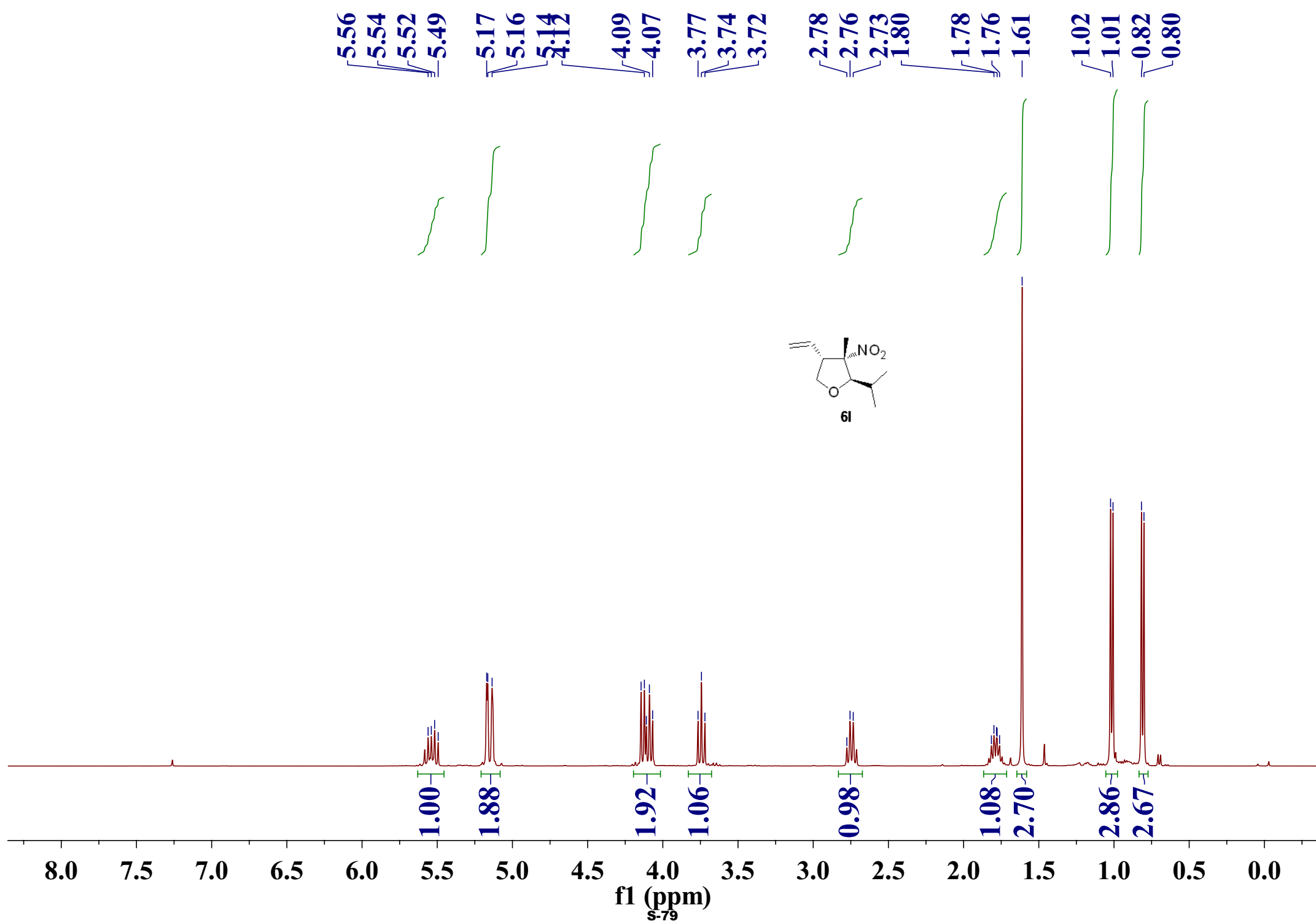
<Chromatogram>

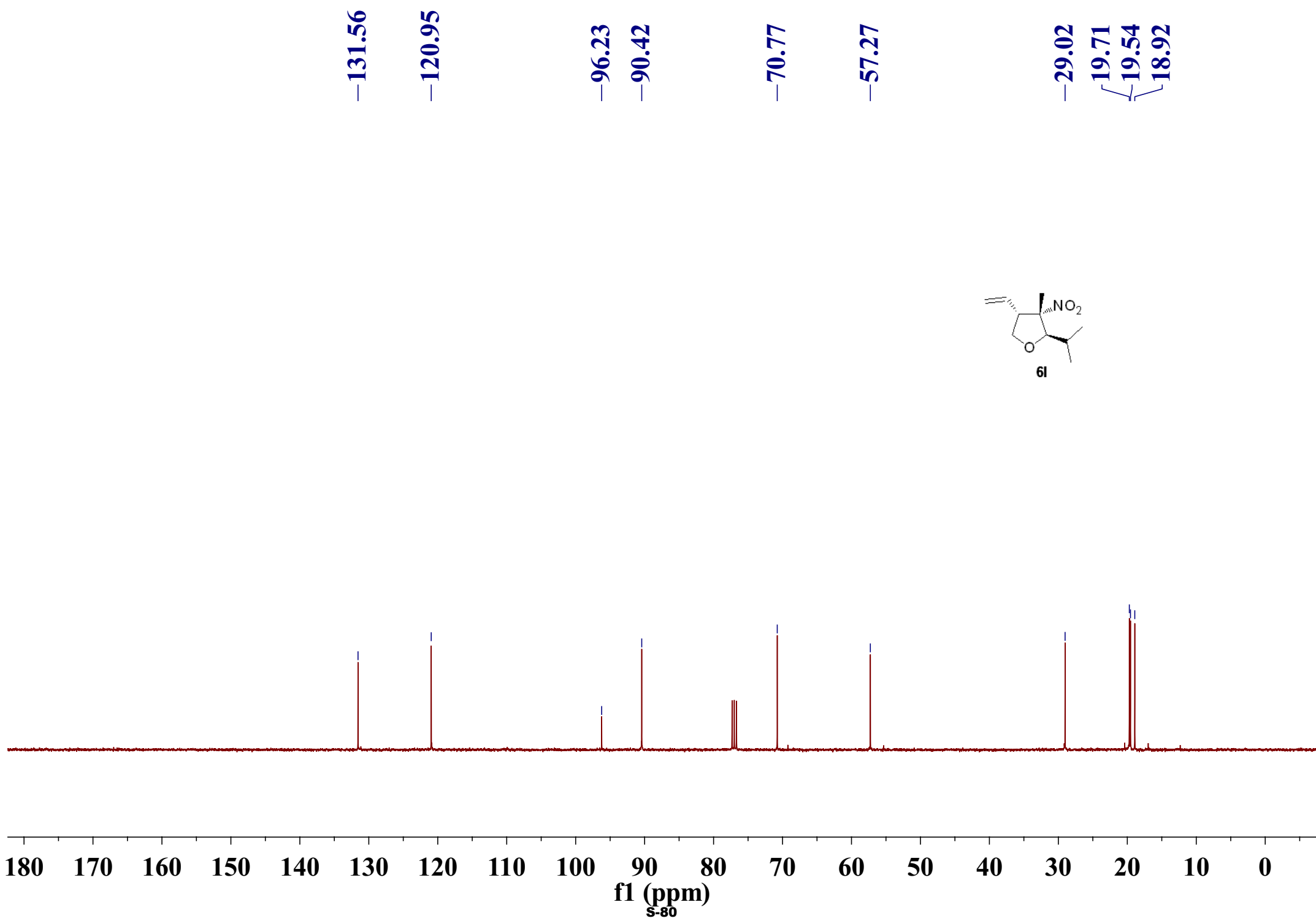


PeakTable

Detector A Ch1 214nm

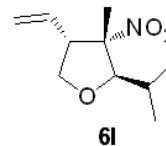
Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.554	67218	5759	0.497	0.533
2	9.374	13464297	1075111	99.503	99.467
Total		13531515	1080871	100.000	100.000



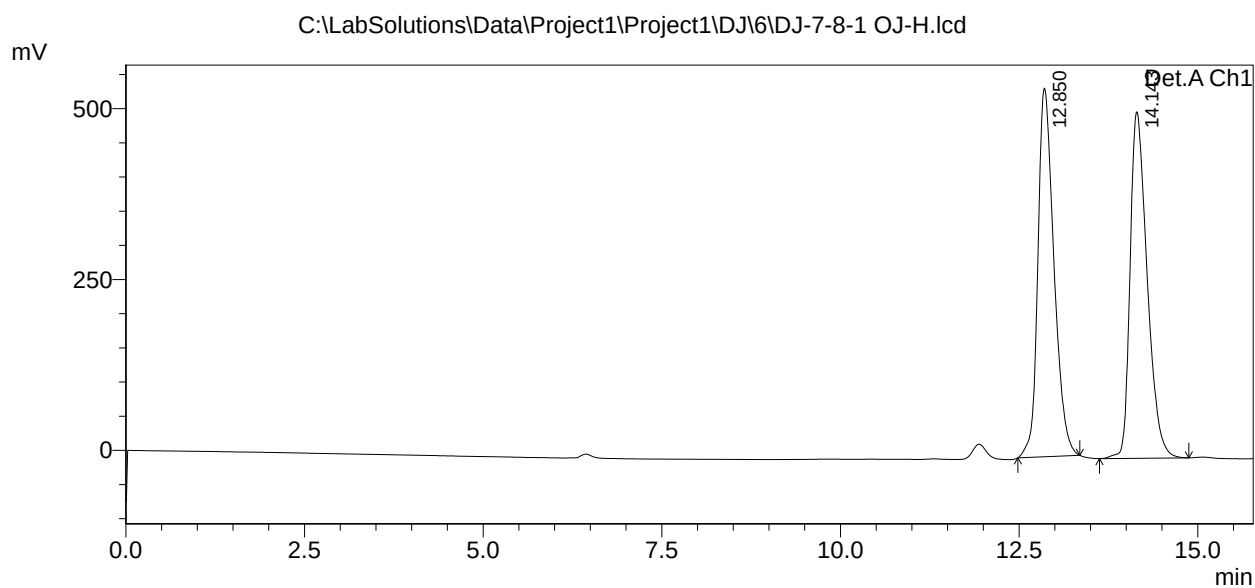


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\DJ-7-8-1 OJ-H.lcd
 Acquired by : Admin
 Sample Name : DJ-7-8-1 OJ-H
 Sample ID : OJ-H,99.9/0.1,0.5,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-7-8-1 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2017-3-2 15:41:23
 Data Processed : 2017-3-2 15:57:11



<Chromatogram>



1 Det.A Ch1/214nm

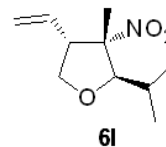
PeakTable

Detector A Ch1 214nm

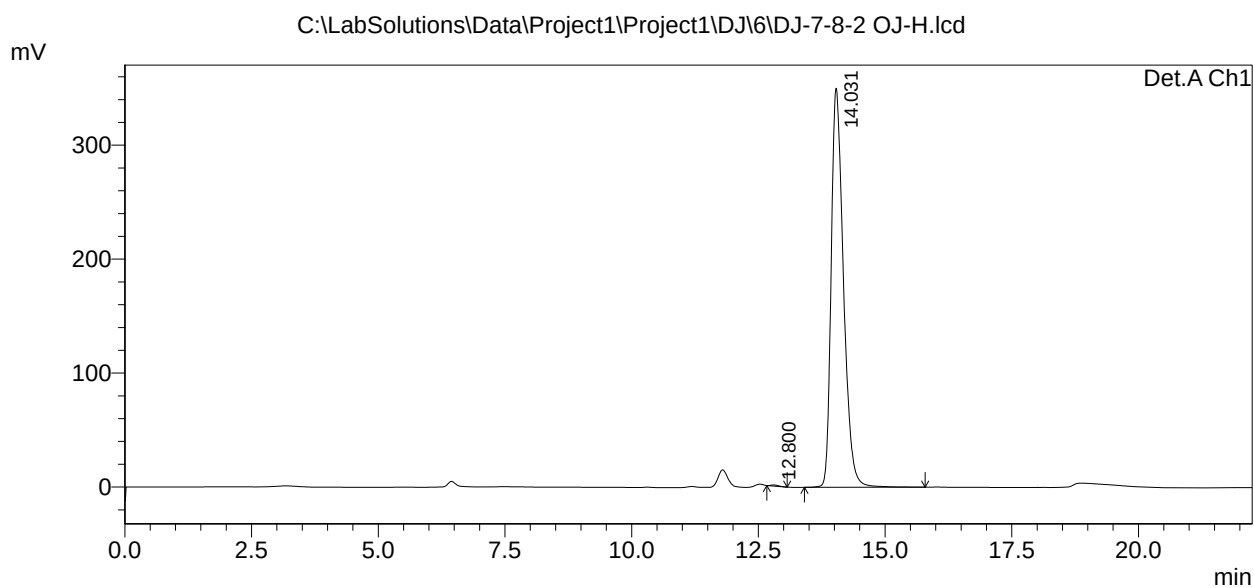
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.850	8438007	539429	50.001	51.546
2	14.143	8437535	507069	49.999	48.454
Total		16875543	1046499	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\DJ-7-8-2 OJ-H.lcd
 Acquired by : Admin
 Sample Name : DJ-7-8-2 OJ-H
 Sample ID : OJ-H,99.9/0.1,0.5,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-7-8-2 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2017-3-2 16:02:17
 Data Processed : 2017-3-2 16:24:32



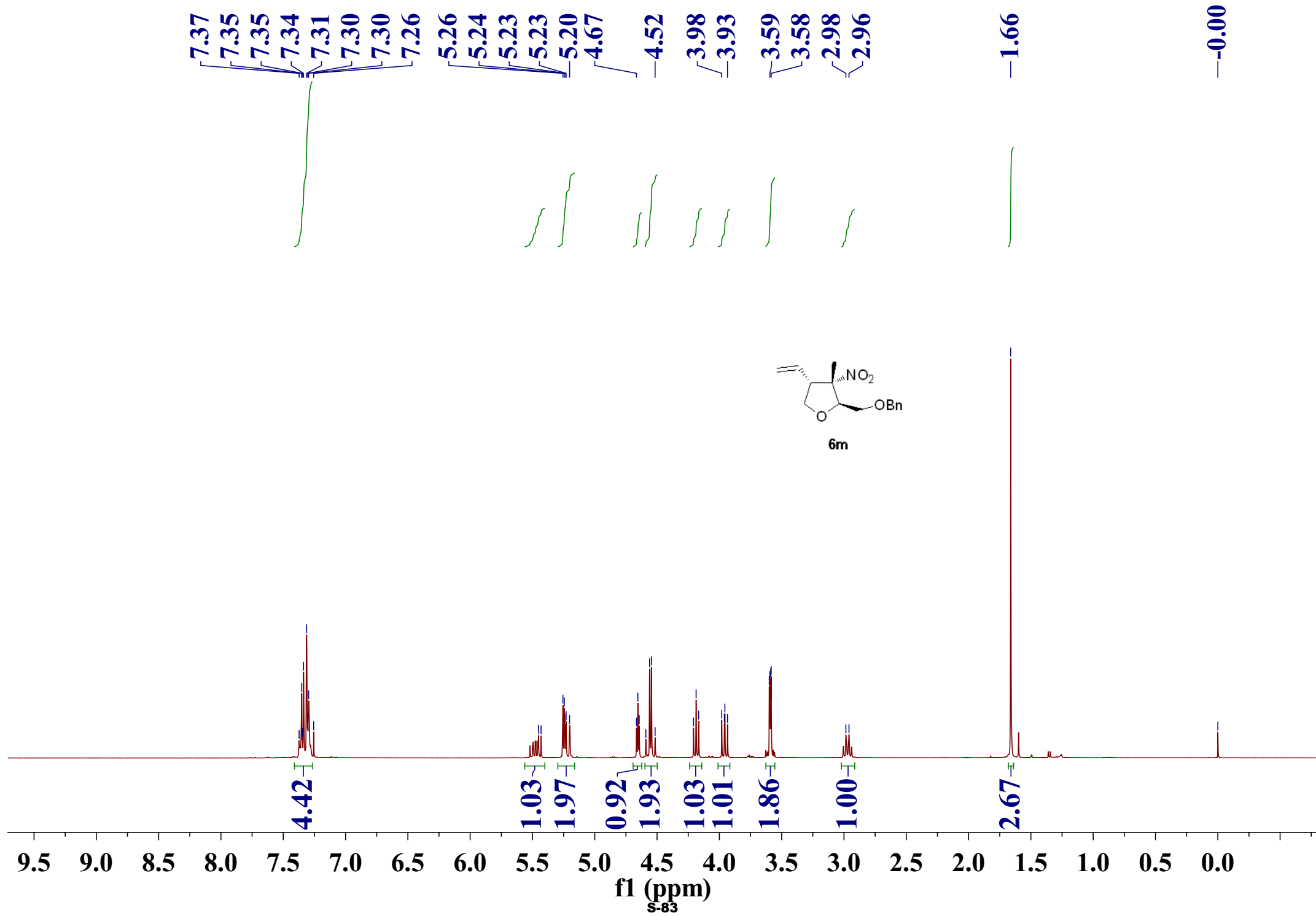
<Chromatogram>

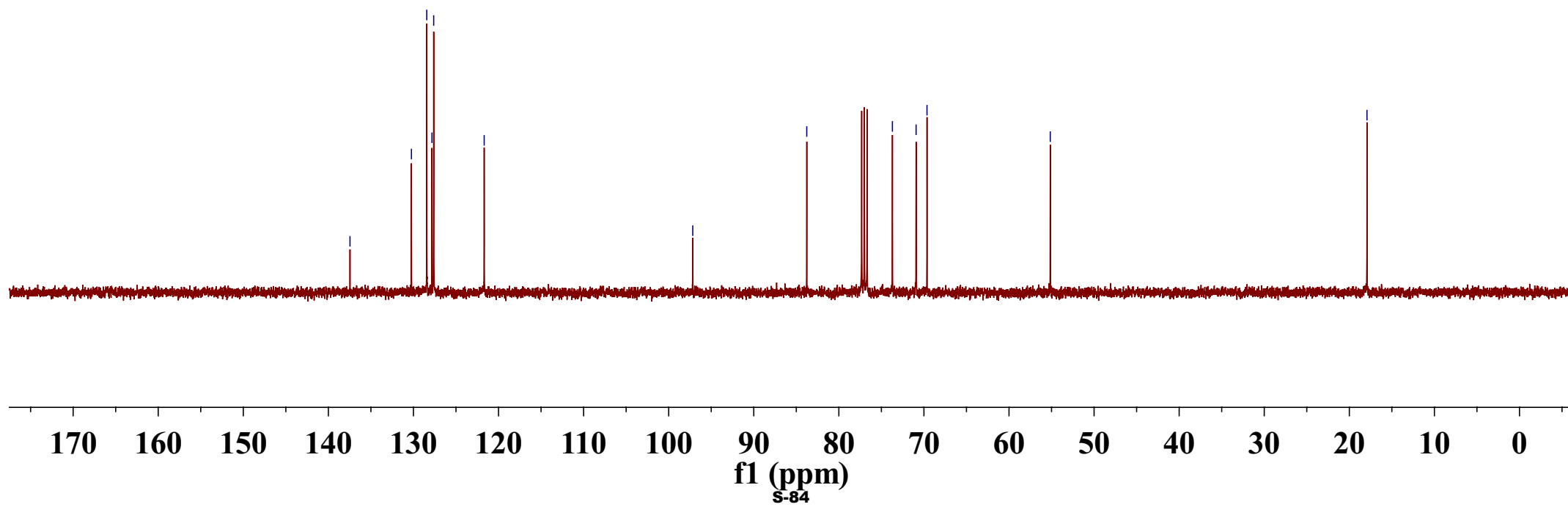
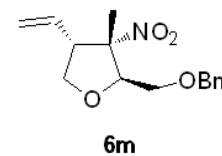
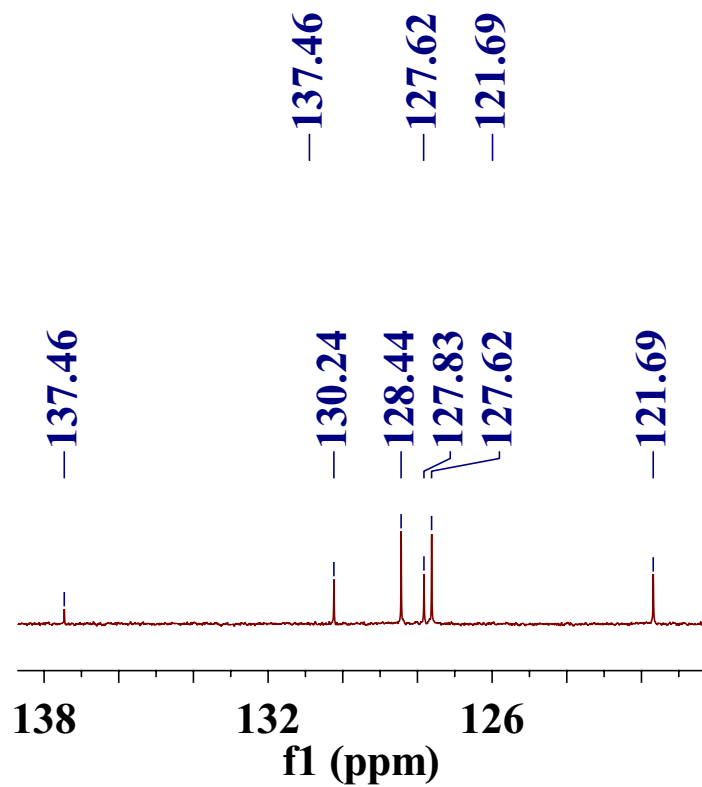


PeakTable

Detector A Ch1 214nm

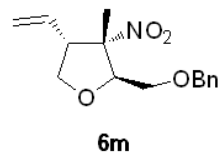
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.800	10460	988	0.177	0.281
2	14.031	5909130	350301	99.823	99.719
Total		5919590	351289	100.000	100.000



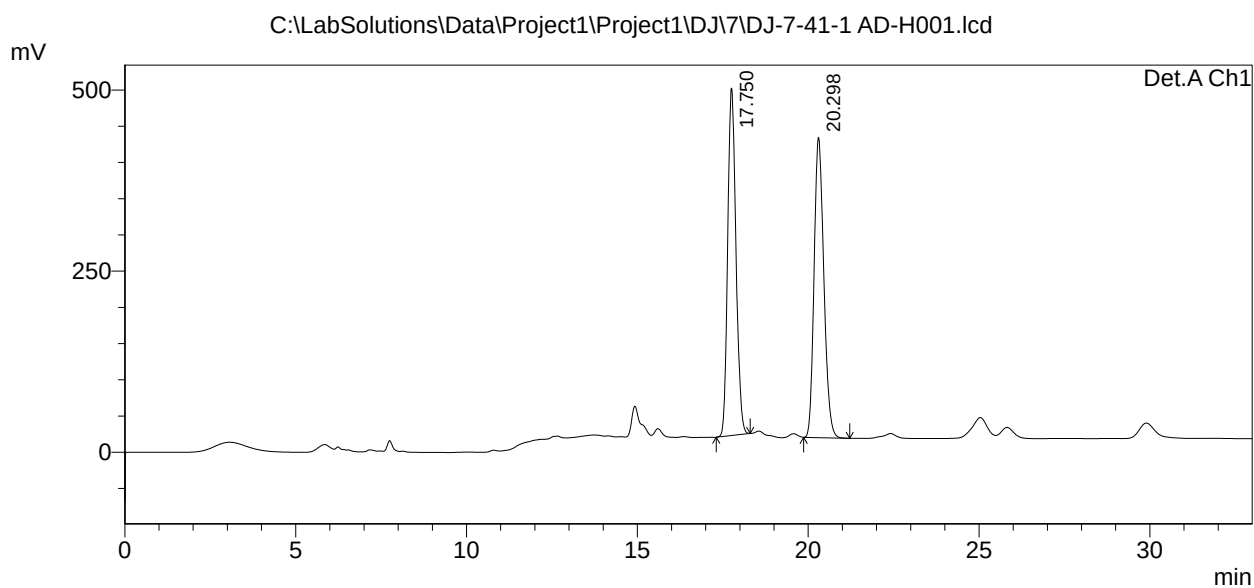


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\7\DJ-7-41-1 AD-H001.lcd
 Acquired by : Admin
 Sample Name : DJ-7-41-1 AD-H
 Sample ID : AD-H,98/2,0.5,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-7-41-1 AD-H001.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2017-4-8 17:20:41
 Data Processed : 2017-4-8 17:53:41



<Chromatogram>



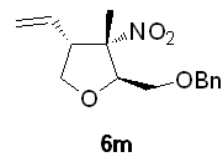
PeakTable

Detector A Ch1 214nm

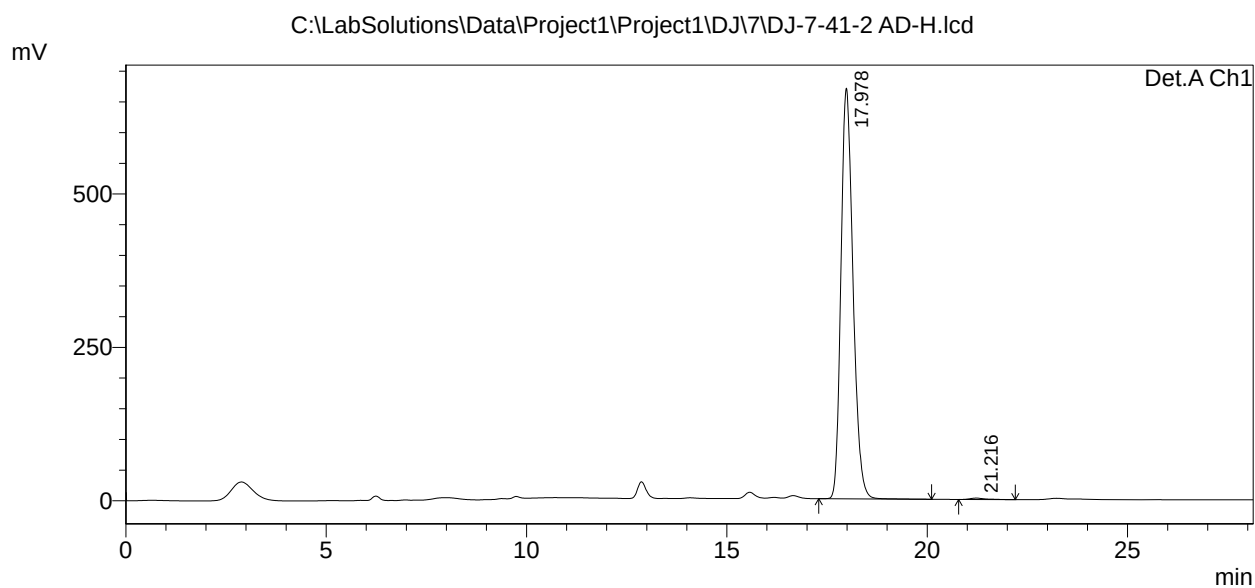
Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.750	8059631	479449	49.537	53.635
2	20.298	8210295	414468	50.463	46.365
Total		16269926	893917	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\7\DJ-7-41-2 AD-H.lcd
 Acquired by : Admin
 Sample Name : DJ-7-41-2 AD-H
 Sample ID : AD-H,98/2,0.5,214
 Vail # :
 Injection Volume : 2 uL
 Data File Name : DJ-7-41-2 AD-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2017-4-8 17:55:11
 Data Processed : 2017-4-8 18:23:20



<Chromatogram>

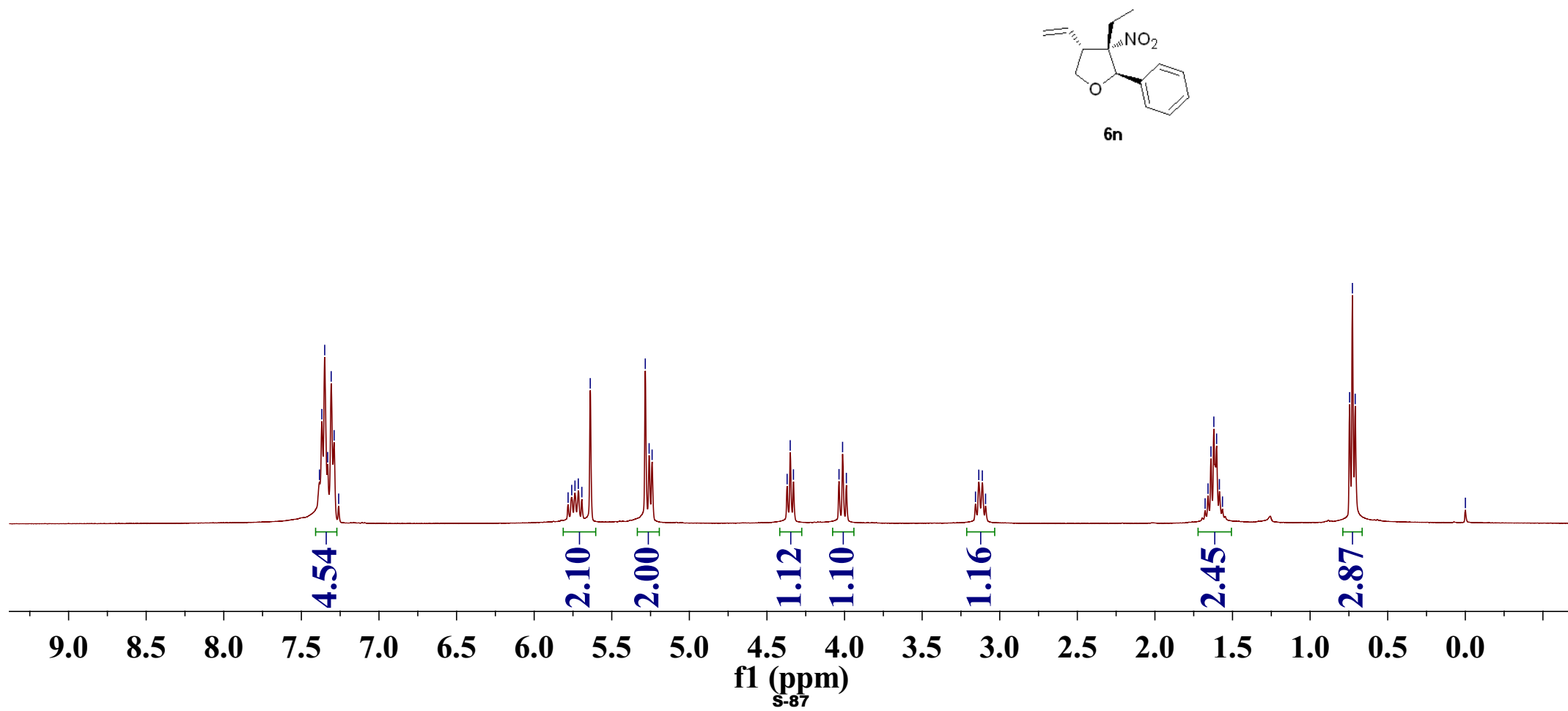


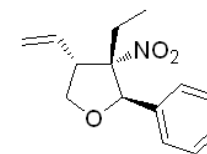
1 Det.A Ch1/214nm

PeakTable

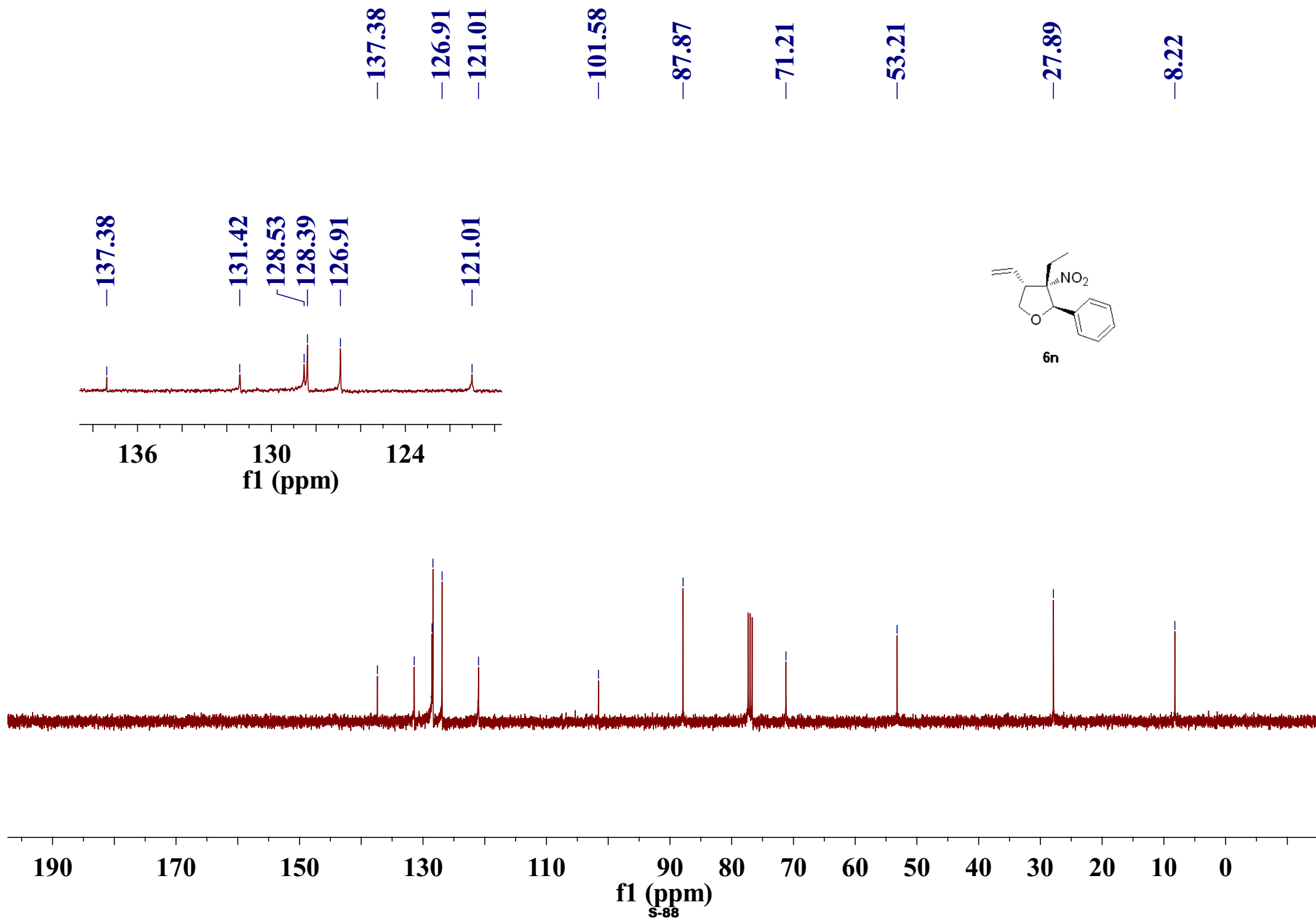
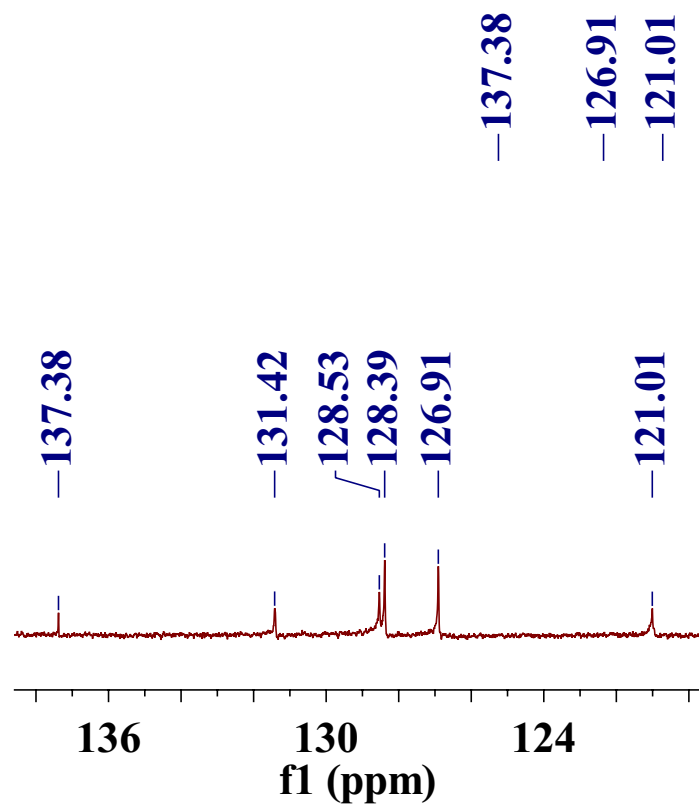
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.978	14009157	669282	99.537	99.652
2	21.216	65218	2336	0.463	0.348
Total		14074375	671618	100.000	100.000





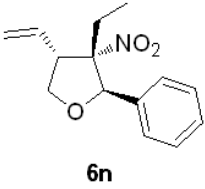
6n



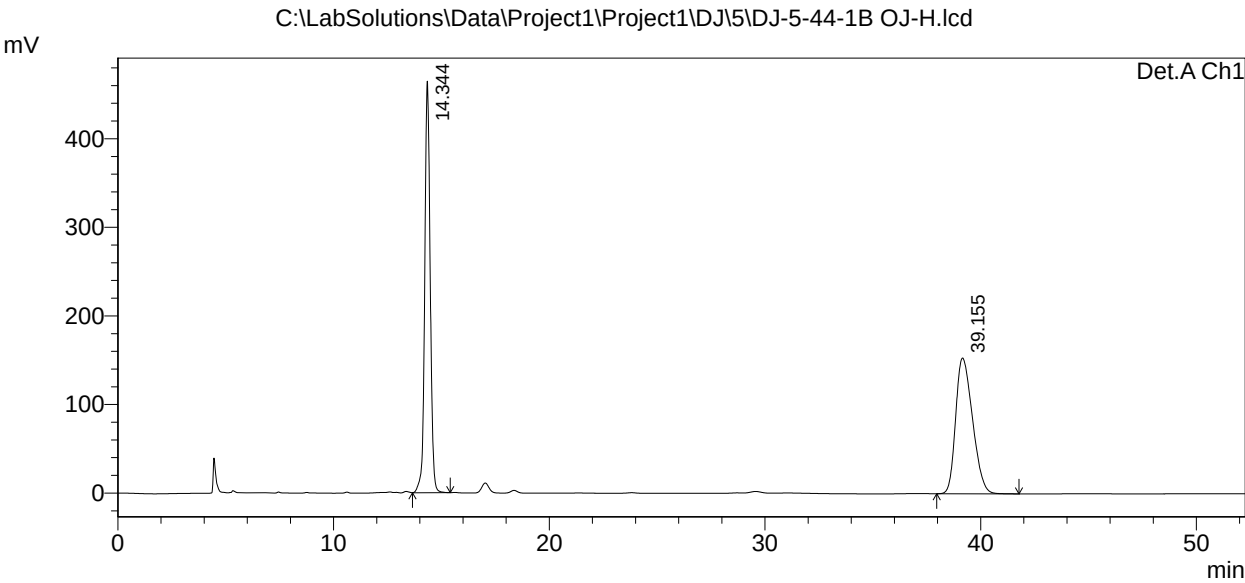
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\5\DJ-5-44-1B OJ-H.lcd

Acquired by : Admin
Sample Name : DJ-5-44-1B OJ-H
Sample ID : OJ-H,98/2,0.7,214
Vial # :
Injection Volume : 2 uL
Data File Name : DJ-5-44-1B OJ-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2016-10-19 17:38:29
Data Processed : 2016-10-21 8:39:27



<Chromatogram>



1 Det.A Ch1/214nm

PeakTable

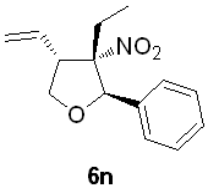
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.344	8229272	464636	49.723	75.192
2	39.155	8320805	153293	50.277	24.808
Total		16550076	617929	100.000	100.000

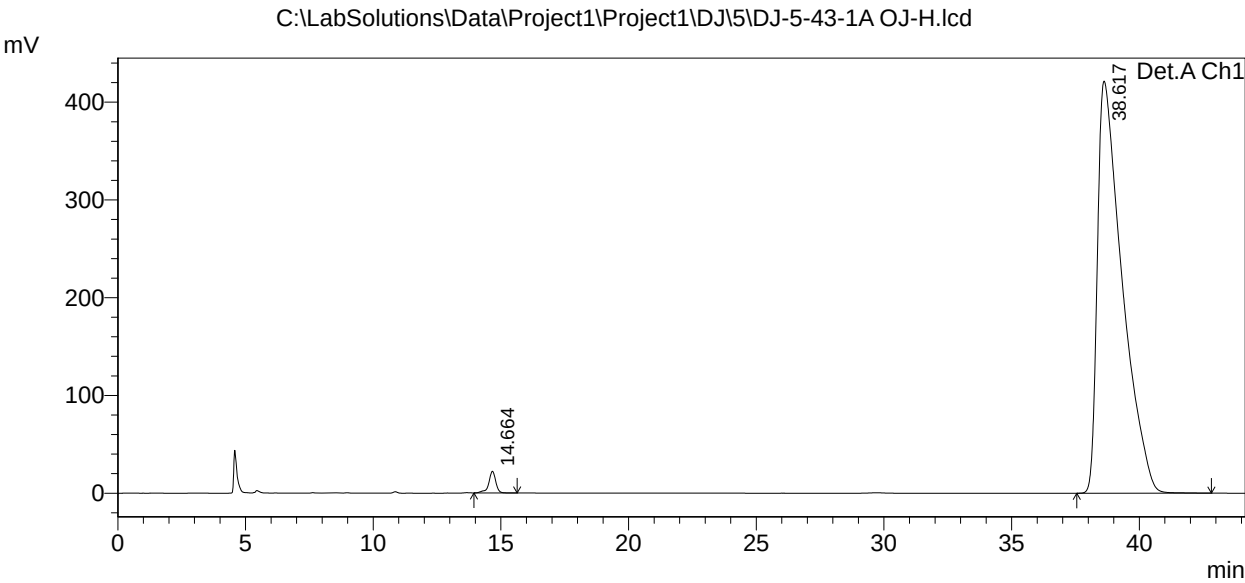
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\5\DJ-5-43-1A OJ-H.lcd

Acquired by : Admin
Sample Name : DJ-5-43-1A OJ-H
Sample ID : OJ-H,98/2,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : DJ-5-43-1A OJ-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2016-10-19 18:33:19
Data Processed : 2016-10-21 8:41:14



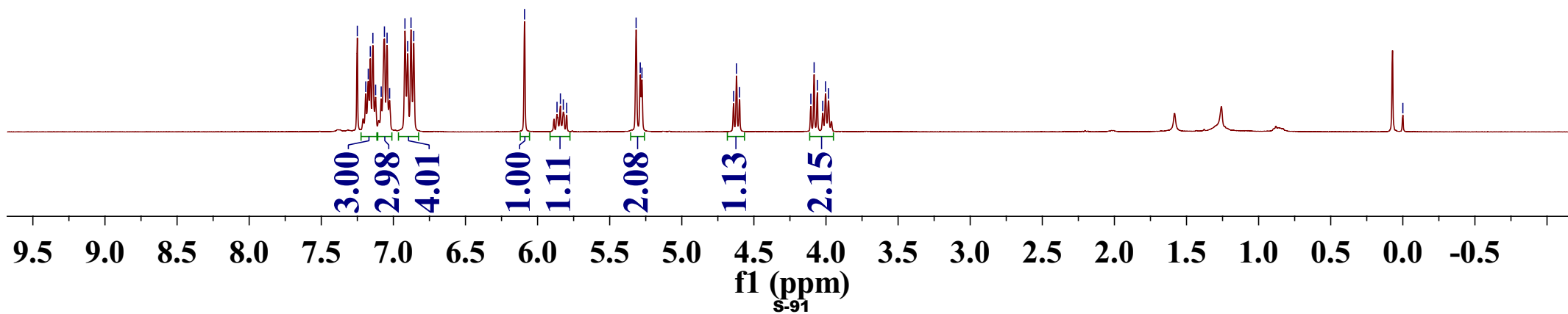
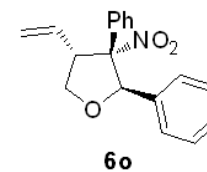
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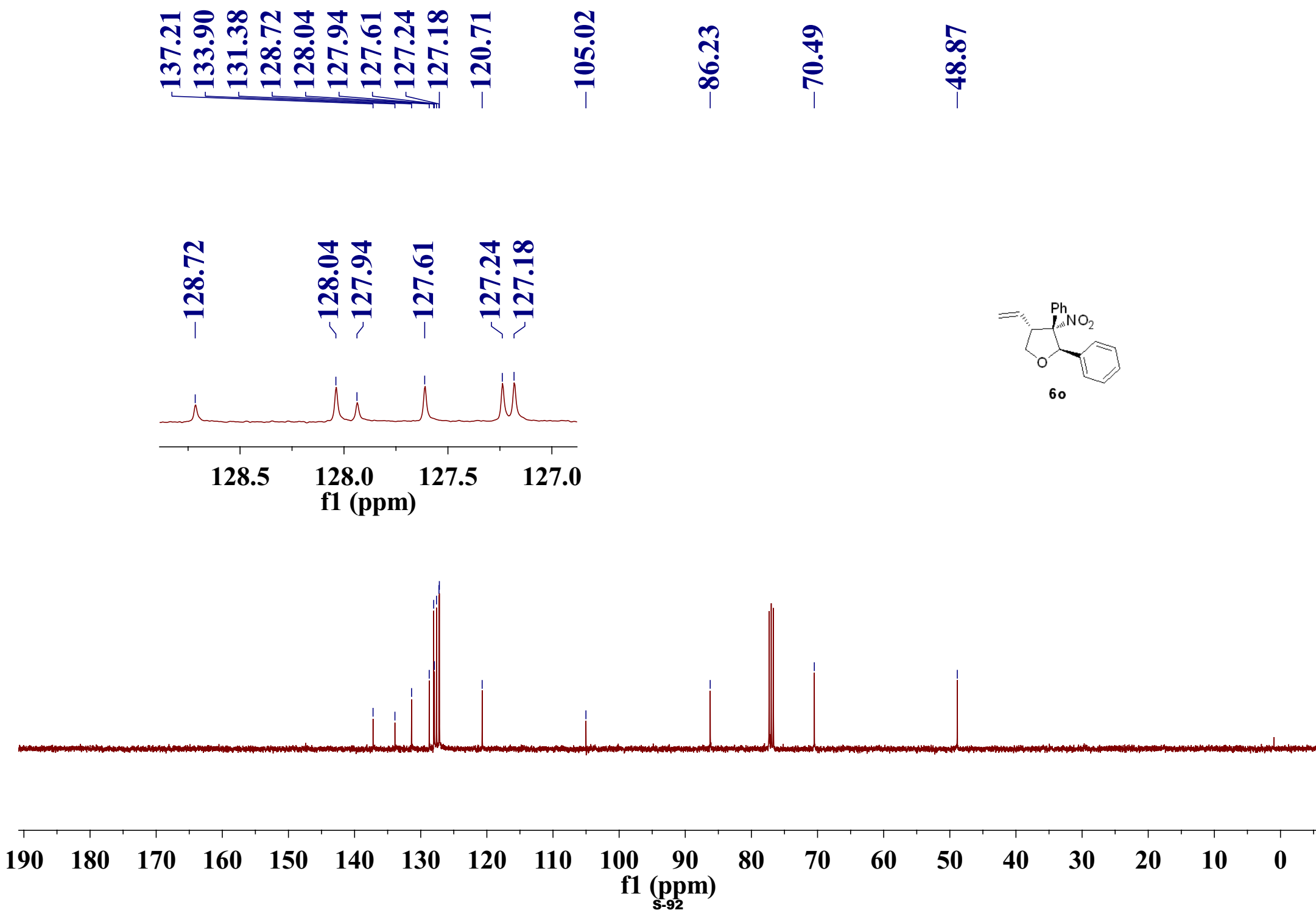


PeakTable

Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.664	425206	22211	1.474	5.005
2	38.617	28423039	421552	98.526	94.995
Total		28848245	443763	100.000	100.000

7.14
7.12
7.08
7.06
7.04
7.03
6.92
6.90
6.88
6.86
6.09
5.82
5.80
5.32
5.28
4.60
4.10
4.08
4.06
4.02
4.00
3.98
-0.00

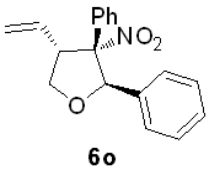




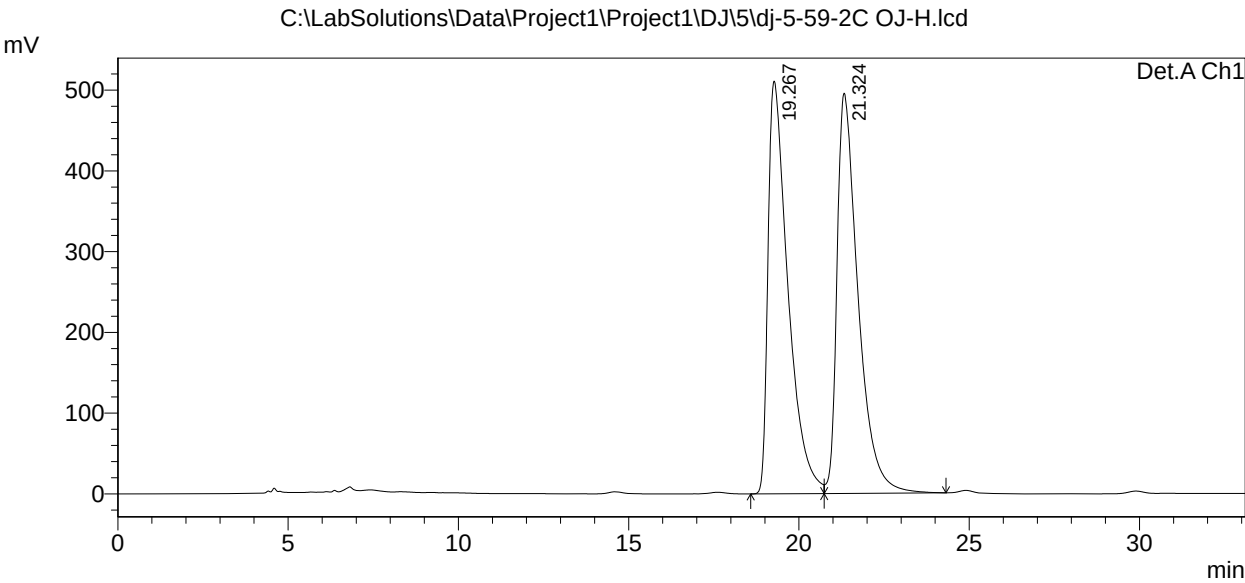
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\5\dj-5-59-2C OJ-H.lcd

Acquired by : Admin
Sample Name : dj-5-59-2C OJ-H
Sample ID : OJ-H,85/15,0.7,214
Vial # :
Injection Volume : 2 uL
Data File Name : dj-5-59-2C OJ-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2016-11-5 15:58:55
Data Processed : 2016-11-5 16:32:03



<Chromatogram>



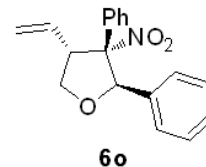
1 Det.A Ch1/214nm

PeakTable

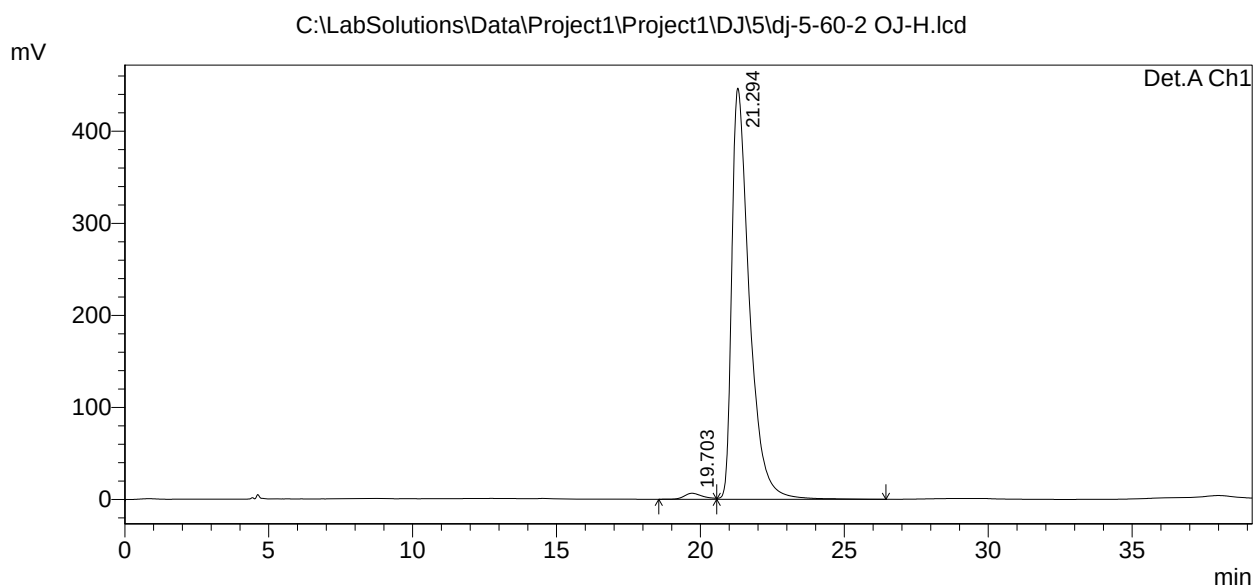
Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.267	20828292	511103	49.411	50.768
2	21.324	21324651	495636	50.589	49.232
Total		42152943	1006739	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\5\dj-5-60-2 OJ-H.lcd
 Acquired by : Admin
 Sample Name : dj-5-60-2 OJ-H
 Sample ID : OJ-H,85/15,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-5-60-2 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-11-5 15:16:10
 Data Processed : 2016-11-5 16:46:31



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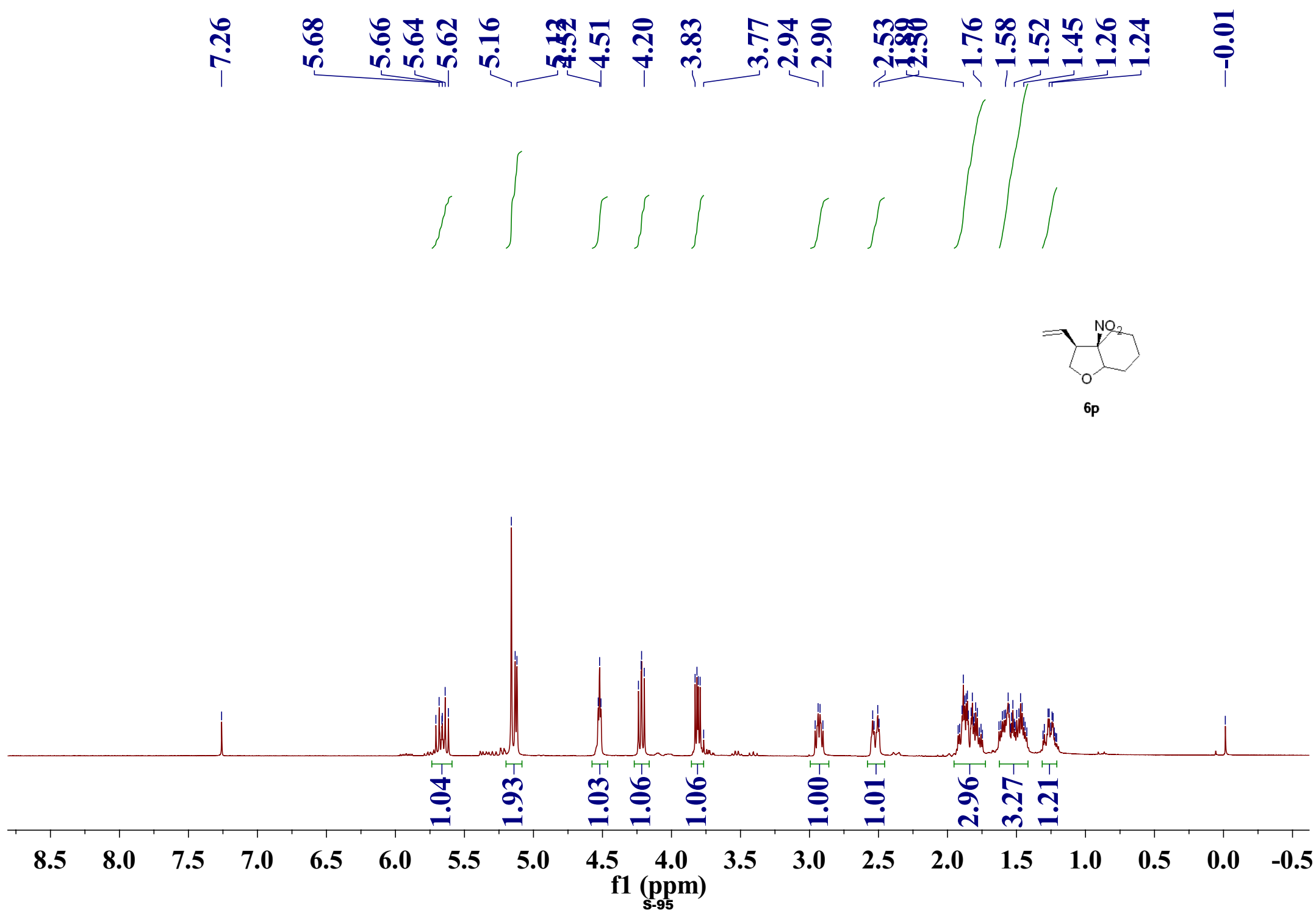


1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.703	291973	6512	1.516	1.437
2	21.294	18965725	446545	98.484	98.563
Total		19257698	453057	100.000	100.000



—132.94

—120.10

—94.29

—76.32

—70.51

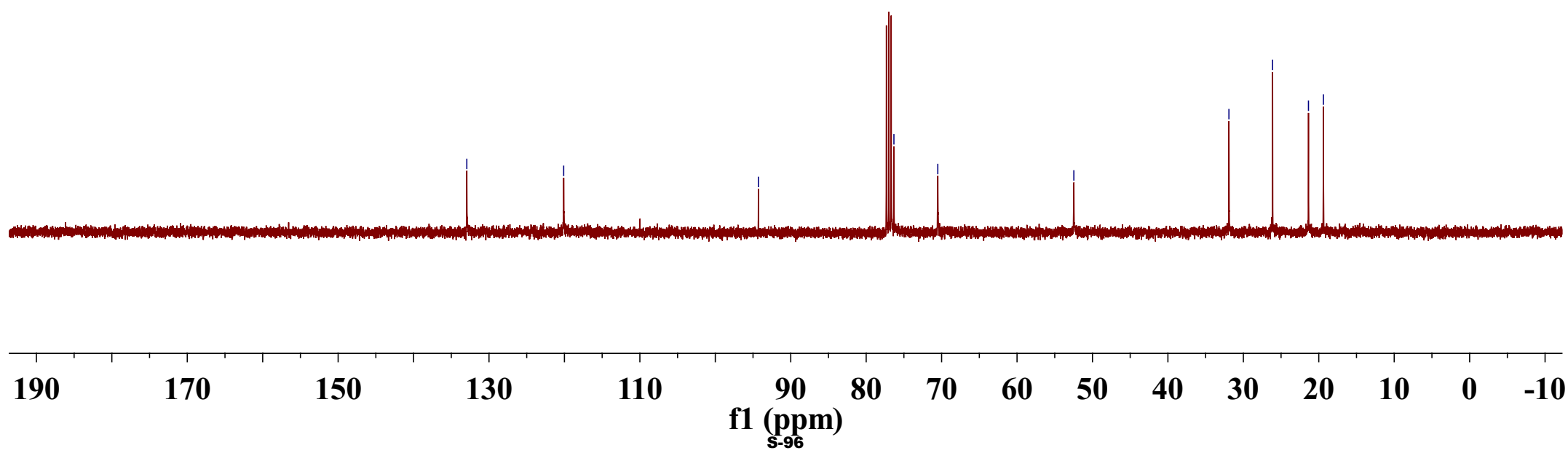
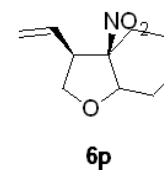
—52.47

—31.91

—26.12

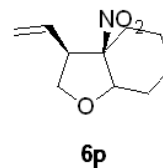
—21.37

—19.38

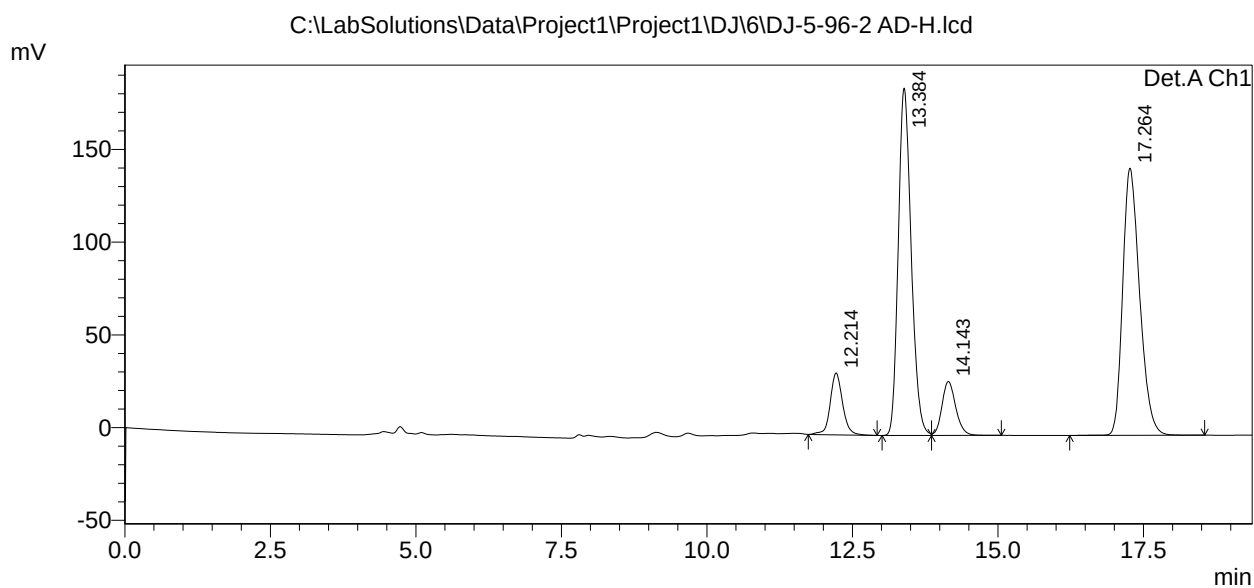


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\DJ-5-96-2 AD-H.lcd
 Acquired by : Admin
 Sample Name : DJ-5-96-2 AD-H
 Sample ID : AD-H,99/1,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-5-96-2 AD-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-12-6 10:34:53
 Data Processed : 2016-12-6 10:54:17



<Chromatogram>



1 Det.A Ch1/214nm

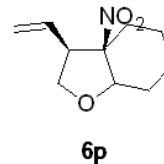
PeakTable

Detector A Ch1 214nm

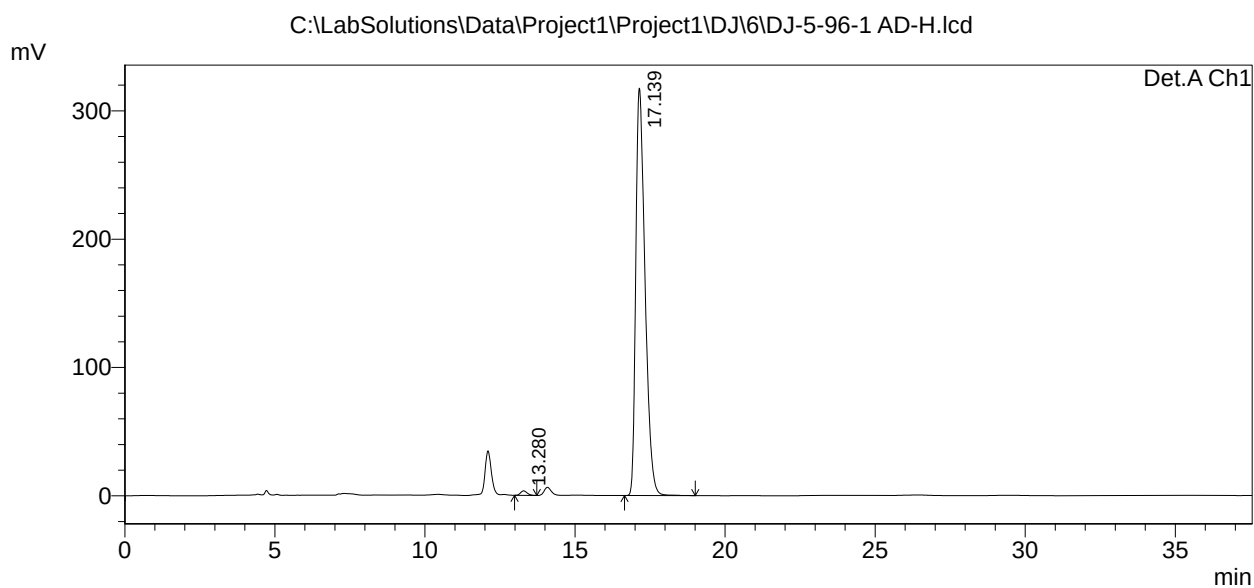
Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.214	492864	33365	7.260	8.472
2	13.384	2898559	187285	42.696	47.554
3	14.143	478009	29107	7.041	7.391
4	17.264	2919382	144083	43.003	36.584
Total		6788815	393840	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\DJ-5-96-1 AD-H.lcd
 Acquired by : Admin
 Sample Name : DJ-5-96-1 AD-H
 Sample ID : AD-H,99/1,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-5-96-1 AD-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-12-6 10:57:04
 Data Processed : 2016-12-6 11:34:38



<Chromatogram>

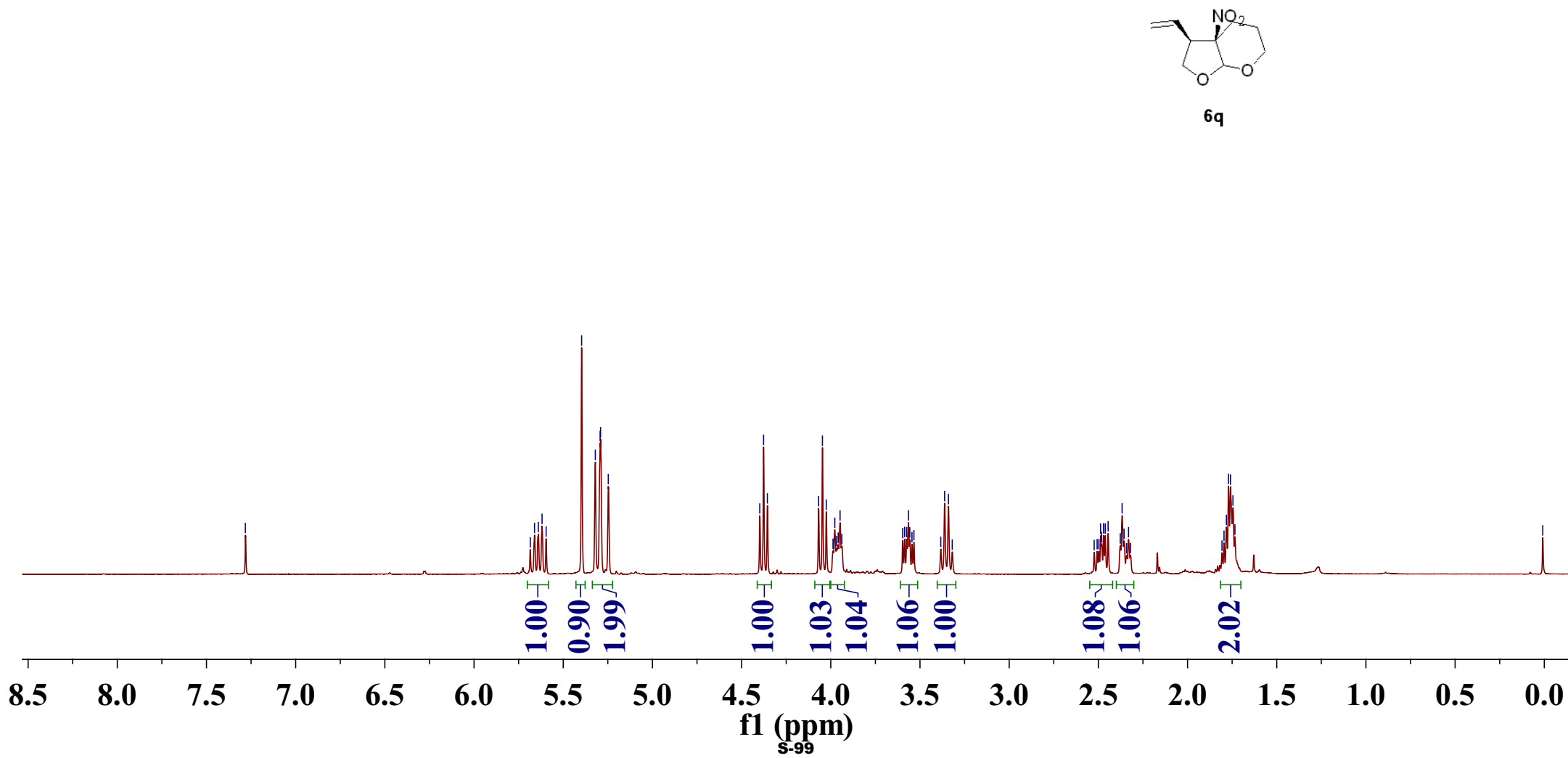


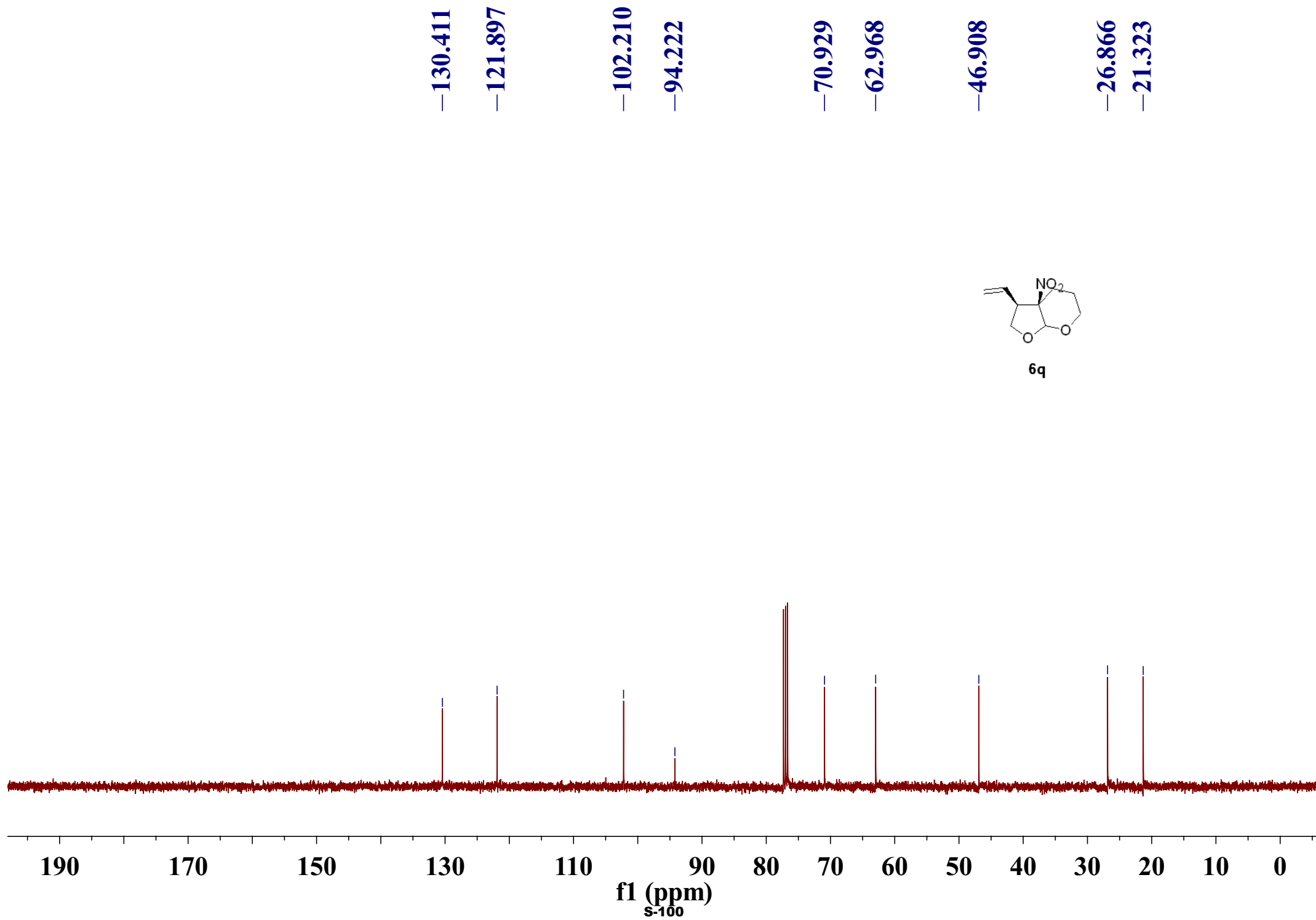
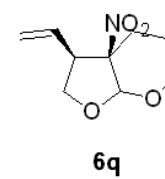
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

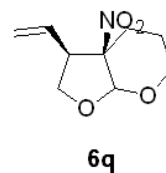
Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.280	53794	3505	0.784	1.092
2	17.139	6806384	317476	99.216	98.908
Total		6860178	320981	100.000	100.000



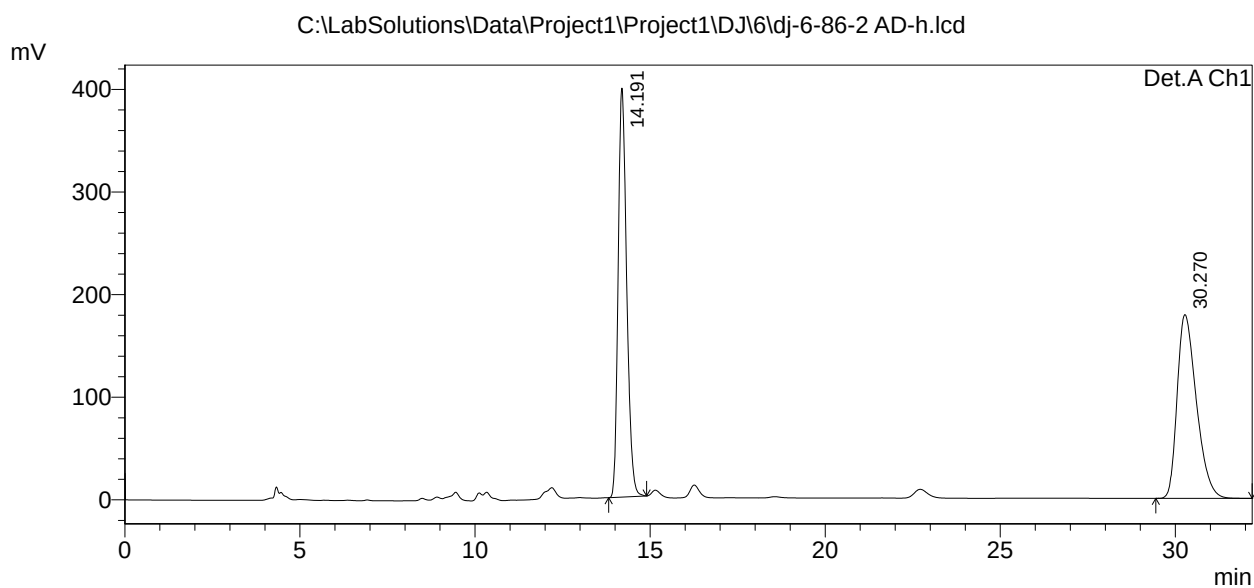


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\dj-6-86-2 AD-h.lcd
 Acquired by : Admin
 Sample Name : dj-6-86-2 AD-h
 Sample ID : AD-H,95/5,0.7,214
 Vail # :
 Injection Volume : 2 uL
 Data File Name : dj-6-86-2 AD-h.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2017-2-15 20:14:42
 Data Processed : 2017-2-15 20:46:53



<Chromatogram>



1 Det.A Ch1/214nm

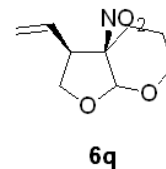
PeakTable

Detector A Ch1 214nm

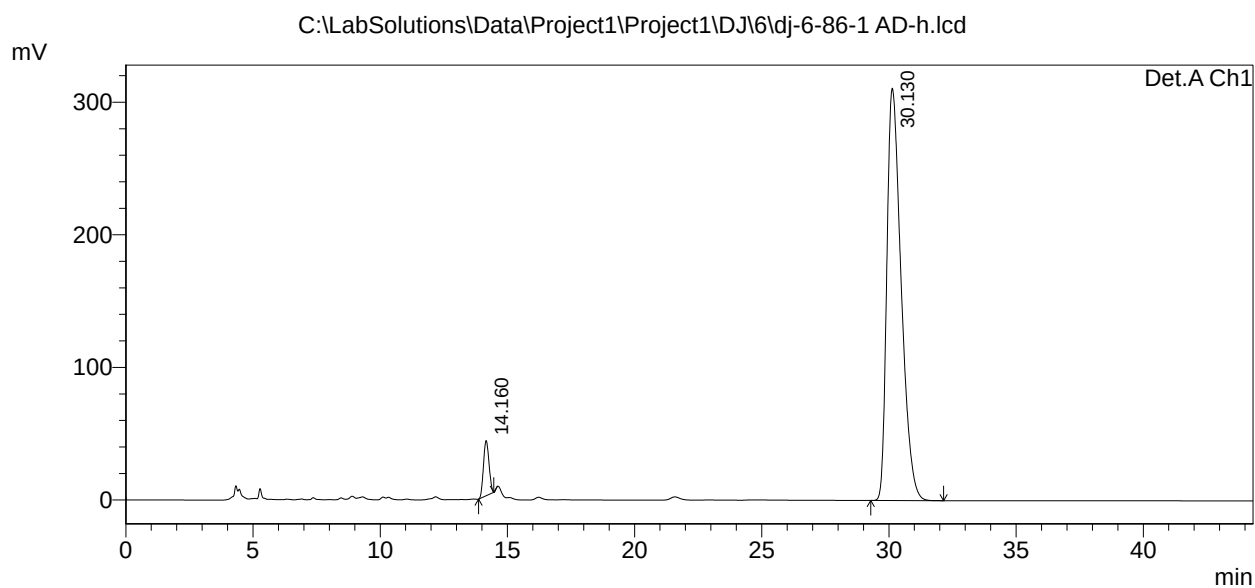
Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.191	6768879	398634	49.778	69.000
2	30.270	6829298	179093	50.222	31.000
Total		13598177	577726	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\dj-6-86-1 AD-h.lcd
 Acquired by : Admin
 Sample Name : dj-6-86-1 AD-h
 Sample ID : AD-H,95/5,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-6-86-1 AD-h.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2017-2-15 20:49:25
 Data Processed : 2017-2-15 21:33:45



<Chromatogram>

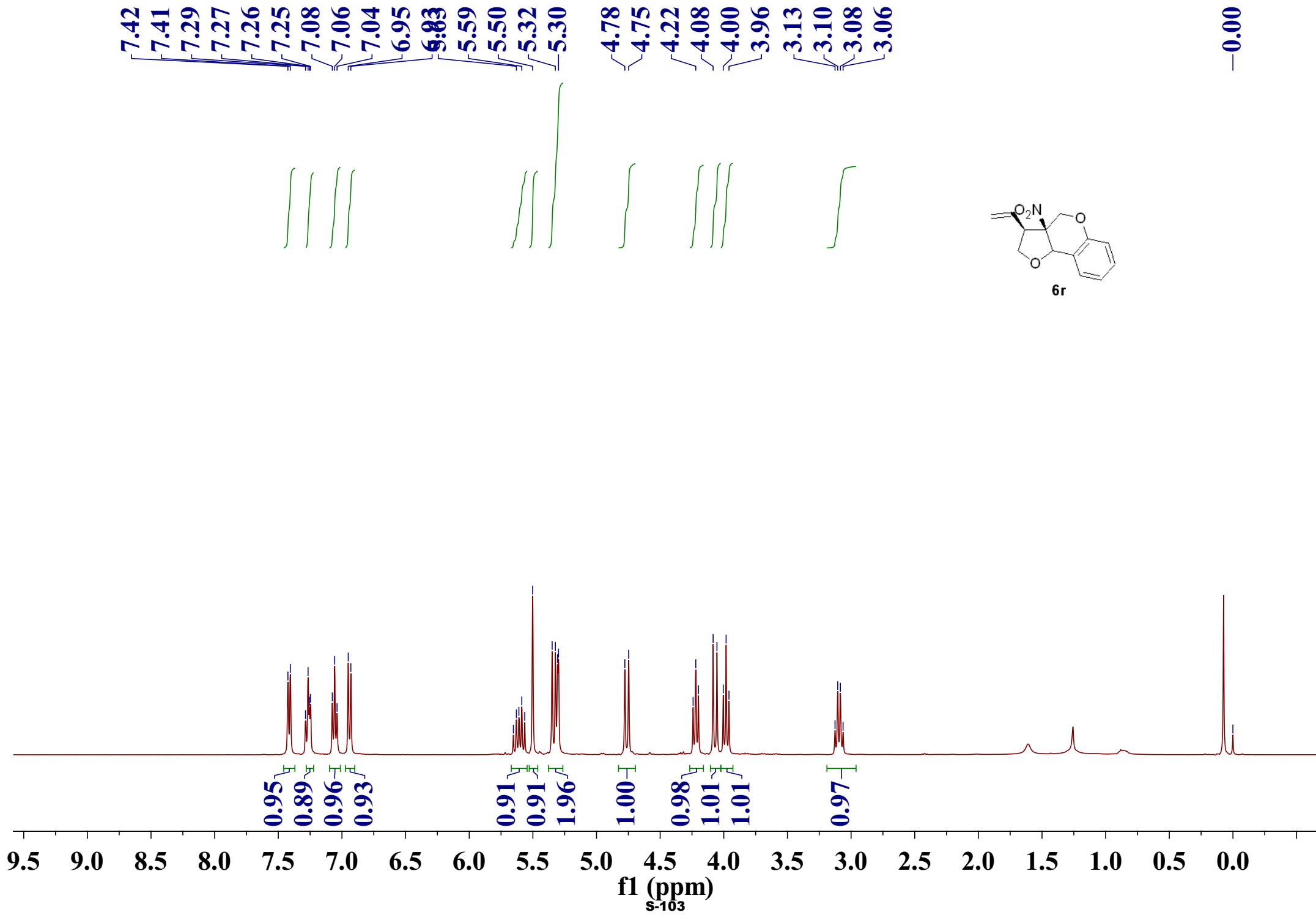


1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.160	629601	41604	4.927	11.798
2	30.130	12147829	311038	95.073	88.202
Total		12777429	352642	100.000	100.000



—153.59

130.42

130.22

129.90

122.62

122.42

119.87

117.23

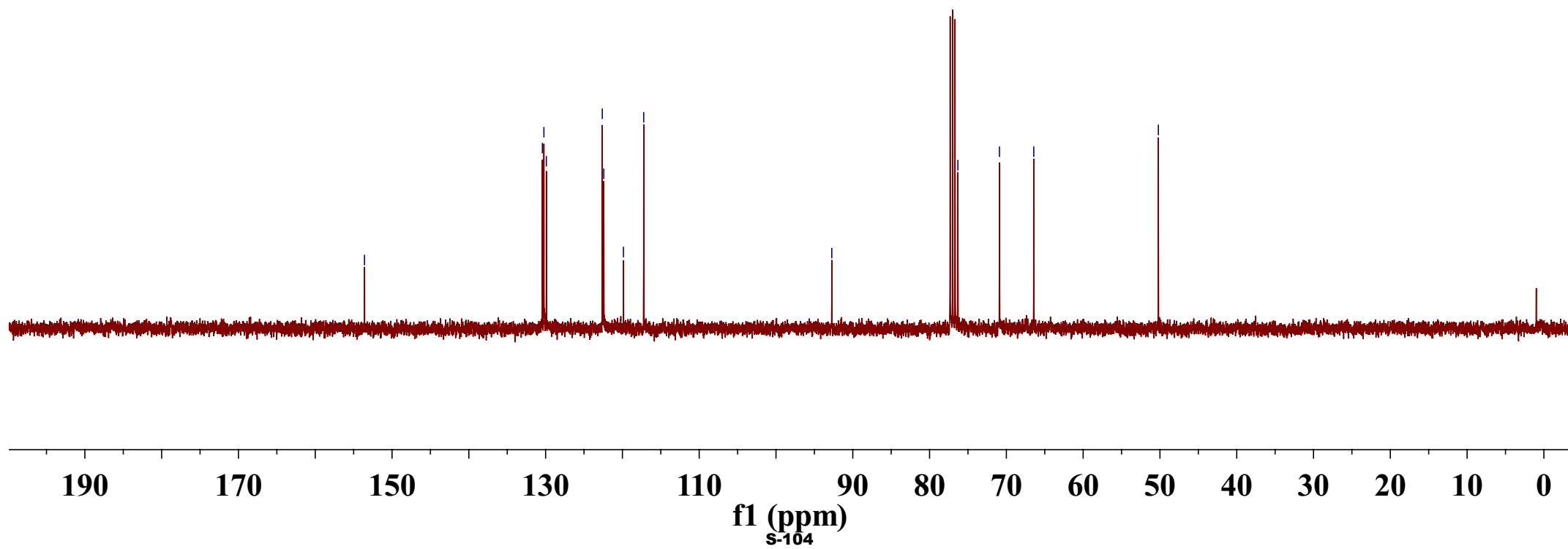
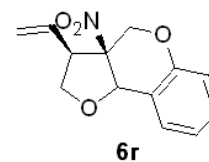
—92.73

—76.31

—70.90

—66.43

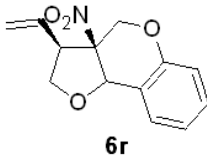
—50.20



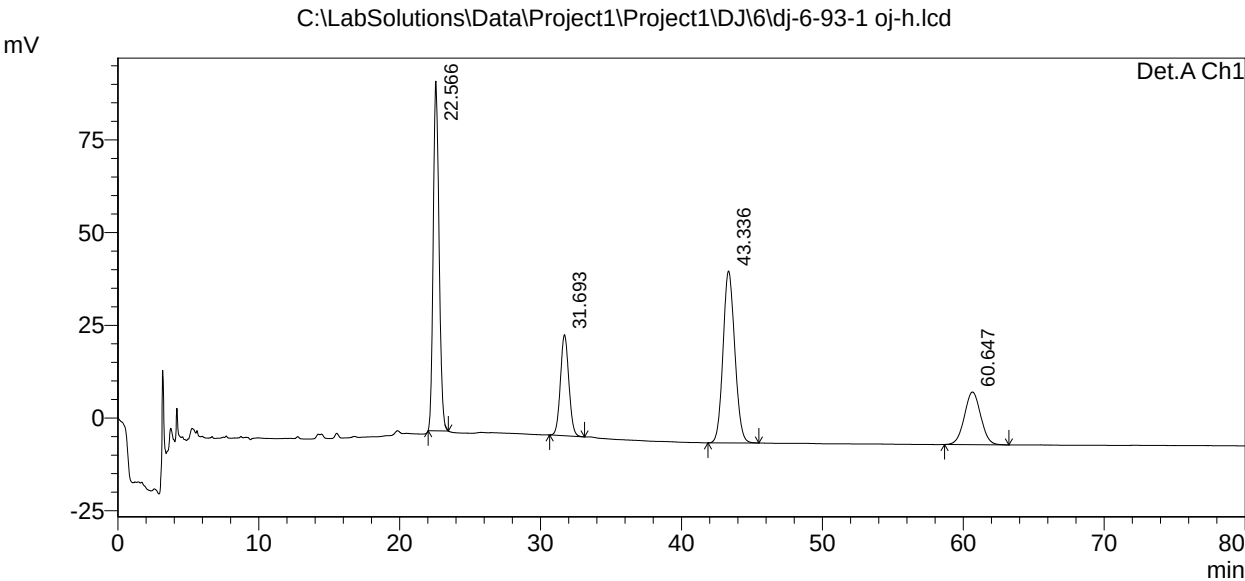
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\6\dj-6-93-1 oj-h.lcd

Acquired by : Admin
Sample Name : dj-6-93-1 OJ-H
Sample ID : OJ-H,90/10,1,214
Vial # :
Injection Volume : 2 uL
Data File Name : dj-6-93-1 oj-h.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2017-2-21 16:19:04
Data Processed : 2017-2-21 17:45:43



<Chromatogram>



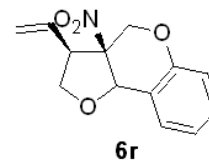
1 Det.A Ch1/214nm

PeakTable

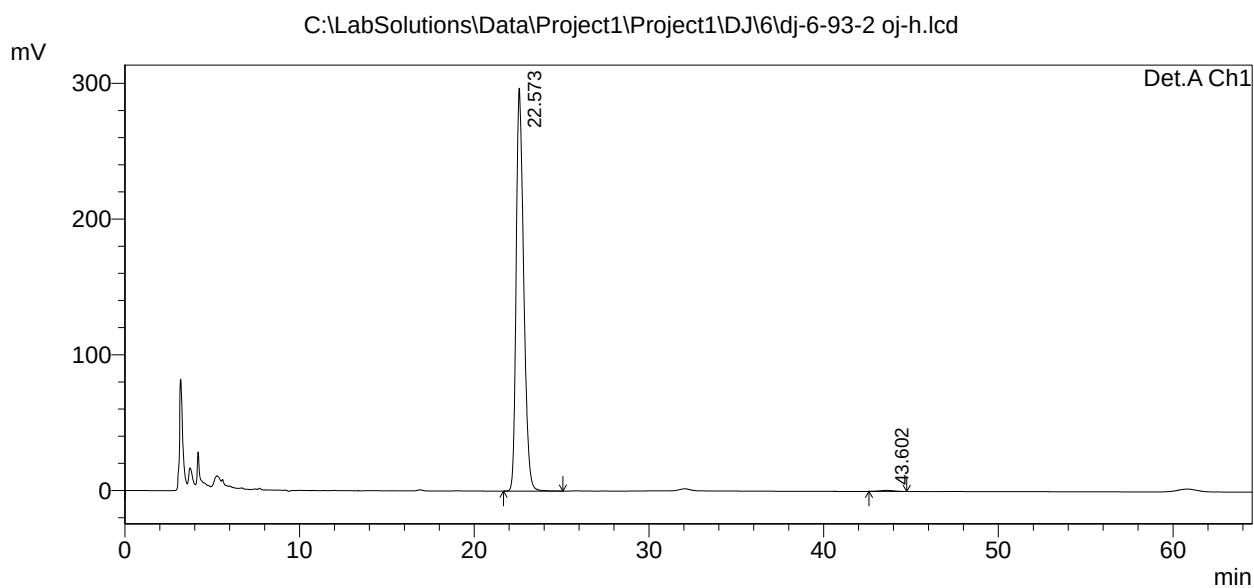
Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.566	2719607	94306	35.381	51.770
2	31.693	1130620	27266	14.709	14.968
3	43.336	2690798	46392	35.006	25.467
4	60.647	1145571	14199	14.903	7.795
Total		7686596	182164	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\dj-6-93-2 oj-h.lcd
 Acquired by : Admin
 Sample Name : dj-6-93-2 OJ-H
 Sample ID : OJ-H,90/10,1,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-6-93-2 oj-h.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2017-2-21 17:48:50
 Data Processed : 2017-2-21 18:53:24



<Chromatogram>

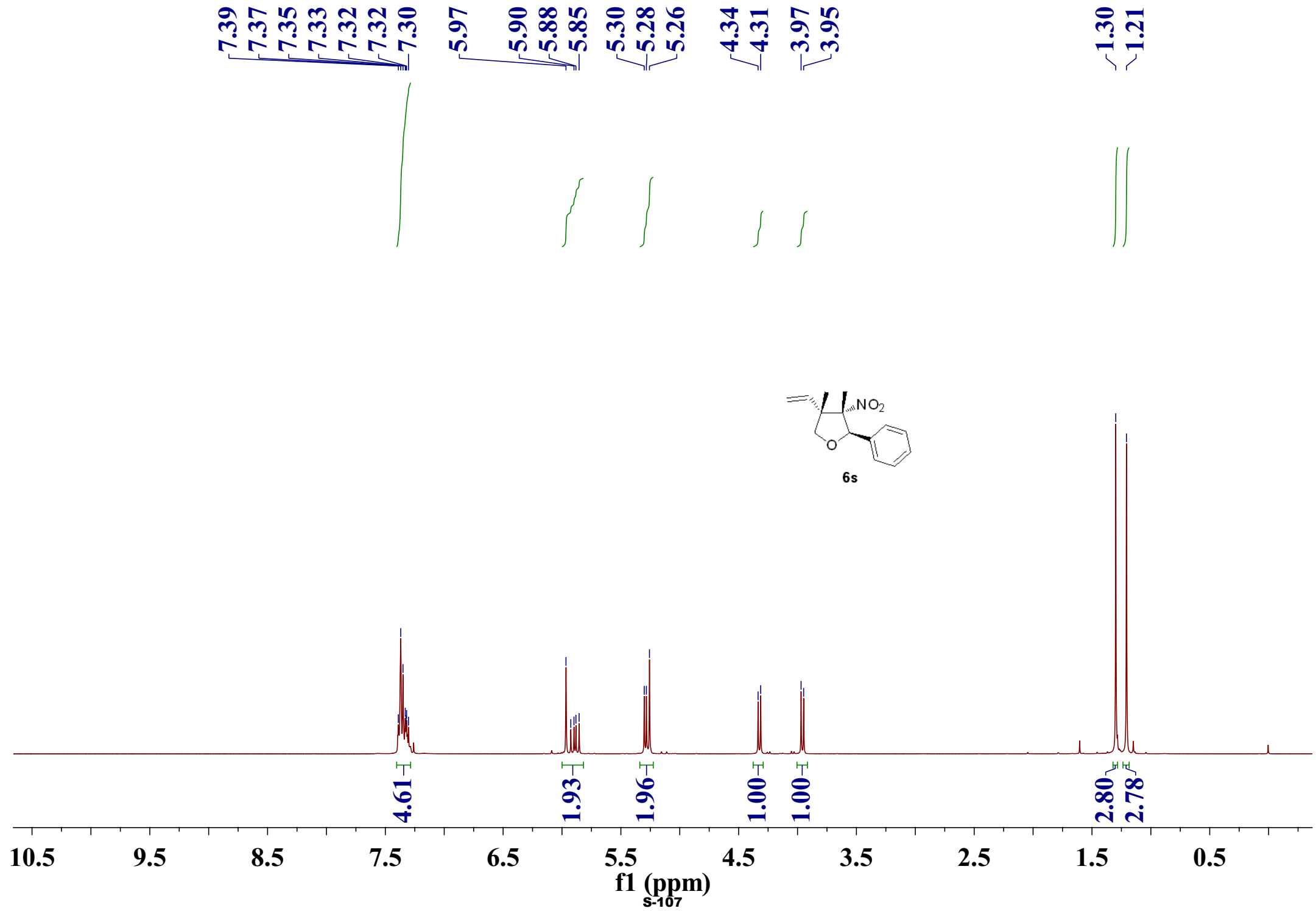


1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	22.573	8914057	296894	99.525	99.738
2	43.602	42499	779	0.475	0.262
Total		8956556	297673	100.000	100.000



137.82
137.37
128.27
128.21
126.70
117.02

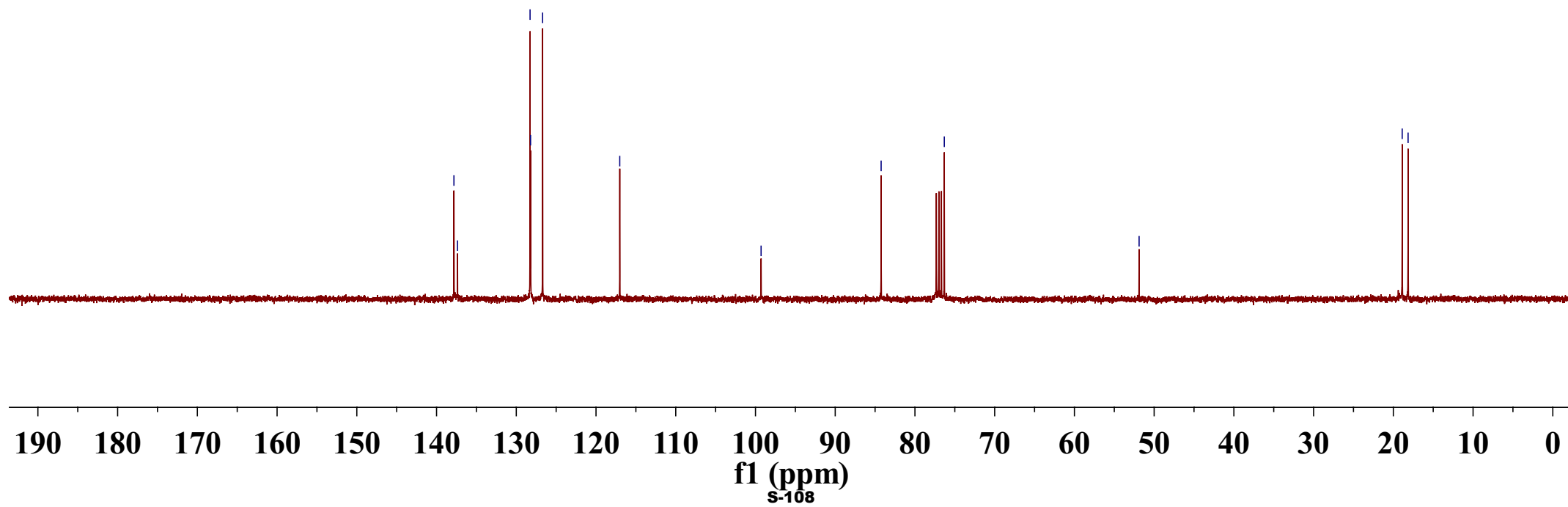
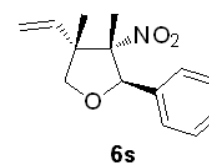
99.30

84.24

76.32

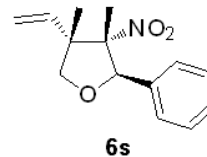
51.89

18.89
18.15

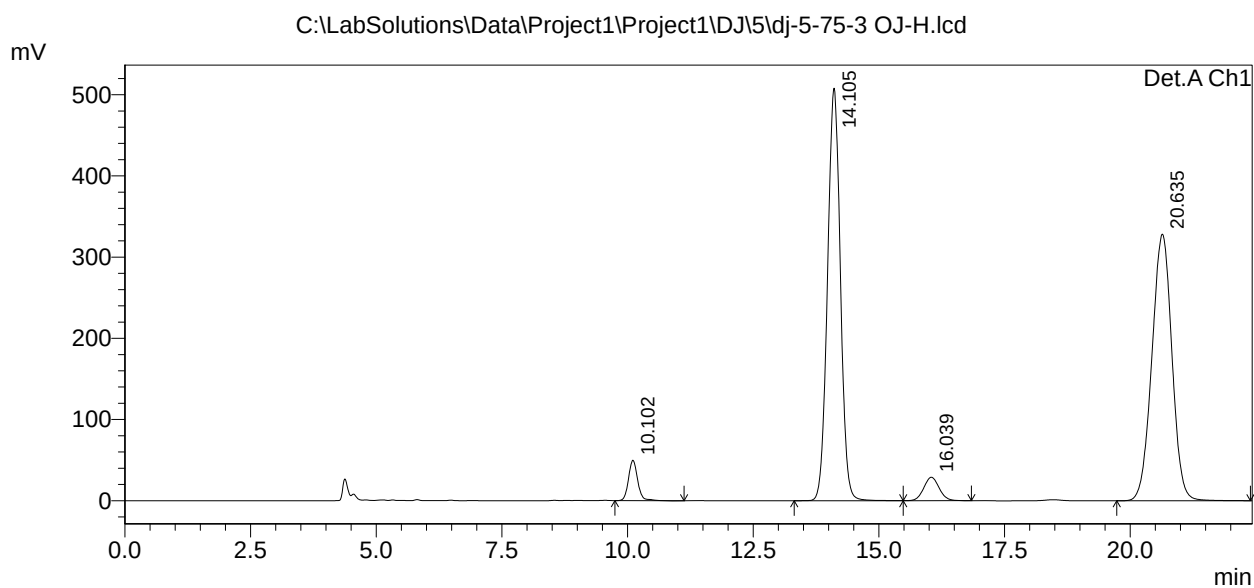


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\5\dj-5-75-3 OJ-H.lcd
 Acquired by : Admin
 Sample Name : dj-5-75-3 OJ-H
 Sample ID : OJ-H,92/8,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-5-75-3 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-11-11 13:21:50
 Data Processed : 2016-11-11 13:44:16



<Chromatogram>



1 Det.A Ch1/214nm

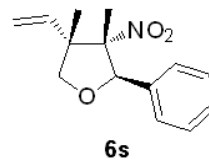
PeakTable

Detector A Ch1 214nm

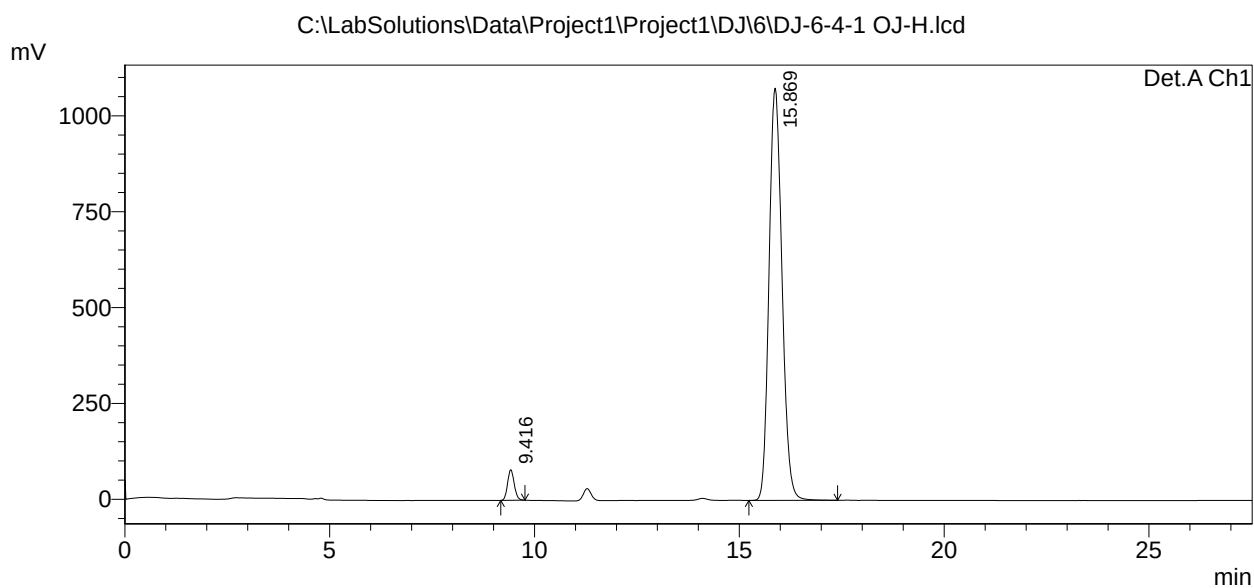
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.102	630695	49748	3.251	5.436
2	14.105	9063733	508170	46.724	55.527
3	16.039	615454	28890	3.173	3.157
4	20.635	9088729	328375	46.852	35.881
Total		19398611	915183	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\6\DJ-6-4-1 OJ-H.lcd
 Acquired by : Admin
 Sample Name : DJ-6-4-1 OJ-H
 Sample ID : OJ-H,92/8,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : DJ-6-4-1 OJ-H.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2016-12-5 21:13:56
 Data Processed : 2016-12-5 21:41:28



<Chromatogram>

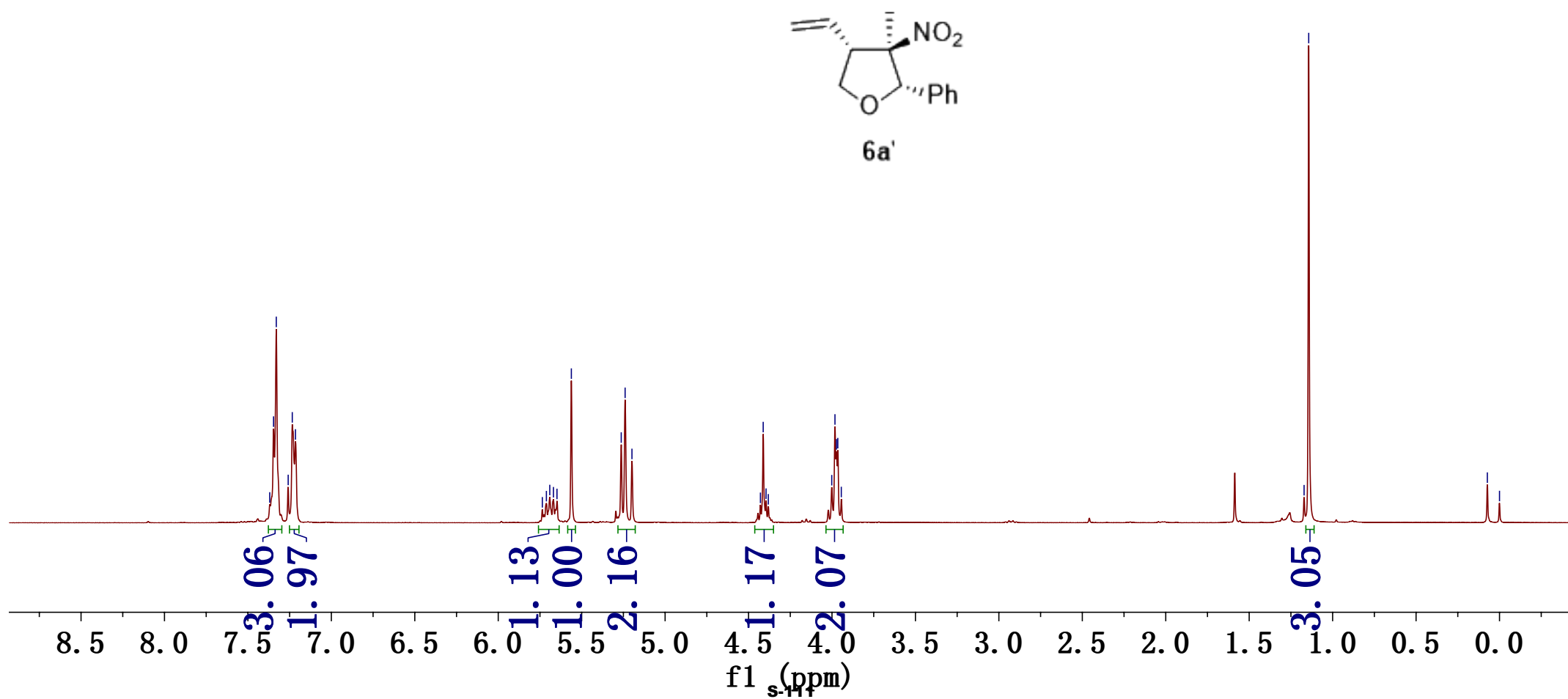


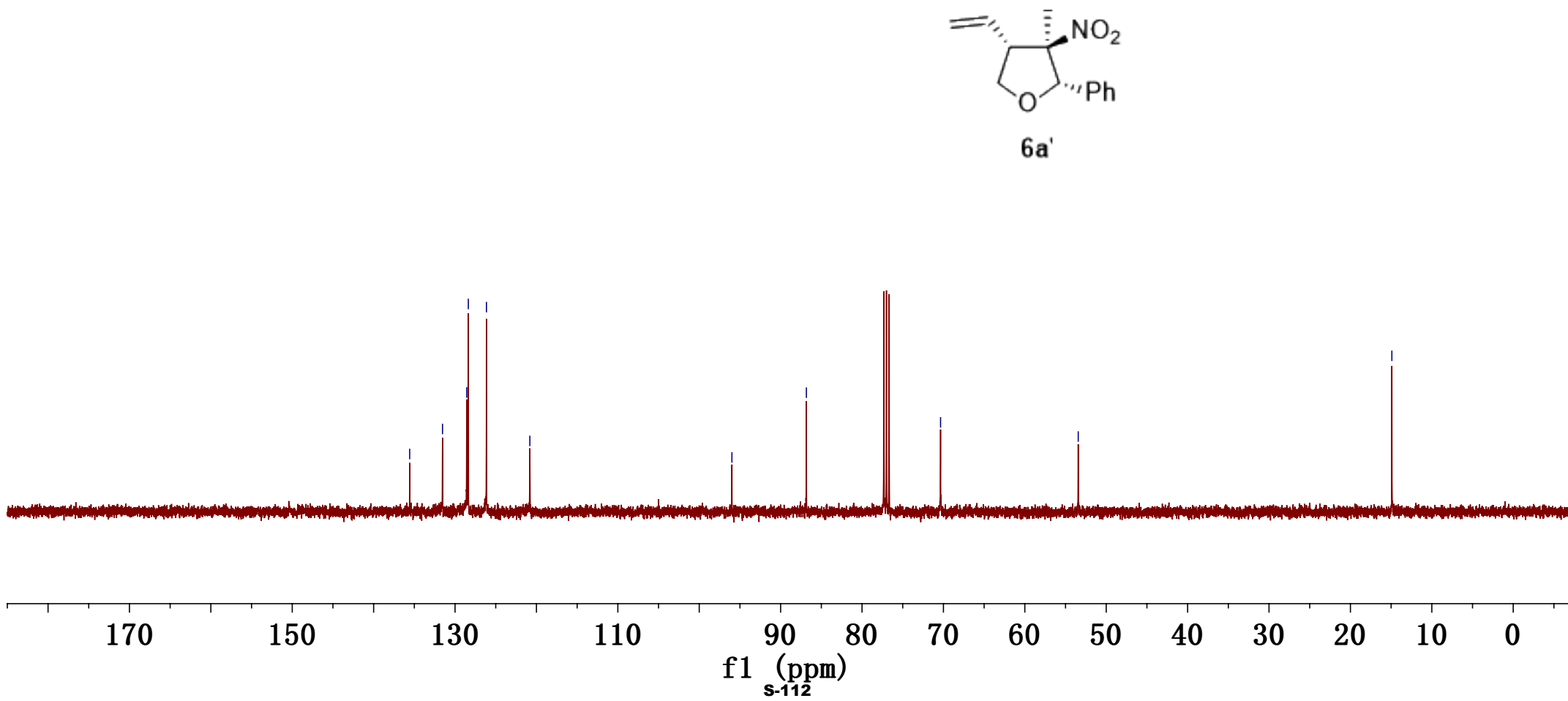
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

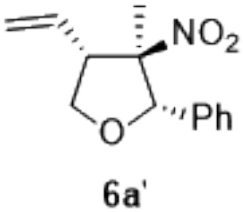
Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.416	897798	79599	3.657	6.894
2	15.869	23651057	1074988	96.343	93.106
Total		24548855	1154587	100.000	100.000



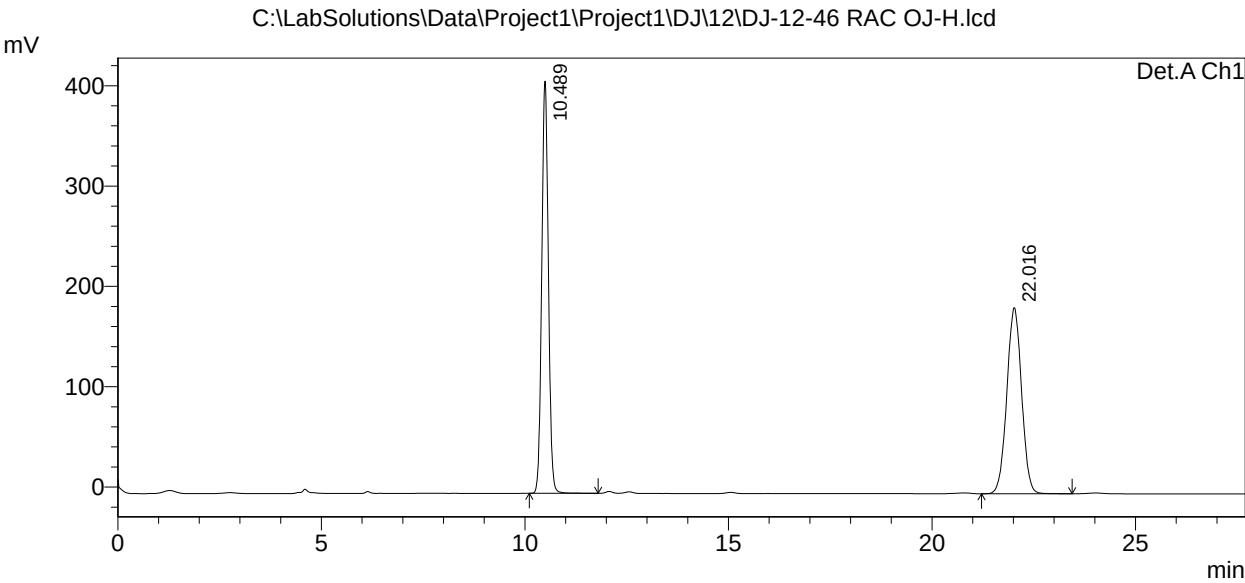


==== Shimadzu LCsolution Analysis Report ====

Acquired by : Admin
Sample Name : DJ-12-46 RAC OJ-H
Sample ID : OJ-H,90/10,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : DJ-12-46 RAC OJ-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2018-7-8 11:28:25
Data Processed : 2018-7-8 11:56:06



<Chromatogram>



1 Det.A Ch1/214nm

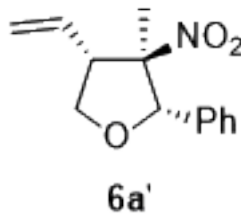
PeakTable

Detector A Ch1 214nm

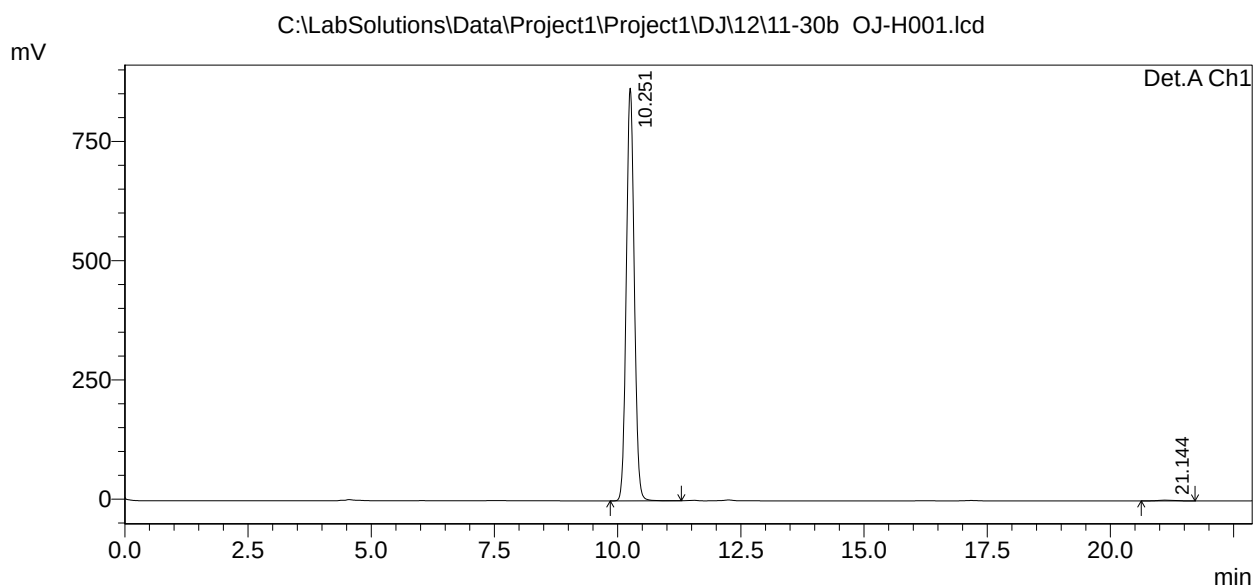
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.489	4653704	410846	49.879	68.900
2	22.016	4676331	185444	50.121	31.100
Total		9330036	596290	100.000	100.000

==== Shimadzu LcSolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\12\11-30b OJ-H001.lcd
 Acquired by : Admin
 Sample Name : 11-30b OJ-H
 Sample ID : OJ-H,90/10,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : 11-30b OJ-H001.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2018-7-5 22:15:49
 Data Processed : 2018-7-5 22:38:43



<Chromatogram>

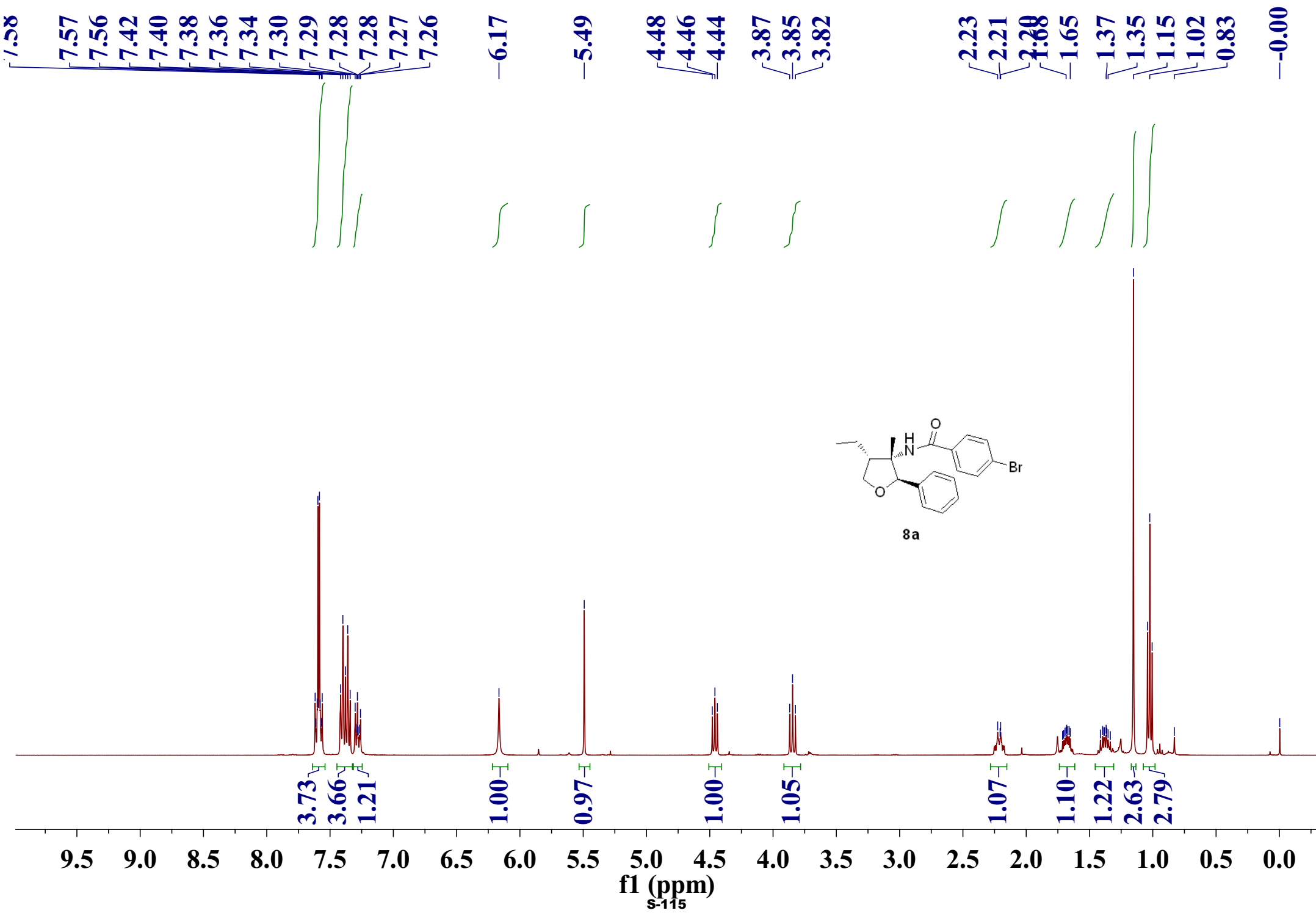


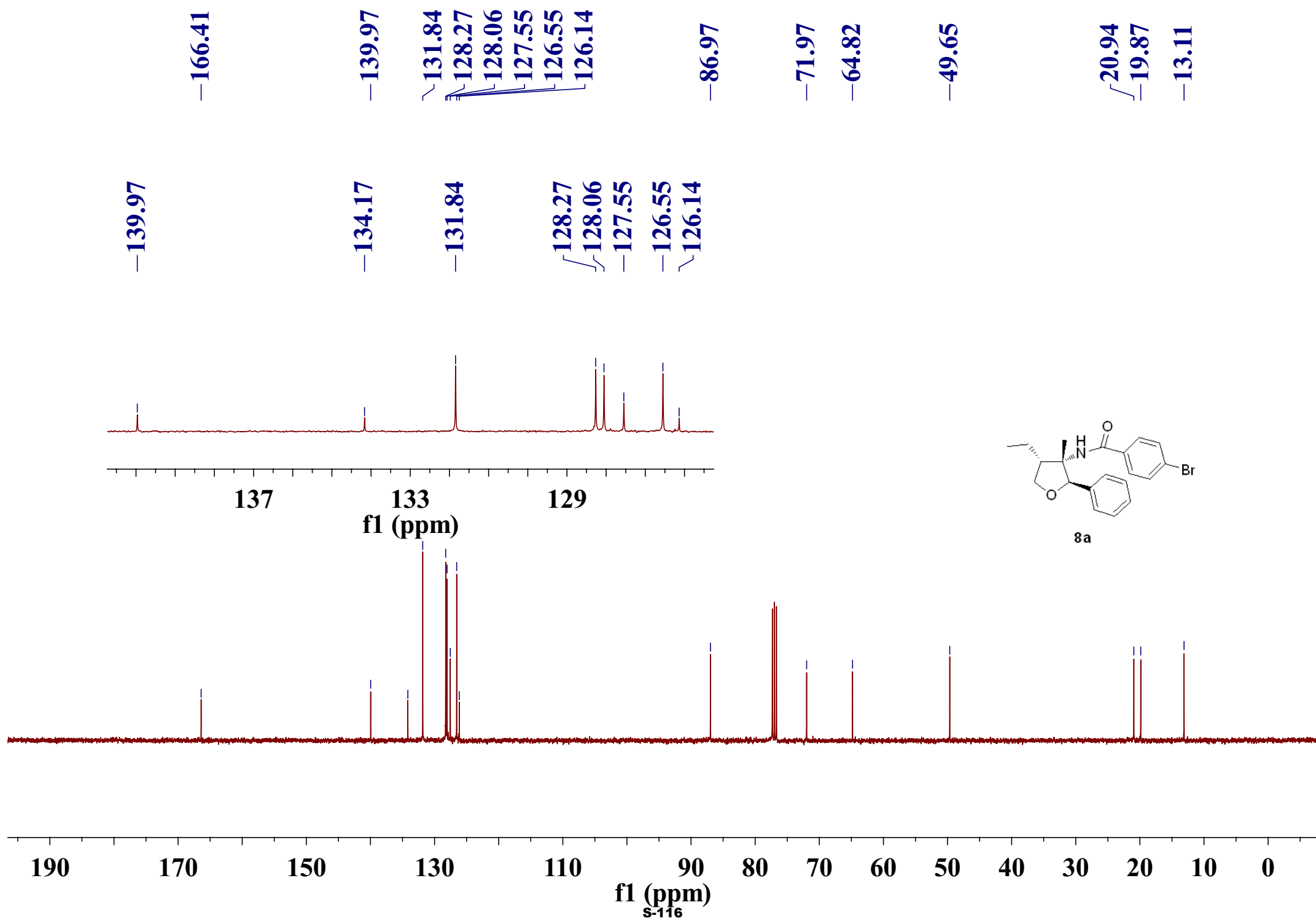
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

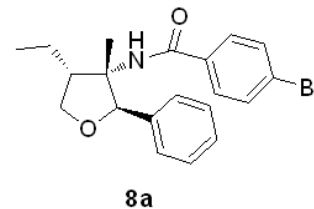
Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.251	9709021	865362	99.591	99.806
2	21.144	39911	1685	0.409	0.194
Total		9748932	867047	100.000	100.000



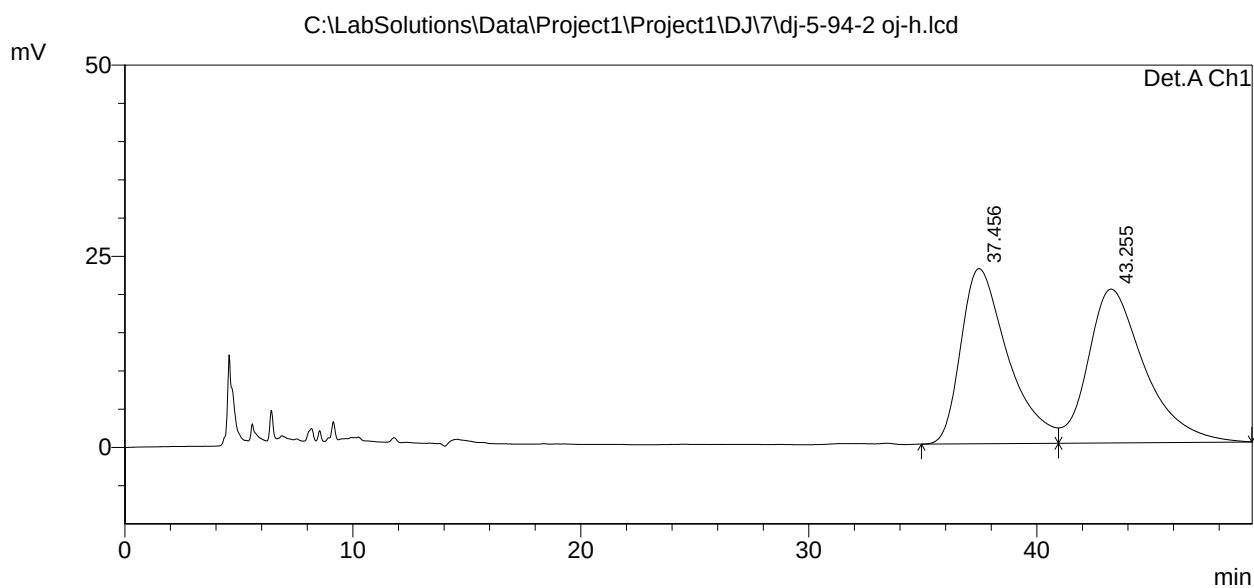


==== Shimadzu LCsolution Analysis Report =====

C:\LabSolutions\Data\Project1\Project1\DJ\7\dj-5-94-2 oj-h.lcd
 Acquired by : Admin
 Sample Name : dj-5-94-2 oj-h
 Sample ID : oj-H,90/10,0.7,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-5-94-2 oj-h.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2017-3-16 9:26:19
 Data Processed : 2017-3-16 10:42:28



<Chromatogram>



1 Det.A Ch1/214nm

PeakTable

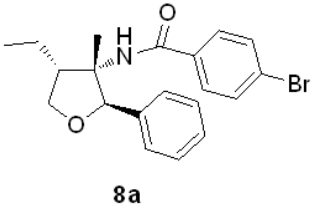
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	37.456	3287713	22916	48.710	53.244
2	43.255	3461903	20123	51.290	46.756
Total		6749617	43039	100.000	100.000

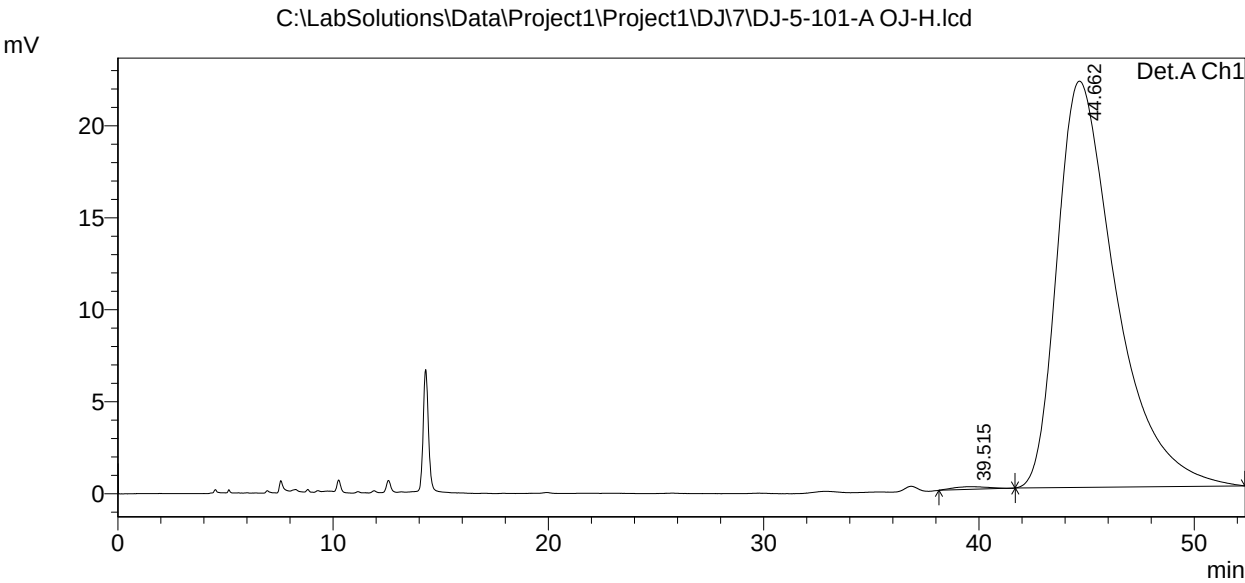
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\7\DJ-5-101-A OJ-H.lcd

Acquired by : Admin
Sample Name : DJ-5-101-A OJ-H
Sample ID : OJ-H,90/10,0.7,214
Vail # :
Injection Volume : 2 uL
Data File Name : DJ-5-101-A OJ-H.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2017-4-12 9:31:22
Data Processed : 2017-4-12 10:23:45



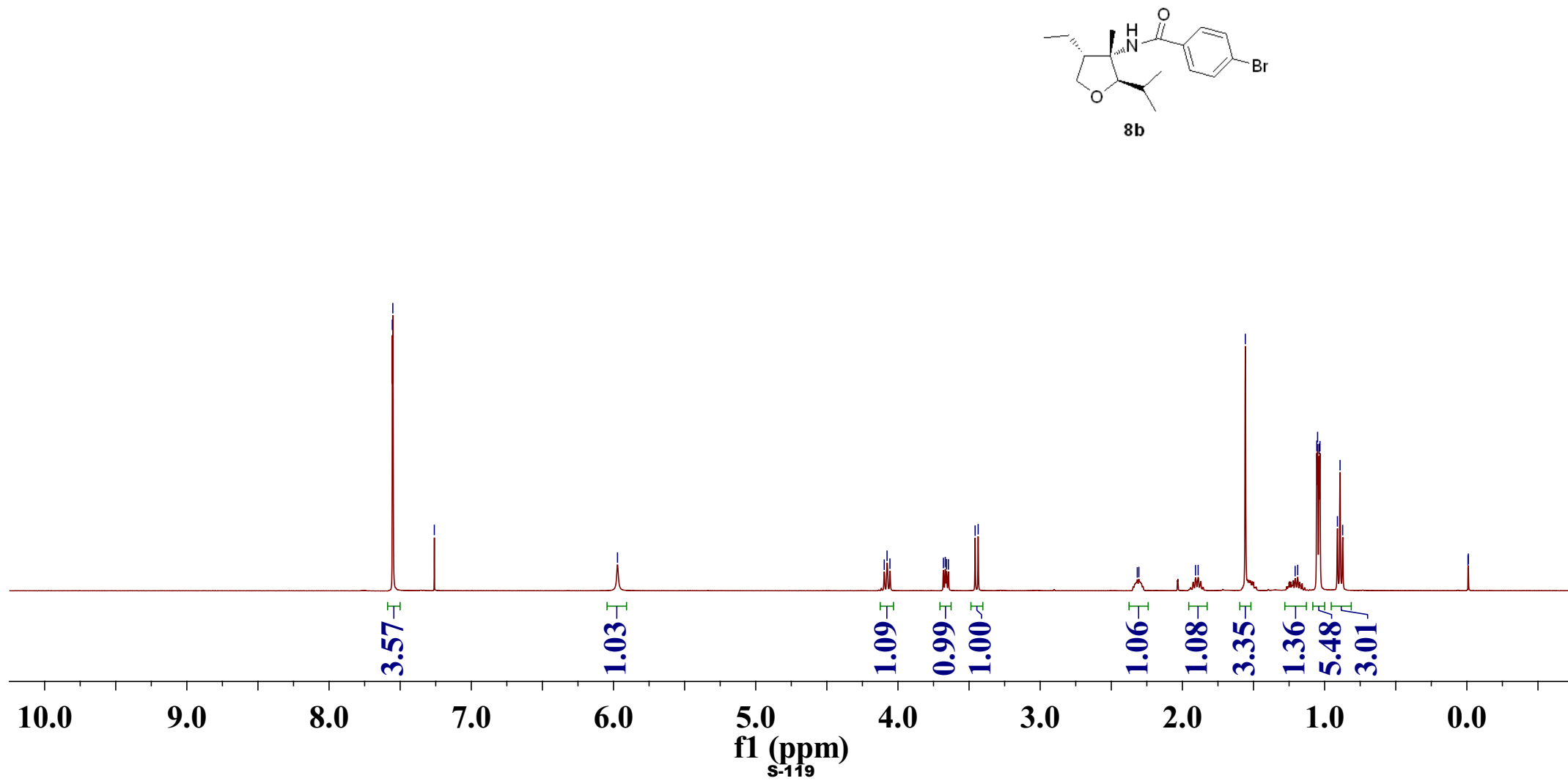
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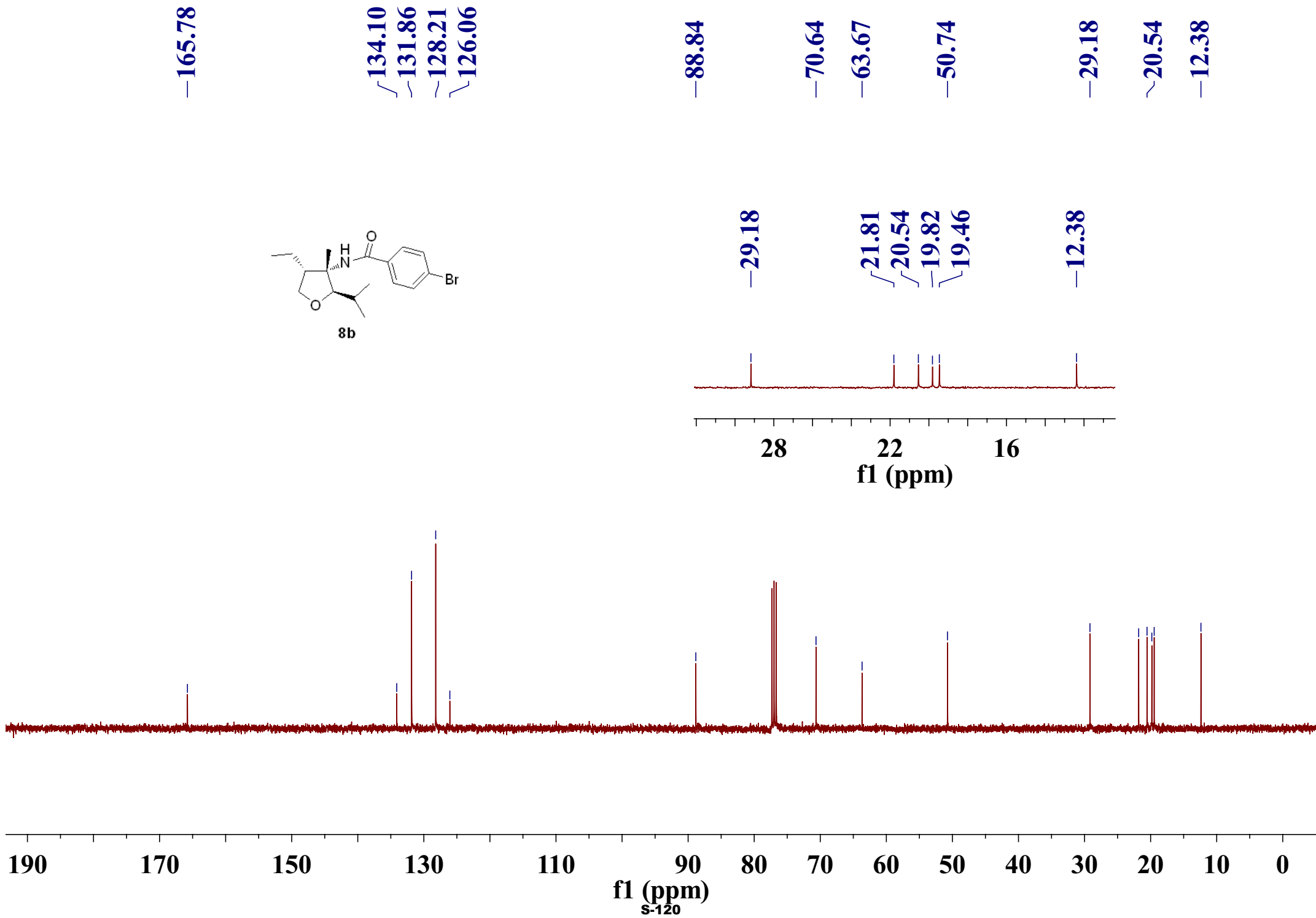


PeakTable

Detector A Ch1 254nm

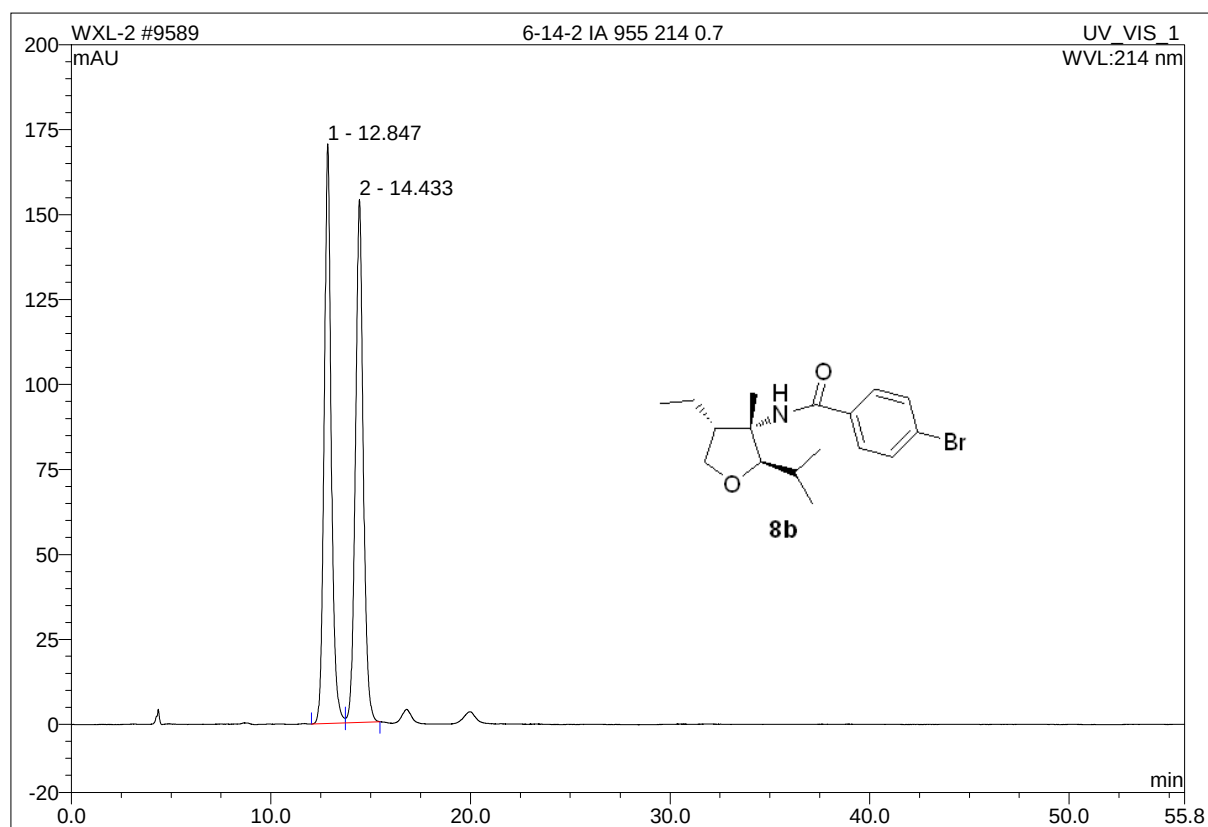
Peak#	Ret. Time	Area	Height	Area %	Height %
1	39.515	15815	147	0.378	0.660
2	44.662	4165031	22077	99.622	99.340
Total		4180845	22223	100.000	100.000





9589 6-14-2 IA 955 214 0.7

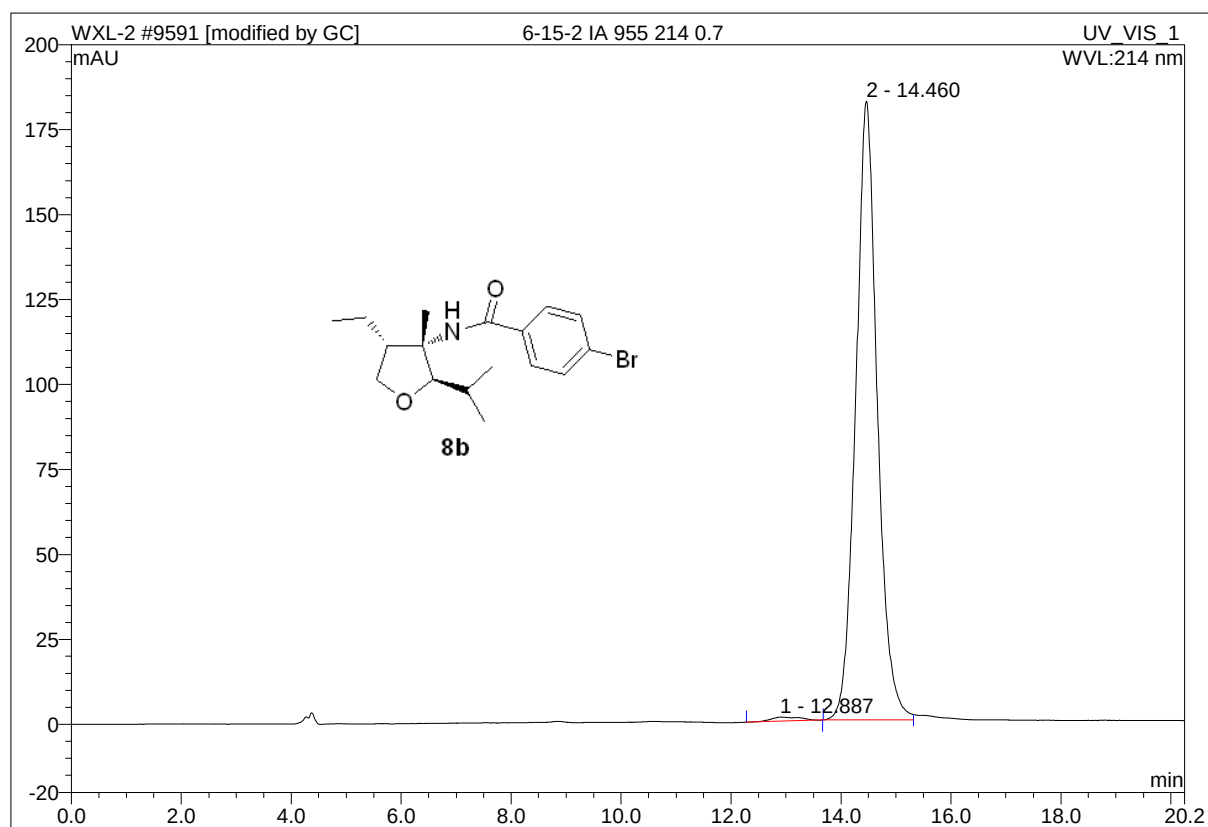
Sample Name:	6-14-2 IA 955 214 0.7	Injection Volume:	2.0
Vial Number:	GB2	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	214
Control Program:	WXL-2014	Bandwidth:	n.a.
Quantif. Method:	WXL	Dilution Factor:	1.0000
Recording Time:	2016/12/15 13:13	Sample Weight:	1.0000
Run Time (min):	55.77	Sample Amount:	1.0000



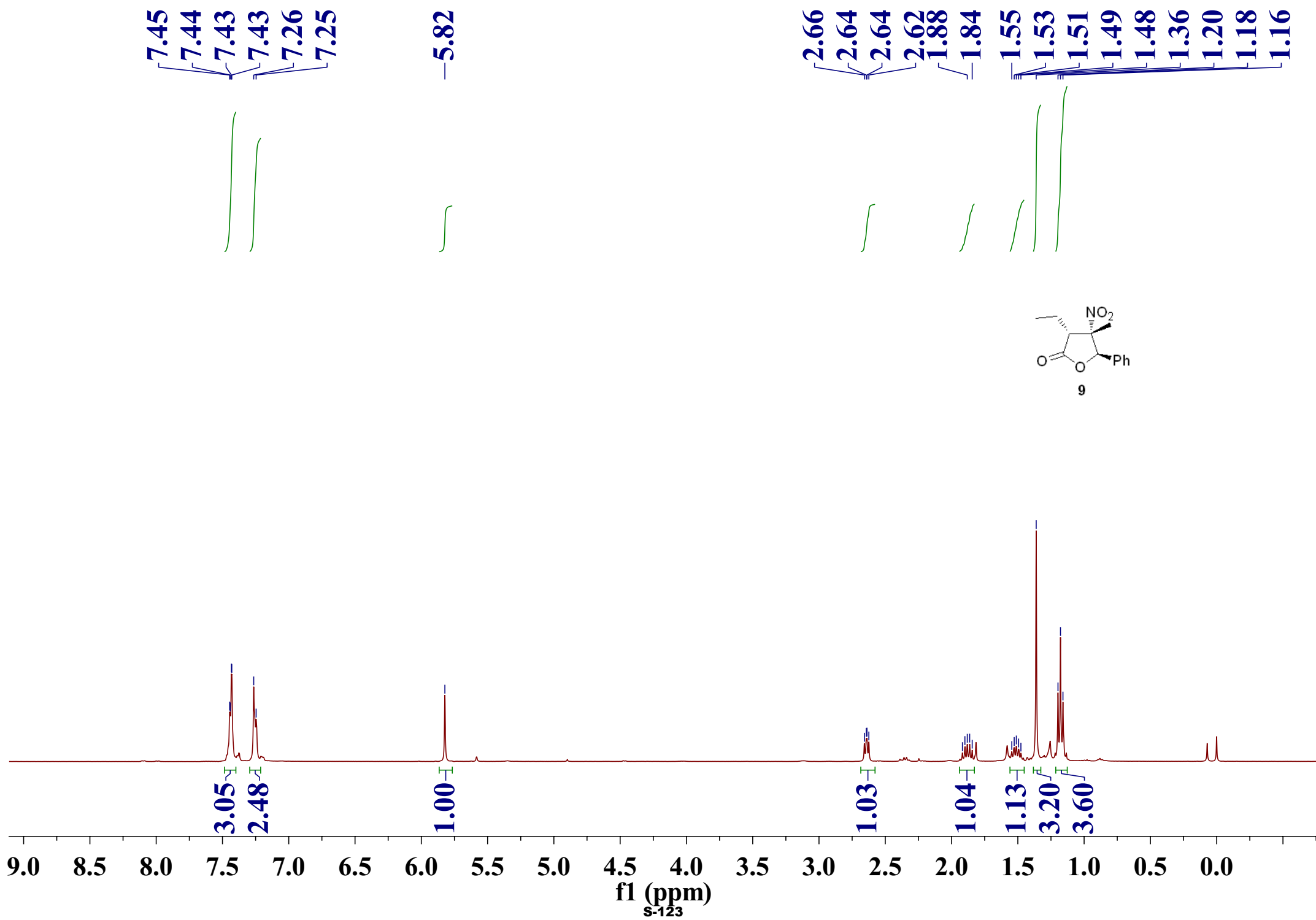
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.85	n.a.	170.544	70.100	50.06	n.a.	BM
2	14.43	n.a.	153.964	69.929	49.94	n.a.	MB
Total:			324.508	140.029	100.00	0.000	

9591 6-15-2 IA 955 214 0.7

Sample Name:	6-15-2 IA 955 214 0.7	Injection Volume:	2.0
Vial Number:	GB3	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	214
Control Program:	WXL-2014	Bandwidth:	n.a.
Quantif. Method:	WXL	Dilution Factor:	1.0000
Recording Time:	2016/12/15 18:54	Sample Weight:	1.0000
Run Time (min):	20.25	Sample Amount:	1.0000



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.89	n.a.	1.217	0.720	0.86	n.a.	BMB*
2	14.46	n.a.	182.115	82.838	99.14	n.a.	BM *
Total:			183.332	83.558	100.00	0.000	



—173.90

—133.99

—129.68

—129.10

—126.07

—94.55

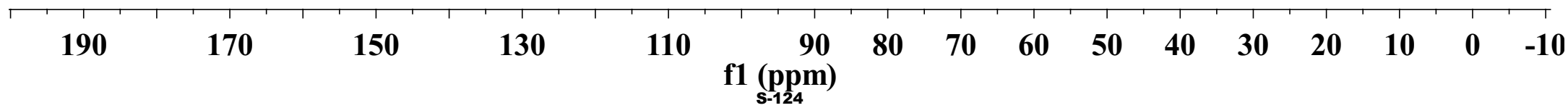
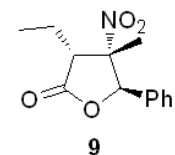
—83.83

—49.61

—20.27

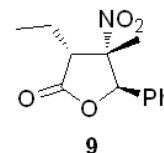
—18.98

—12.14

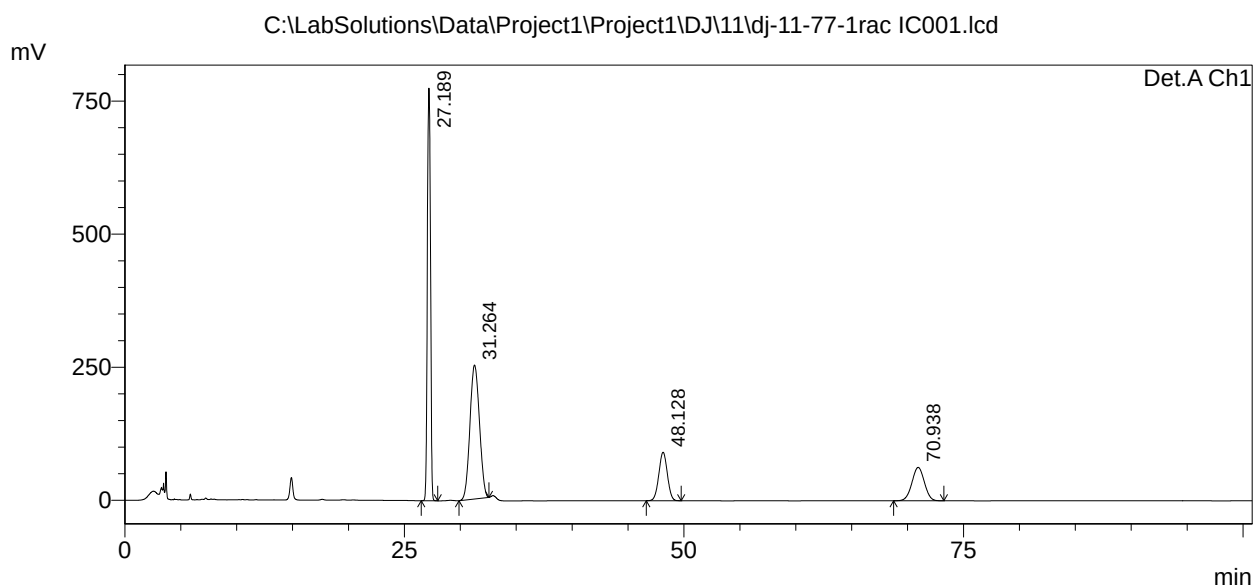


==== Shimadzu LCsolution Analysis Report =====

Acquired by : Admin
 Sample Name : dj-11-77-1RAC IC
 Sample ID : IC,97/3,1.0,214
 Vial # :
 Injection Volume : 2 uL
 Data File Name : dj-11-77-1rac IC001.lcd
 Method File Name : 123.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2018-5-4 13:53:54
 Data Processed : 2018-5-4 15:34:43



<Chromatogram>



1 Det.A Ch1/214nm

PeakTable

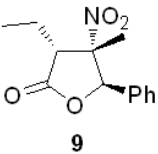
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.189	15403046	775160	38.482	65.646
2	31.264	14952047	251839	37.355	21.328
3	48.128	4823049	91099	12.049	7.715
4	70.938	4848923	62715	12.114	5.311
Total		40027064	1180812	100.000	100.000

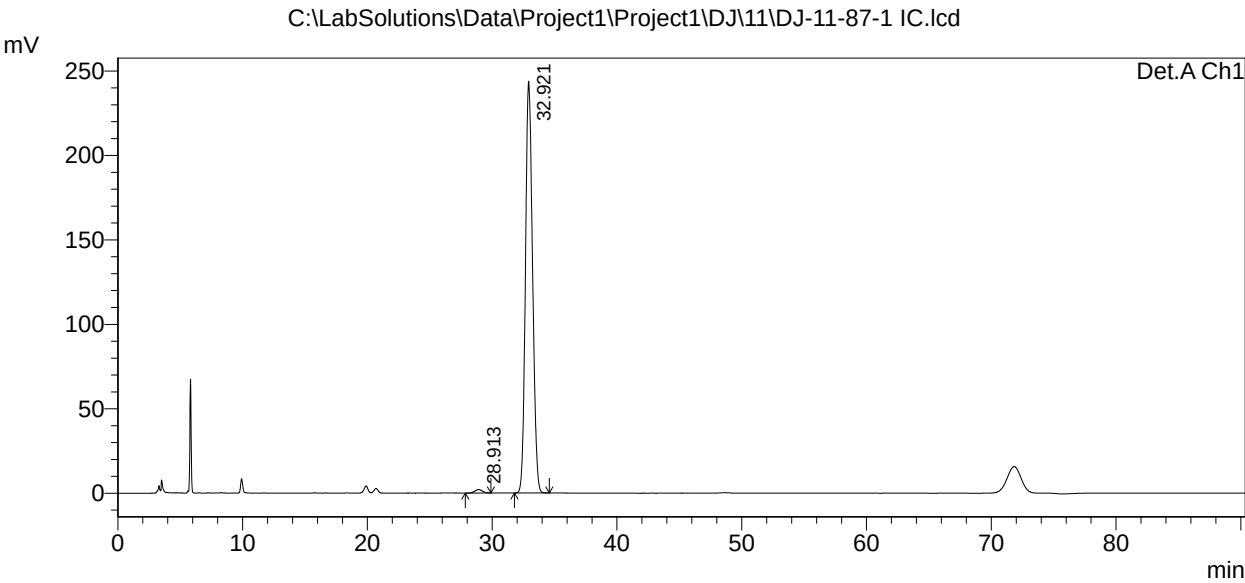
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\11\DJ-11-87-1 IC.lcd

Acquired by : Admin
Sample Name : DJ-11-87-1 IC
Sample ID : IC,97/3,1.0,214
Vial # :
Injection Volume : 2 uL
Data File Name : DJ-11-87-1 IC.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2018-5-9 17:21:37
Data Processed : 2018-5-9 18:51:58

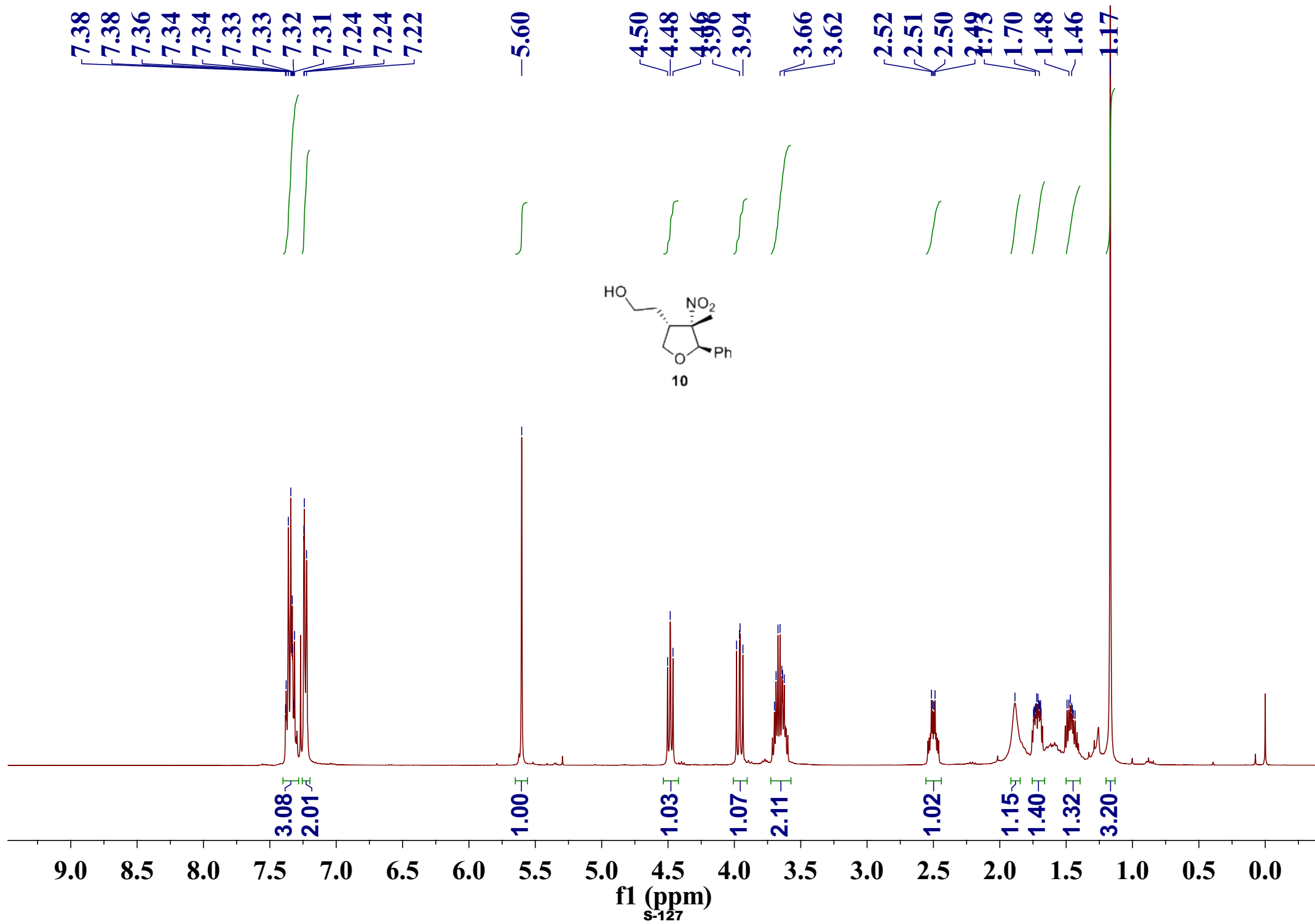


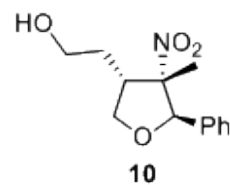
<Chromatogram>



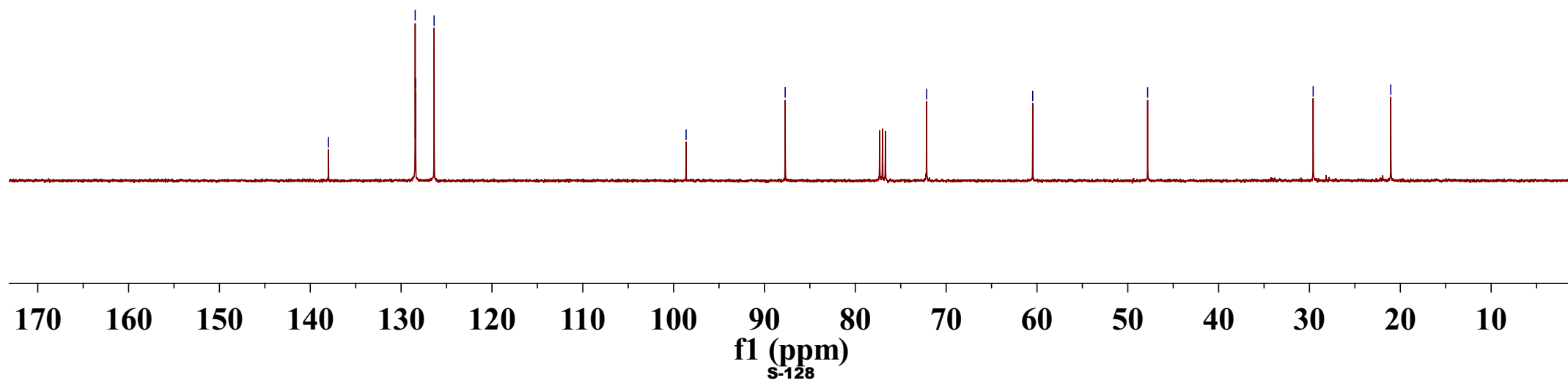
PeakTable

Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.913	89889	2069	0.923	0.841
2	32.921	9648969	243868	99.077	99.159
Total		9738858	245937	100.000	100.000





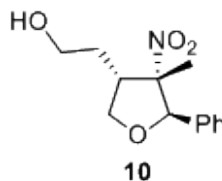
—138.00
 { 128.45
 { 128.41
 { 126.37
 —98.62
 —87.72
 —72.15
 —60.47
 —47.82
 —29.59
 —21.05



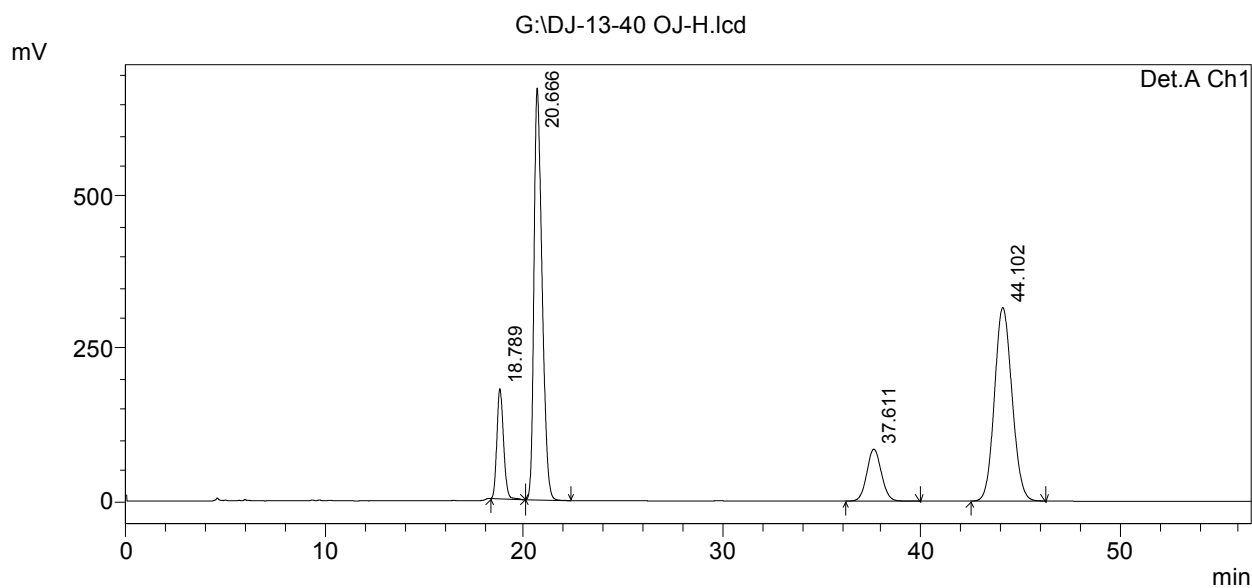
==== Shimadzu LCsolution Analysis Report =====

G:\DJ-13-40 OJ-H.lcd

Acquired by : Admin
 Sample Name : DJ-13-40 OJ-H
 Sample ID : OJ-H,85/15,0.7,215
 Vial # :
 Injection Volume : 1 uL
 Data File Name : DJ-13-40 OJ-H.lcd
 Method File Name : 1.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2018-10-22 19:24:52
 Data Processed : 2018-10-22 20:21:28



<Chromatogram>



PeakTable

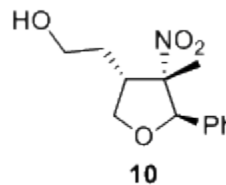
Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.789	4226100	180657	8.957	14.347
2	20.666	19129657	675763	40.544	53.664
3	37.611	4332790	85273	9.183	6.772
4	44.102	19493744	317545	41.316	25.217
Total		47182292	1259237	100.000	100.000

==== Shimadzu LCsolution Analysis Report =====

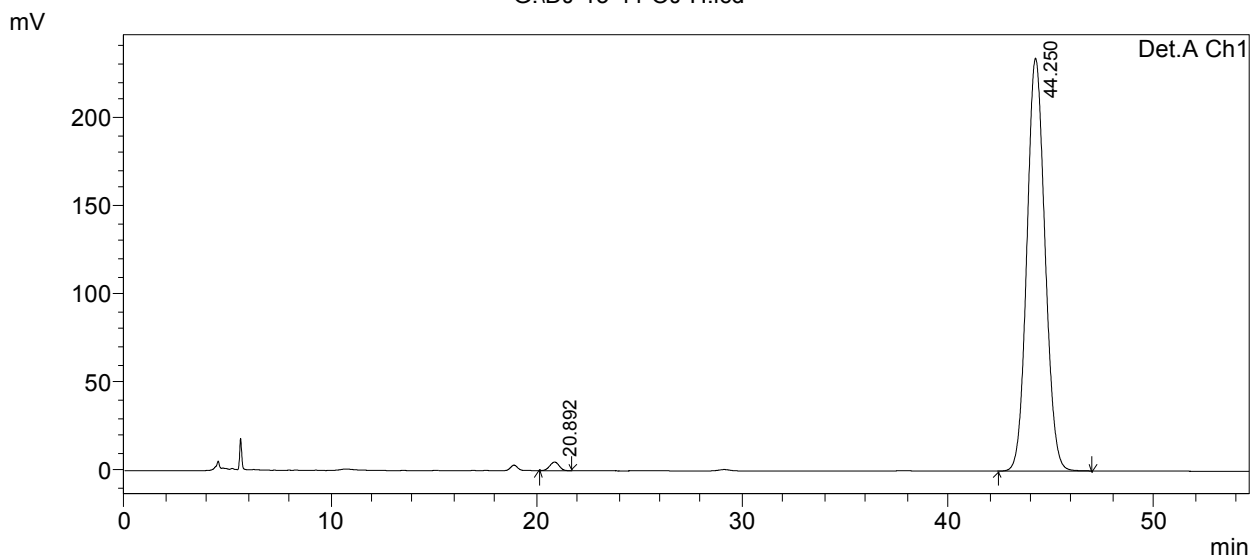
G:\DJ-13-41 OJ-H.lcd

Acquired by : Admin
 Sample Name : DJ-13-41 OJ-H
 Sample ID : OJ-H,85/15,0.7,215
 Vial # :
 Injection Volume : 1 uL
 Data File Name : DJ-13-41 OJ-H.lcd
 Method File Name : 1.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2018-10-22 20:26:59
 Data Processed : 2018-10-22 21:21:37



<Chromatogram>

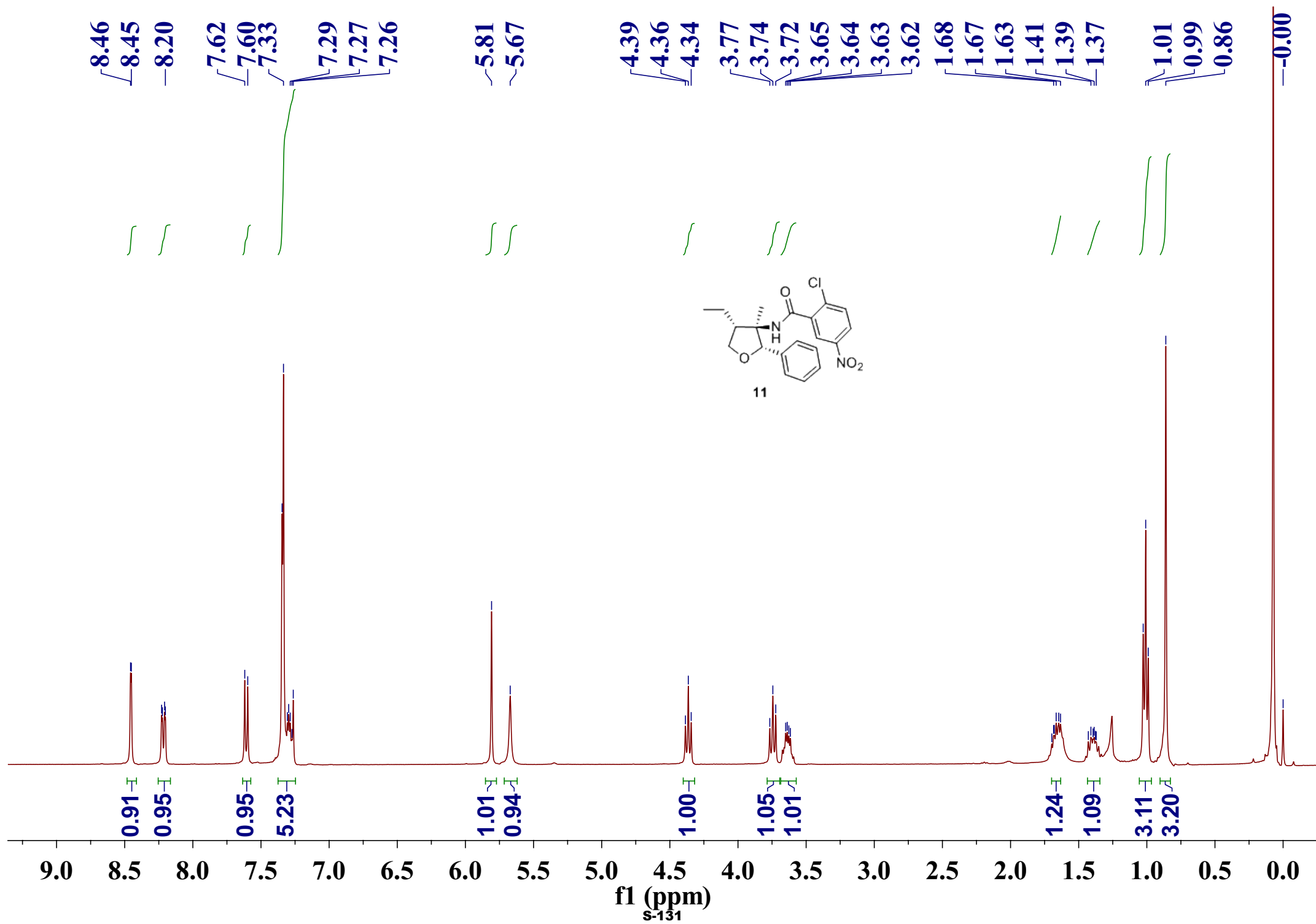
G:\DJ-13-41 OJ-H.lcd

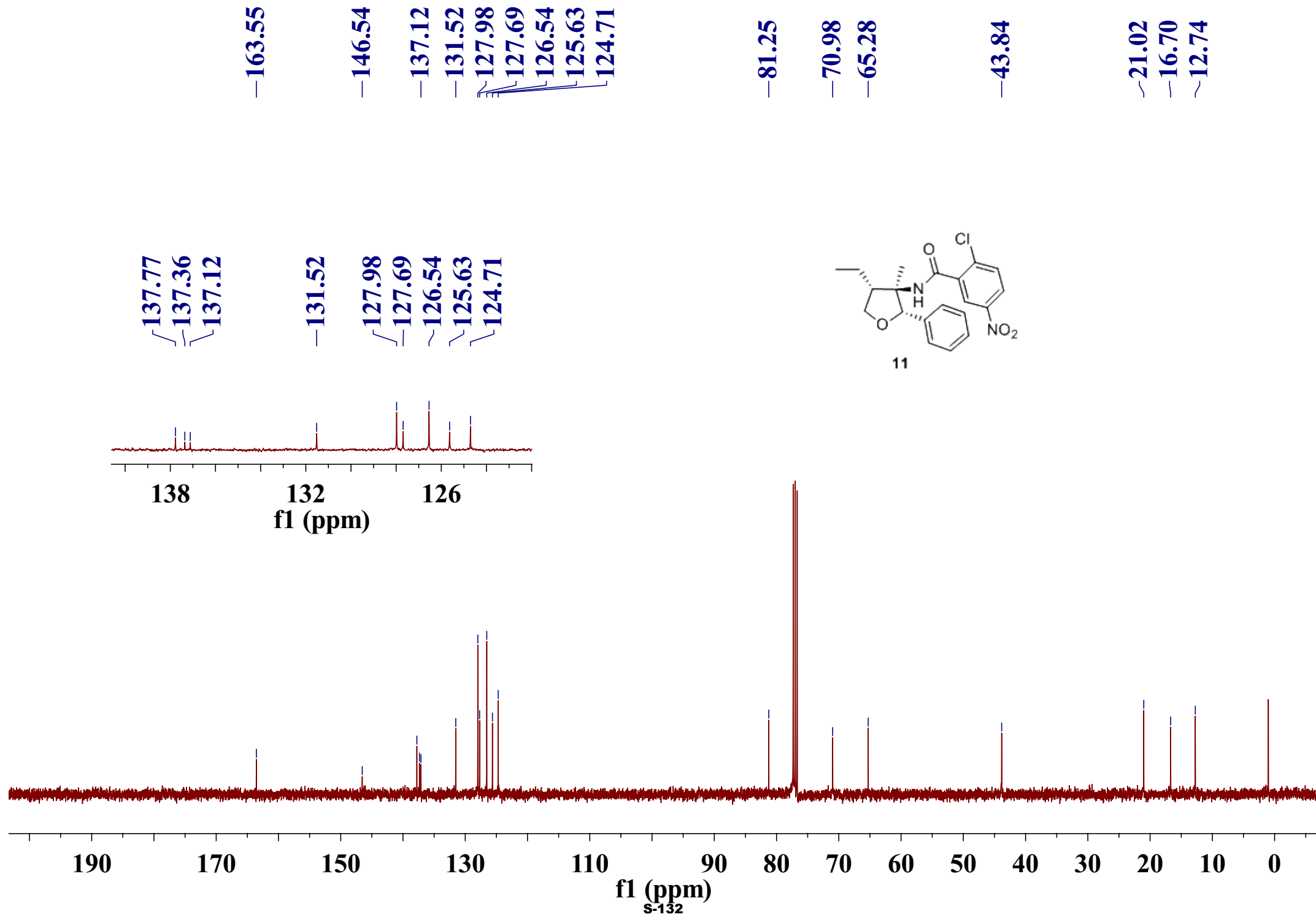


PeakTable

Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	20.892	155359	4873	1.076	2.042
2	44.250	14278244	233719	98.924	97.958
Total		14433603	238592	100.000	100.000





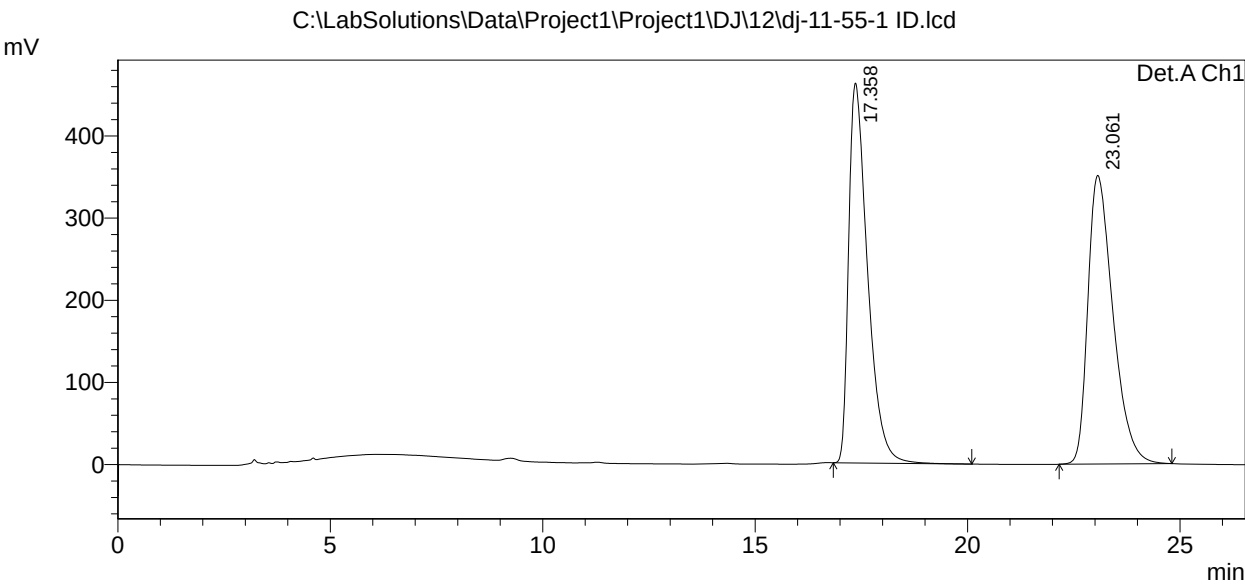
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\12\dj-11-55-1 ID.lcd

Acquired by : Admin
Sample Name : dj-11-55-1 ID
Sample ID : ID,80/20,1.0,214
Vail # :
Injection Volume : 2 uL
Data File Name : dj-11-55-1 ID.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2018-7-13 8:21:11
Data Processed : 2018-7-13 8:47:43

CC[C@H]1O[C@@H](NC(=O)c2cc([N+](=O)[O-])cc(Cl)c2)[C@H](c3ccccc3)[C@H]1O
11

<Chromatogram>



PeakTable

Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.358	14287557	462353	49.719	56.822
2	23.061	14448789	351332	50.281	43.178
Total		28736346	813685	100.000	100.000

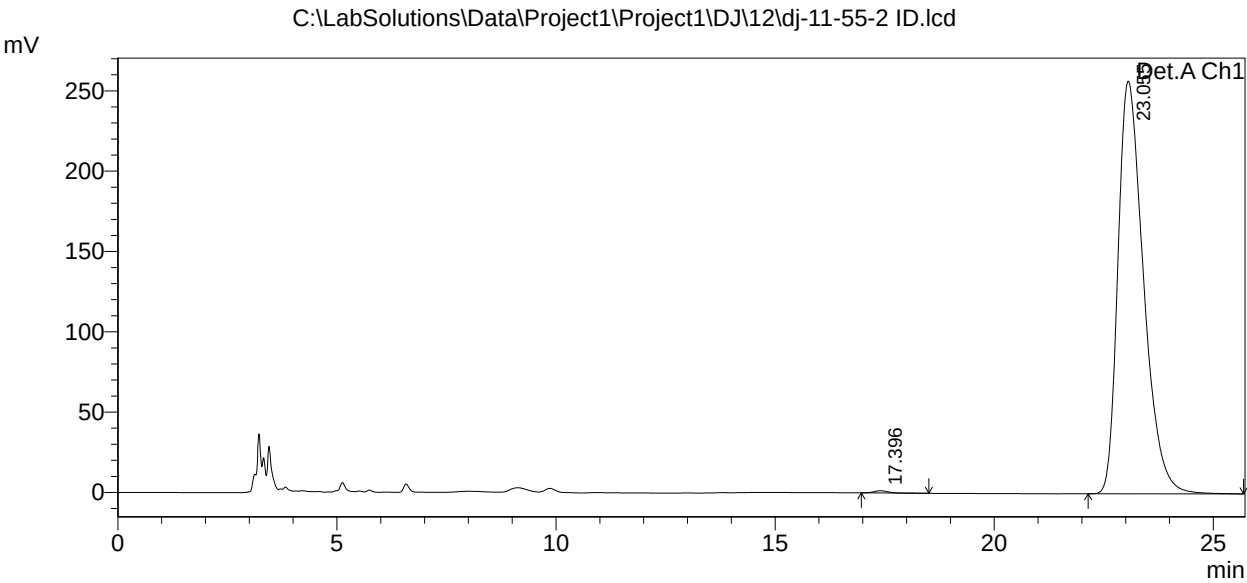
==== Shimadzu LCsolution Analysis Report ====

C:\LabSolutions\Data\Project1\Project1\DJ\12\dj-11-55-2 ID.lcd

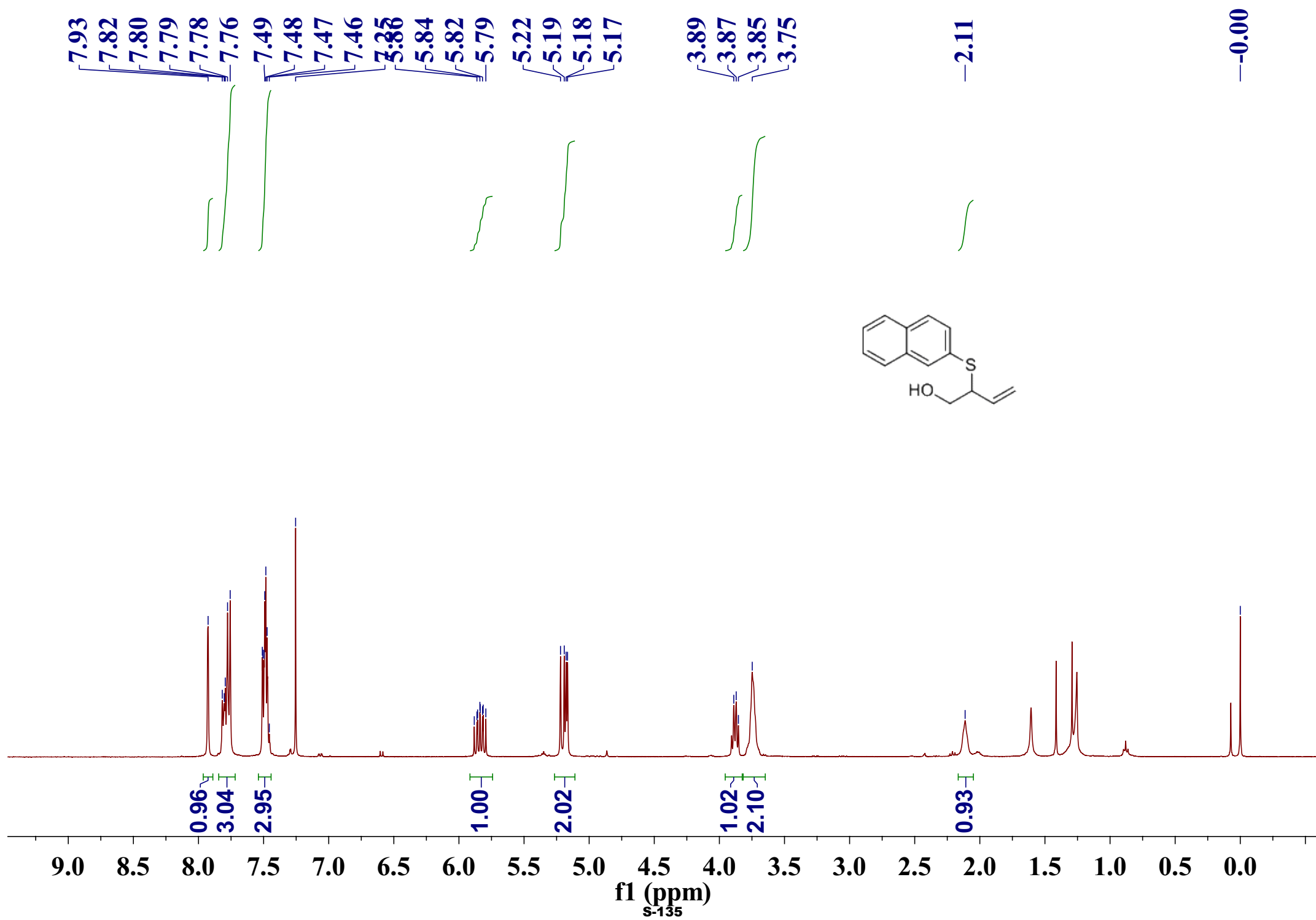
Acquired by : Admin
Sample Name : dj-11-55-2 ID
Sample ID : ID,80/20,1.0,214
Vail # :
Injection Volume : 2 uL
Data File Name : dj-11-55-2 ID.lcd
Method File Name : 123.lcm
Batch File Name :
Report File Name : Default.lcr
Data Acquired : 2018-7-13 8:49:37
Data Processed : 2018-7-13 9:15:22

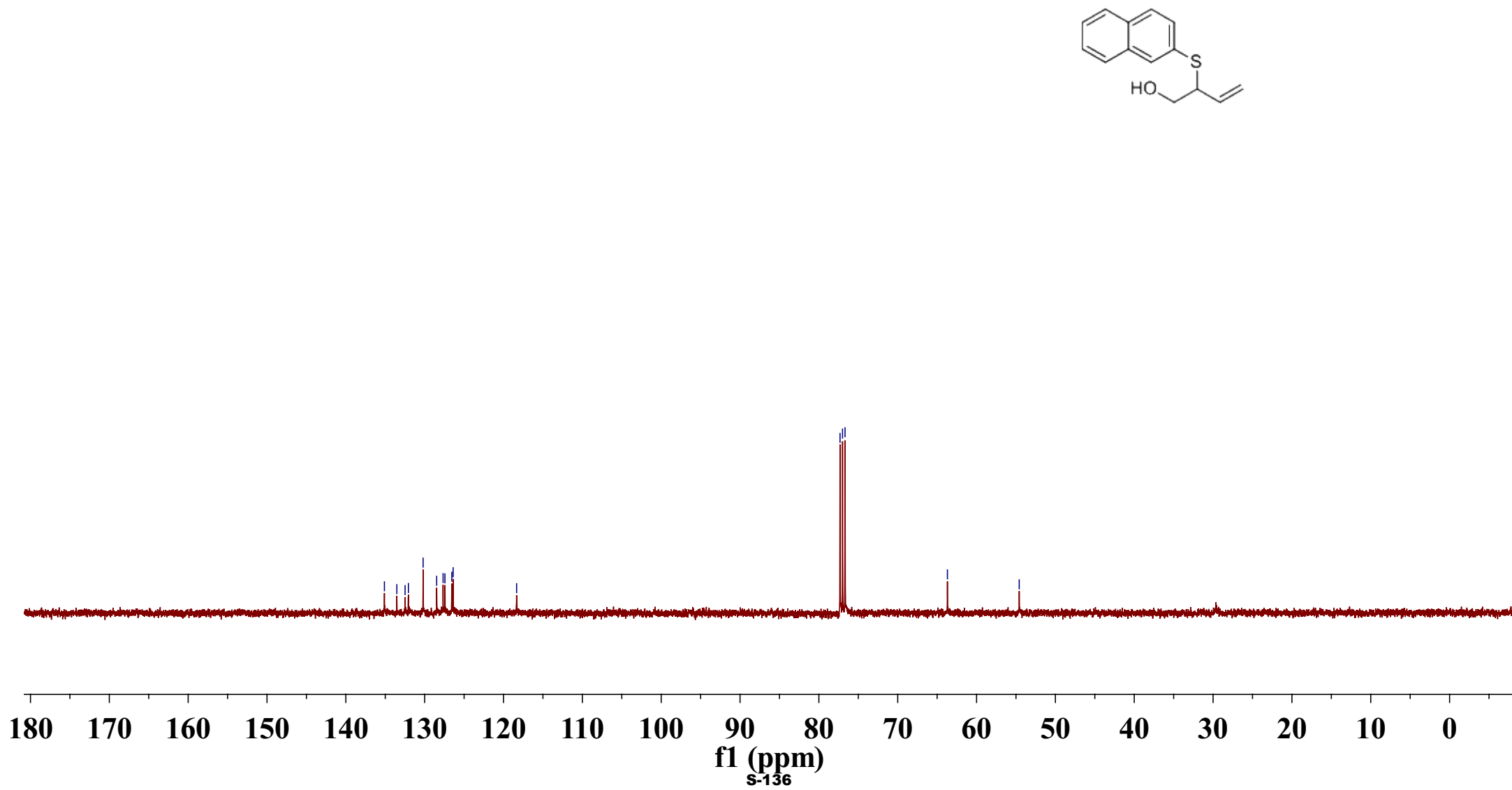
CC[C@H]1O[C@@H](NC(=O)c2cc(Cl)cc([N+](=O)[O-])c2)[C@H](c3ccccc3)[C@@H]1O
11

<Chromatogram>



PeakTable					
Detector A Ch1 214nm					
Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.396	33272	1395	0.318	0.540
2	23.055	10423089	256912	99.682	99.460
Total		10456361	258307	100.000	100.000

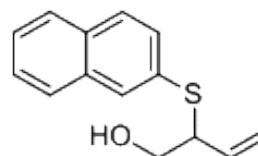




==== Shimadzu LCsolution Analysis Report =====

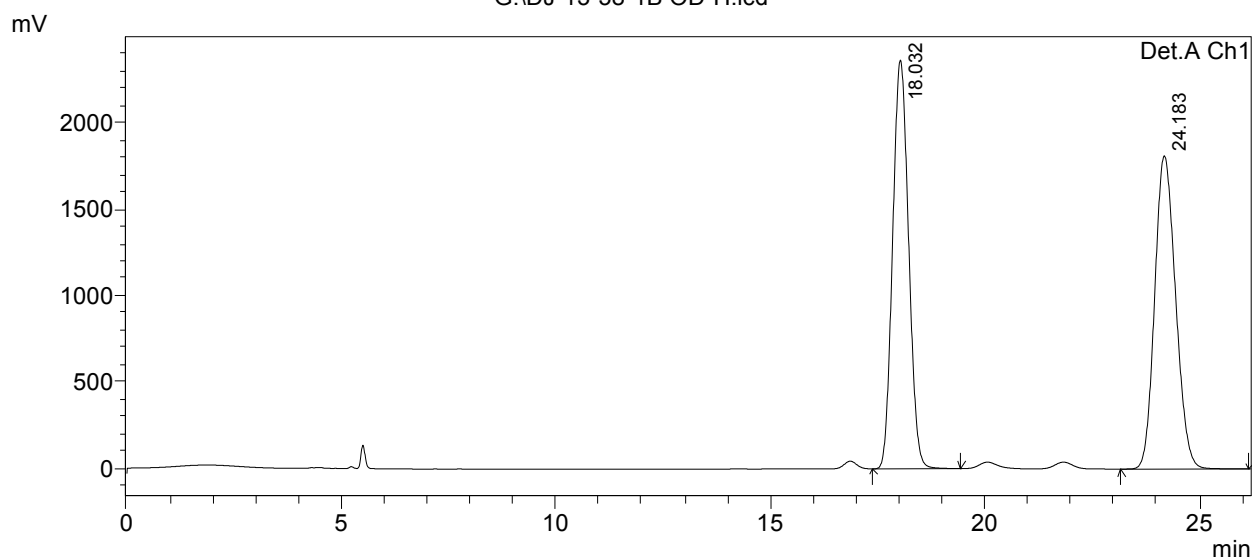
G:\DJ-13-38-1B OD-H.lcd

Acquired by : Admin
 Sample Name : DJ-13-38-1B OD-H
 Sample ID : OD-H,92/8,0.7,215
 Vial # :
 Injection Volume : 1 uL
 Data File Name : DJ-13-38-1B OD-H.lcd
 Method File Name : 1.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2018-10-20 9:47:36
 Data Processed : 2018-10-20 10:13:50



<Chromatogram>

G:\DJ-13-38-1B OD-H.lcd



1 Det.A Ch1/215nm

PeakTable

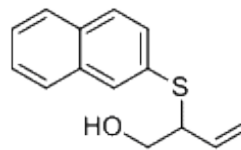
Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	18.032	61106203	2364341	49.870	56.616
2	24.183	61424665	1811766	50.130	43.384
Total		122530868	4176108	100.000	100.000

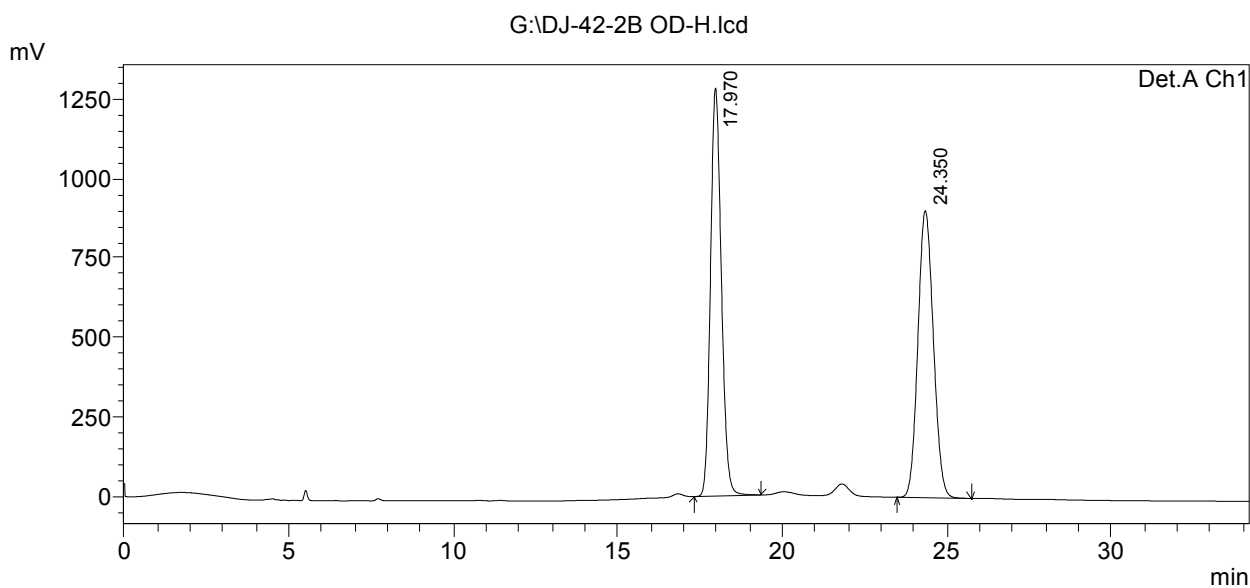
==== Shimadzu LCsolution Analysis Report =====

G:\DJ-42-2B OD-H.lcd

Acquired by : Admin
 Sample Name : DJ-42-2B OD-H
 Sample ID : OD-H,92/8,0.7,215
 Vial # :
 Injection Volume : 1 uL
 Data File Name : DJ-42-2B OD-H.lcd
 Method File Name : 1.lcm
 Batch File Name :
 Report File Name : Default.lcr
 Data Acquired : 2018-10-24 19:47:25
 Data Processed : 2018-10-24 20:21:37



<Chromatogram>



PeakTable

Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	17.970	29340903	1283121	49.881	58.695
2	24.350	29481237	902954	50.119	41.305
Total		58822139	2186075	100.000	100.000