Supporting Information for
α-Arylation of Alkylamines with Sulfonylarenes through a Radical Chain Mechanism

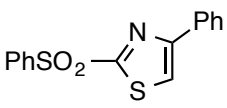
Yuko Ikeda, Ryota Ueno, Yuto Akai and Eiji Shirakawa

General Remarks. All manipulations of oxygen- and moisture-sensitive materials were conducted in a glove box under a nitrogen atmosphere. Nuclear magnetic resonance spectra were taken on a JEOL JNM ECZ500R spectrometer (^{1}H, 500 MHz and ^{13}C, 125 MHz) or a JEOL ECA300 spectrometer (^{1}H, 300 MHz). High-resolution mass spectra were obtained with a Bruker Daltonics micrOTOF-Q spectrometer (ESI). GC spectra were taken on Shimadzu GC-2014. GC-MS spectra were taken on Shimadzu GCMS-QP2010 SE. GC and GC-MS were equipped with capillary column SGE BPX5. Preparative recycling gel permeation chromatography (GPC) was performed with JAI LC-908 equipped with JAIGEL-1H and -2H using chloroform as an eluent. Medium pressure liquid chromatography (MPLC) was performed with YAMAZEN EPCLC-W-Prep 2XY using silica gel 60 N (spherical neutral, 40–50 μm). Unless otherwise noted, reagents were commercially available and used without further purification. *tert*-Butyl(dimethyl)amine (**2b**),[1] 2-methoxyethyl(dimethyl)amine (**2g**),[2] [2-(methoxycarbonyl)ethyl](dimethyl)amine (**2i**),[3] butyl(*tert*-butyldimethylsilyl)amine (**4o**),[4] (*tert*-butyldimethylsilyl)isobutylamine (**4p**),[4] (*tert*-butyldimethylsilyl)-(2-methoxyethyl)amine (**4q**),[4] (*tert*-butyldimethylsilyl)[2-(*tert*-butyldimethylsilyloxy)-ethyl]amine (**4r**),[4] *N*,*N*'-bis(*tert*-butyldimethylsilyl)ethylenediamine (**4s**),[4] (*tert*-butyldimethylsilyl)[2-(ethoxycarbonyl)ethyl]amine (**4t**),[4] and di-*tert*-butyl hyponitrite (*t*-BuON=NO*t*-Bu)[5] were prepared according to literature procedures.

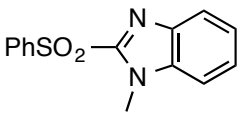
Synthesis of Sulfonylarenes. 2-(Benzenesulfonyl)benzothiazoles (**2a**, **2h**, **2i**), 2-(benzenesulfonyl)thiazoles (**2b**, **2c**, **2g**), 2- and 4-(benzenesulfonyl)benzonitrile (**2j**, **2k**), methyl 4-(benzenesulfonyl)benzoate (**2l**), 2-(benzenesulfonyl)pyrimidine (**2n**), 2-(benzenesulfonyl)pyridine (**2o**), and 1-(benzenesulfonyl)isoquinoline (**2p**) were prepared by the reaction of the corresponding haloheteroarenes or aryl fluorides with sodium benzenesulfinate.[6] 2-(Benzenesulfonyl)-5-phenyloxazole (**2d**) was prepared through deprotonation from 5-phenyloxazole by butyllithium, phenylthiolation with

diphenyl disulfide, and oxidation by ammonium molybdate.[7] 2-(Benzenesulfonyl)benzimidazole and 2-(benzenesulfonyl)-1-methylbenzimidazole (**2e**, **2f**) were prepared according to the literature procedure.[8] 1-(Benzenesulfonyl)naphthalene (**2m**) was prepared according to the literature procedure.[9] 2-[3,3-Bis(ethoxycarbonyl)-5-hexenesulfonyl]benzothiazole (**2"a**) was prepared through successive allylation and bromoethylation of diethyl malonate, nucleophilic substitution of the resulting alkyl bromide with 2-mercaptobenzothiazole, and oxidation by ammonium molybdate.

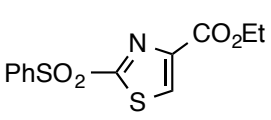
Spectrum Data of Sulfonylarenes



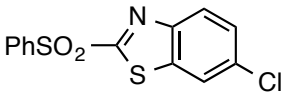
2-(Benzenesulfonyl)-4-phenylthiazole (2c). A pale orange solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (t, *J* = 8.6 Hz, 1 H), 7.42 (t, *J* = 8.0 Hz, 2 H), 7.58 (t, *J* = 8.0 Hz, 2 H), 7.66 (t, *J* = 8.0 Hz, 1 H), 7.76 (s, 1 H), 7.86 (d, *J* = 8.0 Hz, 2 H), 8.16 (d, *J* = 8.6 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 119.1, 126.8, 128.9, 129.0, 129.3, 129.6, 133.0, 134.4, 139.1, 158.5, 166.7. HRMS (ESI) Calcd for $C_{15}H_{11}NO_2S_2$: $[M+Na]^+$, 324.0123. Found: m/z 324.0124.



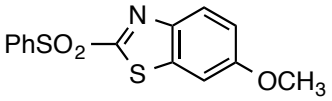
2-(Benzenesulfonyl)-1-methylbenzimidazole (2f). A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.13 (s, 3 H), 7.35 (t, *J* = 7.7 Hz, 1 H), 7.38–7.49 (m, 2 H), 7.59 (t, *J* = 8.0 Hz, 2 H), 7.68 (t, *J* = 8.0 Hz, 1 H), 7.85 (d, *J* = 8.0 Hz, 1 H), 8.13 (d, *J* = 8.0 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 31.9, 110.6, 122.2, 124.1, 126.1, 128.8, 129.6, 134.6, 136.4, 139.2, 141.3, 148.6. HRMS (ESI) Calcd for $C_{14}H_{12}N_2O_2S$: $[M+Na]^+$, 295.0512. Found: m/z 295.0513.



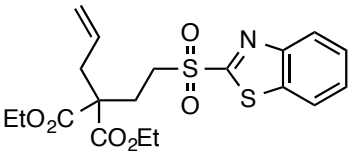
2-(Benzenesulfonyl)-4-(ethoxycarbonyl)thiazole (2g). A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.37 (t, *J* = 7.2 Hz, 3 H), 4.40 (q, *J* = 7.2 Hz, 2 H), 7.59 (t, *J* = 7.8 Hz, 2 H), 7.68 (t, *J* = 7.4 Hz, 1 H), 8.14 (d, *J* = 7.5 Hz, 2 H), 8.39 (s, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.4, 62.2, 129.1, 129.7, 132.6, 134.8, 138.3, 149.6, 160.3, 167.9. HRMS (ESI) Calcd for $C_{12}H_{11}NO_4S_2$: $[M+Na]^+$, 320.0022. Found: m/z 320.0025.



2-(Benzenesulfonyl)-6-chlorobenzothiazole (2h). A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 8.9, 2.0 Hz, 1 H), 7.60 (t, *J* = 8.0 Hz, 2 H), 7.69 (t, *J* = 8.6 Hz, 1 H), 7.95 (d, *J* = 2.0 Hz, 1 H), 8.06 (d, *J* = 8.6 Hz, 1 H), 8.16 (d, *J* = 8.6 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 121.9, 126.5, 128.8, 129.2, 129.8, 134.4, 134.9, 138.2, 138.3, 151.5, 168.0. HRMS (ESI) Calcd for $C_{13}H_8NO_2S_2Cl$: $[M+Na]^+$, 331.9577. Found: m/z 331.9577.



2-(Benzenesulfonyl)-6-methoxybenzothiazole (2i). A pale pink solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.89 (s, 3 H), 7.16 (dd, *J* = 9.2, 2.3 Hz, 1 H), 7.34 (d, *J* = 2.3 Hz, 1 H), 7.57 (t, *J* = 8.0 Hz, 2 H), 7.65 (t, *J* = 8.0 Hz, 1 H), 8.02 (d, *J* = 9.2 Hz, 1 H), 8.15 (d, *J* = 8.3 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 56.1, 103.5, 118.2, 126.4, 128.9, 129.6, 134.5, 139.0, 139.2, 147.6, 159.8, 164.0. HRMS (ESI) Calcd for $C_{14}H_{11}NO_3S_2$: $[M+Na]^+$, 328.0073. Found: m/z 328.0066.

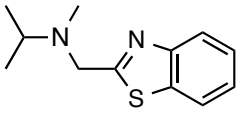


2-[3,3-Bis(ethoxycarbonyl)-5-hexenesulfonyl]benzothia zole (2"a). A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.22 (t, *J* = 7.2 Hz, 6 H), 2.32–2.41 (m, 2 H), 2.64 (d, *J* = 7.5 Hz, 2 H), 3.55–3.63 (m, 2 H), 4.11–4.23 (m, 4 H), 5.05 (d, *J* = 10.3 Hz, 1 H), 5.11 (dd, *J* = 17.2, 1.7 Hz, 1 H), 5.57 (ddt, *J* = 17.2, 10.3, 7.5 Hz, 1 H), 7.61 (t, *J* = 7.7 Hz, 1 H), 7.65 (t, *J* = 7.8 Hz, 1 H), 8.03 (d, *J* = 8.0 Hz, 1 H), 8.21 (d, *J* = 8.1 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.2, 25.7, 38.0, 50.7, 56.2, 62.0, 120.3, 122.5, 125.6, 127.9, 128.2, 131.3, 137.0, 152.8, 165.3, 170.0. HRMS (ESI) Calcd for $C_{19}H_{23}NO_6S_2$: $[M+Na]^+$, 448.0859. Found: m/z 448.0863.

α-Arylation of Alkylamines with Sulfonylarenes: General Procedure (Tables 1–4). To a 4 mL vial equipped with a stir bar in a glove box were added successively an amine (**1**: 0.45 mmol), a sulfonylarene (**2**: 0.25 mmol), methanol (0.50 mL) and *t*-BuON=NO*t*-Bu (8.7 mg, 0.050 mmol). The vial was taken out of the glove box and stirred at 50 °C for 8 h. The reaction mixture was poured into sat. $NaHCO_3$ aq. (15 mL), extracted with ethyl acetate (3 x 15 mL), and dried over Na_2SO_4. After filtration and concentration, the crude mixture was subjected to silica gel chromatography to give the corresponding product (**3**).

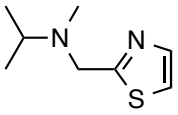
Spectrum Data of the α-Arylation Products

Table 1

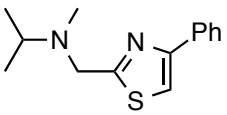


(2-Benzothiazolylmethyl)(isopropyl)(methyl)amine (3aa). A yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.10 (d, J = 6.9 Hz, 6 H), 2.36 (s, 3 H), 3.00 (sept, J = 6.7 Hz, 1 H), 3.95 (s, 2 H), 7.34 (t, J = 7.4 Hz, 1 H), 7.44 (t, J = 7.2 Hz, 1 H), 7.86 (d, J = 7.9 Hz, 1 H), 7.94 (d, J = 7.9 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.2, 38.0, 54.0, 55.7, 121.8, 122.7, 124.7, 125.8, 135.5, 153.7, 175.9. HRMS (ESI) Calcd for $C_{12}H_{16}N_2S$: $[M+H]^+$, 221.1107. Found: m/z 221.1115.

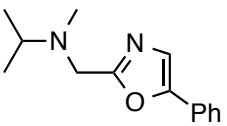
Table 2



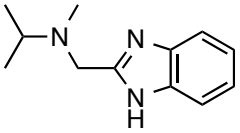
Isopropyl(methyl)(2-thiazolylmethyl)amine (3ab). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.07 (d, J = 6.3 Hz, 6 H), 2.30 (s, 3 H), 2.94 (sept, J = 6.3 Hz, 1 H), 3.85 (s, 2 H), 7.25 (d, J = 2.9 Hz, 1 H), 7.68 (d, J = 2.9 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.2, 37.8, 53.8, 55.0, 119.4, 142.4, 173.8. HRMS (ESI) Calcd for $C_8H_{14}N_2S$: $[M+H]^+$, 171.0950. Found: m/z 171.0956.



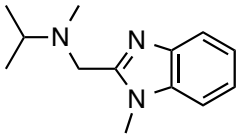
Isopropyl(methyl)[2-(4-phenylthiazolyl)methyl]amine (3ac). A pale yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.10 (d, J = 6.3 Hz, 6 H), 2.36 (s, 3 H), 3.00 (sept, J = 6.3 Hz, 1 H), 3.91 (s, 2 H), 7.31 (t, J = 7.5 Hz, 1 H), 7.38–7.45 (m, 3 H), 7.88 (d, J = 8.1 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.2, 38.0, 53.9, 55.2, 113.2, 126.3, 128.0, 128.8, 134.9, 155.2, 174.4. HRMS (ESI) Calcd for $C_{14}H_{18}N_2S$: $[M+H]^+$, 247.1263. Found: m/z 247.1272.



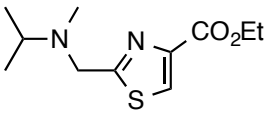
Isopropyl(methyl)[2-(5-phenyloxazolyl)methyl]amine (3ad). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.10 (d, J = 6.3 Hz, 6 H), 2.36 (s, 3 H), 2.90 (sept, J = 6.3 Hz, 1 H), 3.79 (s, 2 H), 7.26 (1 H), 7.30 (t, J = 7.5 Hz, 1 H), 7.40 (t, J = 8.0 Hz, 2 H), 7.64 (d, J = 8.6 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.6, 38.1, 50.4, 53.5, 122.0, 124.4, 128.2, 128.4, 129.0, 151.7, 162.2. HRMS (ESI) Calcd for $C_{14}H_{18}N_2O$: $[M+H]^+$, 231.1492. Found: m/z 231.1500.



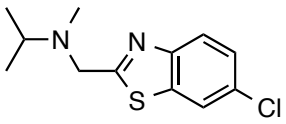
(2-Benzimidazolylmethyl)(isopropyl)(methyl)amine (3ae). A pale yellow solid. ^{1}H NMR (500 MHz, DMSO-d_6) δ 1.04 (d, J = 6.3 Hz, 6 H), 2.18 (s, 3 H), 2.88 (sept, J = 6.3 Hz, 1 H), 3.76 (s, 2 H), 7.07–7.16 (m, 2 H), 7.43–7.54 (m, 2 H). ^{13}C NMR (125 MHz, DMSO-d_6) δ 17.7, 37.0, 51.3, 52.9, 121.3, 153.3. HRMS (ESI) Calcd for $C_{12}H_{17}N_3$: $[M+H]^+$, 204.1495. Found: m/z 204.1499.



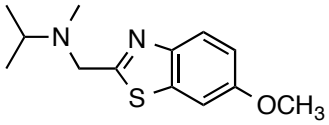
Isopropyl(methyl)[2-(1-methylbenzimidazolyl)methyl]amine (3af). A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.09 (d, J = 6.9 Hz, 6 H), 2.17 (s, 3 H), 2.90 (sept, J = 6.9 Hz, 1 H), 3.84 (s, 2 H), 3.86 (s, 3 H), 7.23 (*t*, J = 7.5 Hz, 1 H), 7.26 (*t*, J = 6.9 Hz, 1 H), 7.33 (d, J = 8.0 Hz, 1 H), 7.72 (d, J = 7.5 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 17.7, 30.2, 36.4, 51.5, 53.5, 109.1, 119.6, 121.8, 122.4, 136.6, 142.4, 152.8. HRMS (ESI) Calcd for $C_{13}H_{19}N_3$: $[M+H]^+$, 218.1652. Found: m/z 218.1660.



[2-(4-Ethoxycarbonylthiazolyl)methyl](isopropyl)(methyl)-amine (3ag). A pale yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.05 (d, J = 7.2 Hz, 6 H), 1.39 (t, J = 6.9 Hz 3 H), 2.30 (s, 3 H), 2.94 (sept, J = 6.5 Hz, 1 H), 3.85 (s, 2 H), 4.40 (q, J = 6.9 Hz 2 H), 8.11 (s, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.5, 18.2, 37.9, 54.0, 54.9, 61.4, 128.3, 147.0, 161.8, 176.3. HRMS (ESI) Calcd for $C_{11}H_{18}N_2O_2S$: $[M+H]^+$, 243.1162. Found: m/z 243.1162.



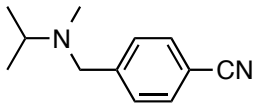
[2-(6-Chlorobenzothiazolyl)methyl](isopropyl)(methyl)-amine (3ah). A pale orange solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.10 (d, J = 6.3 Hz, 6 H), 2.35 (s, 3 H), 2.99 (sept, J = 6.3 Hz, 1 H), 3.92 (s, 2 H), 7.39 (dd, J = 8.6, 1.7 Hz, 1 H), 7.83 (s, 1 H), 7.83 (d, J = 8.6 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.2, 38.0, 54.1, 55.6, 121.5, 123.4, 126.5, 130.6, 136.8, 152. 3, 177. 0. HRMS (ESI) Calcd for $C_{12}H_{15}N_2SCl$: $[M+H]^+$, 255.0717. Found: m/z 255.0721.



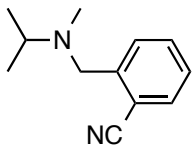
Isopropyl[2-(6-Methoxybenzothiazolyl)methyl](methyl)-amine (3ai). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ

1.10 (d, J = 6.3 Hz, 6 H), 2.35 (s, 3 H), 3.00 (sept, J = 6.3 Hz, 1 H), 3.87 (s, 3 H), 3.91 (s, 2 H), 7.03 (dd, J = 8.6, 2.3 Hz, 1 H), 7.31 (d, J = 2.3 Hz, 1 H), 7.81 (d, J = 8.6 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.1, 37.9, 53.9, 55.6, 55.9, 104.5, 115.0, 123.2, 136.9, 148.1, 157.4, 172.9. HRMS (ESI) Calcd for $C_{13}H_{18}N_2OS$: $[M+H]^+$, 251.1213. Found: m/z 251.1220.

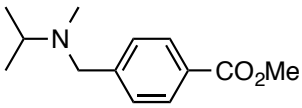
Table 3



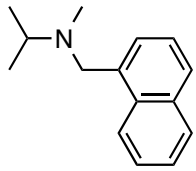
[(4-Cyanophenyl)methyl](methyl)(isopropyl)amine (3aj). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.06 (d, J = 6.9 Hz, 6 H), 2.13 (s, 3 H), 2.87 (sept, J = 6.9 Hz, 1 H), 3.54 (s, 2 H), 7.45 (d, J = 8.6 Hz, 2 H), 7.59 (d, J = 8.6 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.0, 37.1, 53.6, 57.3, 110.6, 119.3, 129.3, 132.2, 146.5. HRMS (ESI) Calcd for $C_{12}H_{16}N_2$: $[M+H]^+$, 189.1386. Found: m/z 189.1388.



[(2-Cyanophenyl)methyl](isopropyl)(methyl)amine (3ak). A pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.09 (d, J = 6.9 Hz, 6 H), 2.15 (s, 3 H), 2.95 (sept, J = 6.9 Hz, 1 H), 3.71 (s, 2 H), 7.32 (t, J = 7.5 Hz, 1 H), 7.53 (t, J = 7.5 Hz, 1 H), 7.58 (d, J = 7.5 Hz, 1 H), 7.62 (d, J = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.0, 36.6, 54.0, 55.8, 112.7, 118.1, 127.3, 129.9, 132.7, 133.0, 144.6. HRMS (ESI) Calcd for $C_{12}H_{16}N_2$: $[M+H]^+$, 189.1386. Found: m/z 189.1393.

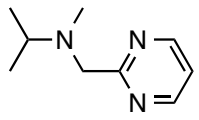


Isopropyl[4-(methoxycarbonyl)phenylmethyl](methyl)-amine (3al). A pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.07 (d, J = 6.3 Hz, 6 H), 2.14 (s, 3 H), 2.88 (sept, J = 6.3 Hz, 1 H), 3.55 (s, 2 H), 3.90 (s, 3 H), 7.41 (d, J = 8.6 Hz, 2 H), 7.97 (d, J = 8.6 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.0, 37.1, 52.1, 53.5, 57.4, 128.7, 128.8, 129.7, 146.1, 167.3. HRMS (ESI) Calcd for $C_{13}H_{19}NO_2$: $[M+H]^+$, 222.1489. Found: m/z 222.1482.

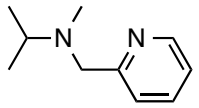


Isopropyl(methyl)[(1-Naphtyl)methyl]amine (3am). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.15 (d, J = 6.3 Hz, 6 H), 2.17 (s, 3 H), 3.02 (sept, J = 6.3 Hz, 1 H), 3.96 (s, 2 H), 7.41 (t, J = 7.5 Hz, 1 H)

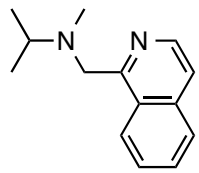
7.44–7.55 (m, 3 H), 7.76 (d, J = 8.0 Hz, 1 H), 7.85 (d, J = 8.0 Hz, 1 H), 8.31 (d, J = 8.6 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 17.9, 36.5, 53.7, 56.4, 124.6, 125.3, 125.6, 125.9, 127.3, 127.8, 128.6, 132.7, 134.0, 135.7. HRMS (ESI) Calcd for $C_{15}H_{19}N$: $[M+H]^+$, 214.1590. Found: m/z 214.1599.



Isopropyl(methyl)[(2-pyrimidyl)methyl]amine (3an). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.08 (d, J = 6.9 Hz, 6 H), 2.28 (s, 3 H), 2.94 (sept, J = 6.9 Hz, 1 H), 3.81 (s, 2 H), 7.14 (t, J = 5.2 Hz, 1 H), 8.70 (d, J = 5.2 Hz, 2 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.1, 38.1, 54.1, 59.9, 119.2, 157.3, 169.4. HRMS (ESI) Calcd for $C_9H_{15}N_3$: $[M+H]^+$, 166.1339. Found: m/z 166.1335.

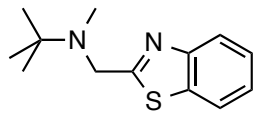


Isopropyl(methyl)[(2-pyridyl)methyl]amine (3ao). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.07 (d, J = 6.3 Hz, 6 H), 2.19 (s, 3 H), 2.90 (sept, J = 6.3 Hz, 1 H), 3.66 (s, 2 H), 7.12 (dd, J = 7.5, 4.6 Hz, 1 H), 7.44 (d, J = 7.5 Hz, 1 H), 7.63 (t, J = 7.5 Hz, 1 H), 8.51 (d, J = 4.6 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.1, 37.4, 53.8, 59.4, 121.9, 123.0, 136.5, 149.1, 160.7. HRMS (ESI) Calcd for $C_{10}H_{16}N_2$: $[M+H]^+$, 165.1386. Found: m/z 165.1382.



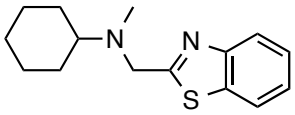
Isopropyl[(2-isoquinolyl)methyl](methyl)amine (3ap). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.15 (d, J = 6.3 Hz, 6 H), 2.17 (s, 3 H), 3.02 (sept, J = 6.3 Hz, 1 H), 4.13 (s, 2 H), 7.55 (d, J = 5.7 Hz, 1 H), 7.57 (t, J = 7.5 Hz, 1 H) 7.64 (t, J = 6.9 Hz, 1 H), 7.79 (d, J = 8.0 Hz, 1 H), 8.43 (d, J = 5.7 Hz, 1 H), 8.52 (d, J = 8.6 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 17.8, 36.7, 54.2, 58.9, 120.5, 126.4, 127.0, 127.1, 127.9, 130.0, 136.5, 141.6, 159.4. HRMS (ESI) Calcd for $C_{14}H_{18}N_2$: $[M+H]^+$, 215.1543. Found: m/z 215.1545.

Table 4

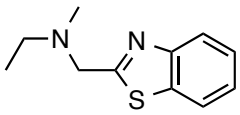


(2-Benzothiazolylmethyl)(*tert*-butyl)(methyl)amine (3ba). A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.18 (s, 9 H), 2.35 (s, 3 H), 3.96 (s, 2 H), 7.33 (t, J = 7.4 Hz, 1 H), 7.43 (t, J = 8.0 Hz, 1 H), 7.85 (d, J = 8.0 Hz, 1 H), 7.92 (d, J = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 26.4, 36.8, 54.0, 54.7, 121.8, 122.6, 124.5, 125.7, 135.5, 154.0, 178.1. HRMS (ESI)

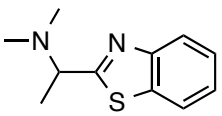
Calcd for $C_{13}H_{18}N_2S$: $[M+H]^+$, 235.1263. Found: m/z 235.1262.



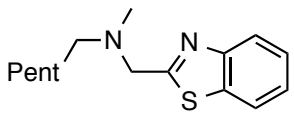
(2-Benzothiazolylmethyl)(cyclohexyl)(methyl)amine (3ca). A pale yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.05–1.17 (m, 1 H), 1.18–1.35 (m, 4 H), 1.63 (d, *J* = 13.2 Hz, 1 H), 1.81 (d, *J* = 12.0 Hz, 2 H), 1.91 (d, *J* = 10.3 Hz, 2 H), 2.41 (s, 3 H), 2.48–2.57 (m, 1 H), 4.00 (s, 2 H), 7.34 (t, *J* = 7.7 Hz, 1 H), 7.43 (t, *J* = 7.5 Hz, 1 H), 7.86 (d, *J* = 8.0 Hz, 1 H), 7.94 (d, *J* = 8.1 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 26.0, 26.3, 29.0, 38.8, 56.0, 63.0, 121.9, 122.7, 124.7, 125.7, 135.5, 153.7, 176.4. HRMS (ESI) Calcd for $C_{15}H_{20}N_2S$: $[M+H]^+$, 261.1420. Found: m/z 261.1420.



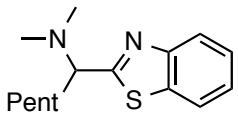
(2-Benzothiazolylmethyl)(ethyl)(methyl)amine (3da). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.14 (t, *J* = 7.2 Hz, 3 H), 2.39 (s, 3 H), 2.60 (q, *J* = 7.2 Hz, 2 H), 3.95 (s, 2 H), 7.35 (t, *J* = 7.5 Hz, 1 H), 7.44 (t, *J* = 7.7 Hz, 1 H), 7.87 (d, *J* = 8.0 Hz, 1 H), 7.96 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 12.7, 42.5, 51.8, 59.6, 121.8, 122.8, 124.9, 125.9, 135.5, 153.4, 173.6. HRMS (ESI) Calcd for $C_{11}H_{14}N_2S$: $[M+H]^+$, 207.0950. Found: m/z 207.0953.



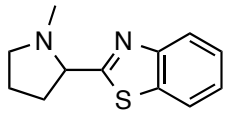
[1-(2-Benzothiazolyl)ethyl](dimethyl)amine (3'da). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.53 (d, *J* = 6.3 Hz, 3 H), 2.37 (s, 6 H), 3.97 (q, *J* = 6.3 Hz, 1 H), 7.36 (t, *J* = 7.5 Hz, 1 H), 7.45 (t, *J* = 7.7 Hz, 1 H), 7.87 (d, *J* = 8.0 Hz, 1 H), 7.98 (d, *J* = 8.1 Hz, 1 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 16.4, 42.5, 63.5, 121.9, 123.0, 124.9, 125.8, 135.5, 153.2, 177.5. HRMS (ESI) Calcd for $C_{11}H_{14}N_2S$: $[M+H]^+$, 207.0950. Found: m/z 207.0957.



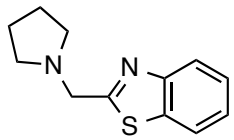
(2-Benzothiazolylmethyl)(hexyl)(methyl)amine (3ea). A pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.88 (t, *J* = 7.2 Hz, 3 H), 1.24–1.39 (m, 6 H), 1.53 (quint, *J* = 7.5 Hz, 2 H), 2.38 (s, 3 H), 2.52 (t, *J* = 7.5 Hz, 2 H), 3.94 (s, 2 H), 7.35 (t, *J* = 8.0 Hz, 1 H), 7.45 (t, *J* = 8.3 Hz, 1 H), 7.87 (d, *J* = 8.0 Hz, 1 H), 7.96 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.2, 22.8, 27.0, 27.6, 31.9, 43.0, 58.0, 60.1, 121.9, 122.8, 124.8, 125.9, 135.6, 153.4, 174.0. HRMS (ESI) Calcd for $C_{15}H_{22}N_2S$: $[M+H]^+$, 263.1576. Found: m/z 263.1584.



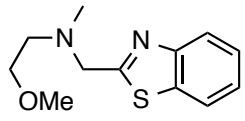
[1-(2-Benzothiazolyl)pentyl](dimethyl)amine (3'ea). A pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.85 (t, *J* = 6.9 Hz, 3 H), 1.20–1.44 (m, 6 H), 1.84–2.03 (m, 2 H), 2.36 (s, 6 H), 3.83 (dd, *J* = 8.9, 5.4 Hz, 1 H), 7.37 (t, *J* = 7.7 Hz, 1 H), 7.46 (t, *J* = 7.7 Hz, 1 H), 7.88 (d, *J* = 8.0 Hz, 1 H), 8.02 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.2, 22.6, 26.3, 32.0, 33.3, 42.6, 68.3, 121.8, 123.1, 125.0, 125.9, 135.2, 153.0, 173.8. HRMS (ESI) Calcd for $C_{15}H_{22}N_2S$: $[M+H]^+$, 263.1576. Found: m/z 263.1579.



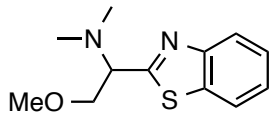
2-(1-Methyl-2-pyrrolidinyl)benzothiazole (3fa). A pale yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.80–2.06 (m, 3 H), 2.37–2.49 (m, 2 H), 2.44 (s, 3 H), 3.27 (t, *J* = 7.5 Hz, 1 H), 3.80 (dd, *J* = 8.9, 6.6 Hz, 1 H), 7.34 (t, *J* = 8.0 Hz, 1 H), 7.44 (t, *J* = 7.7 Hz, 1 H), 7.87 (d, *J* = 7.5 Hz, 1 H), 7.95 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 23.7, 34.6, 41.4, 57.1, 68.4, 122.0, 122.7, 124.7, 125.8, 135.2, 153.8, 179.1. HRMS (ESI) Calcd for $C_{12}H_{14}N_2S$: $[M+H]^+$, 219.0950. Found: m/z 219.0945.



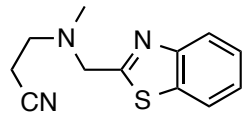
2-(1-Pyrrolidinylmethyl)benzothiazole (3'fa). A pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.79–1.92 (m, 4 H), 2.65–2.81 (m, 4 H), 4.10 (s, 2 H), 7.36 (t, *J* = 7.7 Hz, 1 H), 7.45 (t, *J* = 7.5 Hz, 1 H), 7.87 (d, *J* = 8.0 Hz, 1 H), 7.98 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 24.0, 54.6, 58.2, 121.8, 122.9, 124.9, 125.9, 135.5, 153.3, 172.7. HRMS (ESI) Calcd for $C_{12}H_{14}N_2S$: $[M+H]^+$, 219.0950. Found: m/z 219.0950.



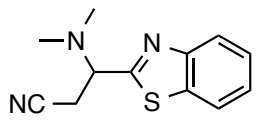
(2-Benzothiazolylmethyl)(2-methoxyethyl)(methyl)amine (3ga). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.47 (s, 3 H), 2.78 (t, *J* = 5.7 Hz, 2 H), 3.36 (s, 3 H), 3.57 (t, *J* = 5.7 Hz, 2 H), 4.05 (s, 2 H), 7.36 (t, *J* = 7.7 Hz, 1 H), 7.45 (t, *J* = 7.7 Hz, 1 H), 7.87 (d, *J* = 8.0 Hz, 1 H), 7.96 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 43.5, 56.8, 59.0, 60.2, 71.1, 121.9, 122.9, 124.9, 125.9, 135.6, 153.4, 172.9. HRMS (ESI) Calcd for $C_{12}H_{16}N_2OS$: $[M+H]^+$, 237.1056. Found: m/z 237.1054.



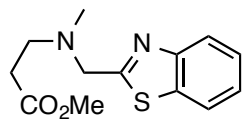
2-[1-(Dimethylamino)-2-methoxyethyl]benzothiazole (3'ga). This product could not be isolated in a pure form. The following data were obtained from a spectrum of a mixture with **3ga (3'ga**: **3ga** = 40:60). ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.46 (s, 6 H), 3.40 (s, 3 H), 3.89 (dd, *J* = 10.3, 6.3 Hz, 1 H), 3.99 (dd, *J* = 9.7, 4.9 Hz, 1 H), 4.12 (t, *J* = 5.7 Hz, 1 H), 7.37 (t, *J* = 6.6 Hz, 1 H), 7.46 (t, *J* = 7.2 Hz, 1 H), 7.88 (d, *J* = 6.3 Hz, 1 H), 8.00 (d, *J* = 8.6 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 42.8, 59.3, 67.0, 70.7, 121.8, 123.2, 125.0, 125.1, 153.1. GC-MS m/z (% relative intensity, ion) 191 (100, M – $MeOCH_2$), 150 (90), 42 (40).



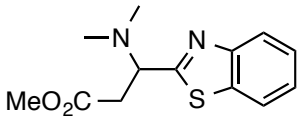
(2-Benzothiazolylmethyl)(2-cyanoethyl)(methyl)amine (3ha). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.48 (s, 3 H), 2.58 (t, *J* = 6.9 Hz, 2 H), 2.90 (t, *J* = 6.9 Hz, 2 H), 4.05 (s, 2 H), 7.37 (t, *J* = 7.5 Hz, 1 H), 7.46 (t, *J* = 7.7 Hz, 1 H), 7.88 (d, *J* = 8.0 Hz, 1 H), 7.97 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 16.7, 42.4, 52.7, 59.6, 118.4, 122.0, 123.0, 125.2, 126.1, 135.5, 153.3, 171.5. HRMS (ESI) Calcd for $C_{12}H_{13}N_3S$: $[M+H]^+$, 232.0903. Found: m/z 232.0910.



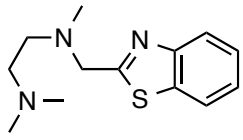
2-[2-Cyano-1-(dimethylamino)ethyl]benzothiazole (3'ha). A pale orange solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.49 (s, 6 H), 3.00 (dd, *J* = 16.9, 7.2 Hz, 1 H), 3.26 (dd, *J* = 16.9, 6.0 Hz, 1 H), 4.43 (t, *J* = 6.6 Hz, 1 H), 7.40 (t, *J* = 8.0 Hz, 1 H), 7.48 (t, *J* = 8.0 Hz, 1 H), 7.89 (d, *J* = 8.0 Hz, 1 H), 8.00 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 17.3, 41.5, 63.8, 118.4, 121.9, 123.5, 125.5, 126.2, 135.8, 153.0, 170.6. HRMS (ESI) Calcd for $C_{12}H_{13}N_3S$: $[M+H]^+$, 232.0903. Found: m/z 232.0901.



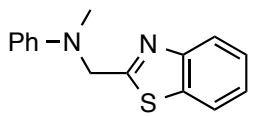
(2-Benzothiazolylmethyl)(2-methoxycarbonylethyl)(methyl)-amine (3ia). A pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.41 (s, 3 H), 2.58 (t, *J* = 6.9 Hz, 2 H), 2.91 (t, *J* = 6.9 Hz, 2 H), 3.70 (s, 3 H), 3.98 (s, 2 H), 7.36 (t, *J* = 7.5 Hz, 1 H), 7.45 (t, *J* = 7.5 Hz, 1 H), 7.86 (d, *J* = 8.0 Hz, 1 H), 7.96 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 33.0, 42.6, 51.8, 53.3, 59.8, 121.9, 122.9, 125.0, 125.9, 135.5, 153.4, 172.8, 172.9. HRMS (ESI) Calcd for $C_{13}H_{16}N_2O_2S$: $[M+H]^+$, 265.1005. Found: m/z 265.0997.



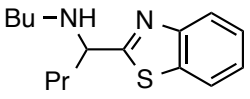
Methyl 2-benzothiazolyl-2-(dimethylamino)propanoate (3'ia). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.40 (bs, 6 H), 2.85–3.04 (m, 1 H), 3.10–3.22 (m, 1 H), 3.72 (s, 3 H), 4.53–4.71 (m, 1 H), 7.37 (t, *J* = 7.5 Hz, 1 H), 7.45 (t, *J* = 7.7 Hz, 1 H), 7.87 (d, *J* = 8.0 Hz, 1 H), 7.97 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 33.6, 41.7, 52.1, 63.7, 121.8, 123.3, 125.1, 125.9, 135.8, 153.1, 172.4, 172.7. HRMS (ESI) Calcd for $C_{13}H_{16}N_2O_2S$: $[M+H]^+$, 265.1005. Found: m/z 265.1003.



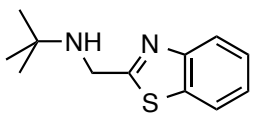
***N*-(2-Benzothiazolylmethyl)-*N*,*N*',*N*'-trimethylethylenediamine (3ja).** An orange solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.28 (s, 6 H), 2.43 (s, 3 H), 2.54 (t, *J* = 6.9 Hz, 2 H), 2.69 (t, *J* = 6.9 Hz, 2 H), 4.00 (s, 2 H), 7.35 (t, *J* = 7.5 Hz, 1 H), 7.44 (t, *J* = 7.7 Hz, 1 H), 7.86 (d, *J* = 8.0 Hz, 1 H), 7.96 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 43.3, 45.8, 55.5, 57.4, 60.4, 121.9, 122.9, 124.9, 125.9, 135.5, 153.4, 172.9. HRMS (ESI) Calcd for $C_{13}H_{19}N_3S$: $[M+H]^+$, 250.1372. Found: m/z 250.1382.



***N*-(2-Benzothiazolylmethyl)-*N*-methylaniline (3ka).** A pale yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.16 (s, 3 H), 4.89 (s, 2 H), 6.81 (t, *J* = 7.5 Hz, 1 H), 6.85 (d, *J* = 8.0 Hz, 2 H), 7.26 (t, *J* = 8.0 Hz, 2 H), 7.36 (t, *J* = 8.0 Hz, 1 H), 7.47 (t, *J* = 8.0 Hz, 1 H), 7.81 (d, *J* = 8.0 Hz, 1 H), 8.00 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 39.6, 56.5, 113.3, 118.3, 121.9, 122.8, 125.1, 126.1, 129.5, 135.2, 148.9, 153.7, 173.1. HRMS (ESI) Calcd for $C_{15}H_{14}N_2S$: $[M+H]^+$, 255.0950. Found: m/z 255.0950.

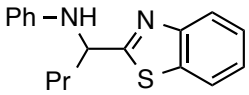


[1-(2-Benzothiazolyl)butyl](butyl)amine (3la).[10] A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.89 (t, *J* = 7.5 Hz, 3 H), 0.94 (t, *J* = 7.5 Hz, 3 H), 1.27–1.53 (m, 6 H), 1.75–1.90 (m, 2 H), 2.57–2.68 (m, 2 H), 4.09 (t, *J* = 6.6 Hz, 1 H), 7.35 (t, *J* = 8.0 Hz, 1 H), 7.45 (t, *J* = 8.0 Hz, 1 H), 7.88 (d, *J* = 8.0 Hz, 1 H), 7.97 (d, *J* = 8.0 Hz, 1 H).



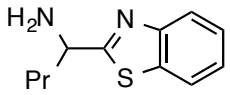
(2-Benzothiazolylmethyl)(*tert*-butyl)amine (3ma). This product could not be isolated in a pure form. The following data were

obtained from a spectrum of a mixture with **2a (3ma**:**2a** = 90:10). ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.21 (s, 9 H), 4.21 (s, 2 H), 7.35 (t, *J* = 7.7 Hz, 1 H), 7.44 (t, *J* = 8.0 Hz, 1 H), 7.86 (d, *J* = 8.0 Hz, 1 H), 7.95 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 28.9, 45.2, 52.3, 121.9, 122.8, 124.9, 126.0, 135.3, 153.4. GC-MS m/z (% relative intensity, ion) 220 (10, M), 205 (100), 148 (92), 136 (15). HRMS (ESI) Calcd for $C_{12}H_{16}N_2S$: $[M+H]^+$, 221.1107. Found: m/z 221.1109.

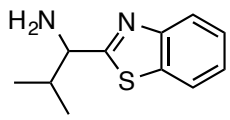


***N*-[1-(2-Benzothiazolyl)butyl]aniline (3na).** A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.99 (t, *J* = 7.5 Hz, 3 H), 1.47–1.66 (m, 2 H), 1.92–2.02 (m, 1 H), 2.05–2.15 (m, 1 H), 4.27 (d, *J* = 5.2 Hz, 1 H), 4.81 (dt, *J* = 8.0, 5.4 Hz, 1 H), 6.65 (d, *J* = 8.0 Hz, 2 H), 6.73 (t, *J* = 7.5 Hz, 1 H), 7.14 (t, *J* = 8.0 Hz, 2 H), 7.34 (t, *J* = 8.0 Hz, 1 H), 7.46 (t, *J* = 7.2 Hz, 1 H), 7.81 (d, *J* = 8.0 Hz, 1 H), 8.00 (d, *J* = 8.6 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.0, 19.4, 39.6, 57.4, 113.5, 118.7, 122.0, 122.9, 124.9, 126.0, 129.4, 135.1, 146.8, 153.8, 178.7. HRMS (ESI) Calcd for $C_{17}H_{18}N_2S$: $[M+H]^+$, 283.1263. Found: m/z 283.1264.

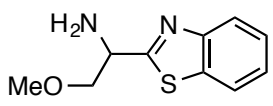
α-Arylation of Primary Alkylamines through tert-Butyldimethylsilyl Protection–Deprotection (Table 5): Representative Procedure (Table 5, Entry 4). To a 4 mL vial equipped with a stir bar in a glove box were added successively (*tert*-butyldimethylsilyl)[2-(*tert*-butyldimethylsilyloxy)ethyl]amine (**4r**: 130.3 mg, 0.450 mmol),[4] 2-(benzenesulfonyl)benzothiazole (**2a**: 68.8 mg, 0.250 mmol), acetonitrile (0.50 mL) and *t*-BuON=NO*t*-Bu (21.8 mg, 0.125 mmol). The vial was taken out of the glove box and stirred at 50 °C for 24 h. The reaction mixture was poured into sat. $NaHCO_3$ aq. (15 mL), extracted with ethyl acetate (3 x 15 mL), and dried over Na_2SO_4. After filtration and concentration, the crude mixture was subjected to silica gel chromatography (hexane/ethyl acetate = 82:18 to 61:39, MPLC) to give 1-(2-Benzothiazolyl)-2-(*tert*-butyldimethylsilyloxy)ethylamine (**3ra**: 61.6 mg, 80% yield).



1-(2-Benzothiazolyl)butylamine (3oa). A white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.97 (t, *J* = 7.5 Hz, 3 H), 1.39–1.59 (m, 2 H), 1.75–1.85 (m, 1 H), 1.86 (bs, 2 H), 1.93–2.03 (m, 1 H), 4.37 (dd, *J* = 8.0, 5.7 Hz, 1 H), 7.36 (t, *J* = 8.3 Hz, 1 H), 7.46 (t, *J* = 8.3 Hz, 1 H), 7.88 (d, *J* = 8.0 Hz, 1 H), 7.97 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.0, 19.3, 40.8, 54.8, 121.9, 122.9, 124.9, 126.0, 134.9, 153.5, 179.1. HRMS (ESI) Calcd for $C_{11}H_{14}N_2S$: $[M+H]^+$, 207.0950. Found: m/z 207.0945.

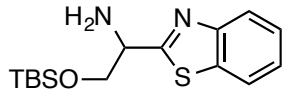


1-(2-Benzothiazolyl)-2-methylpropylamine (3pa). A pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.97 (d, *J* = 6.9 Hz, 3 H), 1.03 (d, *J* = 6.9 Hz, 3 H), 1.80 (bs, 2 H), 2.24–2.35 (m, 1 H), 4.18 (d, *J* = 5.2 Hz, 1 H), 7.35 (t, *J* = 7.5 Hz, 1 H), 7.45 (t, *J* = 7.5 Hz, 1 H), 7.87 (d, *J* = 8.0 Hz, 1 H), 7.97 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 17.2, 19.8, 34.9, 60.3, 121.8, 122.9, 124.8, 126.0, 135.0, 153.4, 178.2. HRMS (ESI) Calcd for $C_{11}H_{14}N_2S$: $[M+H]^+$, 207.0950. Found: m/z 207.0950.

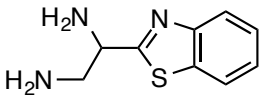


1-(2-Benzothiazolyl)-2-methoxyethylamine (3qa). An orange oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.05 (bs, 2 H), 3.42 (s, 3 H), 3.67 (dd, *J* = 9.2, 7.5 Hz, 1 H), 3.86 (dd, *J* = 9.2, 4.0 Hz, 1 H), 4.58 (dd, *J* = 7.5, 4.2 Hz, 1 H), 7.36 (t, *J* = 8.0 Hz, 1 H), 7.45 (t, *J* = 8.0 Hz, 1 H), 7.88 (d, *J* = 8.0 Hz, 1 H), 7.97

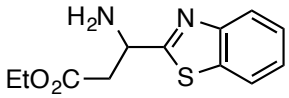
(d, J = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 54.5, 59.2, 76.8, 121.9, 122.9, 124.9, 126.1, 135.1, 153.5, 175.5. HRMS (ESI) Calcd for $C_{10}H_{12}N_2OS$: $[M+H]^+$, 209.0743. Found: m/z 209.0749.



1-(2-Benzothiazolyl)-2-(*tert*-butyldimethylsilyloxy)-ethylamine (3ra). An orange oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 0.03 (s, 3 H), 0.07 (s, 3 H), 0.88 (s, 9 H), 2.07 (bs, 2 H), 3.85 (dd, J = 9.2, 7.5 Hz, 1 H), 4.07 (dd, J = 9.7, 4.0 Hz, 1 H), 4.40–4.54 (m, 1 H), 7.36 (t, J = 7.5 Hz, 1 H), 7.45 (t, J = 7.5 Hz, 1 H), 7.89 (d, J = 8.0 Hz, 1 H), 7.97 (d, J = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ –5.32, –5.27, 18.4, 26.0, 56.5, 67.6, 121.9, 122.8, 124.8, 126.0, 135.1, 153.5, 175.9. HRMS (ESI) Calcd for $C_{15}H_{24}N_2OSSi$: $[M+H]^+$, 309.1451. Found: m/z 309.1447.

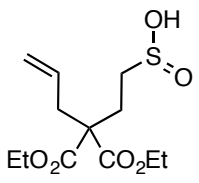


1-(2-Benzothiazolyl)ethylenediamine (3sa). A yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.88 (bs, 4 H), 3.11 (dd, J = 13.2, 6.3 Hz, 1 H), 3.19 (dd, J = 12.6, 3.4 Hz, 1 H), 4.25–4.39 (m, 1 H), 7.35 (t, J = 7.5 Hz, 1 H), 7.45 (t, J = 7.5 Hz, 1 H), 7.87 (d, J = 8.0 Hz, 1 H), 7.96 (d, J = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 48.8, 56.9, 121.9, 122.9, 124.9, 126.1, 135.0, 153.5, 176.8. HRMS (ESI) Calcd for $C_9H_{11}N_3S$: $[M+H]^+$, 194.0746. Found: m/z 194.0751.

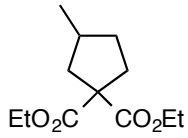


1-(2-Benzothiazolyl)-2-(ethoxycarbonyl)ethylamine (3ta). An orange oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.25 (t, J = 6.9 Hz, 3 H), 2.03 (bs, 2 H), 2.86 (dd, J = 16.0, 8.6 Hz, 1 H), 3.15 (dd, J = 16.0, 4.0 Hz, 1 H), 4.12–4.23 (m, 2 H), 4.74 (dd, J = 8.6, 4.0 Hz, 1 H), 7.36 (t, J = 7.5 Hz, 1 H), 7.46 (t, J = 7.5 Hz, 1 H), 7.88 (d, J = 8.0 Hz, 1 H), 7.96 (d, J = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.3, 42.5, 51.7, 61.0, 121.9, 123.0, 125.0, 126.1, 135.2, 153.5, 171.4, 176.7. HRMS (ESI) Calcd for $C_{12}H_{14}N_2O_2S$: $[M+H]^+$, 251.0849. Found: m/z 251.0850.

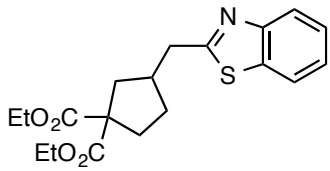
Involvement of Sulfonyl Radicals as Leaving Groups (Scheme 2). To a 4 mL vial equipped with a stir bar in a glove box were added successively isopropyl(dimethyl)amine (**1a**: 39.2 mg, 0.450 mmol), 2-[3,3-bis(ethoxycarbonyl)-5-hexenesulfonyl]benzothiazole (**2"a**: 106.4 mg, 0.250 mmol), methanol (0.50 mL) and *t*-BuON=NO*t*-Bu (8.7 mg, 0.050 mmol). The vial was taken out of the glove box and stirred under 50 °C for 8 h. The reaction mixture was poured into sat. $NaHCO_3$ aq. (15 mL), extracted with ethyl acetate (3 x 15 mL), dried over Na_2SO_4, filtered and concentrated. An aliquot of the crude mixture was subjected to GC analysis using nonane to determine the yield of (2-benzothiazolylmethyl)(isopropyl)(methyl)amine (**3aa**: the same compound as obtained in Table 1) to be 61%. The rest of the crude mixture was subjected to silica gel chromatography (hexane/ethyl acetate = 96:4 to 75:25, MPLC) to give diethyl 3-methylcylclopentane-1,1-dicarboxylate (**6**), contaminated with 2-methoxybenzothiazole (**6**: 2-methoxybenzothiazole = 40:60), and 2-[3,3-bis(ethoxycarbonyl)cyclopentylmethyl]benzothiazole (**7**), contaminated with **3aa** (**7**:**3aa** = 90:10). The yields of **6** and **7** were estimated to be 5% and 4%, respectively. The yield of 3,3-bis(ethoxycarbonyl)-5-hexenesulfinic acid (**5**) was determined by the following procedure: the aqueous layer, which was obtained by the above extraction process, was acidified with HCl aq., extracted with ethyl acetate (3 x 15 mL), dried over Na_2SO_4, filtered and concentrated to give **5** but not in a pure form, contaminated with ethyl acetate and a compound similar to **5**. Due to instability of **5**, further purification was not performed and the yield of **5** was estimated to be *ca*. 70%, assuming that the unknown compound has the same molecular weight as **5**.



3,3-Bis(ethoxycarbonyl)-5-hexenesulfinic acid (5). This product could not be isolated in a pure form. The following data were obtained from a spectrum of a mixture with ethyl acetate and a compound similar to **5**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.26 (t, *J* = 7.2 Hz, 6 H), 2.20–2.25 (m, 2 H), 2.66 (d, *J* = 7.5 Hz, 2 H), 2.79–2.84 (m, 2 H), 4.15–4.24 (m, 4 H), 5.14 (d, *J* = 10.6 Hz, 1 H), 5.15 (d, *J* = 17.2, 1 H), 5.57 (ddt, *J* = 16.9, 10.3, 7.5 Hz, 1 H).



Diethyl 3-methylcylclopentane-1,1-dicarboxylate (6).[11] This product could not be isolated in a pure form. The following data were obtained from a spectrum of a mixture with 2-methoxybenzothiazole (**6**: 2-methoxybenzothiazole = 40:60). ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.01 (d, *J* = 6.3 Hz, 3 H), 1.20–1.30 (m, 1 H), 1.24 (t, *J* = 6.9 Hz, 6 H), 1.66 (dd, *J* = 13.5, 10.0 Hz, 1 H), 1.81–1.89 (m, 1 H), 2.00–2.09 (m, 1 H), 2.10–2.18 (m, 1 H), 2.28–2.35 (m, 1 H), 2.44 (dd, *J* = 13.2, 6.9 Hz, 1 H), 4.17 (q, *J* = 6.9 Hz, 4 H).



2-[3,3-Bis(ethoxycarbonyl)cyclopentylmethyl]-benzothiazole (7). This product could not be isolated in a pure form. The following data were obtained from a spectrum of a mixture with **3aa** (**7**:**3aa** = 90:10). ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.21–1.27 (m, 6 H), 1.45–1.55 (m, 1 H), 1.91–2.03 (m, 2 H), 2.16–2.25 (m, 1 H), 2.33–2.40 (m, 1 H), 2.52–2.65 (m, 2 H), 3.11–3.24 (m, 2 H), 4.14–4.21 (m, 4 H), 7.35 (t, *J* = 8.3 Hz, 1 H), 7.45 (t, *J* = 8.3 Hz, 1 H), 7.84 (d, *J* = 8.0 Hz, 1 H), 7.96 (d, *J* = 8.0 Hz, 1 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 14.2, 32.1, 33.8, 39.6, 40.1, 40.4, 60.1, 61.56, 61.61, 121.6, 122.8, 124.9, 126.1, 135.3, 153.4, 170.6, 172.5, 172.6. GC-MS m/z (% relative intensity, ion) 361 (31, M), 316 (14), 288 (11), 214 (14), 149 (100). HRMS (ESI) Calcd for $C_{19}H_{23}NO_4S$: $[M+Na]^+$, 384.1240. Found: m/z 384.1255.

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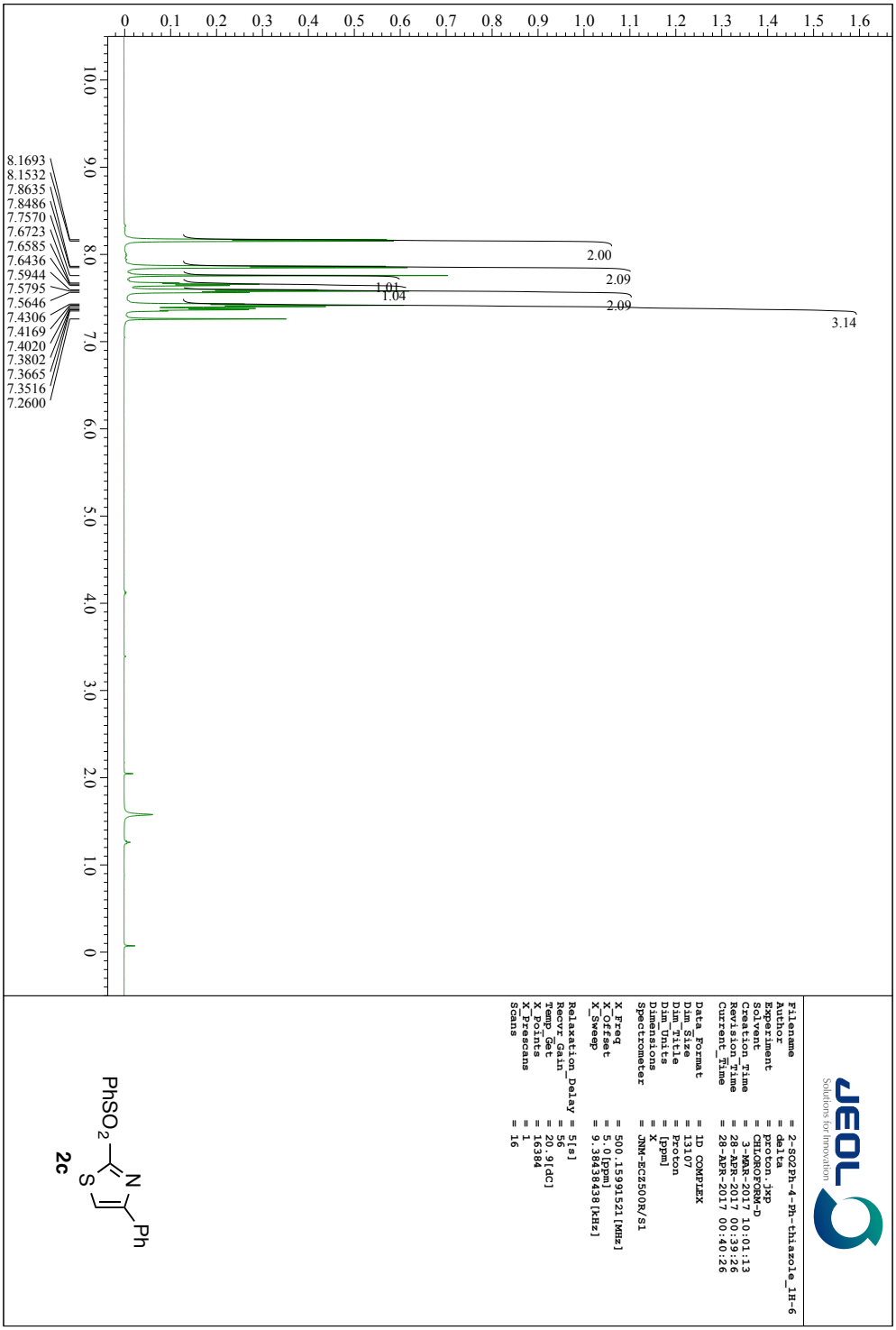
NMR Spectra of the Products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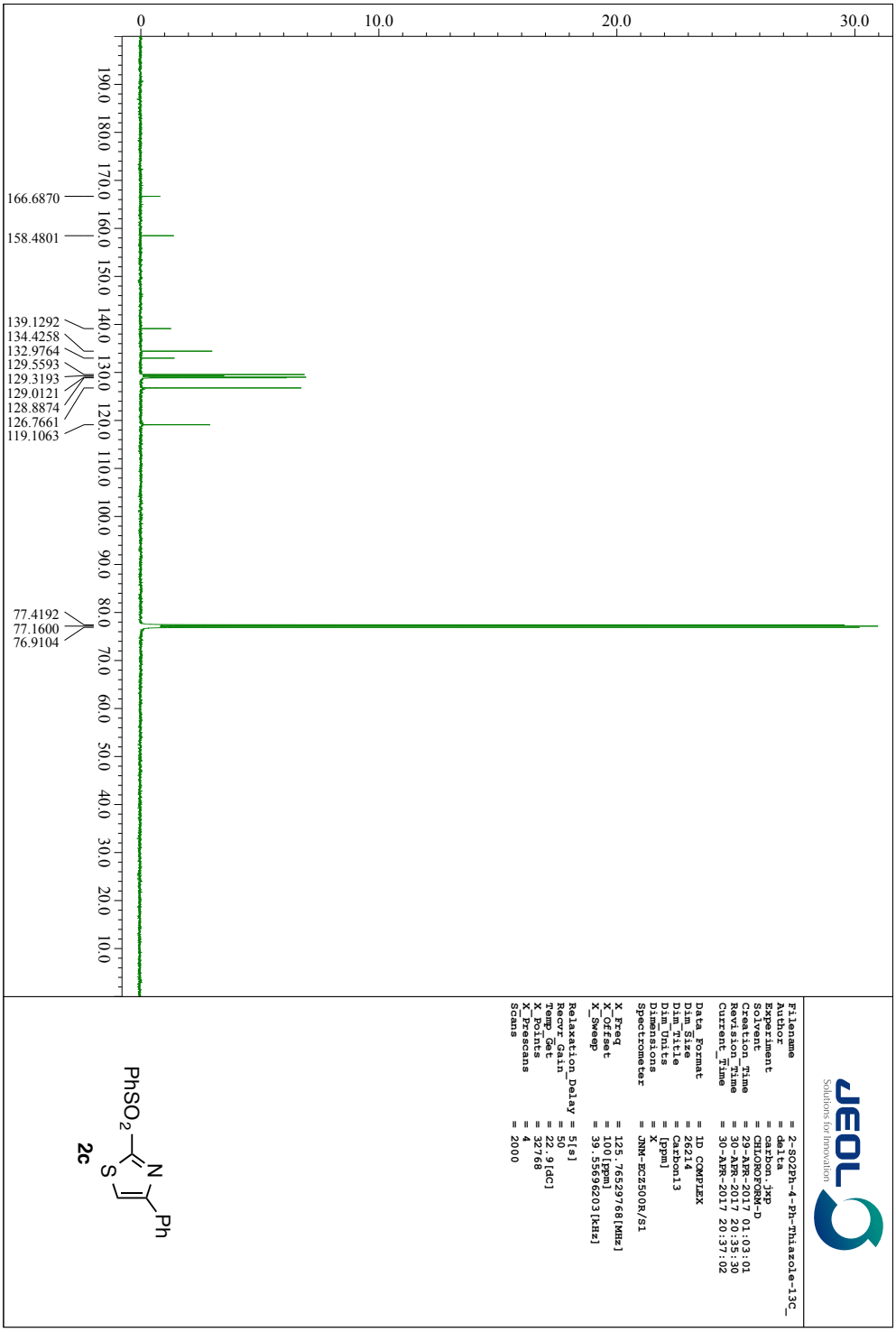
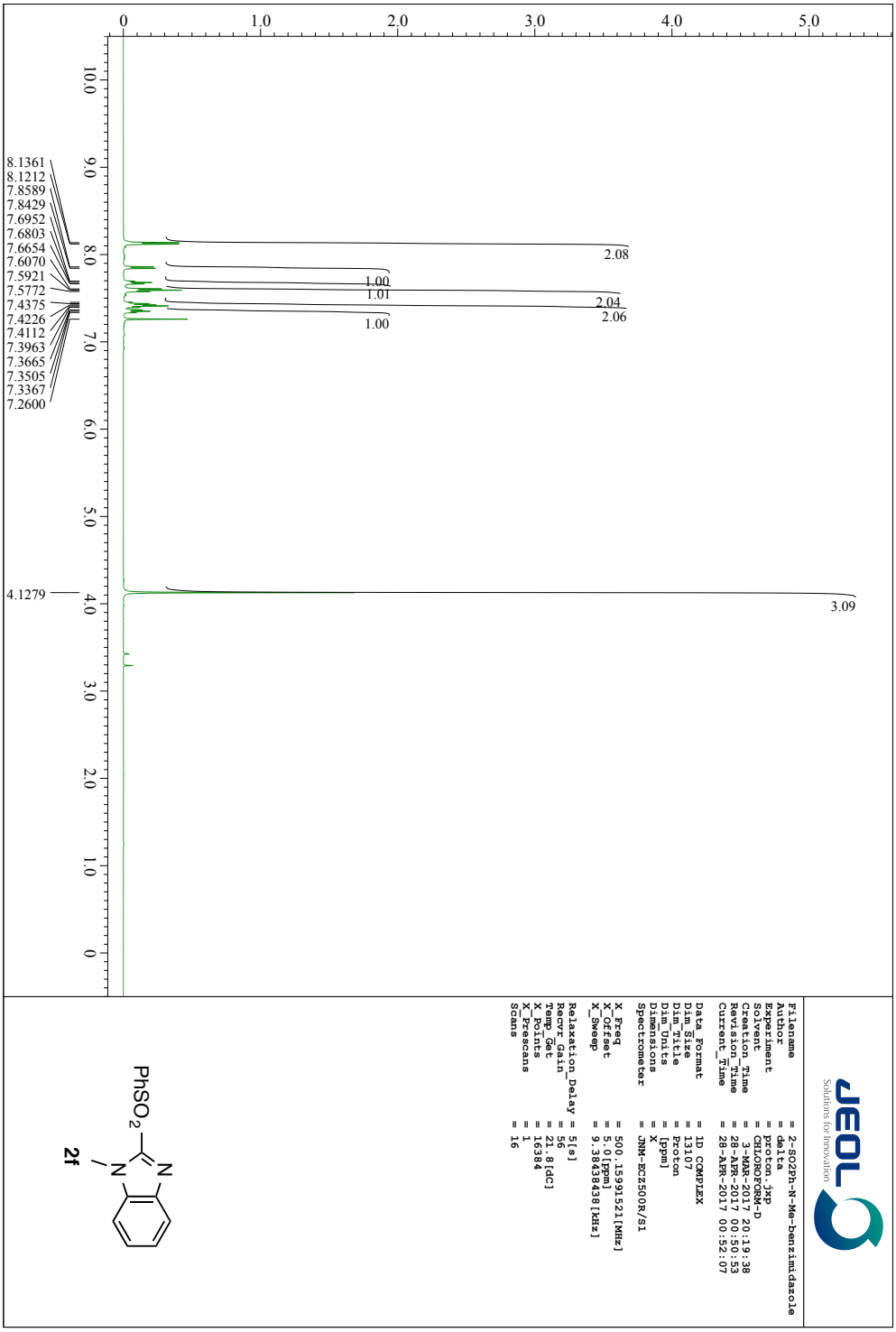
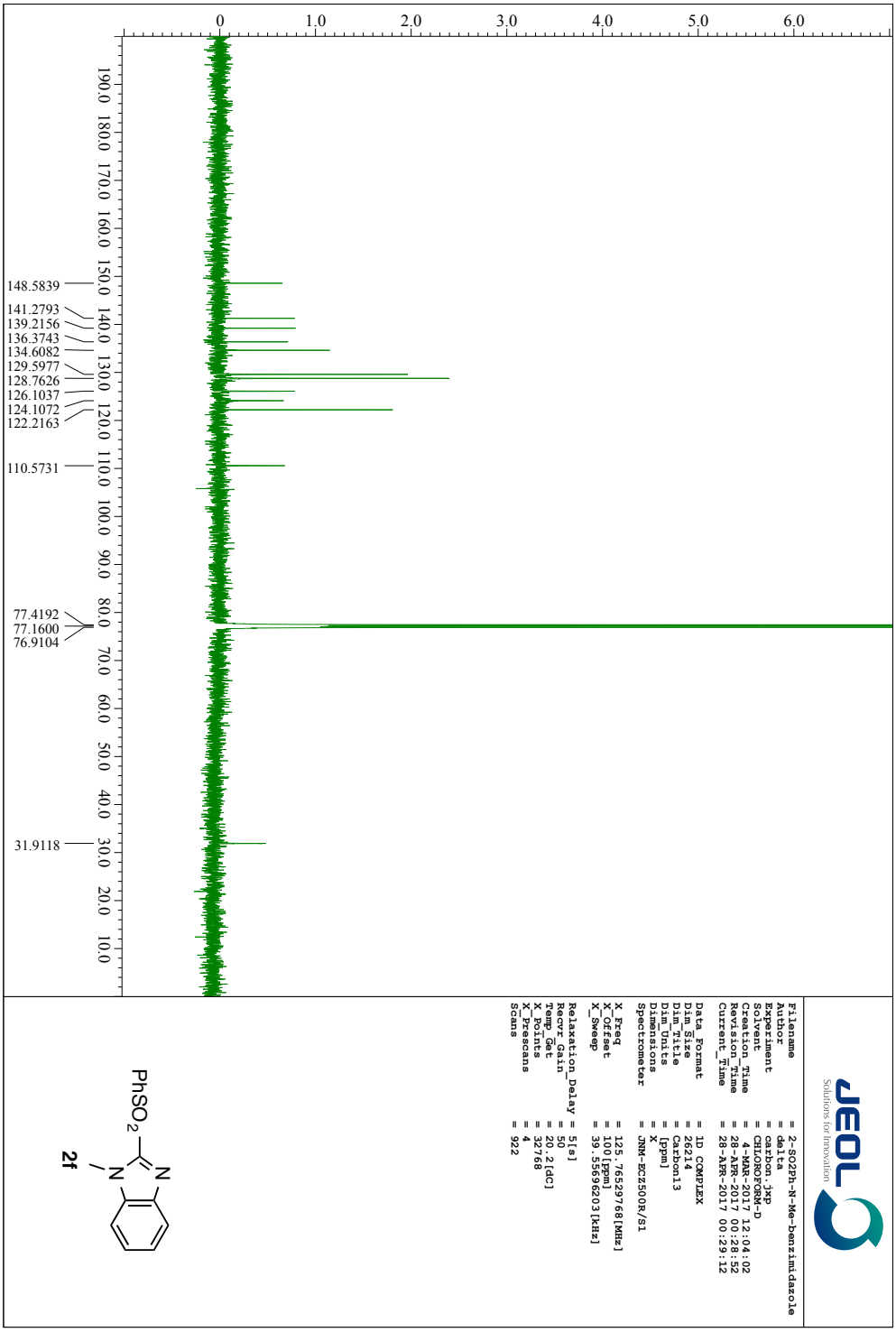
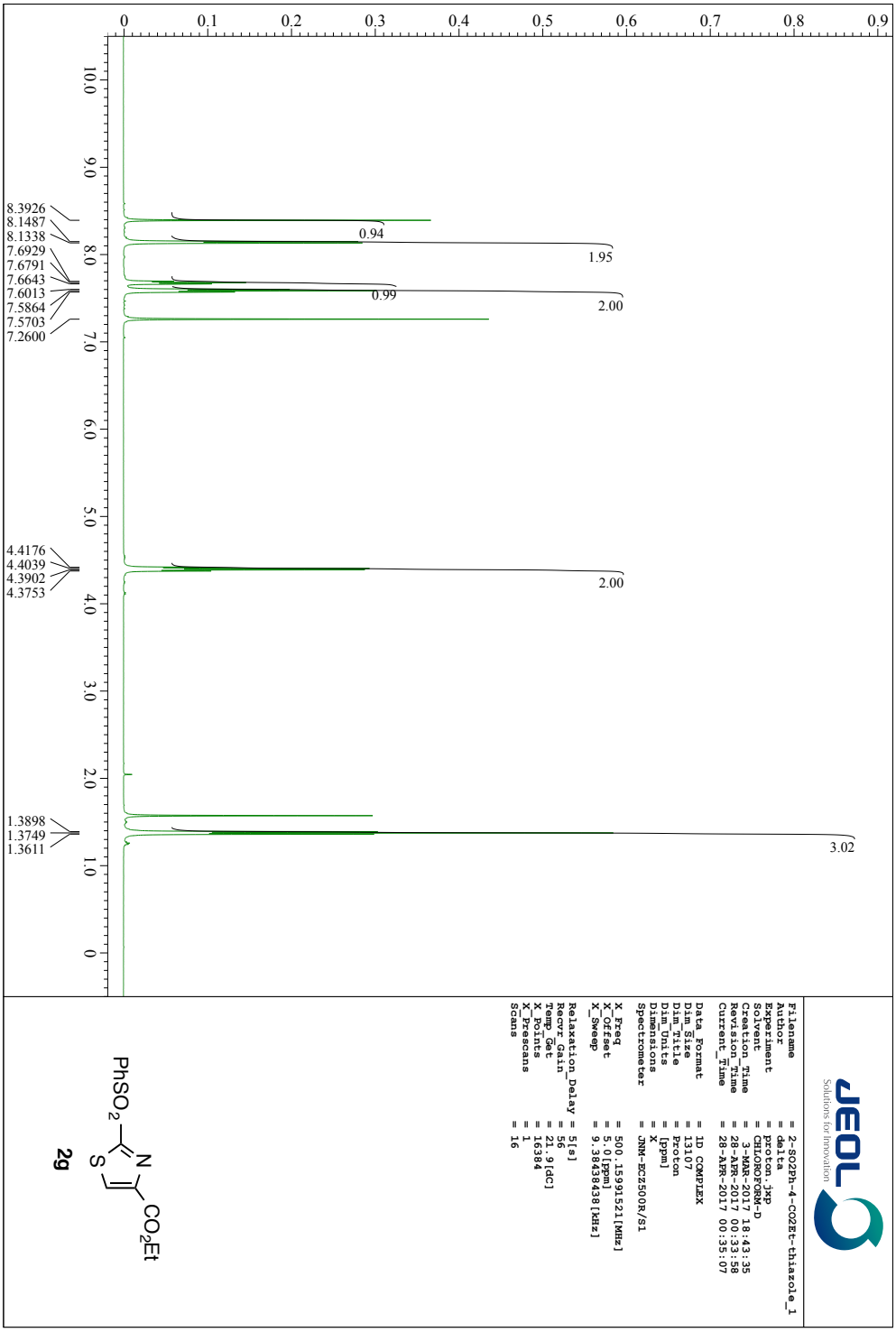
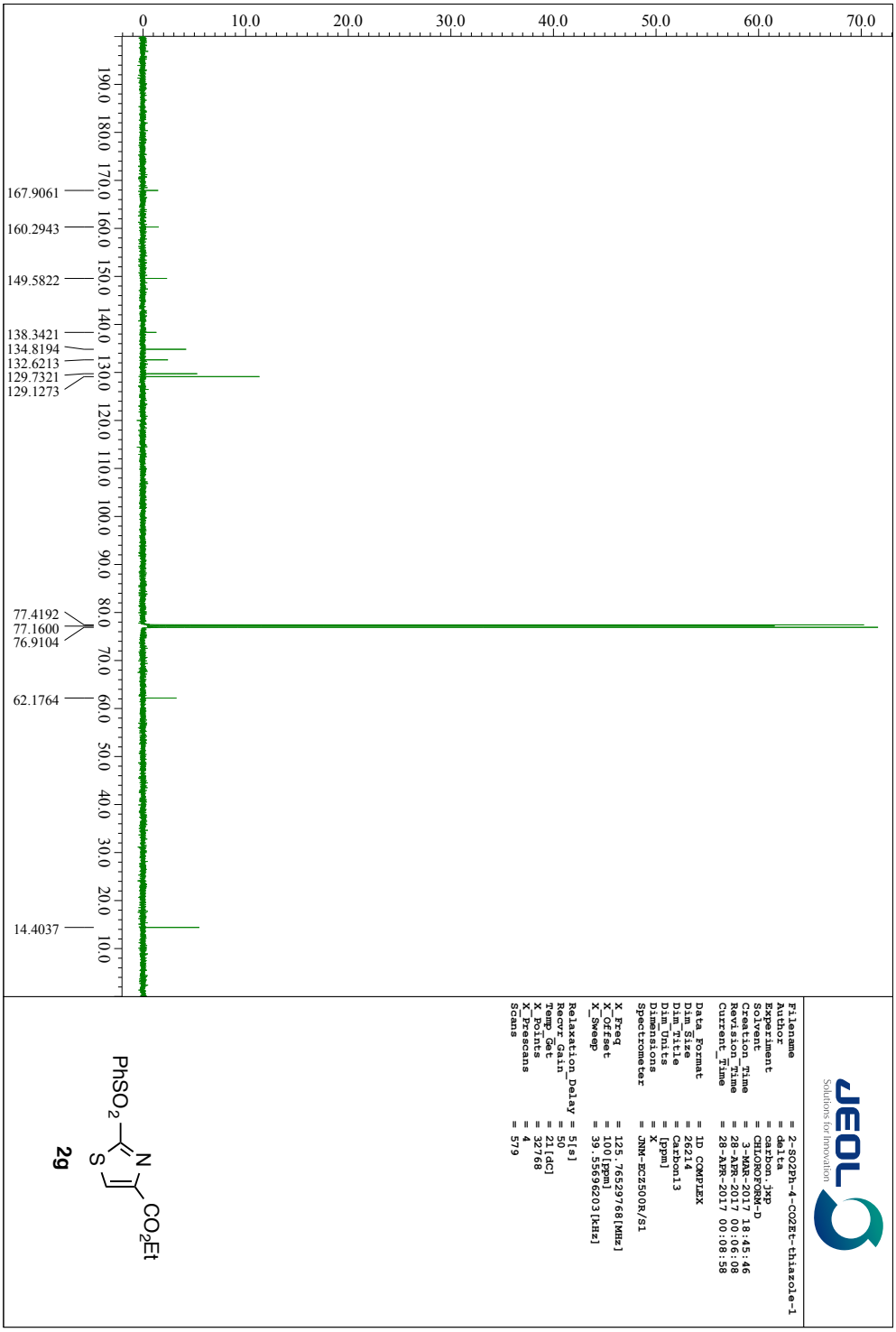
Ph
2c

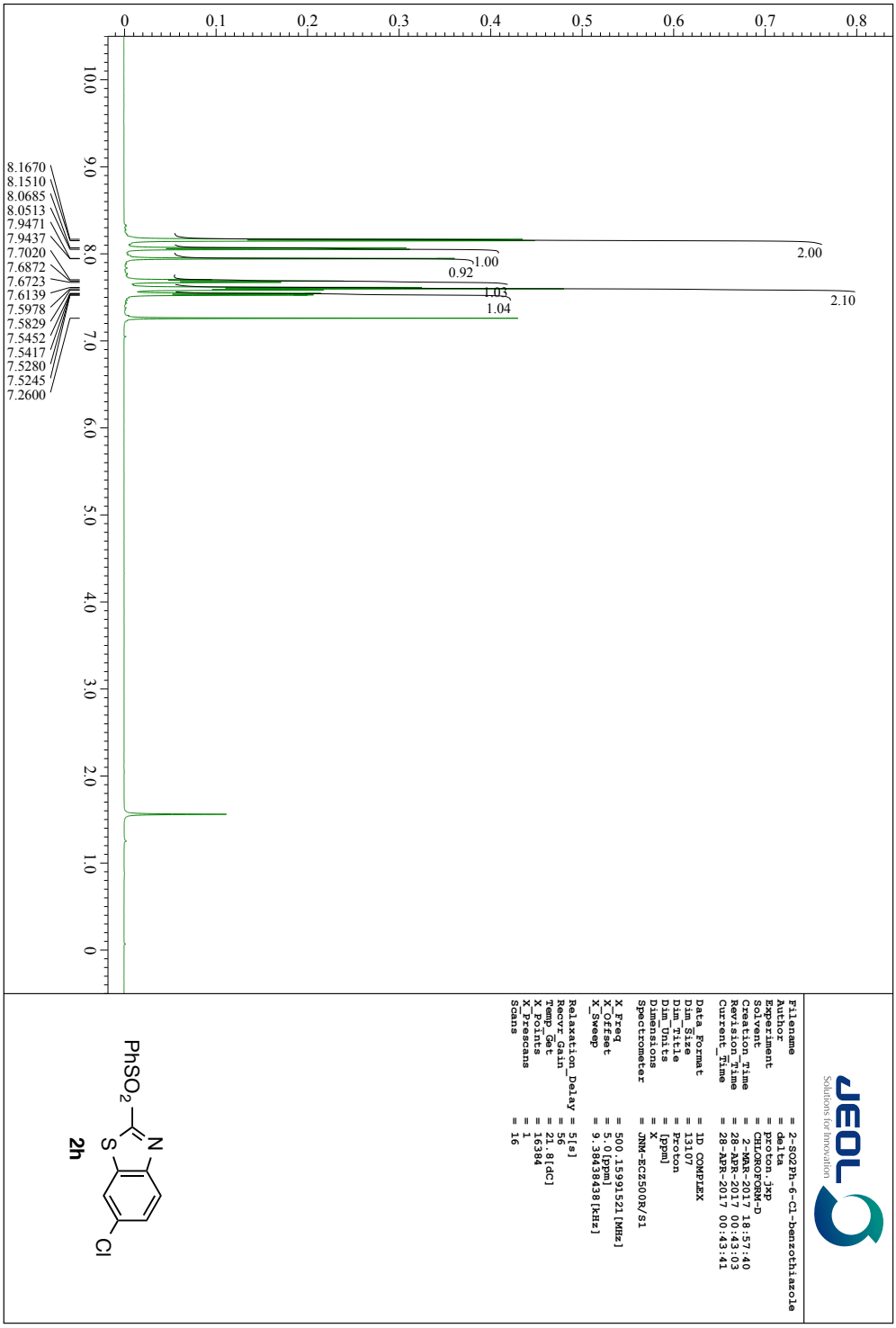

JEOL
Solutions for Innovation
Filename = 2-SO2Ph-4-Ph-Thiazole-13C_
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 29-APR-2017 01:03:01
Revision_Time = 30-APR-2017 20:35:30
Current_Time = 30-APR-2017 20:37:02
Data_Format = 1D COMPLEX
Dim_Size = 32214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765297681[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.556962031[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 20.9[dC]
Temp_Deg_C = 32768
X_Points = 4
X_Prescans = 2000
Scans
0
10.0
20.0
30.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
166.6870
158.4801
139.1292
134.4258
132.9764
129.5593
129.3193
129.0121
128.8874
126.7661
119.1063
77.4192
77.1600
76.9104
PhSO2
N
S
Ph
2c

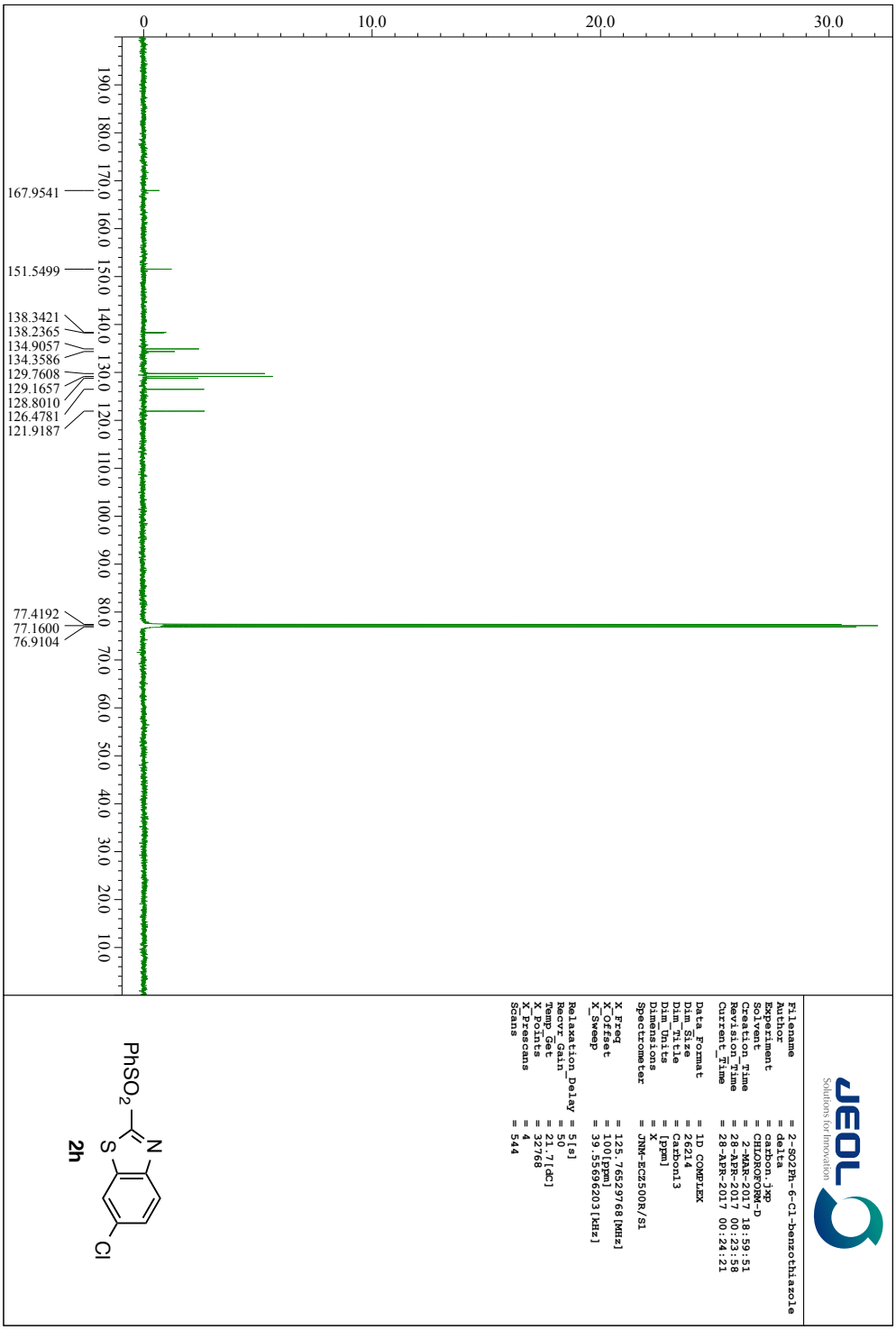

8.1361
8.1212
7.8589
7.8429
7.6952
7.6803
7.6654
7.6070
7.5921
7.5772
7.4375
7.4226
7.4112
7.3963
7.3665
7.3505
7.3367
7.2600
4.1279
2.08
1.00
1.01
2.04
2.06
1.00
3.09
Filename = 2-SO2Ph-N-Me-benzimidazole
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 3-MAR-2017 20:19:38
Revision_Time = 28-APR-2017 00:50:53
Current_Time = 28-APR-2017 00:52:07
Data_Format = 1D COMPLEX
Dim_Size = 19107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 26
Temp_Chc = 25.8[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
PhSO2
2f

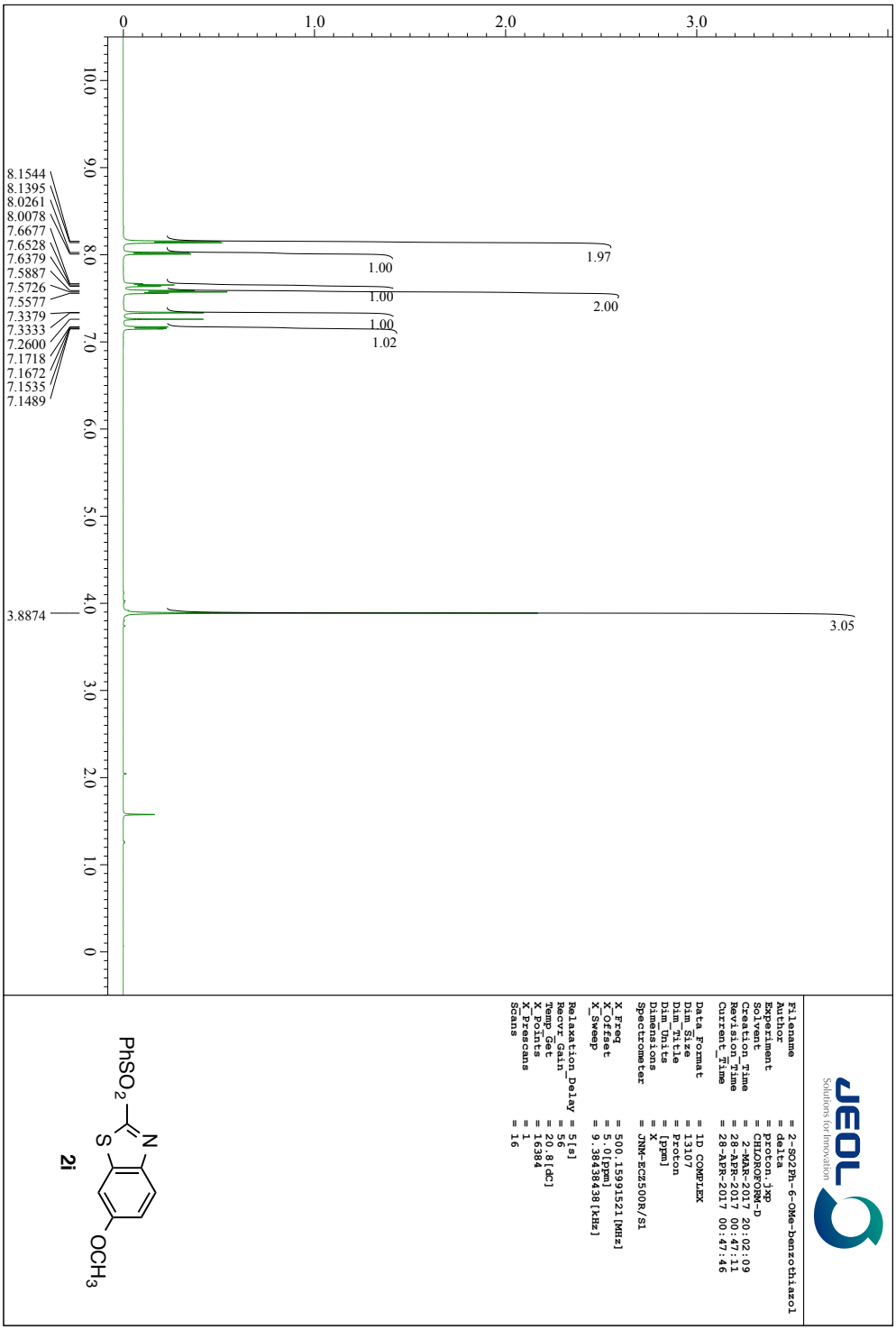

148.5839
141.2793
139.2156
136.3743
134.6082
129.5977
128.7626
126.1037
124.1072
122.2163
110.5731
77.4192
77.1600
76.9104
31.9118
Filename = 2-SO2Ph-N-Me-benzimidazole
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-MAR-2017 12:04:02
Revision_Time = 28-APR-2017 00:28:52
Current_Time = 28-APR-2017 00:29:12
Data_Format = 1D COMPLEX
Dim_Size = 32214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765297681[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.556962O3[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50.2[dC]
Temp_Deg_C = 32768
X_Points = 4
X_Prescans = 922
Scans
PhSO2
2f

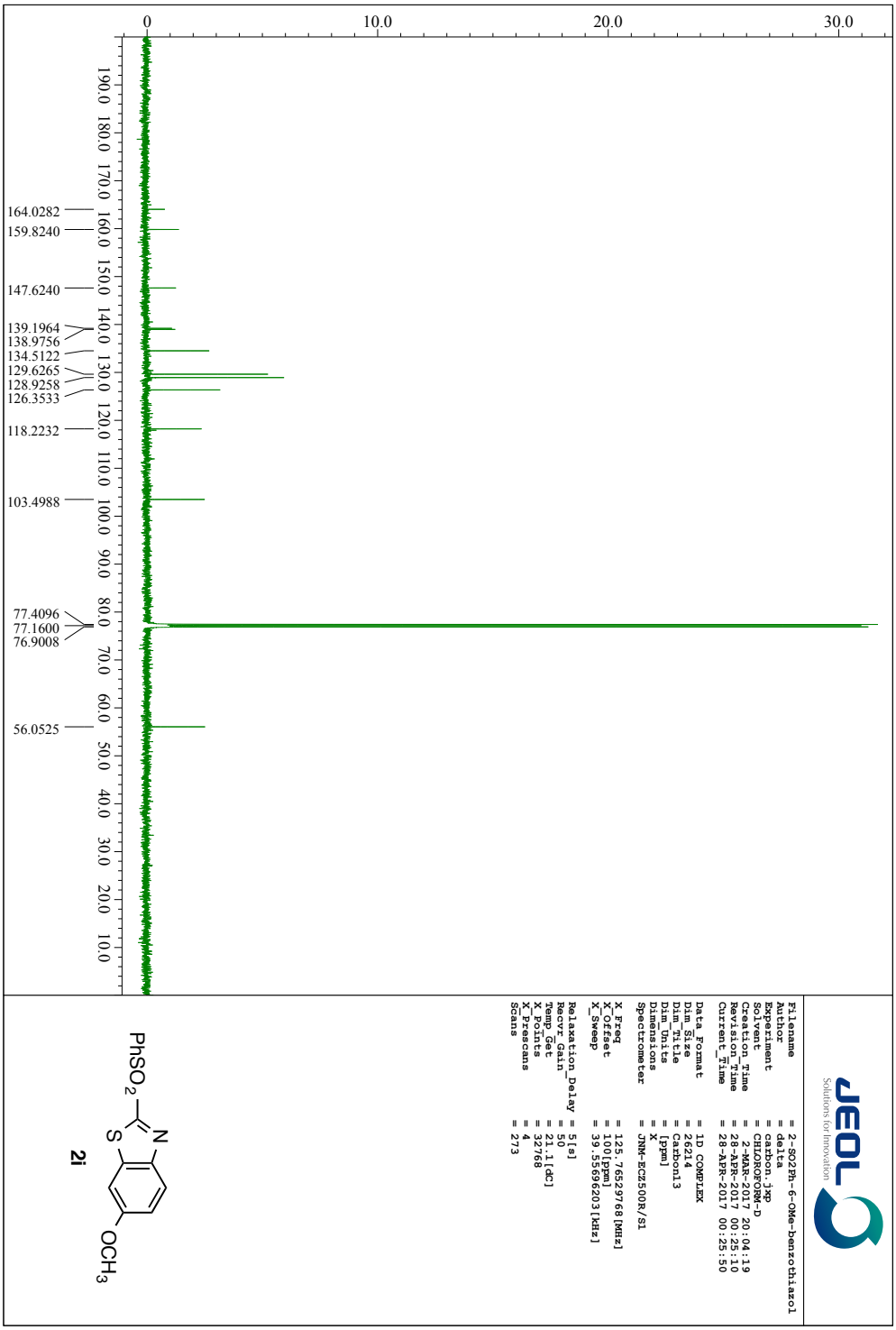

Filename = 2-SO2Ph-4-CO2Et-thiazole_1
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 3-MAR-2017 18:43:35
Revision_Time = 28-APR-2017 00:33:58
Current_Time = 28-APR-2017 00:35:07
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 26
Temp_Comment = 25.9[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
8.3926
8.1487
8.1338
7.6929
7.6791
7.6643
7.6013
7.5864
7.5703
7.2600
4.4176
4.4039
4.3902
4.3753
1.3898
1.3749
1.3611
0.94
1.95
0.99
2.00
2.00
3.02
PhSO2
N
S
CO2Et
2g

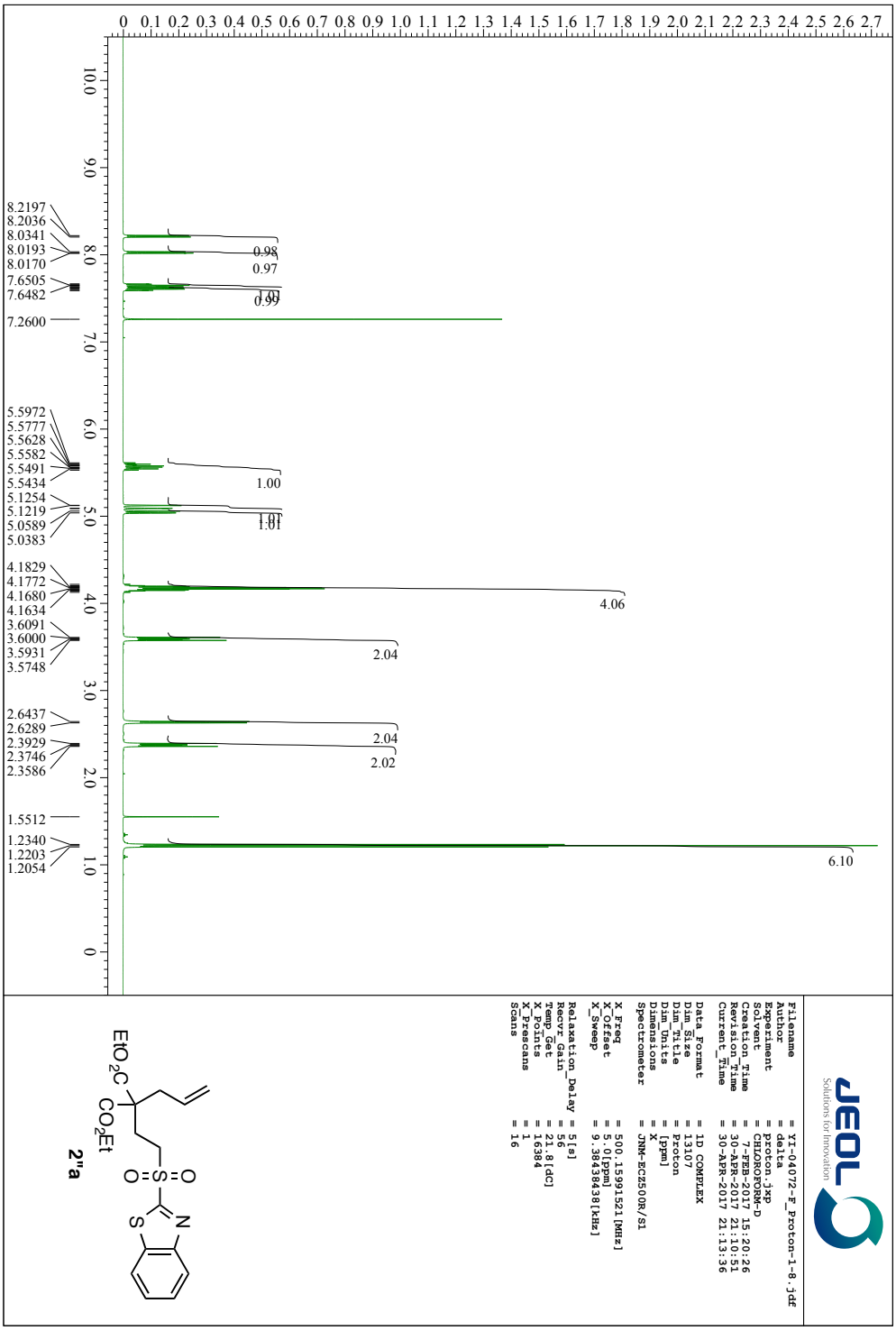

JEOL
Solutions for Innovation
Filename = 2-SO2Ph-4-CO2Et-thiazole-1
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 3-MAR-2017 18:45:46
Revision_Time = 28-APR-2017 00:06:08
Current_Time = 28-APR-2017 00:08:58
Data_Format = 1D COMPLEX
Dim_Size = 32214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765297681MHz]
X_Offset = 100[ppm]
X_Sweep = 39.556962031kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 20 [dC]
Temp_Calc = 21[dC]
X_Points = 32768
X_Prescans = 4
Scans = 579
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
167.9061
160.2943
149.5822
138.3421
134.8194
132.6213
129.7321
129.1273
77.4192
77.1600
76.9104
62.1764
14.4037
PhSO2
N
S
CO2Et
2g

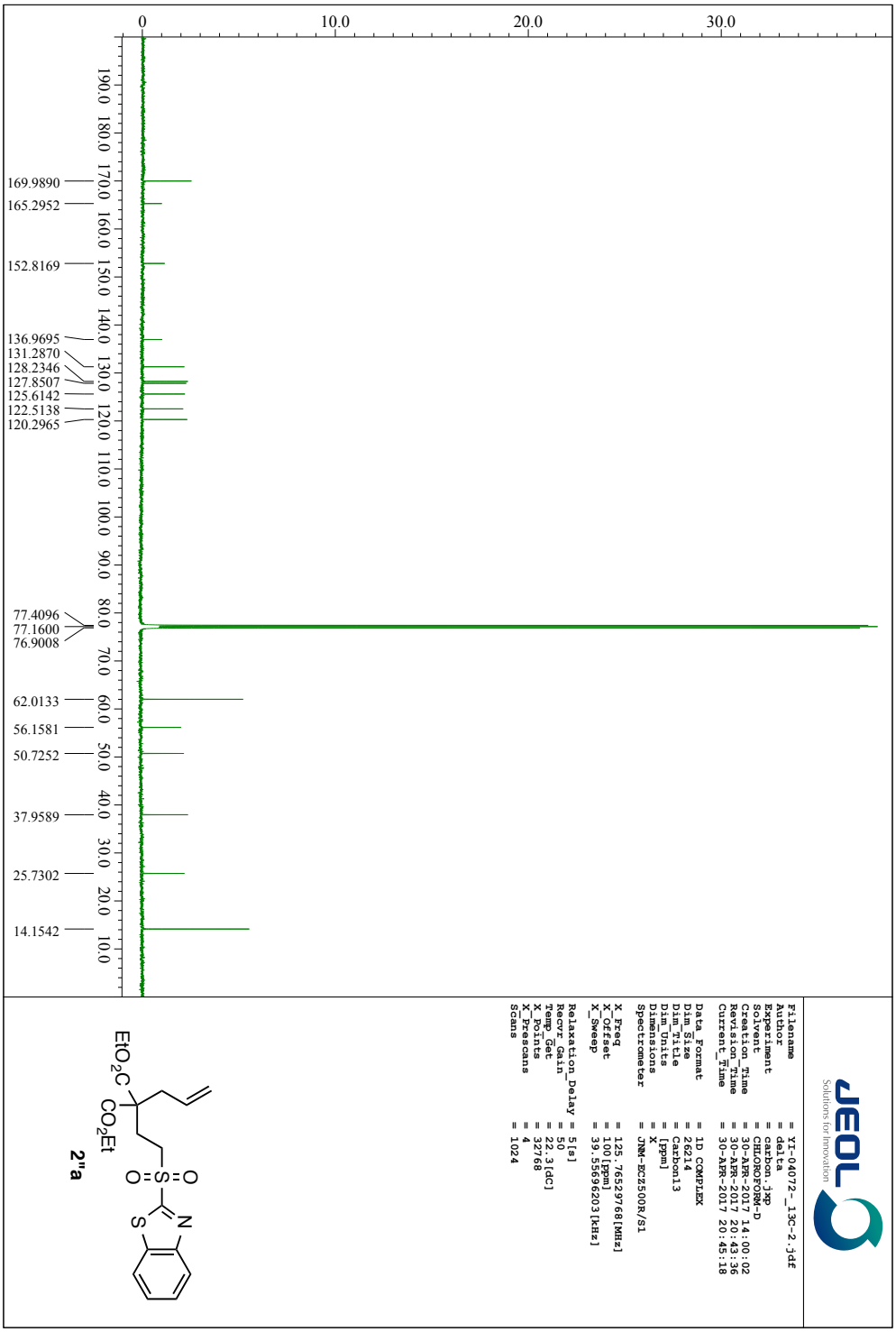

8.1670
8.1510
8.0685
8.0513
7.9471
7.9437
7.7020
7.6872
7.6723
7.6139
7.5978
7.5829
7.5452
7.5417
7.5280
7.5245
7.2600
2.00
1.00
0.92
1.03
1.04
2.10
Filename = 2-SO2Ph-6-Cl-benzothiazole
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 2-MAR-2017 18:57:40
Revision_Time = 28-APR-2017 00:43:03
Current_Time = 28-APR-2017 00:43:41
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 56
Temp_Get = 21.8[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
PhSO2
N
S
Cl
2h


JEOL
Solutions for Innovation
Filename = 2-SO2Ph-6-Cl-benzothiazole
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 2-MAR-2017 18:59:51
Revision_Time = 28-APR-2017 00:23:58
Current_Time = 28-APR-2017 00:24:21
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 51.7[dB]
Temp_Get = 21.7[dC]
X_Points = 32768
X_Prescans = 4
Scans = 544
0
10.0
20.0
30.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
167.9541
151.5499
138.3421
138.2365
134.9057
134.3586
129.7608
129.1657
128.8010
126.4781
121.9187
77.4192
77.1600
76.9104
PhSO2
N
S
Cl
2h


8.1544
8.1395
8.0261
8.0078
7.6677
7.6528
7.6379
7.5887
7.5726
7.5577
7.3379
7.3333
7.2600
7.1718
7.1672
7.1535
7.1489
3.8874
1.97
1.00
2.00
1.00
1.00
1.02
3.05
Filename = 2-SO2Ph-6-OMe-benzothiazol
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 2-MAR-2017 20:02:09
Revision_Time = 28-APR-2017 00:47:11
Current_Time = 28-APR-2017 00:47:46
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 58.8[dB]
Temp_Get = 20.8[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
PhSO2
N
S
OCH3
2i


JEOL
Solutions for Innovation
Filename = 2-SO2Ph-6-OMe-benzothiazol
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 2-MAR-2017 20:04:19
Revision_Time = 28-APR-2017 00:25:10
Current_Time = 28-APR-2017 00:25:50
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 51.1[dC]
Temp_Get = 21.1[dC]
X_Points = 32768
X_Prescans = 4
Scans = 273
164.0282
159.8240
147.6240
139.1964
138.9756
134.5122
129.6265
128.9258
126.3533
118.2232
103.4988
77.4096
77.1600
76.9008
56.0525
PhSO2
N
S
OCH3
2i


8.2197
8.2036
8.0341
8.0193
8.0170
7.6505
7.6482
7.2600
5.5972
5.5777
5.5628
5.5582
5.5491
5.5434
5.1254
5.1219
5.0589
5.0383
4.1829
4.1772
4.1680
4.1634
3.6091
3.6000
3.5931
3.5748
2.6437
2.6289
2.3929
2.3746
2.3586
1.5512
1.2340
1.2203
1.2054
0.98
0.97
1.00
0.99
1.00
1.01
4.06
2.04
2.04
2.02
6.10
Filename = YI-04072-F_Proton-1-8.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 7-FEB-2017 15:20:26
Revision_Time = 30-APR-2017 21:10:51
Current_Time = 30-APR-2017 21:13:36
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 59.8[dB]
Temp_Get = 21.8[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
EtO2C
CO2Et
2"a


JEOL
Solutions for Innovation
Filename = YI-04072-_13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 30-APR-2017 14:00:02
Revision_Time = 30-APR-2017 20:43:36
Current_Time = 30-APR-2017 20:45:18
Data_Format = 1D COMPLEX
Dim_Size = 262144
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765297681[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50.3[dC]
Temp_Get = 22
X_Points = 32768
X_Prescans = 4
Scans = 1024
169.9890
165.2952
152.8169
136.9695
131.2870
128.2346
127.8507
125.6142
122.5138
120.2965
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62.0133
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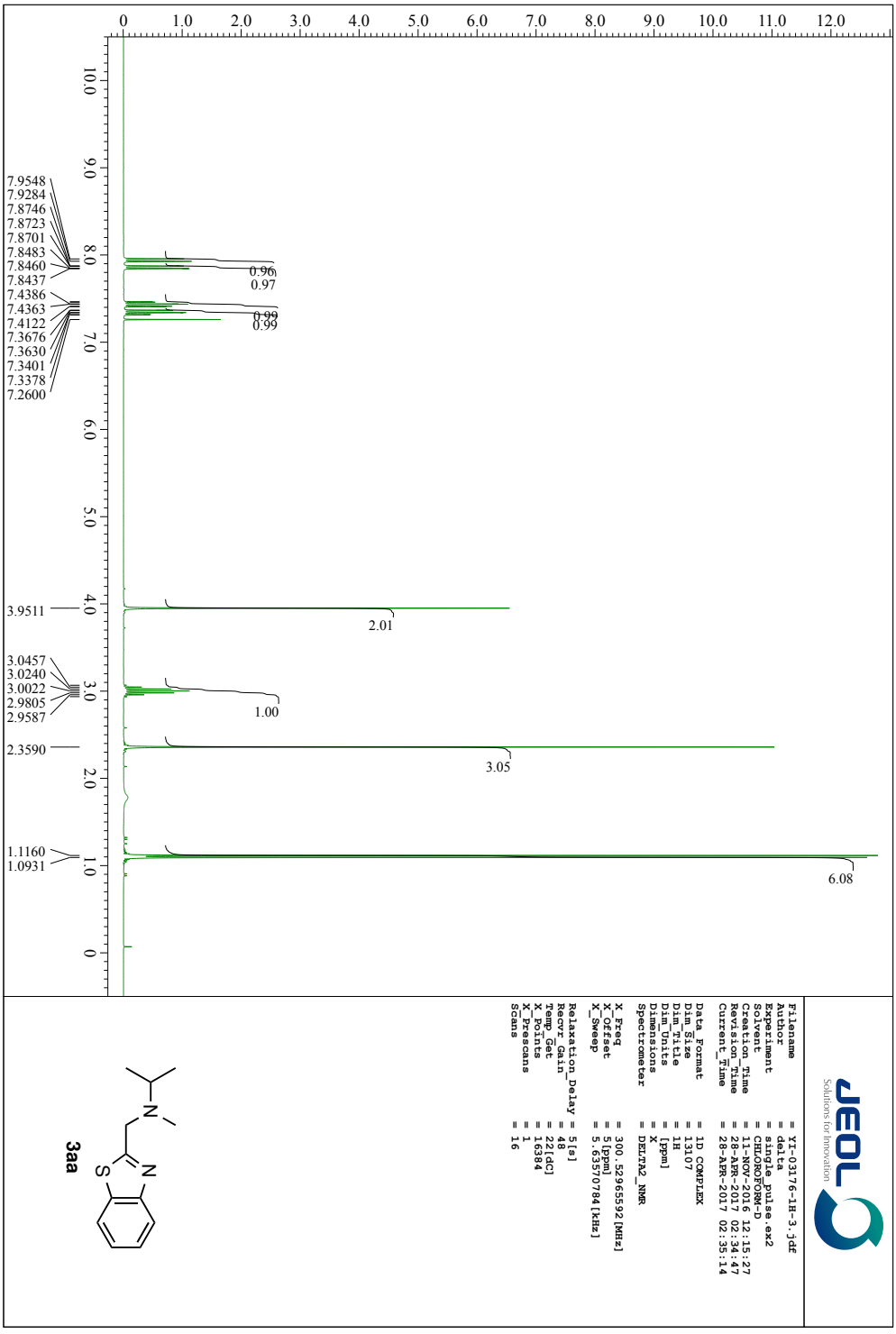
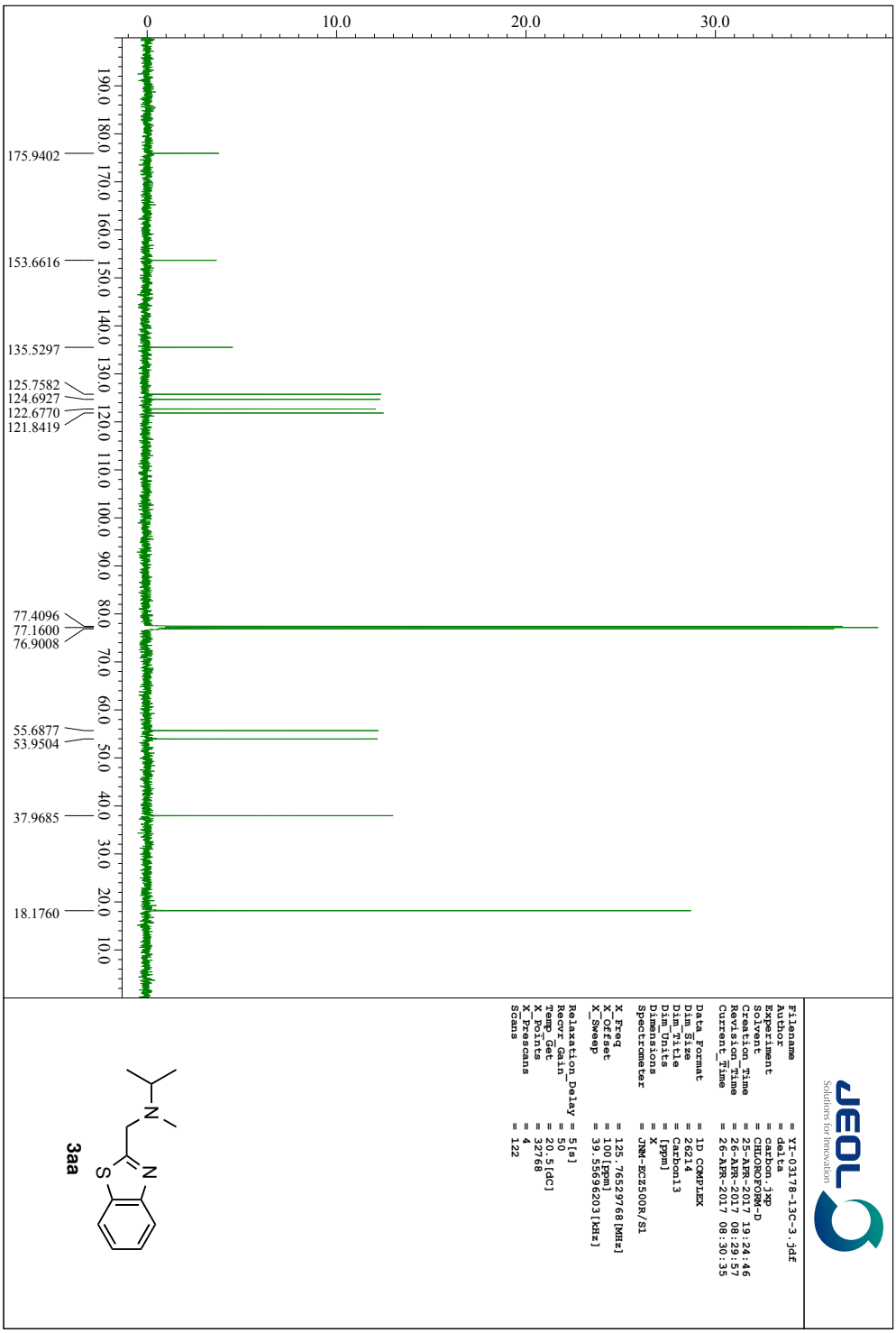
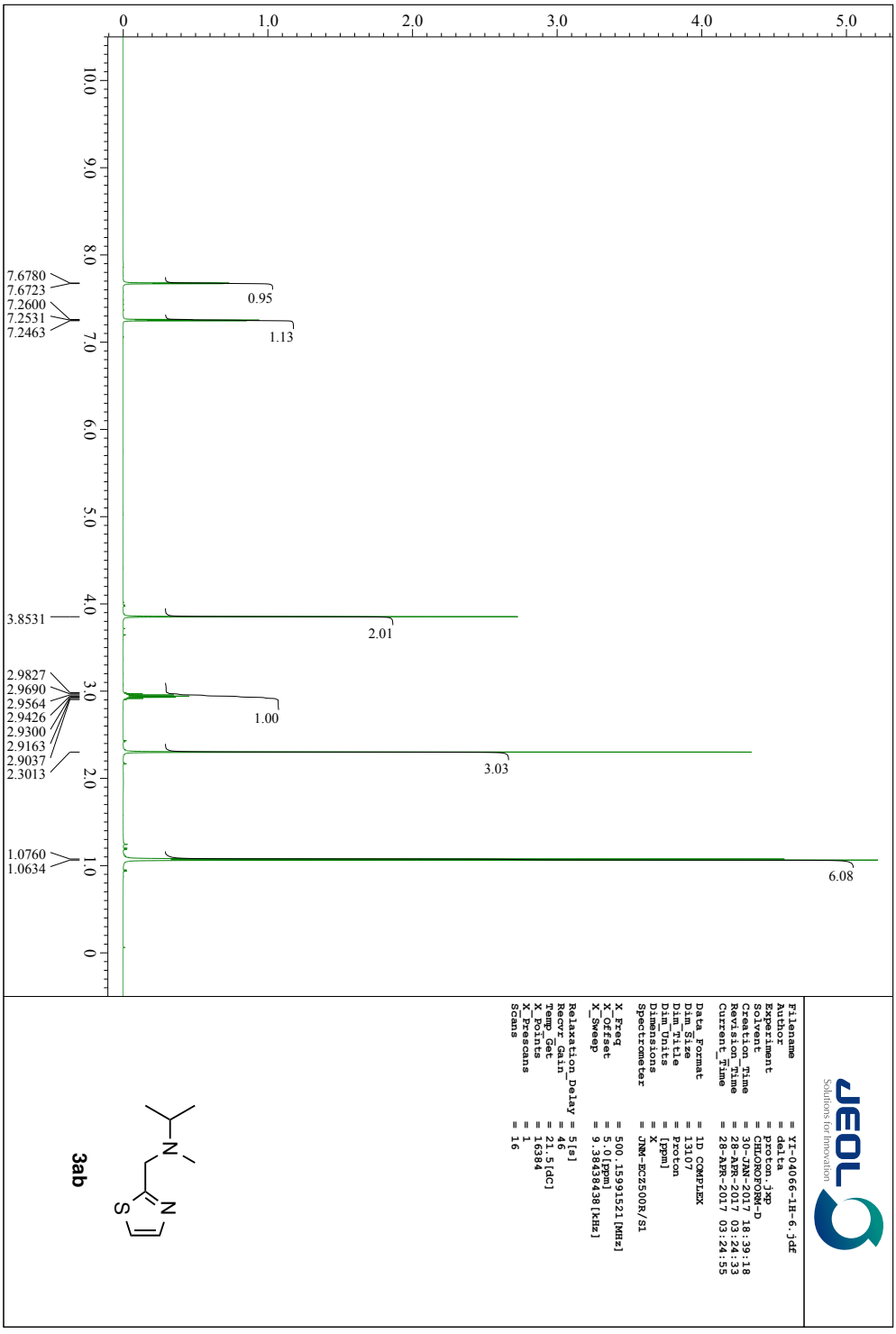
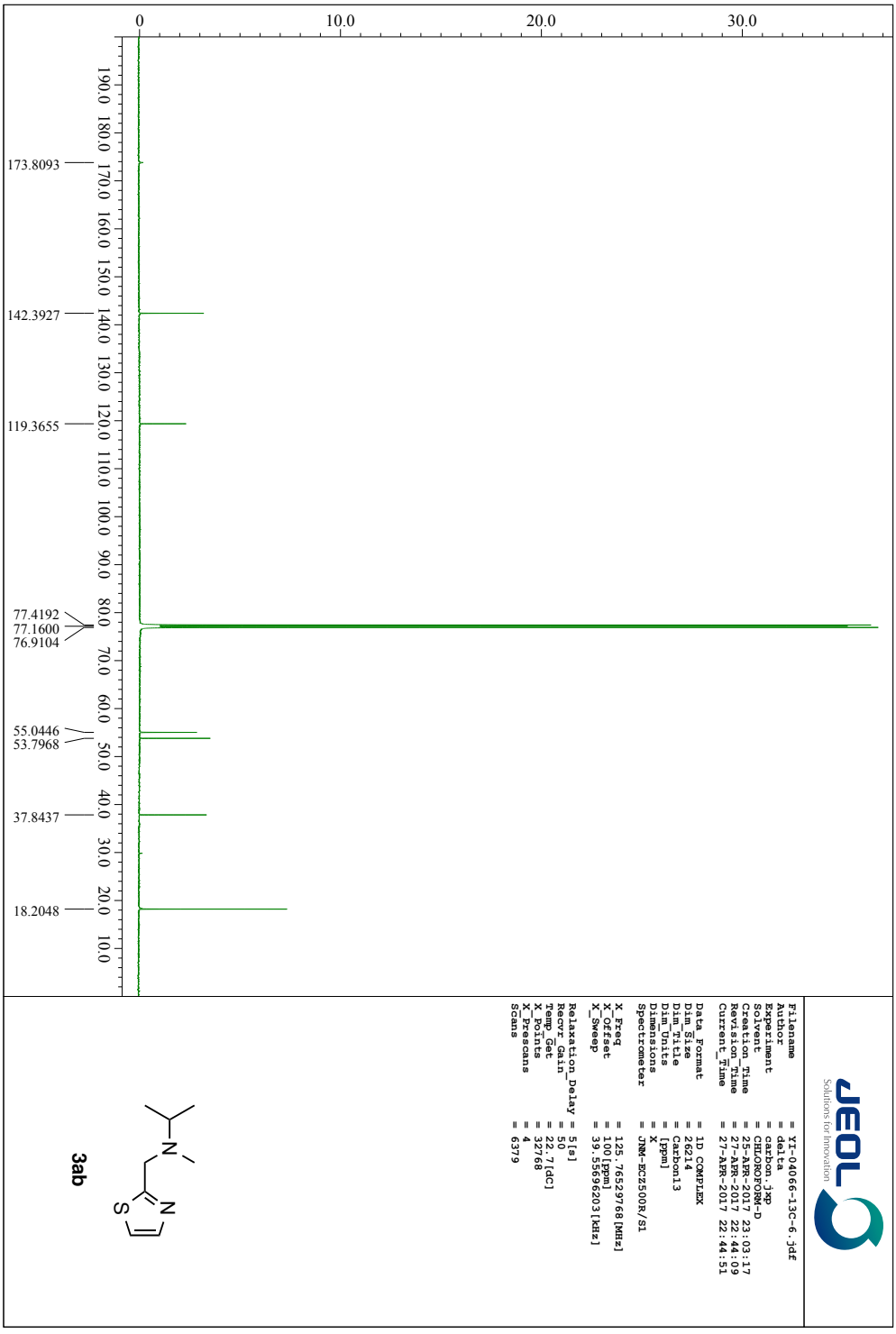
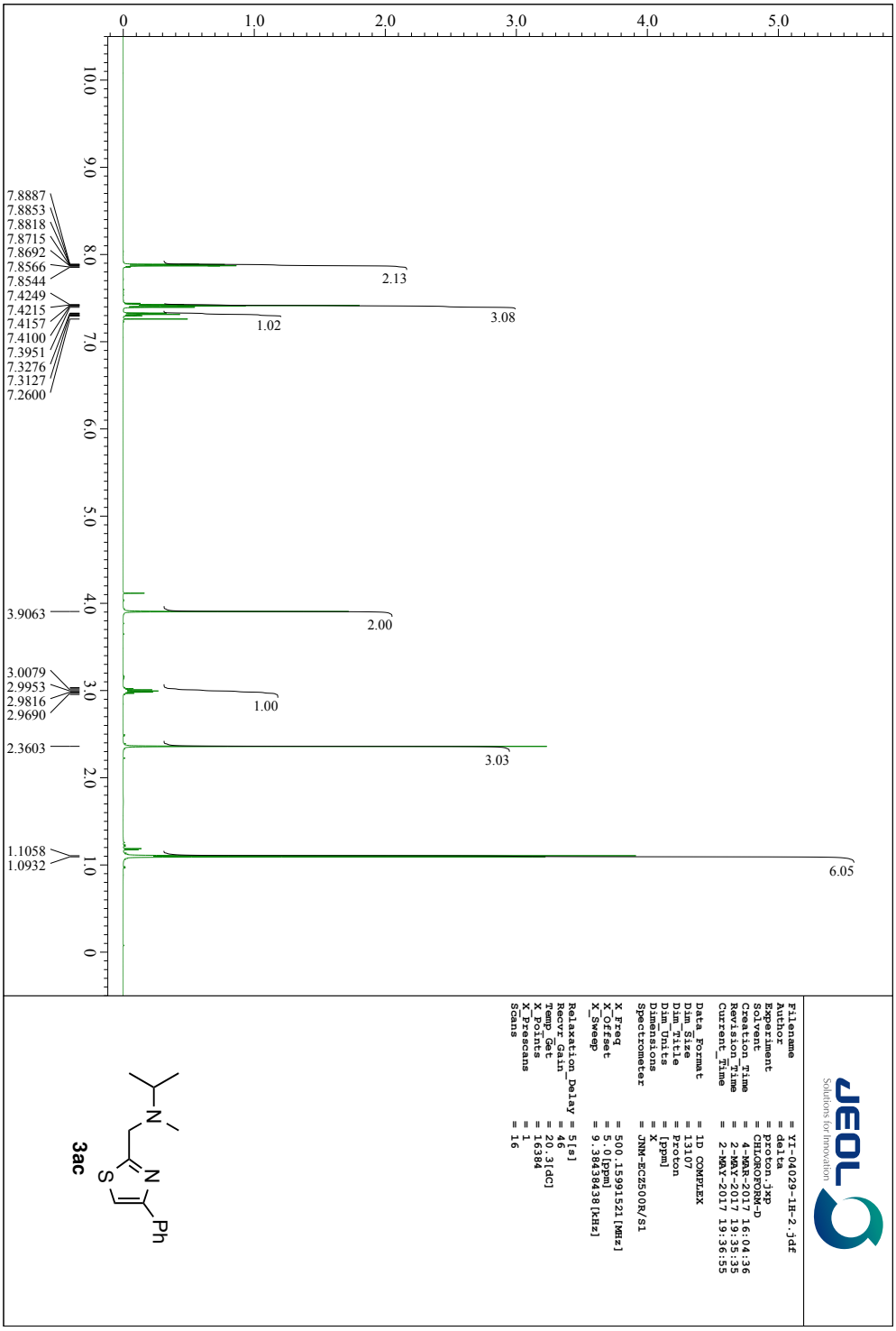
50.7252
37.9589
25.7302
14.1542
2"a

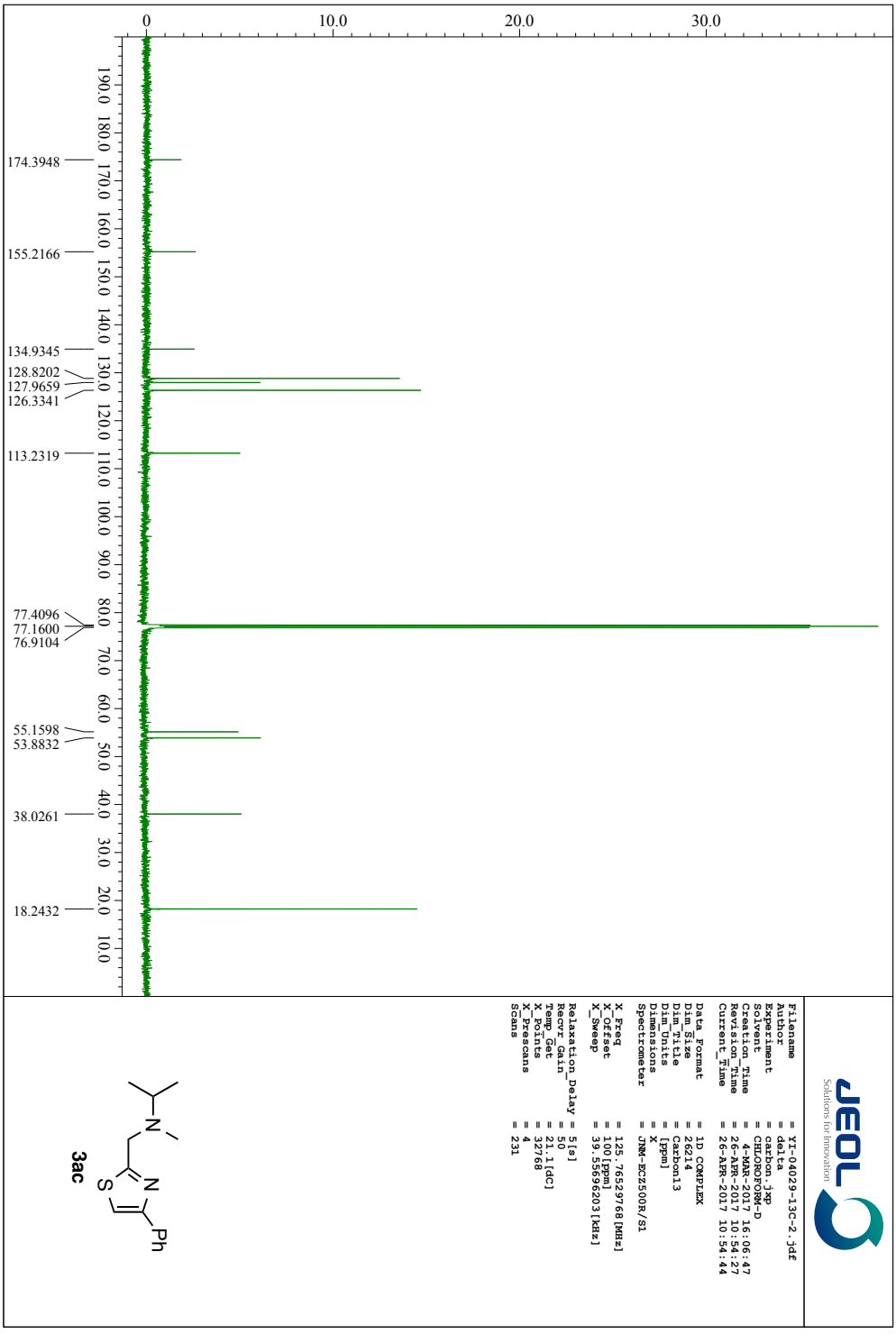

7.9548
7.9284
7.8746
7.8723
7.8701
7.8483
7.8460
7.8437
7.4386
7.4363
7.4122
7.3676
7.3630
7.3401
7.3378
7.2600
3.9511
3.0457
3.0240
3.0022
2.9805
2.9587
2.3590
1.1160
1.0931
0.96
0.97
0.99
0.99
2.01
1.00
3.05
6.08
JEOL
Solutions for Innovation
Filename = YI-03176-1H-3.jdf
Author = delta
Experiment = single_pulse.ex2
Solvent = CHLOROFORM-D
Creation_Time = 11-NOV-2016 12:15:27
Revision_Time = 28-APR-2017 02:34:47
Current_Time = 28-APR-2017 02:35:14
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
X_Freq = 300.52965592 [MHz]
X_Offset = 5 [ppm]
X_Sweep = 5.63570784 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 48
Temp_C = 22 [dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3aa

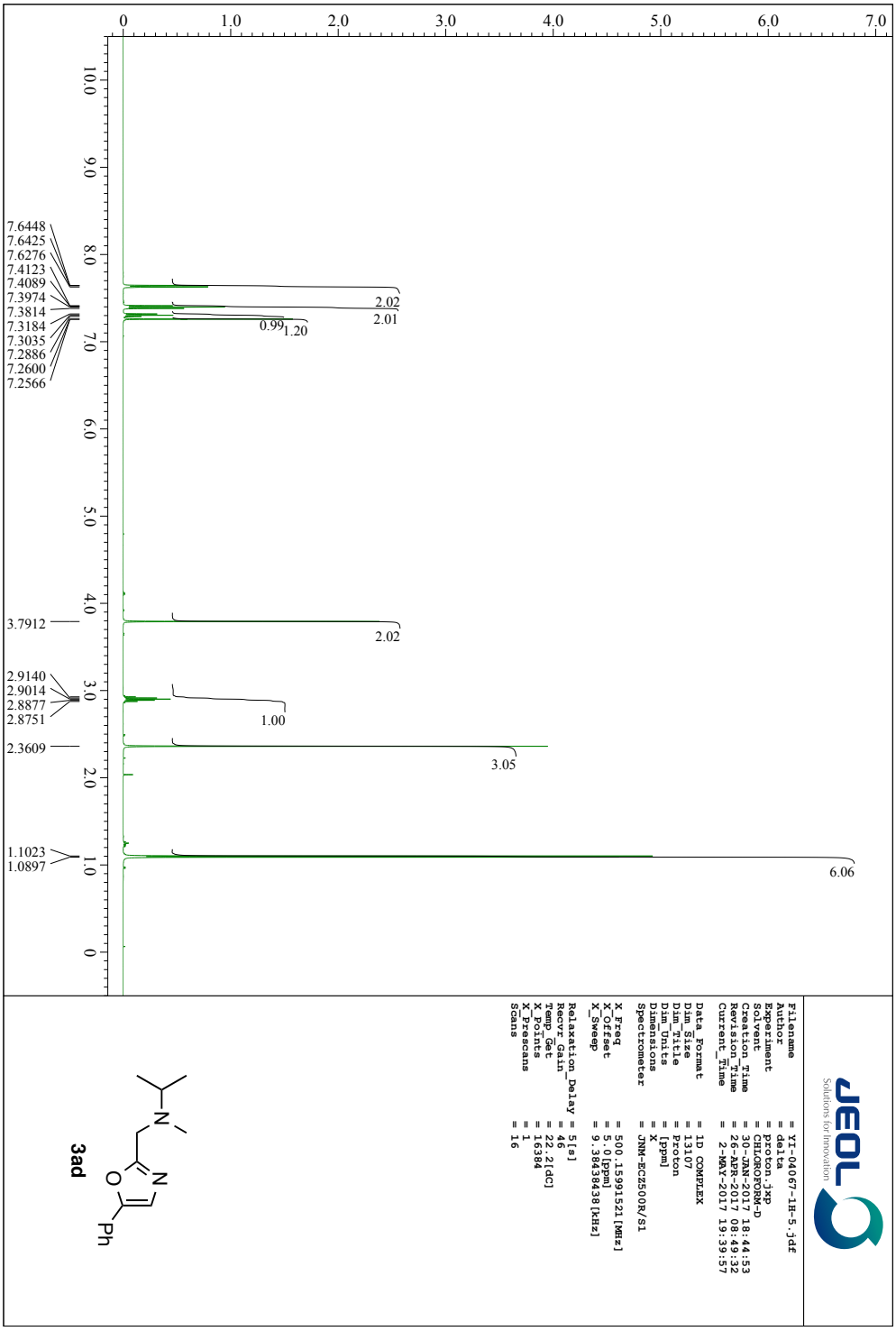

0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
175.9402
153.6616
135.5297
125.7582
124.6927
122.6770
121.8419
77.4096
77.1600
76.9008
55.6877
53.9504
37.9685
18.1760
JEOL
Solutions for Innovation
Filename = YI-03178-13C-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 25-APR-2017 19:24:46
Revision_Time = 26-APR-2017 08:29:57
Current_Time = 26-APR-2017 08:30:35
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.7652976 8 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 50.5 [dC]
Temp_Comte = 20
X_Points = 32768
X_Prescans = 4
Scans = 122
3aa
N
S
N

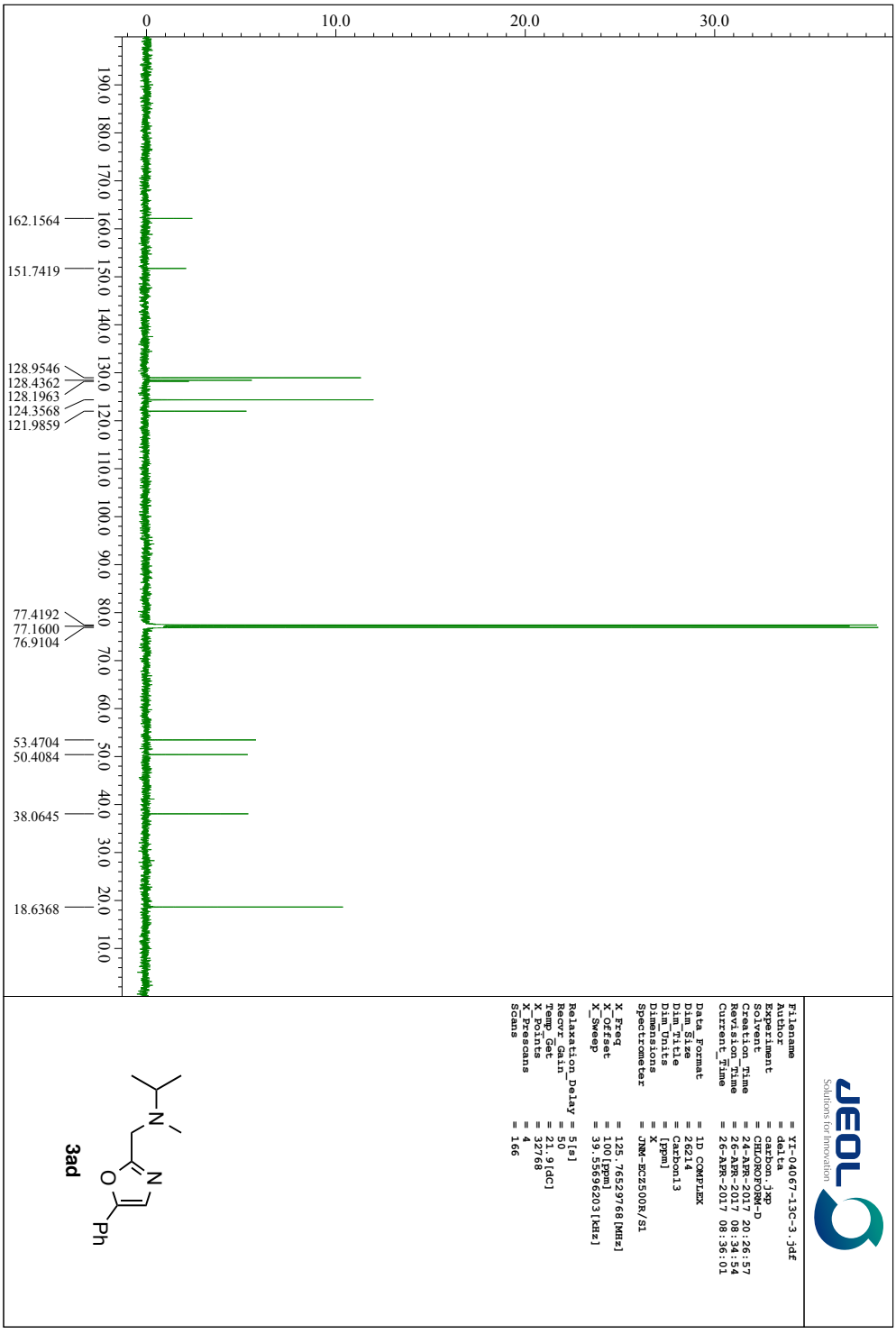

7.6780
7.6723
7.2600
7.2531
7.2463
3.8531
2.9827
2.9690
2.9564
2.9426
2.9300
2.9163
2.9037
2.3013
1.0760
1.0634
0.95
1.13
2.01
1.00
3.03
6.08
Filename = YI-04066-1H-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 30-JAN-2017 18:39:18
Revision_Time = 28-APR-2017 03:24:33
Current_Time = 28-APR-2017 03:24:55
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 40
Temp_C = 21.5 [dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3ab

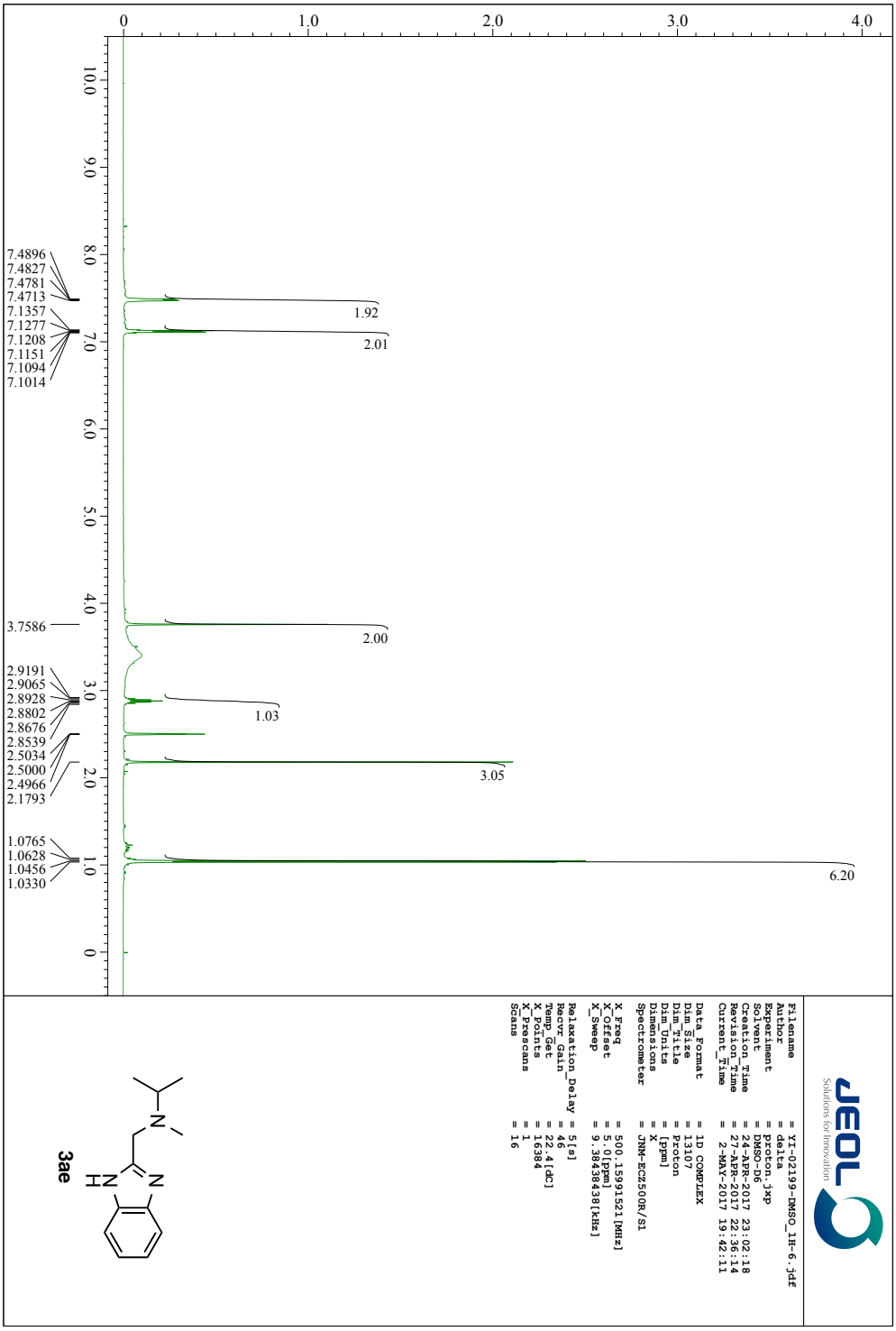

0
10.0
20.0
30.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
173.8093
142.3927
119.3655
77.4192
77.1600
76.9104
55.0446
53.7968
37.8437
18.2048
JEOL
Solutions for Innovation
Filename = YI-04066-13C-6.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 25-APR-2017 23:03:17
Revision_Time = 27-APR-2017 22:44:09
Current_Time = 27-APR-2017 22:44:51
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.7652976B [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 50.7 [dC]
Temp_C = 22
X_Points = 32768
X_Prescans = 4
Scans = 6379
3ab
N
S
N

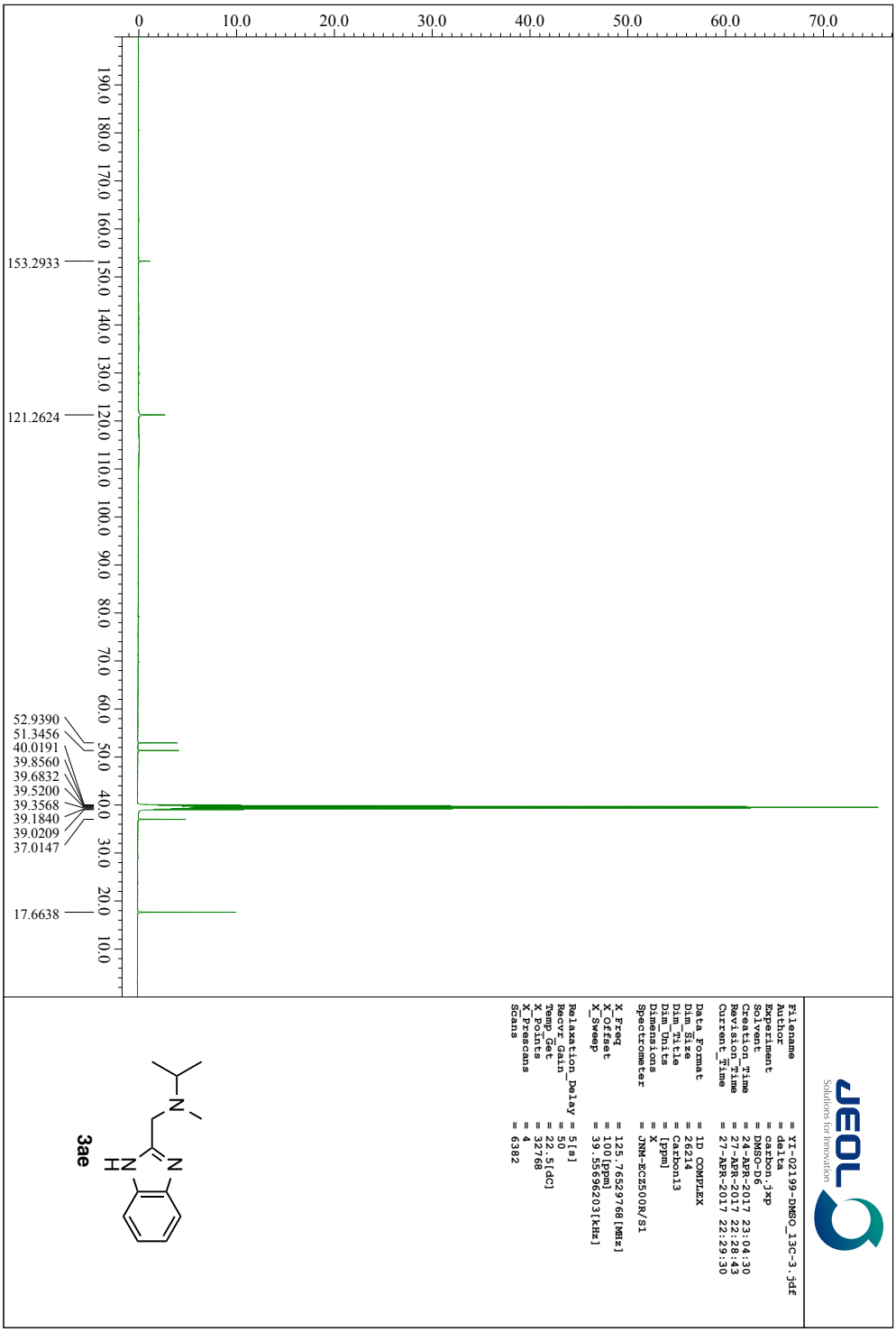

7.8887
7.8853
7.8818
7.8715
7.8692
7.8566
7.8544
7.4249
7.4215
7.4157
7.4100
7.3951
7.3276
7.3127
7.2600
3.9063
3.0079
2.9953
2.9816
2.9690
2.3603
1.1058
1.0932
2.13
3.08
1.02
2.00
1.00
3.03
6.05
Filename = YI-04029-1H-2.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-MAR-2017 16:04:36
Revision_Time = 2-MAY-2017 19:35:35
Current_Time = 2-MAY-2017 19:36:55
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 26.3[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3ac
N
S
N
Ph

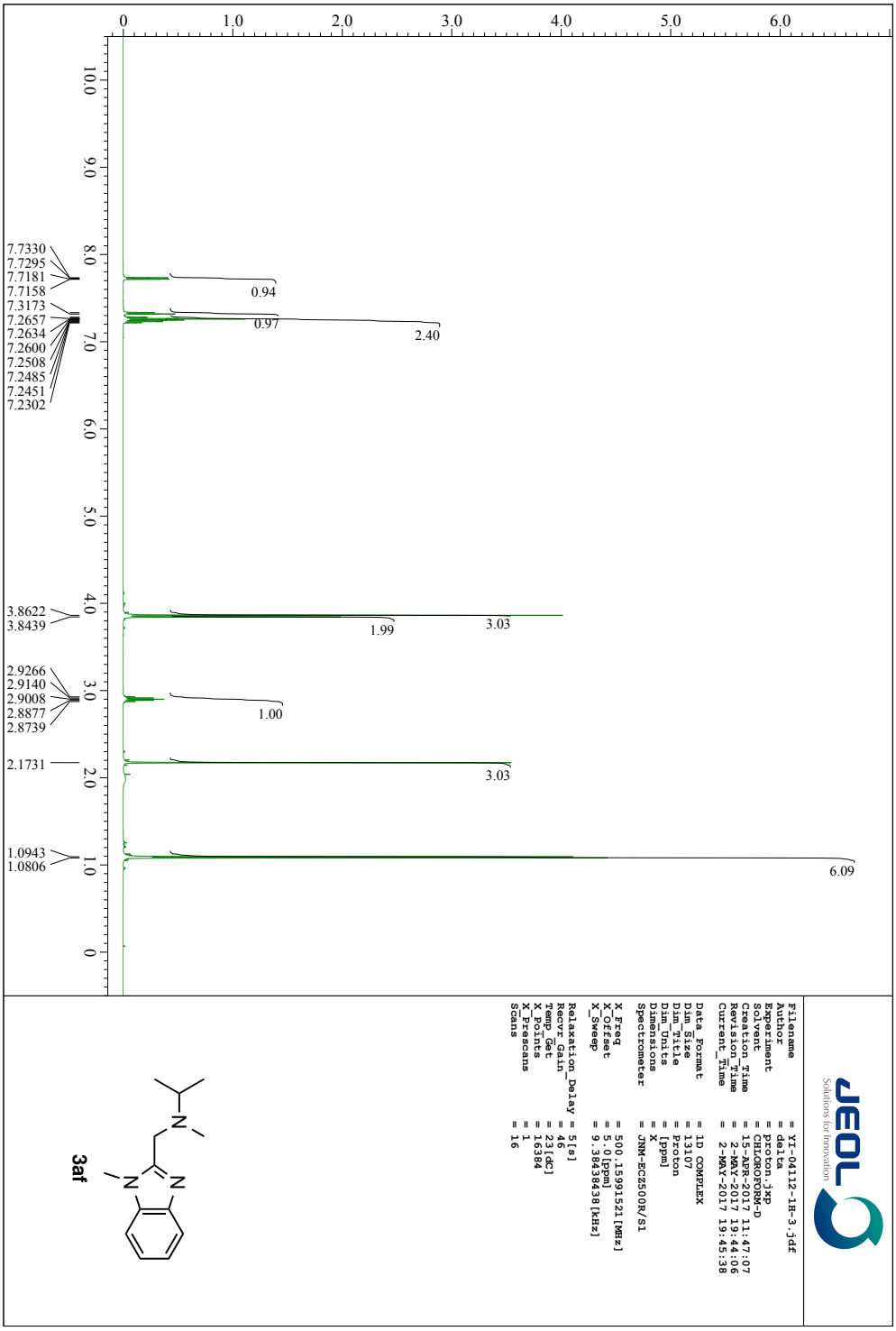

JEOL
Solutions for Innovation
Filename = YI-04029-13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-MAR-2017 16:06:47
Revision_Time = 26-APR-2017 10:54:27
Current_Time = 26-APR-2017 10:54:44
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.7652976 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 50
Temp_Get = 21.1 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 231
174.3948
155.2166
134.9345
128.8202
127.9659
126.3341
113.2319
77.4096
77.1600
76.9104
55.1598
53.8832
38.0261
18.2432
3ac
N
S
N
Ph

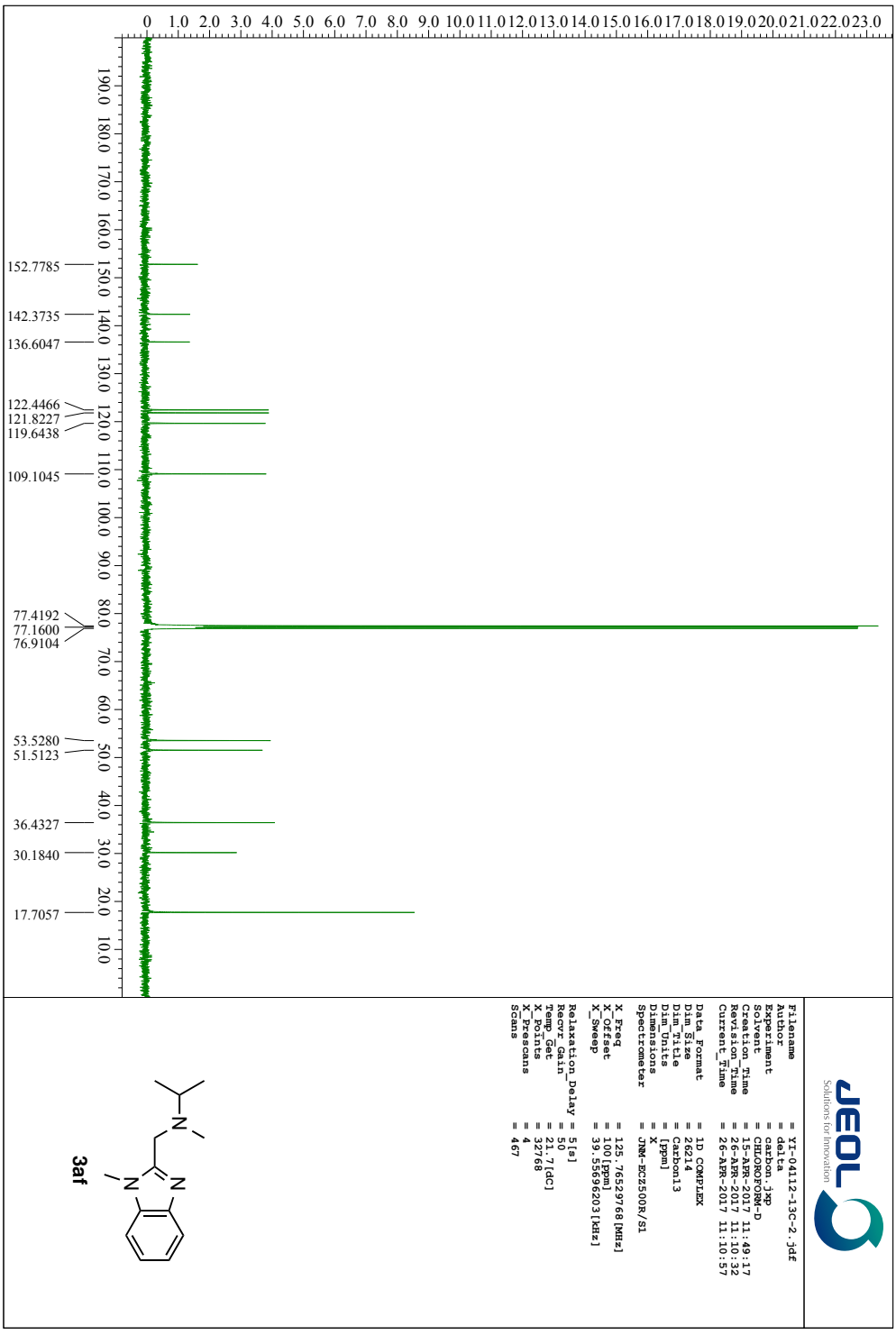

7.6448
7.6425
7.6276
7.4123
7.4089
7.3974
7.3814
7.3184
7.3035
7.2886
7.2600
7.2566
3.7912
2.9140
2.9014
2.8877
2.8751
2.3609
1.1023
1.0897
2.02
2.01
0.99
1.20
2.02
1.00
3.05
6.06
Filename = YI-04067-1H-5.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 30-JAN-2017 18:44:53
Revision_Time = 26-APR-2017 08:49:32
Current_Time = 2-MAY-2017 19:39:57
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.2[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3ad
N
N
O
Ph

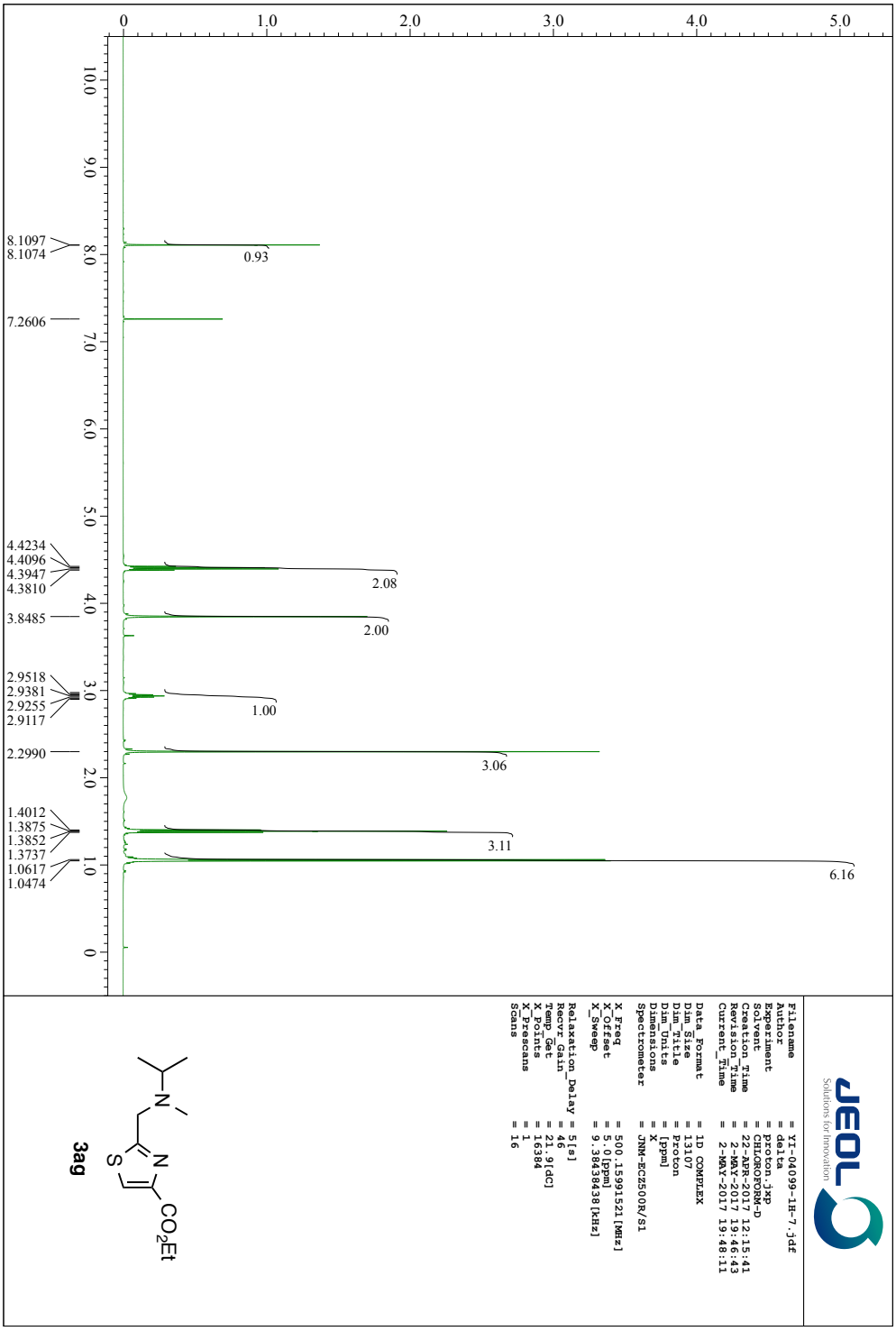

JEOL
Solutions for Innovation
Filename = YI-04067-13C-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 24-APR-2017 20:26:57
Revision_Time = 26-APR-2017 08:34:54
Current_Time = 26-APR-2017 08:36:01
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.7652976 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 50
Temp_C = 21.9 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 166
0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
162.1564
151.7419
128.9546
128.4362
128.1963
124.3568
121.9859
77.4192
77.1600
76.9104
53.4704
50.4084
38.0645
18.6368
3ad
N
N
O
Ph

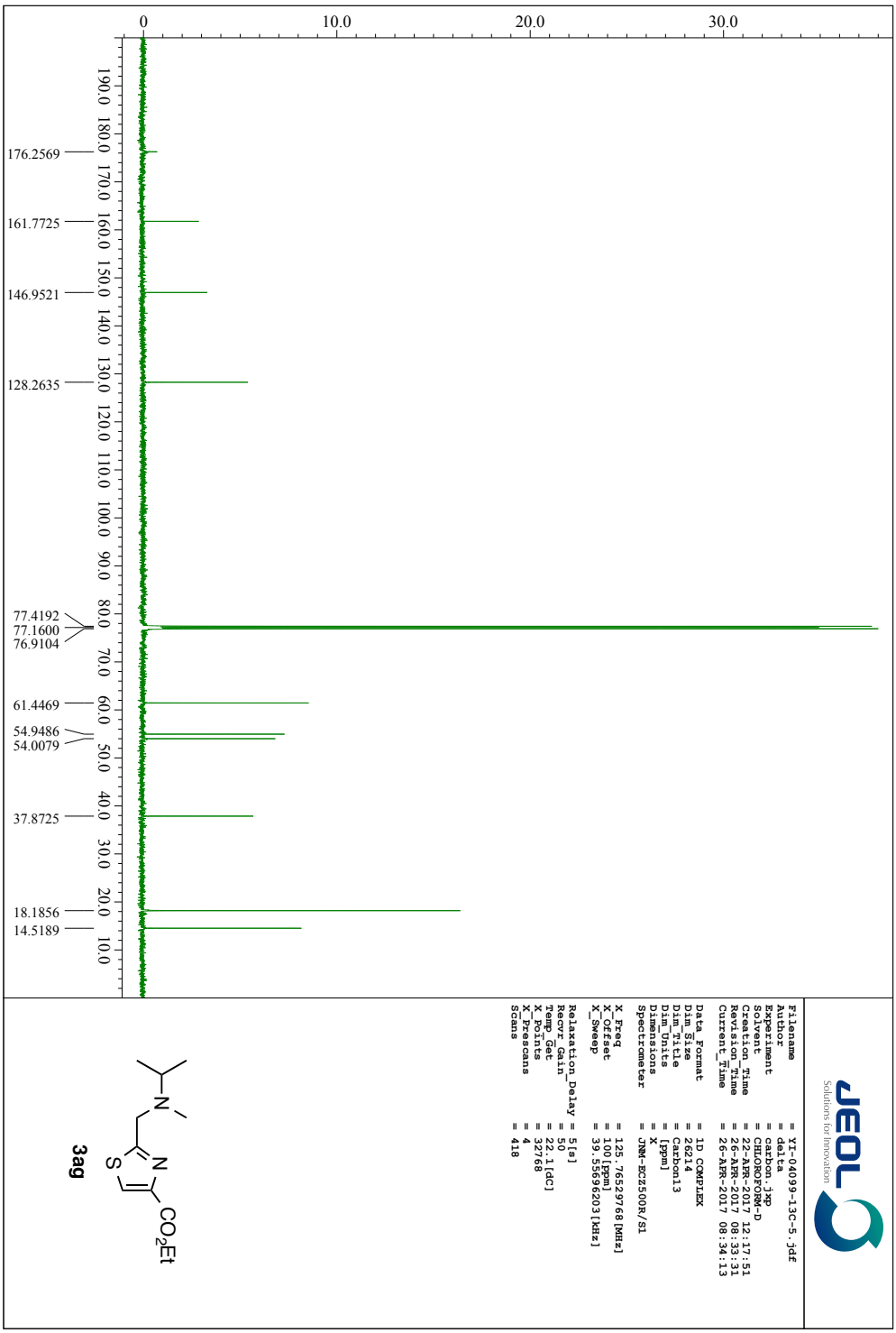

7.4896
7.4827
7.4781
7.4713
7.1357
7.1277
7.1208
7.1151
7.1094
7.1014
3.7586
2.9191
2.9065
2.8928
2.8802
2.8676
2.8539
2.5034
2.5000
2.4966
2.1793
1.0765
1.0628
1.0456
1.0330
1.92
2.01
2.00
1.03
3.05
6.20
Filename = YI-02199-DMSO_1H-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = DMSO-D6
Creation_Time = 24-APR-2017 23:02:18
Revision_Time = 27-APR-2017 22:36:14
Current_Time = 2-MAY-2017 19:42:11
Data_Format = 1D COMPLEX
Dim_Size = 12107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.4[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3ae

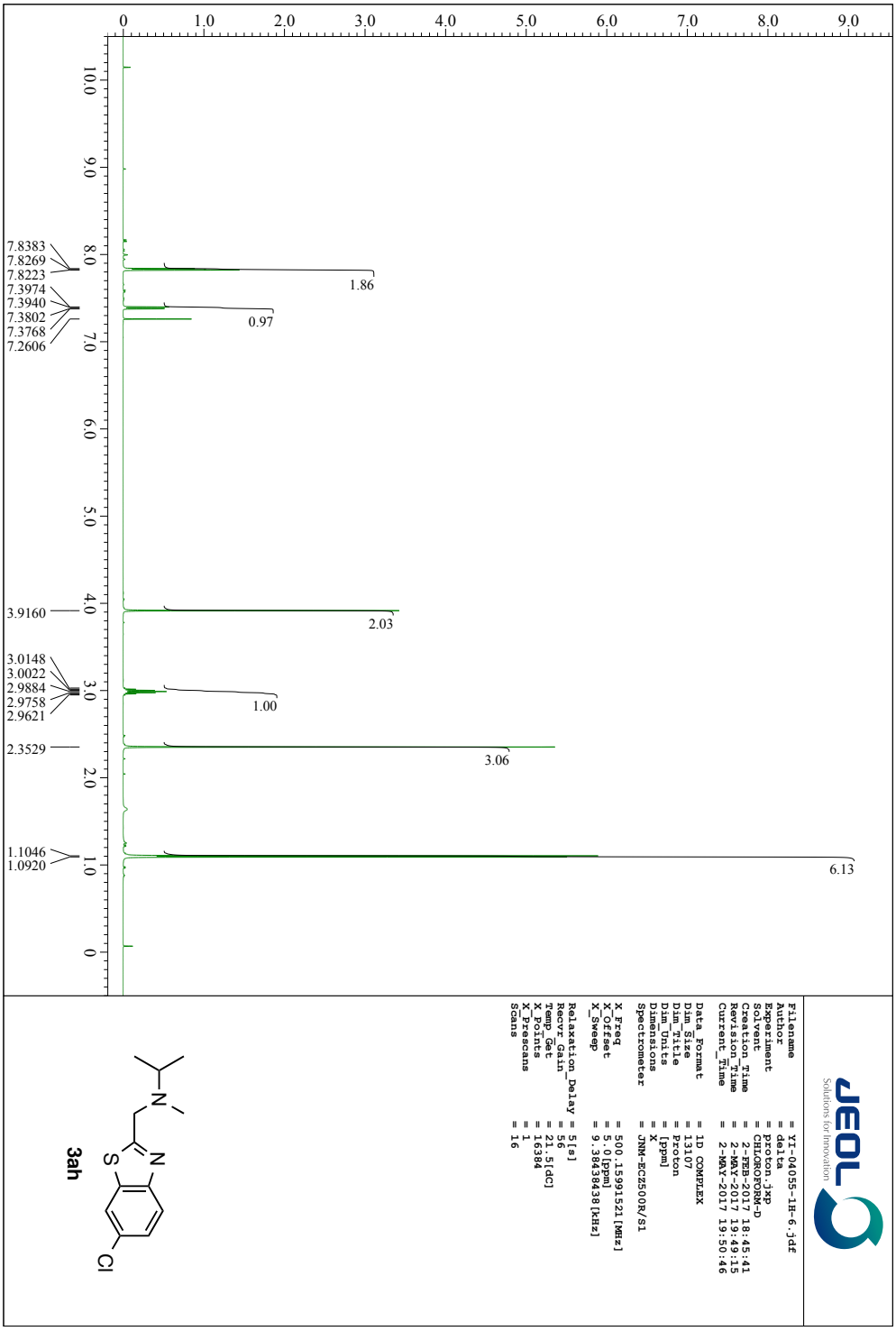

0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
153.2933
121.2624
52.9390
51.3456
40.0191
39.8560
39.6832
39.5200
39.3568
39.1840
39.0209
37.0147
17.6638
JEOL
Solutions for Innovation
Filename = YI-02199-DMSO_13C-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = DMSO-D6
Creation_Time = 24-APR-2017 23:04:30
Revision_Time = 27-APR-2017 22:28:43
Current_Time = 27-APR-2017 22:29:30
Data_Format = 1D COMPLEX
Dim_Size = 2F214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[KHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Comments = 22.5[dC]
X_Points = 32768
X_Prescans = 4
Scans = 6382
3ae

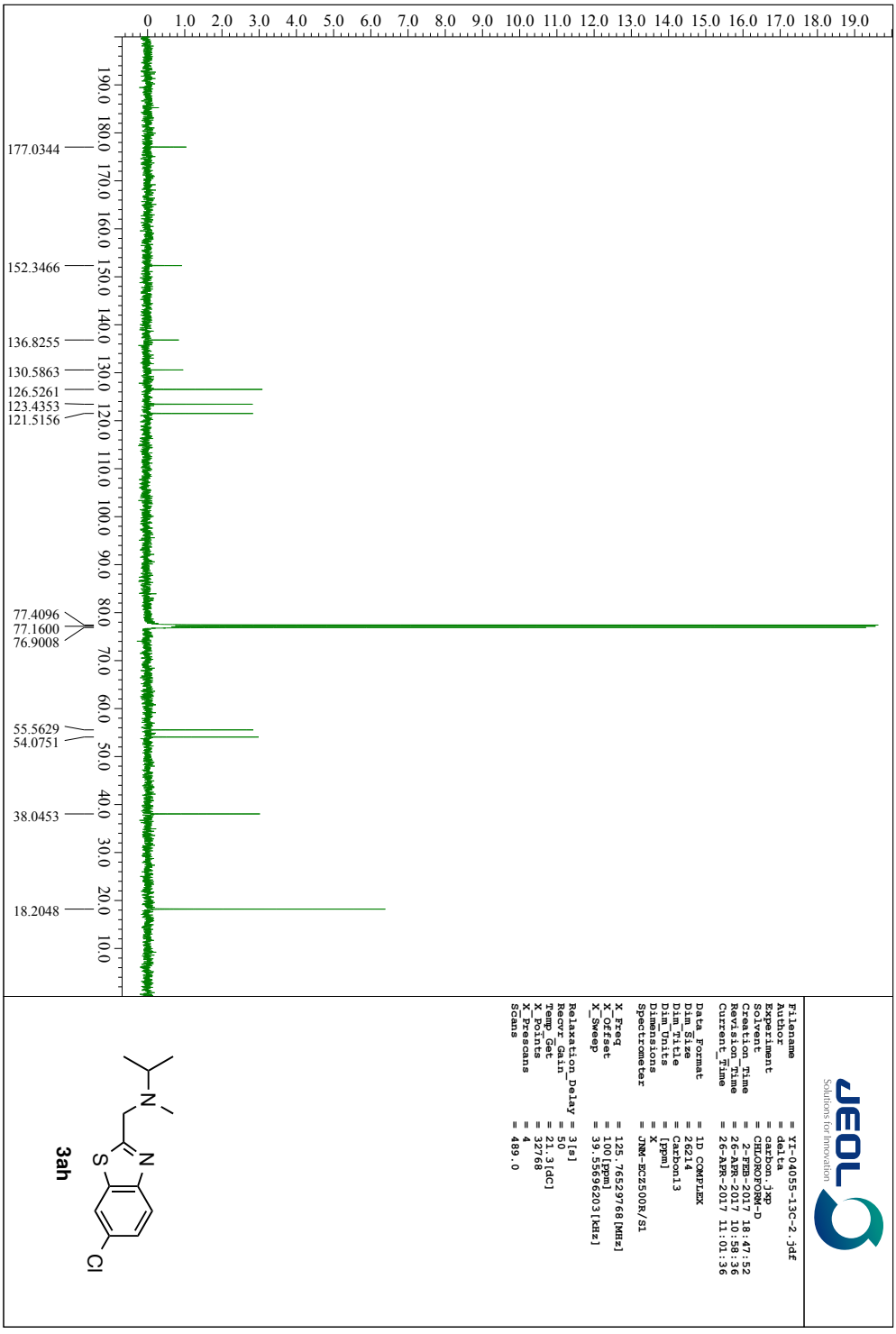

7.7330
7.7295
7.7181
7.7158
7.3173
7.2657
7.2634
7.2600
7.2508
7.2485
7.2451
7.2302
3.8622
3.8439
2.9266
2.9140
2.9008
2.8877
2.8739
2.1731
1.0943
1.0806
0.94
0.97
2.40
1.99
3.03
1.00
3.03
6.09
3af
Filename = YI-04112-1H-3.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 15-APR-2017 11:47:07
Revision_Time = 2-MAY-2017 19:44:06
Current_Time = 2-MAY-2017 19:45:38
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16

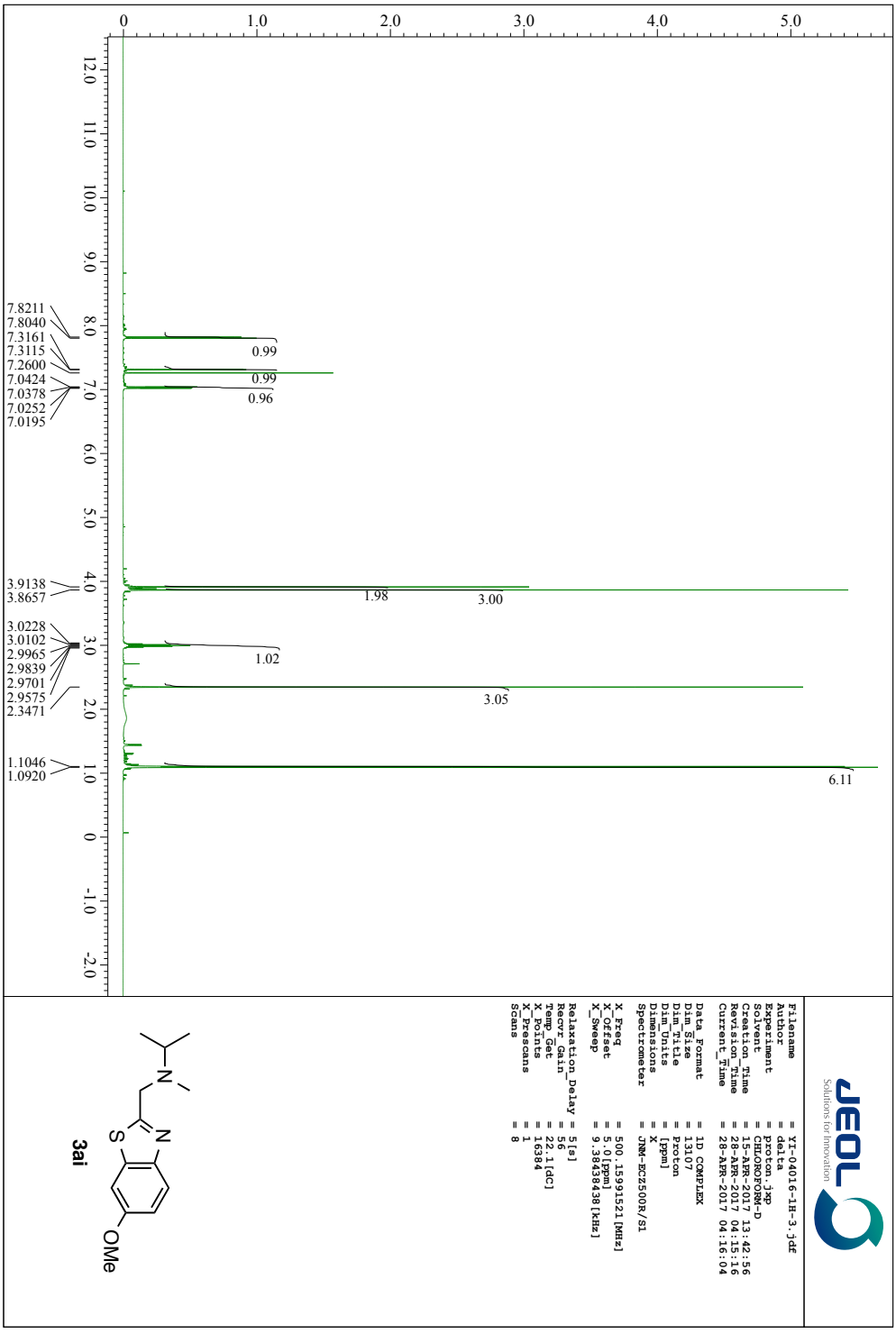

JEOL
Solutions for Innovation
Filename = YI-04112-13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 15-APR-2017 11:49:17
Revision_Time = 26-APR-2017 11:10:32
Current_Time = 26-APR-2017 11:10:57
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.7652976 8 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 50
Temp = 21.7 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 467
152.7785
142.3735
136.6047
122.4466
121.8227
119.6438
109.1045
77.4192
77.1600
76.9104
53.5280
51.5123
36.4327
30.1840
17.7057
3af

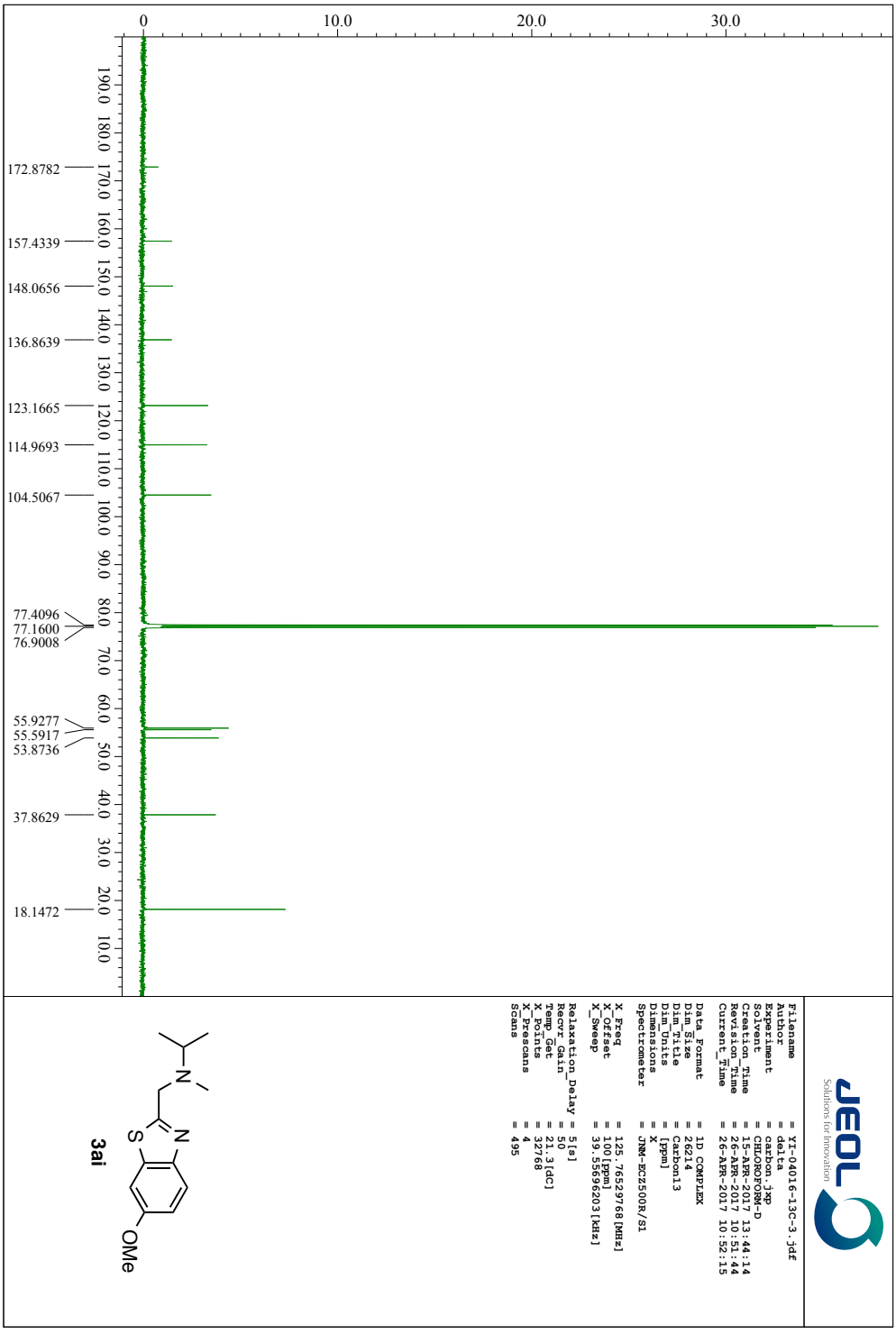

8.1097
8.1074
7.2606
4.4234
4.4096
4.3947
4.3810
3.8485
2.9518
2.9381
2.9255
2.9117
2.2990
1.4012
1.3875
1.3852
1.3737
1.0617
1.0474
0.93
2.08
2.00
1.00
3.06
3.11
6.16
JEOL
Solutions for Innovation
Filename = YI-04099-1H-7.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 22-APR-2017 12:15:41
Revision_Time = 2-MAY-2017 19:46:43
Current_Time = 2-MAY-2017 19:48:11
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.9[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3ag

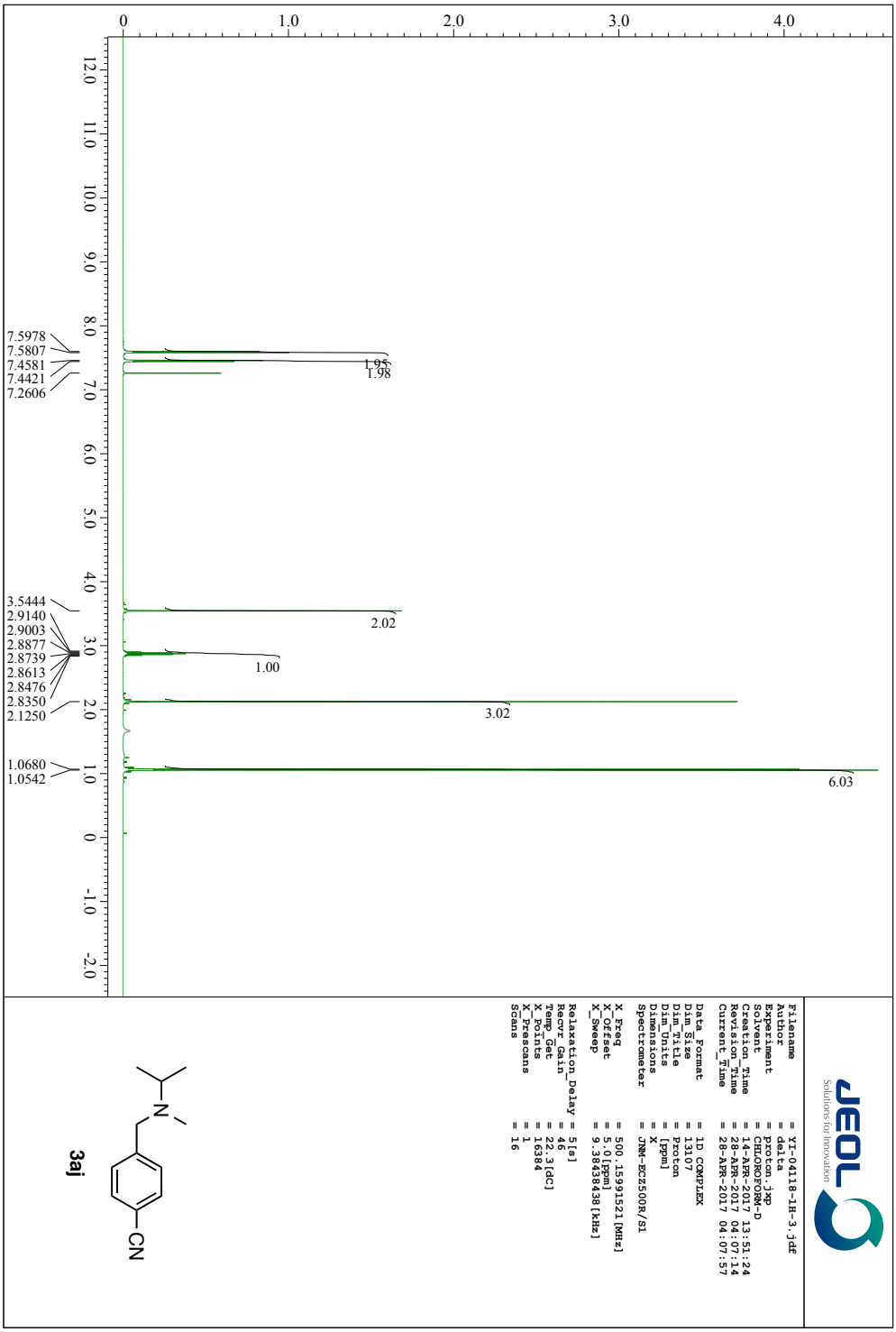

0
10.0
20.0
30.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
176.2569
161.7725
146.9521
128.2635
77.4192
77.1600
76.9104
61.4469
54.9486
54.0079
37.8725
18.1856
14.5189
JEOL
Solutions for Innovation
Filename = YI-04099-13C-5.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 22-APR-2017 12:17:51
Revision_Time = 26-APR-2017 08:33:31
Current_Time = 26-APR-2017 08:34:13
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.7652976 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 22.1 [dC]
Temp_C = 32768
X_Points = 4
X_Prescans = 418
Scans
N
S
N
CO2Et
3ag

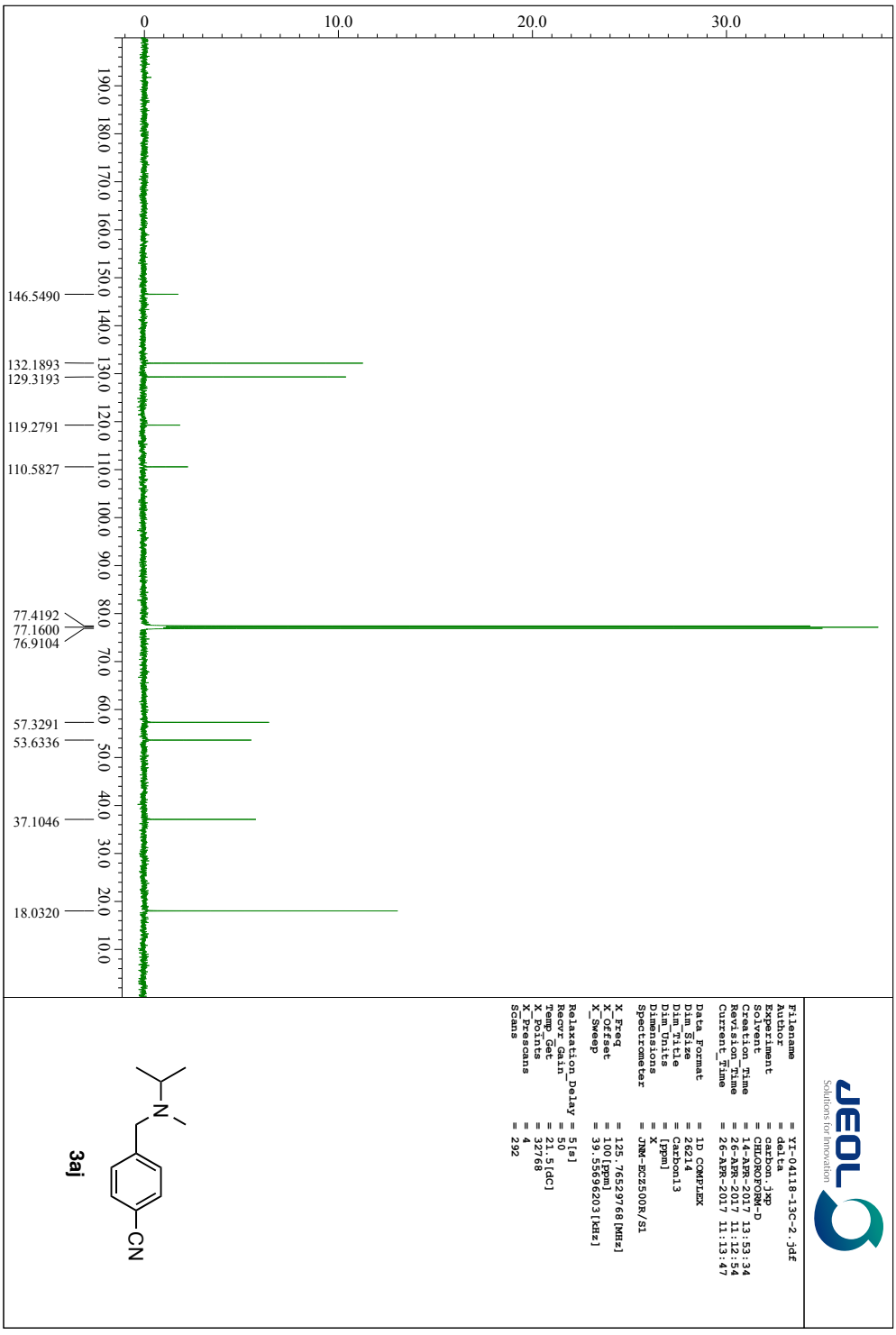

7.8383
7.8269
7.8223
7.3974
7.3940
7.3802
7.3768
7.2606
3.9160
3.0148
3.0022
2.9884
2.9758
2.9621
2.3529
1.1046
1.0920
1.86
0.97
2.03
1.00
3.06
6.13
Filename = YI-04055-1H-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 2-FEB-2017 18:45:41
Revision_Time = 2-MAY-2017 19:49:15
Current_Time = 2-MAY-2017 19:50:46
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.5[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3ah

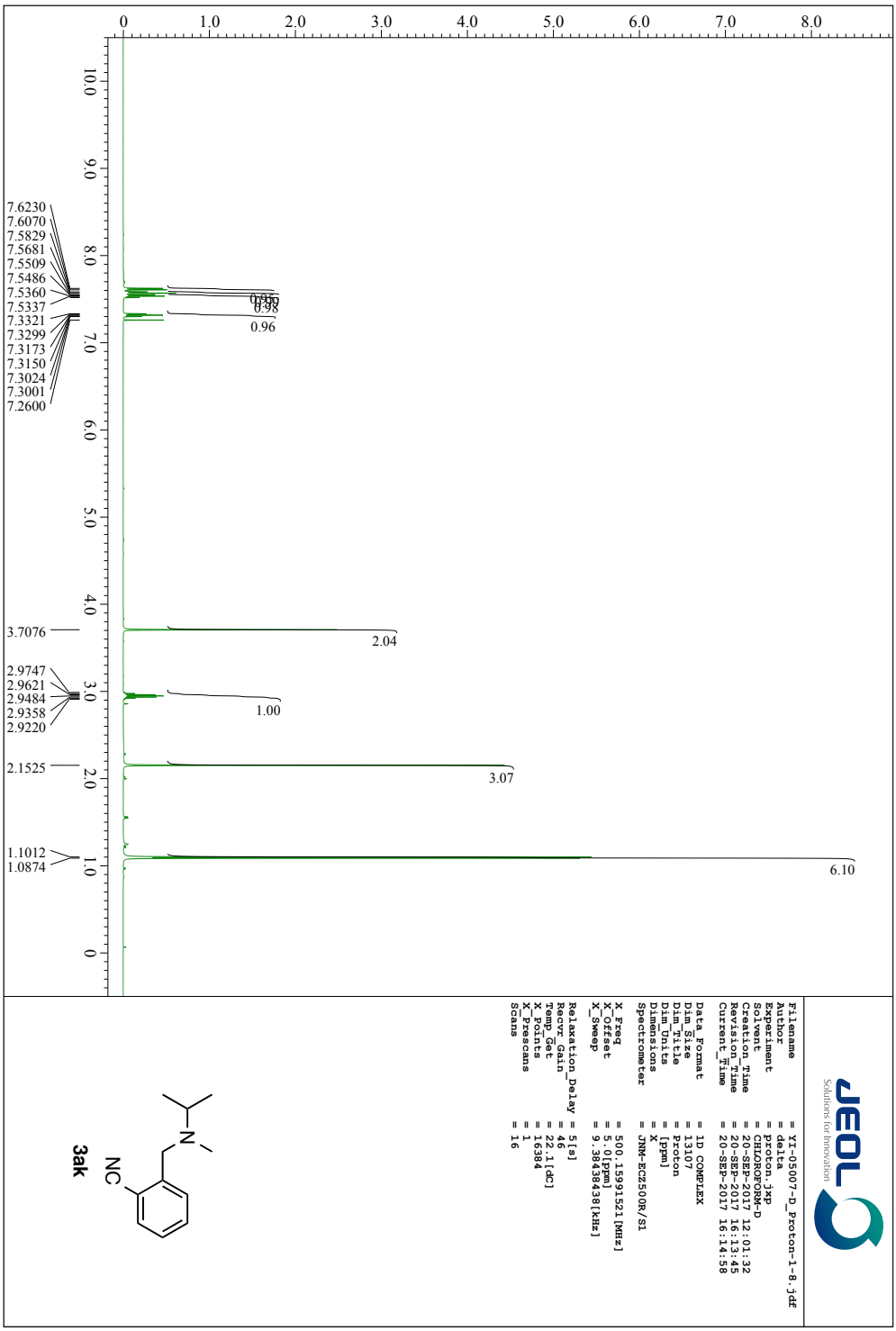

JEOL
Solutions for Innovation
Filename = YI-04055-13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 2-FEB-2017 18:47:52
Revision_Time = 26-APR-2017 10:58:36
Current_Time = 26-APR-2017 11:01:36
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.7652976B [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 3 [s]
Recvr_Gain = 50
Temp_C = 21.3 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 489.0
177.0344
152.3466
136.8255
130.5863
126.5261
123.4353
121.5156
77.4096
77.1600
76.9008
55.5629
54.0751
38.0453
18.2048
3ah
S
N
N
Cl

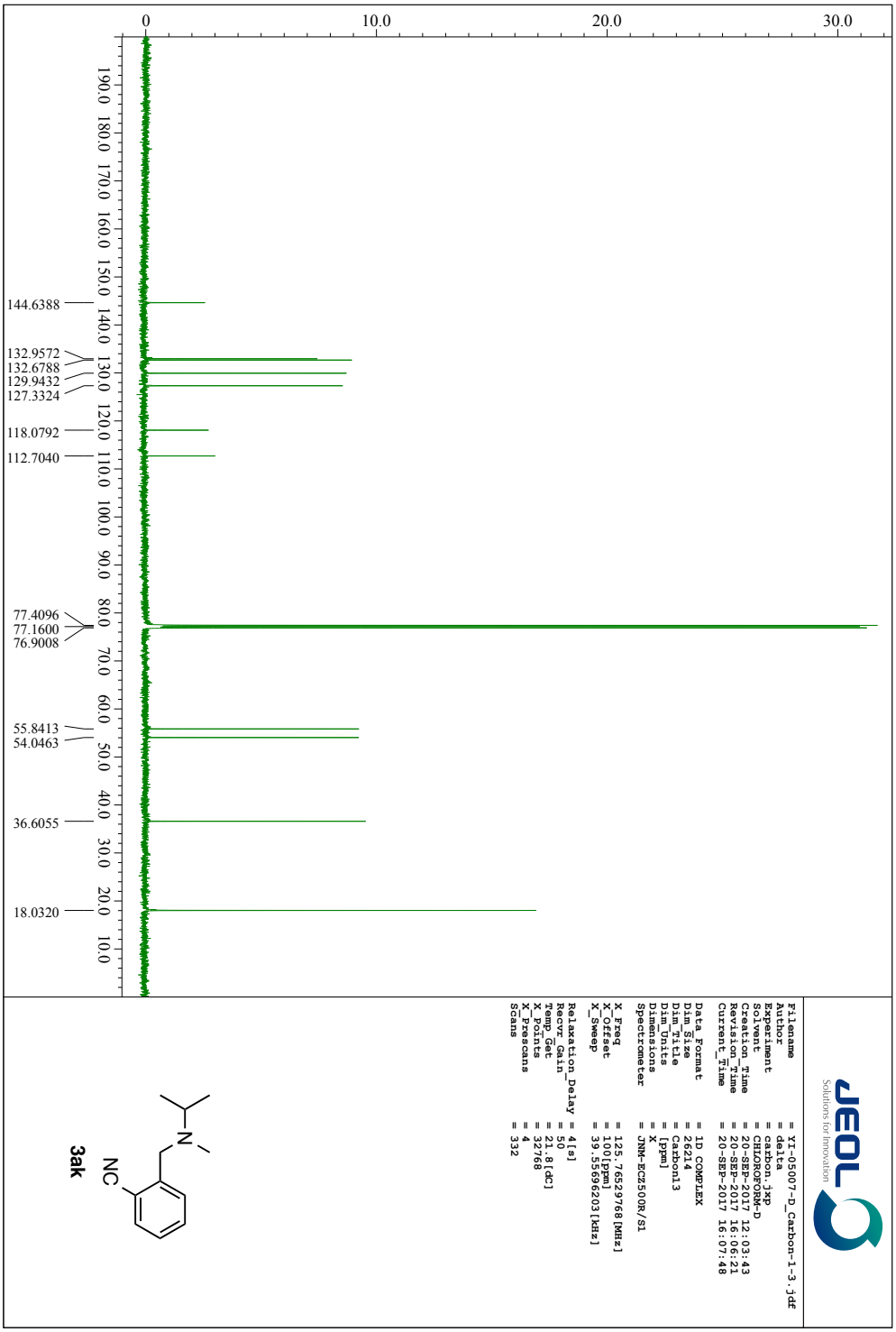

7.8211
7.8040
7.3161
7.3115
7.2600
7.0424
7.0378
7.0252
7.0195
3.9138
3.8657
3.0228
3.0102
2.9965
2.9839
2.9701
2.9575
2.3471
1.1046
1.0920
0.99
0.99
0.96
1.98
3.00
1.02
3.05
6.11
Solutions for Innovation
Filename = YI-04016-1H-3.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 15-APR-2017 13:42:56
Revision_Time = 28-APR-2017 04:15:16
Current_Time = 28-APR-2017 04:16:04
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 56
Temp_C_Gain = 22.1 [dC]
X_Points = 16384
X_Prescans = 1
Scans = 8
N
S
N
OMe
3ai

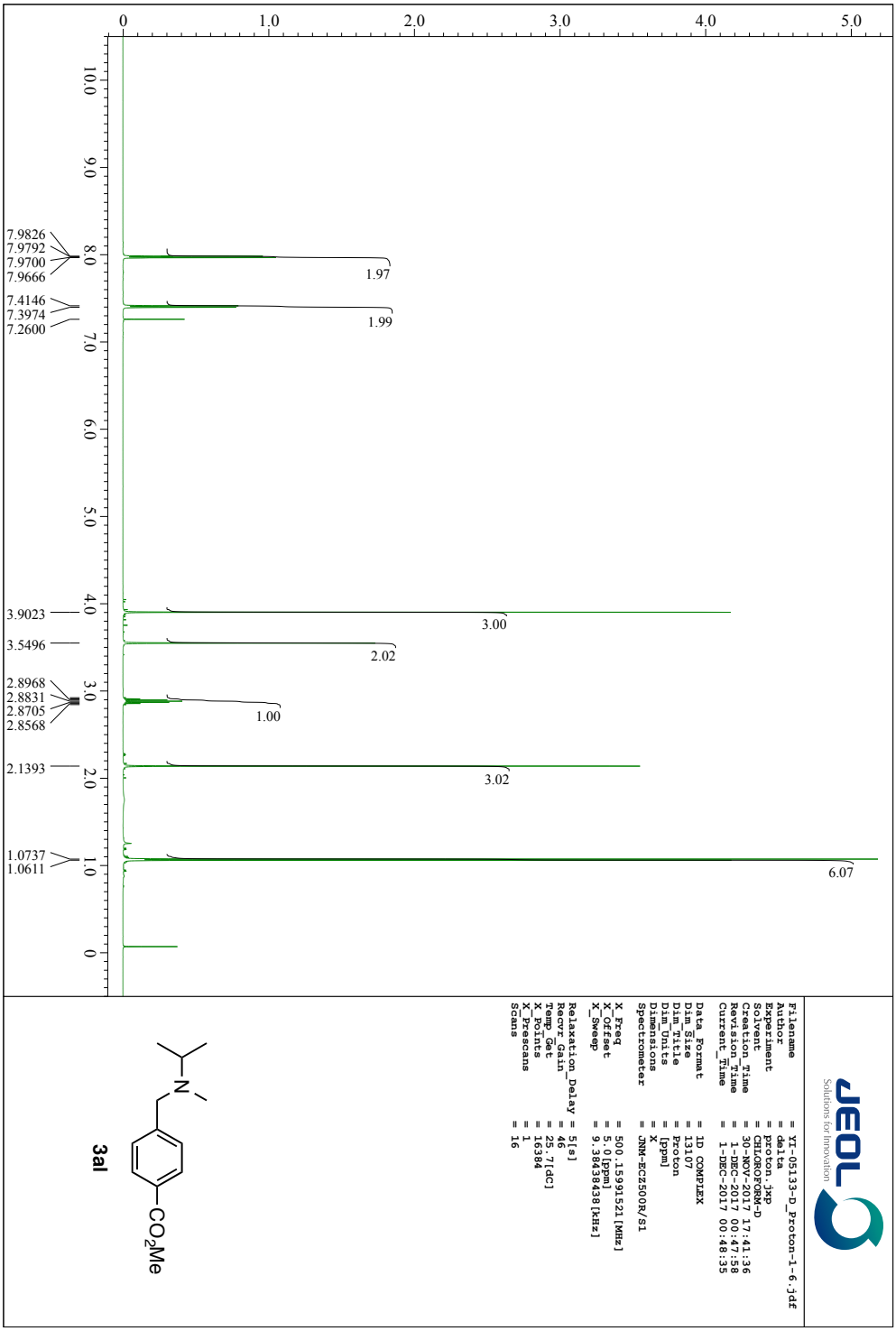

JEOL
Solutions for Innovation
Filename = YI-04016-13C-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 15-APR-2017 13:44:14
Revision_Time = 26-APR-2017 10:51:44
Current_Time = 26-APR-2017 10:52:15
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.7652976 8[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_C = 21.3[dC]
X_Points = 32768
X_Prescans = 4
Scans = 495
172.8782
157.4339
148.0656
136.8639
123.1665
114.9693
104.5067
77.4096
77.1600
76.9008
55.9277
55.5917
53.8736
37.8629
18.1472
N
S
N
OMe
3ai

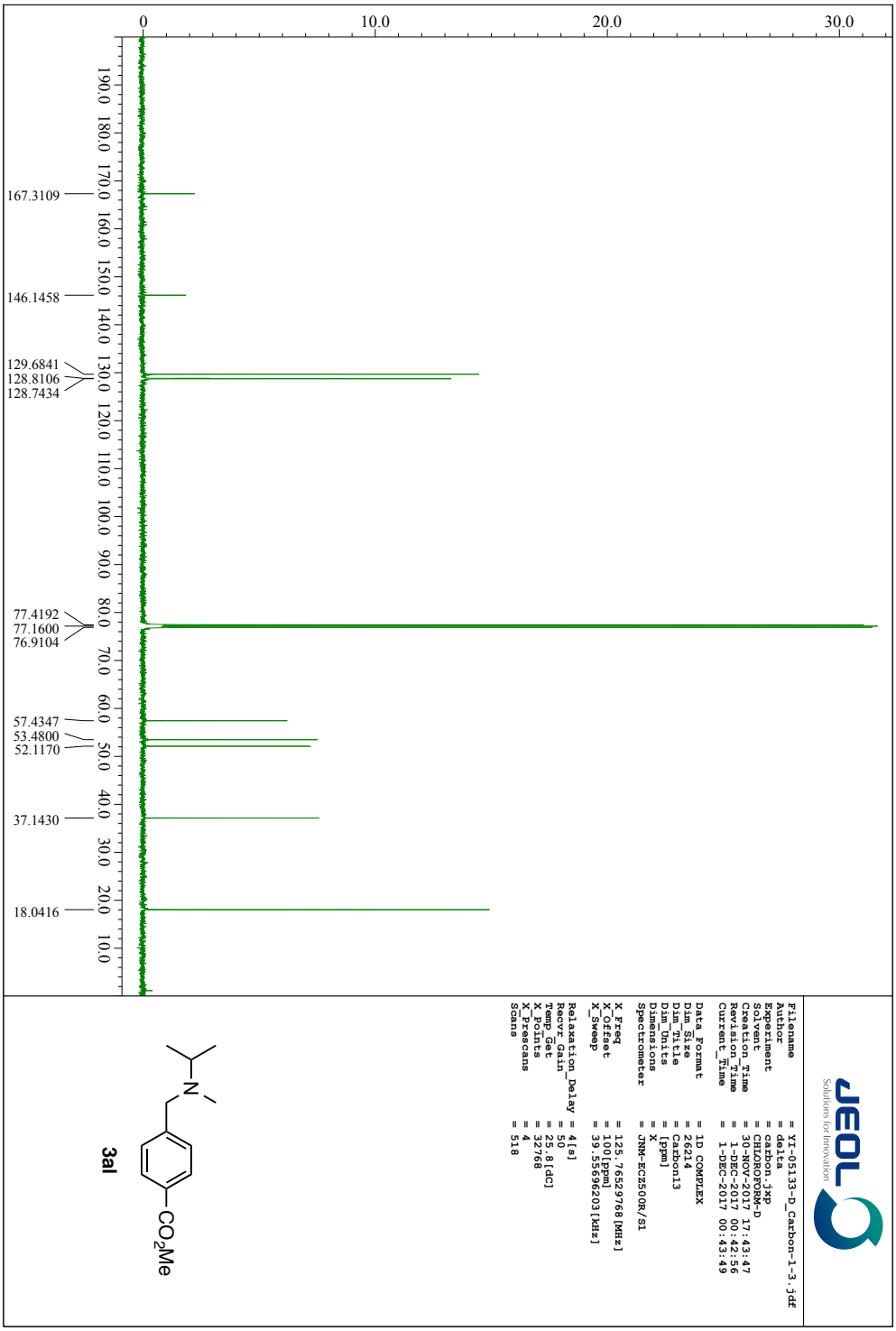

7.5978
7.5807
7.4581
7.4421
7.2606
3.5444
2.9140
2.9003
2.8877
2.8739
2.8613
2.8476
2.8350
2.1250
1.0680
1.0542
1.95
1.98
2.02
1.00
3.02
6.03
Filename = YI-04118-1H-3.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 14-APR-2017 13:51:24
Revision_Time = 28-APR-2017 04:07:14
Current_Time = 28-APR-2017 04:07:57
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 46
Temp_C_Gain = 22.3 [dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
N
CN
3aj

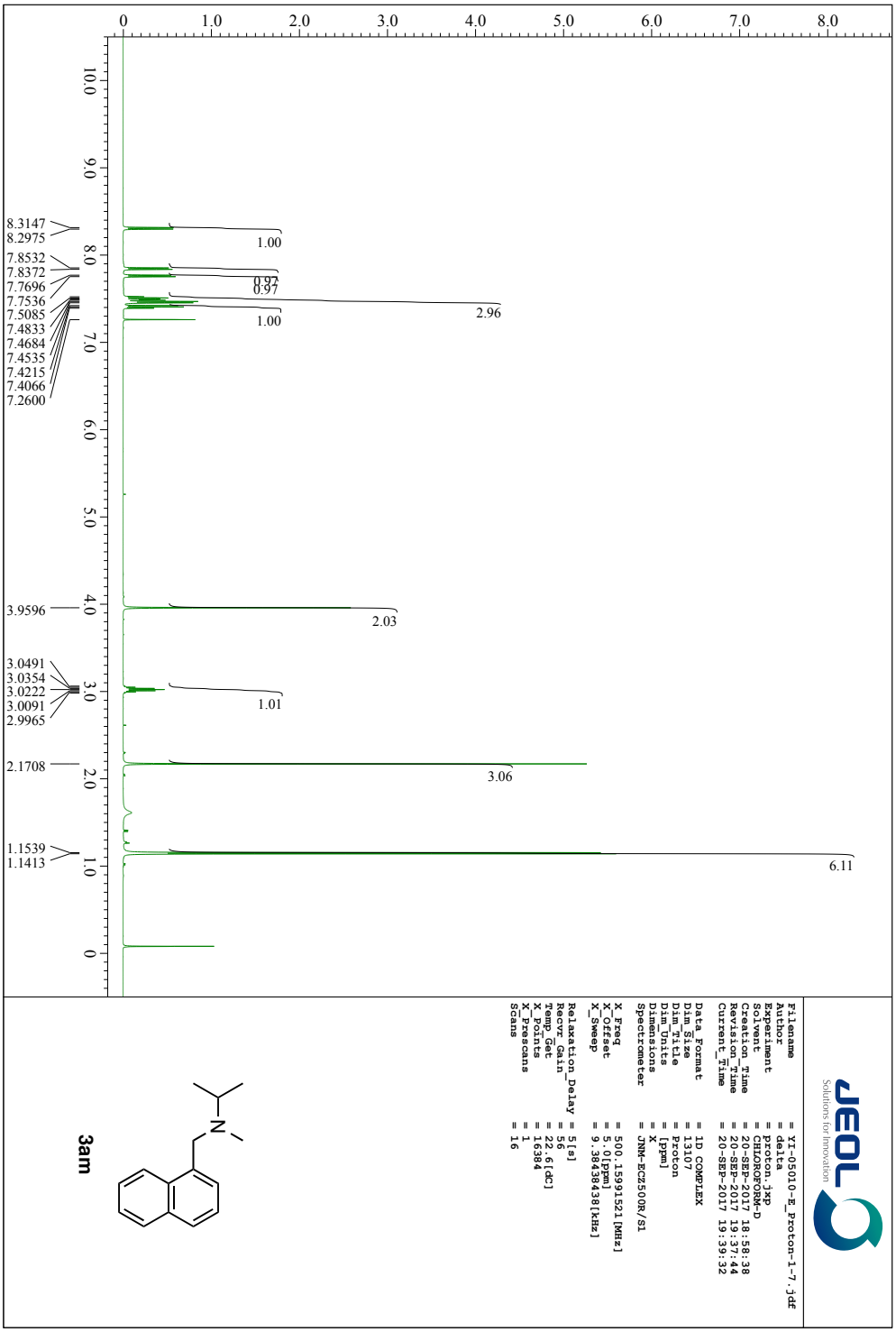

0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
146.5490
132.1893
129.3193
119.2791
110.5827
77.4192
77.1600
76.9104
57.3291
53.6336
37.1046
18.0320
Filename = YI-04118-13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 14-APR-2017 13:53:34
Revision_Time = 26-APR-2017 11:12:54
Current_Time = 26-APR-2017 11:13:47
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.7652976 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 50
Temp_C = 21.5 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 292
N
CN
3aj

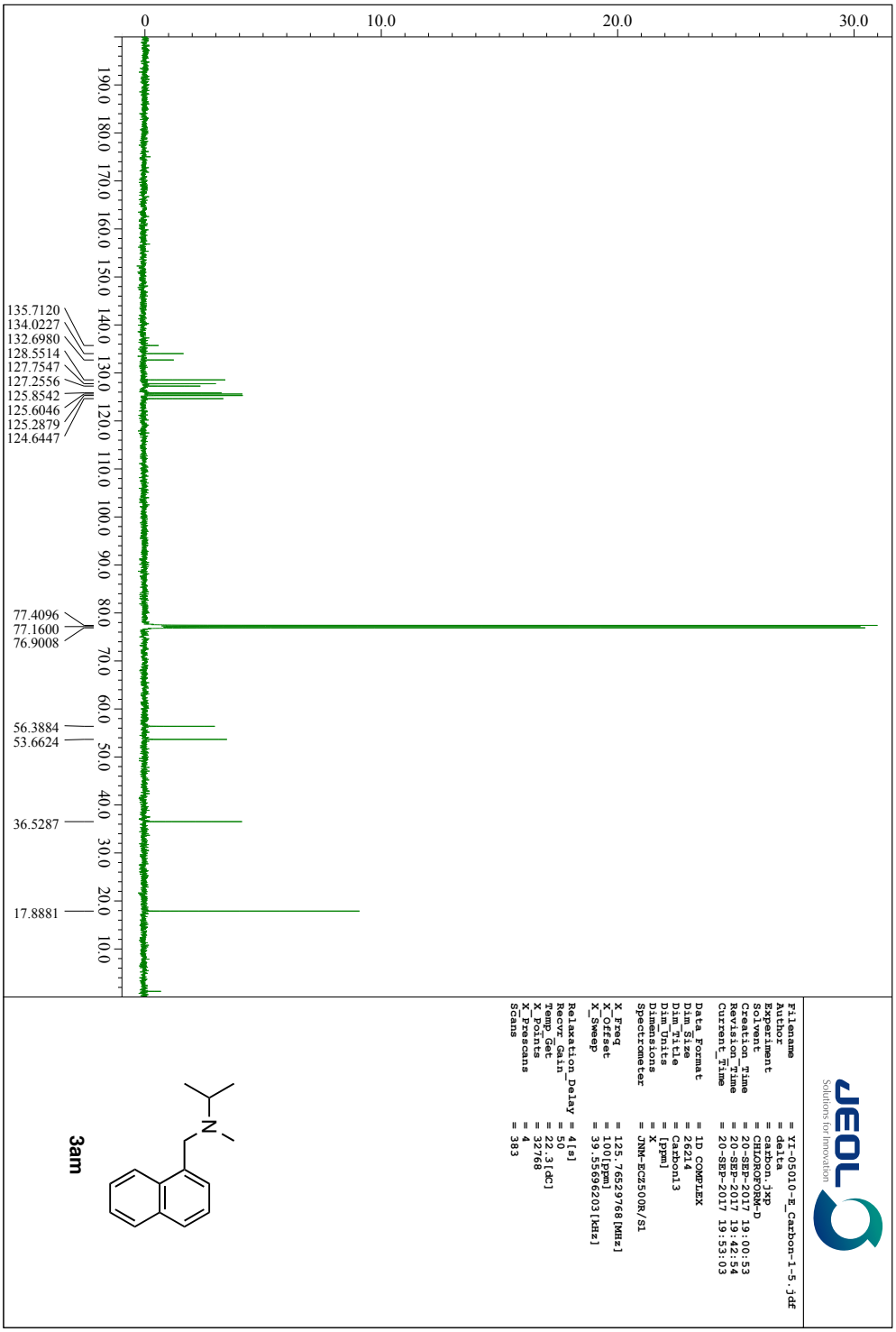

7.6230
7.6070
7.5829
7.5681
7.5509
7.5486
7.5360
7.5337
7.3321
7.3299
7.3173
7.3150
7.3024
7.3001
7.2600
3.7076
2.9747
2.9621
2.9484
2.9358
2.9220
2.1525
1.1012
1.0874
0.96
2.04
1.00
3.07
6.10
3ak
NC
N
Filename = YI-05007-D_Proton-1-8.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 20-SEP-2017 12:01:32
Revision_Time = 20-SEP-2017 16:13:45
Current_Time = 20-SEP-2017 16:14:58
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 46
Temp_Get = 22.1[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16

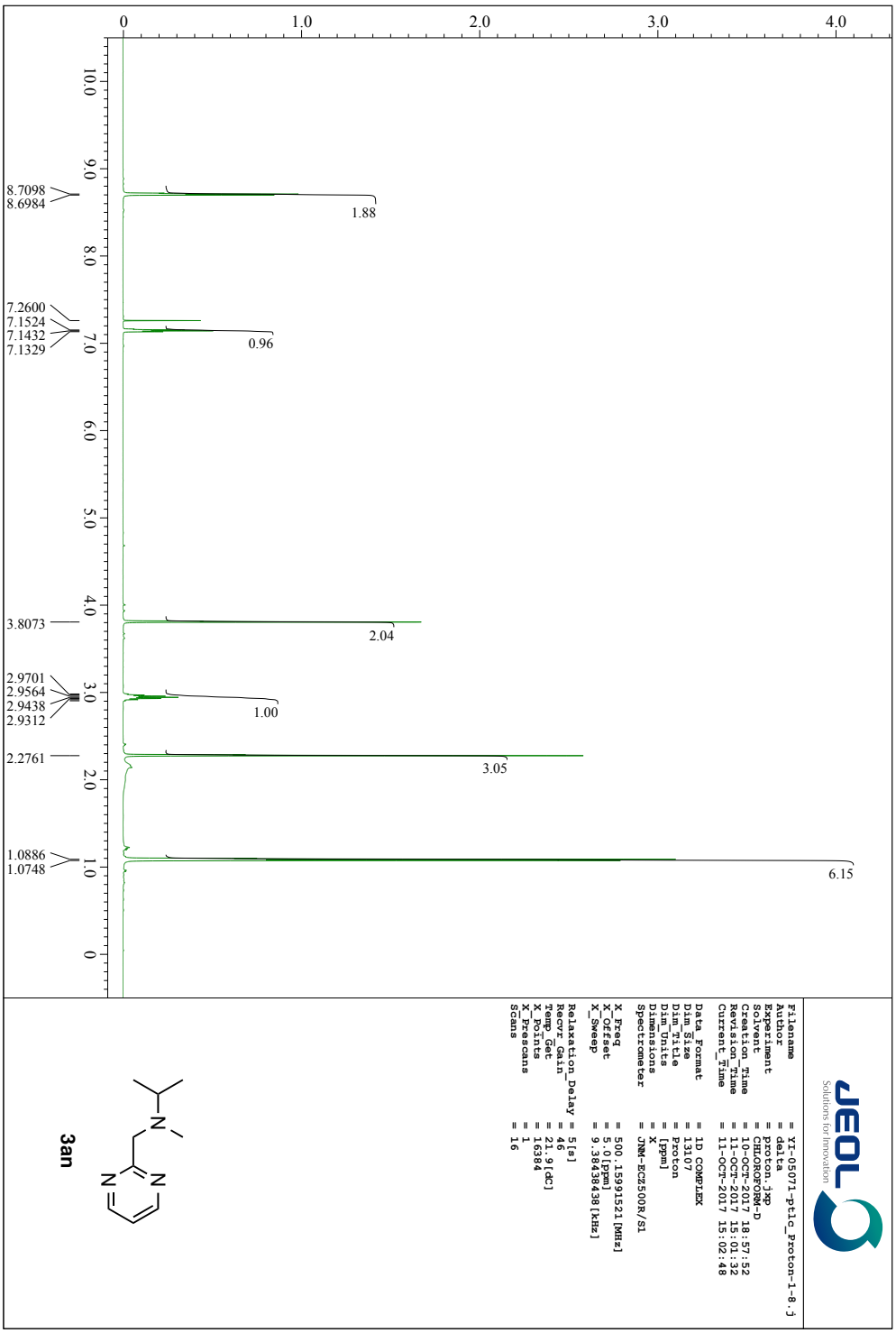

0
10.0
20.0
30.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
144.6388
132.9572
132.6788
129.9432
127.3324
118.0792
112.7040
77.4096
77.1600
76.9008
55.8413
54.0463
36.6055
18.0320
JEOL
Solutions for Innovation
Filename = YI-05007-D_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 20-SEP-2017 12:03:43
Revision_Time = 20-SEP-2017 16:06:21
Current_Time = 20-SEP-2017 16:07:48
Data_Format = 1D COMPLEX
Dim_Size = 2621
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[KHz]
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Comment = 21.8[dC]
Temp_Set = 32768
X_Points = 4
X_Prescans = 332
SCans
N
NC
3ak

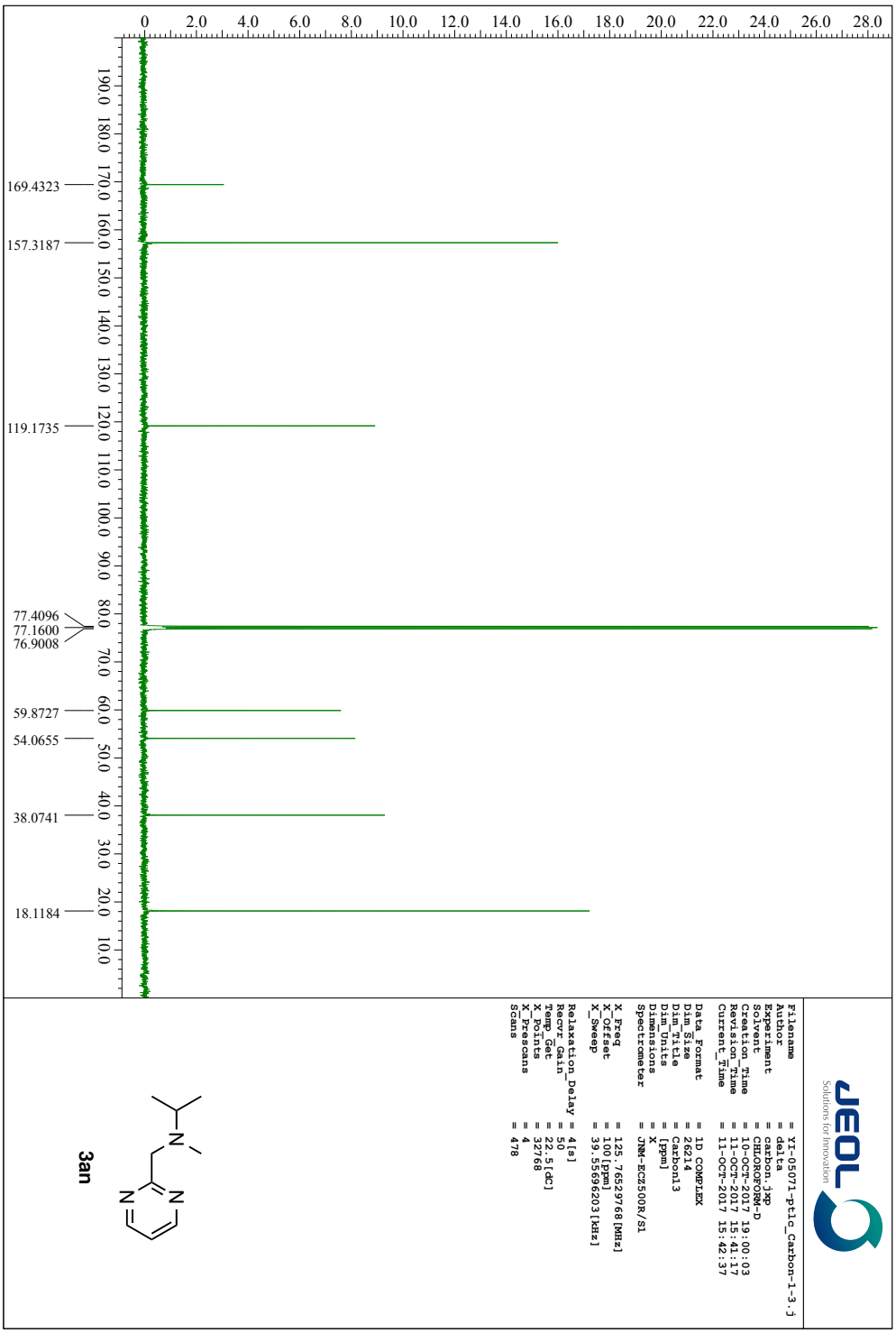

7.9826
7.9792
7.9700
7.9666
7.4146
7.3974
7.2600
3.9023
3.5496
2.8968
2.8831
2.8705
2.8568
2.1393
1.0737
1.0611
1.97
1.99
3.00
2.02
1.00
3.02
6.07
Filename = YI-05133-D_Proton-1-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 30-NOV-2017 17:41:36
Revision_Time = 1-DEC-2017 00:47:58
Current_Time = 1-DEC-2017 00:48:35
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 48
Temp_Comment = 25.7[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
N
CO2Me
3al

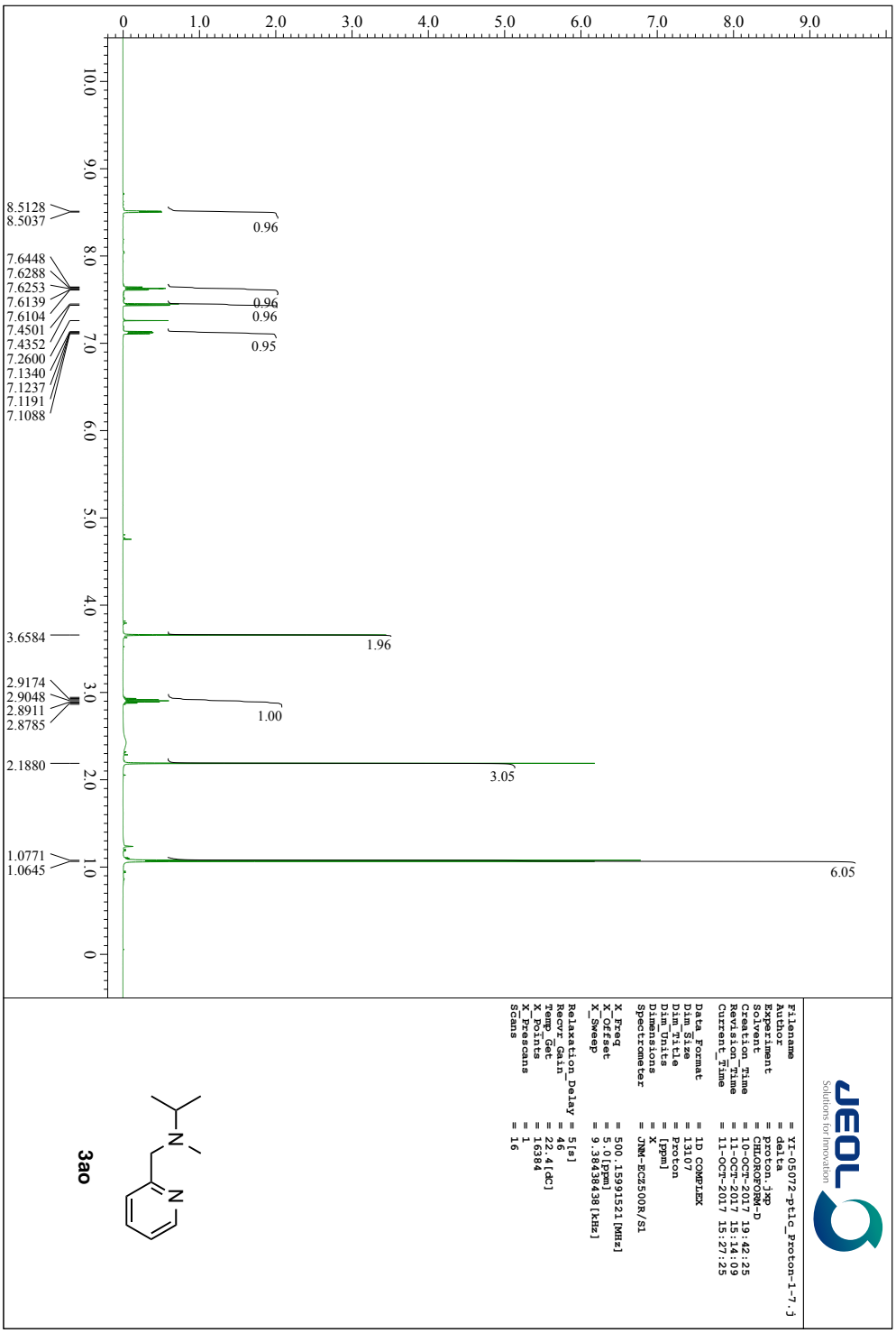

0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
167.3109
146.1458
129.6841
128.8106
128.7434
77.4192
77.1600
76.9104
57.4347
53.4800
52.1170
37.1430
18.0416
JEOL
Solutions for Innovation
Filename = YI-05133-D_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 30-NOV-2017 17:43:47
Revision_Time = 1-DEC-2017 00:42:56
Current_Time = 1-DEC-2017 00:43:49
Data_Format = 1D COMPLEX
Dim_Size = 32214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 4[s]
Recvr_Gain = 59.8[dB]
Temp_Get = 25.0[degC]
X_Points = 32768
X_Prescans = 4
Scans = 518
N
CO2Me
3al

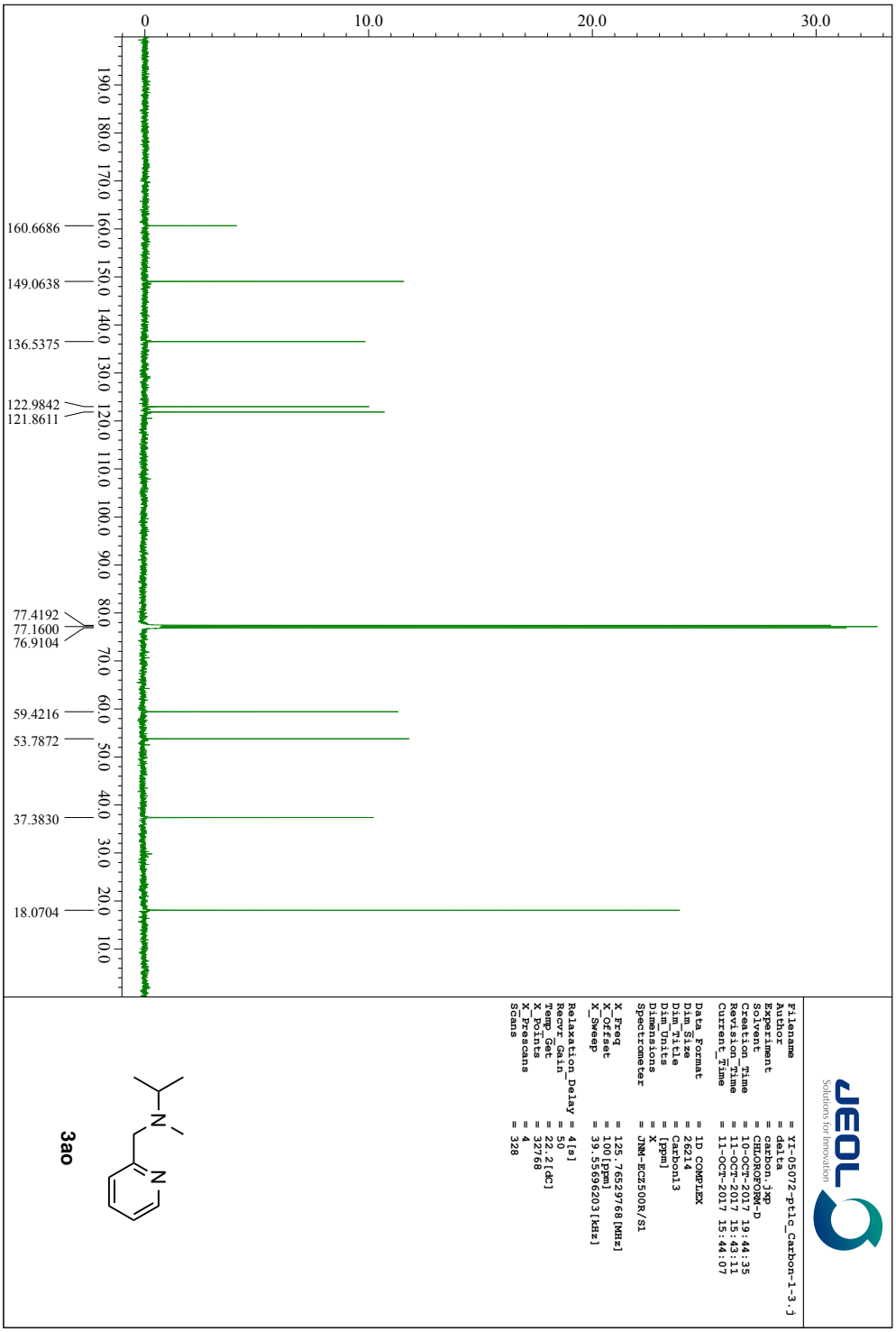

8.3147
8.2975
7.8532
7.8372
7.7696
7.7536
7.5085
7.4833
7.4684
7.4535
7.4215
7.4066
7.2600
3.9596
3.0491
3.0354
3.0222
3.0091
2.9965
2.1708
1.1539
1.1413
1.00
0.92
0.97
1.00
2.96
2.03
1.01
3.06
6.11
3am
Filename = YI-05010-E_Proton-1-7.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 20-SEP-2017 18:58:38
Revision_Time = 20-SEP-2017 19:37:44
Current_Time = 20-SEP-2017 19:39:32
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 52
Temp_Get = 22.6[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16

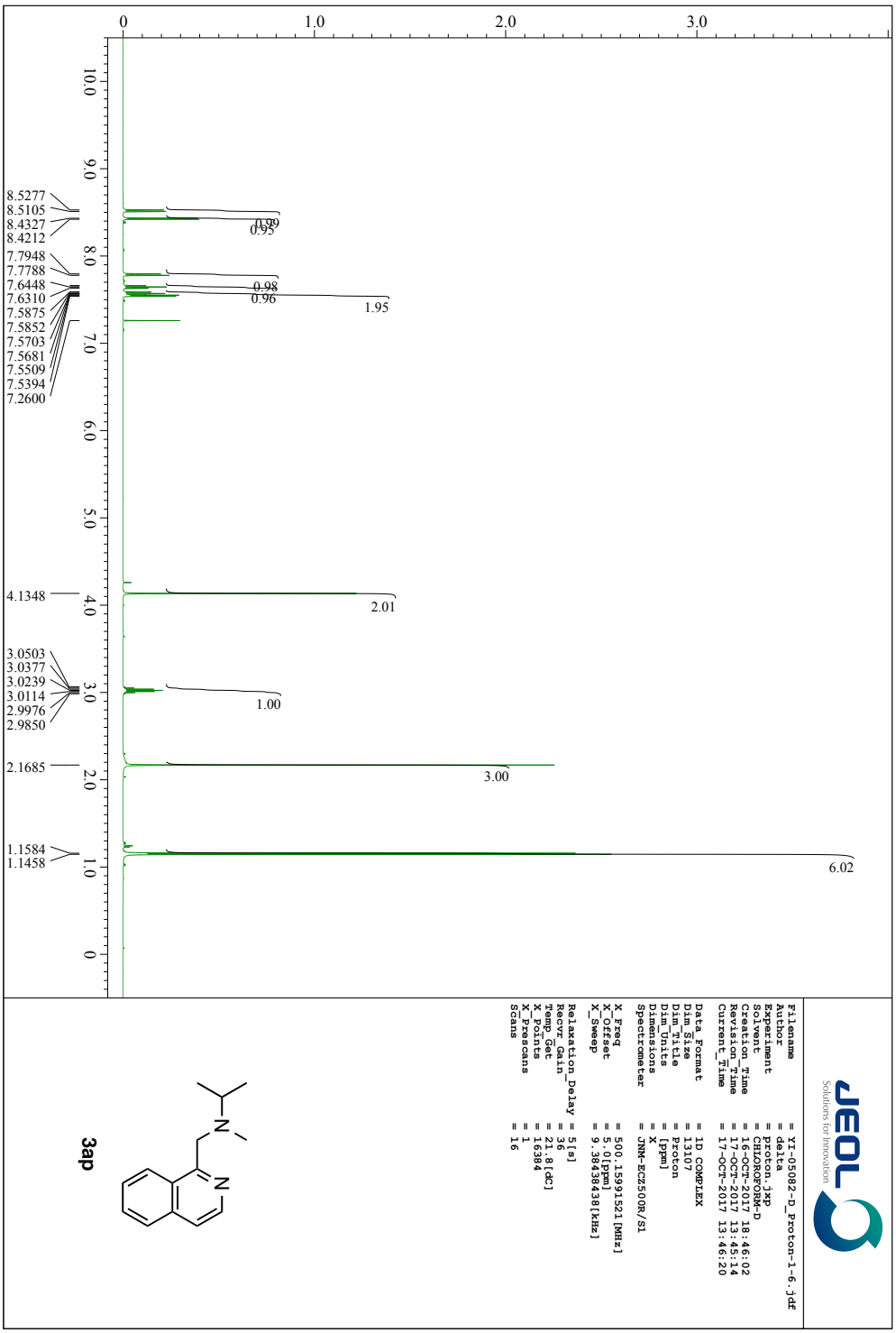

JEOL
Solutions for Innovation
Filename = YI-05010-E_Carbon-1-5.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 20-SEP-2017 19:00:53
Revision_Time = 20-SEP-2017 19:42:54
Current_Time = 20-SEP-2017 19:53:03
Data_Format = 1D COMPLEX
Dim_Size = 2621
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[KHz]
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Deg_C = 23.3[dC]
X_Points = 32768
X_Prescans = 4
Scans = 383
135.7120
134.0227
132.6980
128.5514
127.7547
127.2556
125.8542
125.6046
125.2879
124.6447
77.4096
77.1600
76.9008
56.3884
53.6624
36.5287
17.8881
3am

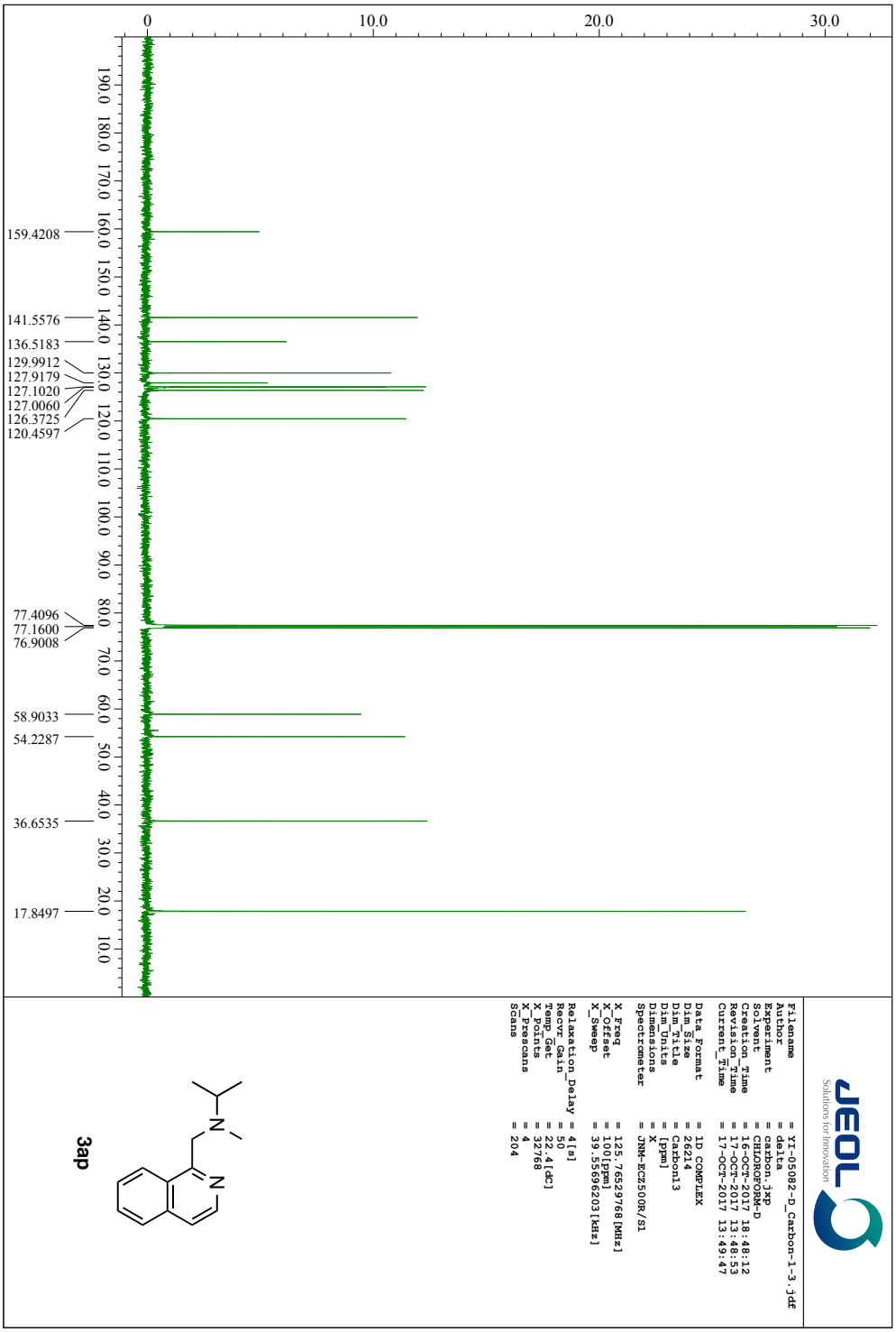

8.7098
8.6984
7.2600
7.1524
7.1432
7.1329
3.8073
2.9701
2.9564
2.9438
2.9312
2.2761
1.0886
1.0748
1.88
0.96
2.04
1.00
3.05
6.15
Filename = YI-05071-ptlc_Proton-1-8.j
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 10-OCT-2017 18:57:52
Revision_Time = 11-OCT-2017 15:01:32
Current_Time = 11-OCT-2017 15:02:48
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 21.9 [dB]
Temp_Set = 21
X_Points = 16384
X_Prescans = 1
Scans = 16
3an

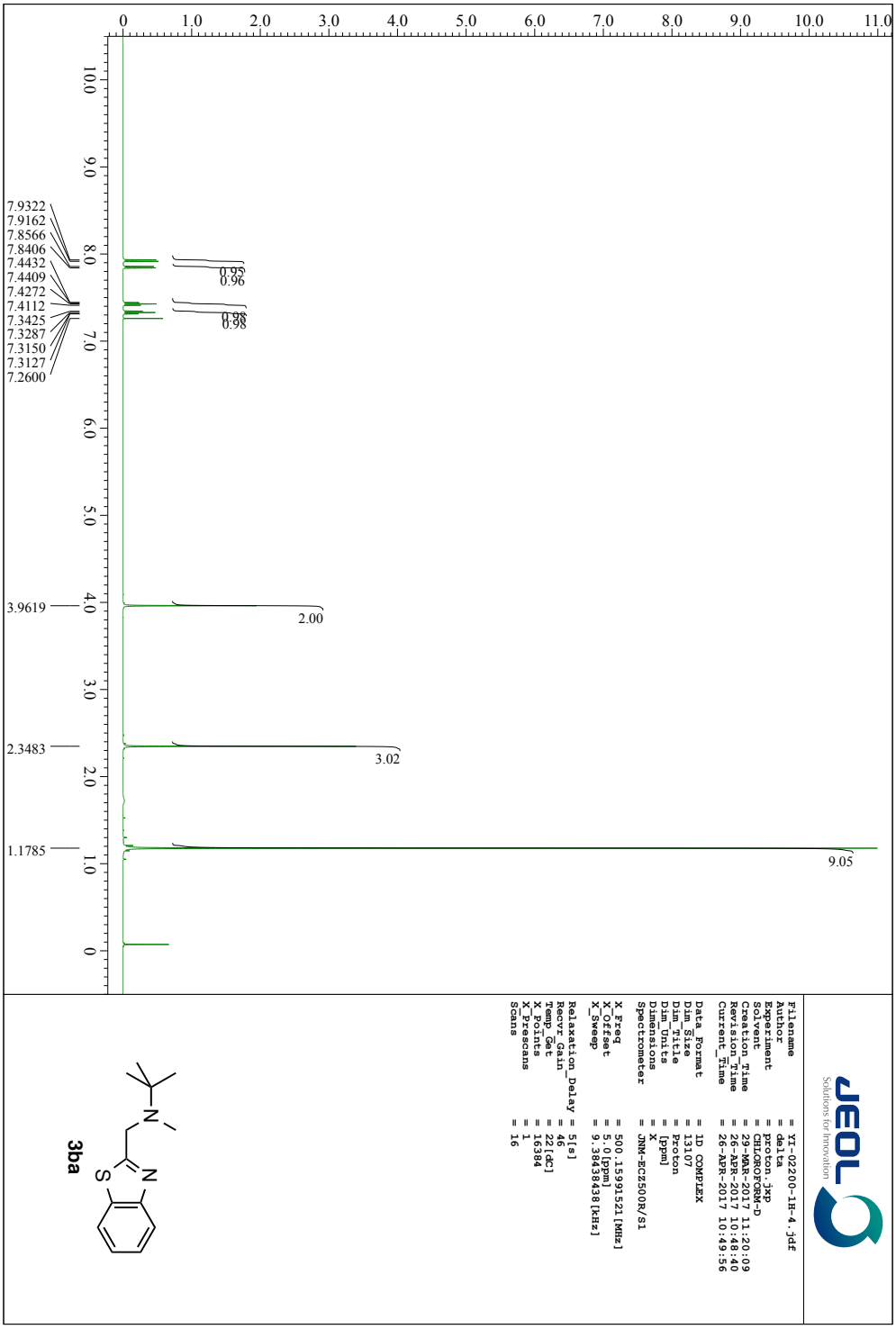

JEOL
Solutions for Innovation
Filename = YI-05071-ptic_Carbon-1-3.j
Author =
Experiment = delta
Solvent = carbon.jxp
Creation_Time = CHLOROFORM-D
Revision_Time = 10-OCT-2017 19:00:03
Current_Time = 11-OCT-2017 15:41:17
Data_Format = 1D COMPLEX
Dim_Size = 2621
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[KHz]
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Deg_C = 22.5[dC]
X_Points = 32768
X_Prescans = 4
Scans = 478
169.4323
157.3187
119.1735
77.4096
77.1600
76.9008
59.8727
54.0655
38.0741
18.1184
3an

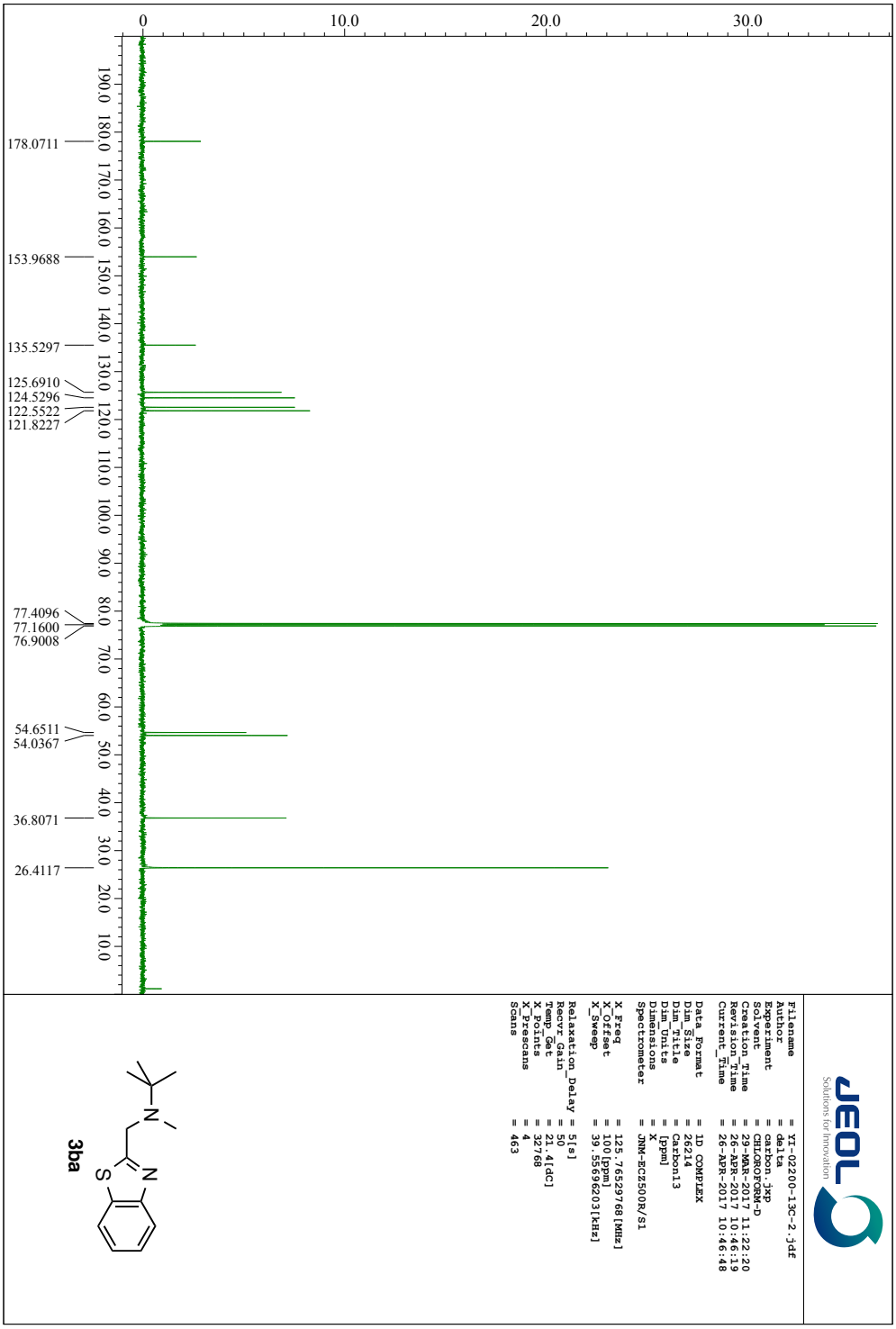

8.5128
8.5037
7.6448
7.6288
7.6253
7.6139
7.6104
7.4501
7.4352
7.2600
7.1340
7.1237
7.1191
7.1088
3.6584
2.9174
2.9048
2.8911
2.8785
2.1880
1.0771
1.0645
0.96
0.96
0.96
0.95
1.96
1.00
3.05
6.05
Filename = YI-05072-ptic_Proton-1-7.j
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 10-OCT-2017 19:42:25
Revision_Time = 11-OCT-2017 15:14:09
Current_Time = 11-OCT-2017 15:27:25
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 22.4 [dB]
Temp_Set = 22
X_Points = 16384
X_Prescans = 1
Scans = 16
3ao

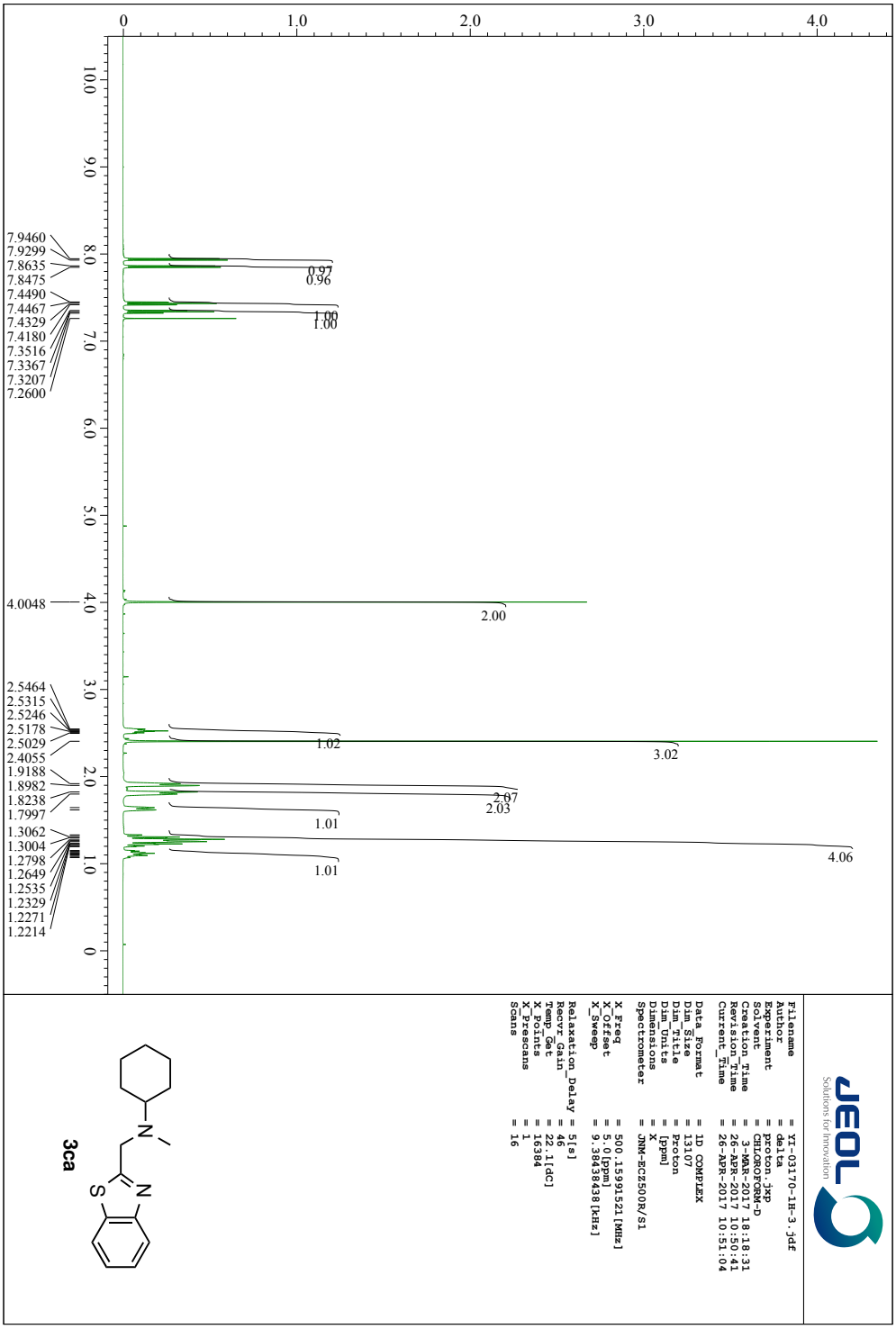

JEOL
Solutions for Innovation
Filename = YI-05072-ptic_Carbon-1-3.j
Author =
Experiment = delta
Solvent = carbon.jxp
Creation_Time = CHLOROFORM-D
Revision_Time = 10-OCT-2017 19:44:35
Current_Time = 11-OCT-2017 15:43:11
Data_Format = 11-OCT-2017 15:44:07
Dim_Size = 1D COMPLEX
Dim_Title = 2821
Dim_Units = Carbon13
Dimensions = [ppm]
Spectrometer = X
X_Freq = JNM-ECZ500R/S1
X_Offset = 125.76529768 [MHz]
X_Sweep = 100[ppm]
Relaxation_Delay = 39.55696203[KHz]
Recvr_Gain = 4[s]
Temp_Deg_C = 50
X_Points = 21.2[dC]
X_Prescans = 32768
Scans = 4
= 328
3ao
160.6686
149.0638
136.5375
122.9842
121.8611
77.4192
77.1600
76.9104
59.4216
53.7872
37.3830
18.0704

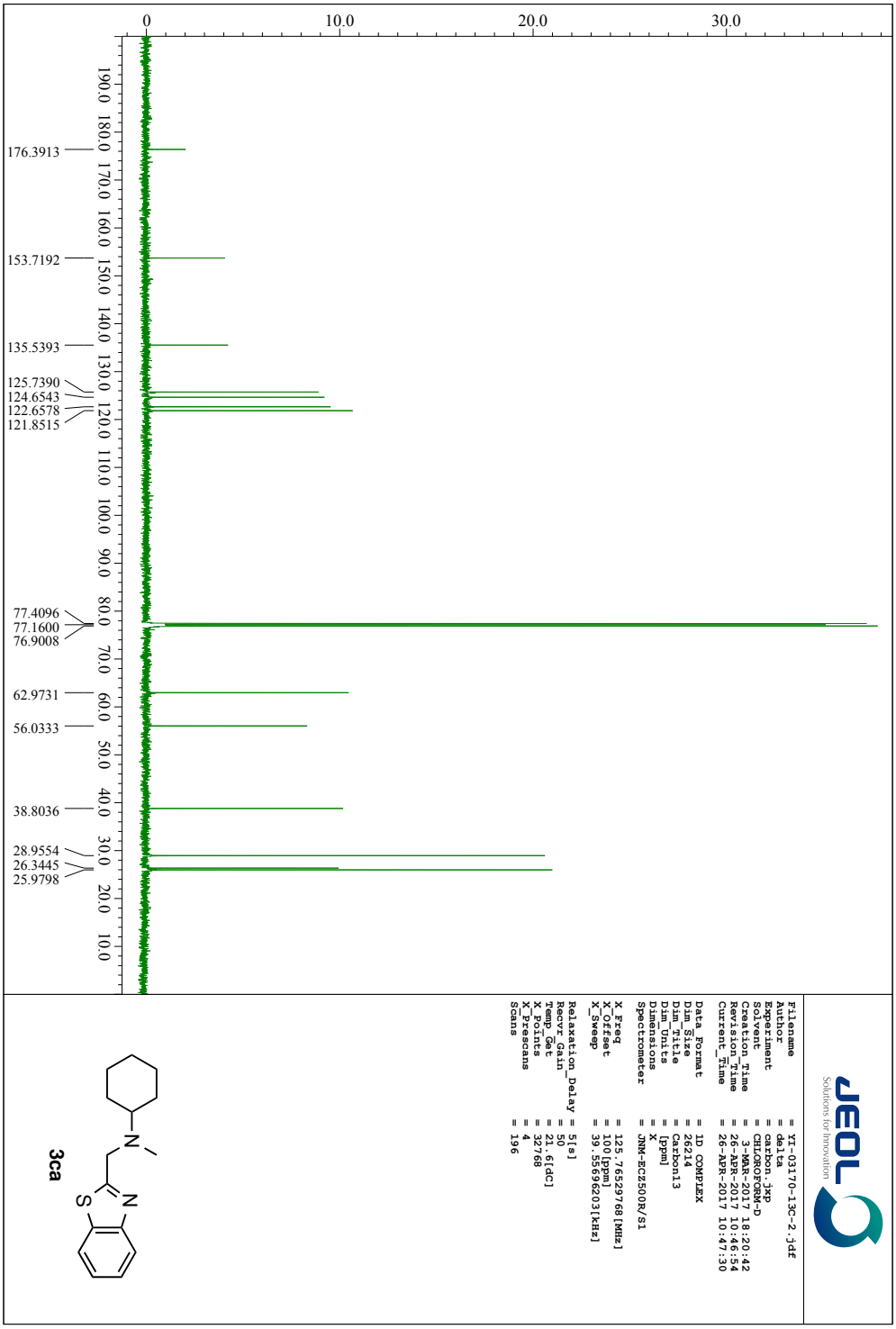

8.5277
8.5105
8.4327
8.4212
7.7948
7.7788
7.6448
7.6310
7.5875
7.5852
7.5703
7.5681
7.5509
7.5394
7.2600
4.1348
3.0503
3.0377
3.0239
3.0114
2.9976
2.9850
2.1685
1.1584
1.1458
0.99
0.95
0.98
0.96
1.95
2.01
1.00
3.00
6.02
JEOL
Solutions for Innovation
Filename = YI-05082-D_Proton-1-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 16-OCT-2017 18:46:02
Revision_Time = 17-OCT-2017 13:45:14
Current_Time = 17-OCT-2017 13:46:20
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 22.8[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3ap

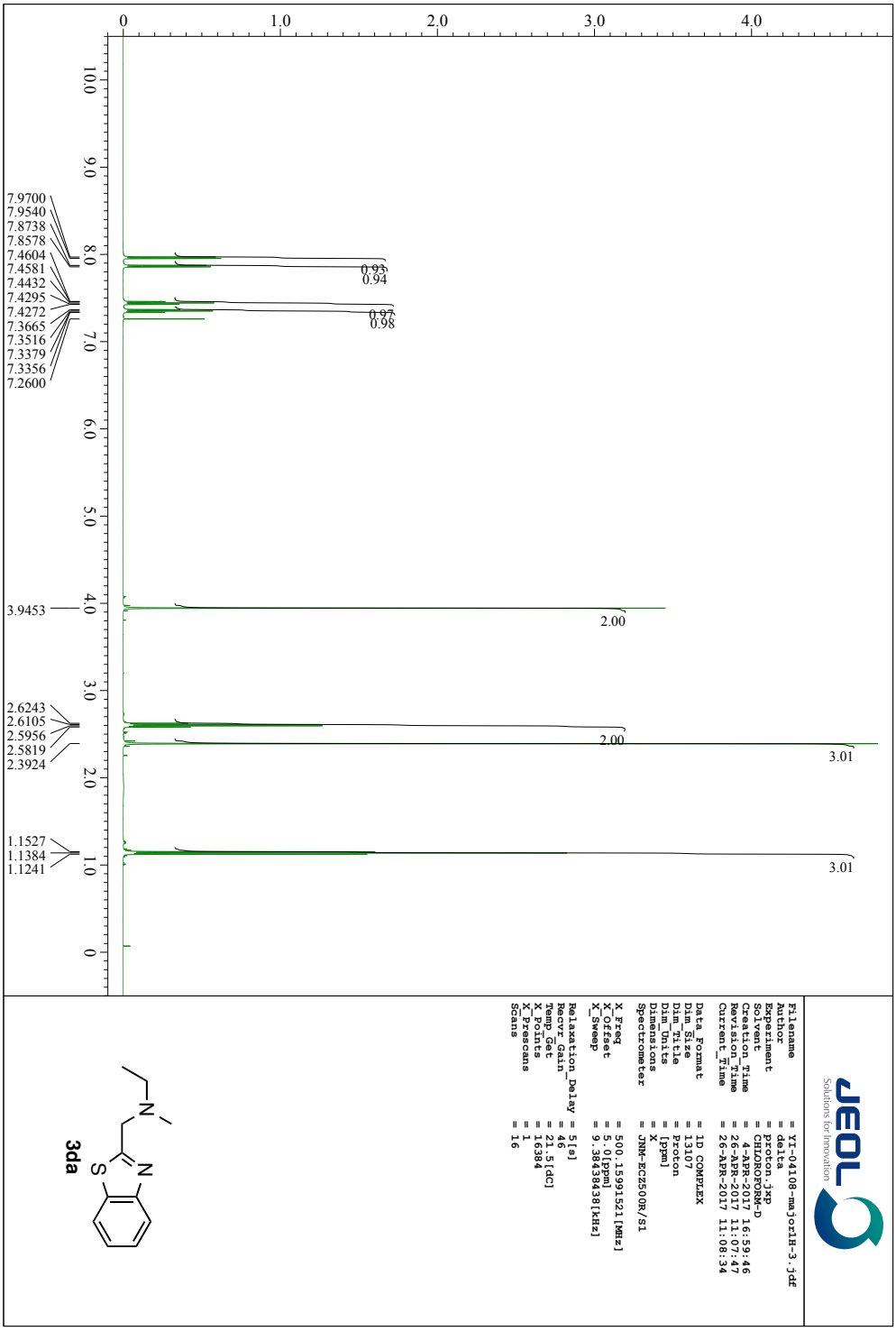

0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
159.4208
141.5576
136.5183
129.9912
127.9179
127.1020
127.0060
126.3725
120.4597
77.4096
77.1600
76.9008
58.9033
54.2287
36.6535
17.8497
JEOL
Solutions for Innovation
Filename = YI-05082-D_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 16-OCT-2017 18:48:12
Revision_Time = 17-OCT-2017 13:48:53
Current_Time = 17-OCT-2017 13:49:47
Data_Format = 1D COMPLEX
Dim_Size = 2224
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[KHz]
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Deg_C = 24[dC]
X_Points = 32768
X_Prescans = 4
Scans = 204
3ap

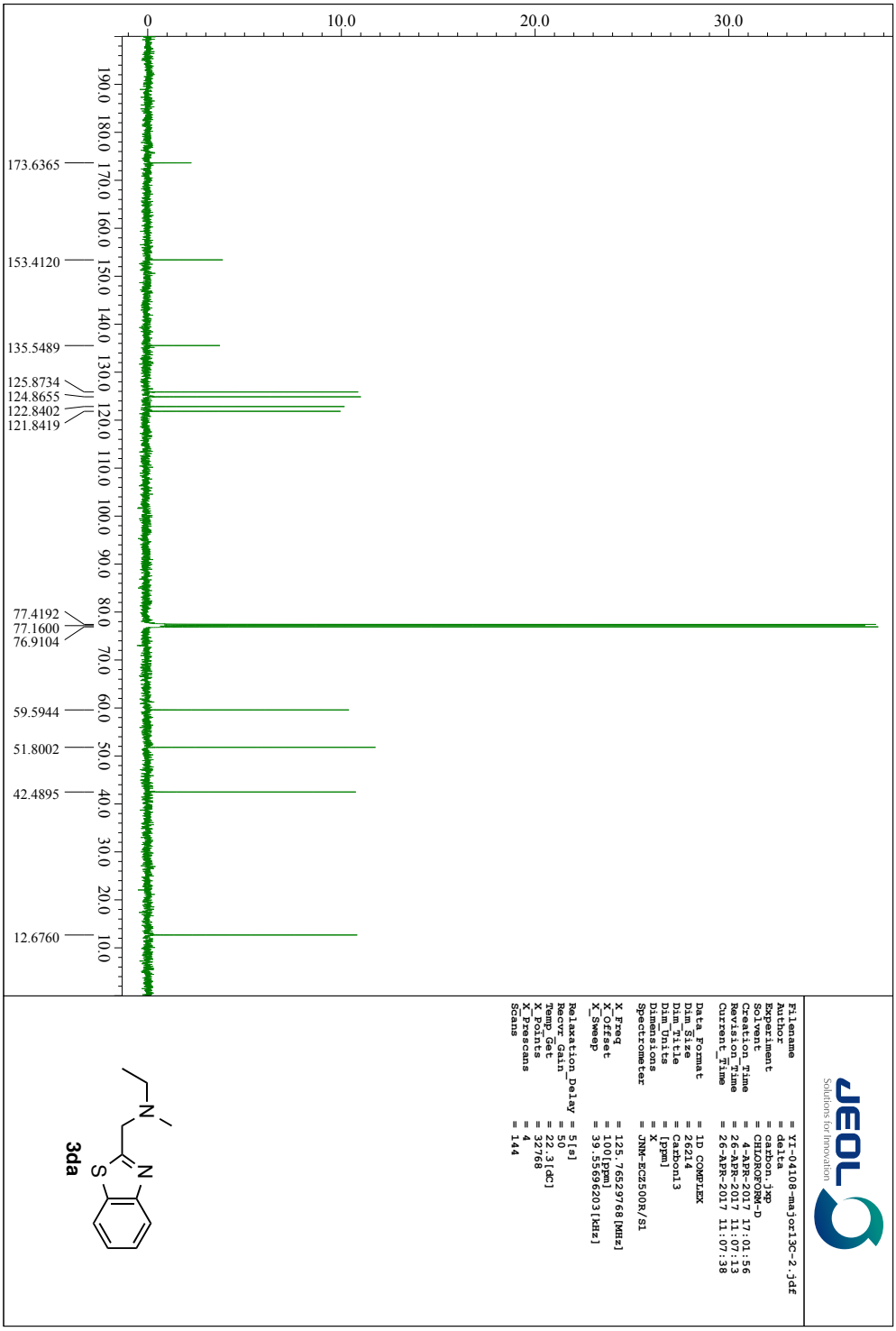

7.9322
7.9162
7.8566
7.8406
7.4432
7.4409
7.4272
7.4112
7.3425
7.3287
7.3150
7.3127
7.2600
3.9619
2.3483
1.1785
0.95
0.96
0.98
0.98
2.00
3.02
9.05
3ba
Filename = YI-02200-1H-4.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 29-MAR-2017 11:20:09
Revision_Time = 26-APR-2017 10:48:40
Current_Time = 26-APR-2017 10:49:56
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16

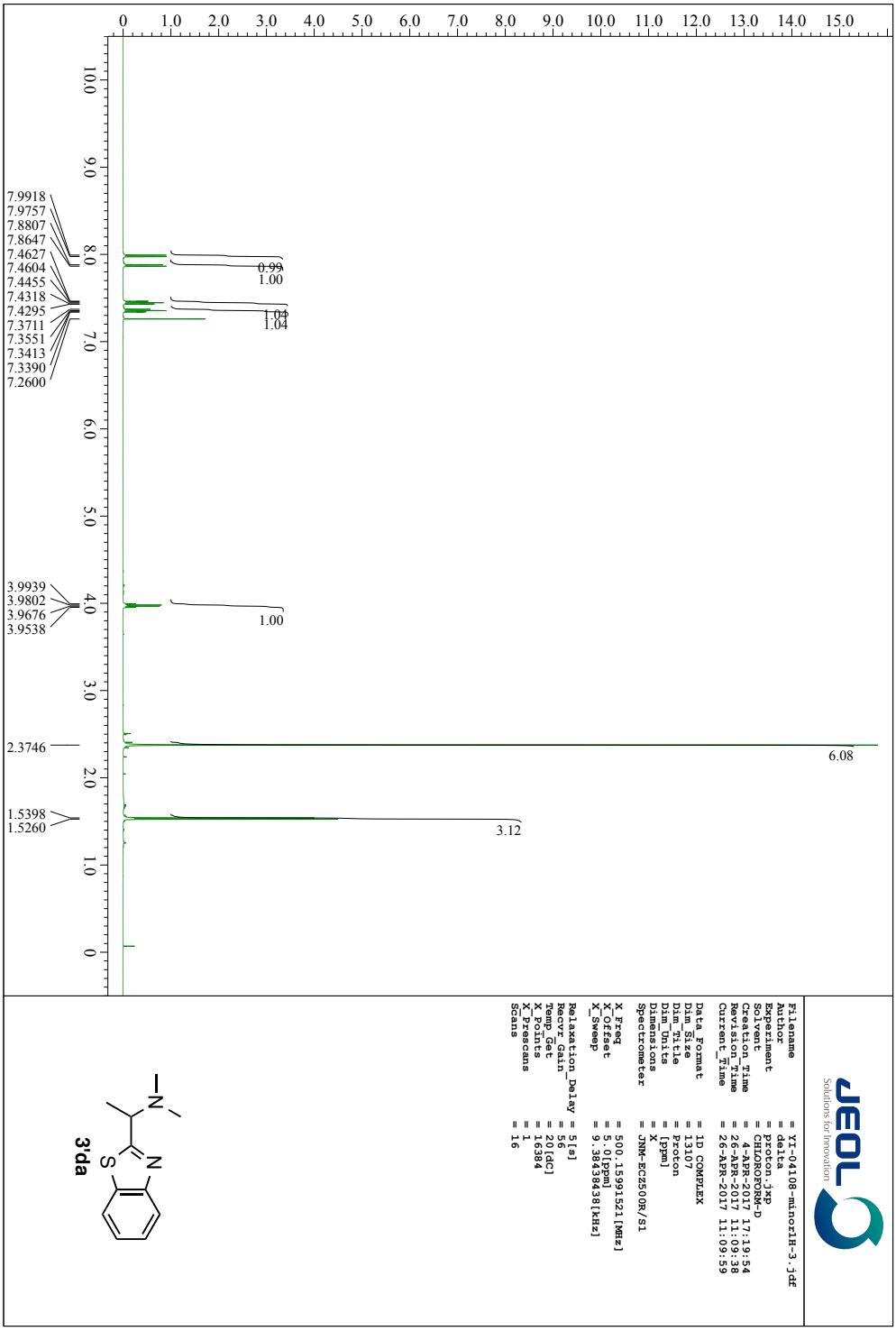

JEOL
Solutions for Innovation
Filename = YI-02200-13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 29-MAR-2017 11:22:20
Revision_Time = 26-APR-2017 10:46:19
Current_Time = 26-APR-2017 10:46:48
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765297681 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 50
Temp_Control = 21.4 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 463
178.0711
153.9688
135.5297
125.6910
124.5296
122.5522
121.8227
77.4096
77.1600
76.9008
54.6511
54.0367
36.8071
26.4117
3ba

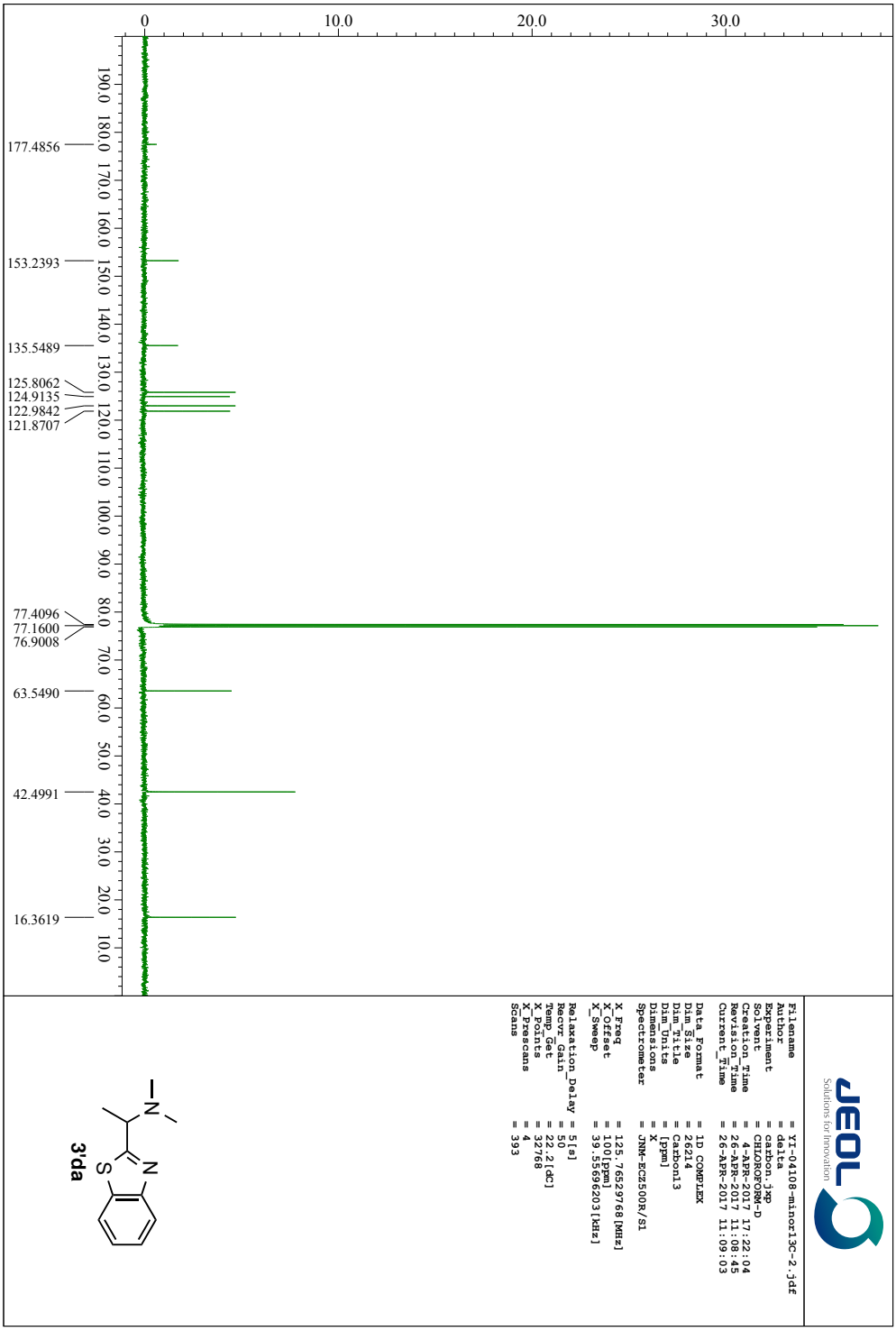

7.9460
7.9299
7.8635
7.8475
7.4490
7.4467
7.4329
7.4180
7.3516
7.3367
7.3207
7.2600
4.0048
2.5464
2.5315
2.5246
2.5178
2.5029
2.4055
1.9188
1.8982
1.8238
1.7997
1.3062
1.3004
1.2798
1.2649
1.2535
1.2329
1.2271
1.2214
0.97
0.96
1.00
1.00
2.00
1.02
3.02
2.07
2.03
1.01
4.06
1.01
3ca
Filename = YI-03170-1H-3.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 3-MAR-2017 18:18:31
Revision_Time = 26-APR-2017 10:50:41
Current_Time = 26-APR-2017 10:51:04
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Repetitions = 16
Temp_Control = 22.1[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16

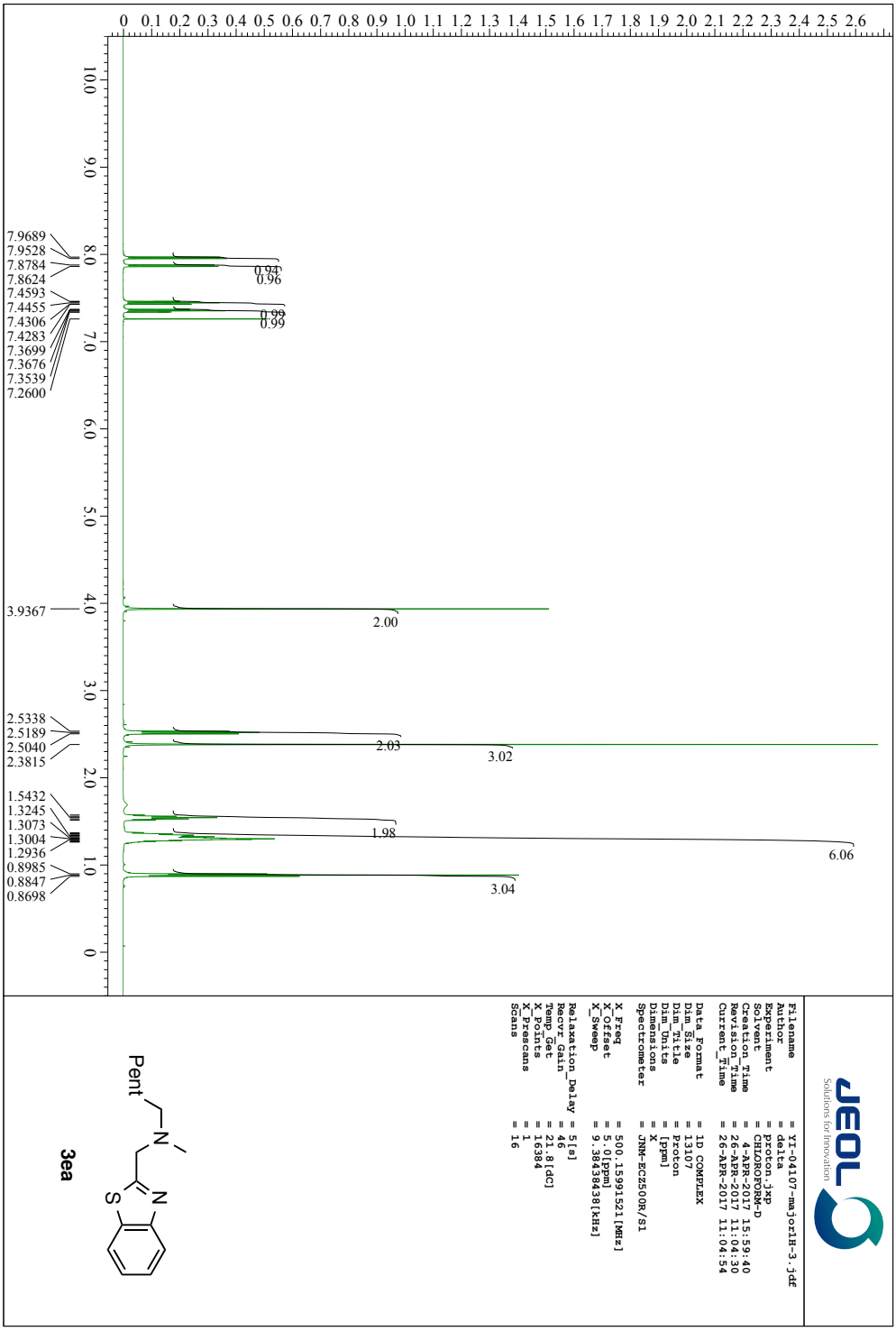

JEOL
Solutions for Innovation
Filename = YI-03170-13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 3-MAR-2017 18:20:42
Revision_Time = 26-APR-2017 10:46:54
Current_Time = 26-APR-2017 10:47:30
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765297681 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.556962031 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 50
Temp_Comment = 21.6 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 196
3ca
176.3913
153.7192
135.5393
125.7390
124.6543
122.6578
121.8515
77.4096
77.1600
76.9008
62.9731
56.0333
38.8036
28.9554
26.3445
25.9798

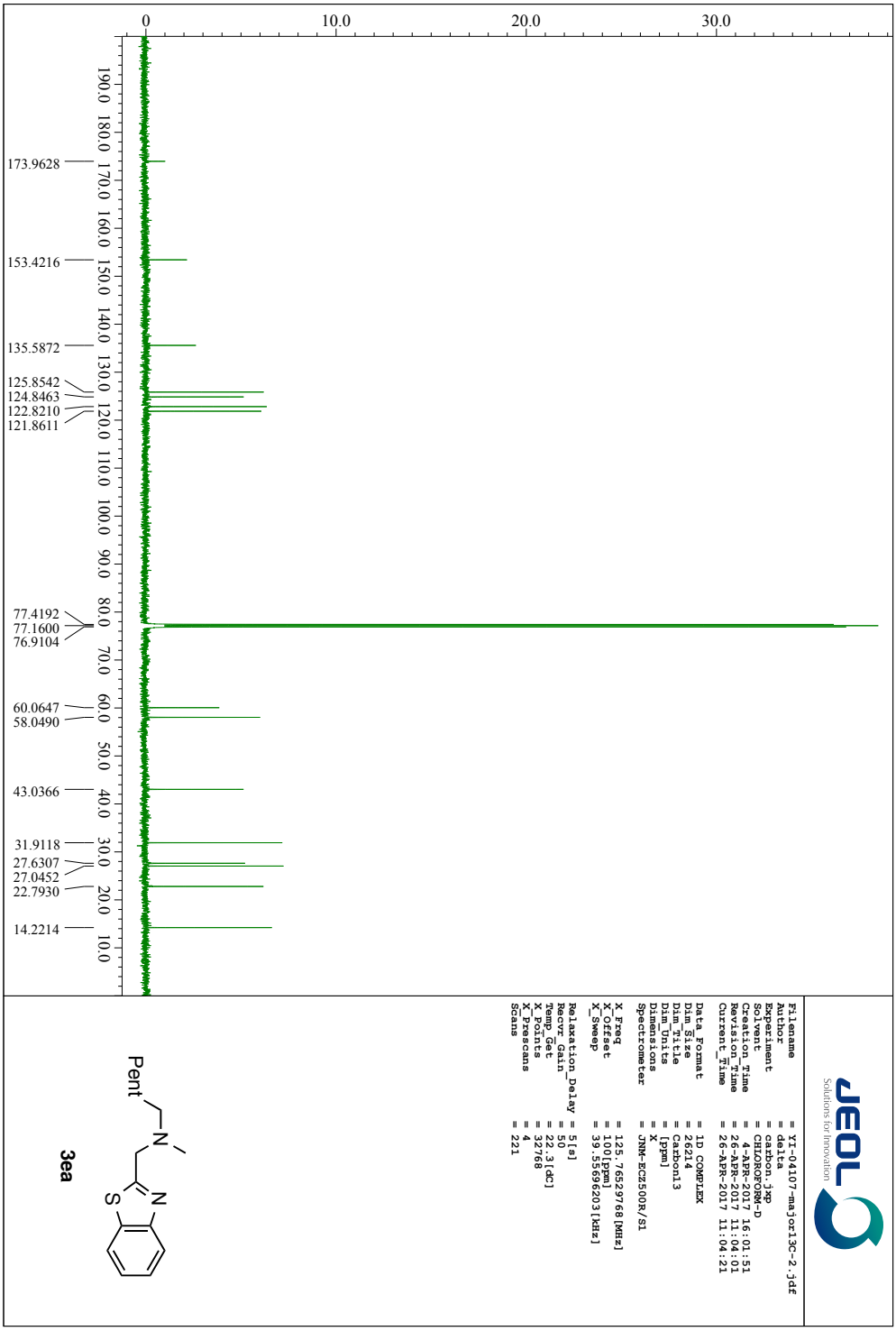

7.9700
7.9540
7.8738
7.8578
7.4604
7.4581
7.4432
7.4295
7.4272
7.3665
7.3516
7.3379
7.3356
7.2600
3.9453
2.6243
2.6105
2.5956
2.5819
2.3924
1.1527
1.1384
1.1241
0.93
0.94
0.97
0.98
2.00
2.00
3.01
3.01
3da
Filename = YI-04108-majorH-3.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-APR-2017 16:59:46
Revision_Time = 26-APR-2017 11:07:47
Current_Time = 26-APR-2017 11:08:34
Data_Format = 1D COMPLEX
Dim_Size = 12107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.5[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16

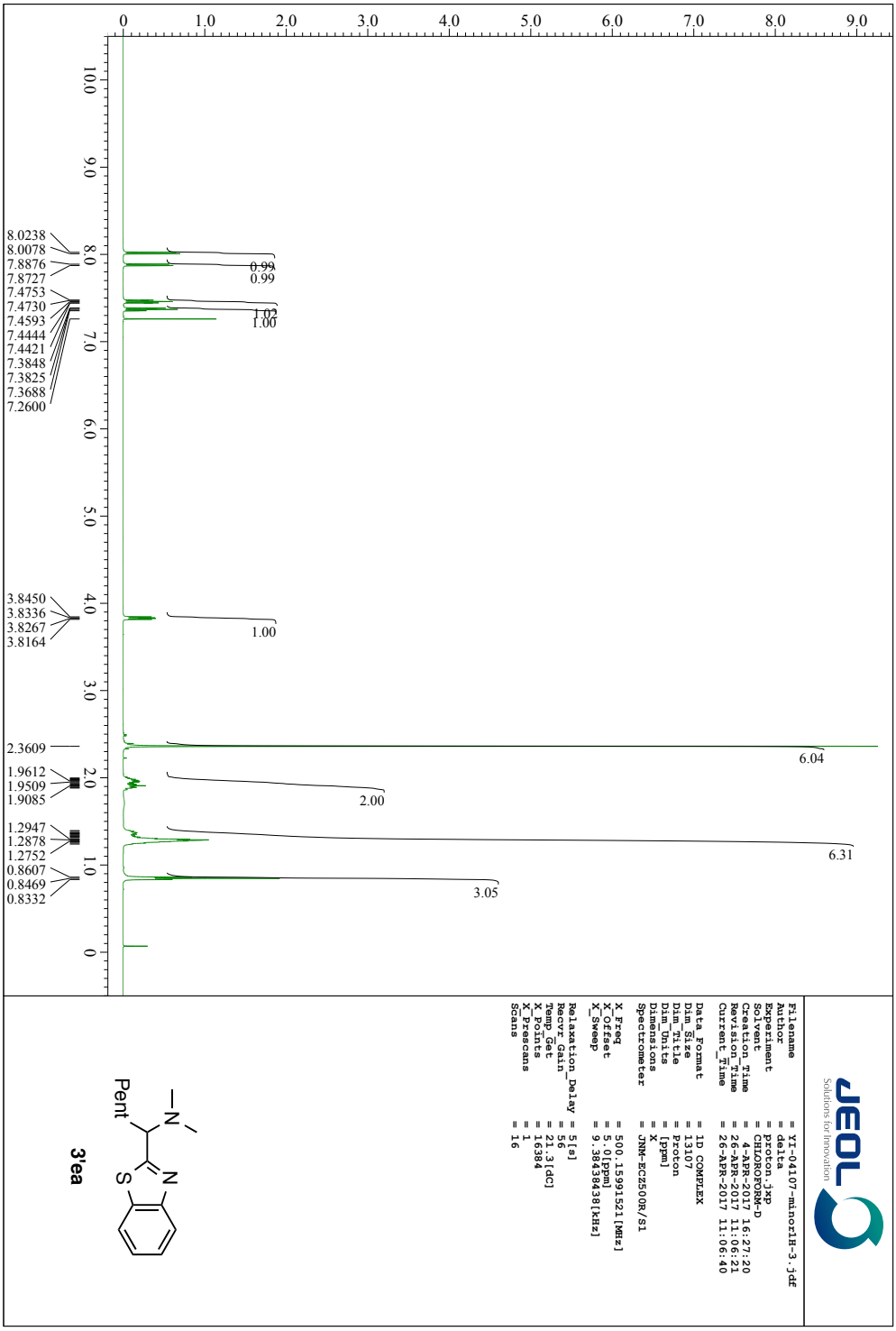

0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
173.6365
153.4120
135.5489
125.8734
124.8655
122.8402
121.8419
77.4192
77.1600
76.9104
59.5944
51.8002
42.4895
12.6760
JEOL
Solutions for Innovation
Filename = YI-04108-major13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-APR-2017 17:01:56
Revision_Time = 26-APR-2017 11:07:13
Current_Time = 26-APR-2017 11:07:38
Data_Format = 1D COMPLEX
Dim_Size = 2F214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50.3[dC]
Temp_Get = 22.3[dC]
X_Points = 32768
X_Prescans = 4
Scans = 144
N
S
N
3da

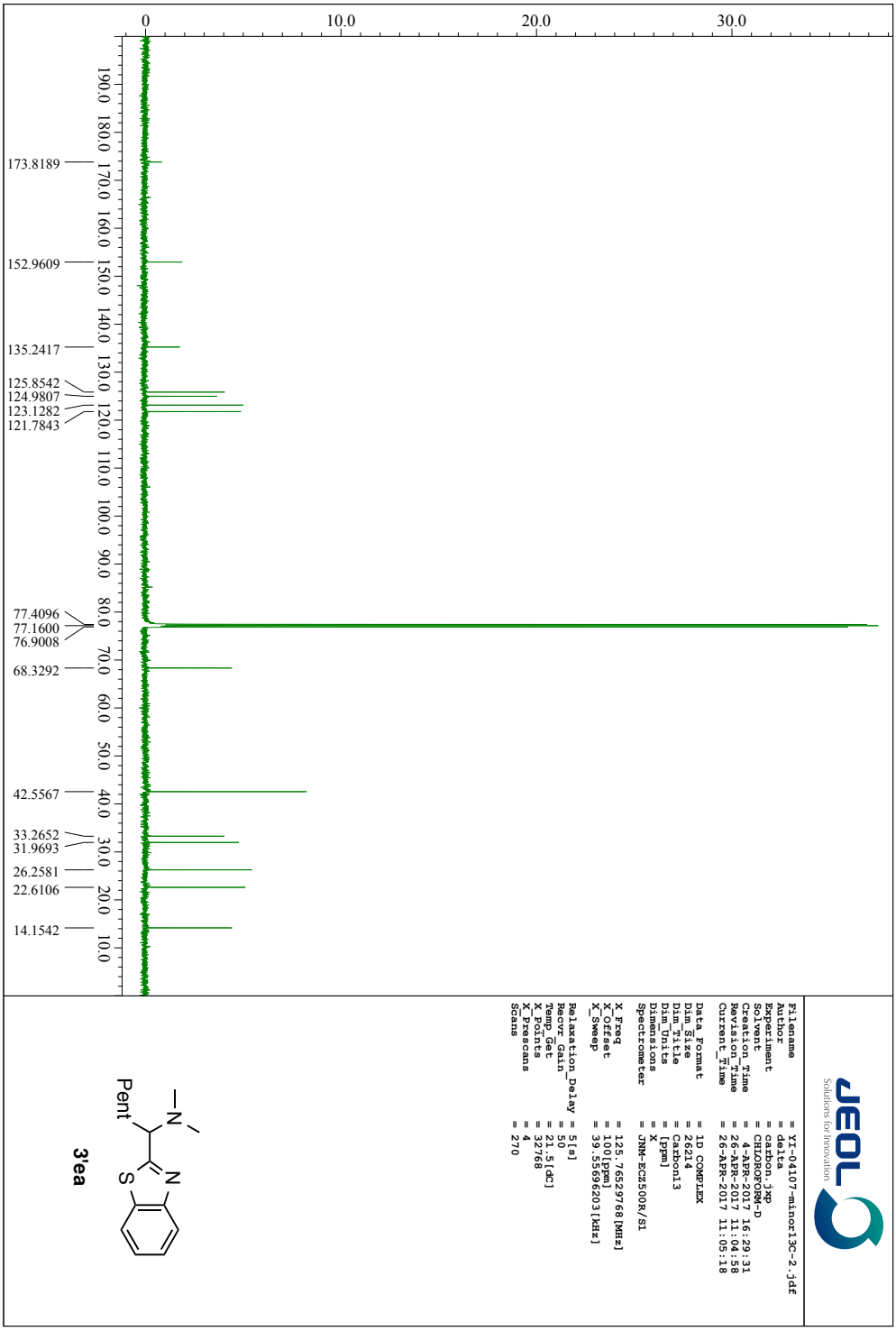

7.9918
7.9757
7.8807
7.8647
7.4627
7.4604
7.4455
7.4318
7.4295
7.3711
7.3551
7.3413
7.3390
7.2600
3.9939
3.9802
3.9676
3.9538
2.3746
1.5398
1.5260
0.99
1.00
1.04
1.04
1.00
6.08
3.12
Filename = YI-04108-minorH-3.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-APR-2017 17:19:54
Revision_Time = 26-APR-2017 11:09:38
Current_Time = 26-APR-2017 11:09:59
Data_Format = 1D COMPLEX
Dim_Size = 12107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 20[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3'da

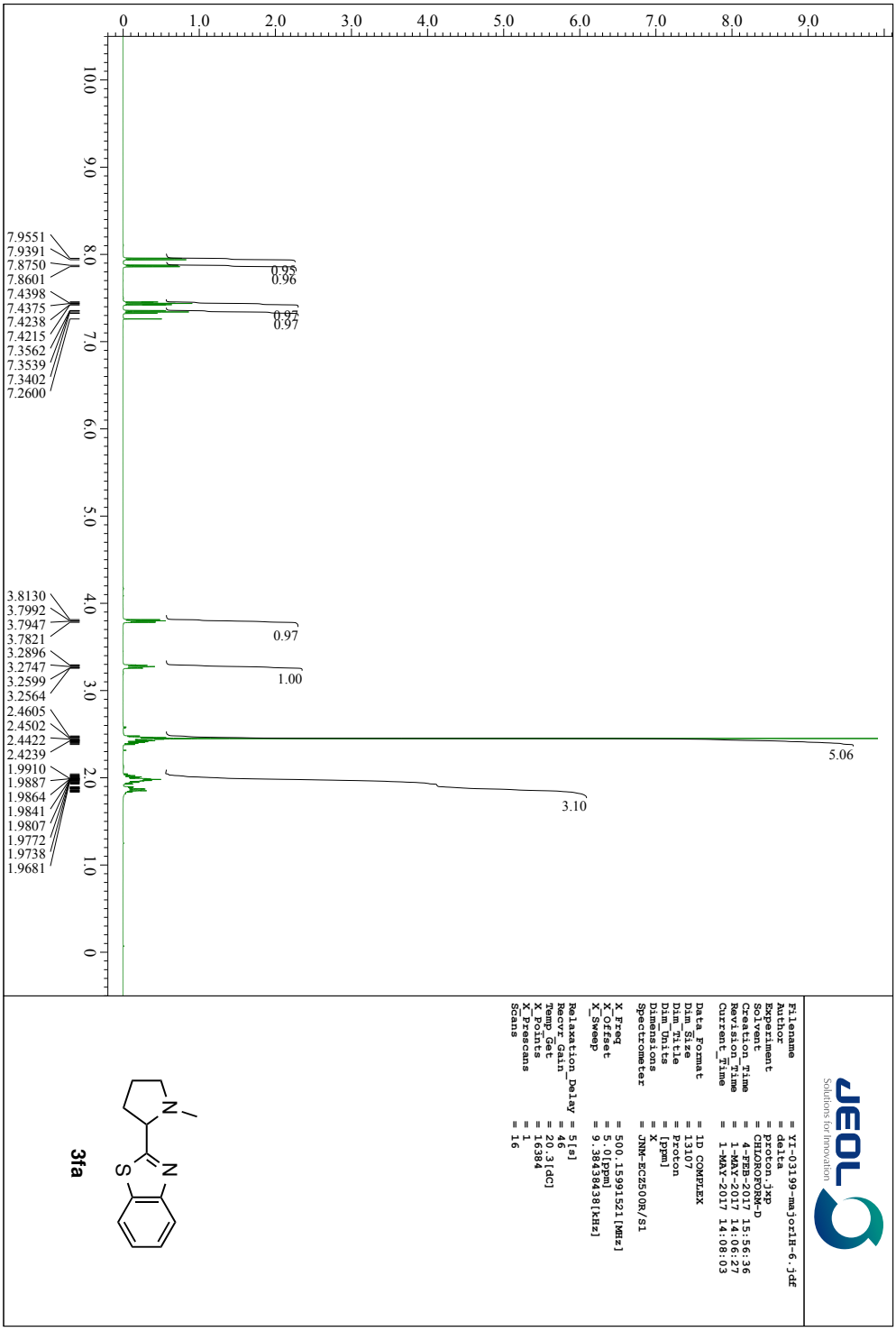

0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
177.4856
153.2393
135.5489
125.8062
124.9135
122.9842
121.8707
77.4096
77.1600
76.9008
63.5490
42.4991
16.3619
JEOL
Solutions for Innovation
Filename = YI-04108-minor13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-APR-2017 17:22:04
Revision_Time = 26-APR-2017 11:08:45
Current_Time = 26-APR-2017 11:09:03
Data_Format = 1D COMPLEX
Dim_Size = 2F214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765299768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[KHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50.0
Temp_C = 22.2[dC]
X_Points = 32768
X_Prescans = 4
Scans = 393
N
S
N
3'da


7.9689
7.9528
7.8784
7.8624
7.4593
7.4455
7.4306
7.4283
7.3699
7.3676
7.3539
7.2600
3.9367
2.5338
2.5189
2.5040
2.3815
1.5432
1.3245
1.3073
1.3004
1.2936
0.8985
0.8847
0.8698
0.94
0.96
0.99
0.99
2.00
2.03
3.02
1.98
6.06
3.04
Pent
N
S
N
3ea
Filename = YI-04107-majorH-3.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-APR-2017 15:59:40
Revision_Time = 26-APR-2017 11:04:30
Current_Time = 26-APR-2017 11:04:54
Data_Format = 1D COMPLEX
Dim_Size = 12107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.8[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16


JEOL
Solutions for Innovation
Filename = YI-04107-major13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-APR-2017 16:01:51
Revision_Time = 26-APR-2017 11:04:01
Current_Time = 26-APR-2017 11:04:21
Data_Format = 1D COMPLEX
Dim_Size = 2E214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[KHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50.3[dC]
Temp_Comments = 22.3[dC]
X_Points = 32768
X_Prescans = 4
Scans = 221
0
10.0
20.0
30.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
173.9628
153.4216
135.5872
125.8542
124.8463
122.8210
121.8611
77.4192
77.1600
76.9104
60.0647
58.0490
43.0366
31.9118
27.6307
27.0452
22.7930
14.2214
Pent
N
S
N
3ea


8.0238
8.0078
7.8876
7.8727
7.4753
7.4730
7.4593
7.4444
7.4421
7.3848
7.3825
7.3688
7.2600
3.8450
3.8336
3.8267
3.8164
2.3609
1.9612
1.9509
1.9085
1.2947
1.2878
1.2752
0.8607
0.8469
0.8332
0.99
0.99
1.02
1.00
1.00
6.04
2.00
6.31
3.05
Filename = YI-04107-minorH-3.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-APR-2017 16:27:20
Revision_Time = 26-APR-2017 11:06:21
Current_Time = 26-APR-2017 11:06:40
Data_Format = 1D COMPLEX
Dim_Size = 12107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.3[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
Pent
N
S
N
3'ea


0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
173.8189
152.9609
135.2417
125.8542
124.9807
123.1282
121.7843
77.4096
77.1600
76.9008
68.3292
42.5567
33.2652
31.9693
26.2581
22.6106
14.1542
JEOL
Solutions for Innovation
Filename = YI-04107-minor13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-APR-2017 16:29:31
Revision_Time = 26-APR-2017 11:04:58
Current_Time = 26-APR-2017 11:05:18
Data_Format = 1D COMPLEX
Dim_Size = 2F214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_C = 21.5[dC]
X_Points = 32768
X_Prescans = 4
Scans = 270
Pent
N
S
N
3'ea


7.9551
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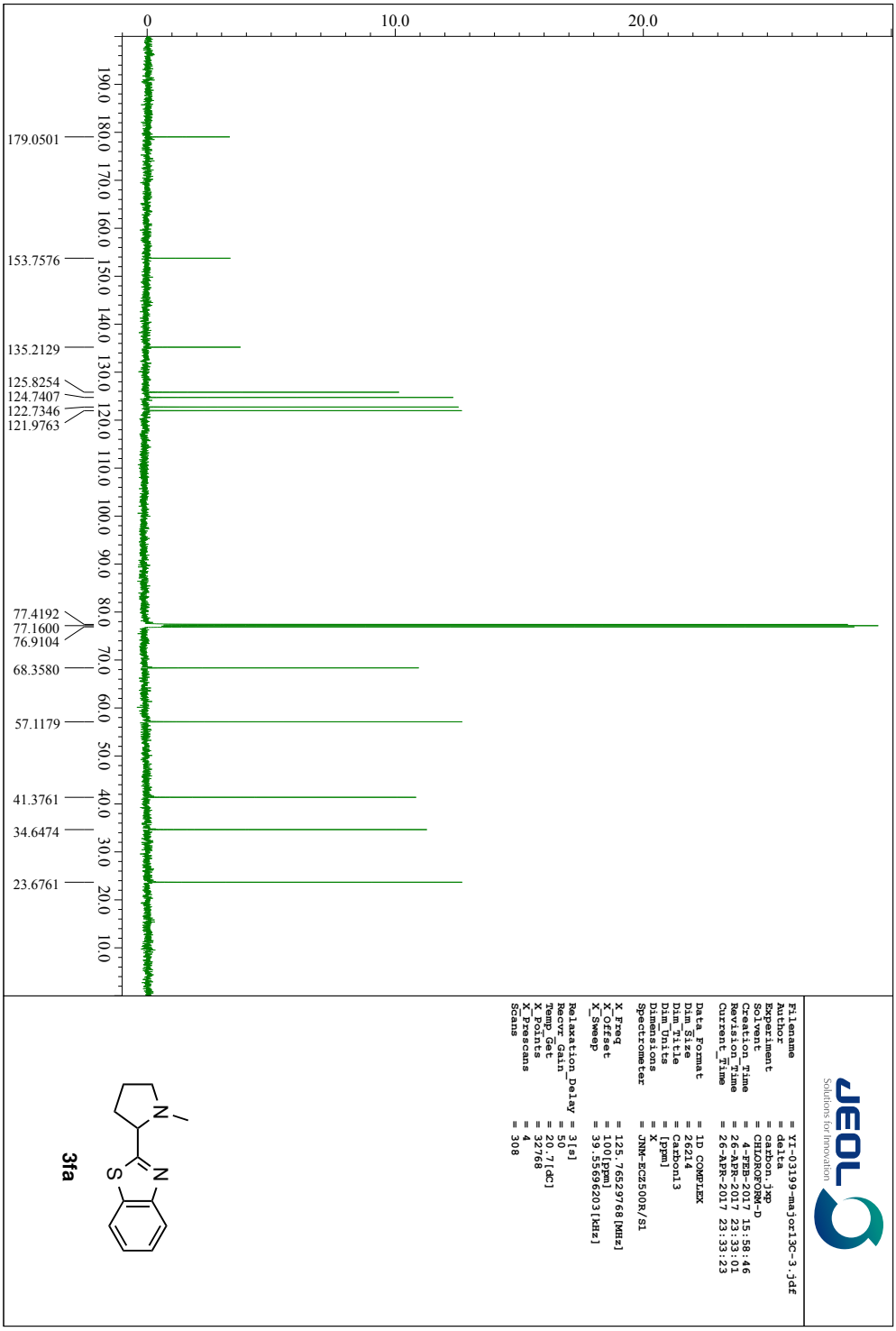
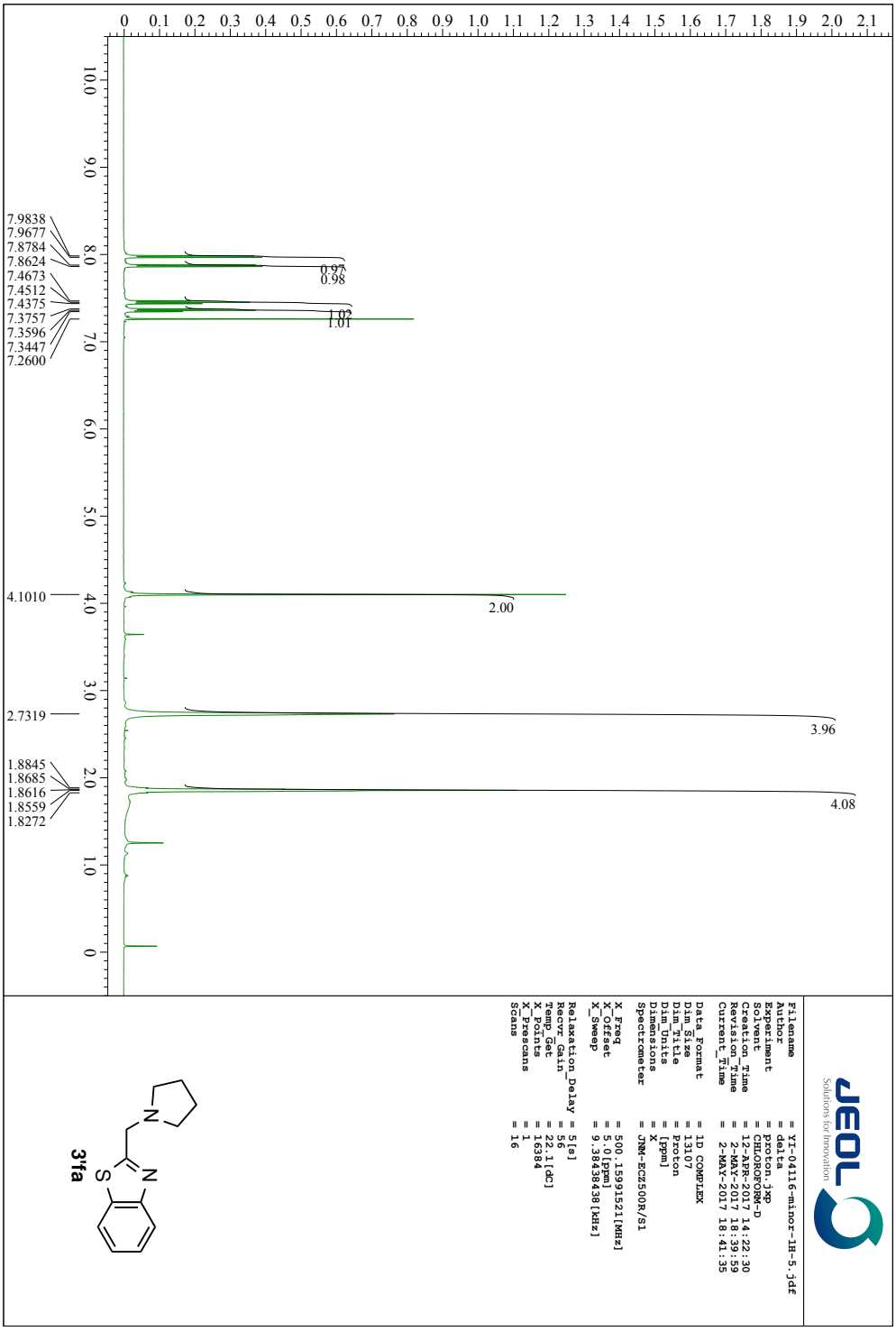
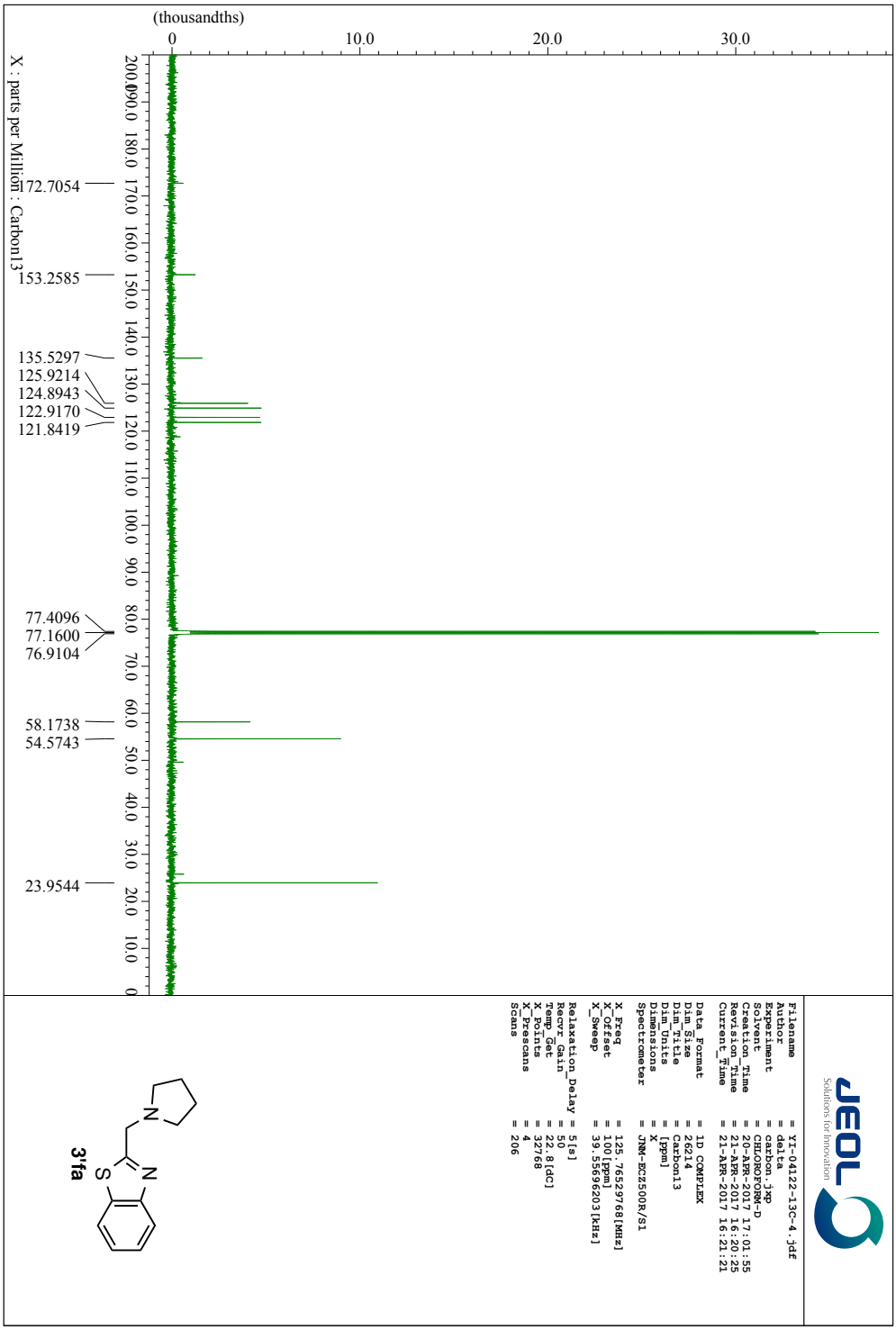
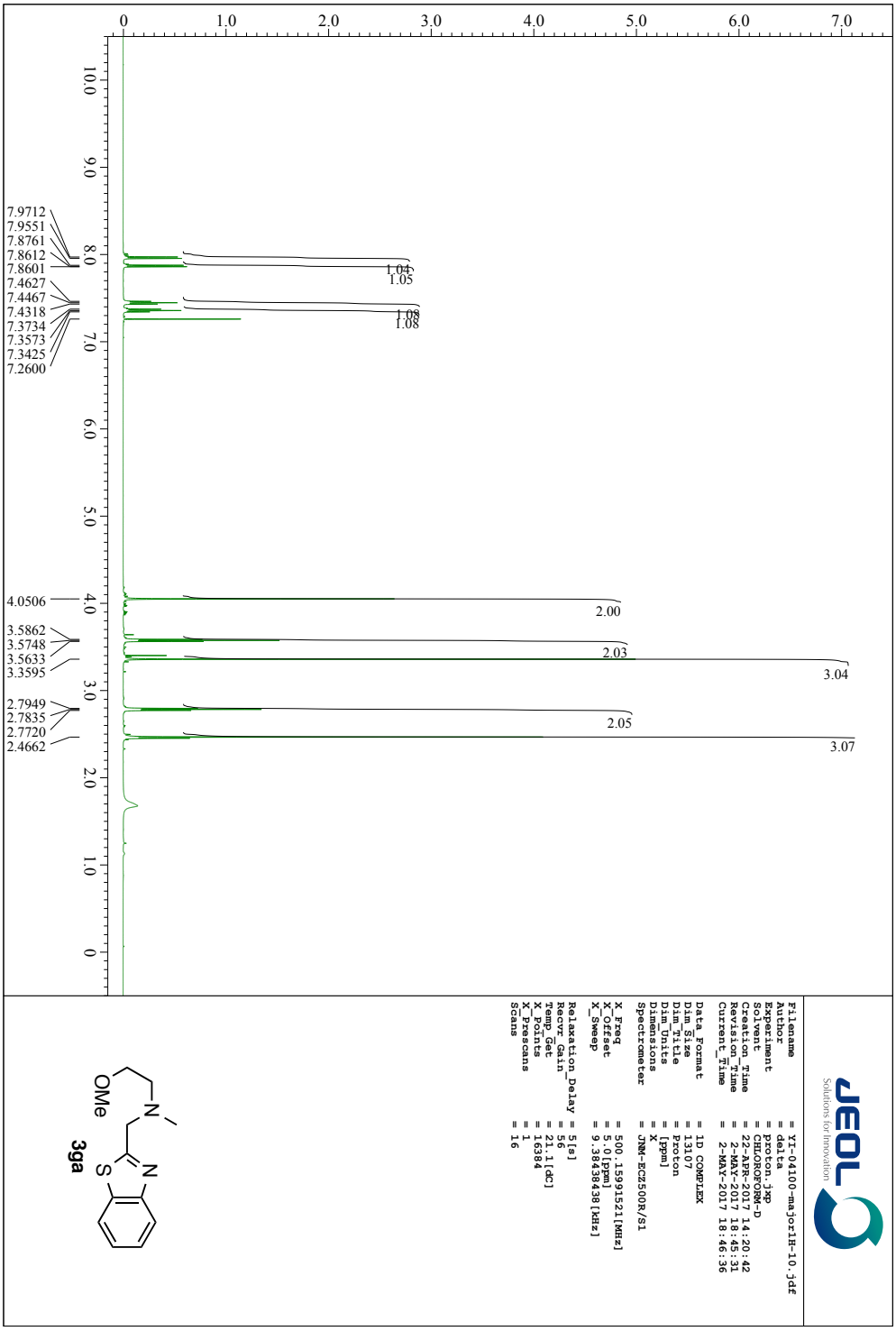
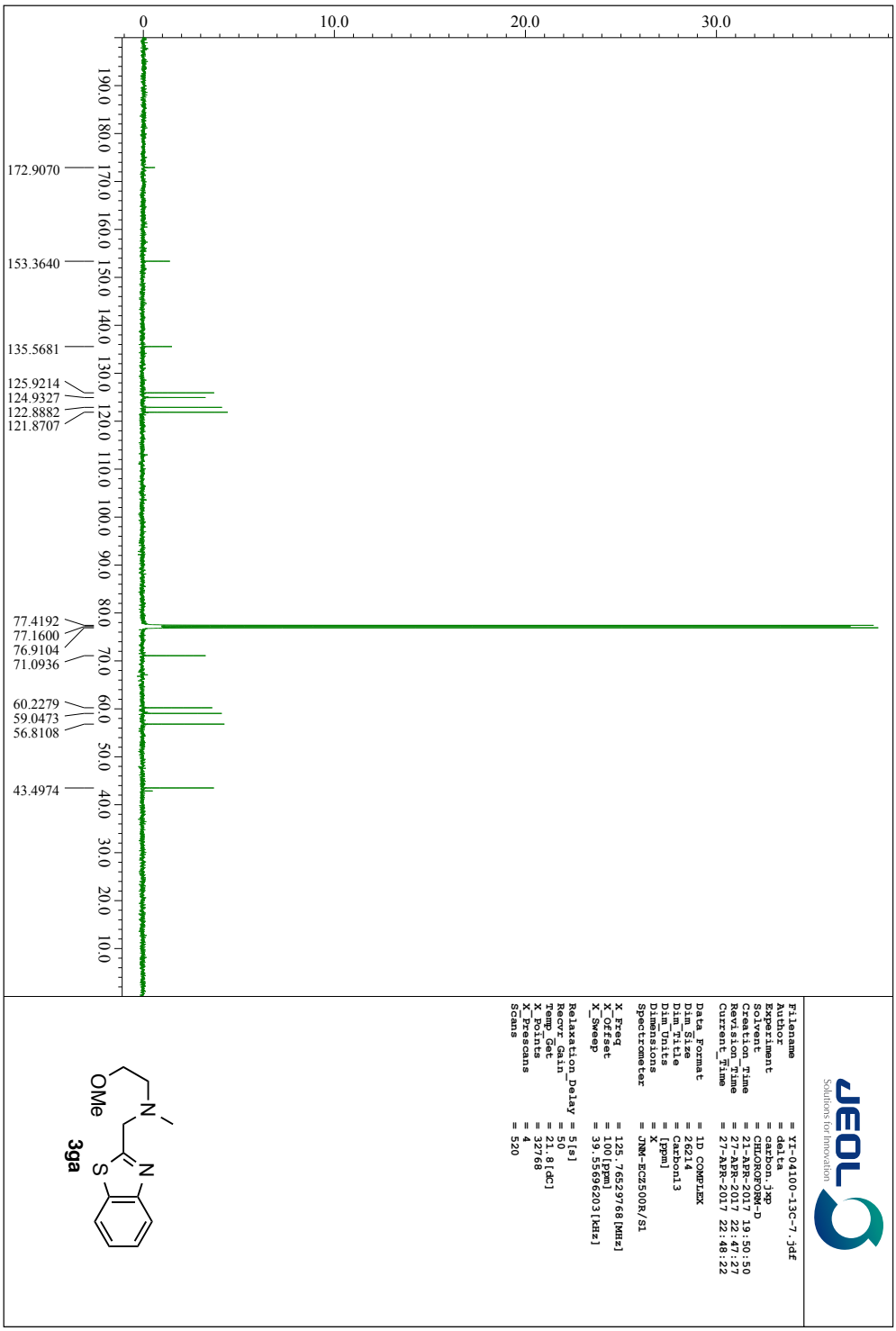
7.8750
7.8601
7.4398
7.4375
7.4238
7.4215
7.3562
7.3539
7.3402
7.2600
3.8130
3.7992
3.7947
3.7821
3.2896
3.2747
3.2599
3.2564
2.4605
2.4502
2.4422
2.4239
1.9910
1.9887
1.9864
1.9841
1.9807
1.9772
1.9738
1.9681
0.95
0.96
0.97
0.97
0.97
1.00
5.06
3.10
Filename = YI-03199-majorH-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-FEB-2017 15:56:36
Revision_Time = 1-MAY-2017 14:06:27
Current_Time = 1-MAY-2017 14:08:03
Data_Format = 1D COMPLEX
Dim_Size = 12107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 20.3[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3fa

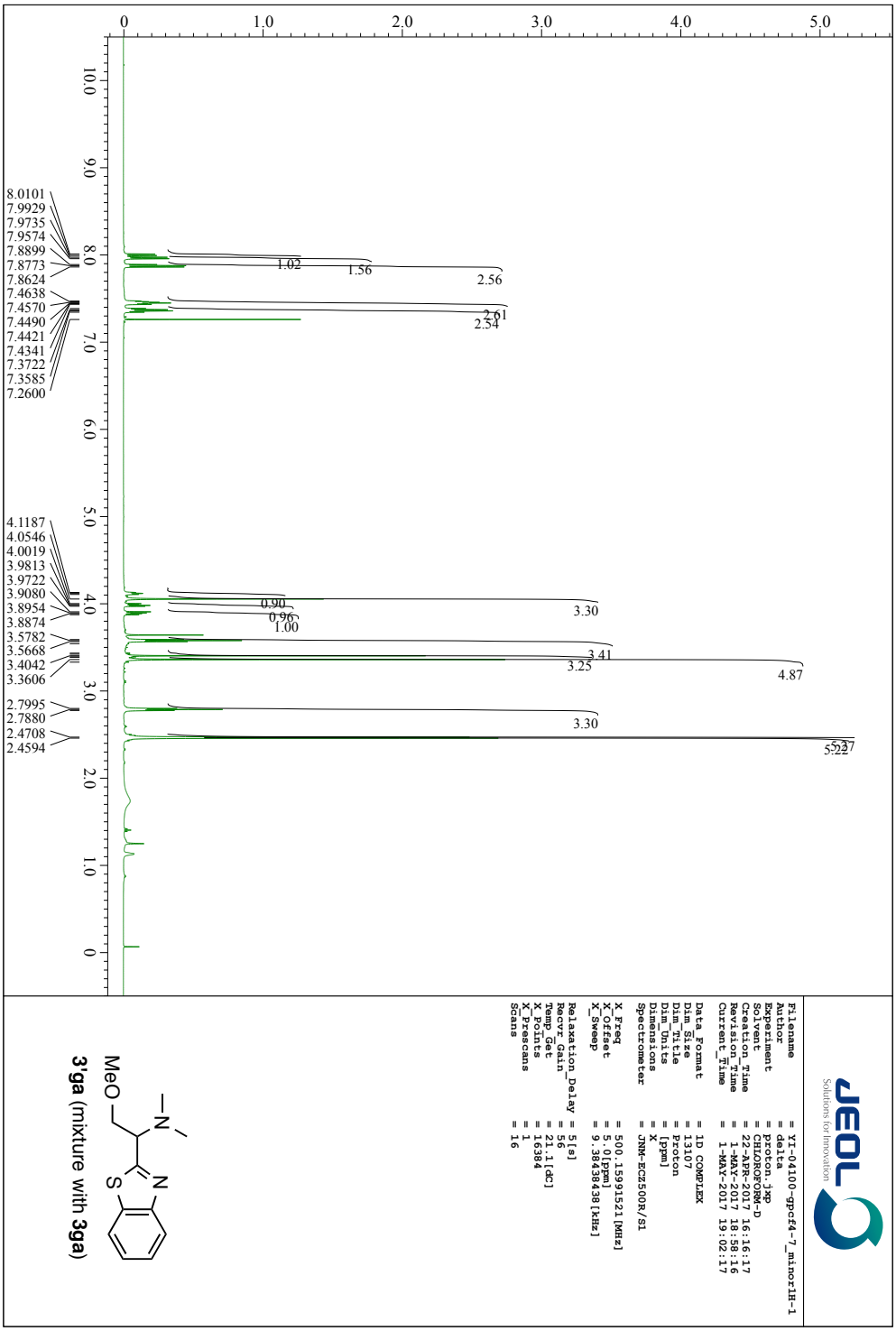

0
10.0
20.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
179.0501
153.7576
135.2129
125.8254
124.7407
122.7346
121.9763
77.4192
77.1600
76.9104
68.3580
57.1179
41.3761
34.6474
23.6761
JEOL
Solutions for Innovation
Filename = YI-03199-major13C-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-FEB-2017 15:58:46
Revision_Time = 26-APR-2017 23:33:01
Current_Time = 26-APR-2017 23:33:23
Data_Format = 1D COMPLEX
Dim_Size = 2F214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 3[s]
Recvr_Gain = 50.7[dC]
Temp_Comte = 20.7[dC]
X_Points = 32768
X_Prescans = 4
Scans = 308
3fa

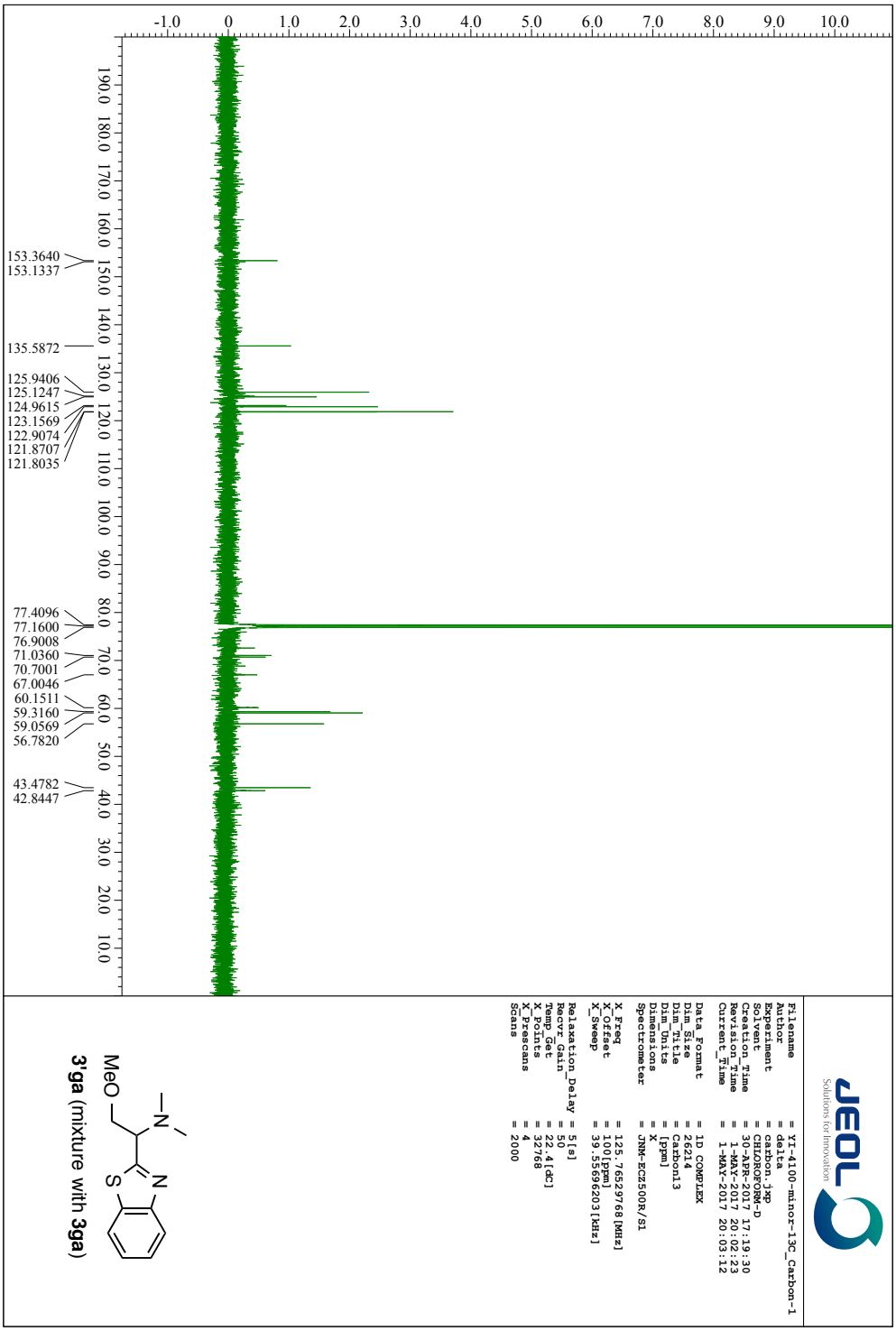

7.9838
7.9677
7.8784
7.8624
7.4673
7.4512
7.4375
7.3757
7.3596
7.3447
7.2600
4.1010
2.7319
1.8845
1.8685
1.8616
1.8559
1.8272
0.97
0.98
1.02
1.01
2.00
3.96
4.08
JEOL
Solutions for Innovation
Filename = YI-04116-minor-1H-5.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 12-APR-2017 14:22:30
Revision_Time = 2-MAY-2017 18:39:59
Current_Time = 2-MAY-2017 18:41:35
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.1[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3'1a

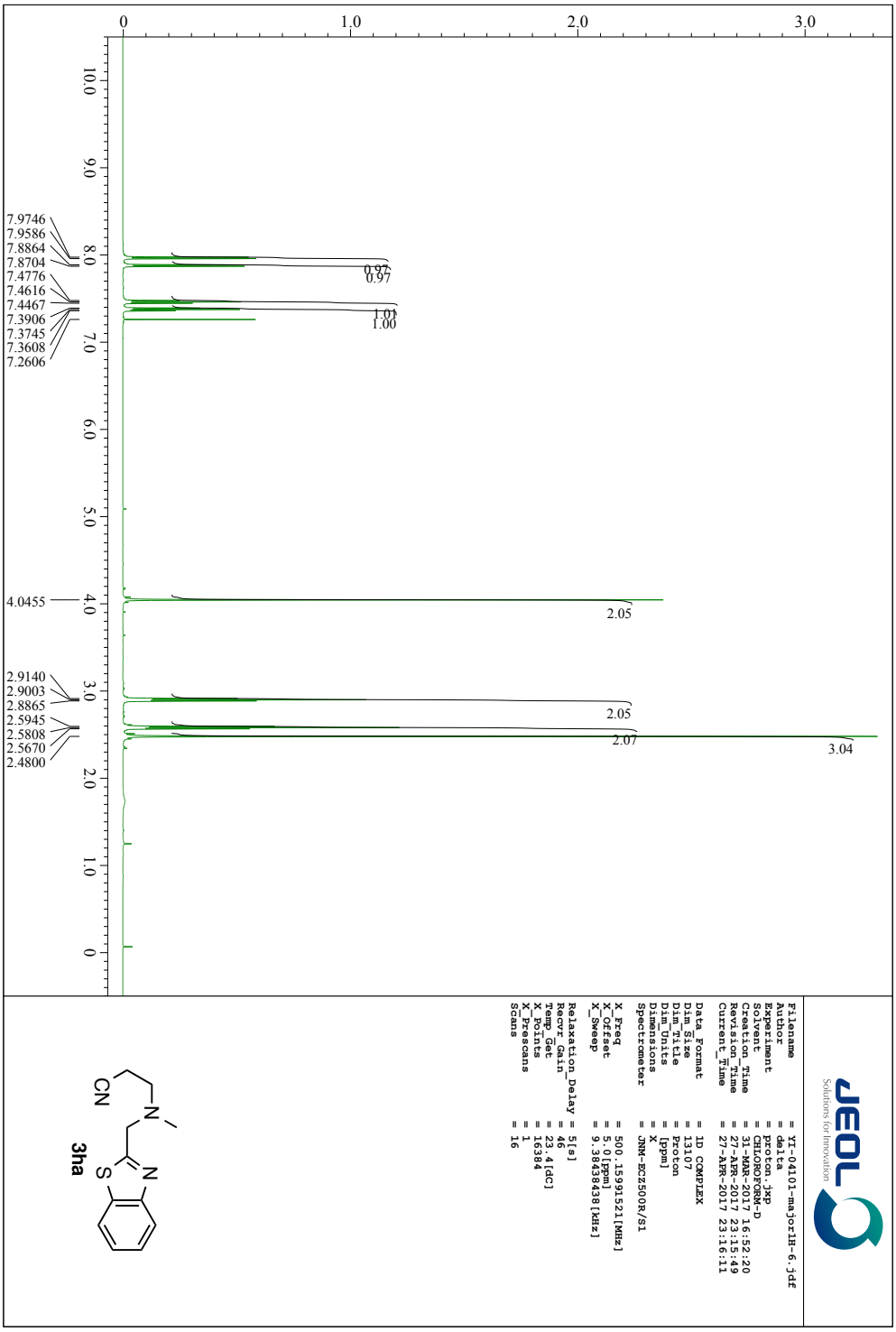

(thousandths)
0
10.0
20.0
30.0
X : parts per Million : Carbon13
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
172.7054
153.2585
135.5297
125.9214
124.8943
122.9170
121.8419
77.4096
77.1600
76.9104
58.1738
54.5743
23.9544
Filename = YI-04122-13C-4.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 20-APR-2017 17:01:55
Revision_Time = 21-APR-2017 16:20:25
Current_Time = 21-APR-2017 16:21:21
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765297681[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50.8[dC]
Temp_Get = 22
X_Points = 32768
X_Prescans = 4
Scans = 206
N
S
N
3'1a

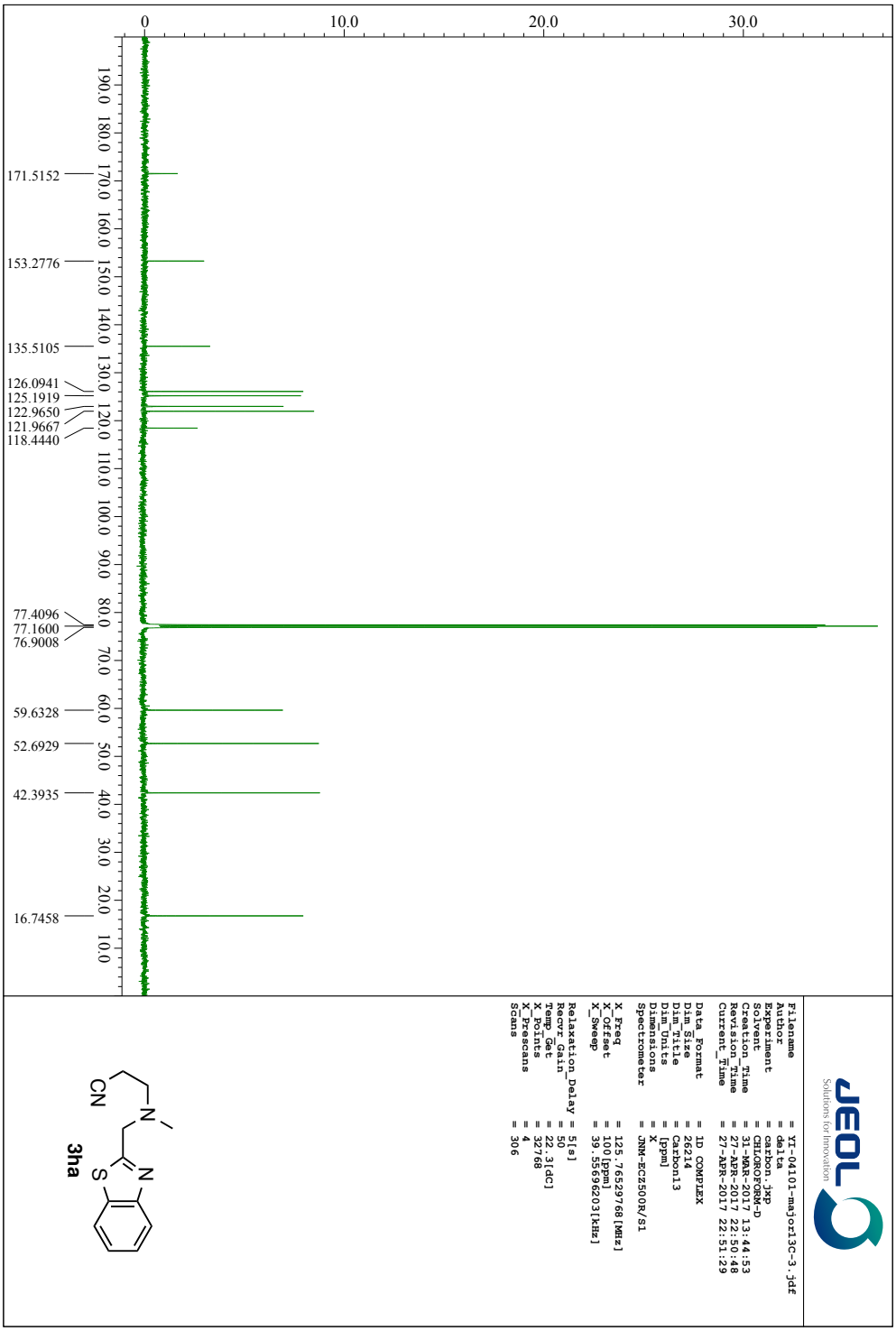

7.9712
7.9551
7.8761
7.8612
7.8601
7.4627
7.4467
7.4318
7.3734
7.3573
7.3425
7.2600
4.0506
3.5862
3.5748
3.5633
3.3595
2.7949
2.7835
2.7720
2.4662
1.04
1.05
1.08
1.08
2.00
2.03
3.04
2.05
3.07
Filename = YI-04100-majorIH-10.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 22-APR-2017 14:20:42
Revision_Time = 2-MAY-2017 18:45:31
Current_Time = 2-MAY-2017 18:46:36
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.1[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
OMe
N
S
N
3ga

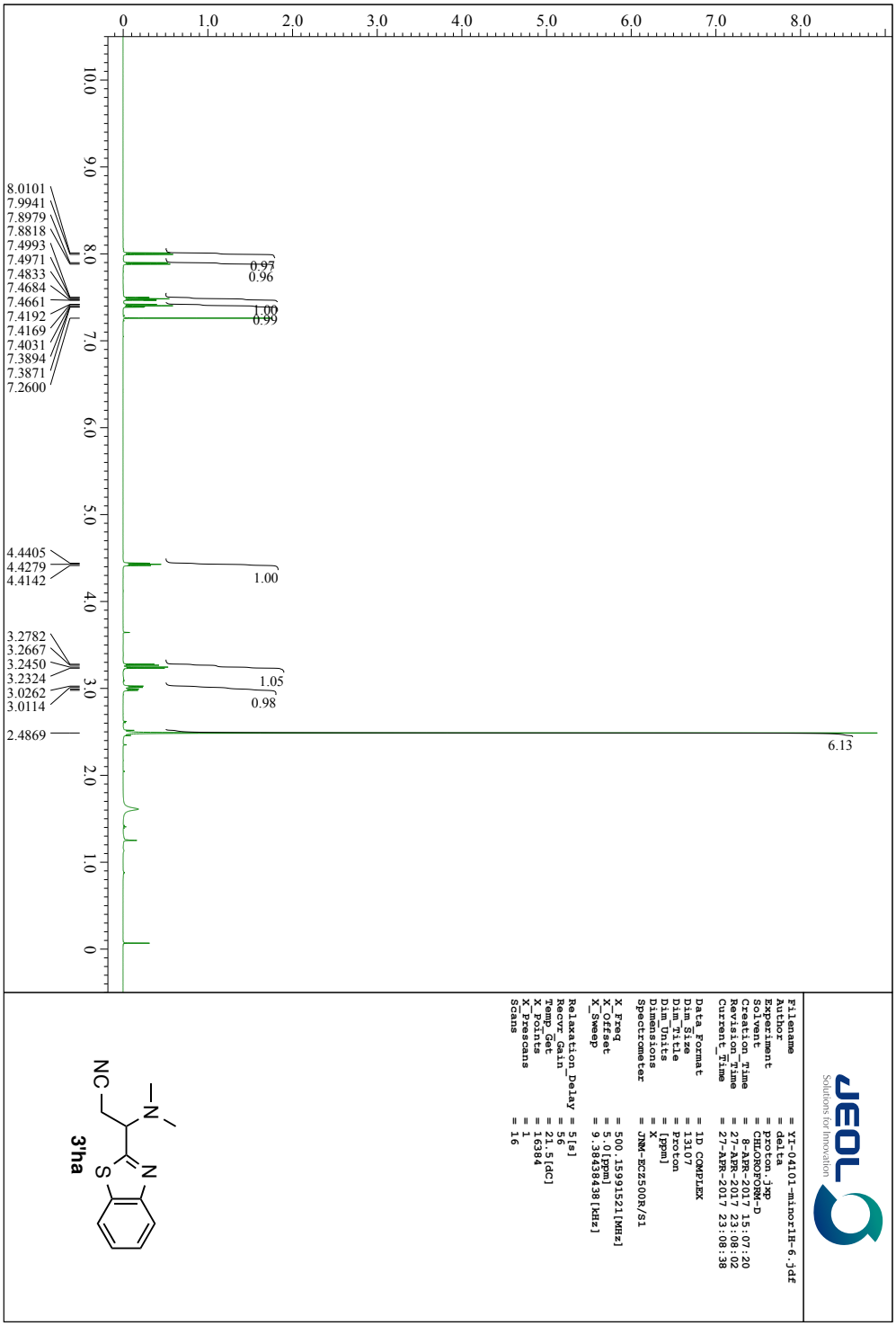

0
10.0
20.0
30.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
172.9070
153.3640
135.5681
125.9214
124.9327
122.8882
121.8707
77.4192
77.1600
76.9104
71.0936
60.2279
59.0473
56.8108
43.4974
JEOL
Solutions for Innovation
Filename = YI-04100-13C-7.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 21-APR-2017 19:50:50
Revision_Time = 27-APR-2017 22:47:27
Current_Time = 27-APR-2017 22:48:22
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765297 68 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50.8[dC]
Temp_Get = 21
X_Points = 32768
X_Prescans = 4
Scans = 520
OMe
N
S
N
3ga

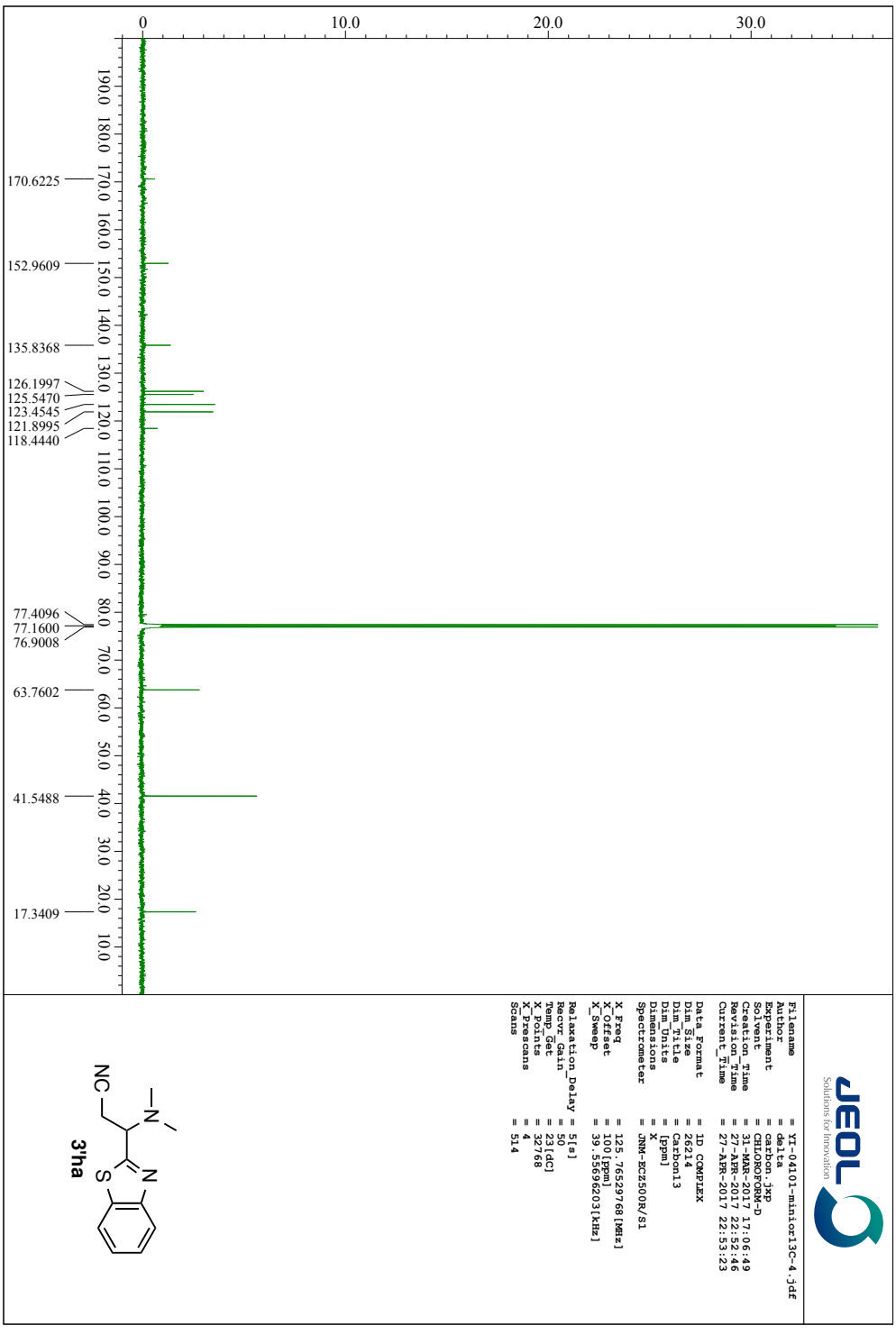

JEOL
Solutions for Innovation
Filename = YI-04100-ppcf4-7_minorIH-1
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 22-APR-2017 16:16:17
Revision_Time = 1-MAY-2017 18:58:16
Current_Time = 1-MAY-2017 19:02:17
Data_Format = 1D COMPLEX
Dim_Size = 32107
Dim_Title = proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 58
Temp_Get = 25.1 [dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
MeO
S
N
N
3'ga (mixture with 3ga)

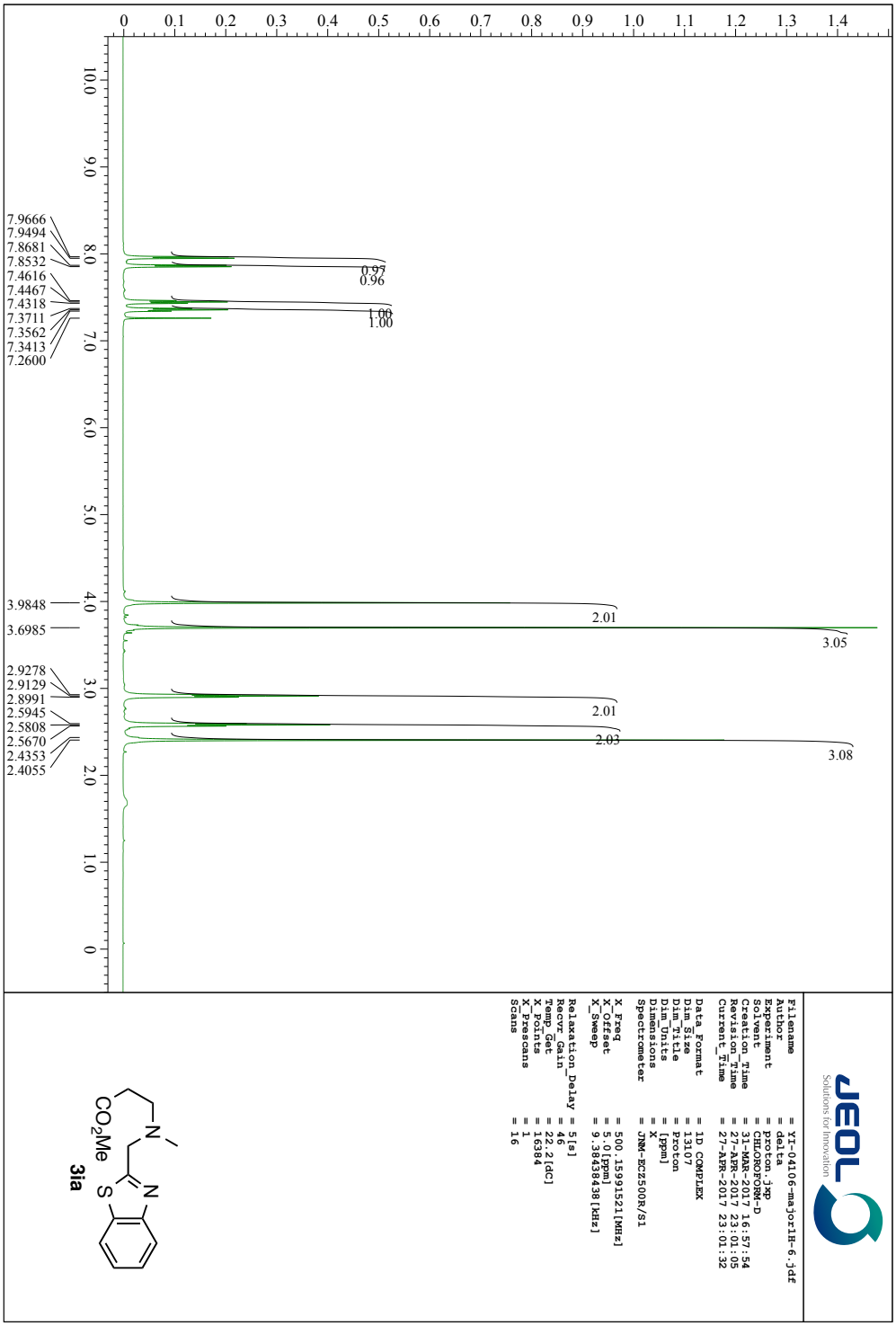

JEOL
Solutions for Innovation
Filename = YI-4100-minor-13C_Carbon-1
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 30-APR-2017 17:19:30
Revision_Time = 1-MAY-2017 20:02:23
Current_Time = 1-MAY-2017 20:03:12
Data_Format = 1D COMPLEX
Data_Size = 32214
Dim_Size = Carbon13
Dim_Title = [ppm]
Dim_Units = X
Dimensions = JNM-ECZ500R/S1
Spectrometer
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50.4[dC]
Temp_Get = 22.4[dC]
X_Points = 32768
X_Prescans = 4
Scans = 2000
153.3640
153.1337
135.5872
125.9406
125.1247
124.9615
123.1569
122.9074
121.8707
121.8035
77.4096
77.1600
76.9008
71.0360
70.7001
67.0046
60.1511
59.3160
59.0569
56.7820
43.4782
42.8447
MeO
N
S
N
3'ga (mixture with 3ga)

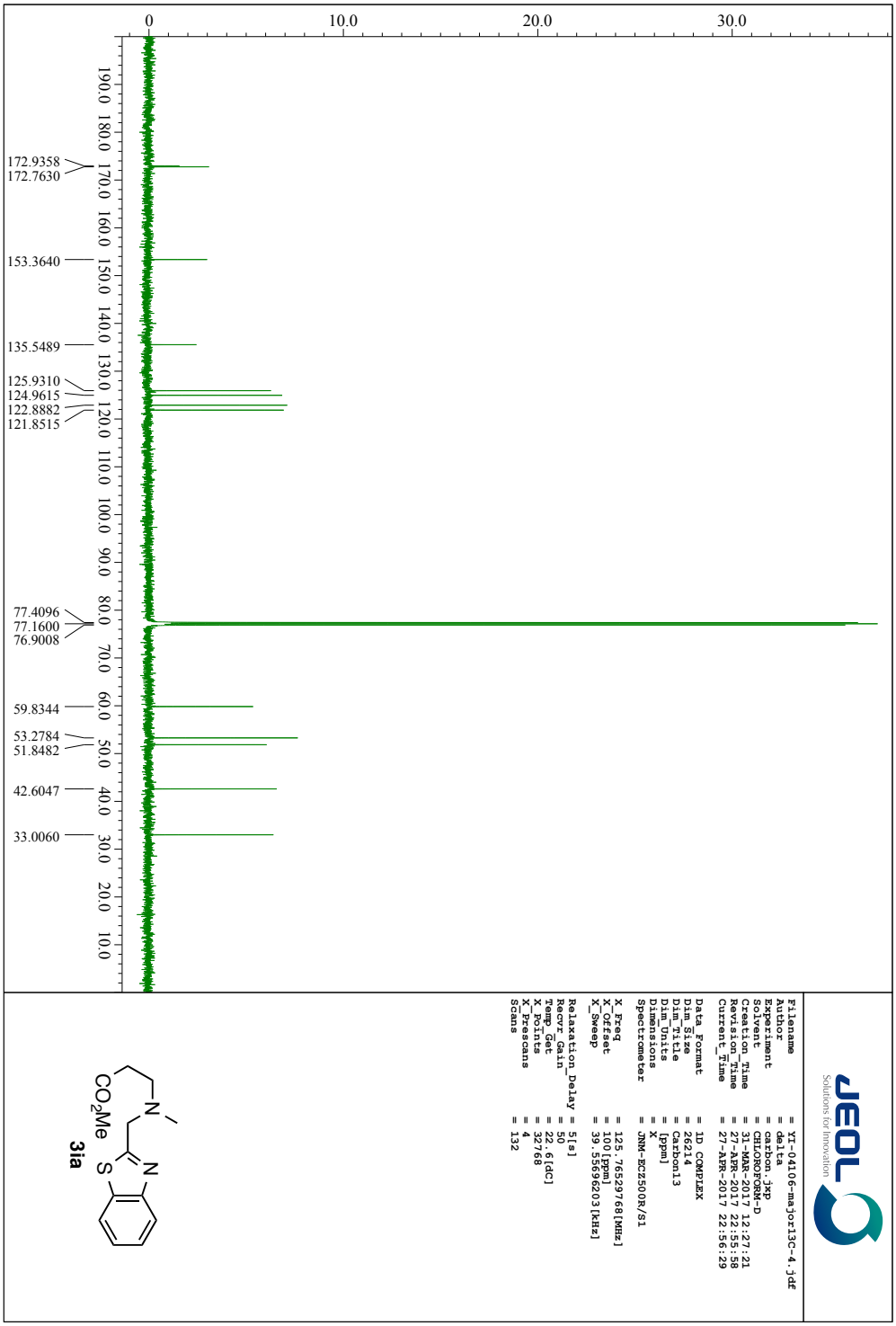

7.9746
7.9586
7.8864
7.8704
7.4776
7.4616
7.4467
7.3906
7.3745
7.3608
7.2606
4.0455
2.9140
2.9003
2.8865
2.5945
2.5808
2.5670
2.4800
0.97
0.97
1.01
1.00
2.05
2.05
2.07
3.04
Filename = YI-04101-majorIH-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 31-MAR-2017 16:52:20
Revision_Time = 27-APR-2017 23:15:49
Current_Time = 27-APR-2017 23:16:11
Data_Format = 1D COMPLEX
Dim_Size = 19107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 28
Temp_Get = 23.4[dC]
X_Points = 19384
X_Prescans = 1
Scans = 16
3ha

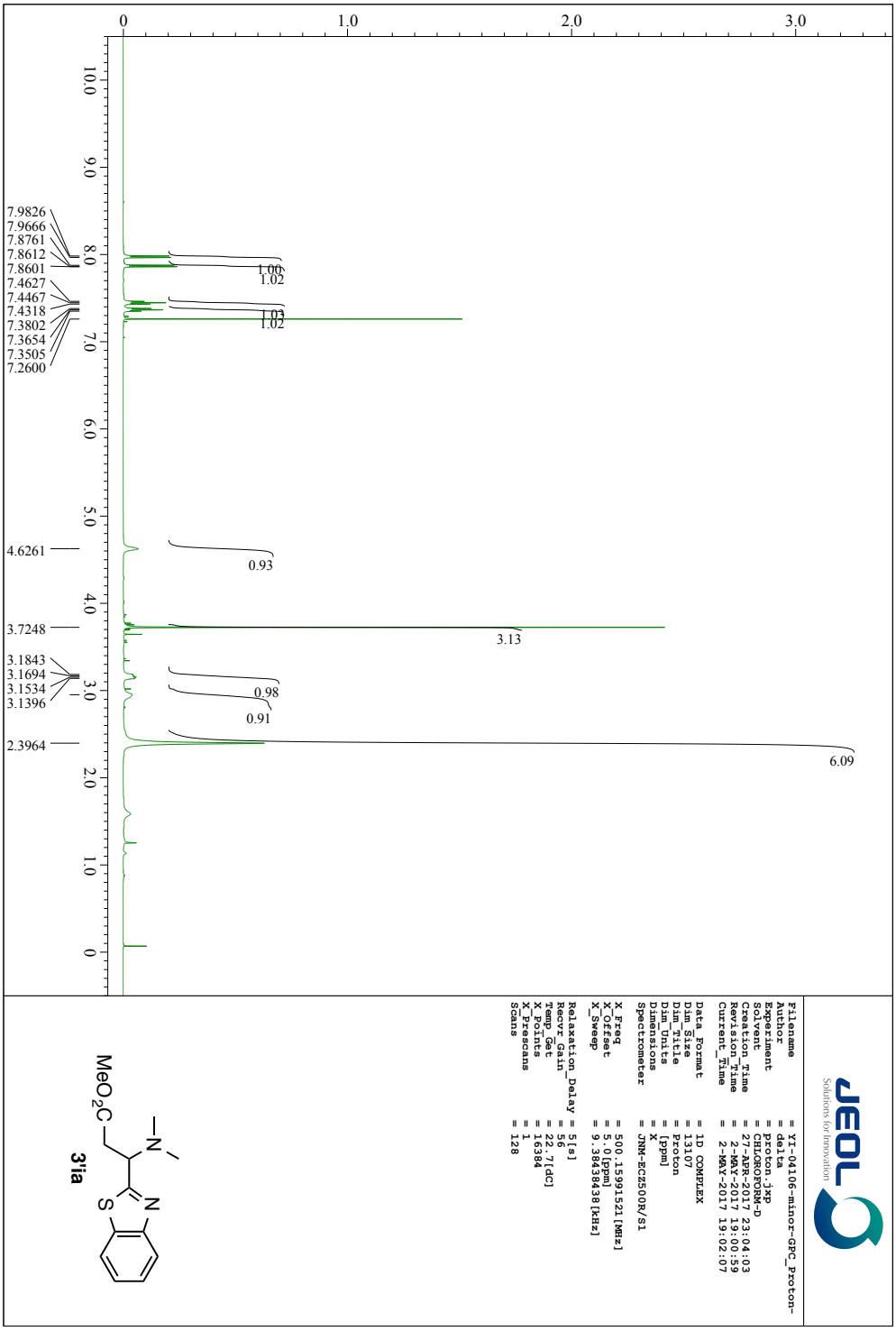

0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
171.5152
153.2776
135.5105
126.0941
125.1919
122.9650
121.9667
118.4440
77.4096
77.1600
76.9008
59.6328
52.6929
42.3935
16.7458
JEOL
Solutions for Innovation
Filename = YI-04101-major13C-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 31-MAR-2017 13:44:53
Revision_Time = 27-APR-2017 22:50:48
Current_Time = 27-APR-2017 22:51:29
Data_Format = 1D COMPLEX
Dim_Size = 32214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 50
Temp_Get = 22.3 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 306
CN
N
N
S
3ha

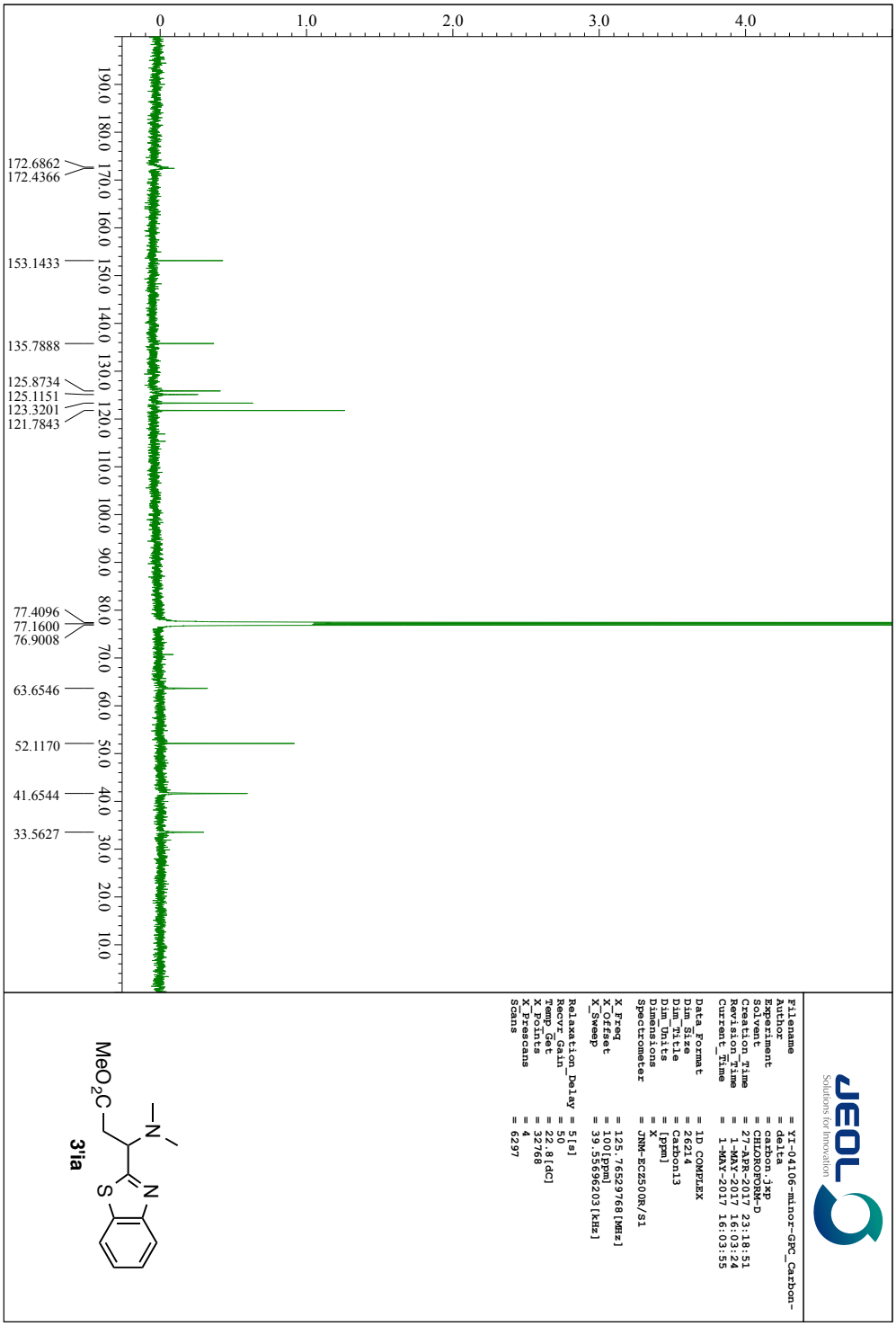

8.0101
7.9941
7.8979
7.8818
7.4993
7.4971
7.4833
7.4684
7.4661
7.4192
7.4169
7.4031
7.3894
7.3871
7.2600
4.4405
4.4279
4.4142
3.2782
3.2667
3.2450
3.2324
3.0262
3.0114
2.4869
0.97
0.96
1.00
0.99
1.00
1.05
0.98
6.13
Filename = YI-04101-minorIH-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 8-APR-2017 15:07:20
Revision_Time = 27-APR-2017 23:08:02
Current_Time = 27-APR-2017 23:08:38
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.01[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 56
Temp_Get = 21.5[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3'ha

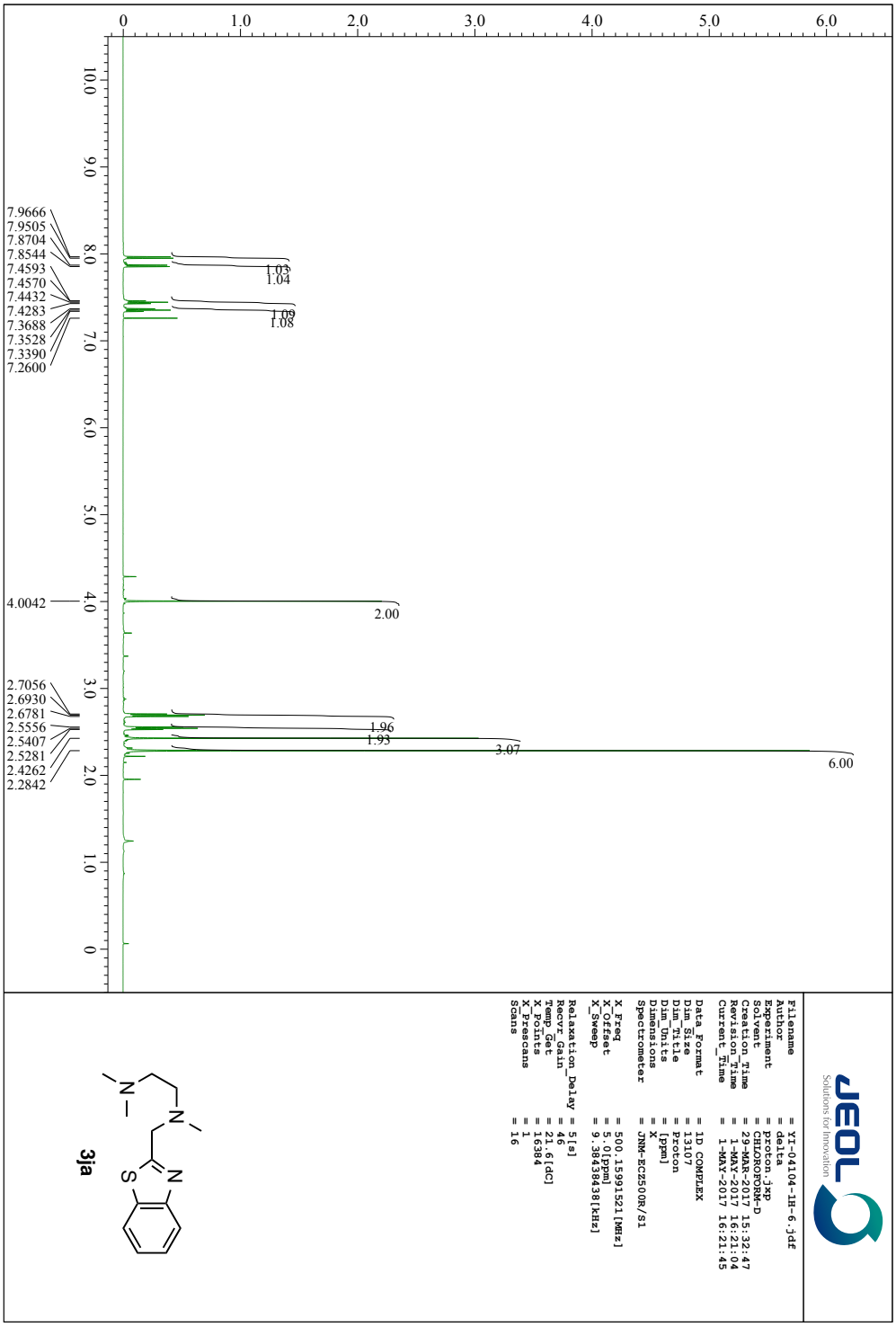

0
10.0
20.0
30.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
170.6225
152.9609
135.8368
126.1997
125.5470
123.4545
121.8995
118.4440
77.4096
77.1600
76.9008
63.7602
41.5488
17.3409
Solutions for Innovation
Filename = YI-04101-minisor13C-4.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 31-MAR-2017 17:06:49
Revision_Time = 27-APR-2017 22:52:46
Current_Time = 27-APR-2017 22:53:23
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 23[dC]
Temp_Gain = 32768
X_Points = 4
X_Prescans = 514
Scans
NC
N
S
N
3'ha

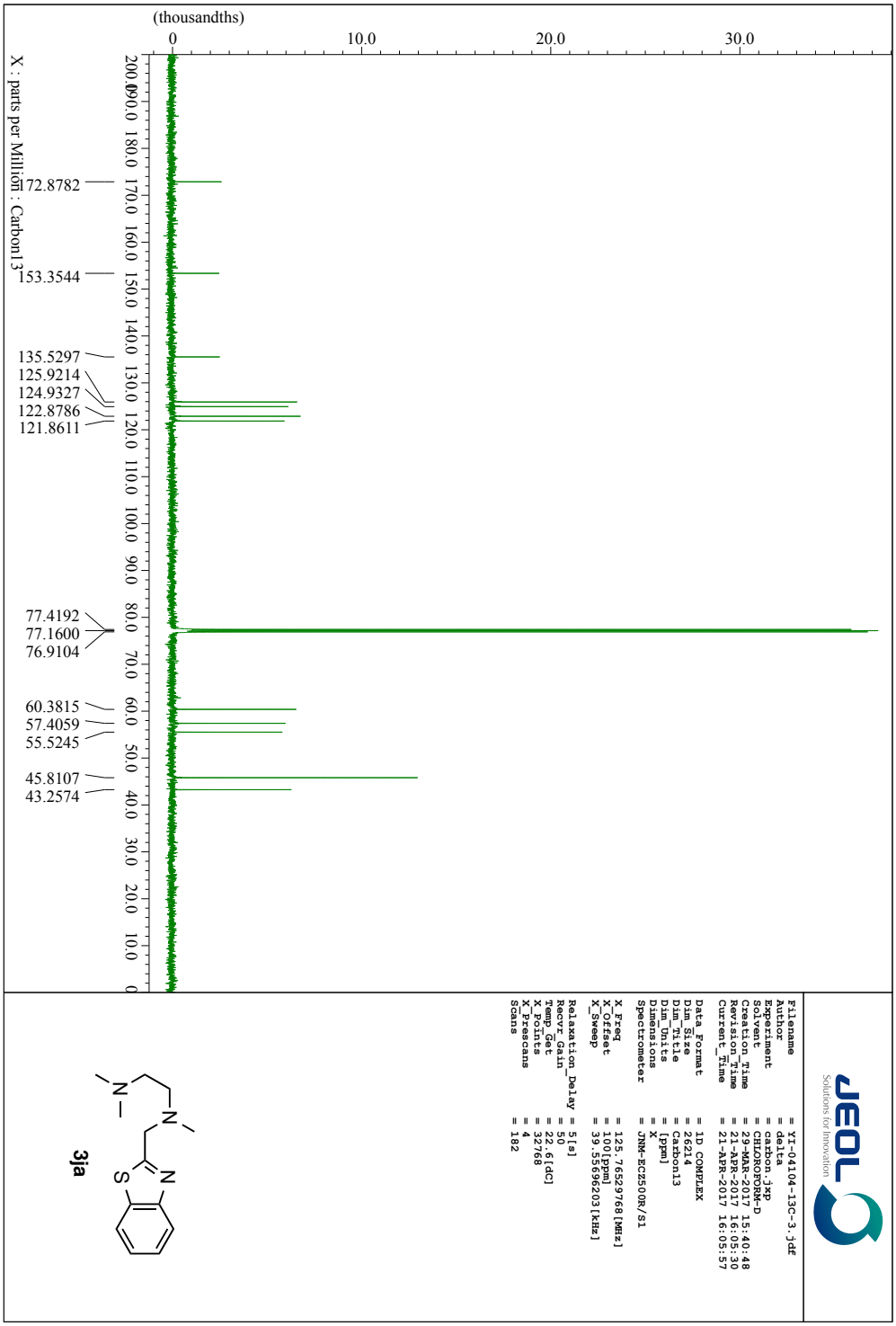

7.9666
7.9494
7.8681
7.8532
7.4616
7.4467
7.4318
7.3711
7.3562
7.3413
7.2600
3.9848
3.6985
2.9278
2.9129
2.8991
2.5945
2.5808
2.5670
2.4353
2.4055
0.97
0.96
1.00
1.00
2.01
3.05
2.01
2.03
3.08
Filename = YI-04106-majorIH-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 31-MAR-2017 16:57:54
Revision_Time = 27-APR-2017 23:01:05
Current_Time = 27-APR-2017 23:01:32
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 46
Temp_Get = 22.2[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
JEOL
Solutions for Innovation
CO2Me
3ia

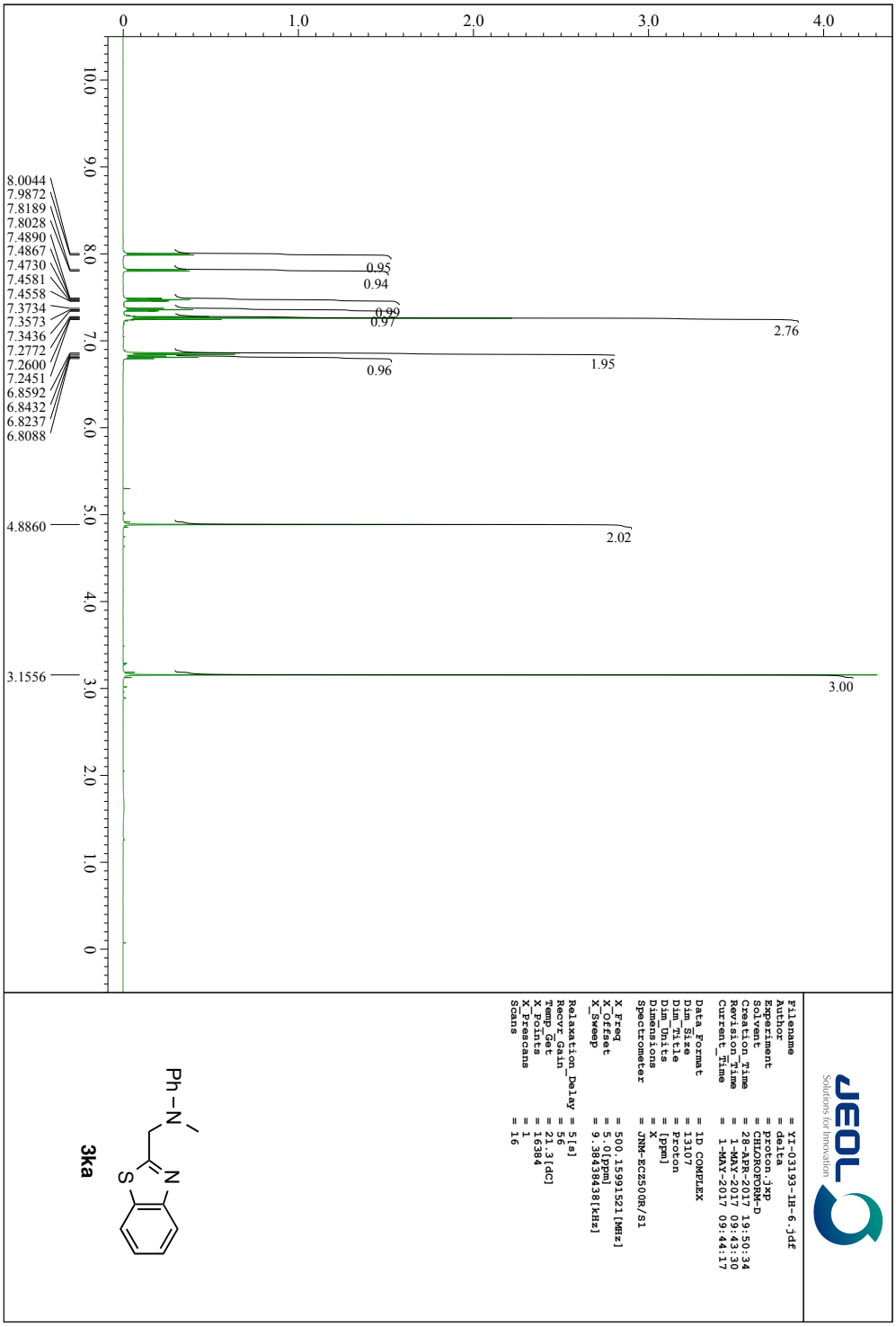

JEOL
Solutions for Innovation
Filename = YT-04106-major13C-4.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 31-MAR-2017 12:27:21
Revision_Time = 27-APR-2017 22:55:58
Current_Time = 27-APR-2017 22:56:29
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 50
Temp_Get = 22.6[dC]
X_Points = 32768
X_Prescans = 4
Scans = 132
172.9358
172.7630
153.3640
135.5489
125.9310
124.9615
122.8882
121.8515
77.4096
77.1600
76.9008
59.8344
53.2784
51.8482
42.6047
33.0060
CO2Me
3ia

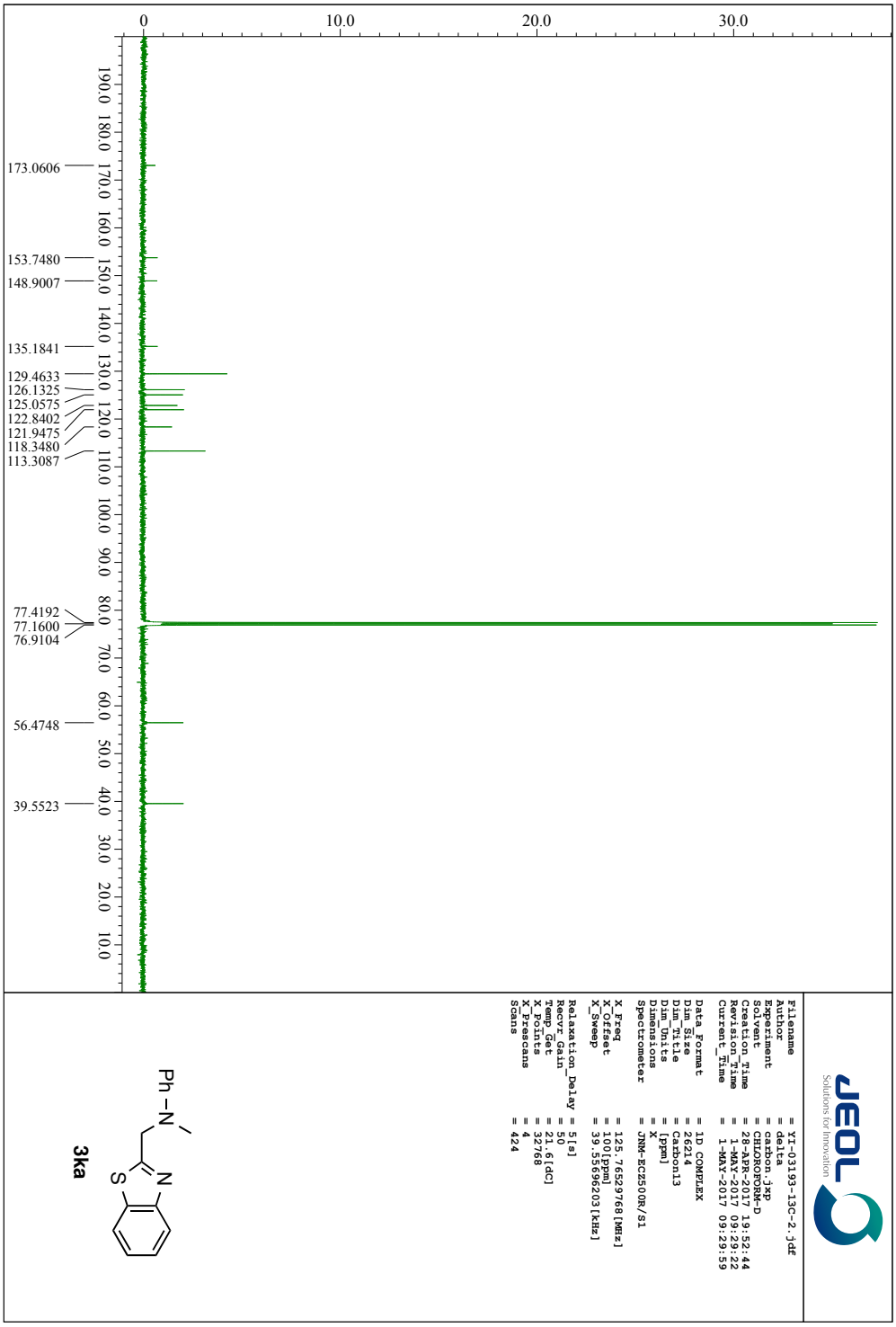

7.9826
7.9666
7.8761
7.8612
7.8601
7.4627
7.4467
7.4318
7.3802
7.3654
7.3505
7.2600
4.6261
3.7248
3.1843
3.1694
3.1534
3.1396
2.3964
1.00
1.02
1.03
1.02
0.93
3.13
0.98
0.91
6.09
Filename = YI-04106-minor-GPC_Proton-
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 27-APR-2017 23:04:03
Revision_Time = 2-MAY-2017 19:00:59
Current_Time = 2-MAY-2017 19:02:07
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 22.7 [dB]
Temp_Comment =
X_Points = 16384
X_Prescans = 1
Scans = 128
MeO2C
N
S
N
3'ia

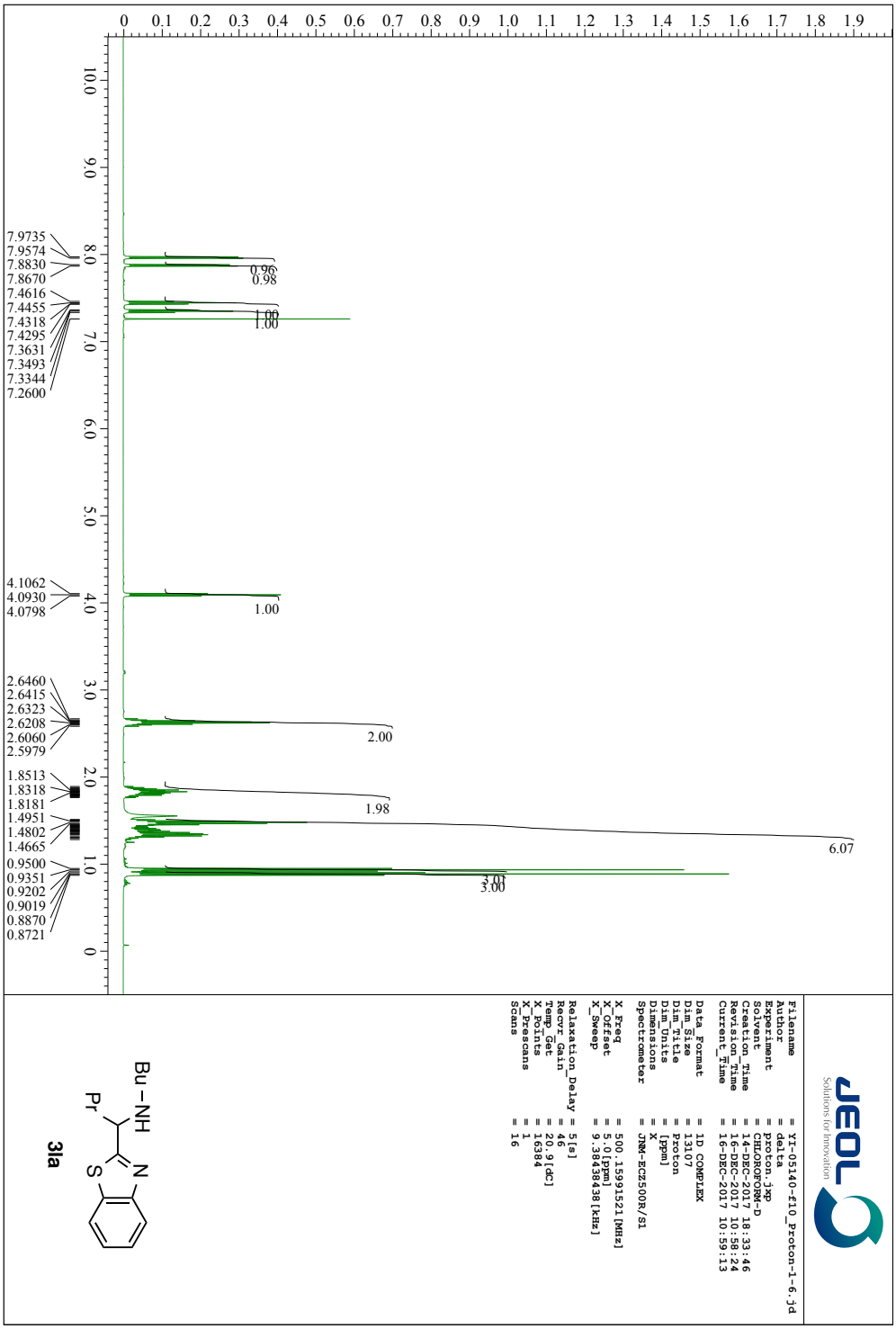

0
1.0
2.0
3.0
4.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
172.6862
172.4366
153.1433
135.7888
125.8734
125.1151
123.3201
121.7843
77.4096
77.1600
76.9008
63.6546
52.1170
41.6544
33.5627
JEOL
Solutions for Innovation
Filename = YI-04106-minor-GPC_Carbon-
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 27-APR-2017 23:18:51
Revision_Time = 1-MAY-2017 16:03:24
Current_Time = 1-MAY-2017 16:03:55
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 50
Temp_Get = 22.8[dC]
X_Points = 32768
X_Prescans = 4
Scans = 6297
MeO2C
N
S
N
3ia

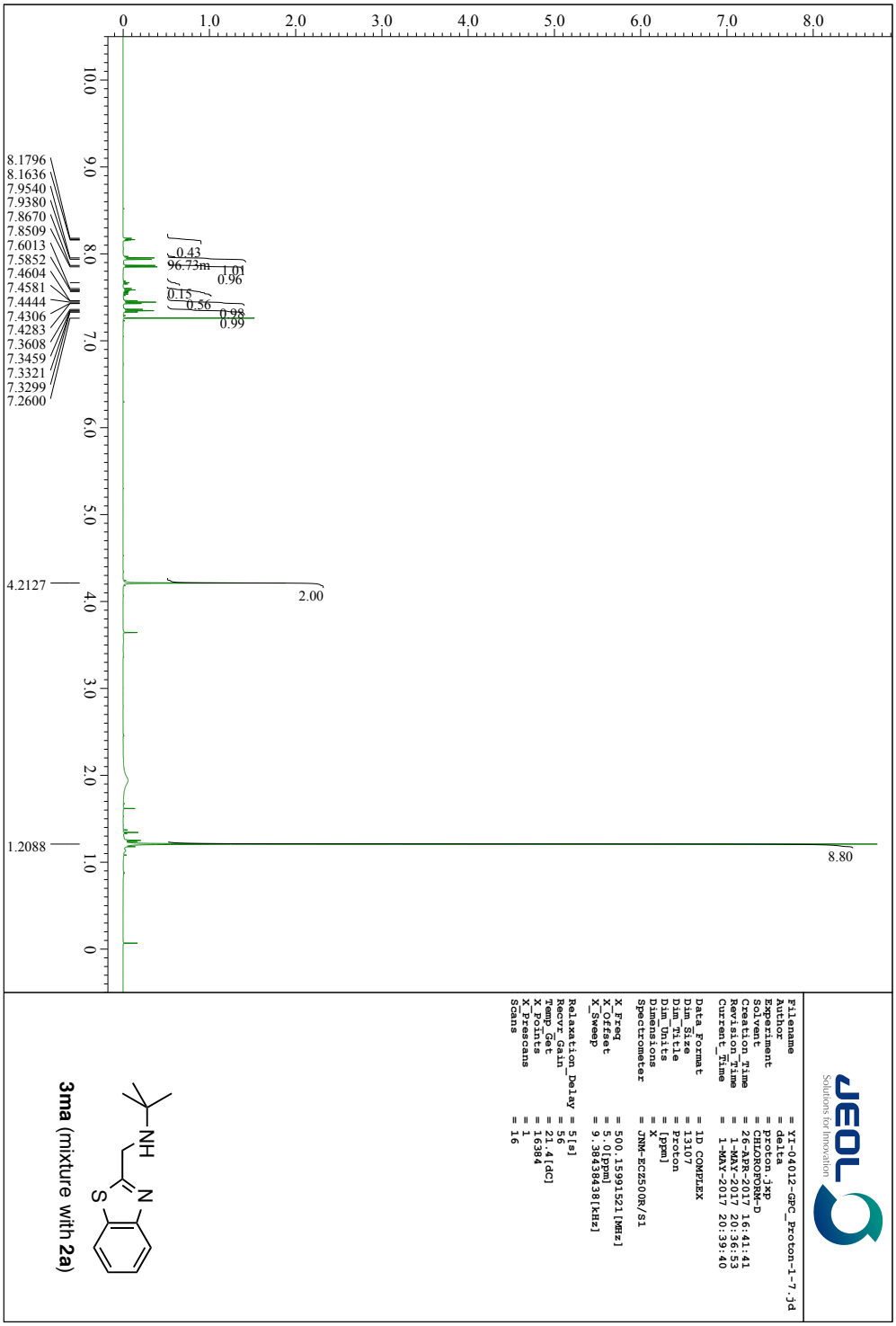

7.9666
7.9505
7.8704
7.8544
7.4593
7.4570
7.4432
7.4283
7.3688
7.3528
7.3390
7.2600
4.0042
2.7056
2.6930
2.6781
2.5556
2.5407
2.5281
2.4262
2.2842
1.03
1.04
1.09
1.08
2.00
1.96
1.93
3.07
6.00
Filename = YI-04104-1H-6.jdf
Author = deita
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 29-MAR-2017 15:32:47
Revision_Time = 1-MAY-2017 16:21:04
Current_Time = 1-MAY-2017 16:21:45
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.01[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 46
Temp_Get = 21.6[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3ja

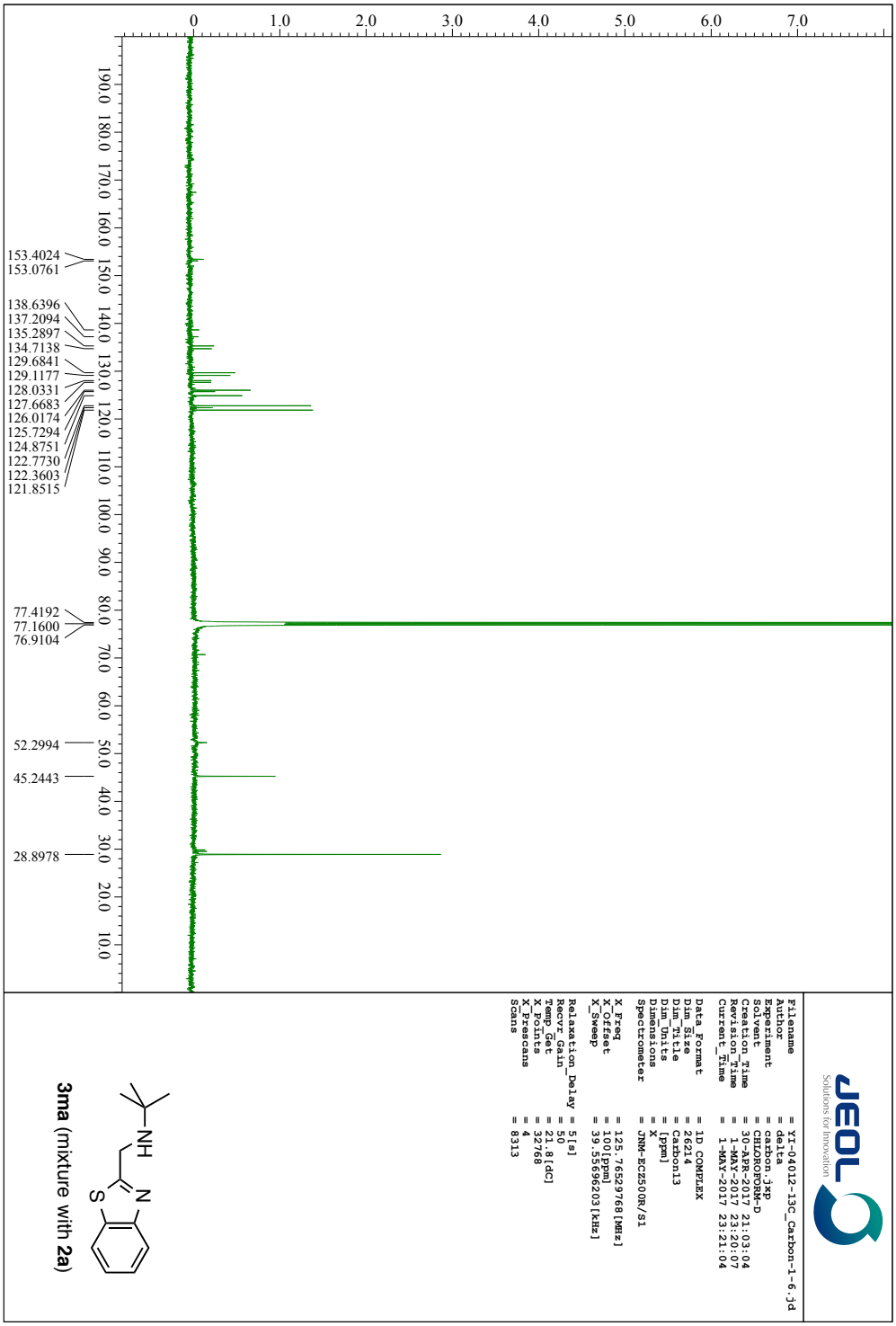

(thousandths)
0
10.0
20.0
30.0
X : parts per Million : Carbon13
172.8782
153.3544
135.5297
125.9214
124.9327
122.8786
121.8611
77.4192
77.1600
76.9104
60.3815
57.4059
55.5245
45.8107
43.2574
JEOL
Solutions for Innovation
Filename = YI-04104-13C-3.jdf
Author = deita
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 29-MAR-2017 15:40:48
Revision_Time = 21-APR-2017 16:05:30
Current_Time = 21-APR-2017 16:05:57
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Set = 22.6[dC]
X_Points = 32768
X_Prescans = 4
Scans = 182
3ja

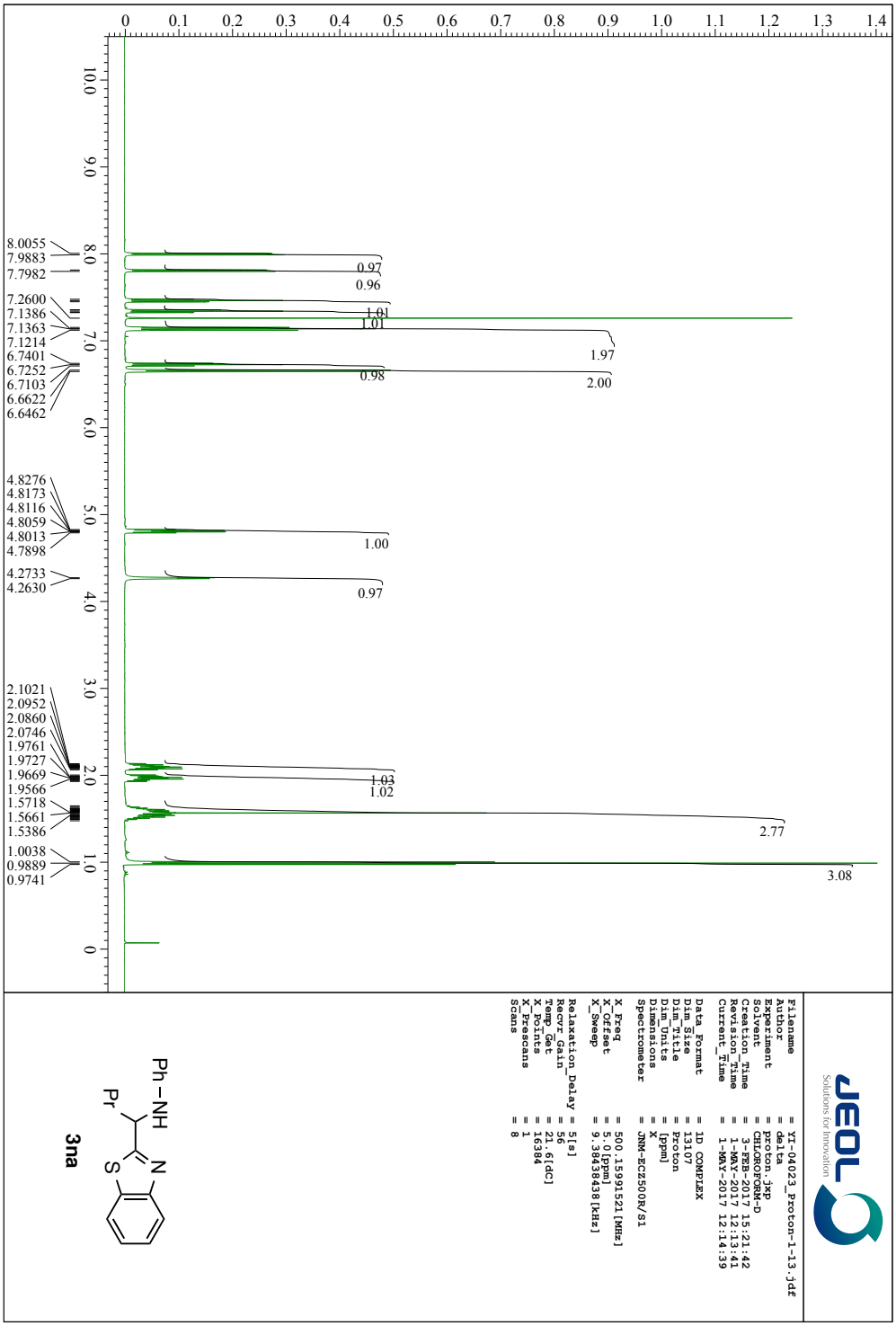

8.0044
7.9872
7.8189
7.8028
7.4890
7.4867
7.4730
7.4581
7.4558
7.3734
7.3573
7.3436
7.2772
7.2600
7.2451
6.8592
6.8432
6.8237
6.8088
4.8860
3.1556
0.95
0.94
0.99
0.97
2.76
0.96
1.95
2.02
3.00
Filename = YI-03193-1H-6.jdf
Author = deita
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 28-APR-2017 19:50:34
Revision_Time = 1-MAY-2017 09:43:30
Current_Time = 1-MAY-2017 09:44:17
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.01[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 56
Temp_Set = 21.3[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
Ph–N
S
N
3ka

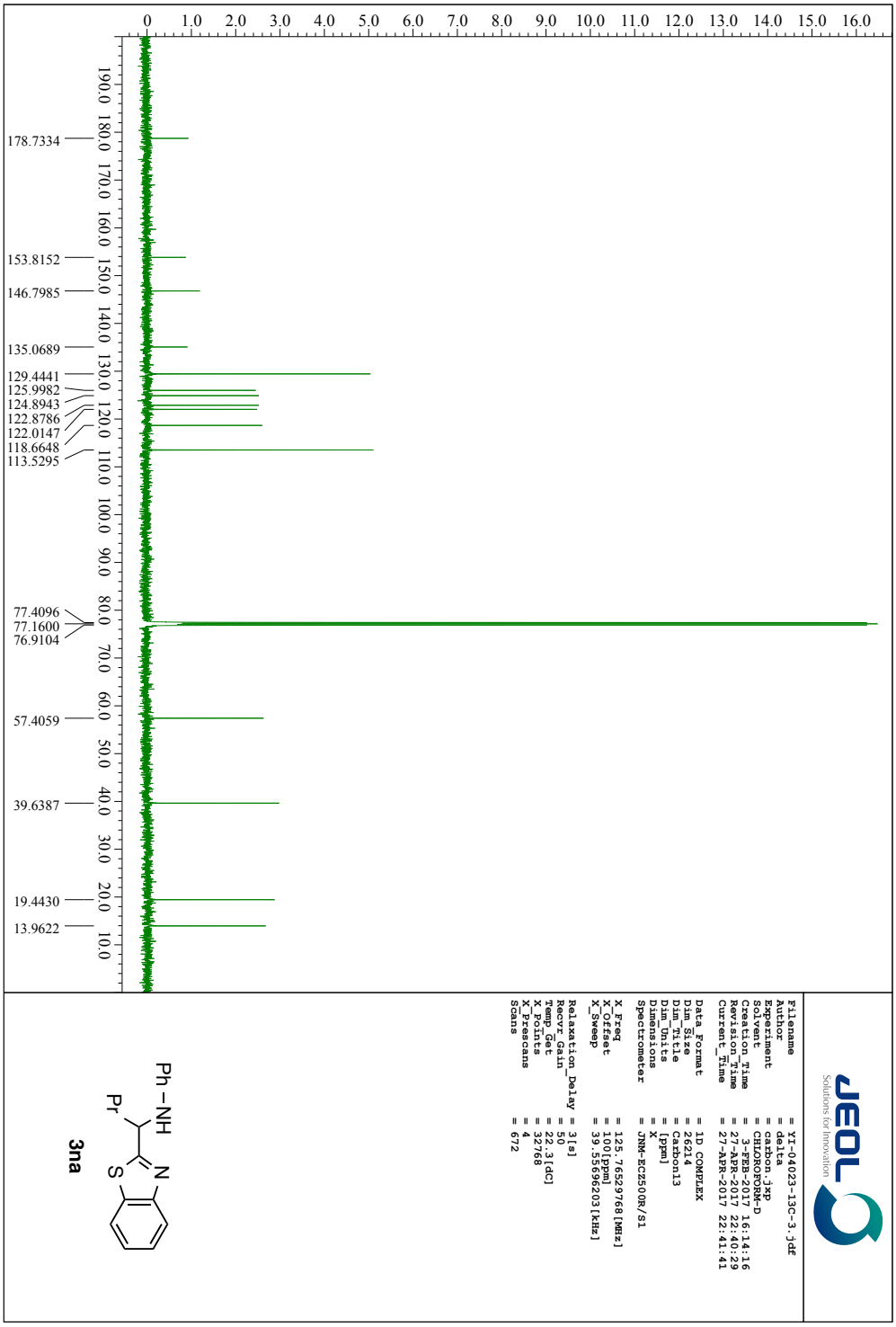

0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
173.0606
153.7480
148.9007
135.1841
129.4633
126.1325
125.0575
122.8402
121.9475
118.3480
113.3087
77.4192
77.1600
76.9104
56.4748
39.5523
JEOL
Solutions for Innovation
Filename = YI-03193-13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 28-APR-2017 19:52:44
Revision_Time = 1-MAY-2017 09:29:22
Current_Time = 1-MAY-2017 09:29:59
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 50
Temp_Set = 21.6[dC]
X_Points = 32768
X_Prescans = 4
Scans = 424
Ph–N
N
S
3ka

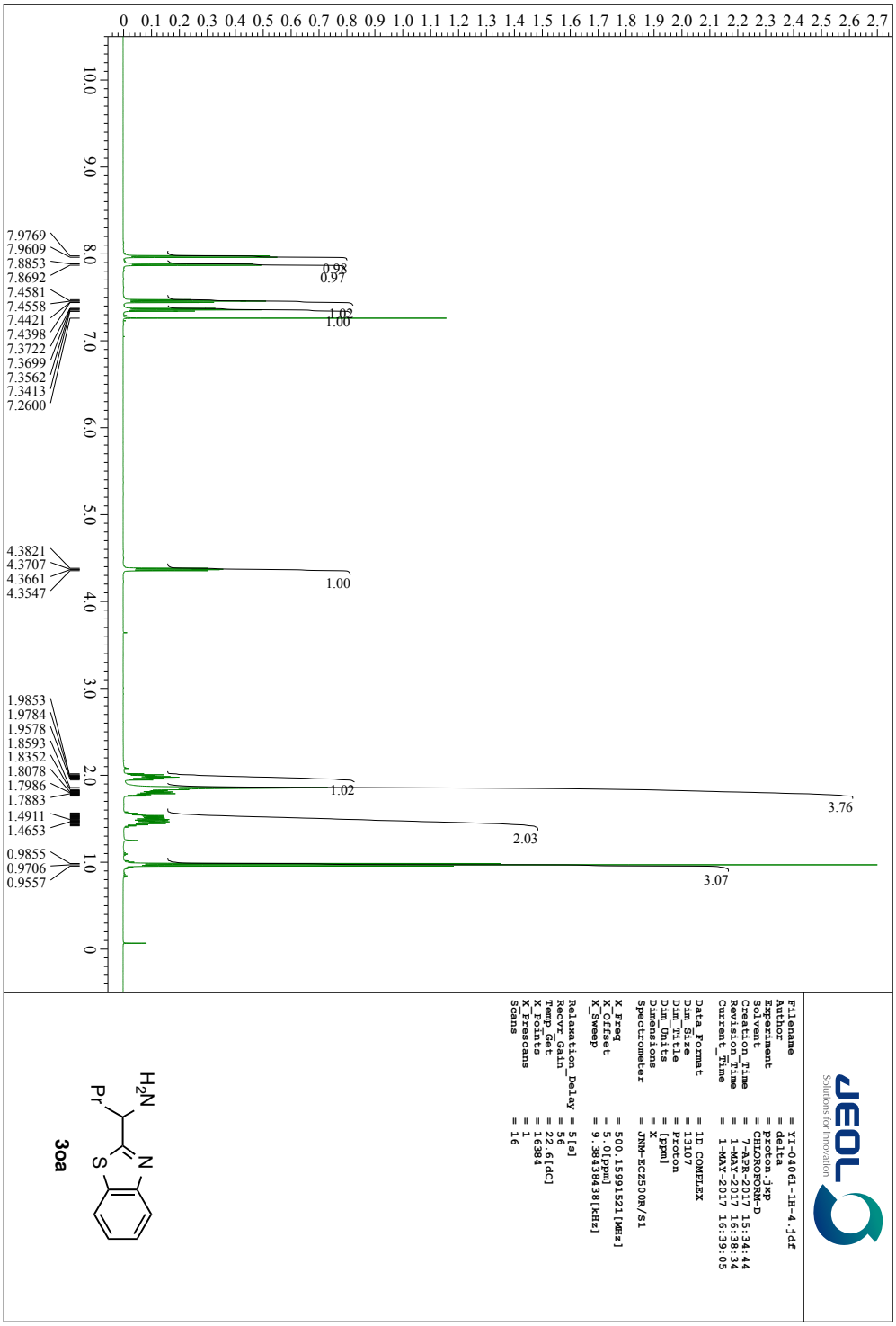

Filename = YI-05140-f10_Proton-1-6.jd
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 14-DEC-2017 18:33:46
Revision_Time = 16-DEC-2017 10:58:24
Current_Time = 16-DEC-2017 10:59:13
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 46
Temp_Get = 20.9[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
Bu–NH
Pr
N
S
3la

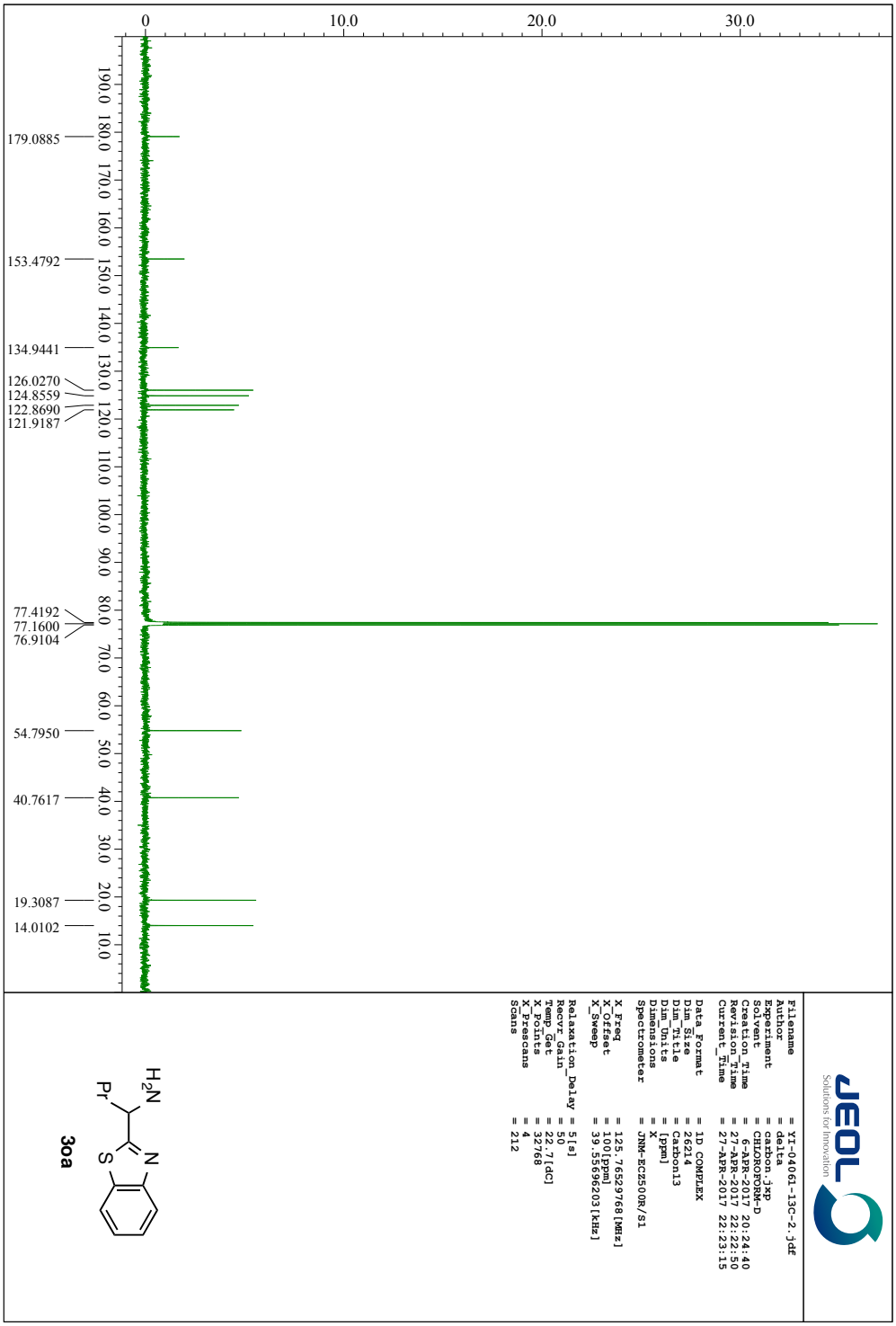

8.1796
8.1636
7.9540
7.9380
7.8670
7.8509
7.6013
7.5852
7.4604
7.4581
7.4444
7.4306
7.4283
7.3608
7.3459
7.3321
7.3299
7.2600
4.2127
1.2088
8.80
2.00
0.43
96.73m
1.01
0.96
0.15
0.56
0.98
0.99
Filename = YI-04012-GPC_Proton-1-7.jd
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 26-APR-2017 16:41:41
Revision_Time = 1-MAY-2017 20:36:53
Current_Time = 1-MAY-2017 20:39:40
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 56
Temp_Set = 21.4[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
Solutions for Innovation
3ma (mixture with 2a)

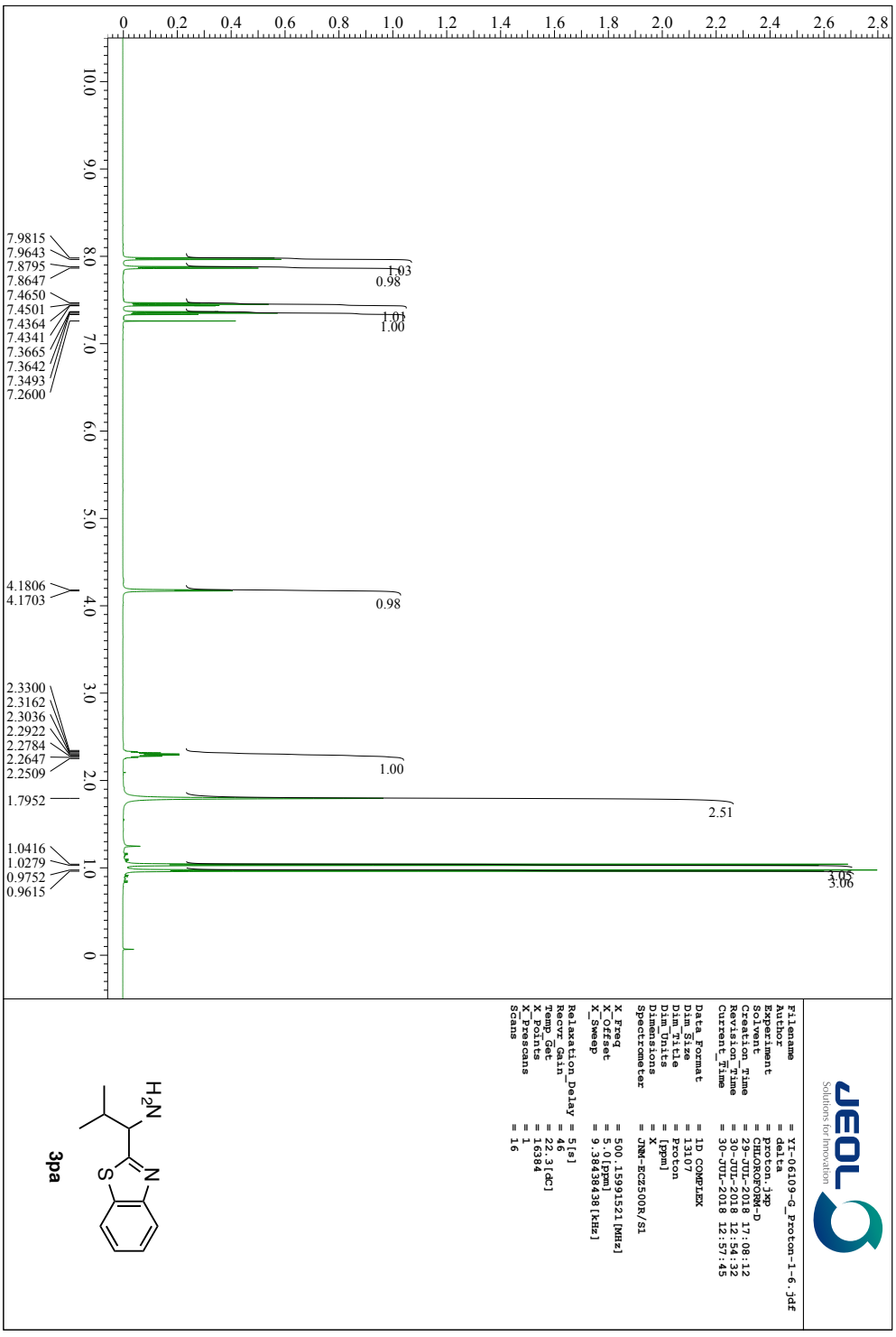

JEOL
Solutions for Innovation
Filename = YT-04012-13C_Carbon-1-6.jd
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 30-APR-2017 21:03:04
Revision_Time = 1-MAY-2017 23:20:07
Current_Time = 1-MAY-2017 23:21:04
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 50
Temp_Get = 21.8[dC]
X_Points = 32768
X_Prescans = 4
Scans = 8313
153.4024
153.0761
138.6396
137.2094
135.2897
134.7138
129.6841
129.1177
128.0331
127.6683
126.0174
125.7294
124.8751
122.7730
122.3603
121.8515
77.4192
77.1600
76.9104
52.2994
45.2443
28.8978
NH
N
S
3ma (mixture with 2a)

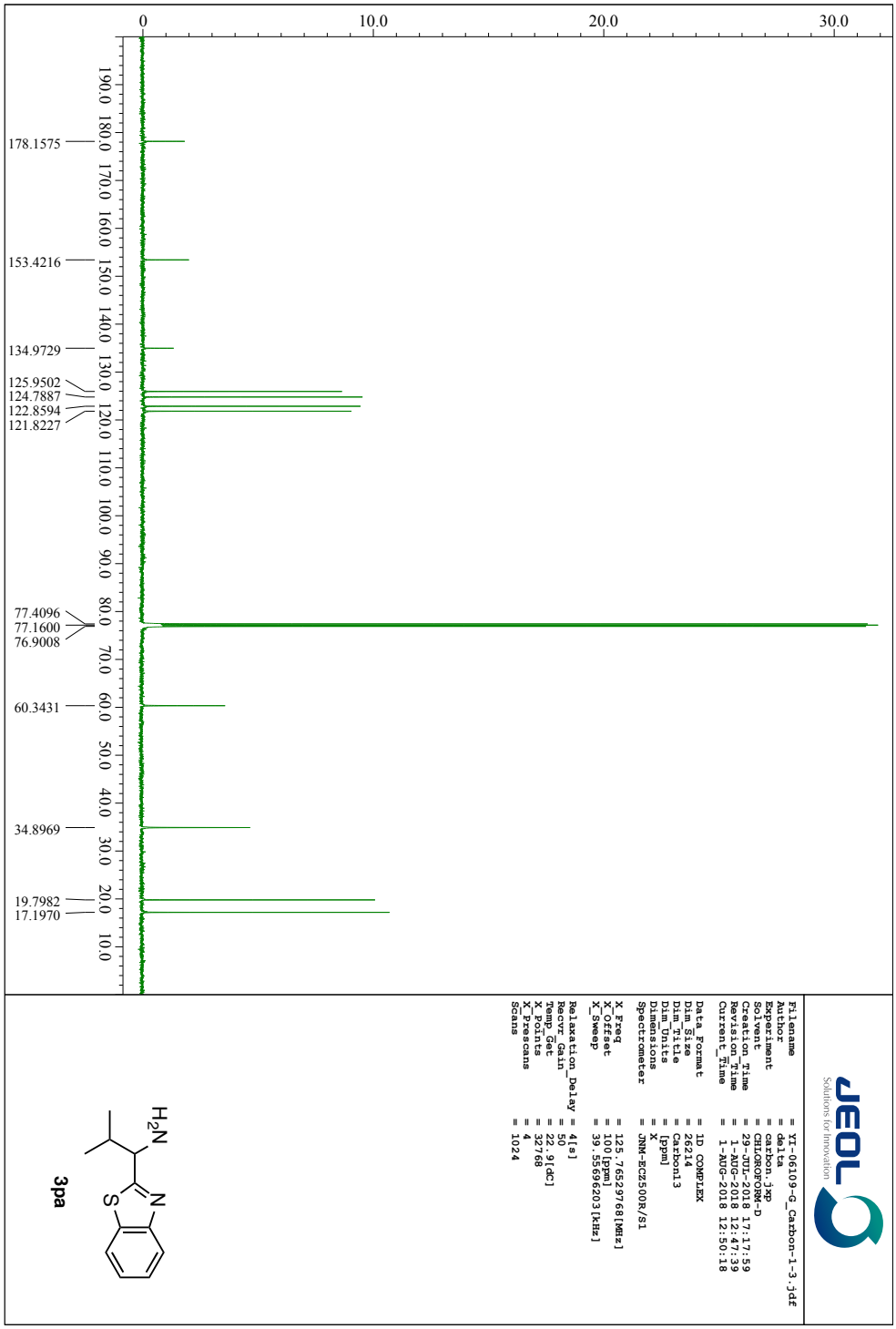

8.0055
7.9883
7.7982
7.2600
7.1386
7.1363
7.1214
6.7401
6.7252
6.7103
6.6622
6.6462
4.8276
4.8173
4.8116
4.8059
4.8013
4.7898
4.2733
4.2630
2.1021
2.0952
2.0860
2.0746
1.9761
1.9727
1.9669
1.9566
1.5718
1.5661
1.5386
1.0038
0.9889
0.9741
0.97
0.96
1.01
1.01
1.97
0.98
2.00
1.00
0.97
1.03
1.02
2.77
3.08
Filename = YT-04023_Proton-1-13.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 3-FEB-2017 15:21:42
Revision_Time = 1-MAY-2017 12:13:41
Current_Time = 1-MAY-2017 12:14:39
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 56
Temp_Get = 21.6[dC]
X_Points = 16384
X_Prescans = 1
Scans = 8
Ph–NH
Pr
N
S
3na

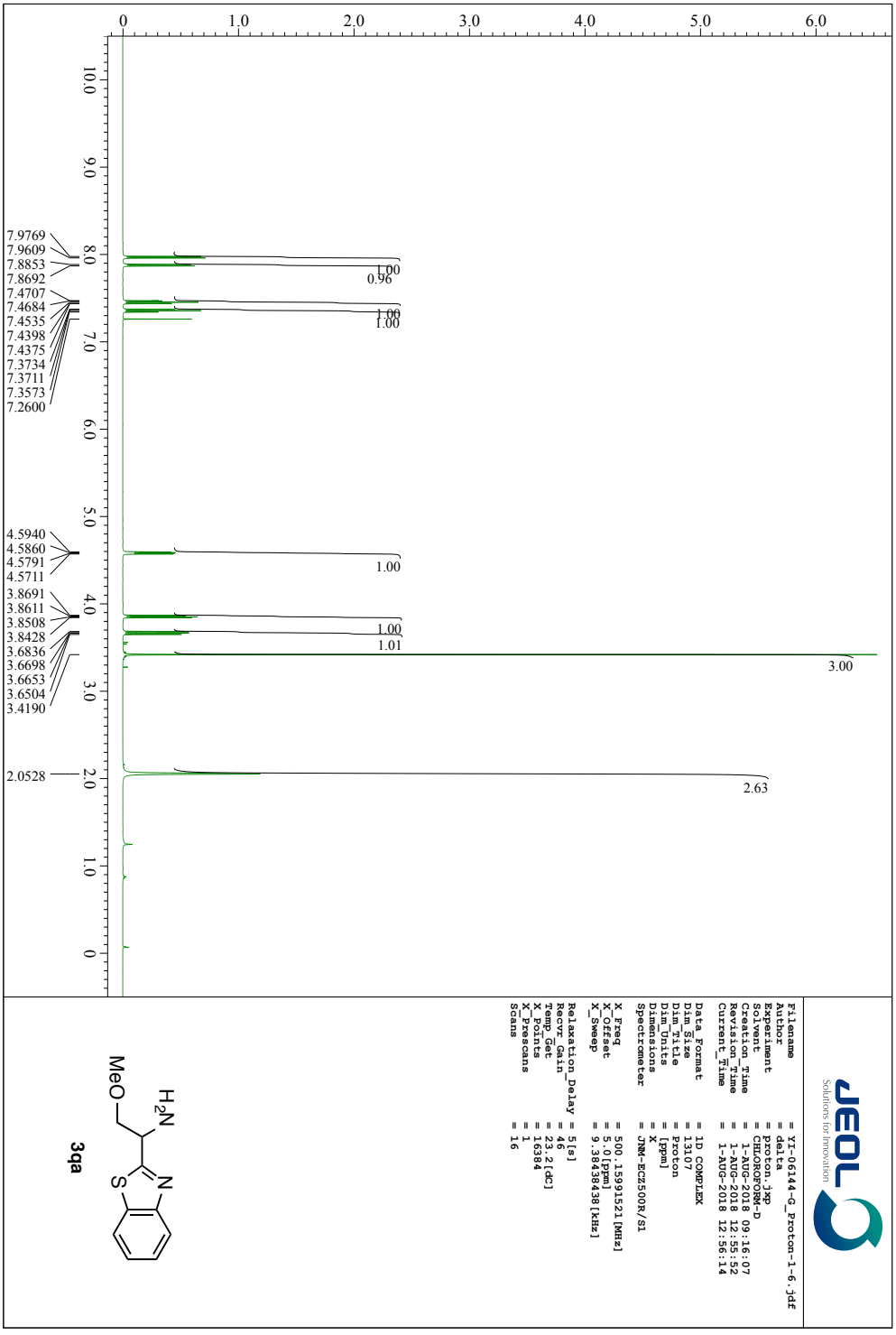

JEOL
Solutions for Innovation
Filename = YI-04023-13C-3.jdf
Author = deita
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 3-FEB-2017 16:14:16
Revision_Time = 27-APR-2017 22:40:29
Current_Time = 27-APR-2017 22:41:41
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 3[s]
Receiver_Gain = 50
Temp_Set = 22.3[dC]
X_Points = 32768
X_Prescans = 4
Scans = 672
Ph–NH
Pr
S
N
3na
178.7334
153.8152
146.7985
135.0689
129.4441
125.9982
124.8943
122.8786
122.0147
118.6648
113.5295
77.4096
77.1600
76.9104
57.4059
39.6387
19.4430
13.9622

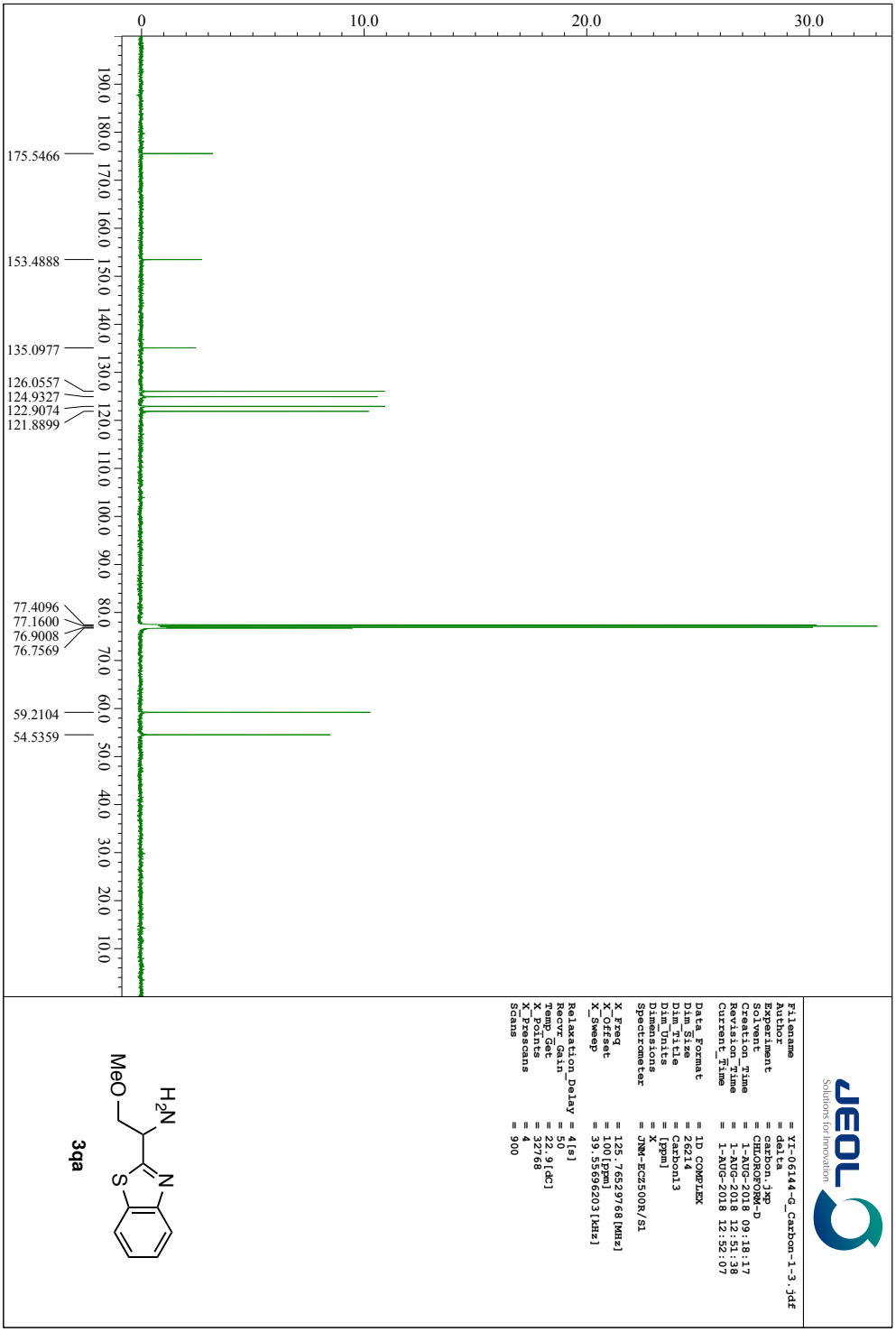

7.9769
7.9609
7.8853
7.8692
7.4581
7.4558
7.4421
7.4398
7.3722
7.3699
7.3562
7.3413
7.2600
4.3821
4.3707
4.3661
4.3547
1.9853
1.9784
1.9578
1.8593
1.8352
1.8078
1.7986
1.7883
1.4911
1.4653
0.9855
0.9706
0.9557
0.98
0.97
1.08
1.00
1.00
1.02
3.76
2.03
3.07
Filename = YI-04061-1H-4.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 7-APR-2017 15:34:44
Revision_Time = 1-MAY-2017 16:38:34
Current_Time = 1-MAY-2017 16:39:05
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.01[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 56
Temp_Get = 22.6[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
JEOL
Solutions for Innovation
3oa

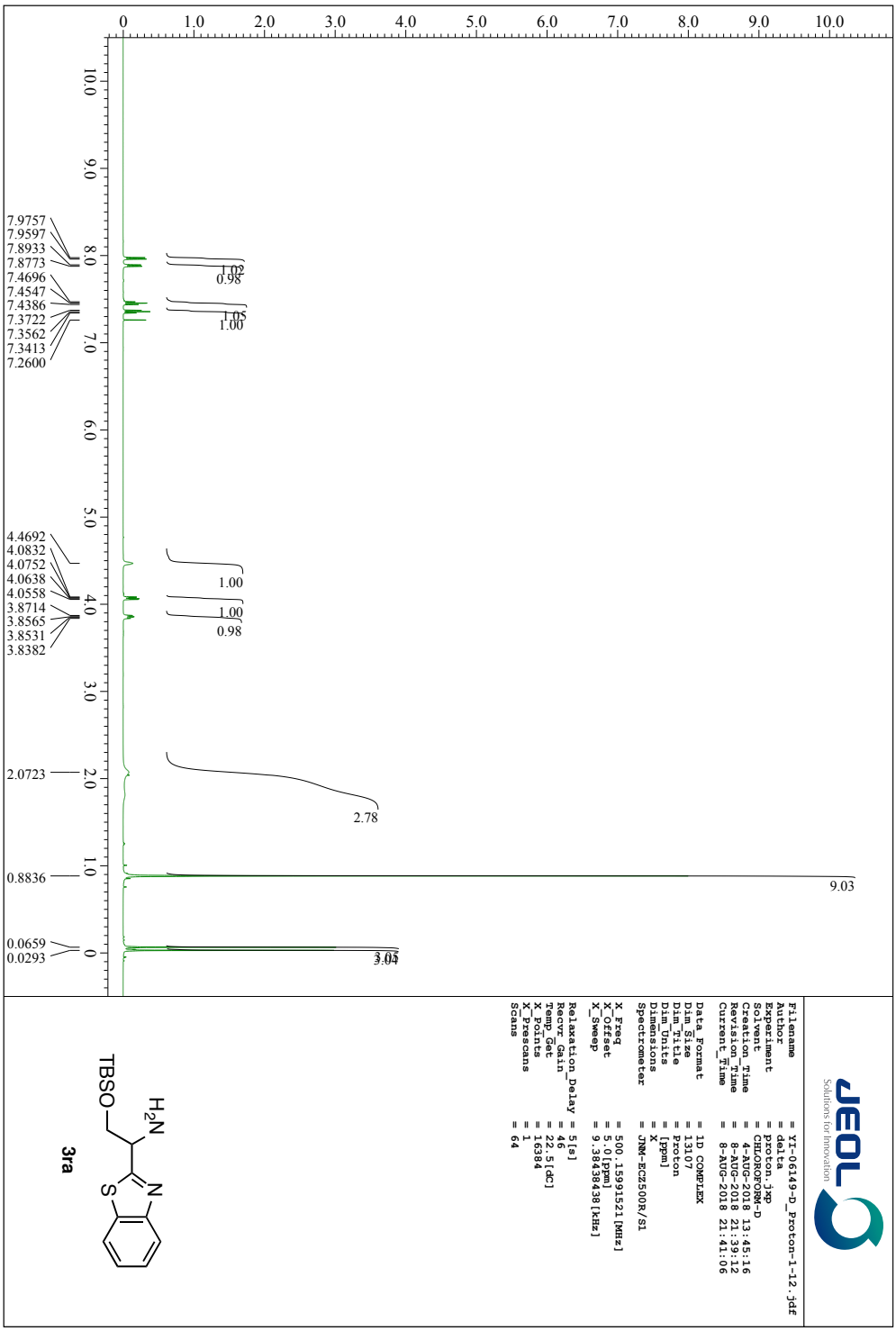

JEOL
Solutions for Innovation
Filename = YI-04061-13C-2.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 6-APR-2017 20:24:40
Revision_Time = 27-APR-2017 22:22:50
Current_Time = 27-APR-2017 22:23:15
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100[ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 50
Temp_Set = 22.7[dC]
X_Points = 32768
X_Prescans = 4
Scans = 212
179.0885
153.4792
134.9441
126.0270
124.8559
122.8690
121.9187
77.4192
77.1600
76.9104
54.7950
40.7617
19.3087
14.0102
Pr
H2N
S
N
3oa

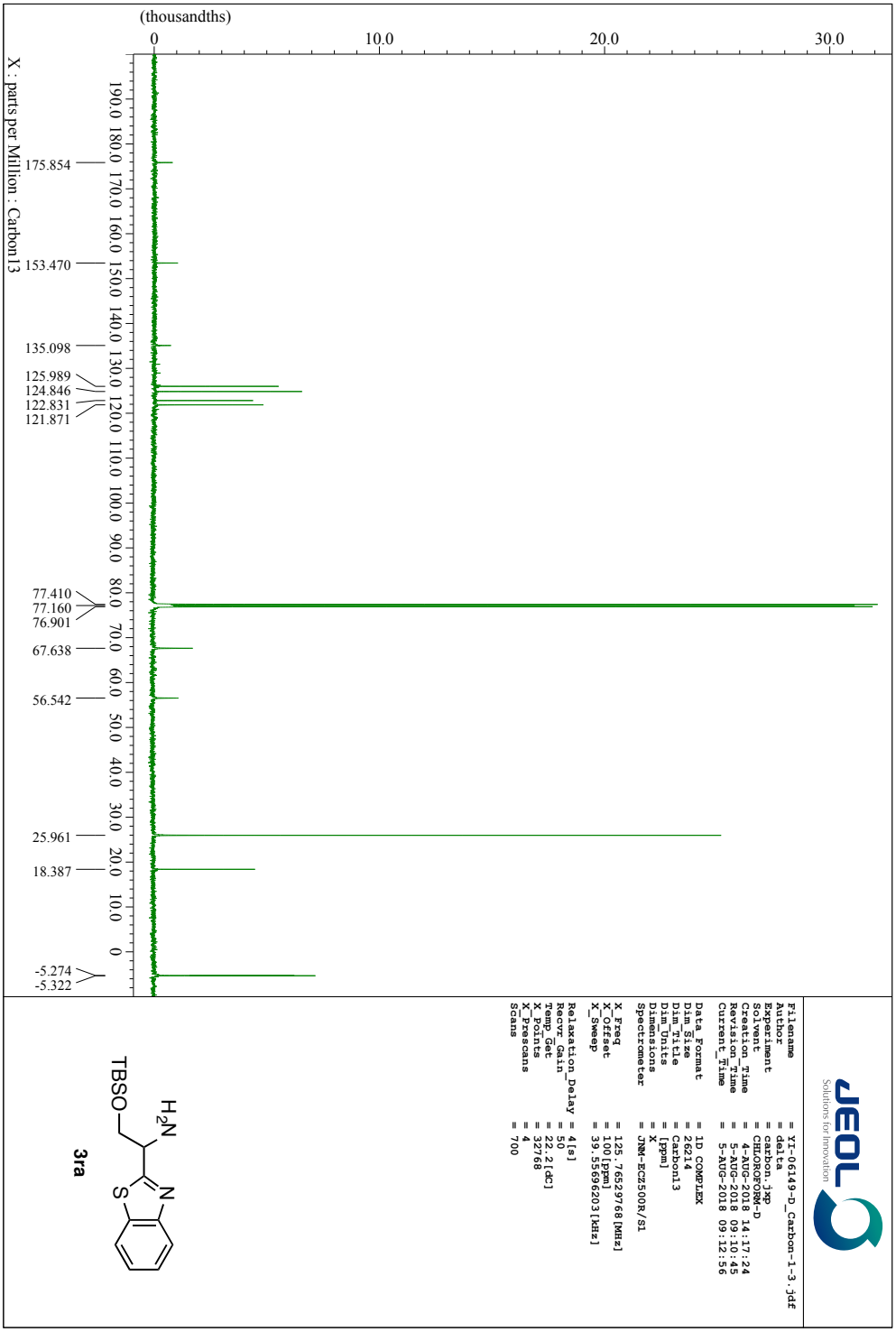

7.9815
7.9643
7.8795
7.8647
7.4650
7.4501
7.4364
7.4341
7.3665
7.3642
7.3493
7.2600
4.1806
4.1703
2.3300
2.3162
2.3036
2.2922
2.2784
2.2647
2.2509
1.7952
1.0416
1.0279
0.9752
0.9615
1.03
0.98
1.01
1.00
0.98
1.00
2.51
3.05
3.06
Filename = YI-06109-G_Proton-1-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 29-JUL-2018 17:08:12
Revision_Time = 30-JUL-2018 12:54:32
Current_Time = 30-JUL-2018 12:57:45
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 46
Temp_Get = 22.3 [dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3pa

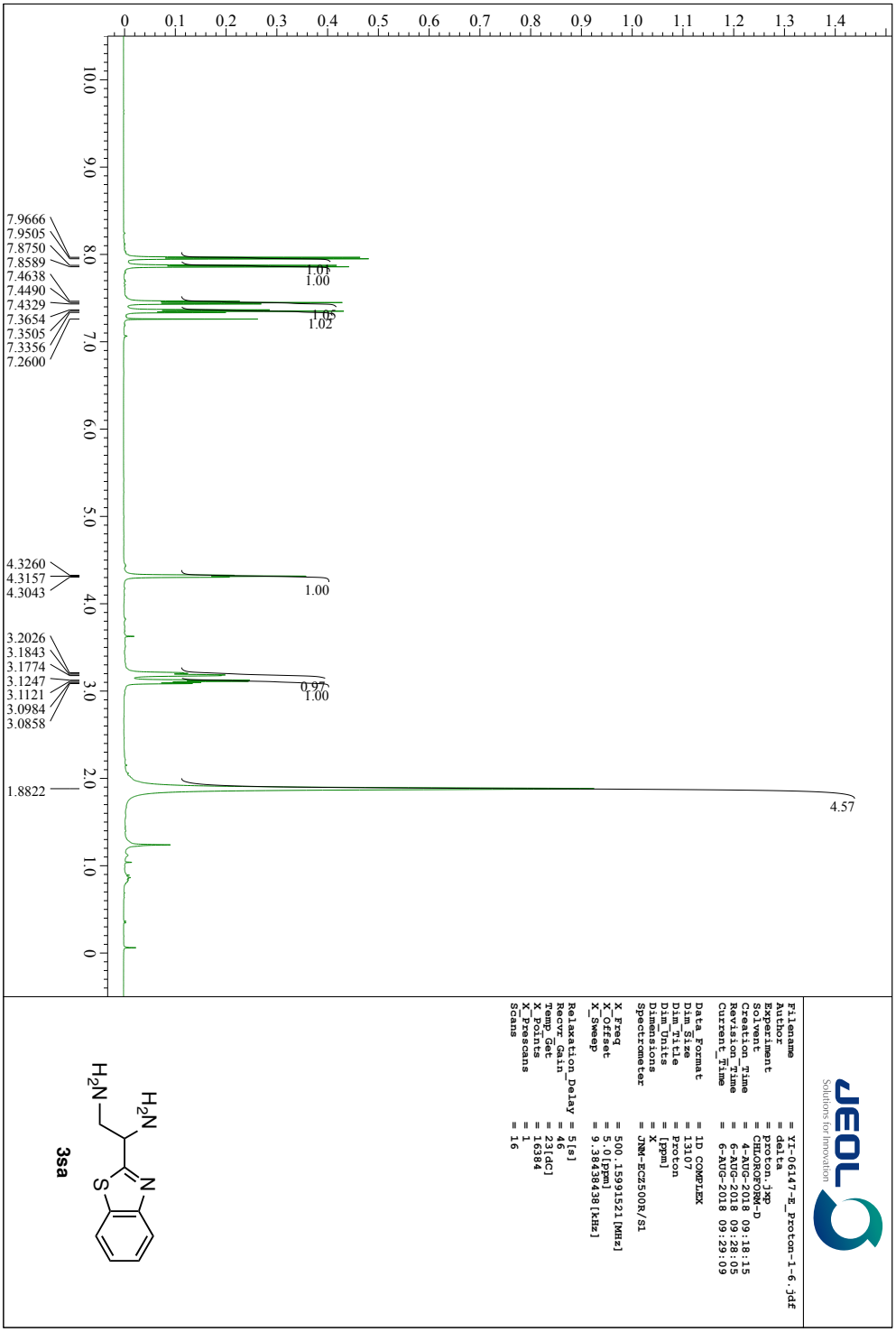

JEOL
Solutions for Innovation
Filename = YI-06109-G_Carbon-1-3.jdf
Author
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 29-JUL-2018 17:17:59
Revision_Time = 1-AUG-2018 12:47:39
Current_Time = 1-AUG-2018 12:50:18
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768[MHz]
X_Offset = 100.[PPM]
X_Sweep = 39.15896203[kHz]
Relaxation_Delay = 4[s]
Recvr_Gain = 50
Temp_Get = 22.9[dC]
X_Points = 32768
X_Prescans = 4
Scans = 1024
178.1575
153.4216
134.9729
125.9502
124.7887
122.8594
121.8227
77.4096
77.1600
76.9008
60.3431
34.8969
19.7982
17.1970
3pa

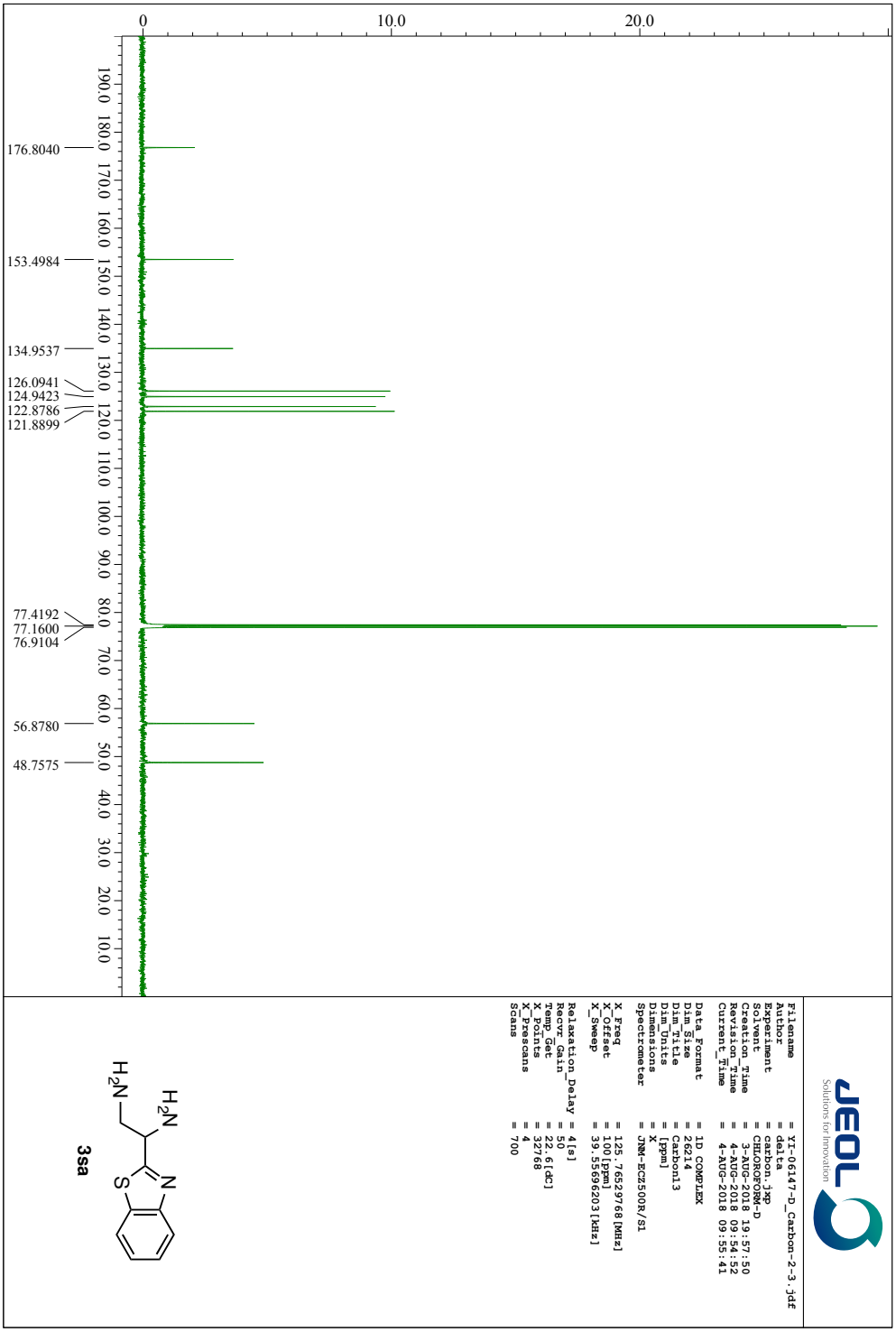

7.9769
7.9609
7.8853
7.8692
7.4707
7.4684
7.4535
7.4398
7.4375
7.3734
7.3711
7.3573
7.2600
4.5940
4.5860
4.5791
4.5711
3.8691
3.8611
3.8508
3.8428
3.6836
3.6698
3.6653
3.6504
3.4190
2.0528
1.00
0.96
1.00
1.00
1.00
1.00
1.01
3.00
2.63
Filename = YI-06144-G_Proton-1-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 1-AUG-2018 09:16:07
Revision_Time = 1-AUG-2018 12:55:52
Current_Time = 1-AUG-2018 12:56:14
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 46
Temp_Get = 25.2 [dC]
X_Points = 125304
X_Prescans = 1
Scans = 16
MeO
H2N
S
N
3qa

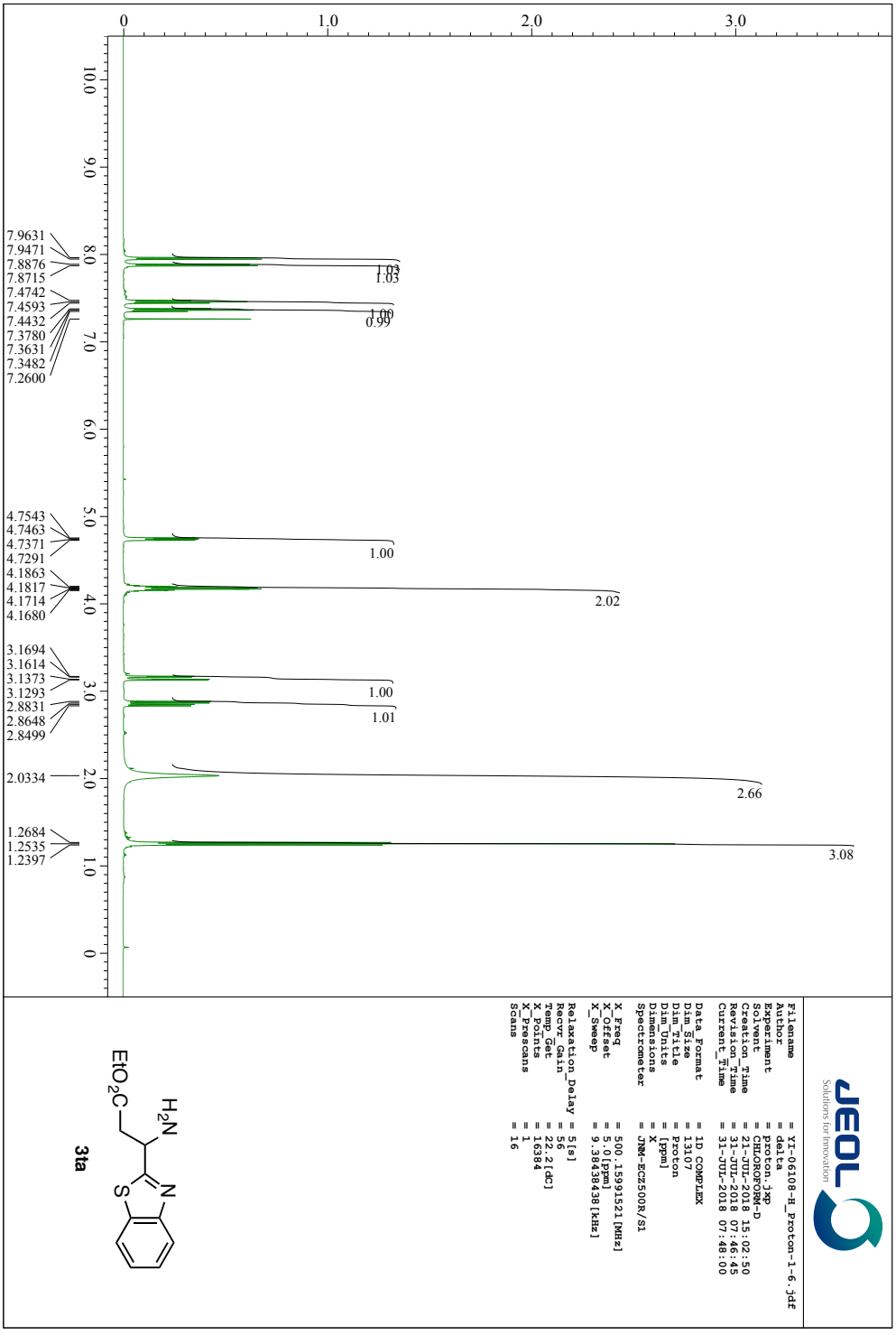

JEOL
Solutions for Innovation
Filename = YI-06144-G_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 1-AUG-2018 09:18:17
Revision_Time = 1-AUG-2018 12:51:38
Current_Time = 1-AUG-2018 12:52:07
Data_Format = 1D COMPLEX
Dim_Size = 16214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [KHz]
Relaxation_Delay = 4 [s]
Recvr_Gain = 50
Temp_Set = 22.9 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 900
175.5466
153.4888
135.0977
126.0557
124.9327
122.9074
121.8899
77.4096
77.1600
76.9008
76.7569
59.2104
54.5359
MeO
H2N
S
N
3qa

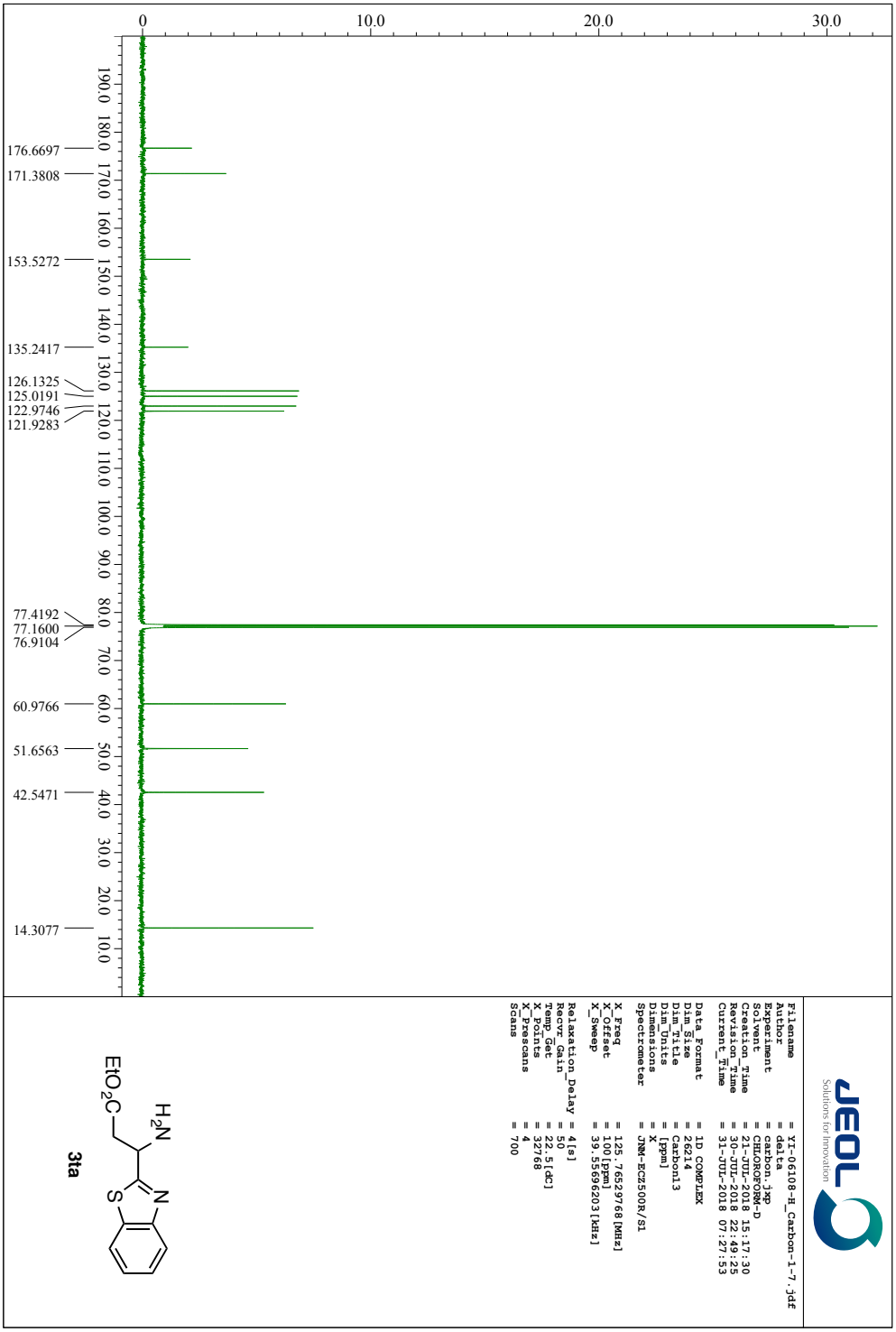

7.9757
7.9597
7.8933
7.8773
7.4696
7.4547
7.4386
7.3722
7.3562
7.3413
7.2600
4.4692
4.0832
4.0752
4.0638
4.0558
3.8714
3.8565
3.8531
3.8382
2.0723
0.8836
0.0659
0.0293
1.02
0.98
1.05
1.00
1.00
1.00
0.98
2.78
9.03
3.05
Filename = YI-06149-D_Proton-1-12.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-AUG-2018 13:45:16
Revision_Time = 8-AUG-2018 21:39:12
Current_Time = 8-AUG-2018 21:41:06
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 46
Temp_Get = 22.5[dC]
X_Points = 16384
X_Prescans = 1
Scans = 64
TBSO
H2N
N
S
3ra

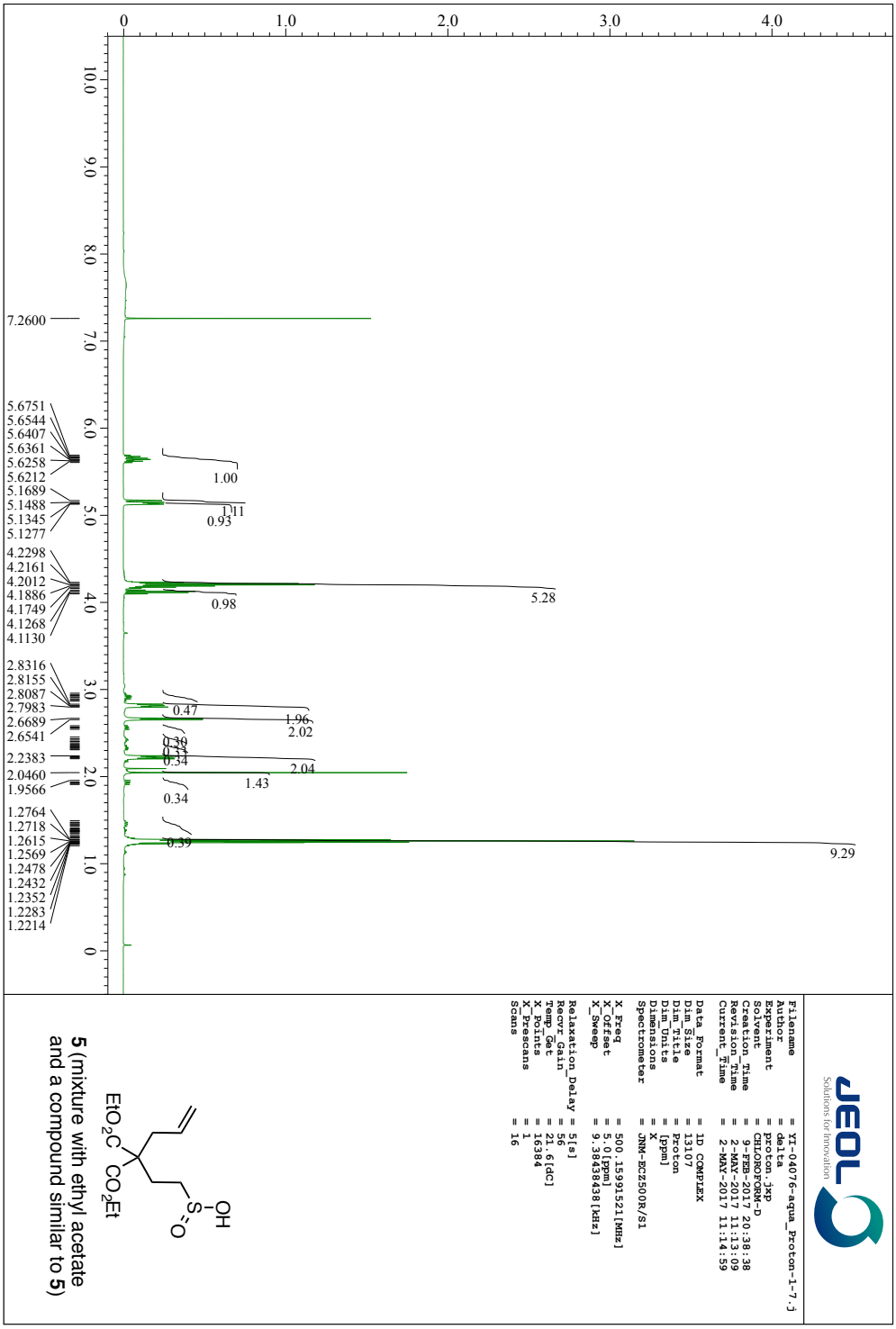

(thousandths)
0
10.0
20.0
30.0
X : parts per Million : Carbon13
175.854
153.470
135.098
125.989
124.846
122.831
121.871
77.410
77.160
76.901
67.638
56.542
25.961
18.387
-5.274
-5.322
Filename = YI-06149-D_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-AUG-2018 14:17:24
Revision_Time = 5-AUG-2018 09:10:45
Current_Time = 5-AUG-2018 09:12:56
Data_Format = 1D COMPLEX
Dim_Size = 24214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [KHz]
Relaxation_Delay = 4 [s]
Recvr_Gain = 50
Temp_Get = 22.2 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 700
TBSO
H2N
S
N
3ra


7.9666
7.9505
7.8750
7.8589
7.4638
7.4490
7.4329
7.3654
7.3505
7.3356
7.2600
4.3260
4.3157
4.3043
3.2026
3.1843
3.1774
3.1247
3.1121
3.0984
3.0858
1.8822
4.57
1.01
1.00
1.05
1.02
1.00
0.97
1.00
Filename = YI-06147-E_Proton-1-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 4-AUG-2018 09:18:15
Revision_Time = 6-AUG-2018 09:28:05
Current_Time = 6-AUG-2018 09:29:09
Data_Format = 1D COMPLEX
Dim_Size = 131072
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 46
Temp_Get = 23 [dC]
X_Points = 12304
X_Prescans = 1
Scans = 16
3sa

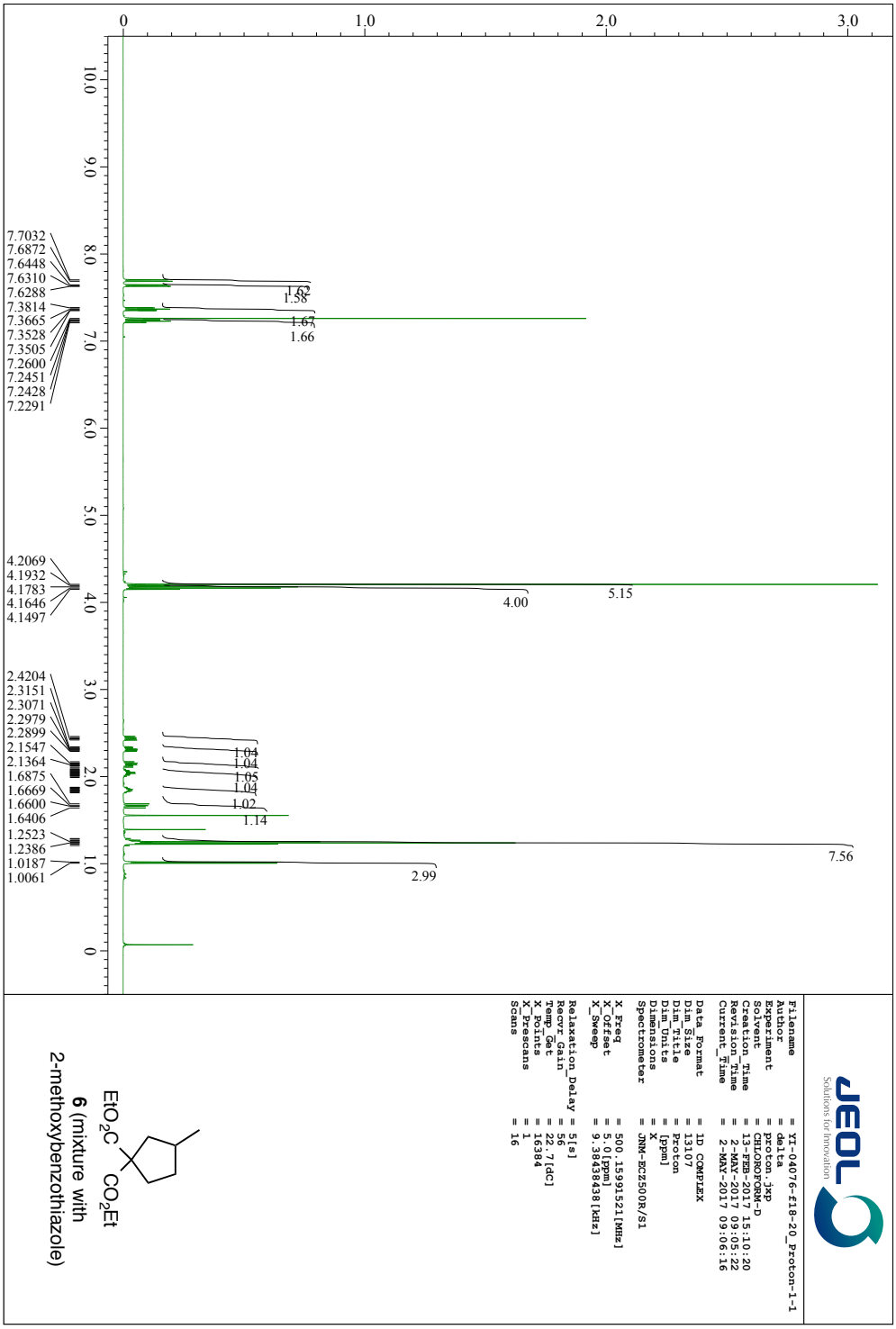

0
10.0
20.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
176.8040
153.4984
134.9537
126.0941
124.9423
122.8786
121.8899
77.4192
77.1600
76.9104
56.8780
48.7575
JEOL
Solutions for Innovation
Filename = YI-06147-D_Carbon-2-3.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 3-AUG-2018 19:57:50
Revision_Time = 4-AUG-2018 09:54:52
Current_Time = 4-AUG-2018 09:55:41
Data_Format = 1D COMPLEX
Dim_Size = 24214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [KHz]
Relaxation_Delay = 4 [s]
Recvr_Gain = 50
Temp_Get = 22.6 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 700
H2N
H2N
S
N
3sa

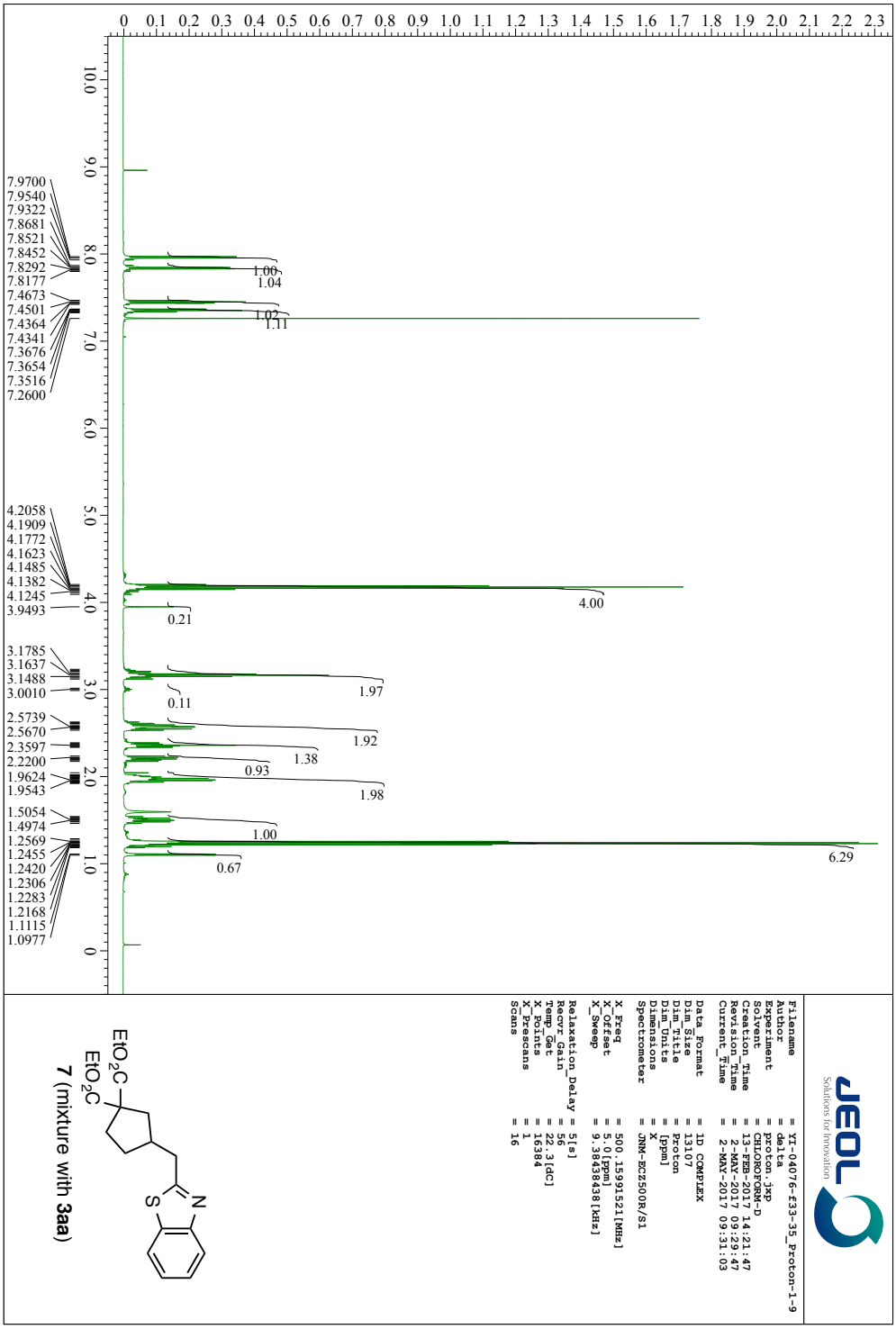

Filename = YI-06108-H_Proton-1-6.jdf
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 21-JUL-2018 15:02:50
Revision_Time = 31-JUL-2018 07:46:45
Current_Time = 31-JUL-2018 07:48:00
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521 [MHz]
X_Offset = 5.0 [ppm]
X_Sweep = 9.38438438 [kHz]
Relaxation_Delay = 5 [s]
Recvr_Gain = 56
Temp_Get = 22.2 [dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
3ta
7.9631
7.9471
7.8876
7.8715
7.4742
7.4593
7.4432
7.3780
7.3631
7.3482
7.2600
4.7543
4.7463
4.7371
4.7291
4.1863
4.1817
4.1714
4.1680
3.1694
3.1614
3.1373
3.1293
2.8831
2.8648
2.8499
2.0334
1.2684
1.2535
1.2397
1.03
1.03
1.00
0.99
1.00
2.02
1.00
1.01
2.66
3.08

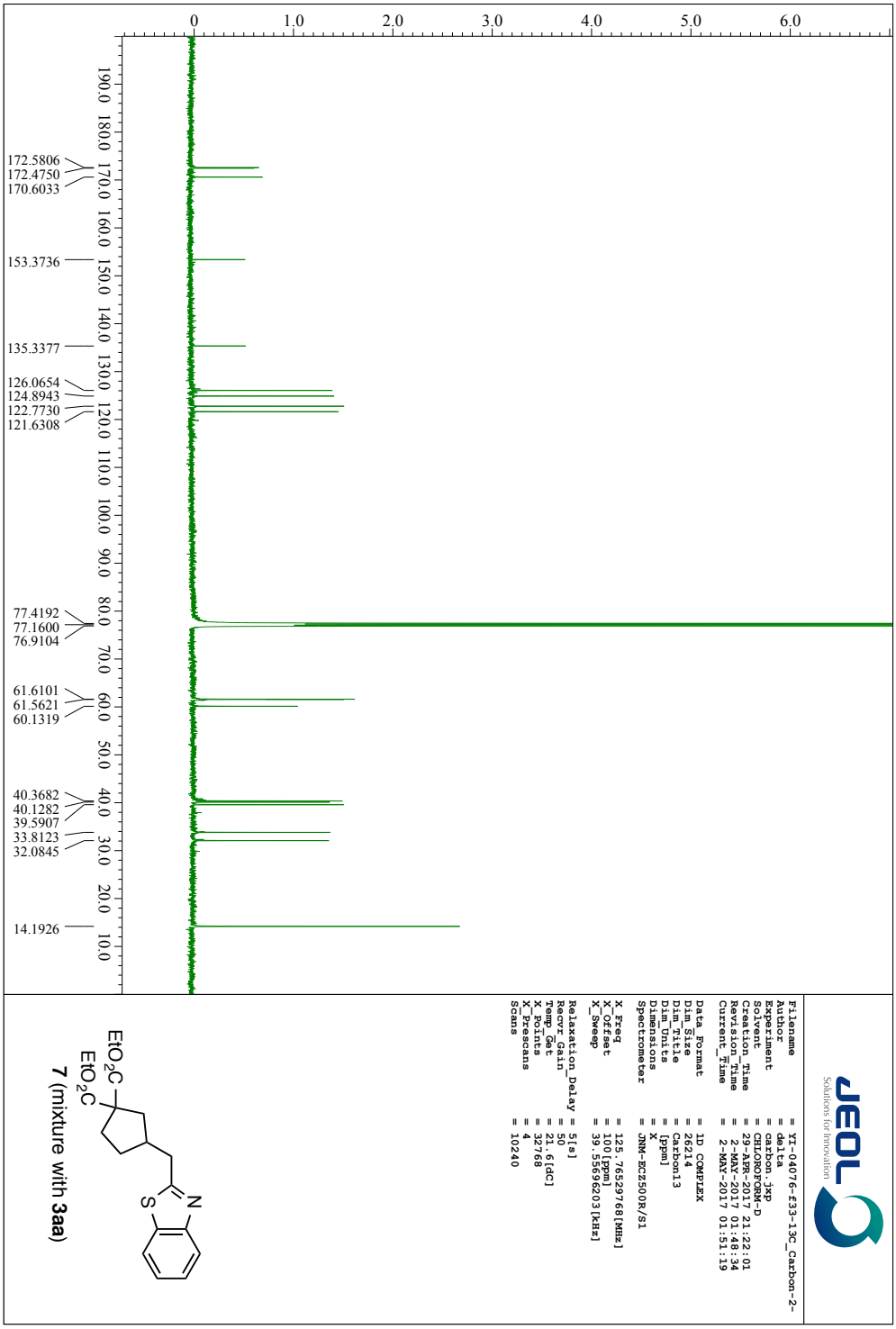

0
10.0
20.0
30.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
176.6697
171.3808
153.5272
135.2417
126.1325
125.0191
122.9746
121.9283
77.4192
77.1600
76.9104
60.9766
51.6563
42.5471
14.3077
JEOL
Solutions for Innovation
Filename = YI-06108-H_Carbon-1-7.jdf
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 21-JUL-2018 15:17:30
Revision_Time = 30-JUL-2018 22:49:25
Current_Time = 31-JUL-2018 07:27:53
Data_Format = 1D COMPLEX
Dim_Size = 16214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.76529768 [MHz]
X_Offset = 100 [ppm]
X_Sweep = 39.55696203 [kHz]
Relaxation_Delay = 4 [s]
Recvr_Gain = 50
Temp_Get = 22.5 [dC]
X_Points = 32768
X_Prescans = 4
Scans = 700
EtO2C
H2N
S
N
3ta



5 (mixture with ethyl acetate and a compound similar to **5**)


Filename = YT-04076-f18-20_Proton-1-1
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 13-FEB-2017 15:10:20
Revision_Time = 2-MAY-2017 09:05:22
Current_Time = 2-MAY-2017 09:06:16
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-EC2500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 56
Temp_Get = 22.7[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
EtO2C CO2Et
6 (mixture with
2-methoxybenzothiazole)


7.9700
7.9540
7.9322
7.8681
7.8521
7.8452
7.8292
7.8177
7.4673
7.4501
7.4364
7.4341
7.3676
7.3654
7.3516
7.2600
4.2058
4.1909
4.1772
4.1623
4.1485
4.1382
4.1245
3.9493
3.1785
3.1637
3.1488
3.0010
2.5739
2.5670
2.3597
2.2200
1.9624
1.9543
1.5054
1.4974
1.2569
1.2455
1.2420
1.2306
1.2283
1.2168
1.1115
1.0977
1.00
1.04
1.02
1.11
4.00
0.21
0.11
1.97
1.92
1.38
0.93
1.98
1.00
0.67
6.29
Filename = YT-04076-f33-35_Proton-1-9
Author = delta
Experiment = proton.jxp
Solvent = CHLOROFORM-D
Creation_Time = 13-FEB-2017 14:21:47
Revision_Time = 2-MAY-2017 09:29:47
Current_Time = 2-MAY-2017 09:31:03
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Sweep = 9.38438438[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 56
Temp_Get = 22.3[dC]
X_Points = 16384
X_Prescans = 1
Scans = 16
JEOL
Solutions for Innovation
EtO2C
EtO2C
7 (mixture with 3aa)
S
N


JEOL
Solutions for Innovation
Filename = YT-04076-f33-13C_Carbon-2-
Author = delta
Experiment = carbon.jxp
Solvent = CHLOROFORM-D
Creation_Time = 29-APR-2017 21:22:01
Revision_Time = 2-MAY-2017 01:48:34
Current_Time = 2-MAY-2017 01:51:19
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
X_Freq = 125.765297681[MHz]
X_Offset = 100[ppm]
X_Sweep = 39.556962031[kHz]
Relaxation_Delay = 5[s]
Receiver_Gain = 50.6[dC]
Temp_Get = 21.6[dC]
X_Points = 32768
X_Prescans = 4
Scans = 10240
172.5806
172.4750
170.6033
153.3736
135.3377
126.0654
124.8943
122.7730
121.6308
77.4192
77.1600
76.9104
61.6101
61.5621
60.1319
40.3682
40.1282
39.5907
33.8123
32.0845
14.1926
EtO2C
EtO2C
S
N
7 (mixture with 3aa)