Support Information

Regioselective One-pot Three Component Synthesis of Chiral 2-Iminoselenazolines by Sonication

Wong-Jin Chang[1], Manohar V. Kulkarni[1], and Chung-Ming Sun*[1,2]

[1]*Department of Applied Chemistry, National Chiao-Tung University, Hsinchu 300-10, Taiwan* [2]*Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, 100, Shih-Chuan 1st Road, Kaohsiung, 807-08, Taiwan*

E-mail : cmsun@mail.nctu.edu.tw

General Information

All reactions were performed under an inert atmosphere with unpurified reagents and dry solvents. Analytical thin-layer chromatography (TLC) was performed using 0.25 mm silica gel coated Kiselgel 60 F254 plates. Flash chromatography was performed using the indicated solvent and silica gel 60 (Merck, 230-400 mesh). 1H NMR (400MHz), ^{1}H NMR (600 MHz) and ^{13}C NMR (100 MHz), ^{13}C NMR (150 MHz) spectra were recorded on a VARIAN VNMRS-600 NMR spectrometer and VARIAN VNMRS-400 NMR spectrometer ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were recorded on a Bruker DRX-300 NMR. Chemical shifts are reported in parts per million (ppm) on the scale from an internal standard. Mass spectra were recorded on an electrospray ionization (Impact HD, EVOQ, Bruker), samples being introduced by infusion method using the electrospray ionization (ESI) technique. High-resolution mass spectra (HRMS) were recorded on a MAT-95XL high resolution mass spectrometer. IR spectra were recorded with a HORIBA FREEXACT-II FT-720 spectrometer and Bruker Tensor 27. Optical rotations are reported as $[\alpha]^{D}_{20}$.

Materials:

All starting materials were purchased from Alfa, Aldrich and Acros and used directly.

General Procedure for the Preparation of isoselenocyanates 1a-1f

A mixture of amine (1 eq) and ethyl formate (15ml) was sonicated for 120 minutes (TLC). Excess of ethyl formate was removed on a rotavapor to obtain N-formylanilne. Formation of these intermediates was confirmed by 1H-NMR. To this compound was added, triphosgene (0.5 eq) and triethyl amine (5 eq). This mixture was refluxed in dichloromethane 10 ml for 8 hrs (TLC). To this solution selenium powder (3 eq) was added and refluxing was continued for further 8 hrs (TLC). The solid was removed by filter paper and solvent was removed by rotavaporand the product was purified was column chromatography. This is a modified procedure from the reported one by reference 1 and reference 2. The following isoselenocyanates 1a and 1f have been prepared. The spectral data for these compounds is in agreement with the reported values in the literature.

General Procedure for the Preparation of 2-Iminoselenazolines 5a-5l

Chiral aminoester hydrochlorides **2** (1eq) were treated with saturated Sodium bicarbonate solution in water and free base was liberated. This was extracted in dichloromethane, which was removed later on a rotavapor. To the free aminoester **2** was added, isoselenocyanate **1** (1.5eq) and the mixture was sonicated in dry acetonitrile. Time for sonication was 15 min. The reaction was monitored by TLC. To

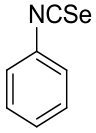
the reaction mixture was added bromoketone **4** (1.5 eq). And the sonication was continued further. The time for sonication in the second stage Varied between 40 min (TLC). At the end of the reaction, acetonitrile was removed on a rotavapor and the compounds were purified by column chromatography. Compounds prepared by this method along with their spectral data for 2-iminoselenazole **5a-5l** (Scheme1) is as follows:

General Procedure for the Preparation of 2-Iminoselenazolines 7a-7f

Chiral aminoester hydrochlorides **2** (1eq) were treated with saturated Sodium bicarbonate solution in water and free base was liberated. This was extracted in dichloromethane, which was removed later on a rotavapor. To the free aminoester **2** was added, isoselenocyanate **1** (1.5eq) and the mixture was sonicated in dry acetonitrile. Time for sonication was 15 min. The reaction was monitored by TLC. To the reaction mixture was added bromoketone **6** (1.5 eq). And the sonication was continued further. The time for sonication in the second stage Varied between 90 min (TLC). At the end of the reaction, acetonitrile was removed on a rotavapor and the compounds were purified by column chromatography. Compounds prepared by this method along with their spectral data for 2-iminoselenazole **7a-7f** (Scheme1) is as follows:

General Procedure for the Preparation of 2-Iminoselenazolines 9a-9c

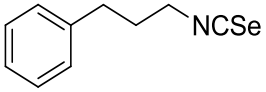
Chiral aminoester hydrochlorides **2** (1eq) were treated with saturated Sodium bicarbonate solution in water and free base was liberated. This was extracted in dichloromethane, which was removed later on a rotavapor. To the free aminoester **2** was added, isoselenocyanate **1** (1.5eq) and the mixture was sonicated in dry acetonitrile. Time for sonication was 15 min. The reaction was monitored by TLC. To the reaction mixture was added bromoketone **8** (1.5 eq). And the sonication was continued further. The time for sonication in the second stage Varied between 60 min (TLC). At the end of the reaction, acetonitrile was removed on a rotavapor and the compounds were purified by column chromatography. Compounds prepared by this method along with their spectral data for 2-iminoselenazole **9a-9c** (Scheme1) is as follows:



1a

Isoselenocyanatobenzene (1a)

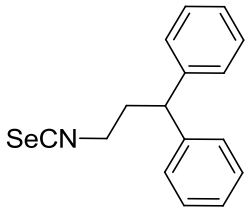
See reference 1



1b

(3-isoselenocyanatopropyl)benzene (1b)

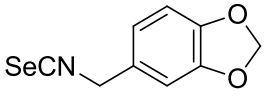
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.31 (m, *J* = 2H), 7.26-7.18 (m, *J* = 3H), 3.55 (t, *J* = 6.5 Hz, 2H), 2.76 (t, *J* = 7.4 Hz, 2H), 2.12-1.90 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 128.4, 128.2, 126.2, 44.3, 32.1, 30.6; IR (KBr, *v*) 3055, 2947, 2927, 2146, 1453, 700cm^{-1}; MS(EI-MS) *m/z* : 225; HRMS : calcd for $C_{10}H_{11}NSe$ m/z: 225.0057; Found : 205.0371



1c

(3-isoselenocyanatopropane-1,1-diyl)dibenzene (1c)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.29 (m, 4H), 7.25-7.19 (m, 6H), 4.08 (t, *J* = 8.0 Hz, 1H), 3.51 (t, *J* = 6.6 Hz, 2H), 2.45 (dt, *J* = 7.9, 6.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 128.8, 127.7, 126.8, 47.8, 43.8, 34.9; IR (KBr, *v*) 3025, 2922, 2139, 1492, 1450, 698cm^{-1}; MS(EI-MS) *m/z* : 301; HRMS : calcd for $C_{16}H_{15}NSe$ m/z: 301.0370; Found : 301.0365

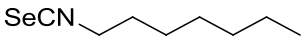


1d

5-(isoselenocyanatomethyl)benzo[d][1,3]dioxole (1d)

^{1}H NMR (400 MHz, $CDCl_3$) δ6.71-6.70 (m, 3H), 5.89 (s, 2H), 4.62 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.64, 147.33, 126.09, 120.33, 108.00, 107.11, 101.04, 48.51; IR (KBr, *v*) 2896, 2137, 1501, 1445, 1251, 1038cm^{-1}; MS(EI-MS) *m/z* : 241; HRMS :

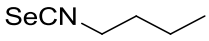
calcd for $C_9H_7NO_2Se$ m/z: 240.9642; Found : 240.9635



1e

1-isoselenocyanatoheptane (1e)

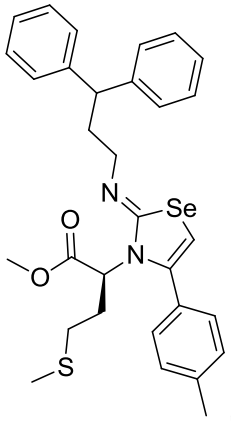
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.47 (t, *J* = 6.7 Hz, 2H), 1.69-1.48 (m, 2H), 1.36-1.00 (m, 8H), 0.72 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 45.6, 31.5, 29.5, 28.3, 26.4, 22.4, 14.0; IR (KBr, *v*) 2955, 2927, 2857, 2143, 1455, 1344cm^{-1}; MS(EI-MS) *m/z* : 205; HRMS : calcd for $C_8H_{15}NSe$ m/z: 205.0370; Found : 205.0371



1f

1-isoselenocyanatobutane (1f)

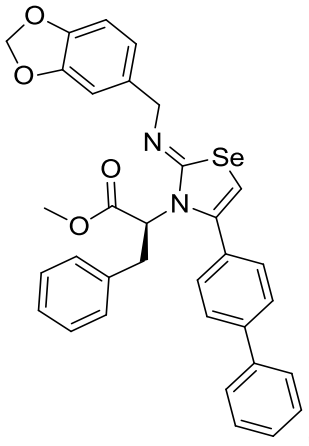
See reference 2



5a

(S,Z)-methyl 2-(2-((3,3-diphenylpropyl)imino)-4-(p-tolyl)-1,3-selenazol-3(2H)-yl)-4-(methylthio)butanoate (5a)

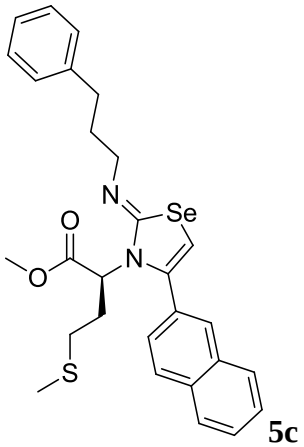
^{1}H NMR (600 MH$_Z$, $CDCl_3$) δ 7.19-7.14 (m, 8H), 7.12-7.10 (m, 2H), 7.04-7.01 (m,4H), 6.08 (s, 1H), 3.79 (t, *J* = 7.7 Hz, 1H), 3.76-3.71 (m, 4H), 3.65-3.61 (m, 2H), 2.66-2.62 (m, 1H), 2.60-2.56 (m, 1H), 2.45 (s, 3H), 2.34-2.19 (m, 4H), 2.09 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.0, 161.0, 144.2, 143.6, 141.6, 138.6, 130.3, 129.2, 128.8, 128.3, 128.2, 127.6, 127.5, 126.0, 94.0, 69.00, 51.9, 48.6, 45.3, 33.3, 33.2, 30.8, 21.3, 15.5; IR (KBr, *v*) 3026, 2949, 2918, 1742, 1608, 1451, 1435, 702cm^{-1}; MS (ESI-MS) *m/z* : 579 $(M+H)^+$; HRMS : calcd for $C_{30}H_{31}BrN_2O_2SSe$ m/z: 578.1506; Found : 579.1583 $(M+H)^+$; $[\alpha]^{18}{}_D$ -67.57 (c 0.03, CH_2Cl_2); HPLC: t_R = 12.344 min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang500801



5b

(S,Z)-methyl 2-(4-([1,1'-biphenyl]-4-yl)-2-((benzo[d][1,3]dioxol-5-ylmethyl)imino)-1,3-selenazol-3(2H)-yl)-3-phenylpropanoate (5b)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61-7.55 (m, 2H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.45-7.43 (m, 2H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.26-7.17 (m, 7H), 6.56 (d, *J* = 8.0 Hz, 2H), 6.26 (d, *J* = 7.9 Hz, 1H), 6.13 (s, 1H), 5.89 (dd, *J* = 4.2, 1.3 Hz, 2H), 4.99 (d, *J* = 15.1 Hz, 1H), 4.82 (d, *J* = 15.2 Hz, 1H), 3.71 (s, 4H), 3.29 (dd, *J* = 13.3, 5.0 Hz, 1H), 3.11 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 194.6, 172.6, 161.3, 147.4, 146.4, 146.1, 141.6, 140.1, 139.7, 138.1, 133.9, 131.9, 131.7, 129.5, 129.4, 129.3, 128.9, 128.8, 128.3, 128.2, 127.7, 127.3, 127.2, 127.0, 126.9, 126.3, 120.7, 108.1, 107.7, 100.8, 94.96, 72.3, 51.9, 49.2, 40.1, 28.7; IR (KBr, *v*) 3029, 2950, 1740, 1603, 1489, 1445, 1247, 1039, 699cm^{-1}; MS (ESI-MS) *m/z* : 457 $(M+H)^+$; HRMS : calcd for $C_{33}H_{28}N_2O_4Se$ m/z: 597.1292; Found : 597.1290 $(M+H)^+$; $[\alpha]^{18}{}_D$ -217.89 (c 0.04, CH_2Cl_2); HPLC: t_R = 58.344min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang603201

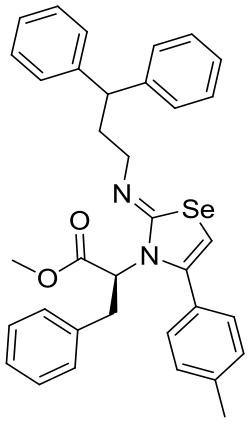


5c

(S,Z)-methyl 4-(methylthio)-2-(4-(naphthalen-2-yl)-2-((3-phenylpropyl)imino)-1,3-selenazol-3(2H)-yl)butanoate (5c)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89-7.78 (m, 4H), 7.55-7.53 (m, 2H), 7.34 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.02-6.97 (m, 3H), 6.89 (dd, *J* = 7.4, 2.0Hz, 1H), 6.19 (s, 1H), 3.88-3.84 (m, 1H), 3.77-3.72 (m, 4H), 3.65-3.63 (m, 1H), 2.66-2.57 (m, 2H), 2.35-2.22 (m, 2H), 2.23-2.20 (m, 2H), 2.10 (s, 3H), 2.03−1.73 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 173.0, 161.3, 141.9, 141.1, 133.1, 133.0, 130.7, 128.3, 128.2, 128.1, 128.1, 128.0,

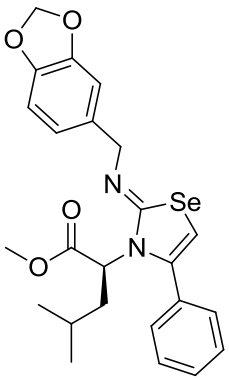
127.8, 126.8, 126.7, 126.1, 125.6, 95.0, 69.2, 52.0, 46.0, 33.3, 32.7, 30.8, 29.1, 15.5; IR (KBr, *v*) 3106, 3058, 2948, 2918, 1742, 1612, 1434, 1267, 750, 479cm^{-1}; MS (ESI-MS) *m/z* : 539 $(M+H)^+$; HRMS : calcd for $C_{28}H_{30}N_2O_2SSe$ m/z: 538.1193; Found : 539.1274 $(M+H)^+$; $[\alpha]^{18}{}_D$ -83.38 (c 0.03, CH_2Cl_2); HPLC: t_R = 17.646min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang501202



5d

(S,Z)-methyl 2-(2-((3,3-diphenylpropyl)imino)-4-(p-tolyl)-1,3-selenazol-3(2H)-yl)-3-Phenylpropanoate (5d)

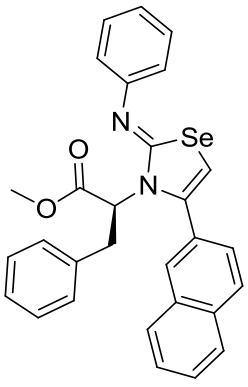
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14-7.11 (m 2H), 7.07-6.94 (m, 13H), 6.91 (d, *J* = 4.0Hz, 2H), 6.83 (d, *J* = 3.9Hz, 2H), 5.86 (s, 1H), 3.70-3.63 (m, 2H), 3.61-3.57 (m, 1H), 3.55 (s, 3H), 3.43-3.40 (m, 1H), 3.23-3.19 (m, 1H), 3.07-3.03 (m,1H), 2.28 (s, 3H), 2.06-1.98 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.9, 160.9, 144.4, 143.8, 141.6, 138.7, 138.3, 130.4, 129.5, 129.3, 128.9, 128.4, 128.4, 128.3, 128.2, 127.7, 126.4, 126.1, 126.0, 94.1, 72.2, 51.9, 48.9, 45.4, 40.2, 33.1, 21.4; IR (KBr, *v*) 3027, 2949, 1743, 1603, 1452, 1263, 700cm^{-1}; MS (ESI-MS) *m/z* : 595 $(M+H)^+$; HRMS : calcd for $C_{35}H_{34}N_2O_2Se$ m/z: 594.1786; Found : 595.1858 $(M+H)^+$; $[\alpha]^{19}{}_D$ -55.93 (c 0.05, CH_2Cl_2); HPLC: t_R = 16.488min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang609104



5e

(S,Z)-methyl 2-(2-((benzo[d][1,3]dioxol-5-ylmethyl)imino)-4-phenyl-1,3-selenazol-3(2H)-yl)-4-methylpentanoate (5e)

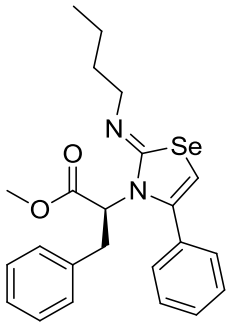
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.28 (m, 3H), 7.19 (dd, *J* = 8.0, 1.4 Hz, 2H), 6.63 (d, *J* = 1.5 Hz, 1H), 6.60-6.51 (m, 1H), 6.28 (dd, *J* = 8.0, 1.4 Hz, 1H), 6.13 (s, 1H), 5.88 (s, 2H), 4.87 (s, 2H), 3.73 (s, 3H), 3.50 (dd, *J* = 9.1, 4.9 Hz, 1H), 1.83 (ddd, *J* = 14.0, 9.1, 5.2 Hz, 1H), 1.71 (ddd, *J* = 13.4, 8.7, 4.9 Hz, 1H), 1.63-1.51 (m, 1H), 0.89 (dd, *J* = 15.9, 6.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.7, 160.6, 147.4, 146.3, 141.9, 133.2, 131.9, 129.1, 128.8, 128.3, 120.7, 108.2, 107.6, 100.8, 94.6, 69.1, 51.7, 49.1, 42.8, 24.7, 23.2, 21.8; IR (KBr, *v*) 2954, 2869, 1742, 1616, 1490, 1445, 1246, 1039, 701 cm^{-1}; MS (ESI-MS) *m/z* : 487 $(M+H)^+$; $[\alpha]^{20}_D$ +16.60 (c 0.02, CH_2Cl_2); HRMS : calcd for $C_{24}H_{27}N_2O_4Se$ m/z: 487.1131 Found : 487.1131 $(M+H)^+$; HPLC: t_R = 13.596min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang703201



5f

(S,Z)-methyl 2-(4-(naphthalen-2-yl)-2-(phenylimino)-1,3-selenazol-3(2H)-yl)-3-phenylpropanoate (5f)

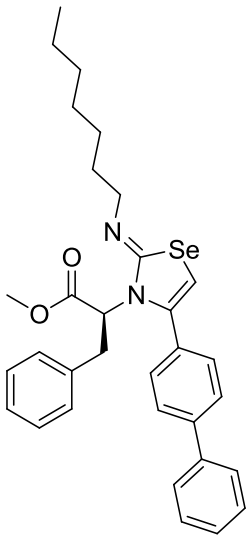
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95-7.83 (m, 1H), 7.80-7.67 (m, 2H), 7.61-7.51 (m, 2H), 7.48 (dd, *J* = 19.3, 11.3 Hz, 2H), 7.36 (d, *J* = 7.3 Hz, 1H), 7.29-7.10 (m, 5H), 7.10-6.85 (m, 4H), 6.07-5.85 (m, 1H), 4.65-4.50 (m, 1H), 4.04 (dd, *J* = 13.8, 11.3 Hz, 1H), 3.92 (s, 3H), 3.25 (dd, *J* = 13.9, 3.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.0, 156.8, 152.5, 142.0, 138.1, 133.5, 133.2, 130.3, 130.1, 130.0, 129.4, 129.0, 128.7, 128.4, 128.2, 127.3, 127.1, 127.0, 126.5, 124.1, 121.2, 94.8, 61.6, 53.1, 33.5; IR (KBr, *v*) 3058, 3029, 2948, 2927, 1716, 1616, 1585, 1407, 1223, 754, 698cm^{-1}; MS (ESI-MS) *m/z* : 513 $(M+H)^+$; HRMS : calcd for $C_{29}H_{24}N_2O_2Se$ m/z: 512.1003; Found : 513.1077 $(M+H)^+$; $[\alpha]^{18}_D$ -80.06 (c 0.04, CH_2Cl_2); HPLC: t_R = 16.444min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang504802



5g

(S,Z)-methyl 2-(2-(butylimino)-4-phenyl-1,3-selenazol-3(2H)-yl)-3-phenylpropanoate (5g)

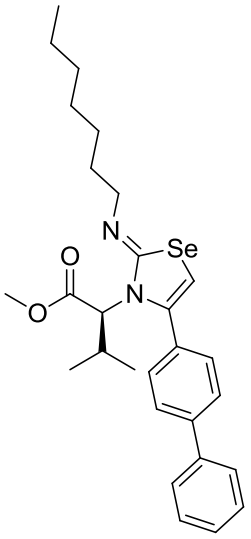
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.35 (m, 3H), 7.35-7.24 (m, 5H), 7.24-7.13 (m, 1H), 6.14-5.98 (m, 1H), 3.95-3.78 (m, 1H), 3.71 (s, 3H), 3.67-3.53 (m, 1H), 3.33 (dd, *J* = 13.4, 5.9 Hz, 1H), 3.16 (dd, *J* = 13.2, 7.8 Hz, 1H), 1.48-1.25 (m, 2H), 1.16-0.94 (m, 2H), 0.71 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 161.0, 141.9, 138.2, 133.4, 129.4, 128.8, 128.6, 128.3, 128.0, 126.2, 94.3, 72.2, 51.7, 45.9, 40.0, 29.7, 19.5, 13.5; IR (KBr, *v*) 2956, 2931, 1744,1614, 1443, 1272,1154,700cm^{-1}; MS (ESI-MS) *m/z* : 443 $(M+H)^+$; HRMS : calcd for $C_{23}H_{26}N_2O_2Se$ m/z: 443.1232 ; Found : 443.1234 $(M+H)^+$; $[\alpha]^{20}_D$ -366.75 (c 0.05, CH_2Cl_2); HPLC: t_R = 15.468min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang705801



5h

(S,Z)-methyl 2-(4-([1,1'-biphenyl]-4-yl)-2-(heptylimino)-1,3-selenazol-3(2H)-yl)-3-phenylpropanoate (5h)

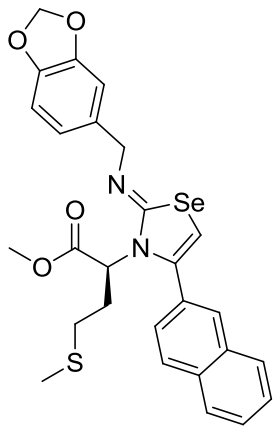
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.6-7.60 (m, 4H), 7.52-7.44 (m, 2H), 7.44-7.35 (m, 3H), 7.35−7.16 (m, 5H), 6.12 (s, 1H), 3.96-3.80 (m, 1H), 3.75−3.60 (m, 5H), 3.34 (dd, *J* = 13.4, 5.9 Hz, 1H), 3.24-3.10 (m, 1H), 1.53-1.36 (m, 2H), 1.27-1.01 (m, 8H), 0.84 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 161.1, 141.8, 141.5, 140.2, 138.3, 129.6, 129.3, 128.9, 128.2, 127.7, 127.1, 127.0, 126.3, 94.6, 72.4, 51.9, 46.4, 40.2, 31.6, 28.7, 27.7, 26.4, 22.6, 14.1; IR (KBr, *v*) 3061, 3030, 2952, 2927, 2856, 1745, 1602, 1487, 1435, 1272, 915, 756, 698cm^{-1}; MS (ESI-MS) *m/z* : 561(M+H)$^{+}$; HRMS calcd for $C_{32}H_{37}N_2O_2Se$ m/z: 561.2015 Found : 561.2022 (M+H)$^{+}$; $[\alpha]^{20}_{D}$ +30.88 (c 0.03, CH_2Cl_2); HPLC: t_R = 18.924min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang705601



5i

(S,Z)-methyl 2-(4-([1,1'-biphenyl]-4-yl)-2-(heptylimino)-1,3-selenazol-3(2H)-yl)-3-methylbutanoate (5i)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.55 (m, 4H), 7.53-7.32 (m, 5H), 6.13 (s, 1H), 3.97-3.84 (m, 1H), 3.74 (s, 3H), 3.70-3.57 (m, 1H), 3.18 (d, *J* = 6.2 Hz, 1H), 2.32 (dd, *J* = 13.1, 6.6 Hz, 1H), 1.59-1.37 (m, 2H), 1.32-0.95 (m, 8H), 0.81 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 160.3, 141.9, 141.5, 140.2, 132.6, 129.3, 129.0, 128.9, 127.7, 127.2, 127.1, 127.0, 94.3, 77.4, 77.3, 77.0, 76.7, 51.7, 46.4, 32.8, 31.5, 29.7, 28.7, 27.9, 26.4, 22.5, 19.7, 18.7, 14.0; IR (KBr, *v*) 3031, 2956, 2928, 2856, 1745, 1720, 1604, 1488, 1372, 1273, 1298, 847, 759, 698cm^{-1}; MS (ESI-MS) *m/z* : 513 $(M+H)^+$; HRMS : calcd for $C_{28}H_{37}N_2O_2Se$ m/z: 513.2015 Found : 513.2021 $(M+H)^+$; $[\alpha]^{20}{}_D$ -57.35 (c 0.01, CH_2Cl_2); HPLC: t_R = 9.524min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang705501

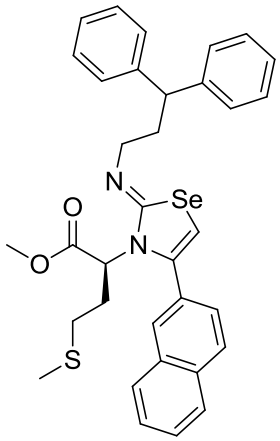


5j

(S,Z)-methyl 2-(2-((benzo[d][1,3]dioxol-5-ylmethyl)imino)-4-(naphthalen-2-yl)-1,3-selenazol-3(2H)-yl)-4-(methylthio)butanoate (5j)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89-7.73 (m, 3H), 7.71 (s, 1H), 7.57-7.45 (m, 2H), 7.28 (dd, *J* = 8.4, 1.7 Hz, 1H), 6.69 (d, *J* = 1.6 Hz, 1H), 6.57 (d, *J* = 8.0 Hz, 1H), 6.29 (dd, *J* = 7.9, 1.5 Hz, 1H), 6.26 (s, 1H), 5.88 (s, 2H), 5.01-4.77 (m, 2H), 3.76 (s, 3H), 3.66 (dd, *J* = 7.9, 4.9 Hz, 1H), 2.56-2.36 (m, 2H), 2.26-2.12 (m, 2H), 2.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 161.5, 147.5, 146.4, 141.9, 133.1, 132.8, 131.7, 130.36, 128.6, 128.1, 128.0, 127.7, 126.8, 126.6, 126.2, 120.5, 108.0, 107.6, 100.8, 95.3, 68.9, 52.0, 49.4, 33.1, 30.5, 15.4; IR (KBr, *v*) 3108, 3056, 2949, 2915, 1739, 1614, 1502, 1489, 1444, 1246, 1039, 936,479cm^{-1}; MS (ESI-MS) *m/z* : 555 $(M+H)^+$; HRMS : calcd for $C_{27}H_{26}N_2O_4SSe$ m/z: 555.0851 Found : 555.0863$(M+H)^+$;

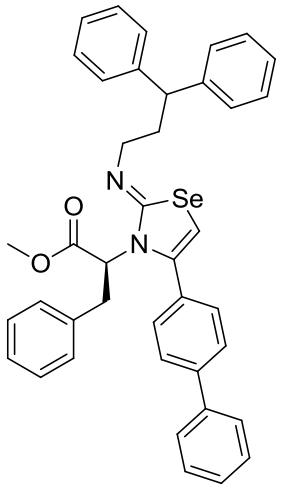
$[\alpha]^{21}{}_{D}$ -77.40 (c 0.01, CH_2Cl_2); HPLC: t_R = 29.064min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang703001 *



5k

(S,Z)-methyl 2-(2-((3,3-diphenylpropyl)imino)-4-(naphthalen-2-yl)-1,3-selenazol-3(2H)-yl)-4-(methylthio)butanoate (5k)

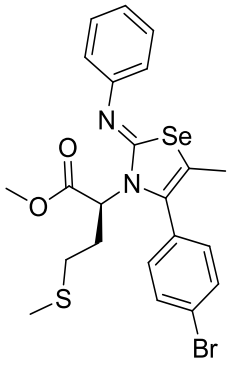
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, *J* = 11.5, 4.3 Hz, 1H), 7.87-7.75 (m, 3H), 7.63-7.56 (m, 2H), 7.30 (dt, *J* = 12.9, 6.5 Hz, 2H), 7.02-6.83 (m, 9H), 6.21 (s, 1H), 3.85-3.71 (m, 4H), 3.71-3.58 (m, 2H), 2.72-2.52 (m, 2H), 2.39-2.17 (m, 4H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 161.0, 144.1, 143.4, 141.6, 133.2, 133.0, 130.6, 128.4, 128.3, 128.2, 128.2, 128.1, 127.8, 127.5, 127.4, 126.9, 126.7, 126.1, 126.0, 94.9, 77.3, 77.0, 76.7, 69.1, 52.0, 48.6, 45.5, 33.3, 30.8, 15.5; IR (KBr, *v*) 3105, 3058, 2950, 2923, 1740, 1612, 1261, 1031, 751, 702, 479cm^{-1}; MS (ESI-MS) *m/z* : 615 $(M+H)^+$; HRMS : calcd for $C_{34}H_{34}N_2O_2SSe$ m/z: 614.1579 Found : 615.1598$(M+H)^+$; $[\alpha]^{20}{}_{D}$ -689.50 (c 0.01, CH_2Cl_2); HPLC: t_R = 19.716min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang706301



5l

(S,Z)-methyl 2-(4-([1,1'-biphenyl]-4-yl)-2-((3,3-diphenylpropyl)imino)-1,3-selenazol-3(2H)-yl)-3-phenylpropanoate (5l)

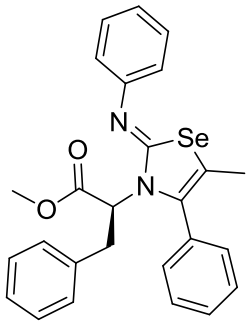
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 5.1, 3.3 Hz, 2H), 7.60-7.47 (m, 4H), 7.47-7.37 (m, 1H), 7.34-7.23 (m, 4H), 7.23-7.01 (m, 9H), 7.01-6.87 (m, 2H), 6.11 (s, 1H), 3.95-3.78 (m, 2H), 3.72 (s, 3H), 3.65-3.51 (m, 1H), 3.35 (dd, *J* = 13.5, 5.6 Hz, 1H), 3.19 (dd, *J* = 13.5, 8.0 Hz, 1H), 2.27-2.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 160.8, 144.2, 143.6, 141.5, 141.2, 140.2, 138.2, 132.0, 129.4, 129.2, 128.9, 128.3, 128.3, 128.1, 127.7, 127.5, 127.5, 127.1, 127.0, 126.2, 126.0, 126.0, 94.6, 72.2, 51.9, 48.7, 45.3, 40.1, 33.0; MS (ESI-MS) *m/z* : 657 $(M+H)^+$; IR (KBr, *v*) HRMS : calcd for $C_{40}H_{37}N_2O_2Se$ m/z: 657.2015 Found : 657.2024 $(M+H)^+$; HPLC: t_R =30.432 min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang704201 *



7a

(S,Z)-methyl 2-(4-(4-bromophenyl)-5-methyl-2-(phenylimino)-1,3-selenazol-3(2H)-yl)-4-(methylthio)butanoate (7a)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (t, *J* = 7.0 Hz, 2H), 7.34-7.24 (m, 3H), 7.18 (d, *J* = 8.0 Hz, 1H), 7.08-7.02 (m, 1H), 6.96 (dd, *J* = 8.2, 0.9 Hz, 2H), 4.34 (s, 1H), 3.77 (s, 3H), 2.66 (d, *J* = 8.7 Hz, 1H), 2.45-2.37 (m, 2H), 2.34-2.24 (m, 1H), 1.99 (overlap s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.7, 152.0, 134.4, 132.3, 132.1, 131.9, 130.3, 129.4, 123.6, 123.4, 120.6, 58.5, 52.5, 30.7, 27.5, 15.2, 15.2; IR (KBr, *v*) 3057, 3028, 2949, 2916, 1745, 1606, 1579, 1489, 1331, 1230, 1070, 1011, 833, 696, 517cm^{-1}; MS (ESI-MS) *m/z* : 539 $(M+H)^+$; HRMS : calcd for $C_{22}H_{23}BrN_2O_2SSe$ m/z: 537.9829; Found : 538.9912 $(M+H)^+$; $[\alpha]^{21}{}_D$ -108.9 (c 0.01, CH_2Cl_2); HPLC: t_R = 21.06min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang501601



7b

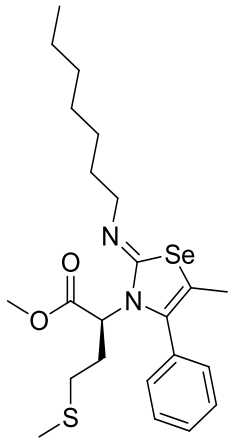
(S,Z)-methyl 2-(5-methyl-4-phenyl-2-(phenylimino)-1,3-selenazol-3(2H)-yl)-3-phenylpropanoate (7b)

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48-7.21 (m, 9H), 7.12 (t, *J* = 11.5 Hz, 4H), 7.00 (dd, *J* = 10.5, 7.3 Hz, 2H), 5.90 (d, *J* = 7.5 Hz, 1H), 4.28 (dd, *J* = 10.8, 3.8 Hz, 1H), 3.97 (dd, *J* = 13.7, 11.0 Hz, 1H), 3.85 (d, *J* = 7.5 Hz, 3H), 3.25 (dd, *J* = 13.8, 3.8 Hz, 1H), 1.87 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.3, 156.2, 152.8, 138.5, 136.3, 131.6, 131.3, 130.4, 130.2, 129.9, 129.2, 128.8, 127.0, 123.8, 121.2, 106.4, 78.0, 77.5, 77.1, 61.9, 52.9, 33.6, 15.4; IR (KBr, *v*) 3060, 3028, 1720, 1581,1396, 1070, 1011, 760,700cm^{-1}; MS (ESI-MS) *m/z* : 477 $(M+H)^+$; HRMS : calcd for $C_{26}H_{24}N_2O_2Se$ m/z: 477.1081; Found : 477.1083 $(M+H)^+$; $[\alpha]^{20}{}_D$ +368.4 (c 0.05, CH_2Cl_2); HPLC: t_R = 10.22min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang501801

7c

(S,Z)-methyl 2-(2-(butylimino)-5-methyl-4-phenyl-1,3-selenazol-3(2H)-yl)-3-phenylpropanoate (7c)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.33 (m, 3H), 7.33-7.12 (m, 7H), 3.77-3.60 (m, 4H), 3.47-3.35 (m, 1H), 3.31 (dd, *J* = 13.4, 5.9 Hz, 1H), 3.14 (dd, *J* = 13.2, 7.8 Hz, 1H), 1.97 (s, 3H), 1.46-1.22 (m, 2H), 1.11-0.94 (m, 2H), 0.69 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 160.0, 138.3, 136.1, 132.0, 130.1, 129.4, 128.6, 128.4, 128.3, 128.0, 126.1, 106.5, 72.4, 51.7, 46.1, 40.1, 29.8, 19.5, 14.8, 13.5; IR (KBr, *v*) 3028, 2956, 2871, 1744, 1614, 1443, 1272, 1154, 700cm^{-1}; MS (ESI-MS) *m/z* : 457 $(M+H)^+$; HRMS : calcd for $C_{24}H_{29}N_2O_2Se$ m/z: 457.1389 ; Found : 457.1397 $(M+H)^+$; $[\alpha]^{19}_D$ -81.18 (c 0.04, CH_2Cl_2); HPLC: t_R = 15.468min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang705701

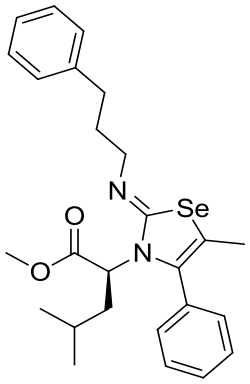


7d

(S,Z)-methyl 2-(2-(heptylimino)-5-methyl-4-phenyl-1,3-selenazol-3(2H)-yl)-4-(methylthio)butanoate (7d)

1H NMR (400 MHz, $CDCl_3$) δ 7.46-7.28 (m, 3H), 7.19 (d, *J* = 6.5 Hz, 2H), 3.67 (s, 3H), 3.63-3.52 (m, 2H), 3.42-3.35 (m, 1H), 2.62-2.49 (m, 2H), 2.20-2.09 (m, 2H),

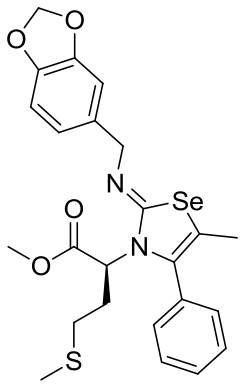
2.05 (s, 3H), 1.94 (m, 3H), 1.45-1.32 (m, 2H), 1.16-0.96 (m, 8H), 0.77 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 160.2, 136.0, 131.9, 130.00, 128.5, 128.4, 128.3, 106.5, 69.1, 51.7, 46.2, 33.1, 31.3, 30.6, 28.4, 27.5, 26.2, 22.3, 15.3, 14.7, 13.8; IR (KBr, *v*) 2952, 2925, 2855, 1743, 1633, 1601, 1435, 1271, 1157, 777, 707cm^{-1}; MS (ESI-MS) *m/z* : 483 $(M+H)^+$; HRMS : calcd for $C_{23}H_{35}N_2O_2SSe$ m/z: 483.1579 Found : 483.1582 $(M+H)^+$; $[\alpha]^{20}{}_D$ -24.08 (c 0.03, CH_2Cl_2);HPLC: t_R = 8.696min, 9:1hexane/2-propanol, flow: 0.5ml/min. Chang705201



7e

(S,Z)-methyl 4-methyl-2-(5-methyl-4-phenyl-2-((3-phenylpropyl)imino)-1,3-selenazol-3(2H)-yl) pentanoate (7e)

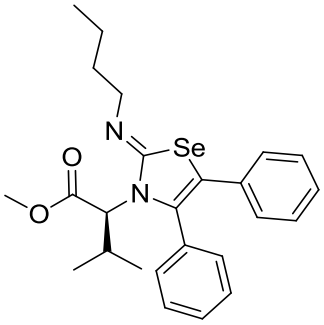
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.31 (m, 2H), 7.31-7.07 (m, 4H), 7.02-6.88 (m, 2H), 3.72 (s, 4H), 3.53-3.49 (m, 2H), 2.40 (dd, *J* = 15.1, 7.7 Hz, 2H), 2.00 (s, 3H), 1.94-1.66 (m, 5H), 0.96 (dd, *J* = 21.5, 4.5 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.9, 159.4, 141.5, 136.0, 132.0, 130.1, 128.5, 128.1, 128.0, 125.5, 106.5, 69.4, 51.8, 46.1, 43.0, 32.7, 29.2, 24.9, 23.2, 21.9, 14.9; IR (KBr, *v*) 3084, 2953, 2888, 1744, 1634, 1603, 1451, 1271, 700cm^{-1}; MS (ESI-MS) *m/z* : 485 $(M+H)^+$; HRMS : calcd for $C_{26}H_{32}N_2O_2Se$ m/z: 485.1702 Found : 485.1704 $(M+H)^+$; $[\alpha]^{20}{}_D$ -68.63 (c 0.04, CH_2Cl_2); HPLC: t_R = 9.321min, 9:1hexane/2-propanol, flow: 0.5ml/min. Chang704901



7f

(S,Z)-methyl 2-(2-((benzo[d][1,3]dioxol-5-ylmethyl)imino)-5-methyl-4-phenyl-1,3-selenazol-3(2H)-yl)-4-(methylthio)butanoate (7f)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.27 (m, 3H), 7.06 (s, 2H), 6.59-6.53 (m, 2H), 6.21 (dd, *J* = 8.0, 1.4 Hz, 1H), 5.85 (s, 2H), 4.71 (s, 2H), 3.72 (s, 3H), 3.60 (dd, *J* = 8.1, 4.8 Hz, 1H), 2.58-2.33 (m, 2H), 2.19-2.06 (m, 2H), 2.05 (s, 3H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 160.7, 147.2, 146.2, 135.8, 131.9, 131.4, 130.3, 128.5, 128.2, 120.3, 107.9, 107.4, 107.2, 100.6, 69.0, 51.8, 49.1, 33.0, 30.5, 15.3, 14.8; IR (KBr, *v*) 3057, 2949, 2914, 1740, 1601, 1489, 1444, 1246, 1039, 479cm^{-1}; MS (ESI-MS) *m/z* : 519 $(M+H)^+$; HRMS : calcd for $C_{24}H_{26}N_2O_4SSe$ m/z: 519.0851 Found : 519.0855 $(M+H)^+$; $[\alpha]^{20}_D$ -76.94 (c 0.04, CH_2Cl_2); HPLC: t_R = 15.924min, 9:1hexane/2-propanol, flow: 0.5ml/min. Chang702901

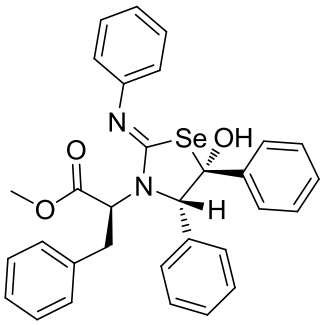


9a

(S,Z)-methyl 2-(2-(butylimino)-4,5-diphenyl-1,3-selenazol-3(2H)-yl)-3-methylbutanoate (9a)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.34 (m, 3H), 7.28-7.26 (m, 2H), 7.08-7.00 (m, 3H), 6.93-6.91 (m, 2H), 3.83-3.76 (m, 1H), 3.74 (s, 3H), 3.55-3.47 (m, 1H), 3.26 (d, *J* = 6.2 Hz, 1H), 2.39-2.31 (m, 1H), 1.60-1.48 (m, 2H), 1.17-1.07 (m, 2H), 1.03 (t, *J* = 7.3, 6H), 0.73 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 158.3, 136.4, 134.5, 132.4, 130.4, 129.6, 128.6, 128.5, 128.3, 127.8, 125.9, 110.4, 76.5, 51.4, 45.9,

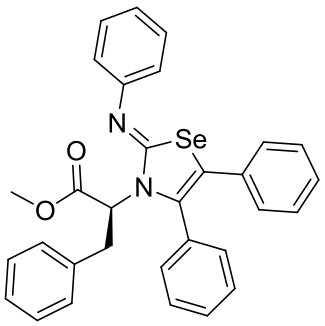
32.5, 29.9, 19.5, 19.5, 18.4, 13.4; IR (KBr, *v*) 3057, 3022, 2959, 2932, 1744, 1619, 1465, 1380, 1300, 1253, 1170, 1026, 757, 696cm^{-1}; MS(ESI-MS) *m/z* : 471(M+H)$^{+}$; HRMS : calcd for $C_{25}H_{31}N_2O_2Se$ m/z: 471.1545 ; Found : 471.1549(M+H)$^{+}$; $[\alpha]^{19}{}_{D}$ -13.45 (c 0.01, CH_2Cl_2); HPLC: t_R = 8.200min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang706001



9b

(S)-methyl 2-((4S,5S,Z)-5-hydroxy-4,5-diphenyl-2-(phenylimino)-1,3-selenazolidin-3-yl)-3-phenylpropanoate (9b)

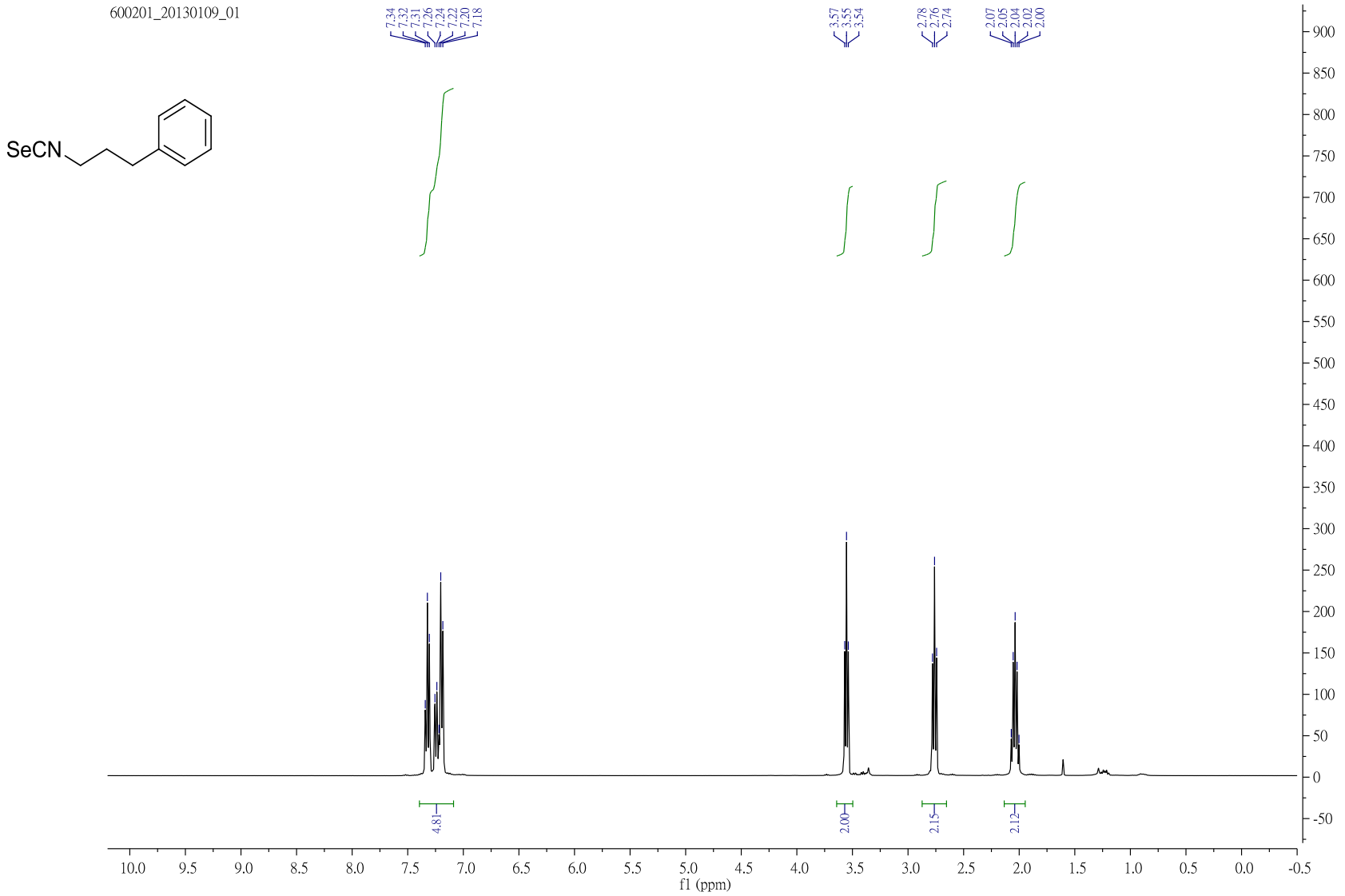
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43-7.34 (m, 2H), 7.34-7.23 (m, 4H), 7.23-7.06 (m, 10H), 7.06-6.96 (m, 4H), 6.03 (s, 1H), 5.16 (s, 1H), 3.87-3.80 (m, 4H), 3.75-3.69 (m, 1H), 3.47 (dd, *J* = 13.6, 6.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ^{13}C NMR (75 MHz, $CDCl_3$) δ 174.6, 156.0, 151.7, 139.4, 138.7, 133.3, 130.5, 130.0, 129.0, 128.3, 128.3, 128.2, 127.8, 127.6, 126.5, 124.0, 121.2, 95.9, 62.5, 56.7, 53.1, 35.4; IR (KBr, *v*) 3330, 3060, 3029, 2951, 2849, 1707, 1627, 1591, 1489, 1448, 1266, 1216, 698cm^{-1}; MS (ESI-MS) *m/z* : 539 (M+H)$^{+}$; HRMS : calcd for $C_{31}H_{28}N_2O_3Se$ m/z: 577.1343; Found : 577.1346 (M+H)$^{+}$; $[\alpha]^{21}{}_{D}$ -78.50 (c 0.01, CH_2Cl_2); HPLC: t_R = 17.6487min, 9:1hexane/2-propanol, flow: 0.5ml/min. chang505101



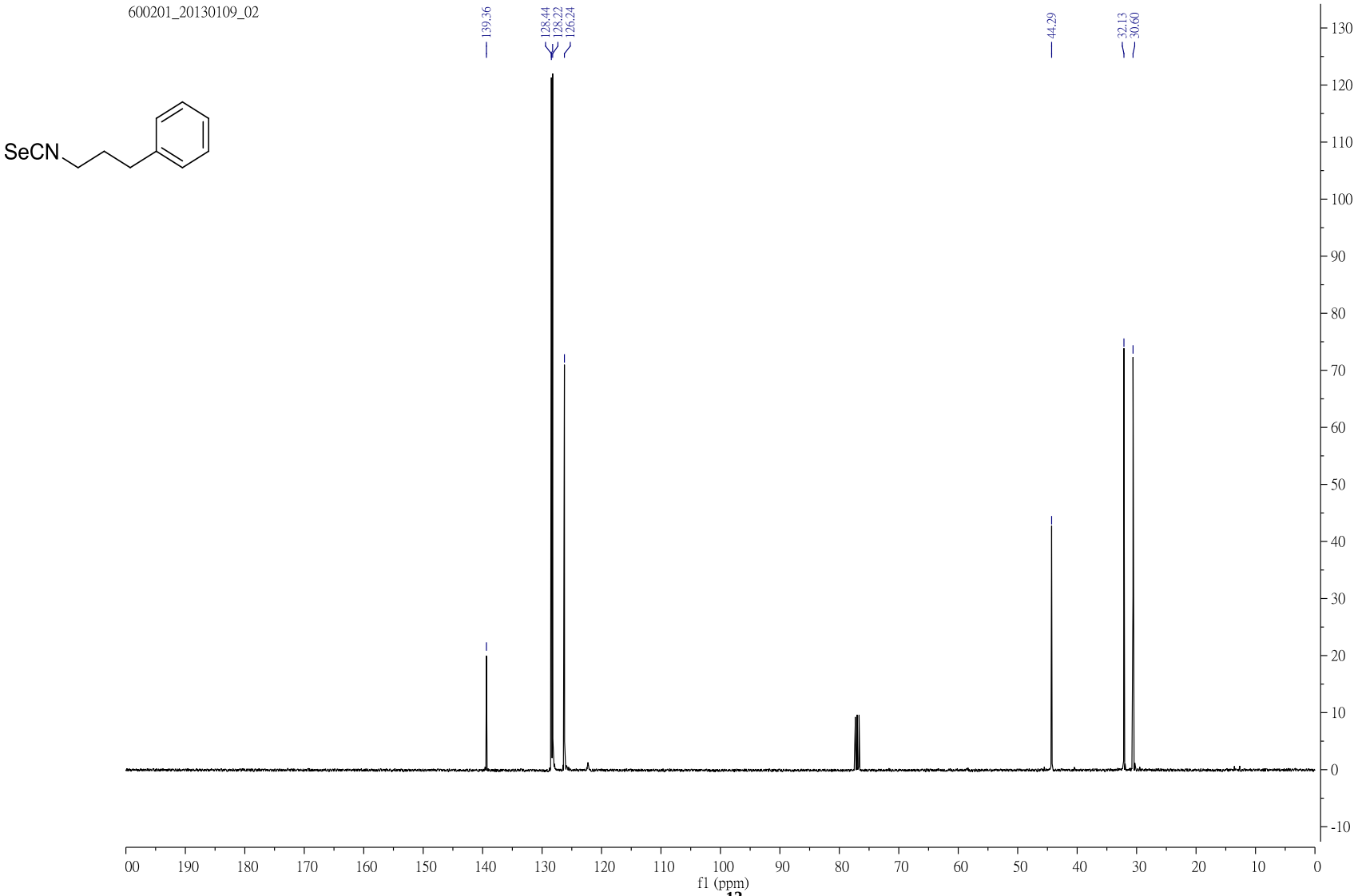
9c

(S,Z)-methyl 2-(4,5-diphenyl-2-(phenylimino)-1,3-selenazol-3(2H)-yl)-3-phenylpropanoate (9c)

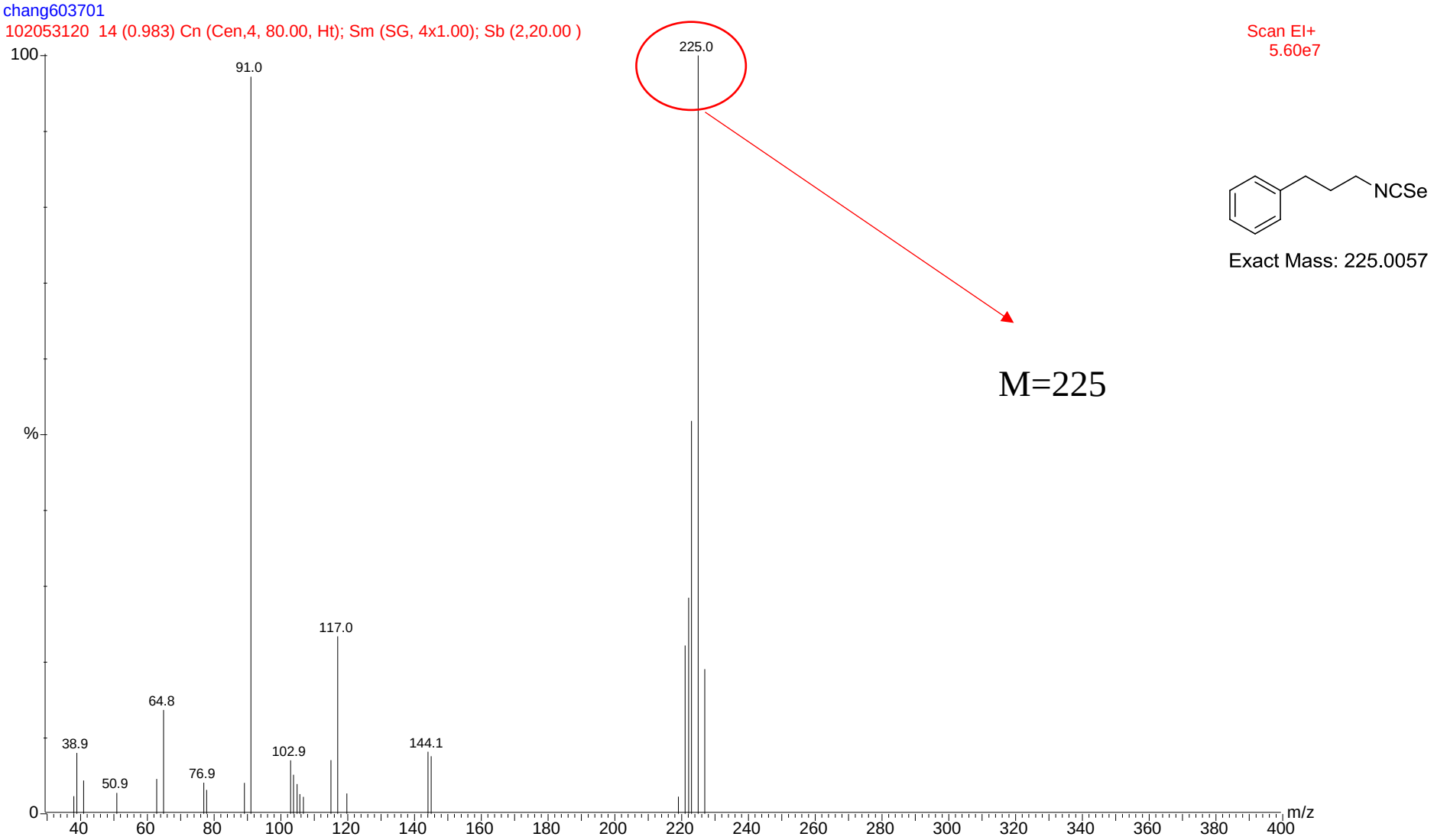
Copies of the NMR spectra


600201_20130109_01
SeCN
7.34
7.32
7.31
7.26
7.24
7.22
7.20
7.18
3.57
3.55
3.54
2.78
2.76
2.74
2.07
2.05
2.04
2.02
2.00
4.81
2.00
2.15
2.12
f1 (ppm)

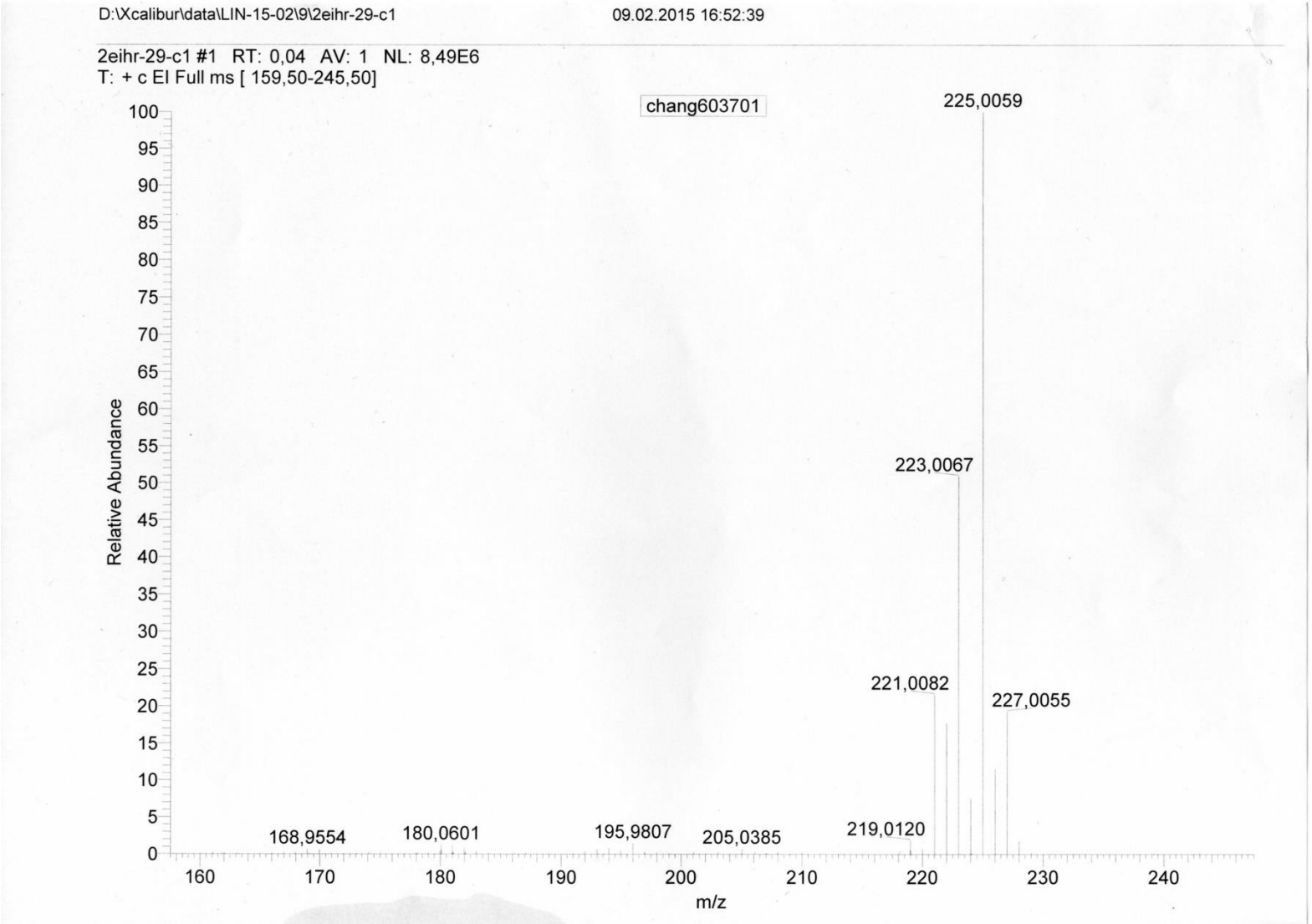
1b H^1-NMR


600201_20130109_02
SeCN
139.36
128.44
128.22
126.24
44.29
32.13
30.60
f1 (ppm)

1b C^{13}-NMR


chang603701
102053120 14 (0.983) Cn (Cen,4, 80.00, Ht); Sm (SG, 4x1.00); Sb (2,20.00)
Scan EI+
5.60e7
225.0
91.0
117.0
64.8
38.9
102.9
144.1
76.9
50.9
100
%
0
m/z
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
NCSe
Exact Mass: 225.0057
M=225

1b LR-MS

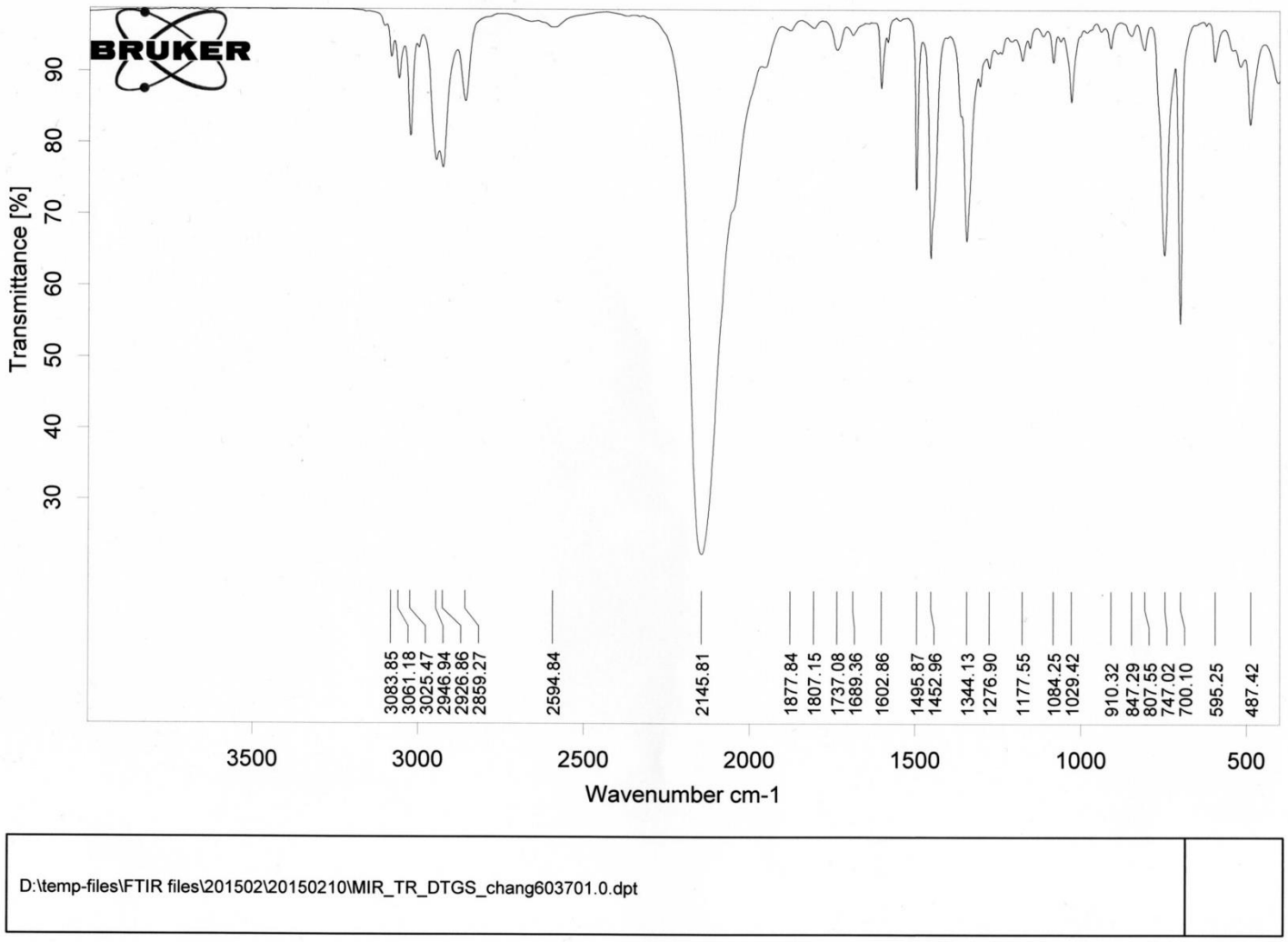

D:\Xcalibur\data\LIN-15-02\9\2eihr-29-c1
09.02.2015 16:52:39
2eihr-29-c1 #1 RT: 0,04 AV: 1 NL: 8,49E6
T: + c EI Full ms [159,50-245,50]
chang603701
225,0059
223,0067
221,0082
227,0055
219,0120
168,9554
180,0601
195,9807
205,0385
Relative Abundance
m/z

1b HR-MS

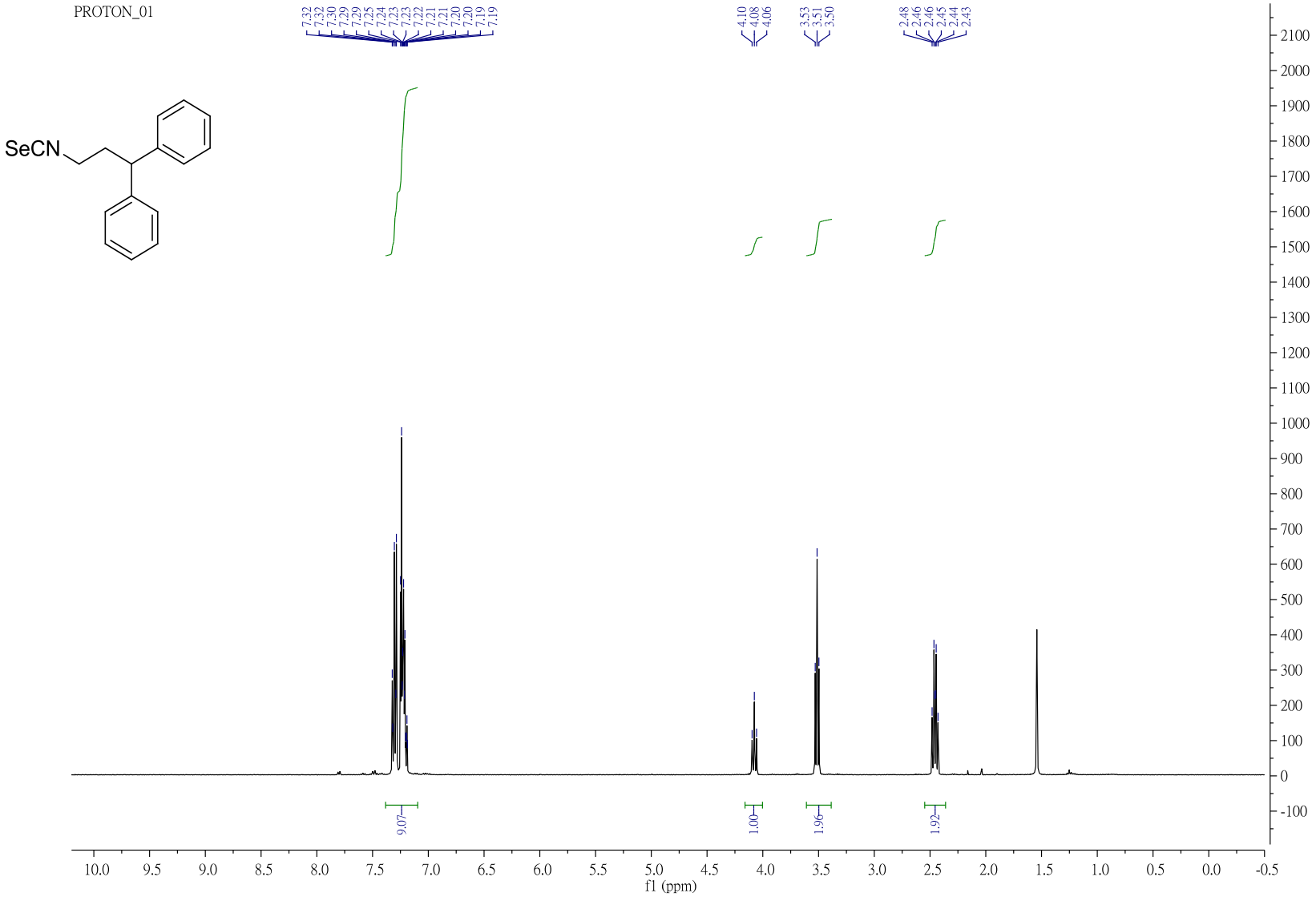
Isotope:	Min. .. Max.		
12 C	0....15		
1 H	0....30		
14 N	0....3		
80 Se	0....1		
78 Se	0....1		
Tolerance Window:	+- 3.00 mmu		
Db/Ring Equiv:	0.. 100	N-Rule:	Do not use
Fits:	3	Charge:	0

File : D:\Xcalibur\data\LIN-15-02\9\2eihr-29-c1.RAW
Full ms [159.500 - 245.500] - Range: 159.500 - 245.500
Scan No. 1 of 10

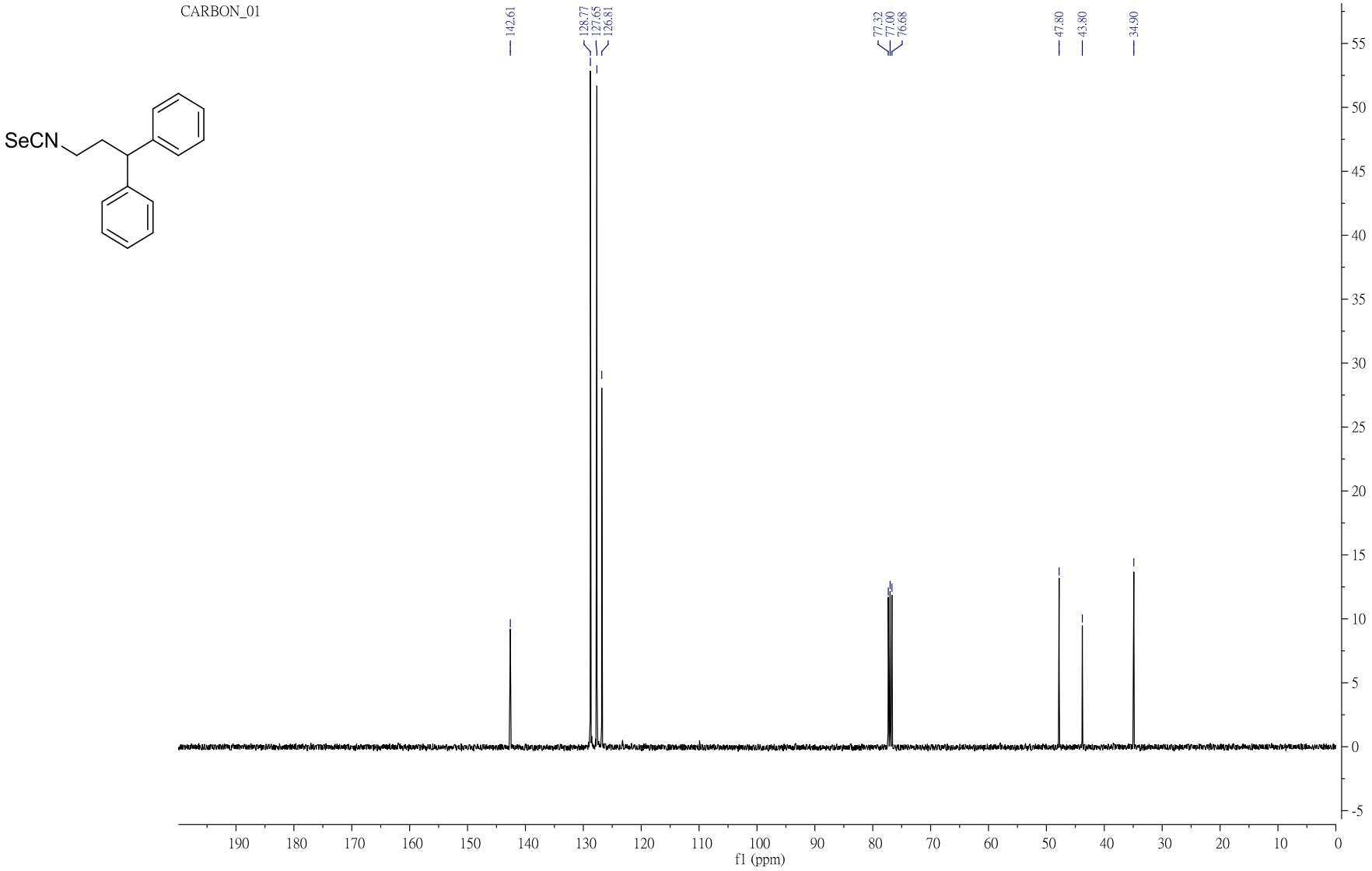
Mass	Relative Intensity	Delta [mmu]	Composition
161.0847	0.3		
168.9554	0.7	-0.2	$C_{7} H_{5} Se_{1}$
169.9629	0.6	-0.6	$C_{7} H_{6} Se_{1}$
179.9655	0.4	1.2	$C_{8} H_{6} {}^{78}Se_{1}$
180.0601	1.2		
180.0844	0.5		
180.9904	1.2		
181.9641	0.8	0.6	$C_{8} H_{6} Se_{1}$
182.0564	0.4		
182.9702	0.4	-1.1	$C_{8} H_{7} Se_{1}$
191.9835	0.4		
192.9842	0.6		
193.9805	0.8	0.6	$C_{6} H_{8} {}^{78}Se_{1}$
194.9747	0.6	-0.5	$C_{6} H_{7} N_{1} {}^{78}Se_{1}$
195.9807	1.4	1.6	$C_{8} H_{8} Se_{1}$
		-2.3	$C_{8} H_{8} N_{1} {}^{78}Se_{1}$
196.9728	0.3	-1.6	$C_{8} H_{7} N_{1} Se_{1}$
203.0365	0.3	-1.2	$C_{8} H_{15} N_{1} {}^{78}Se_{1}$
		2.6	$C_{9} H_{15} Se_{1}$
205.0385	0.7	1.5	$C_{8} H_{15} N_{1} Se_{1}$
		-2.4	$C_{7} H_{15} N_{2} {}^{78}Se_{1}$
207.9833	0.3	0.3	$C_{8} H_{8} N_{1} {}^{78}Se_{1}$
218.1176	0.4		
218.9833	0.5		
219.0120	1.8		
220.0011	0.7		
221.0082	21.6		
222.0094	17.8	0.2	$C_{15} N_{1}$
		-1.8	$C_{11} H_{12} {}^{78}Se_{1}$
223.0067	50.9	0.3	$C_{10} H_{11} N_{1} {}^{78}Se_{1}$
224.0065	7.5		
225.0059	100.0	0.2	$C_{10} H_{11} N_{1} Se_{1}$
226.0085	11.5		
227.0055	19.3		
228.0098	1.7		


BRUKER
Transmittance [%]
90
80
70
60
50
40
30
3083.85
3061.18
3025.47
2946.94
2926.86
2859.27
2594.84
2145.81
1877.84
1807.15
1737.08
1689.36
1602.86
1495.87
1452.96
1344.13
1276.90
1177.55
1084.25
1029.42
910.32
847.29
807.55
747.02
700.10
595.25
487.42
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201502\20150210\MIR_TR_DTGS_chang603701.0.dpt
Page 1/1

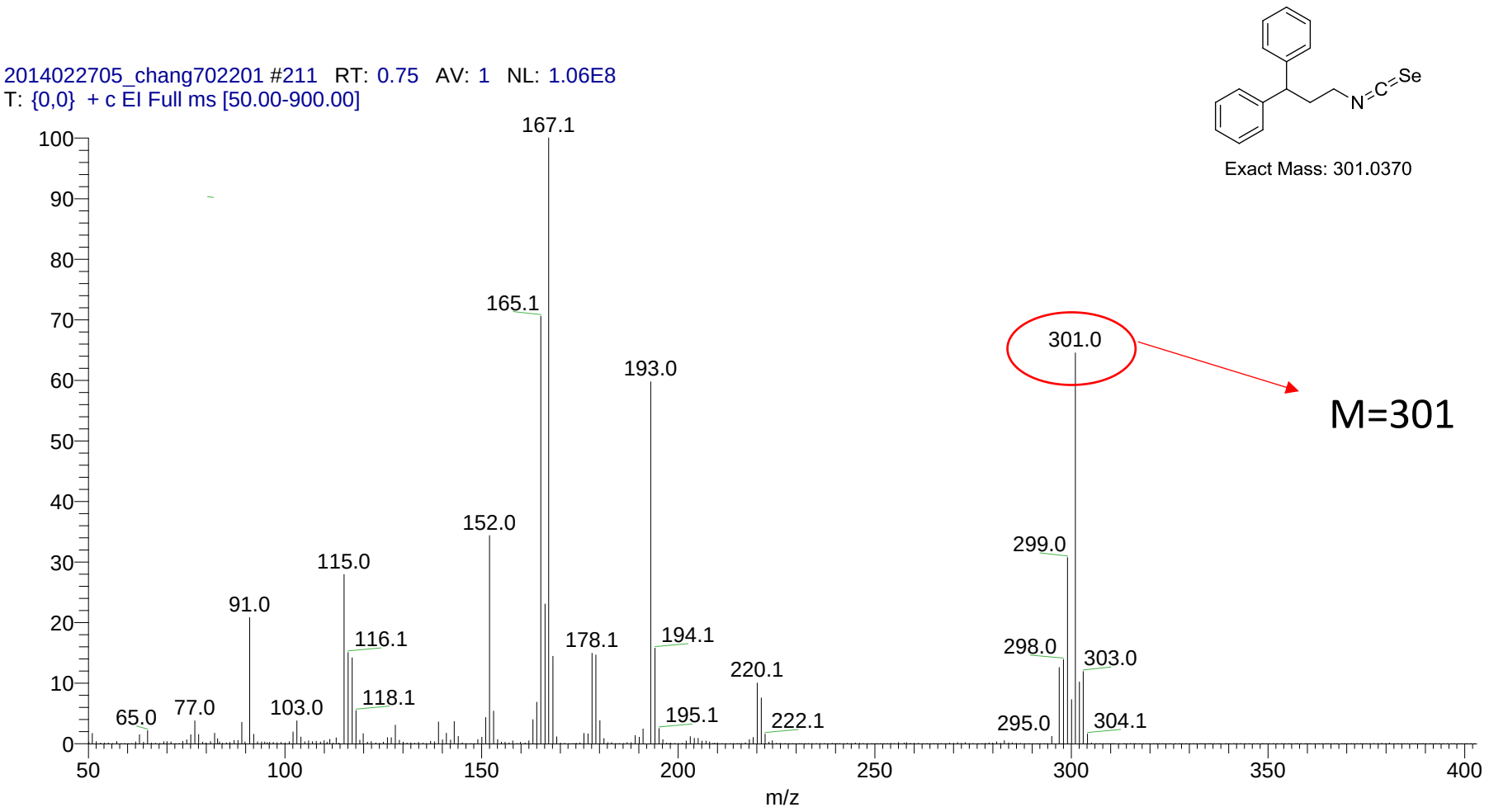
1b FT-IR


PROTON_01
SeCN
7.32
7.32
7.30
7.29
7.29
7.25
7.24
7.23
7.23
7.22
7.21
7.21
7.20
7.20
7.19
7.19
4.10
4.08
4.06
3.53
3.51
3.50
2.48
2.46
2.46
2.45
2.44
2.43
9.07
1.00
1.96
1.92
f1 (ppm)

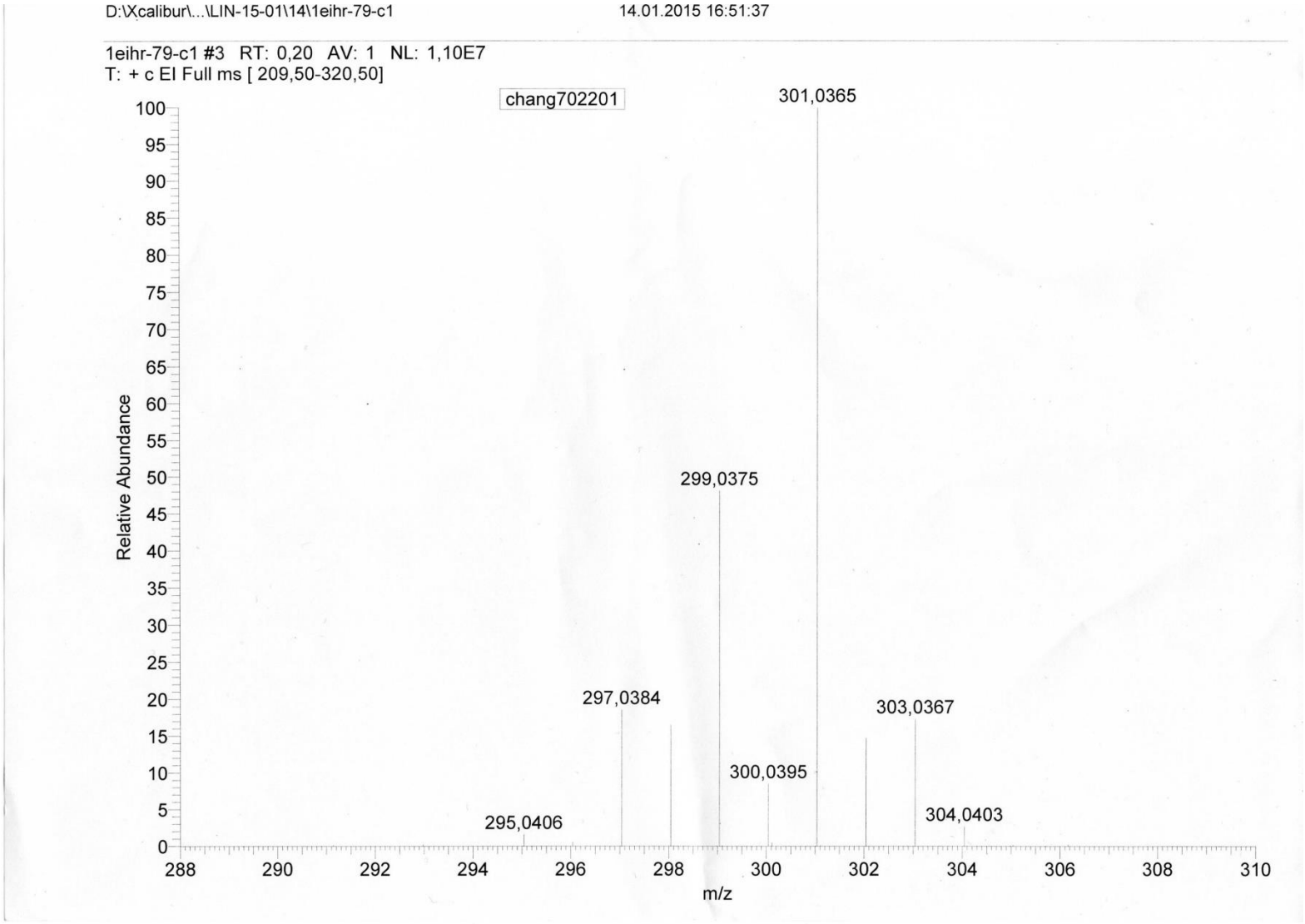
1c H^1-NMR


CARBON_01
SeCN
142.61
128.77
127.65
126.81
77.32
77.00
76.68
47.80
43.80
34.90
f1 (ppm)

1c C^{13}-NMR


2014022705_chang702201 #211 RT: 0.75 AV: 1 NL: 1.06E8
T: {0,0} + c EI Full ms [50.00-900.00]
Exact Mass: 301.0370
M=301
m/z

1c LR-MS

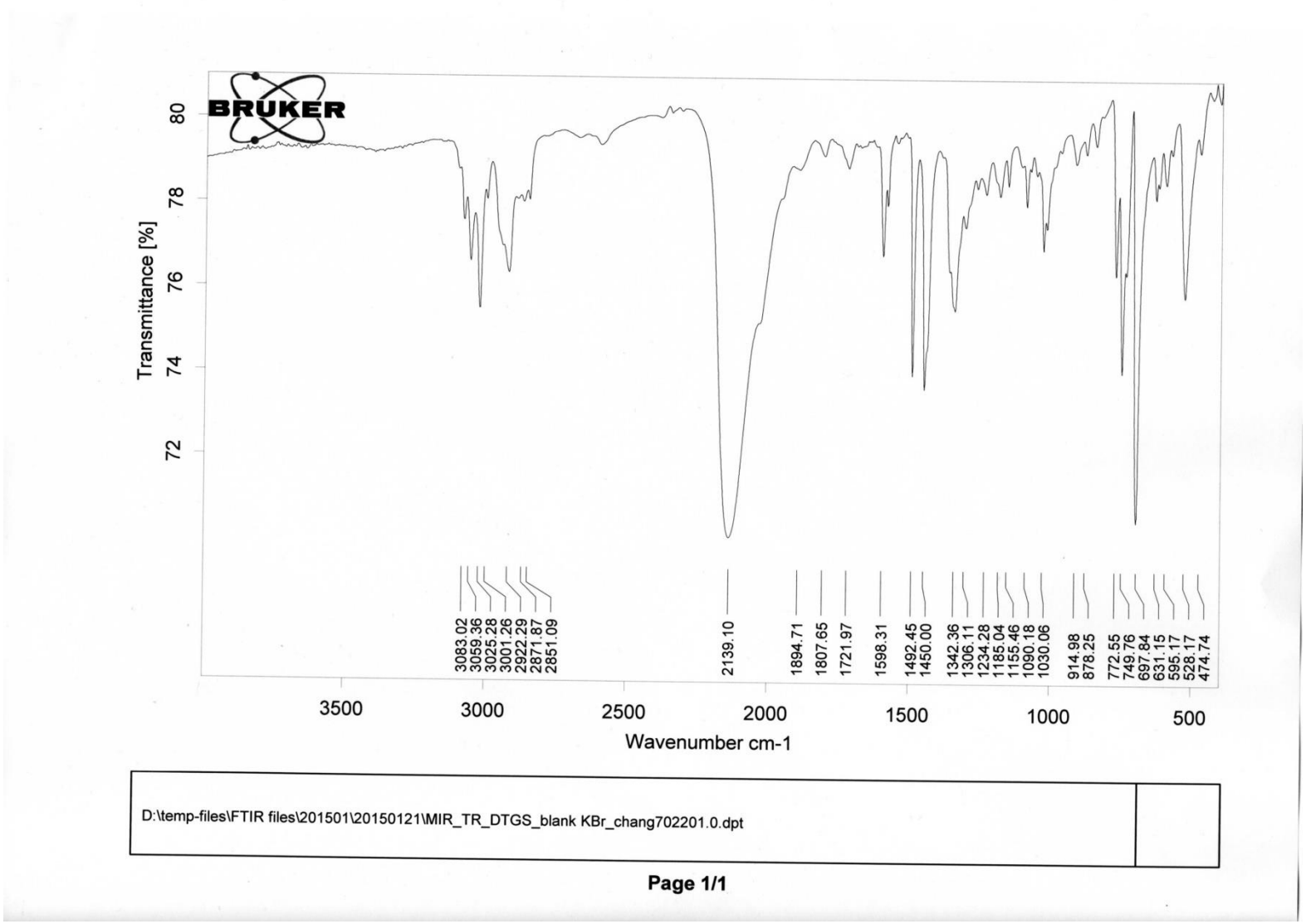

D:\Xcalibur\...\LIN-15-01\14\1eihr-79-c1
14.01.2015 16:51:37
1eihr-79-c1 #3 RT: 0,20 AV: 1 NL: 1,10E7
T: + c EI Full ms [209,50-320,50]
chang702201
301,0365
299,0375
297,0384
303,0367
300,0395
304,0403
295,0406
Relative Abundance
m/z
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
288
290
292
294
296
298
300
302
304
306
308
310

1c HR-MS

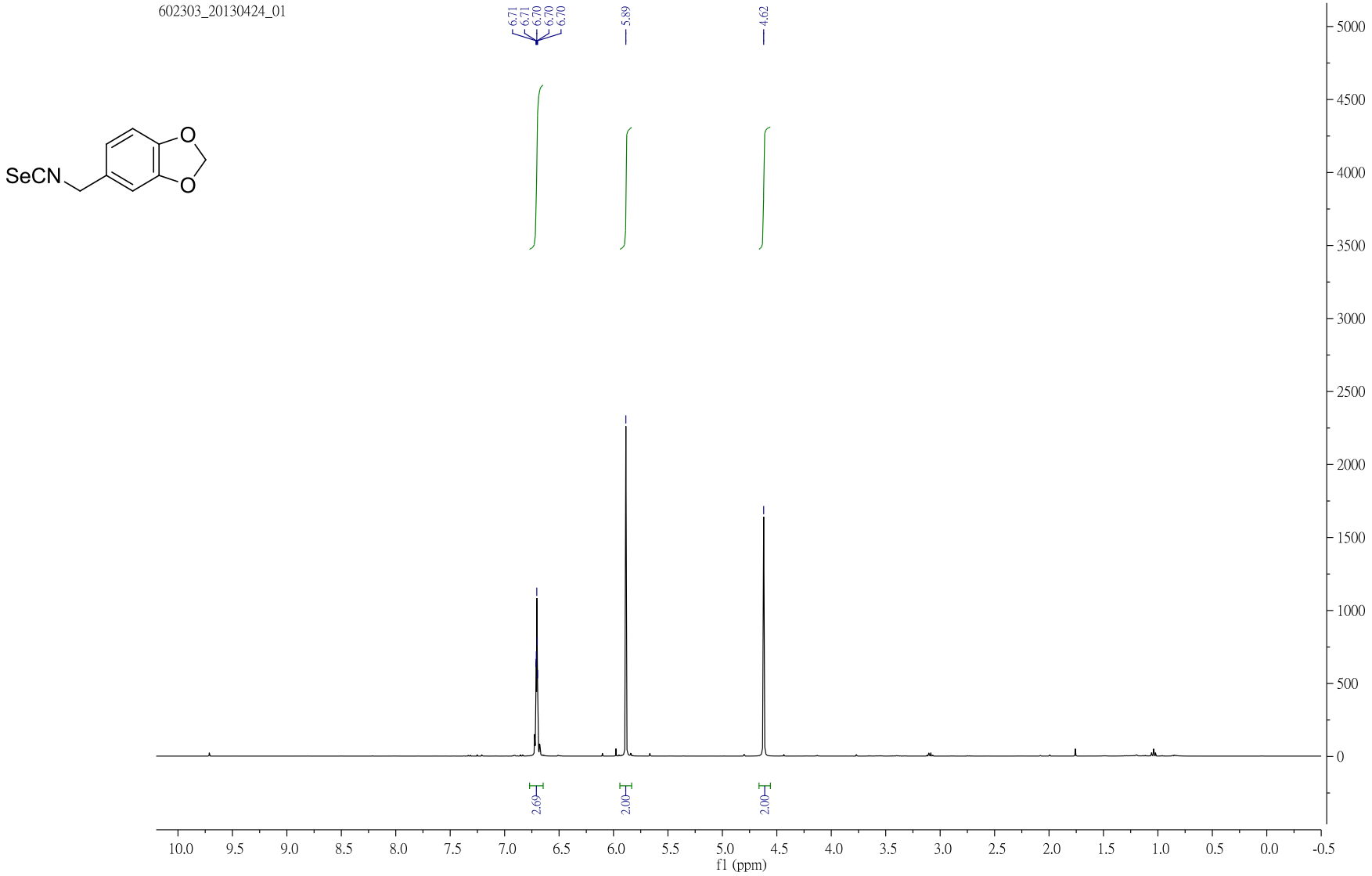
Isotope:	Min. .. Max.		
12 C	0....20		
1 H	0....25		
14 N	0....1		
80 Se	0....1		
78 Se	0....1		
Tolerance Window:	+- 3.00 mmu		
Db/Ring Equiv:	0.. 100	N-Rule:	Do not use
Fits:	3	Charge:	0

File : D:\Xcalibur\data\LIN-15-01\14\leihr-79-c1.RAW
Full ms [209.500 - 320.500] - Range: 209.500 - 320.500
Scan No. 3 of 10

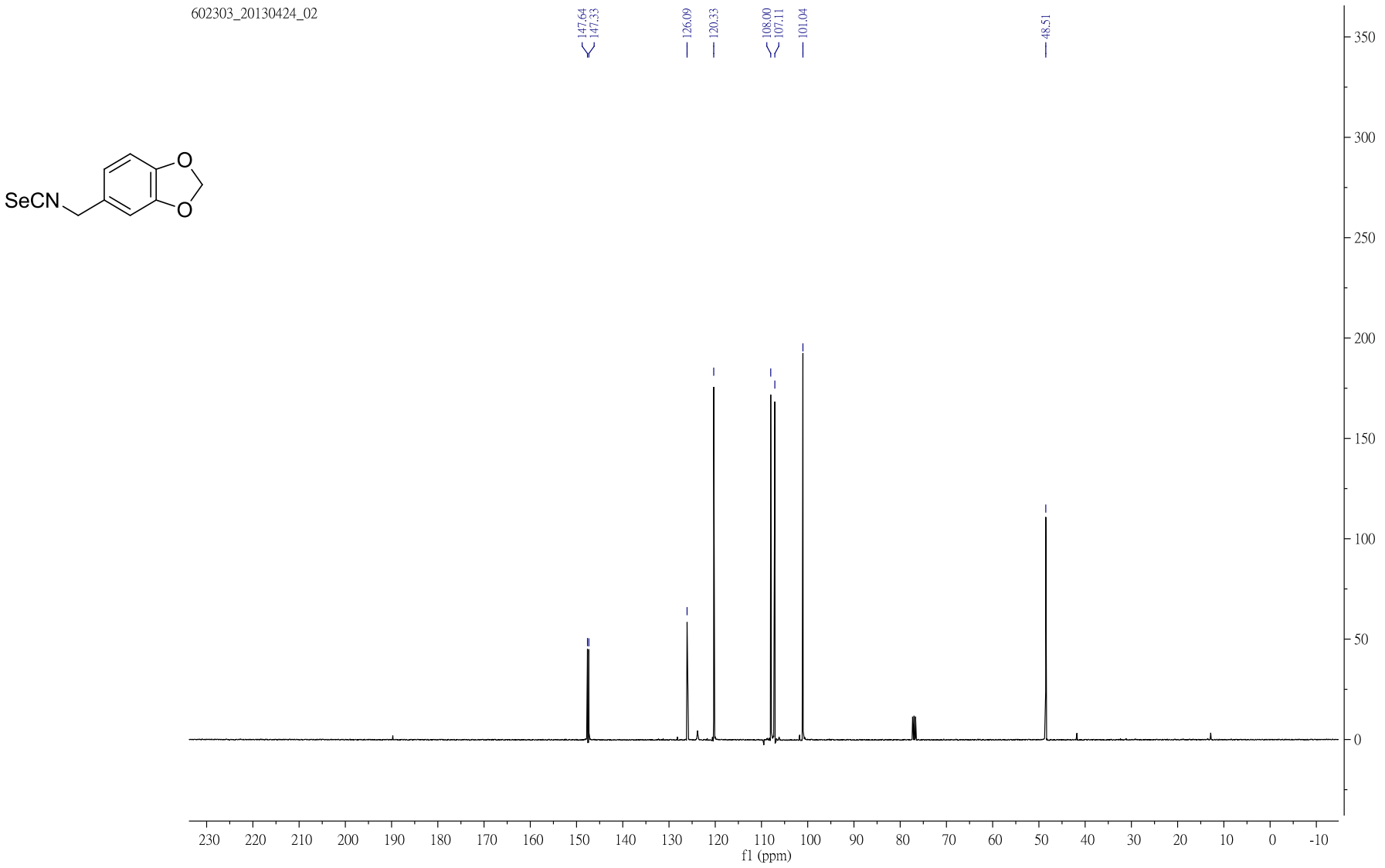
Mass	Relative Intensity	Delta [mmu]	Composition
218.0942	0.7	-2.8	$C_{16} H_{12} N_1$
218.9842	2.6		
219.1038	1.0	-1.0	$C_{16} H_{13} N_1$
220.1105	20.8	-2.1	$C_{16} H_{14} N_1$
221.1191	14.1	-1.4	$C_{16} H_{15} N_1$
222.1220	2.2		
222.9758	1.1		
224.9730	1.1		
242.9855	1.0	-2.3	$C_{13} H_9 {}^{78}Se_1$
249.0925	0.9		
250.0983	0.6		
257.0954	0.7	-1.8	$C_{13} H_{23} {}^{78}Se_1$
295.0406	1.6		
296.0394	0.6		
297.0384	18.6		
298.0398	16.5	-2.7	$C_{17} H_{16} {}^{78}Se_1$
299.0375	48.1	-0.3	$C_{16} H_{15} N_1 {}^{78}Se_1$
300.0395	8.5	-2.2	$C_{17} H_{16} Se_1$
301.0365	100.0	-0.5	$C_{16} H_{15} N_1 Se_1$
302.0401	14.7		
303.0367	17.4		
304.0403	2.7		


BRUKER
Transmittance [%]
80
78
76
74
72
3083.02
3059.36
3025.28
3001.26
2922.29
2871.87
2851.09
2139.10
1894.71
1807.65
1721.97
1598.31
1492.45
1450.00
1342.36
1306.11
1234.28
1185.04
1155.46
1090.18
1030.06
914.98
878.25
772.55
749.76
697.84
631.15
595.17
528.17
474.74
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang702201.0.dpt
Page 1/1

1c FT-IR


602303_20130424_01
SeCN
O
O
6.71
6.71
6.70
6.70
6.70
5.89
4.62
2.69
2.00
2.00
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
10.0
9.5
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
-0.5
f1 (ppm)

1d H^1-NMR

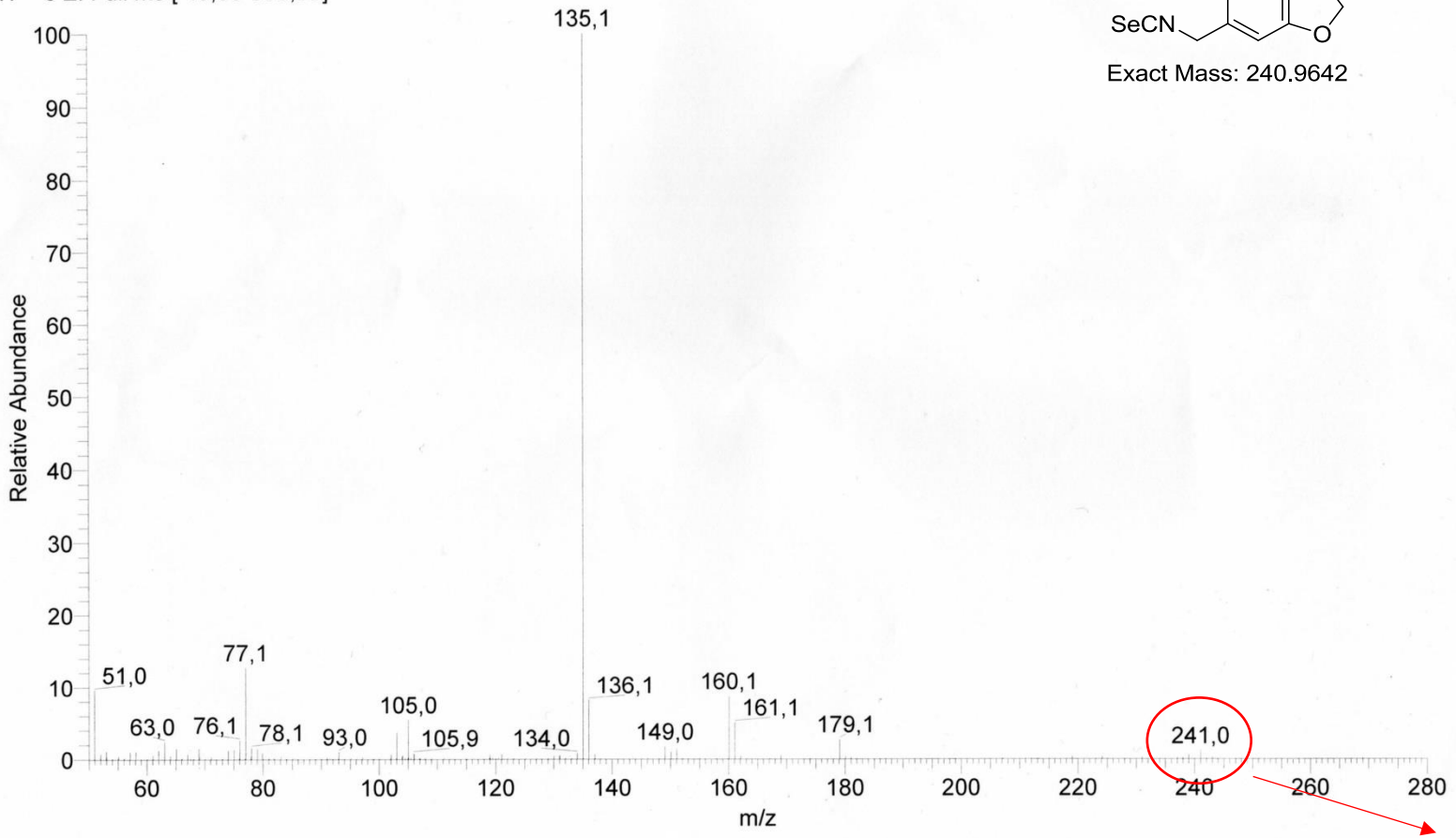

602303_20130424_02
147.64
147.33
126.09
120.33
108.00
107.11
101.04
48.51
SeCN
O
O
350
300
250
200
150
100
50
0
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

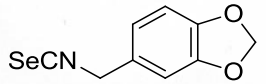
1d C^{13}-NMR

D:\Xcalibur\data\LIN-15-01\21\1eilr-35 21.01.2015 15:47:05 chang503301
FINNIGAN MAT-95XL

1eilr-35
Type: Unknown ID: Row: 1
Sample Name: chang503301
Comments: FINNIGAN MAT-95XL
Study::
Client::
Operator:: sclin
:
:

1eilr-35 #1 RT: 0,08 AV: 1 NL: 1,48E7
T: + c EI Full ms [49,50-500,50]

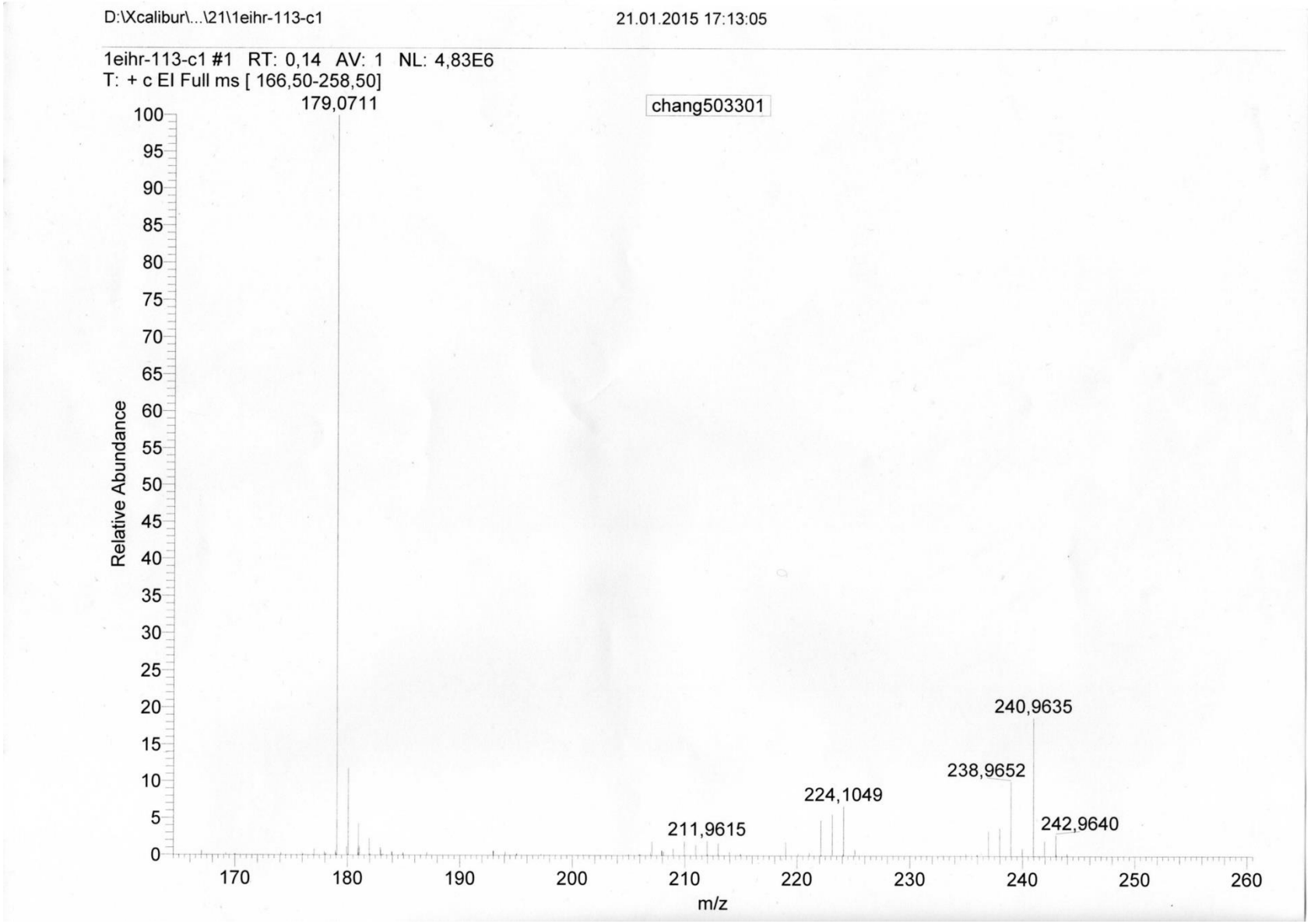




Exact Mass: 240.9642

M=241

1d LR-MS

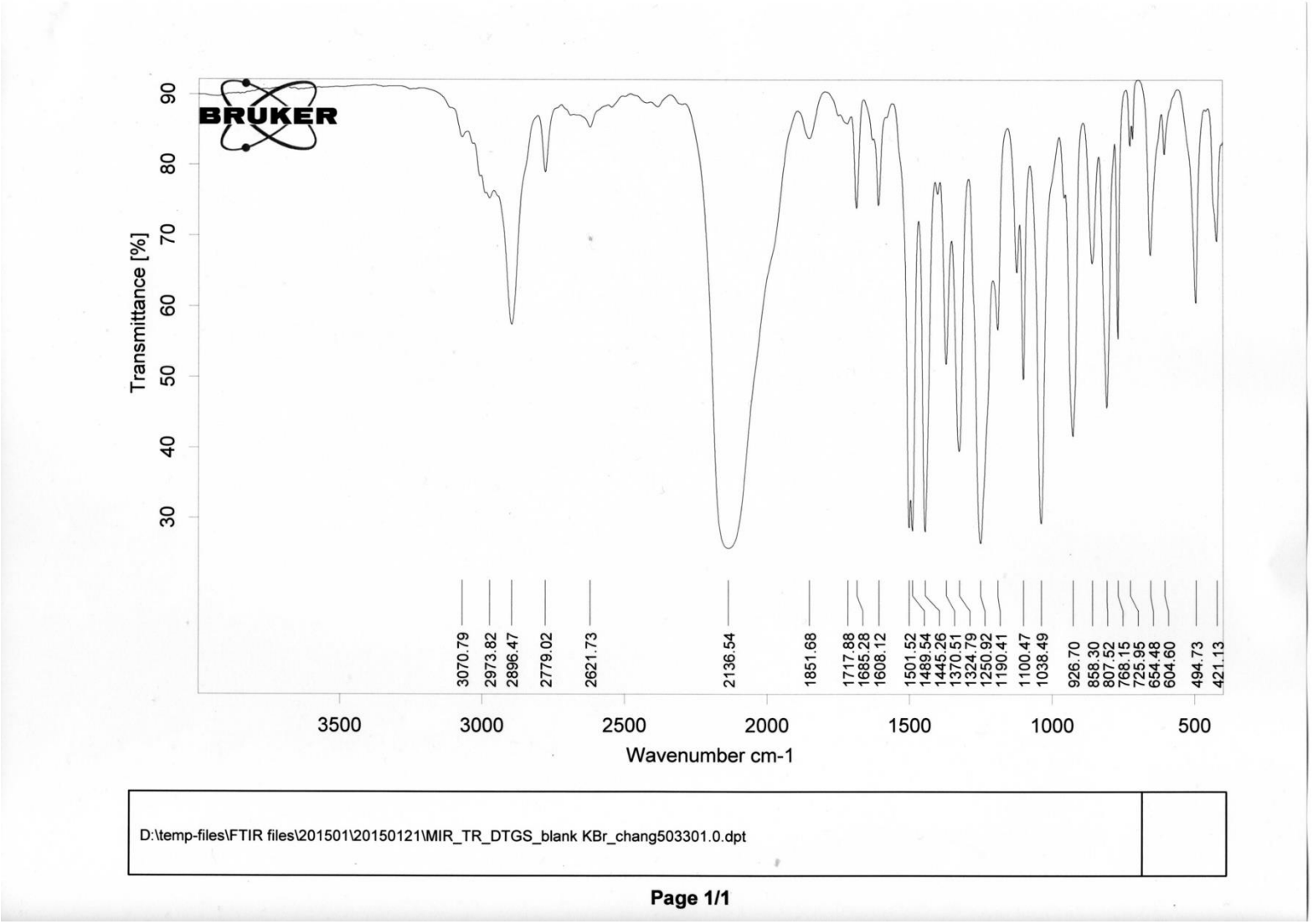

D:\Xcalibur\...\21\1eihr-113-c1
21.01.2015 17:13:05
1eihr-113-c1 #1 RT: 0,14 AV: 1 NL: 4,83E6
T: + c EI Full ms [166,50-258,50]
chang503301
179,0711
240,9635
238,9652
224,1049
242,9640
211,9615
Relative Abundance
m/z

1d HR-MS

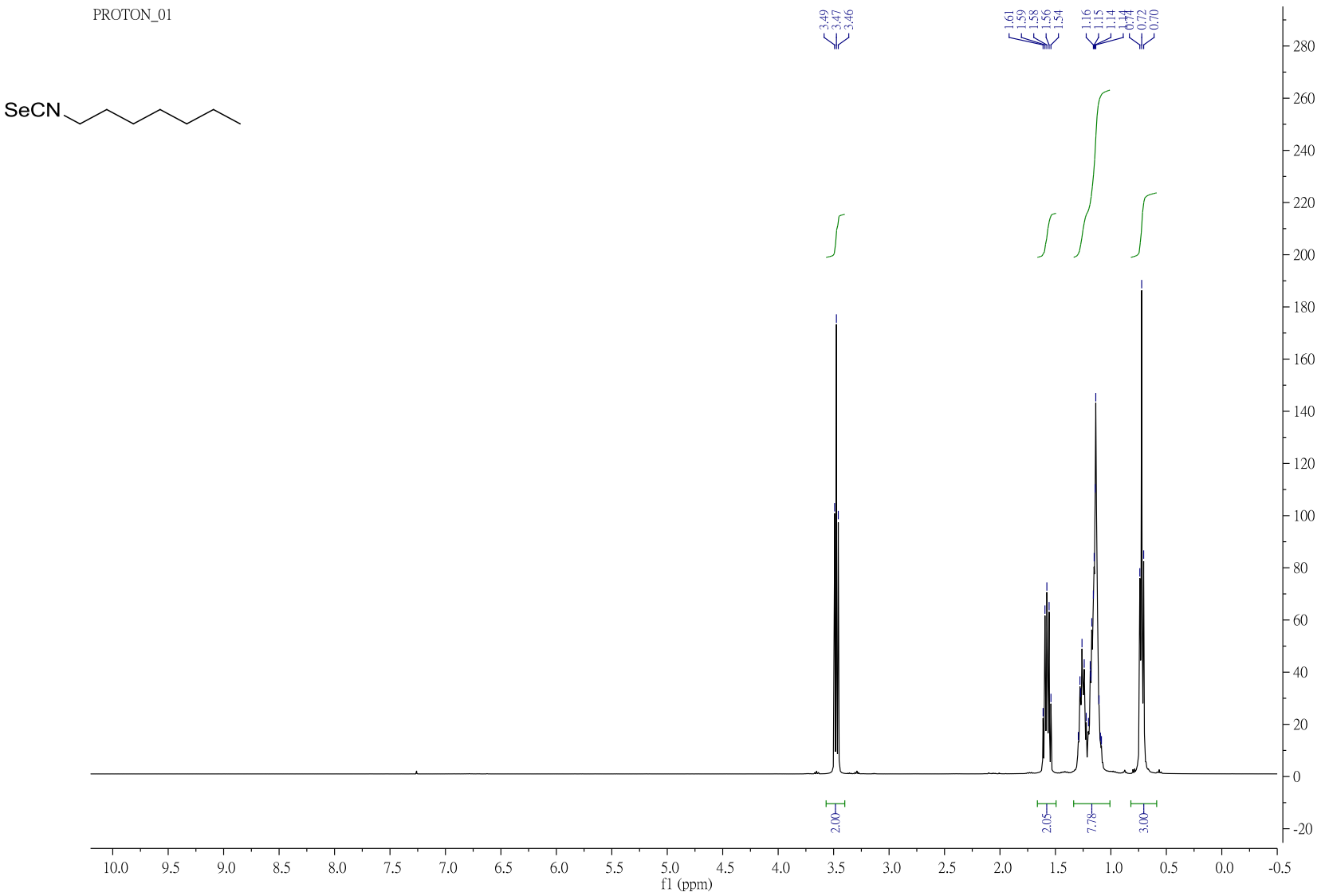
Isotope:	Min. .. Max.		
12 C	0....10		
1 H	0....18		
14 N	0....1		
16 O	0....3		
80 Se	0....1		
78 Se	0....1		
Tolerance Window:	+- 3.00 mmu		
Db/Ring Equiv:	0.. 100	N-Rule:	Do not use
Fits:	3	Charge:	0

File : D:\Xcalibur\data\LIN-15-01\21\leihr-113-c1.RAW
Full ms [166.500 - 258.500] - Range: 166.500 - 258.500
Scan No. 1 of 9

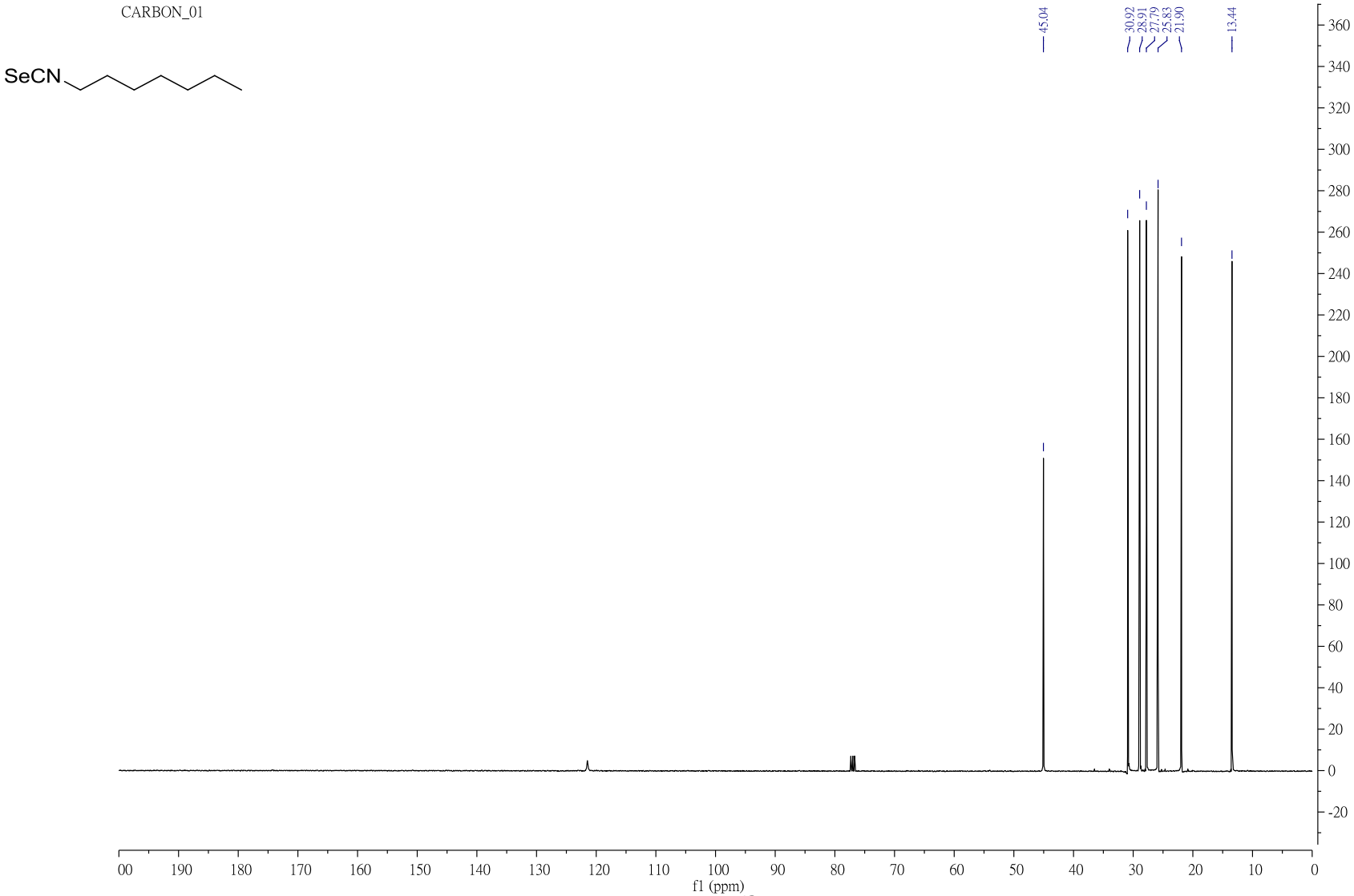
Mass	Relative Intensity	Delta [mmu]	Composition
179.0711	100.0	0.3	$C_{10} H_{11} O_1$
179.9498	1.2	0.8	$C_4 H_6 O_1 {}^{78}Se_1$
		-1.8	$C_7 H_4 N_1 {}^{78}Se_1$
		2.0	$C_8 H_4 Se_1$
180.0743	11.8		
180.9894	4.2		
181.0772	1.2		
181.9509	2.3	-0.0	$C_7 H_4 N_1 Se_1$
		-1.2	$C_3 H_6 O_3 N_1 {}^{78}Se_1$
		2.7	$C_4 H_6 O_3 Se_1$
182.9355	1.1	0.6	$C_7 H_3 O_1 Se_1$
207.0803	1.9		
209.9451	1.9	-0.7	$C_8 H_4 O_1 N_1 Se_1$
210.9511	1.4	-2.6	$C_8 H_5 O_1 N_1 Se_1$
211.9615	2.0	0.0	$C_8 H_6 O_1 N_1 Se_1$
212.9463	1.7	0.9	$C_8 H_5 O_2 Se_1$
		-3.0	$C_7 H_5 O_2 N_1 {}^{78}Se_1$
218.9848	1.9		
222.1025	4.8		
223.1101	5.7		
224.1049	6.7		
236.9658	3.4		
237.9654	3.8		
238.9652	10.1	0.2	$C_9 H_7 O_2 N_1 {}^{78}Se_1$
239.9653	1.0		
240.9635	18.8	-0.7	$C_9 H_7 O_2 N_1 Se_1$
241.9657	2.1	1.0	$C_9 H_8 O_3 {}^{78}Se_1$
242.9640	2.9		


BRUKER
Transmittance [%]
90
80
70
60
50
40
30
3070.79
2973.82
2896.47
2779.02
2621.73
2136.54
1851.68
1717.88
1685.28
1608.12
1501.52
1489.54
1445.26
1370.51
1324.79
1250.92
1190.41
1100.47
1038.49
926.70
858.30
807.52
768.15
725.95
654.48
604.60
494.73
421.13
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang503301.0.dpt
Page 1/1

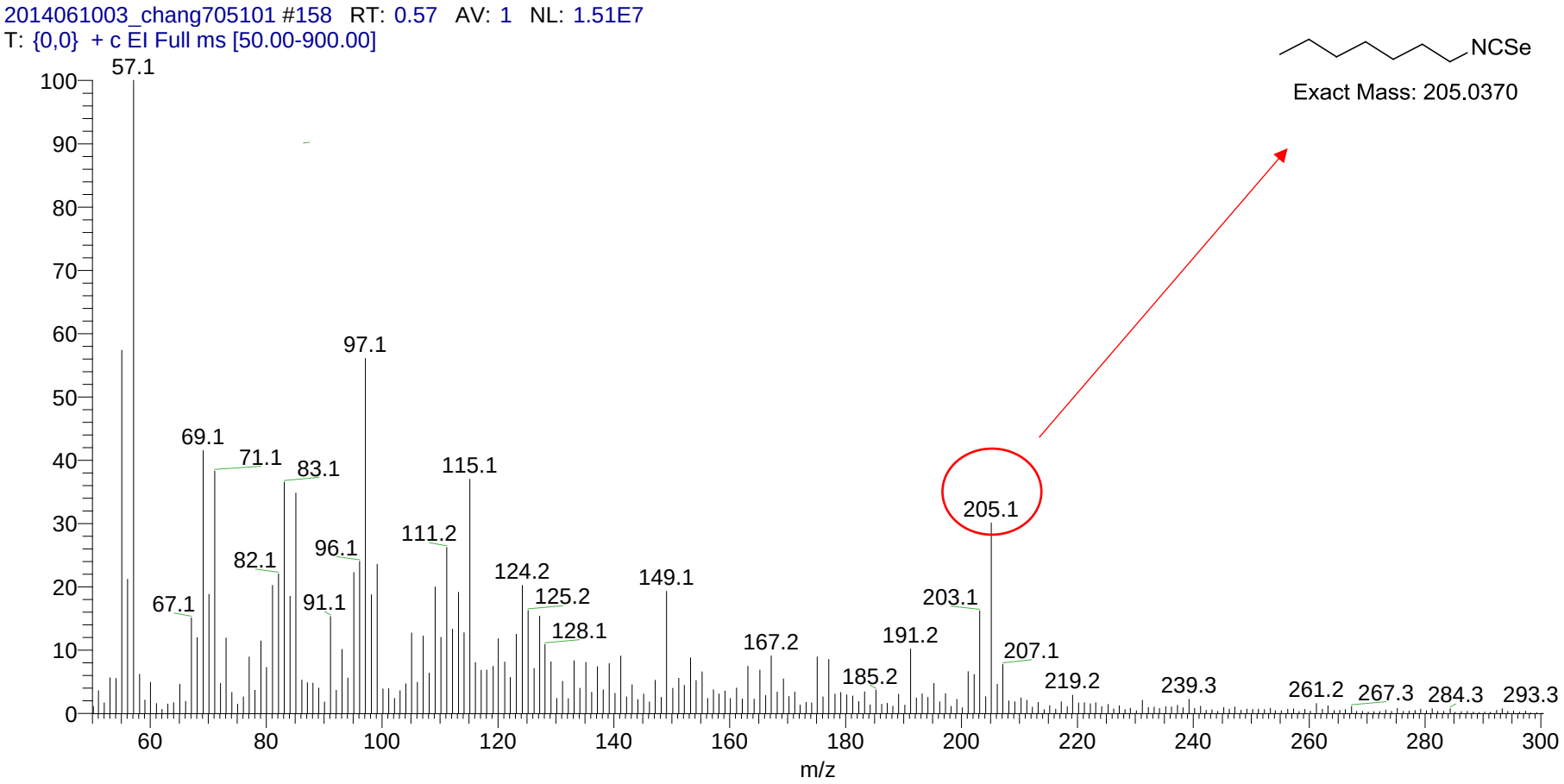
1d FT-RT


PROTON_01
SeCN
3.49
3.47
3.46
1.61
1.59
1.58
1.56
1.54
1.16
1.15
1.14
0.72
0.70
2.00
2.05
7.78
3.00
f1 (ppm)

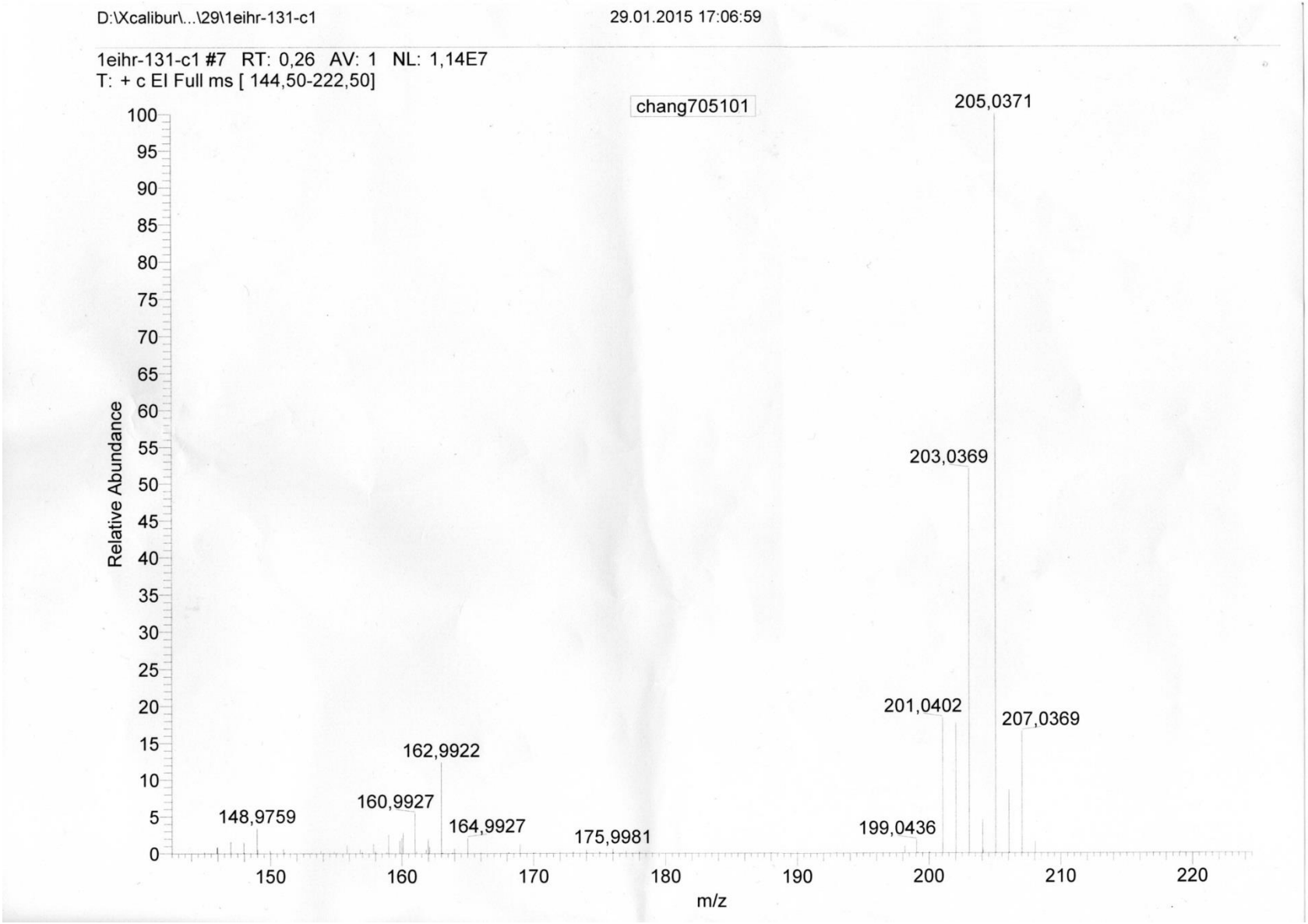
1e H^1-NMR


CARBON_01
SeCN
45.04
30.92
28.91
27.79
25.83
21.90
13.44
360
340
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

1e C^{13}-NMR


2014061003_chang705101 #158 RT: 0.57 AV: 1 NL: 1.51E7
T: {0,0} + c EI Full ms [50.00-900.00]
NCSe
Exact Mass: 205.0370
57.1
97.1
69.1
71.1
83.1
115.1
205.1
111.2
82.1
96.1
124.2
149.1
67.1
91.1
125.2
203.1
128.1
191.2
167.2
207.1
185.2
219.2
239.3
261.2
267.3
284.3
293.3
m/z

1e LR-MS

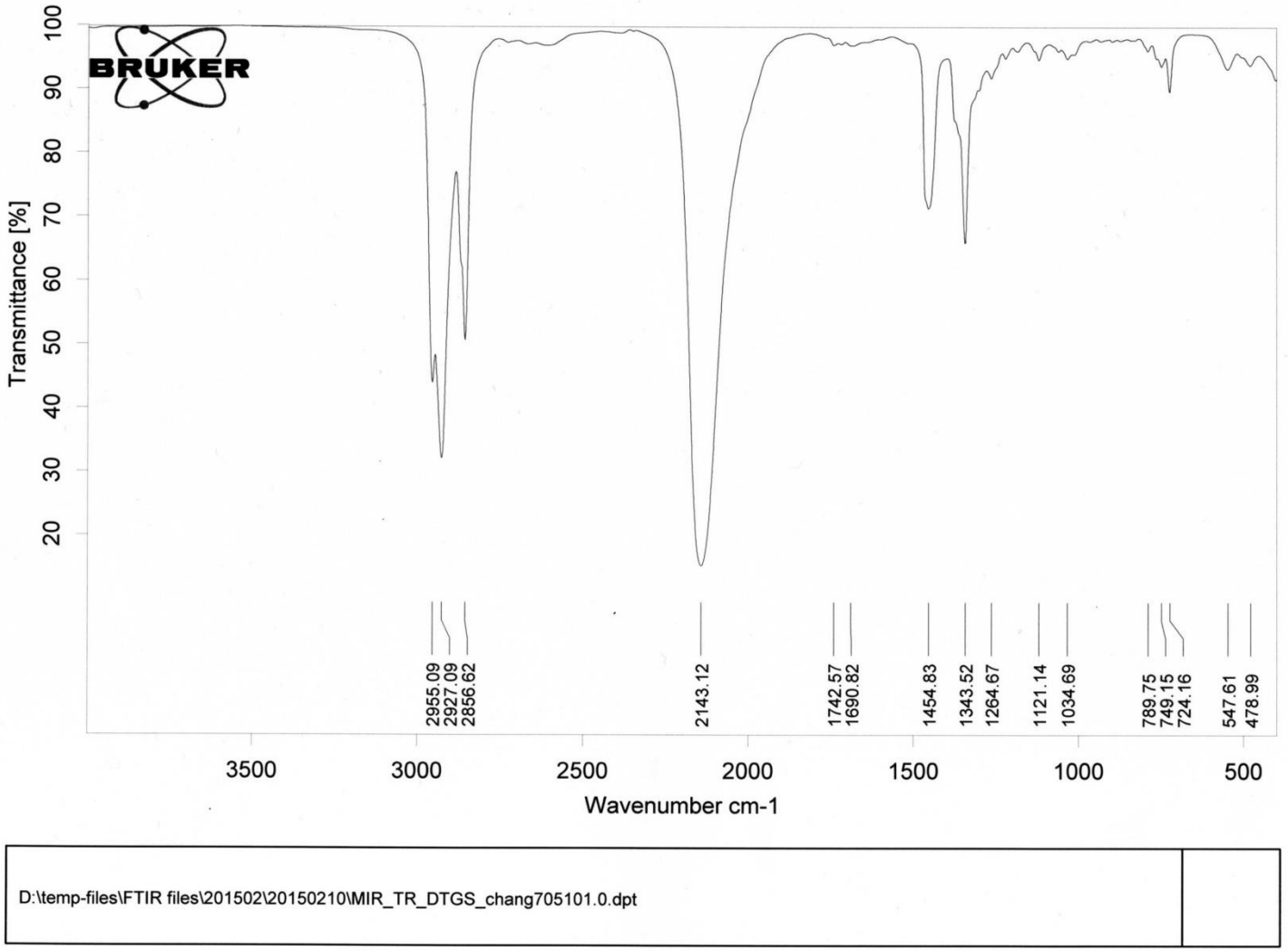

D:\Xcalibur\...\29\1eihr-131-c1
29.01.2015 17:06:59
1eihr-131-c1 #7 RT: 0,26 AV: 1 NL: 1,14E7
T: + c EI Full ms [144,50-222,50]
chang705101
205,0371
203,0369
201,0402
207,0369
162,9922
160,9927
148,9759
164,9927
175,9981
199,0436
Relative Abundance
m/z
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
150
160
170
180
190
200
210
220

1e HR-MS

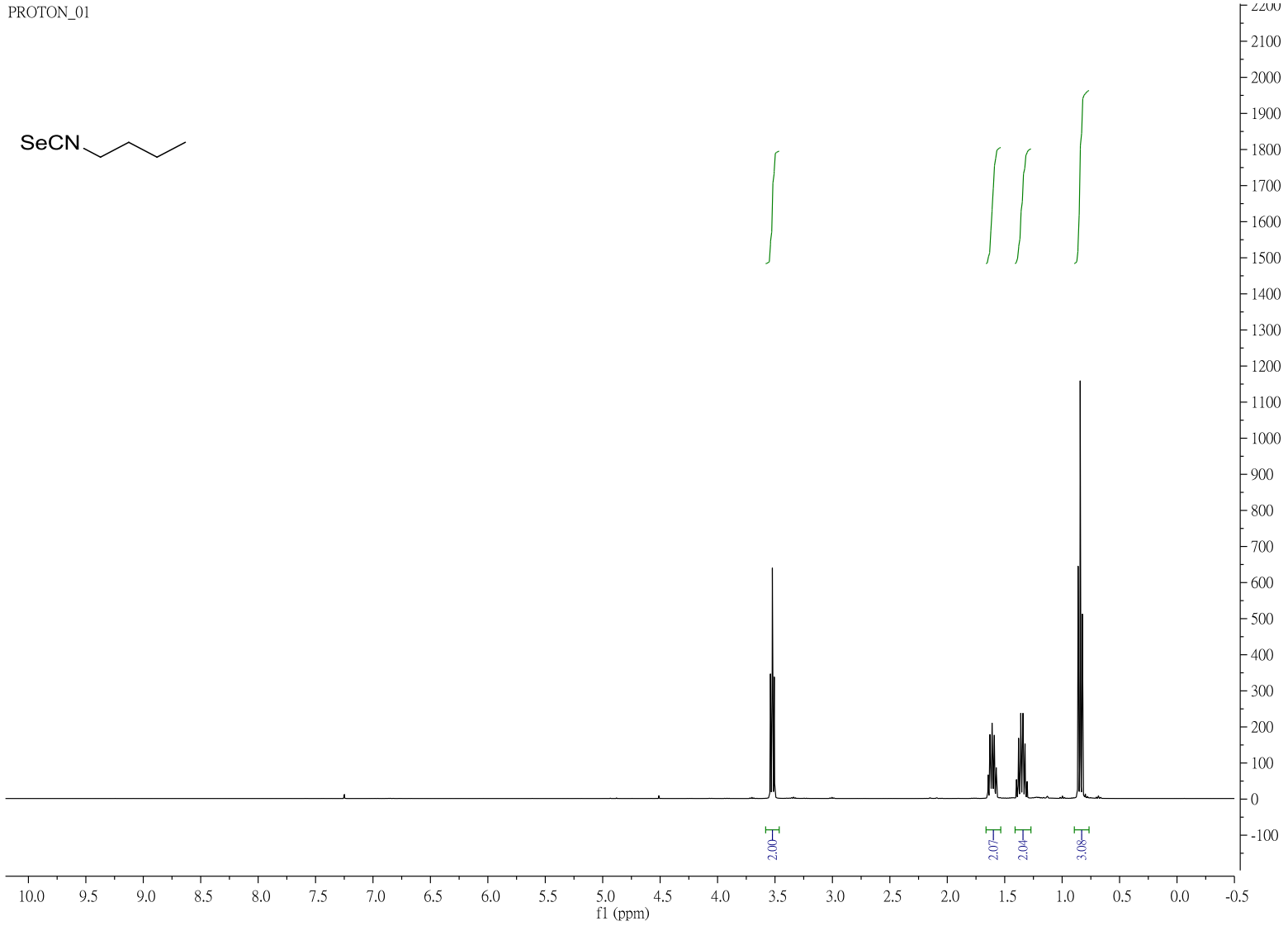
Isotope:	Min. .. Max.		
12 C	0....10		
1 H	0....20		
80 Se	0....1		
78 Se	0....1		
14 N	0....1		
Tolerance Window:	+- 3.00 mmu		
Db/Ring Equiv:	0.. 100	N-Rule:	Do not use
Fits:	3	Charge:	0

File : D:\Xcalibur\data\LIN-15-01\29\1eihr-131-c1.RAW
Full ms [144.500 - 222.500] - Range: 144.500 - 222.500
Scan No. 7 of 7

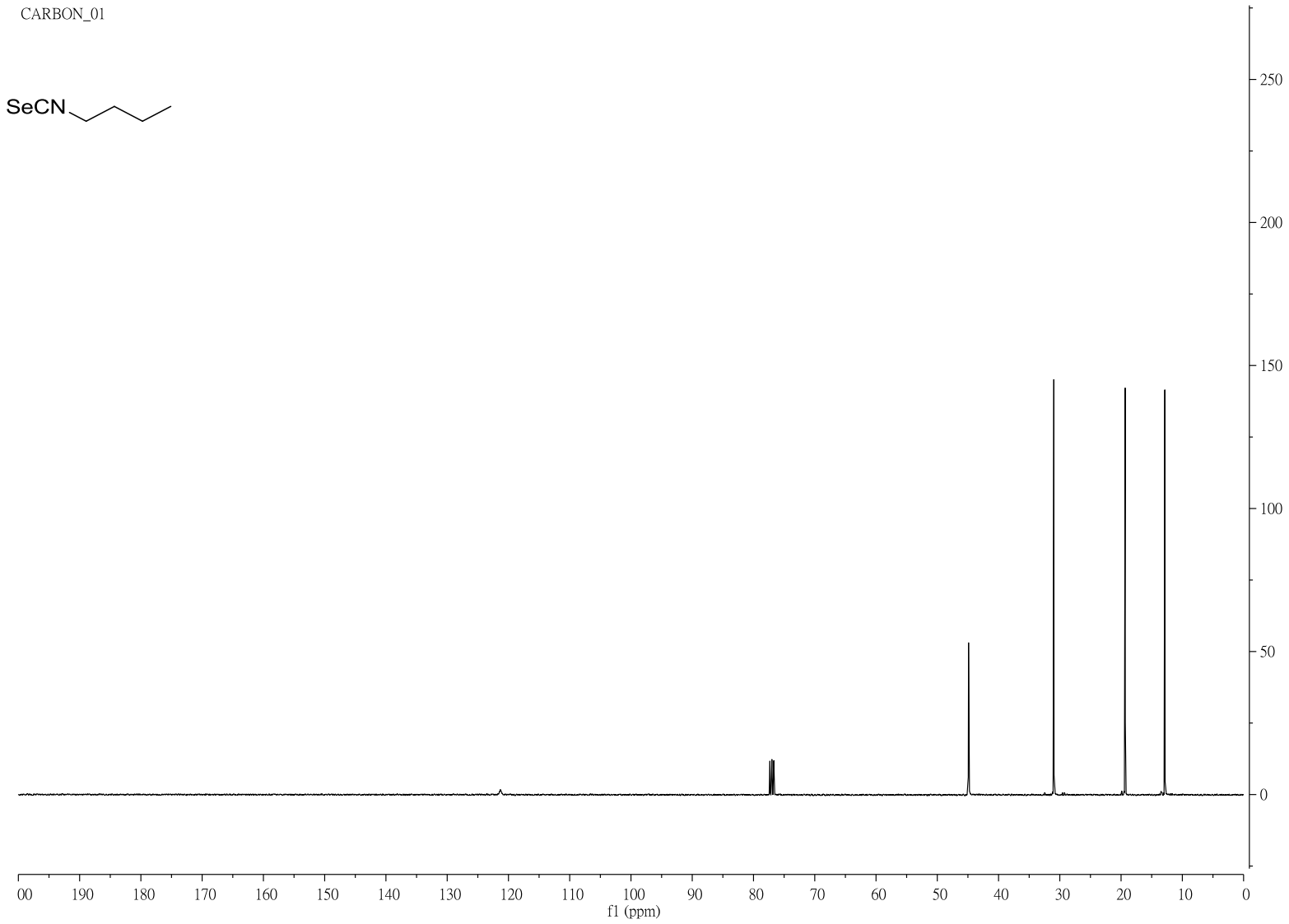
Mass	Relative Intensity	Delta [mmu]	Composition
145.9512	0.7	0.3	$C_4 H_4 N_1 Se_1$
145.9674	0.9	0.0	$C_4 H_6 N_1 {}^{78}Se_1$
145.9775	0.8	-2.4	$C_5 H_8 {}^{78}Se_1$
146.9773	1.6	2.1	$C_4 H_7 N_1 {}^{78}Se_1$
147.9689	1.5	2.4	$C_4 H_6 N_1 Se_1$
148.9759	3.4	1.6	$C_4 H_7 N_1 Se_1$
149.0264	0.6		
150.9759	0.6		
155.8378	1.1		
156.8389	0.6		
157.8366	1.3	2.8	$^{78}Se_1 Se_1$
158.9937	2.6		
159.8356	1.7		
159.9947	2.1	-0.8	$C_6 H_{10} {}^{78}Se_1$
160.0921	2.9		
160.9927	5.5	1.9	$C_5 H_9 N_1 {}^{78}Se_1$
161.8359	0.5		
161.9855	2.0		
162.0883	0.9		
162.9922	12.4	2.2	$C_5 H_9 N_1 Se_1$
163.9945	0.7		
164.9927	2.1		
168.9909	1.3		
175.9981	0.6	0.3	$C_6 H_{10} N_1 Se_1$
198.1498	1.0		
199.0436	1.8		
201.0402	18.4		
202.0400	17.7	-2.5	$C_9 H_{16} {}^{78}Se_1$
203.0369	52.0	-0.8	$C_8 H_{15} N_1 {}^{78}Se_1$
204.0400	4.5	-1.7	$C_9 H_{16} Se_1$
205.0371	100.0	0.2	$C_8 H_{15} N_1 Se_1$
206.0404	8.6		
207.0369	16.6		
208.0397	1.5		


BRUKER
Transmittance [%]
100
90
80
70
60
50
40
30
20
2955.09
2927.09
2856.62
2143.12
1742.57
1690.82
1454.83
1343.52
1264.67
1121.14
1034.69
789.75
749.15
724.16
547.61
478.99
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201502\20150210\MIR_TR_DTGS_chang705101.0.dpt
Page 1/1

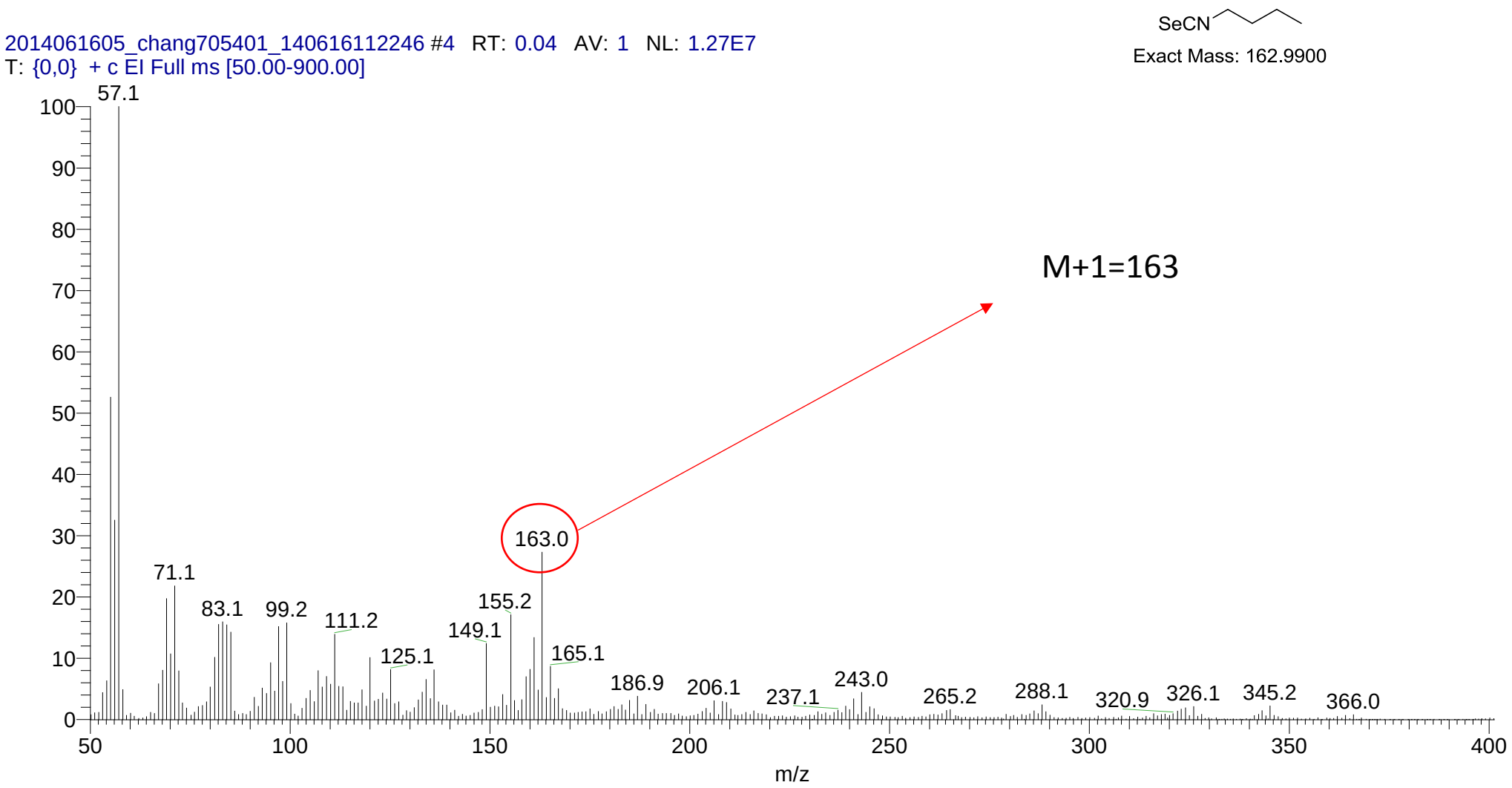
1e FT-IR



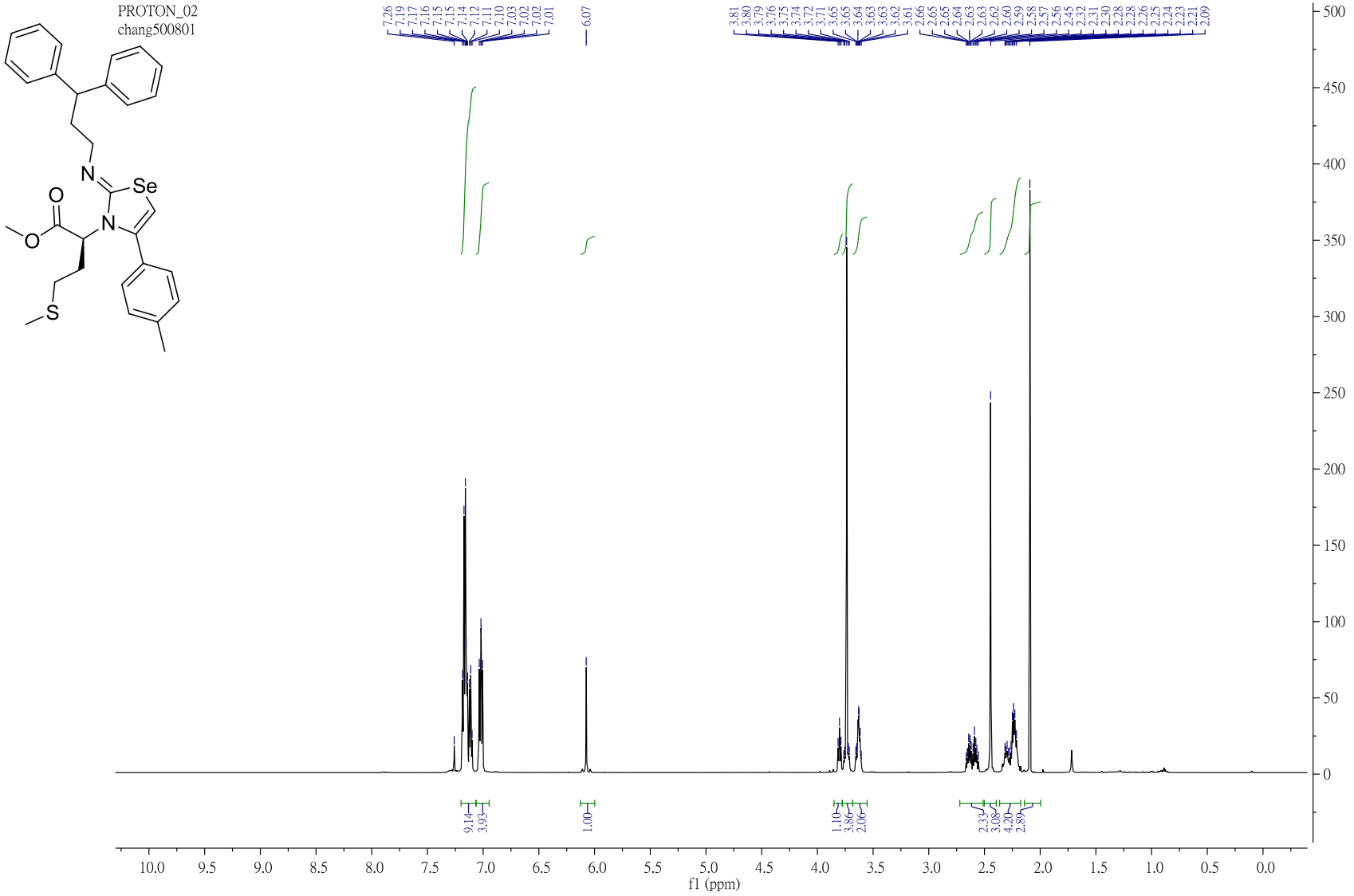
1f H^1-NMR


CARBON_01
SeCN
250
200
150
100
50
0
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

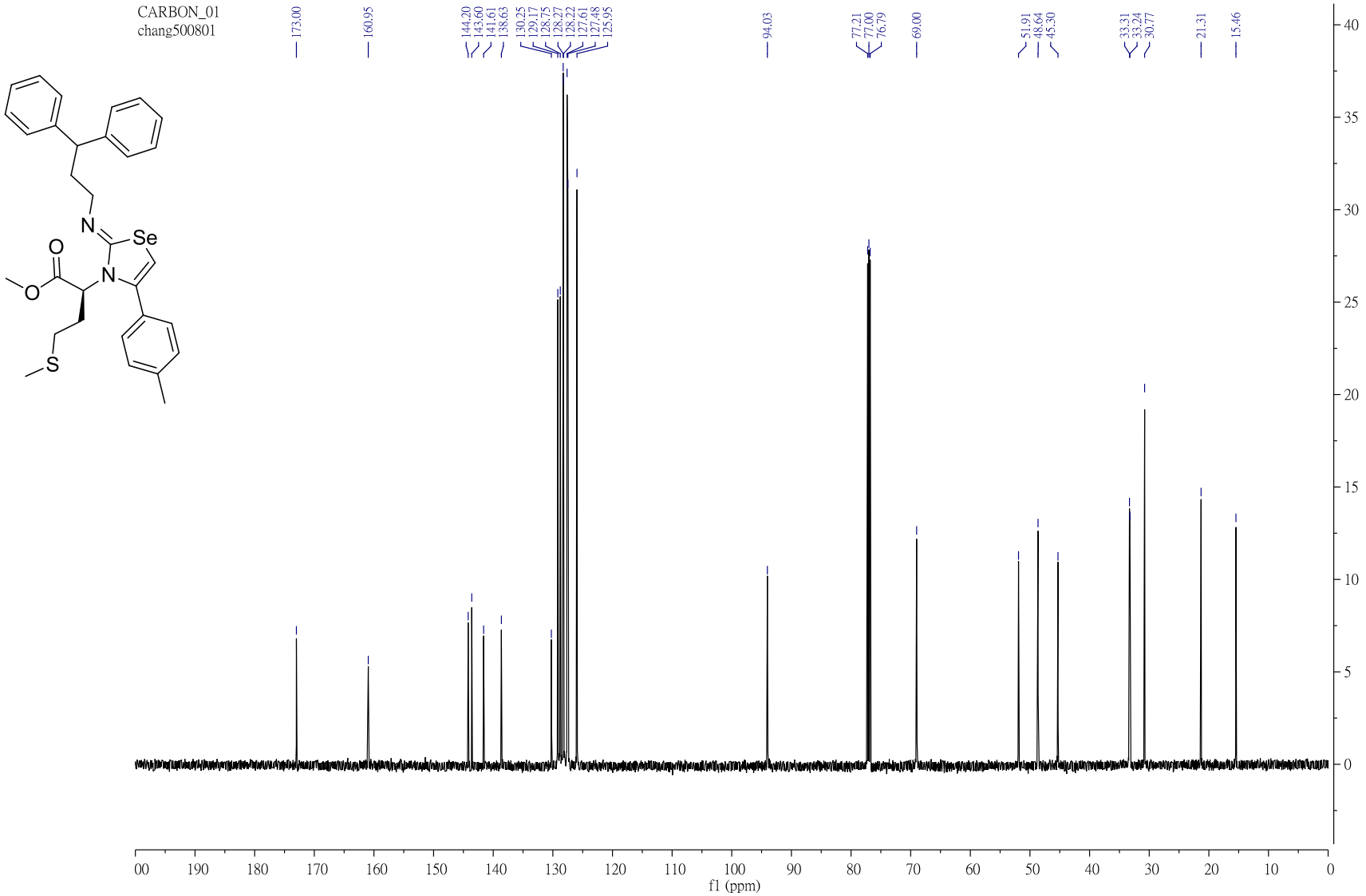
1f C^{13}-NMR


SeCN
Exact Mass: 162.9900
2014061605_chang705401_140616112246 #4 RT: 0.04 AV: 1 NL: 1.27E7
T: {0,0} + c EI Full ms [50.00-900.00]
M+1=163
57.1
71.1
83.1
99.2
111.2
125.1
149.1
155.2
163.0
165.1
186.9
206.1
237.1
243.0
265.2
288.1
320.9
326.1
345.2
366.0
m/z

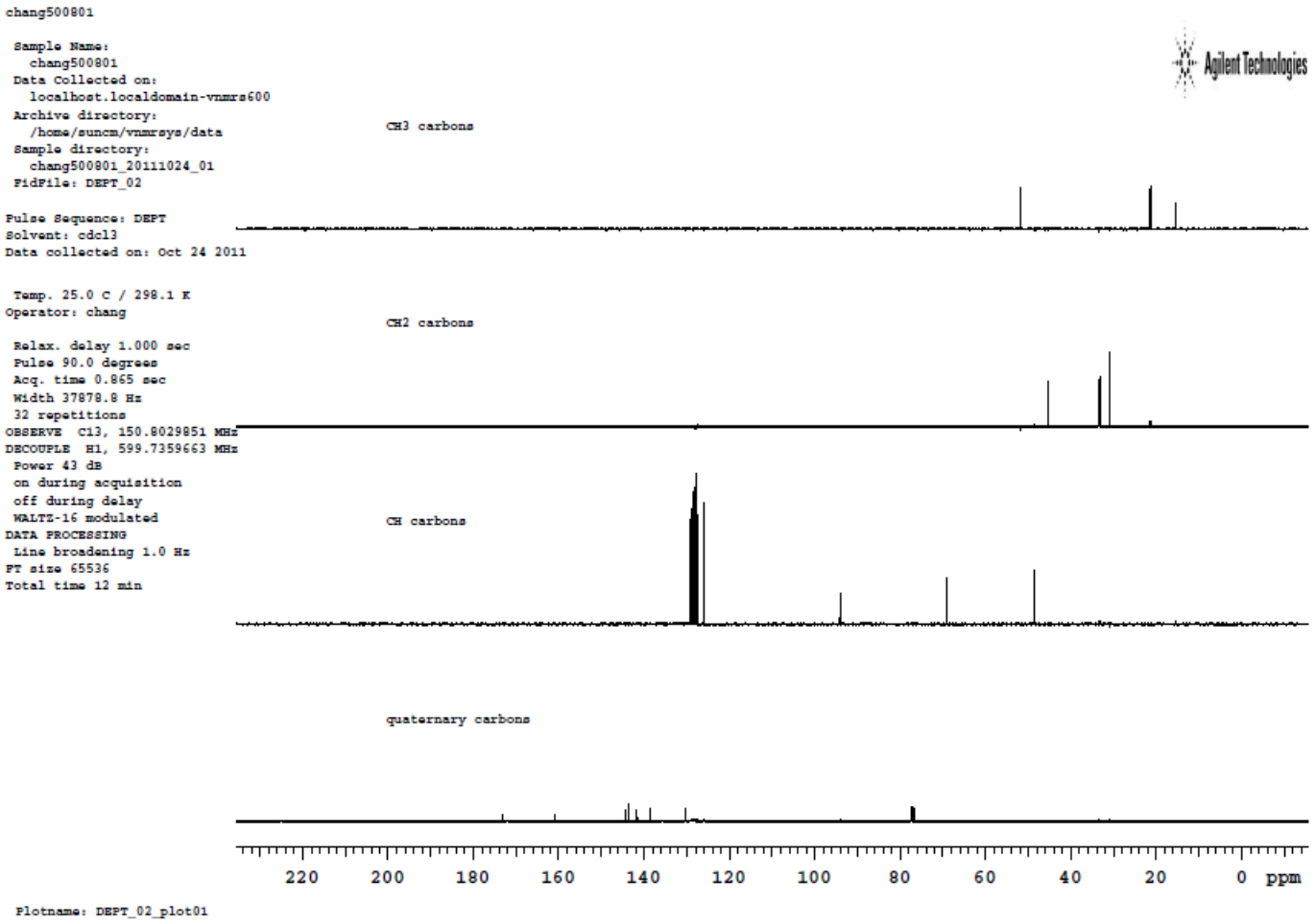
1f LR-MS



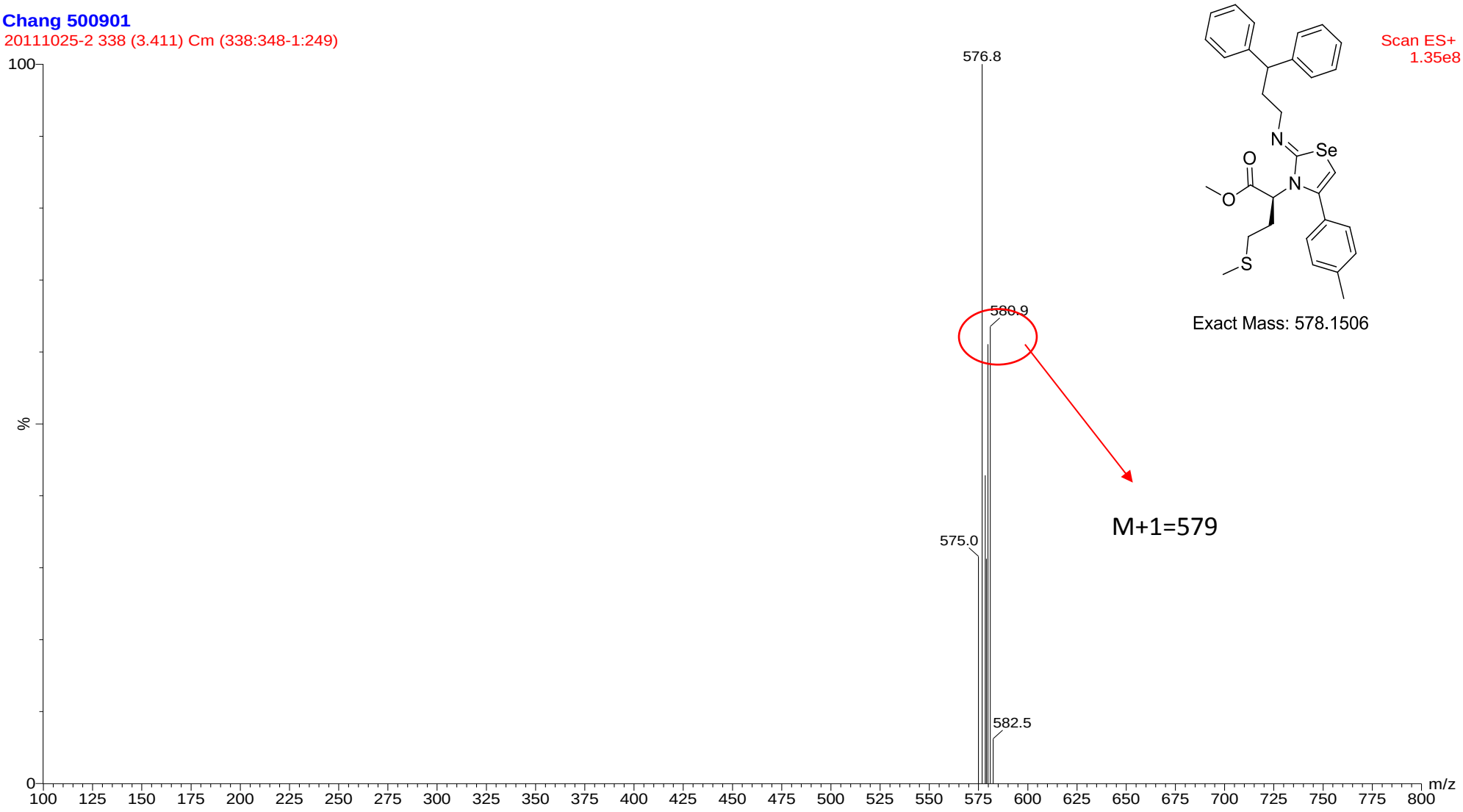
5a H^1-NMR


CARBON_01
chang500801
173.00
160.95
144.20
143.60
141.61
138.63
130.25
129.17
128.75
128.27
128.22
127.61
127.48
125.95
94.03
77.21
77.00
76.79
69.00
51.91
48.64
45.30
33.31
33.24
30.77
21.31
15.46
f1 (ppm)

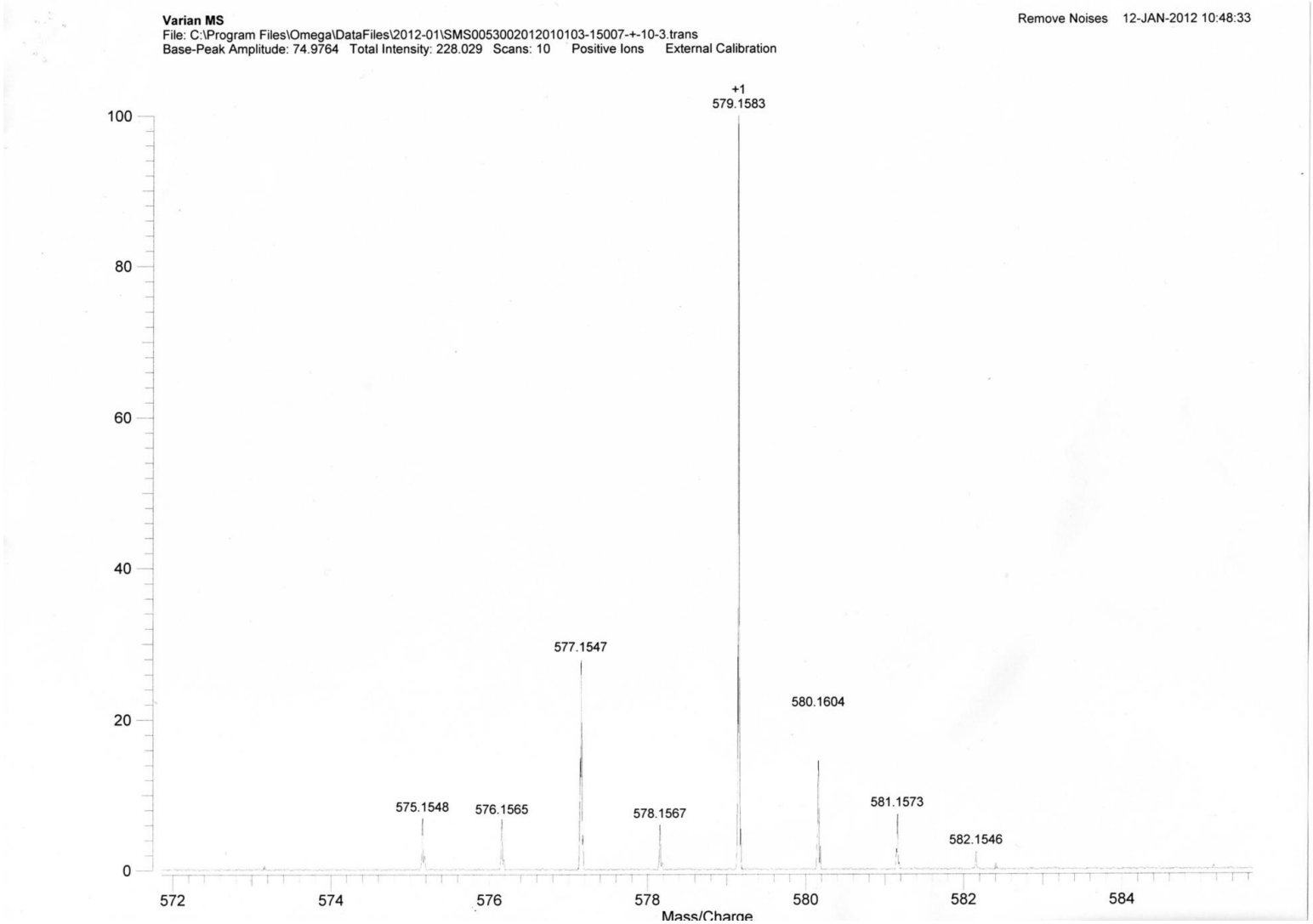
5a C^{13}-NMR

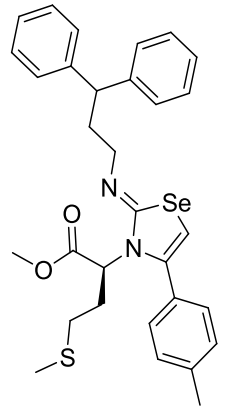

chang500801
Sample Name:
chang500801
Data Collected on:
localhost.localdomain-vnmrs600
Archive directory:
/home/suncm/vnmrsys/data
Sample directory:
chang500801_20111024_01
FidFile: DEPT_02
Pulse Sequence: DEPT
Solvent: cdcl3
Data collected on: Oct 24 2011
Temp. 25.0 C / 298.1 K
Operator: chang
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
32 repetitions
OBSERVE C13, 150.8029851 MHz
DECOUPLE H1, 599.7359663 MHz
Power 43 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 12 min
CH3 carbons
CH2 carbons
CH carbons
quaternary carbons
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Plotname: DEPT_02_plot01

5a DEPT


Chang 500901
20111025-2 338 (3.411) Cm (338:348-1:249)
Scan ES+
1.35e8
100
%
0
576.8
580.9
575.0
582.5
M+1=579
Exact Mass: 578.1506
N
Se
O
N
O
S
100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725 750 775 800
m/z

5a LR-MS





Exact Mass: 578.1506

5a HR-MS

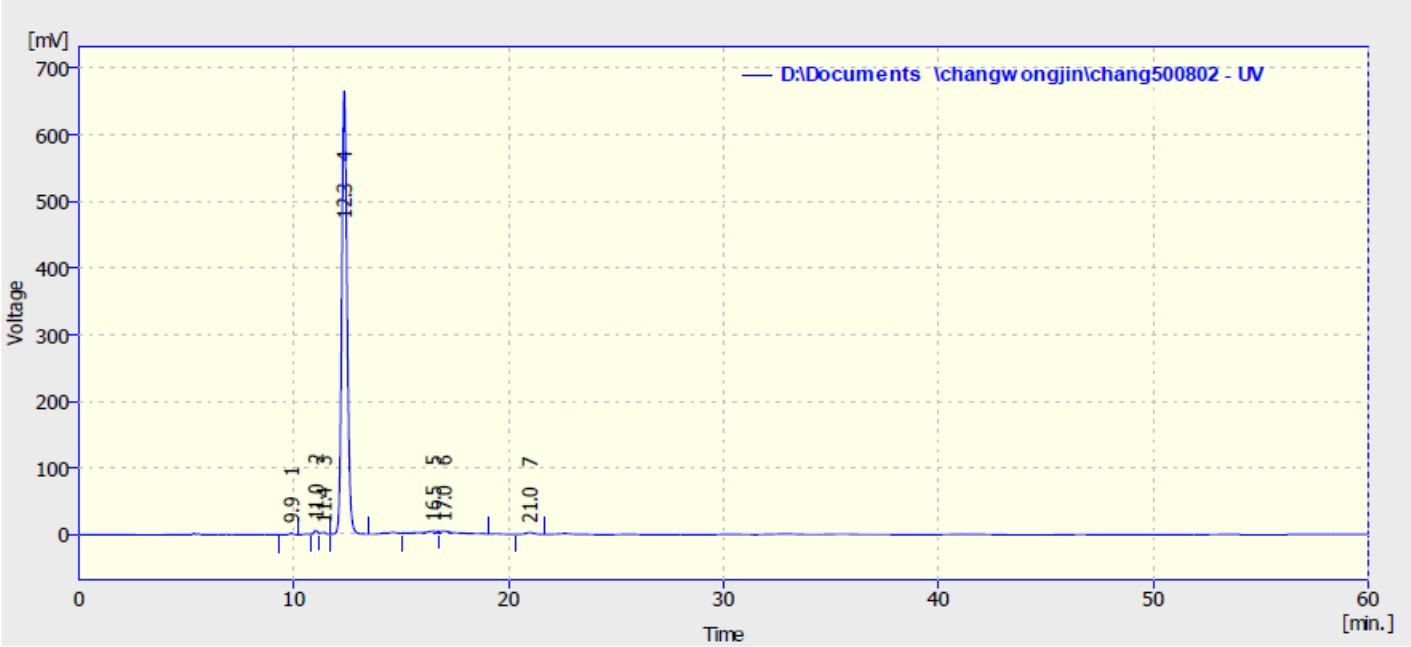
Monoisotopic Mass List - Varian ESI FTMS with Omega v9.1.20

File: C:\Program Files\Omega\DataFiles\2012-01\SMS0053002012010103-15007-+-10-3.trans
Acquired: 12-JAN-2012 10:48:33

Mass	*Ampl.*	*Rel. Ampl.*
107.00091	0.5	0.51
109.12527	0.3	0.35
128.24300	0.5	0.54
179.19543	0.5	0.56
192.04721	0.3	0.38
192.05102	0.7	0.75
217.13208	0.4	0.39
245.25071	0.4	0.46
245.25301	1.0	1.09
287.57089	0.8	0.87
287.58002	0.5	0.60
288.57782	1.8	1.97
306.81349	0.4	0.47
306.81837	0.4	0.42
344.01505	0.6	0.68
344.01699	0.6	0.69
344.02681	0.6	0.61
344.04321	0.5	0.59
344.06459	1.0	1.07
344.07354	0.6	0.70
359.31384	2.7	2.92
375.10890	0.4	0.45
375.28736	1.0	1.14
394.44883	0.7	0.72
394.62020	0.5	0.57
407.29773	2.6	2.91
412.25496	0.7	0.72
415.34370	0.4	0.44
423.27131	0.7	0.77
426.32896	0.6	0.60
429.23177	0.5	0.56
434.23306	0.5	0.58
436.18325	18.1	19.83
437.32612	3.5	3.81
450.20961	0.6	0.66
452.15618	7.8	8.62
452.16763	0.6	0.64

Mass	*Ampl.*	*Rel. Ampl.*
453.29030	1.1	1.25
478.24083	0.5	0.57
515.32430	0.7	0.77
516.52432	0.8	0.85
516.58577	0.5	0.53
516.60415	0.6	0.65
531.30235	1.2	1.26
567.28011	0.5	0.59
572.14926	0.5	0.54
574.14692	10.0	11.00
574.17072	2.5	2.79
576.14212	15.3	16.81
576.14684	20.5	22.56
576.16788	4.3	4.74
577.14128	2.4	2.63
578.13647	22.3	24.52
578.15046	91.0	100.00
578.16702	7.4	8.13
580.13944	3.7	4.12
580.14485	5.8	6.35
581.39565	0.6	0.70
584.15410	0.4	0.44
594.13672	0.4	0.43
600.12270	0.4	0.46
658.06300	0.9	1.02
658.55330	0.6	0.70
696.63929	1.6	1.81

5a HR-MS

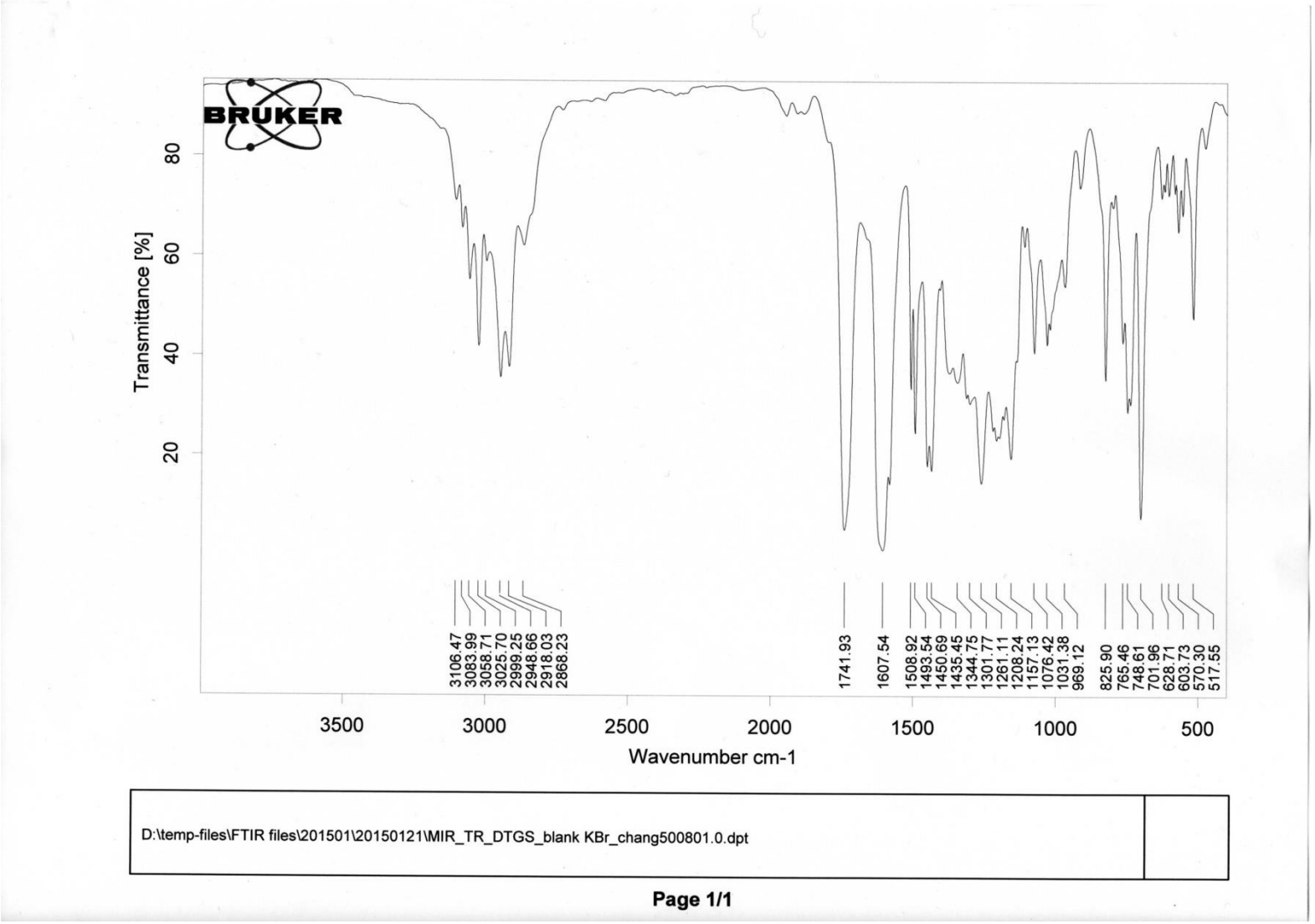


Result Table (Uncal - D:\Documents \changwongjin\chang500802 - UV)

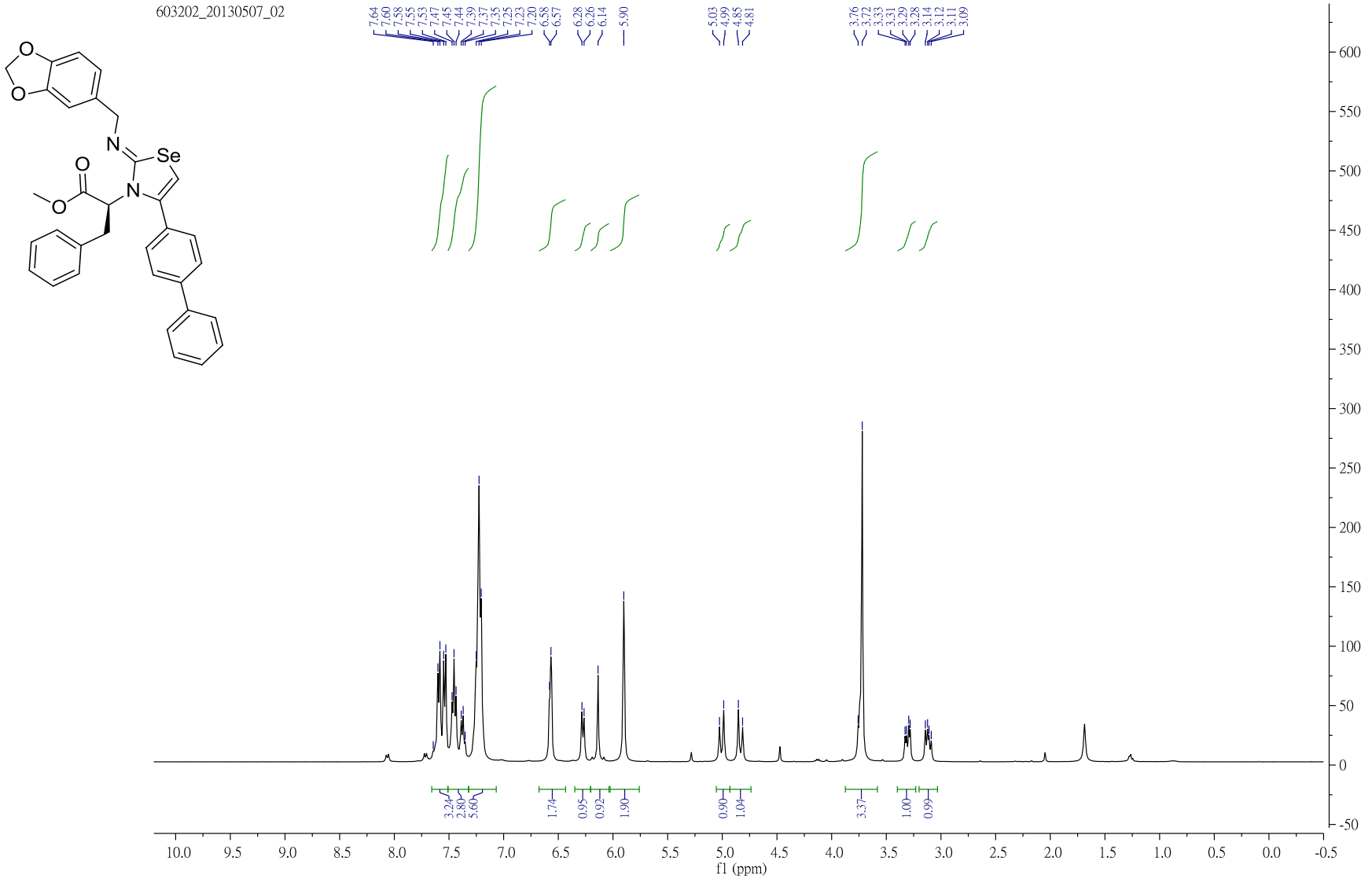
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	9.884	25.193	2.248	0.2	0.3
2	11.020	74.003	5.942	0.6	0.9
3	11.404	50.088	3.160	0.4	0.5
4	12.344	11499.032	664.988	95.3	96.9
5	16.492	160.982	3.639	1.3	0.5
6	16.980	181.835	3.782	1.5	0.6
7	20.988	76.680	2.545	0.6	0.4
	Total	12067.813	686.305	100.0	100.0

5a chiral HPLC

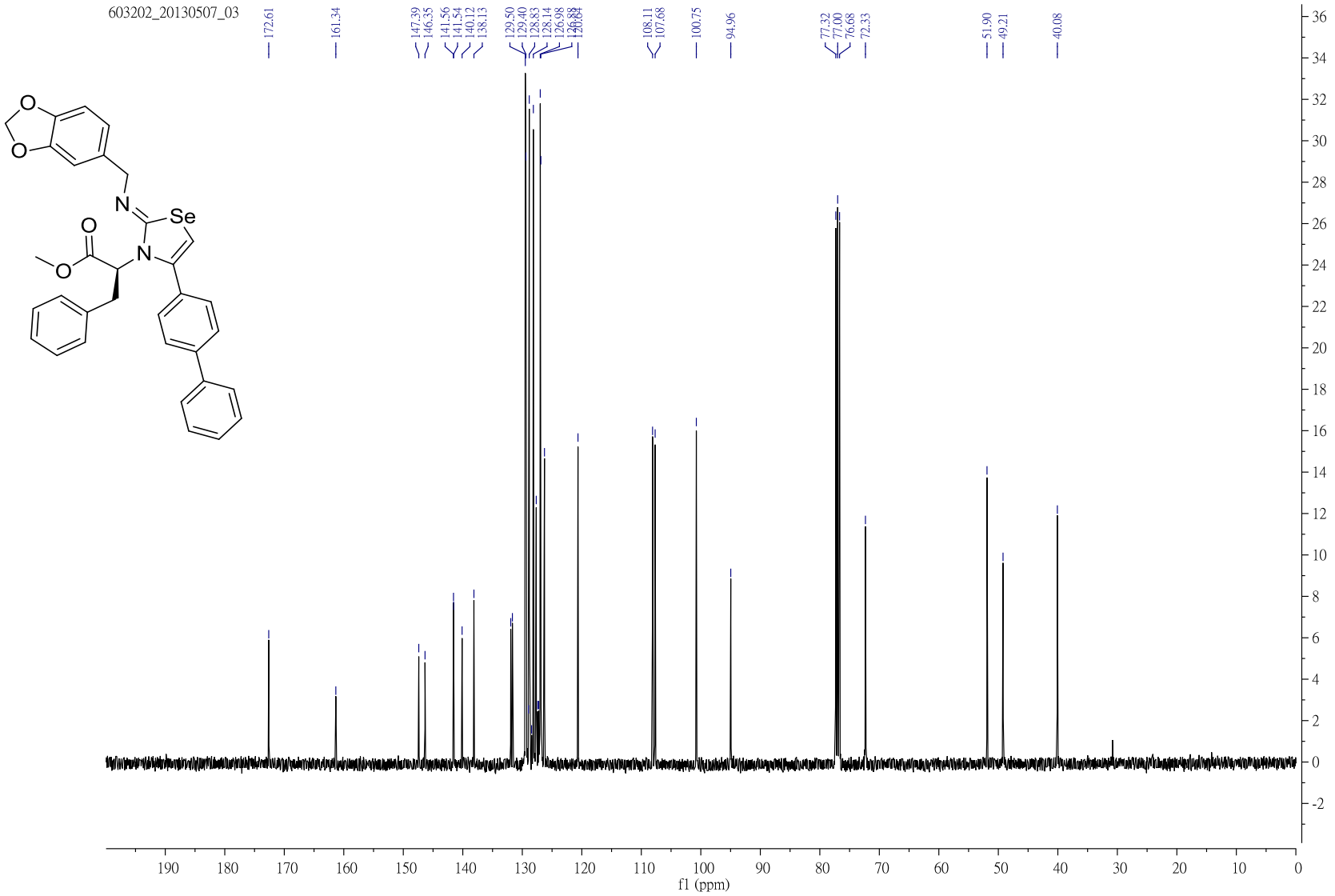
```
SAMPLE : ----------
ID #   : 002
LAMP λ : 589 nm
CONC   : 0.03000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-------------------------
SPECIFIC ROTATION [α]
 COUNT  [α](°)  TEMP(°C)
  01   - 64.3340   18.2
  02   - 65.8339   18.2
  03   - 66.8340   18.2
  04   - 67.3339   18.2
  05   - 67.8340   18.2
  06   - 68.1673   18.2
  07   - 68.6672   18.3
  08   - 68.6672   18.3
  09   - 68.8339   18.3
  10   - 69.1672   18.3
-------------------------
MEAN     = - 67.5673°
σ(N-1)   =    1.5299°
C.V.     = -  2.2643%
```


BRUKER
Transmittance [%]
20
40
60
80
3106.47
3083.99
3058.71
3025.70
2999.25
2948.66
2918.03
2868.23
1741.93
1607.54
1508.92
1493.54
1450.69
1435.45
1344.75
1301.77
1261.11
1208.24
1157.13
1076.42
1031.38
969.12
825.90
765.46
748.61
701.96
628.71
603.73
570.30
517.55
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang500801.0.dpt
Page 1/1

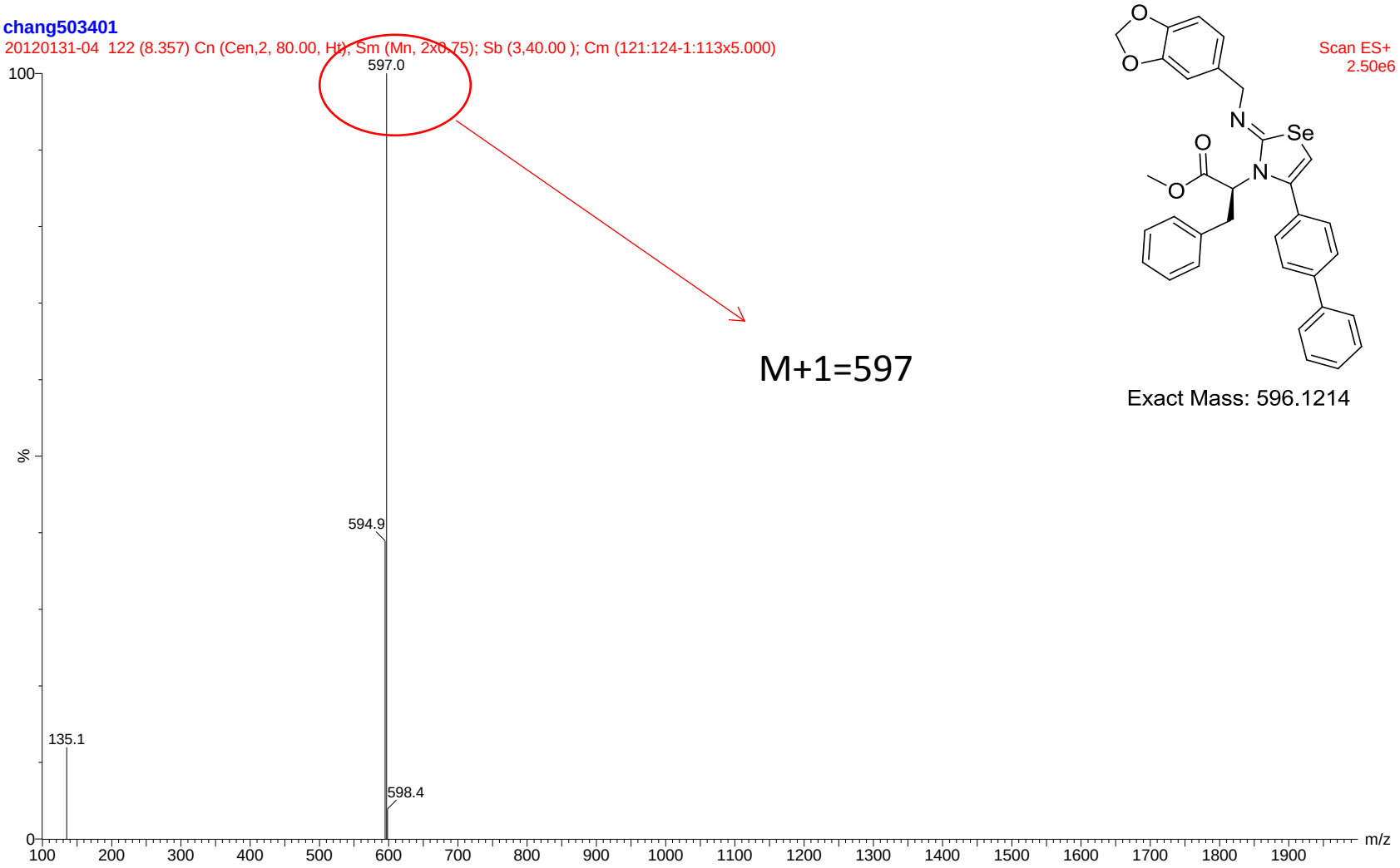
5a FT-IR


603202_20130507_02
7.64
7.60
7.58
7.55
7.53
7.47
7.45
7.44
7.39
7.37
7.35
7.25
7.23
7.20
6.58
6.57
6.28
6.26
6.14
5.90
5.03
4.99
4.85
4.81
3.76
3.72
3.33
3.31
3.29
3.28
3.14
3.12
3.11
3.09
O
O
N
Se
O
N
O
3.24
2.80
5.60
1.74
0.95
0.92
1.90
0.90
1.04
3.37
1.00
0.99
f1 (ppm)

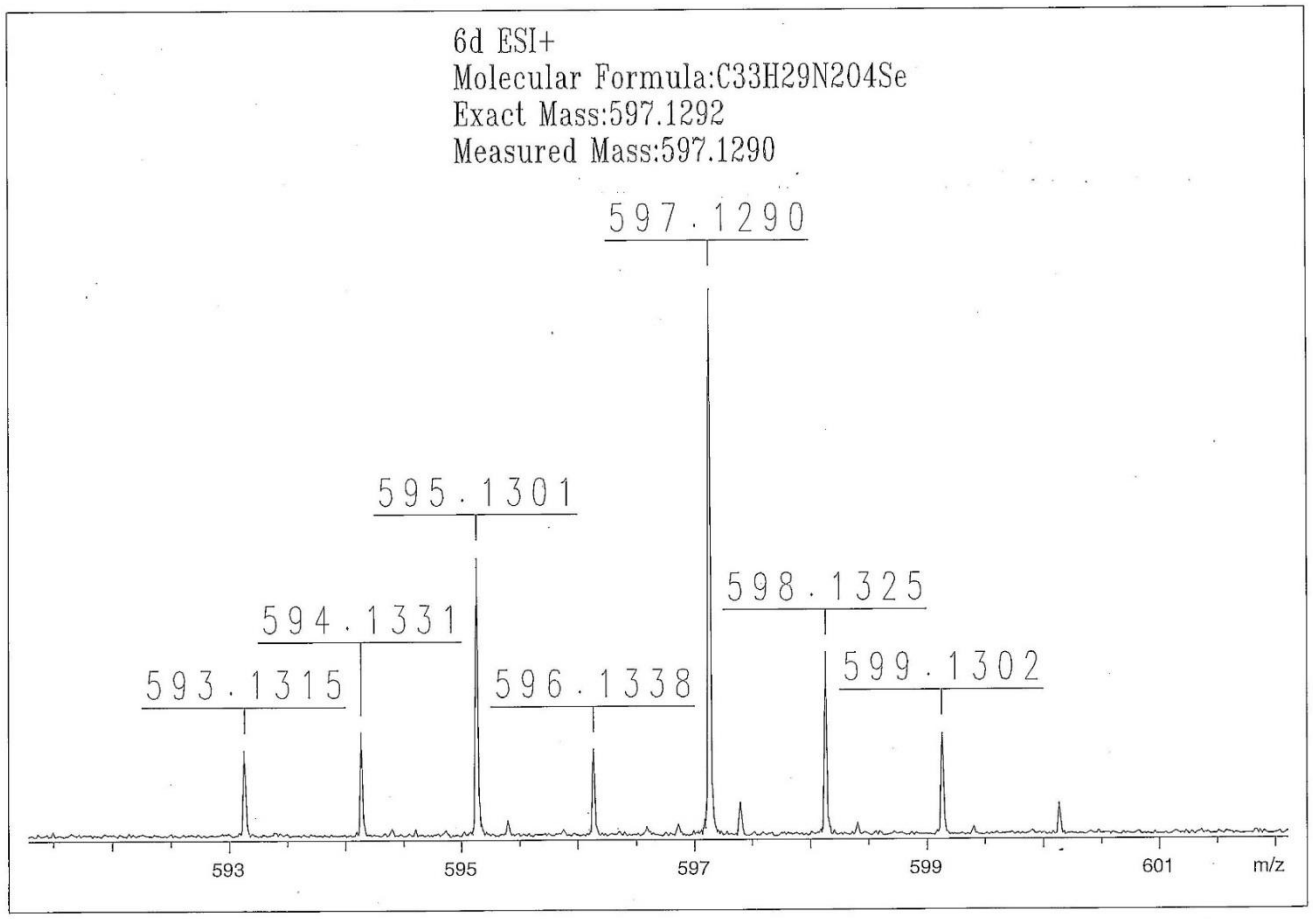
5b H^1NMR


603202_20130507_03
172.61
161.34
147.39
146.35
141.56
141.54
140.12
138.13
129.50
129.40
128.83
128.14
126.98
108.11
107.68
100.75
94.96
77.32
77.00
76.68
72.53
51.90
49.21
40.08
O
O
N
Se
O
N
O
f1 (ppm)

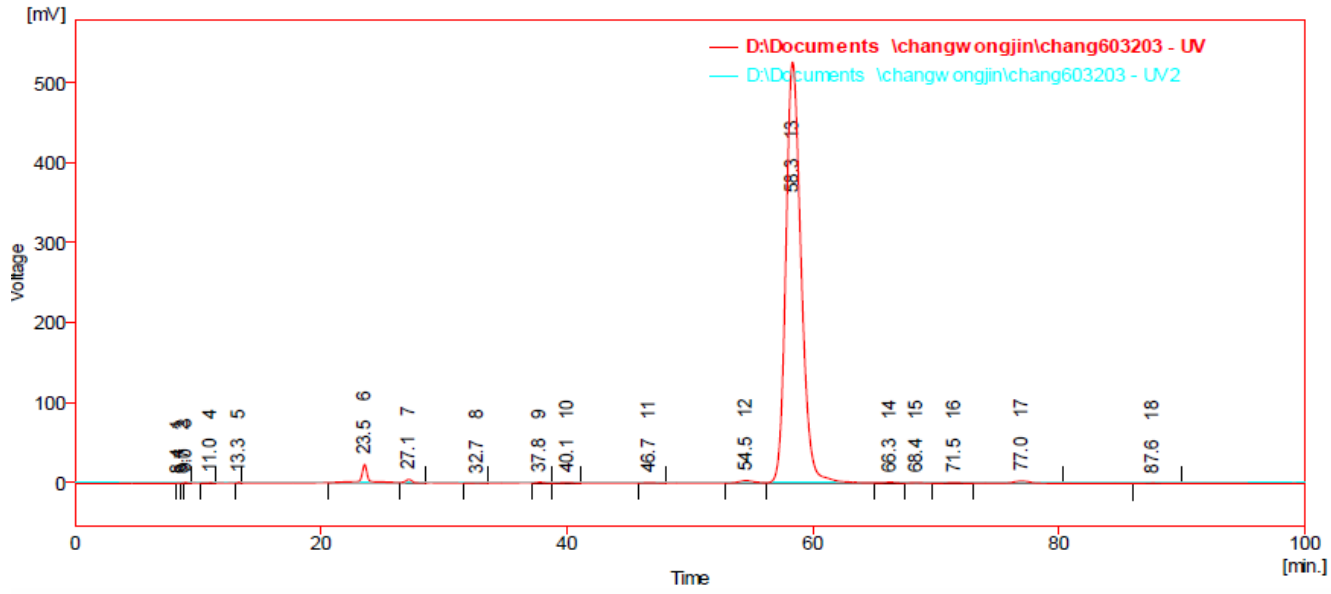
5b C^{13}NMR


chang503401
20120131-04 122 (8.357) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (121:124-1:113x5.000)
Scan ES+
2.50e6
597.0
M+1=597
Exact Mass: 596.1214
100
%
0
594.9
135.1
598.4
100
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
1600
1700
1800
1900
m/z

5b LR-MS


6d ESI+
Molecular Formula:C33H29N2O4Se
Exact Mass:597.1292
Measured Mass:597.1290
597.1290
595.1301
598.1325
594.1331
599.1302
593.1315
596.1338
593
595
597
599
601
m/z
/d=/Data/yu/6d/4/pdata/1 Administrator Thu Aug 1 15:25:45 2013

5b HR-MS



Result Table (Uncal - D:|Documents |changwongjin|chang603203 - UV)

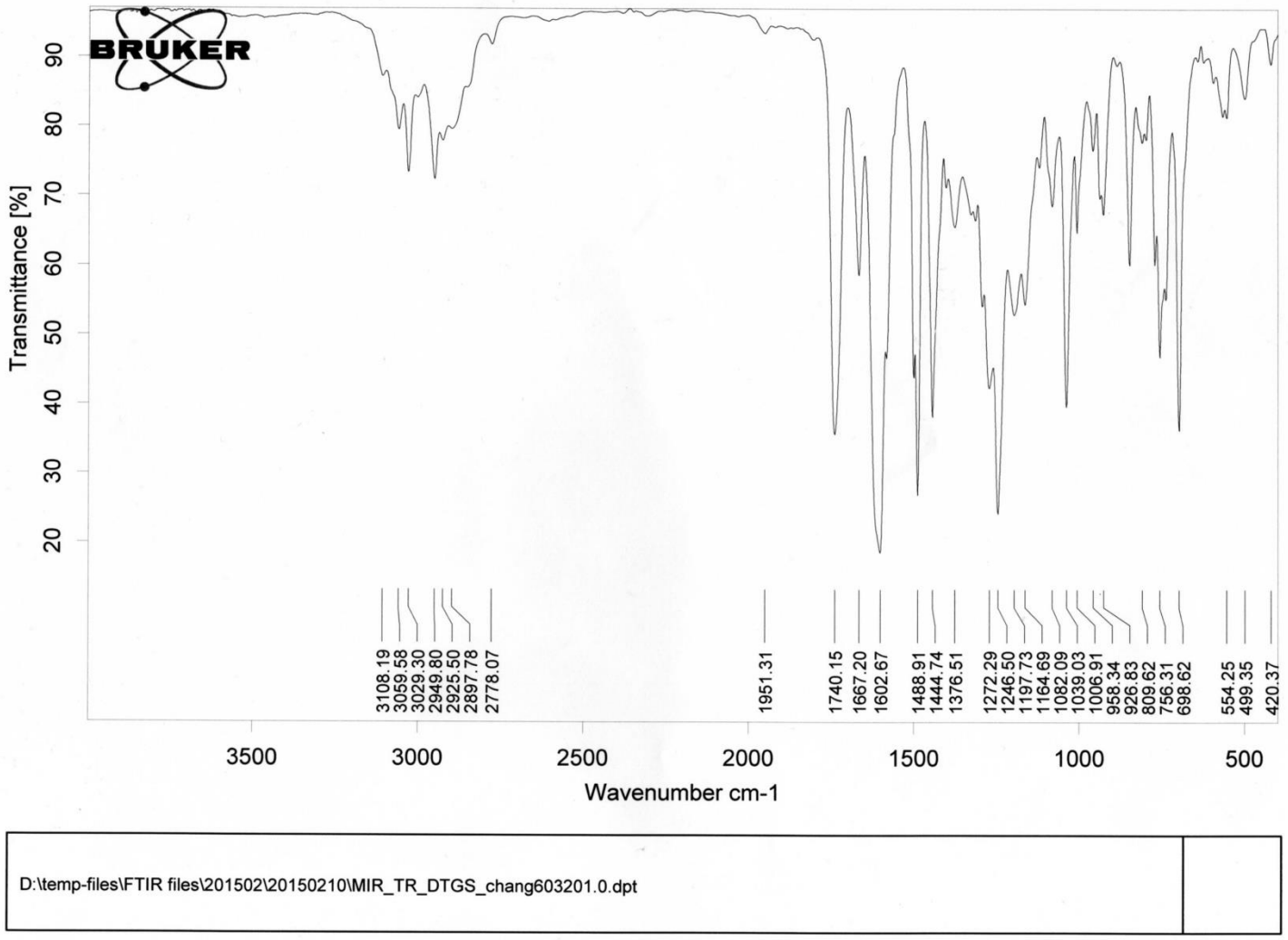
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	8.356	3.179	0.307	0.0	0.1
2	8.724	2.685	0.269	0.0	0.0
3	8.968	14.837	1.075	0.0	0.2
4	11.028	15.909	1.019	0.0	0.2
5	13.312	15.732	1.113	0.0	0.2
6	23.540	851.844	22.864	1.8	4.0
7	27.140	158.060	4.313	0.3	0.8
8	32.720	19.286	0.359	0.0	0.1
9	37.772	32.365	0.867	0.1	0.2
10	40.064	37.008	0.708	0.1	0.1
11	46.704	34.257	0.547	0.1	0.1
12	54.544	248.861	2.877	0.5	0.5
13	58.344	45448.384	526.052	95.8	92.6
14	66.292	102.885	1.079	0.2	0.2
15	68.432	65.018	0.864	0.1	0.2
16	71.504	77.580	0.784	0.2	0.1
17	76.976	283.044	2.770	0.6	0.5
18	87.632	27.622	0.282	0.1	0.0
	Total	47438.556	568.147	100.0	100.0

Result Table (Uncal - D:|Documents |changwongjin|chang603203 - UV2)

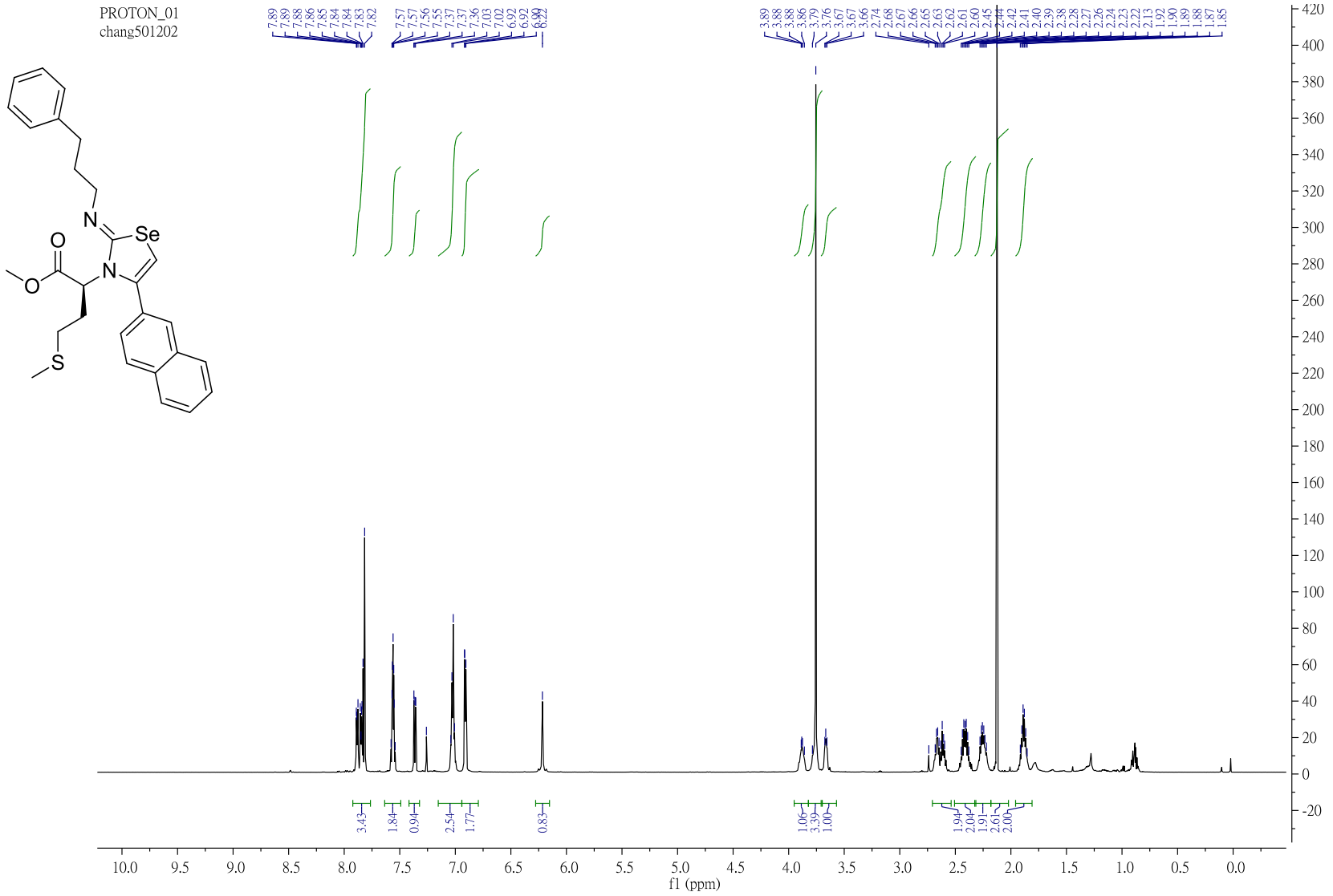
Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
No peak to report				

5b chiral HPLC

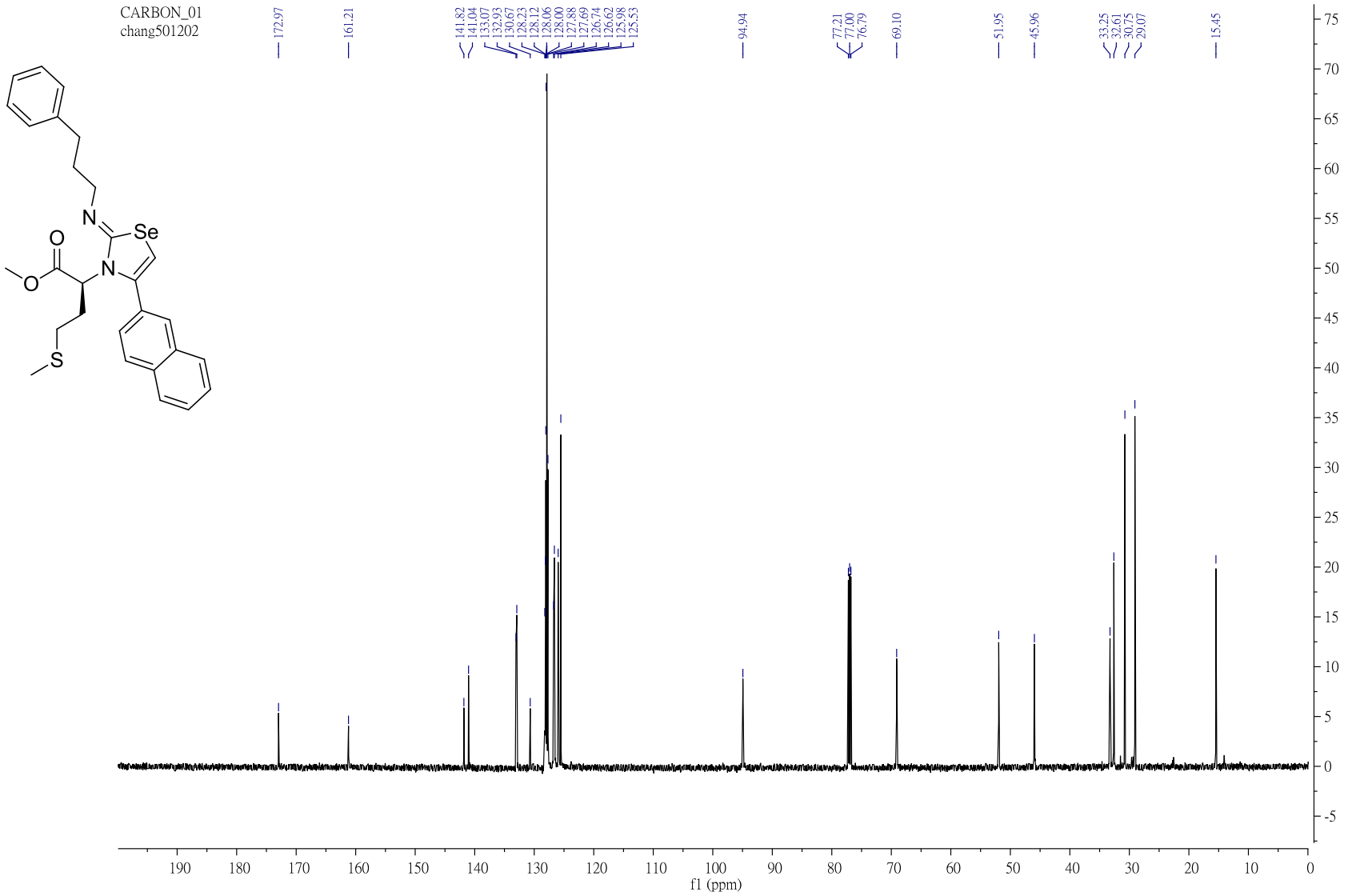
```
SAMPLE : ----------
ID #   : 001
LAMP λ : 589 nm
CONC   : 0.04000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-----------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01   -215.6260   18.1
  02   -216.1260   18.2
  03   -217.0010   18.2
  04   -216.6260   18.2
  05   -216.7510   18.2
  06   -217.7510   18.2
  07   -219.2510   18.2
  08   -219.2510   18.2
  09   -219.6260   18.2
  10   -220.8760   18.2
-----------------------
MEAN     = -217.8880°
σ(N-1)   =    1.7504°
C.V.     = - 0.80337%
```


BRUKER
Transmittance [%]
20
30
40
50
60
70
80
90
3108.19
3059.58
3029.30
2949.80
2925.50
2897.78
2778.07
1951.31
1740.15
1667.20
1602.67
1488.91
1444.74
1376.51
1272.29
1246.50
1197.73
1164.69
1082.09
1039.03
1006.91
958.34
926.83
809.62
756.31
698.62
554.25
499.35
420.37
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201502\20150210\MIR_TR_DTGS_chang603201.0.dpt
Page 1/1

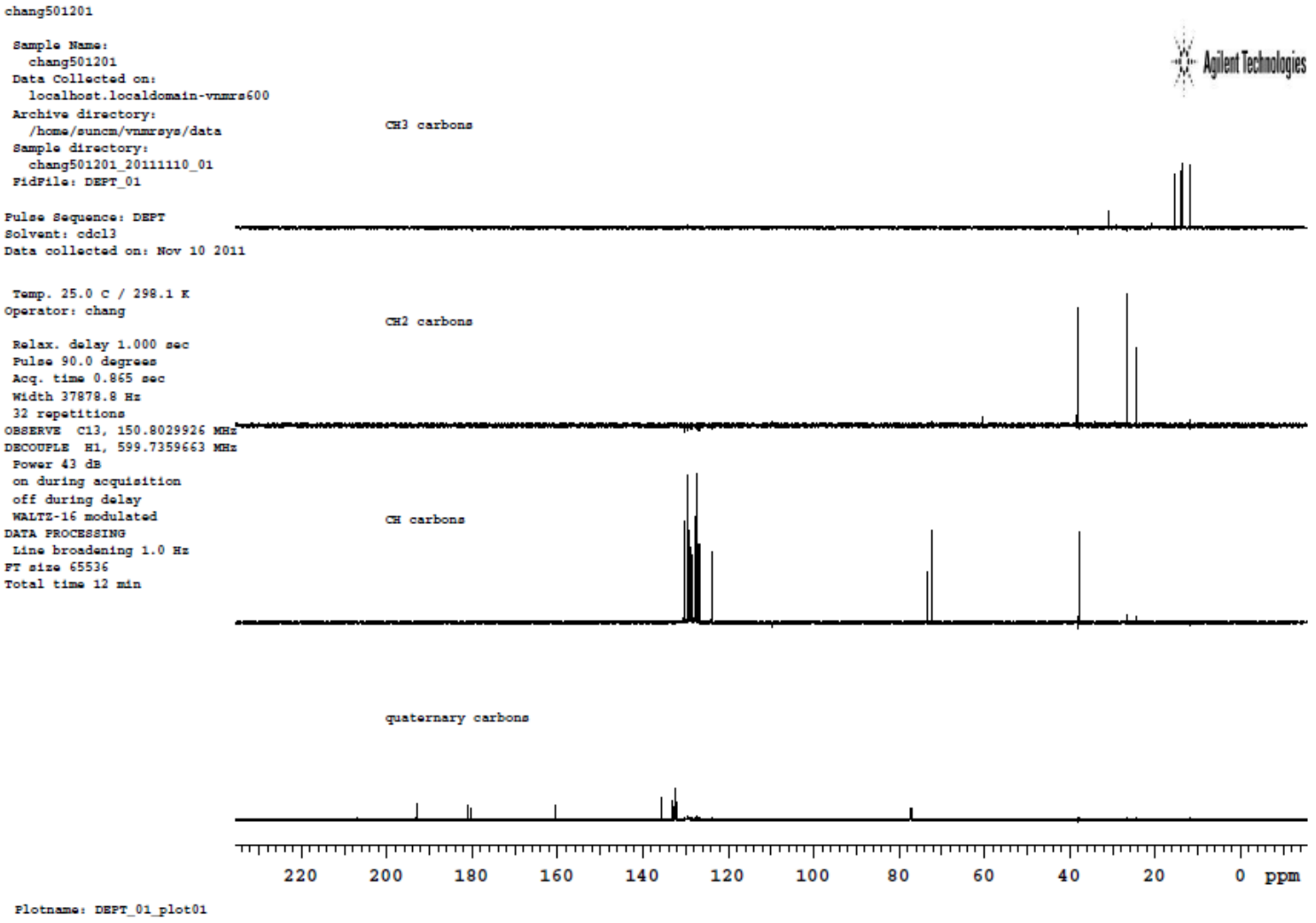
5b FT-IR



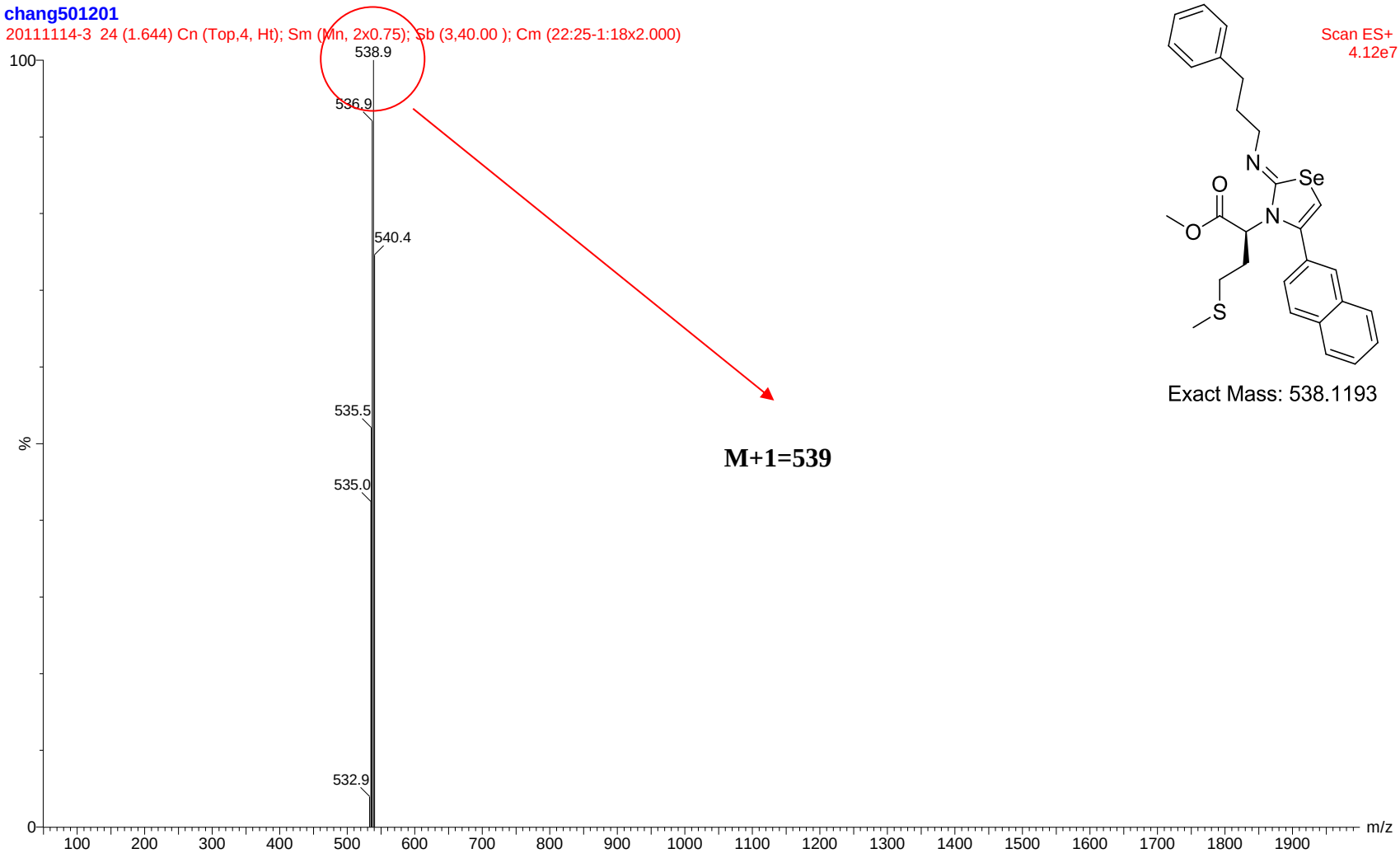
5c H^1NMR


CARBON_01
chang501202
172.97
161.21
141.82
141.04
133.07
132.93
130.67
128.23
128.12
128.06
128.00
127.88
127.69
126.74
126.62
125.98
125.53
94.94
77.21
77.00
76.79
69.10
51.95
45.96
33.25
32.61
30.75
29.07
15.45
N
Se
O
O
N
S
f1 (ppm)

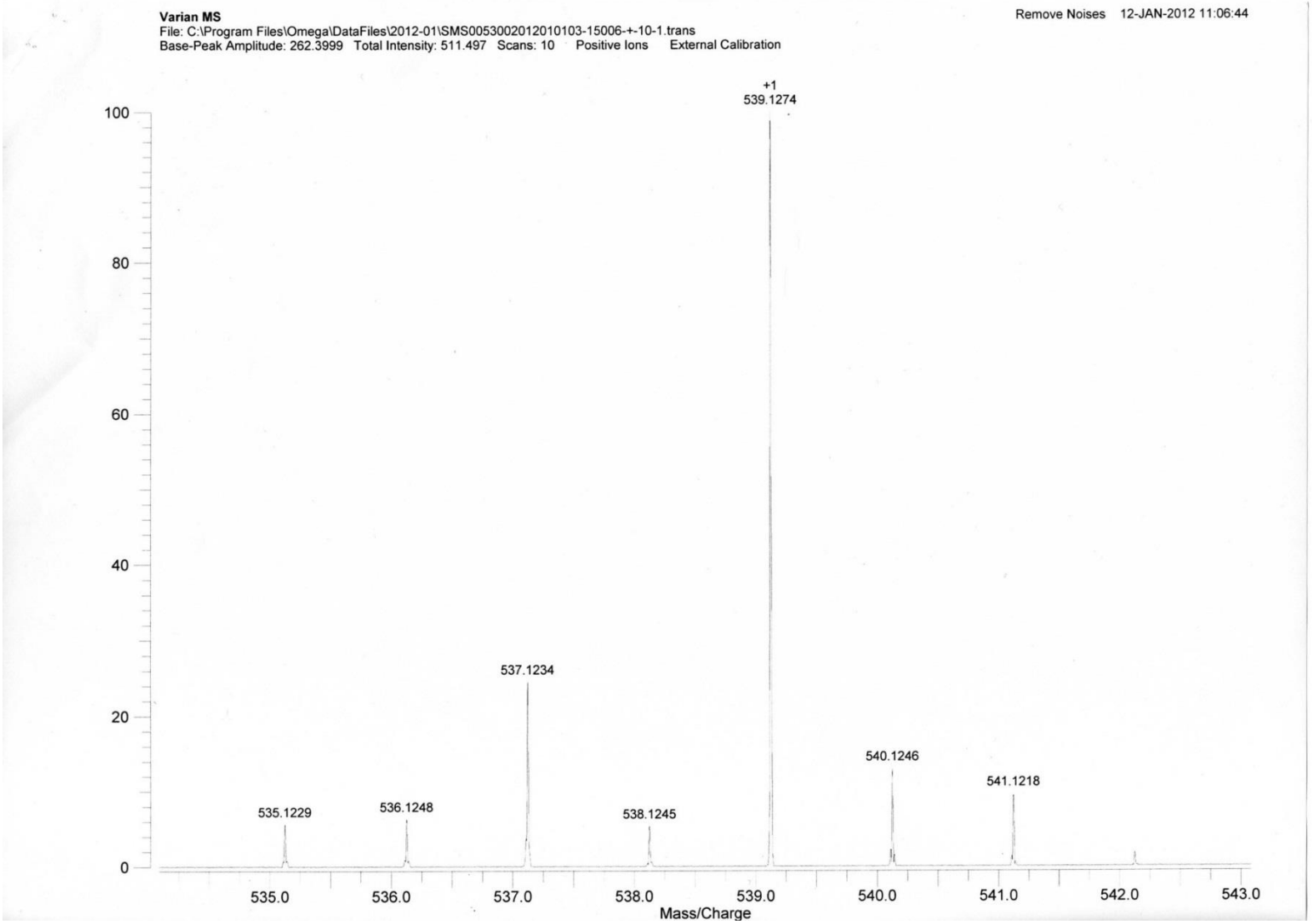
5c C^{13}NMR


chang501201
Sample Name:
chang501201
Data Collected on:
localhost.localdomain-vnmrs600
Archive directory:
/home/suncm/vnmrsys/data
Sample directory:
chang501201_20111110_01
FidFile: DEPT_01
Pulse Sequence: DEPT
Solvent: cdcl3
Data collected on: Nov 10 2011
Temp. 25.0 C / 298.1 K
Operator: chang
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
32 repetitions
OBSERVE C13, 150.8029926 MHz
DECOUPLE H1, 599.7359663 MHz
Power 43 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 12 min
Agilent Technologies
CH3 carbons
CH2 carbons
CH carbons
quaternary carbons
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Plotname: DEPT_01_plot01

5c DEPT


chang501201
20111114-3 24 (1.644) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (22:25-1:18x2.000)
Scan ES+
4.12e7
538.9
536.9
540.4
535.5
535.0
532.9
100
%
0
m/z
100 200 300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 1700 1800 1900
M+1=539
N
Se
O
O
N
S
Exact Mass: 538.1193

5c LR-MS


Varian MS
File: C:\Program Files\Omega\DataFiles\2012-01\SMS0053002012010103-15006-+-10-1.trans
Base-Peak Amplitude: 262.3999 Total Intensity: 511.497 Scans: 10 Positive Ions External Calibration
Remove Noises 12-JAN-2012 11:06:44
+1
539.1274
537.1234
540.1246
541.1218
535.1229
536.1248
538.1245
100
80
60
40
20
0
535.0
536.0
537.0
538.0
539.0
540.0
541.0
542.0
543.0
Mass/Charge

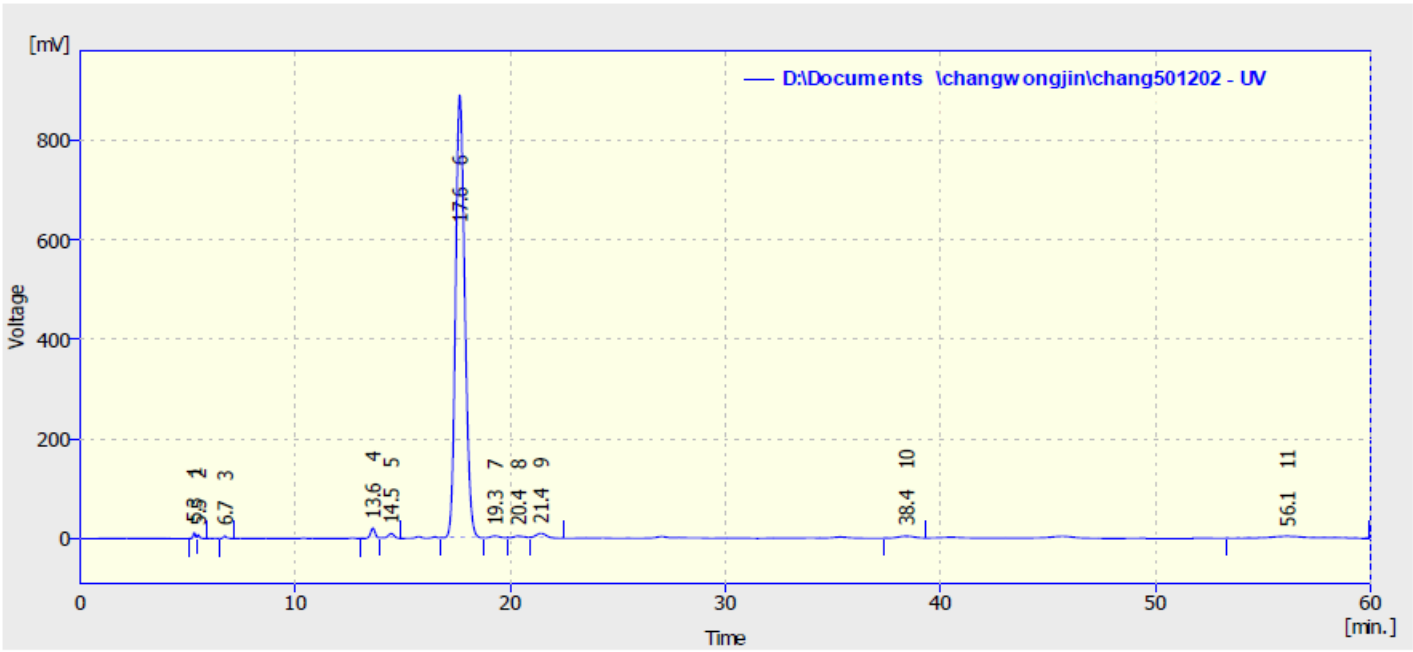
5c HR-MS

Mass/Intensity Table - Varian ESI FTMS with Omega v9.1.20

File: C:\Program Files\Omega\DataFiles\2012-01\SMS0053002012010103-15006-+-10-1.trans
Acquired: 12-JAN-2012 11:06:44
Accumulated Transients: 10
Mode: Positive Ions
Threshold: 0.35%

External CAL
Total Peak Area: 4941.1468
Total Intensity: 511.4965

m/z	Rel. Abund.	Resolution
179.04792	0.32	123900
179.71486	0.94	136200
268.56894	0.56	110100
269.56957	2.23	70300
345.10088	0.46	65400
345.11237	0.45	58100
360.31923	0.53	67600
437.18884	5.22	54100
438.19046	0.97	54700
438.33090	0.54	55800
453.16158	2.01	55500
535.12288	5.70	47100
535.13841	0.85	32600
536.11055	0.92	35700
536.12477	6.36	47700
536.14038	0.84	33800
537.11022	3.81	33900
537.12345	24.53	46000
538.10963	0.50	50600
538.12446	5.40	46600
538.14073	0.64	31000
539.12739	100.00	44400
540.10960	2.13	45900
540.12464	13.01	49200
540.14008	1.56	46100
541.10743	1.37	44700
541.12185	9.63	48700
541.13785	0.64	42300
542.12297	1.77	45300
659.05260	0.62	27200
697.64444	0.44	31600



Result Table (Uncal - D:|Documents |changwongjin|chang501202 - UV)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	5.304	83.097	11.850	0.3	1.2
2	5.484	60.351	7.343	0.2	0.8
3	6.724	49.096	4.875	0.2	0.5
4	13.612	314.587	20.748	1.1	2.1
5	14.464	209.177	9.709	0.7	1.0
6	17.648	26669.174	889.464	92.7	91.6
7	19.288	136.842	4.170	0.5	0.4
8	20.372	151.700	4.244	0.5	0.4
9	21.428	338.807	9.698	1.2	1.0
10	38.424	199.907	4.108	0.7	0.4
11	56.140	554.114	4.324	1.9	0.4
	Total	28766.853	970.534	100.0	100.0

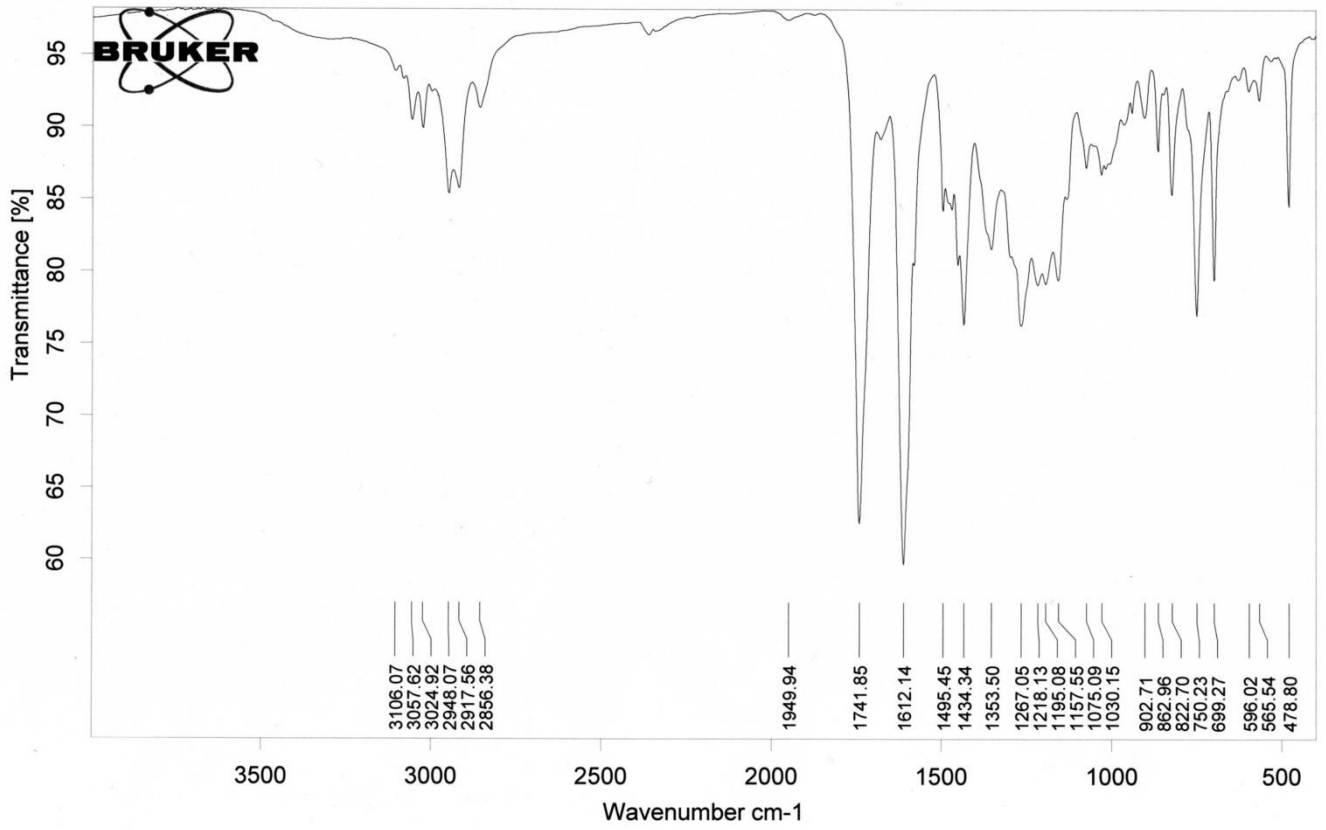
5c chiral HPLC

SAMPLE : 5c
ID # : 002
LAMP λ : 589 nm
CONC : 0.03000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL: 1 min

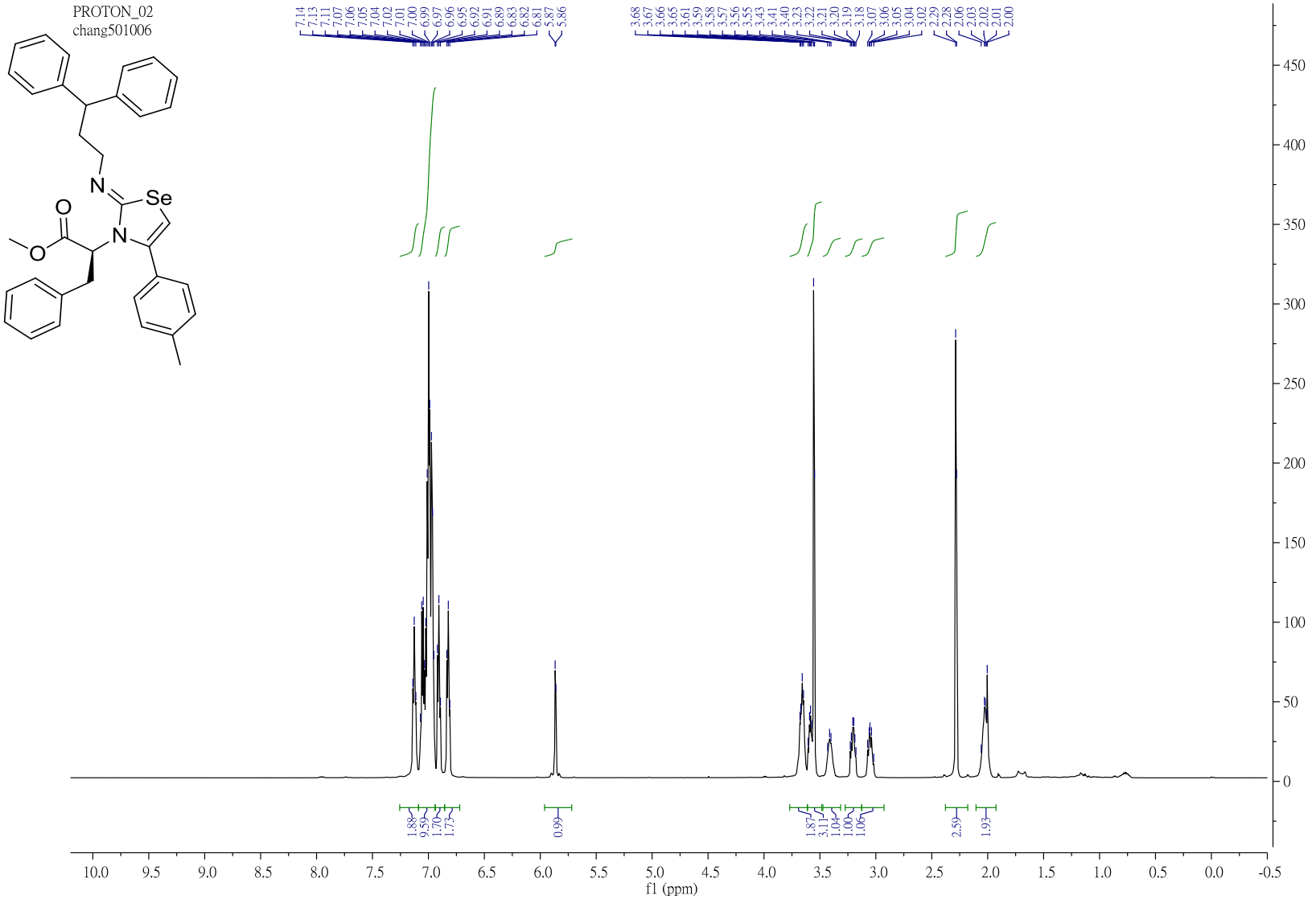
SPECIFIC ROTATION [α]

COUNT	[α](°)	TEMP(°C)
01	- 80.5002	19.2
02	- 81.8336	19.2
03	- 82.6669	19.2
04	- 82.5002	19.2
05	- 83.3336	19.2
06	- 84.0003	19.2
07	- 84.1669	19.2
08	- 84.5003	19.2
09	- 84.8336	19.2
10	- 85.5003	19.2

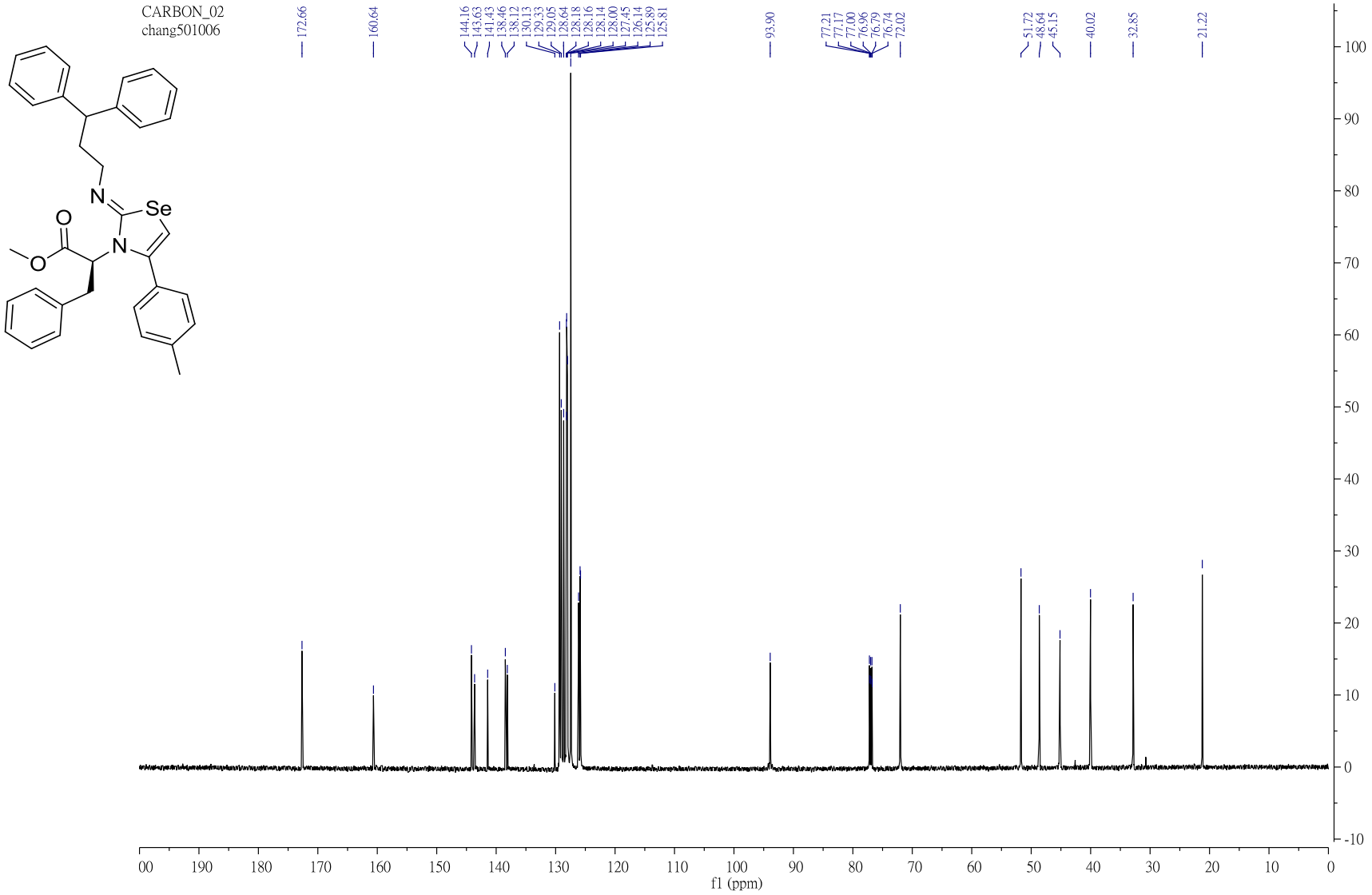
MEAN = - 83.3836°
σ(N-1) = 1.5215°
C.V. = - 1.8247%


BRUKER
Transmittance [%]
95
90
85
80
75
70
65
60
3106.07
3057.62
3024.92
2948.07
2917.56
2856.38
1949.94
1741.85
1612.14
1495.45
1434.34
1353.50
1267.05
1218.13
1195.08
1157.55
1075.09
1030.15
902.71
862.96
822.70
750.23
699.27
596.02
565.54
478.80
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang501202.0.dpt
Page 1/1

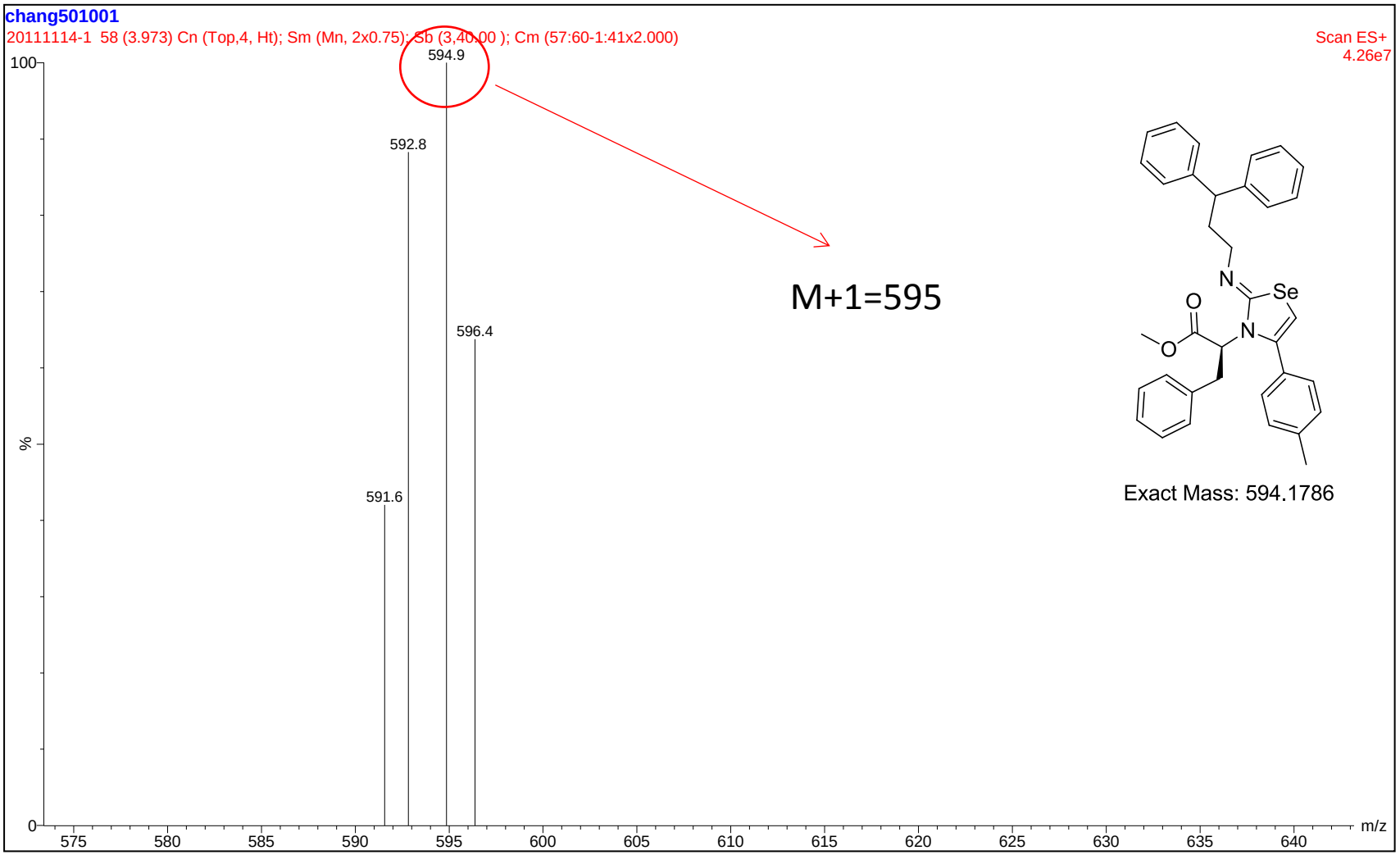
5c FT-IR


PROTON_02
chang501006
N
Se
O
O
N
7.14 7.13 7.11 7.07 7.06 7.05 7.04 7.02 7.01 7.00 6.99 6.97 6.96 6.95 6.92 6.91 6.89 6.83 6.82 6.81 5.87 5.86
3.68 3.67 3.66 3.65 3.61 3.59 3.58 3.57 3.56 3.55 3.43 3.41 3.40 3.23 3.22 3.21 3.20 3.19 3.18 3.07 3.06 3.05 3.04 3.02 2.29 2.28 2.06 2.03 2.02 2.01 2.00
1.88 9.59 1.70 1.75 0.99 1.87 3.11 1.04 1.00 1.06 2.59 1.93
f1 (ppm)

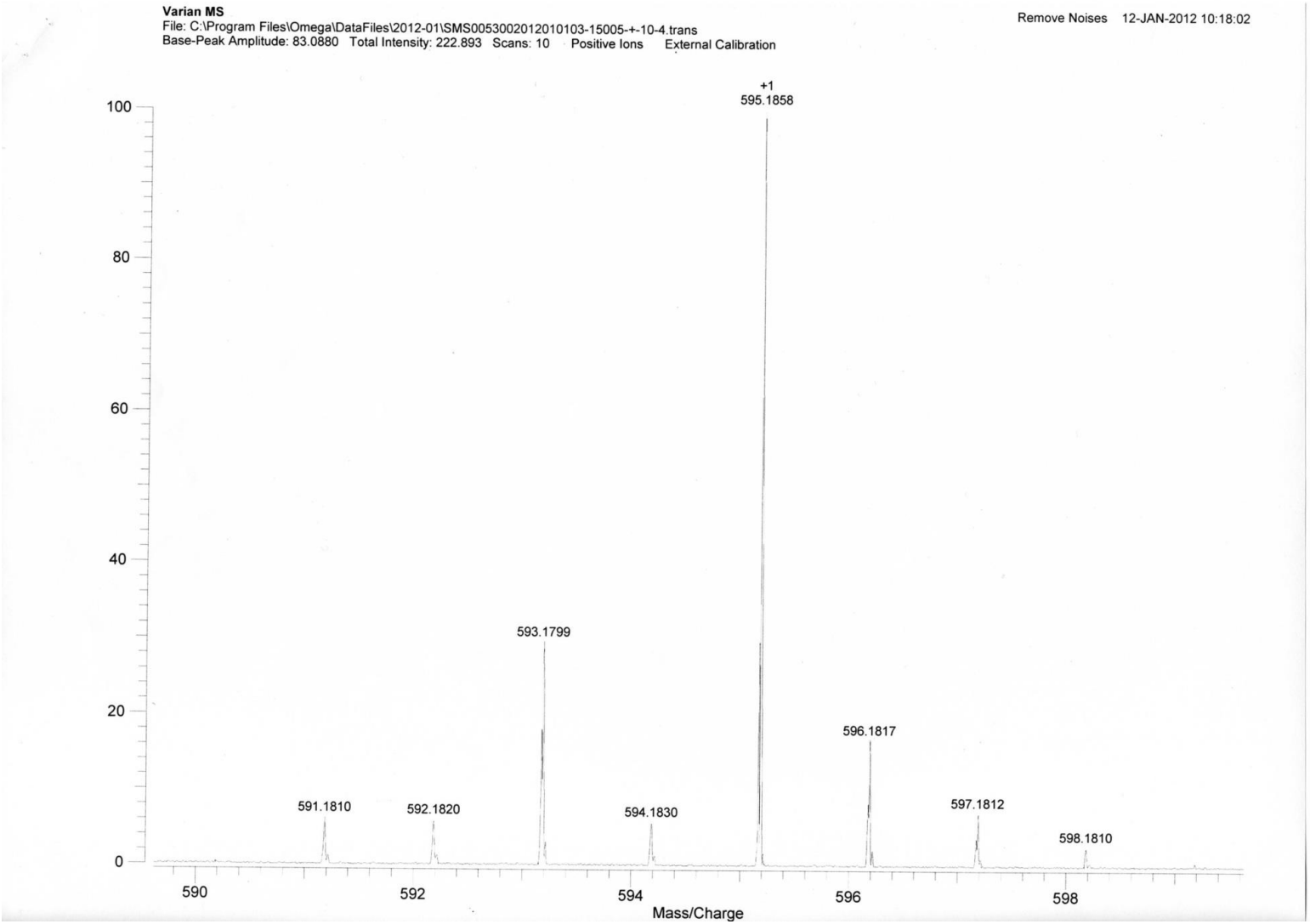
5d H^1NMR


CARBON_02
chang501006
172.66
160.64
144.16
143.63
141.43
138.46
138.12
130.13
129.33
129.05
128.64
128.18
128.16
128.14
128.00
127.45
126.14
125.89
125.81
93.90
77.21
77.17
77.00
76.96
76.79
76.74
72.02
51.72
48.64
45.15
40.02
32.85
21.22
N
Se
O
N
O
f1 (ppm)

5d C^{13}NMR


chang501001
20111114-1 58 (3.973) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (57:60-1:41x2.000)
Scan ES+
4.26e7
100
%
0
594.9
592.8
596.4
591.6
M+1=595
N
Se
O
N
O
Exact Mass: 594.1786
575
580
585
590
595
600
605
610
615
620
625
630
635
640
m/z

5d LR-MS


Varian MS
File: C:\Program Files\Omega\DataFiles\2012-01\SMS0053002012010103-15005-+-10-4.trans
Base-Peak Amplitude: 83.0880 Total Intensity: 222.893 Scans: 10 Positive Ions External Calibration
Remove Noises 12-JAN-2012 10:18:02
+1
595.1858
593.1799
596.1817
591.1810
592.1820
594.1830
597.1812
598.1810
100
80
60
40
20
0
590
592
594
596
598
Mass/Charge

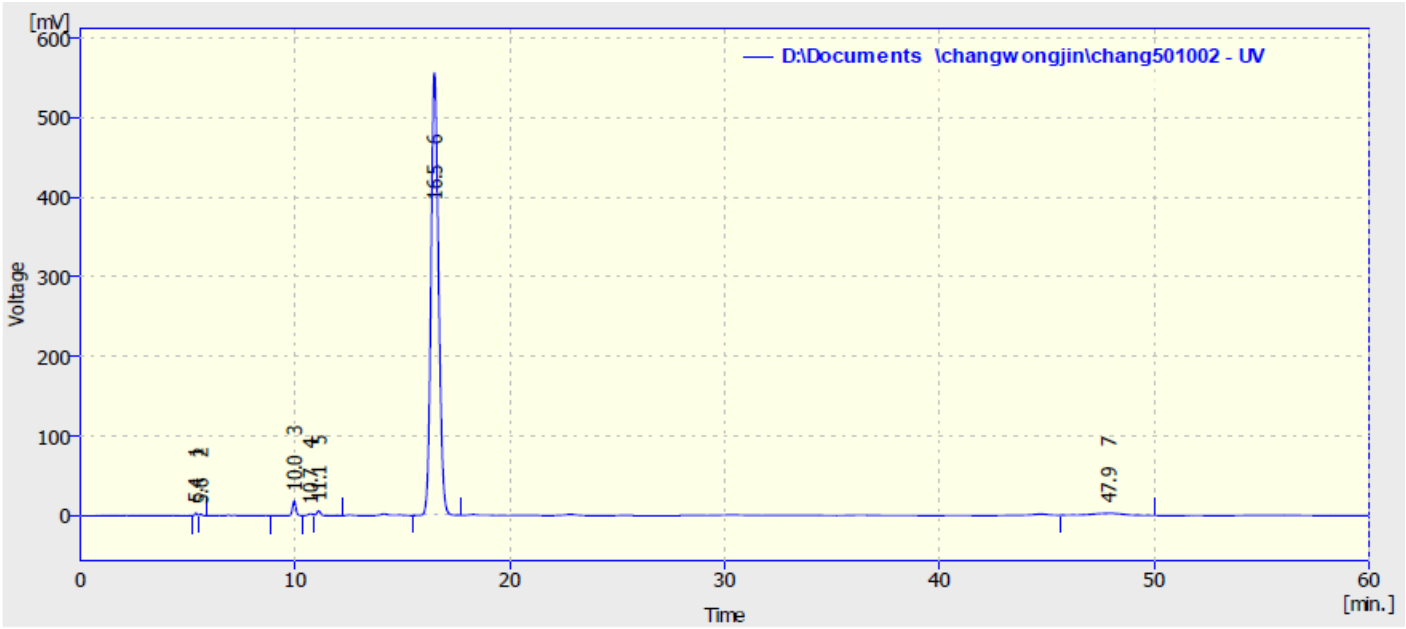
5d HR-MS

Mass/Intensity Table - Varian ESI FTMS with Omega v9.1.20

File: C:\Program Files\Omega\DataFiles\2012-01\SMS0053002012010103-15005-+-10-4.trans
Acquired: 12-JAN-2012 10:18:02
Accumulated Transients: 10
Mode: Positive Ions
Threshold: 0.50%

External CAL
Total Peak Area: 1992.7401
Total Intensity: 222.8925

m/z	Rel. Abund.	Resolution
246.25534	0.67	96300
296.59192	1.33	58500
296.60124	0.79	82800
297.59272	1.68	51400
297.59907	1.28	90300
298.09329	0.93	69200
344.97208	0.71	70400
344.97948	1.78	67800
344.98564	1.44	47400
344.98998	0.75	45400
345.02916	0.65	63200
360.32091	0.67	71800
395.26225	0.61	66300
395.43721	0.97	62700
413.26255	0.70	59100
437.18959	2.34	51000
438.33323	1.09	55200
453.16278	1.28	50400
589.18296	0.66	35600
591.18103	5.99	27700
591.21167	1.22	28300
592.18197	5.73	26200
592.21088	1.26	25000
593.17360	16.70	30800
593.17993	29.93	48600
593.20823	3.12	45200
594.18304	5.55	27100
594.21094	1.30	30400
595.16917	32.64	63100
595.18582	100.00	46200
595.20955	1.72	64300
596.17418	8.12	30500
596.18167	16.52	43600
596.21425	2.15	44800
597.17211	3.37	29600
597.18118	6.90	45200
597.20994	1.02	41500
598.18104	2.48	31300
658.56719	0.78	37200
659.05107	0.76	21000
659.53327	0.67	29400

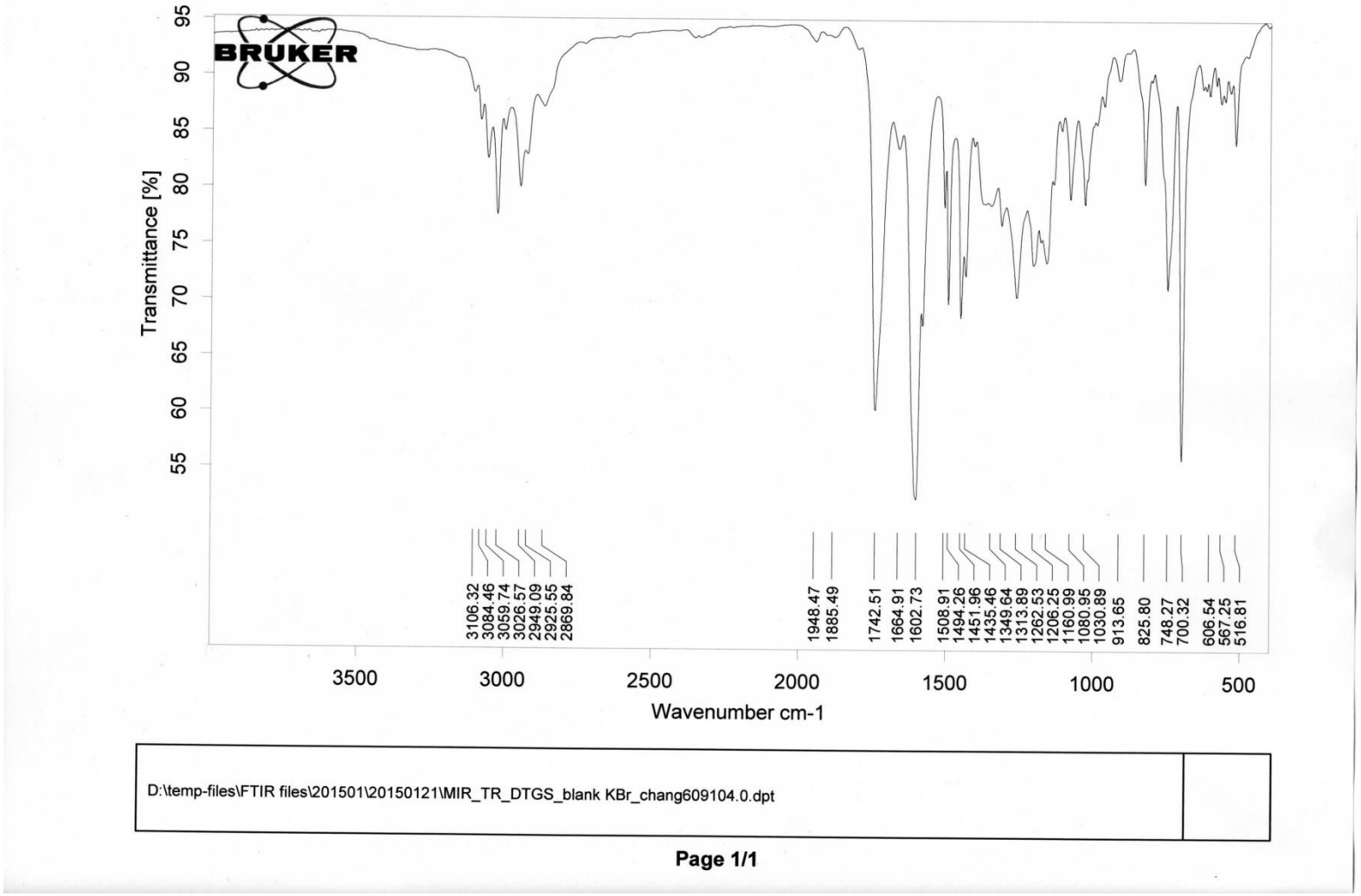


Result Table (Uncal - D:|Documents |changwongjin|chang501002 - UV)

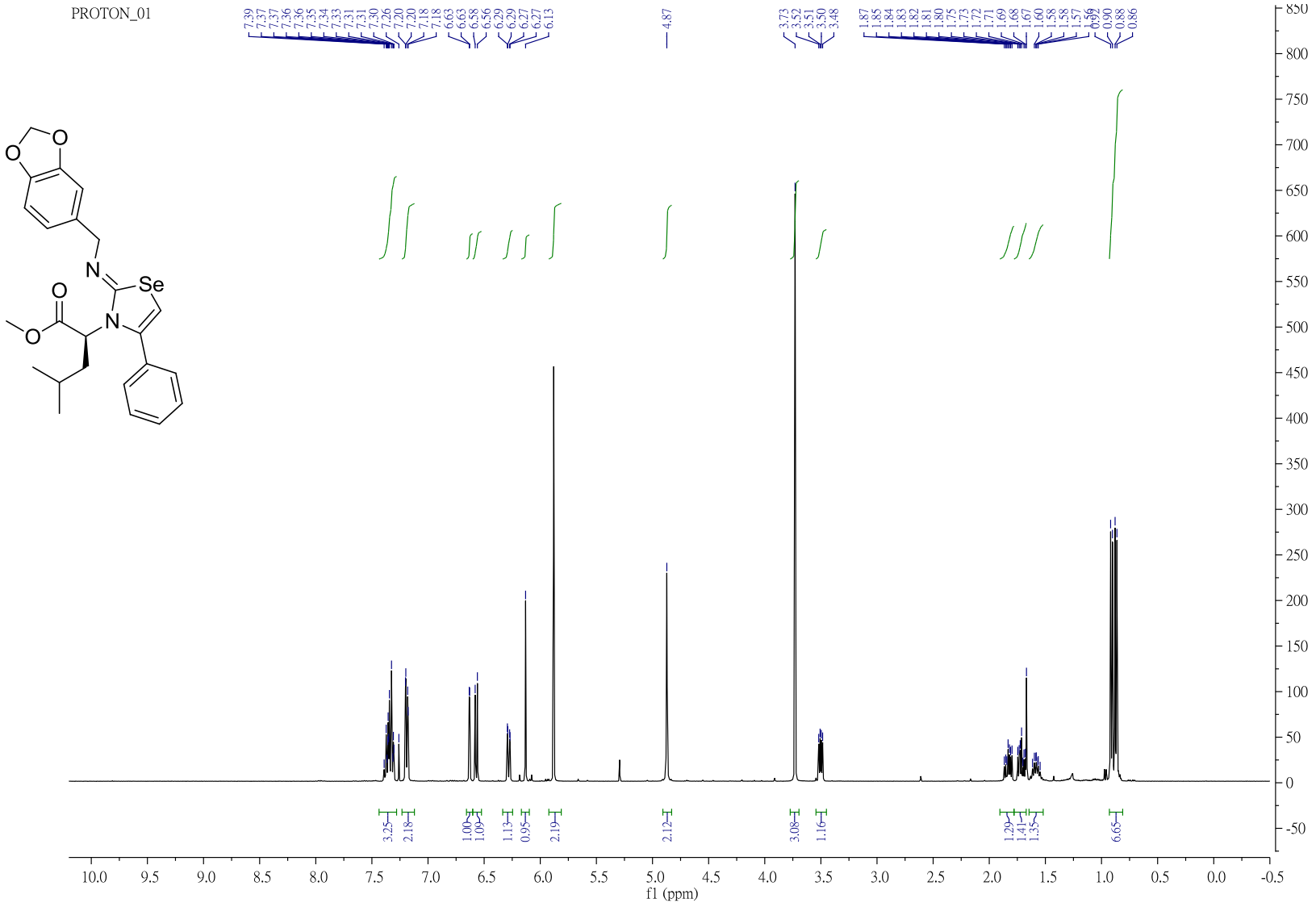
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	5.380	24.336	3.401	0.2	0.6
2	5.604	17.284	2.042	0.1	0.3
3	9.960	204.851	18.503	1.4	3.1
4	10.712	35.424	2.342	0.2	0.4
5	11.100	76.162	6.011	0.5	1.0
6	16.488	13651.457	556.116	95.7	94.1
7	47.880	251.772	2.691	1.8	0.5
	Total	14261.287	591.105	100.0	100.0

5d chiral HPLC

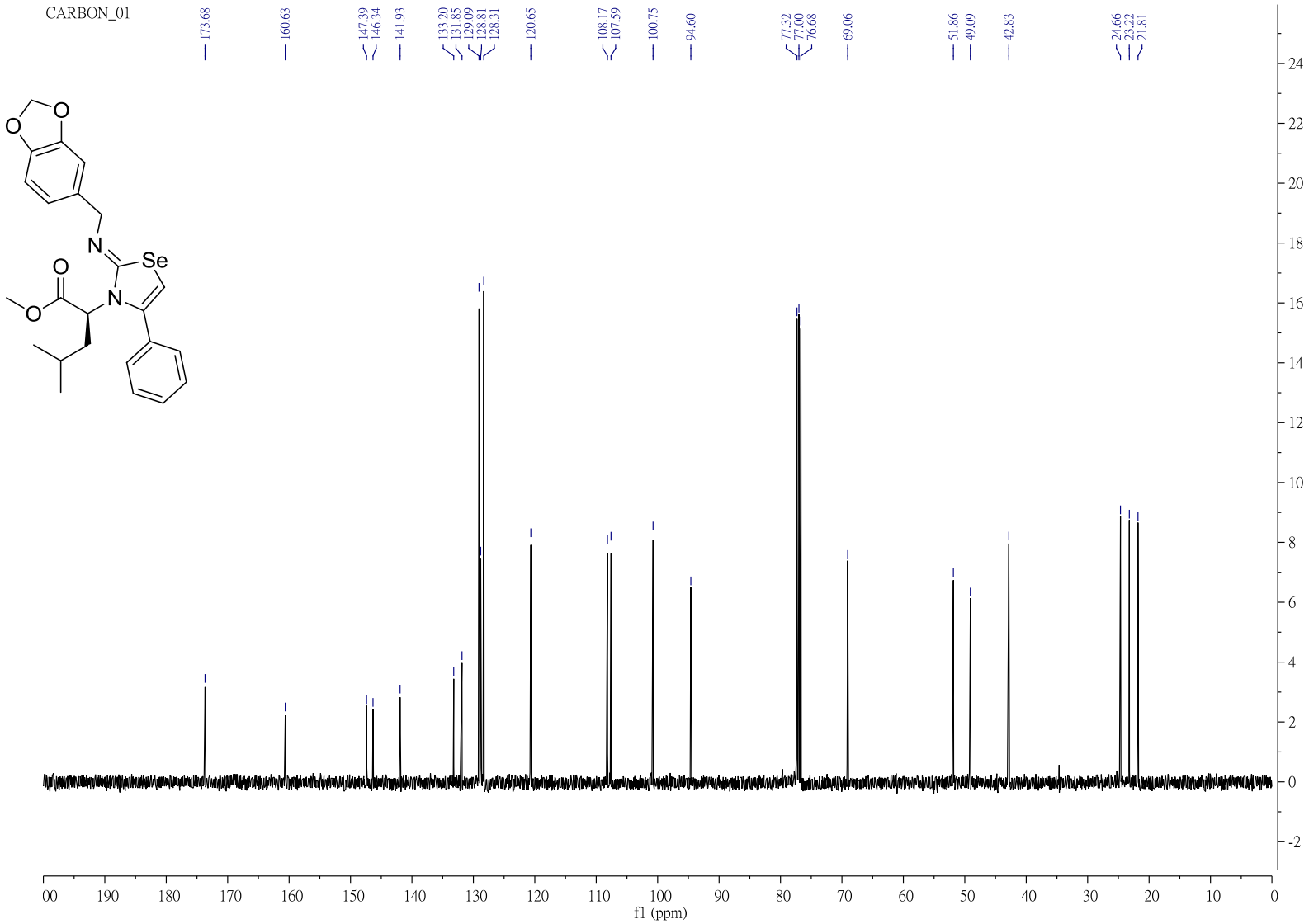
```
SAMPLE : ____________
ID #   : 003
LAMP λ : 589 nm
CONC   : 0.05000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-------------------------
SPECIFIC ROTATION [α]
 COUNT  [α](°)  TEMP(°C)
  01   - 53.4002   19.2
  02   - 55.1002   19.2
  03   - 55.9003   19.2
  04   - 55.8003   19.2
  05   - 55.8003   19.2
  06   - 56.1002   19.2
  07   - 56.2002   19.2
  08   - 56.7002   19.2
  09   - 57.0002   19.3
  10   - 57.3002   19.3
-------------------------
MEAN     = - 55.9302°
σ(N-1)   =    1.0975°
C.V.     = -  1.9622%
```


BRUKER
Transmittance [%]
95
90
85
80
75
70
65
60
55
3106.32
3084.46
3059.74
3026.57
2949.09
2925.55
2869.84
1948.47
1885.49
1742.51
1664.91
1602.73
1508.91
1494.26
1451.96
1435.46
1349.64
1313.89
1262.53
1206.25
1160.99
1080.95
1030.89
913.65
825.80
748.27
700.32
606.54
567.25
516.81
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang609104.0.dpt
Page 1/1

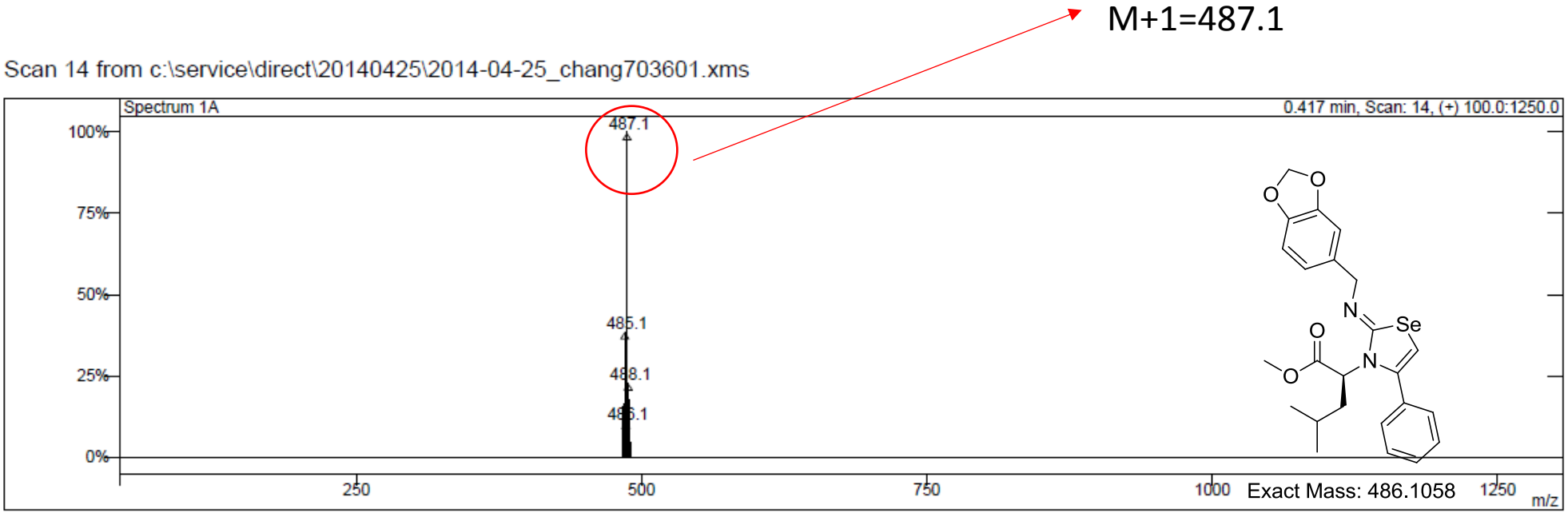
5d FT-IR


PROTON_01
7.39
7.37
7.37
7.36
7.36
7.35
7.34
7.33
7.31
7.31
7.30
7.26
7.20
7.20
7.18
7.18
6.63
6.63
6.58
6.56
6.29
6.29
6.27
6.27
6.13
4.87
3.73
3.52
3.51
3.50
3.48
1.87
1.85
1.84
1.83
1.82
1.81
1.80
1.75
1.73
1.72
1.71
1.69
1.68
1.67
1.60
1.58
1.58
1.57
0.92
0.90
0.88
0.86
O
O
O
N
Se
O
N
O
3.25
2.18
1.00
1.09
1.13
0.95
2.19
2.12
3.08
1.16
1.29
1.41
1.35
6.65
f1 (ppm)

5e H[1]NMR


CARBON_01
173.68
160.63
147.39
146.34
141.93
133.20
131.85
129.09
128.81
128.31
120.65
108.17
107.59
100.75
94.60
77.32
77.00
76.68
69.06
51.86
49.09
42.83
24.66
23.22
21.81
O
O
O
N
Se
O
N
f1 (ppm)

5e C^{13}NMR



Spectrum from ...vice\direct\20140425\2014-04-25_chang703601.xms
Scan No: 14, Time: 0.417 minutes
No averaging. Background corrected.
Name: HESI-FS-POS
Comment: 0.417 min. Scan: 14 (+) 100.0:1250.0 RIC: 2454431205
Pair Count: 8 MW: 0 Formula: None
CAS No: None Acquired Range: 100.0 - 1250.0 m/z

5e LR-MS

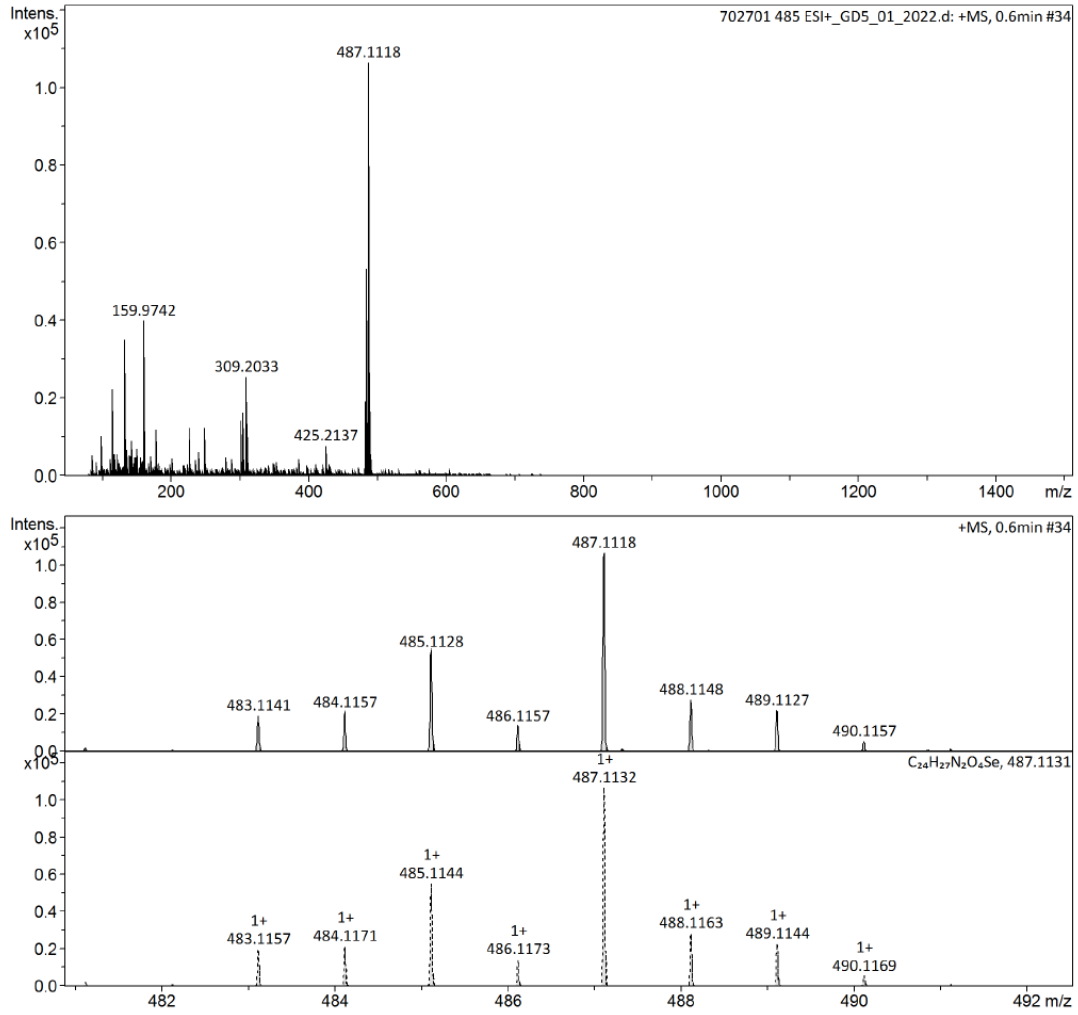
Display Report

Analysis Info

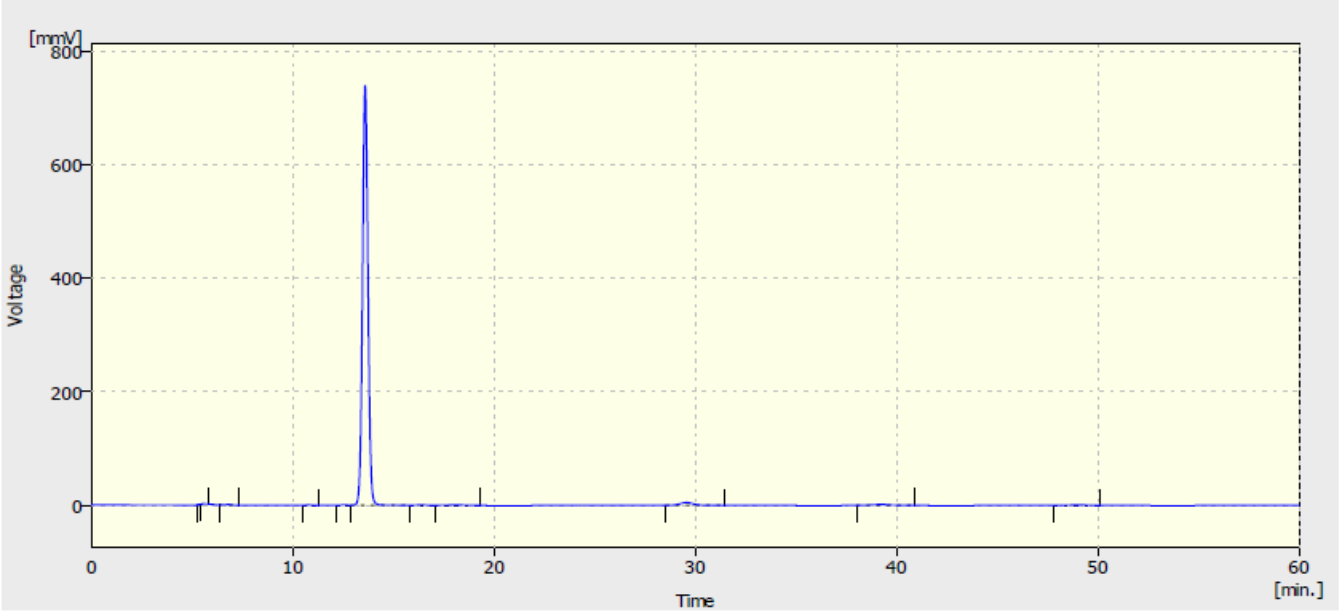
Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\702701 485 ESI+_GD5_01_2022.d	Acquisition Date	6/26/2014 9:52:30 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	702701 485 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



5e HR-MS

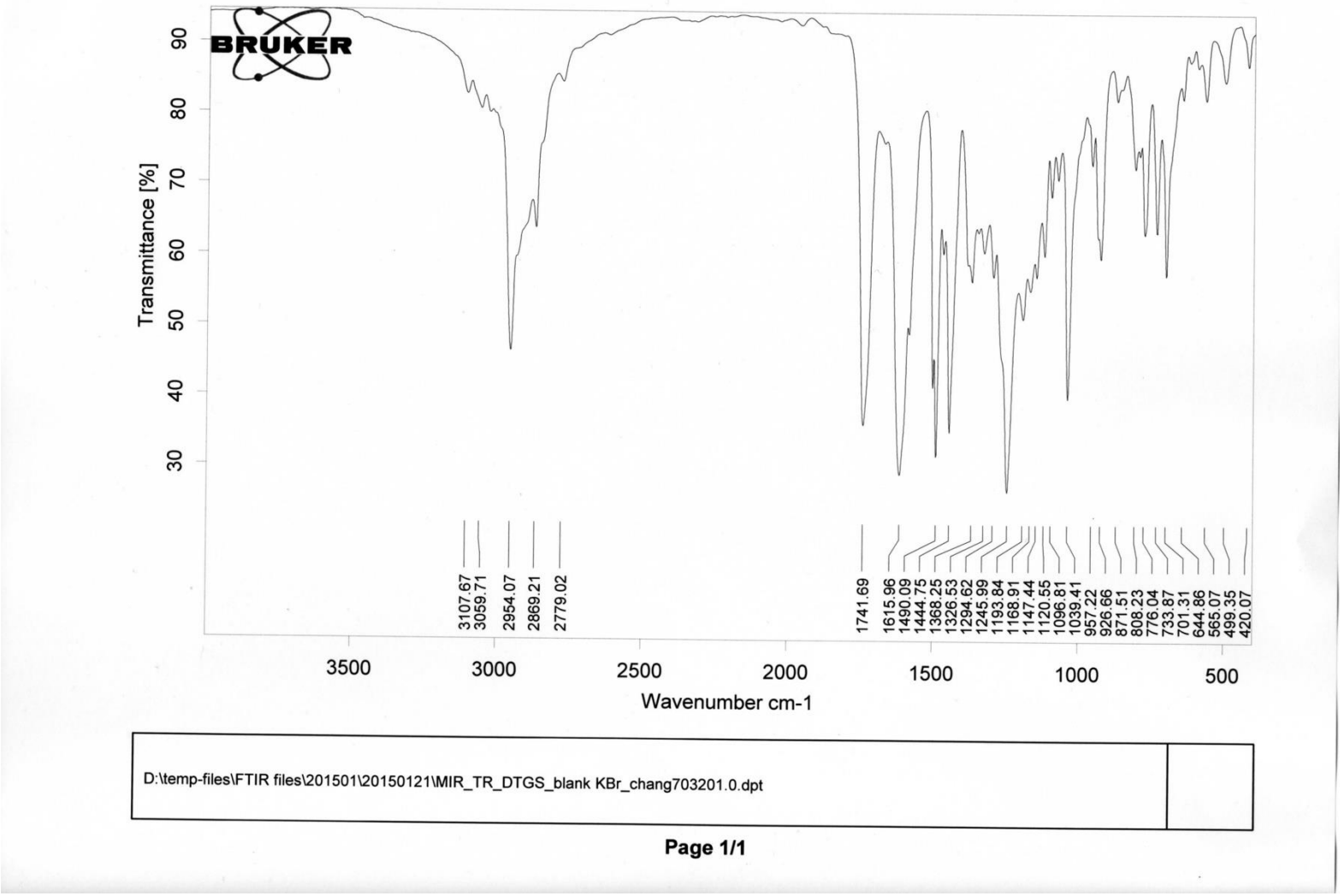


Result Table (Uncal - D:|Documents |changwongjin|chang703603)

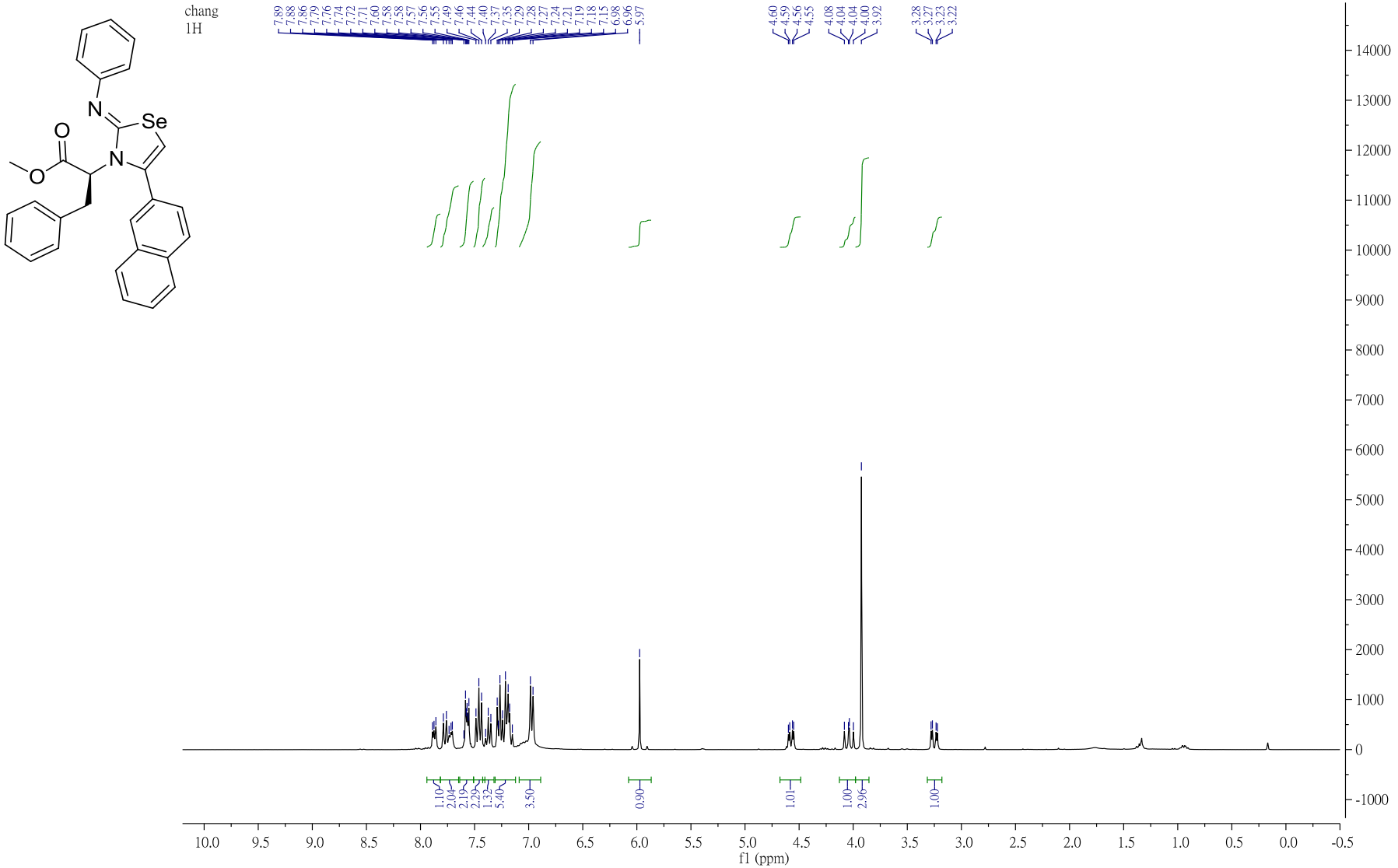
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.336	5.330	0.924	0.0	0.1	0.09
2	5.536	21.229	1.739	0.1	0.2	0.32
3	6.792	23.004	1.117	0.2	0.1	0.34
4	10.764	12.813	0.958	0.1	0.1	0.21
5	12.572	19.964	1.124	0.1	0.1	0.28
6	13.596	13972.431	739.565	96.7	98.1	0.29
7	16.376	24.355	1.061	0.2	0.1	0.32
8	18.248	33.287	0.601	0.2	0.1	0.93
9	29.564	216.935	4.753	1.5	0.6	0.70
10	39.224	75.595	1.499	0.5	0.2	0.77
11	49.016	47.948	0.836	0.3	0.1	0.91
	Total	14452.892	754.177	100.0	100.0	

5e chair HPLC

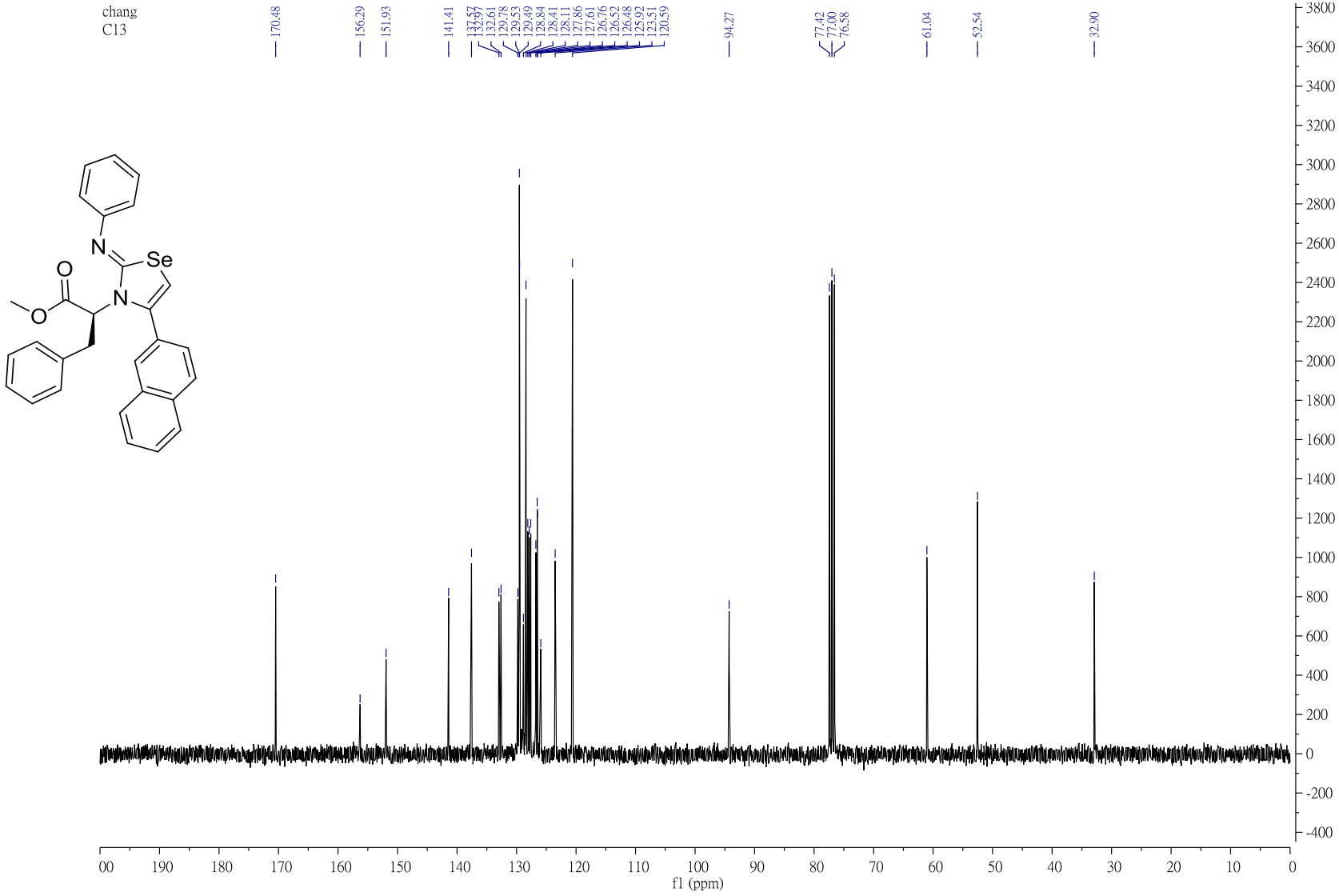
```
SAMPLE  : ____________
ID #    : 017
LAMP λ  : 589 nm
CONC    : 0.02000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
------------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01    + 18.4999   19.9
  02    + 20.2499   19.9
  03    + 19.2499   19.9
  04    + 18.4999   19.9
  05    + 18.2499   19.9
  06    + 15.9999   19.9
  07    + 15.4999   19.9
  08    + 13.4999   19.9
  09    + 13.4999   19.9
  10    + 12.7499   19.9
------------------------
MEAN     = + 16.5999°
σ(N-1)   =    2.7059°
C.V.     = + 16.3010%
```


BRUKER
Transmittance [%]
90
80
70
60
50
40
30
3107.67
3059.71
2954.07
2869.21
2779.02
1741.69
1615.96
1490.09
1444.75
1368.25
1326.53
1294.62
1245.99
1193.84
1168.91
1147.44
1120.55
1096.81
1039.41
957.22
926.66
871.51
808.23
776.04
733.87
701.31
644.86
565.07
499.35
420.07
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang703201.0.dpt
Page 1/1

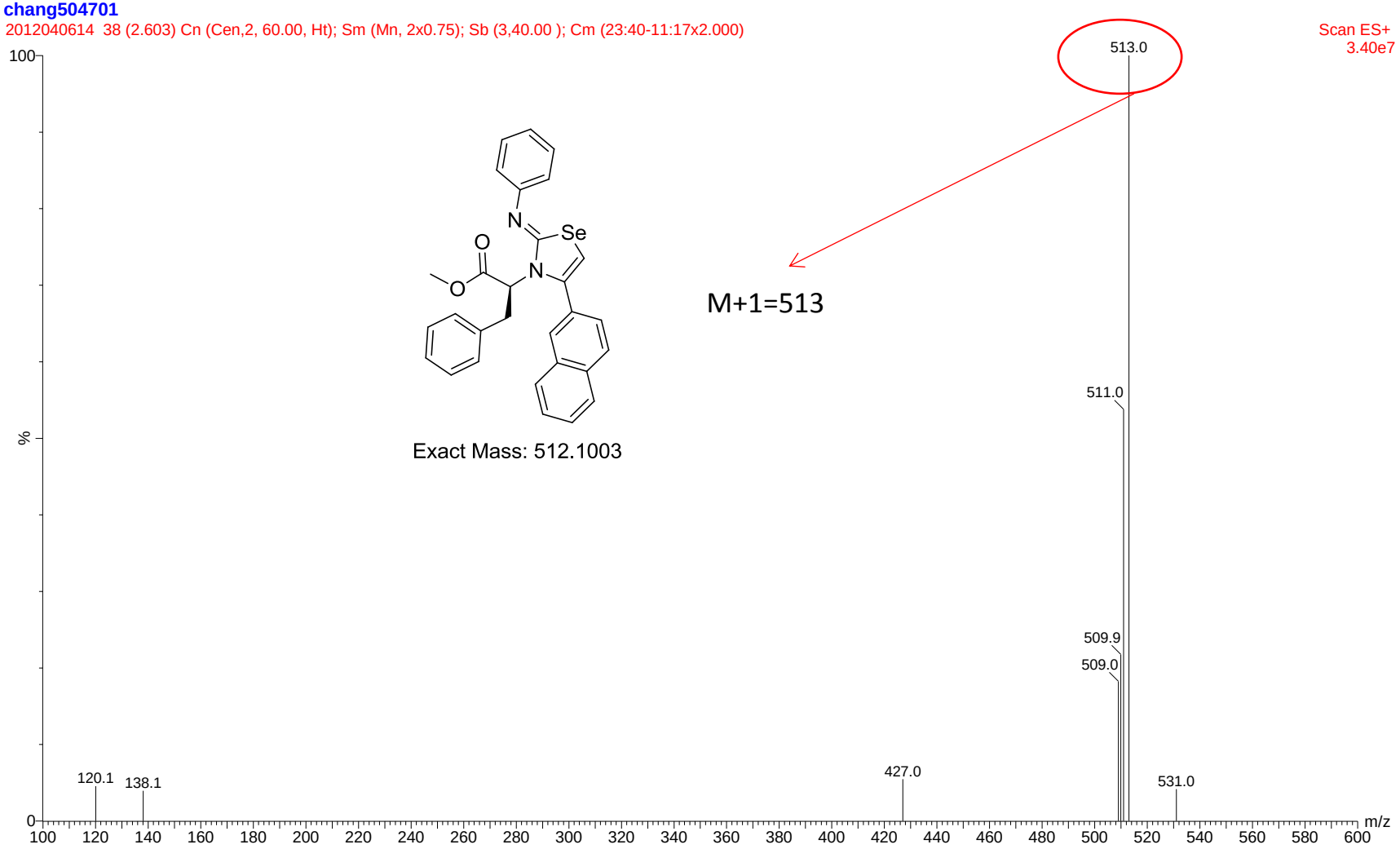
5e FT-IR


chang
1H
7.89
7.88
7.86
7.79
7.76
7.74
7.72
7.71
7.60
7.58
7.58
7.57
7.56
7.55
7.49
7.46
7.44
7.40
7.37
7.35
7.29
7.28
7.27
7.24
7.21
7.19
7.18
7.15
6.98
6.96
5.97
4.60
4.59
4.56
4.55
4.08
4.04
4.04
4.00
3.92
3.28
3.27
3.23
3.22
1.10
2.04
2.19
2.29
1.32
5.40
3.50
0.90
1.01
1.00
2.96
1.00
f1 (ppm)

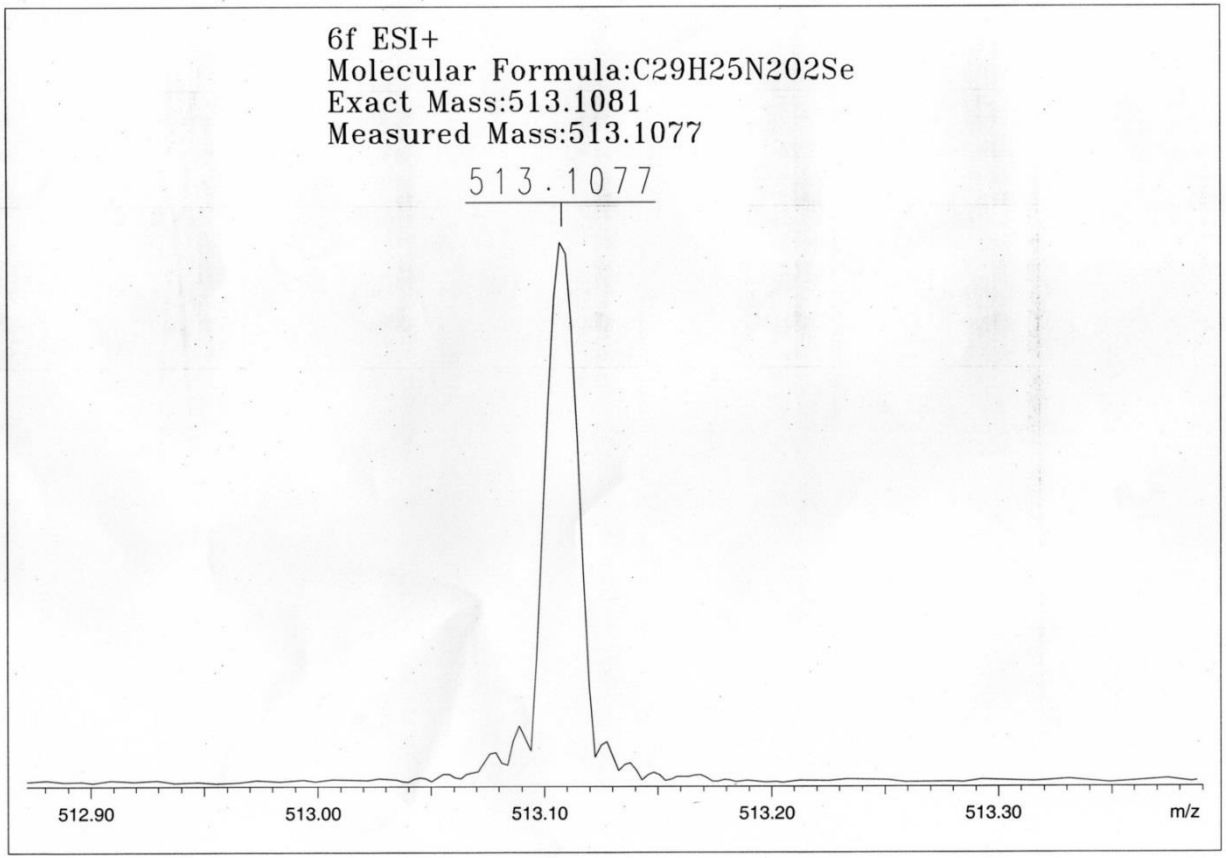
5f H[1]NMR


chang
C13
170.48
156.29
151.93
141.41
137.57
132.97
132.61
129.78
129.53
129.49
128.84
128.41
128.11
127.86
127.61
126.76
126.52
126.48
125.92
123.51
120.59
94.27
77.42
77.00
76.58
61.04
52.54
32.90
f1 (ppm)

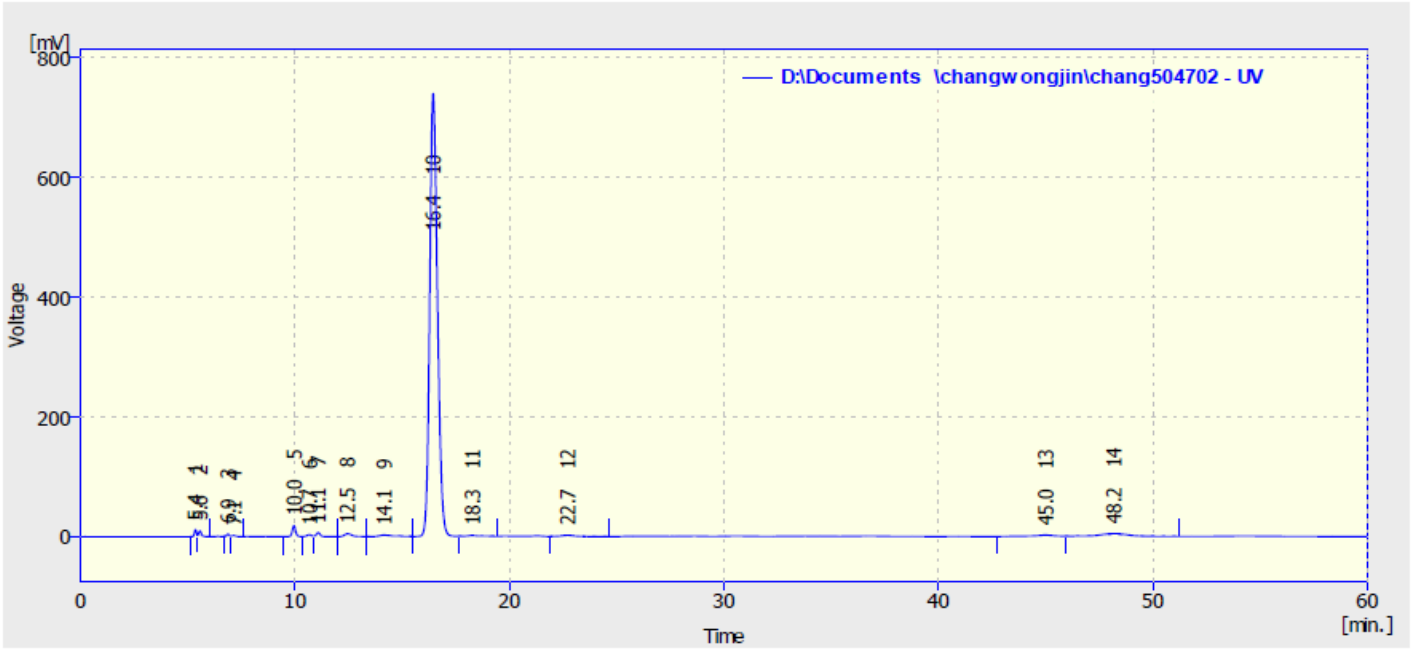
5f C^{13}NMR


chang504701
2012040614 38 (2.603) Cn (Cen,2, 60.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (23:40-11:17x2.000)
Scan ES+
3.40e7
513.0
M+1=513
Exact Mass: 512.1003
511.0
509.9
509.0
427.0
531.0
120.1
138.1
%
m/z

5f LR-MS


6f ESI+
Molecular Formula:C29H25N2O2Se
Exact Mass:513.1081
Measured Mass:513.1077
513.1077
512.90
513.00
513.10
513.20
513.30
m/z
/d=/Data/yu/6f/2/pdata/1 Administrator Wed Mar 13 12:24:39 2013

5f HR-MS

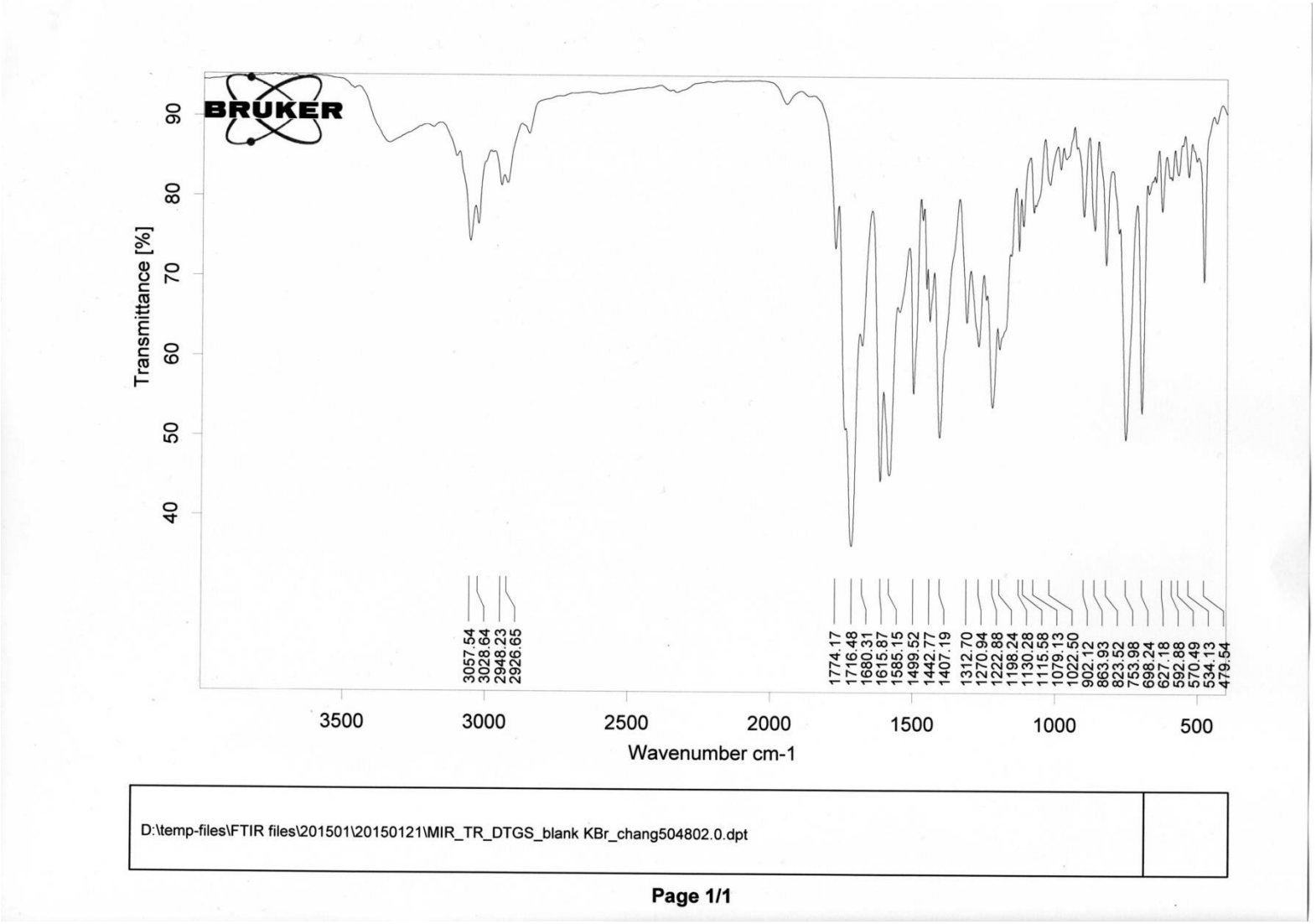


Result Table (Uncal - D:|Documents |changwongjin|chang504702 - UV)

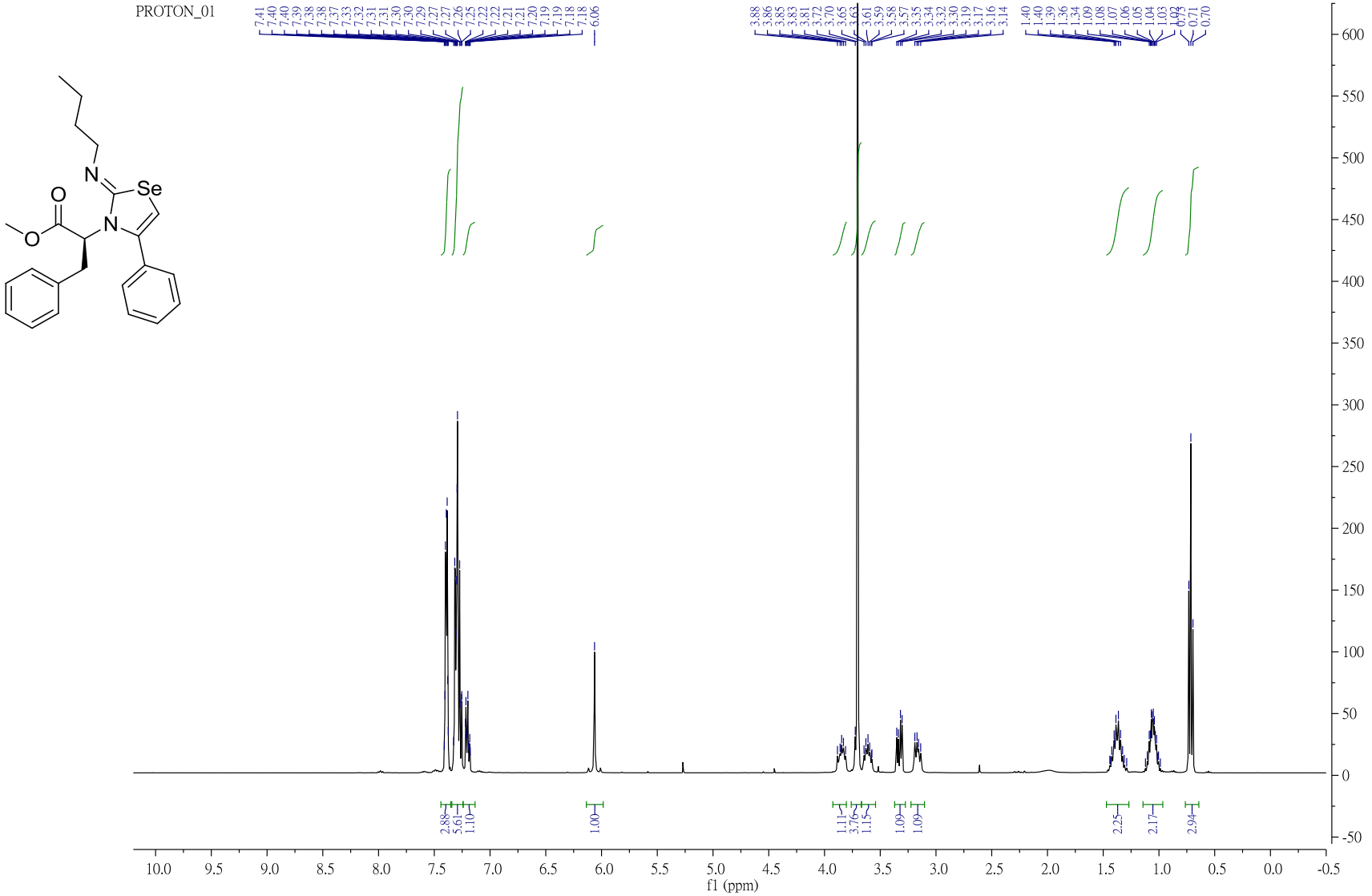
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	5.360	84.494	11.888	0.4	1.5
2	5.576	88.819	9.501	0.4	1.2
3	6.880	33.937	4.293	0.2	0.5
4	7.148	21.741	1.776	0.1	0.2
5	9.956	199.560	18.178	1.0	2.2
6	10.672	48.946	3.116	0.2	0.4
7	11.092	86.050	6.647	0.4	0.8
8	12.452	108.955	4.559	0.5	0.6
9	14.148	106.838	2.443	0.5	0.3
10	16.444	18479.281	739.517	92.2	91.0
11	18.264	72.691	1.650	0.4	0.2
12	22.708	89.729	2.220	0.4	0.3
13	45.004	159.266	2.264	0.8	0.3
14	48.172	458.907	4.756	2.3	0.6
	Total	20039.214	812.808	100.0	100.0

5f chiral HPLC

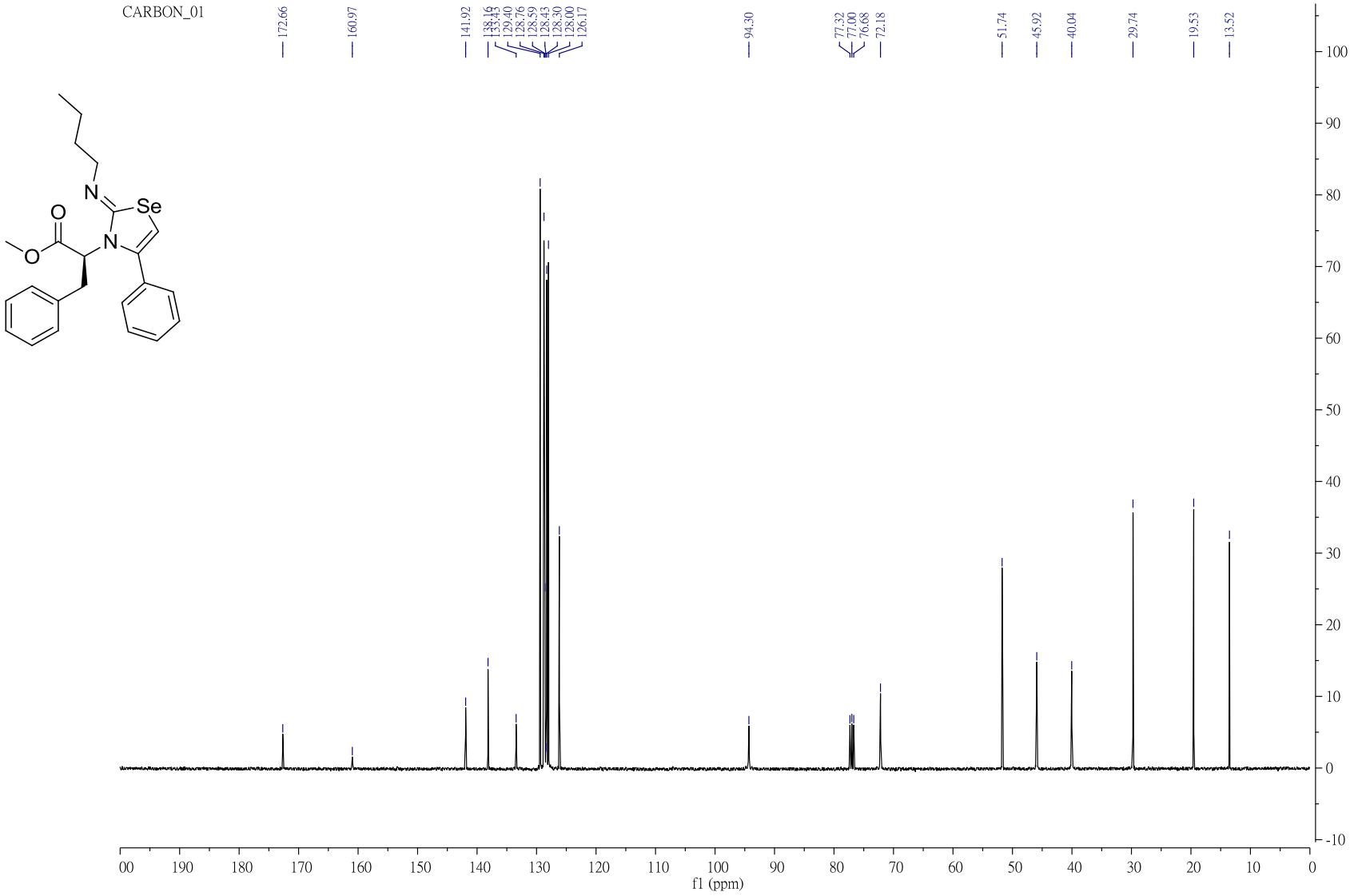
```
SAMPLE : ____________
ID #   : 005
LAMP λ : 589 nm
CONC   : 0.04000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
------------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01   - 76.5002   19.3
  02   - 77.3752   19.3
  03   - 78.8752   19.3
  04   - 79.6252   19.3
  05   - 80.2502   19.3
  06   - 80.1252   19.3
  07   - 81.0002   19.3
  08   - 81.5002   19.3
  09   - 82.1252   19.4
  10   - 83.2502   19.4
------------------------
MEAN     = - 80.0627°
σ(N-1)   =   2.0793°
C.V.     = -  2.5971%
```


BRUKER
Transmittance [%]
90
80
70
60
50
40
3057.54
3028.64
2948.23
2926.65
1774.17
1716.48
1680.31
1615.87
1585.15
1499.52
1442.77
1407.19
1312.70
1270.94
1222.88
1198.24
1130.28
1115.58
1079.13
1022.50
902.12
863.93
823.52
753.98
698.24
627.18
592.88
570.49
534.13
479.54
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang504802.0.dpt
Page 1/1

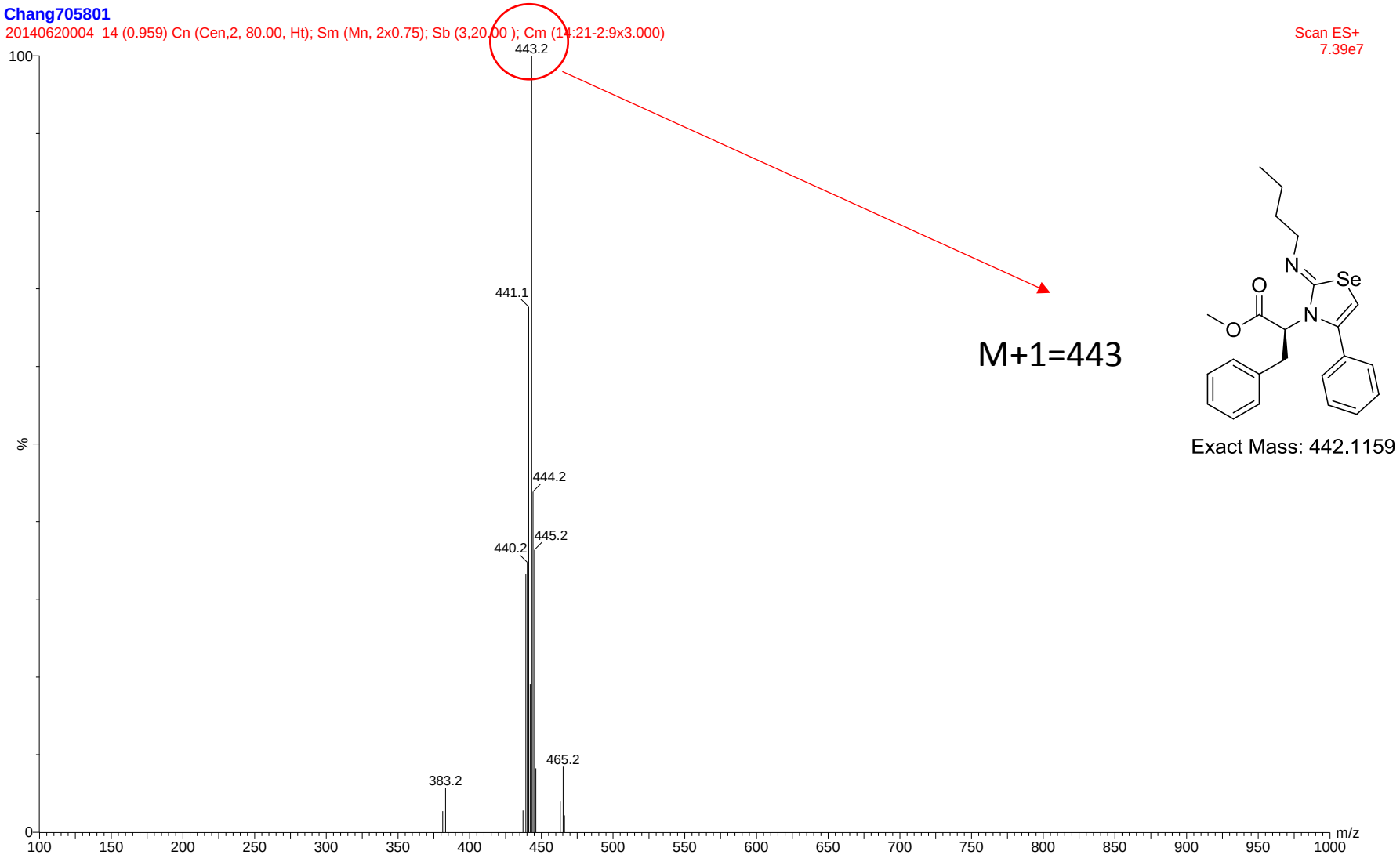
5f FT-IR



5g H^1NMR


CARBON_01
172.66
160.97
141.92
138.16
133.45
129.40
128.76
128.59
128.43
128.30
128.00
126.17
94.30
77.32
77.00
76.68
72.18
51.74
45.92
40.04
29.74
19.53
13.52
O
O
N
Se
N
f1 (ppm)

5g C^{13}NMR


Chang705801
20140620004 14 (0.959) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,20.00); Cm (14:21-2:9x3.000)
Scan ES+
7.39e7
100
%
0
443.2
441.1
444.2
440.2
445.2
465.2
383.2
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z
M+1=443
N
Se
O
N
O
Exact Mass: 442.1159

5g LR-MS

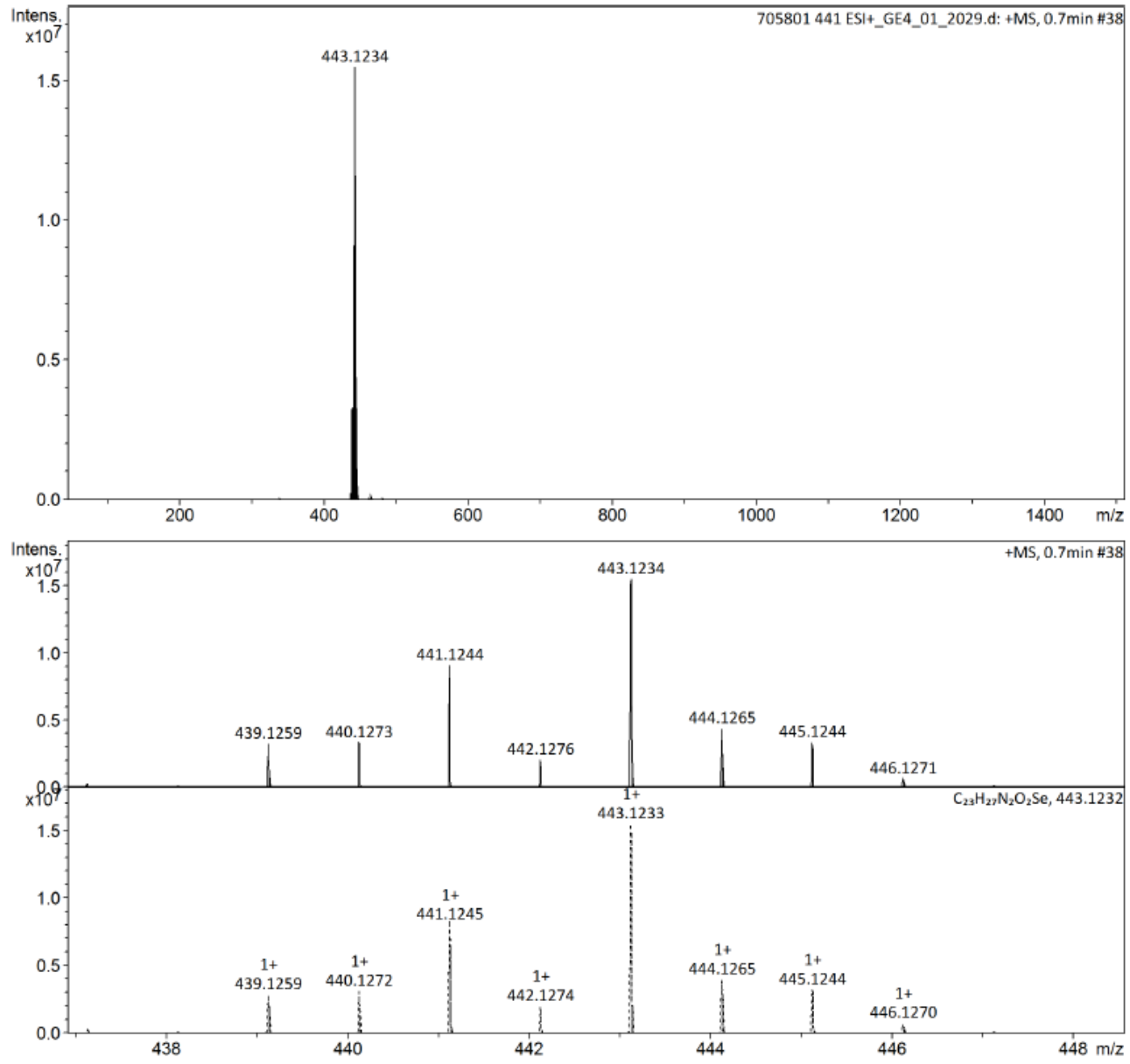
Display Report

Analysis Info

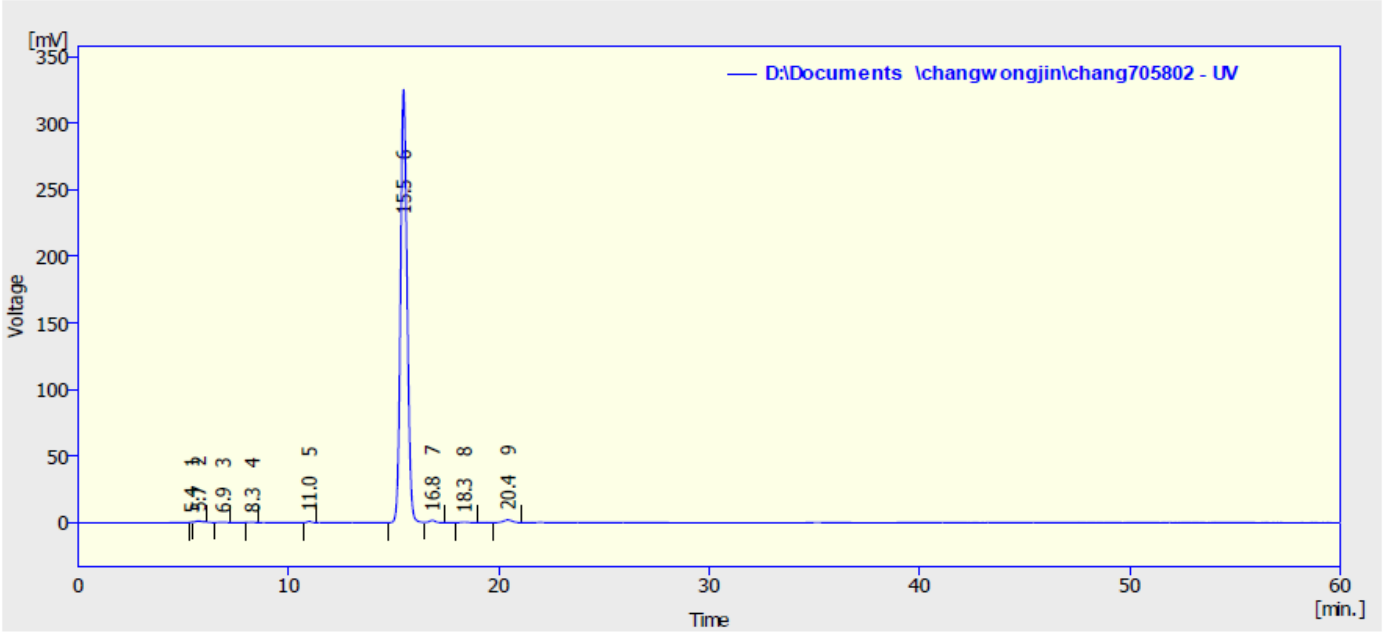
Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\705801 441 ESI+_GE4_01_2029.d	Acquisition Date	6/26/2014 10:22:43 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	705801 441 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



5g HR-MS

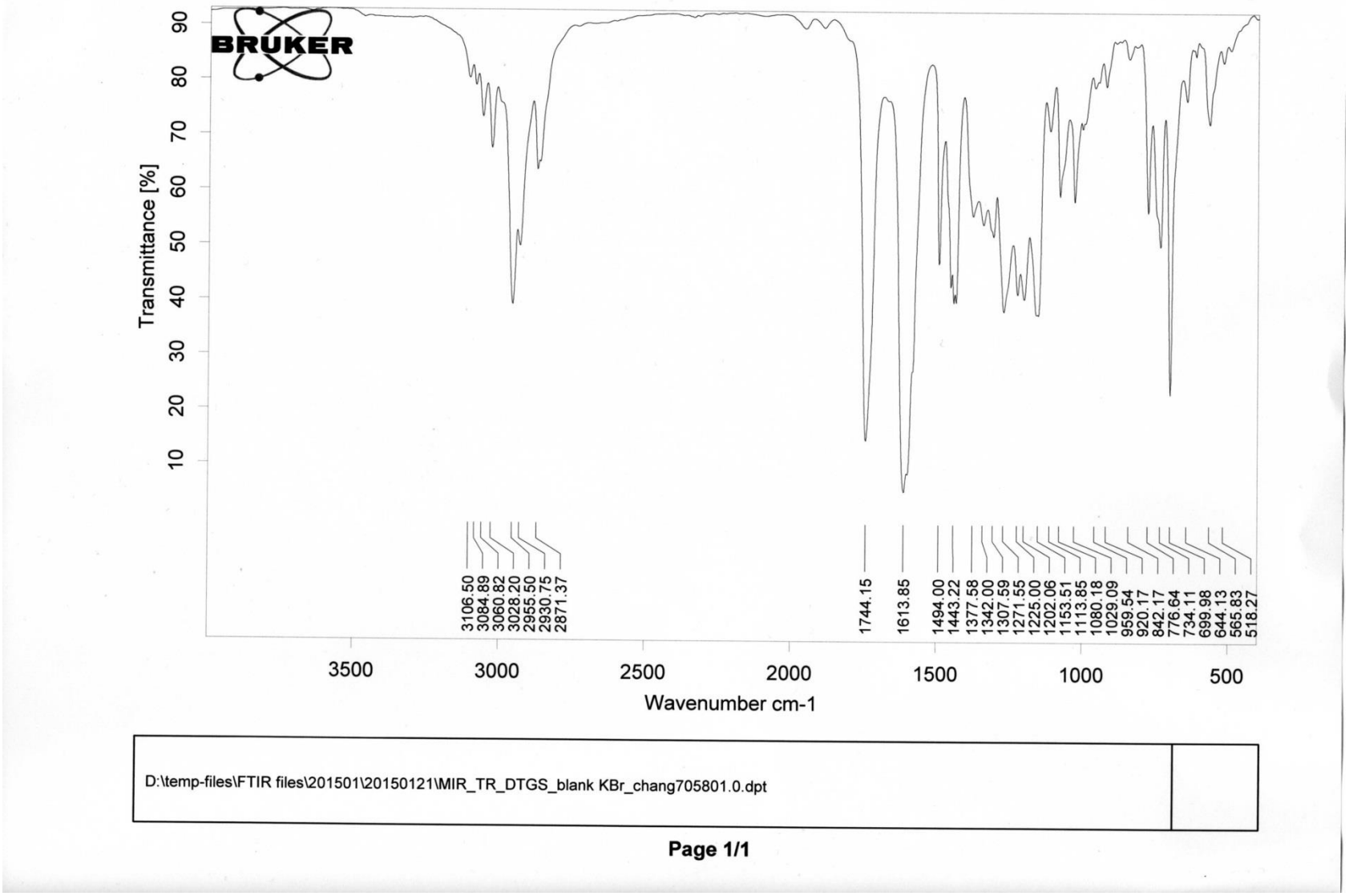


Result Table (Uncal - D:|Documents |changwongjin|chang705802 - UV)

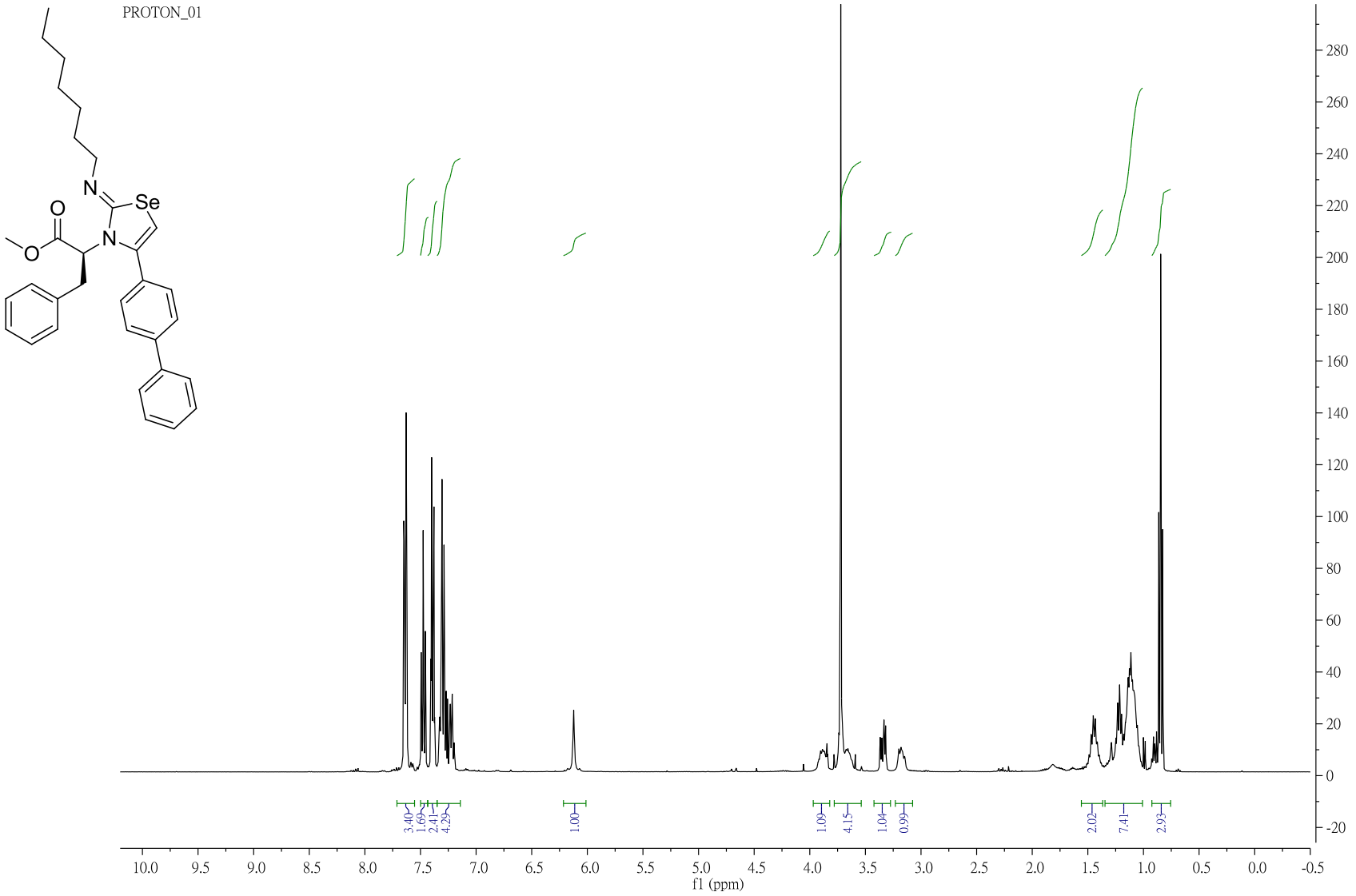
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.392	2.026	0.345	0.0	0.1	0.10
2	5.724	18.635	0.939	0.3	0.3	0.33
3	6.896	5.986	0.261	0.1	0.1	0.39
4	8.264	4.579	0.260	0.1	0.1	0.29
5	10.988	11.450	0.916	0.2	0.3	0.20
6	15.468	7098.171	324.964	98.0	97.9	0.34
7	16.840	34.370	1.693	0.5	0.5	0.31
8	18.348	9.593	0.407	0.1	0.1	0.37
9	20.436	58.700	2.012	0.8	0.6	0.46
	Total	7243.511	331.798	100.0	100.0	

5g chair HPLC

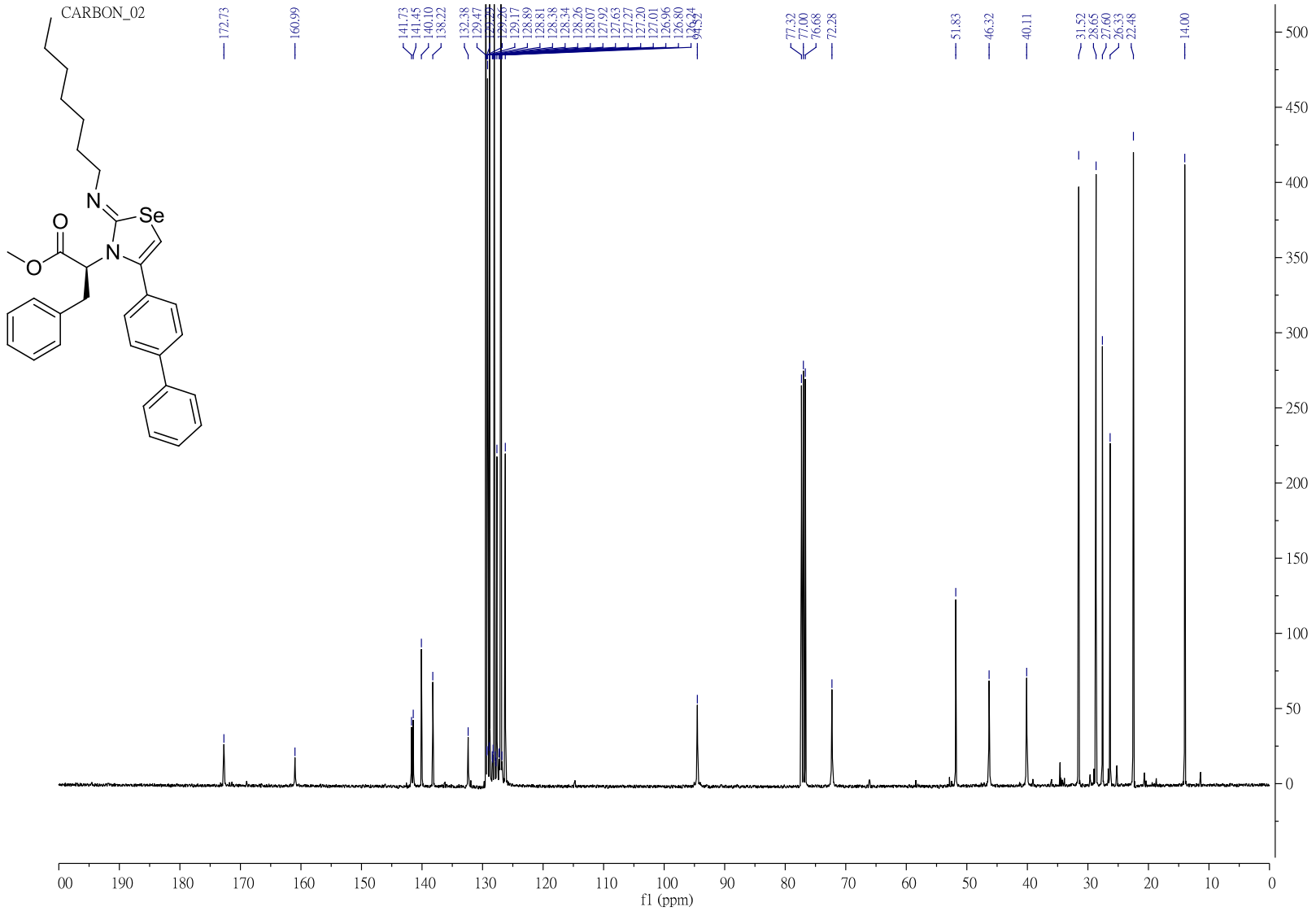
```
SAMPLE : ____________
ID #   : 013
LAMP λ : 589 nm
CONC   : 0.05000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-------------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01   -365.9000   20.4
  02   -366.0000   20.4
  03   -366.2000   20.4
  04   -366.4000   20.4
  05   -366.7000   20.4
  06   -366.8000   20.4
  07   -367.0000   20.4
  08   -367.2000   20.4
  09   -367.5000   20.4
  10   -367.8000   20.4
-------------------------
MEAN     = -366.7500°
σ(N-1)   =   0.63640°
C.V.     = - 0.17352%
```


BRUKER
Transmittance [%]
10
20
30
40
50
60
70
80
90
3106.50
3084.89
3060.82
3028.20
2955.50
2930.75
2871.37
1744.15
1613.85
1494.00
1443.22
1377.58
1342.00
1307.59
1271.55
1225.00
1202.06
1153.51
1113.85
1080.18
1029.09
959.54
920.17
842.17
776.64
734.11
699.98
644.13
565.83
518.27
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang705801.0.dpt
Page 1/1

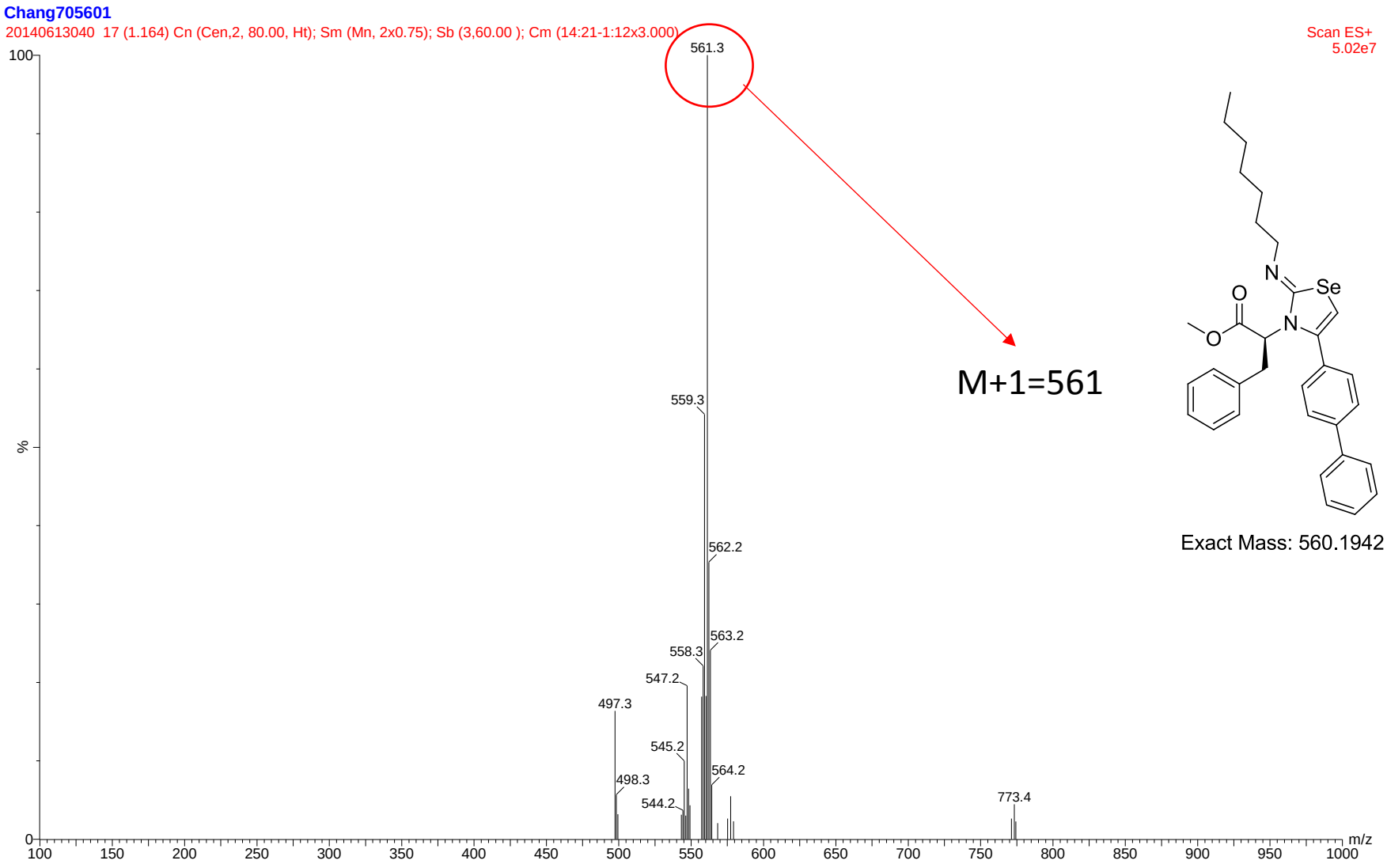
5g FT-IR


PROTON_01
O
O
N
Se
N
3.40
1.69
2.41
4.29
1.00
1.09
4.15
1.04
0.99
2.02
7.41
2.93
f1 (ppm)

5h H^1NMR


CARBON_02
172.73
160.99
141.73
141.45
140.10
138.22
132.38
129.47
129.17
128.89
128.81
128.38
128.34
128.26
128.07
127.92
127.63
127.27
127.20
127.01
126.96
126.80
126.24
94.32
77.32
77.00
76.68
72.28
51.83
46.32
40.11
31.52
28.65
27.60
26.33
22.48
14.00
f1 (ppm)

5h C^{13}NMR


Chang705601
20140613040 17 (1.164) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,60.00); Cm (14:21-1:12x3.000)
Scan ES+
5.02e7
100
%
0
561.3
559.3
562.2
563.2
558.3
547.2
497.3
545.2
564.2
498.3
544.2
773.4
m/z
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
M+1=561
N
Se
O
N
O
Exact Mass: 560.1942

5h LR-MS

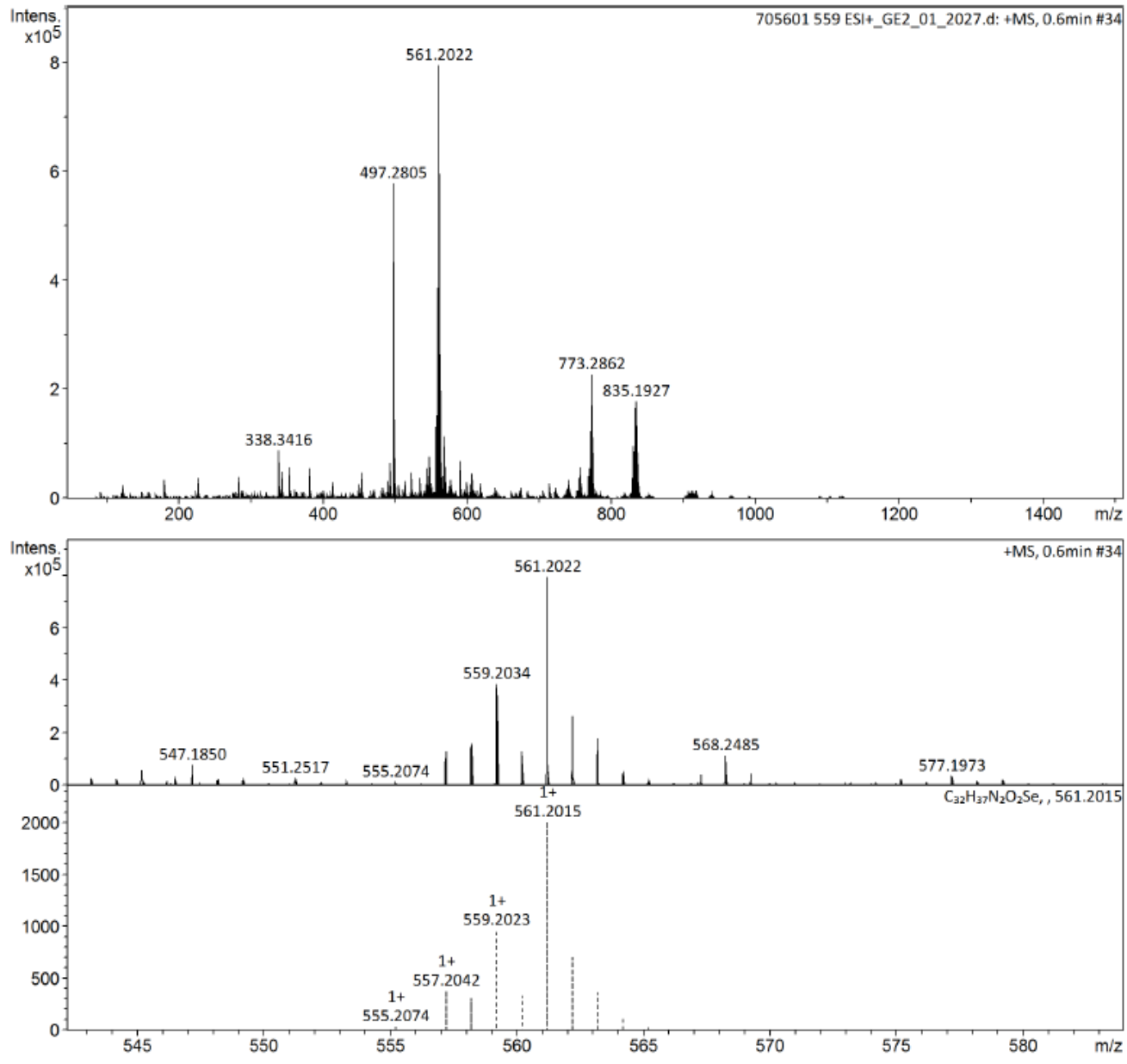
Display Report

Analysis Info

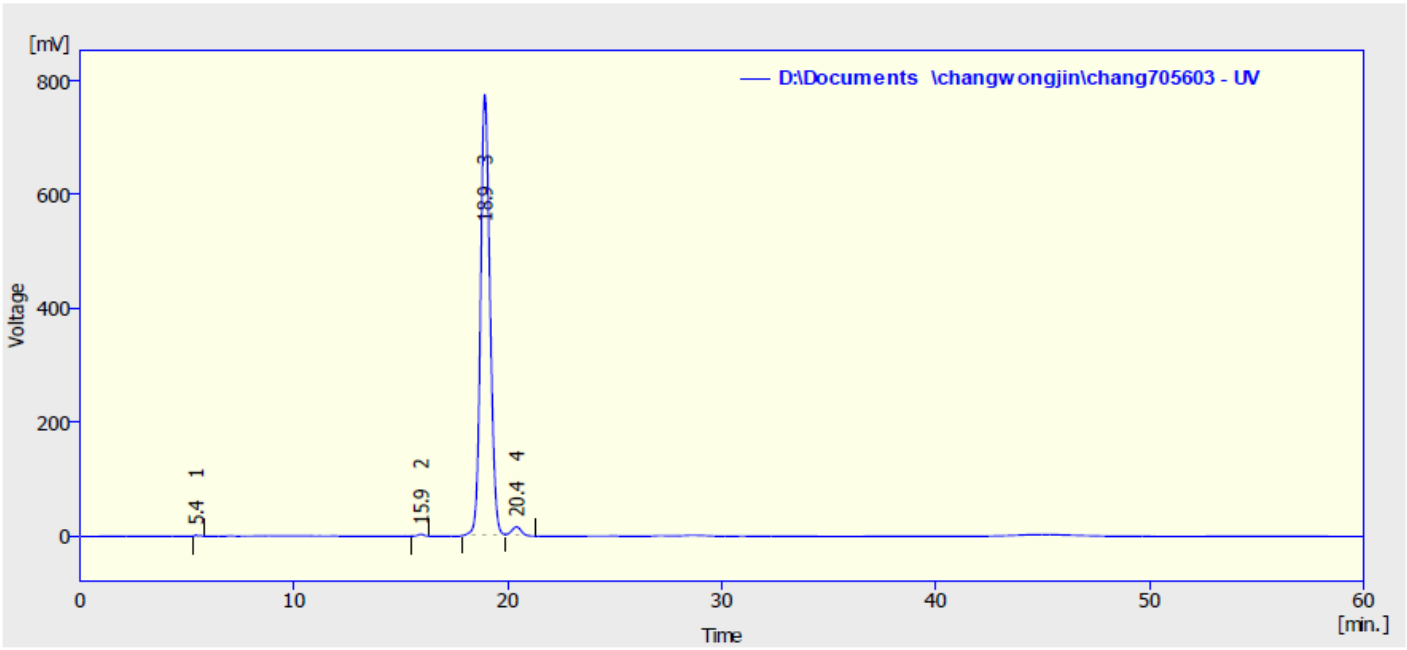
Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\705601 559 ESI+_GE2_01_2027.d	Acquisition Date	6/26/2014 10:14:05 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	705601 559 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



5h HR-MS

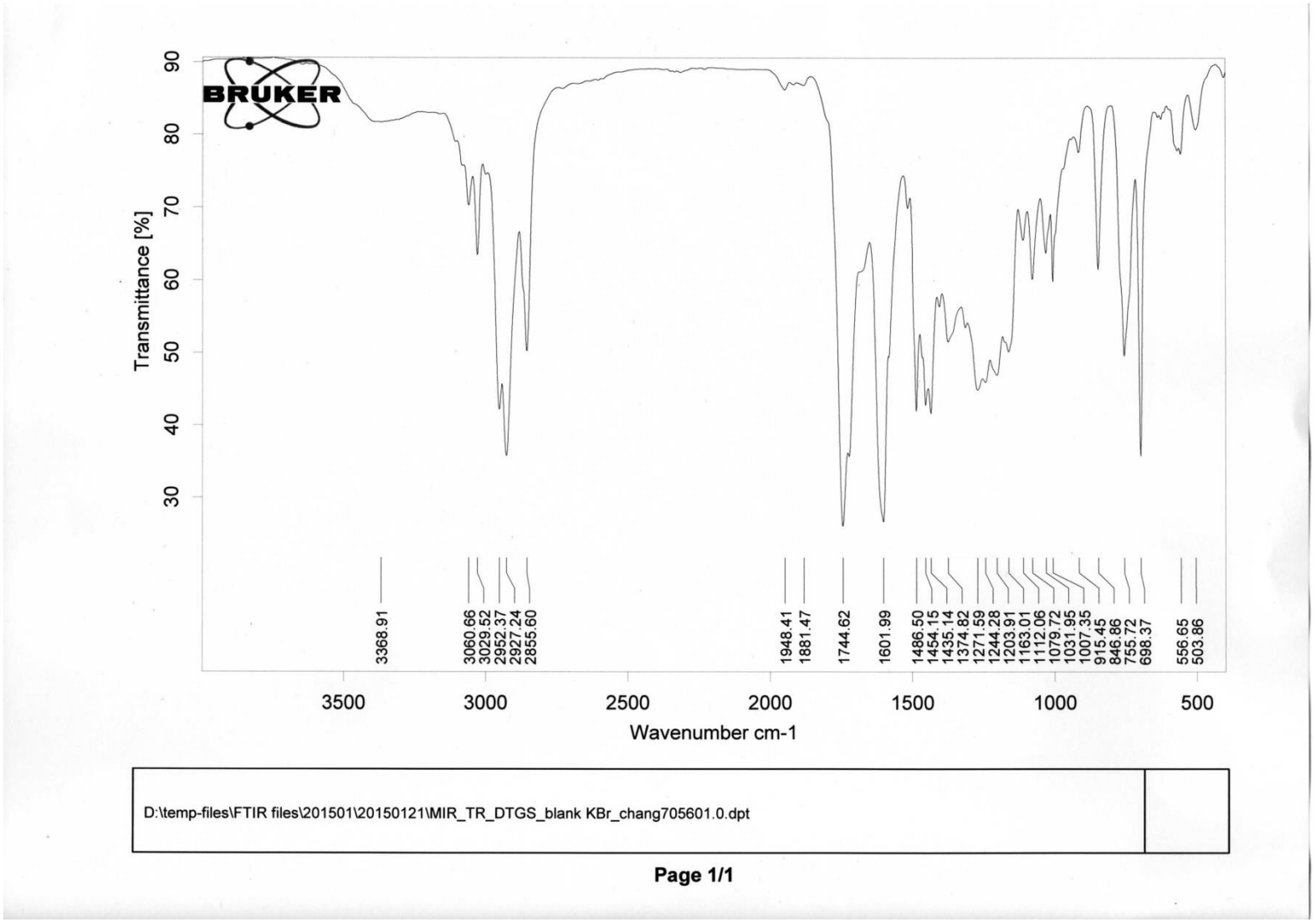


Result Table (Uncal - D:|Documents |changwongjin|chang705603 - UV)

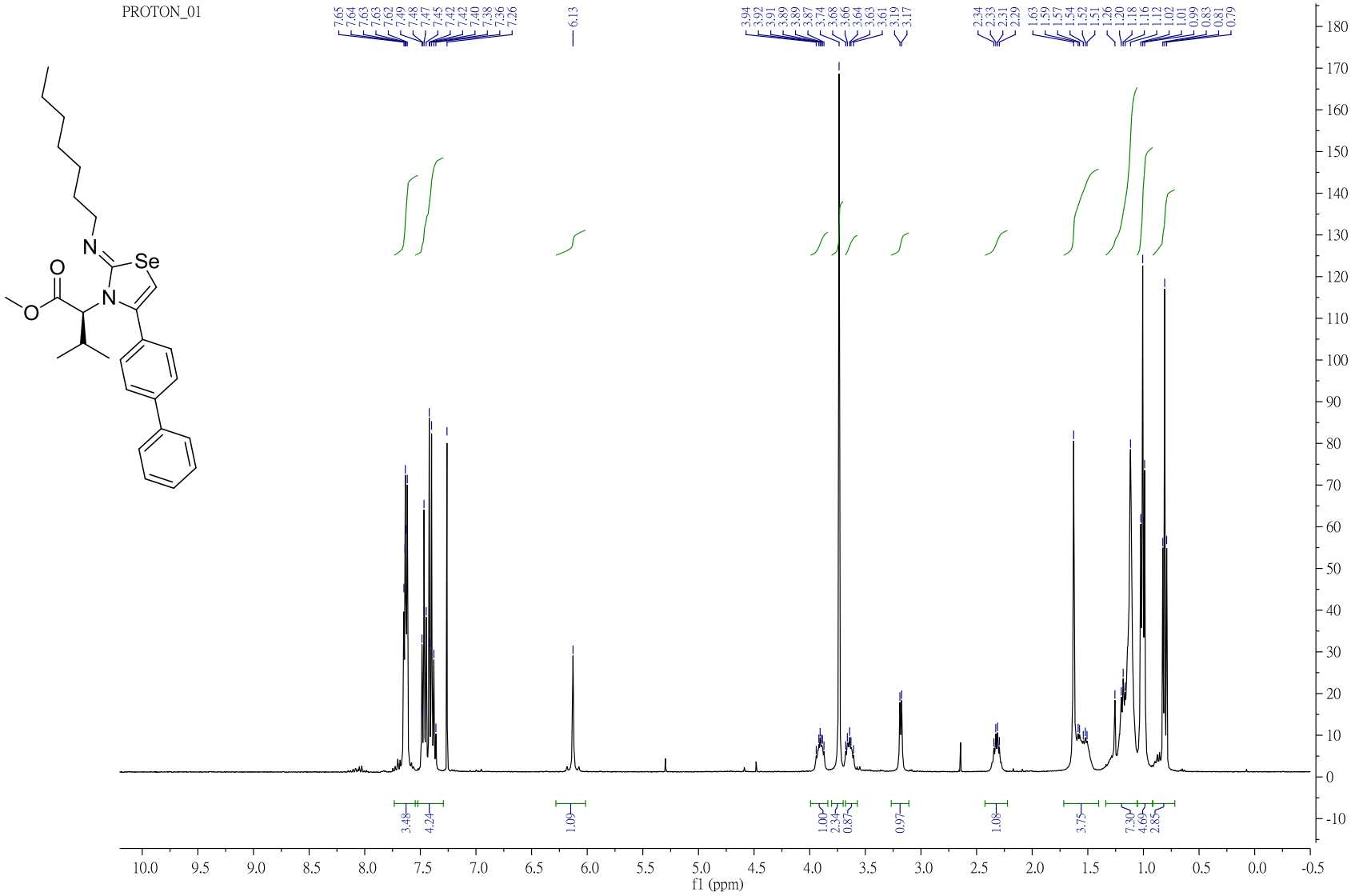
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	5.424	28.846	2.324	0.1	0.3
2	15.940	67.280	3.514	0.3	0.4
3	18.924	23859.500	774.547	97.4	97.2
4	20.408	534.313	16.218	2.2	2.0
	Total	24489.938	796.604	100.0	100.0

5h chiral HPLC

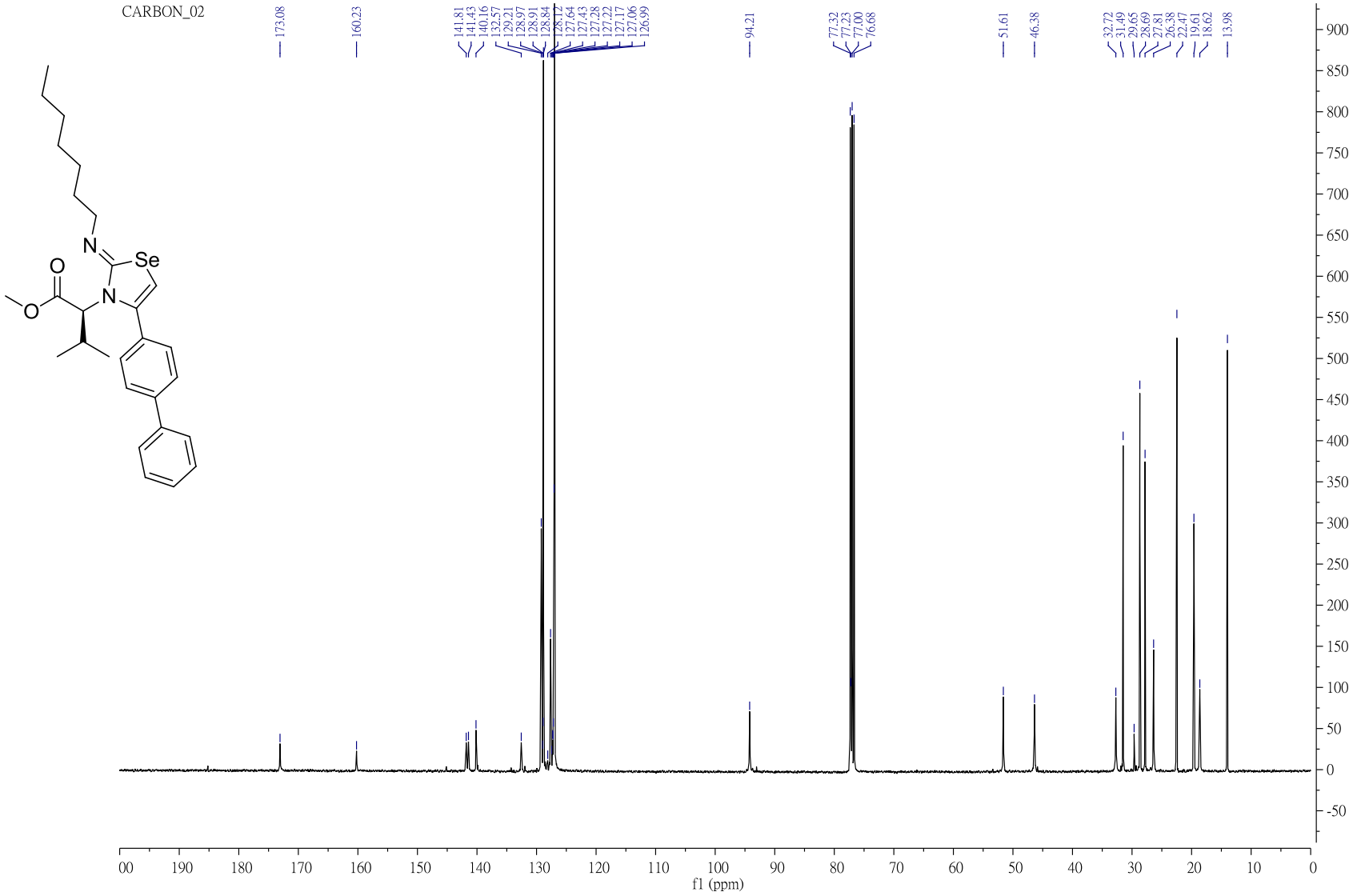
```
SAMPLE : ____________
ID #   : 014
LAMP λ : 589 nm
CONC   : 0.03000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
------------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01   + 34.5000   20.1
  02   + 33.5000   20.1
  03   + 32.6667   20.1
  04   + 32.1667   20.1
  05   + 31.5000   20.1
  06   + 30.0000   20.1
  07   + 29.6667   20.1
  08   + 29.0000   20.1
  09   + 28.3333   20.1
  10   + 27.5000   20.1
------------------------
MEAN     = + 30.8833°
σ(N-1)   =    2.3307°
C.V.     = +  7.5469%
```


BRUKER
Transmittance [%]
90
80
70
60
50
40
30
3368.91
3060.66
3029.52
2952.37
2927.24
2855.60
1948.41
1881.47
1744.62
1601.99
1486.50
1454.15
1435.14
1374.82
1271.59
1244.28
1203.91
1163.01
1112.06
1079.72
1031.95
1007.35
915.45
846.86
755.72
698.37
556.65
503.86
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang705601.0.dpt
Page 1/1

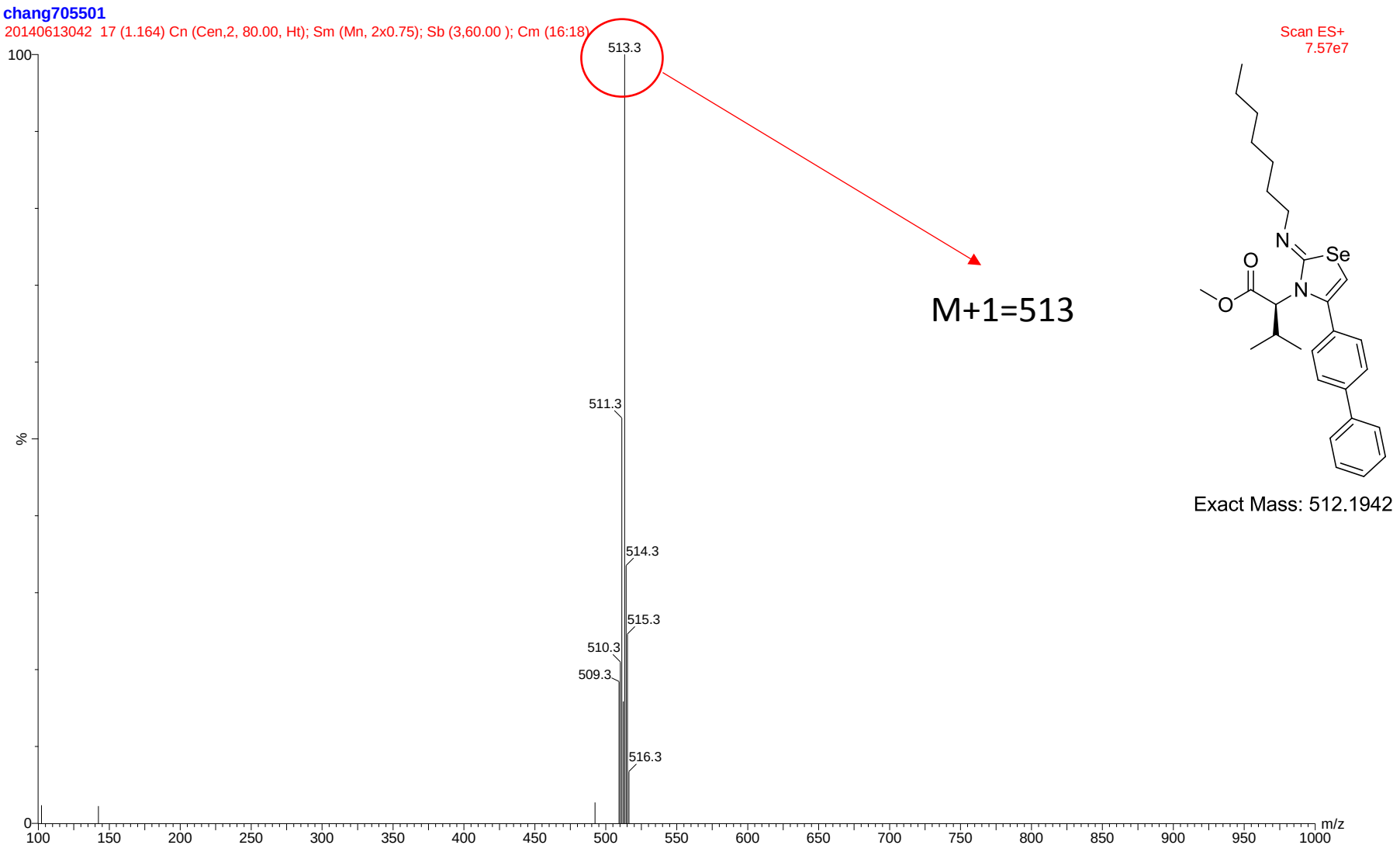
5h FT-IR


PROTON_01
7.65 7.64 7.63 7.63 7.62 7.49 7.48 7.47 7.45 7.42 7.42 7.40 7.38 7.36 7.26
6.13
3.94 3.92 3.91 3.89 3.89 3.87 3.74 3.68 3.66 3.64 3.63 3.61 3.19 3.17
2.34 2.33 2.31 2.29
1.63 1.59 1.57 1.54 1.52 1.51 1.26 1.20 1.18 1.16 1.12 1.02 1.01 0.99 0.83 0.81 0.79
N
Se
O
O
N
3.48 4.24 1.09 1.00 2.34 0.87 0.97 1.08 3.75 7.30 4.69 2.85
f1 (ppm)

5i H^1NMR


CARBON_02
173.08
160.23
141.81
141.43
140.16
132.57
129.21
128.97
128.91
128.84
128.12
127.64
127.43
127.28
127.22
127.17
127.06
126.99
94.21
77.32
77.23
77.00
76.68
51.61
46.38
32.72
31.49
29.65
28.69
27.81
26.38
22.47
19.61
18.62
13.98
f1 (ppm)

5i C^{13}NMR


chang705501
20140613042 17 (1.164) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,60.00); Cm (16:18)
Scan ES+
7.57e7
513.3
M+1=513
511.3
514.3
515.3
510.3
509.3
516.3
%
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
N
Se
O
N
O
Exact Mass: 512.1942

5i LR-MS

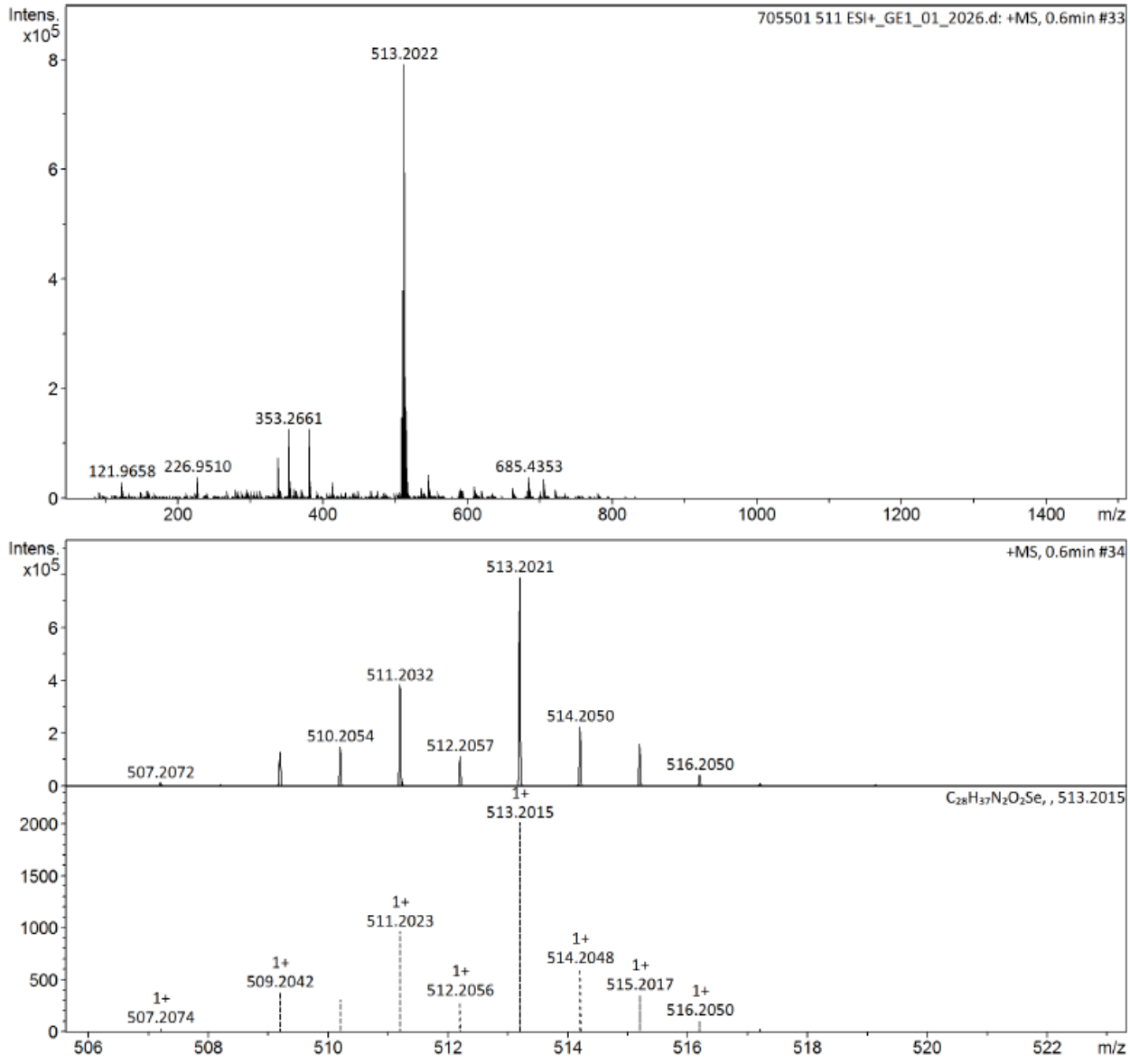
Display Report

Analysis Info

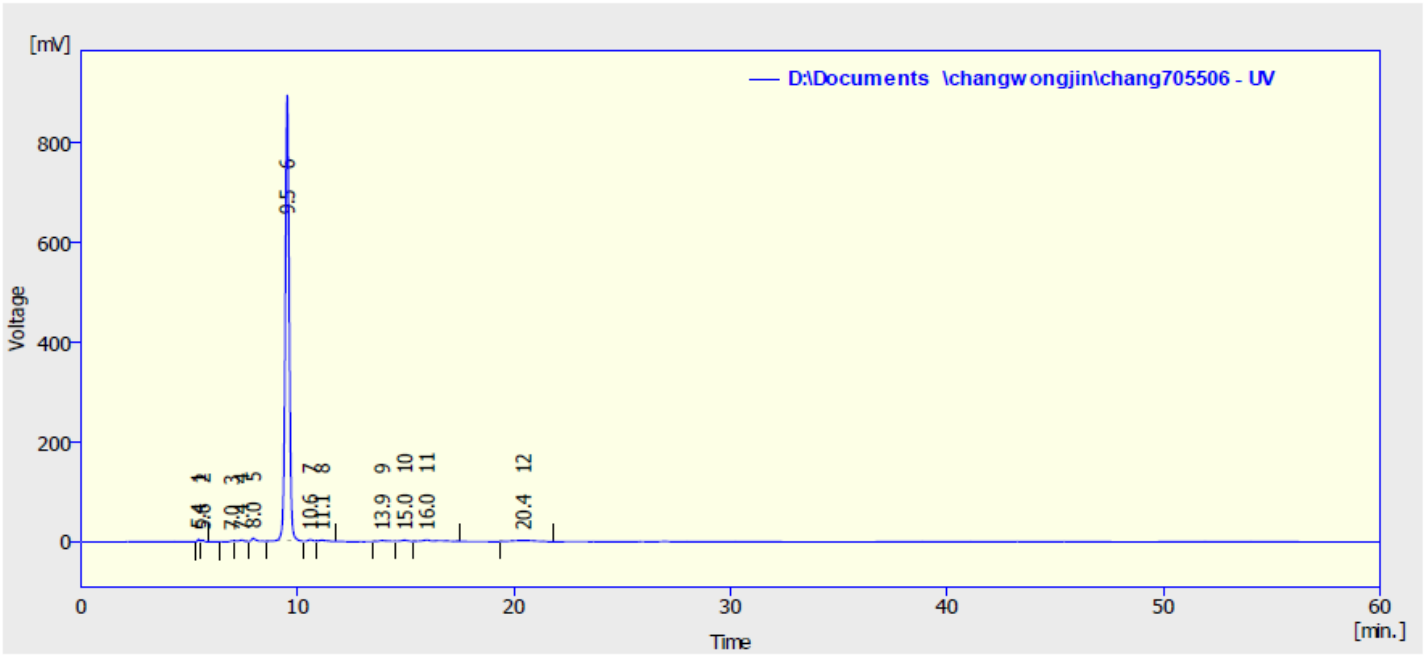
Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\705501 511 ESI+_GE1_01_2026.d	Acquisition Date	6/26/2014 10:09:48 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	705501 511 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



5i HR-MS

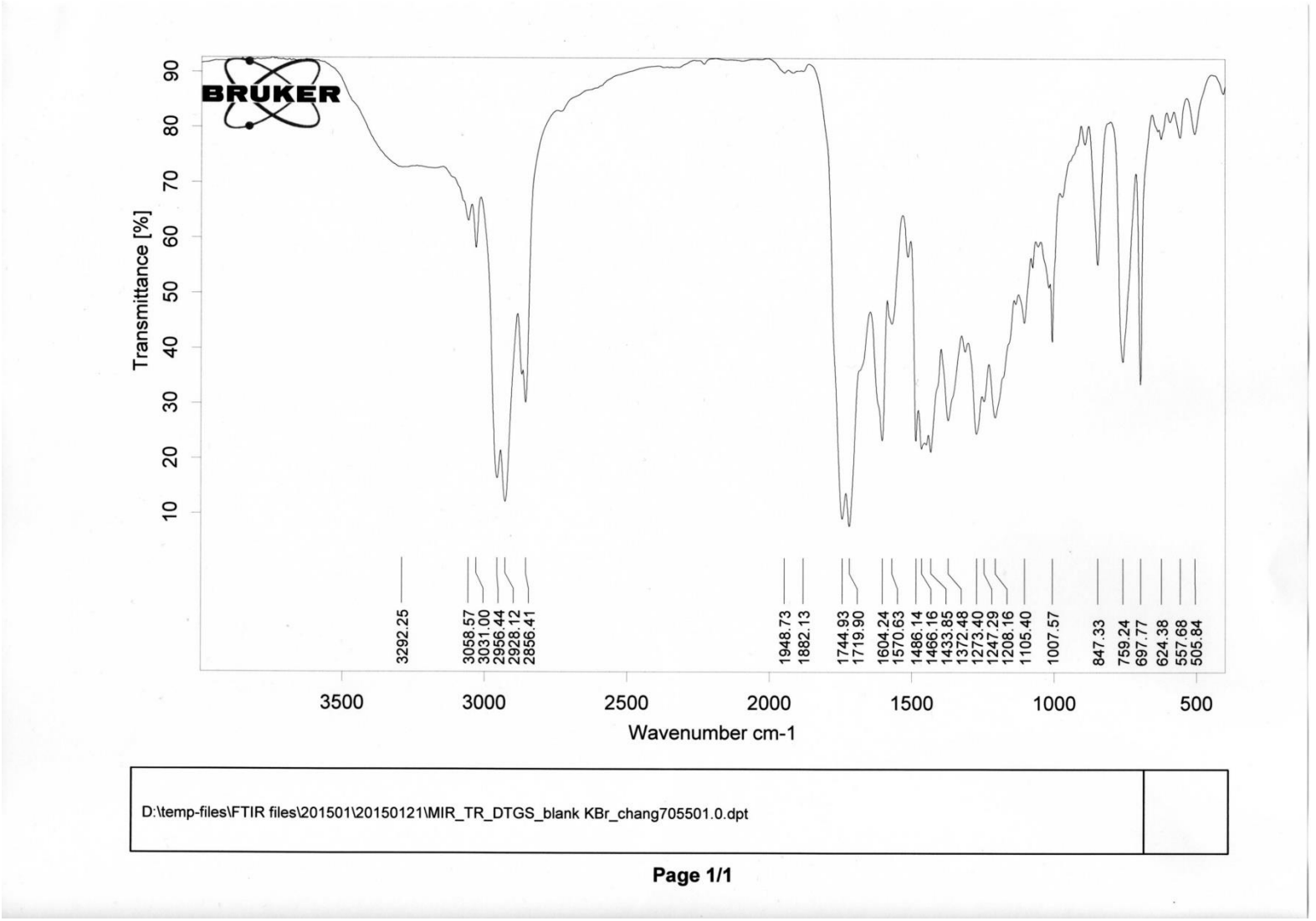


Result Table (Uncal - D:|Documents |changwongjin|chang705506 - UV)

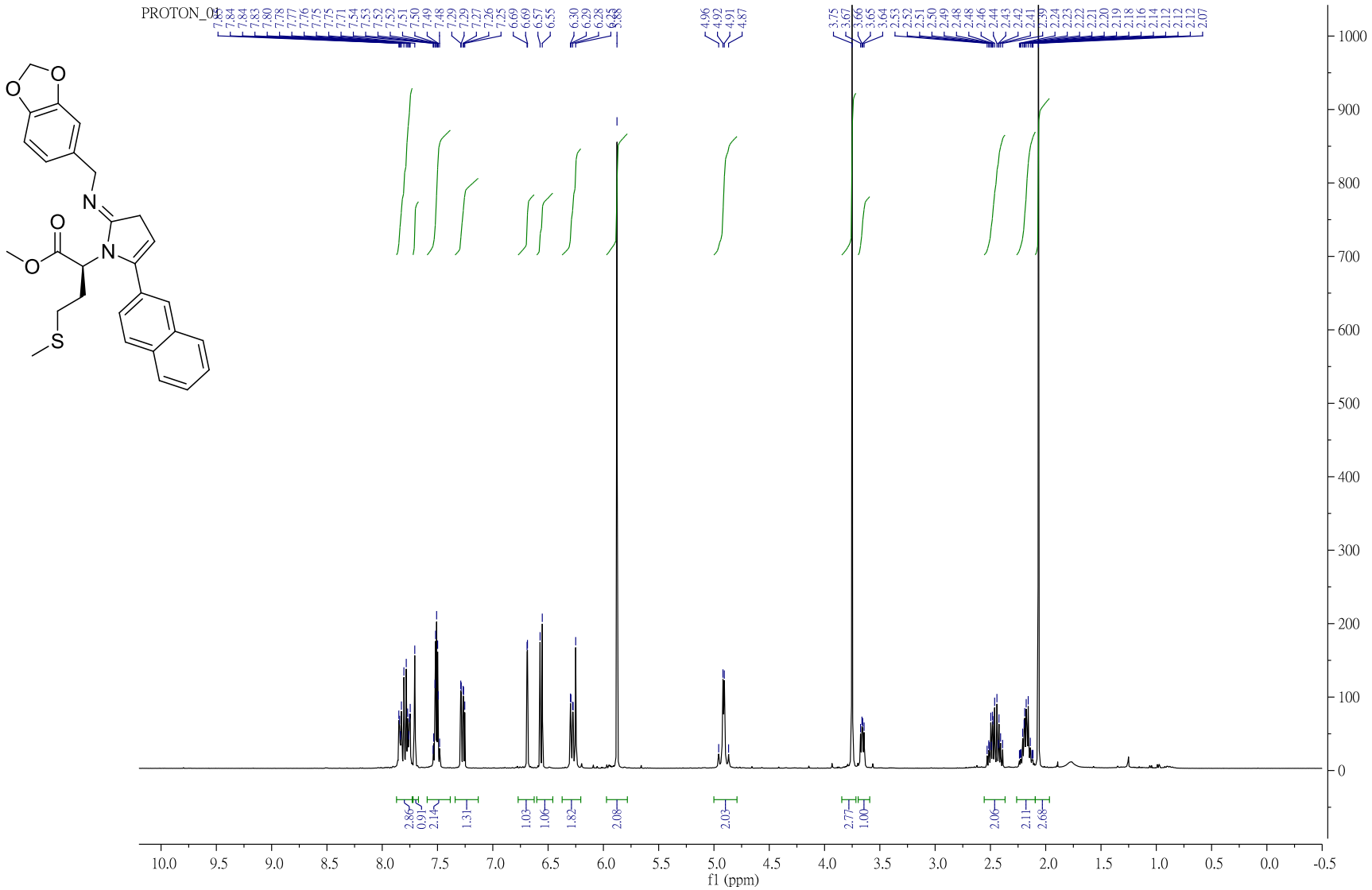
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	5.432	34.671	4.961	0.3	0.5
2	5.620	25.345	3.294	0.2	0.4
3	6.960	18.772	2.024	0.2	0.2
4	7.420	65.870	3.479	0.5	0.4
5	7.952	114.559	6.852	0.9	0.7
6	9.524	11636.346	894.311	93.4	96.1
7	10.596	67.423	3.571	0.5	0.4
8	11.124	65.766	2.577	0.5	0.3
9	13.900	59.594	1.964	0.5	0.2
10	14.952	65.942	2.530	0.5	0.3
11	15.976	131.323	3.033	1.1	0.3
12	20.428	167.693	2.367	1.3	0.3
	Total	12453.303	930.962	100.0	100.0

5i chiral HPLC

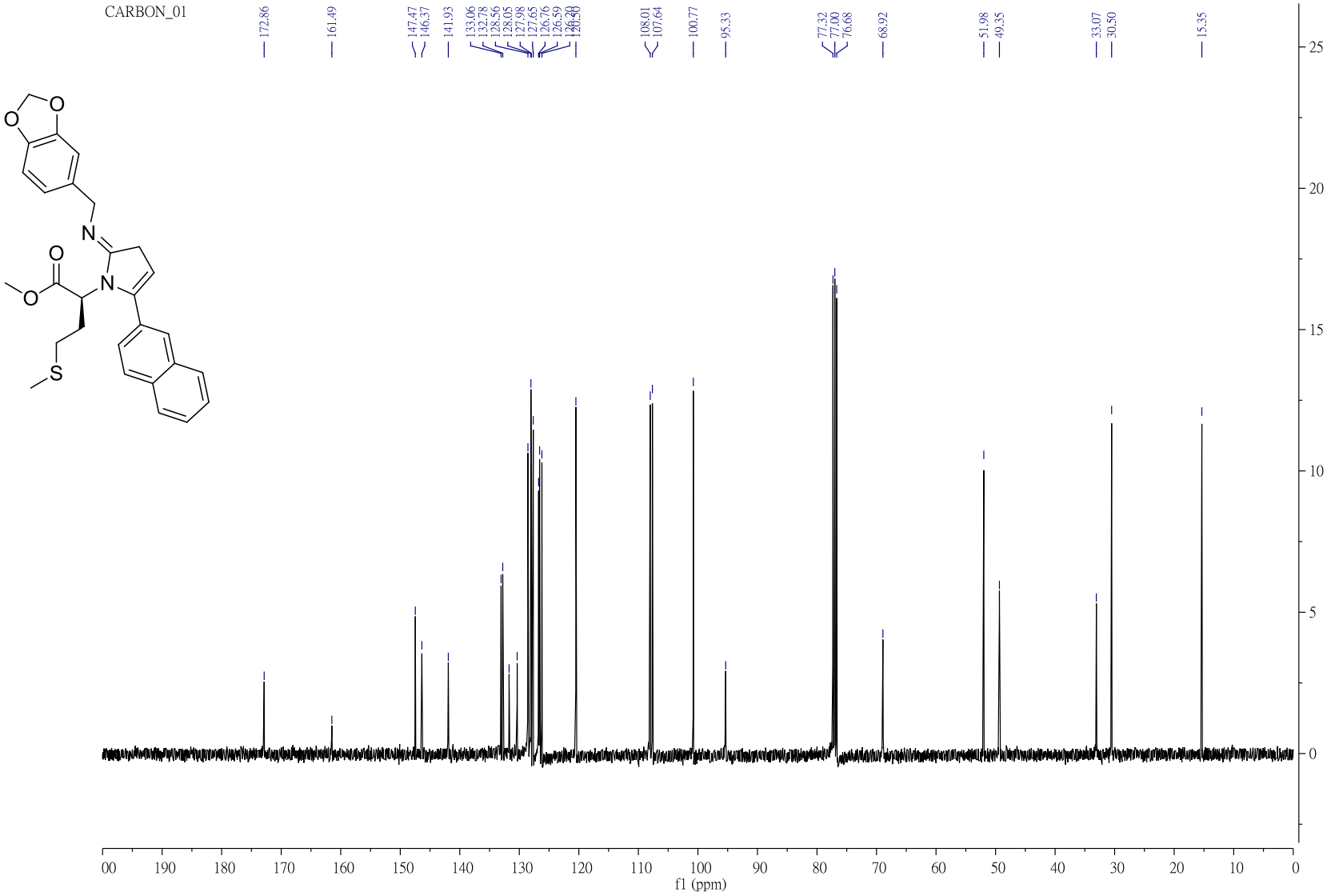
```
SAMPLE  : ____________
ID #    : 009
LAMP λ  : 589 nm
CONC    : 0.01000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
------------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01    - 54.4997   20.6
  02    - 55.9997   20.6
  03    - 54.4997   20.6
  04    - 55.4997   20.6
  05    - 56.4997   20.6
  06    - 57.4997   20.6
  07    - 58.9997   20.6
  08    - 58.4997   20.6
  09    - 59.4997   20.6
  10    - 61.9997   20.6
------------------------
MEAN     = - 57.3497°
σ(N-1)   =    2.4158°
C.V.     = -  4.2124%
```


BRUKER
Transmittance [%]
10
20
30
40
50
60
70
80
90
3292.25
3058.57
3031.00
2956.44
2928.12
2856.41
1948.73
1882.13
1744.93
1719.90
1604.24
1570.63
1486.14
1466.16
1433.85
1372.48
1273.40
1247.29
1208.16
1105.40
1007.57
847.33
759.24
697.77
624.38
557.68
505.84
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang705501.0.dpt
Page 1/1

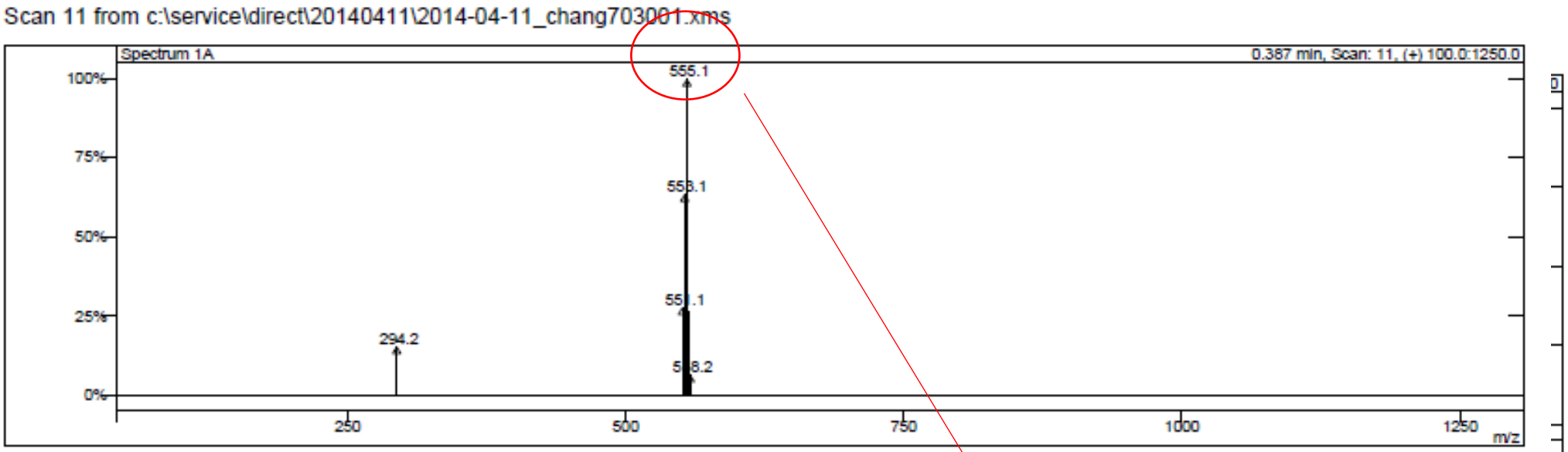
5i FT-IR



5j H^1NMR


CARBON_01
172.86
161.49
147.47
146.37
141.93
133.06
132.78
128.56
128.05
127.98
127.65
126.76
126.59
108.01
107.64
100.77
95.33
77.32
77.00
76.68
68.92
51.98
49.35
33.07
30.50
15.35
O
O
N
O
O
N
S
f1 (ppm)

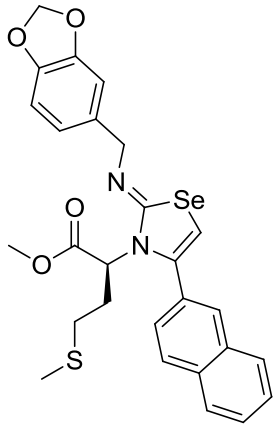
5j C^{13}NMR



Spectrum from ...vice\direct\20140411\2014-04-11_chang703001.xms
Scan No: 11, Time: 0.387 minutes
No averaging. Not background corrected.
Name: HESI-FS-POS
Comment: 0.387 min. Scan: 11 (+) 100.0:1250.0 RIC: 5066589784
Pair Count: 9 MW: 0 Formula: None
CAS No: None Acquired Range: 100.0 - 1250.0 m/z

CAS No: None Acquired Range: 100.0 - 1250.0 m/z

M+1=555



Exact Mass: 554.0778

5j LR-MS

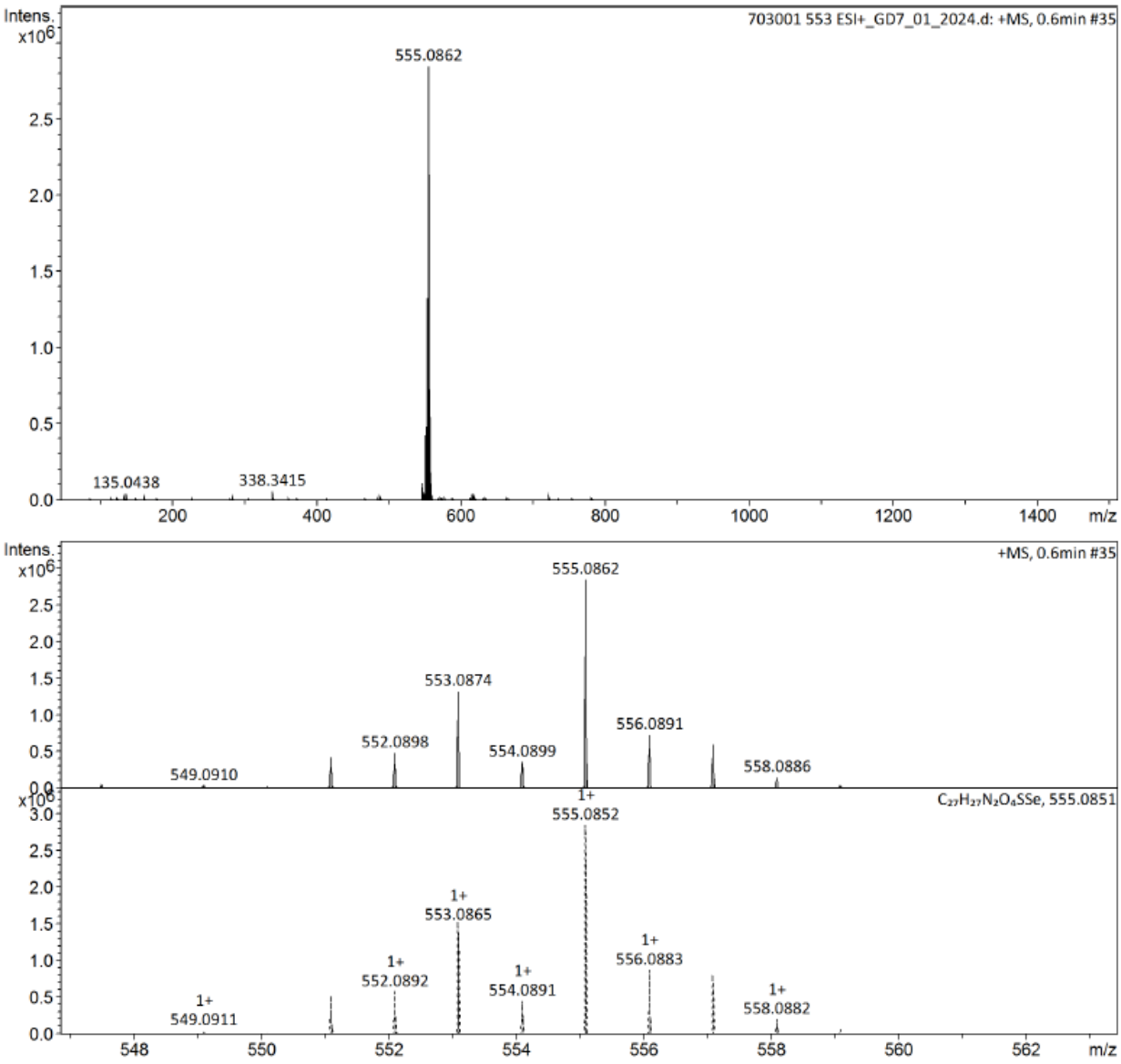
Display Report

Analysis Info

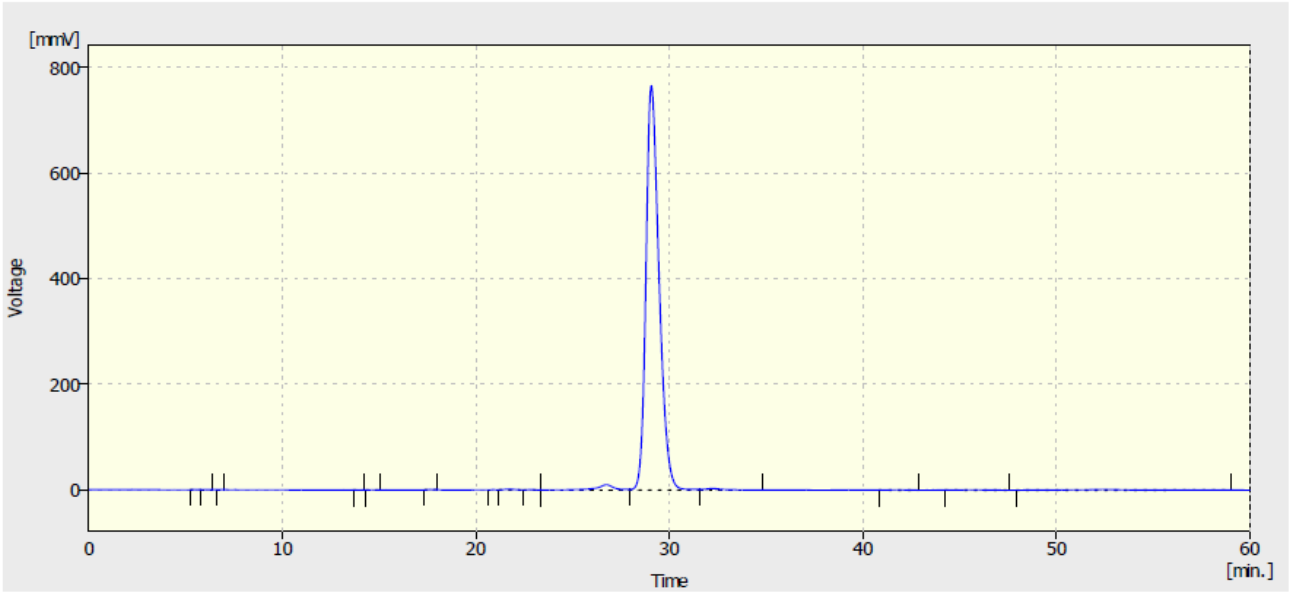
Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\703001 553 ESI+_GD7_01_2024.d	Acquisition Date	6/26/2014 10:01:10 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	703001 553 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



5j HR-MS



Result Table (Uncal - D:|Documents |changwongjin|chang703004)

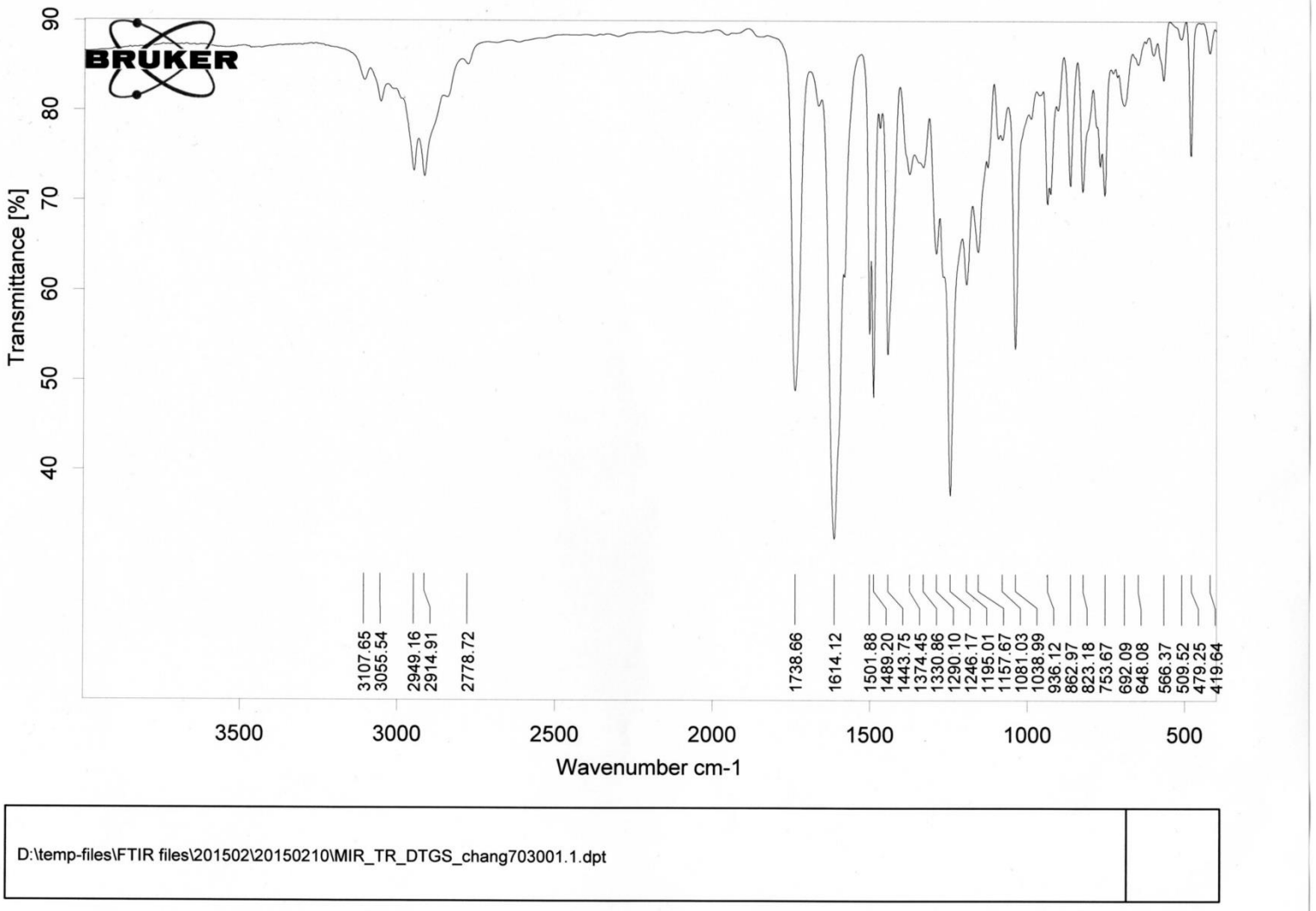
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.636	4.736	0.292	0.0	0.0	0.26
2	5.912	8.531	0.647	0.0	0.1	0.15
3	6.800	2.411	0.229	0.0	0.0	0.17
4	13.904	4.384	0.288	0.0	0.0	0.26
5	14.676	11.532	0.595	0.0	0.1	0.32
6	17.676	10.448	0.605	0.0	0.1	0.31
7	20.892	5.665	0.267	0.0	0.0	0.36
8	21.696	57.932	1.500	0.2	0.2	0.62
9	22.848	17.078	0.686	0.0	0.1	0.40
10	26.744	657.107	10.082	1.8	1.3	0.75
11	29.064	36021.664	765.503	96.4	97.3	0.72
12	32.232	212.306	2.950	0.6	0.4	1.16
13	41.828	33.622	0.704	0.1	0.1	0.76
14	45.672	53.936	0.658	0.1	0.1	1.28

Result Table (Uncal - D:|Documents |changwongjin|chang703004)

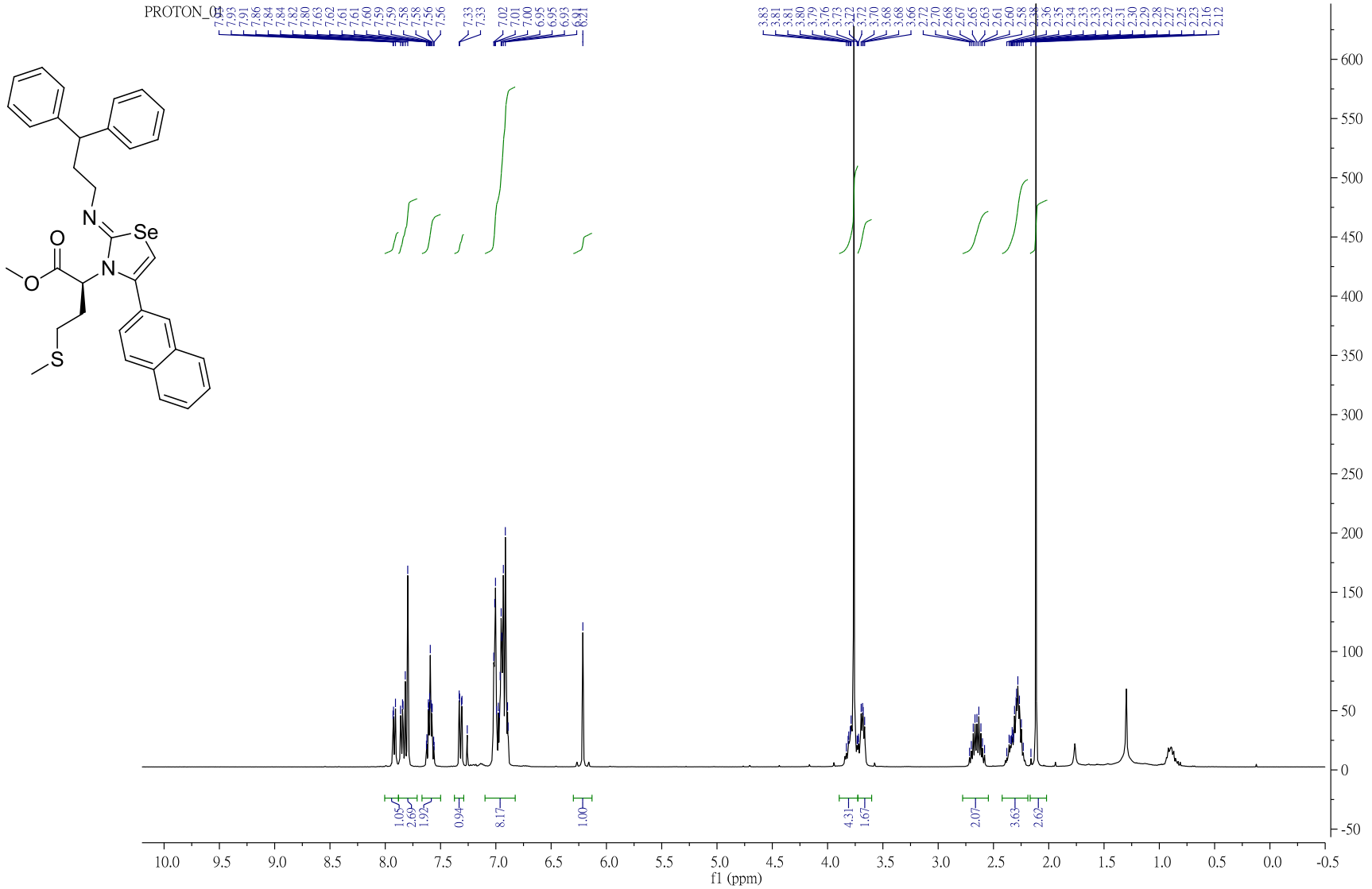
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
15	52.436	253.251	1.391	0.7	0.2	1.64
	Total	37354.603	786.397	100.0	100.0	

5j chiral HPLC

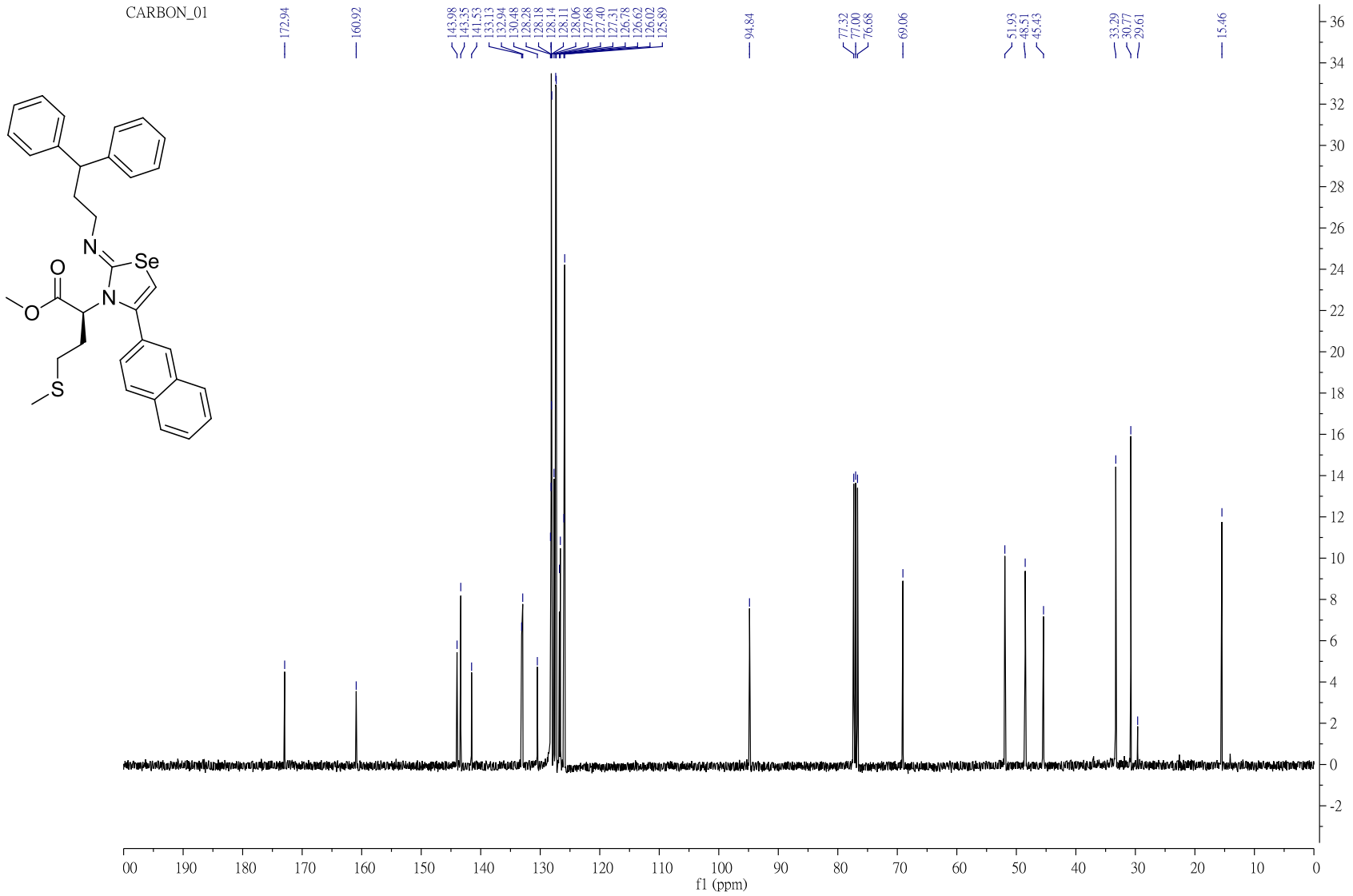
```
SAMPLE : ----------
ID #   : 001
LAMP λ : 589 nm
CONC   : 0.01000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-------------------------
SPECIFIC ROTATION [α]
 COUNT  [α](°)  TEMP(°C)
  01   - 71.4997   20.8
  02   - 71.4997   20.8
  03   - 71.4997   20.8
  04   - 72.4997   20.8
  05   - 75.9997   20.8
  06   - 76.9997   20.8
  07   - 79.4997   20.8
  08   - 83.9997   20.8
  09   - 84.4997   20.8
  10   - 85.9997   20.7
-------------------------
MEAN    = - 77.3997°
σ(N-1)  =    5.8013°
C.V.    = -  7.4953%
```


BRUKER
Transmittance [%]
90
80
70
60
50
40
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3107.65
3055.54
2949.16
2914.91
2778.72
1738.66
1614.12
1501.88
1489.20
1443.75
1374.45
1330.86
1290.10
1246.17
1195.01
1157.67
1081.03
1038.99
936.12
862.97
823.18
753.67
692.09
648.08
566.37
509.52
479.25
419.64
D:\temp-files\FTIR files\201502\20150210\MIR_TR_DTGS_chang703001.1.dpt
Page 1/1

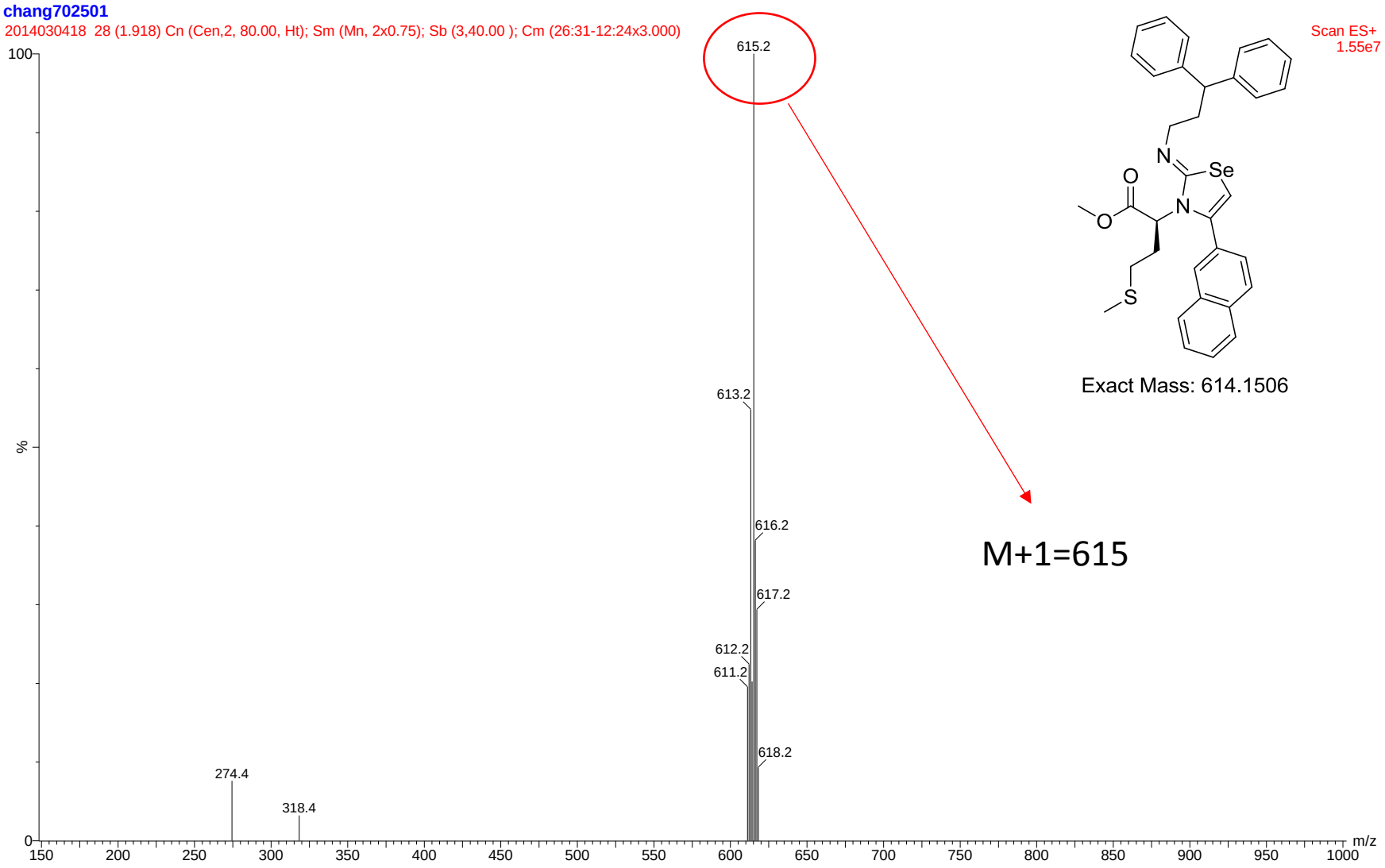
5j FT-IR



5k H^1-NMR


CARBON_01
172.94
160.92
143.98
143.35
141.53
133.13
132.94
130.48
128.28
128.18
128.14
128.11
128.06
127.68
127.40
127.31
126.78
126.62
126.02
125.89
94.84
77.32
77.00
76.68
69.06
51.93
48.51
45.43
33.29
30.77
29.61
15.46
O
O
N
Se
N
S
f1 (ppm)

5k C^{13}-NMR


chang702501
2014030418 28 (1.918) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (26:31-12:24x3.000)
Scan ES+
1.55e7
615.2
613.2
616.2
617.2
612.2
611.2
618.2
274.4
318.4
100
%
0
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
m/z
N
Se
O
O
N
S
Exact Mass: 614.1506
M+1=615

5k LR-MS

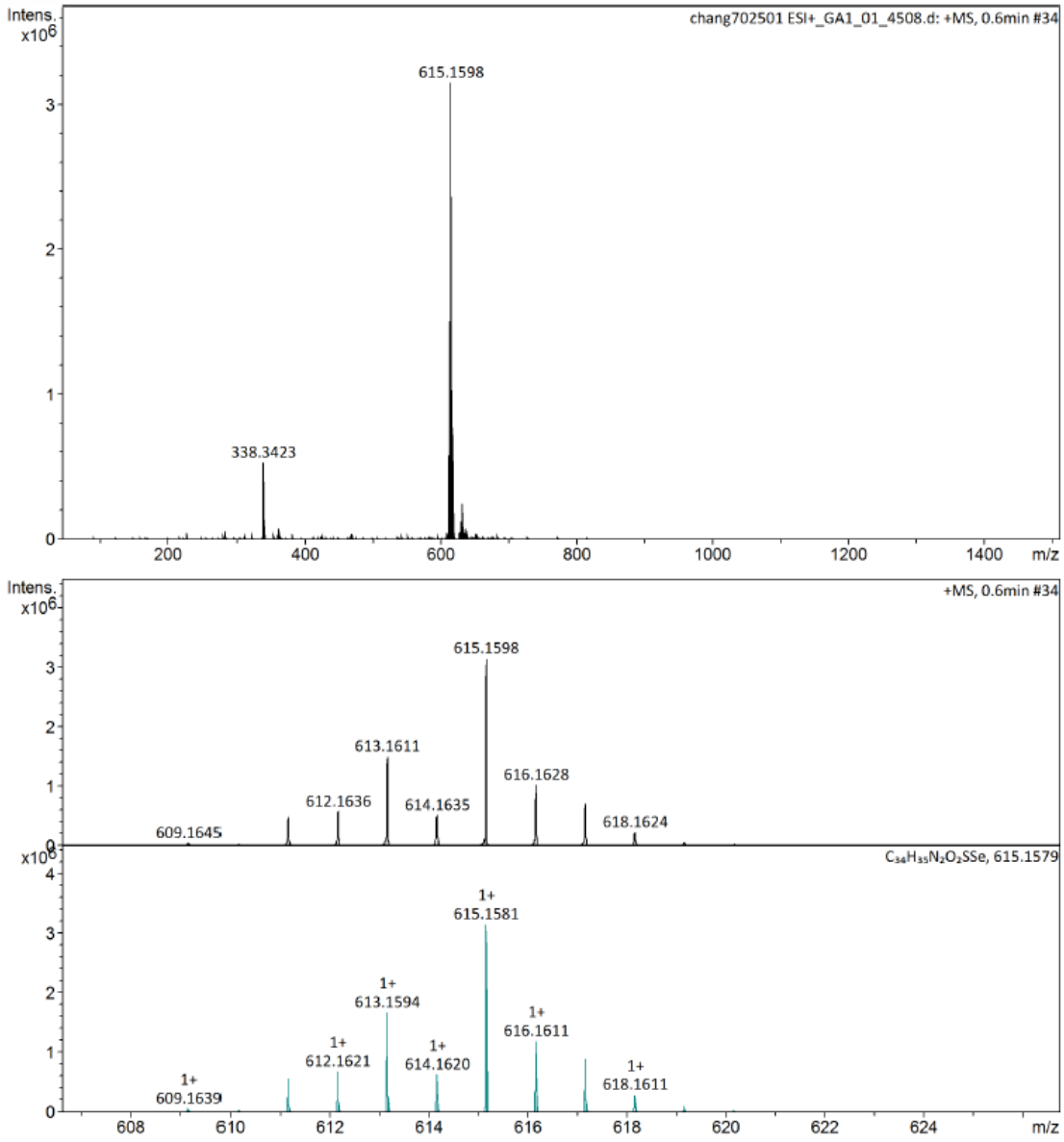
Display Report

Analysis Info

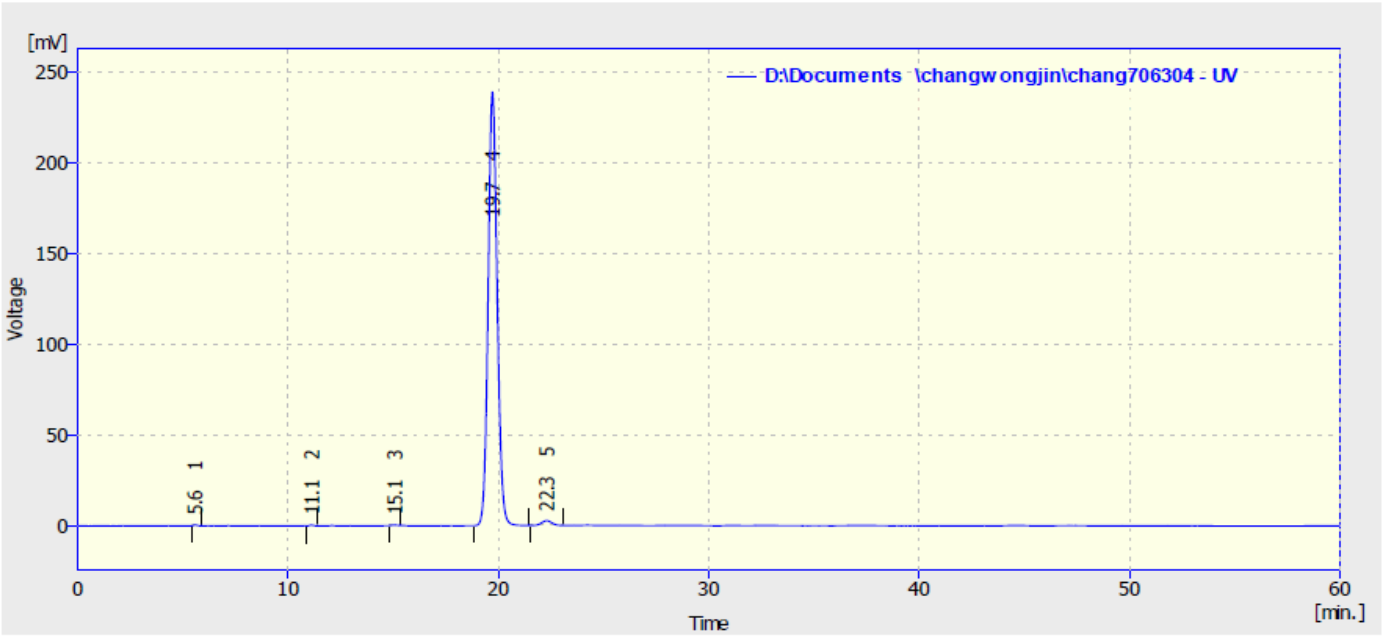
Analysis Name	F:\Q-TOF\20150115\chang702501 ESI+_GA1_01_4508.d	Acquisition Date	1/15/2015 4:37:29 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	chang702501 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



5k HR-MS

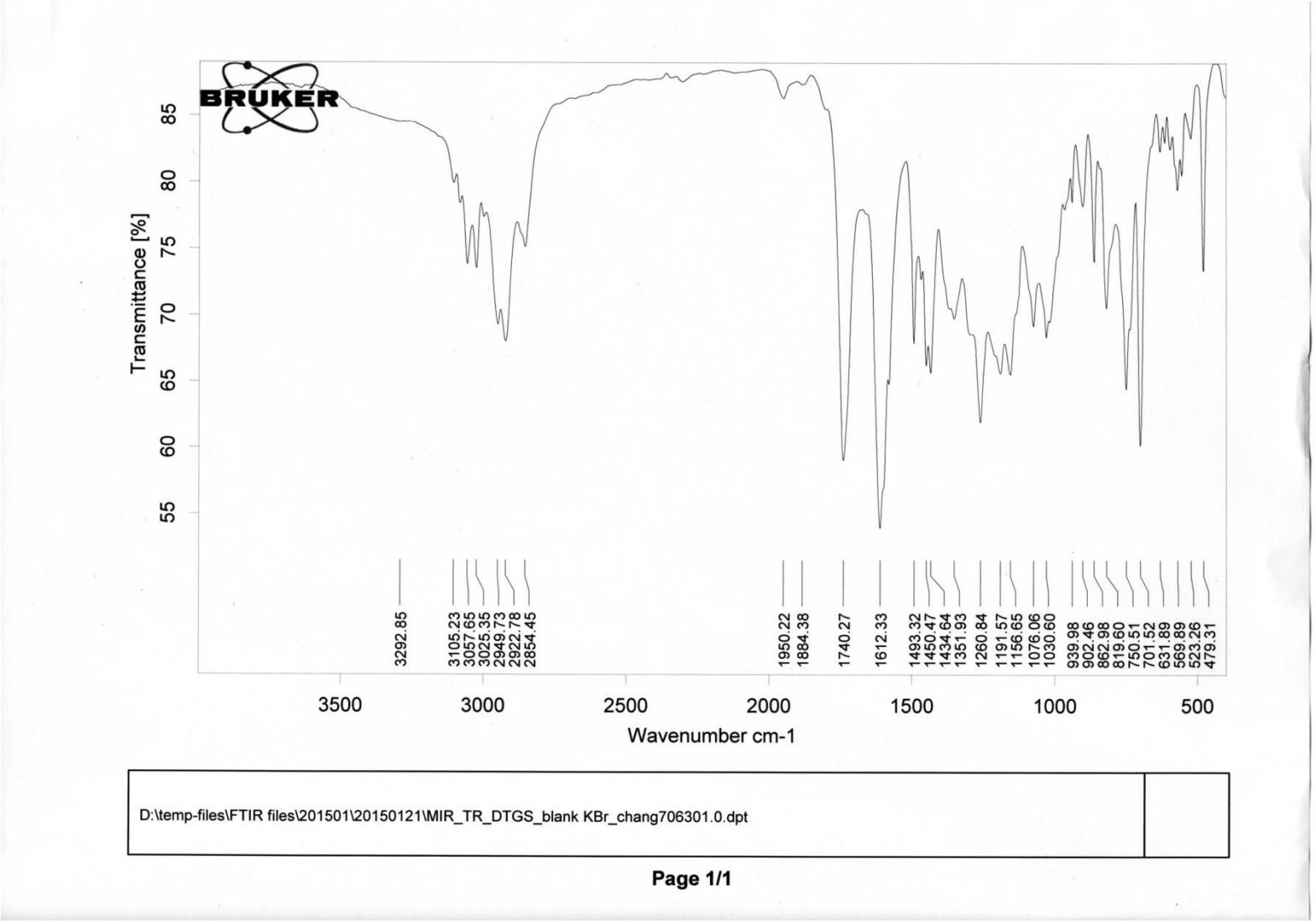


Result Table (Uncal - D:\Documents \changwongjin\chang706304 - UV)

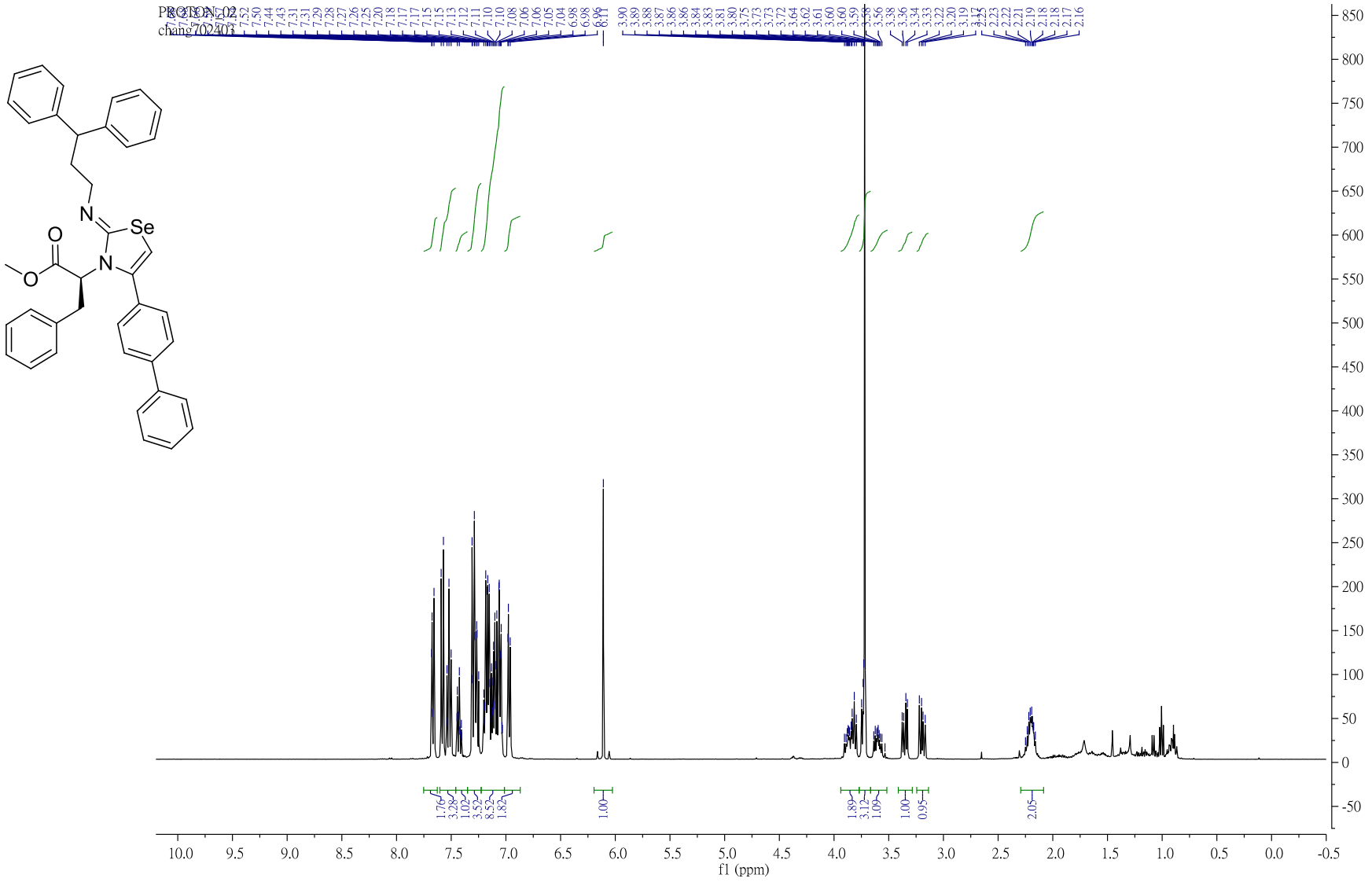
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	5.580	4.604	0.485	0.1	0.2
2	11.120	4.719	0.396	0.1	0.2
3	15.064	4.019	0.251	0.1	0.1
4	19.716	7114.447	238.552	98.6	98.4
5	22.284	91.103	2.674	1.3	1.1
	Total	7218.892	242.357	100.0	100.0

5k chiral HPLC

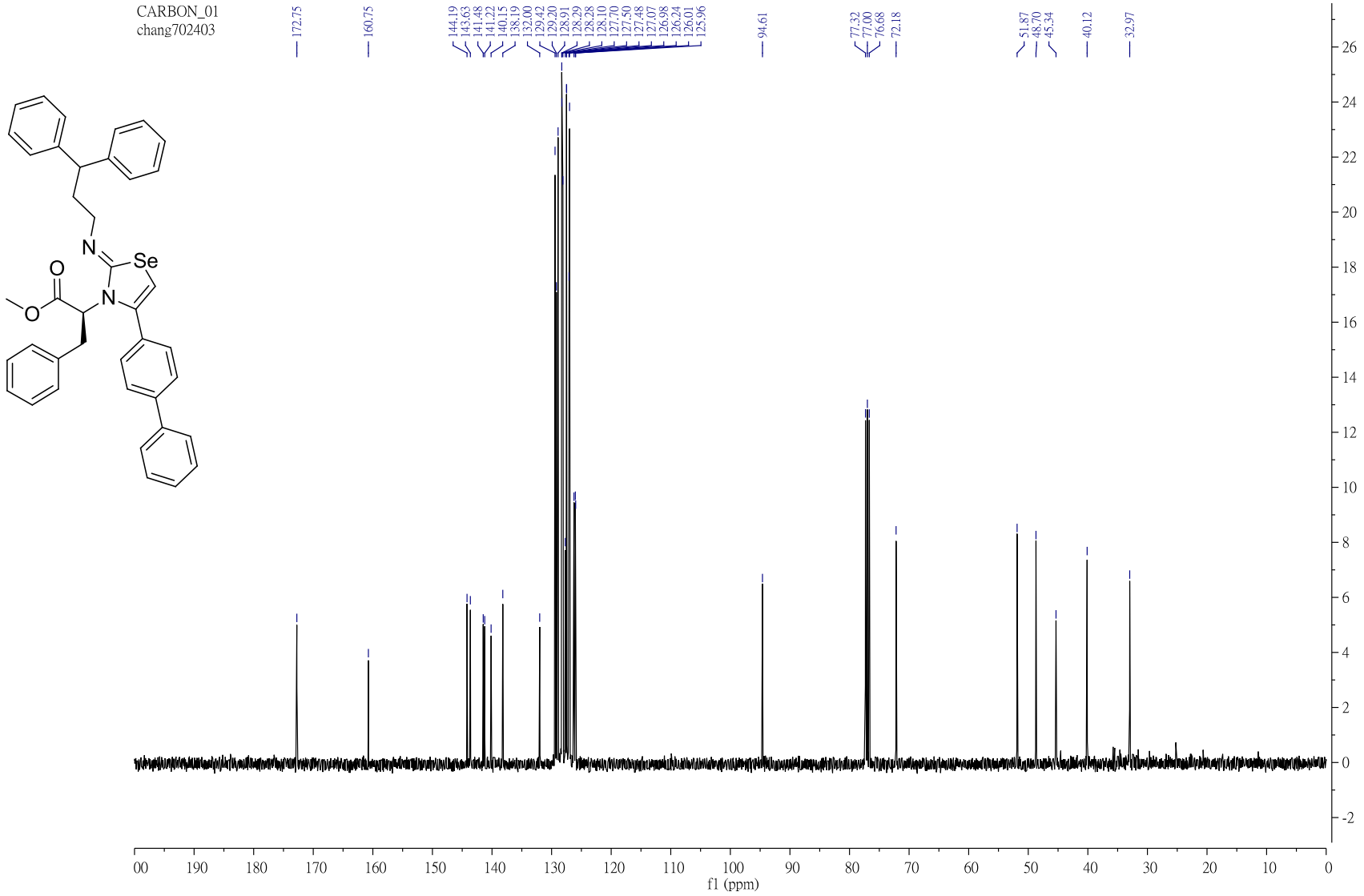
```
SAMPLE : ___________
ID #   : 019
LAMP λ : 589 nm
CONC   : 0.01000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-----------------------
SPECIFIC ROTATION [α]
 COUNT  [α](°)  TEMP(°C)
  01   -682.0000   19.9
  02   -685.5000   19.9
  03   -687.0000   19.9
  04   -688.0000   19.9
  05   -687.0000   19.9
  06   -692.5000   19.9
  07   -693.0000   19.9
  08   -692.0000   19.9
  09   -693.0000   19.9
  10   -695.0000   19.9
-----------------------
MEAN     = -689.5000°
σ(N-1)   =    4.1766°
C.V.     = - 0.60575%
```


BRUKER
Transmittance [%]
85
80
75
70
65
60
55
3292.85
3105.23
3057.65
3025.35
2949.73
2922.78
2854.45
1950.22
1884.38
1740.27
1612.33
1493.32
1450.47
1434.64
1351.93
1260.84
1191.57
1156.65
1076.06
1030.60
939.98
902.46
862.98
819.60
750.51
701.52
631.89
569.89
523.26
479.31
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang706301.0.dpt
Page 1/1

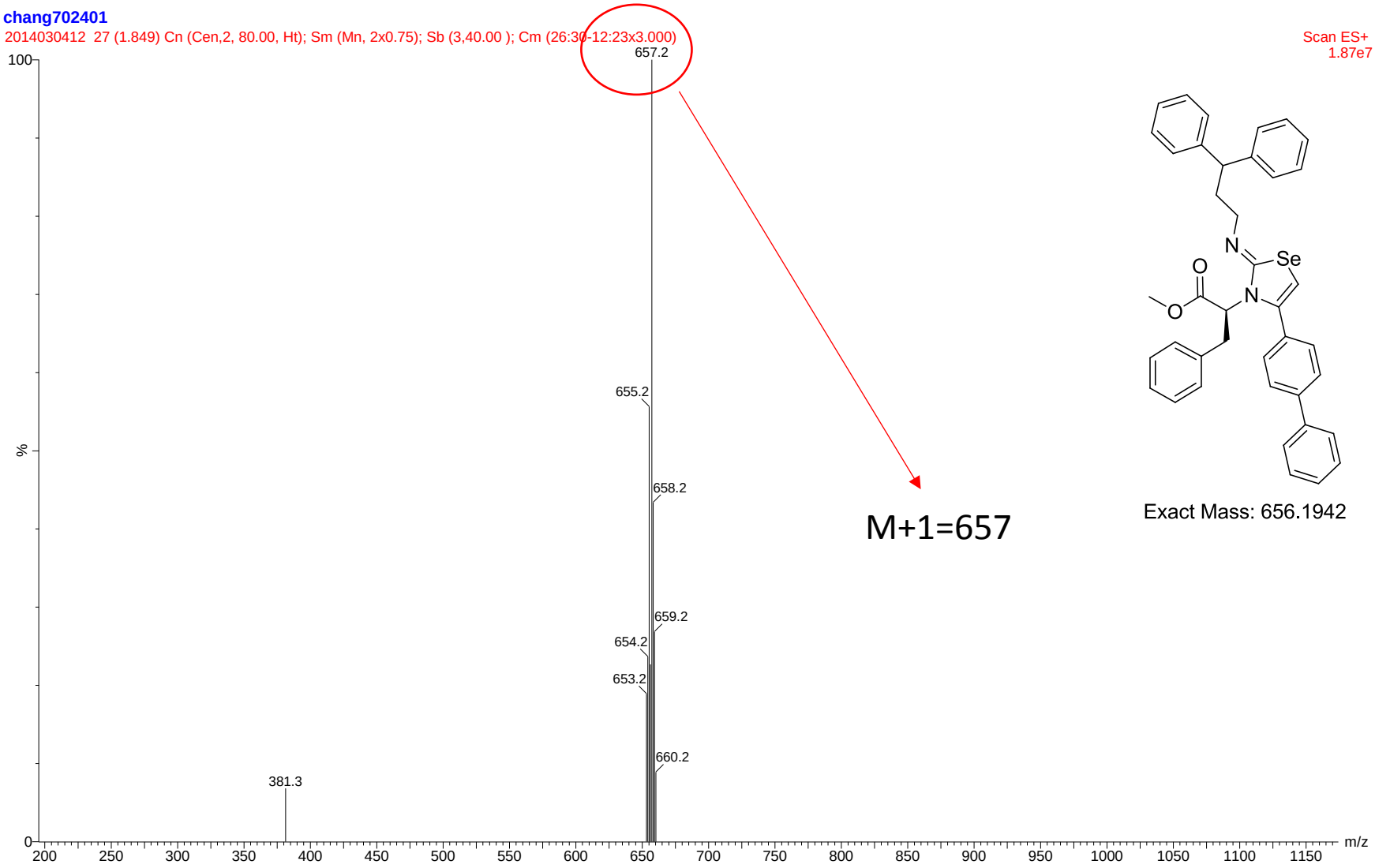
5k FT-IR



5l H^1NMR


CARBON_01
chang702403
172.75
160.75
144.19
143.63
141.48
141.22
140.15
138.19
132.00
129.42
129.20
128.91
128.29
128.28
128.10
127.70
127.50
127.48
127.07
126.98
126.24
126.01
125.96
94.61
77.32
77.00
76.68
72.18
51.87
48.70
45.34
40.12
32.97
N
Se
O
N
O
f1 (ppm)

5l C^{13}NMR


chang702401
2014030412 27 (1.849) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (26:30-12:23x3.000)
Scan ES+
1.87e7
100
%
0
657.2
655.2
658.2
659.2
654.2
653.2
660.2
381.3
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
1050
1100
1150
m/z
M+1=657
N
Se
O
N
O
Exact Mass: 656.1942

5l LR-MS

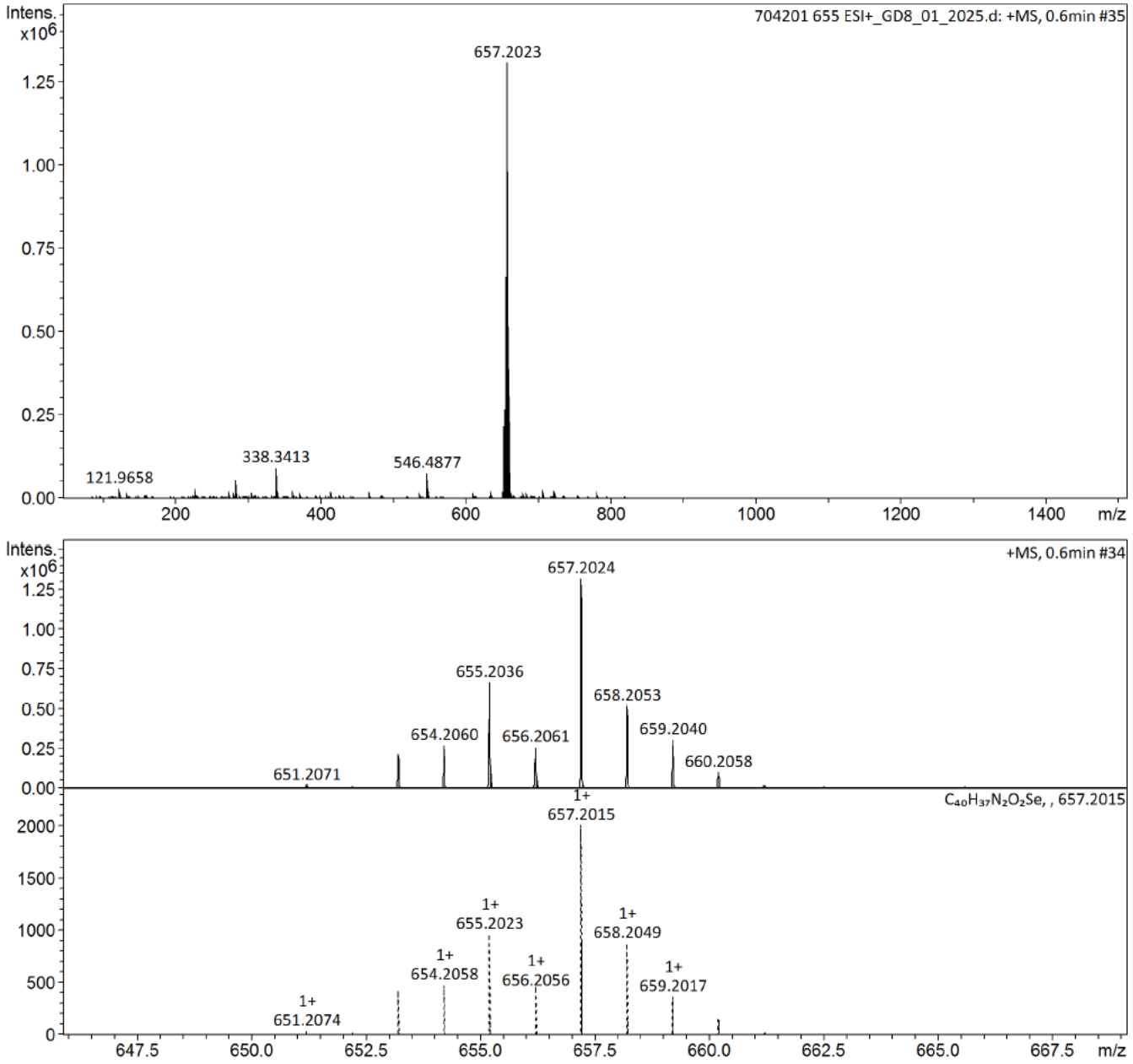
Display Report

Analysis Info

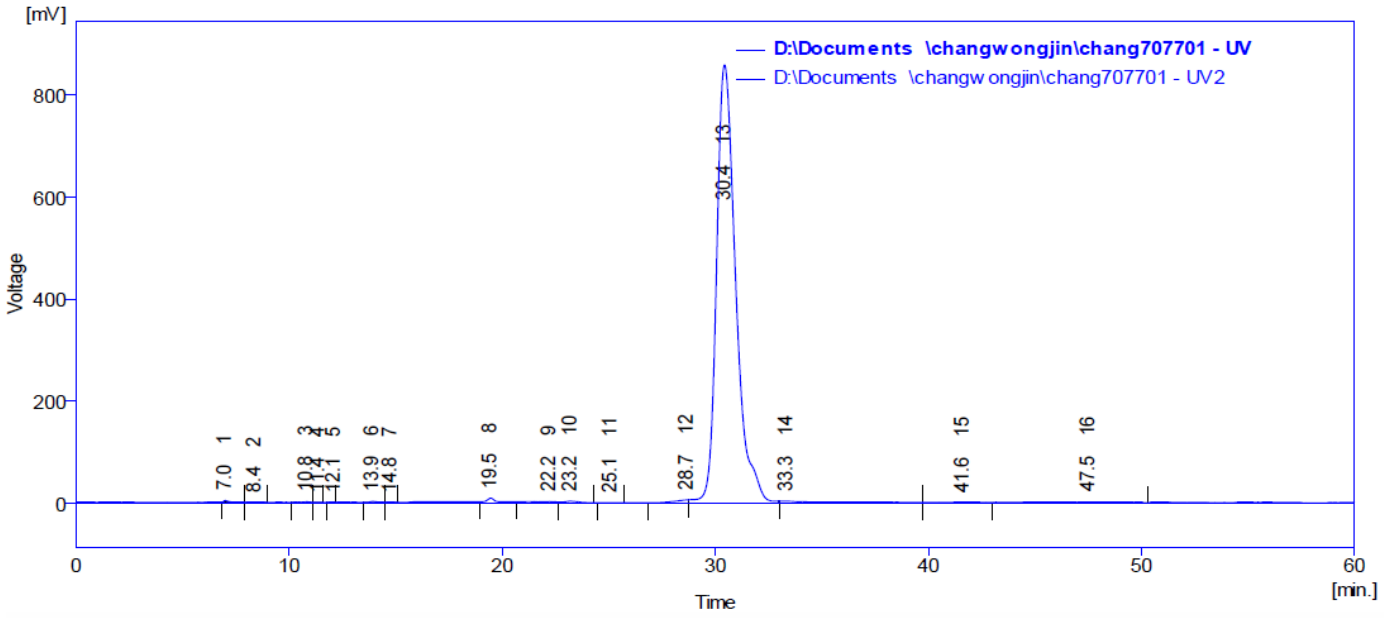
Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\704201 655 ESI+_GD8_01_2025.d	Acquisition Date	6/26/2014 10:05:30 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	704201 655 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



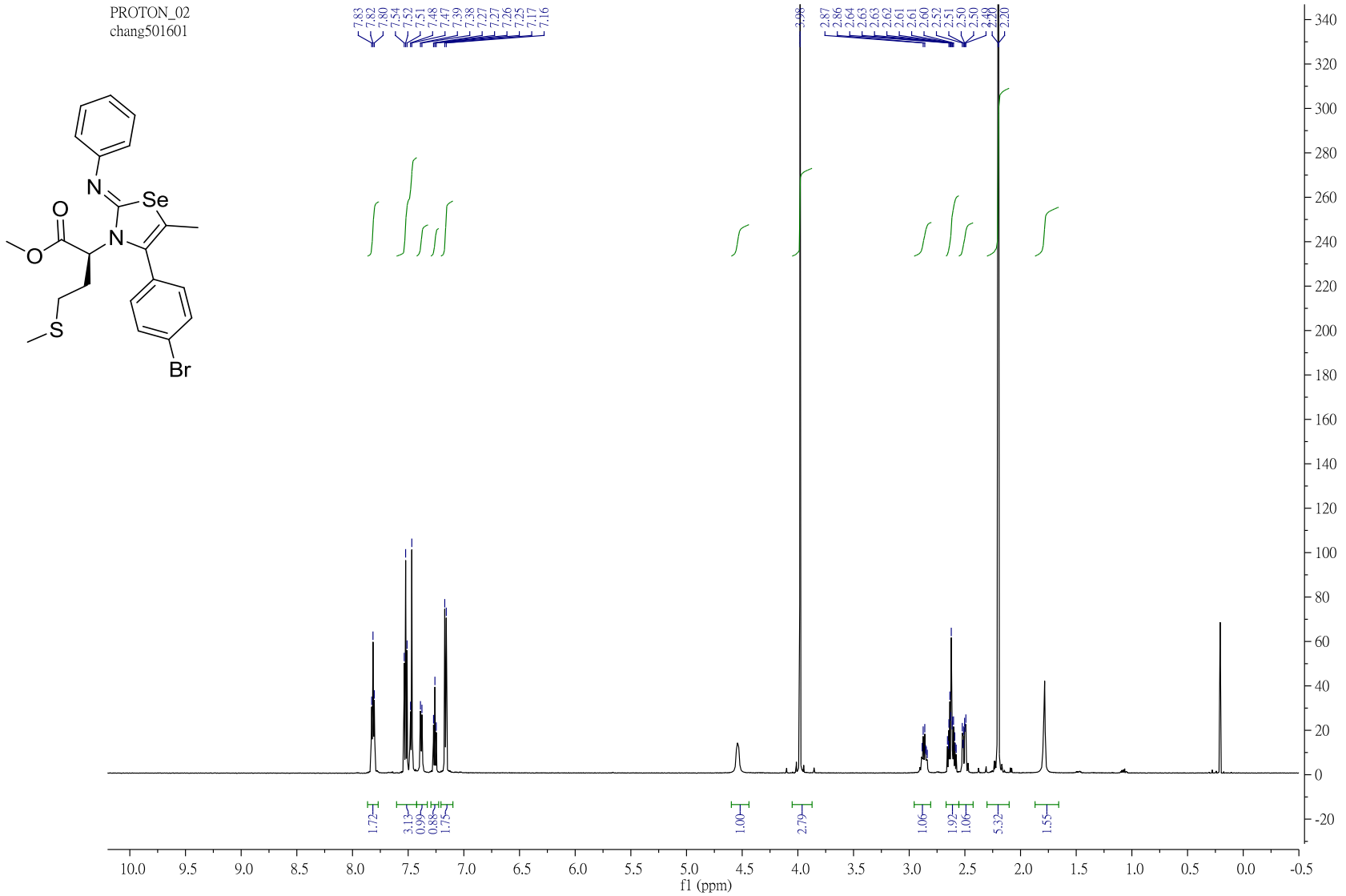
5l HR-MS



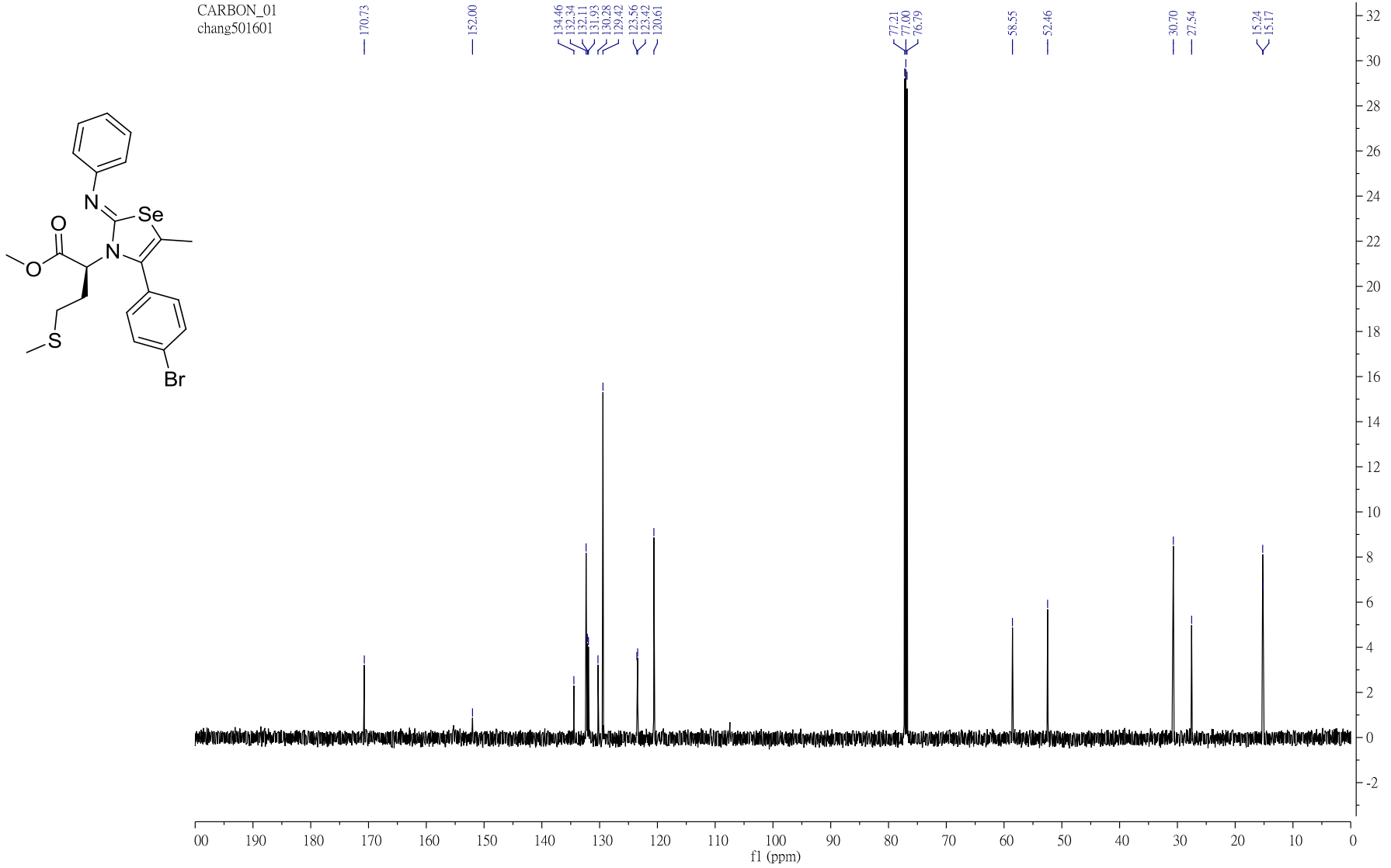
Result Table (Uncal - D:\Documents \changwongjin\chang707701 - UV)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	6.992	50.714	3.013	0.1	0.3
2	8.380	28.267	0.820	0.0	0.1
3	10.820	21.773	0.949	0.0	0.1
4	11.380	8.434	0.472	0.0	0.1
5	12.104	12.814	0.674	0.0	0.1
6	13.912	47.136	2.248	0.1	0.3
7	14.752	19.912	0.729	0.0	0.1
8	19.456	340.494	9.129	0.6	1.0
9	22.212	226.305	2.453	0.4	0.3
10	23.204	154.527	3.470	0.3	0.4
11	25.092	17.675	0.455	0.0	0.1
12	28.676	273.995	6.022	0.5	0.7
13	30.432	53679.511	858.846	94.6	95.7
14	33.348	755.568	3.707	1.3	0.4
15	41.628	282.268	1.827	0.5	0.2
16	47.524	817.538	2.261	1.4	0.3
	Total	56736.931	897.078	100.0	100.0

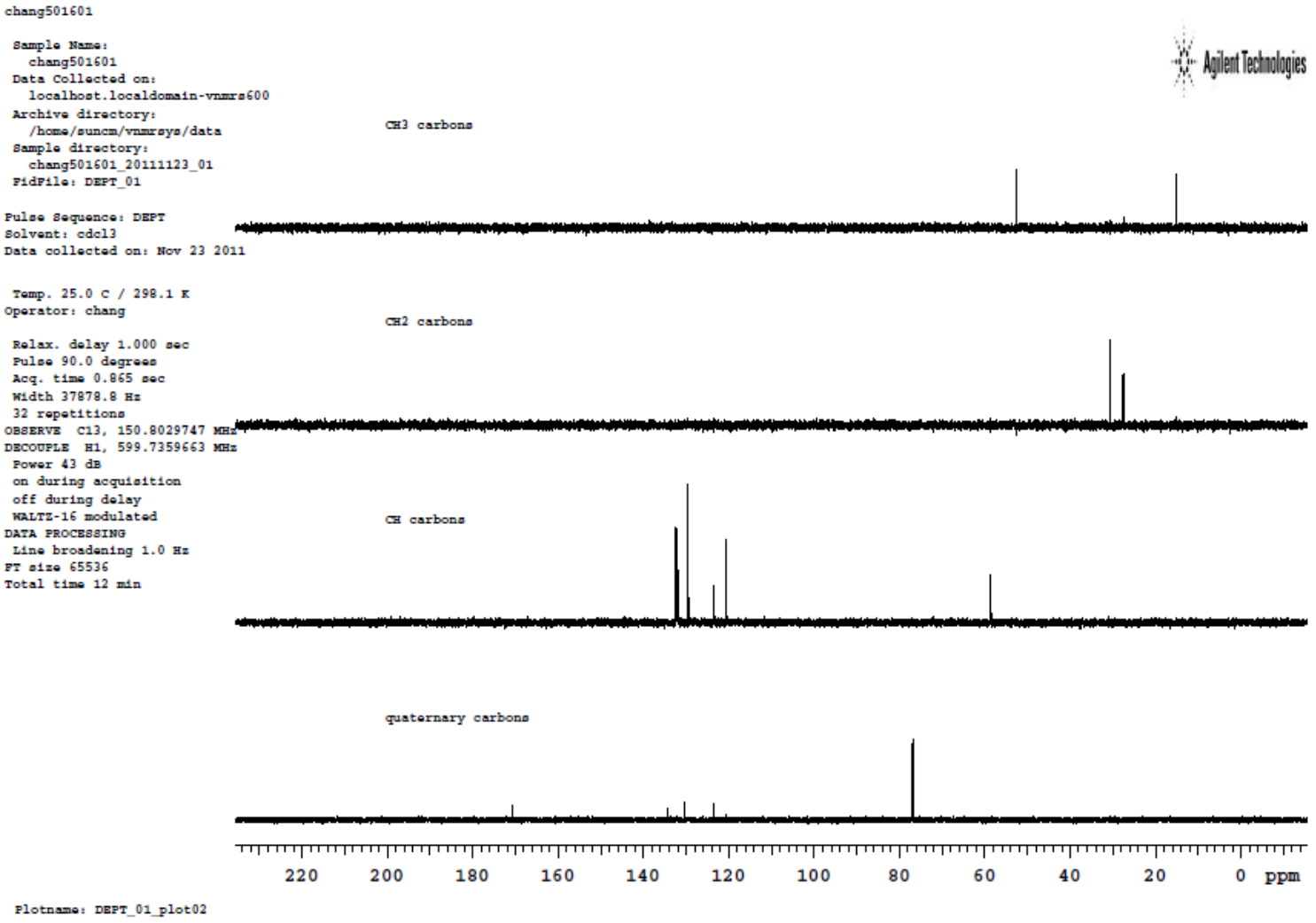
5l chiral HPLC



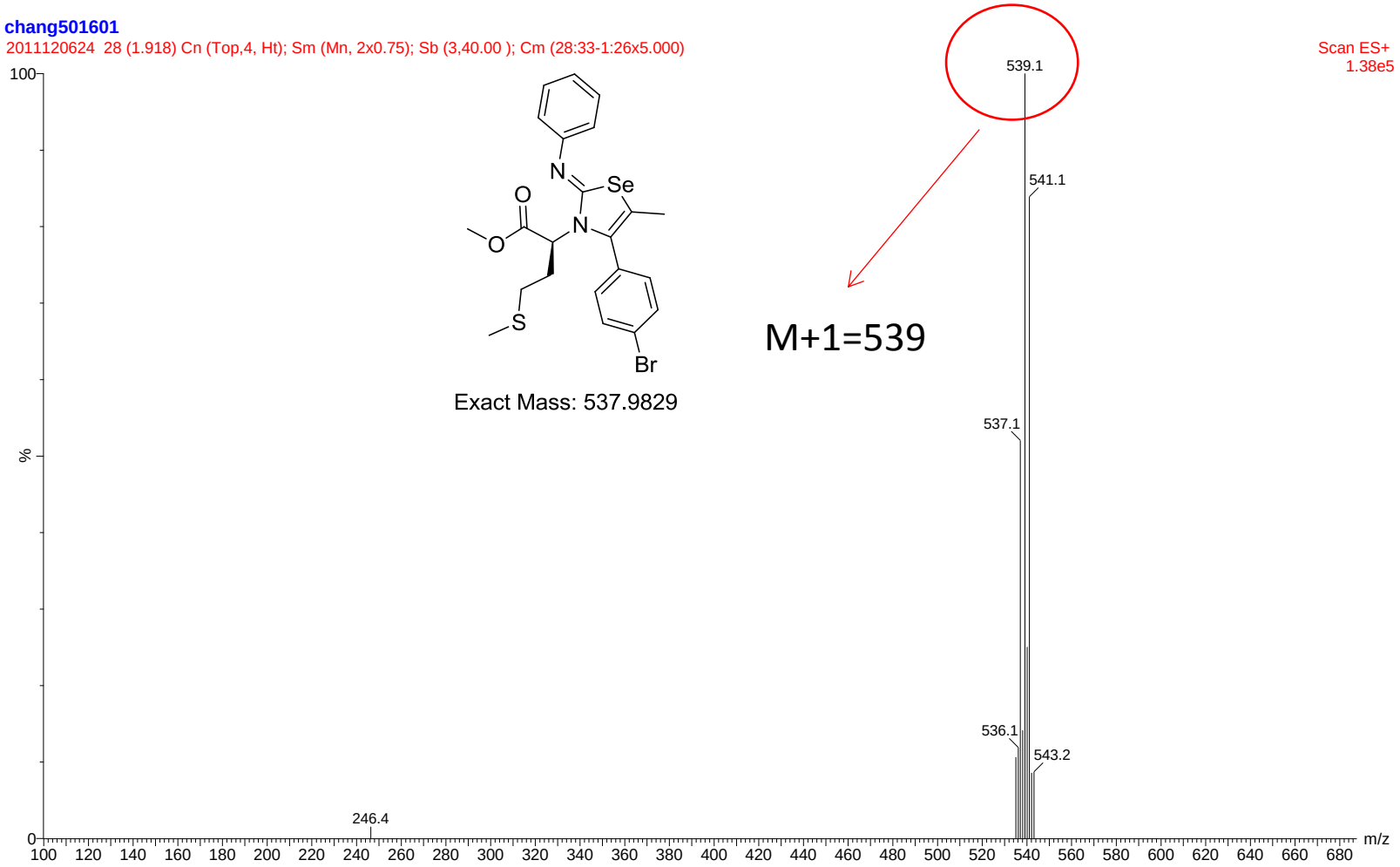
7a H^1NMR


CARBON_01
chang501601
170.73
152.00
134.46
132.34
132.11
131.93
130.28
129.42
123.56
123.42
120.61
77.21
77.00
76.79
58.55
52.46
30.70
27.54
15.24
15.17
N
Se
O
N
O
S
Br
f1 (ppm)

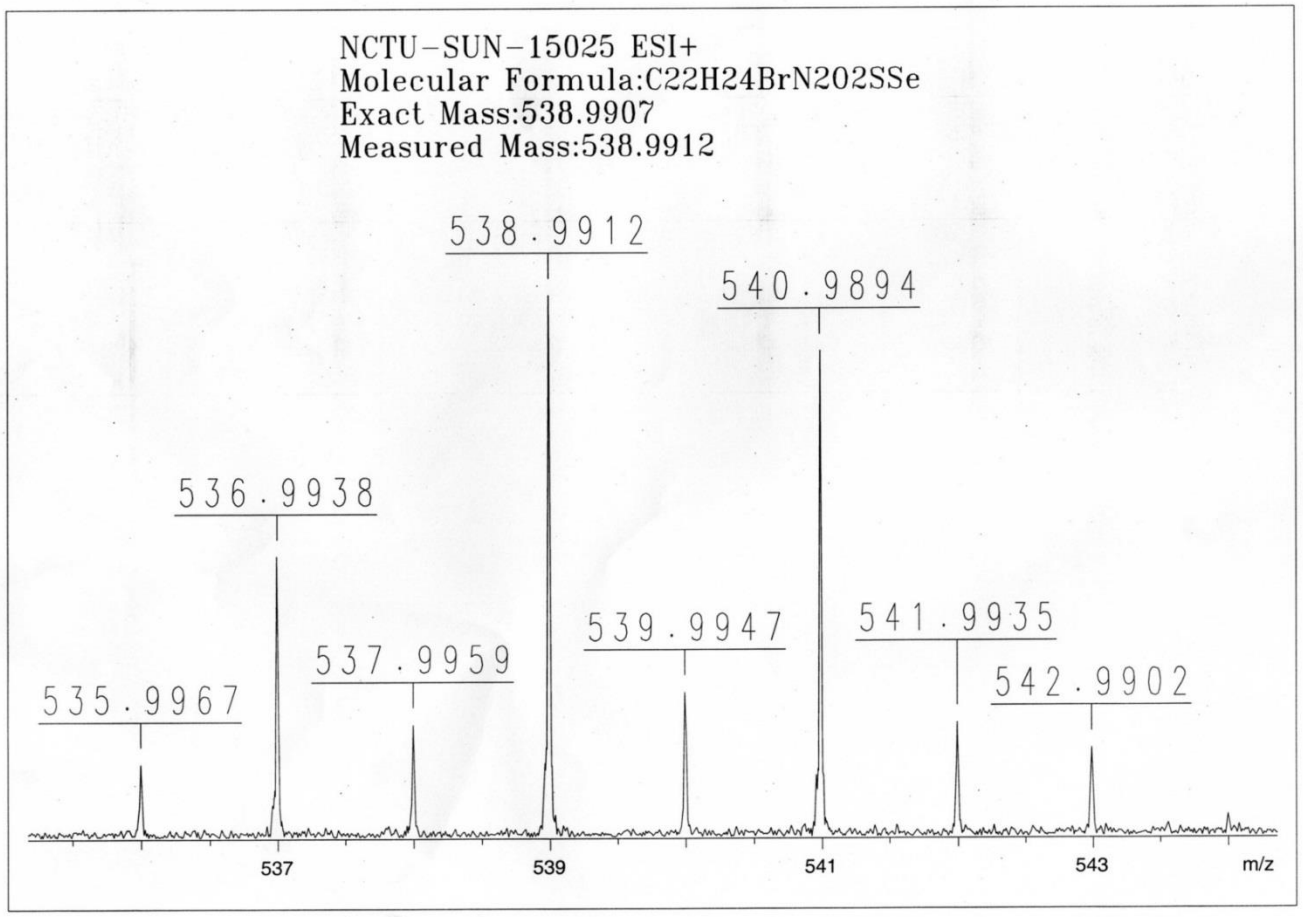
7a C^{13}NMR


chang501601
Sample Name:
chang501601
Data Collected on:
localhost.localdomain-vnmrs600
Archive directory:
/home/suncm/vnmrsys/data
Sample directory:
chang501601_20111123_01
FidFile: DEPT_01
Pulse Sequence: DEPT
Solvent: cdcl3
Data collected on: Nov 23 2011
Temp. 25.0 C / 298.1 K
Operator: chang
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 0.865 sec
Width 37878.8 Hz
32 repetitions
OBSERVE C13, 150.8029747 MHz
DECOUPLE H1, 599.7359663 MHz
Power 43 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 12 min
Agilent Technologies
CH3 carbons
CH2 carbons
CH carbons
quaternary carbons
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Plotname: DEPT_01_plot02

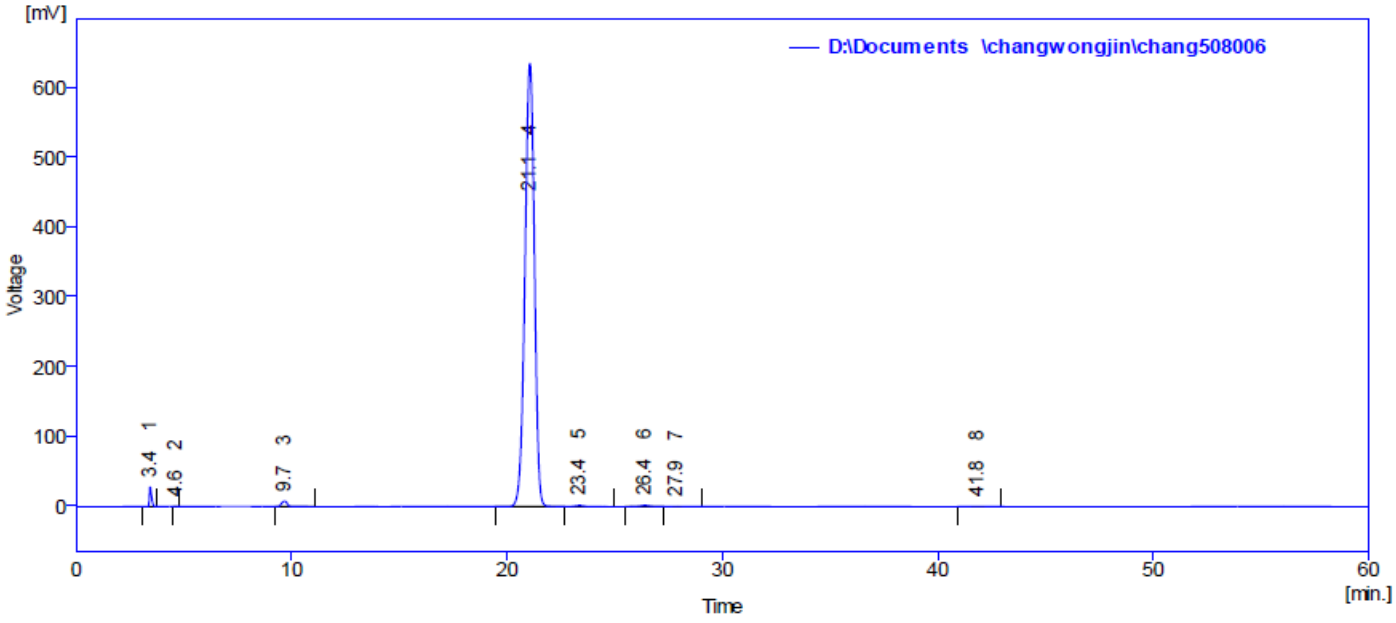
7a DEPT


chang501601
2011120624 28 (1.918) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (28:33-1:26x5.000)
Scan ES+
1.38e5
100
%
0
539.1
541.1
537.1
536.1
543.2
246.4
M+1=539
Exact Mass: 537.9829
N
Se
O
O
N
S
Br
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680
m/z

7a LR-MS


NCTU-SUN-15025 ESI+
Molecular Formula:C22H24BrN2O2SSe
Exact Mass:538.9907
Measured Mass:538.9912
538.9912
540.9894
536.9938
539.9947
541.9935
537.9959
542.9902
535.9967
537
539
541
543
m/z
/d=/Data/yu/NCTUSUN15025/2/pdata/1 Administrator Wed Mar 13 11:13:15 2013

7a HR-MS



Result Table (Uncal - D:|Documents |changwongjin|chang508006)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	3.428	199.038	28.366	1.0	4.2
2	4.620	3.022	0.431	0.0	0.1
3	9.676	147.879	7.759	0.7	1.1
4	21.060	19390.209	635.996	97.3	93.9
5	23.368	66.168	1.908	0.3	0.3
6	26.392	68.653	2.015	0.3	0.3
7	27.864	20.406	0.551	0.1	0.1
8	41.828	27.180	0.538	0.1	0.1
	Total	19922.555	677.563	100.0	100.0

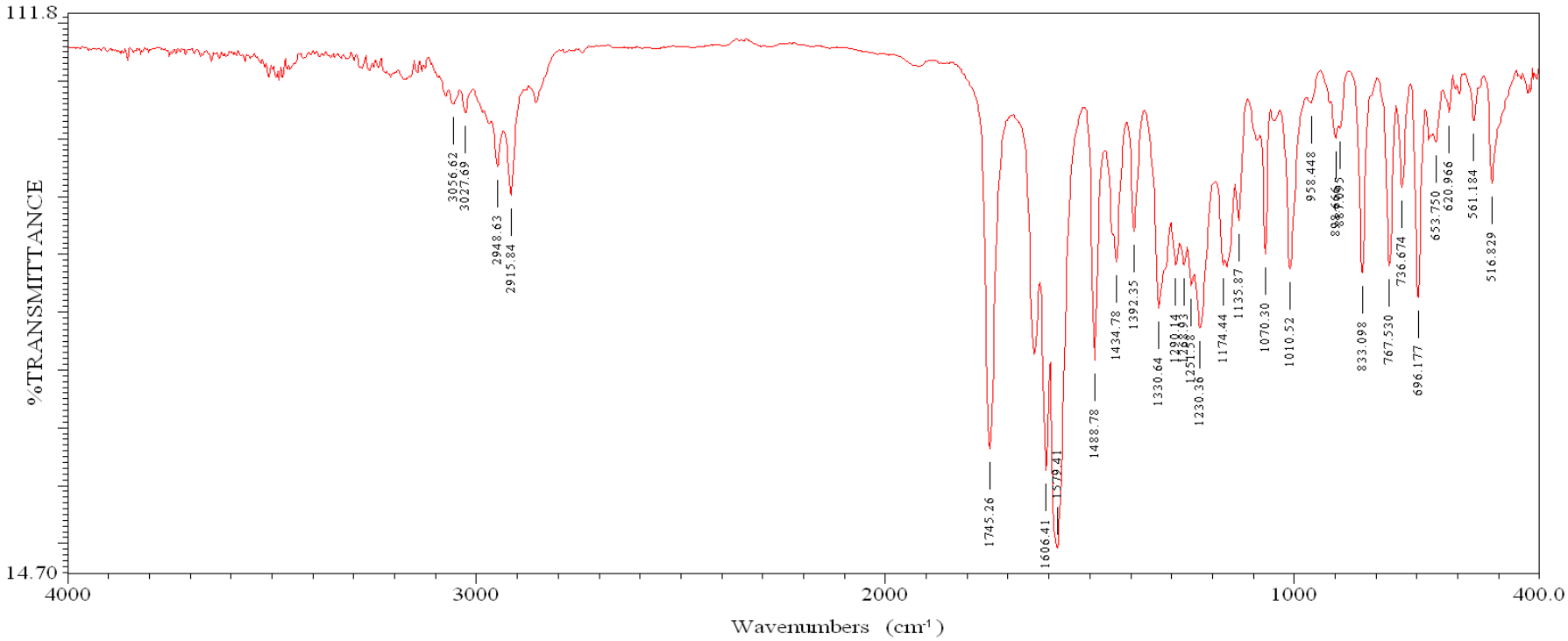
7a chiral HPLC

SAMPLE :
ID # : 005
LAMP λ : 589 nm
CONC : 0.01000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL: 1 min

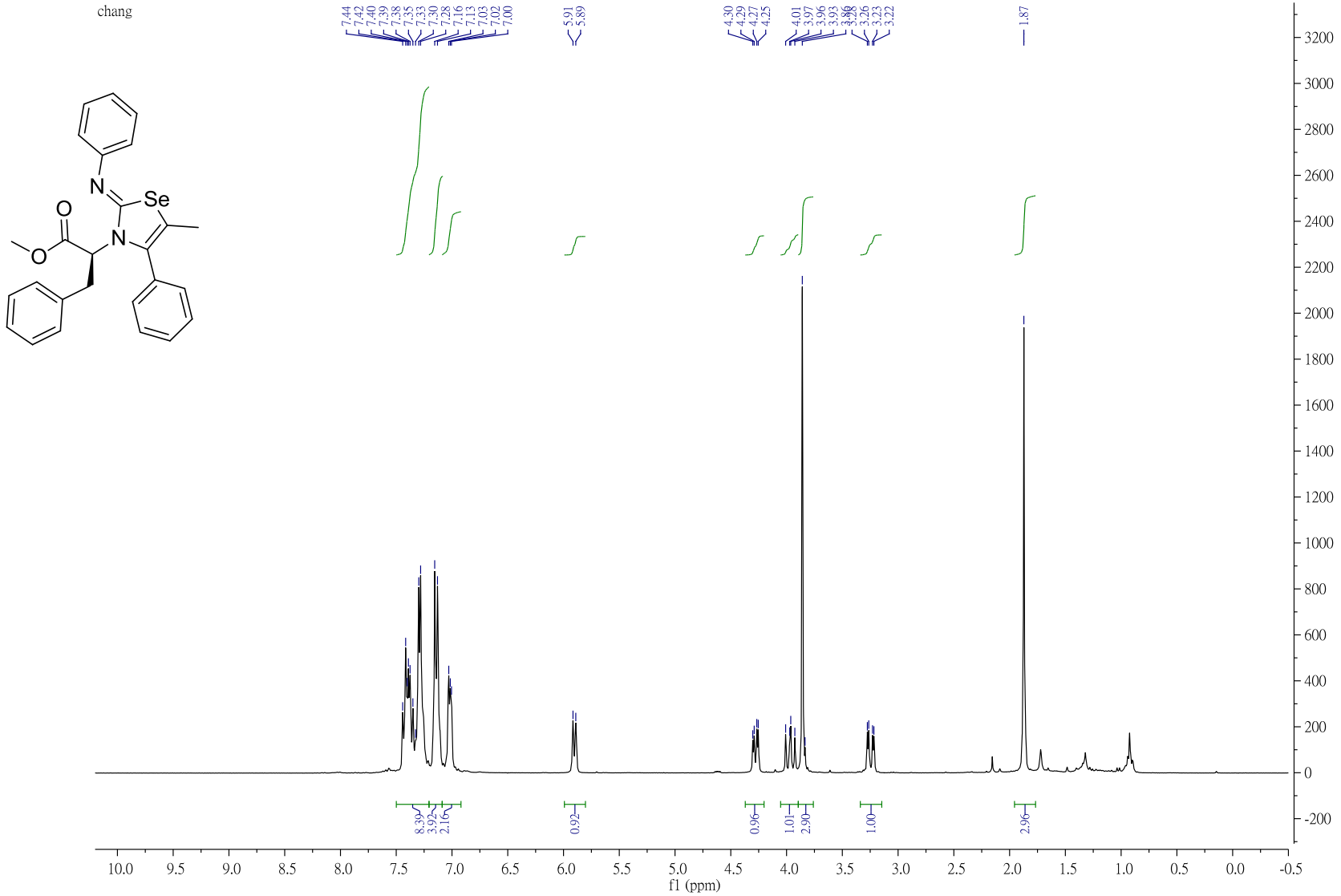
SPECIFIC ROTATION [α]

COUNT	[α](°)	TEMP(°C)
01	- 98.4995	21.3
02	-100.5000	21.3
03	-102.5000	21.3
04	-105.5000	21.3
05	-107.5000	21.3
06	-110.0000	21.3
07	-112.5000	21.3
08	-114.5000	21.3
09	-117.5000	21.3
10	-120.0000	21.3

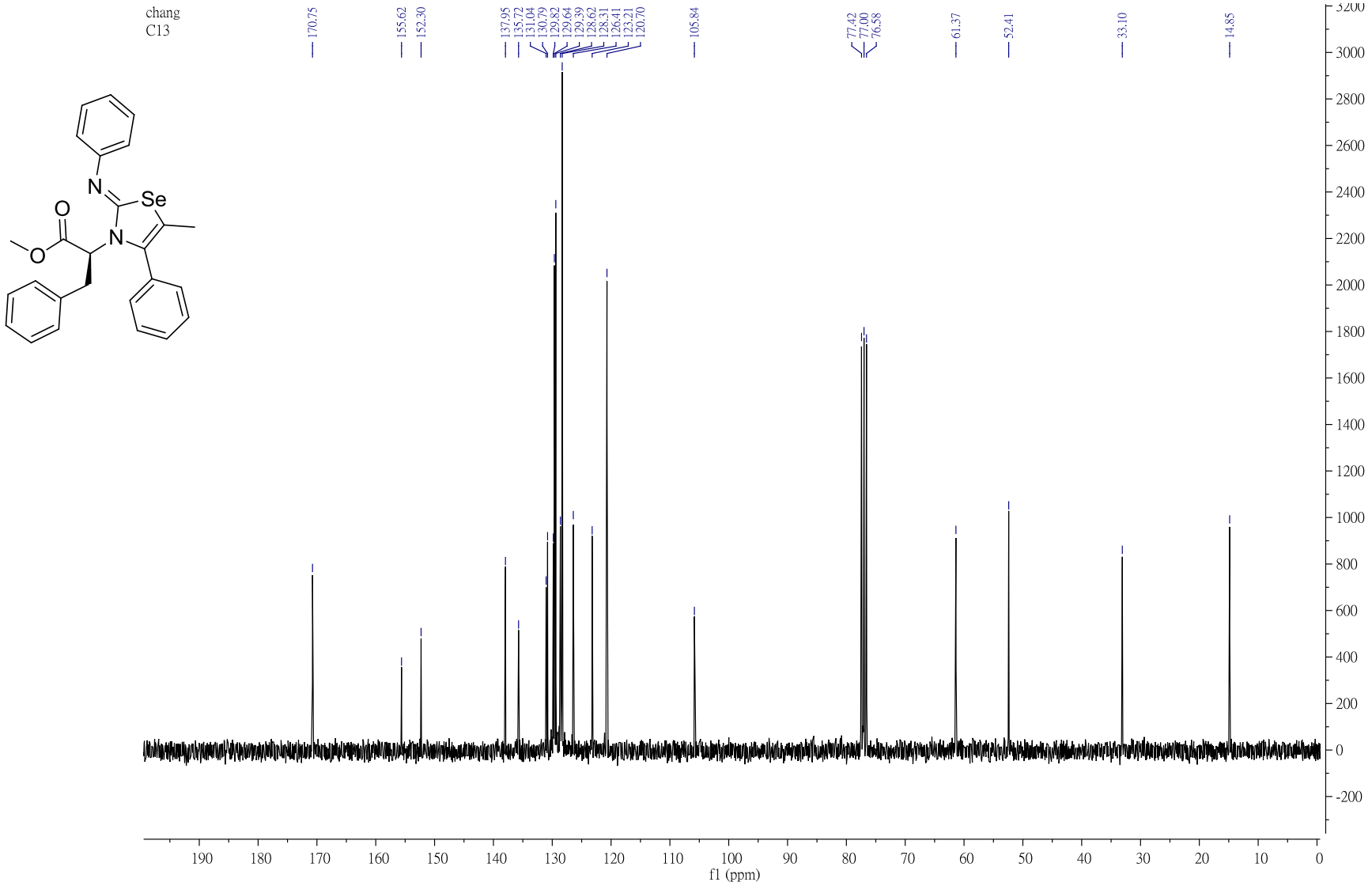
MEAN = -108.9000°
σ(N-1) = 7.2717°
C.V. = - 6.6774%


111.8
14.70
%TRANSMITTANCE
4000
3000
2000
1000
400.0
Wavenumbers (cm-1)
3056.62
3027.69
2948.63
2915.84
1745.26
1606.41
1579.41
1488.78
1434.78
1392.35
1330.64
1290.14
1268.93
1251.58
1230.38
1174.44
1135.87
1070.30
1010.52
958.448
833.098
767.530
736.674
696.177
653.750
620.966
561.184
516.829

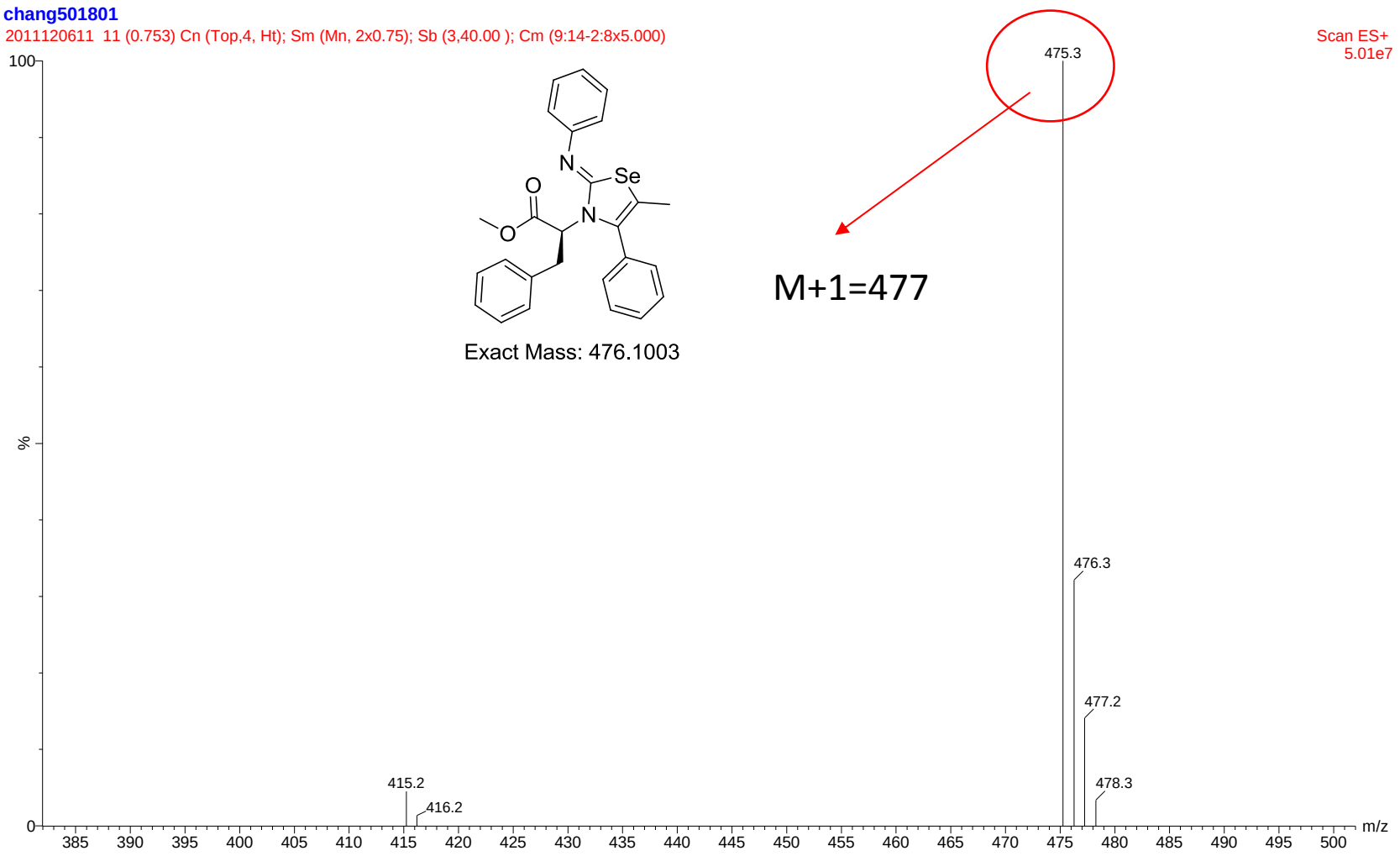
7a FT-IR


chang
7.44
7.42
7.40
7.39
7.38
7.35
7.33
7.30
7.28
7.16
7.13
7.03
7.02
7.00
5.91
5.89
4.30
4.29
4.27
4.25
4.01
3.97
3.96
3.93
3.26
3.23
3.22
1.87
N
Se
O
N
O
8.39
3.92
2.16
0.92
0.96
1.01
2.90
1.00
2.96
f1 (ppm)

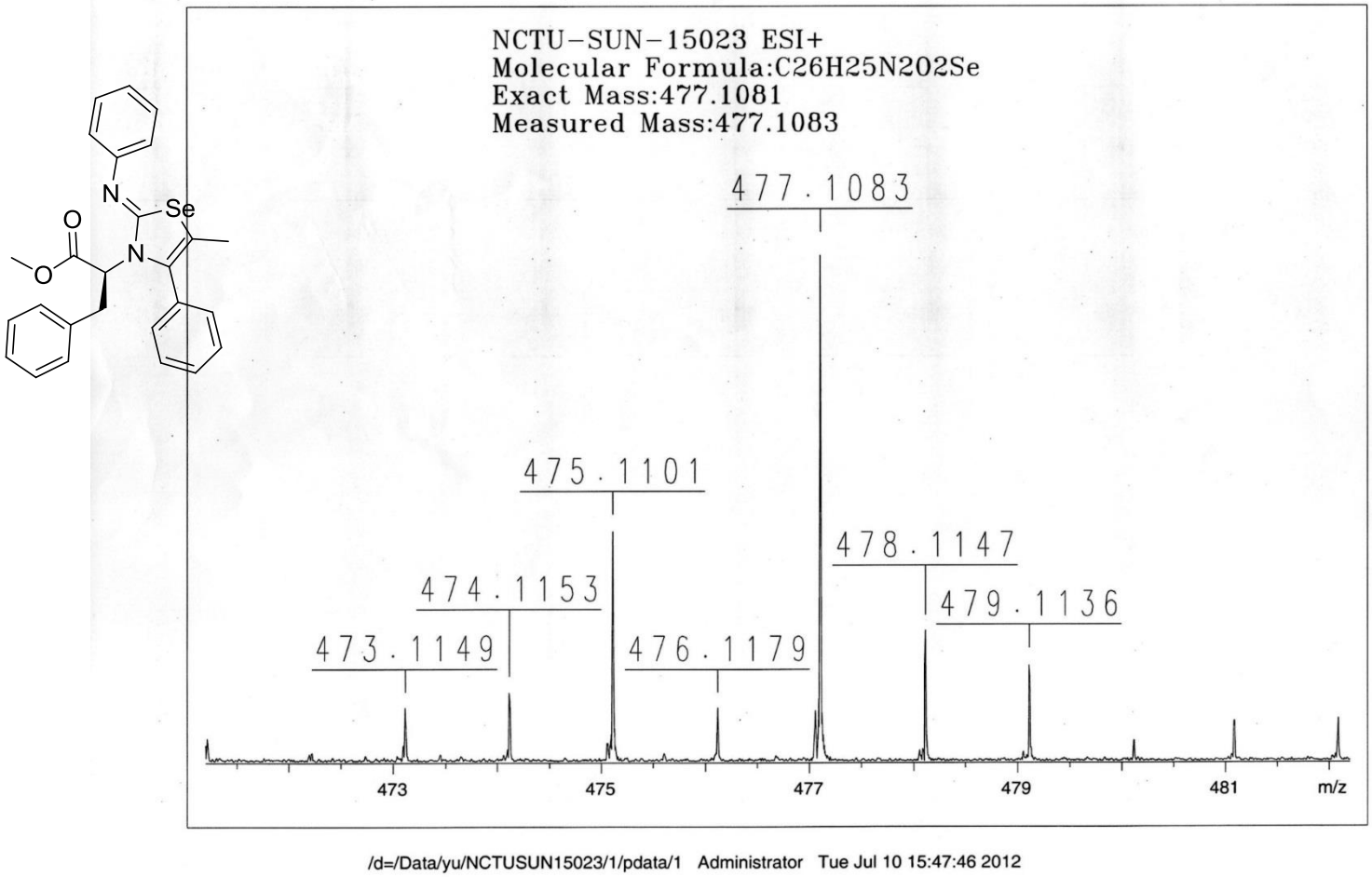
7b H[1]NMR


chang
C13
170.75
155.62
152.30
137.95
135.72
131.04
130.79
129.82
129.64
129.39
128.62
128.31
126.41
123.21
120.70
105.84
77.42
77.00
76.58
61.37
52.41
33.10
14.85
N
Se
O
N
O
f1 (ppm)

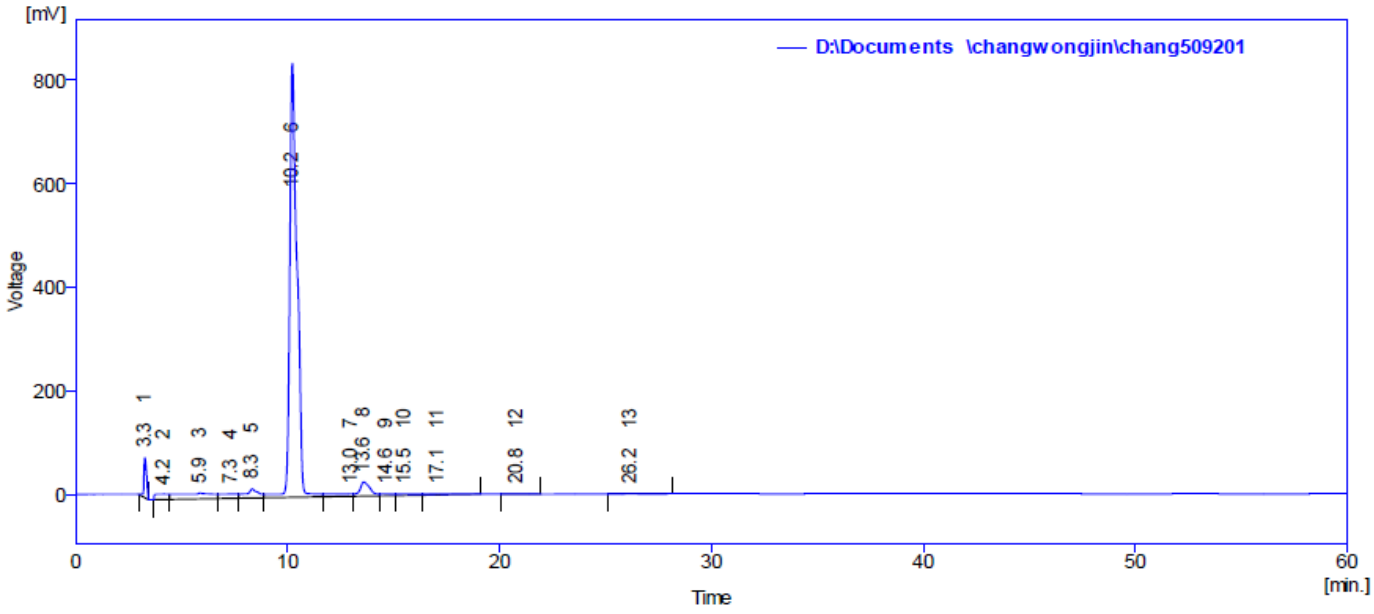
7b C^{13}NMR


chang501801
2011120611 11 (0.753) Cn (Top,4, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (9:14-2:8x5.000)
Scan ES+
5.01e7
100
%
0
N
Se
O
O
N
Exact Mass: 476.1003
M+1=477
475.3
476.3
477.2
478.3
415.2
416.2
385 390 395 400 405 410 415 420 425 430 435 440 445 450 455 460 465 470 475 480 485 490 495 500
m/z

7b LR-MS


NCTU-SUN-15023 ESI+
Molecular Formula:C26H25N2O2Se
Exact Mass:477.1081
Measured Mass:477.1083
477.1083
475.1101
478.1147
474.1153
479.1136
473.1149
476.1179
473
475
477
479
481
m/z
/d=/Data/yu/NCTUSUN15023/1/pdata/1 Administrator Tue Jul 10 15:47:46 2012

7b HR-MS

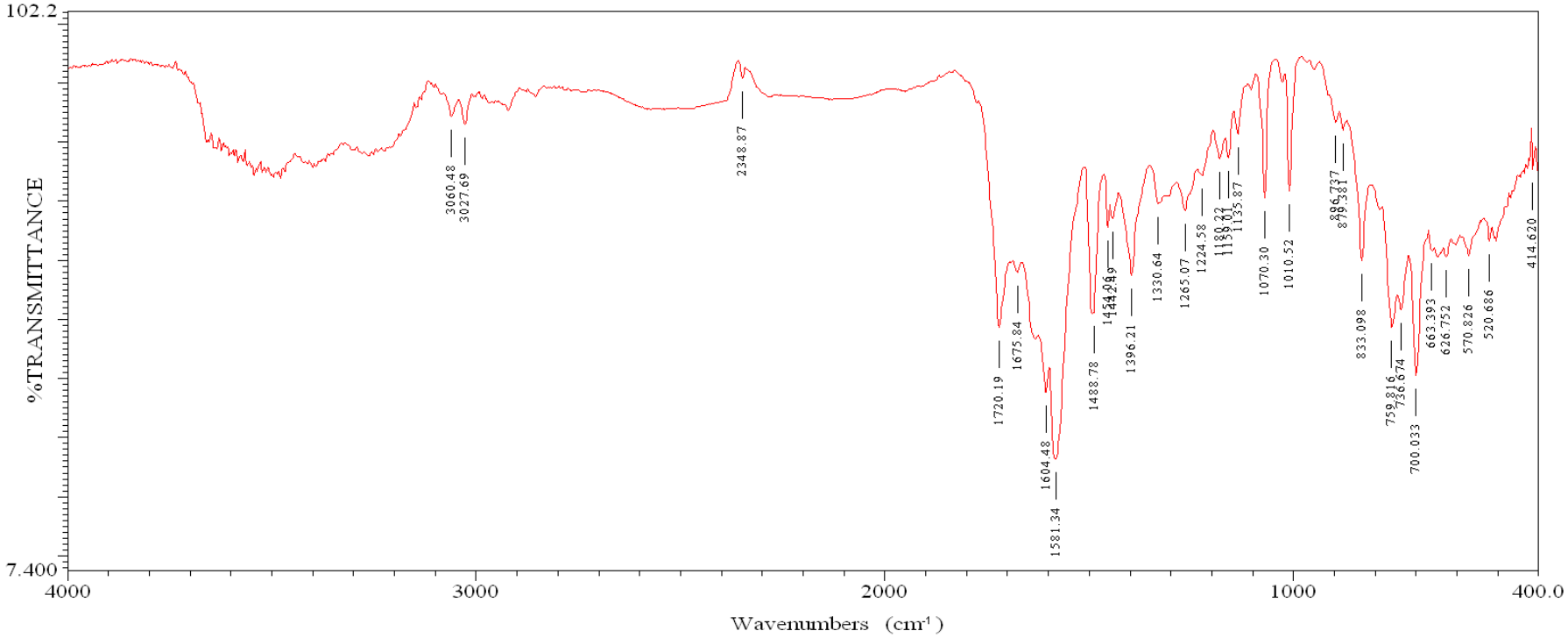


Result Table (Uncal - D:\Documents \changwongjin\chang509201)

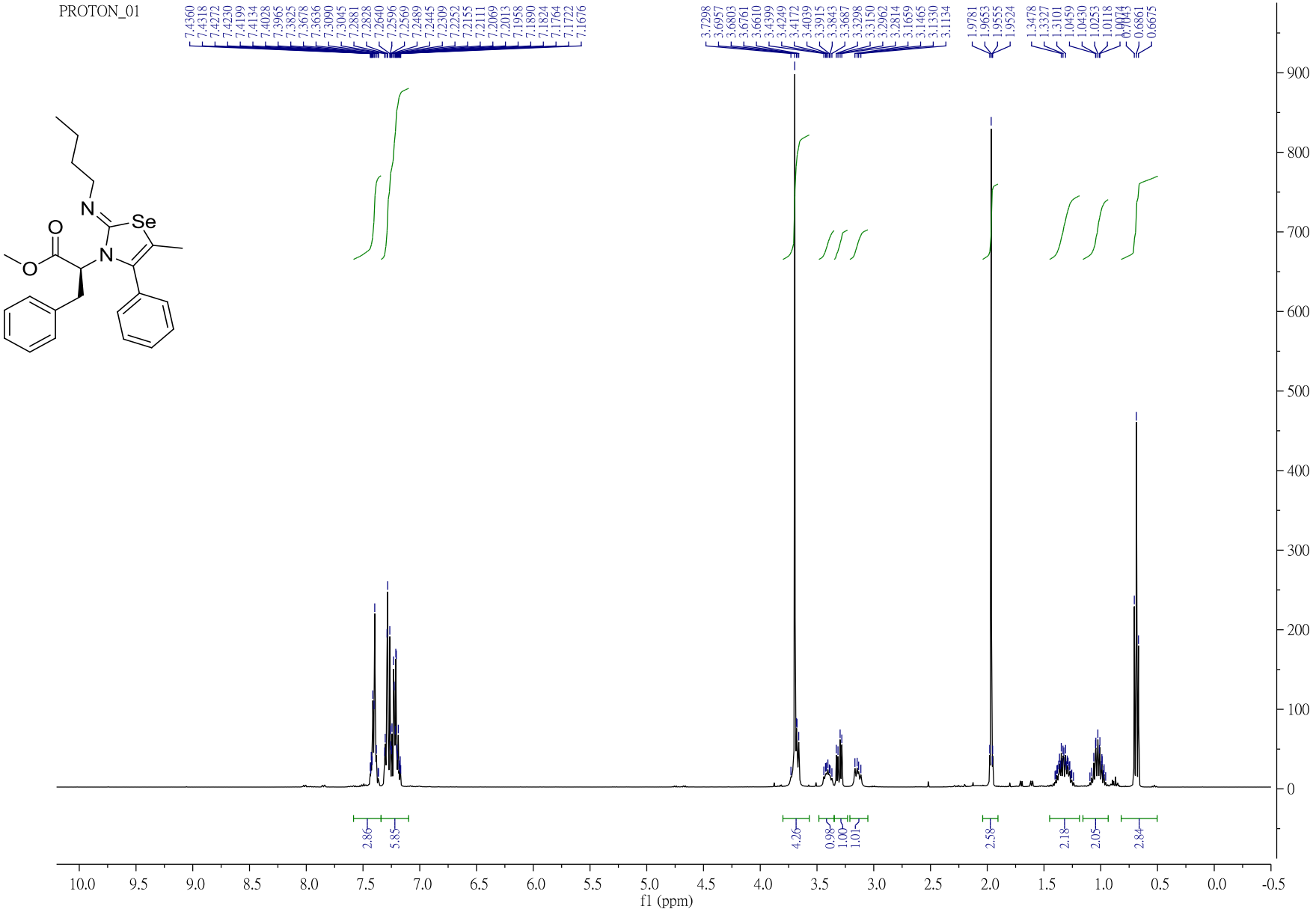
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	3.256	673.615	77.152	2.6	7.7
2	4.152	446.343	10.512	1.7	1.0
3	5.856	1317.987	11.498	5.1	1.1
4	7.316	491.999	8.530	1.9	0.8
5	8.324	732.115	17.630	2.8	1.8
6	10.220	20107.981	836.984	78.1	83.3
7	12.980	435.720	4.753	1.7	0.5
8	13.592	921.613	27.433	3.6	2.7
9	14.648	159.601	3.685	0.6	0.4
10	15.508	202.112	3.165	0.8	0.3
11	17.064	186.026	1.960	0.7	0.2
12	20.804	23.091	0.438	0.1	0.0
13	26.188	38.056	0.502	0.1	0.0
	Total	25736.259	1004.239	100.0	100.0

7b chiral HPLC

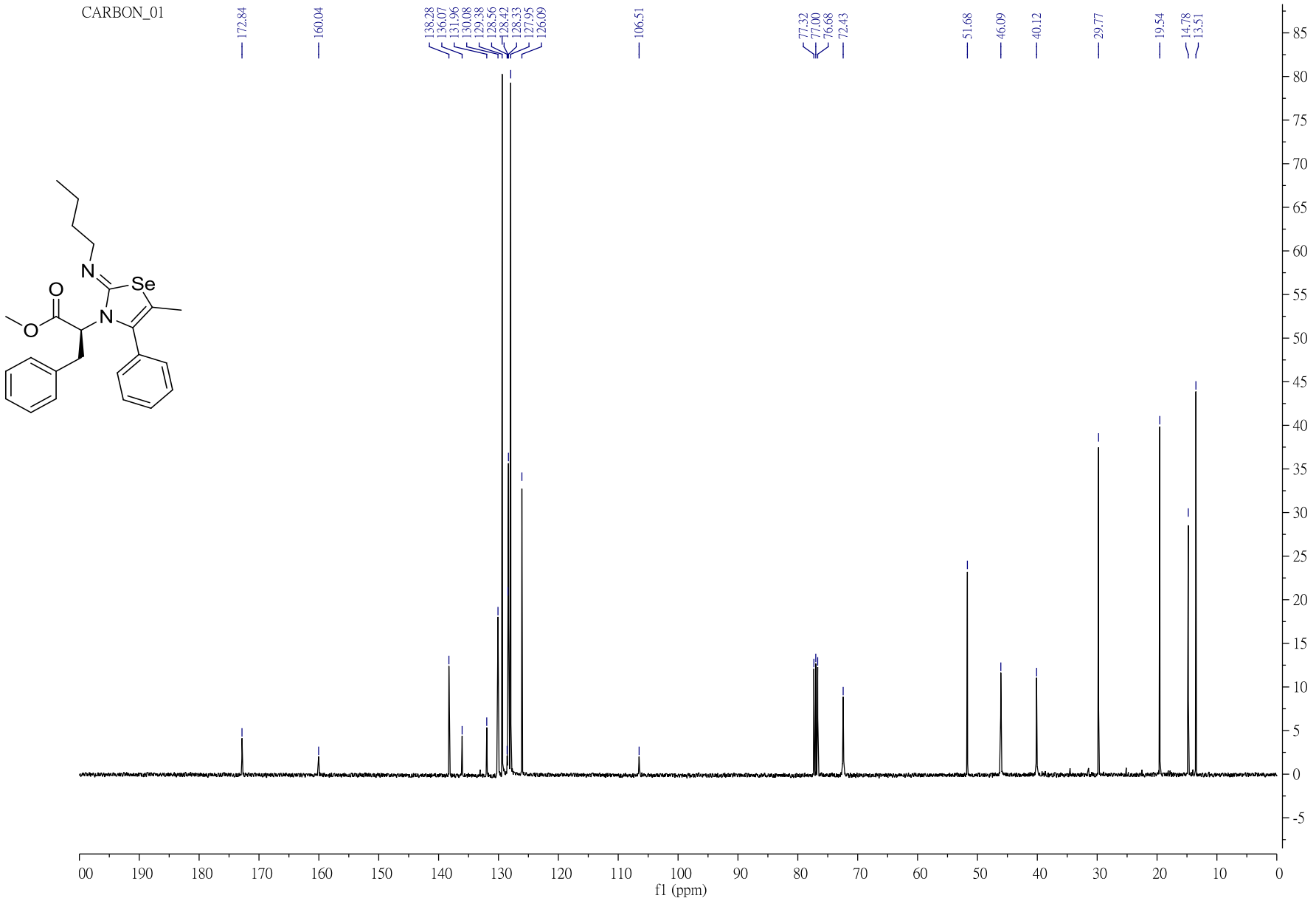
```
SAMPLE  : ____________
ID #    : 001
LAMP λ  : 589 nm
CONC    : 0.05000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-----------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01   +368.4000   21.1
  02   +368.7000   21.1
  03   +368.4000   21.1
  04   +367.7000   21.1
  05   +367.8000   21.1
  06   +367.4000   21.1
  07   +366.9000   21.1
  08   +366.6000   21.1
  09   +366.4000   21.1
  10   +365.9000   21.1
-----------------------
MEAN     = +367.4200°
σ(N-1)   =   0.94727°
C.V.     = + 0.25782%
```


102.2
%TRANSMITTANCE
7.400
4000
3000
2000
1000
400.0
Wavenumbers (cm-1)
3060.48
3027.69
2348.87
1720.19
1675.84
1604.48
1581.34
1488.78
1454.29
1396.21
1330.64
1265.07
1224.58
1135.87
1070.30
1010.52
833.098
759.816
736.674
700.033
663.393
626.752
570.826
520.686
414.620

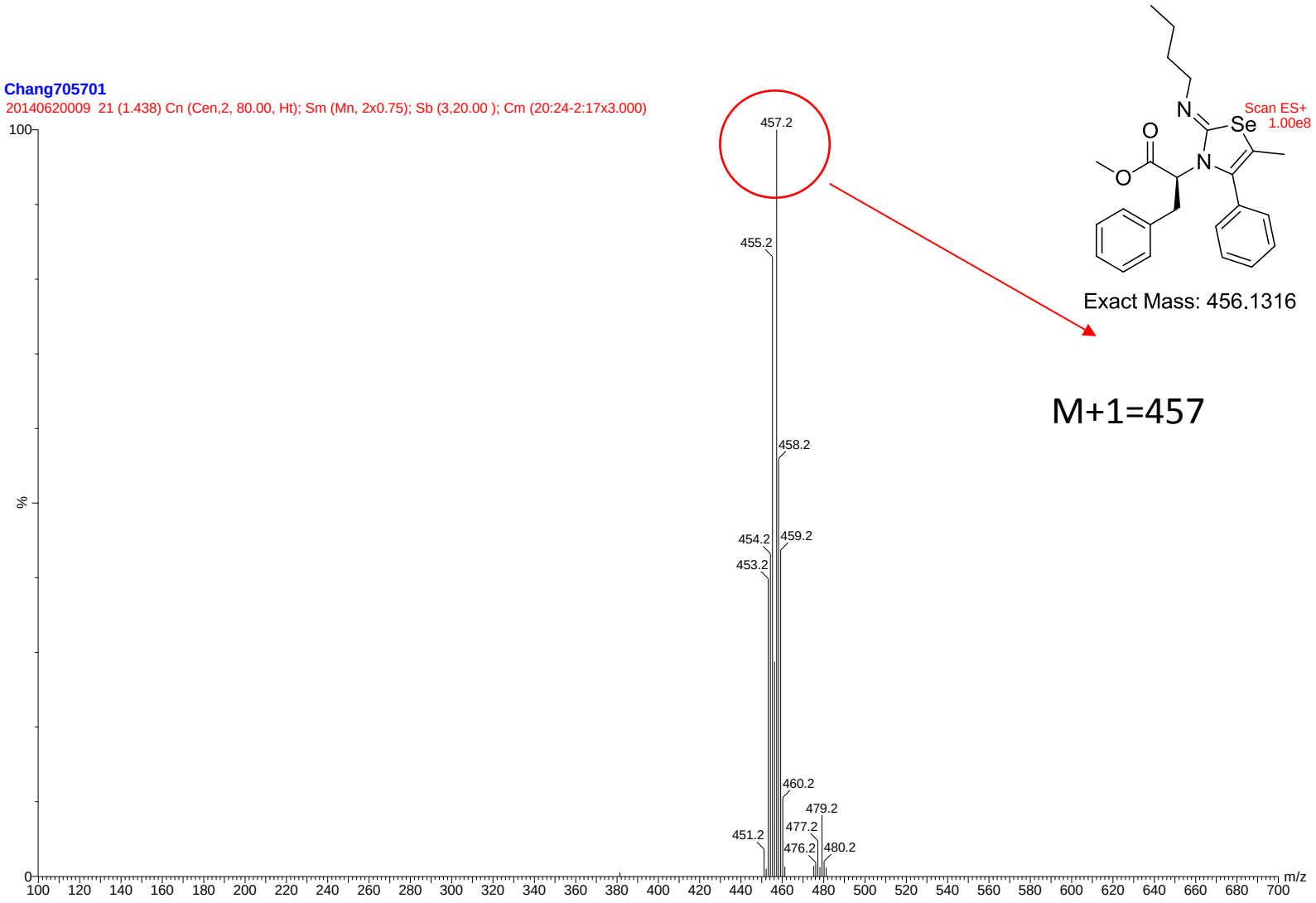
7b FT-IR


PROTON_01
7.4360 7.4318 7.4272 7.4230 7.4199 7.4134 7.4028 7.3965 7.3825 7.3678 7.3636 7.3090 7.3045 7.2881 7.2828 7.2640 7.2596 7.2569 7.2489 7.2445 7.2309 7.2252 7.2155 7.2111 7.2069 7.2013 7.1958 7.1890 7.1824 7.1764 7.1722 7.1676
3.7298 3.6957 3.6803 3.6761 3.6610 3.4399 3.4249 3.4172 3.4039 3.3915 3.3843 3.3687 3.3298 3.3150 3.2962 3.2814 3.1659 3.1465 3.1330 3.1134
1.9781 1.9653 1.9555 1.9524
1.3478 1.3327 1.3101 1.0459 1.0430 1.0253 1.0118 0.7043 0.6861 0.6675
O
O
N
Se
N
2.86 5.85 4.26 0.98 1.00 1.01 2.58 2.18 2.05 2.84
f1 (ppm)

7c H^1NMR


CARBON_01
172.84
160.04
138.28
136.07
131.96
130.08
129.38
128.56
128.42
128.33
127.95
126.09
106.51
77.32
77.00
76.68
72.43
51.68
46.09
40.12
29.77
19.54
14.78
13.51
N
Se
O
O
N
f1 (ppm)

7c C^{13}NMR


Chang705701
20140620009 21 (1.438) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,20.00); Cm (20:24-2:17x3.000)
Scan ES+
1.00e8
Exact Mass: 456.1316
M+1=457
%
m/z
457.2
455.2
458.2
454.2
459.2
453.2
460.2
479.2
477.2
451.2
476.2
480.2

7c LR-MS

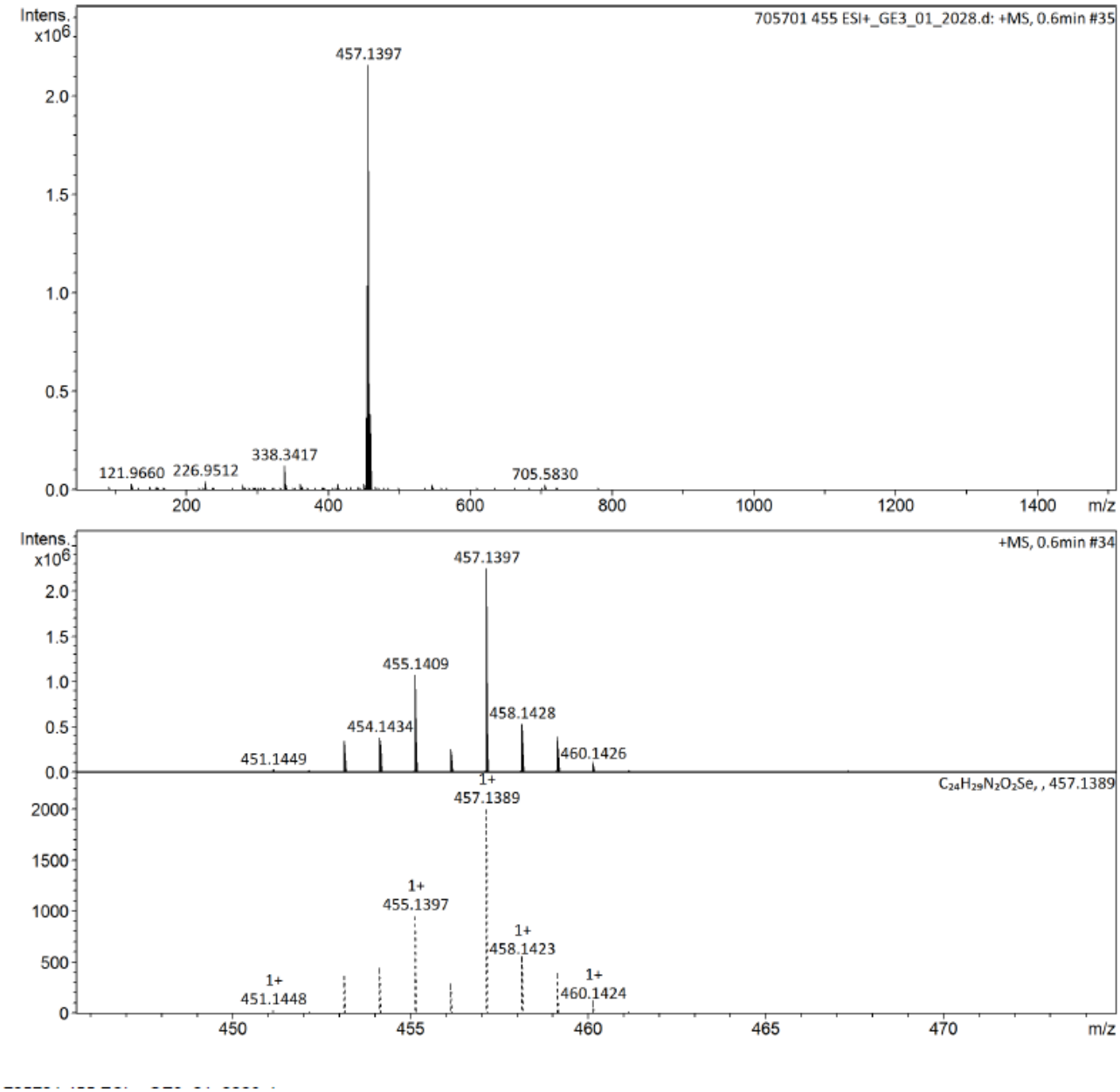
Display Report

Analysis Info

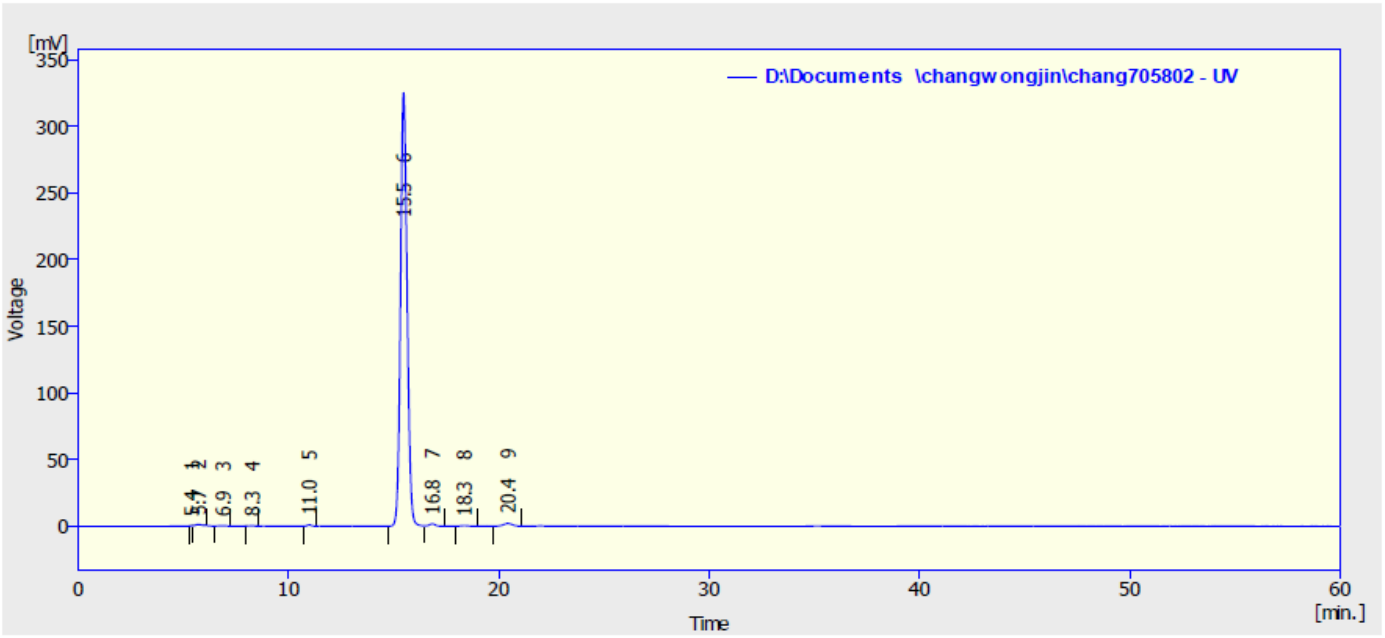
Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\705701 455 ESI+_GE3_01_2028.d	Acquisition Date	6/26/2014 10:18:25 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	705701 455 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



7c HR-MS

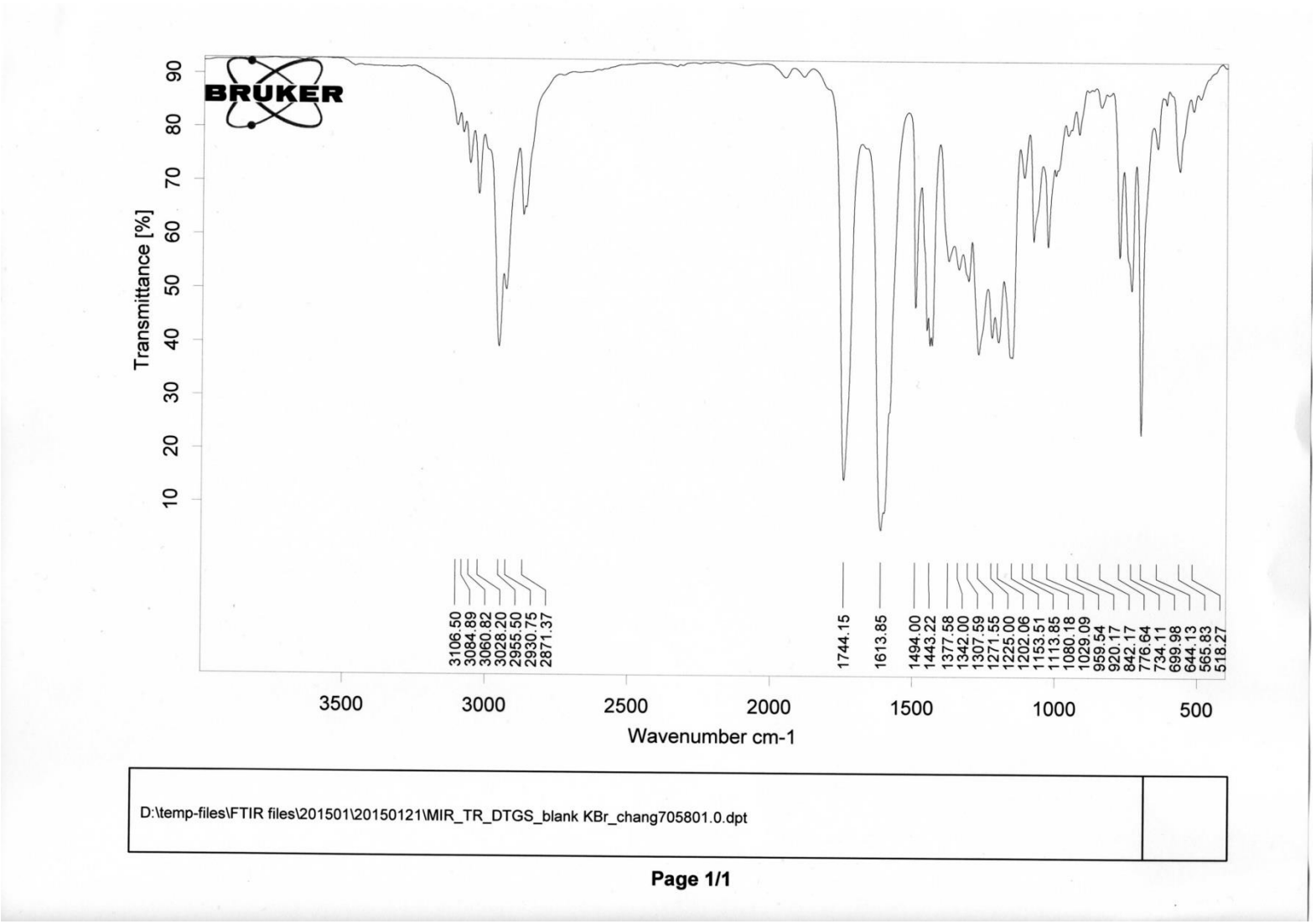


Result Table (Uncal - D:|Documents |changwongjin|chang705802 - UV)

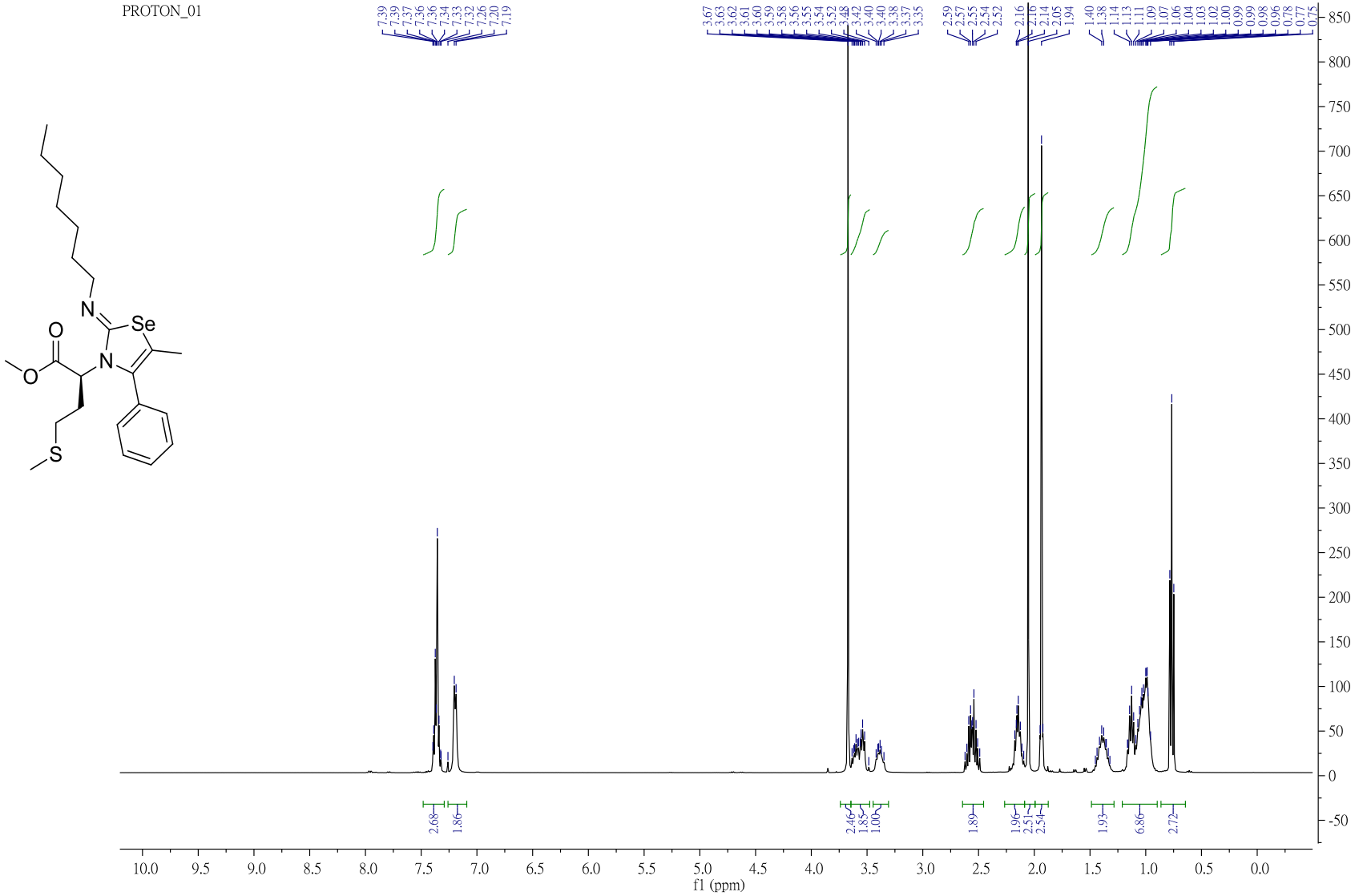
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.392	2.026	0.345	0.0	0.1	0.10
2	5.724	18.635	0.939	0.3	0.3	0.33
3	6.896	5.986	0.261	0.1	0.1	0.39
4	8.264	4.579	0.260	0.1	0.1	0.29
5	10.988	11.450	0.916	0.2	0.3	0.20
6	15.468	7098.171	324.964	98.0	97.9	0.34
7	16.840	34.370	1.693	0.5	0.5	0.31
8	18.348	9.593	0.407	0.1	0.1	0.37
9	20.436	58.700	2.012	0.8	0.6	0.46
	Total	7243.511	331.798	100.0	100.0	

7c chiral HPLC

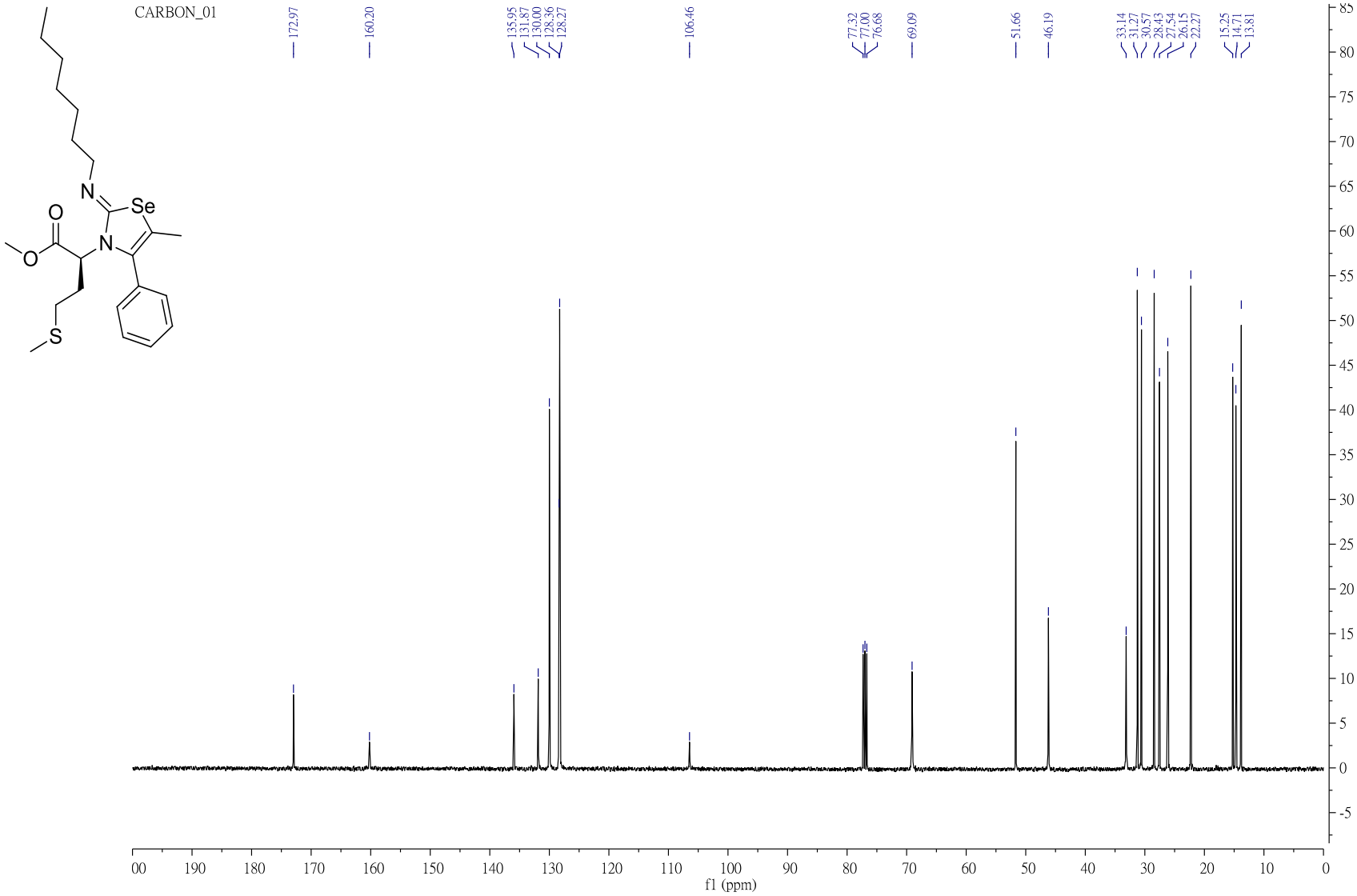
```
SAMPLE : ____________
ID #   : 007
LAMP λ : 589 nm
CONC   : 0.04000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
------------------------
SPECIFIC ROTATION [α]
 COUNT  [α](°)  TEMP(°C)
  01   - 80.7502   19.3
  02   - 81.0002   19.3
  03   - 80.8752   19.4
  04   - 81.1252   19.4
  05   - 81.1252   19.4
  06   - 81.1252   19.4
  07   - 81.0002   19.4
  08   - 81.3752   19.4
  09   - 81.5002   19.4
  10   - 81.8752   19.4
------------------------
MEAN     = - 81.1752°
σ(N-1)   =   0.32913°
C.V.     = - 0.40546%
```


BRUKER
Transmittance [%]
10
20
30
40
50
60
70
80
90
3106.50
3084.89
3060.82
3028.20
2955.50
2930.75
2871.37
1744.15
1613.85
1494.00
1443.22
1377.58
1342.00
1307.59
1271.55
1225.00
1202.06
1153.51
1113.85
1080.18
1029.09
959.54
920.17
842.17
776.64
734.11
699.98
644.13
565.83
518.27
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang705801.0.dpt
Page 1/1

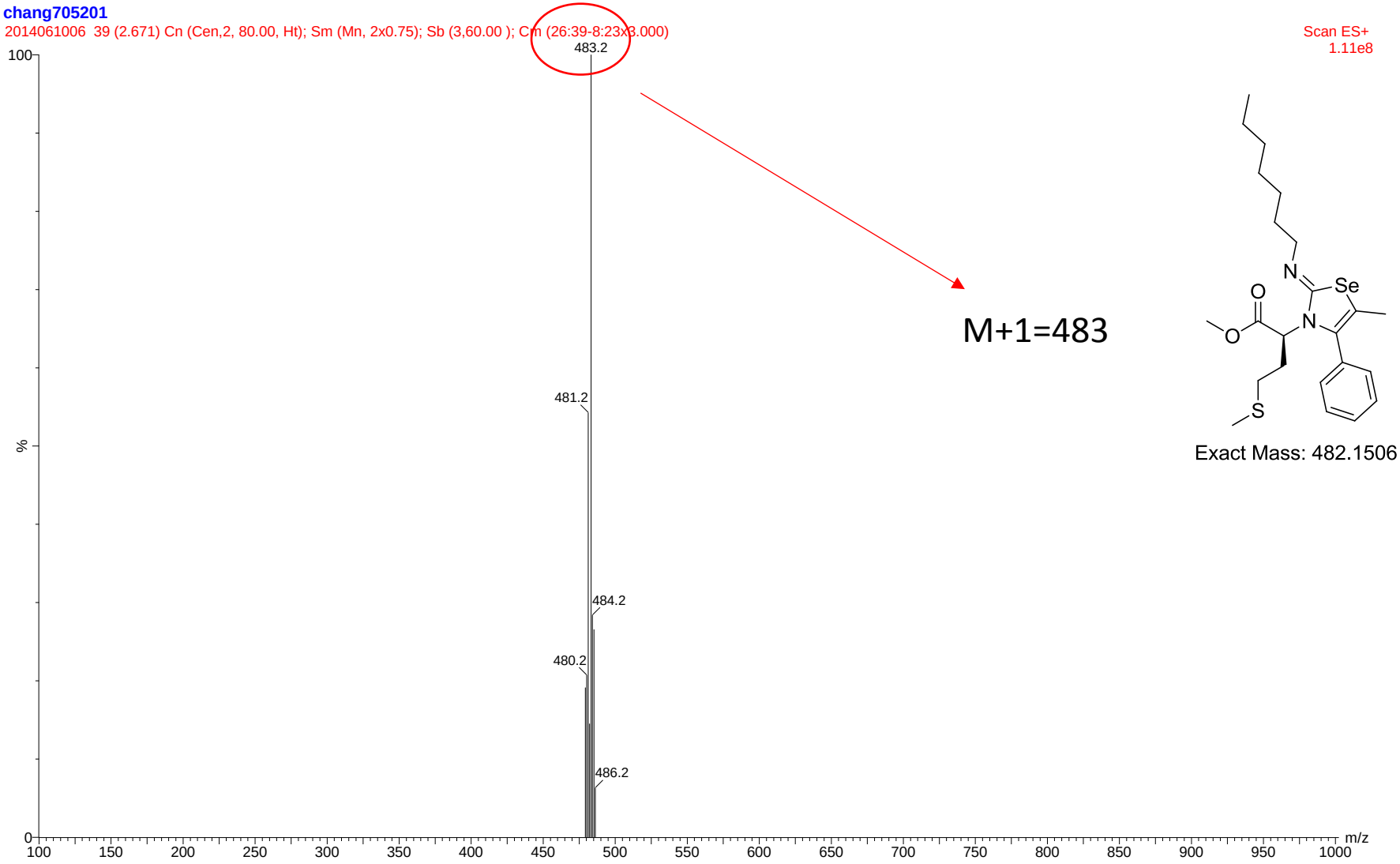
7c FT-IR



7d H^1NMR


CARBON_01
172.97
160.20
135.95
131.87
130.00
128.36
128.27
106.46
77.32
77.00
76.68
69.09
51.66
46.19
33.14
31.27
30.57
28.43
27.54
26.15
22.27
15.25
14.71
13.81
O
O
N
Se
N
S
f1 (ppm)

7d C^{13}NMR


chang705201
2014061006 39 (2.671) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,60.00); Cm (26:39-8:23x3.000)
Scan ES+
1.11e8
483.2
481.2
484.2
480.2
486.2
100
%
0
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
m/z
M+1=483
N
Se
O
O
N
S
Exact Mass: 482.1506

7d LR-MS

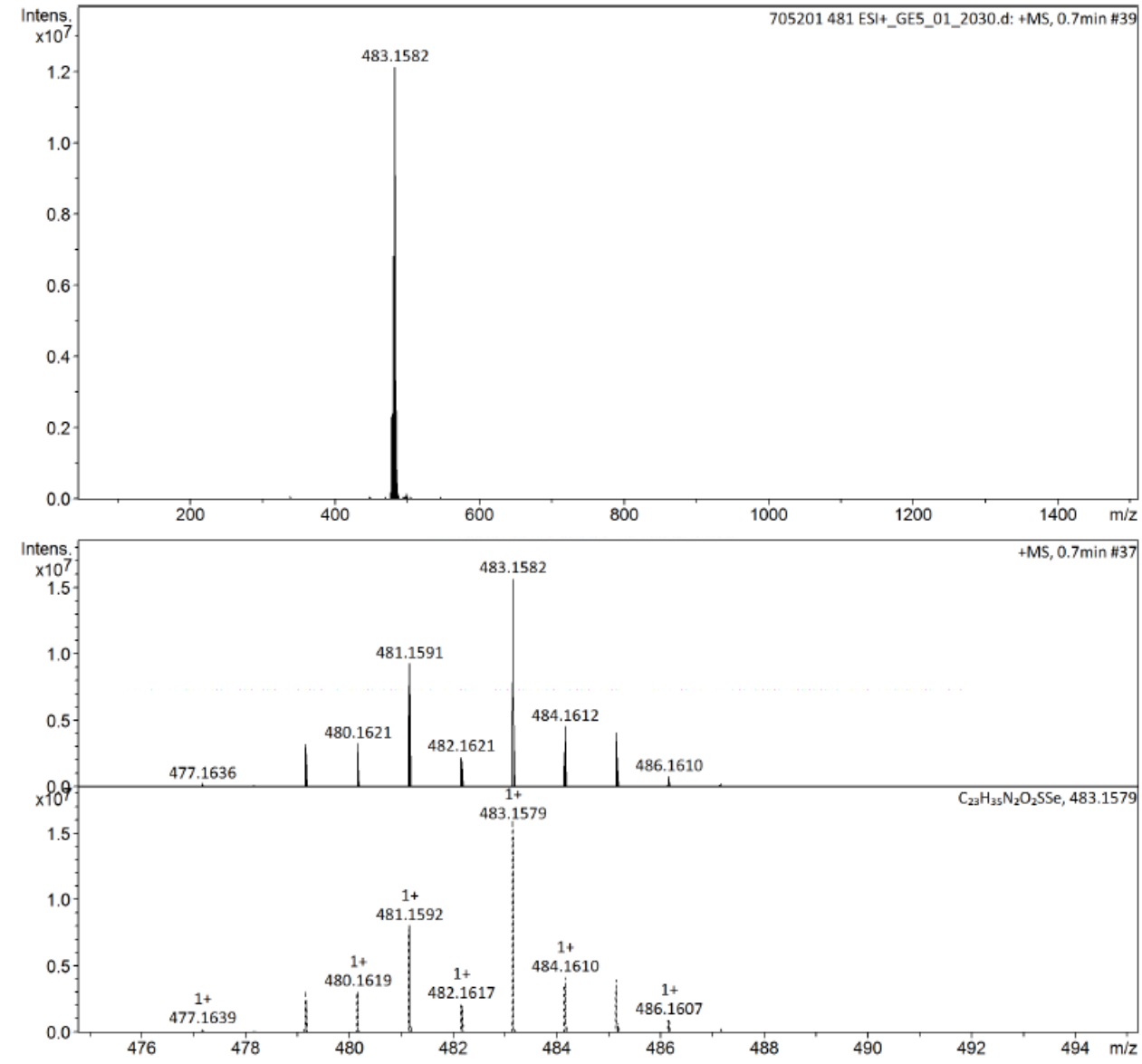
Display Report

Analysis Info

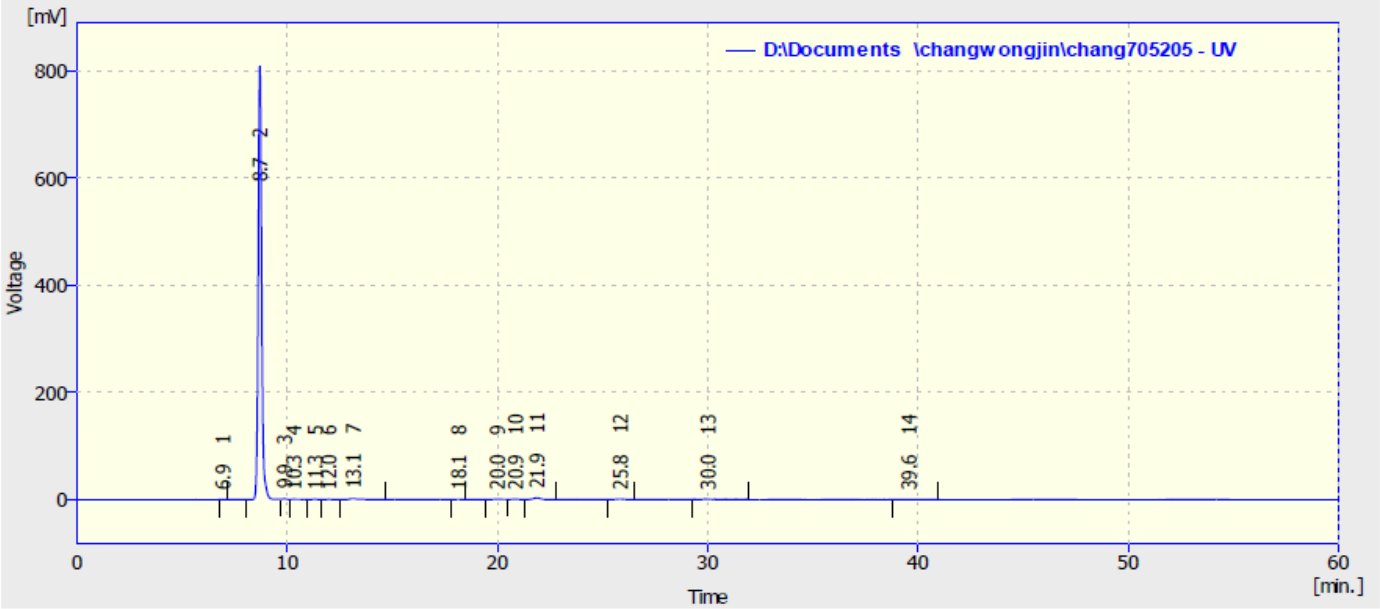
Acquisition Date	6/26/2014 10:27:01 AM		
Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\705201 481 ESI+_GE5_01_2030.d		
Method	Small molecule.m	Operator	NCTU
Sample Name	705201 481 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



7d HR-MS

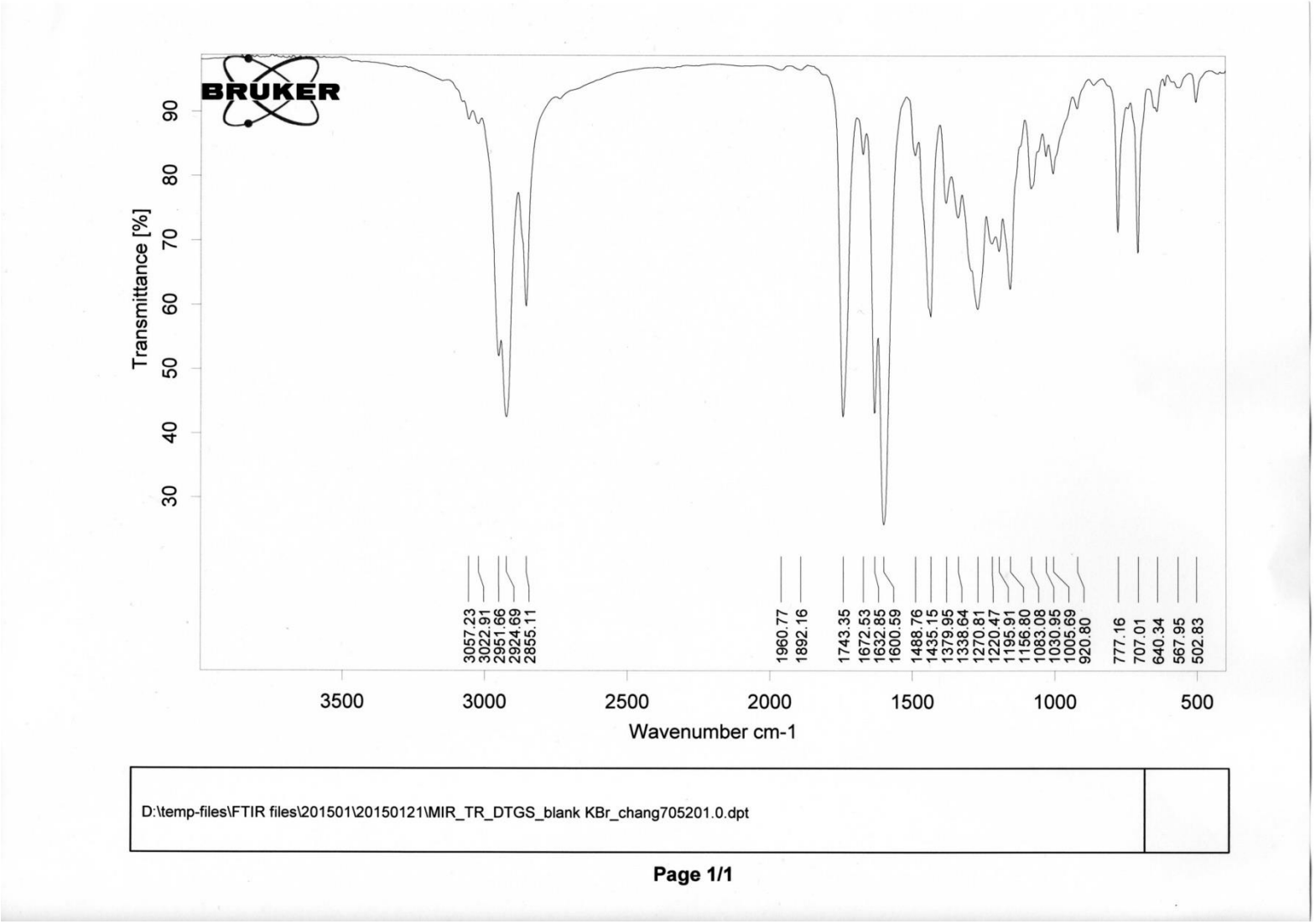


Result Table (Uncal - D:|Documents |changwongjin|chang705205 - UV)

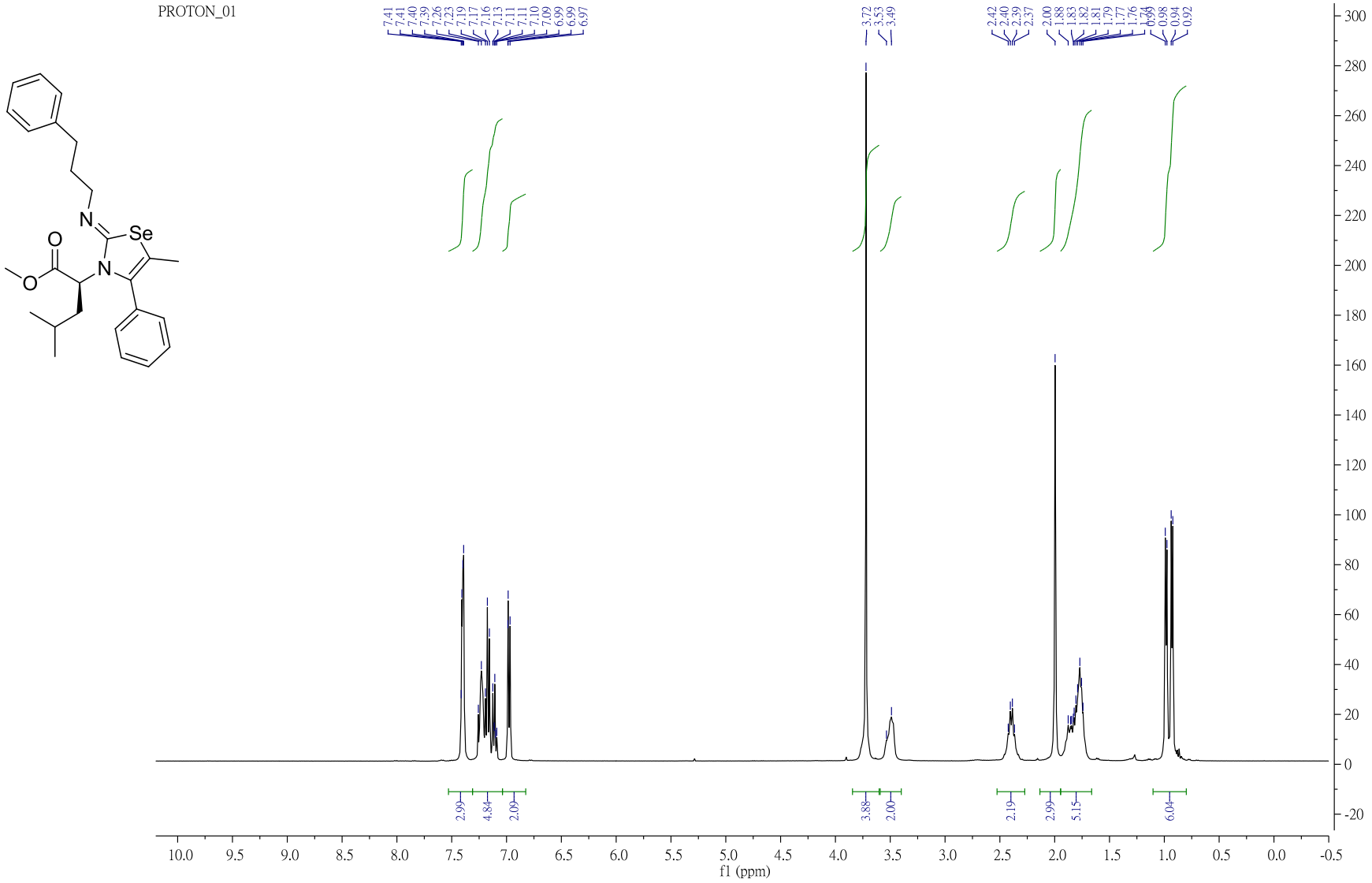
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	6.928	3.283	0.369	0.0	0.0
2	8.696	9183.891	808.124	96.0	98.3
3	9.868	25.468	1.750	0.3	0.2
4	10.304	22.994	0.897	0.2	0.1
5	11.316	14.248	0.802	0.1	0.1
6	11.984	11.135	0.679	0.1	0.1
7	13.136	70.963	2.142	0.7	0.3
8	18.148	8.988	0.462	0.1	0.1
9	19.996	28.385	0.825	0.3	0.1
10	20.856	21.280	0.858	0.2	0.1
11	21.876	82.160	3.243	0.9	0.4
12	25.840	31.916	1.111	0.3	0.1
13	30.000	39.641	0.738	0.4	0.1
14	39.556	24.507	0.350	0.3	0.0
	Total	9568.859	822.351	100.0	100.0

7d chiral HPLC

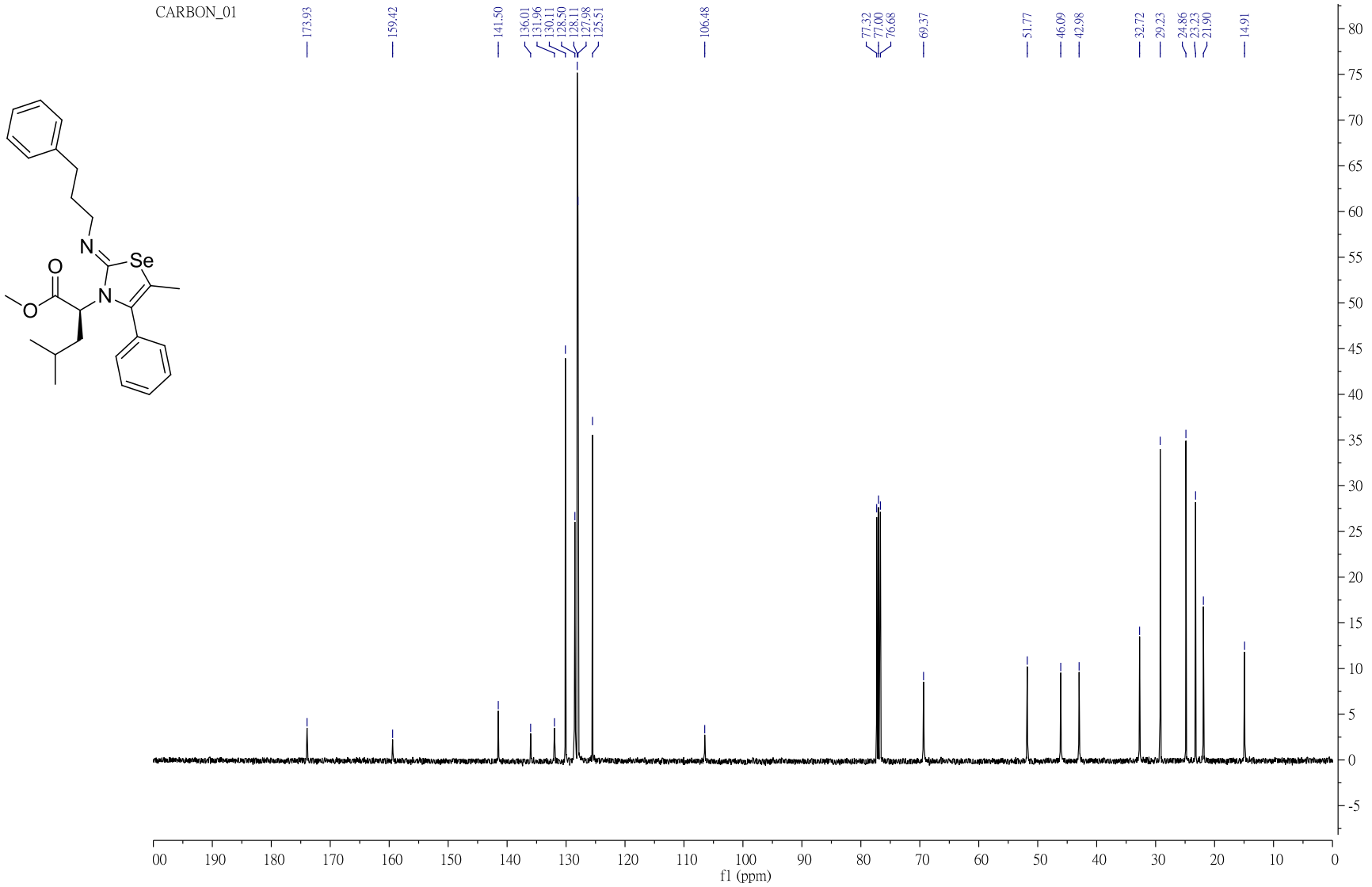
```
SAMPLE :
ID #   : 012
LAMP λ : 589 nm
CONC   : 0.03000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-----------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01    - 23.3332   20.2
  02    - 23.4999   20.2
  03    - 23.6665   20.2
  04    - 23.4999   20.2
  05    - 23.6665   20.2
  06    - 23.9999   20.2
  07    - 24.1665   20.2
  08    - 24.9999   20.2
  09    - 24.9999   20.2
  10    - 24.9999   20.2
-----------------------
MEAN     = - 24.0832°
σ(N-1)   =   0.67700°
C.V.     = -  2.8111%
```


BRUKER
Transmittance [%]
90
80
70
60
50
40
30
3057.23
3022.91
2951.66
2924.69
2855.11
1960.77
1892.16
1743.35
1672.53
1632.85
1600.59
1488.76
1435.15
1379.95
1338.64
1270.81
1220.47
1195.91
1156.80
1083.08
1030.95
1005.69
920.80
777.16
707.01
640.34
567.95
502.83
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang705201.0.dpt
Page 1/1

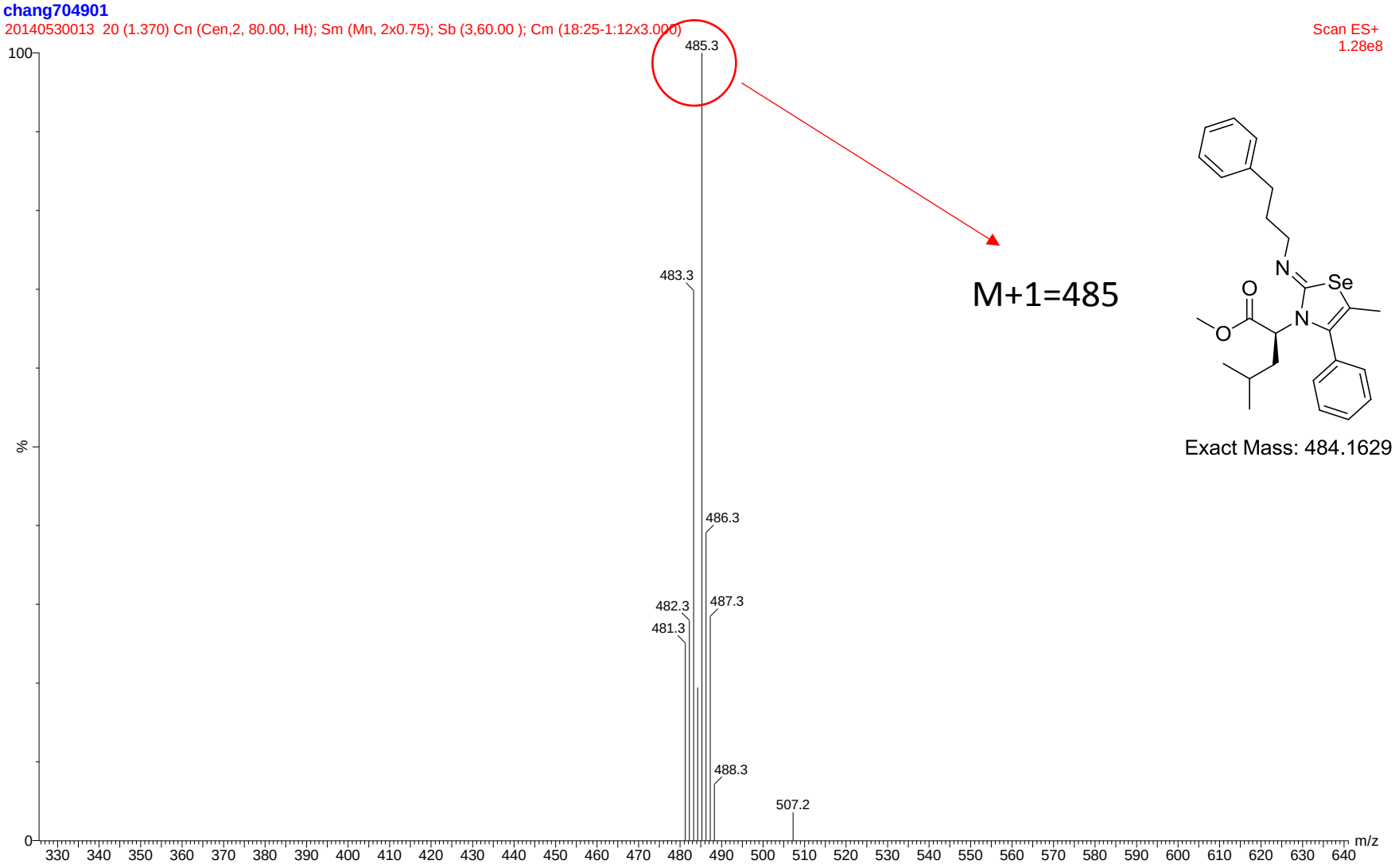
7d FT-IR


PROTON_01
7.41
7.41
7.40
7.39
7.26
7.23
7.19
7.17
7.16
7.13
7.11
7.11
7.10
7.09
6.99
6.99
6.97
3.72
3.53
3.49
2.42
2.40
2.39
2.37
2.00
1.88
1.83
1.82
1.81
1.79
1.77
1.76
0.99
0.98
0.94
0.92
N
Se
O
N
O
2.99
4.84
2.09
3.88
2.00
2.19
2.99
5.15
6.04
f1 (ppm)

7e H^1NMR


CARBON_01
173.93
159.42
141.50
136.01
131.96
130.11
128.50
128.11
127.98
125.51
106.48
77.32
77.00
76.68
69.37
51.77
46.09
42.98
32.72
29.23
24.86
23.23
21.90
14.91
f1 (ppm)

7e C^{13}NMR


chang704901
20140530013 20 (1.370) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,60.00); Cm (18:25-1:12x3.000)
Scan ES+
1.28e8
100
%
0
485.3
483.3
486.3
482.3
487.3
481.3
488.3
507.2
330 340 350 360 370 380 390 400 410 420 430 440 450 460 470 480 490 500 510 520 530 540 550 560 570 580 590 600 610 620 630 640
m/z
M+1=485
O
N
Se
N
O
Exact Mass: 484.1629

7e LR-MS

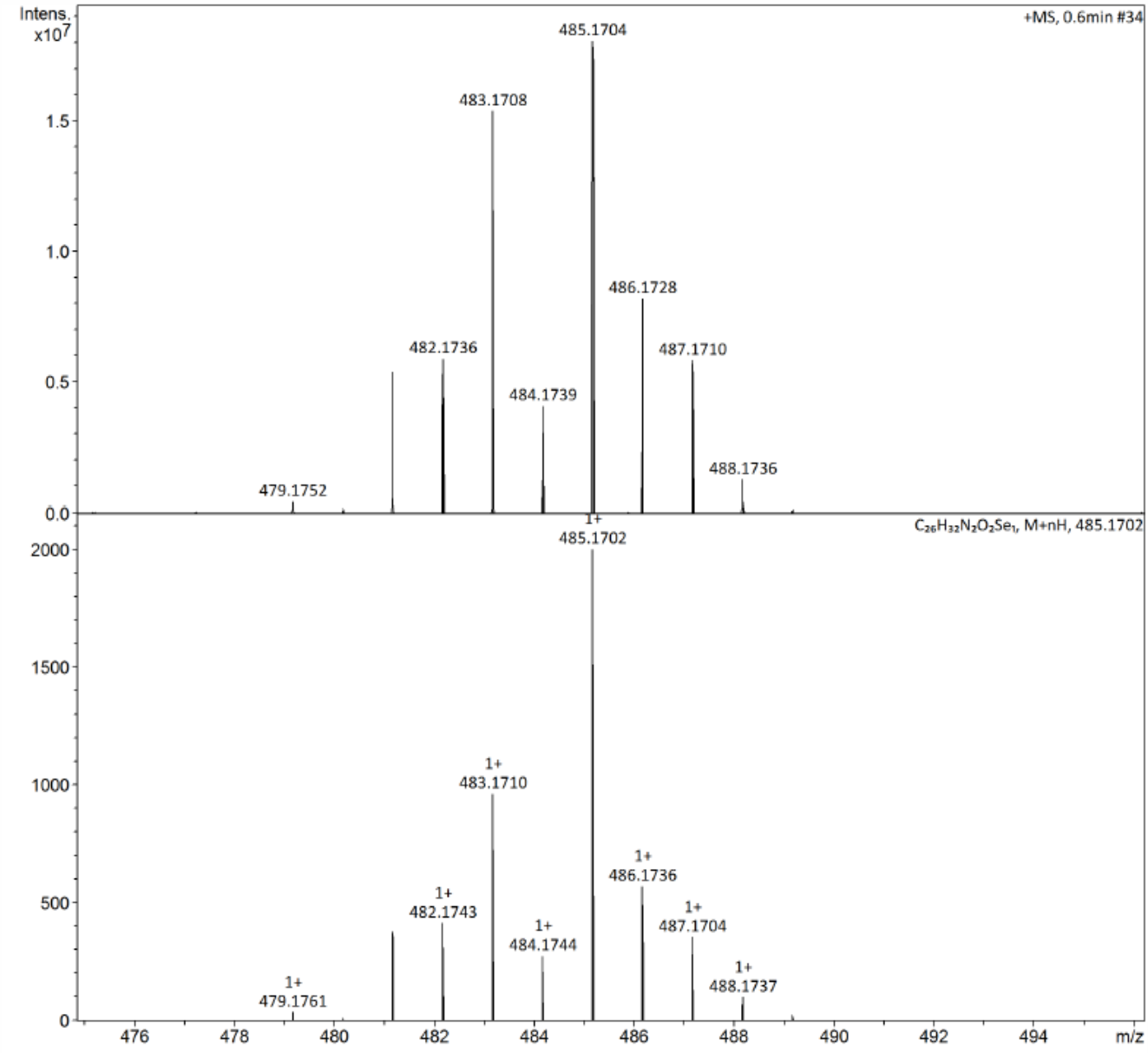
Display report

Analysis Info

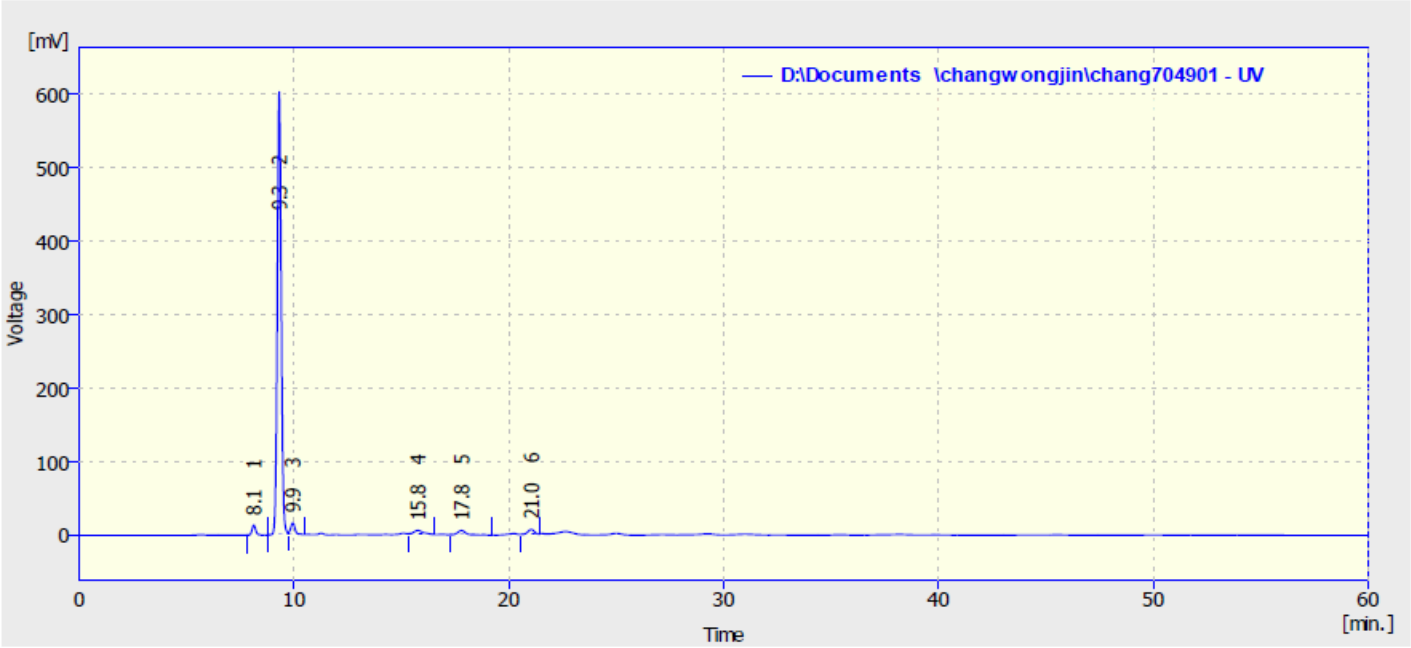
Analysis Name	D:\Data\NCTU SERVICE\Data\20140909\704901 ESI+_RD6_01_2943.d	Acquisition Date	9/9/2014 2:08:36 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	704901 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



7e HR-MS



Result Table (Uncal - D:\Documents \changwongjin\chang704901 - UV)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	8.128	161.901	13.616	1.9	2.1
2	9.312	7724.511	602.451	90.2	92.7
3	9.944	236.772	16.015	2.8	2.5
4	15.768	150.536	5.016	1.8	0.8
5	17.796	151.670	6.019	1.8	0.9
6	21.044	136.273	6.651	1.6	1.0
	Total	8561.663	649.769	100.0	100.0

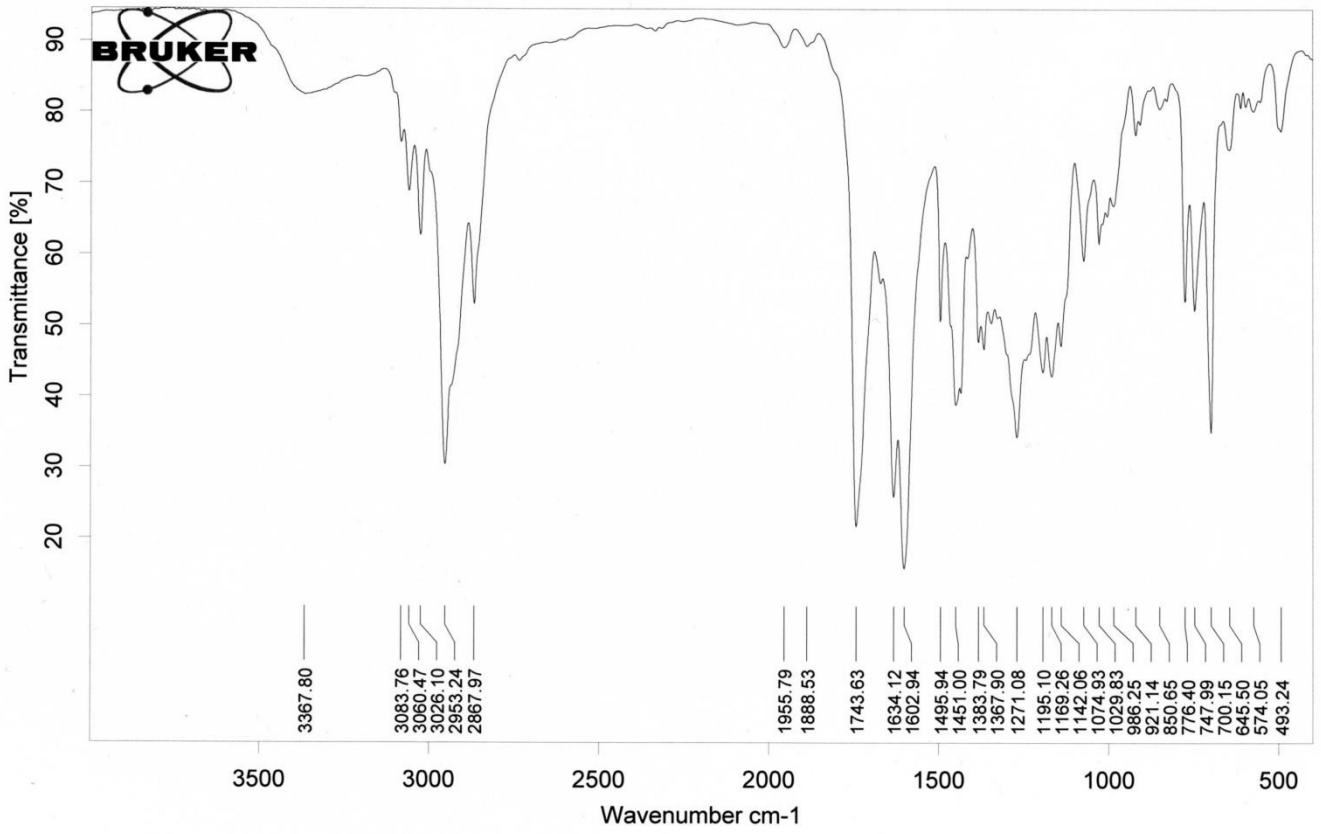
7e chiral HPLC

SAMPLE :
ID # : 018
LAMP λ : 589 nm
CONC : 0.04000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL: 1 min

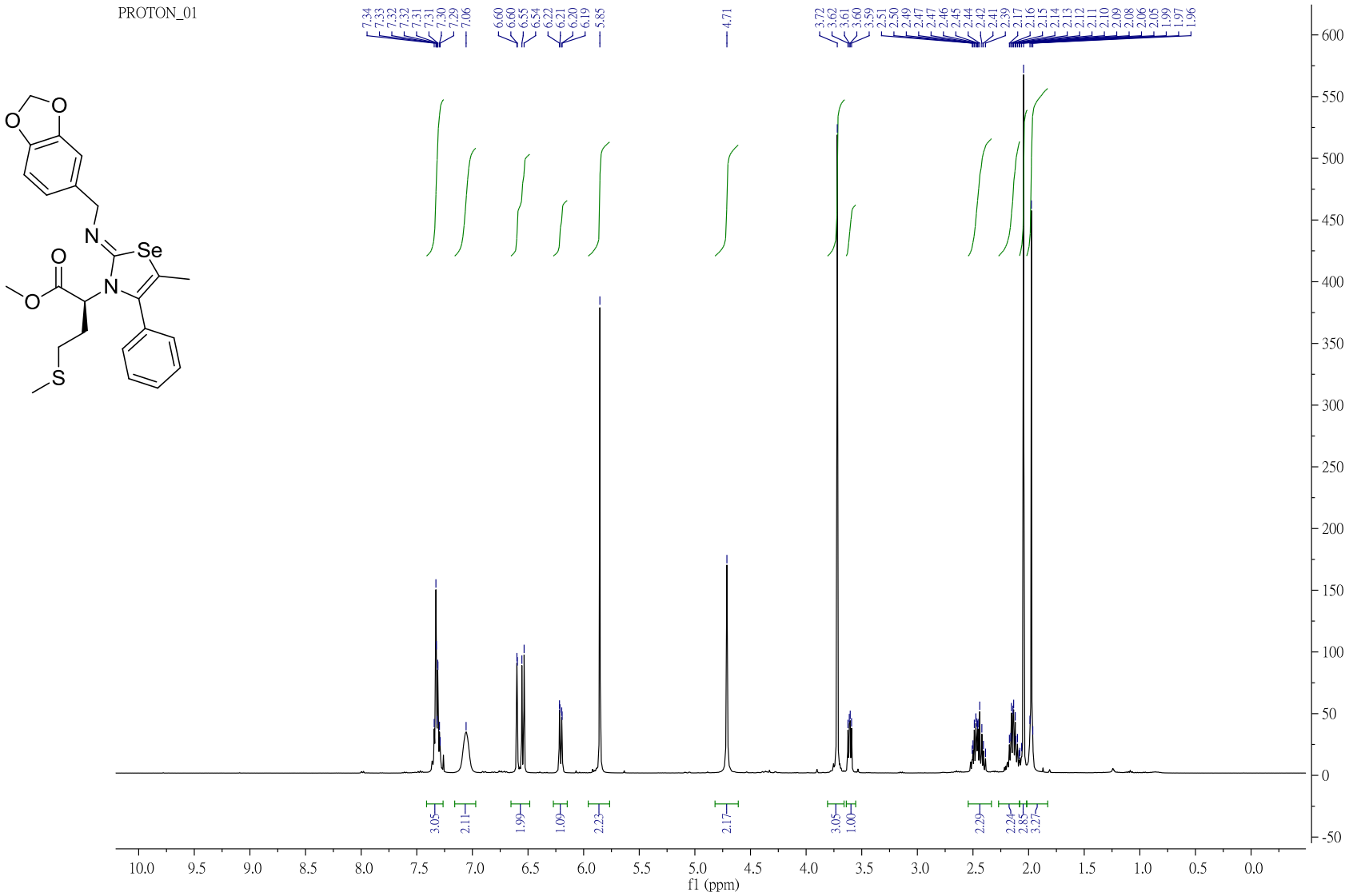
SPECIFIC ROTATION [α]

COUNT	[α](°)	TEMP(°C)
01	- 65.0000	20.0
02	- 66.2500	20.0
03	- 66.3750	20.0
04	- 67.5000	20.0
05	- 69.2500	20.0
06	- 69.0000	20.0
07	- 69.8750	20.0
08	- 70.1250	20.0
09	- 71.6250	20.0
10	- 71.2500	20.0

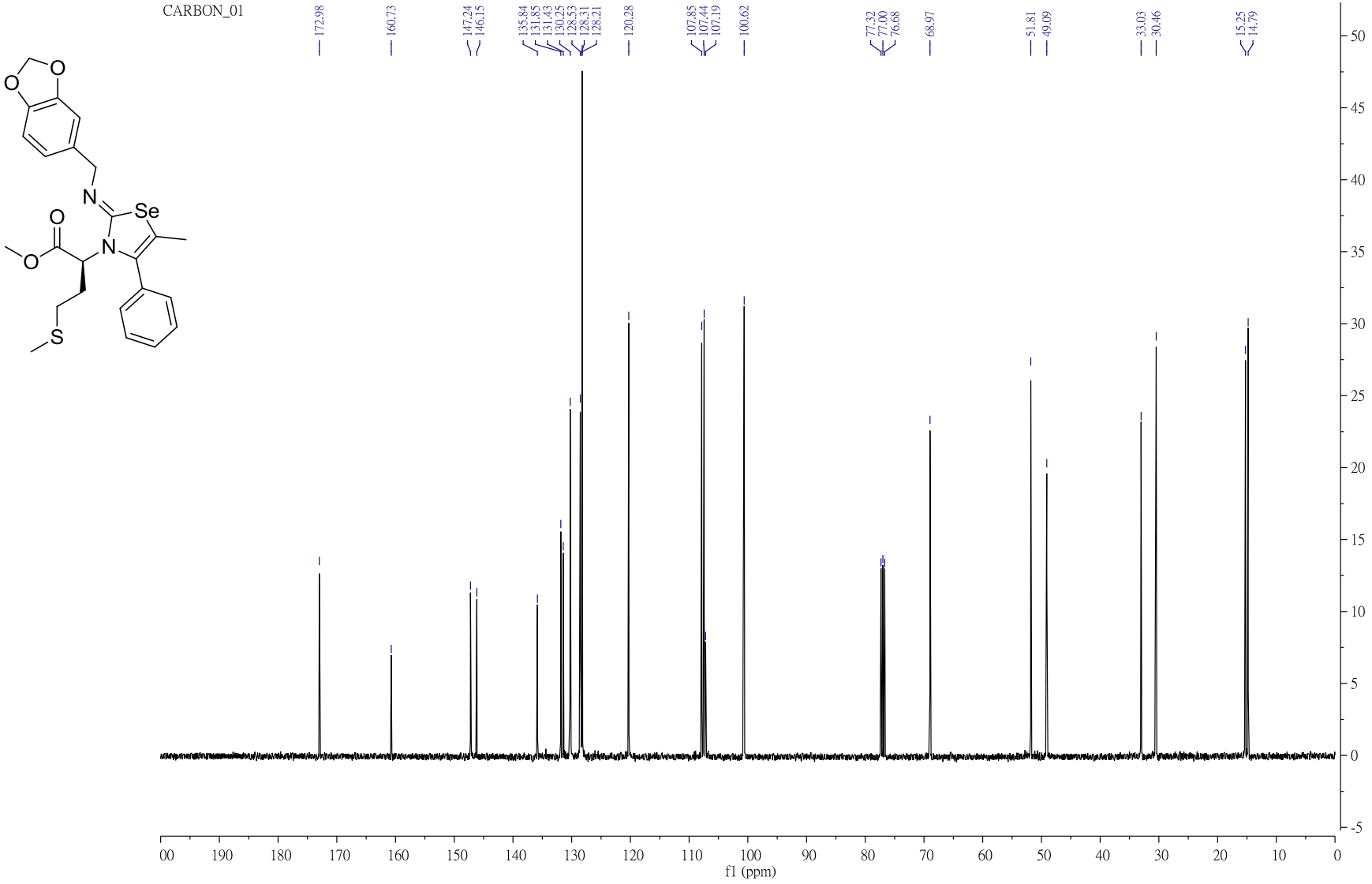
MEAN = - 68.6250°
σ(N-1) = 2.2445°
C.V. = - 3.2708%


BRUKER
Transmittance [%]
90
80
70
60
50
40
30
20
3367.80
3083.76
3060.47
3026.10
2953.24
2867.97
1955.79
1888.53
1743.63
1634.12
1602.94
1495.94
1451.00
1383.79
1367.90
1271.08
1195.10
1169.26
1142.06
1074.93
1029.83
986.25
921.14
850.65
776.40
747.99
700.15
645.50
574.05
493.24
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang704901.0.dpt
Page 1/1

7e FT-IR



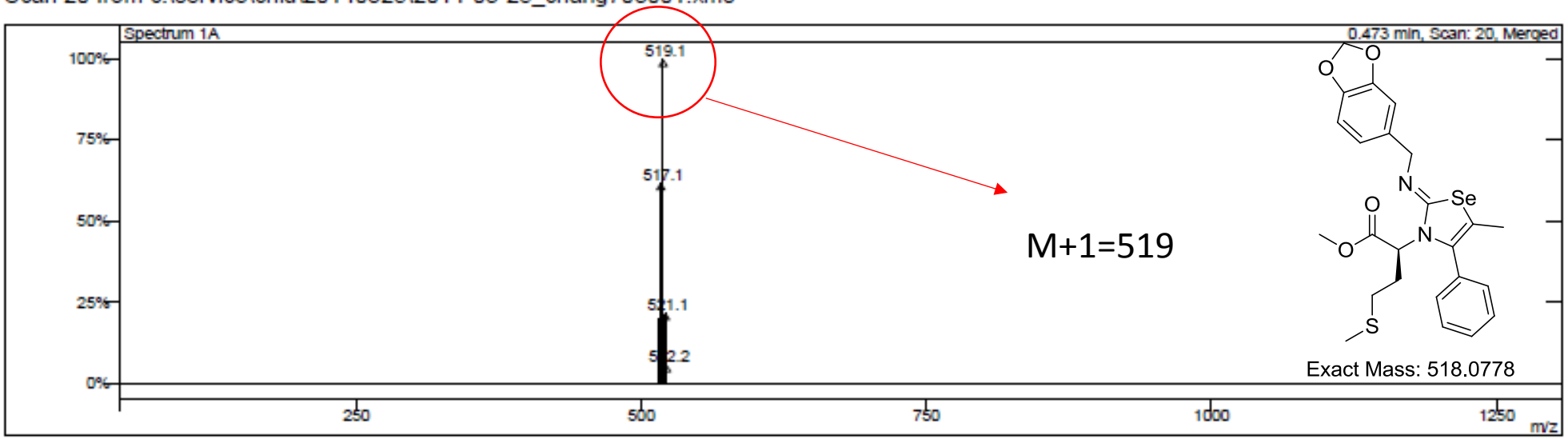
7f H^1NMR


CARBON_01
172.98
160.73
147.24
146.15
135.84
131.85
131.43
130.25
128.53
128.31
128.21
120.28
107.85
107.44
107.19
100.62
77.32
77.00
76.68
68.97
51.81
49.09
33.03
30.46
15.25
14.79
O
O
N
Se
O
O
N
S
f1 (ppm)

7f C^{13}NMR

Print Date: 25 Mar 2014 10:49:07

Scan 20 from c:\service\chiu\20140325\2014-03-25_chang703001.xms



Spectrum from ...ervice\chiu\20140325\2014-03-25_chang703001.xms
Scan No: 20, Time: 0.473 minutes
No averaging. Background corrected.
Comment: 0.473 min. Scan: 20 Merged RIC: 4712584837
Pair Count: 8 MW: 0 Formula: None
CAS No: None Acquired Range: 100.0 - 1250.0 m/z

7f LR-MS

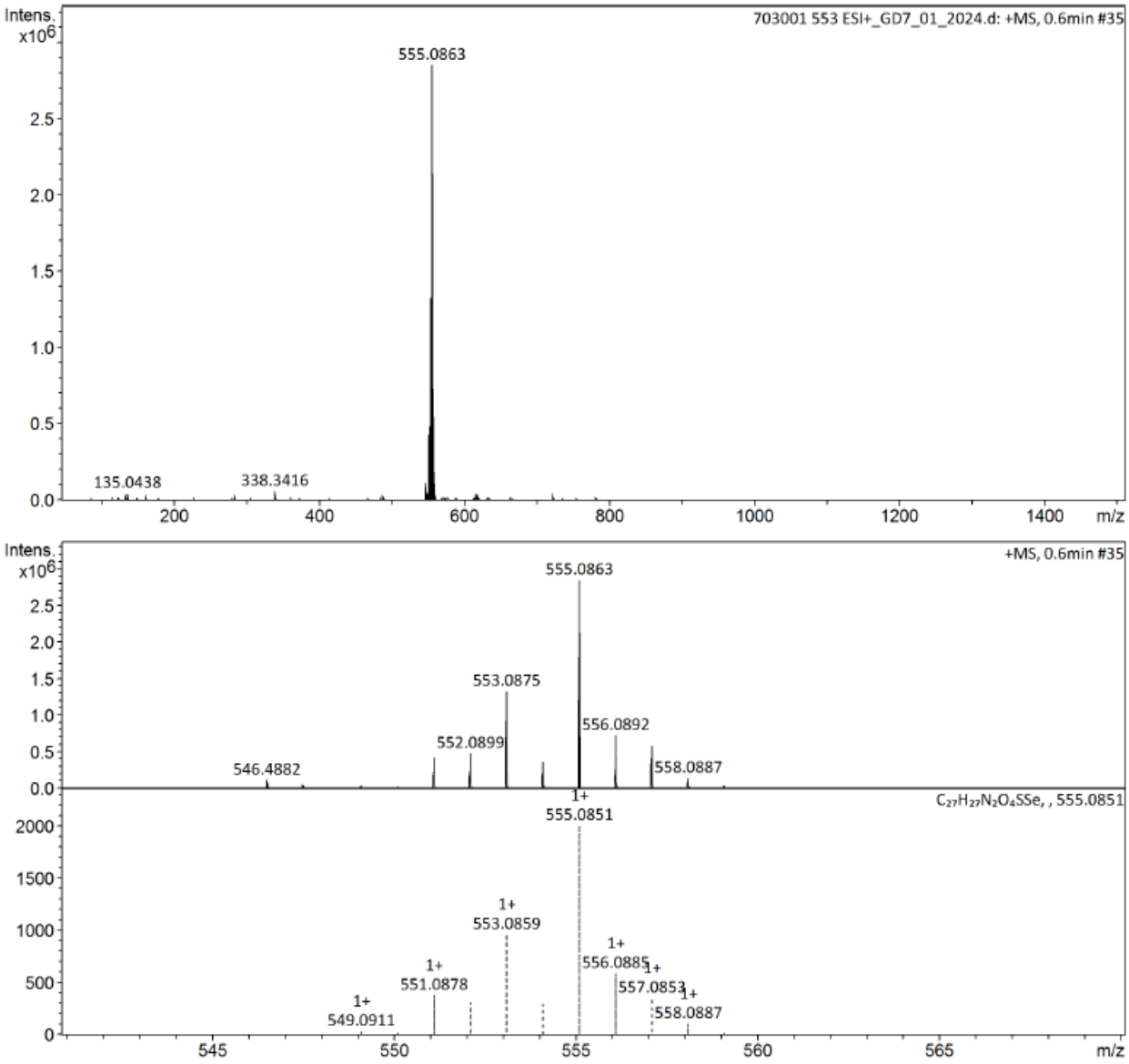
Display Report

Analysis Info

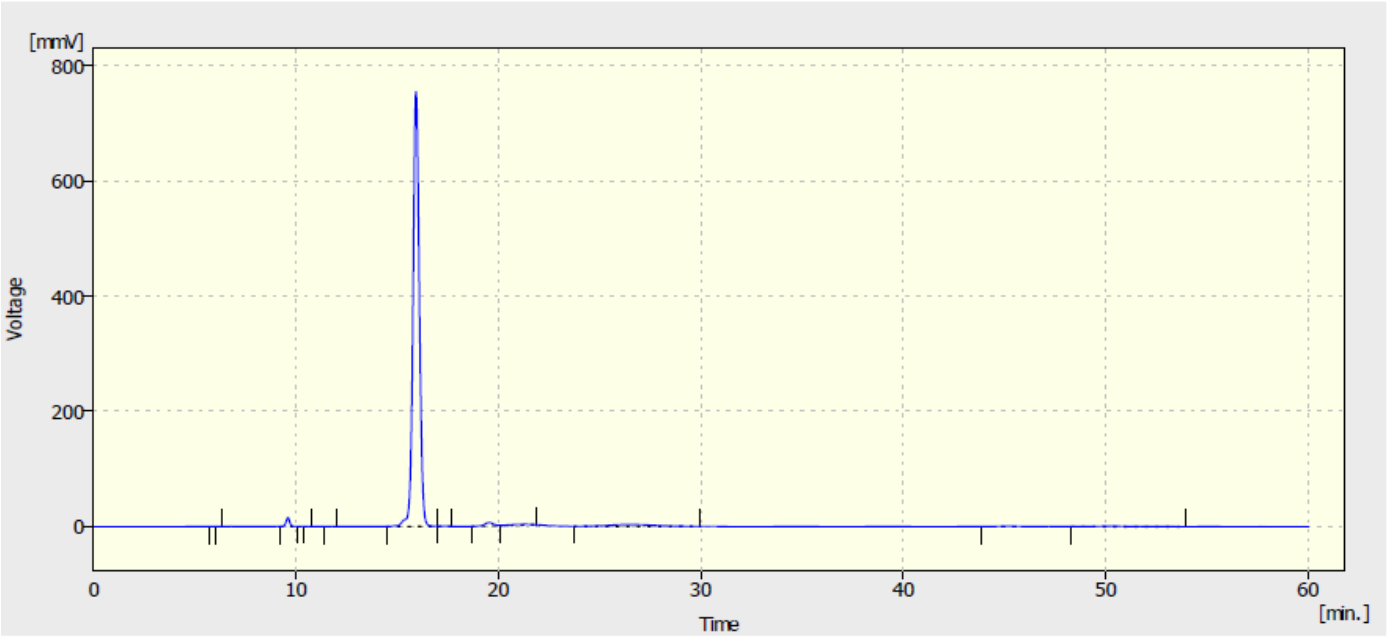
Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\703001 553 ESI+_GD7_01_2024.d	Acquisition Date	6/26/2014 10:01:10 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	703001 553 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



7f HR-MS

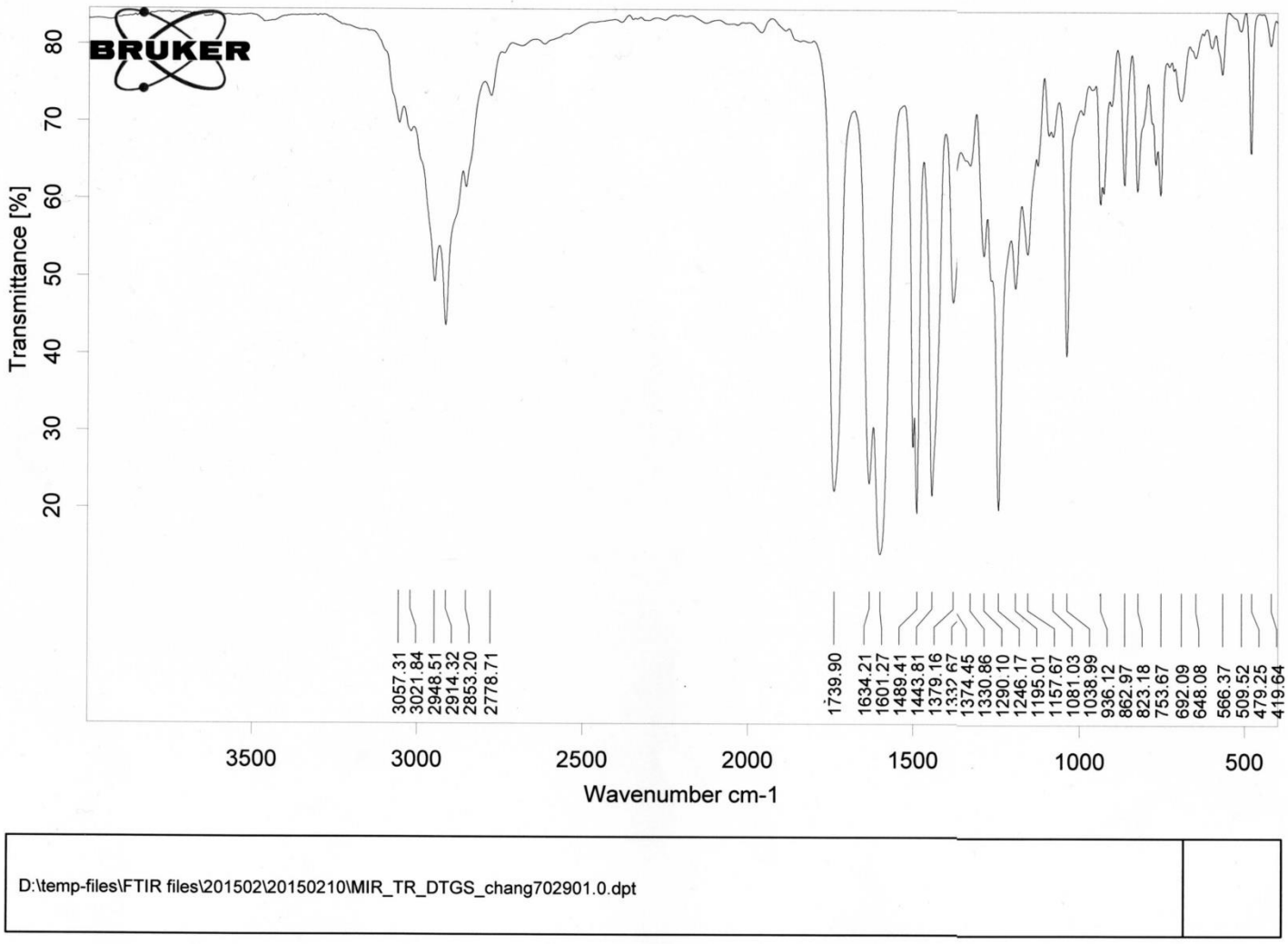


Result Table (Uncal - D:|Documents |changwongjin|chang702906)

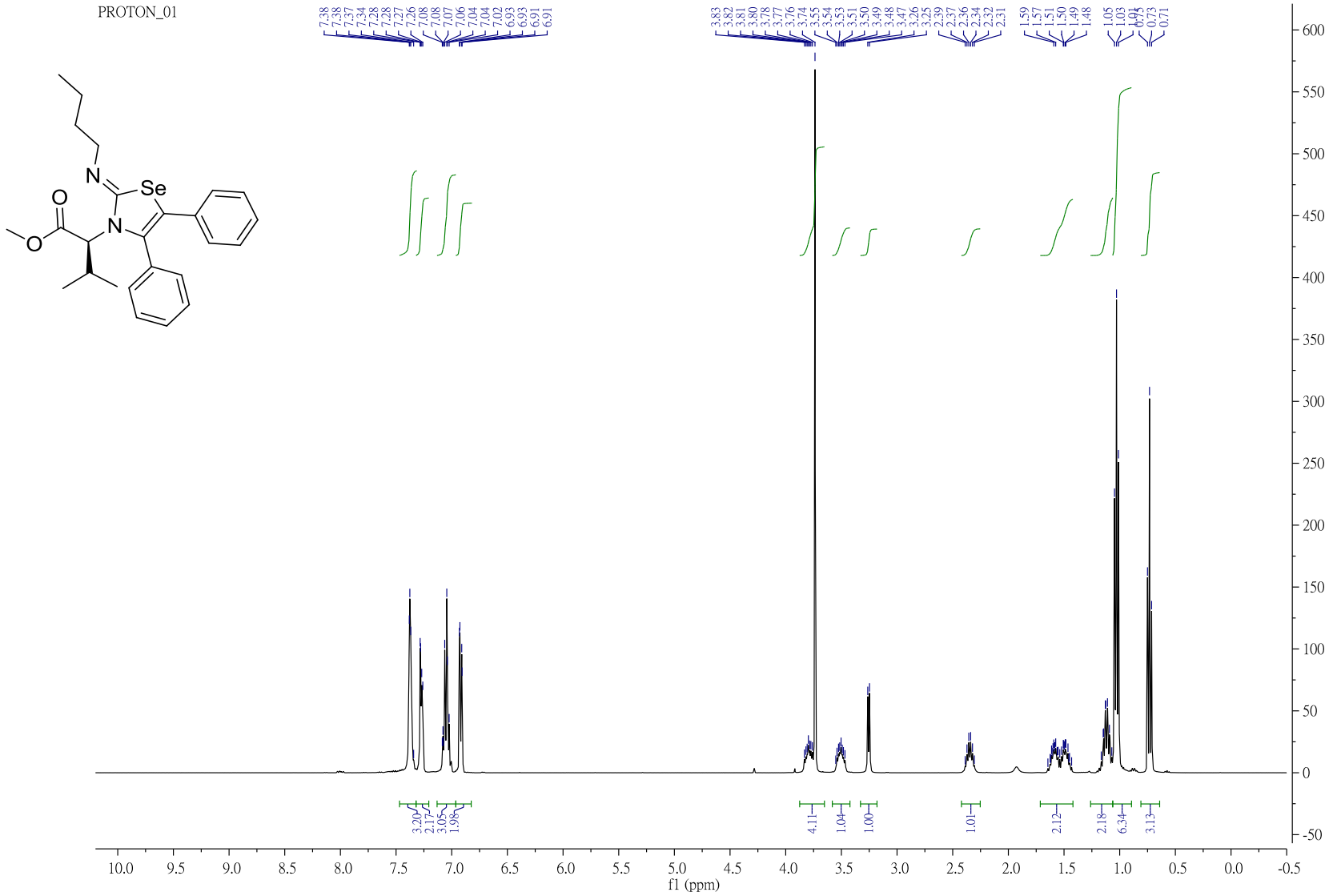
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.888	2.396	0.317	0.0	0.0	0.12
2	6.096	4.101	0.520	0.0	0.1	0.12
3	9.592	198.936	15.595	1.1	2.0	0.19
4	10.204	6.123	0.471	0.0	0.1	0.25
5	10.532	4.036	0.341	0.0	0.0	0.19
6	11.800	3.878	0.303	0.0	0.0	0.19
7	15.924	16435.199	754.252	93.2	96.0	0.33
8	17.344	16.303	0.878	0.1	0.1	0.31
9	19.536	185.924	6.029	1.1	0.8	0.46
10	21.308	104.960	1.402	0.6	0.2	0.98
11	26.428	495.375	3.195	2.8	0.4	2.40
12	45.240	81.921	1.010	0.5	0.1	1.01
13	50.260	95.109	0.960	0.5	0.1	1.39
	Total	17634.260	785.271	100.0	100.0	

7f chiral HPLC

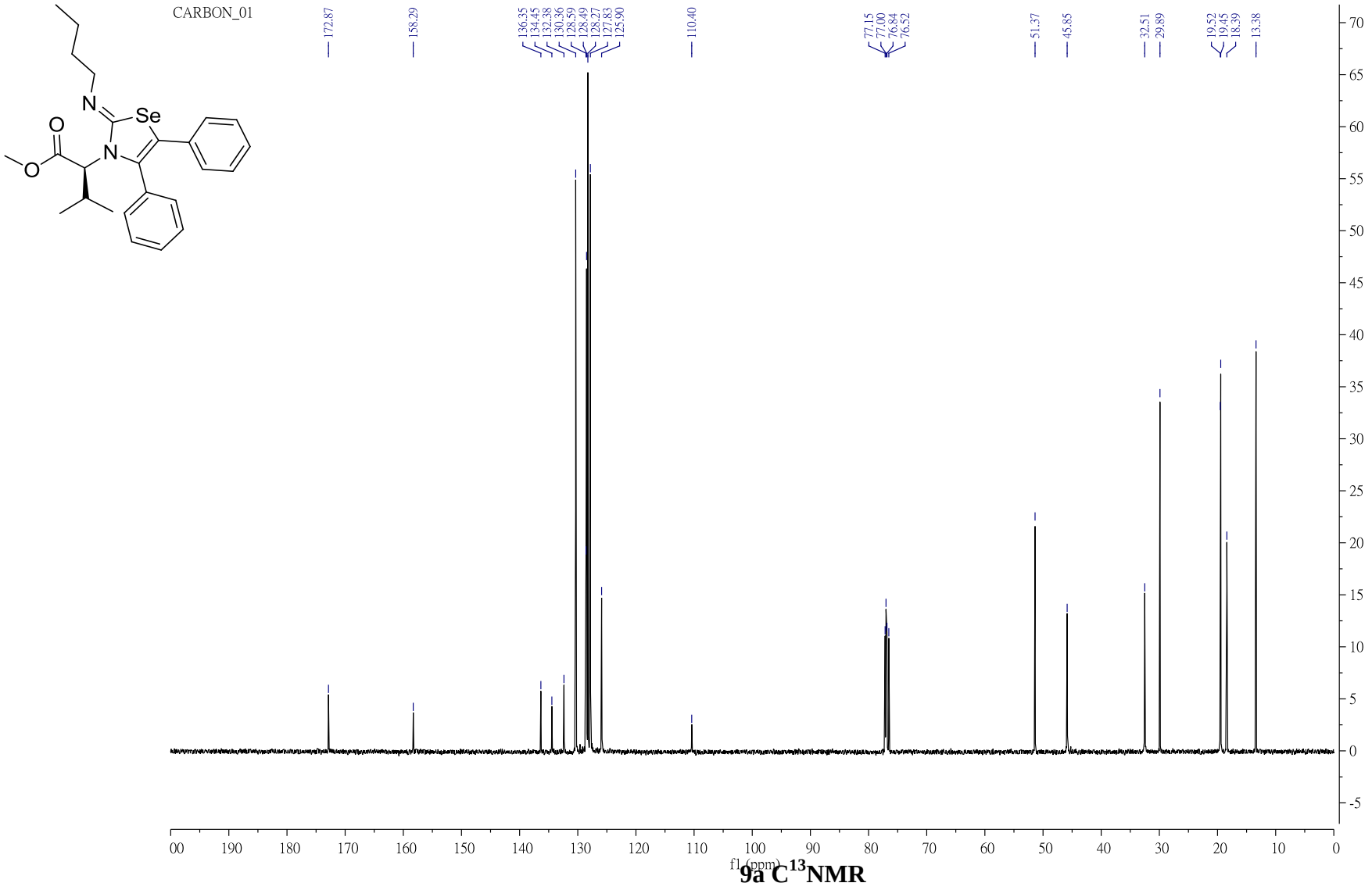
```
SAMPLE : ____________
ID #   : 002
LAMP λ : 589 nm
CONC   : 0.04000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-------------------------
SPECIFIC ROTATION [α]
 COUNT  [α](°)  TEMP(°C)
  01   - 74.3747   20.6
  02   - 75.2497   20.6
  03   - 75.7497   20.6
  04   - 76.1247   20.6
  05   - 76.8747   20.6
  06   - 77.3747   20.6
  07   - 77.7497   20.6
  08   - 78.2497   20.6
  09   - 78.6247   20.6
  10   - 78.9997   20.7
-------------------------
MEAN     = - 76.9372°
σ(N-1)   =    1.5334°
C.V.     = -  1.9931%
```


BRUKER
Transmittance [%]
20
30
40
50
60
70
80
3057.31
3021.84
2948.51
2914.32
2853.20
2778.71
1739.90
1634.21
1601.27
1489.41
1443.81
1379.16
1332.67
1374.45
1330.86
1290.10
1246.17
1195.01
1157.67
1081.03
1038.99
936.12
862.97
823.18
753.67
692.09
648.08
566.37
509.52
479.25
419.64
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201502\20150210\MIR_TR_DTGS_chang702901.0.dpt
Page 1/1

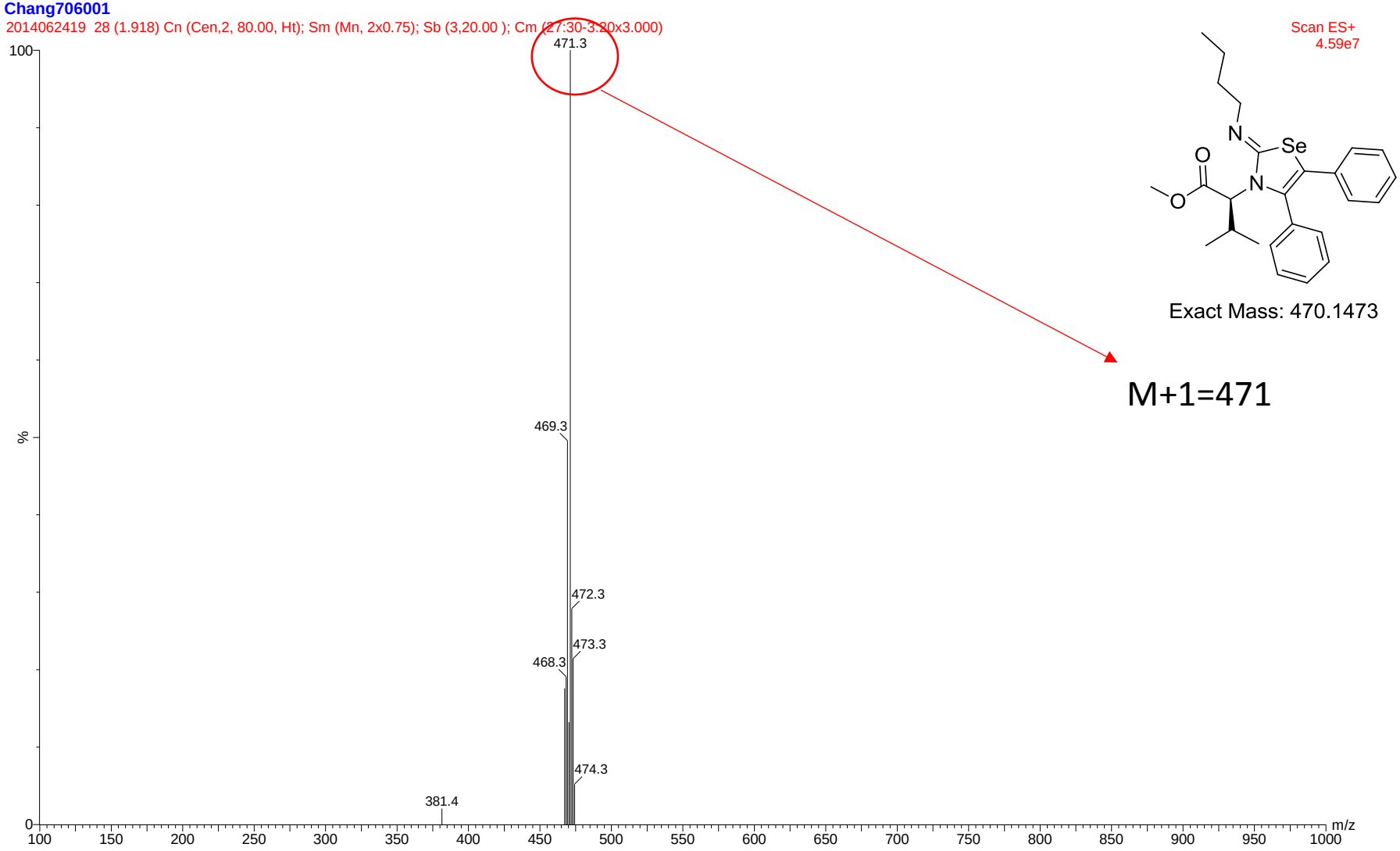
7f FT-IR


PROTON_01
N
Se
O
O
N
7.38
7.38
7.37
7.34
7.28
7.28
7.27
7.26
7.08
7.08
7.07
7.06
7.04
7.04
7.02
6.93
6.91
6.91
3.83
3.82
3.81
3.80
3.78
3.77
3.76
3.74
3.55
3.54
3.53
3.51
3.50
3.49
3.48
3.47
3.26
3.25
2.39
2.37
2.36
2.34
2.32
2.31
1.59
1.57
1.51
1.50
1.49
1.48
1.05
1.03
0.75
0.73
0.71
3.20
2.17
3.05
1.98
4.11
1.04
1.00
1.01
2.12
2.18
6.34
3.13
f1 (ppm)

9a H[1]NMR


CARBON_01
172.87
158.29
136.35
134.45
132.38
130.36
128.59
128.49
128.27
127.83
125.90
110.40
77.15
77.00
76.84
76.52
51.37
45.85
32.51
29.89
19.52
19.45
18.39
13.38
O
N
Se
N
O
f1 (ppm)

9a C^{13}NMR


Chang706001
2014062419 28 (1.918) Cn (Cen,2, 80.00, Ht); Sm (Mn, 2x0.75); Sb (3,20.00); Cm (27:30-3.20x3.000)
Scan ES+
4.59e7
100
%
0
471.3
469.3
472.3
473.3
468.3
474.3
381.4
m/z
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
N
Se
O
N
O
Exact Mass: 470.1473
M+1=471

9a LR-MS

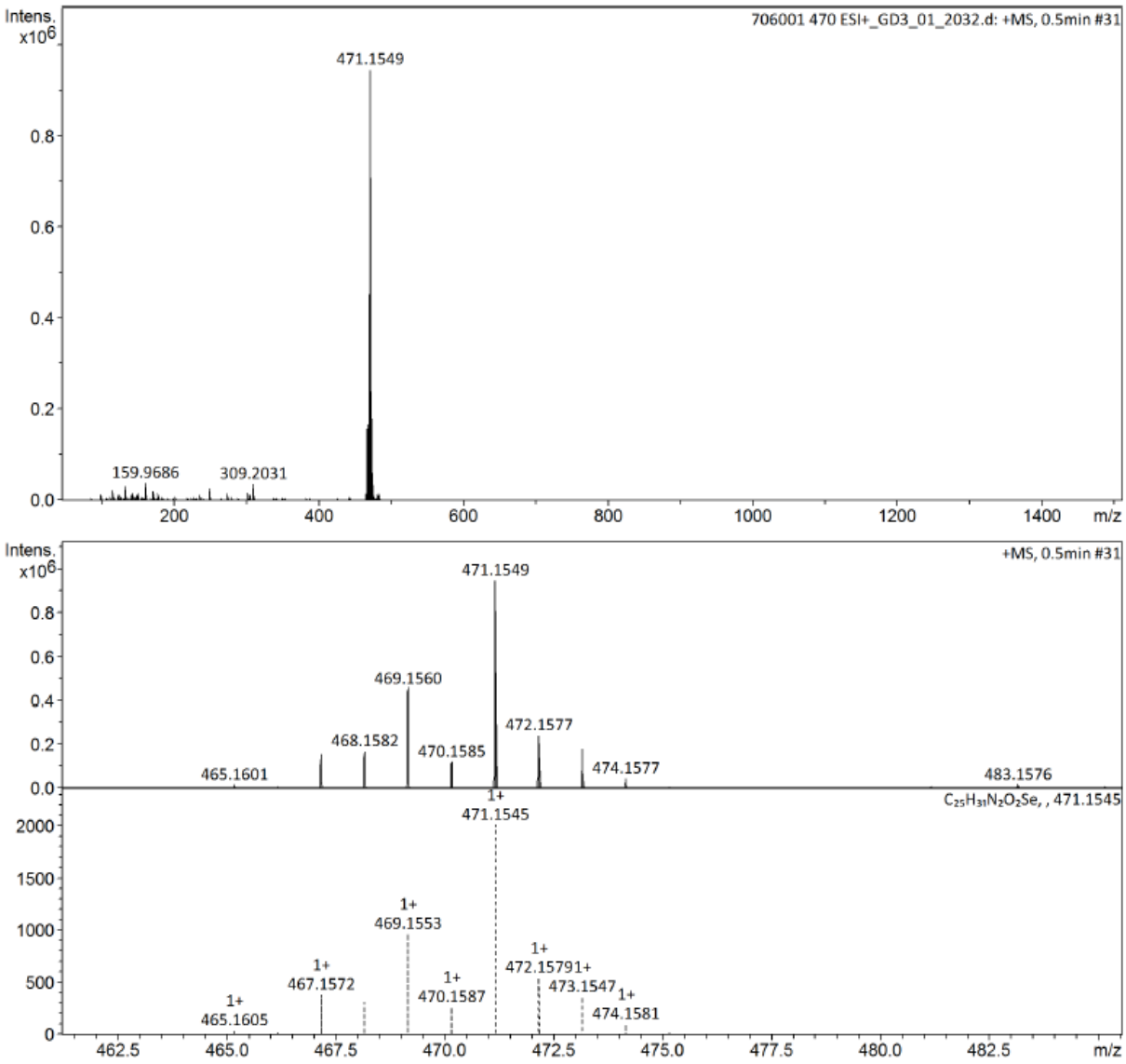
Display Report

Analysis Info

Analysis Name	D:\Data\NCTU SERVICE\Data\20140626\706001 470 ESI+_GD3_01_2032.d	Acquisition Date	6/26/2014 3:14:43 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	706001 470 ESI+	Instrument	impact HD 1819696.00164
Comment			

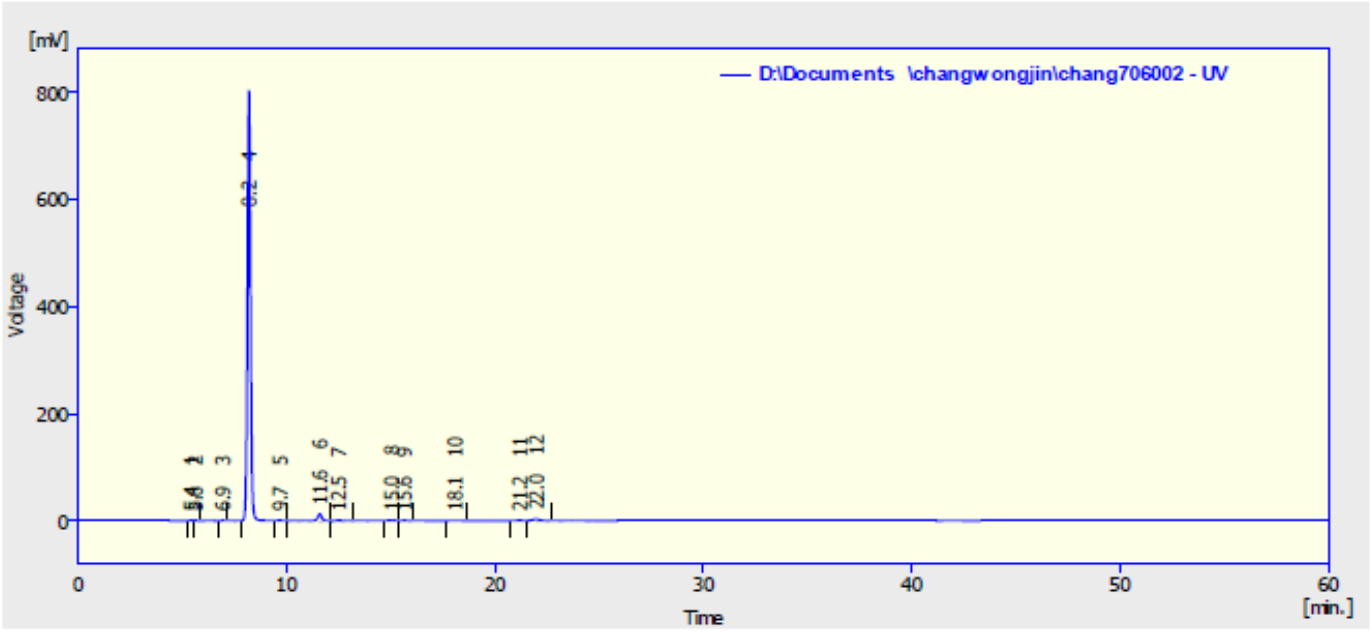
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



706001 470 ESI+_GD3_01_2032.d

9a HR-MS



Result Table (Uncal - D:\Documents \changwongjin\chang706002 - UV)

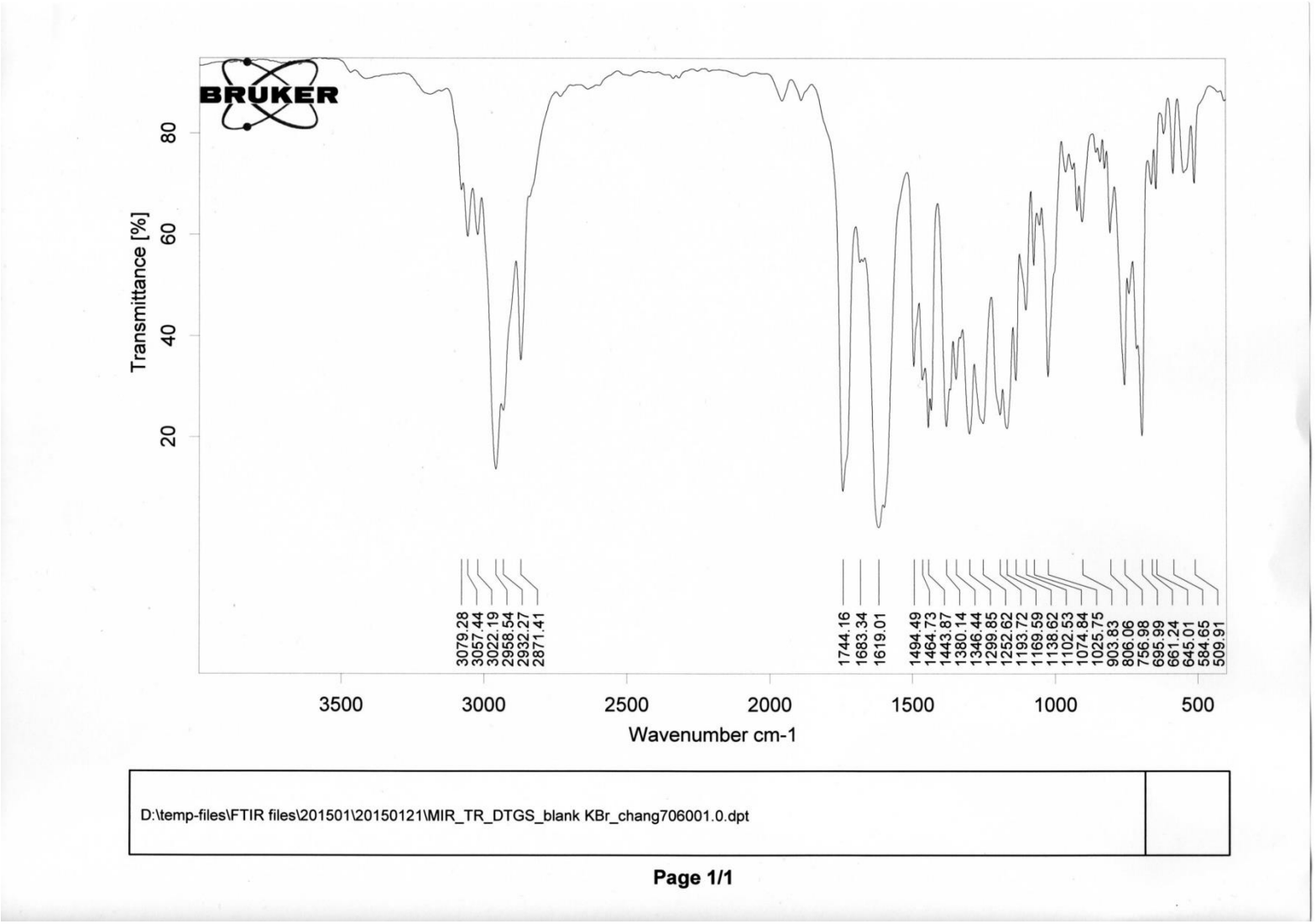
	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.404	7.641	1.097	0.1	0.1	0.11
2	5.604	6.279	0.771	0.1	0.1	0.13
3	6.932	4.144	0.485	0.0	0.1	0.13
4	8.200	8342.581	803.542	96.5	97.6	0.16
5	9.668	8.078	0.643	0.1	0.1	0.19
6	11.600	167.943	12.305	1.9	1.5	0.20
7	12.492	10.123	0.404	0.1	0.0	0.38
8	15.036	15.208	0.875	0.2	0.1	0.28
9	15.628	3.510	0.202	0.0	0.0	0.30
10	18.076	8.306	0.338	0.1	0.0	0.38
11	21.208	11.359	0.424	0.1	0.1	0.47
12	21.984	62.796	2.519	0.7	0.3	0.38
	Total	8647.971	823.605	100.0	100.0	

Result Table (Uncal - D:\Documents \changwongjin\chang706002 - UV2)

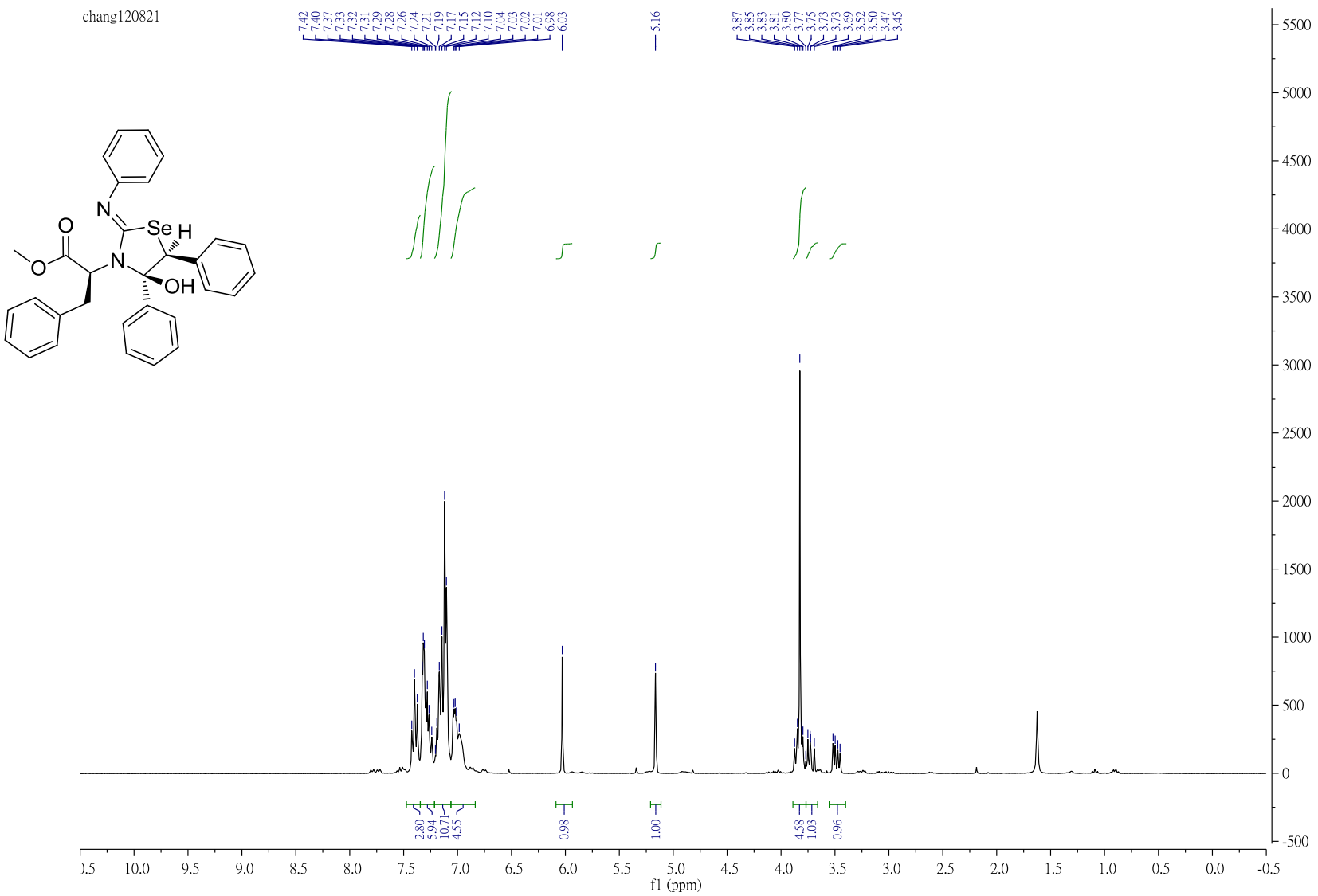
Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
No peak to report					

9a chiral HPLC

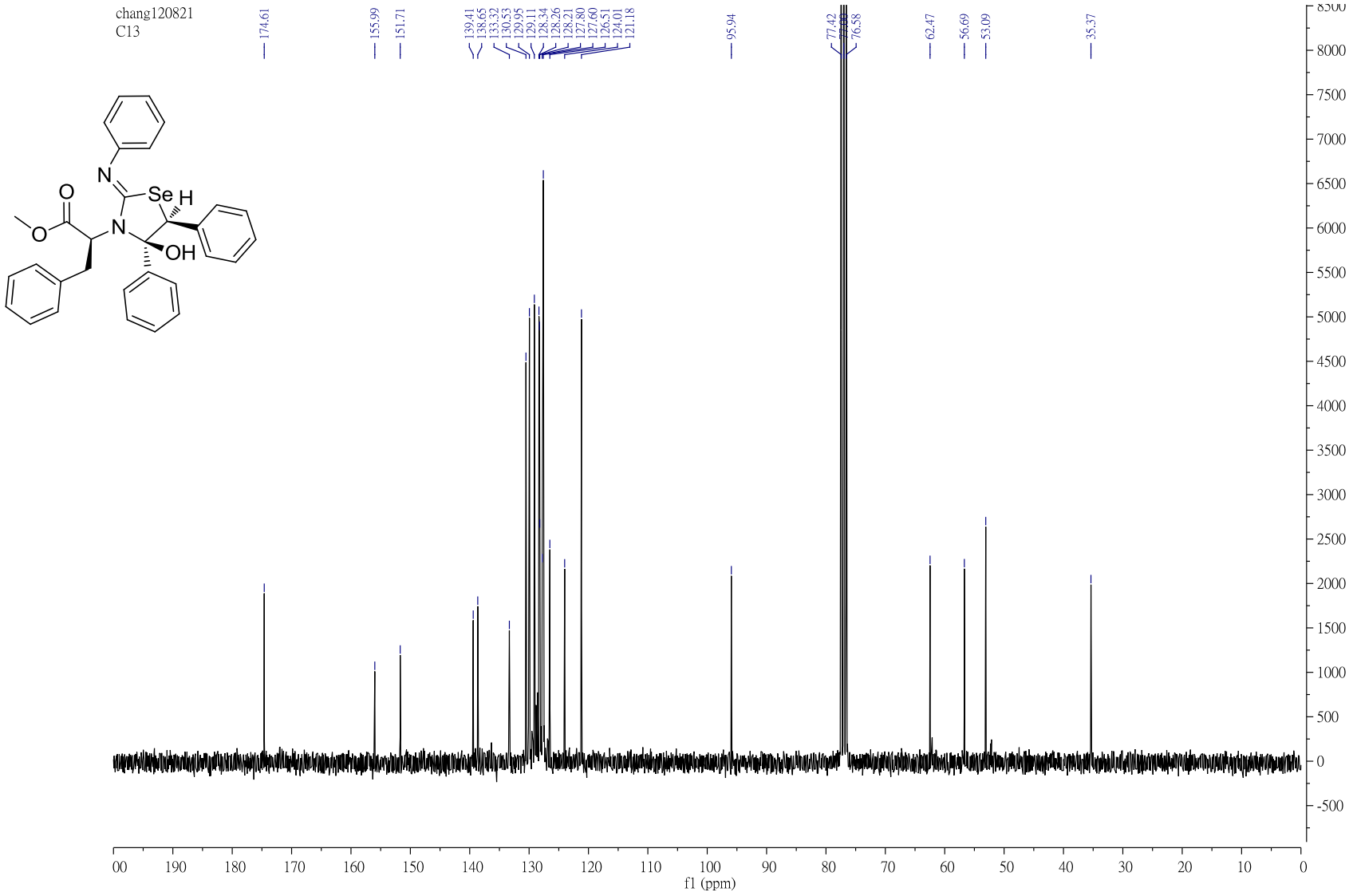
```
SAMPLE :
ID #    : 008
LAMP λ  : 589 nm
CONC    : 0.01000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-----------------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01   - 11.5002   19.4
  02   - 14.0002   19.4
  03   - 13.5002   19.4
  04   - 10.5002   19.4
  05   - 12.5002   19.4
  06   - 14.0001   19.5
  07   - 14.0001   19.5
  08   - 14.5001   19.5
  09   - 15.0001   19.5
  10   - 15.0001   19.5
-----------------------------
MEAN     = - 13.4502°
σ(N-1)   =    1.4990°
C.V.     = - 11.1452%
```


BRUKER
Transmittance [%]
20
40
60
80
3079.28
3057.44
3022.19
2958.54
2932.27
2871.41
1744.16
1683.34
1619.01
1494.49
1464.73
1443.87
1380.14
1346.44
1299.85
1252.62
1193.72
1169.59
1138.62
1102.53
1074.84
1025.75
903.83
806.06
756.98
695.99
661.24
645.01
584.65
509.91
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang706001.0.dpt
Page 1/1

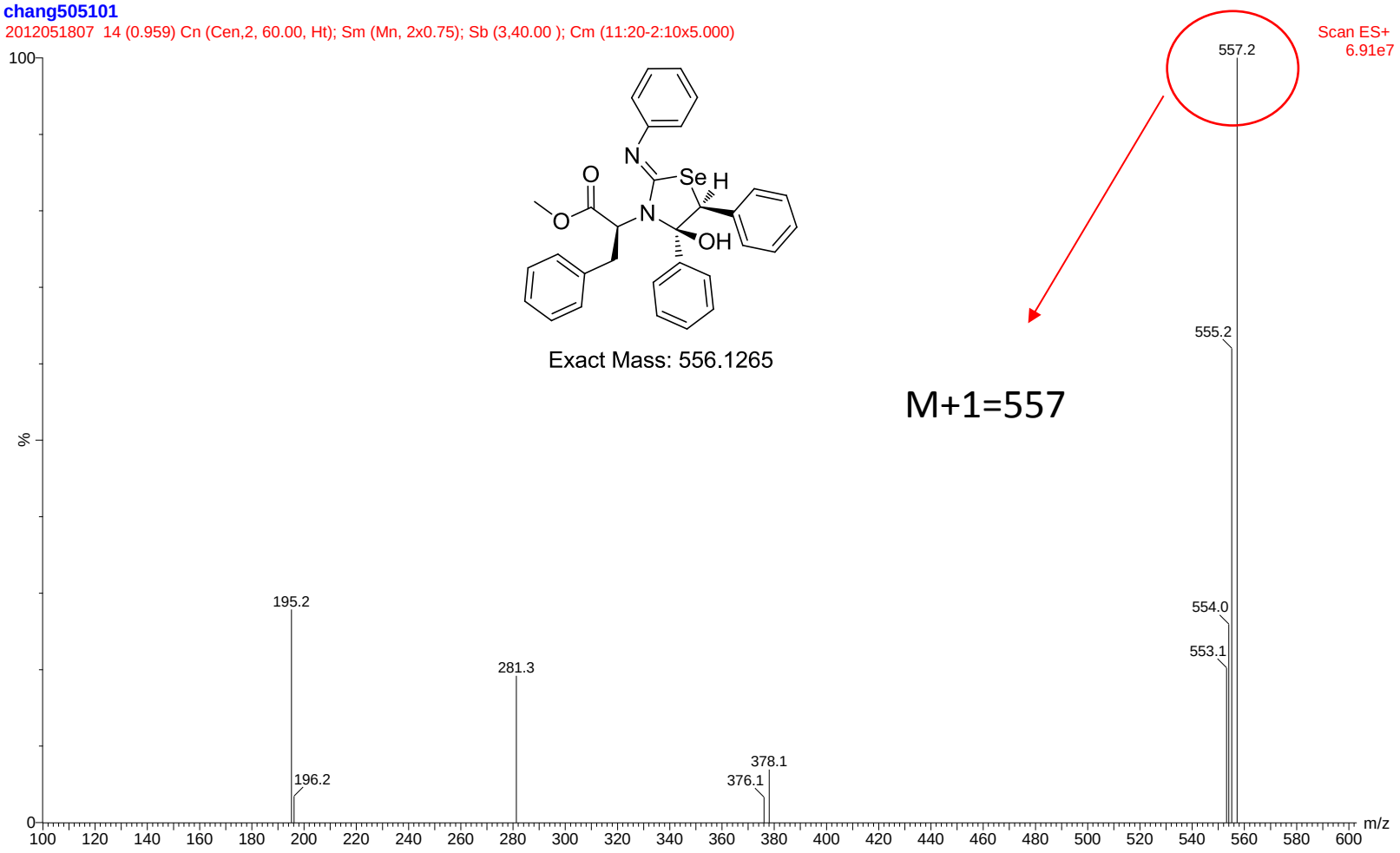
9a FT-IR


chang120821
7.42
7.40
7.37
7.33
7.32
7.31
7.29
7.28
7.26
7.24
7.21
7.19
7.17
7.15
7.12
7.10
7.04
7.03
7.02
7.01
6.98
6.03
5.16
3.87
3.85
3.83
3.81
3.80
3.77
3.75
3.73
3.73
3.69
3.52
3.50
3.47
3.45
N
Se
H
O
O
N
OH
2.80
5.94
10.71
4.55
0.98
1.00
4.58
1.03
0.96
f1 (ppm)

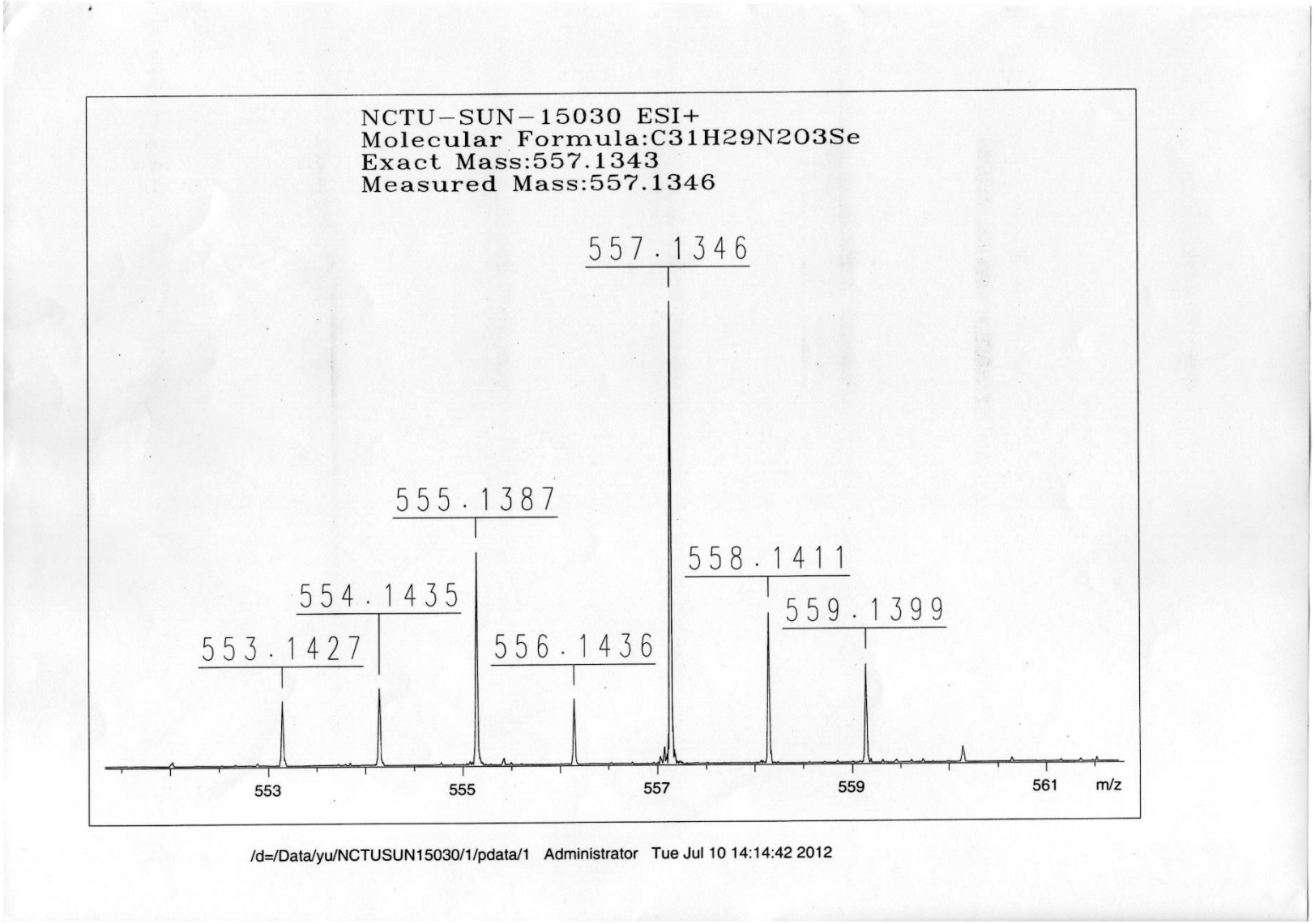
9b H[1]NMR


chang120821
C13
174.61
155.99
151.71
139.41
138.65
133.32
130.53
129.95
129.11
128.34
128.26
128.21
127.80
127.60
126.51
124.01
121.18
95.94
77.42
76.58
62.47
56.69
53.09
35.37
O
O
N
Se
H
N
OH
f1 (ppm)

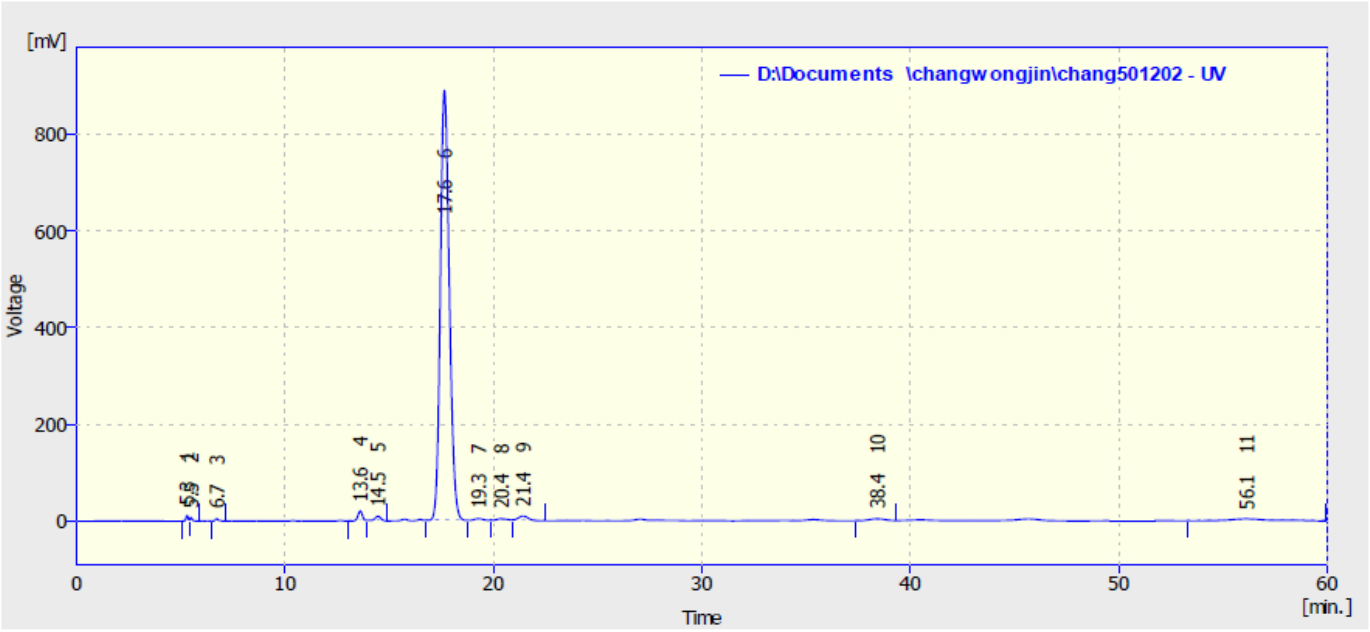
9b C^{13}NMR


chang505101
2012051807 14 (0.959) Cn (Cen,2, 60.00, Ht); Sm (Mn, 2x0.75); Sb (3,40.00); Cm (11:20-2:10x5.000)
Scan ES+
6.91e7
557.2
555.2
554.0
553.1
195.2
196.2
281.3
376.1
378.1
100
%
0
m/z
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600
N
Se H
O
O
N
OH
Exact Mass: 556.1265
M+1=557

9b LR-MS


NCTU-SUN-15030 ESI+
Molecular Formula:C31H29N2O3Se
Exact Mass:557.1343
Measured Mass:557.1346
557.1346
555.1387
558.1411
554.1435
559.1399
553.1427
556.1436
553
555
557
559
561
m/z
/d=/Data/yu/NCTUSUN15030/1/pdata/1 Administrator Tue Jul 10 14:14:42 2012

9b HR-MS

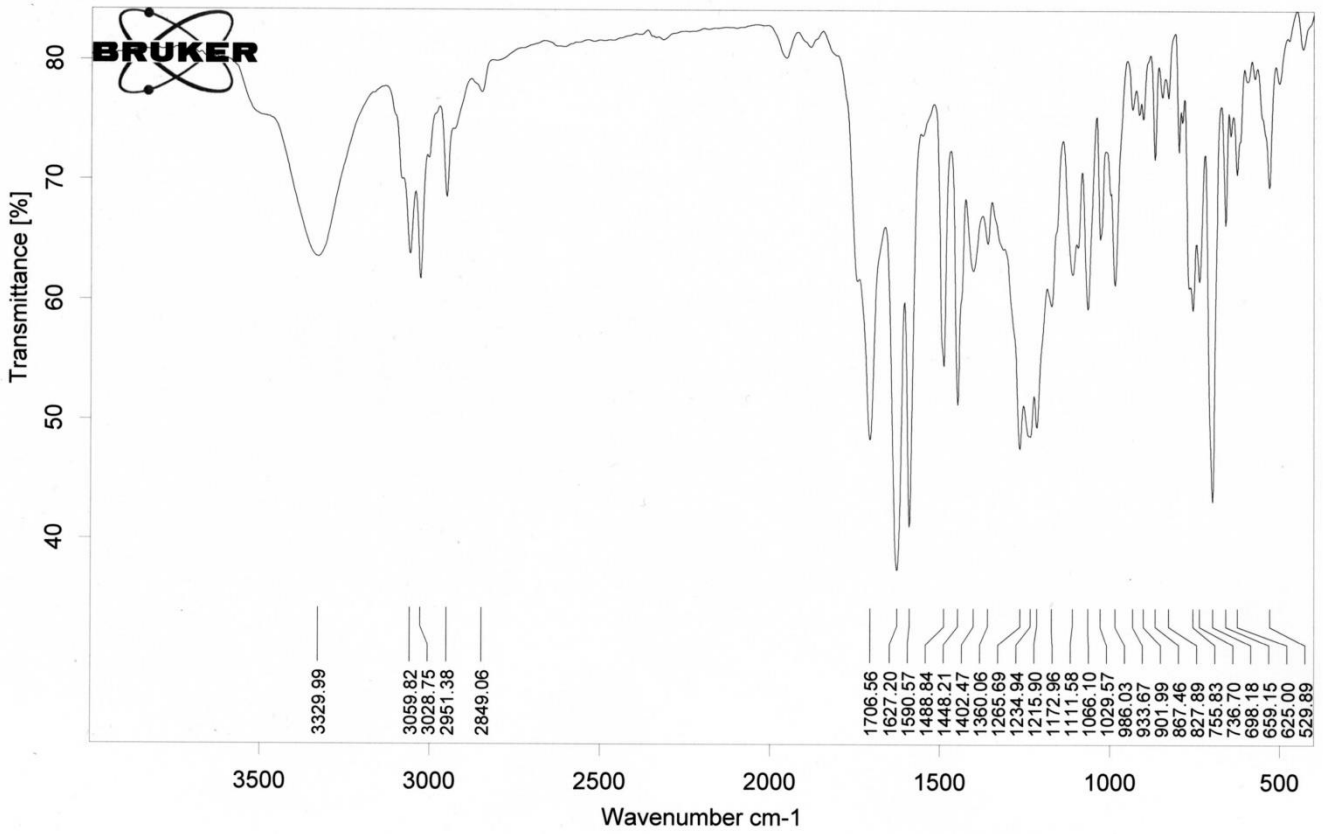


Result Table (Uncal - D:\Documents \changwongjin\chang501202 - UV)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]
1	5.304	83.097	11.850	0.3	1.2
2	5.484	60.351	7.343	0.2	0.8
3	6.724	49.096	4.875	0.2	0.5
4	13.612	314.587	20.748	1.1	2.1
5	14.464	209.177	9.709	0.7	1.0
6	17.648	26669.174	889.464	92.7	91.6
7	19.288	136.842	4.170	0.5	0.4
8	20.372	151.700	4.244	0.5	0.4
9	21.428	338.807	9.698	1.2	1.0
10	38.424	199.907	4.108	0.7	0.4
11	56.140	554.114	4.324	1.9	0.4
	Total	28766.853	970.534	100.0	100.0

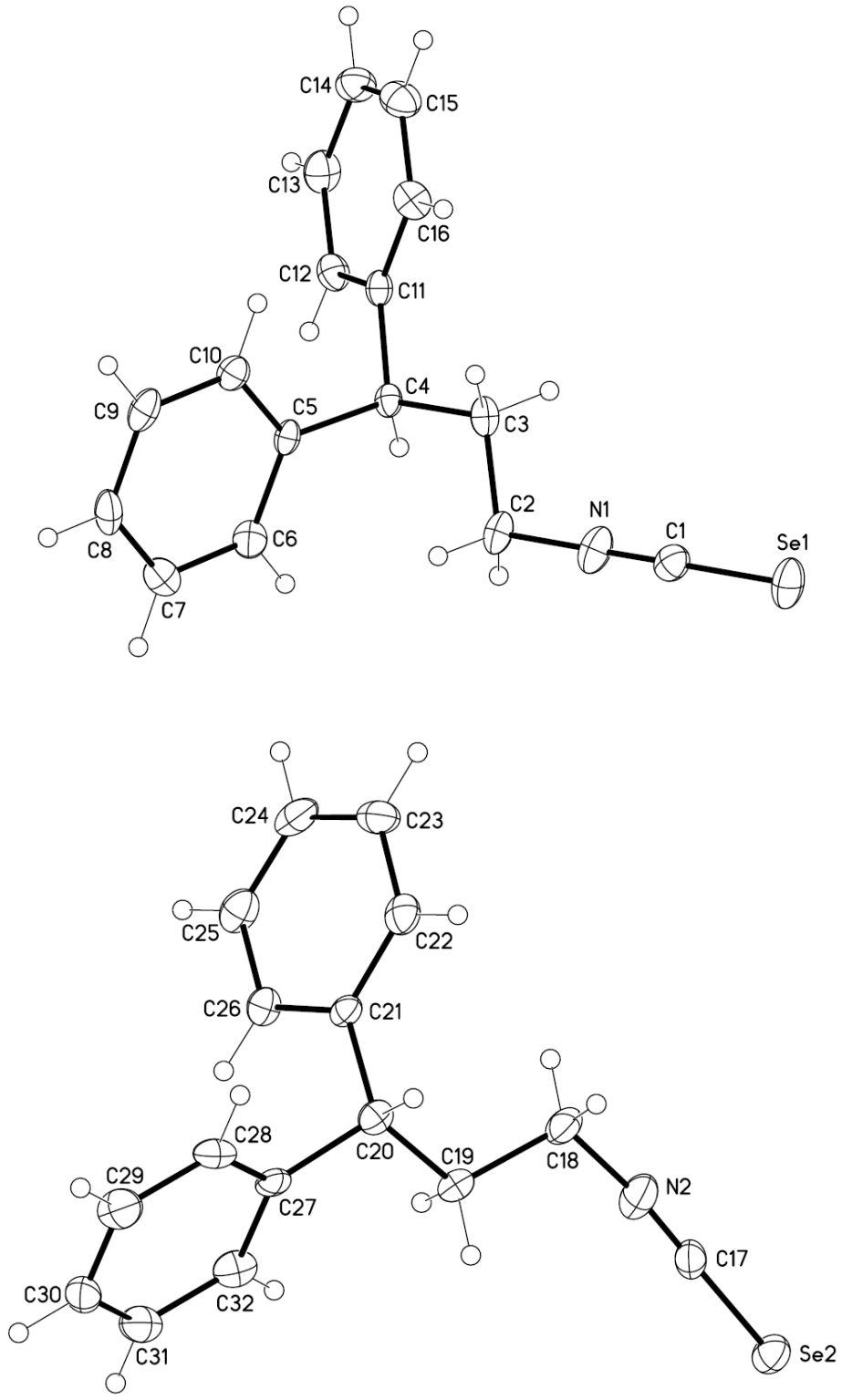
9b chiral HPLC

```
SAMPLE  : ____________
ID #    : 011
LAMP λ  : 589 nm
CONC    : 0.01000 g/ml
CELL LG: 010 mm
TEMP CORR: +0.00037
INTERVAL:  1 min
-----------------------
SPECIFIC ROTATION [α]
 COUNT   [α](°)  TEMP(°C)
  01   - 77.9998   20.4
  02   - 76.9998   20.4
  03   - 77.4998   20.5
  04   - 78.9998   20.5
  05   - 76.4998   20.5
  06   - 79.4998   20.5
  07   - 77.9998   20.5
  08   - 78.9997   20.6
  09   - 79.9997   20.6
  10   - 80.4997   20.6
-----------------------
MEAN     = - 78.4998°
σ(N-1)   =   1.3123°
C.V.     = -  1.6717%
```


BRUKER
Transmittance [%]
80
70
60
50
40
3329.99
3059.82
3028.75
2951.38
2849.06
1706.56
1627.20
1590.57
1488.84
1448.21
1402.47
1360.06
1265.69
1234.94
1215.90
1172.96
1111.58
1066.10
1029.57
986.03
933.67
901.99
867.46
827.89
755.83
736.70
698.18
659.15
625.00
529.89
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
D:\temp-files\FTIR files\201501\20150121\MIR_TR_DTGS_blank KBr_chang505101.0.dpt
Page 1/1

9b FT-IR

X-ray data



X-Ray ORTEP diagram of (3-isoselenocyanatopropane-1,1-diyl)dibenzene 1f

Table 1. Crystal data and structure refinement for mo_140308LT_0m.

Identification code	mo_140308lt_0m
Empirical formula	C32 H30 N2 Se2
Formula weight	600.50

Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	a = 14.8679(9) Å α= 90°.
b = 10.0040(6) Å	β= 98.871(2)°.
c = 18.5854(11) Å	γ = 90°.
Volume	2731.3(3) Å^3
Z	4
Density (calculated)	1.460 Mg/m^3
Absorption coefficient	2.731 mm^{-1}
F(000)	1216
Crystal size	0.30 x 0.30 x 0.10 mm^3
Theta range for data collection	1.636 to 26.381°.
Index ranges	-16<=h<=18, -12<=k<=12, -23<=l<=23
Reflections collected	19190
Independent reflections	5560 [R(int) = 0.0286]
Completeness to theta = 25.242°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.7832
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5560 / 0 / 325
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0272, wR2 = 0.0575
R indices (all data)	R1 = 0.0409, wR2 = 0.0615
Extinction coefficient	n/a
Largest diff. peak and hole	0.427 and -0.371 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for mo_140308LT_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

x	y	z	U(eq)	
Se(1)	5341(1)	12366(1)	799(1)	29(1)
Se(2)	4032(1)	-4739(1)	994(1)	24(1)
N(1)	5844(1)	9571(2)	1029(1)	28(1)
N(2)	3541(1)	-1922(2)	994(1)	29(1)
C(1)	5644(2)	10679(2)	940(1)	22(1)
C(2)	6123(2)	8202(2)	1144(1)	23(1)
C(3)	6322(2)	7871(2)	1954(1)	19(1)
C(4)	6500(1)	6364(2)	2075(1)	15(1)
C(5)	7317(1)	5923(2)	1730(1)	15(1)
C(6)	7184(2)	5391(2)	1028(1)	21(1)
C(7)	7917(2)	5061(2)	685(1)	24(1)
C(8)	8799(2)	5232(2)	1044(1)	24(1)
C(9)	8942(2)	5748(2)	1745(1)	22(1)
C(10)	8205(2)	6092(2)	2084(1)	19(1)
C(11)	6589(1)	5955(2)	2870(1)	16(1)
C(12)	6320(2)	4670(2)	3036(1)	20(1)
C(13)	6390(2)	4242(2)	3751(1)	24(1)
C(14)	6739(2)	5088(2)	4314(1)	25(1)
C(15)	7018(2)	6359(2)	4157(1)	26(1)
C(16)	6943(2)	6795(2)	3442(1)	21(1)
C(17)	3733(2)	-3044(2)	998(1)	22(1)
C(18)	3312(2)	-533(2)	1073(1)	24(1)
C(19)	3492(2)	-134(2)	1876(1)	19(1)
C(20)	3328(2)	1367(2)	1990(1)	18(1)
C(21)	2347(1)	1751(2)	1717(1)	16(1)
C(22)	2096(2)	2272(2)	1015(1)	22(1)
C(23)	1187(2)	2576(2)	751(1)	26(1)
C(24)	531(2)	2373(2)	1197(1)	27(1)
C(25)	772(2)	1890(2)	1892(1)	26(1)
C(26)	1671(2)	1583(2)	2147(1)	21(1)
C(27)	3603(1)	1769(2)	2787(1)	18(1)
C(28)	3842(2)	3087(2)	2945(1)	22(1)
C(29)	4083(2)	3515(2)	3660(1)	28(1)
C(30)	4092(2)	2616(2)	4225(1)	28(1)
C(31)	3860(2)	1305(2)	4074(1)	26(1)

C(32)	3616(2)	878(2)	3361(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for mo_140308LT_0m.

Se(1)-C(1)	1.756(2)
Se(2)-C(17)	1.754(2)
N(1)-C(1)	1.153(3)
N(1)-C(2)	1.437(3)
N(2)-C(17)	1.158(3)
N(2)-C(18)	1.444(3)
C(2)-C(3)	1.526(3)
C(2)-H(1)	0.9900
C(2)-H(15)	0.9900
C(3)-C(4)	1.541(3)
C(3)-H(3)	0.9900
C(3)-H(2)	0.9900
C(4)-C(11)	1.519(3)
C(4)-C(5)	1.524(3)
C(4)-H(14)	1.0000
C(5)-C(10)	1.391(3)
C(5)-C(6)	1.393(3)
C(6)-C(7)	1.385(3)
C(6)-H(8)	0.9500
C(7)-C(8)	1.387(3)
C(7)-H(4)	0.9500
C(8)-C(9)	1.386(3)
C(8)-H(5)	0.9500
C(9)-C(10)	1.390(3)
C(9)-H(6)	0.9500
C(10)-H(7)	0.9500
C(11)-C(16)	1.394(3)
C(11)-C(12)	1.395(3)
C(12)-C(13)	1.385(3)
C(12)-H(13)	0.9500
C(13)-C(14)	1.383(3)
C(13)-H(9)	0.9500
C(14)-C(15)	1.382(3)
C(14)-H(10)	0.9500
C(15)-C(16)	1.387(3)
C(15)-H(11)	0.9500
C(16)-H(12)	0.9500
C(18)-C(19)	1.528(3)

C(18)-H(29)	0.9900
C(18)-H(30)	0.9900
C(19)-C(20)	1.542(3)
C(19)-H(17)	0.9900
C(19)-H(16)	0.9900
C(20)-C(21)	1.519(3)
C(20)-C(27)	1.528(3)
C(20)-H(28)	1.0000
C(21)-C(26)	1.387(3)
C(21)-C(22)	1.402(3)
C(22)-C(23)	1.399(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.389(3)
C(23)-H(18)	0.9500
C(24)-C(25)	1.374(3)
C(24)-H(19)	0.9500
C(25)-C(26)	1.381(3)
C(25)-H(20)	0.9500
C(26)-H(21)	0.9500
C(27)-C(28)	1.385(3)
C(27)-C(32)	1.389(3)
C(28)-C(29)	1.390(3)
C(28)-H(27)	0.9500
C(29)-C(30)	1.381(3)
C(29)-H(26)	0.9500
C(30)-C(31)	1.374(3)
C(30)-H(25)	0.9500
C(31)-C(32)	1.386(3)
C(31)-H(24)	0.9500
C(32)-H(23)	0.9500

C(1)-N(1)-C(2)	178.2(2)
C(17)-N(2)-C(18)	173.8(2)
N(1)-C(1)-Se(1)	179.7(2)
N(1)-C(2)-C(3)	111.16(17)
N(1)-C(2)-H(1)	109.4
C(3)-C(2)-H(1)	109.4
N(1)-C(2)-H(15)	109.4
C(3)-C(2)-H(15)	109.4
H(1)-C(2)-H(15)	108.0

C(2)-C(3)-C(4)	110.99(16)
C(2)-C(3)-H(3)	109.4
C(4)-C(3)-H(3)	109.4
C(2)-C(3)-H(2)	109.4
C(4)-C(3)-H(2)	109.4
H(3)-C(3)-H(2)	108.0
C(11)-C(4)-C(5)	112.11(16)
C(11)-C(4)-C(3)	113.05(16)
C(5)-C(4)-C(3)	110.65(16)
C(11)-C(4)-H(14)	106.9
C(5)-C(4)-H(14)	106.9
C(3)-C(4)-H(14)	106.9
C(10)-C(5)-C(6)	118.5(2)
C(10)-C(5)-C(4)	121.66(18)
C(6)-C(5)-C(4)	119.79(18)
C(7)-C(6)-C(5)	120.9(2)
C(7)-C(6)-H(8)	119.6
C(5)-C(6)-H(8)	119.6
C(6)-C(7)-C(8)	120.1(2)
C(6)-C(7)-H(4)	119.9
C(8)-C(7)-H(4)	119.9
C(9)-C(8)-C(7)	119.7(2)
C(9)-C(8)-H(5)	120.2
C(7)-C(8)-H(5)	120.2
C(8)-C(9)-C(10)	120.0(2)
C(8)-C(9)-H(6)	120.0
C(10)-C(9)-H(6)	120.0
C(9)-C(10)-C(5)	120.82(19)
C(9)-C(10)-H(7)	119.6
C(5)-C(10)-H(7)	119.6
C(16)-C(11)-C(12)	118.32(18)
C(16)-C(11)-C(4)	123.08(18)
C(12)-C(11)-C(4)	118.59(17)
C(13)-C(12)-C(11)	121.02(19)
C(13)-C(12)-H(13)	119.5
C(11)-C(12)-H(13)	119.5
C(14)-C(13)-C(12)	120.0(2)
C(14)-C(13)-H(9)	120.0
C(12)-C(13)-H(9)	120.0
C(15)-C(14)-C(13)	119.6(2)

C(15)-C(14)-H(10)	120.2
C(13)-C(14)-H(10)	120.2
C(14)-C(15)-C(16)	120.6(2)
C(14)-C(15)-H(11)	119.7
C(16)-C(15)-H(11)	119.7
C(15)-C(16)-C(11)	120.47(19)
C(15)-C(16)-H(12)	119.8
C(11)-C(16)-H(12)	119.8
N(2)-C(17)-Se(2)	179.2(2)
N(2)-C(18)-C(19)	109.99(17)
N(2)-C(18)-H(29)	109.7
C(19)-C(18)-H(29)	109.7
N(2)-C(18)-H(30)	109.7
C(19)-C(18)-H(30)	109.7
H(29)-C(18)-H(30)	108.2
C(18)-C(19)-C(20)	112.39(16)
C(18)-C(19)-H(17)	109.1
C(20)-C(19)-H(17)	109.1
C(18)-C(19)-H(16)	109.1
C(20)-C(19)-H(16)	109.1
H(17)-C(19)-H(16)	107.9
C(21)-C(20)-C(27)	110.87(17)
C(21)-C(20)-C(19)	111.39(17)
C(27)-C(20)-C(19)	111.45(16)
C(21)-C(20)-H(28)	107.6
C(27)-C(20)-H(28)	107.6
C(19)-C(20)-H(28)	107.6
C(26)-C(21)-C(22)	118.0(2)
C(26)-C(21)-C(20)	121.42(18)
C(22)-C(21)-C(20)	120.54(19)
C(23)-C(22)-C(21)	120.7(2)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(24)-C(23)-C(22)	119.3(2)
C(24)-C(23)-H(18)	120.4
C(22)-C(23)-H(18)	120.4
C(25)-C(24)-C(23)	120.4(2)
C(25)-C(24)-H(19)	119.8
C(23)-C(24)-H(19)	119.8
C(24)-C(25)-C(26)	120.0(2)

C(24)-C(25)-H(20)	120.0
C(26)-C(25)-H(20)	120.0
C(25)-C(26)-C(21)	121.6(2)
C(25)-C(26)-H(21)	119.2
C(21)-C(26)-H(21)	119.2
C(28)-C(27)-C(32)	118.36(18)
C(28)-C(27)-C(20)	118.54(17)
C(32)-C(27)-C(20)	123.09(18)
C(27)-C(28)-C(29)	121.03(19)
C(27)-C(28)-H(27)	119.5
C(29)-C(28)-H(27)	119.5
C(30)-C(29)-C(28)	119.9(2)
C(30)-C(29)-H(26)	120.1
C(28)-C(29)-H(26)	120.1
C(31)-C(30)-C(29)	119.6(2)
C(31)-C(30)-H(25)	120.2
C(29)-C(30)-H(25)	120.2
C(30)-C(31)-C(32)	120.6(2)
C(30)-C(31)-H(24)	119.7
C(32)-C(31)-H(24)	119.7
C(31)-C(32)-C(27)	120.5(2)
C(31)-C(32)-H(23)	119.7
C(27)-C(32)-H(23)	119.7

Symmetry transformations used to generate equivalent atoms:

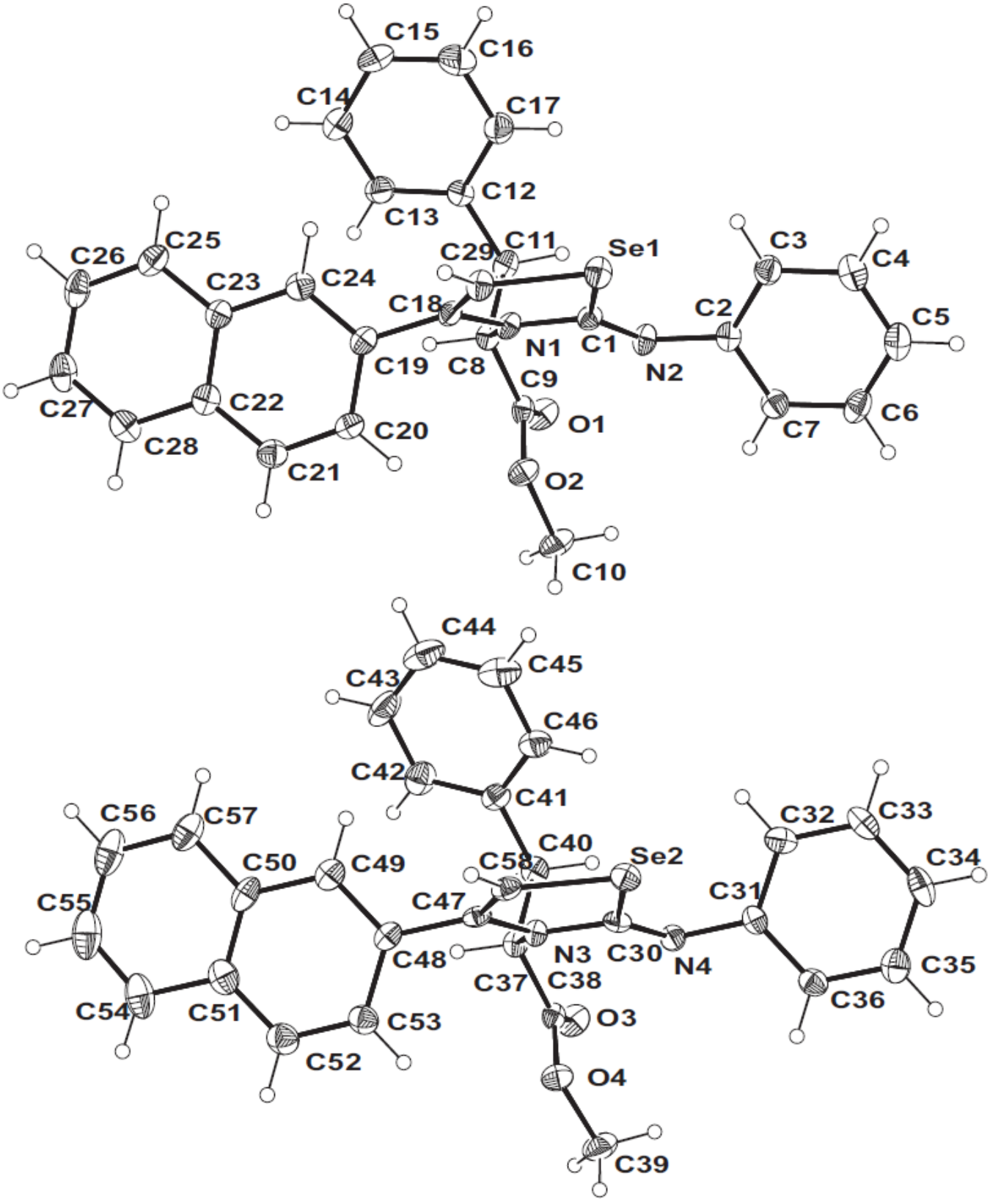
Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for mo_140308LT_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(1)	27(1)	19(1)	43(1)	8(1)	10(1)	6(1)
Se(2)	24(1)	20(1)	27(1)	-3(1)	3(1)	2(1)
N(1)	26(1)	20(1)	38(1)	7(1)	2(1)	5(1)
N(2)	26(1)	26(1)	35(1)	-8(1)	6(1)	3(1)
C(1)	17(1)	26(1)	22(1)	3(1)	4(1)	0(1)
C(2)	20(1)	16(1)	31(1)	4(1)	2(1)	5(1)
C(3)	16(1)	16(1)	27(1)	0(1)	6(1)	2(1)
C(4)	10(1)	14(1)	20(1)	-2(1)	2(1)	0(1)
C(5)	14(1)	10(1)	21(1)	3(1)	3(1)	1(1)
C(6)	19(1)	19(1)	25(1)	-2(1)	2(1)	-1(1)
C(7)	27(1)	23(1)	24(1)	-3(1)	7(1)	1(1)
C(8)	23(1)	20(1)	32(1)	5(1)	14(1)	8(1)
C(9)	13(1)	23(1)	32(1)	8(1)	3(1)	2(1)
C(10)	18(1)	17(1)	20(1)	3(1)	3(1)	1(1)
C(11)	11(1)	18(1)	22(1)	0(1)	5(1)	2(1)
C(12)	18(1)	18(1)	24(1)	-3(1)	4(1)	-1(1)
C(13)	26(1)	18(1)	30(1)	3(1)	7(1)	-1(1)
C(14)	25(1)	31(1)	19(1)	3(1)	5(1)	1(1)
C(15)	24(1)	29(1)	23(1)	-6(1)	2(1)	-4(1)
C(16)	20(1)	20(1)	25(1)	-2(1)	7(1)	-5(1)
C(17)	18(1)	29(1)	18(1)	-6(1)	4(1)	1(1)
C(18)	24(1)	19(1)	29(1)	-4(1)	2(1)	7(1)
C(19)	16(1)	17(1)	24(1)	1(1)	3(1)	3(1)
C(20)	15(1)	17(1)	22(1)	1(1)	5(1)	-1(1)
C(21)	15(1)	13(1)	19(1)	-3(1)	1(1)	1(1)
C(22)	29(1)	15(1)	25(1)	-3(1)	6(1)	-1(1)
C(23)	30(1)	20(1)	25(1)	-1(1)	-7(1)	3(1)
C(24)	19(1)	20(1)	39(1)	-8(1)	-3(1)	5(1)
C(25)	19(1)	25(1)	34(1)	-6(1)	5(1)	-1(1)
C(26)	22(1)	19(1)	22(1)	-3(1)	5(1)	0(1)
C(27)	11(1)	20(1)	21(1)	0(1)	-1(1)	4(1)
C(28)	20(1)	22(1)	23(1)	8(1)	0(1)	3(1)
C(29)	26(1)	22(1)	33(1)	-5(1)	-4(1)	-1(1)
C(30)	20(1)	43(1)	20(1)	-6(1)	-2(1)	10(1)
C(31)	20(1)	37(1)	24(1)	10(1)	8(1)	4(1)

C(32)	17(1)	22(1)	30(1)	4(1)	4(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10 ^{3}) for mo_140308LT_0m.

x	y	z	U(eq)	
H(1)	6675	8040	920	28
H(15)	5635	7607	904	28
H(3)	5798	8142	2191	23
H(2)	6862	8382	2183	23
H(14)	5957	5885	1811	18
H(8)	6582	5253	782	25
H(4)	7816	4716	203	29
H(5)	9302	4997	811	29
H(6)	9545	5866	1993	27
H(7)	8308	6447	2564	22
H(13)	6084	4079	2652	24
H(9)	6199	3366	3855	29
H(10)	6787	4798	4805	30
H(11)	7263	6940	4543	31
H(12)	7135	7672	3342	25
H(29)	2662	-387	876	29
H(30)	3682	32	793	29
H(17)	4130	-356	2079	23
H(16)	3089	-661	2146	23
H(28)	3723	1876	1696	21
H(22)	2549	2420	714	27
H(18)	1020	2918	272	31
H(19)	-89	2570	1020	32
H(20)	322	1767	2197	31
H(21)	1830	1249	2628	25
H(27)	3842	3709	2558	27
H(26)	4240	4424	3760	34
H(25)	4258	2902	4715	34
H(24)	3867	685	4463	32
H(23)	3457	-31	3265	27



X-Ray ORTEP diagram of 2-iminoselenazole 5f

Table 1. Crystal data and structure refinement for ch13687.

Identification code	ch13687	
Empirical formula	C29 H24 N2 O2 Se	
Formula weight	511.46	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 8.7794(3) Å	α= 90°.
	b = 14.6701(4) Å	β= 90°.
	c = 37.5122(10) Å	γ = 90°.
Volume	4831.4(2) Å^3	
Z	8	
Density (calculated)	1.406 Mg/m^3	
Absorption coefficient	1.583 mm^{-1}	
F(000)	2096	
Crystal size	0.78 x 0.74 x 0.67 mm^3	
Theta range for data collection	2.70 to 25.00°.	
Index ranges	-3<=h<=9, -17<=k<=17, -44<=l<=44	
Reflections collected	19306	
Independent reflections	8037 [R(int) = 0.0336]	
Completeness to theta = 24.99°	95.9 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.4168 and 0.3714	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8037 / 0 / 613	
Goodness-of-fit on F^2	1.011	
Final R indices [I>2sigma(I)]	R1 = 0.0350, wR2 = 0.0679	
R indices (all data)	R1 = 0.0453, wR2 = 0.0708	
Absolute structure parameter	0.023(7)	
Largest diff. peak and hole	0.279 and -0.581 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for ch13687. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7308(4)	489(2)	9791(1)	28(1)
C(2)	7920(4)	18(2)	10373(1)	30(1)
C(3)	6801(4)	414(2)	10581(1)	38(1)
C(4)	6487(5)	67(3)	10917(1)	48(1)
C(5)	7285(5)	-663(3)	11049(1)	48(1)
C(6)	8414(5)	-1043(2)	10847(1)	45(1)
C(7)	8753(4)	-711(2)	10513(1)	37(1)
C(8)	9257(4)	1037(2)	9375(1)	27(1)
C(9)	10458(4)	327(2)	9464(1)	32(1)
C(10)	11072(5)	-1226(2)	9462(1)	52(1)
C(11)	9619(4)	1958(2)	9547(1)	36(1)
C(12)	8559(4)	2697(2)	9414(1)	32(1)
C(13)	8632(5)	3001(2)	9064(1)	44(1)
C(14)	7650(5)	3666(3)	8941(1)	54(1)
C(15)	6603(6)	4049(3)	9170(1)	58(1)
C(16)	6534(5)	3765(3)	9518(1)	63(1)
C(17)	7502(5)	3090(3)	9638(1)	47(1)
C(18)	6551(4)	741(2)	9195(1)	29(1)
C(19)	6951(4)	771(2)	8808(1)	32(1)
C(20)	7774(4)	21(2)	8663(1)	36(1)
C(21)	8126(5)	2(2)	8309(1)	40(1)
C(22)	7709(4)	721(2)	8084(1)	35(1)
C(23)	6907(4)	1481(2)	8226(1)	33(1)
C(24)	6524(4)	1473(2)	8596(1)	36(1)
C(25)	6564(5)	2214(2)	8003(1)	45(1)
C(26)	6961(5)	2201(3)	7652(1)	46(1)
C(27)	7718(5)	1452(3)	7504(1)	47(1)
C(28)	8084(4)	730(2)	7712(1)	42(1)
C(29)	5154(4)	621(2)	9324(1)	32(1)
C(30)	7617(4)	7512(2)	8536(1)	29(1)
C(31)	7189(4)	7385(2)	9142(1)	30(1)
C(32)	8126(5)	6678(2)	9253(1)	44(1)
C(33)	8614(5)	6625(3)	9601(1)	52(1)
C(34)	8178(5)	7282(3)	9845(1)	48(1)
C(35)	7227(5)	7975(3)	9742(1)	43(1)

C(36)	6724(4)	8030(2)	9393(1)	36(1)
C(37)	5638(4)	7206(2)	8093(1)	30(1)
C(38)	4427(4)	7803(2)	8264(1)	30(1)
C(39)	3846(5)	9289(2)	8464(1)	52(1)
C(40)	5370(4)	6193(2)	8184(1)	36(1)
C(41)	6532(4)	5584(2)	8011(1)	37(1)
C(42)	6332(5)	5266(2)	7666(1)	50(1)
C(43)	7424(6)	4701(3)	7511(1)	63(1)
C(44)	8687(6)	4443(3)	7699(1)	63(1)
C(45)	8908(5)	4760(3)	8035(1)	60(1)
C(46)	7828(5)	5325(2)	8190(1)	45(1)
C(47)	8325(4)	7638(2)	7930(1)	27(1)
C(48)	7896(4)	7742(2)	7544(1)	30(1)
C(49)	8359(4)	7117(2)	7296(1)	38(1)
C(50)	7991(4)	7239(2)	6927(1)	39(1)
C(51)	7206(5)	8027(3)	6824(1)	45(1)
C(52)	6758(5)	8664(2)	7080(1)	45(1)
C(53)	7058(4)	8521(2)	7432(1)	38(1)
C(54)	6846(5)	8149(3)	6452(1)	59(1)
C(55)	7195(5)	7484(4)	6217(1)	67(1)
C(56)	7945(5)	6690(4)	6324(1)	62(1)
C(57)	8356(5)	6568(3)	6673(1)	51(1)
C(58)	9715(4)	7712(2)	8059(1)	31(1)
N(1)	7714(3)	724(2)	9448(1)	28(1)
N(2)	8332(3)	322(2)	10027(1)	33(1)
N(3)	7164(3)	7512(2)	8182(1)	26(1)
N(4)	6649(3)	7443(2)	8787(1)	30(1)
O(1)	11720(3)	514(2)	9567(1)	46(1)
O(2)	9994(3)	-514(1)	9382(1)	39(1)
O(3)	3198(3)	7533(2)	8357(1)	45(1)
O(4)	4852(3)	8677(1)	8273(1)	38(1)
Se(1)	5124(1)	435(1)	9819(1)	35(1)
Se(2)	9790(1)	7614(1)	8558(1)	34(1)

Table 3. Bond lengths [Å] and angles [°] for ch13687.

C(1)-N(2)	1.285(4)
C(1)-N(1)	1.379(4)
C(1)-Se(1)	1.922(3)
C(2)-C(3)	1.383(5)
C(2)-C(7)	1.399(4)
C(2)-N(2)	1.420(4)
C(3)-C(4)	1.385(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.373(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.366(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.375(4)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-N(1)	1.457(4)
C(8)-C(9)	1.520(5)
C(8)-C(11)	1.530(4)
C(8)-H(8)	1.0000
C(9)-O(1)	1.205(4)
C(9)-O(2)	1.335(4)
C(10)-O(2)	1.442(4)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.513(5)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(17)	1.379(5)
C(12)-C(13)	1.389(4)
C(13)-C(14)	1.380(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.376(6)
C(14)-H(14)	0.9500
C(15)-C(16)	1.372(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.381(5)
C(16)-H(16)	0.9500

C(17)-H(17)	0.9500
C(18)-C(29)	1.331(5)
C(18)-N(1)	1.395(4)
C(18)-C(19)	1.491(4)
C(19)-C(24)	1.354(4)
C(19)-C(20)	1.424(4)
C(20)-C(21)	1.365(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.399(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.421(5)
C(22)-C(28)	1.437(4)
C(23)-C(25)	1.396(4)
C(23)-C(24)	1.430(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.362(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.398(5)
C(26)-H(26)	0.9500
C(27)-C(28)	1.355(5)
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
C(29)-Se(1)	1.875(3)
C(29)-H(29)	0.9500
C(30)-N(4)	1.272(4)
C(30)-N(3)	1.388(4)
C(30)-Se(2)	1.916(3)
C(31)-C(32)	1.389(5)
C(31)-C(36)	1.397(4)
C(31)-N(4)	1.415(4)
C(32)-C(33)	1.373(5)
C(32)-H(32)	0.9500
C(33)-C(34)	1.384(5)
C(33)-H(33)	0.9500
C(34)-C(35)	1.372(5)
C(34)-H(34)	0.9500
C(35)-C(36)	1.381(5)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-N(3)	1.451(4)

C(37)-C(38)	1.518(4)
C(37)-C(40)	1.543(4)
C(37)-H(37)	1.0000
C(38)-O(3)	1.202(4)
C(38)-O(4)	1.335(4)
C(39)-O(4)	1.449(4)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-C(41)	1.503(5)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-C(46)	1.375(5)
C(41)-C(42)	1.388(5)
C(42)-C(43)	1.394(6)
C(42)-H(42)	0.9500
C(43)-C(44)	1.368(6)
C(43)-H(43)	0.9500
C(44)-C(45)	1.355(6)
C(44)-H(44)	0.9500
C(45)-C(46)	1.388(5)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
C(47)-C(58)	1.318(5)
C(47)-N(3)	1.404(4)
C(47)-C(48)	1.502(4)
C(48)-C(49)	1.369(4)
C(48)-C(53)	1.422(5)
C(49)-C(50)	1.433(5)
C(49)-H(49)	0.9500
C(50)-C(51)	1.400(5)
C(50)-C(57)	1.406(5)
C(51)-C(52)	1.397(5)
C(51)-C(54)	1.441(5)
C(52)-C(53)	1.363(5)
C(52)-H(52)	0.9500
C(53)-H(53)	0.9500
C(54)-C(55)	1.349(6)
C(54)-H(54)	0.9500
C(55)-C(56)	1.397(6)

C(55)-H(55)	0.9500
C(56)-C(57)	1.369(5)
C(56)-H(56)	0.9500
C(57)-H(57)	0.9500
C(58)-Se(2)	1.878(3)
C(58)-H(58)	0.9500

N(2)-C(1)-N(1)	120.6(3)
N(2)-C(1)-Se(1)	130.7(2)
N(1)-C(1)-Se(1)	108.6(2)
C(3)-C(2)-C(7)	118.6(3)
C(3)-C(2)-N(2)	124.5(3)
C(7)-C(2)-N(2)	116.8(3)
C(2)-C(3)-C(4)	120.1(3)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	120.8(4)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(6)-C(5)-C(4)	119.2(4)
C(6)-C(5)-H(5)	120.4
C(4)-C(5)-H(5)	120.4
C(5)-C(6)-C(7)	121.2(4)
C(5)-C(6)-H(6)	119.4
C(7)-C(6)-H(6)	119.4
C(6)-C(7)-C(2)	120.0(3)
C(6)-C(7)-H(7)	120.0
C(2)-C(7)-H(7)	120.0
N(1)-C(8)-C(9)	112.8(3)
N(1)-C(8)-C(11)	113.1(3)
C(9)-C(8)-C(11)	111.6(3)
N(1)-C(8)-H(8)	106.2
C(9)-C(8)-H(8)	106.2
C(11)-C(8)-H(8)	106.2
O(1)-C(9)-O(2)	124.4(3)
O(1)-C(9)-C(8)	123.5(3)
O(2)-C(9)-C(8)	111.8(3)
O(2)-C(10)-H(10A)	109.5
O(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5

O(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-C(8)	111.4(3)
C(12)-C(11)-H(11A)	109.3
C(8)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11B)	109.3
C(8)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
C(17)-C(12)-C(13)	118.3(3)
C(17)-C(12)-C(11)	120.8(3)
C(13)-C(12)-C(11)	120.9(3)
C(14)-C(13)-C(12)	120.8(4)
C(14)-C(13)-H(13)	119.6
C(12)-C(13)-H(13)	119.6
C(15)-C(14)-C(13)	119.9(4)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(16)-C(15)-C(14)	119.8(4)
C(16)-C(15)-H(15)	120.1
C(14)-C(15)-H(15)	120.1
C(15)-C(16)-C(17)	120.1(4)
C(15)-C(16)-H(16)	119.9
C(17)-C(16)-H(16)	119.9
C(16)-C(17)-C(12)	121.0(4)
C(16)-C(17)-H(17)	119.5
C(12)-C(17)-H(17)	119.5
C(29)-C(18)-N(1)	115.0(3)
C(29)-C(18)-C(19)	125.2(3)
N(1)-C(18)-C(19)	119.3(3)
C(24)-C(19)-C(20)	120.3(3)
C(24)-C(19)-C(18)	121.8(3)
C(20)-C(19)-C(18)	117.9(3)
C(21)-C(20)-C(19)	120.2(3)
C(21)-C(20)-H(20)	119.9
C(19)-C(20)-H(20)	119.9
C(20)-C(21)-C(22)	120.7(3)
C(20)-C(21)-H(21)	119.6
C(22)-C(21)-H(21)	119.6
C(21)-C(22)-C(23)	119.8(3)

C(21)-C(22)-C(28)	122.2(3)
C(23)-C(22)-C(28)	118.0(3)
C(25)-C(23)-C(22)	119.2(3)
C(25)-C(23)-C(24)	122.6(3)
C(22)-C(23)-C(24)	118.2(3)
C(19)-C(24)-C(23)	120.8(3)
C(19)-C(24)-H(24)	119.6
C(23)-C(24)-H(24)	119.6
C(26)-C(25)-C(23)	120.9(4)
C(26)-C(25)-H(25)	119.5
C(23)-C(25)-H(25)	119.5
C(25)-C(26)-C(27)	121.1(3)
C(25)-C(26)-H(26)	119.5
C(27)-C(26)-H(26)	119.5
C(28)-C(27)-C(26)	119.9(3)
C(28)-C(27)-H(27)	120.1
C(26)-C(27)-H(27)	120.1
C(27)-C(28)-C(22)	120.9(4)
C(27)-C(28)-H(28)	119.5
C(22)-C(28)-H(28)	119.5
C(18)-C(29)-Se(1)	113.2(3)
C(18)-C(29)-H(29)	123.4
Se(1)-C(29)-H(29)	123.4
N(4)-C(30)-N(3)	121.1(3)
N(4)-C(30)-Se(2)	129.8(2)
N(3)-C(30)-Se(2)	109.0(2)
C(32)-C(31)-C(36)	118.4(3)
C(32)-C(31)-N(4)	121.7(3)
C(36)-C(31)-N(4)	119.7(3)
C(33)-C(32)-C(31)	120.8(4)
C(33)-C(32)-H(32)	119.6
C(31)-C(32)-H(32)	119.6
C(32)-C(33)-C(34)	120.2(4)
C(32)-C(33)-H(33)	119.9
C(34)-C(33)-H(33)	119.9
C(35)-C(34)-C(33)	119.8(3)
C(35)-C(34)-H(34)	120.1
C(33)-C(34)-H(34)	120.1
C(34)-C(35)-C(36)	120.3(4)
C(34)-C(35)-H(35)	119.8

C(36)-C(35)-H(35)	119.8
C(35)-C(36)-C(31)	120.4(3)
C(35)-C(36)-H(36)	119.8
C(31)-C(36)-H(36)	119.8
N(3)-C(37)-C(38)	111.8(3)
N(3)-C(37)-C(40)	112.9(3)
C(38)-C(37)-C(40)	110.9(3)
N(3)-C(37)-H(37)	107.0
C(38)-C(37)-H(37)	107.0
C(40)-C(37)-H(37)	107.0
O(3)-C(38)-O(4)	124.0(3)
O(3)-C(38)-C(37)	124.1(3)
O(4)-C(38)-C(37)	111.7(3)
O(4)-C(39)-H(39A)	109.5
O(4)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
O(4)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(41)-C(40)-C(37)	111.9(3)
C(41)-C(40)-H(40A)	109.2
C(37)-C(40)-H(40A)	109.2
C(41)-C(40)-H(40B)	109.2
C(37)-C(40)-H(40B)	109.2
H(40A)-C(40)-H(40B)	107.9
C(46)-C(41)-C(42)	117.9(4)
C(46)-C(41)-C(40)	121.0(3)
C(42)-C(41)-C(40)	121.1(4)
C(41)-C(42)-C(43)	120.1(4)
C(41)-C(42)-H(42)	119.9
C(43)-C(42)-H(42)	119.9
C(44)-C(43)-C(42)	120.4(4)
C(44)-C(43)-H(43)	119.8
C(42)-C(43)-H(43)	119.8
C(45)-C(44)-C(43)	120.1(4)
C(45)-C(44)-H(44)	120.0
C(43)-C(44)-H(44)	120.0
C(44)-C(45)-C(46)	119.8(4)
C(44)-C(45)-H(45)	120.1
C(46)-C(45)-H(45)	120.1

C(41)-C(46)-C(45)	121.7(4)
C(41)-C(46)-H(46)	119.2
C(45)-C(46)-H(46)	119.2
C(58)-C(47)-N(3)	115.8(3)
C(58)-C(47)-C(48)	125.3(3)
N(3)-C(47)-C(48)	118.7(3)
C(49)-C(48)-C(53)	119.4(3)
C(49)-C(48)-C(47)	120.8(3)
C(53)-C(48)-C(47)	119.7(3)
C(48)-C(49)-C(50)	120.5(3)
C(48)-C(49)-H(49)	119.8
C(50)-C(49)-H(49)	119.8
C(51)-C(50)-C(57)	120.3(4)
C(51)-C(50)-C(49)	118.7(3)
C(57)-C(50)-C(49)	121.0(4)
C(52)-C(51)-C(50)	120.1(3)
C(52)-C(51)-C(54)	121.4(4)
C(50)-C(51)-C(54)	118.5(4)
C(53)-C(52)-C(51)	120.6(4)
C(53)-C(52)-H(52)	119.7
C(51)-C(52)-H(52)	119.7
C(52)-C(53)-C(48)	120.7(3)
C(52)-C(53)-H(53)	119.7
C(48)-C(53)-H(53)	119.7
C(55)-C(54)-C(51)	119.5(4)
C(55)-C(54)-H(54)	120.3
C(51)-C(54)-H(54)	120.3
C(54)-C(55)-C(56)	121.5(4)
C(54)-C(55)-H(55)	119.3
C(56)-C(55)-H(55)	119.3
C(57)-C(56)-C(55)	120.5(4)
C(57)-C(56)-H(56)	119.7
C(55)-C(56)-H(56)	119.7
C(56)-C(57)-C(50)	119.7(4)
C(56)-C(57)-H(57)	120.2
C(50)-C(57)-H(57)	120.2
C(47)-C(58)-Se(2)	113.2(2)
C(47)-C(58)-H(58)	123.4
Se(2)-C(58)-H(58)	123.4
C(1)-N(1)-C(18)	116.8(3)

C(1)-N(1)-C(8)	119.6(3)
C(18)-N(1)-C(8)	123.2(3)
C(1)-N(2)-C(2)	120.8(3)
C(30)-N(3)-C(47)	115.9(3)
C(30)-N(3)-C(37)	118.9(3)
C(47)-N(3)-C(37)	123.9(3)
C(30)-N(4)-C(31)	118.5(3)
C(9)-O(2)-C(10)	115.0(3)
C(38)-O(4)-C(39)	116.0(3)
C(29)-Se(1)-C(1)	85.75(15)
C(58)-Se(2)-C(30)	85.94(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$)for ch13687. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

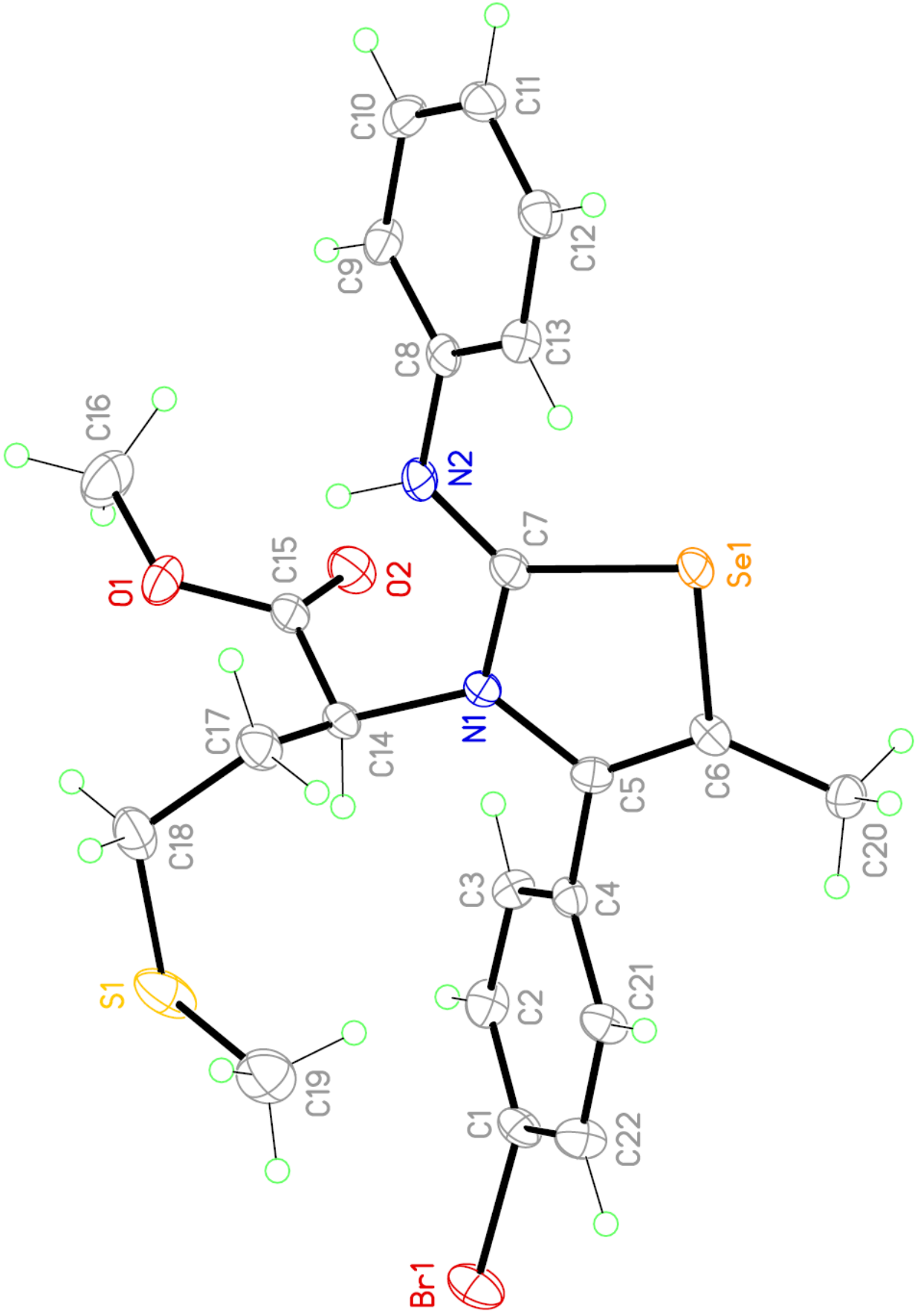
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	27(2)	26(2)	31(2)	4(2)	1(2)	0(2)
C(2)	25(2)	34(2)	30(2)	2(2)	-3(2)	-9(2)
C(3)	40(2)	41(2)	34(2)	3(2)	-2(2)	1(2)
C(4)	46(3)	60(3)	37(2)	-1(2)	3(2)	-6(2)
C(5)	55(3)	54(3)	33(2)	7(2)	-3(2)	-14(2)
C(6)	53(3)	43(2)	39(2)	11(2)	-15(2)	-4(2)
C(7)	33(2)	44(2)	35(2)	0(2)	-4(2)	4(2)
C(8)	17(2)	34(2)	29(2)	4(2)	0(1)	-3(1)
C(9)	27(2)	42(2)	28(2)	8(2)	5(2)	-3(2)
C(10)	45(3)	42(2)	68(3)	12(2)	-5(2)	16(2)
C(11)	32(2)	37(2)	38(2)	8(2)	-4(2)	-6(2)
C(12)	29(2)	31(2)	37(2)	-1(2)	2(2)	-4(2)
C(13)	46(3)	40(2)	47(2)	4(2)	6(2)	7(2)
C(14)	63(3)	50(2)	50(2)	10(2)	-2(2)	8(2)
C(15)	58(3)	47(2)	70(3)	7(2)	-6(2)	22(2)
C(16)	54(3)	66(3)	68(3)	-7(2)	10(2)	17(3)
C(17)	46(3)	52(2)	44(2)	5(2)	3(2)	6(2)
C(18)	29(2)	29(2)	29(2)	6(1)	-1(2)	5(2)
C(19)	23(2)	35(2)	37(2)	5(2)	-4(2)	-1(2)
C(20)	37(2)	31(2)	40(2)	2(2)	-2(2)	4(2)
C(21)	41(3)	36(2)	43(2)	-1(2)	1(2)	-1(2)
C(22)	28(2)	36(2)	39(2)	4(2)	-1(2)	-11(2)
C(23)	25(2)	37(2)	35(2)	2(2)	-4(2)	-1(2)
C(24)	28(2)	39(2)	40(2)	0(2)	-2(2)	2(2)
C(25)	44(3)	41(2)	49(2)	9(2)	-10(2)	3(2)
C(26)	52(3)	48(2)	38(2)	15(2)	-10(2)	-18(2)
C(27)	50(3)	55(2)	35(2)	8(2)	0(2)	-23(2)
C(28)	40(3)	43(2)	41(2)	-5(2)	6(2)	-14(2)
C(29)	19(2)	43(2)	34(2)	4(1)	-5(2)	0(2)
C(30)	24(2)	24(2)	38(2)	2(2)	-3(2)	4(2)
C(31)	26(2)	35(2)	29(2)	6(2)	0(2)	-6(2)
C(32)	46(3)	35(2)	50(2)	4(2)	-2(2)	6(2)
C(33)	57(3)	53(2)	45(2)	17(2)	-11(2)	8(2)
C(34)	48(3)	63(3)	33(2)	20(2)	-6(2)	-15(2)
C(35)	42(3)	49(2)	38(2)	2(2)	6(2)	-9(2)

C(36)	30(2)	38(2)	39(2)	5(2)	2(2)	3(2)
C(37)	22(2)	36(2)	31(2)	0(2)	4(1)	-4(2)
C(38)	22(2)	40(2)	28(2)	-3(2)	-6(2)	2(2)
C(39)	44(3)	50(2)	61(3)	-15(2)	1(2)	16(2)
C(40)	31(2)	37(2)	38(2)	1(2)	4(2)	-5(2)
C(41)	40(2)	27(2)	42(2)	-1(2)	10(2)	-6(2)
C(42)	55(3)	46(2)	50(2)	-8(2)	-1(2)	-10(2)
C(43)	91(4)	42(2)	55(3)	-21(2)	22(3)	-10(3)
C(44)	66(4)	36(2)	86(3)	-11(2)	27(3)	0(2)
C(45)	51(3)	40(2)	89(3)	-2(2)	8(3)	3(2)
C(46)	50(3)	33(2)	54(2)	-2(2)	2(2)	2(2)
C(47)	25(2)	17(2)	38(2)	-2(1)	7(2)	-1(2)
C(48)	22(2)	31(2)	35(2)	-5(2)	9(2)	-8(2)
C(49)	32(2)	41(2)	42(2)	-4(2)	6(2)	-6(2)
C(50)	26(2)	51(2)	39(2)	-15(2)	11(2)	-11(2)
C(51)	39(3)	51(2)	46(2)	10(2)	7(2)	-12(2)
C(52)	48(3)	39(2)	49(2)	5(2)	3(2)	-6(2)
C(53)	39(3)	34(2)	41(2)	4(2)	2(2)	-4(2)
C(54)	52(3)	85(3)	41(2)	13(2)	1(2)	-20(2)
C(55)	50(3)	112(4)	41(2)	-1(3)	5(2)	-23(3)
C(56)	41(3)	102(4)	42(2)	-20(2)	9(2)	-15(3)
C(57)	39(3)	67(3)	48(2)	-17(2)	9(2)	-5(2)
C(58)	27(2)	28(2)	39(2)	-2(1)	9(2)	5(2)
N(1)	18(2)	33(2)	32(2)	8(1)	-3(1)	2(1)
N(2)	25(2)	43(2)	32(2)	9(1)	-4(1)	-3(2)
N(3)	21(2)	31(2)	26(1)	-1(1)	2(1)	-4(1)
N(4)	24(2)	37(2)	29(2)	2(1)	4(1)	4(1)
O(1)	23(2)	49(2)	65(2)	9(1)	-5(1)	-2(1)
O(2)	31(1)	35(1)	49(1)	5(1)	-4(1)	2(1)
O(3)	26(2)	54(2)	56(2)	-6(2)	9(1)	-6(2)
O(4)	30(2)	35(1)	49(1)	-3(1)	1(1)	1(1)
Se(1)	23(1)	47(1)	35(1)	7(1)	3(1)	0(1)
Se(2)	24(1)	38(1)	39(1)	1(1)	-2(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for ch13687.

	x	y	z	U(eq)
H(3)	6247	924	10494	46
H(4)	5709	339	11057	57
H(5)	7054	-902	11278	57
H(6)	8975	-1544	10939	54
H(7)	9553	-977	10378	45
H(8)	9317	1135	9111	32
H(10A)	10639	-1817	9393	78
H(10B)	11295	-1226	9717	78
H(10C)	12014	-1121	9328	78
H(11A)	9521	1905	9809	43
H(11B)	10684	2129	9492	43
H(13)	9368	2749	8906	53
H(14)	7696	3859	8700	65
H(15)	5931	4510	9087	70
H(16)	5819	4033	9676	75
H(17)	7439	2894	9879	57
H(20)	8079	-467	8814	43
H(21)	8660	-506	8214	48
H(24)	5964	1967	8695	43
H(25)	6048	2729	8097	53
H(26)	6719	2708	7505	55
H(27)	7975	1450	7258	56
H(28)	8595	223	7610	50
H(29)	4262	629	9181	39
H(32)	8434	6224	9087	52
H(33)	9253	6137	9673	62
H(34)	8536	7253	10084	58
H(35)	6913	8420	9910	52
H(36)	6057	8508	9324	43
H(37)	5522	7269	7829	36
H(39A)	4262	9909	8455	78
H(39B)	3760	9092	8712	78
H(39C)	2837	9282	8352	78
H(40A)	5414	6111	8446	43

H(40B)	4340	6012	8103	43
H(42)	5450	5434	7535	60
H(43)	7290	4493	7273	75
H(44)	9409	4042	7595	75
H(45)	9800	4595	8163	72
H(46)	7988	5537	8427	54
H(49)	8927	6598	7369	46
H(52)	6238	9202	7008	55
H(53)	6704	8945	7605	46
H(54)	6366	8693	6373	71
H(55)	6924	7557	5974	81
H(56)	8172	6231	6154	74
H(57)	8886	6032	6743	61
H(58)	10591	7806	7915	38



X-Ray ORTEP diagram of 2-iminoselenazole 7a

Table 1. Crystal data and structure refinement for mo_111153lt_0m.

Identification code	mo_111153lt_0m	
Empirical formula	C22 H24 Br N2 O2 S Se	
Formula weight	539.36	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 11.244(2) Å	α= 90°.
	b = 7.6728(14) Å	β= 98.983(4)°.
	c = 12.837(2) Å	γ = 90°.
Volume	1093.9(3) $Å^3$	
Z	2	
Density (calculated)	1.637 Mg/m^3	
Absorption coefficient	3.659 mm^{-1}	
F(000)	542	
Crystal size	0.25 x 0.12 x 0.12 mm^3	
Theta range for data collection	1.61 to 26.52°.	
Index ranges	-14<=h<=14, -9<=k<=5, -15<=l<=16	
Reflections collected	8706	
Independent reflections	3751 [R(int) = 0.0186]	
Completeness to theta = 26.52°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.8045	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3751 / 1 / 265	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0185, wR2 = 0.0409	
R indices (all data)	R1 = 0.0210, wR2 = 0.0414	
Absolute structure parameter	0.004(6)	
Largest diff. peak and hole	0.271 and -0.617 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for mo_111153lt_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	-4860(1)	3670(1)	4803(1)	25(1)
Se(1)	425(1)	3910(1)	10640(1)	18(1)
S(1)	-350(1)	6482(1)	5437(1)	31(1)
N(2)	2288(2)	3680(3)	9304(1)	19(1)
O(2)	1153(2)	1076(2)	7488(1)	24(1)
N(1)	293(2)	3932(3)	8530(1)	17(1)
O(1)	2327(2)	2973(2)	6794(1)	25(1)
C(1)	-3684(2)	3664(4)	6044(2)	17(1)
C(2)	-2803(2)	2392(3)	6174(2)	19(1)
C(3)	-1922(2)	2455(3)	7055(2)	17(1)
C(4)	-1893(2)	3785(4)	7795(2)	15(1)
C(5)	-919(2)	3886(3)	8709(2)	15(1)
C(6)	-1070(2)	3877(4)	9725(2)	16(1)
C(7)	1175(2)	3827(4)	9398(2)	17(1)
C(8)	3216(2)	3555(3)	10169(2)	16(1)
C(9)	4159(2)	2398(3)	10094(2)	19(1)
C(10)	5085(2)	2197(3)	10924(2)	21(1)
C(11)	5131(2)	3172(3)	11833(2)	21(1)
C(12)	4220(2)	4364(3)	11907(2)	22(1)
C(13)	3268(2)	4571(3)	11083(2)	18(1)
C(14)	663(2)	4135(3)	7486(2)	16(1)
C(15)	1400(2)	2533(4)	7287(2)	19(1)
C(16)	3066(3)	1513(4)	6580(3)	37(1)
C(17)	1221(3)	5915(4)	7355(2)	22(1)
C(18)	1144(3)	6480(3)	6200(2)	26(1)
C(19)	-1076(3)	8127(4)	6116(2)	33(1)
C(20)	-2206(2)	3737(4)	10191(2)	20(1)
C(21)	-2812(2)	5028(3)	7654(2)	18(1)
C(22)	-3714(2)	4965(3)	6787(2)	22(1)

Table 3. Bond lengths [Å] and angles [°] for mo_111153lt_0m.

Br(1)-C(1)	1.905(2)
Se(1)-C(6)	1.895(2)
Se(1)-C(7)	1.9174(19)
S(1)-C(19)	1.800(3)
S(1)-C(18)	1.808(3)
N(2)-C(7)	1.281(3)
N(2)-C(8)	1.403(3)
N(2)-H(2)	0.8800
O(2)-C(15)	1.190(3)
N(1)-C(7)	1.373(3)
N(1)-C(5)	1.418(2)
N(1)-C(14)	1.473(3)
O(1)-C(15)	1.344(3)
O(1)-C(16)	1.446(3)
C(1)-C(2)	1.382(3)
C(1)-C(22)	1.385(3)
C(2)-C(3)	1.383(3)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.391(3)
C(3)-H(3)	0.9500
C(4)-C(21)	1.397(3)
C(4)-C(5)	1.476(3)
C(5)-C(6)	1.342(3)
C(6)-C(20)	1.496(3)
C(8)-C(9)	1.398(3)
C(8)-C(13)	1.402(3)
C(9)-C(10)	1.377(4)
C(9)-H(9)	0.9500
C(10)-C(11)	1.380(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.387(3)
C(11)-H(11)	0.9500
C(12)-C(13)	1.392(4)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(14)-C(17)	1.523(4)
C(14)-C(15)	1.526(3)
C(14)-H(14)	1.0000

C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.534(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.384(3)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500

C(6)-Se(1)-C(7)	86.96(9)
C(19)-S(1)-C(18)	101.01(13)
C(7)-N(2)-C(8)	123.28(17)
C(7)-N(2)-H(2)	118.4
C(8)-N(2)-H(2)	118.4
C(7)-N(1)-C(5)	117.25(16)
C(7)-N(1)-C(14)	118.30(16)
C(5)-N(1)-C(14)	124.41(17)
C(15)-O(1)-C(16)	113.9(2)
C(2)-C(1)-C(22)	121.3(2)
C(2)-C(1)-Br(1)	119.58(18)
C(22)-C(1)-Br(1)	119.11(19)
C(1)-C(2)-C(3)	118.9(2)
C(1)-C(2)-H(2A)	120.6
C(3)-C(2)-H(2A)	120.6
C(2)-C(3)-C(4)	121.4(2)
C(2)-C(3)-H(3)	119.3
C(4)-C(3)-H(3)	119.3
C(3)-C(4)-C(21)	118.3(2)
C(3)-C(4)-C(5)	121.1(2)
C(21)-C(4)-C(5)	120.6(2)
C(6)-C(5)-N(1)	115.37(18)

C(6)-C(5)-C(4)	125.57(17)
N(1)-C(5)-C(4)	119.01(16)
C(5)-C(6)-C(20)	129.38(19)
C(5)-C(6)-Se(1)	111.57(14)
C(20)-C(6)-Se(1)	118.92(14)
N(2)-C(7)-N(1)	121.41(17)
N(2)-C(7)-Se(1)	130.09(16)
N(1)-C(7)-Se(1)	108.50(13)
C(9)-C(8)-C(13)	118.5(2)
C(9)-C(8)-N(2)	117.9(2)
C(13)-C(8)-N(2)	123.6(2)
C(10)-C(9)-C(8)	120.5(2)
C(10)-C(9)-H(9)	119.7
C(8)-C(9)-H(9)	119.7
C(9)-C(10)-C(11)	121.1(2)
C(9)-C(10)-H(10)	119.4
C(11)-C(10)-H(10)	119.4
C(10)-C(11)-C(12)	119.0(2)
C(10)-C(11)-H(11)	120.5
C(12)-C(11)-H(11)	120.5
C(11)-C(12)-C(13)	120.8(2)
C(11)-C(12)-H(12)	119.6
C(13)-C(12)-H(12)	119.6
C(12)-C(13)-C(8)	120.0(2)
C(12)-C(13)-H(13)	120.0
C(8)-C(13)-H(13)	120.0
N(1)-C(14)-C(17)	112.1(2)
N(1)-C(14)-C(15)	107.76(19)
C(17)-C(14)-C(15)	117.3(2)
N(1)-C(14)-H(14)	106.3
C(17)-C(14)-H(14)	106.3
C(15)-C(14)-H(14)	106.3
O(2)-C(15)-O(1)	124.2(2)
O(2)-C(15)-C(14)	124.7(2)
O(1)-C(15)-C(14)	111.0(2)
O(1)-C(16)-H(16A)	109.5
O(1)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
O(1)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5

H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-C(18)	113.5(2)
C(14)-C(17)-H(17A)	108.9
C(18)-C(17)-H(17A)	108.9
C(14)-C(17)-H(17B)	108.9
C(18)-C(17)-H(17B)	108.9
H(17A)-C(17)-H(17B)	107.7
C(17)-C(18)-S(1)	115.57(19)
C(17)-C(18)-H(18A)	108.4
S(1)-C(18)-H(18A)	108.4
C(17)-C(18)-H(18B)	108.4
S(1)-C(18)-H(18B)	108.4
H(18A)-C(18)-H(18B)	107.4
S(1)-C(19)-H(19A)	109.5
S(1)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
S(1)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(6)-C(20)-H(20A)	109.5
C(6)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(6)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-C(4)	121.0(2)
C(22)-C(21)-H(21)	119.5
C(4)-C(21)-H(21)	119.5
C(21)-C(22)-C(1)	119.0(2)
C(21)-C(22)-H(22)	120.5
C(1)-C(22)-H(22)	120.5

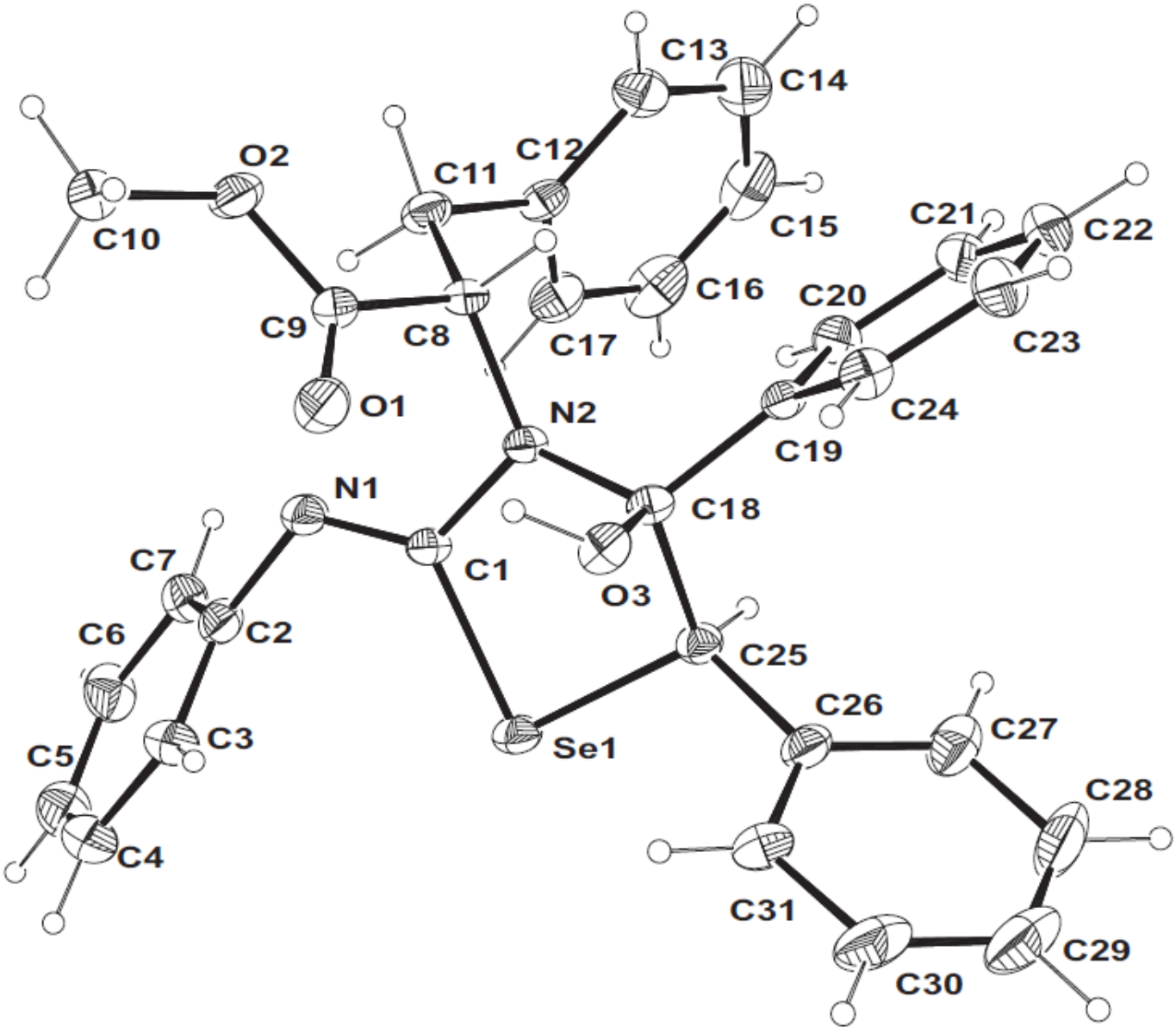
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for mo_111153lt_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	29(1)	26(1)	18(1)	1(1)	-7(1)	-3(1)
Se(1)	17(1)	25(1)	10(1)	1(1)	1(1)	-1(1)
S(1)	48(1)	27(1)	17(1)	0(1)	-3(1)	9(1)
N(2)	18(1)	29(1)	10(1)	-1(1)	3(1)	1(1)
O(2)	29(1)	21(1)	21(1)	2(1)	4(1)	2(1)
N(1)	14(1)	26(1)	11(1)	2(1)	1(1)	2(1)
O(1)	22(1)	29(1)	27(1)	1(1)	12(1)	5(1)
C(1)	20(1)	19(1)	12(1)	0(1)	-2(1)	-2(1)
C(2)	21(1)	20(1)	17(1)	-6(1)	3(1)	-3(1)
C(3)	16(1)	17(1)	19(1)	0(1)	3(1)	2(1)
C(4)	16(1)	15(1)	13(1)	1(1)	3(1)	-2(1)
C(5)	17(1)	12(1)	17(1)	0(1)	1(1)	2(1)
C(6)	19(1)	14(1)	14(1)	0(1)	0(1)	-4(1)
C(7)	20(1)	18(1)	12(1)	-1(1)	1(1)	0(1)
C(8)	15(1)	17(1)	16(1)	3(1)	3(1)	-6(1)
C(9)	16(1)	25(1)	18(1)	-4(1)	5(1)	-3(1)
C(10)	15(1)	23(1)	24(1)	0(1)	4(1)	0(1)
C(11)	16(1)	25(2)	21(1)	5(1)	-1(1)	-3(1)
C(12)	22(1)	26(2)	17(1)	-1(1)	2(1)	-4(1)
C(13)	18(1)	19(1)	18(1)	0(1)	4(1)	-1(1)
C(14)	17(1)	22(2)	10(1)	1(1)	1(1)	2(1)
C(15)	15(1)	32(2)	9(1)	0(1)	-1(1)	0(1)
C(16)	34(2)	36(2)	46(2)	5(2)	20(2)	14(1)
C(17)	25(2)	24(2)	17(2)	-1(1)	2(1)	1(1)
C(18)	35(2)	24(2)	21(1)	5(1)	9(1)	2(1)
C(19)	41(2)	26(2)	33(2)	1(1)	6(1)	8(1)
C(20)	19(1)	24(1)	17(1)	-1(1)	4(1)	2(1)
C(21)	24(1)	16(1)	14(1)	-2(1)	-1(1)	2(1)
C(22)	24(1)	20(1)	21(1)	0(1)	-1(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10 ^{3}) for mo_111153lt_0m.

	x	y	z	U(eq)
H(2)	2480	3655	8666	23
H(2A)	-2803	1490	5668	23
H(3)	-1324	1571	7157	21
H(9)	4162	1744	9466	23
H(10)	5703	1373	10870	25
H(11)	5776	3029	12400	25
H(12)	4247	5048	12527	26
H(13)	2654	5400	11139	22
H(14)	-92	4084	6959	20
H(16A)	2587	711	6089	56
H(16B)	3360	901	7240	56
H(16C)	3753	1937	6267	56
H(17A)	2078	5886	7684	26
H(17B)	809	6794	7735	26
H(18A)	1659	5694	5851	31
H(18B)	1482	7670	6185	31
H(19A)	-576	9180	6197	50
H(19B)	-1181	7693	6814	50
H(19C)	-1864	8404	5708	50
H(20A)	-2242	2591	10522	29
H(20B)	-2901	3878	9633	29
H(20C)	-2219	4650	10723	29
H(21)	-2818	5929	8161	22
H(22)	-4344	5803	6704	26



X-Ray ORTEP diagram of 2-iminoselenazole 9b

Table 1. Crystal data and structure refinement for ch13732. C10(60%), C10'(40%) disorder

Identification code	ch13732	
Empirical formula	C31 H28 N2 O3 Se	
Formula weight	555.51	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 8.6504(3) Å	α= 90°.
	b = 9.7776(4) Å	β= 98.688(2)°.
	c = 16.3783(6) Å	γ = 90°.
Volume	1369.38(9) Å^3	
Z	2	
Density (calculated)	1.347 Mg/m^3	
Absorption coefficient	1.405 mm^{-1}	
F(000)	572	
Crystal size	0.74 x 0.46 x 0.33 mm^3	
Theta range for data collection	1.26 to 25.19°.	
Index ranges	-10<=h<=10, -11<=k<=11, -19<=l<=17	
Reflections collected	9454	
Independent reflections	4712 [R(int) = 0.0241]	
Completeness to theta = 25.19°	98.3 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.6542 and 0.4228	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4712 / 1 / 334	
Goodness-of-fit on F^2	1.082	
Final R indices [I>2sigma(I)]	R1 = 0.0304, wR2 = 0.0683	
R indices (all data)	R1 = 0.0392, wR2 = 0.0730	
Absolute structure parameter	0.014(8)	
Largest diff. peak and hole	0.286 and -0.289 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for ch13732. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7424(3)	10811(4)	7931(2)	37(1)
C(2)	7870(3)	12648(4)	8819(2)	48(1)
C(3)	8712(4)	13595(4)	8444(3)	62(1)
C(4)	9665(4)	14522(5)	8928(3)	79(1)
C(5)	9772(5)	14471(5)	9783(3)	80(1)
C(6)	8912(5)	13555(5)	10149(3)	71(1)
C(7)	7946(4)	12652(4)	9678(2)	56(1)
C(8)	4817(3)	9913(3)	7428(2)	37(1)
C(9)	4294(3)	11273(3)	7027(2)	44(1)
C(10)	2393(7)	13042(6)	6969(4)	47(2)
C(10')	2196(11)	12797(11)	6596(6)	54(3)
C(11)	4176(3)	9646(4)	8246(2)	49(1)
C(12)	4640(3)	8306(4)	8642(2)	45(1)
C(13)	3785(4)	7133(4)	8425(2)	62(1)
C(14)	4248(5)	5886(5)	8799(3)	81(1)
C(15)	5578(6)	5832(6)	9385(3)	88(2)
C(16)	6412(5)	6991(6)	9599(3)	83(1)
C(17)	5970(4)	8210(4)	9235(2)	62(1)
C(18)	7227(3)	9151(3)	6826(2)	37(1)
C(19)	6556(3)	7753(3)	6579(2)	37(1)
C(20)	6470(3)	6738(4)	7167(2)	48(1)
C(21)	5992(4)	5437(4)	6930(2)	57(1)
C(22)	5607(4)	5119(4)	6095(2)	60(1)
C(23)	5692(4)	6109(4)	5526(2)	60(1)
C(24)	6162(3)	7409(4)	5758(2)	46(1)
C(25)	8989(3)	8954(3)	7173(2)	41(1)
C(26)	10006(3)	8612(4)	6532(2)	51(1)
C(27)	10528(4)	7292(5)	6464(3)	71(1)
C(28)	11436(6)	6951(7)	5860(4)	102(2)
C(29)	11811(6)	7909(8)	5331(4)	103(2)
C(30)	11287(5)	9206(7)	5375(3)	92(2)
C(31)	10406(4)	9580(5)	5978(2)	66(1)
N(1)	6856(3)	11687(3)	8358(2)	48(1)
N(2)	6530(2)	9787(3)	7498(2)	35(1)
O(1)	4955(3)	11861(3)	6539(2)	59(1)

O(2)	2969(2)	11720(3)	7257(2)	65(1)
O(3)	7089(2)	10015(2)	6135(1)	45(1)
Se(1)	9588(1)	10637(1)	7798(1)	47(1)

Table 3. Bond lengths [Å] and angles [°] for ch13732.

C(1)-N(1)	1.252(4)
C(1)-N(2)	1.391(4)
C(1)-Se(1)	1.925(3)
C(2)-C(3)	1.379(5)
C(2)-C(7)	1.398(5)
C(2)-N(1)	1.423(4)
C(3)-C(4)	1.390(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.391(6)
C(4)-H(4)	0.9300
C(5)-C(6)	1.360(6)
C(5)-H(5)	0.9300
C(6)-C(7)	1.370(5)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-N(2)	1.474(3)
C(8)-C(9)	1.522(4)
C(8)-C(11)	1.547(5)
C(8)-H(8)	0.9800
C(9)-O(1)	1.198(4)
C(9)-O(2)	1.332(4)
C(10)-O(2)	1.439(6)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(10')-O(2)	1.585(10)
C(10')-H(10D)	0.9600
C(10')-H(10E)	0.9600
C(10')-H(10F)	0.9600
C(11)-C(12)	1.490(5)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.382(5)
C(12)-C(17)	1.392(5)
C(13)-C(14)	1.395(6)
C(13)-H(13)	0.9300
C(14)-C(15)	1.384(6)
C(14)-H(14)	0.9300

C(15)-C(16)	1.360(7)
C(15)-H(15)	0.9300
C(16)-C(17)	1.362(6)
C(16)-H(16)	0.9300
C(17)-H(17)	0.9300
C(18)-O(3)	1.402(3)
C(18)-N(2)	1.471(4)
C(18)-C(19)	1.517(4)
C(18)-C(25)	1.556(4)
C(19)-C(24)	1.378(4)
C(19)-C(20)	1.393(5)
C(20)-C(21)	1.376(6)
C(20)-H(20)	0.9300
C(21)-C(22)	1.393(5)
C(21)-H(21)	0.9300
C(22)-C(23)	1.354(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.371(5)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-C(26)	1.506(4)
C(25)-Se(1)	1.966(3)
C(25)-H(25)	0.9800
C(26)-C(27)	1.377(5)
C(26)-C(31)	1.390(5)
C(27)-C(28)	1.393(6)
C(27)-H(27)	0.9300
C(28)-C(29)	1.349(7)
C(28)-H(28)	0.9300
C(29)-C(30)	1.352(8)
C(29)-H(29)	0.9300
C(30)-C(31)	1.384(6)
C(30)-H(30)	0.9300
C(31)-H(31)	0.9300
O(3)-H(3')	0.8608

N(1)-C(1)-N(2)	122.8(2)
N(1)-C(1)-Se(1)	126.4(2)
N(2)-C(1)-Se(1)	110.7(2)
C(3)-C(2)-C(7)	120.0(3)

C(3)-C(2)-N(1)	122.1(3)
C(7)-C(2)-N(1)	117.9(3)
C(2)-C(3)-C(4)	119.4(4)
C(2)-C(3)-H(3)	120.3
C(4)-C(3)-H(3)	120.3
C(5)-C(4)-C(3)	119.7(4)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(6)-C(5)-C(4)	120.6(4)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(5)-C(6)-C(7)	120.3(4)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(6)-C(7)-C(2)	120.0(4)
C(6)-C(7)-H(7)	120.0
C(2)-C(7)-H(7)	120.0
N(2)-C(8)-C(9)	109.7(2)
N(2)-C(8)-C(11)	113.9(2)
C(9)-C(8)-C(11)	113.5(3)
N(2)-C(8)-H(8)	106.4
C(9)-C(8)-H(8)	106.4
C(11)-C(8)-H(8)	106.4
O(1)-C(9)-O(2)	123.3(3)
O(1)-C(9)-C(8)	124.5(3)
O(2)-C(9)-C(8)	112.1(3)
O(2)-C(10)-H(10A)	109.5
O(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
O(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
O(2)-C(10')-H(10D)	109.5
O(2)-C(10')-H(10E)	109.5
H(10D)-C(10')-H(10E)	109.5
O(2)-C(10')-H(10F)	109.5
H(10D)-C(10')-H(10F)	109.5
H(10E)-C(10')-H(10F)	109.5
C(12)-C(11)-C(8)	114.7(3)
C(12)-C(11)-H(11A)	108.6

C(8)-C(11)-H(11A)	108.6
C(12)-C(11)-H(11B)	108.6
C(8)-C(11)-H(11B)	108.6
H(11A)-C(11)-H(11B)	107.6
C(13)-C(12)-C(17)	118.5(4)
C(13)-C(12)-C(11)	121.3(3)
C(17)-C(12)-C(11)	120.2(3)
C(12)-C(13)-C(14)	120.4(4)
C(12)-C(13)-H(13)	119.8
C(14)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	119.4(5)
C(15)-C(14)-H(14)	120.3
C(13)-C(14)-H(14)	120.3
C(16)-C(15)-C(14)	120.0(5)
C(16)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0
C(15)-C(16)-C(17)	120.9(4)
C(15)-C(16)-H(16)	119.5
C(17)-C(16)-H(16)	119.5
C(16)-C(17)-C(12)	120.8(4)
C(16)-C(17)-H(17)	119.6
C(12)-C(17)-H(17)	119.6
O(3)-C(18)-N(2)	110.8(2)
O(3)-C(18)-C(19)	110.2(2)
N(2)-C(18)-C(19)	113.4(2)
O(3)-C(18)-C(25)	109.2(2)
N(2)-C(18)-C(25)	105.6(2)
C(19)-C(18)-C(25)	107.5(2)
C(24)-C(19)-C(20)	118.1(3)
C(24)-C(19)-C(18)	120.6(3)
C(20)-C(19)-C(18)	121.1(3)
C(21)-C(20)-C(19)	120.5(3)
C(21)-C(20)-H(20)	119.7
C(19)-C(20)-H(20)	119.7
C(20)-C(21)-C(22)	120.1(4)
C(20)-C(21)-H(21)	120.0
C(22)-C(21)-H(21)	120.0
C(23)-C(22)-C(21)	119.1(3)
C(23)-C(22)-H(22)	120.4
C(21)-C(22)-H(22)	120.4

C(22)-C(23)-C(24)	121.1(3)
C(22)-C(23)-H(23)	119.4
C(24)-C(23)-H(23)	119.4
C(23)-C(24)-C(19)	121.1(3)
C(23)-C(24)-H(24)	119.5
C(19)-C(24)-H(24)	119.5
C(26)-C(25)-C(18)	114.6(3)
C(26)-C(25)-Se(1)	114.4(2)
C(18)-C(25)-Se(1)	104.7(2)
C(26)-C(25)-H(25)	107.6
C(18)-C(25)-H(25)	107.6
Se(1)-C(25)-H(25)	107.6
C(27)-C(26)-C(31)	117.9(4)
C(27)-C(26)-C(25)	119.8(4)
C(31)-C(26)-C(25)	122.2(3)
C(26)-C(27)-C(28)	120.5(5)
C(26)-C(27)-H(27)	119.7
C(28)-C(27)-H(27)	119.7
C(29)-C(28)-C(27)	120.4(5)
C(29)-C(28)-H(28)	119.8
C(27)-C(28)-H(28)	119.8
C(28)-C(29)-C(30)	120.1(5)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(29)-C(30)-C(31)	120.8(5)
C(29)-C(30)-H(30)	119.6
C(31)-C(30)-H(30)	119.6
C(30)-C(31)-C(26)	120.2(5)
C(30)-C(31)-H(31)	119.9
C(26)-C(31)-H(31)	119.9
C(1)-N(1)-C(2)	119.1(3)
C(1)-N(2)-C(18)	115.2(2)
C(1)-N(2)-C(8)	117.0(2)
C(18)-N(2)-C(8)	119.8(2)
C(9)-O(2)-C(10)	118.1(3)
C(9)-O(2)-C(10')	108.5(4)
C(10)-O(2)-C(10')	24.4(4)
C(18)-O(3)-H(3')	108.0
C(1)-Se(1)-C(25)	87.03(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$)for ch13732. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	30(1)	44(2)	38(2)	-1(2)	7(1)	-5(2)
C(2)	38(2)	54(2)	52(2)	-14(2)	3(2)	4(2)
C(3)	52(2)	60(3)	75(3)	-6(2)	15(2)	-13(2)
C(4)	63(2)	64(3)	113(4)	-17(3)	21(2)	-18(2)
C(5)	63(2)	75(3)	97(4)	-32(3)	-8(2)	-7(2)
C(6)	75(3)	69(3)	64(3)	-20(2)	-8(2)	-1(2)
C(7)	55(2)	52(2)	59(3)	-10(2)	7(2)	-2(2)
C(8)	28(2)	44(2)	40(2)	2(2)	8(1)	-4(1)
C(9)	32(2)	42(2)	56(2)	-5(2)	3(2)	-1(1)
C(11)	38(2)	56(2)	57(2)	6(2)	18(2)	1(2)
C(12)	39(2)	58(2)	41(2)	5(2)	20(2)	2(2)
C(13)	63(2)	63(3)	64(3)	10(2)	23(2)	-9(2)
C(14)	97(3)	68(4)	90(3)	2(3)	47(3)	-11(3)
C(15)	108(3)	79(4)	88(3)	34(3)	52(3)	36(3)
C(16)	79(3)	108(4)	63(3)	23(3)	14(2)	30(3)
C(17)	57(2)	79(3)	53(2)	4(2)	14(2)	6(2)
C(18)	29(1)	46(2)	35(2)	3(2)	4(1)	-1(1)
C(19)	29(1)	43(2)	41(2)	-1(2)	8(1)	0(1)
C(20)	50(2)	53(2)	41(2)	-2(2)	9(2)	-3(2)
C(21)	60(2)	49(3)	63(2)	6(2)	20(2)	-9(2)
C(22)	60(2)	54(3)	65(3)	-18(2)	11(2)	-10(2)
C(23)	66(2)	72(3)	41(2)	-18(2)	2(2)	-7(2)
C(24)	47(2)	58(2)	32(2)	2(2)	5(2)	0(2)
C(25)	31(1)	45(2)	45(2)	2(2)	3(1)	2(1)
C(26)	33(2)	64(3)	58(2)	-11(2)	9(2)	2(2)
C(27)	59(2)	76(3)	79(3)	-4(2)	11(2)	21(2)
C(28)	83(3)	108(5)	117(4)	-37(4)	27(3)	38(3)
C(29)	72(3)	152(6)	94(4)	-18(4)	41(3)	17(4)
C(30)	68(3)	130(5)	87(3)	-2(3)	45(2)	-4(3)
C(31)	54(2)	76(3)	75(3)	-1(2)	33(2)	-6(2)
N(1)	35(1)	53(2)	55(2)	-14(2)	7(1)	-5(1)
N(2)	28(1)	42(2)	36(2)	-1(1)	5(1)	-2(1)
O(1)	60(1)	52(2)	70(2)	18(1)	25(1)	8(1)
O(2)	38(1)	51(2)	109(2)	21(2)	23(1)	8(1)
O(3)	46(1)	51(1)	39(1)	13(1)	10(1)	9(1)

Se(1)	28(1)	56(1)	56(1)	-7(1)	5(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for ch13732.

	x	y	z	U(eq)
H(3)	8643	13613	7872	74
H(4)	10229	15172	8681	95
H(5)	10438	15070	10109	96
H(6)	8980	13541	10721	85
H(7)	7341	12041	9930	67
H(8)	4374	9200	7042	44
H(10A)	1436	13233	7177	71
H(10B)	2204	13047	6376	71
H(10C)	3155	13728	7162	71
H(10D)	1237	13127	6753	82
H(10E)	1982	12368	6064	82
H(10F)	2900	13550	6571	82
H(11A)	4538	10371	8632	59
H(11B)	3043	9693	8138	59
H(13)	2897	7174	8028	75
H(14)	3667	5098	8655	98
H(15)	5903	5004	9632	105
H(16)	7295	6950	10000	100
H(17)	6564	8989	9385	75
H(20)	6739	6942	7725	57
H(21)	5925	4769	7327	68
H(22)	5295	4238	5931	72
H(23)	5427	5904	4968	72
H(24)	6216	8069	5355	55
H(25)	9069	8196	7568	49
H(27)	10272	6623	6825	85
H(28)	11785	6057	5822	122
H(29)	12431	7677	4934	123
H(30)	11522	9854	4997	110
H(31)	10080	10481	6012	79
H(3')	6450	10663	6209	53

Reference:

1. López, Ó .; Maza, S.; Ulgar, V.; Maya, l.; Fernández-Bolaños, J. *Tetrahedron.* **2009**, *65*, 2556-2566.
2. Galina, K.; Jaroslav, R.; Zdeňka, P.; Zdeněk, N.; Kateřina, V.; Alexandr, H. *Tetrahedron.* **2013**, 6*9*, 8798-8808.