Supporting Information

Pd-Catalyzed Enantioselective Cyclopropanation of Nitriles with Mono Substituted Allyl Carbonates Enabled by the Bulky *N*-Heterocyclic Carbene Ligand

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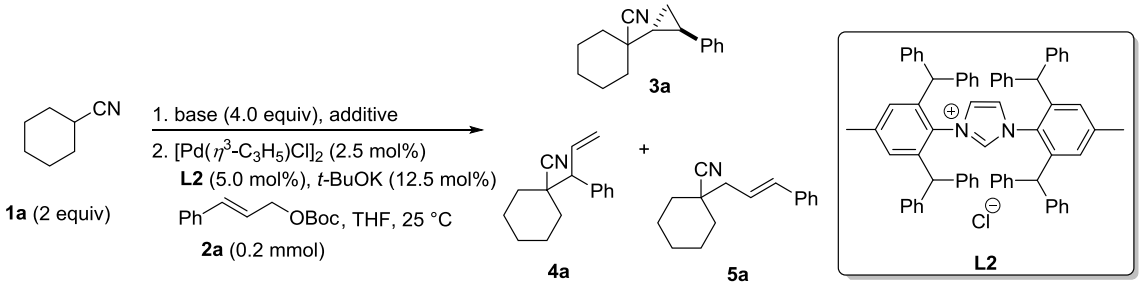
1. General Methods

All reactions were carried out under an atmosphere of argon in flame-dried glassware with magnetic stirring, unless otherwise indicated. Solvents were purified prior to use according to the standard methods. Commercially available reagents were used without further purification. Column chromatography was performed on silica gel (300-400 mesh) using a forced flow of eluent. Analytical thin-layer chromatography was performed with commercial glass plates coated with 0.25 mm silica gel, and spots were visualized with UV and/or by staining with $KMnO_4$. ^1H & ^{13}C-NMR spectra were recorded at room temperature on Varian-400 (400 MHz) and Agilent-400 (400 MHz) instruments. The NMR data were presented as follows: chemical shift in ppm with the proton signal of the residual of chloroform (δ 7.26 for ^1H-NMR) and (δ = 77.0 ppm for ^{13}C-NMR) as internal standards, multiplicity (s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet, br = broad), coupling constant (*J*/Hz), integration. MS and HRMS were measured in EI, ESI, or DART (direct analysis in real-time) mode and the mass analysis mode of the HRMS was TOF. Infrared spectra were recorded from thin films of pure samples. Melting points were measured on an XT-4 micromelting point apparatus.

2. Pd-catalyzed cyclopropanation of nitriles 1 with allyl reagents 2

2.1 Table S1. Screening of reaction conditions for Pd-catalyzed cyclopropanation of nitrile 1a with allyl reagent 2a[a]

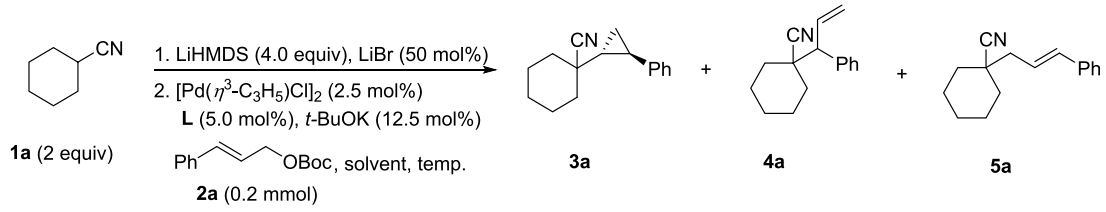


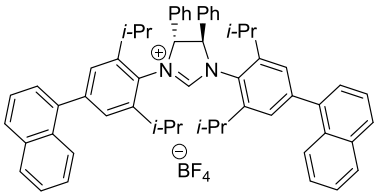
entry	base	additive (mol %)	**3a** (%)[b]	**3a**/(**4a**+**5a**)[b]
1	LiHMDS	-	49	57/43
2	NaHMDS	-	-	-
3	KHMDS	-	-	-
4	LiHMDS	LiBr (50)	68	91/9
5	LiHMDS	LiI (50)	61	80/20

6	LiHMDS	$LiBF_4$ (50)	61	72/28
7	LiHMDS	KCl (50)	50	57/43
8	LiHMDS	KBr (50)	56	64/36
9	LiHMDS	NaBr (50)	57	61/39
10[c]	LiHMDS	AgF (50)	54	64/36
11[c]	LiHMDS	AgCl (50)	54	64/36
12[c]	LiHMDS	$AgNO_3$ (50)	64	66/34
13[c]	LiHMDS	$AgBF_4$ (50)	61	65/35
14[c]	LiHMDS	AgOTf (50)	64	66/34
15[c]	LiHMDS	AgOAc (50)	65	68/32
16[c]	LiHMDS	AgBr (50)	80	89/11
17[c]	LiHMDS	AgBr (25)	80	88/12
18[c,d]	LiHMDS	AgBr (25)	61	88/12

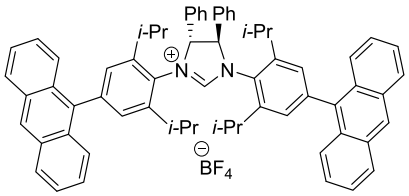
[a]Reaction conditions: **1a**/LiHMDS/**2a**/[Pd(η^3-C_3H_5)Cl]$_2$/**L2**/*t*-BuOK = 2.0/4.0/1.0/0.025/0.05/0.125, 48 h. [b]Determined by ^{1}H NMR using mesitylene as the internal standard. [c]Reaction time: 12 h. [d] without *t*-BuOK.[1]

2.2 Table S2. Screening of reaction conditions for Pd-catalyzed asymmetric cyclopropanation of nitrile 1a with allyl reagent 2a[a]

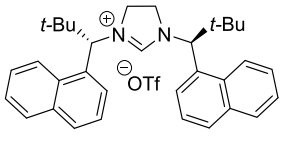




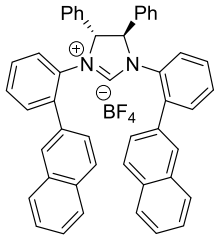
L9



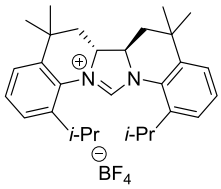
L10



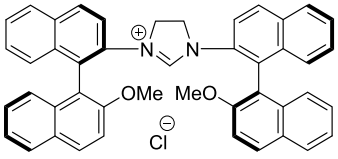
L11



L12



L13



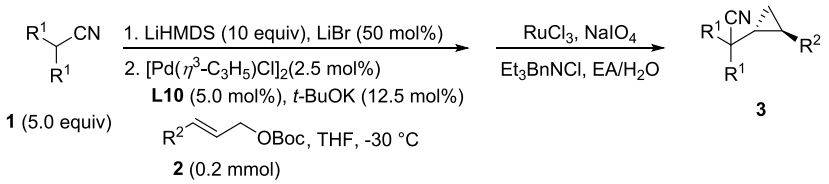
L14

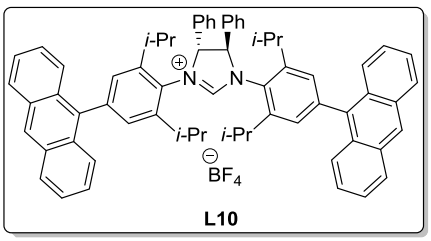
entry	L	solvent	T (℃)	**3a** (%)[b]	**3a**/(**4a**+**5a**)[b]	er of **3a** (%)[c]
1	**L14**	THF	25	-	-	-
2	**L13**	THF	25	13	57/46	50:50
3	**L12**	THF	25	27	28/72	55:45
4	**L11**	THF	25	-	-	-
5	**L9**	THF	25	40	100/0	84:16
6	**L9**	$PhCH_3$	25	18	62/38	77:23
7	**L9**	DME	25	48	79/21	83:17
8	**L9**	dioxane	25	21	54/46	78:22
9	**L9**	Et_2O	25	25	61/39	79:21
10	**L9**	THF	-20	26	100/0	90:10
11	**L10**	THF	-20	24	100/0	91:9
12	**L10**	THF	-30	-	-	-
13[d]	**L10**	THF	-30	74	100/0	94.5:5.5

[a]Reaction conditions: **1a**/LiHMDS/LiBr/**2a**/[Pd(η^3-C_3H_5)Cl]$_2$/**L**/*t*-BuOK = 2.0/4.0/0.5/1.0/0.025/0.05/0.125, 48 h. [b]Determined by ^{1}H NMR using mesitylene as the internal standard. [c]Determined by chiral HPLC. [d][Pd(η^3-C_3H_5)Cl]$_2$ (5.0 mol%), **L10** (10 mol%), **1a** (5.0 equiv), LiHMDS (10 equiv).

2.3 General experimental procedure and characterization of products 3

General experimental procedure





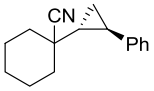
A Schlenk tube was flame dried and flushed with argon. LiBr (8.7 mg, 0.1 mmol), nitriles **1** (1.0 mmol) and THF (1.0 mL) were added. LiHMDS (1.0 M in THF, 2.0 mL, 2.0 mmol) was added at 0 ℃ and stirred at room temperature for 30 min. In a separate flushed flask, [Pd(η^3-C_3H_5)Cl]$_2$ (1.9 mg, 0.005 mmol) and **L10** (9.8 mg, 0.01 mmol)[2] were added

followed by addition of THF (1.0 mL). *t*-BuOK (1.0 M in THF, 25 μL, 0.025 mmol) was added at 0 ℃, and the resulting mixture was stirred at room temperature for 30 min, then added to the nitriles solution. The allylic substrates **2** (0.2 mmol) and another 1.0 mL THF were then added and the mixture was stirred at -30 ℃. After the reaction completed (monitored by TLC), the reaction mixture was quenched with H_2O (0.2 mL). The solution was dried over anhydrous Na_2SO_4 and then filtered through a 0.5 inch plug of silica gel (eluting with EtOAc) to remove the solid. The reaction mixture was concentrated under reduced pressure to afford the crude product. NMR yield and selectivity were determined by ^{1}H NMR using mesitylene as internal standard.

The crude product was dissolved in EtOAc (2.0 mL), and then transferred to a tube and $RuCl_3$ (1.0 mg, 0.005 mmol) and benzyltriethylammonium chloride (10 mg, 0.04 mmol) were added and then $NaIO_4$ (214 mg, 1 mmol) in water (2.0 mL) was added slowly at room temperature. The resulting solution was stirred for additional one hour. EtOAc (8 mL) was added to the reaction mixture. The organic layer was separated and washed with water. The aqueous phase was extracted with EtOAc (3 × 10 mL) and the organic layer was combined, dried (Na_2SO_4), filtered and concentrated in vacuo. Purification by chromatography on silica gel (*n*-hexane/EtOAc 20/1) to yield the desired product.

characterization of products

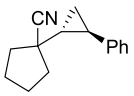
1-((1*R*,2*R*)-2-phenylcyclopropyl)cyclohexane-1-carbonitrile (3a)



3a

$[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ (3.8 mg, 0.01 mmol) and **L10** (19.6 mg, 0.02 mmol) were used. colorless oil, 30.4 mg, yield: 69%, 94:6 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.23 (m, 2H), 7.17-7.14 (m, 1H), 7.08-7.06 (m, 2H), 2.12-2.03 (m, 3H), 1.75-1.73 (m, 3H), 1.67-1.57 (m, 2H), 1.45-1.39 (m, 2H), 1.24-1.17 (m, 2H), 1.11-1.06 (m, 1H), 1.01-0.95 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 141.8, 128.4, 126.1, 125.9, 121.5, 41.8, 36.0, 35.8, 30.2, 25.3, 23.1 (2C), 19.8, 11.9; IR (Neat): 3063, 3028, 2932, 2857, 2233, 2210, 1605, 1499, 1450, 752, 697 cm^{-1}; MS (EI) *m/z* (rel): 225 (M^+, 12), 180 (5), 117 (100), 104 (7), 91 (11), 73 (12), 53 (1); HRMS (EI): calcd for $C_{16}H_{19}N$: 225.1517, found: 225.1524; HPLC (Chiralpak AD-H, Hexane:*i*-Propanol = 98:2, 1 mL/min, 214 nm): t_{minor} = 5.52 min, t_{major} = 6.62 min. $[\alpha]_D^{30}$ = -105.7 (1.0, $CHCl_3$).

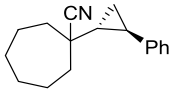
1-((1*R*,2*R*)-2-phenylcyclopropyl)cyclopentane-1-carbonitrile (3b)



3b

colorless oil, 35.8 mg, yield: 90%, 94.5:5.5 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.25 (m, 2H), 7.20-7.16 (m, 1H), 7.10-7.08 (m, 2H), 2.21-2.16 (m, 2H), 2.12-2.07 (m, 1H), 1.90-1.79 (m, 6H), 1.24-1.17 (m, 2H), 1.07-1.02 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 141.6, 128.4, 126.0, 125.9, 123.4, 45.2, 38.1 (2C), 28.4, 24.3 (2C), 20.8, 12.8; IR (Neat): 3027, 3003, 2962, 2874, 2232, 1605, 1498, 1453, 1030, 754, 697 cm^{-1}; MS (EI) *m/z* (rel): 211 (M^+, 12), 184 (5), 141 (7), 117 (100), 104 (13), 91 (12), 77 (3), 51 (2); HRMS (EI): calcd for $C_{15}H_{17}N$: 211.1361, found: 211.1365; HPLC (Chiralpak AD-H, Hexane:*i*-Propanol = 98:2, 1 mL/min, 214 nm): t_{minor} = 5.78 min, t_{major} = 6.40 min. $[\alpha]_D^{29}$= -90.8 (1.0, $CHCl_3$).

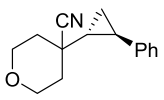
1-((1*R*,2*R*)-2-phenylcyclopropyl)cycloheptane-1-carbonitrile (3c)



3c

colorless oil, 28.4 mg, yield: 61%, 93:7 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.25 (m, 2H), 7.20-7.16 (m, 1H), 7.10-7.08 (m, 2H), 2.20-2.10 (m, 3H), 1.76-1.49 (m, 10H), 1.25-1.15 (m, 2H), 1.05-1.00 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 141.8, 128.4, 126.0, 125.9, 122.3, 44.8, 38.8, 38.6, 31.2, 27.9 (2C), 23.7, 23.6, 20.1, 12.8; IR (Neat): 3063, 3027, 2927, 2857, 2231, 1735, 1604, 1497, 1460, 1255, 1155, 1034, 838, 751, 696 cm^{-1}; MS (EI) *m/z* (rel): 239 (M^+, 3), 154 (2), 122 (6), 117 (100), 115 (18), 104 (13), 91 (17), 77 (5), 57 (38), 41 (13); HRMS (EI): calcd for $C_{17}H_{21}N$: 239.1674, found: 239.1686; HPLC (Chiralpak AD-H, Hexane:*i*-Propanol = 98:2, 1 mL/min, 214 nm): t_{minor} = 5.83 min, t_{major} = 7.06 min. $[\alpha]_D^{30}$= -91.3 (1.0, $CHCl_3$).

4-((1*R*,2*R*)-2-phenylcyclopropyl)tetrahydro-2H-pyran-4-carbonitrile (3d)

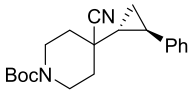


3d

colorless oil, 40.2 mg, yield: 91%, 94:6 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28-7.24 (m,

2H), 7.19-7.15 (m, 1H), 7.08-7.06 (m, 2H), 4.00-3.94 (m, 2H), 3.70 (dt, *J* = 12.0, 2.0 HZ, 2H), 2.16-2.11 (m, 1H), 1.97-1.91 (m, 2H), 1.82-1.74 (m, 2H), 1.25-1.20 (m, 1H), 1.17-1.12 (m, 1H), 1.06-1.01 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 142.6, 129.8, 127.5, 127.4, 121.9, 66.1, 40.9, 36.9, 36.7, 31.1, 21.0, 13.0; IR (Neat): 3063, 2957, 2925, 2852, 2233, 1736, 1604, 1498, 1465, 1443, 1243, 1143, 1103, 1032, 835, 757, 697 cm^{-1}; MS (EI) *m/z* (rel): 227 (M^+, 8), 141 (4), 117 (100), 104 (7), 91 (21), 77 (5), 57 (9), 41 (3); HRMS (EI): calcd for $C_{15}H_{17}NO$: 227.1310, found: 227.1307; HPLC (Chiralpak IC, Hexane:*i*-Propanol = 98:2, 1 mL/min, 214 nm): t_{major} = 14.76 min, t_{minor} = 19.02 min. $[\alpha]_D^{30}$ = -95.2 (1.0, $CHCl_3$).

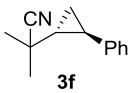
tert-butyl 4-cyano-4-((1*R*,2*R*)-2-phenylcyclopropyl)piperidine-1-carboxylate (3e)



3e

white solid, 45.5 mg, yield: 72%, 90:10 er; mp: 82.4-84.8 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29-7.25 (m, 2H), 7.20-7.16 (m, 1H), 7.08-7.06 (m, 2H), 4.14-4.09 (m, 2H), 3.04 (br, 2H), 2.17-2.12 (m, 1H), 2.03-1.98 (m, 2H), 1.68-1.57 (m, 2H), 1.46 (s, 9H), 1.27-1.21 (m, 1H), 1.14-1.09 (m, 1H), 1.07-1.02 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.4, 141.1, 128.5, 126.1 (2C), 120.2, 80.1, 40.7, 34.8, 29.3, 28.4, 19.8, 11.8; IR (Neat): 3005, 2975, 2864, 2234, 1691, 1605, 1421, 1278, 1159, 863, 760, 697 cm^{-1}; MS (EI) *m/z* (rel): 326 (M^+, 2), 270 (45), 253 (32), 226 (100), 135 (50), 117 (56), 94 (24), 57 (77), 51 (3); HRMS (ESI): calcd for $C_{20}H_{26}N_2NaO_2$ $[M+Na]^+$: 349.1886, found: 349.1887; HPLC (Chiralpak ID, Hexane:*i*-Propanol = 99:1, 1 mL/min, 214 nm): t_{minor} = 28.62 min, t_{major} = 30.71 min. $[\alpha]_D^{30}$ = -49.9 (1.0, $CHCl_3$).

2-methyl-2-((1*R*,2*R*)-2-phenylcyclopropyl)propanenitrile (3f)

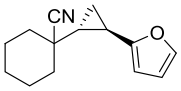


3f

colorless oil, 32.6 mg, yield: 90%, 96:4 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30-7.26 (m, 2H), 7.20-7.16 (m, 1H), 7.11-7.09 (m, 2H), 2.12-2.07 (m, 1H), 1.48 (s, 3H), 1.47 (s, 3H), 1.21-1.11 (m, 2H), 1.06-1.01 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 141.6, 128.4, 126.0 (2C), 122.9, 34.9, 30.8, 26.7 (2C), 20.6, 12.6; IR (Neat): 3029, 2978, 2935, 2236, 1605, 1498, 1466, 753, 697 cm^{-1}; MS (EI) *m/z* (rel): 185 (M^+, 10), 143 (13), 117 (100), 104 (8), 91 (13), 77 (6), 65 (3), 51 (3); HRMS (EI): calcd for $C_{13}H_{15}N$: 185.1204, found:

185.1201; HPLC (Chiralpak OD-H, Hexane:*i*-Propanol = 99:1, 1 mL/min, 214 nm): t_{major} = 7.11 min, t_{minor} = 7.96 min. $[\alpha]_D^{31}$ = -84.8 (1.0, $CHCl_3$).

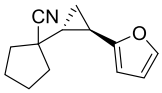
1-((1*R*,2*R*)-2-(furan-2-yl)cyclopropyl)cyclohexane-1-carbonitrile (3g)



3g

The product was isolated from crude product directly without oxidation by $RuCl_3/NaIO_4$**.** colorless oil, 10.3 mg, yield: 25%, 88:12 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.23-7.22 (m, 1H), 6.27-6.25 (m, 1H), 5.98 (d, *J* =3.2 Hz, 1H), 2.13-2.02 (m, 3H), 1.78-1.74 (m, 3H), 1.67-1.57 (m, 2H), 1.49-1.38 (m, 2H), 1.26-1.19 (m, 2H), 1.17-1.11 (m, 1H), 1.07-1.03 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.2, 140.6, 121.2, 110.3, 104.1, 41.4, 35.8, 35.7, 27.8, 25.3, 23.0, 13.2, 10.2; IR (Neat): 3468, 3118, 2933, 2858, 2234, 1700, 1601, 1449, 1400, 1184, 1148, 1014, 919, 798, 732, 700 cm^{-1}; MS (EI) *m/z* (rel): 215 (M^+, 6), 107 (100), 94 (11), 79 (19), 53 (5), 41 (4); HRMS (EI): calcd for $C_{14}H_{17}NO$: 215.1310, found: 215.1315; HPLC (Chiralpak OJ-H, Hexane:*i*-Propanol = 98:2, 1 mL/min, 215 nm): t_{minor} = 7.05 min, t_{major} = 7.48 min. $[\alpha]_D^{29}$ = -41.2 (0.5, $CHCl_3$).

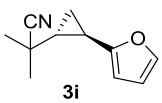
1-((1*R*,2*R*)-2-(furan-2-yl)cyclopropyl)cyclopentane-1-carbonitrile (3h)



3h

The product was isolated from crude product directly without oxidation by $RuCl_3/NaIO_4$**.** colorless oil, 20.4 mg, yield: 50%, 86:14 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24 (s, 1H), 6.28-6.27 (m, 1H), 6.00 (d, *J* = 2.8 Hz, 1H), 2.20-2.16 (m, 2H), 2.12-2.07 (m, 1H), 1.87-1.80 (m, 6H), 1.37-1.32 (m, 1H), 1.15-1.07 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.0, 140.6, 123.1, 110.3, 104.2, 44.7, 38.1, 38.0, 26.0, 24.3, 14.2, 11.1; IR (Neat): 3150, 2962, 2874, 2233, 1600, 1510, 1451, 1249, 1179, 1148, 1078, 1045, 1010, 935, 883, 798, 731, 598 cm^{-1}; MS (EI) *m/z* (rel): 201 (M^+, 13), 191 (4), 107 (100), 94 (21), 79 (24), 53 (4); HRMS (EI): calcd for $C_{13}H_{15}NO$: 201.1154, found: 201.1159; HPLC (Chiralpak ID, Hexane:*i*-Propanol = 97:3, 0.7 mL/min, 214 nm): t_{major} = 14.79 min, t_{minor} = 15.47 min. $[\alpha]_D^{29}$ = -25.5 (1.0, $CHCl_3$).

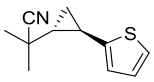
2-((1*R*,2*R*)-2-(furan-2-yl)cyclopropyl)-2-methylpropanenitrile (3i)



3i

The product was isolated from crude product directly without oxidation by $RuCl_3/NaIO_4$**.** colorless oil, 24.6 mg, yield: 71%, 87:13 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.23 (s, 1H), 6.27 (s, 1H), 6.00 (d, J = 2.8 Hz, 1H), 2.10-2.05 (m, 1H), 1.47 (s, 3H), 1.45 (s, 3H), 1.29-1.24 (m, 1H), 1.13-1.05 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 154.9, 140.7, 122.6, 110.3, 104.2, 34.6, 28.5, 26.6 (2C), 13.9, 10.8; IR (Neat): 2979, 2930, 2872, 2237, 1599, 1510, 1460, 1372, 1246, 1183, 1148, 1013, 966, 798, 731, 597 cm^{-1}; MS (EI) *m/z* (rel): 175 (M^+, 51), 117 (7), 107 (100), 94 (24), 79 (75), 77 (57), 65 (12), 63 (5), 57 (1); HRMS (EI): calcd for $C_{11}H_{13}NO$: 175.0997, found: 175.1003; HPLC (Chiralpak IE, Hexane:*i*-Propanol = 99:1, 1 mL/min, 214 nm): t_{minor} = 10.49 min, t_{major} = 10.99 min. $[\alpha]_D^{29}$ = -68.5 (1.0, $CHCl_3$).

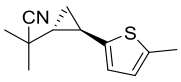
2-methyl-2-((1*R*,2*R*)-2-(thiophen-2-yl)cyclopropyl)propanenitrile (3j)



3j

The product was isolated from crude product directly without oxidation by $RuCl_3/NaIO_4$**.** colorless oil, 31.4 mg, yield: 90%, 94:6 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.06 (dd, J = 5.2, 1.2 Hz, 1H), 6.88 (dd, J = 4.8, 3.2 Hz, 1H), 6.75 (d, J = 3.2 Hz, 1H), 2.28-2.23 (m, 1H), 1.48 (s, 3H), 1.44 (s, 3H), 1.24-1.13 (m, 2H), 1.06-1.01 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 145.9, 126.9, 123.2, 122.6 (2C), 34.8, 31.6, 26.6 (2C), 15.9, 13.7; IR (Neat): 3108, 3074, 2977, 2873, 2236, 1537, 1465, 1442, 1368, 1299, 1251, 1042, 890, 847, 818, 693, 508 cm^{-1}; MS (EI) *m/z* (rel): 191 (M^+, 19), 149 (6), 123 (100), 110 (6), 97 (7), 79 (10), 45 (8); HRMS (EI): calcd for $C_{11}H_{13}NS$: 191.0769, found: 191.0773; HPLC (Chiralpak IC, Hexane:*i*-Propanol = 98:2, 1 mL/min, 215 nm): t_{major} = 6.76 min, t_{minor} = 7.16 min. $[\alpha]_D^{29}$ = -98.5 (1.0, $CHCl_3$).

2-methyl-2-((1*R*,2*R*)-2-(5-methylthiophen-2-yl)cyclopropyl)propanenitrile (3k)

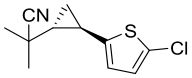


3k

The product was isolated from crude product directly without oxidation by $RuCl_3/NaIO_4$**.** colorless oil, 34.4 mg, yield: 81%, 95:5 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.53-6.50 (m, 2H), 2.39 (s, 3H), 2.18-2.13 (m, 1H), 1.46 (s, 3H), 1.43 (s, 3H), 1.18-1.07 (m, 2H), 1.00-0.96 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 143.4, 137.2, 124.7, 122.9, 122.7, 34.7, 31.3, 26.6 (2C), 16.0, 15.3, 13.3; IR (Neat): 3078, 2918, 2733, 2233, 1501, 1463, 1362, 1292, 1218,1040, 801, 517 cm^{-1}; MS (EI) *m/z* (rel): 205 (M^+, 17), 190 (4), 157 (5),

137 (100), 123 (10), 97 (9), 77 (8), 58 (20); HRMS (EI): calcd for $C_{12}H_{15}NS$: 205.0925, found: 205.0928; HPLC (Chiralpak IC, Hexane:*i*-Propanol = 99:1, 1 mL/min, 215 nm): t_{major} = 8.18 min, t_{minor} = 9.03 min. $[\alpha]_D^{29}$ = -93.1 (1.0, $CHCl_3$).

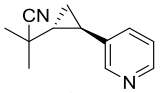
2-((1*R*,2*R*)-2-(5-chlorothiophen-2-yl)cyclopropyl)-2-methylpropanenitrile (3l)



3l

The product was isolated from crude product directly without oxidation by $RuCl_3/NaIO_4$**.** colorless oil, 22.4 mg, yield: 52%, 92:8 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.67 (d, J =3.6 Hz, 1H), 6.52 (dd, J = 3.6, 0.4 Hz, 1H), 2.16-2.11 (m, 1H), 1.47 (s, 3H), 1.43 (s, 3H), 1.21-1.16 (m, 1H), 1.13-1.08 (m, 1H), 1.02-0.98 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 144.4, 126.5, 125.8, 122.7, 122.4, 34.7, 31.2, 26.7, 26.5, 16.0, 13.2; IR (Neat): 2958, 2922, 2852, 1742, 1462, 1259, 1160, 1088, 1022, 798, 664 cm^{-1}; MS (EI) *m/z* (rel): 225 (M^+, 17), 157 (100), 144 (12), 122 (60), 95 (9), 77 (10), 45 (11); HRMS (EI): calcd for $C_{11}H_{12}ClNS$: 225.0379, found: 225.0386; HPLC (Chiralpak IC, Hexane:*i*-Propanol = 99:1, 1 mL/min, 215 nm): t_{major} = 8.01 min, t_{minor} = 8.99 min. $[\alpha]_D^{28}$ = -35.7 (1.0, $CHCl_3$).

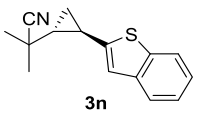
2-methyl-2-((1*R*,2*R*)-2-(pyridin-3-yl)cyclopropyl)propanenitrile (3m)



3m

colorless oil, 17.4 mg, yield: 52%, 88:12 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.45 (s, 2H), 7.36 (d, J = 3.6 Hz, 1H), 7.23-7.20 (m, 1H), 2.10-2.05 (m, 1H), 1.47 (s, 3H), 1.46 (s, 3H), 1.27-1.22 (m, 1H), 1.17-1.12 (m, 1H), 1.08-1.03 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 148.3, 147.5, 136.9, 133.2, 123.3, 122.6, 34.9, 30.8, 26.8, 26.5, 18.2, 12.4; IR (Neat): 3031, 2978, 2935, 2874, 2235, 1573, 1466, 1425, 1247, 1178, 1024, 803, 713, 631 cm^{-1}; MS (EI) *m/z* (rel): 186 (M^+, 10), 171 (9), 157 (15), 118 (100), 105 (18); 91 (24), 63 (12); 51 (13); HRMS (EI): calcd for $C_{12}H_{14}N_2$: 186.1157, found: 186.1158; HPLC (Chiralpak AD-H, Hexane:*i*-Propanol = 98:2, 2 mL/min, 215 nm): t_{major} = 15.11 min, t_{minor} = 20.23 min. $[\alpha]_D^{30}$ = -6.9 (0.5, $CHCl_3$).

2-((1*R*,2*R*)-2-(benzo[b]thiophen-2-yl)cyclopropyl)-2-methylpropanenitrile (3n)

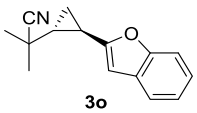


3n

The product was isolated from crude product directly without oxidation by $RuCl_3/NaIO_4$**.**

colorless oil, 21.3 mg, yield: 46%, 86.5:13.5 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.0 Hz, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.31-7.27 (m, 1H), 7.26-7.22 (m, 1H), 6.98 (s, 1H), 2.35-2.31 (m, 1H), 1.50 (s, 3H), 1.46 (s, 3H), 1.31-1.23 (m, 2H), 1.18-1.14 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.5, 140.0, 138.5, 124.3, 123.7, 122.7, 122.5, 122.1, 119.5, 34.8, 31.8, 26.6 (2C), 16.8, 13.7; IR (Neat): 3055, 2977, 2922, 2879, 2237, 1569, 1539, 1455, 1435, 1367, 1249, 1221, 1063, 1032, 926, 815, 746, 723, 569, 433 cm^{-1}; MS (EI) *m/z* (rel): 241 (M^+, 33), 226 (4), 184 (7), 173 (100), 147 (9), 129 (16), 115 (11), 77 (6), 63 (5), 54 (5); HRMS (EI): calcd for $C_{15}H_{15}NS$: 241.0925, found: 241.0930; HPLC (Chiralpak AD-H, Hexane:*i*-Propanol = 98:2, 1 mL/min, 215 nm): t_{minor} = 6.52 min, t_{major} = 7.13 min. $[\alpha]_D^{30}$ = -44.8 (1.0, $CHCl_3$).

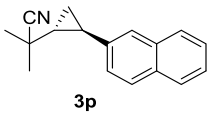
2-((1*R*,2*R*)-2-(benzofuran-2-yl)cyclopropyl)-2-methylpropanenitrile (3o)



3o

The product was isolated from crude product directly without oxidation by $RuCl_3/NaIO_4$**.** colorless oil, 31.2 mg, yield: 70%, 66:34 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47-7.45 (m, 1H), 7.36 (d, J = 7.2 Hz, 1H), 7.22-7.16 (m, 2H), 6.43 (s, 1H), 2.25-2.20 (m, 1H), 1.51-1.42 (m, 7H), 1.32-1.21 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 157.8, 154.2, 128.9, 123.2, 122.7, 122.4, 120.1, 110.6, 101.2, 34.7, 29.0, 26.7, 26.6, 14.5, 11.4; IR (Neat): 3033, 2921, 2236, 1607, 1454, 1368, 1206, 1188, 1078, 968, 925, 889, 783, 745, 452, 433 cm^{-1}; MS (EI) *m/z* (rel): 225 (M^+, 27), 157 (100), 144 (15), 128 (37), 115 (17), 102 (6), 77 (6), 63 (7), 51 (5); HRMS (EI): calcd for $C_{15}H_{15}NO$: 225.1154, found: 225.1158; HPLC (Chiralpak AD-H, Hexane:*i*-Propanol = 98:2, 1 mL/min, 215 nm): t_{minor} = 5.53 min, t_{major} = 5.96 min. $[\alpha]_D^{30}$ = -3.9 (1.0, $CHCl_3$).

2-methyl-2-((1*R*,2*R*)-2-(naphthalen-2-yl)cyclopropyl)propanenitrile (3p)

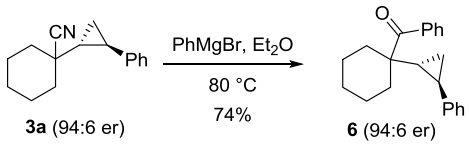


3p

white solid, 23.7 mg, yield: 52%, 90:10 er; mp: 63.9-64.8 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81-7.75 (m, 3H), 7.51 (s, 1H), 7.48-7.40 (m, 2H), 7.22 (d, J = 7.6 Hz, 1H), 2.28-2.24 (m, 1H), 1.51 (s 3H), 1.50 (s, 3H), 1.30-1.21 (m, 2H), 1.19-1.15 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 139.0, 133.4, 132.1, 128.1, 127.6, 127.3, 126.2, 125.3, 124.8, 124.2, 123.0, 35.0, 31.0, 26.8, 26.7, 20.9, 12.6; IR (Neat): 3058, 2980, 2922, 2853, 2235, 2693, 2630, 1597, 1505, 1459, 1367, 1303, 1251, 1023, 964, 886, 811, 742, 475 cm^{-1};

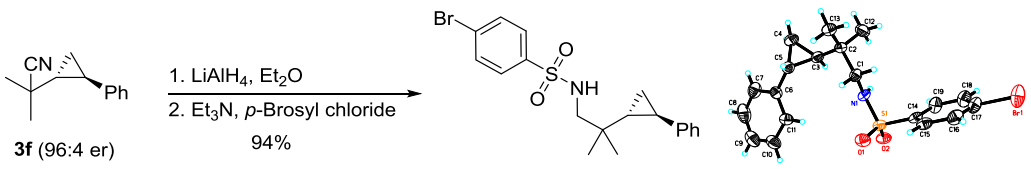
MS (EI) *m/z* (rel): 235 (M^+, 27), 191 (15), 167 (100), 155 (32), 127 (33), 115 (9), 77 (8), 63 (7), 57 (8), 51 (5); HRMS (EI): calcd for $C_{17}H_{17}N$: 235.1361, found: 235.1364; HPLC (Chiralpak IC, Hexane:*i*-Propanol = 99.2:0.8, 1 mL/min, 214 nm): t_{major} = 12.57 min, t_{minor} = 13.31 min. $[\alpha]_D^{29}$ = -50.5 (1.0, $CHCl_3$).

3. The transformation of cyclopropane product



3a (94:6 er) **6** (94:6 er)

To a 10 mL of sealed tube were added cyclopropane **3a** (16.7 mg, 0.074 mmol) and Et_2O (1.0 mL) under argon, followed by PhMgBr (2.5 M in Et_2O, 45 μL, 0.11 mmol) with stirring at 0 ℃. The sealed tube was screw capped and heated to 80 ℃. After stirring for 12 hours, the reaction mixture was quenched with saturated aq NH_4Cl and extracted with Et_2O (3 × 5 mL). The combined organic phase was dried over anhydrous Na_2SO_4 and then concentrated in vacuo. The residue was purified by column chromatography (*n*-hexane/EtOAc 20/1) to give **6** as a colorless oil, 16.7 mg, yield: 75%, 94:6 er; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70-7.68 (m, 2H), 7.45-7.41 (m, 1H), 7.36-7.32 (m, 2H), 7.27-7.23 (m, 2H), 7.17-7.14 (m, 1H), 7.06-7.04 (m, 2H), 2.24-2.18 (m, 2H), 2.07-2.02 (m, 1H), 1.60-1.57 (m, 3H), 1.38-1.32 (m, 3H), 1.25-1.24 (m, 3H), 1.18-1.13 (m, 1H), 107-1.02 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 208.2, 142.5, 139.5, 130.7, 128.3, 127.9, 127.7, 125.8, 125.7, 50.5, 33.5, 33.2, 31.9, 25.9, 23.3 (2C), 20.8, 13.1; IR (Neat): 3066, 2927, 2857, 1667, 1599, 1496, 1449, 1324, 1226, 1159, 1127, 1068, 984, 931, 781, 749, 693 cm^{-1}; MS (EI) *m/z* (rel): 304 (M^+, 10), 243 (5), 200 (34), 131 (14), 117 (100), 105 (82), 91 (73), 77 (43), 67 (11), 55 (16); HRMS (EI): calcd for $C_{12}H_{24}O_2$: 304.1827, found: 304.1833; HPLC (Chiralpak IC, Hexane:*i*-Propanol = 99.3/0.7, 1.0 mL/min, 214 nm): t_{major} = 7.49 min, t_{minor} = 8.07 min. $[\alpha]_D^{29}$ = -44.0 (1.0, $CHCl_3$).

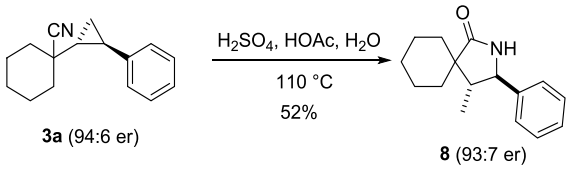


3f (96:4 er) **7** (95:5 er)

To a 10 mL of sealed tube were added $LiAlH_4$ (13.4 mg, 0.35 mmol) and Et_2O (1.0 mL) under argon, followed by cyclopropane **3a** (50 mg, 0.27 mmol) dropwise with stirring at

0 ℃. The sealed tube was screw capped and warmed to room temperature. After stirring for 12 hours, the reaction mixture was quenched carefully with 15% aqueous NaOH solution, until gas evolution had ceased. Then extracted with Et_2O (3 × 5 mL). The combined organic phase was dried over anhydrous Na_2SO_4 and then concentrated in vacuo to give a colorless oil.

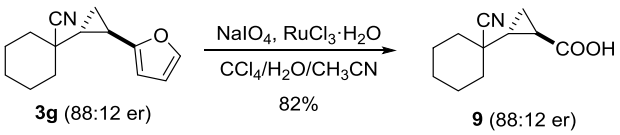
This oil was then dissolved in DCM (1.0 mL), followed by Et_3N (109 μL, 0.78 mmol) and *p*-brosyl chloride (70.0 mg, 0.27 mmol) with stirring at 0 ℃ for 15 min. Then warmed to room temperature and stirred overnight. The reaction mixture was quenched with H_2O and extracted with Et_2O (3 × 10 mL). The combined organic phase was dried over anhydrous Na_2SO_4 and then concentrated in vacuo. The residue was purified by column chromatography (*n*-hexane/EtOAc 5/1) to give **7** as a white solide, 101.9 mg, yield: 94%, 95:5 er; mp: 88.0-89.5 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63-7.58 (m, 4H), 7.28-7.24 (m, 2H), 7.18-7.15 (m, 1H), 7.02-7.00 (m, 2H), 4.64 (br, 1H), 2.85-2.76 (m, 2H), 1.79-1.74 (m, 1H), 0.90-0.87 (m, 1H), 0.84 (s, 3H), 0.83 (s, 3H), 0.82-0.79 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 142.9, 138.9, 132.4, 128.6, 128.5, 127.5, 125.7, 125.6, 54.6, 33.7, 31.6, 23.0, 18.4, 11.0; IR (Neat): 3277, 3083, 2958, 2923, 2857, 1602, 1571, 1466, 1412, 1323, 1275, 1166, 1010, 900, 826, 736, 695, 646, 611, 576, 523 cm^{-1}; MS (ESI) *m/z*: 408 $(M+H)^+$; HRMS (ESI): calcd for $C_{19}H_{23}O_2NBrS$ $[M+H]^+$: 408.0627, found: 408.0629; HPLC (Chiralpak IC, Hexane:*i*-Propanol = 98/2, 0.7 mL/min, 214 nm): t_{major} = 58.50 min, t_{minor} = 62.42 min. $[\alpha]_D^{31}$ = -7.6 (1.0, $CHCl_3$).



3a (94:6 er) **8** (93:7 er)

In a 25 mL round bottomed flask, cyclopropane **3a** (23.0 mg, 0.1 mmol) was added to the mixture of concentrated sulfuric acid (1.0 mL), glacial acetic acid (1.0 mL) and H_2O (1.0 mL) at room temperature. The reaction was then heated to 110 ℃ over night. The mixture was cooled to room temperature and diluted with H_2O (5 mL). Then extracted with EtOAc (3 × 5 mL). The combined organic phase was dried over anhydrous Na_2SO_4 and then concentrated in vacuo. The residue was purified by column chromatography (*n*-hexane/EtOAc 10/1) to give **8** as a white solid, 12.7 mg, yield: 52%, 93:7 er; mp: 165.4-167.3 ℃; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.29 (m, 5H), 5.76 (br, 1H), 4.13 (d, *J* = 9.2 Hz, 1H), 2.26-2.17 (m, 1H), 1.92-1.85 (m, 1H), 1.74-1.24 (m, 9H), 0.97 (d, *J* =

7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 182.1, 141.0,128.7, 128.0, 126.4, 62.1, 52.1, 45.3, 33.4, 28.0, 25.8, 21.9, 21.6, 11.2; IR (Neat): 3166, 3065, 3031, 2922, 2855, 1675, 1446, 1339, 1276, 1233, 1088, 1063, 841, 802, 697, 664 cm^{-1}; MS (EI) *m/z* (rel): 243 (M^+, 38), 228 (17), 202 (10), 188 (100), 175 (22), 160 (13), 117 (11), 106 (25), 91 (15), 81 (15), 77 (11), 67 (9); HRMS (EI): calcd for $C_{16}H_{21}NO$: 243.1623, found: 243.1627; HPLC (Chiralpak AD-H, Hexane:*i*-Propanol = 98/2, 2.0 mL/min, 214 nm): t_{major} = 9.93 min, t_{minor} = 11.19 min. $[\alpha]_D^{29}$ = -19.7 (1.0, $CHCl_3$).



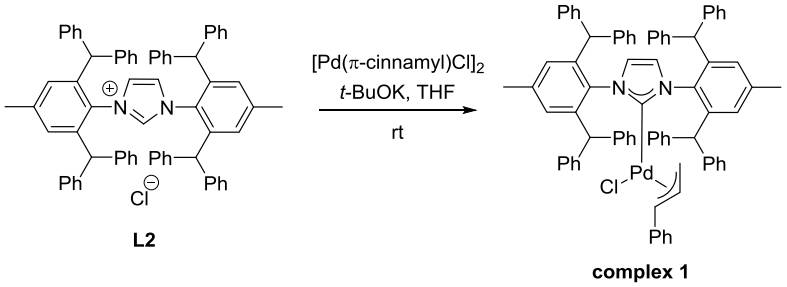
3g (88:12 er) **9** (88:12 er)

To a mixture of furan **3g** (22 mg, 0.1 mmol) and sodium periodate (214 mg, 1.0 mmol) in CCl_4 (0.8 ml)/CH_3CN (0.8 ml)/H_2O (1.0 ml) was added at room temperature $RuCl_3 \cdot H_2O$ (1.2 mg, 5.5 μmol), and the now dark brown mixture was vigorously stirred for 40 min. Then it was diluted with EtOAc (10 ml) and filtered over celite. Then H_2O (10 ml) and HCl (1.0 M, 5 ml) was added, and the phases were separated. The aqueous layer was extracted with EtOAc (3 × 5 ml), and the combined organic phases were dried (Na_2SO_4), filtered, and concentrated in vacuo. The residue was purified by column chromatography (CH_2Cl_2/MeOH/AcOH 95/4/1) to afford **9** as a colorless oil, 15.9 mg, yield: 82%, 88:12 er (determined by chiral GC); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.63 (br, 1H), 1.98 (m, 2H), 1.77-1.74 (m, 3H), 1.60-1.57 (m, 2H), 1.44-1.38 (m, 3H), 1.29-1.09 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 179.7, 120.7, 41.0, 35.8, 35.6, 29.2, 25.1, 23.0 (2C), 17.9, 11.8; IR (Neat): 2934, 2859, 2251, 1699, 1552, 1449, 1423, 1322, 1284, 1226, 1203, 909, 730, 649, 499 cm^{-1}; MS (EI) *m/z* (rel): 193 (M^+, 4), 191 (18), 175 (9), 165 (14), 148 (49), 133 (55), 121 (72), 108 (100), 93 (38), 86 (68), 68 (49), 55 (59); HRMS (EI): calcd for $C_{11}H_{15}NO_2$: 193.1103, found: 193.1105. $[\alpha]_D^{30}$ = -10.7 (0.5, $CHCl_3$).

4. Synthesis of complex 1 and identification of the active intermediate.

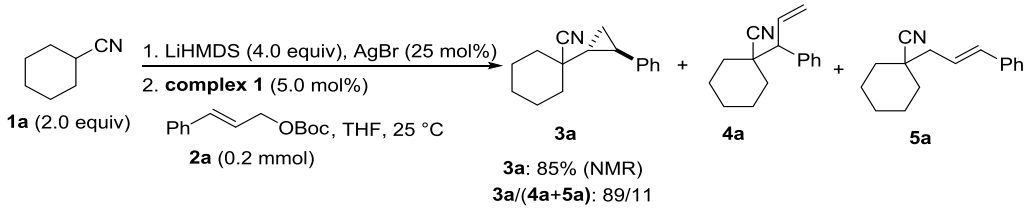
Synthesis of complex 1

L2 was synthesized according to the literature procedure and all analytical data were in good accordance with data reported in the literature.[3]



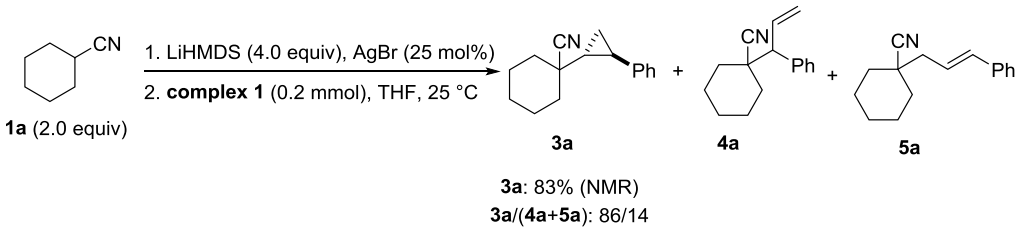
Following the procedure outlined by Chartoire *et al.*,[4] in a vacuum dried 100 mL round bottomed flask equipped with a magnetic stirring bar were added **L2** (522.3 mg, 0.55 mmol) and *t*-BuOK (67 mg, 0.6 mmol) in THF (40 mL). The reaction mixture was stirred for 4 h at room temperature and then [Pd(π-cinnamyl)Cl]$_2$ (130 mg, 0.25 mmol) was added in THF (5.0 mL). The reaction mixture was then stirred overnight at room temperature. After this time, THF was evaporated and the crude product was dissolved in CH_2Cl_2, filtered on a pad of silica covered with celite, and eluted with CH_2Cl_2. After evaporation of the solvents, the complex was precipitated in pentane, filtered and dried to give **complex 1** as an off white solid, 0.51 g, yield 90%. NMR of **complex 1** was in good accordance with the data reported in the literature. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50-7.48 (m, 2H), 7.41-7.37 (m, 2H), 7.34-7.27 (m, 9H), 7.25-7.17 (m, 12H), 7.10-7.06 (m, 12H), 6.85-6.84 (m, 8H), 6.79-6.77 (m, 4H), 6.09 (s, 2H), 5.69 (s, 2H), 5.31 (s, 2H), 5.04-4.96 (m, 1H), 4.61 (d, J = *12.8* Hz, 1H), 2.57 (d, J = 6.4 Hz, 1H), 2.24 (s, 6H), 1.22 (d, J = 10.8 Hz, 1H).

Identification of the active intermediate.



A dry Schlenk tube was flame dried and flushed with argon. AgBr (18.8 mg, 0.1 mmol), nitriles **1** (0.4 mmol) and THF (1.0 mL) were added. LiHMDS (1.0 M in THF, 0.8 mL,

0.8 mmol) was added at 0 ℃ and stirred at room temperature for 30 min. **Complex 1** (11.8 mg, 0.01 mmol) in THF (1.0 mL) was then added to the nitriles solution. The allylic substrates **2a** (0.2 mmol) and another 1.0 mL THF were then added and the mixture was stirred at room temperature. After the reaction completed (monitored by TLC), the reaction mixture was quenched with H_2O (0.2 mL). The solution was dried over anhydrous Na_2SO_4 and then filtered through a 0.5 inch plug of silica gel (eluting with EtOAc) to remove the solid. The reaction mixture was concentrated under reduced pressure to afford the crude product. NMR yield and selectivity were determined by ^1H NMR using mesitylene as internal standard.



A dry Schlenk tube was flame dried and flushed with argon. AgBr (18.8 mg, 0.1 mmol), nitriles **1** (0.4 mmol) and THF (1.0 mL) were added. LiHMDS (1.0 M in THF, 0.8 mL, 0.8 mmol) was added at 0 ℃ and stirred at room temperature for 30 min. **Complex 1** (209.6 mg, 0.2 mmol) in THF (2.0 mL) was then added to the nitriles solution and the mixture was stirred at room temperature. After the reaction completed (monitored by TLC), the reaction mixture was quenched with H_2O (0.2 mL). The solution was dried over anhydrous Na_2SO_4 and then filtered through a 0.5 inch plug of silica gel (eluting with EtOAc) to remove the solid. The reaction mixture was concentrated under reduced pressure to afford the crude product. NMR yield and selectivity were determined by ^1H NMR using mesitylene as internal standard.

5. Crystallographic Data

The structure of **7** was assigned by X-ray crystallographic analysis of a single crystal of **7** (Figure S1).

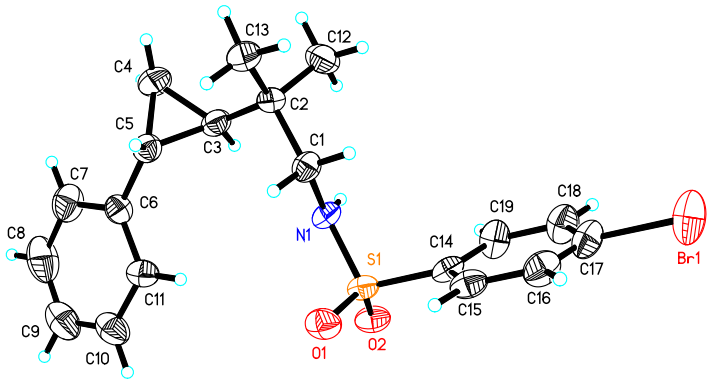


Figure S1

Table 1. Crystal data and structure refinement for mo_d8v18407_0m.

Identification code	mo_d8v18407_0m	
Empirical formula	C19 H22 Br N O2 S	
Formula weight	408.34	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P 1	
Unit cell dimensions	a = 9.4750(9) Å	α= 85.185(3) °.
	b = 9.6439(9) Å	β= 81.590(3) °.
	c = 10.8290(10) Å	γ = 82.894(3) °.
Volume	969.16(16) $Å^3$	
Z	2	
Density (calculated)	1.399 Mg/m^3	
Absorption coefficient	2.239 mm^{-1}	
F(000)	420	
Crystal size	0.200 x 0.170 x 0.130 mm^3	
Theta range for data collection	2.696 to 26.000 °.	
Index ranges	-11<=h<=11, -11<=k<=11, -13<=l<=13	
Reflections collected	37202	
Independent reflections	7458 [R(int) = 0.0496]	

Completeness to theta = 25.242 °	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.4595
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7458 / 5 / 446
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0383, wR2 = 0.0947
R indices (all data)	R1 = 0.0529, wR2 = 0.1027
Absolute structure parameter	0.045(5)
Largest diff. peak and hole	0.372 and -0.431 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_d8v18407_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	8984(1)	4077(1)	13951(1)	118(1)
Br(2)	3731(1)	6659(1)	2288(1)	114(1)
S(1)	7291(1)	3331(1)	8549(1)	50(1)
S(2)	5360(1)	7712(1)	7634(1)	46(1)
N(1)	5568(5)	3549(5)	8665(5)	50(1)
N(2)	7092(5)	7585(5)	7457(4)	48(1)
O(1)	7767(5)	1930(4)	8227(4)	65(1)
O(2)	7792(4)	4482(4)	7744(4)	62(1)
O(3)	4936(4)	6597(4)	8518(4)	54(1)
O(4)	4824(4)	9118(4)	7900(4)	59(1)
C(1)	4744(6)	2503(6)	9424(6)	53(1)
C(2)	3103(6)	2856(6)	9434(5)	53(1)
C(3)	2790(5)	3171(6)	8076(5)	56(1)
C(4)	1429(7)	2897(8)	7668(8)	76(2)
C(5)	2807(5)	2066(5)	7208(5)	56(1)
C(6)	3535(6)	2208(5)	5886(5)	53(1)
C(7)	2768(9)	2426(7)	4892(7)	81(2)
C(8)	3504(14)	2455(10)	3676(8)	105(3)
C(9)	4963(14)	2213(8)	3446(8)	96(3)
C(10)	5709(10)	2000(7)	4438(7)	79(2)
C(11)	5019(7)	2024(6)	5650(6)	59(2)
C(12)	2555(9)	4152(7)	10132(7)	75(2)

C(13)	2449(7)	1593(7)	10115(6)	71(2)
C(14)	7758(6)	3491(5)	10053(6)	49(1)
C(15)	8363(6)	2366(6)	10728(6)	59(2)
C(16)	8726(7)	2545(7)	11897(7)	68(2)
C(17)	8483(8)	3836(7)	12355(7)	70(2)
C(18)	7837(8)	4971(7)	11708(8)	75(2)
C(19)	7485(8)	4804(6)	10553(7)	69(2)
C(20)	7810(6)	8632(6)	6618(6)	56(1)
C(21)	9430(6)	8452(6)	6609(5)	48(1)
C(22)	9761(5)	8715(5)	7888(4)	47(1)
C(23)	11160(8)	8129(9)	8370(7)	77(2)
C(24)	9750(5)	7648(5)	8986(5)	50(1)
C(25)	9114(6)	8065(5)	10238(5)	56(1)
C(26)	9914(9)	7928(8)	11234(7)	86(2)
C(27)	9304(14)	8285(11)	12404(8)	110(3)
C(28)	7893(15)	8755(9)	12631(7)	106(3)
C(29)	7044(10)	8939(7)	11678(7)	82(2)
C(30)	7691(8)	8589(6)	10483(6)	64(2)
C(31)	10101(8)	7028(7)	6136(7)	71(2)
C(32)	9998(8)	9641(7)	5698(6)	69(2)
C(33)	4862(6)	7404(5)	6175(5)	45(1)
C(34)	4261(7)	8501(6)	5453(6)	56(2)
C(35)	3924(7)	8272(7)	4298(7)	66(2)
C(36)	4186(7)	6960(7)	3881(7)	65(2)
C(37)	4757(9)	5848(7)	4604(8)	79(2)
C(38)	5114(8)	6078(6)	5750(7)	66(2)

6. Computational Details and X-Ray Crystal Structure

All calculations were performed with Gaussian 16, A03 program package.[5] Geometry optimizations were performed at the M06 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, Cl. The NPA charges were calculated at the same level of theory. NBO program combined with Gaussian 16 was utilized to calculate NPA charges.

Cartesian Coordinates for Selected Intermediates Shown in Scheme 3

L2	**L3**
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C,0,4.2977180534,-0.3258922281,0.3056031709	C,0,4.3167377606,-0.1404394332,0.1238513283
N,0,3.0076568501,-0.8237906313,0.5001707473	N,0,3.0382956439,-0.6198455584,0.4111408336
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7. References

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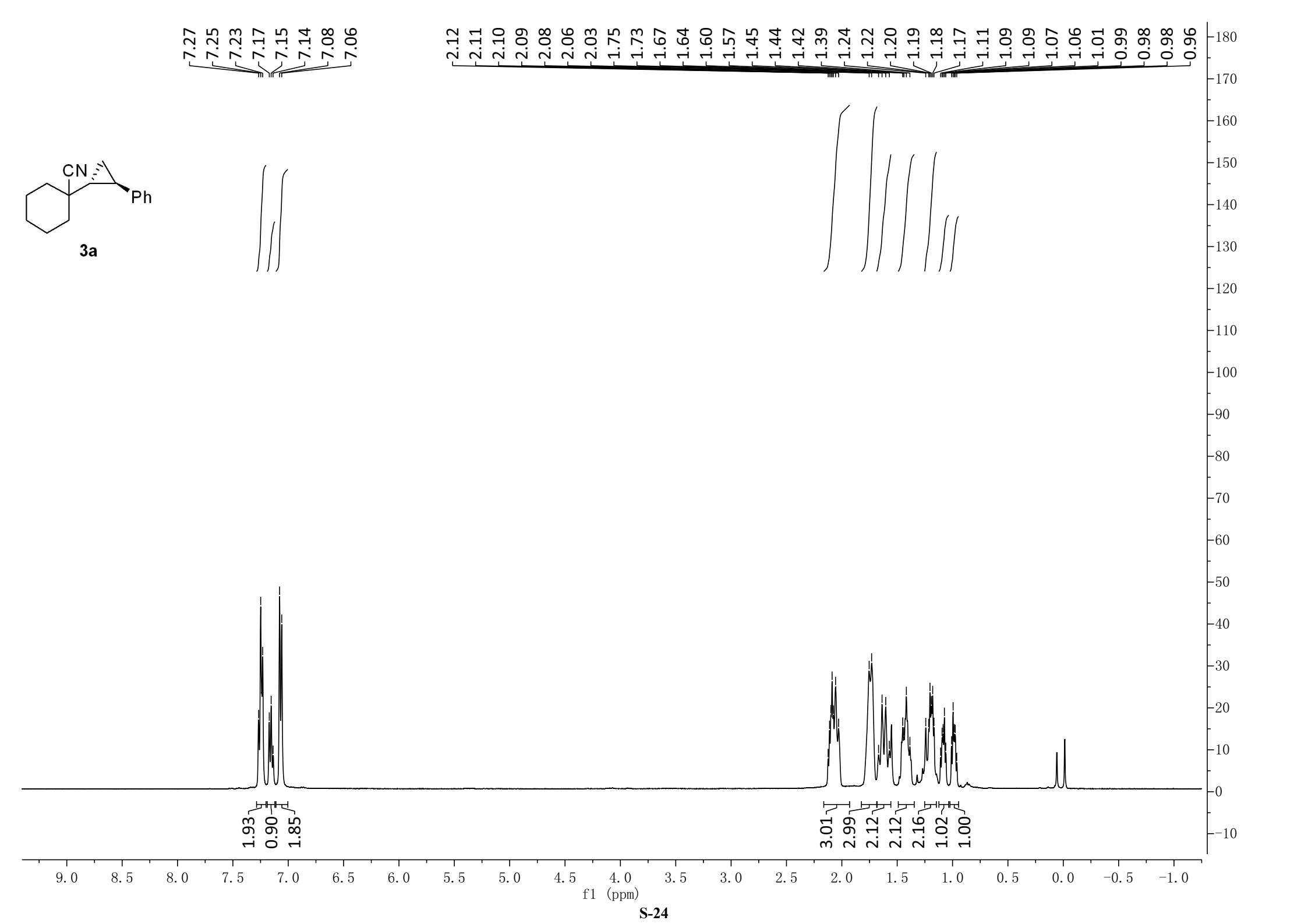
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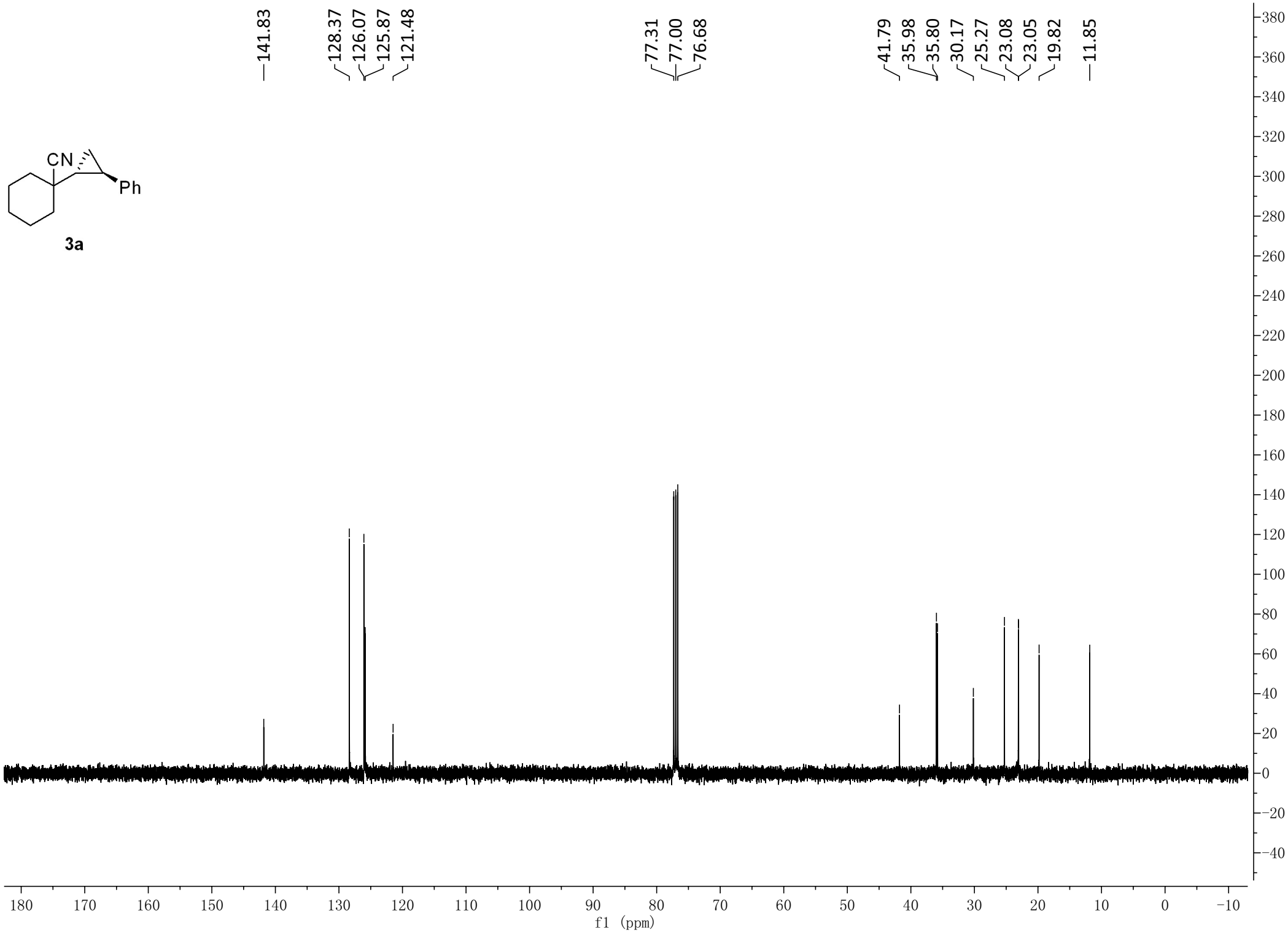
7.23
7.17
7.15
7.14
7.08
7.06
2.12
2.11
2.10
2.09
2.08
2.06
2.03
1.75
1.73
1.67
1.64
1.60
1.57
1.45
1.44
1.42
1.39
1.24
1.22
1.20
1.19
1.18
1.17
1.11
1.09
1.09
1.07
1.06
1.01
0.99
0.98
0.98
0.96
CN
Ph
3a
1.93
0.90
1.85
3.01
2.99
2.12
2.12
2.16
1.02
1.00
f1 (ppm)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128.37
126.07
125.87
121.48
77.31
77.00
76.68
41.79
35.98
35.80
30.17
25.27
23.08
23.05
19.82
11.85
CN
Ph
3a
f1 (ppm)

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

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Vail #	:
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Batch File Name	:
Report File Name	: Default.lcr
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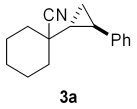
Data Processed	: 2018-7-20 13:07:39



3a

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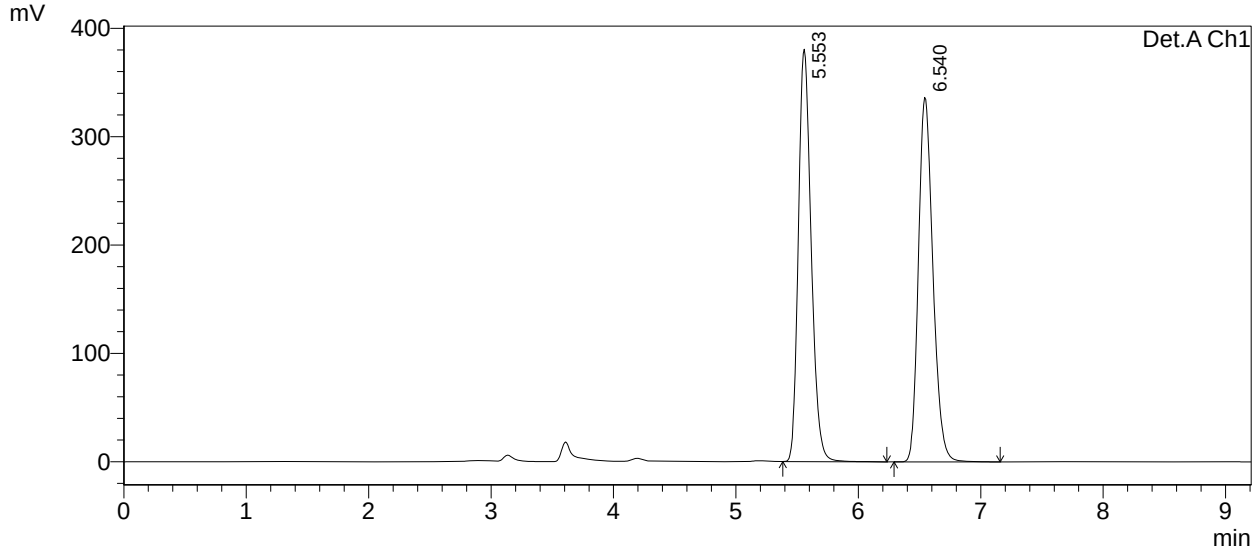

1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.553	2765773	380649	49.998	53.089
2	6.540	2765948	336351	50.002	46.911
Total		5531721	717000	100.000	100.000

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

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Sample ID	: AD-H,98/2,1.0,214
Vail #	:
Injection Volume	: 2 uL
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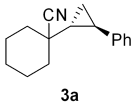

3a

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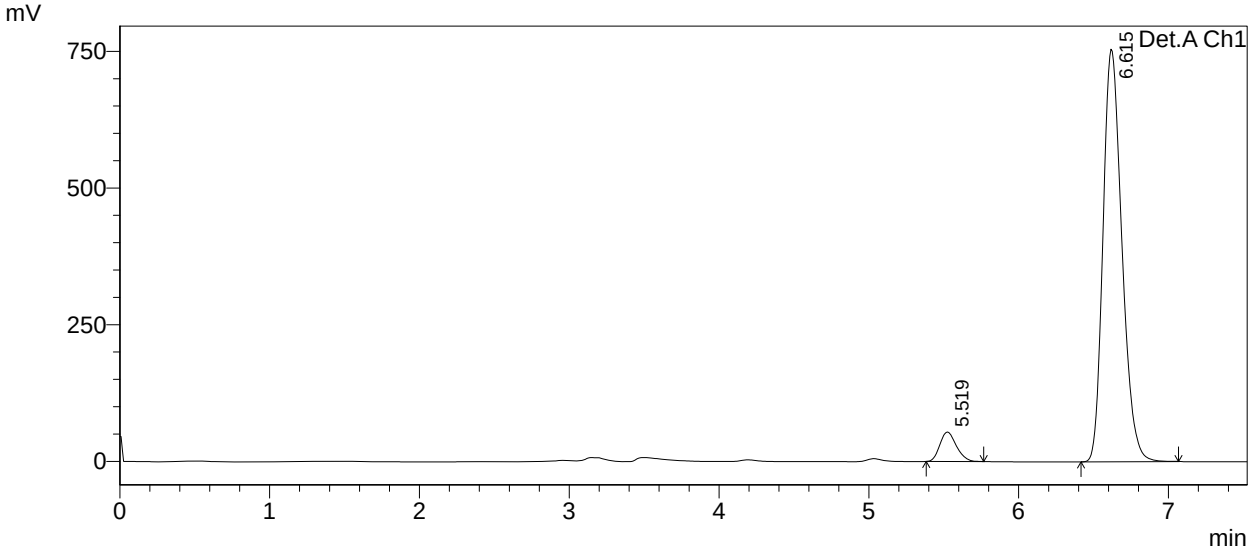
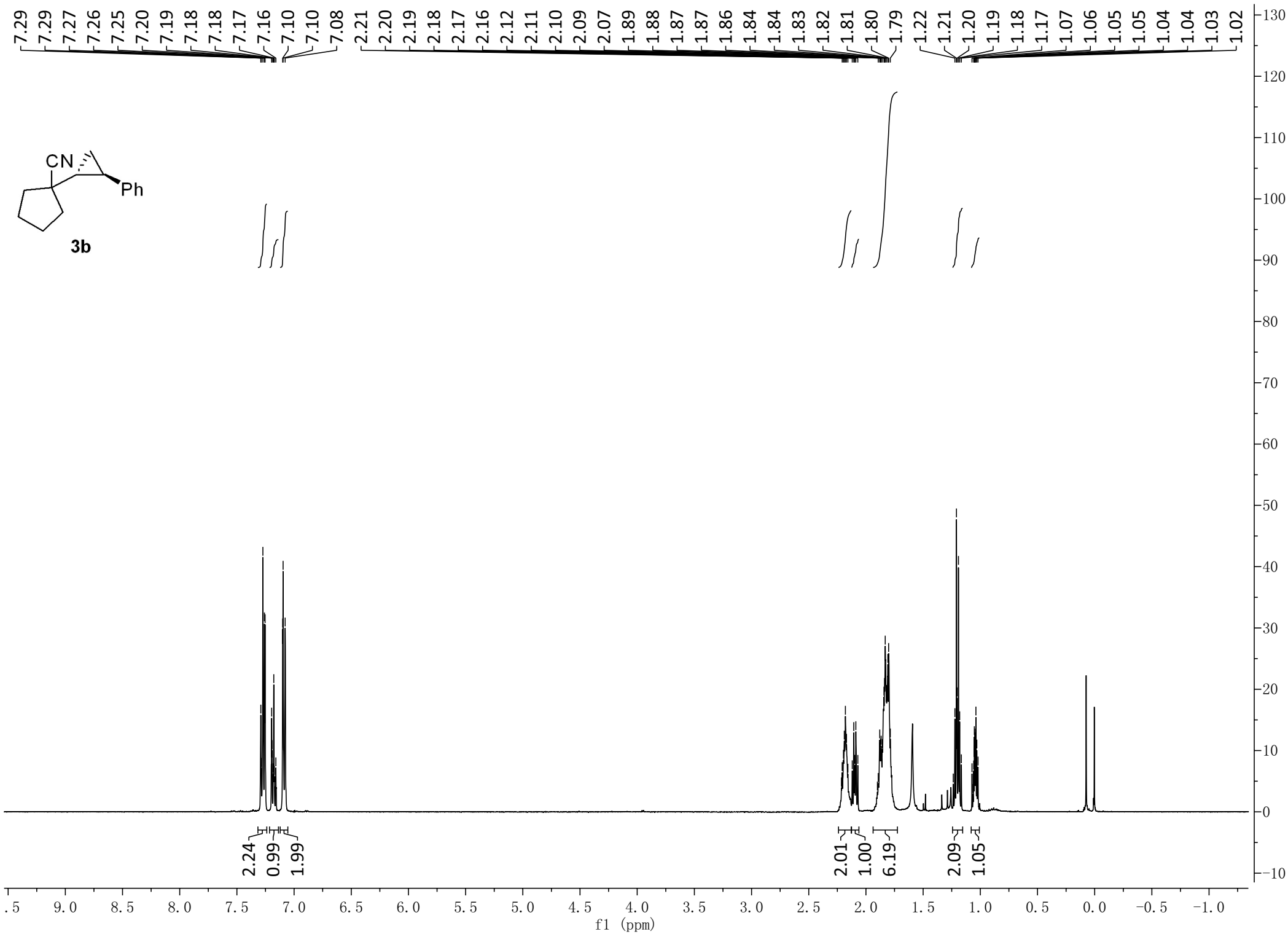


1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.519	414626	53836	5.896	6.657
2	6.615	6617196	754876	94.104	93.343
Total		7031823	808712	100.000	100.000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2.21 2.20 2.19 2.18 2.17 2.16 2.12 2.11 2.10 2.09 2.07 1.89 1.88 1.87 1.87 1.86 1.84 1.84 1.83 1.82 1.81 1.80 1.79
1.22 1.21 1.20 1.19 1.18 1.17 1.07 1.06 1.05 1.05 1.04 1.04 1.03 1.02
CN
Ph
3b
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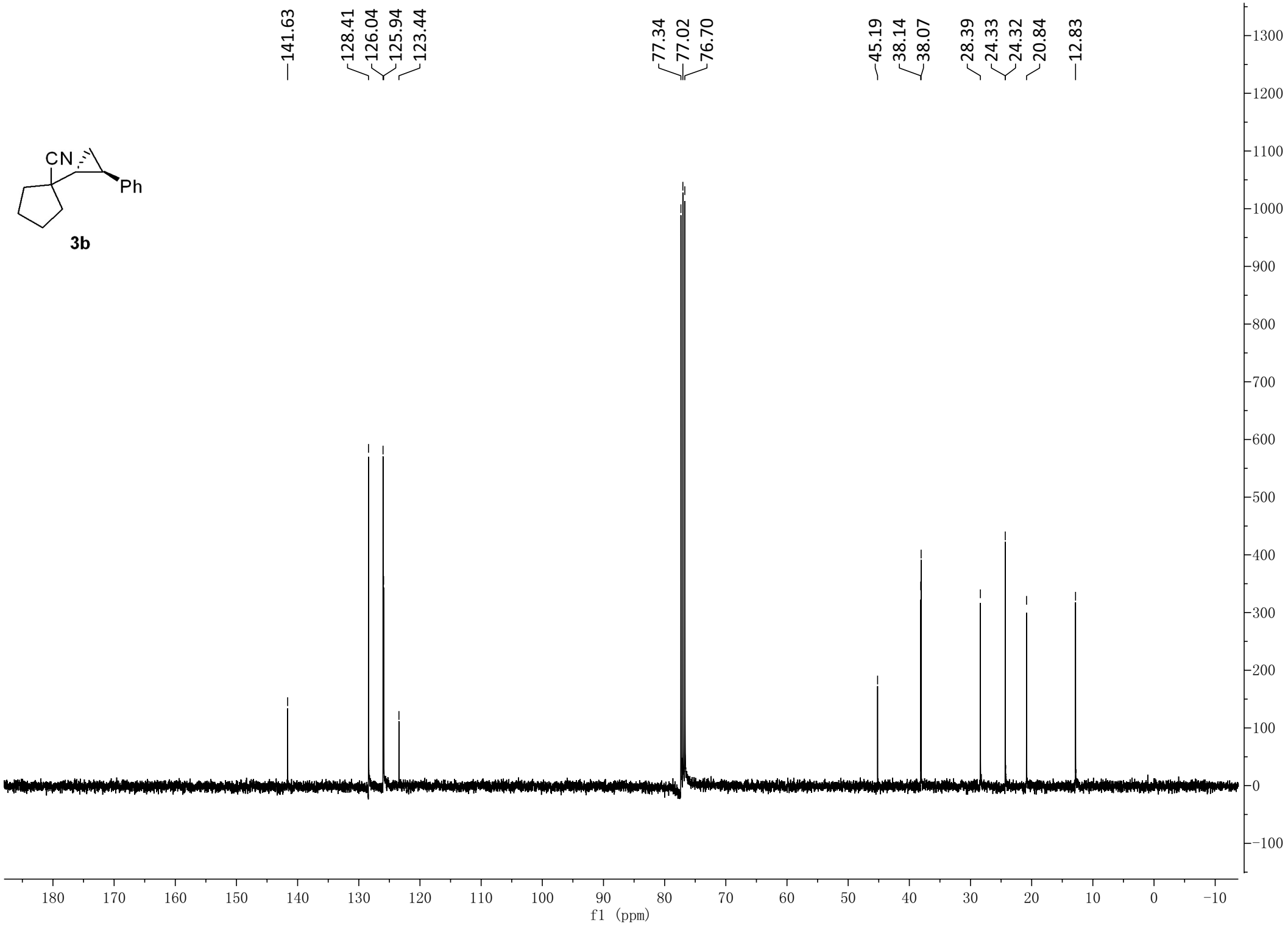
0.99
1.99
2.01
1.00
6.19
2.09
1.05
f1 (ppm)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128.41
126.04
125.94
123.44
77.34
77.02
76.70
45.19
38.14
38.07
28.39
24.33
24.32
20.84
12.83
CN
Ph
3b
f1 (ppm)

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

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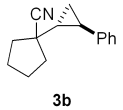
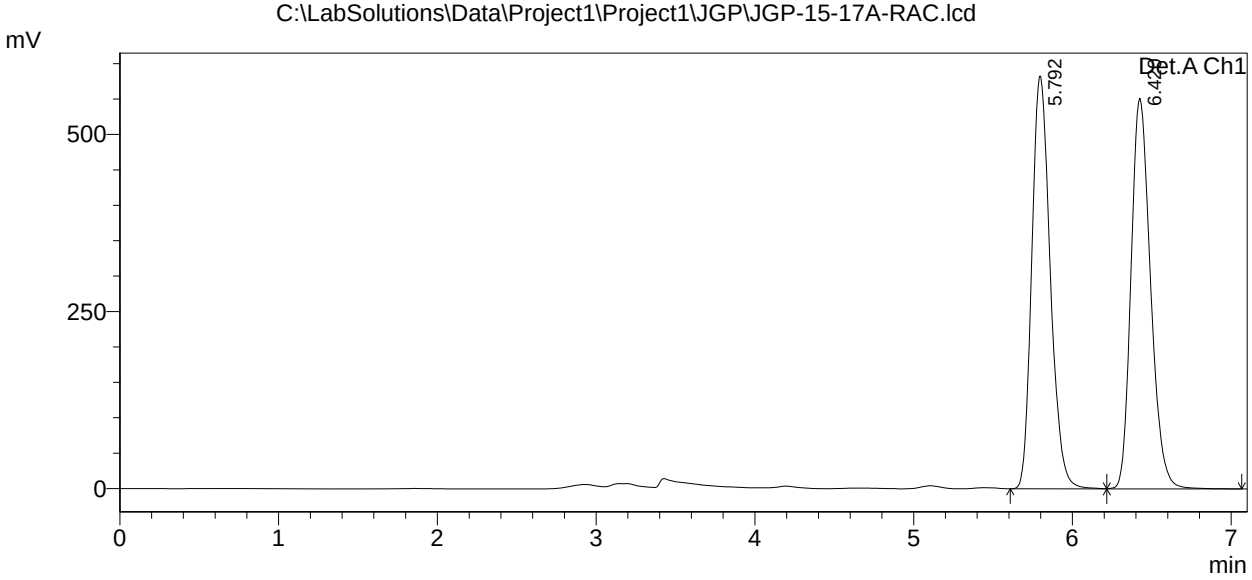


3b

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-17A-RAC.lcd



1 Det.A Ch1/214nm

PeakTable

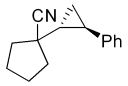
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.792	4710462	582412	50.007	51.362
2	6.420	4709058	551529	49.993	48.638
Total		9419520	1133941	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-17A-1.lcd

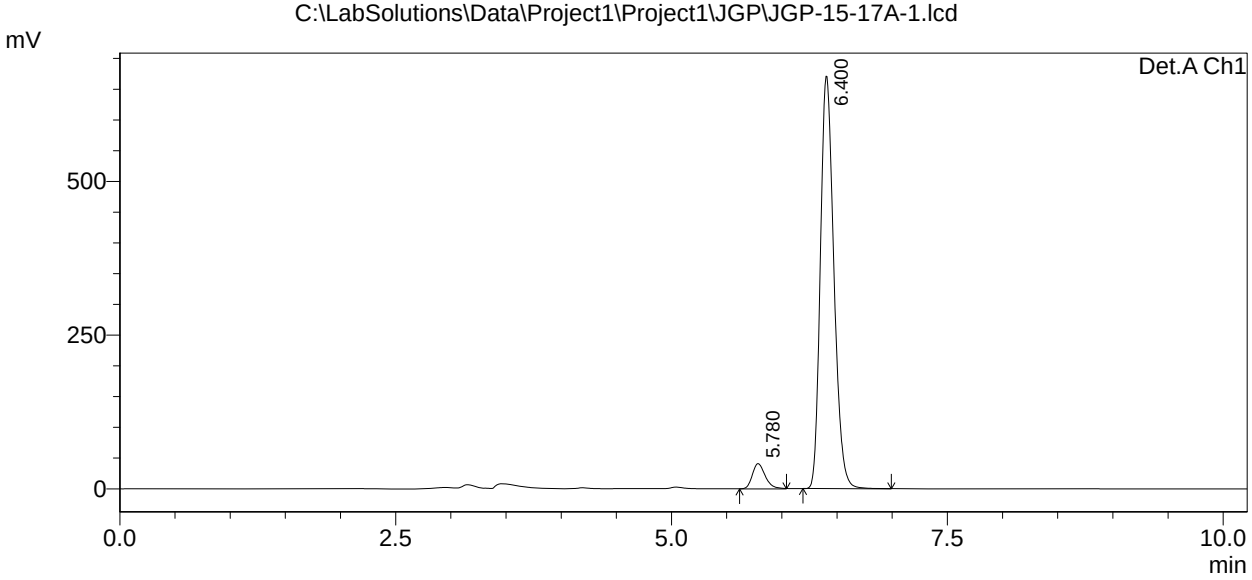
Acquired by	: Admin
Sample Name	: JGP-15-17A-1
Sample ID	: AD-H,98/2,1.0,254
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-17A-1.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-10 15:28:57
Data Processed	: 2018-5-19 9:09:53



3b

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-17A-1.lcd

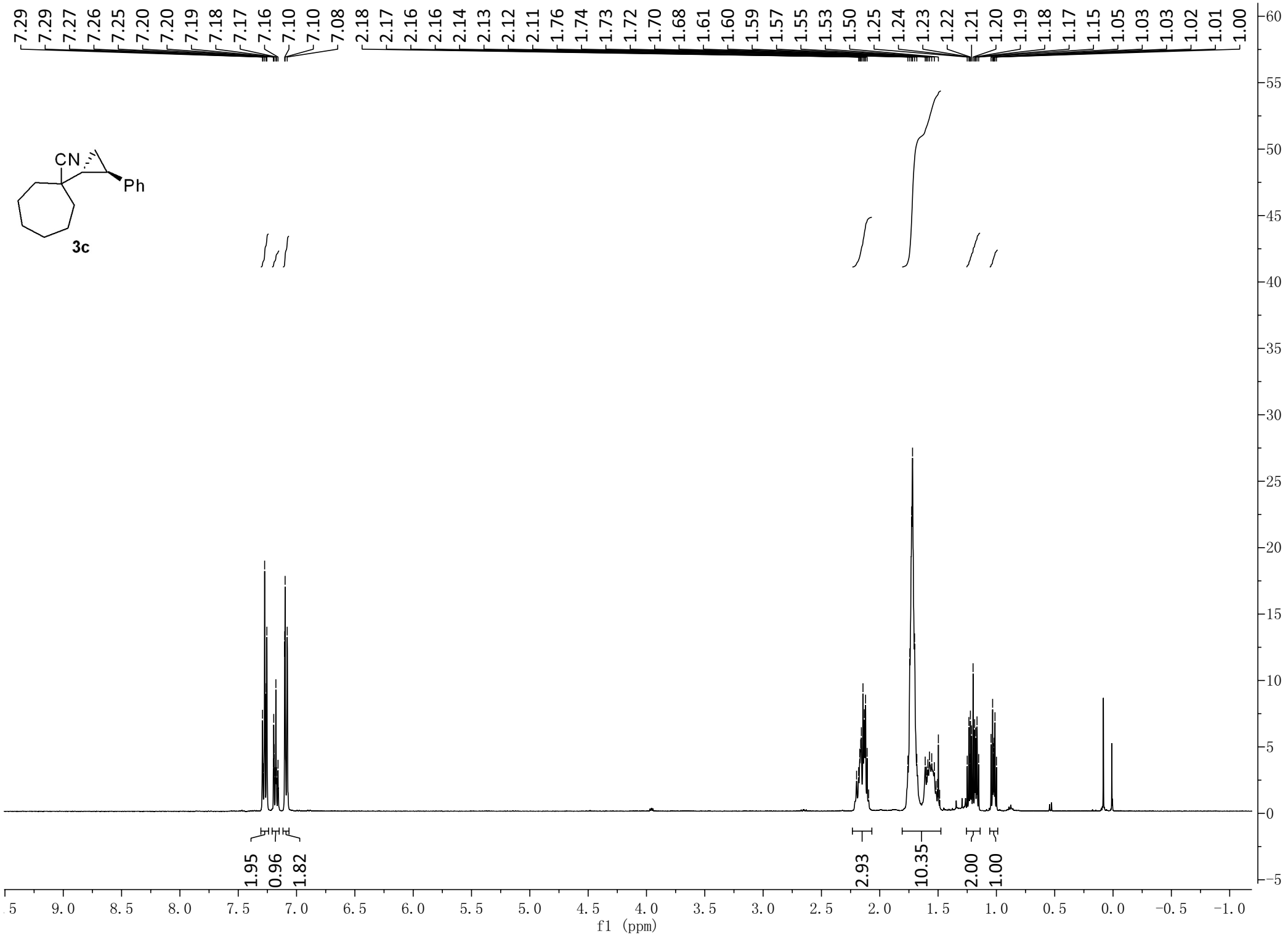


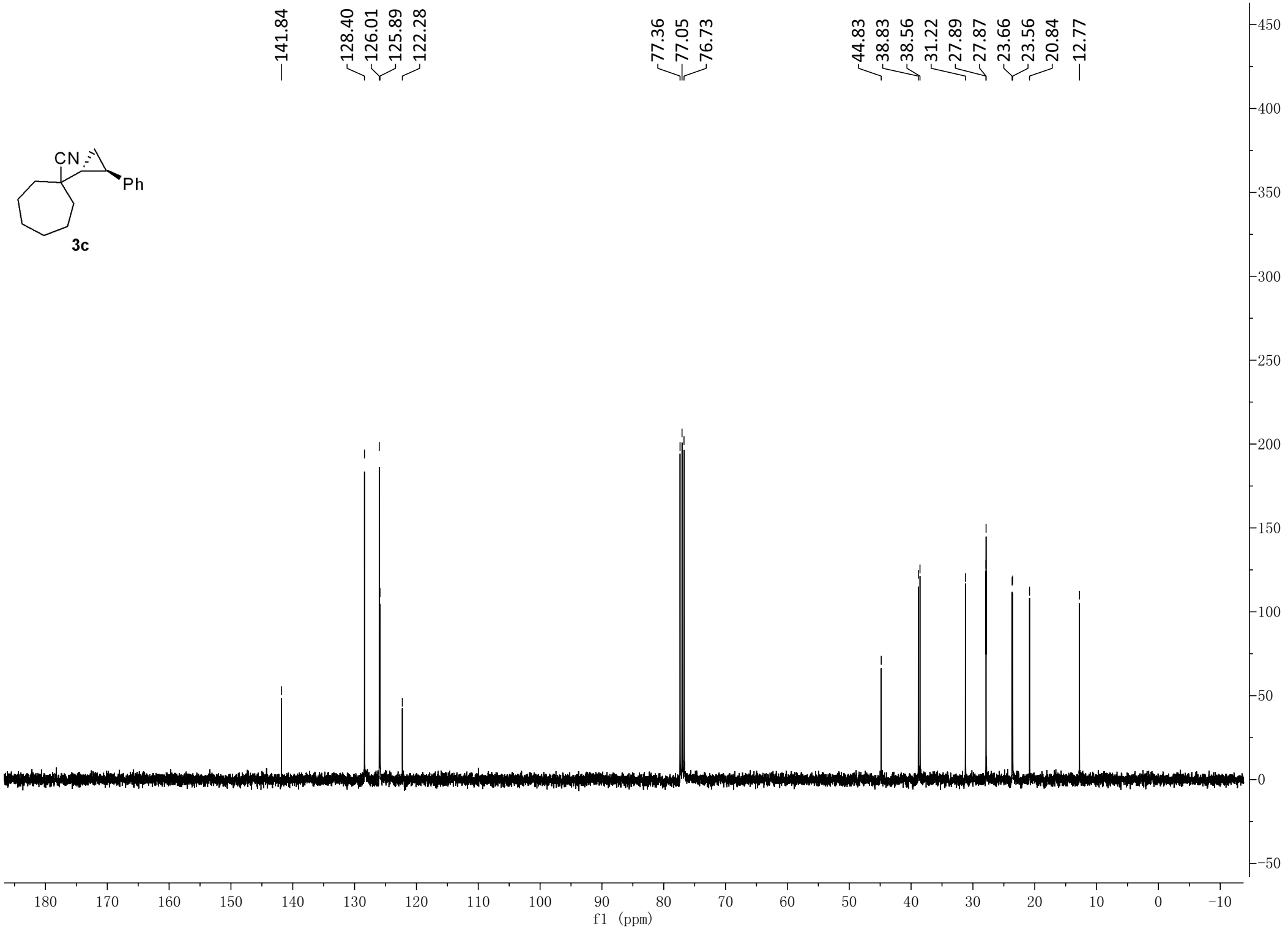
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.780	334928	41045	5.540	5.766
2	6.400	5710309	670782	94.460	94.234
Total		6045238	711827	100.000	100.000

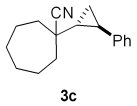

7.29 7.29 7.27 7.26 7.25 7.20 7.20 7.19 7.18 7.17 7.16 7.10 7.10 7.08
2.18 2.17 2.16 2.16 2.14 2.13 2.12 2.11 1.76 1.74 1.73 1.72 1.70 1.68 1.61 1.60 1.59 1.57 1.55 1.53 1.50 1.25 1.24 1.23 1.22 1.21 1.20 1.19 1.18 1.17 1.15 1.05 1.03 1.03 1.02 1.01 1.00
CN
Ph
3c
1.95
0.96
1.82
2.93
10.35
2.00
1.00
f1 (ppm)


141.84
128.40
126.01
125.89
122.28
77.36
77.05
76.73
44.83
38.83
38.56
31.22
27.89
27.87
23.66
23.56
20.84
12.77
CN
Ph
3c
f1 (ppm)

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-18A-RAC.lcd

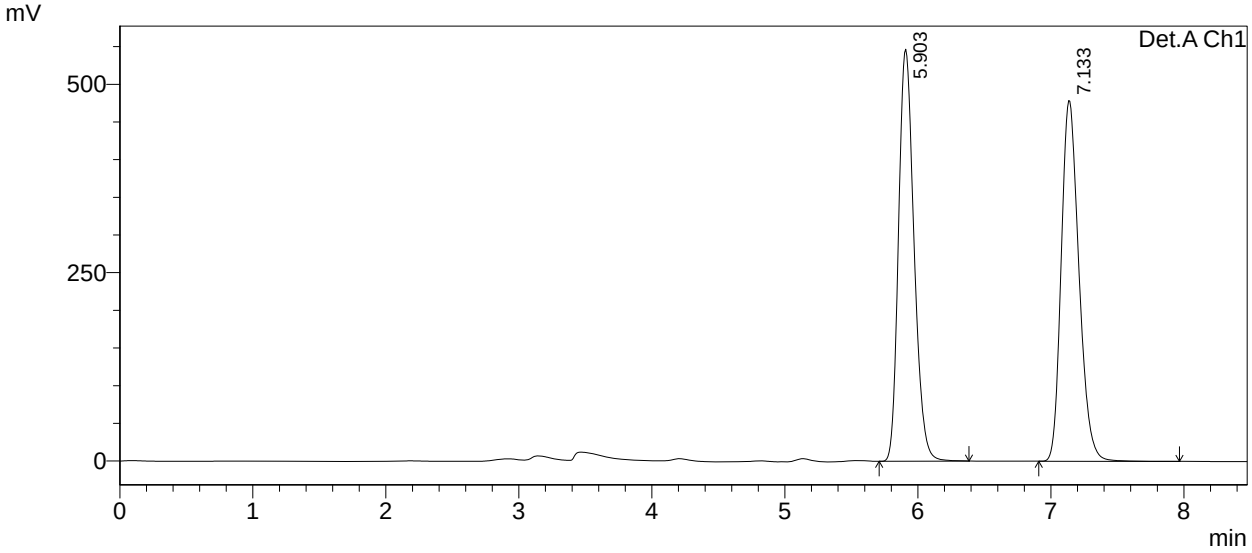
Acquired by	: Admin
Sample Name	: JGP-15-18A-RAC
Sample ID	: AD-H,98/2,1.0,254
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-18A-RAC.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-10 14:52:00
Data Processed	: 2018-5-10 15:00:28



3c

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-18A-RAC.lcd



1 Det.A Ch1/214nm

PeakTable

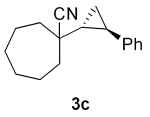
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.903	4425680	547108	49.929	53.327
2	7.133	4438293	478839	50.071	46.673
Total		8863973	1025947	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-18A-1.lcd

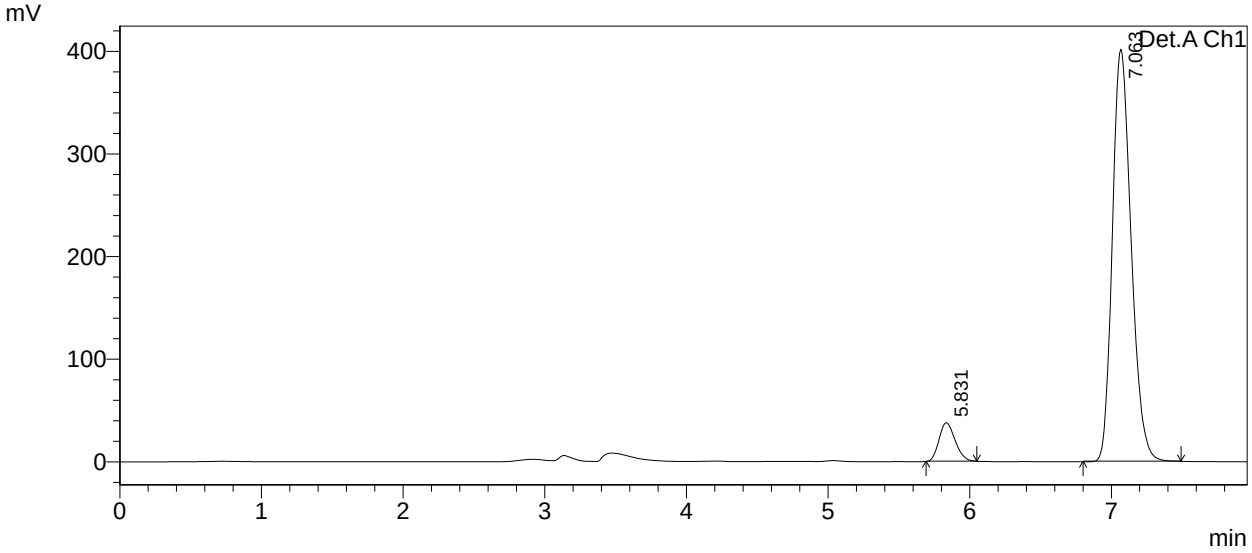
Acquired by	: Admin
Sample Name	: JGP-15-18A-1
Sample ID	: AD-H,98/2,1.0,254
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-18A-1.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-10 15:40:23
Data Processed	: 2018-5-19 9:11:31



3c

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-18A-1.lcd

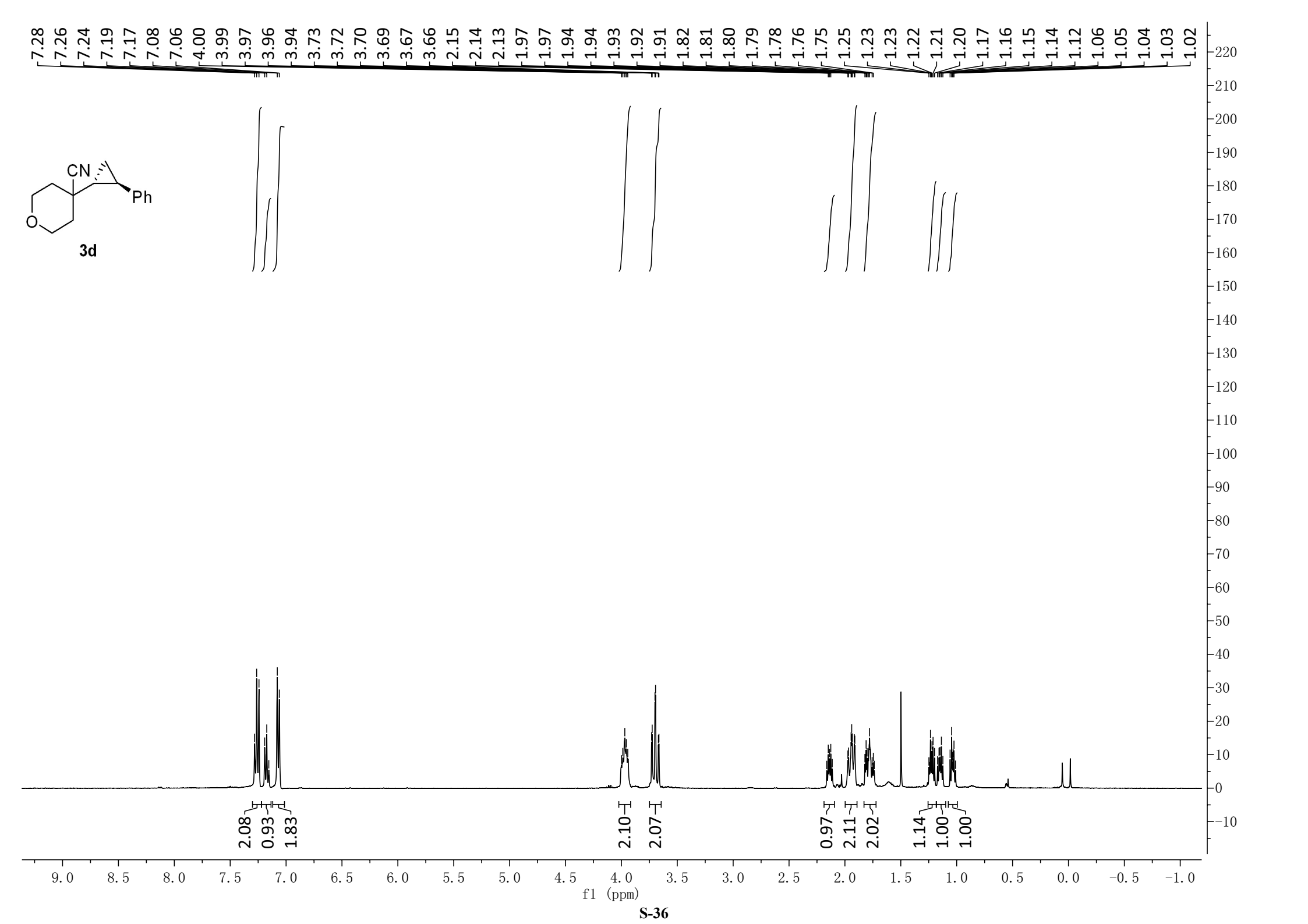


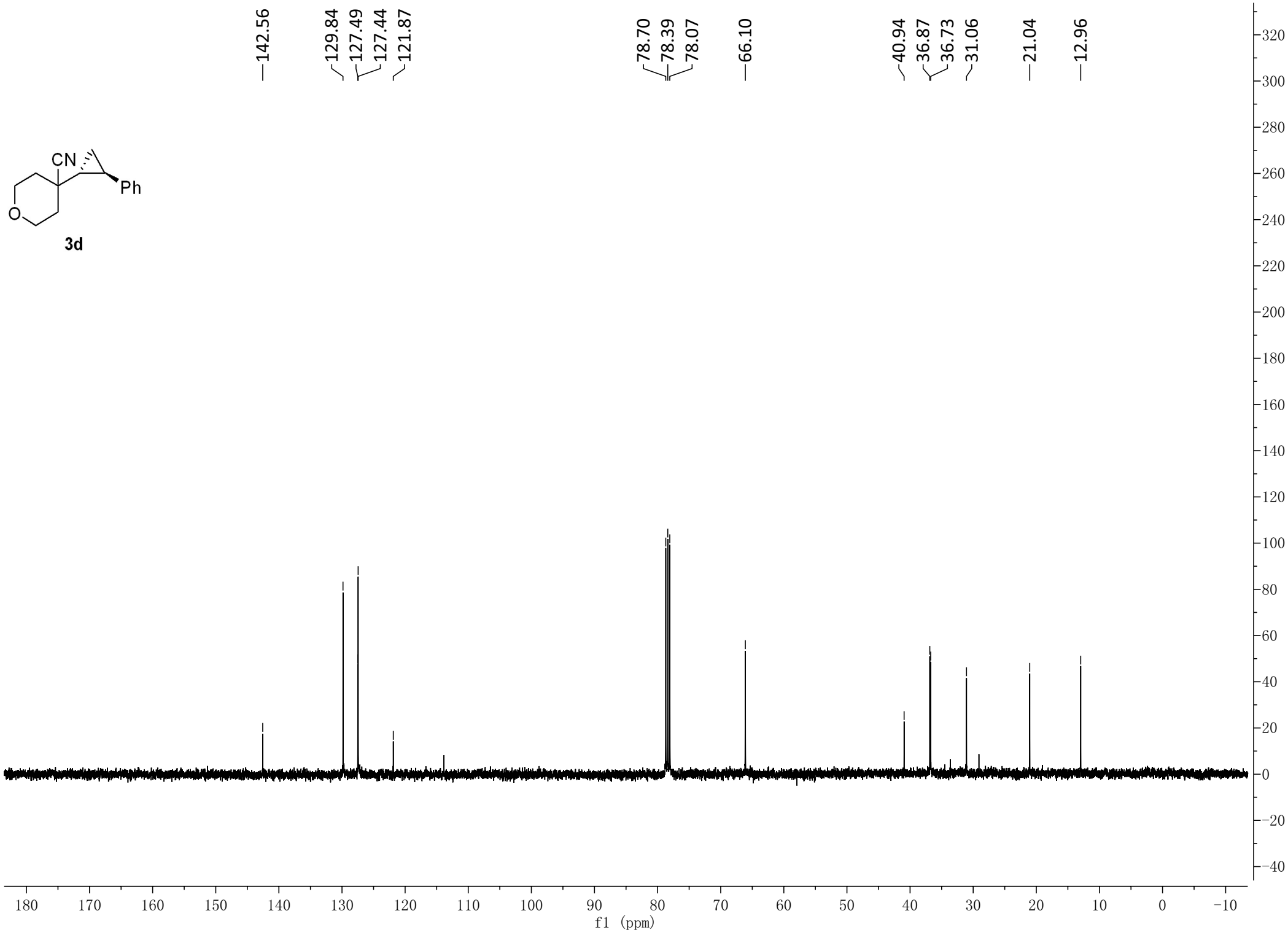
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.831	292076	37347	7.342	8.512
2	7.063	3686239	401430	92.658	91.488
Total		3978314	438776	100.000	100.000

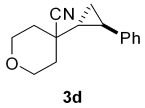

7.28 7.26 7.24 7.19 7.17 7.08 7.06 4.00 3.99 3.97 3.96 3.94 3.73 3.72 3.70 3.69 3.67 3.66 2.15 2.14 2.13 1.97 1.97 1.94 1.94 1.93 1.92 1.91 1.82 1.81 1.80 1.79 1.78 1.76 1.75 1.25 1.23 1.23 1.22 1.21 1.20 1.17 1.16 1.15 1.14 1.12 1.06 1.05 1.04 1.03 1.02
CN
Ph
O
3d
2.08 0.93 1.83 2.10 2.07 0.97 2.11 2.02 1.14 1.00 1.00
f1 (ppm)


142.56
129.84
127.49
127.44
121.87
78.70
78.39
78.07
66.10
40.94
36.87
36.73
31.06
21.04
12.96
CN
Ph
O
3d
f1 (ppm)

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-6A-RAC-5.lcd

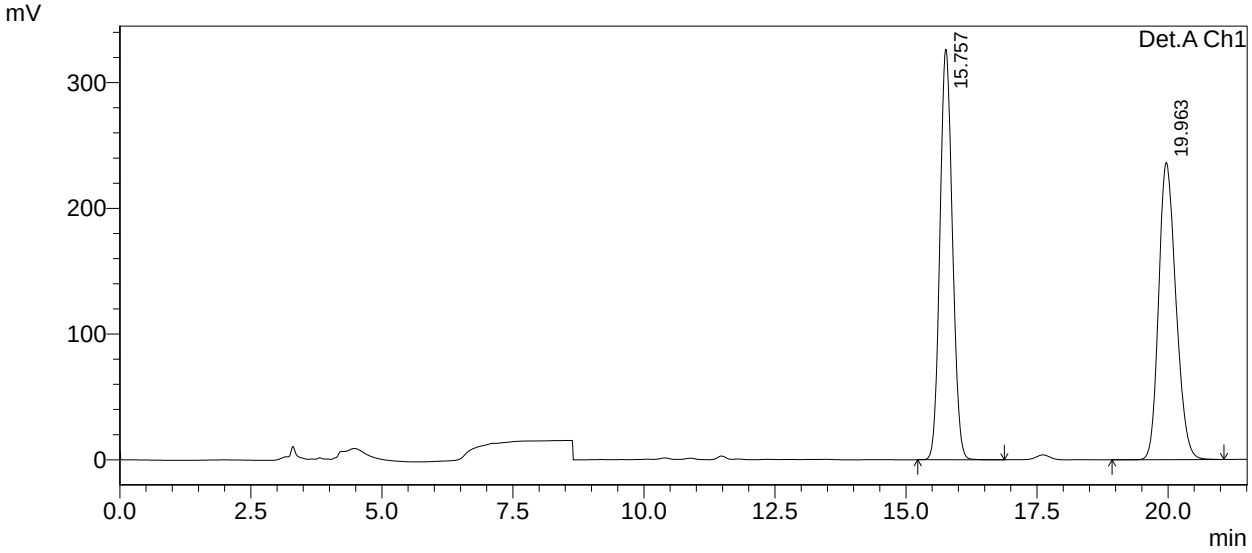
Acquired by	: Admin
Sample Name	: JGP-15-6A-RAC-5
Sample ID	: IC,98/2,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-6A-RAC-5.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-7 16:17:53
Data Processed	: 2018-5-7 16:39:24



3d

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-6A-RAC-5.lcd



1 Det.A Ch1/214nm

PeakTable

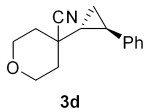
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.757	5427359	326642	49.997	58.010
2	19.963	5428077	236437	50.003	41.990
Total		10855436	563079	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-6A-2.lcd

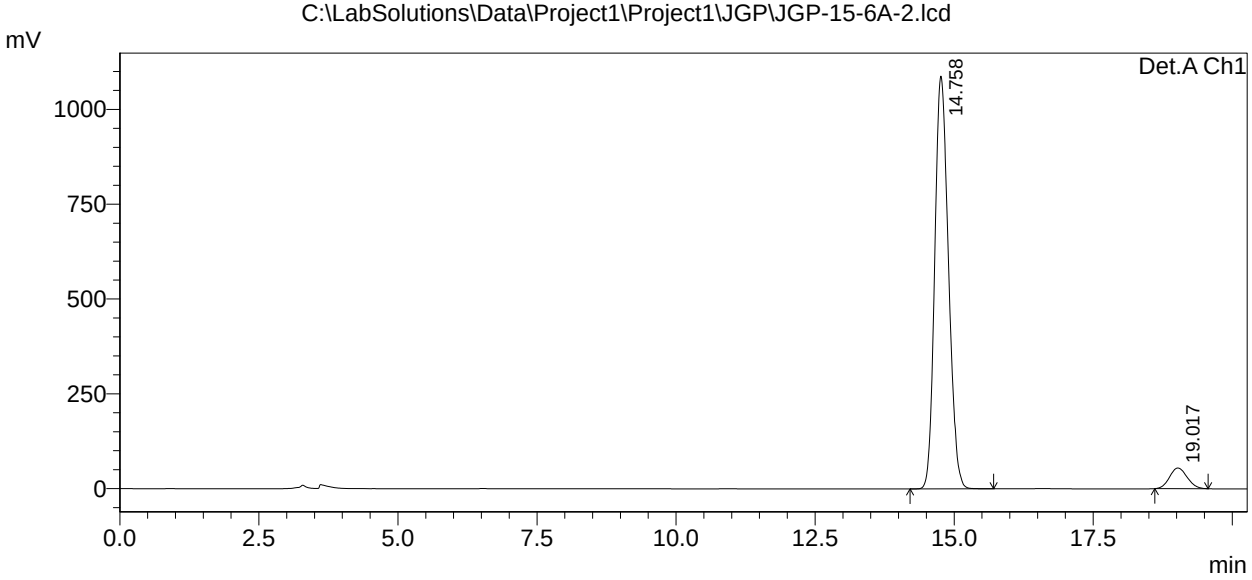
Acquired by	: Admin
Sample Name	: JGP-15-6A-2
Sample ID	: IC,98/2,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-6A-2.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-7 16:40:27
Data Processed	: 2018-5-14 15:28:17



3d

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-6A-2.lcd

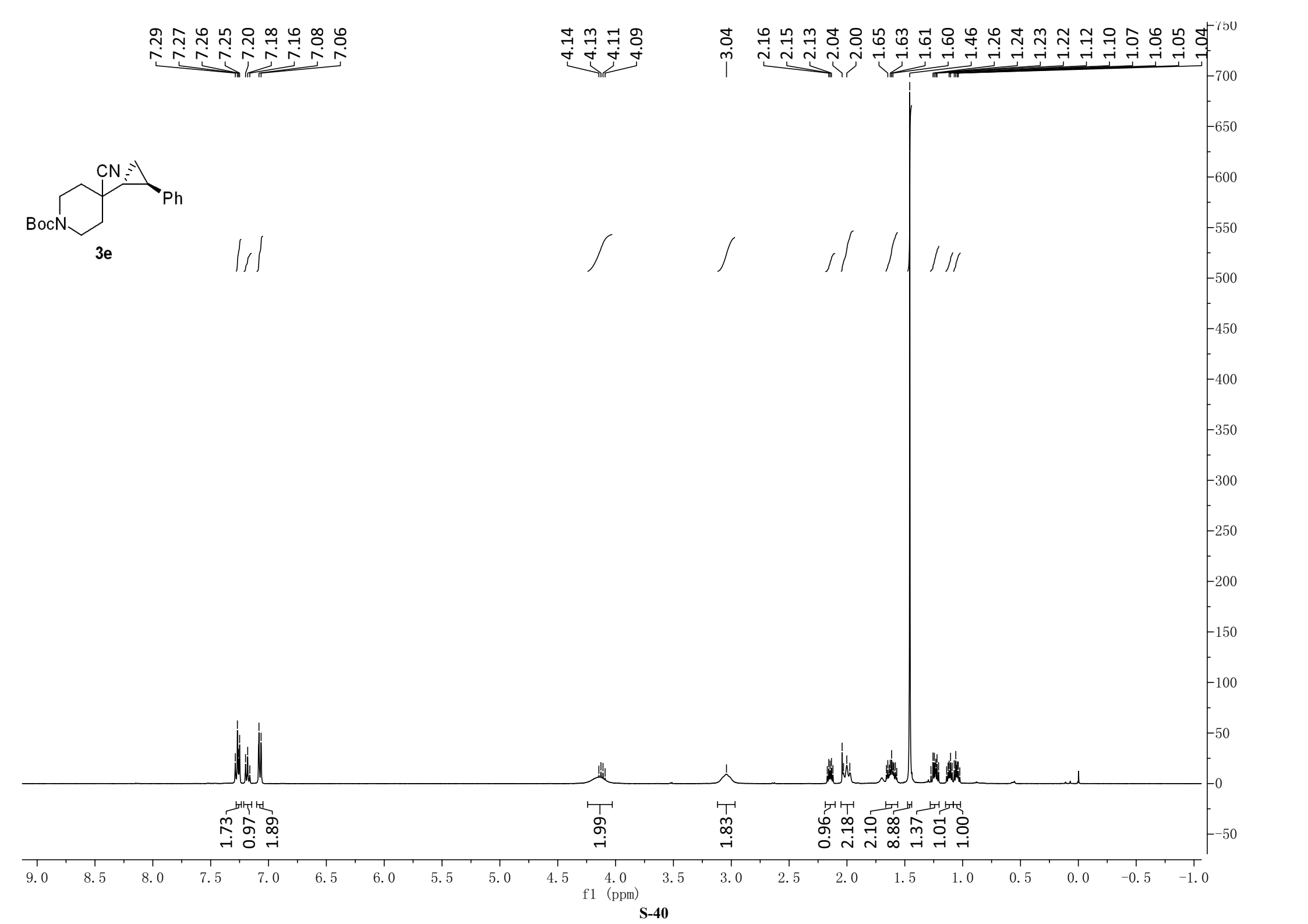


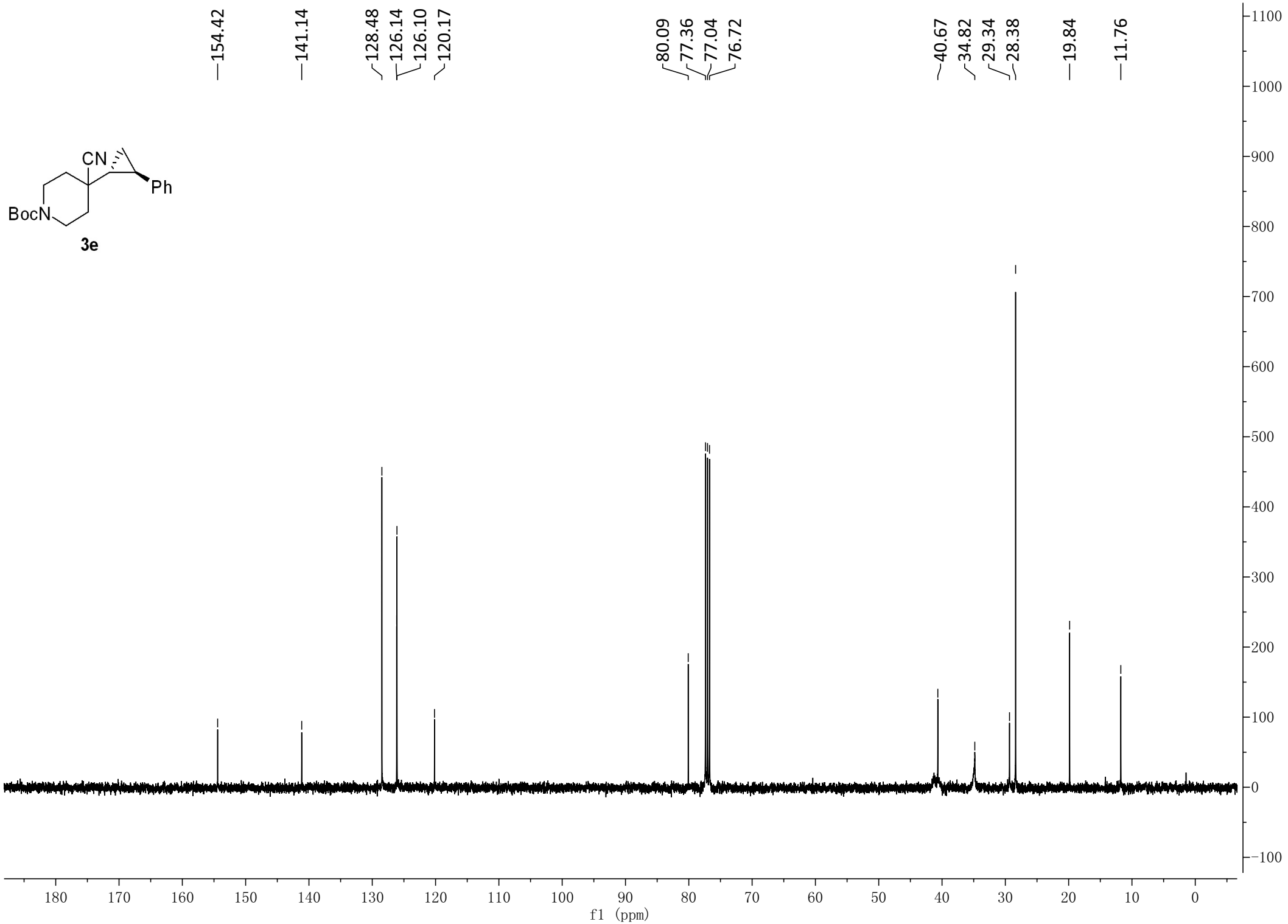
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	14.758	18673299	1088382	93.951	95.220
2	19.017	1202212	54632	6.049	4.780
Total		19875511	1143014	100.000	100.000

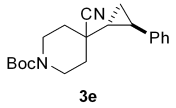

7.29
7.27
7.26
7.25
7.20
7.18
7.16
7.08
7.06
4.14
4.13
4.11
4.09
3.04
2.16
2.15
2.13
2.04
2.00
1.65
1.63
1.61
1.60
1.46
1.26
1.24
1.23
1.22
1.12
1.10
1.07
1.06
1.05
1.04
CN
Ph
BocN
3e
1.73
0.97
1.89
1.99
1.83
0.96
2.18
2.10
8.88
1.37
1.01
1.00
f1 (ppm)


154.42
141.14
128.48
126.14
126.10
120.17
80.09
77.36
77.04
76.72
40.67
34.82
29.34
28.38
19.84
11.76
CN
Ph
BocN
3e
f1 (ppm)

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-5-104A-ID.lcd

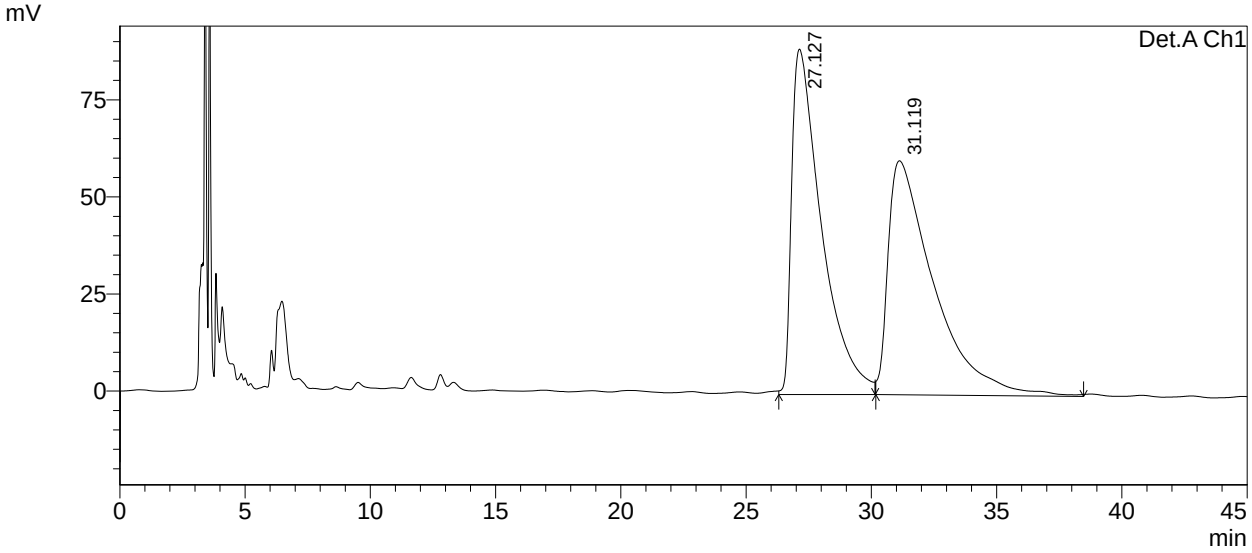
Acquired by	: Admin
Sample Name	: JGP-5-104A
Sample ID	: ID,99/1,1,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-5-104A-ID.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2017-3-2 10:03:53
Data Processed	: 2017-3-2 10:49:38



3e

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-5-104A-ID.lcd



1 Det.A Ch1/214nm

PeakTable

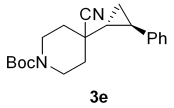
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	27.127	7372052	88944	49.148	59.616
2	31.119	7627774	60251	50.852	40.384
Total		14999827	149195	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-7A-1.lcd

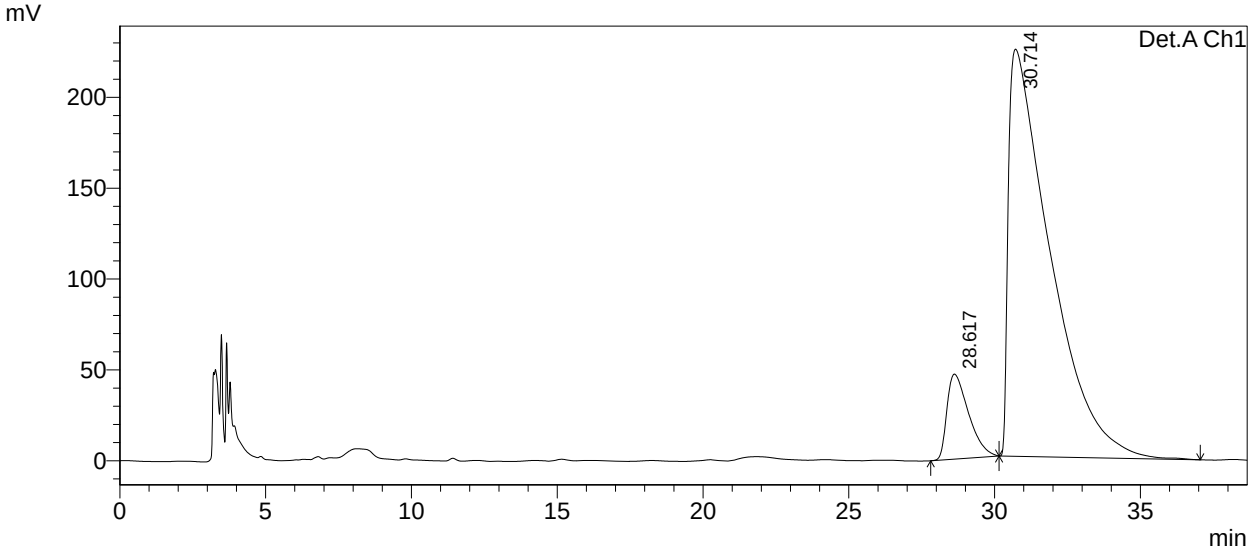
Acquired by	: Admin
Sample Name	: JGP-15-7A-1
Sample ID	: ID,99/1,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-7A-1.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-7 8:02:49
Data Processed	: 2018-5-14 15:45:31



3e

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-7A-1.lcd

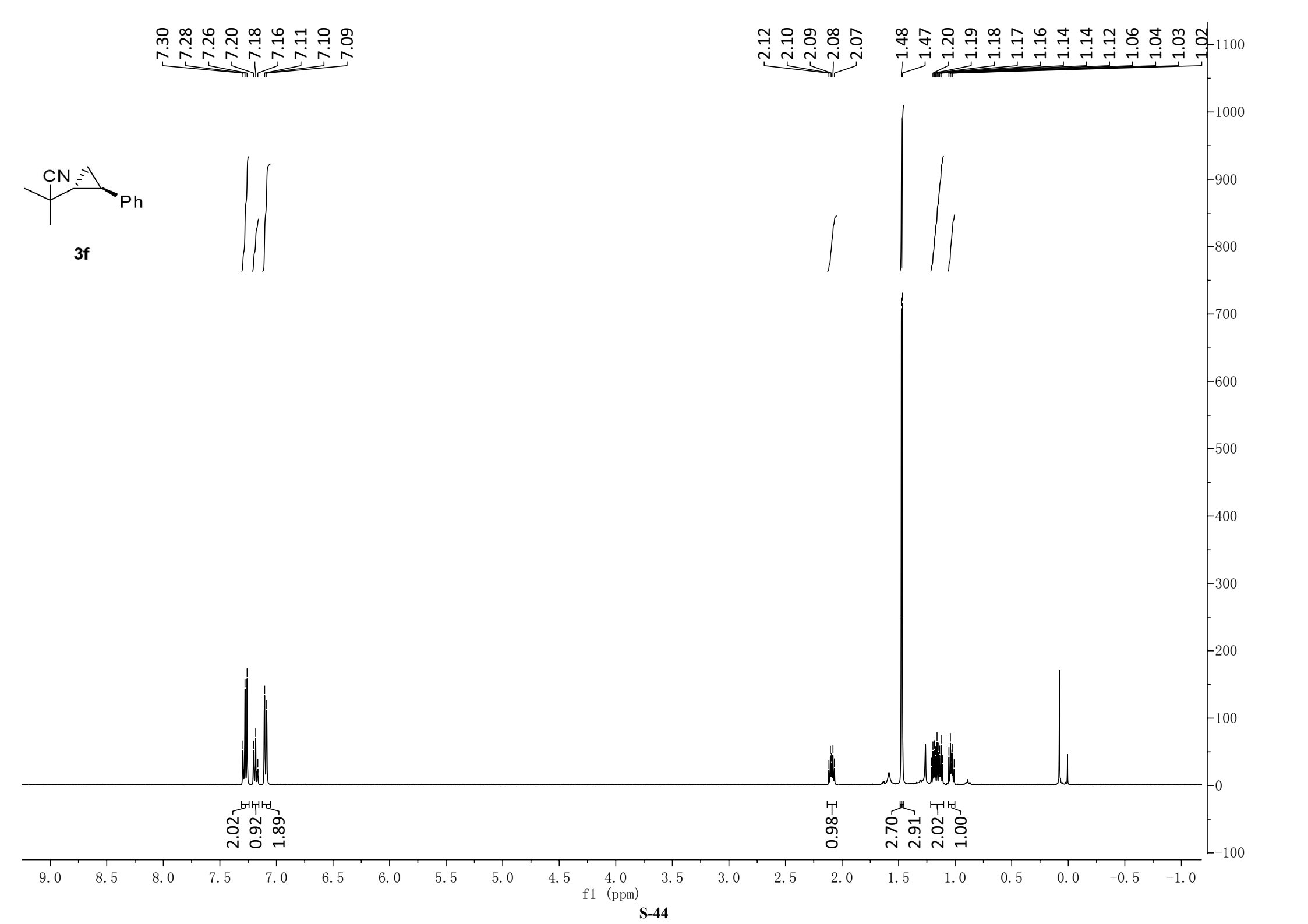


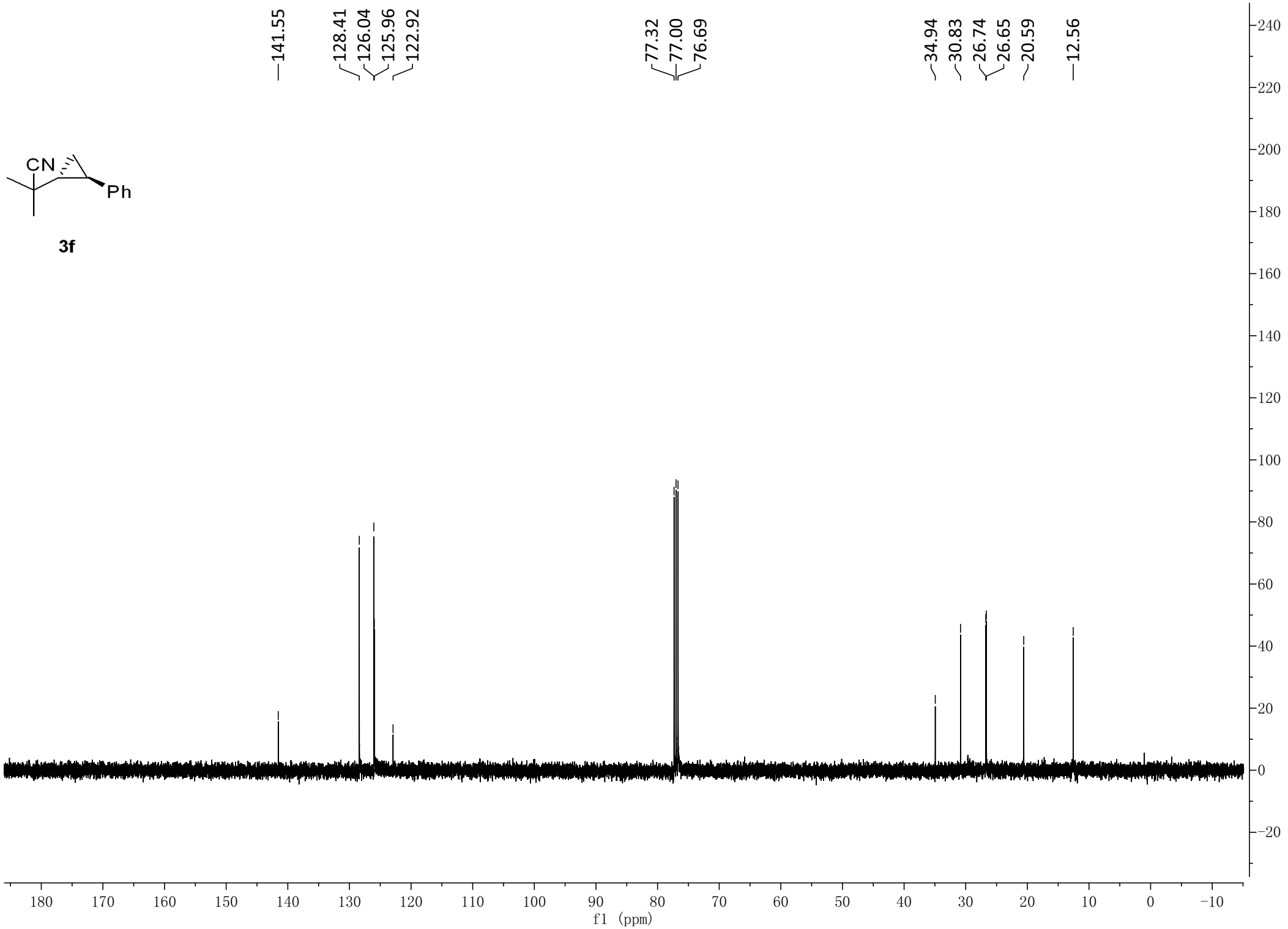
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	28.617	2411461	46793	9.772	17.272
2	30.714	22265609	224125	90.228	82.728
Total		24677070	270918	100.000	100.000

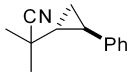

7.30
7.28
7.26
7.20
7.18
7.16
7.11
7.10
7.09
2.12
2.10
2.09
2.08
2.07
1.48
1.47
1.20
1.19
1.18
1.17
1.16
1.14
1.14
1.12
1.06
1.04
1.03
1.02
CN
Ph
3f
2.02
0.92
1.89
0.98
2.70
2.91
2.02
1.00
f1 (ppm)


141.55
128.41
126.04
125.96
122.92
77.32
77.00
76.69
34.94
30.83
26.74
26.65
20.59
12.56
CN
Ph
3f
f1 (ppm)

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-14-69A-RAC-7.lcd

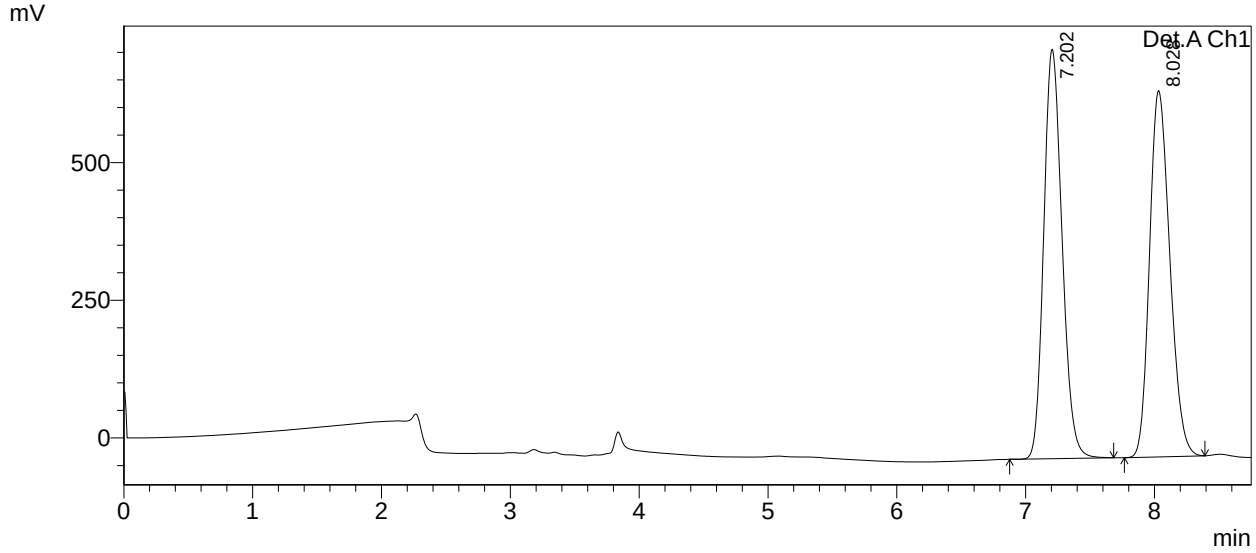
Acquired by	: Admin
Sample Name	: JGP-14-69A-RAC-7
Sample ID	: OD-H,99/1,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-14-69A-RAC-7.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-3-30 12:34:37
Data Processed	: 2018-3-30 12:43:23



3f

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-14-69A-RAC-7.lcd



1 Det.A Ch1/214nm

PeakTable

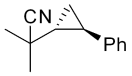
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.202	7367364	743604	50.263	52.776
2	8.028	7290343	665378	49.737	47.224
Total		14657707	1408982	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-2A-1.lcd

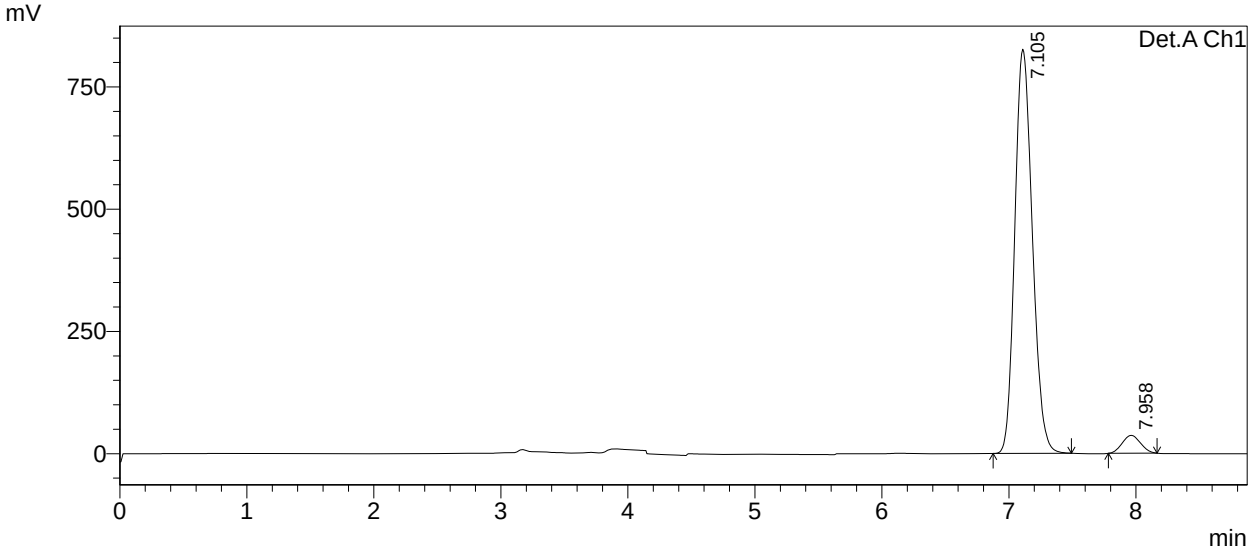
Acquired by	: Admin
Sample Name	: JGP-15-2A-1
Sample ID	: OD-H,99/1,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-2A-1.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-4-28 11:40:43
Data Processed	: 2018-5-14 14:13:38



3f

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-2A-1.lcd

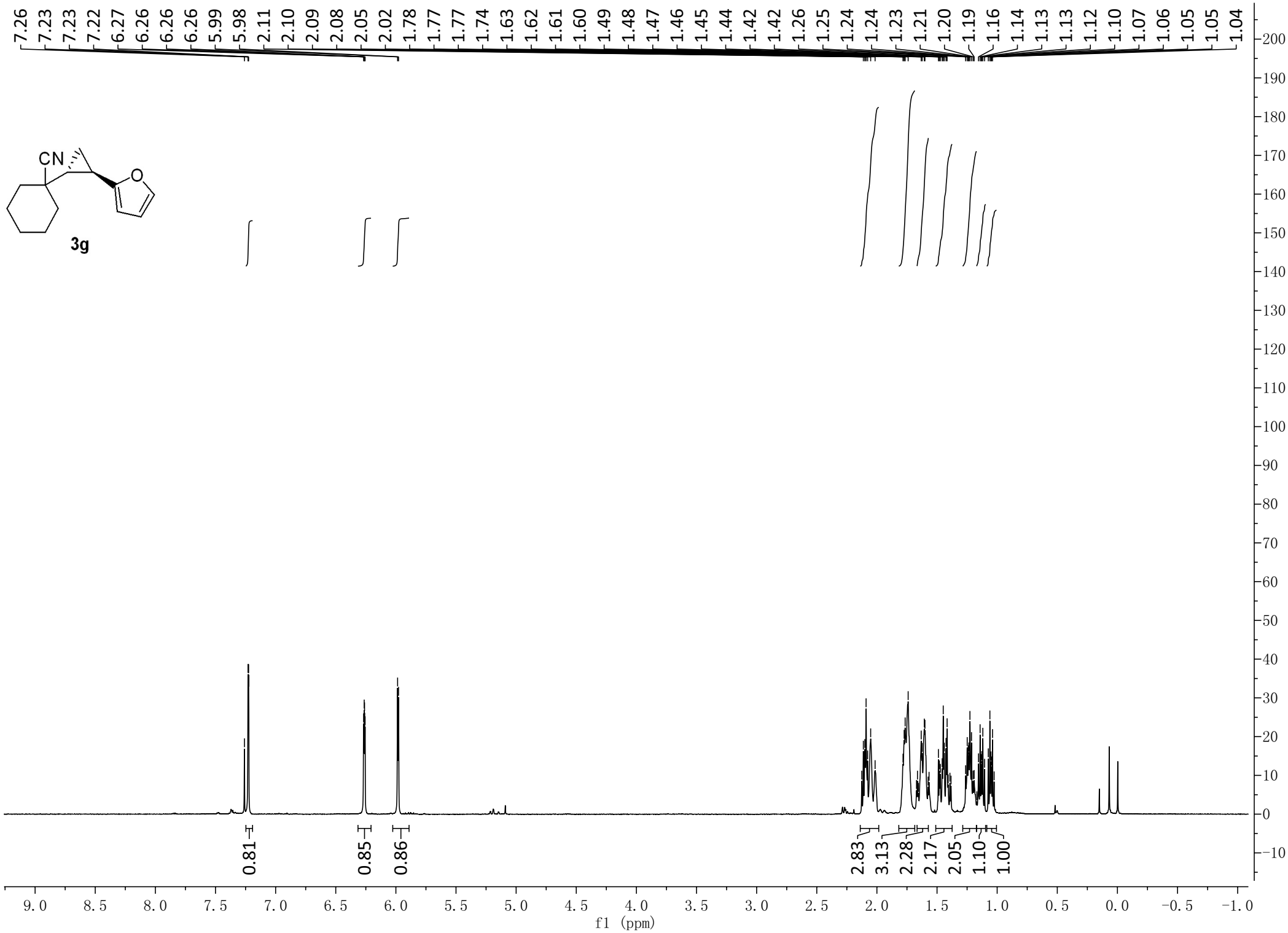


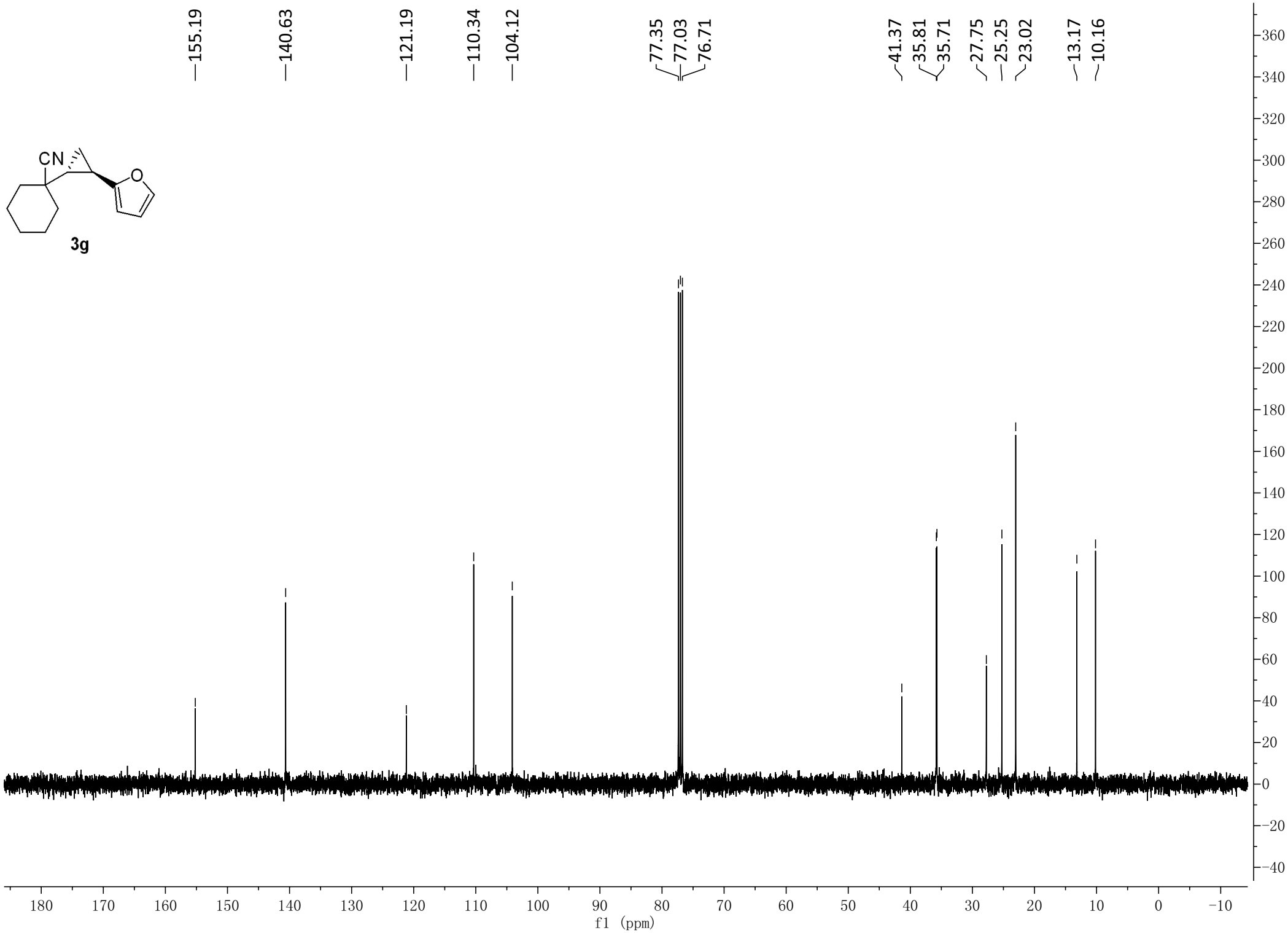
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.105	7945516	826765	95.576	95.752
2	7.958	367810	36676	4.424	4.248
Total		8313326	863441	100.000	100.000

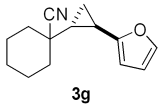

7.26 7.23 7.23 7.22 6.27 6.26 6.26 6.26 5.99 5.98 2.11 2.10 2.09 2.08 2.05 2.02 1.78 1.77 1.77 1.74 1.63 1.62 1.61 1.60 1.49 1.48 1.47 1.46 1.45 1.44 1.42 1.42 1.26 1.25 1.24 1.24 1.23 1.21 1.20 1.19 1.16 1.14 1.13 1.13 1.12 1.10 1.07 1.06 1.05 1.05 1.04
CN
O
3g
0.81
0.85
0.86
2.83
3.13
2.28
2.17
2.05
1.10
1.00
f1 (ppm)


155.19
140.63
121.19
110.34
104.12
77.35
77.03
76.71
41.37
35.81
35.71
27.75
25.25
23.02
13.17
10.16
CN
O
3g
f1 (ppm)

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

G:\JGP-17-24A-RAC-1.lcd

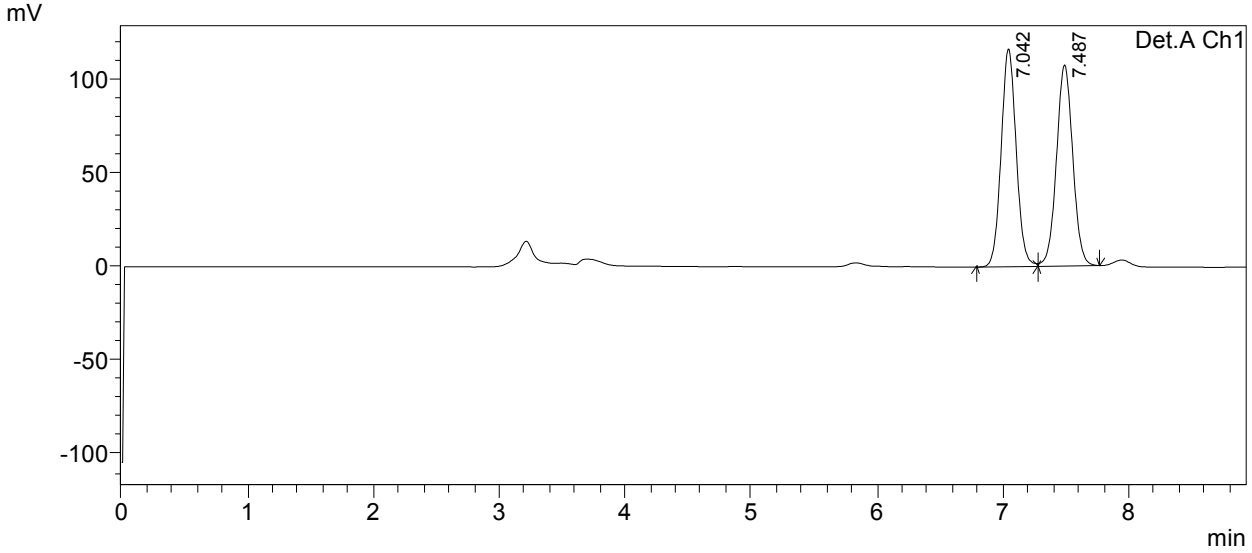
Acquired by	: Admin
Sample Name	: JGP-17-24A-RAC-1
Sample ID	: OJ-H,98/2,1,215
Vail #	:
Injection Volume	: 1 uL
Data File Name	: JGP-17-24A-RAC-1.lcd
Method File Name	: 1.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-11-20 18:01:53
Data Processed	: 2018-11-20 18:10:51



3g

<Chromatogram>

G:\JGP-17-24A-RAC-1.lcd



1 Det.A Ch1/215nm

PeakTable

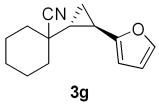
Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.042	968854	116345	50.024	51.943
2	7.487	967942	107641	49.976	48.057
Total		1936796	223986	100.000	100.000

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

G:\JGP-17-24A-1.lcd : Admin

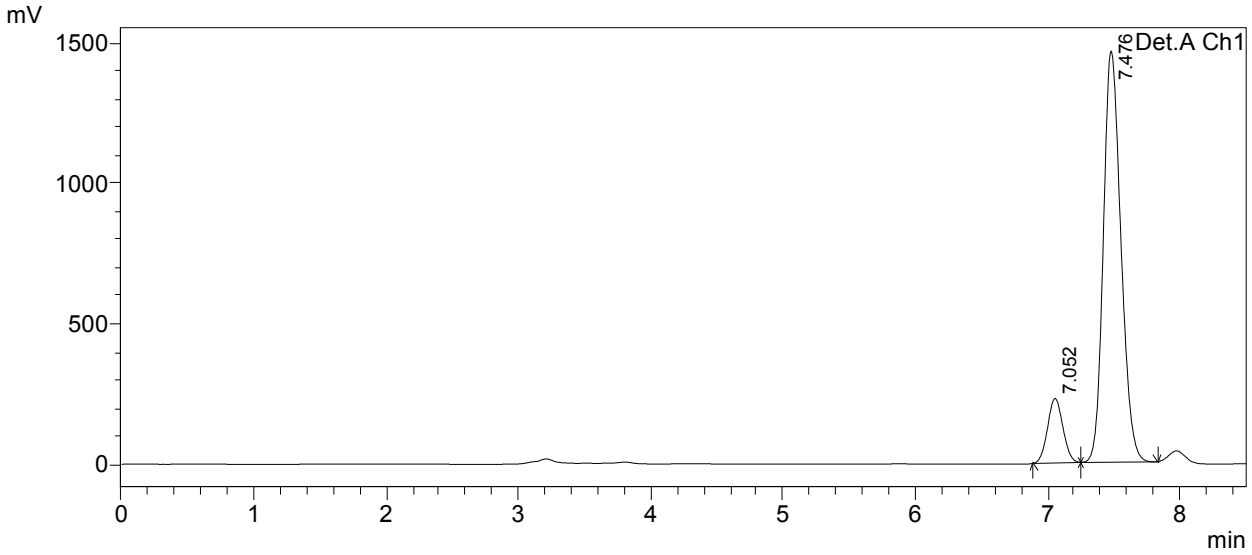
Acquired by	: JGP-17-24A-1
Sample Name	: OJ-H,98/2,1,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-24A-1.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-11-20 18:14:27
Data Acquired	: 2018-11-26 18:53:51
Data Processed	



3g

<Chromatogram>

G:\JGP-17-24A-1.lcd

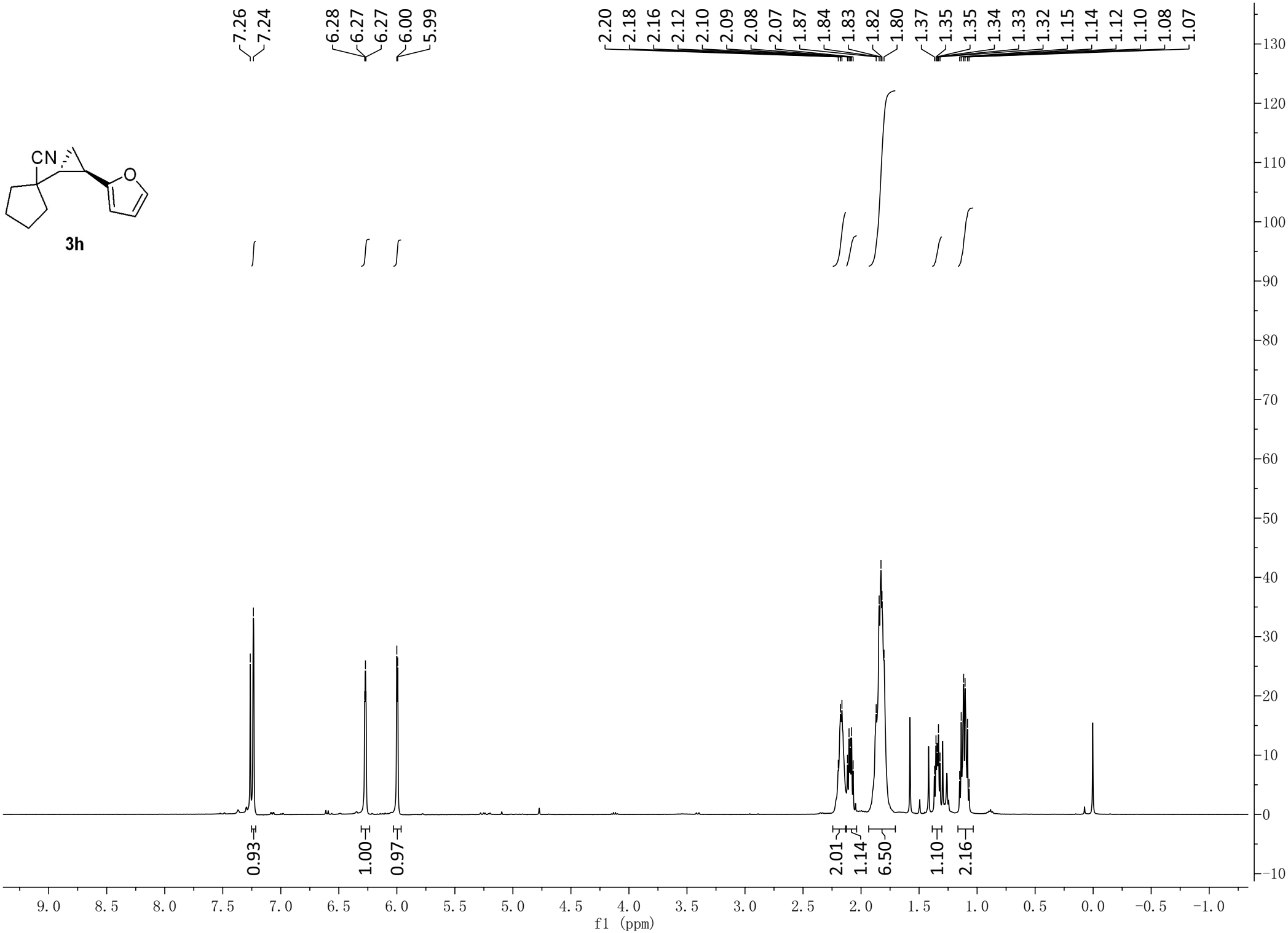


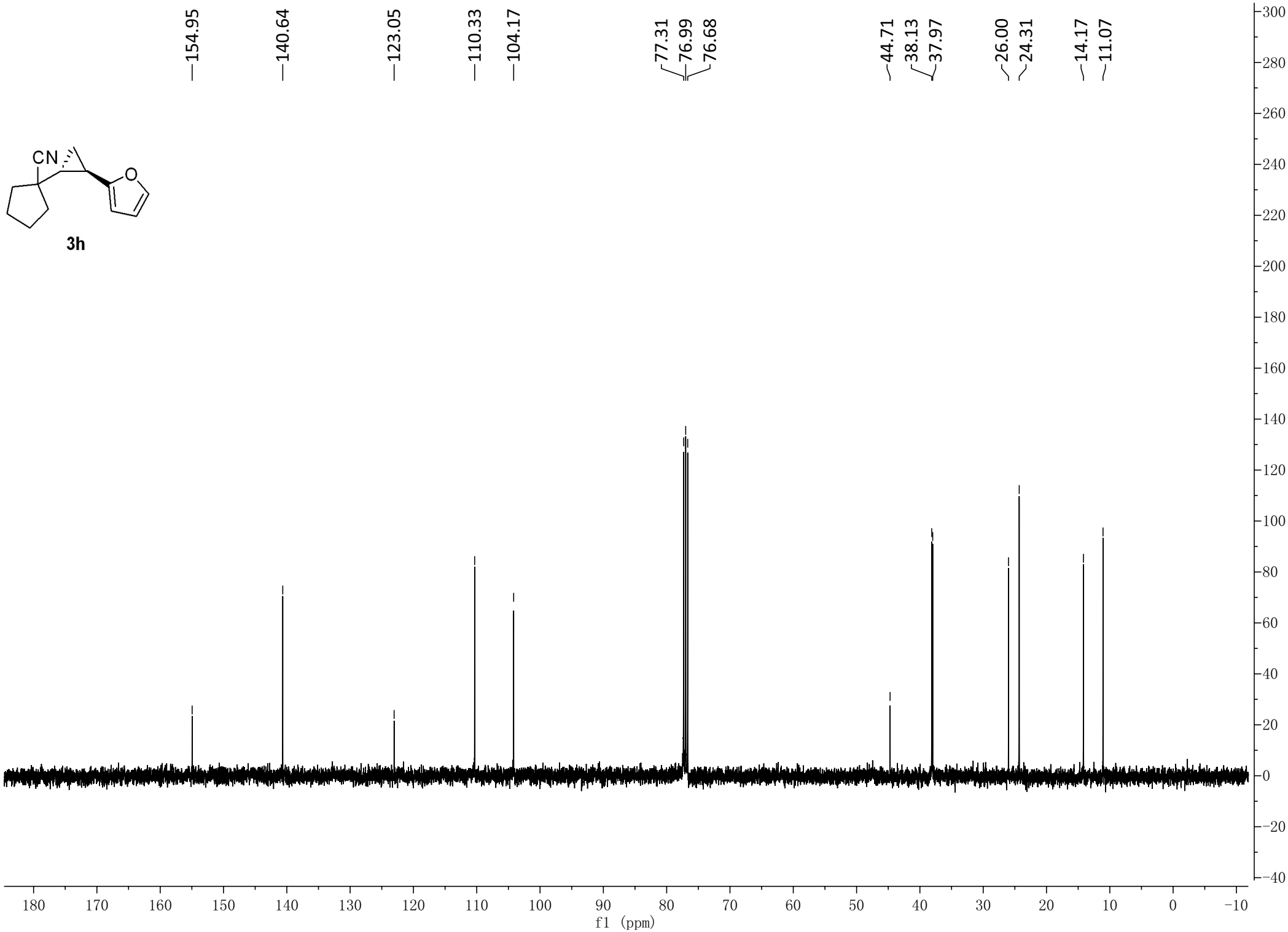
1 Det.A Ch1/215nm

PeakTable

Detector A Ch1 215nm

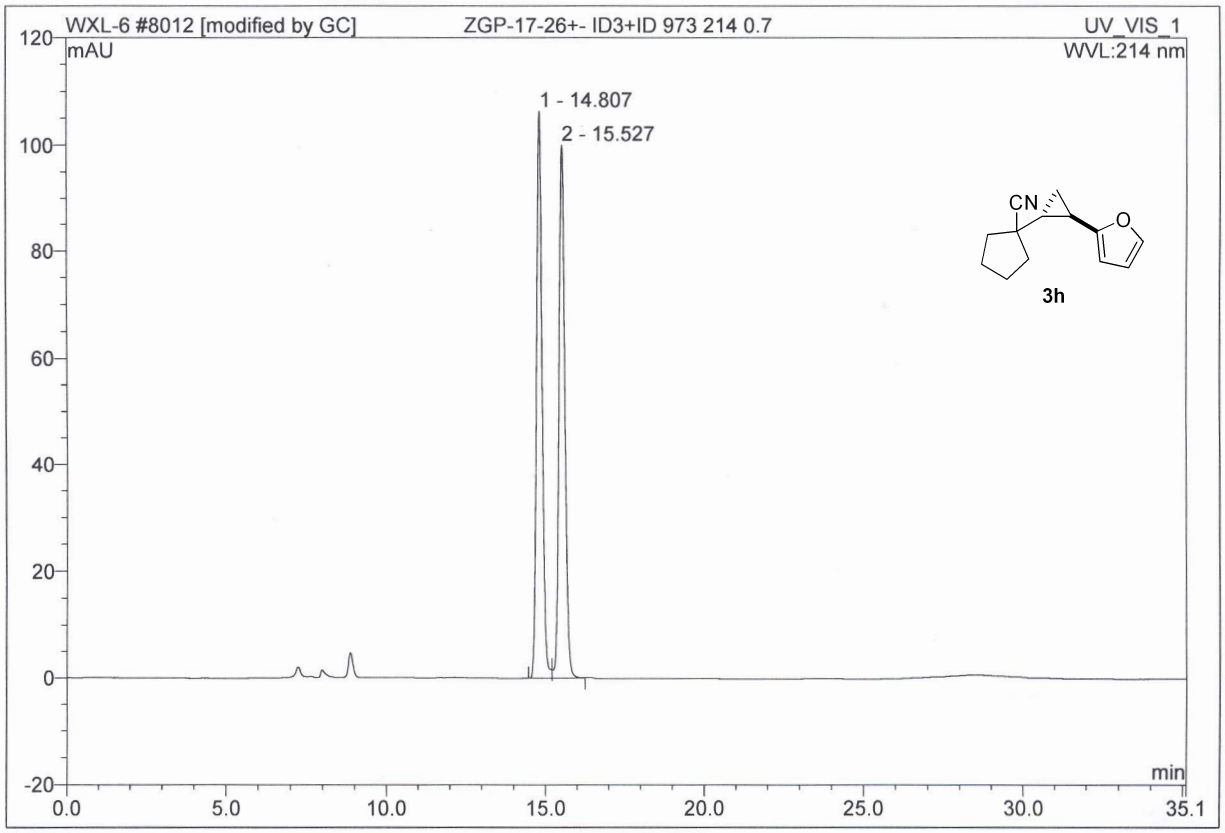
Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.052	1844962	229906	12.013	13.571
2	7.476	13512929	1464149	87.987	86.429
Total		15357891	1694054	100.000	100.000


7.26
7.24
6.28
6.27
6.27
6.00
5.99
2.20
2.18
2.16
2.12
2.10
2.09
2.08
2.07
1.87
1.84
1.83
1.82
1.80
1.37
1.35
1.35
1.34
1.33
1.32
1.15
1.14
1.12
1.10
1.08
1.07
CN
O
3h
0.93
1.00
0.97
2.01
1.14
6.50
1.10
2.16
f1 (ppm)


154.95
140.64
123.05
110.33
104.17
77.31
76.99
76.68
44.71
38.13
37.97
26.00
24.31
14.17
11.07
CN
O
3h
f1 (ppm)

8012 ZGP-17-26+- ID3+ID 973 214 0.7

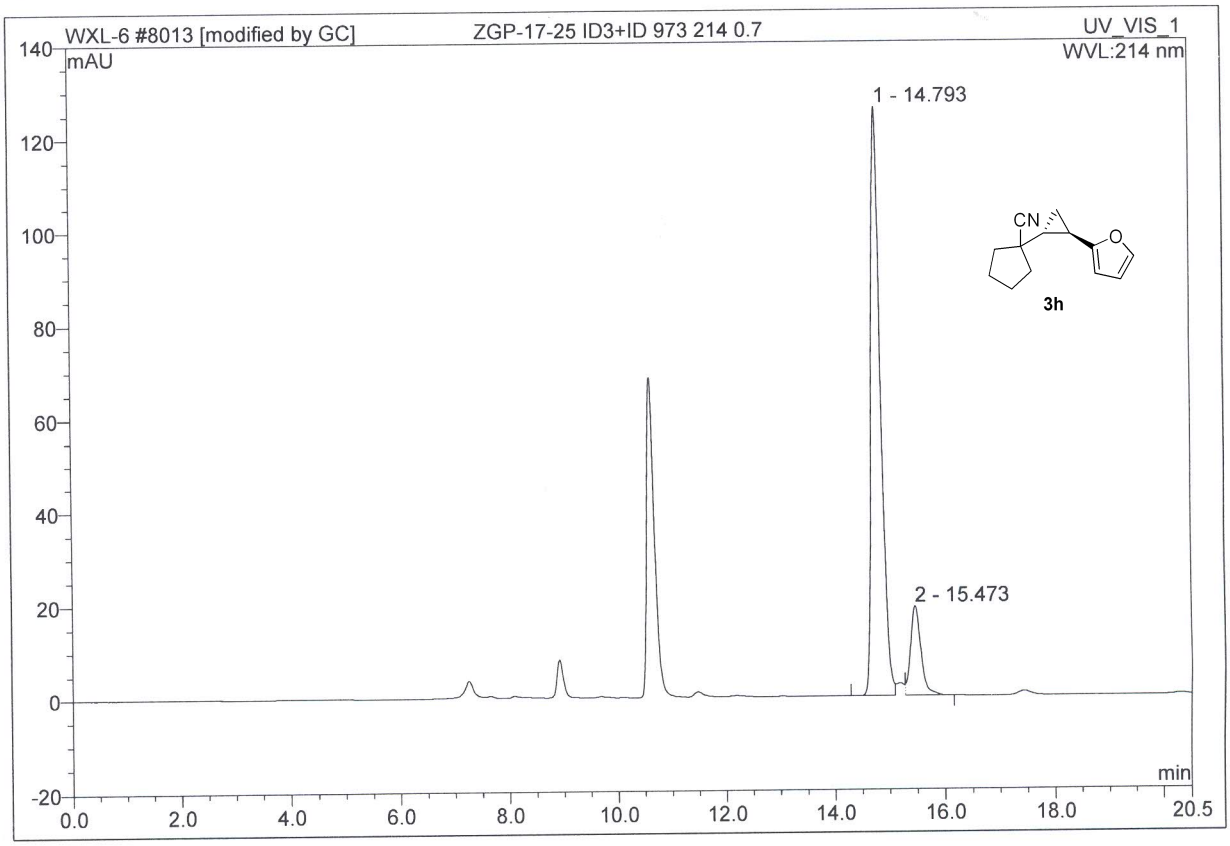
Sample Name:	**ZGP-17-26+- ID3+ID 973 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**GD4**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**201701-4**	*Bandwidth:*	**n.a.**
Quantif. Method:	**201701**	*Dilution Factor:*	**1.0000**
Recording Time:	**2018/11/29 15:01**	*Sample Weight:*	**1.0000**
Run Time (min):	**35.11**	*Sample Amount:*	**1.0000**



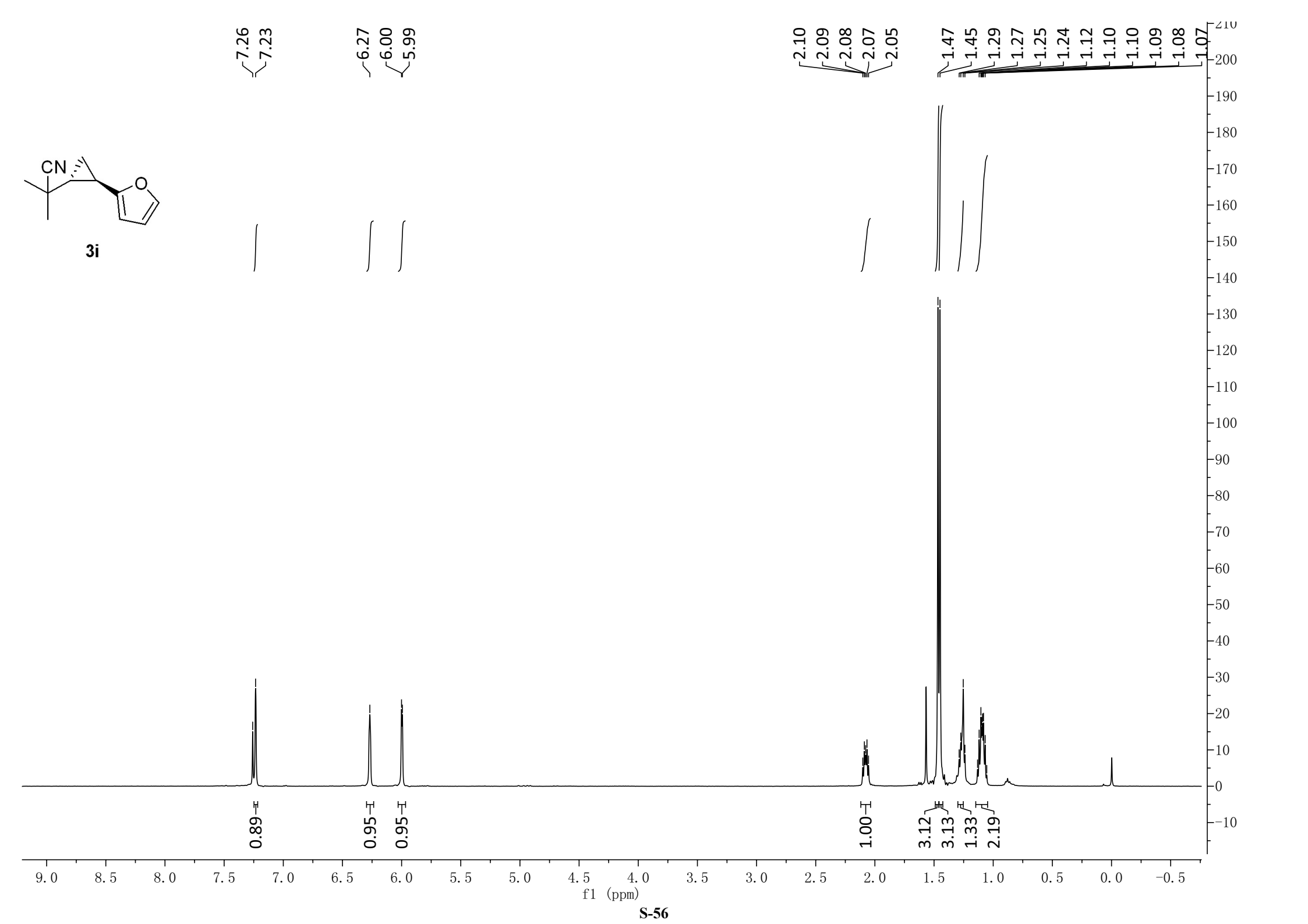
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	14.81	n.a.	106.352	21.831	50.16	n.a.	BM *
2	15.53	n.a.	100.049	21.696	49.84	n.a.	MB*
Total:			206.401	43.526	100.00	0.000	

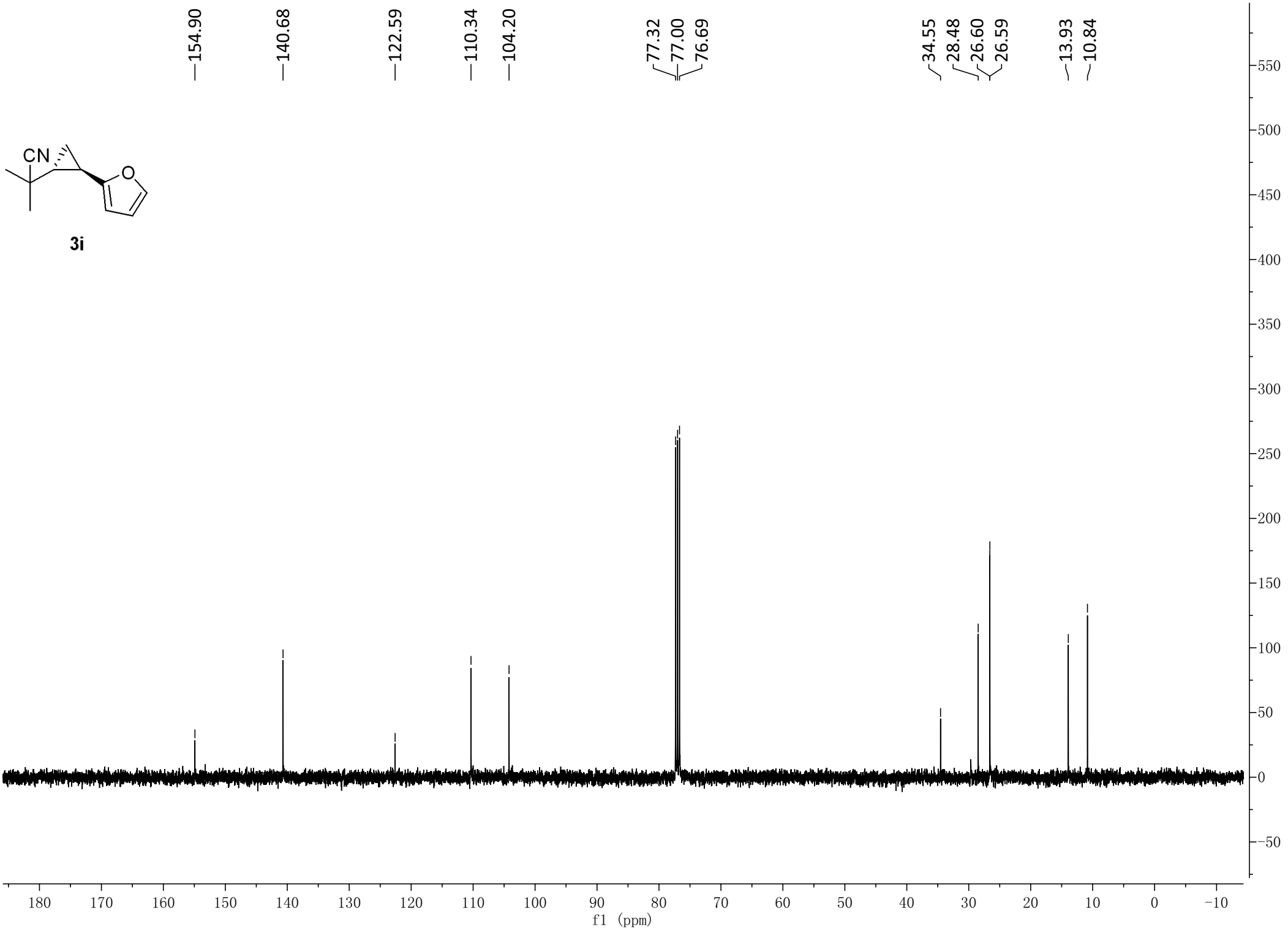
8013 ZGP-17-25 ID3+ID 973 214 0.7

Sample Name:	**ZGP-17-25 ID3+ID 973 214 0.7**	*Injection Volume:*	**2.0**
Vial Number:	**GD5**	*Channel:*	**UV_VIS_1**
Sample Type:	**unknown**	*Wavelength:*	**214**
Control Program:	**201701-4**	*Bandwidth:*	**n.a.**
Quantif. Method:	**201701**	*Dilution Factor:*	**1.0000**
Recording Time:	**2018/11/29 14:39**	*Sample Weight:*	**1.0000**
Run Time (min):	**20.52**	*Sample Amount:*	**1.0000**



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	14.79	n.a.	126.121	25.376	85.95	n.a.	BM *
2	15.47	n.a.	18.995	4.148	14.05	n.a.	MB*
Total:			145.115	29.524	100.00	0.000	

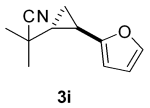

7.26
7.23
6.27
6.00
5.99
2.10
2.09
2.08
2.07
2.05
1.47
1.45
1.29
1.27
1.25
1.24
1.12
1.10
1.10
1.09
1.08
1.07
CN
O
3i
0.89
0.95
0.95
1.00
3.12
3.13
1.33
2.19
f1 (ppm)


154.90
140.68
122.59
110.34
104.20
77.32
77.00
76.69
34.55
28.48
26.60
26.59
13.93
10.84
CN
O
3i
f1 (ppm)

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-12A-8.lcd

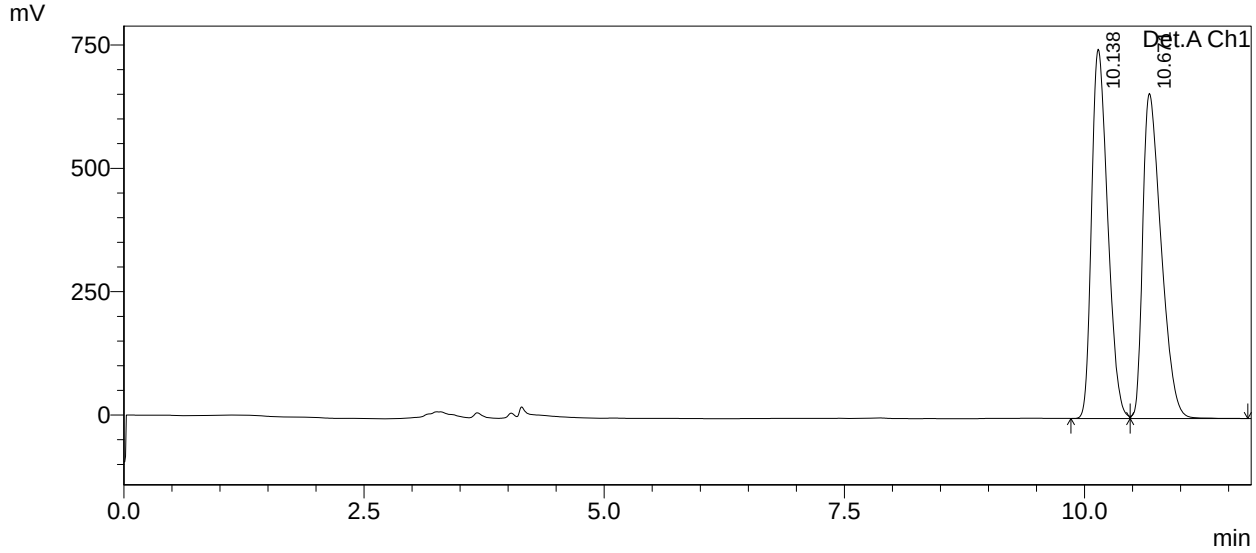
Acquired by	: Admin
Sample Name	: JGP-15-12A-8
Sample ID	: IE,99/1,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-12A-8.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-7 13:45:56
Data Processed	: 2018-5-7 13:57:40



3i

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-12A-8.lcd



1 Det.A Ch1/214nm

PeakTable

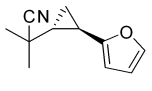
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.138	8728785	748448	49.877	53.187
2	10.671	8771857	658758	50.123	46.813
Total		17500642	1407207	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-16A-1.lcd

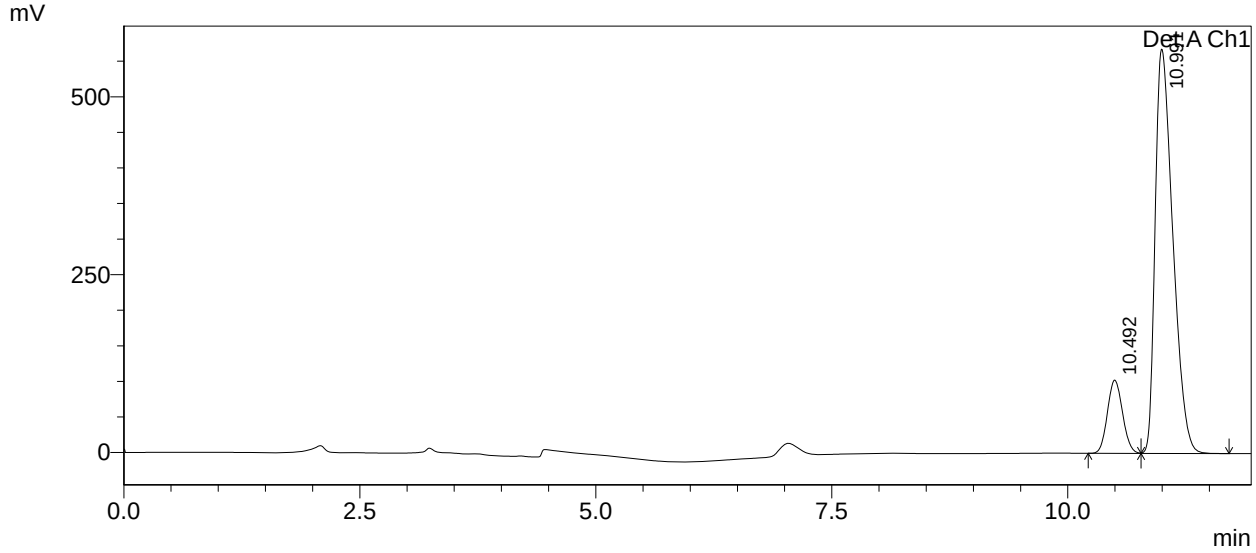
Acquired by	: Admin
Sample Name	: JGP-15-16A-1
Sample ID	: IE,99/1,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-16A-1.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-7 17:21:47
Data Processed	: 2018-5-19 8:38:26



3i

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-16A-1.lcd

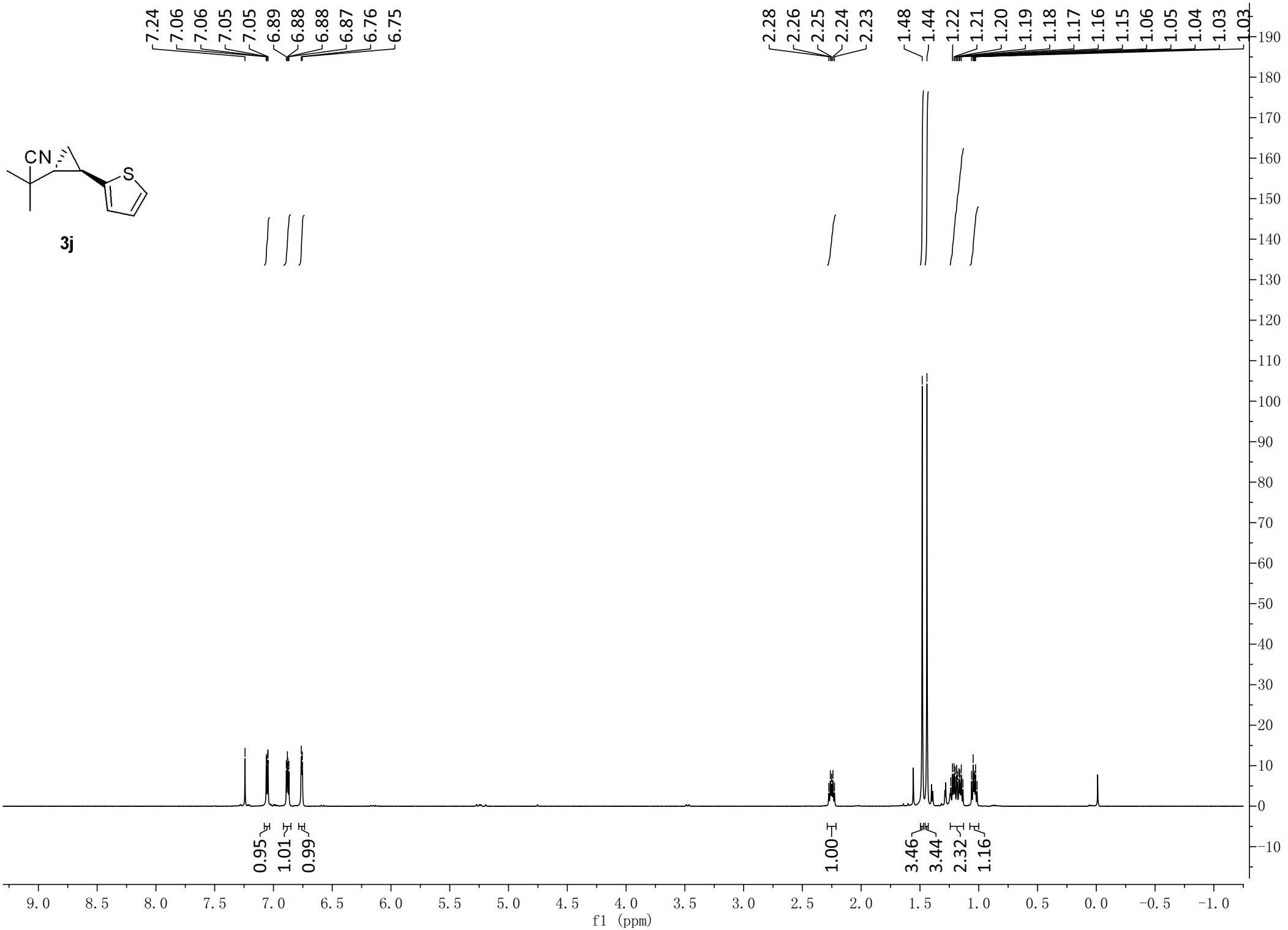


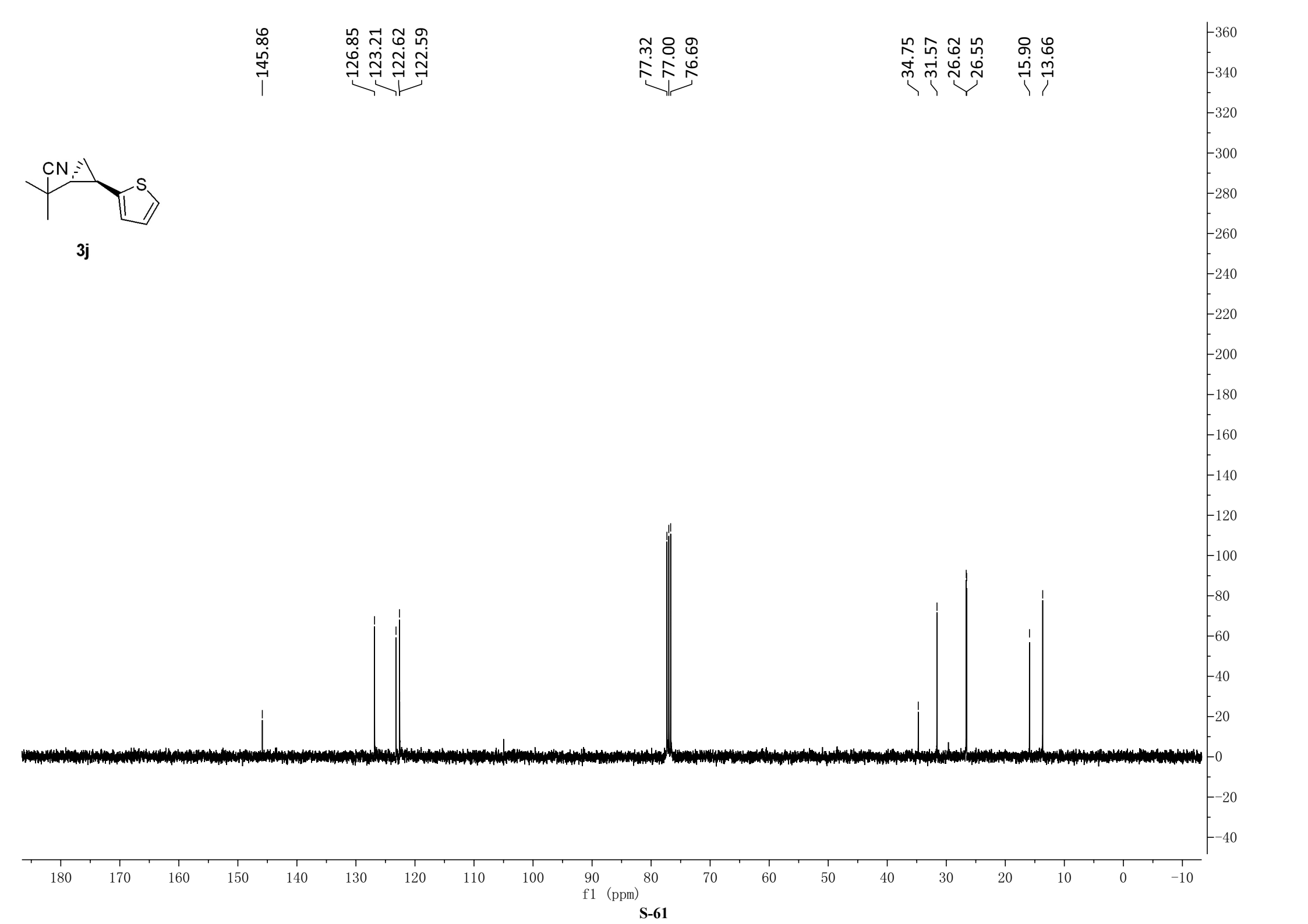
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.492	1149276	102930	13.428	15.333
2	10.991	7409833	568377	86.572	84.667
Total		8559109	671306	100.000	100.000

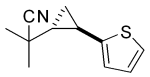

7.24
7.06
7.06
7.05
7.05
6.89
6.88
6.88
6.87
6.76
6.75
2.28
2.26
2.25
2.24
2.23
1.48
1.44
1.22
1.21
1.20
1.19
1.18
1.17
1.16
1.15
1.06
1.05
1.04
1.03
1.03
CN
S
3j
0.95
1.01
0.99
1.00
3.46
3.44
2.32
1.16
f1 (ppm)


145.86
126.85
123.21
122.62
122.59
77.32
77.00
76.69
34.75
31.57
26.62
26.55
15.90
13.66
CN
S
3j
f1 (ppm)

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

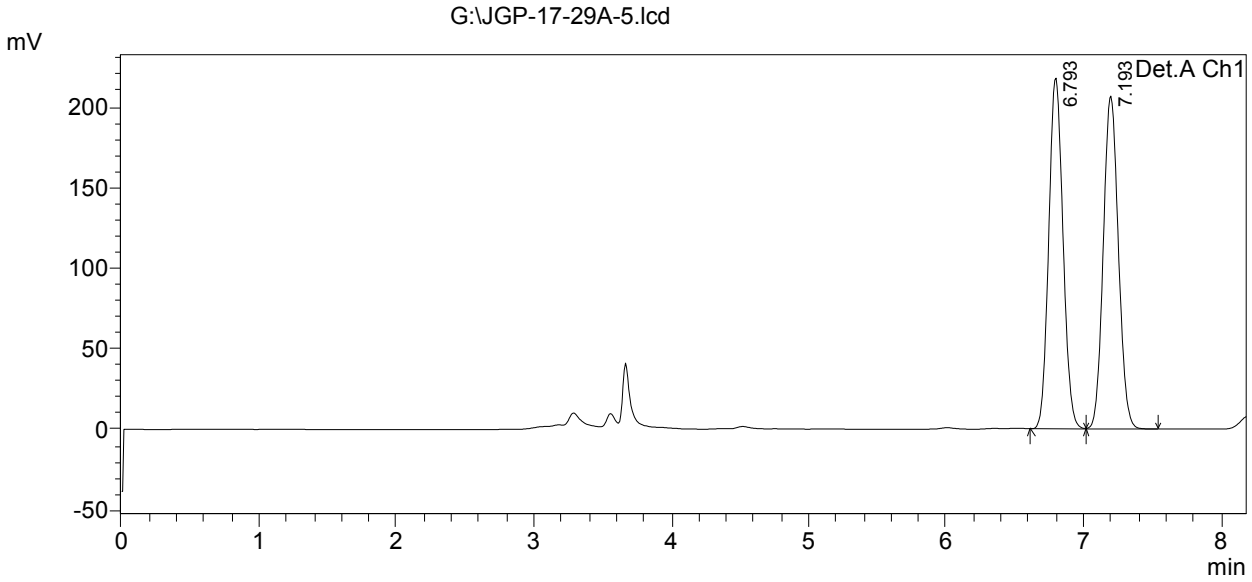
G:\JGP-17-29A-5.lcd : Admin

Acquired by	: JGP-17-29A-5
Sample Name	: IC,98/2,1,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-29A-5.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-11-23 18:29:32
Data Acquired	: 2018-11-23 18:37:44
Data Processed	



3j

<Chromatogram>



1 Det.A Ch1/215nm

PeakTable

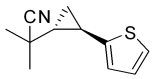
Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.793	1568309	217383	49.913	51.296
2	7.193	1573799	206398	50.087	48.704
Total		3142108	423781	100.000	100.000

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

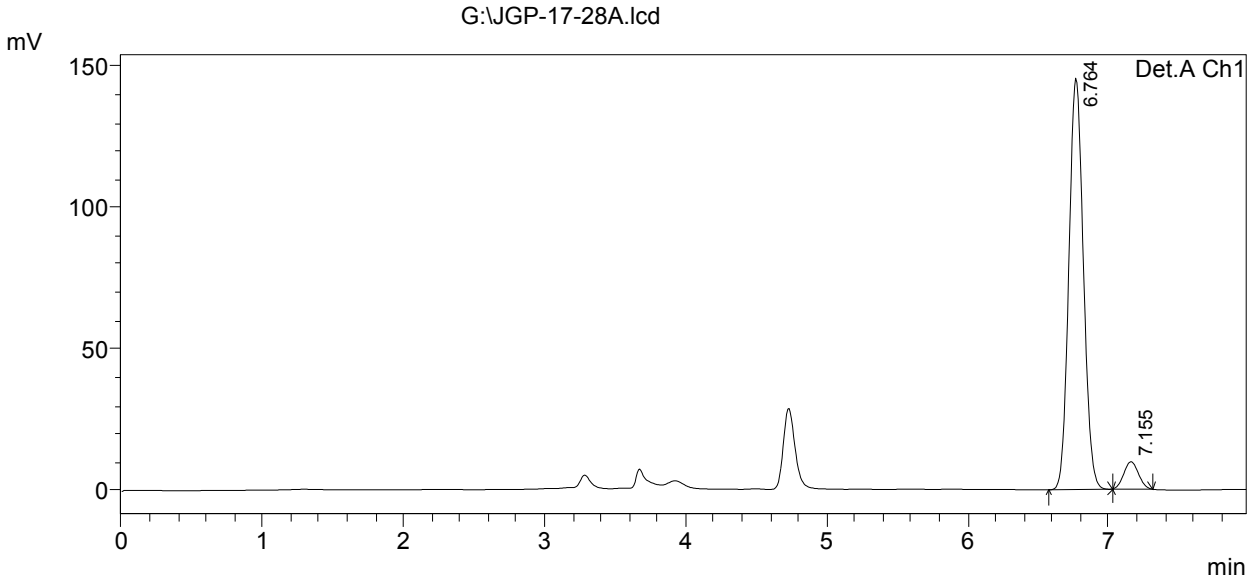
G:\JGP-17-28A.lcd : Admin

Acquired by	: JGP-17-28A
Sample Name	: IC,98/2,1,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-28A.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-11-23 18:40:07
Data Acquired	: 2018-11-26 19:01:46
Data Processed	



3j

<Chromatogram>

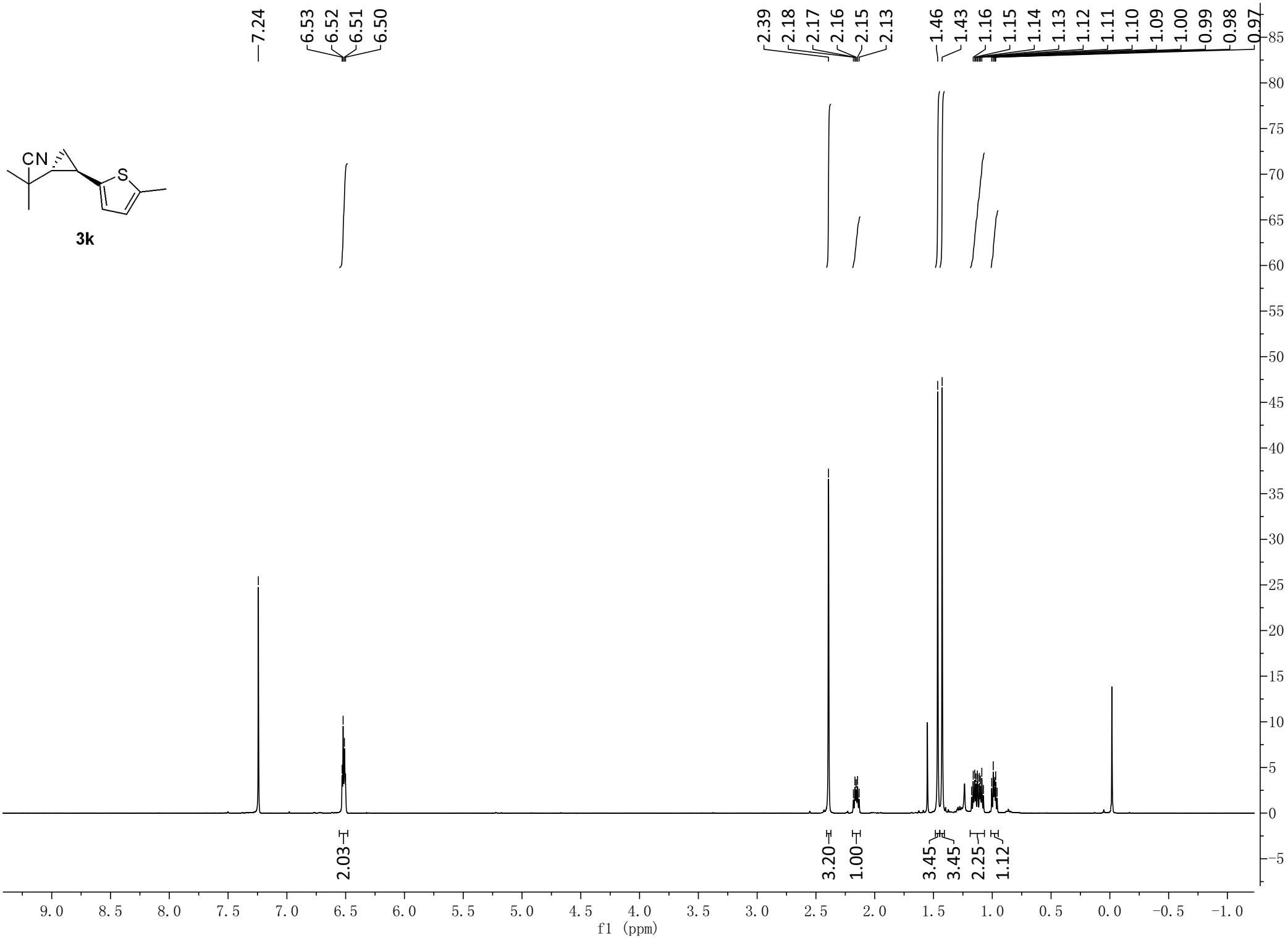


1 Det.A Ch1/215nm

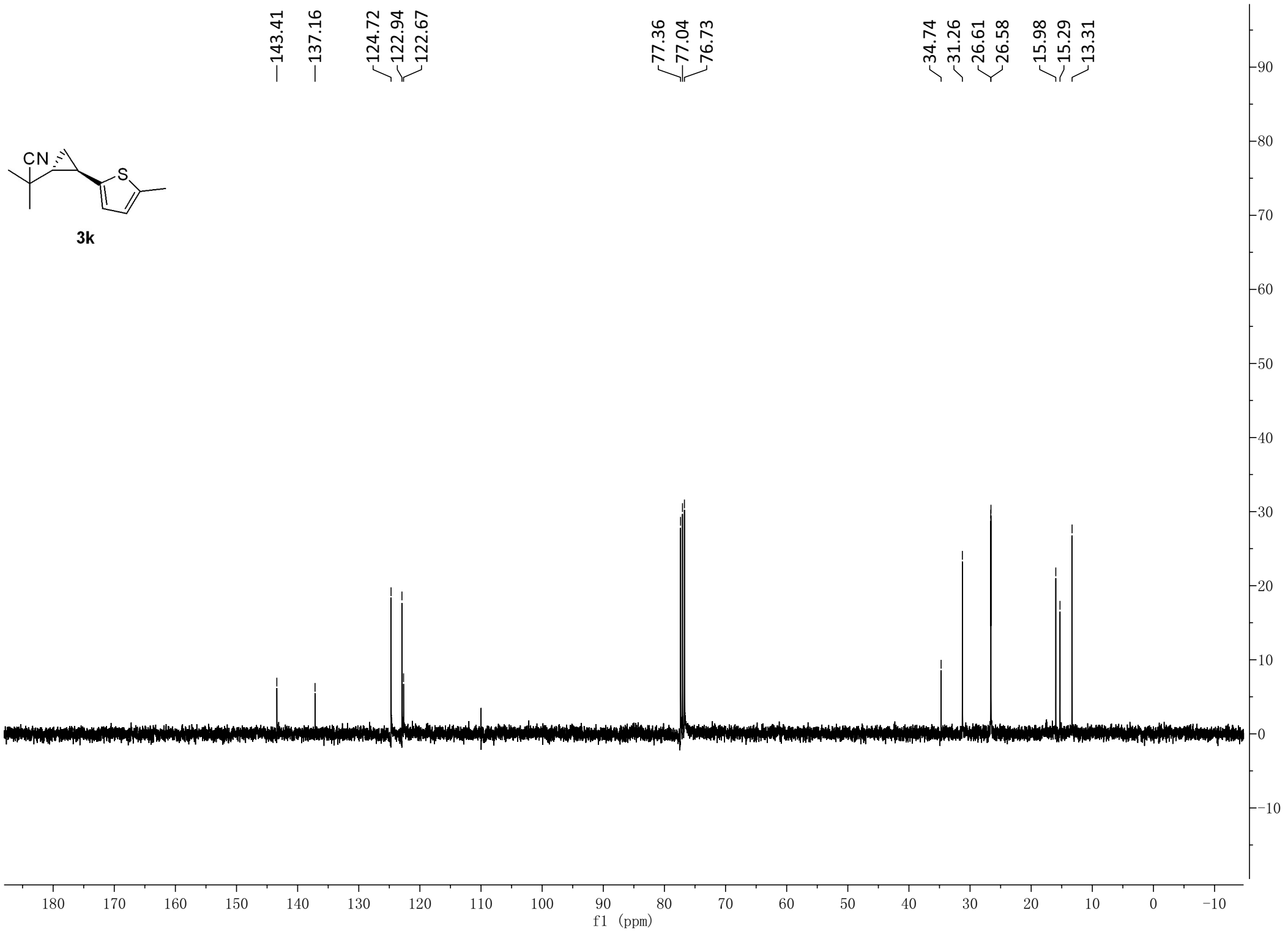
PeakTable

Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.764	1040563	145396	93.686	93.753
2	7.155	70134	9688	6.314	6.247
Total		1110697	155084	100.000	100.000


7.24
6.53
6.52
6.51
6.50
2.39
2.18
2.17
2.16
2.15
2.13
1.46
1.43
1.16
1.15
1.14
1.13
1.12
1.11
1.10
1.09
1.00
0.99
0.98
0.97
CN
S
2.03
3.20
1.00
3.45
3.45
2.25
1.12
f1 (ppm)

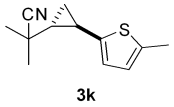
3k


143.41
137.16
124.72
122.94
122.67
77.36
77.04
76.73
34.74
31.26
26.61
26.58
15.98
15.29
13.31
CN
S
3k
f1 (ppm)

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

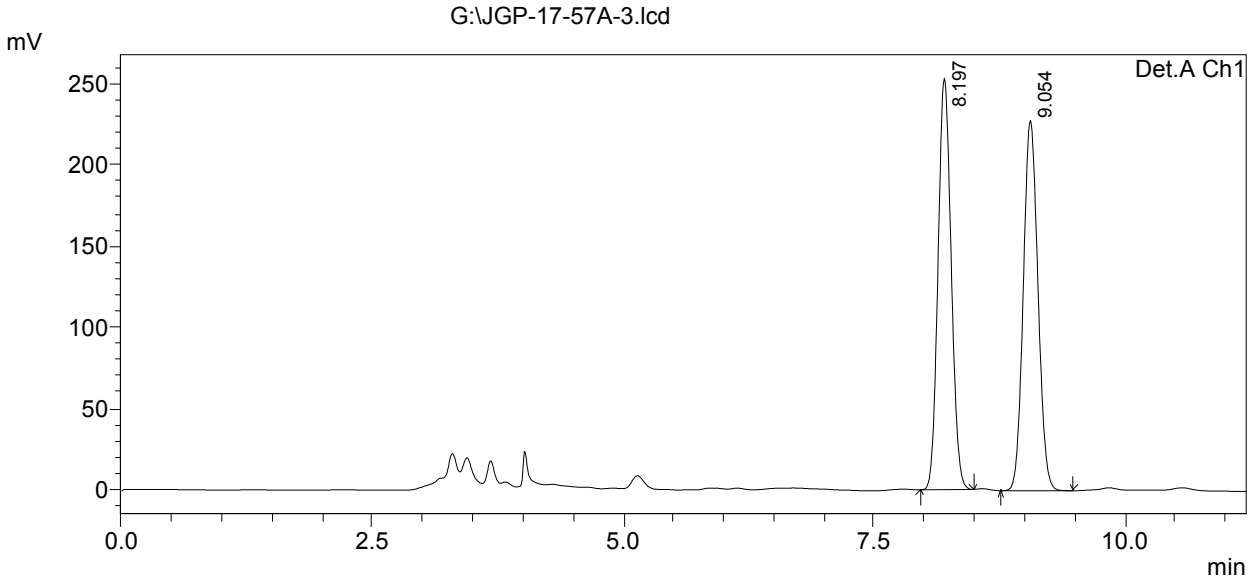
G:\JGP-17-57A-3.lcd : Admin

Acquired by	: JGP-17-57A-3
Sample Name	: IC,99/1,1.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-57A-3.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-13 8:45:19
Data Acquired	: 2018-12-13 8:56:32
Data Processed	



3k

<Chromatogram>



1 Det.A Ch1/215nm

PeakTable

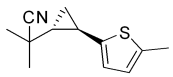
Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.197	2306416	253386	49.923	52.633
2	9.054	2313541	228037	50.077	47.367
Total		4619957	481423	100.000	100.000

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

G:\JGP-17-55A.lcd : Admin

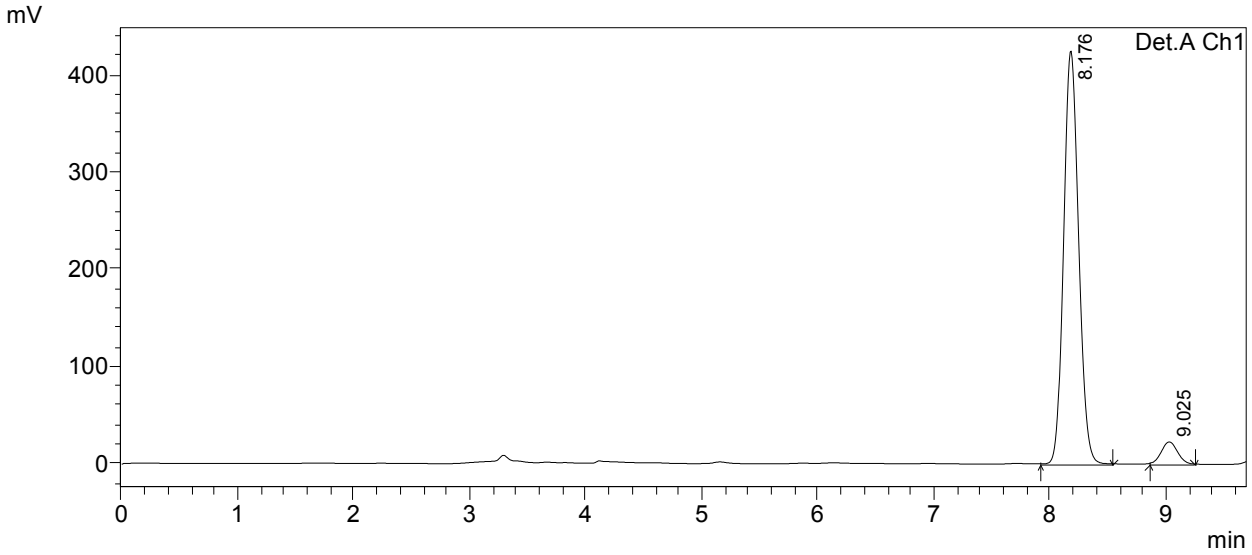
Acquired by	: JGP-17-55A
Sample Name	: IC,99/1,1.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-55A.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-13 8:57:21
Data Acquired	: 2018-12-29 14:42:58
Data Processed	



3k

<Chromatogram>

G:\JGP-17-55A.lcd

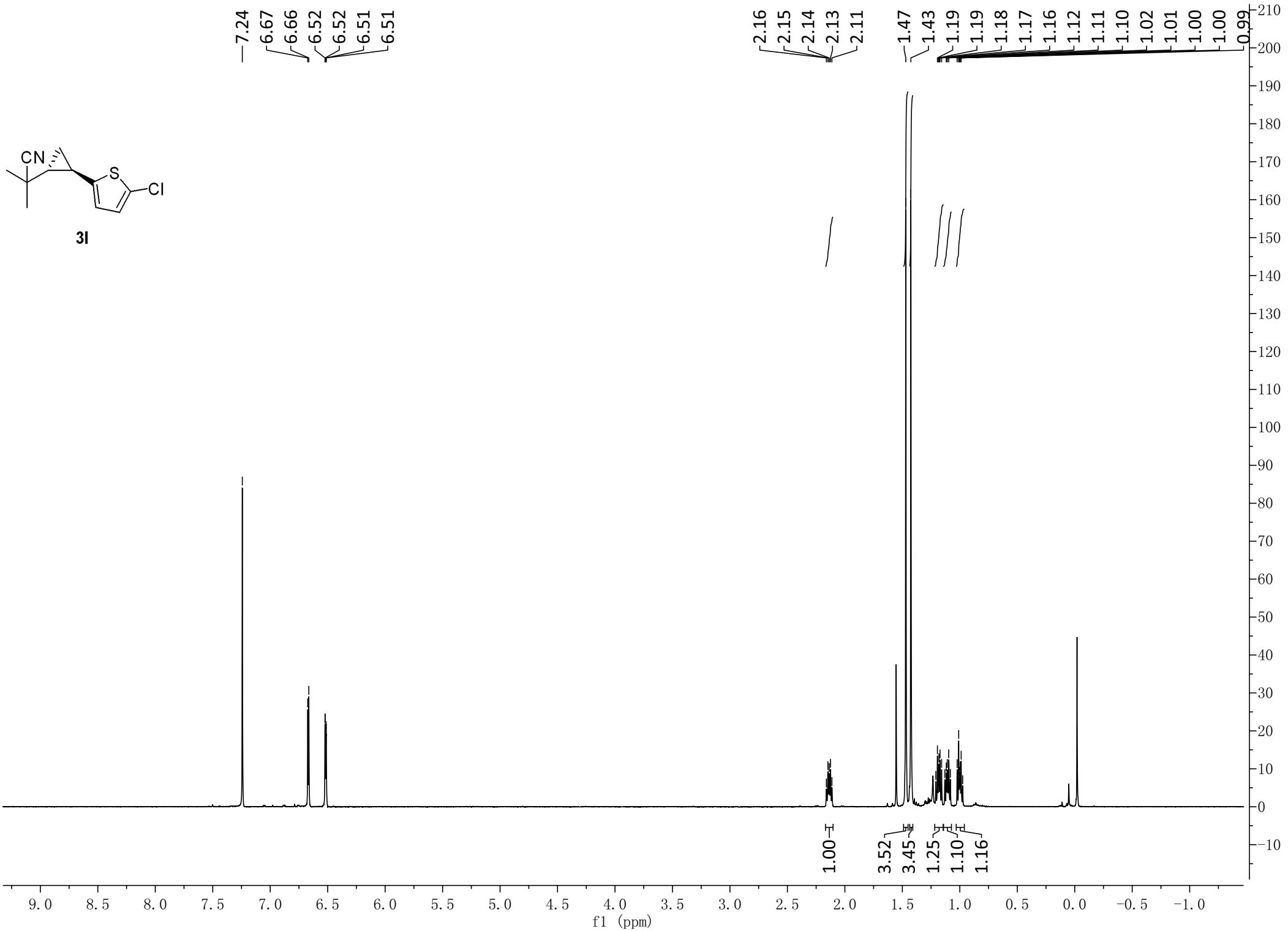


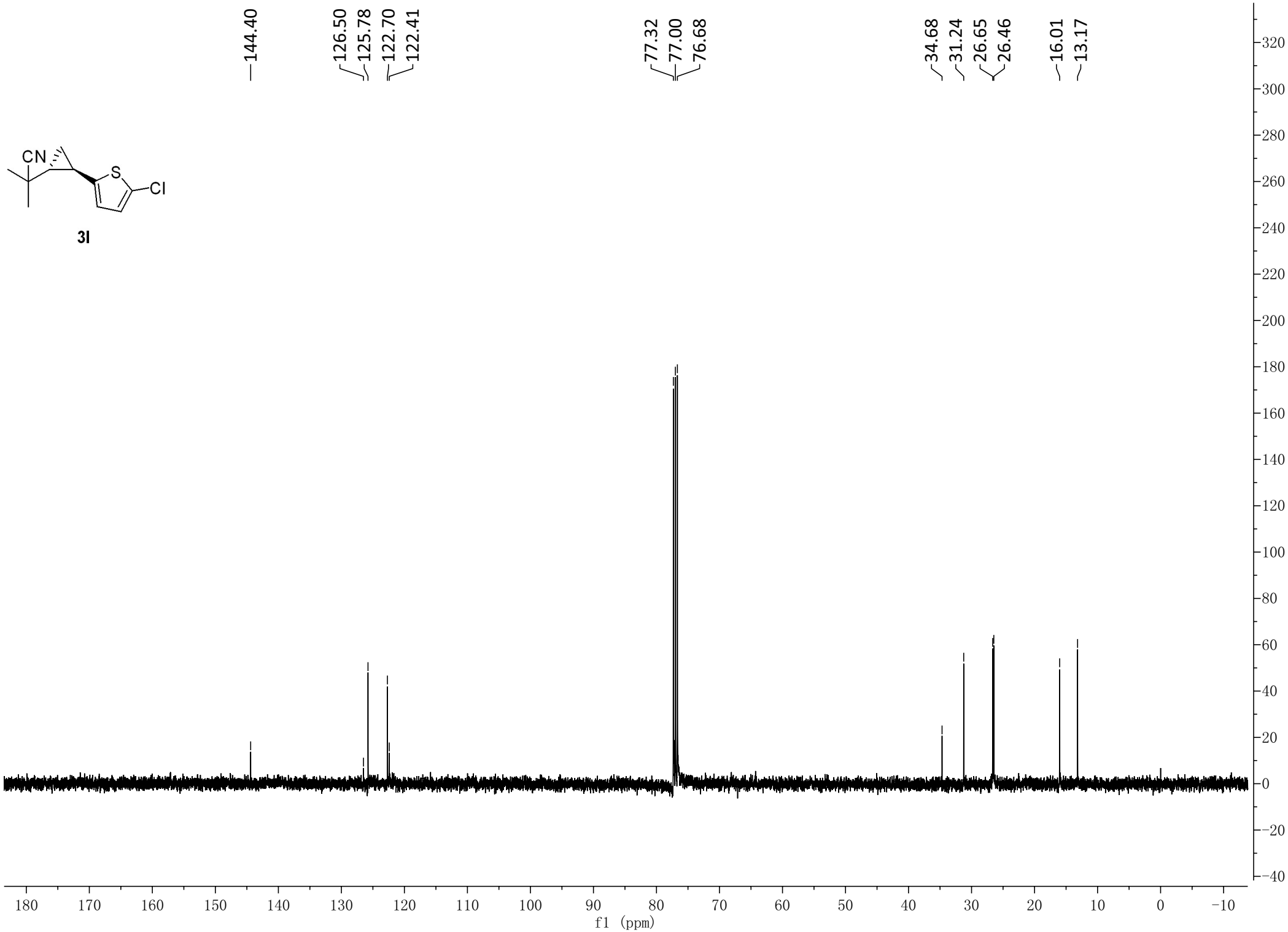
1 Det.A Ch1/215nm

PeakTable

Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.176	3865422	426036	93.994	94.685
2	9.025	246971	23913	6.006	5.315
Total		4112393	449950	100.000	100.000

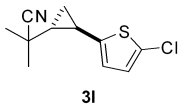

7.24
6.67
6.66
6.52
6.52
6.51
6.51
2.16
2.15
2.14
2.13
2.11
1.47
1.43
1.19
1.19
1.18
1.17
1.16
1.12
1.11
1.10
1.02
1.01
1.00
1.00
0.99
CN
S
Cl
3l
1.00
3.52
3.45
1.25
1.10
1.16
f1 (ppm)


144.40
126.50
125.78
122.70
122.41
77.32
77.00
76.68
34.68
31.24
26.65
26.46
16.01
13.17
CN
S
Cl
3l
f1 (ppm)

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

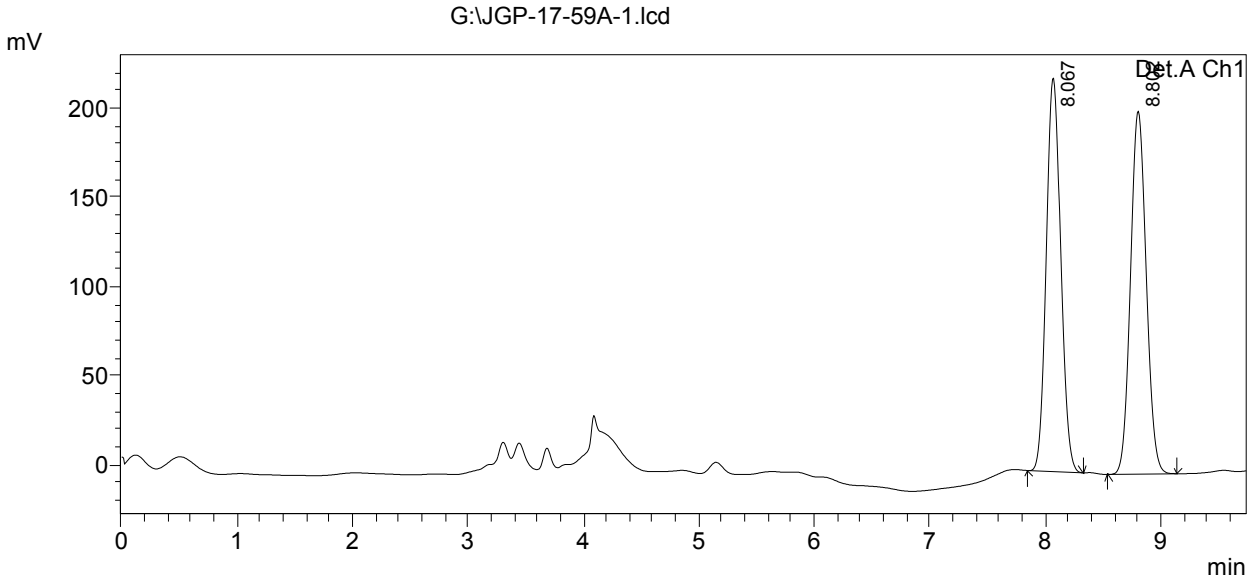
G:\JGP-17-59A-1.lcd : Admin

Acquired by	: JGP-17-59A-1
Sample Name	: IC,99/1,1.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-59A-1.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-13 9:33:34
Data Acquired	: 2018-12-13 9:43:18
Data Processed	



3l

<Chromatogram>



1 Det.A Ch1/215nm

PeakTable

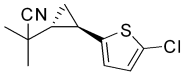
Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.067	1902867	220475	49.637	51.995
2	8.802	1930706	203554	50.363	48.005
Total		3833573	424029	100.000	100.000

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

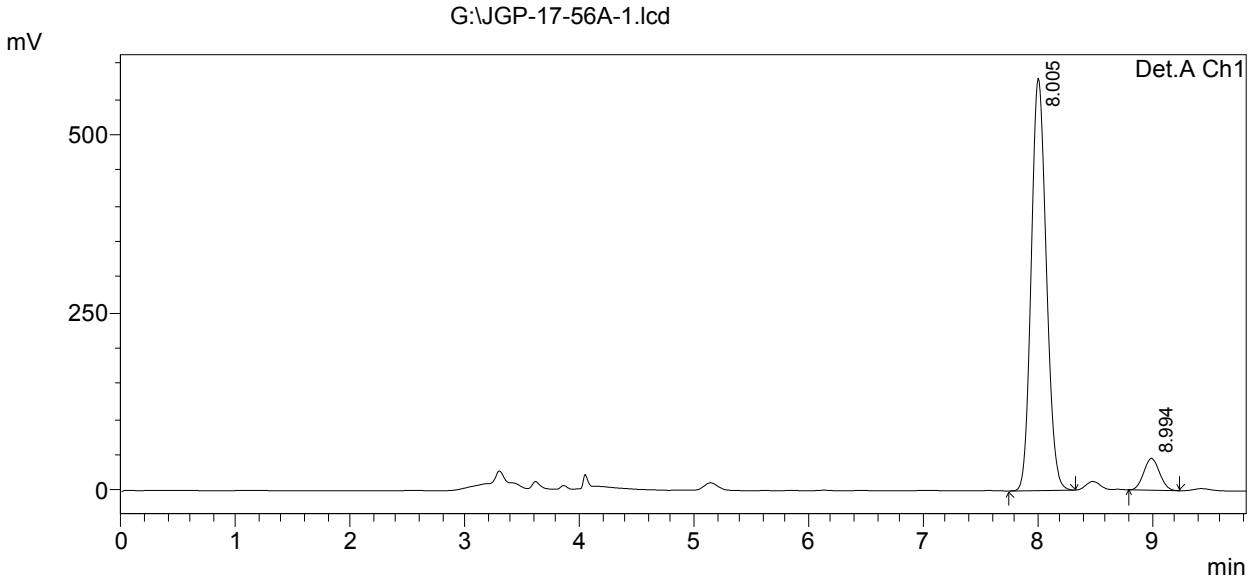
G:\JGP-17-56A-1.lcd : Admin

Acquired by	: JGP-17-56A-1
Sample Name	: IC,99/1,1.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-56A-1.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-13 9:08:26
Data Acquired	: 2018-12-29 14:43:49
Data Processed	



3l

<Chromatogram>

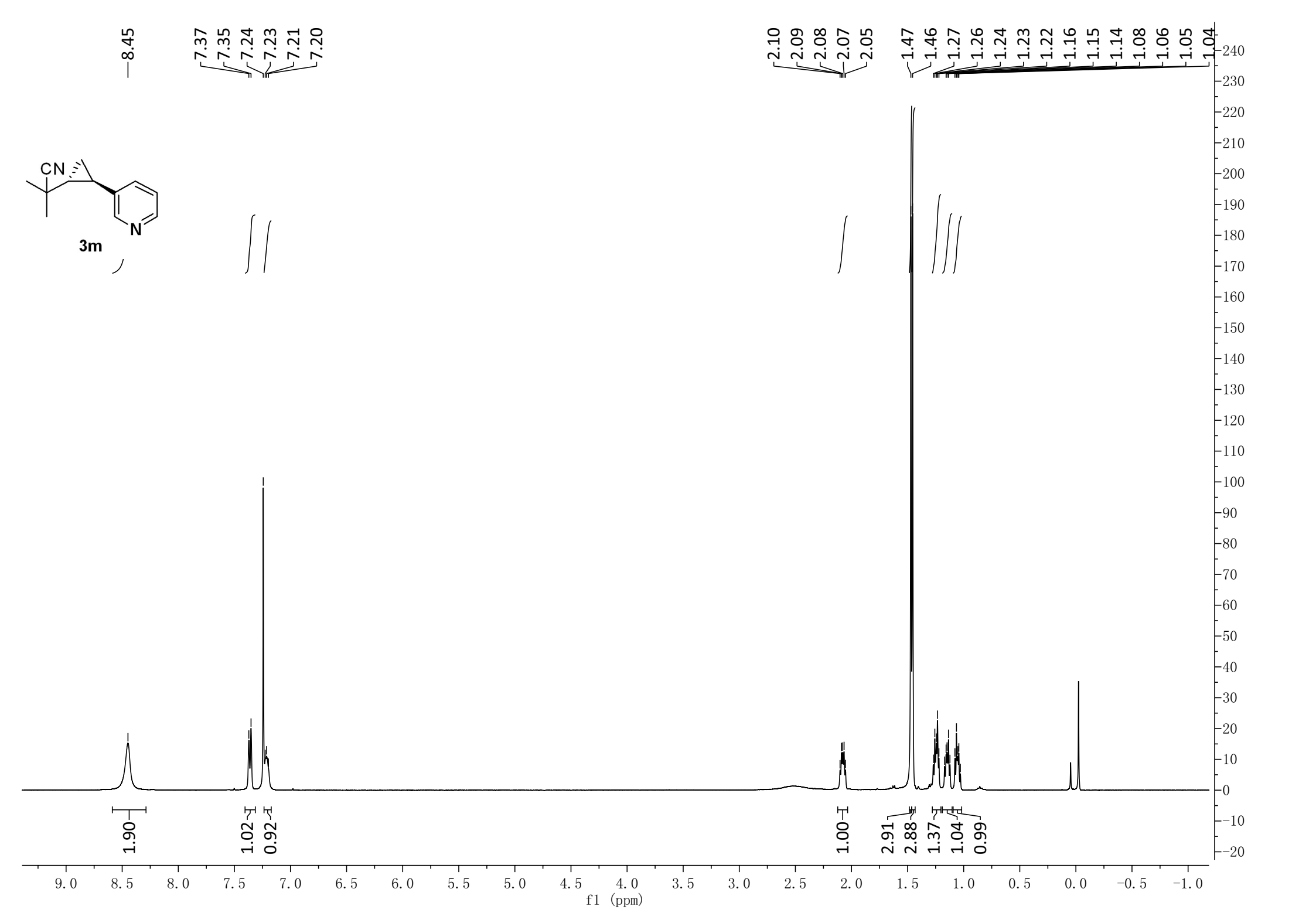


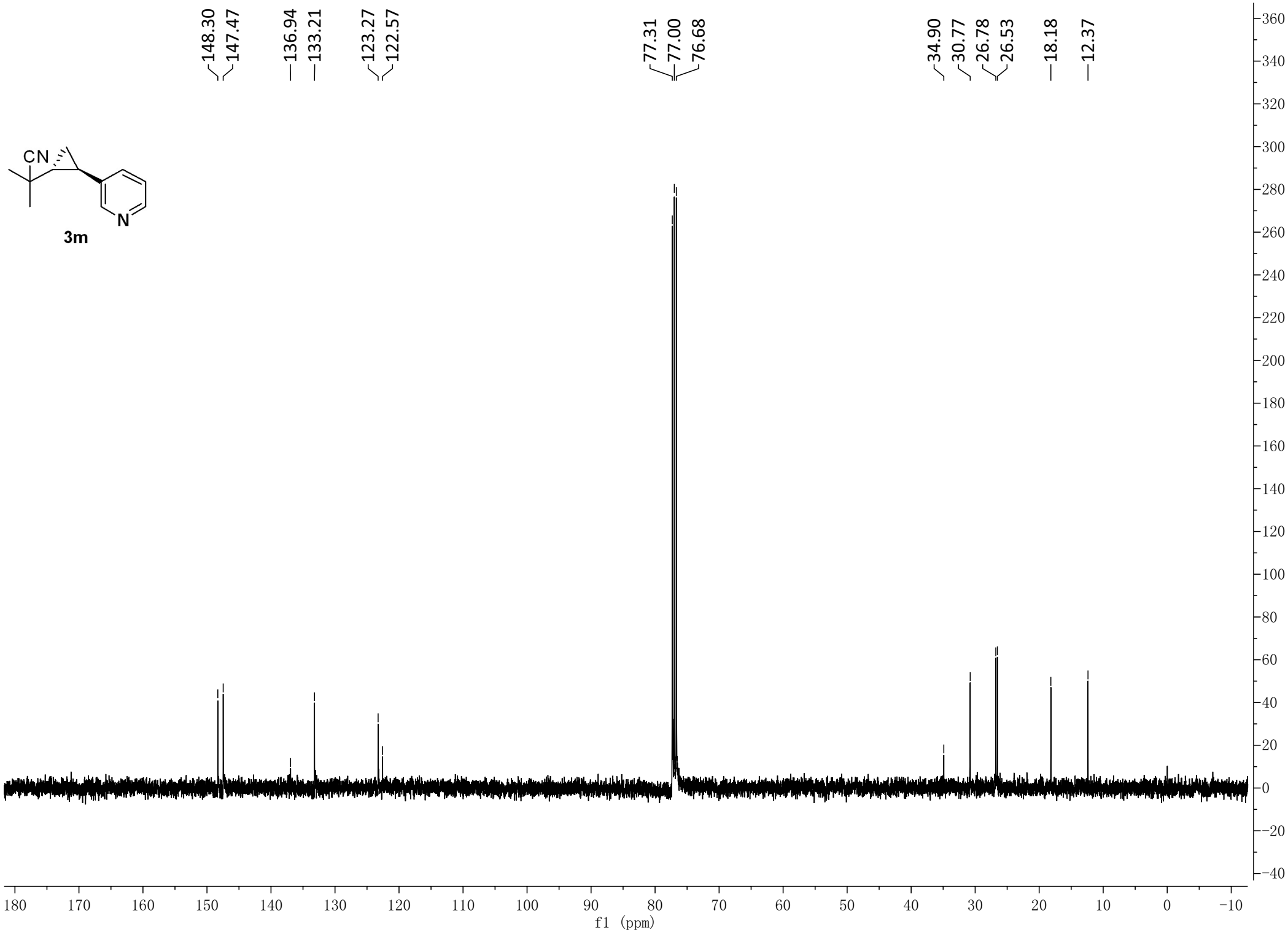
1 Det.A Ch1/215nm

PeakTable

Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	8.005	5279667	579633	92.344	92.795
2	8.994	437720	45004	7.656	7.205
Total		5717388	624638	100.000	100.000

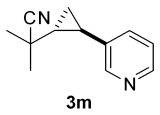

8.45
7.37
7.35
7.24
7.23
7.21
7.20
2.10
2.09
2.08
2.07
2.05
1.47
1.46
1.27
1.26
1.24
1.23
1.22
1.16
1.15
1.14
1.08
1.06
1.05
1.04
CN
N
3m
1.90
1.02
0.92
1.00
2.91
2.88
1.37
1.04
0.99
f1 (ppm)


148.30
147.47
136.94
133.21
123.27
122.57
77.31
77.00
76.68
34.90
30.77
26.78
26.53
18.18
12.37
CN
N
3m
f1 (ppm)

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

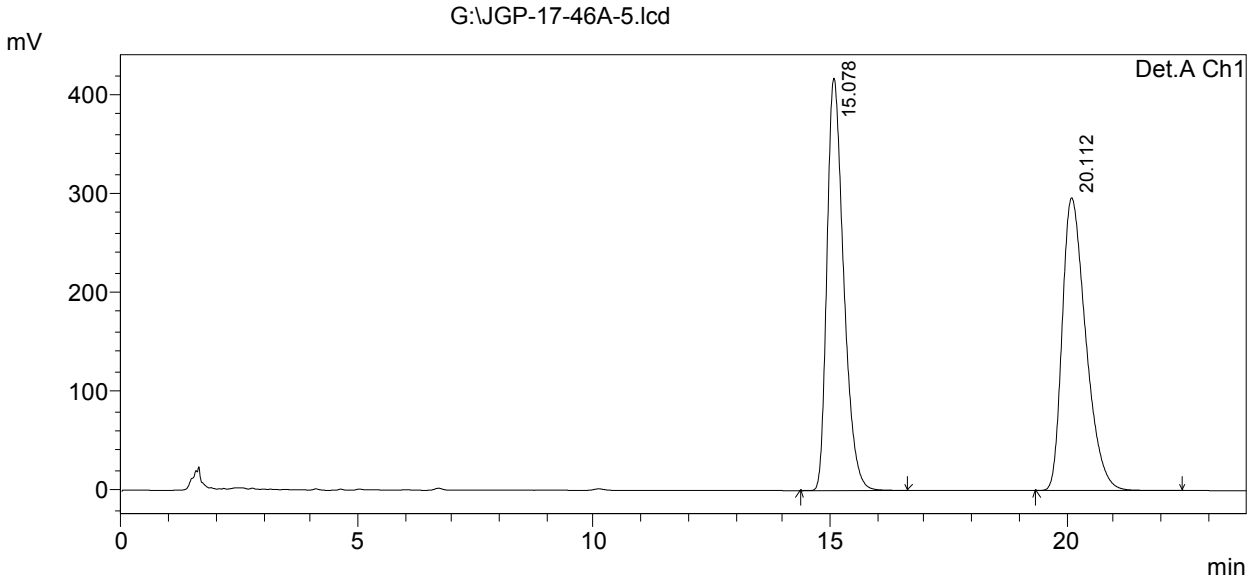
G:\JGP-17-46A-5.lcd : Admin

Acquired by	: JGP-17-46A-5
Sample Name	: AD-H,98/2,2.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-46A-5.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-13 13:57:23
Data Acquired	: 2018-12-13 14:21:12
Data Processed	



3m

<Chromatogram>



1 Det.A Ch1/215nm

PeakTable

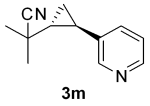
Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.078	10255828	417116	49.980	58.480
2	20.112	10264123	296144	50.020	41.520
Total		20519951	713260	100.000	100.000

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

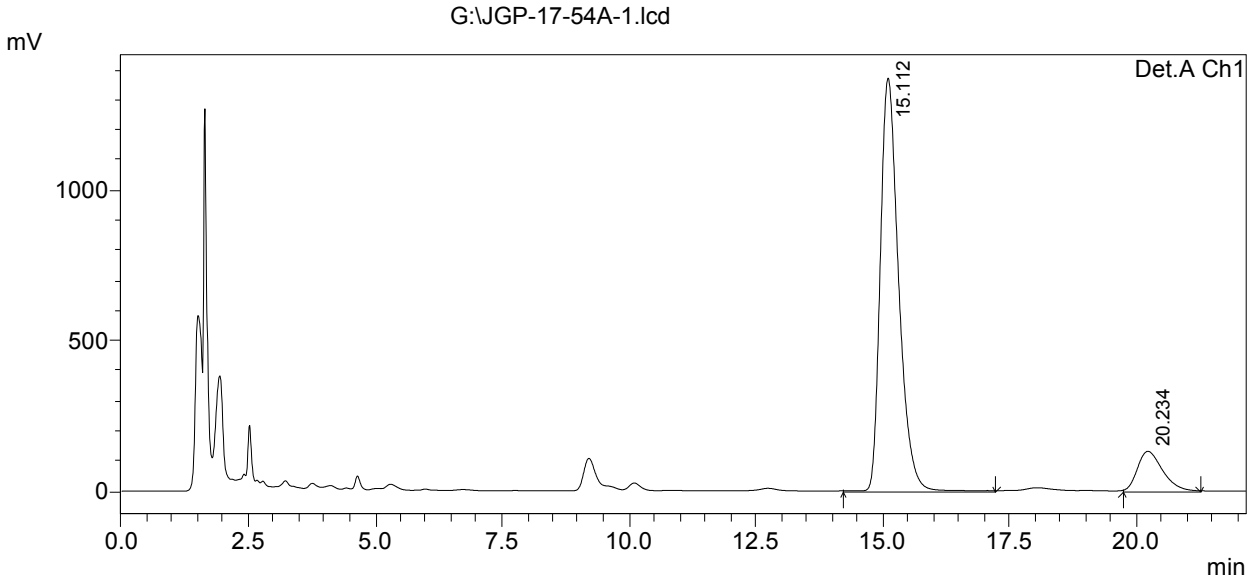
G:\JGP-17-54A-1.lcd : Admin

Acquired by	: JGP-17-54A-1
Sample Name	: AD-H,98/2,2.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-54A-1.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-13 14:23:44
Data Acquired	: 2018-12-29 14:07:44
Data Processed	



3m

<Chromatogram>

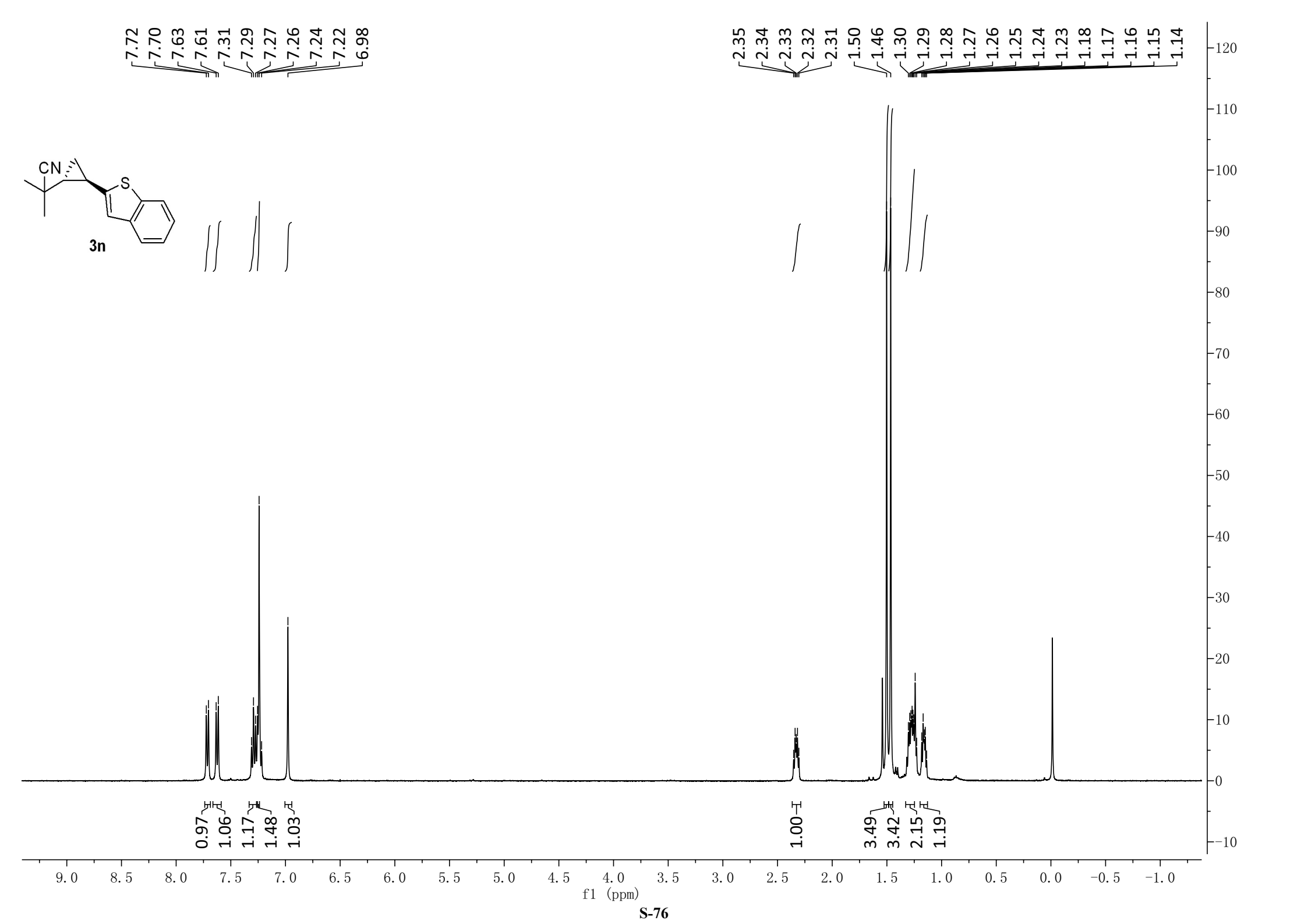


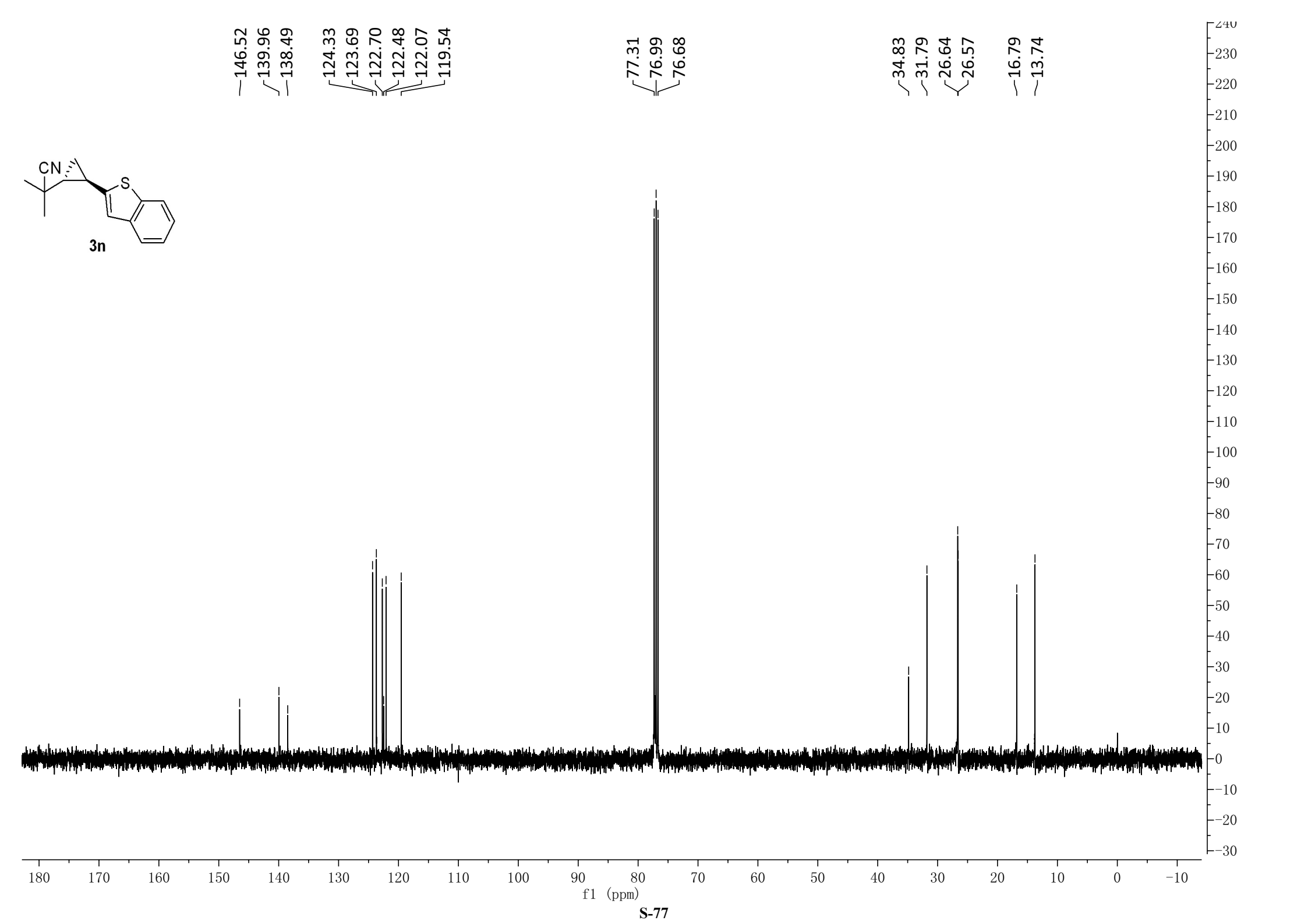
1 Det.A Ch1/215nm

PeakTable

Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	15.112	34980441	1373936	87.767	91.017
2	20.234	4875765	135607	12.233	8.983
Total		39856206	1509543	100.000	100.000

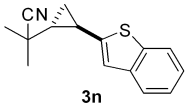

7.72
7.70
7.63
7.61
7.31
7.29
7.27
7.26
7.24
7.22
6.98
2.35
2.34
2.33
2.32
2.31
1.50
1.46
1.30
1.29
1.28
1.27
1.26
1.25
1.24
1.23
1.18
1.17
1.16
1.15
1.14
CN
S
3n
0.97
1.06
1.17
1.48
1.03
1.00
3.49
3.42
2.15
1.19
f1 (ppm)


146.52
139.96
138.49
124.33
123.69
122.70
122.48
122.07
119.54
77.31
76.99
76.68
34.83
31.79
26.64
26.57
16.79
13.74
CN
S
3n
f1 (ppm)

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

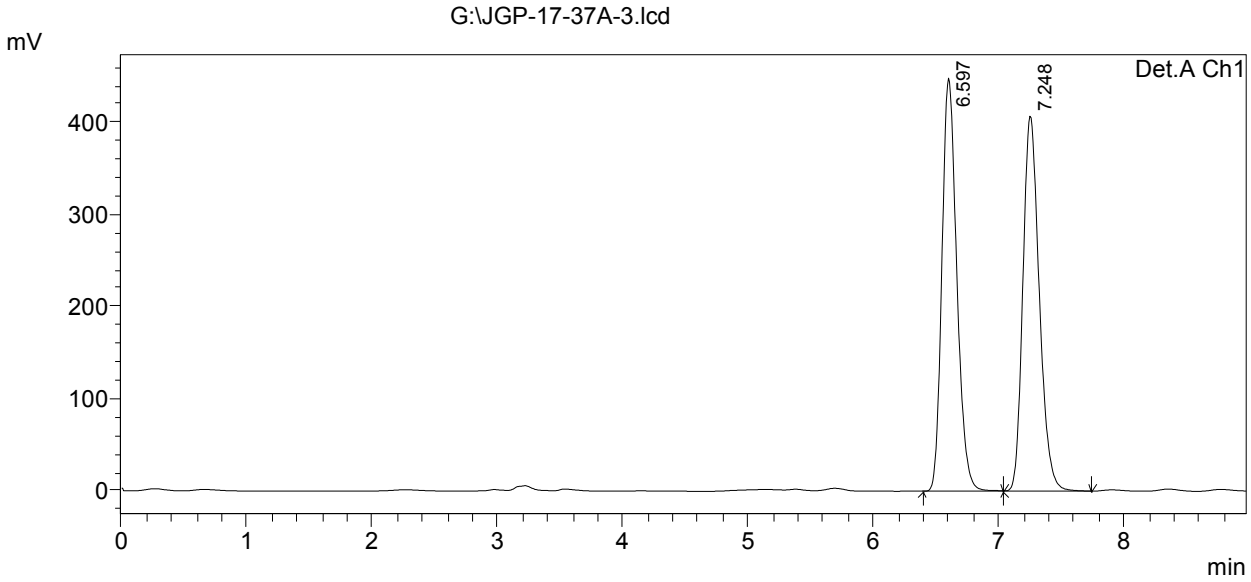
G:\JGP-17-37A-3.lcd : Admin

Acquired by	: JGP-17-37A-3
Sample Name	: AD-H,98/2,1.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-37A-3.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-21 17:40:20
Data Acquired	: 2018-12-21 17:49:19
Data Processed	



3n

<Chromatogram>



1 Det.A Ch1/215nm

PeakTable

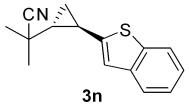
Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.597	3705257	448409	50.000	52.415
2	7.248	3705212	407094	50.000	47.585
Total		7410469	855503	100.000	100.000

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

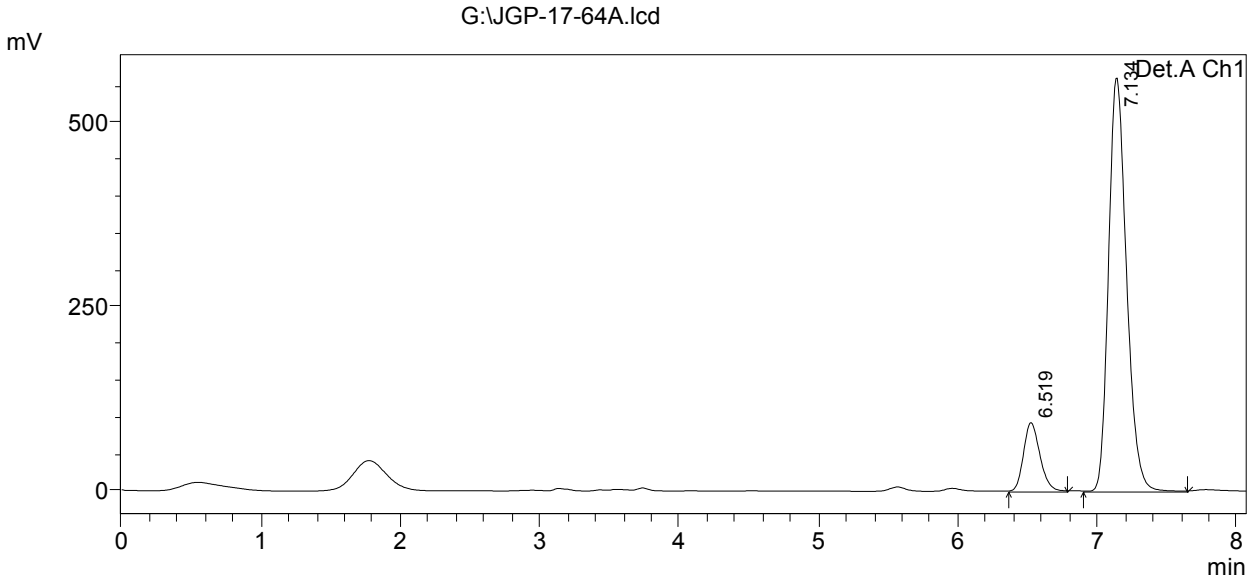
G:\JGP-17-64A.lcd : Admin

Acquired by	: JGP-17-64A
Sample Name	: AD-H,98/2,1.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-64A.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-21 18:52:38
Data Acquired	: 2018-12-28 10:11:48
Data Processed	



3n

<Chromatogram>

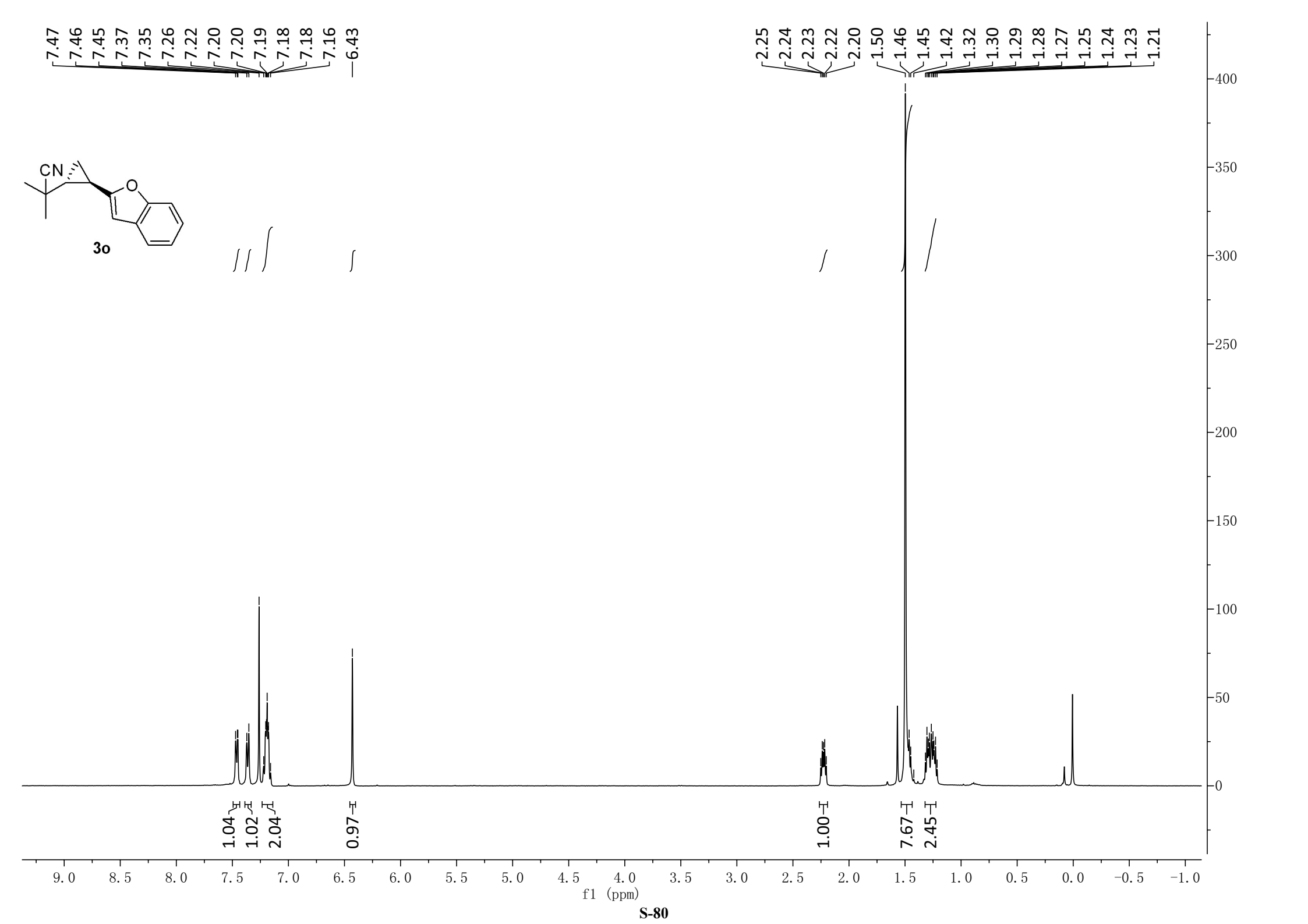


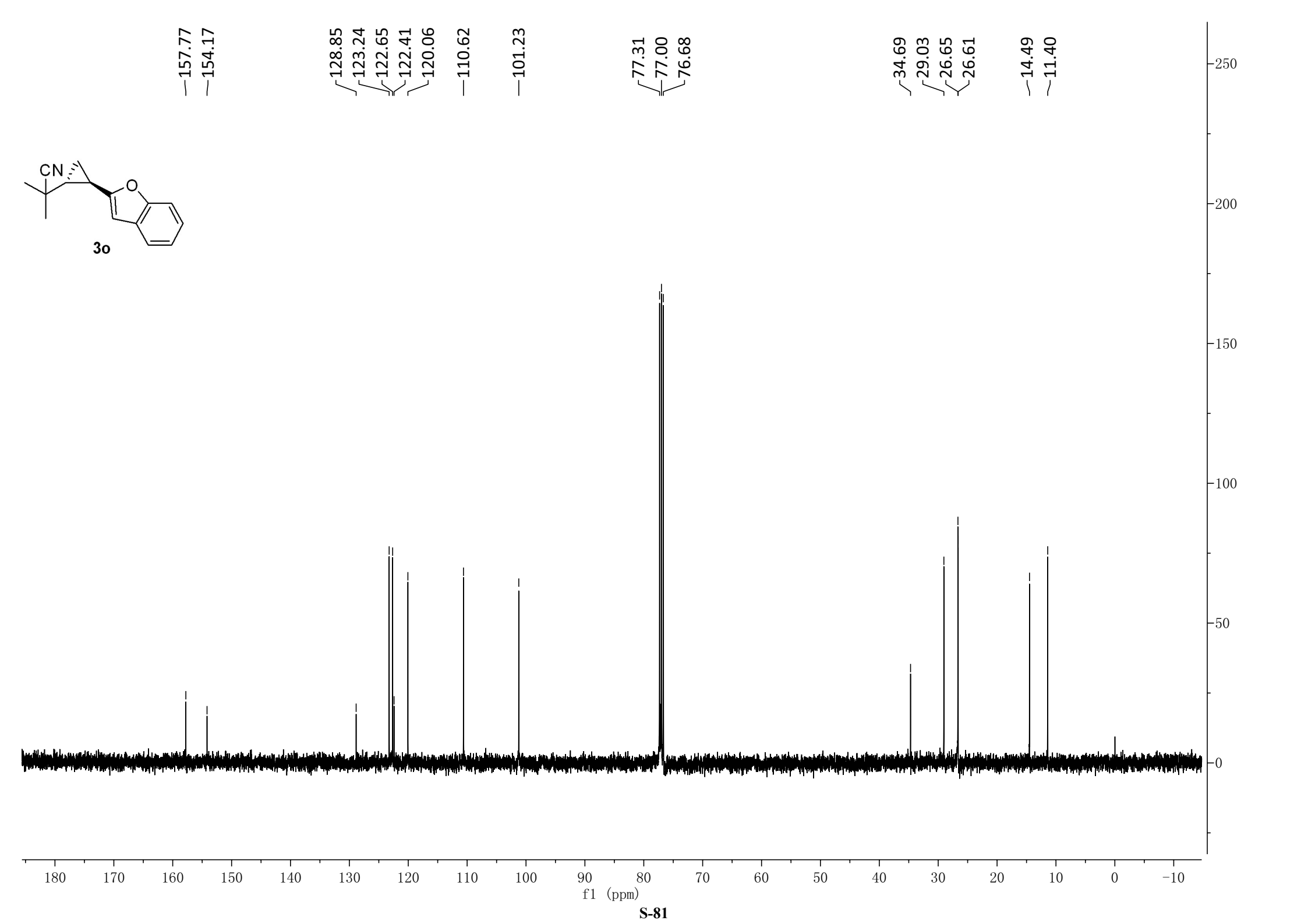
1 Det.A Ch1/215nm

PeakTable

Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	6.519	792449	94524	13.478	14.400
2	7.134	5087320	561907	86.522	85.600
Total		5879769	656431	100.000	100.000

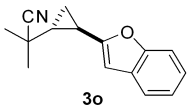

7.47
7.46
7.45
7.37
7.35
7.26
7.22
7.20
7.20
7.19
7.18
7.18
7.16
6.43
2.25
2.24
2.23
2.22
2.20
1.50
1.46
1.45
1.42
1.32
1.30
1.29
1.28
1.27
1.25
1.24
1.23
1.21
CN
O
3o
1.04
1.02
2.04
0.97
1.00
7.67
2.45
f1 (ppm)


157.77
154.17
128.85
123.24
122.65
122.41
120.06
110.62
101.23
77.31
77.00
76.68
34.69
29.03
26.65
26.61
14.49
11.40
CN
O
3o
250
200
150
100
50
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

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

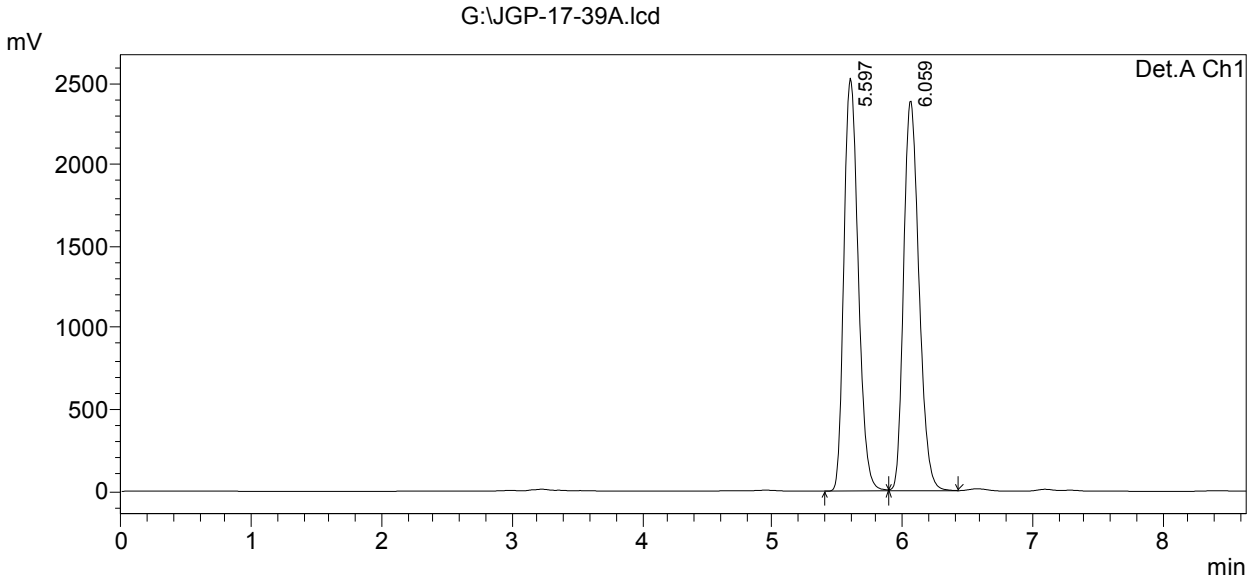
G:\JGP-17-39A.lcd : Admin

Acquired by	: JGP-17-39A
Sample Name	: AD-H,98/2,1.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-39A.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-21 17:50:16
Data Acquired	: 2018-12-21 17:58:55
Data Processed	



3o

<Chromatogram>



1 Det.A Ch1/215nm

PeakTable

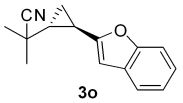
Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.597	19379597	2529216	49.668	51.442
2	6.059	19638731	2387426	50.332	48.558
Total		39018327	4916642	100.000	100.000

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

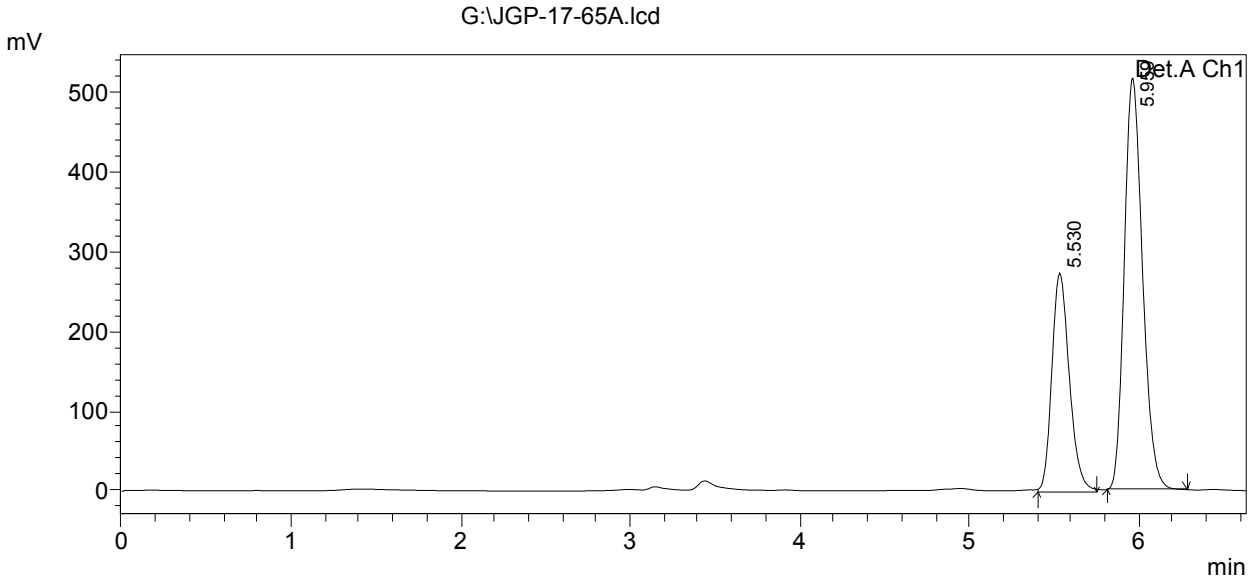
G:\JGP-17-65A.lcd : Admin

Acquired by	: JGP-17-65A
Sample Name	: AD-H,98/2,1.0,215
Sample ID	:
Vail #	: 1 uL
Injection Volume	: JGP-17-65A.lcd
Data File Name	: 1.lcm
Method File Name	:
Batch File Name	: Default.lcr
Report File Name	: 2018-12-21 19:04:04
Data Acquired	: 2018-12-28 10:12:59
Data Processed	



3o

<Chromatogram>

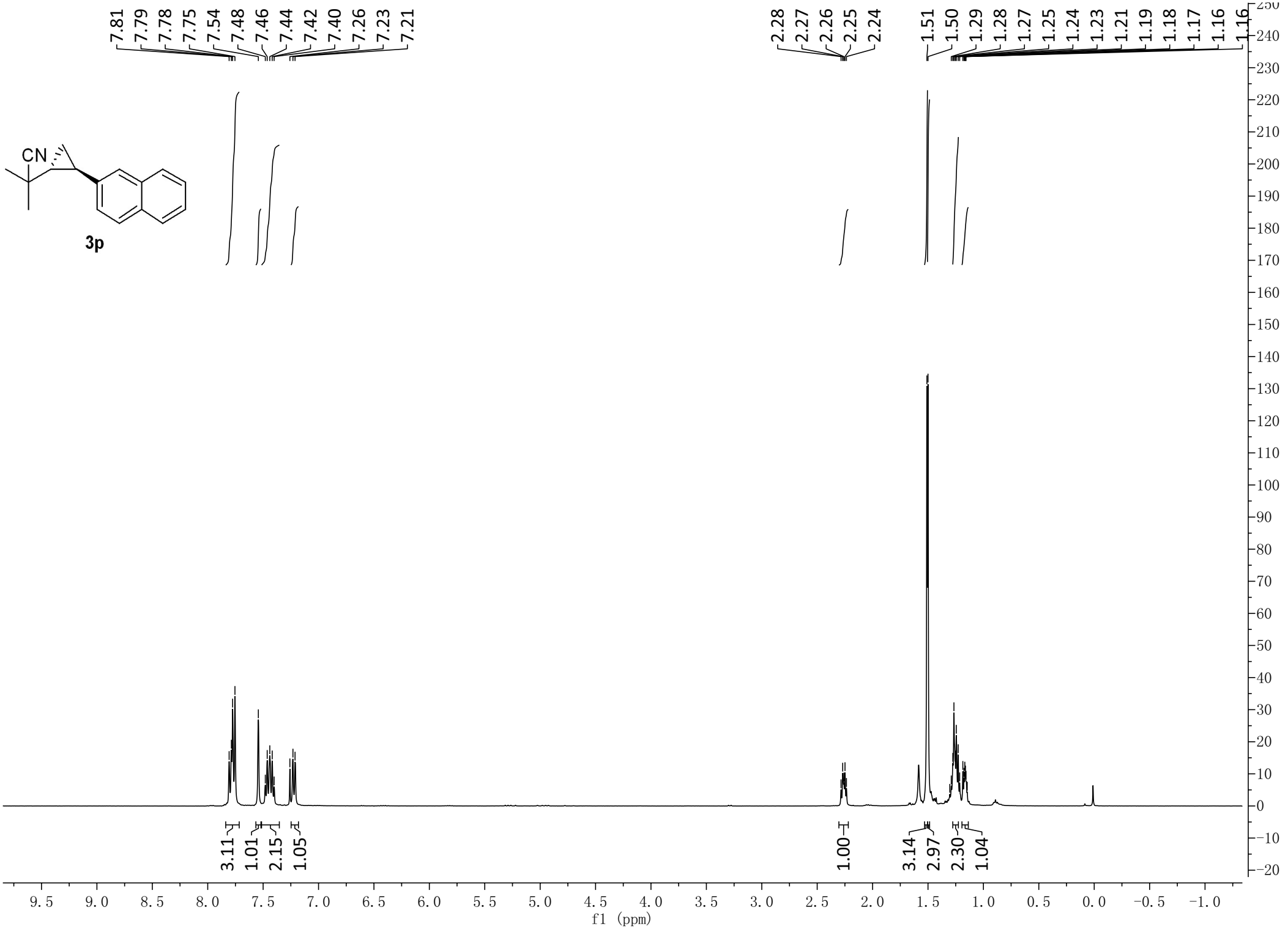


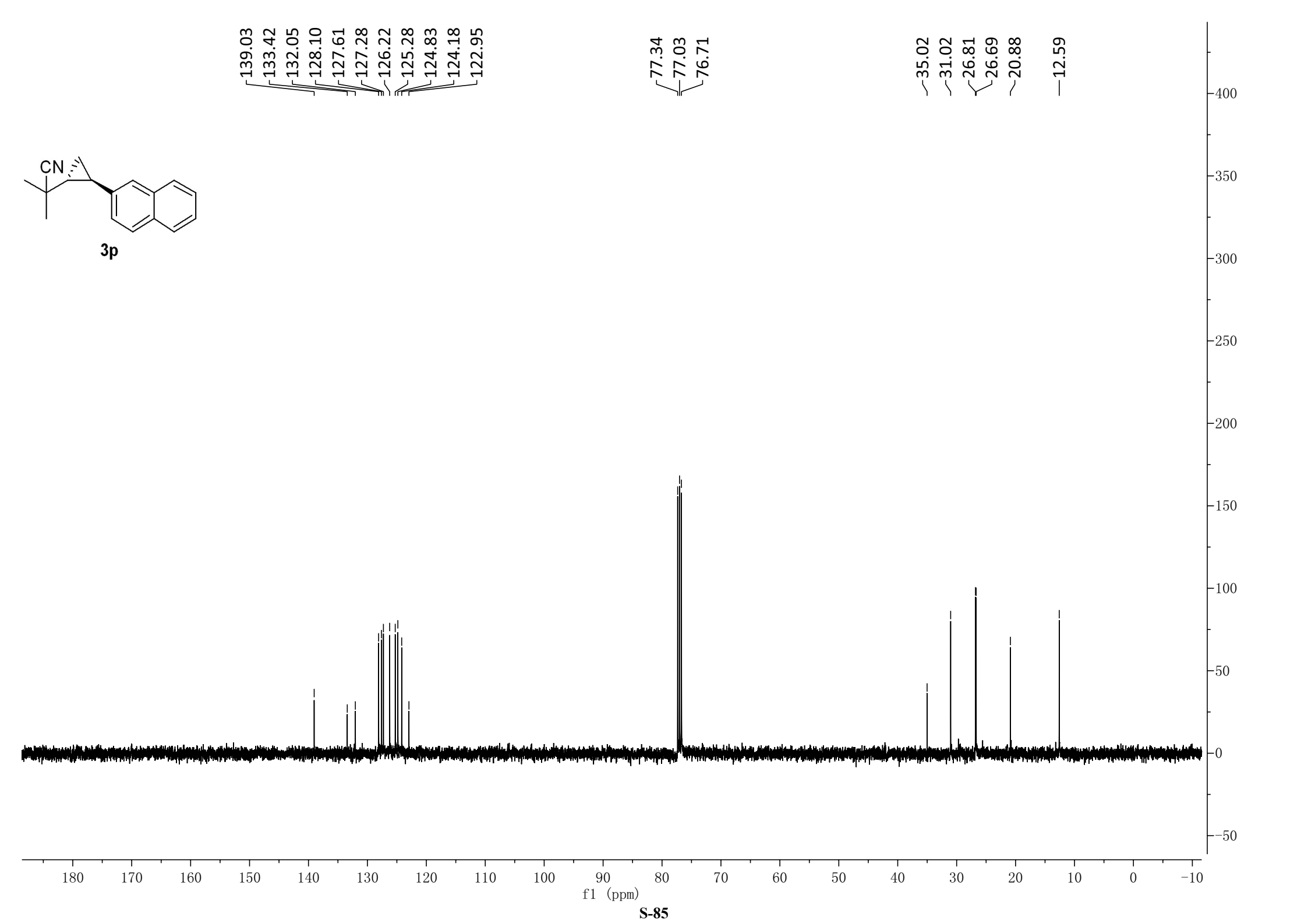
1 Det.A Ch1/215nm

PeakTable

Detector A Ch1 215nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	5.530	1982483	275473	34.053	34.836
2	5.959	3839345	515304	65.947	65.164
Total		5821828	790776	100.000	100.000

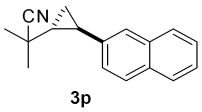

7.81
7.79
7.78
7.75
7.54
7.48
7.46
7.44
7.42
7.40
7.26
7.23
7.21
2.28
2.27
2.26
2.25
2.24
1.51
1.50
1.29
1.28
1.27
1.25
1.24
1.23
1.21
1.19
1.18
1.17
1.16
CN
3p
3.11
1.01
2.15
1.05
1.00
3.14
2.97
2.30
1.04
f1 (ppm)


139.03
133.42
132.05
128.10
127.61
127.28
126.22
125.28
124.83
124.18
122.95
77.34
77.03
76.71
35.02
31.02
26.81
26.69
20.88
12.59
CN
3p
f1 (ppm)

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-11A-4(IC-99.2 0.8-1-214).lcd

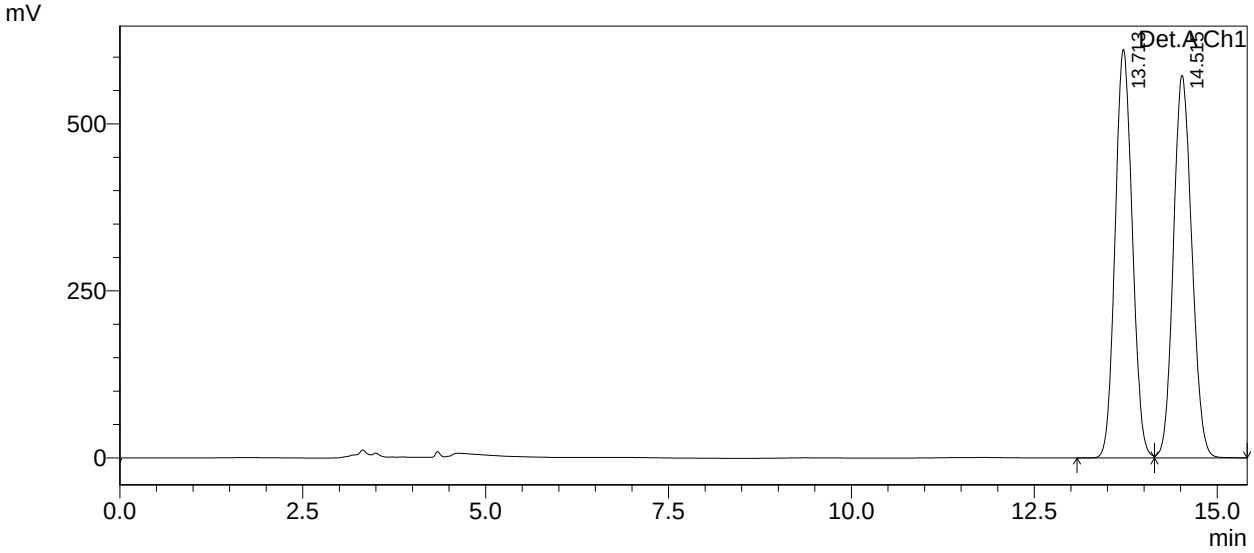
Acquired by	: Admin
Sample Name	: JGP-15-11A-4
Sample ID	: IC,99.2/0.8,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-11A-4(IC-99.2 0.8-1-214).lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-7 12:21:30
Data Processed	: 2018-5-7 12:36:54



3p

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-11A-4(IC-99.2 0.8-1-214).lcd



1 Det.A Ch1/214nm

PeakTable

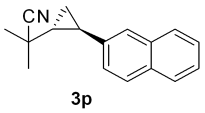
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	13.713	10006905	611985	49.874	51.662
2	14.515	10057506	572618	50.126	48.338
Total		20064412	1184603	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-15A-1.lcd

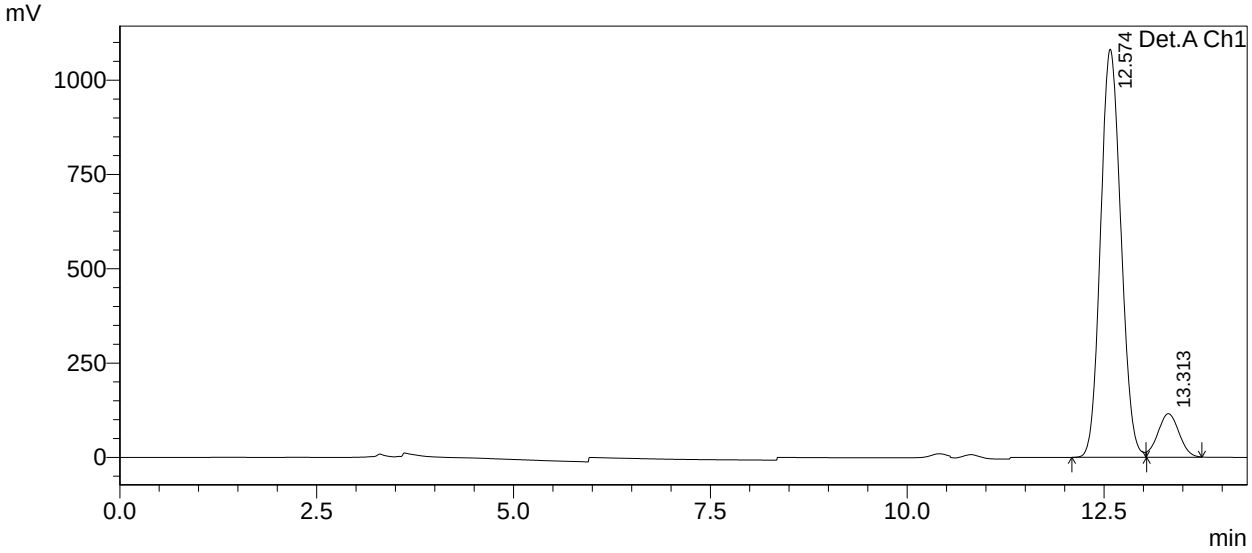
Acquired by	: Admin
Sample Name	: JGP-15-15A-1
Sample ID	: IC,99.2/0.8,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-15A-1.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-7 17:04:09
Data Processed	: 2018-5-19 8:37:14



3p

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-15A-1.lcd

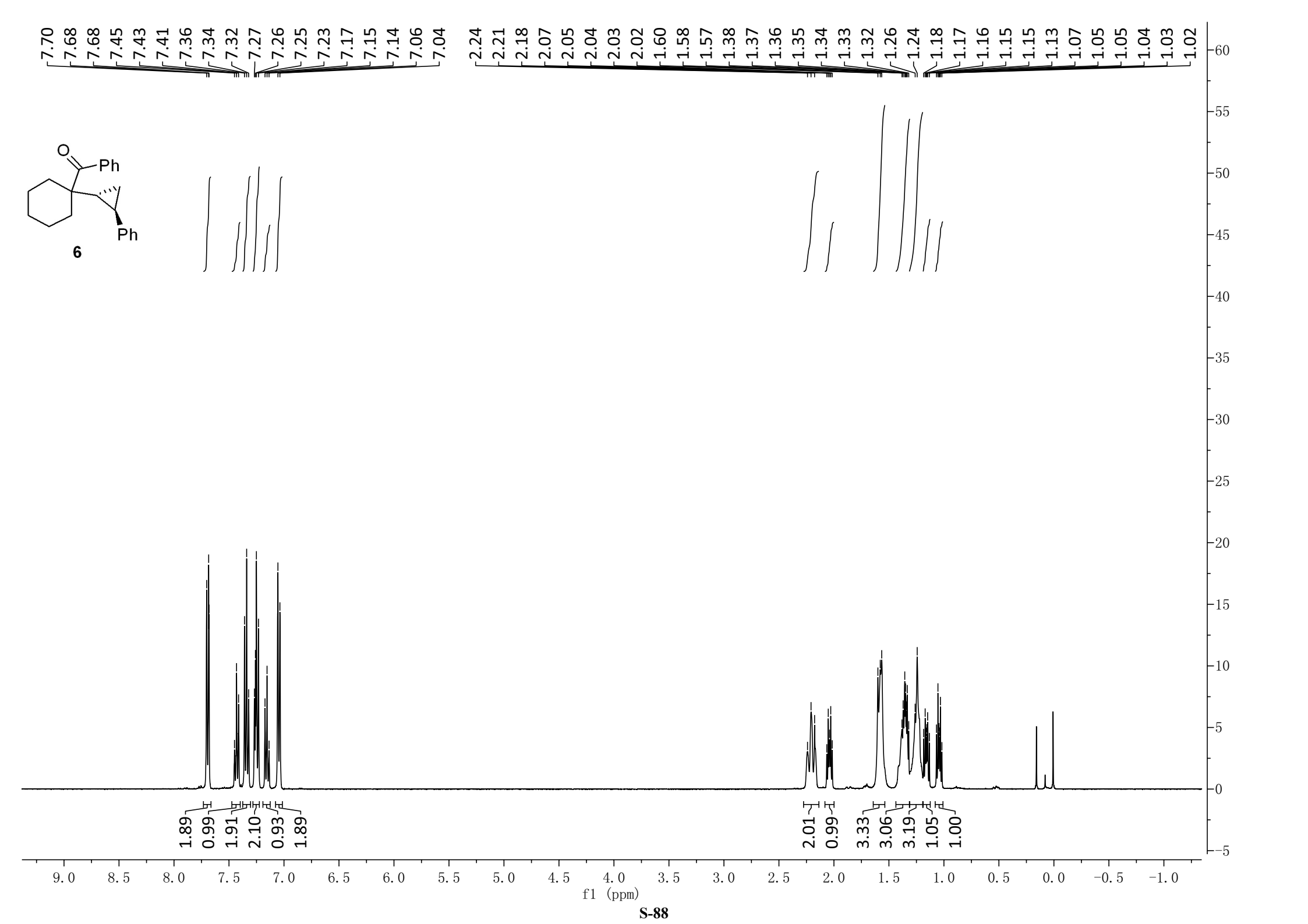


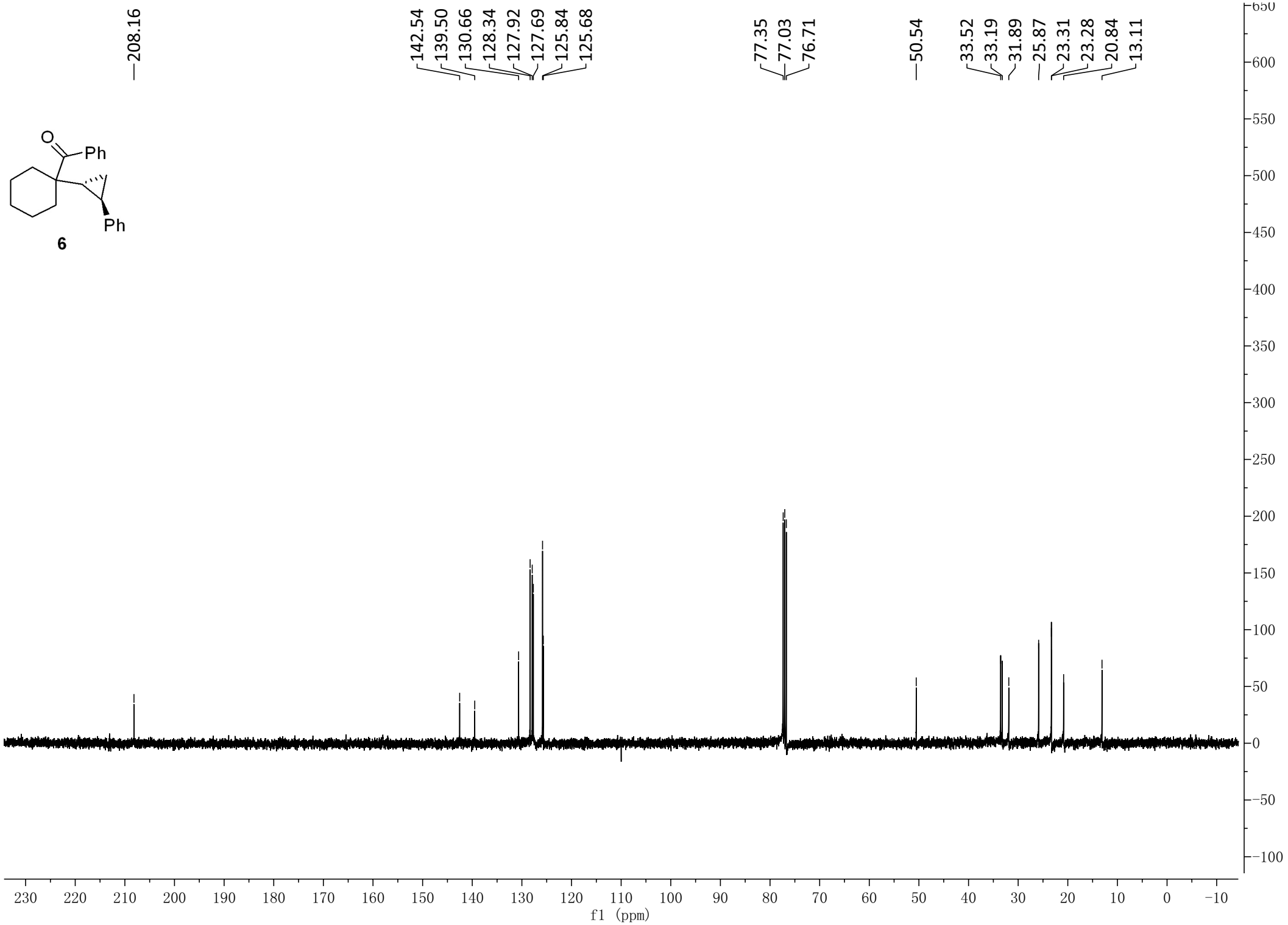
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	12.574	19447446	1081978	90.014	90.355
2	13.313	2157413	115491	9.986	9.645
Total		21604859	1197469	100.000	100.000

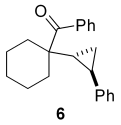

7.70 7.68 7.68 7.45 7.43 7.41 7.36 7.34 7.32 7.27 7.26 7.25 7.23 7.17 7.15 7.14 7.06 7.04
2.24 2.21 2.18 2.07 2.05 2.04 2.03 2.02 1.60 1.58 1.57 1.38 1.37 1.36 1.35 1.34 1.33 1.32 1.26 1.24 1.18 1.17 1.16 1.15 1.15 1.13 1.07 1.05 1.05 1.04 1.03 1.02
O
Ph
Ph
6
1.89 0.99 1.91 2.10 0.93 1.89
2.01 0.99 3.33 3.06 3.19 1.05 1.00
f1 (ppm)


208.16
142.54
139.50
130.66
128.34
127.92
127.69
125.84
125.68
77.35
77.03
76.71
50.54
33.52
33.19
31.89
25.87
23.31
23.28
20.84
13.11
O
Ph
Ph
6
650
600
550
500
450
400
350
300
250
200
150
100
50
0
−50
−100
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-14-38A-RAC-8.lcd

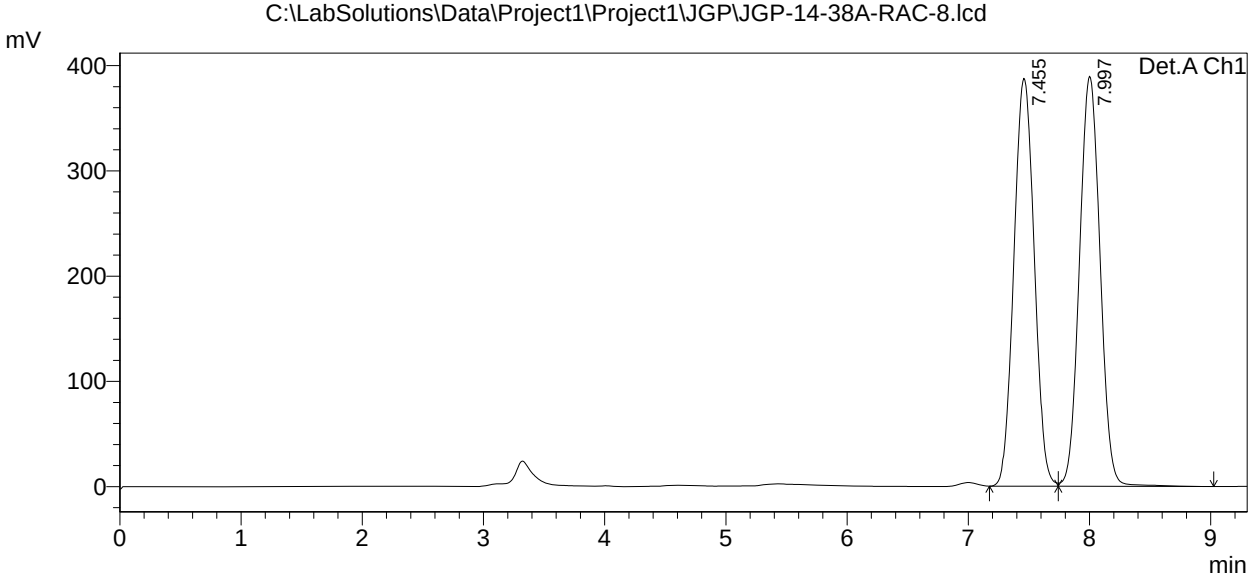
Acquired by	: Admin
Sample Name	: JGP-14-38A-RAC-8
Sample ID	: IC,99.3/0.7,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-14-38A-RAC-8.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-6-1 11:21:10
Data Processed	: 2018-6-1 11:30:28



6

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-14-38A-RAC-8.lcd



1 Det.A Ch1/214nm

PeakTable

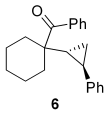
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.455	4528057	387596	49.591	49.861
2	7.997	4602808	389763	50.409	50.139
Total		9130865	777359	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-47A.lcd

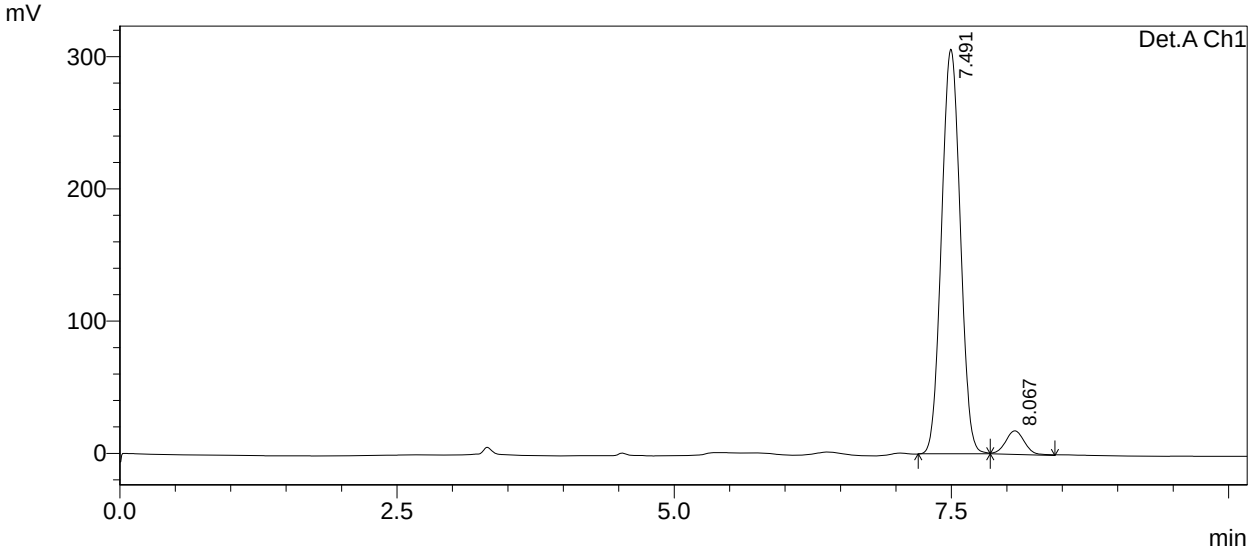
Acquired by	: Admin
Sample Name	: JGP-15-47A
Sample ID	: IC,99.3/0.7,1.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-47A.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-6-1 11:09:15
Data Processed	: 2018-6-4 10:00:46



6

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-47A.lcd

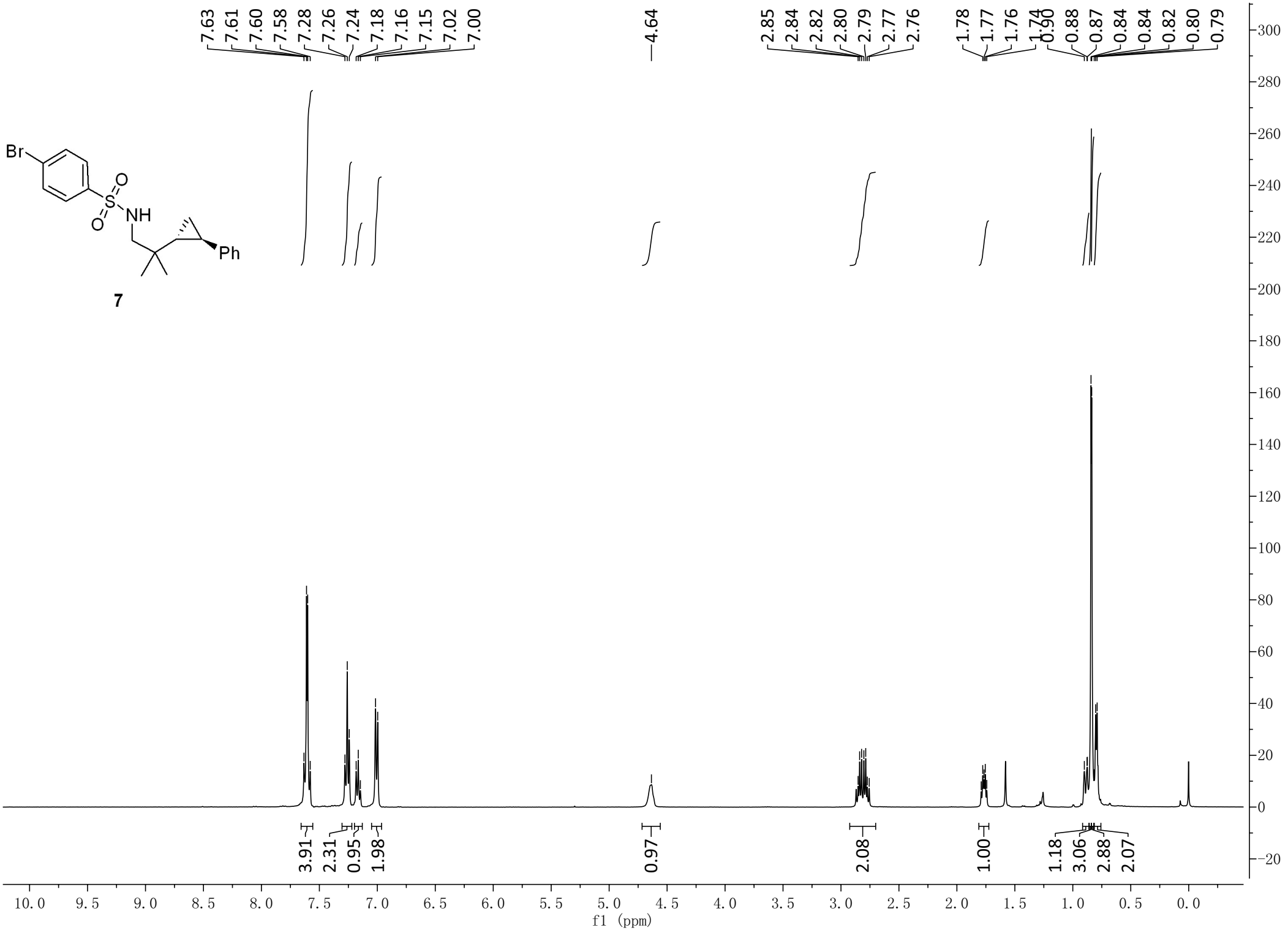


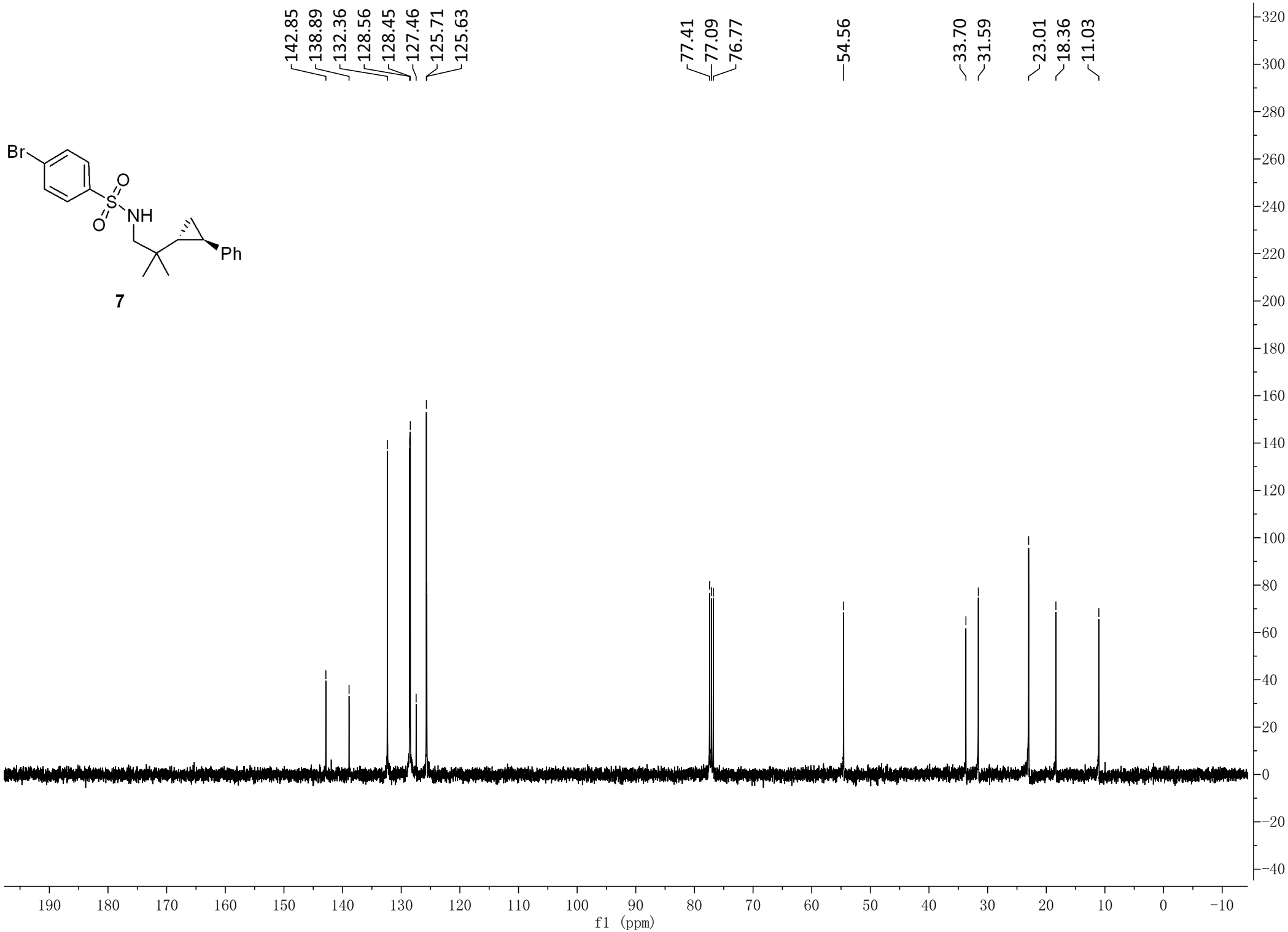
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.491	3595722	306015	94.357	94.475
2	8.067	215061	17895	5.643	5.525
Total		3810783	323910	100.000	100.000

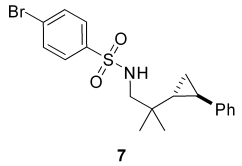

7.63
7.61
7.60
7.58
7.28
7.26
7.24
7.18
7.16
7.15
7.02
7.00
4.64
2.85
2.84
2.82
2.80
2.79
2.77
2.76
1.78
1.77
1.76
1.74
0.90
0.88
0.87
0.84
0.84
0.82
0.80
0.79
Br
O
S
O
NH
Ph
7
3.91
2.31
0.95
1.98
0.97
2.08
1.00
1.18
3.06
2.88
2.07
f1 (ppm)


142.85
138.89
132.36
128.56
128.45
127.46
125.71
125.63
77.41
77.09
76.77
54.56
33.70
31.59
23.01
18.36
11.03
Br
O
S
O
NH
Ph
7
f1 (ppm)

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-22A-6.lcd

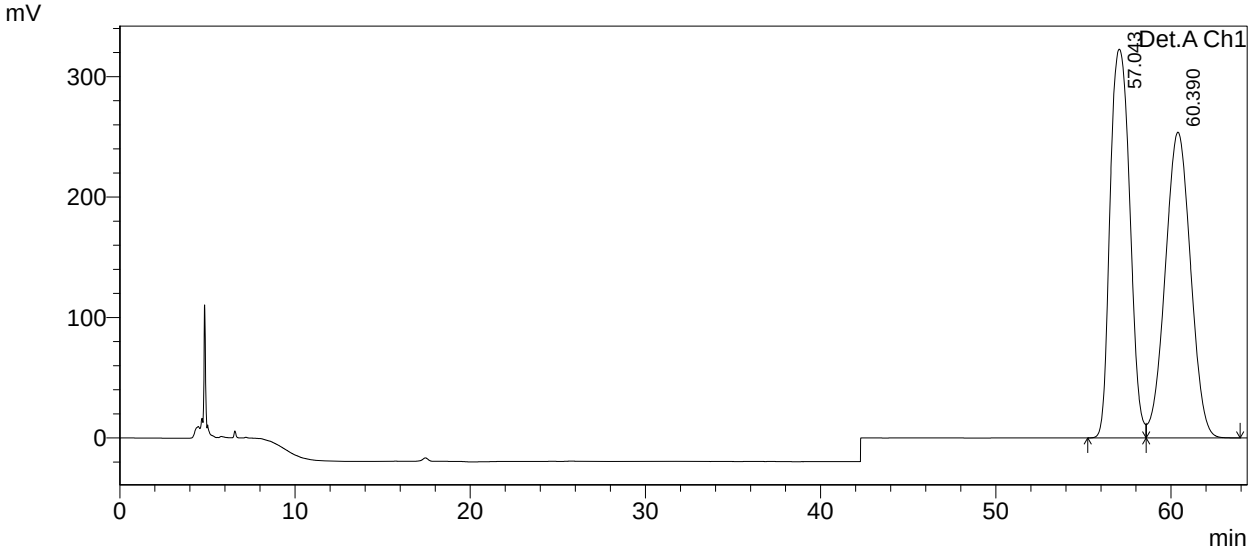
Acquired by	: Admin
Sample Name	: JGP-15-22A-6
Sample ID	: IC,98/2,0.7,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-22A-6.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-14 13:44:05
Data Processed	: 2018-5-14 14:48:26



7

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-22A-6.lcd



1 Det.A Ch1/214nm

PeakTable

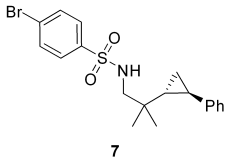
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	57.043	25316876	322791	49.833	55.976
2	60.390	25486473	253864	50.167	44.024
Total		50803349	576656	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-23A-1.lcd

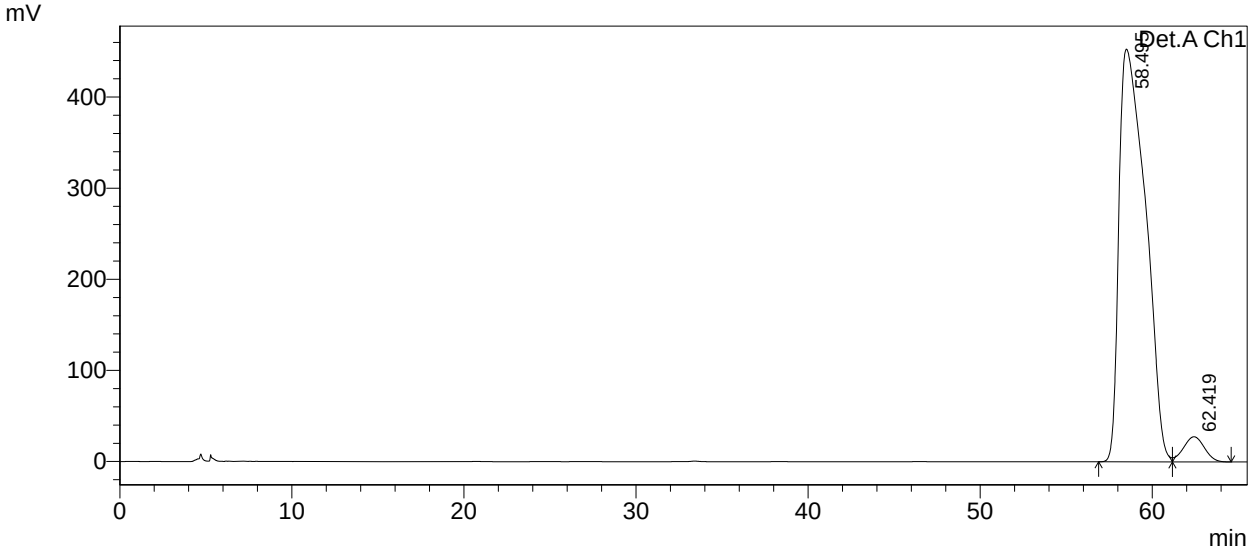
Acquired by	: Admin
Sample Name	: JGP-15-23A-1
Sample ID	: IC,98/2,0.7,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-23A-1.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-5-14 14:52:20
Data Processed	: 2018-5-19 8:43:01



7

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-23A-1.lcd

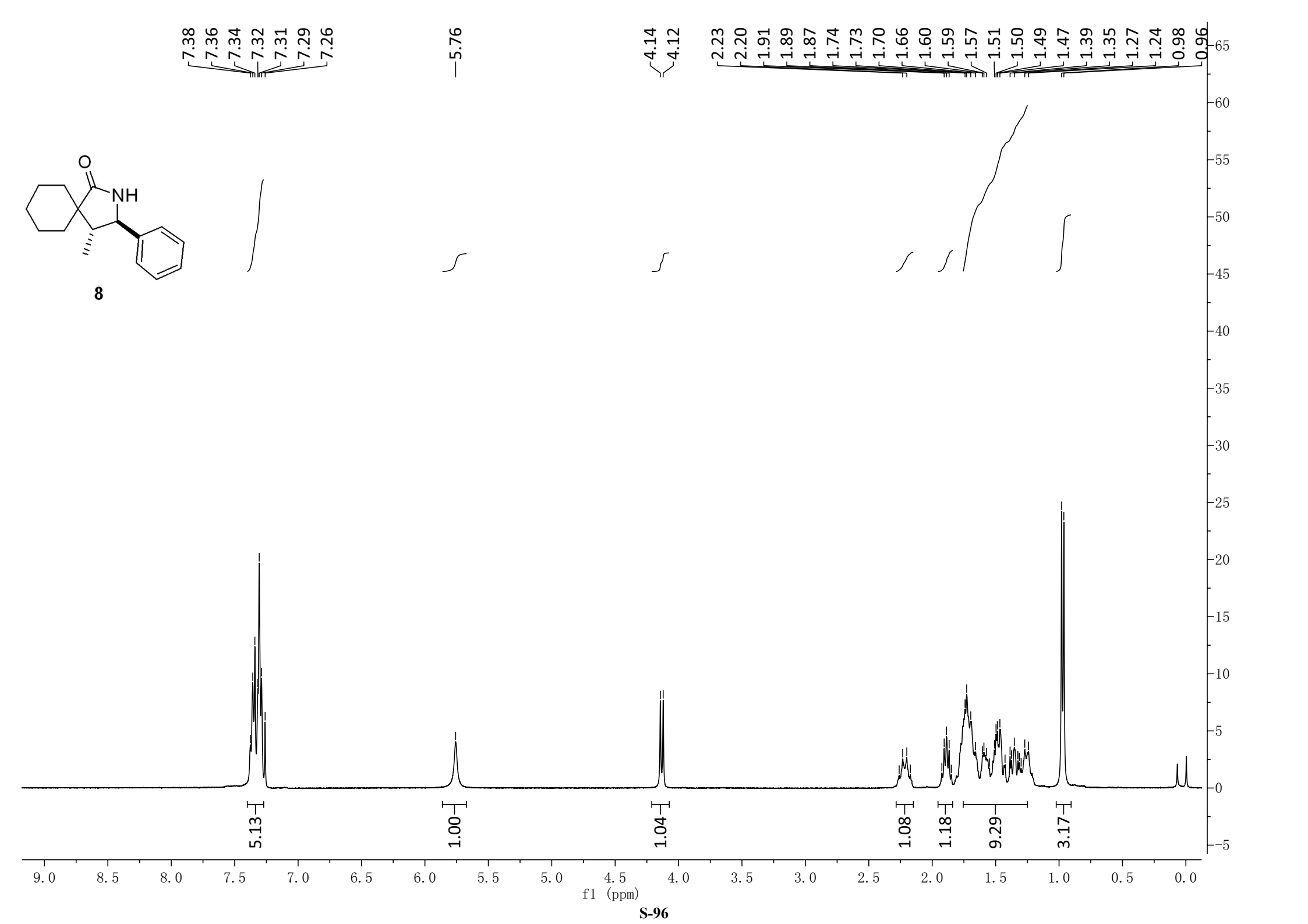


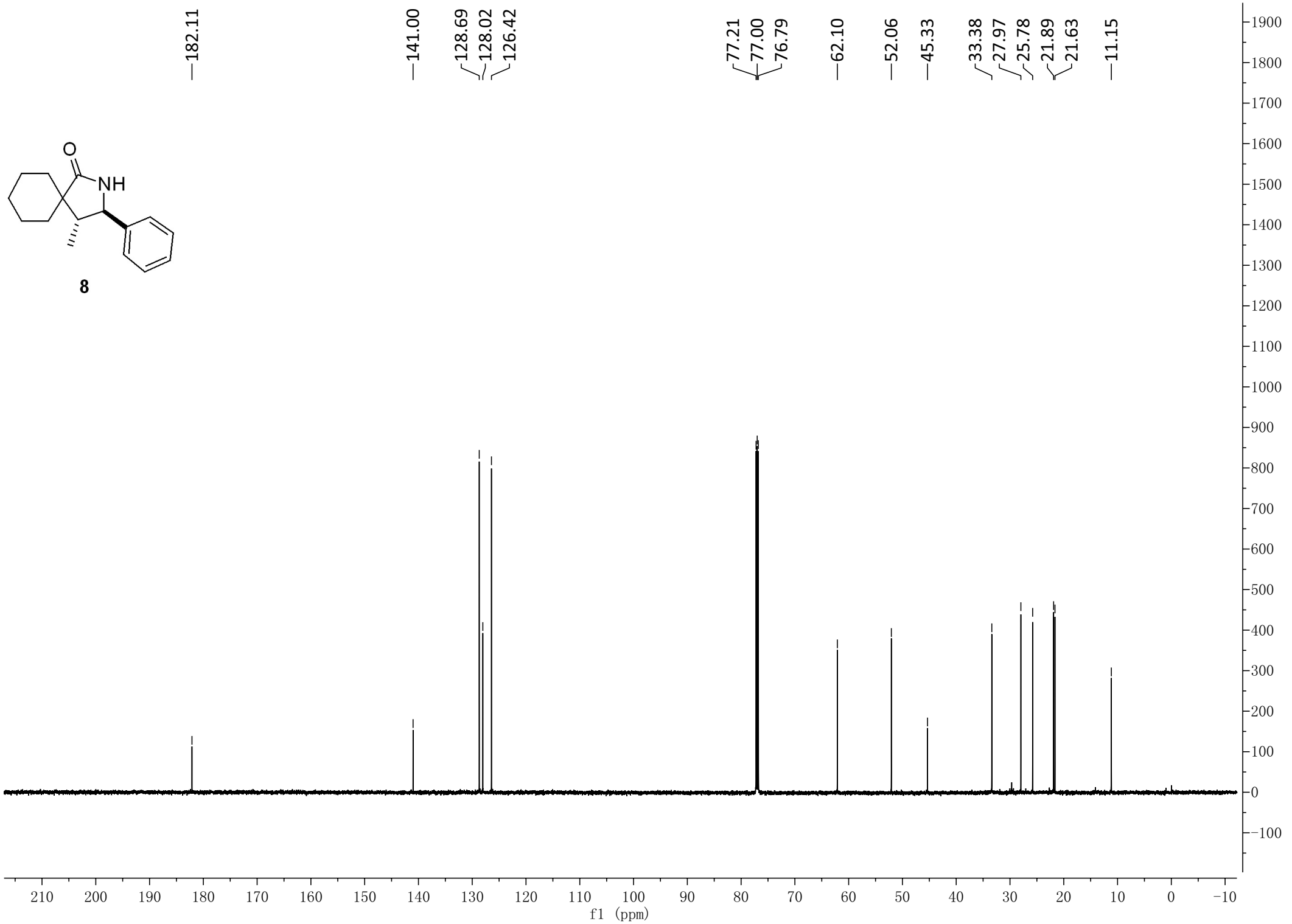
1 Det.A Ch1/214nm

PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	58.495	48469953	452925	95.383	94.251
2	62.419	2346102	27626	4.617	5.749
Total		50816055	480551	100.000	100.000

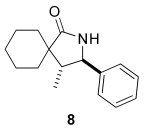

7.38
7.36
7.34
7.32
7.31
7.29
7.26
5.76
4.14
4.12
2.23
2.20
1.91
1.89
1.87
1.74
1.73
1.70
1.66
1.60
1.59
1.57
1.51
1.50
1.49
1.47
1.39
1.35
1.27
1.24
0.98
0.96
O
NH
8
5.13
1.00
1.04
1.08
1.18
9.29
3.17
f1 (ppm)


182.11
141.00
128.69
128.02
126.42
77.21
77.00
76.79
62.10
52.06
45.33
33.38
27.97
25.78
21.89
21.63
11.15
O
NH
8
f1 (ppm)

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-46-RAC-4.lcd

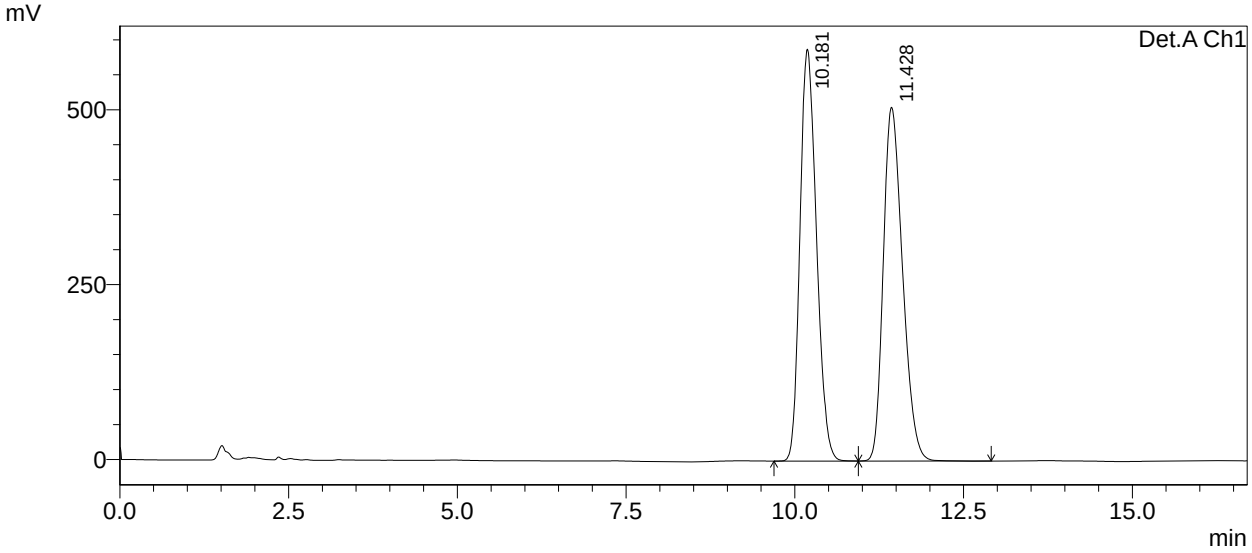
Acquired by	: Admin
Sample Name	: JGP-15-46A-RAC-4
Sample ID	: AD-H,98/2,2.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-46-RAC-4.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-6-2 8:07:25
Data Processed	: 2018-6-2 8:24:10



8

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-46-RAC-4.lcd



1 Det.A Ch1/214nm

PeakTable

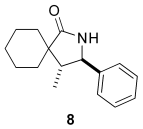
Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	10.181	10021276	588901	49.883	53.795
2	11.428	10068334	505820	50.117	46.205
Total		20089611	1094721	100.000	100.000

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

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-46A-1.lcd

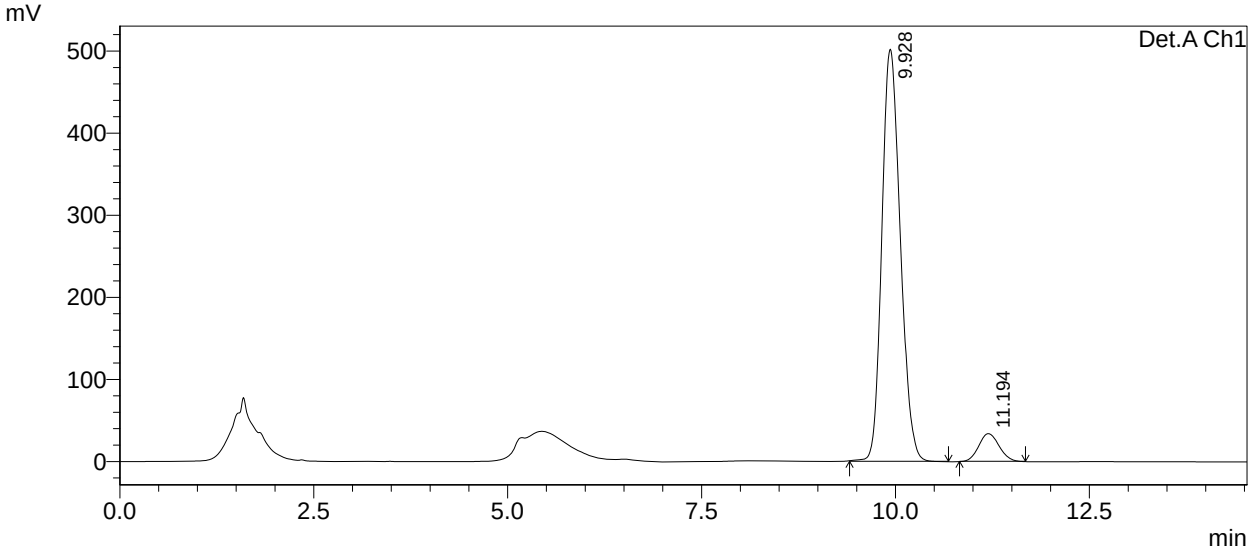
Acquired by	: Admin
Sample Name	: JGP-15-46A-1
Sample ID	: AD-H,98/2,2.0,214
Vail #	:
Injection Volume	: 2 uL
Data File Name	: JGP-15-46A-1.lcd
Method File Name	: 123.lcm
Batch File Name	:
Report File Name	: Default.lcr
Data Acquired	: 2018-6-2 8:43:36
Data Processed	: 2018-6-4 9:55:12



8

<Chromatogram>

C:\LabSolutions\Data\Project1\Project1\JGP\JGP-15-46A-1.lcd

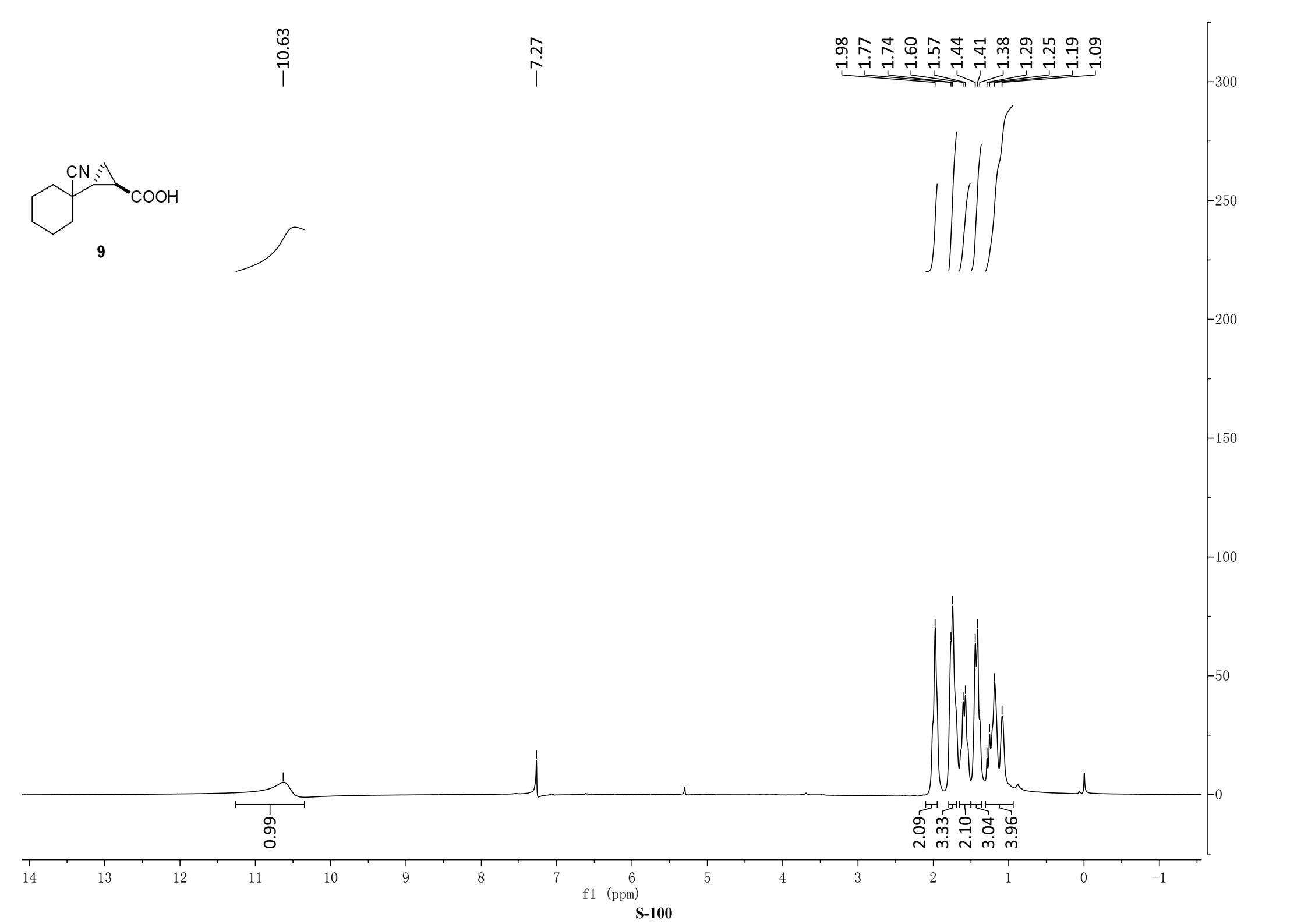


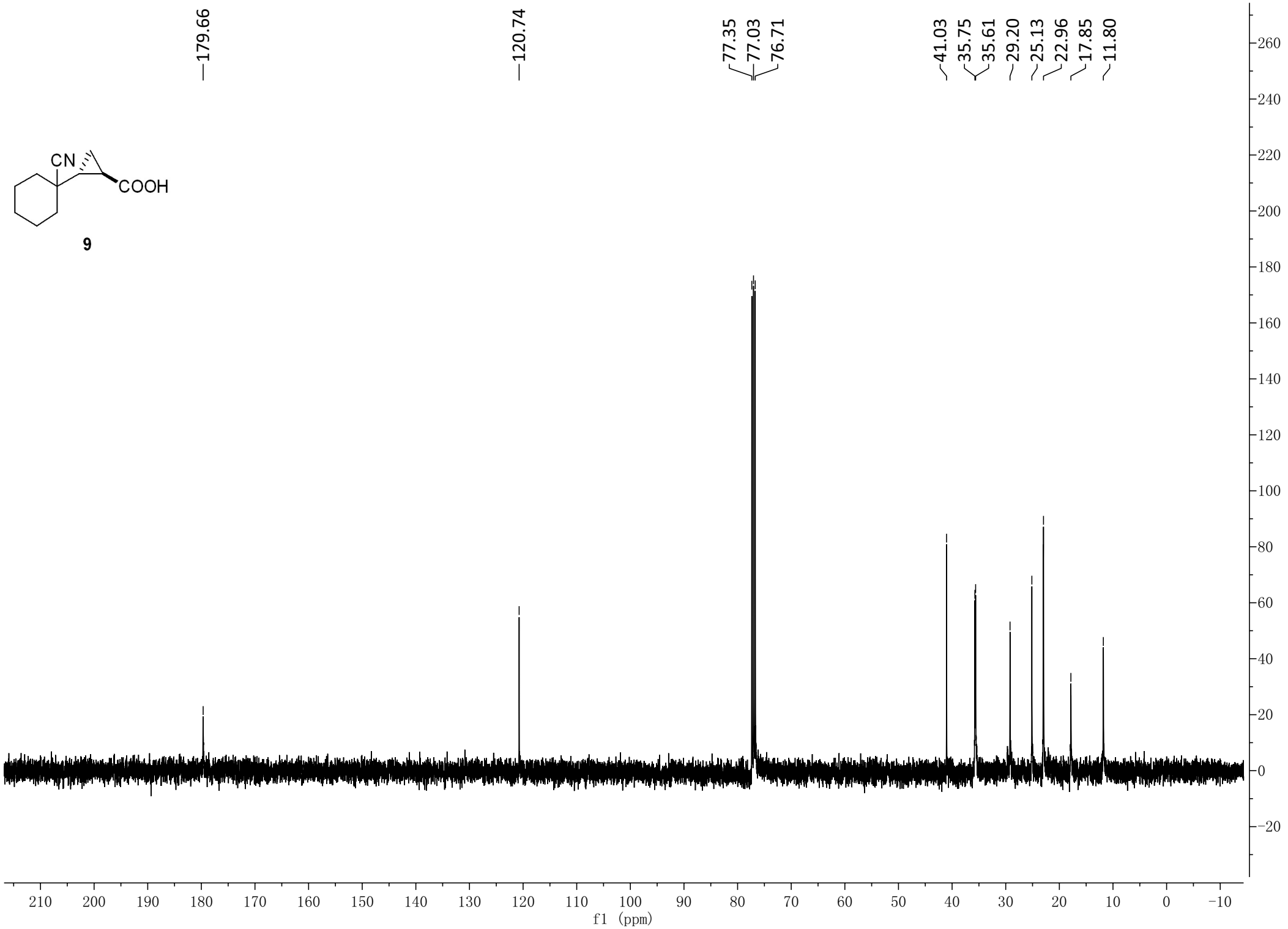
1 Det.A Ch1/214nm

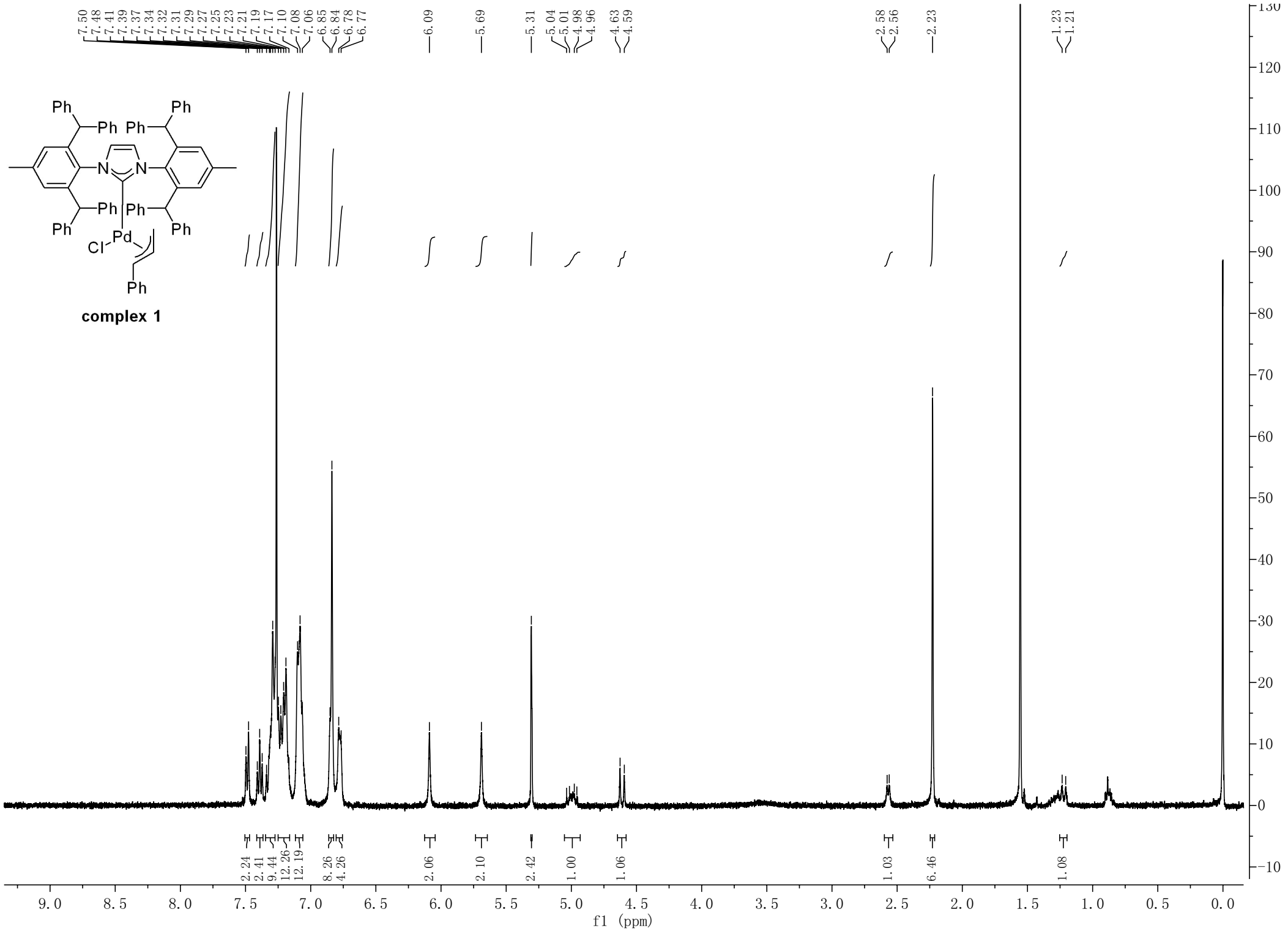
PeakTable

Detector A Ch1 214nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.928	8304155	502050	93.193	93.709
2	11.194	606586	33705	6.807	6.291
Total		8910742	535755	100.000	100.000


10.63
7.27
1.98
1.77
1.74
1.60
1.57
1.44
1.41
1.38
1.29
1.25
1.19
1.09
CN
COOH
9
0.99
2.09
3.33
2.10
3.04
3.96
f1 (ppm)


179.66
120.74
77.35
77.03
76.71
41.03
35.75
35.61
29.20
25.13
22.96
17.85
11.80
CN
COOH
9
f1 (ppm)


7.50
7.48
7.41
7.39
7.37
7.34
7.32
7.31
7.29
7.27
7.25
7.23
7.21
7.19
7.17
7.10
7.08
7.06
6.85
6.84
6.78
6.77
6.09
5.69
5.31
5.04
5.01
4.98
4.96
4.63
4.59
2.58
2.56
2.23
1.23
1.21
Ph
Ph
Ph
Ph
N
N
Ph
Ph
Ph
Ph
Ph
Pd
Cl
Ph
2.24
2.41
9.44
12.26
12.19
8.26
4.26
2.06
2.10
2.42
1.00
1.06
1.03
6.46
1.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

complex 1