**Supporting Information**

# Iron-Catalyzed *ortho*-Selective C−H Borylation of 2-Phenylpyridines and Their Analogs

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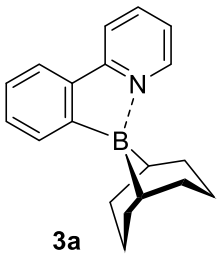
## Contents

**General.**

All reactions were carried out in a grove box or using standard Schlenk techniques under an argon atmosphere. All reagents were purchased from commercial sources and used without further purification unless otherwise noted. Column chromatography was performed with silica gel (10-100 nm). NMR spectra were recorded on JEOL-ECX 500 (500 MHz for $^{1}$H NMR and 125 MHz for $^{13}$C NMR) and JEOL-ECX 400 (400 MHz for $^{1}$H NMR, 100 MHz for $^{13}$C NMR, 368 MHz for $^{19}$F NMR, and 125 MHz for $^{11}$B NMR) spectrometers. Proton and carbon chemical shifts are reported relative to tetramethylsilane (TMS, δ 0.00 ($^{1}$H, $^{13}$C)) or the residual solvent ($CHCl_3$ (δ 7.26), $CH_2Cl_2$ (δ 5.23)) used as an internal reference. Fluorine and boron chemical shifts are reported relative to hexafluorobenzene (δ -164.9) and $BF_3{\cdot}OEt_2$ (δ 0.00) as an external reference, respectively. HRMS were measured on a JEOL JMS-700 spectrometer.

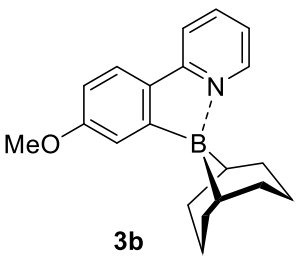
**Typical Procedure for *ortho*-C-H Bolylation of 2-[2-(9-borabicyclo[3.3.1]-9-nonyl)phenyl]pyridine (3a).**



**3a**

2-Phenylpyridine (**1a**, 71.4 μL, 0.500 mmol), 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol), $FeBr_3$ (7.4 mg, 0.025 mmol, 5 mol %), and 1,2-dichloroethane (1.0 mL) were added to a screw-capped test tube (10 mL) under argon atmosphere. The red solution was stirred at 90 °C for 24 h. The reddish yellow precipitate was observed during the reaction. After cooled to room temperature, the reddish dispersion was added to $CH_2Cl_2$ (ca. 10 mL) and stirred for a few minutes. The solution was filtered through a short pad of silica gel to give a yellowish solution. Then, the solvent was evaporated under reduced pressure. Column chromatography on silica gel ($CH_2Cl_2$/hexane = 1/4) afforded **3a** in 93% yield as a white powder (128 mg, 0.470 mmol). The structure of **3a** was identified by comparing these spectroscopic data with those of the reported data.[1]

**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-4-methoxyphenyl]pyridine (3b).**

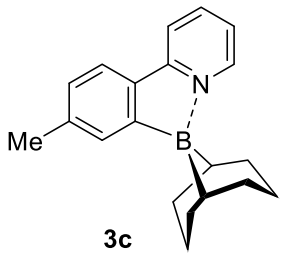


**3b**

The typical procedure of **3a** was applied to (4-methoxylphenyl)pyridine (**1b**, 93.0 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 74% yield as a white crystal (113 mg, 0.370 mmol). The structure of **3b** was identified by comparing these

spectroscopic data with those of the reported data.[1]

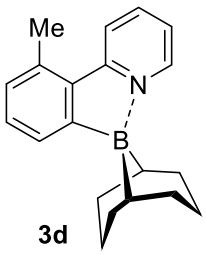
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-4-methylphenyl]pyridine (3c).**



**3c**

The typical procedure of **3a** was applied to (4-methylphenyl)pyridine (**1c**, 85.0 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 51% yield as a white crystal (73.7 mg, 0.255 mmol). The structure of **3c** was identified by comparing these spectroscopic data with those of the reported data.[1]

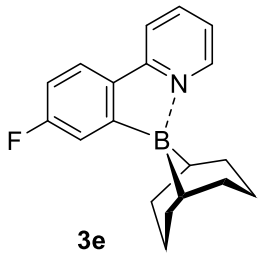
**2-[6-(9-Borabicyclo[3.3.1]-9-nonyl)-2-methylphenyl]pyridine (3d).**



**3d**

The typical procedure of **3a** was applied to 2-(2-methylphenyl)-pyridine (**1d**, 85.0 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 58% yield as a white crystal (83.9 mg, 0.290 mmol). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 9.16 (d, $J$ = 6.0 Hz, 1H), 8.26 (d, $J$ = 8.8 Hz, 1H), 7.95-8.11 (m, 2H), 7.31-7.36 (m, 2H), 7.12 (d, $J$ = 7.2 Hz, 1H), 2.75 (s, 3H), 2.44-2.62 (m, 2H), 2.05-2.32 (m, 4H), 1.76-1.99 (m, 6H), 0.57 (s, 2H); $^{13}$C{$^{1}$H} NMR (100 MHz, $CDCl_3$) δ 158.5, 145.1, 138.6, 134.41, 134.40, 130.5, 128.8, 128.6, 121.8, 119.3, 33.1, 29.7, 24.6, 23.5, 23.4; HRMS (EI$^+$) Calcd for $C_{20}H_{24}BN$ ($M^+$) 289.2002, Found 289.2001; mp. 220-222 °C.

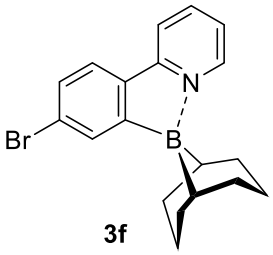
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-4-fluorophenyl]pyridine (3e).**



**3e**

The typical procedure of **3a** was applied to (4-fluorophenyl)pyridine (**1e**, 87.0 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 71% yield as a white crystal (104 mg, 0.360 mmol). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 9.04 (d, $J$ = 5.6 Hz, 1H), 7.96 (d, $J$ = 4.0 Hz, 2H), 7.86 (dd, $J$ = 8.8, 5.6 Hz, 1H), 7.67 (dd, $J$ = 8.8, 2.0 Hz, 1H), 7.31 (dt, $J$ = 6.0, 4.8 Hz, 1H), 7.00 (td, $J$ = 8.8, 2.0 Hz, 1H), 2.42-2.48 (m, 2H), 2.04-2.42 (m, 4H), 1.78-2.09 (m, 6H), 0.67 (s, 2H); $^{13}$C{$^{1}$H} NMR (100 MHz, $CDCl_3$) δ 163.9 (d, $J_{FC}$ = 251 Hz), 157.1, 145.0, 139.0, 131.8, 123.3 (d, $J_{CF}$ = 9.1), 119.8, 119.0 (d, $J_{CF}$ = 19.8 Hz), 117.7, 112.8 (d, $J_{CF}$ = 24.8 Hz), 32.8, 29.5, 24.5, 23.5; HRMS (EI$^+$) Calcd for $C_{19}H_{21}BFN$ ($M^+$) 293.1751, Found 293.1759; mp. 204-206 °C.

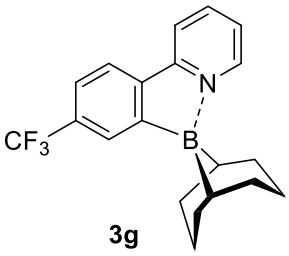
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-4-bromophenyl]pyridine (3f).**



**3f**

The typical procedure of **3a** was applied to (4-bromophenyl)pyridine (**1f**, 117 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 50% yield as a white crystal (88.3 mg, 0.250 mmol). $^{1}$H NMR (400 MHz, DMSO-$d_6$ + $CD_2Cl_2$) δ 9.07 (d, $J$ = 6.0 Hz, 1H), 8.40 (d, $J$ = 8.0 Hz, 1H), 8.23 (t, $J$ = 8.0 Hz, 1H), 8.07 (d, $J$ = 8.0 Hz, 1H), 7.98 (t, $J$ = 2.0 Hz, 1H), 7.61 (td, $J$ = 6.0, 2.0 Hz, 1H), 7.49 (dd, $J$ = 8.0, 2.0 Hz, 1H), 2.03-2.29 (m, 6H), 1.70-1.90 (m, 6H), 0.50 (s, 2H); $^{13}$C{$^{1}$H} NMR (100 MHz, DMSO-$d_6$ + $CD_2Cl_2$) δ 155.7, 144.8, 140.3, 134.8, 134.2, 129.4, 127.8, 123.9, 121.8, 118.7, 32.3, 28.7, 23.9, 22.9; HRMS (EI$^+$) Calcd for $C_{19}H_{21}BBrN$ ($M^+$) 353.0950, Found 353.0948; mp. 307-312 °C.

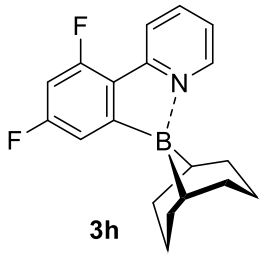
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-4-trifluoromethylphenyl]pyridine (3g).**



**3g**

The typical procedure of **3a** was applied to (4-trifluoromethylphenyl)pyridine (**1g**, 112 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 56% yield as a white crystal (96.1 mg, 0.280 mmol). The structure of **3g** was identified by comparing these spectroscopic data with those of the reported data.[1]

**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-4,6-difluorophenyl]pyridine (3h).**

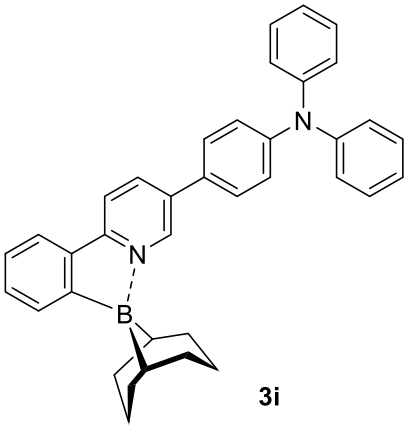


**3h**

The typical procedure of **3a** was applied to (4,6-difluorophenyl)pyridine (**1h**, 96.0 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 63% yield as a white crystal (98.0 mg, 0.315 mmol). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 9.07 (d, $J$ = 6.5 Hz, 1H), 8.27 (d, $J$ = 8.0 Hz, 1H), 8.00 (td, $J$ = 8.0, 1.0 Hz, 1H), 7.49 (dd, $J$ = 9.5, 2.5 Hz, 1H), 7.35 (td, $J$ = 6.5, 1.0 Hz 1H), 6.73 (tt, $J$ = 9.0, 2.0 Hz, 1H), 2.29-2.43 (m, 2H), 2.02-2.28 (m, 4H), 1.74-1.92 (m, 6H), 0.59 (s, 2H); $^{13}$C{$^{1}$H} NMR (125 MHz, $CDCl_3$) δ 163.6 (dd, $J_{FC}$ = 252, 9.5 Hz), 160.4 (dd, $J_{FC}$ = 257, 12.5 Hz), 154.2 (d, $J_{FC}$ = 6.0 Hz), 144.9, 139.4, 121.9 (d, $J_{FC}$ = 13.8 Hz), 120.0, 119.3 (dd, $J_{FC}$ = 6.0, 1.8 Hz), 114.7 (dd, $J_{FC}$ = 19.1, 3.0 Hz), 100.8 (dd, $J_{FC}$ =

27.4, 24.5 Hz), 32.7, 29.3, 24.3, 23.3; HRMS ($EI^+$) Calcd for $C_{19}H_{20}BF_2N$ ($M^+$) 331.1657, Found 331.1656; mp. 181-182 °C.

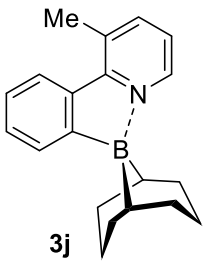
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)phenyl]-5-diphenylaminopyridine (3i).**



**3i**

The typical procedure of **3a** was applied to 2-phenyl-5-diphenylamino-pyridine (**1i**, 200 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 81% yield as a yellowish white crystal (210 mg, 0.405 mmol). $^1H$ NMR (400 MHz, $CD_2Cl_2$) δ 9.26 (s, 1H), 8.18 (dd, *J* = 8.2, 1.8 Hz, 1H), 8.08 (d, *J* = 8.8 Hz, 1H), 8.01 (d, *J* = 7.2 Hz, 1H), 7.94 (d, *J* = 7.2 Hz, 1H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.40 (t, *J* = 7.2 Hz, 1H), 7.30-7.34 (m, 5H), 7.15-7.18 (m, 6H), 7.10 (t, *J* = 7.2 Hz, 2H), 1.77-2.48 (m, 12H), 0.61 (s, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CD_2Cl_2$) δ 156.0, 149.0, 147.7, 143.0, 137.2, 136.2, 133.9, 132.9, 129.83, 129.76, 129.2, 127.9, 125.5, 125.4, 124.1, 123.6, 121.8, 118.2, 33.3, 30.0, 25.0, 23.8; HRMS ($EI^+$) Calcd for $C_{37}H_{35}BN_2$ ($M^+$) 518.2893, Found 518.2890; mp. 268-269 °C.

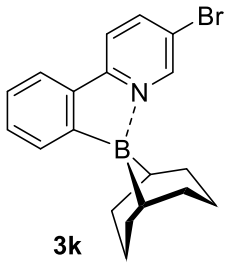
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-phenyl]-3-methylpyridine (3j).**



**3j**

The typical procedure of **3a** was applied to 3-methyl-2-phenylpyridine (**1j**, 85.0 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 51% yield as a white crystal (73.7 mg, 0.255 mmol). $^1H$ NMR (400 MHz, $CDCl_3$) δ 9.05 (d, *J* = 6.0 Hz, 1H), 8.15 (t, *J* = 8.4 Hz, 2H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.6, 0.8 Hz, 1H), 7.36 (td, *J* = 7.6, 1.6 Hz, 1H), 7.24-7.27 (m, 1H), 2.87 (s, 3H), 2.48-2.57 (m, 2H), 2.08-2.33 (m, 4H), 1.78-1.93 (m, 6H), 0.59 (s, 2H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 155.9, 142.7, 141.6, 137.7, 132.6, 131.6, 128.2, 125.7, 125.0, 119.3, 33.2, 29.6, 24.8, 23.4, 22.5; HRMS ($EI^+$) Calcd for $C_{20}H_{24}BN$ ($M^+$) 289.2002, Found 289.2000; mp. 193-195 °C.

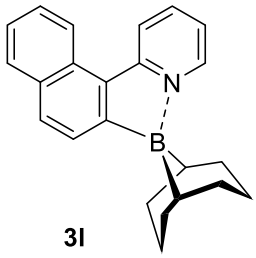
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)phenyl]-5-bromopyridine (3k).**



**3k**

The typical procedure of **3a** was applied to 5-bromo-2-phenylpyridine (**1k**, 117 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 61% yield as a white crystal (108 mg, 0.305 mmol). $^{1}$H NMR (400 MHz, DMSO-$d_6$ + $CD_2Cl_2$) δ 9.03 (d, $J$ = 2.0 Hz, 1H), 8.44 (dd, $J$ = 8.7, 2.0 Hz, 1H), 8.36 (d, $J$ = 8.7 Hz, 1H), 8.11 (d, $J$ = 7.7 Hz, 1H), 7.88 (d, $J$ = 7.7 Hz, 1H), 7.39 (t, $J$ = 6.8 Hz, 1H), 7.31 (t, $J$ = 6.8 Hz, 1H), 2.33-2.36 (m, 2H), 2.01-2.14 (m, 4H), 1.70-1.91 (m, 6H), 0.51 (s, 2H); $^{13}$C{$^{1}$H} NMR (100 MHz DMSO-$d_6$ + $CD_2Cl_2$) δ 144.9, 142.5, 131.8, 129.1, 125.1, 122.2, 119.7, 32.2, 28.8, 23.9, 22.8 [Solubility of **3k** was too low to observe all carbon signals.]; HRMS (EI$^+$) Calcd for $C_{19}H_{21}BBrN$ ($M^+$) 353.0950, Found 353.0951; mp. 270-286 °C.

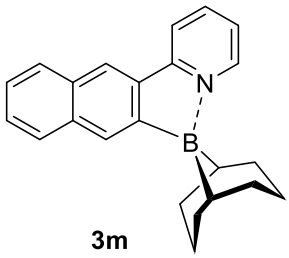
**2-[1-(9-Borabicyclo[3.3.1]-9-nonyl)-naphthyl]pyridine (3l).**



**3l**

The typical procedure of **3a** was applied to 2-(1-naphthyl)pyridine (**1l**, 103 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 79% yield as a white crystal (129 mg, 0.395 mmol). The structure of **3l** was identified by comparing these spectroscopic data with those of the reported data.[1]

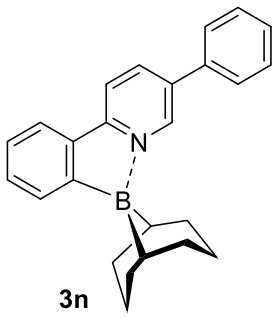
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-naphthyl]pyridine (3m).**



**3m**

The typical procedure of **3a** was applied to 2-(2-naphthyl)pyridine (**3m**, 103 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 85% yield as a white crystal (138 mg, 0.425 mmol). The structure of **3m** was identified by comparing these spectroscopic data with those of the reported data.[1]

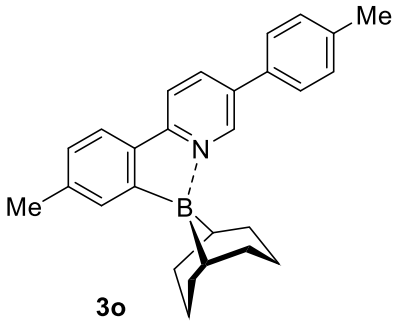
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-phenyl]-5-phenylpyridine (3n).**



**3n**

The typical procedure of **3a** was applied to 2,5-diphenylpyridine (**3n**, 116 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 81% yield as a white crystal (142 mg, 0.405 mmol). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 9.31 (s, 1H), 8.16 (dd, *J* =7.6, 2.0 Hz, 1H), 8.08 (s, 1H), 8.06 (d, *J* = 2.8 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 2H), 7.50 (d, *J* = 6.8 Hz, 1H), 7.45 (t, *J* = 6.8 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 2.40-2.56 (m, 2H), 2.08-2.30 (m, 4H), 1.81-1.98 (m, 6H), 0.69 (s, 2H); $^{13}$C{$^{1}$H} NMR (100 MHz, $CDCl_3$) δ 156.5, 143.3, 137.3, 136.6, 135.7, 133.8, 132.8, 129.7, 129.2, 128.9, 127.0, 125.3, 121.7, 117.8, 33.1, 29.8, 24.8, 24.3, 23.5; HRMS (EI$^+$) Calcd for $C_{25}H_{26}BN$ ($M^+$) 351.2158, Found 351.2154; mp. 198-200 °C.

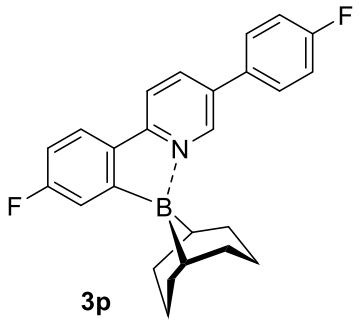
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-4-methylphenyl]-5-(4-methylphenyl)pyridine (3o).**



**3o**

The typical procedure of **3a** was applied to 2,5-di(4-methylphenyl)pyridine (**3o**, 130 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 77% yield as a white crystal (146 mg, 0.385 mmol). $^{1}$H NMR (400 MHz, $CD_2Cl_2$) δ 9.23 (d, *J* = 1.2 Hz, 1H), 8.17 (dd, *J* = 8.0, 1.8 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.82 (s, 1H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 7.6 Hz, 2H), 7.16 (dd, *J* = 8.0, 1.2 Hz, 1H), 2.43-2.51 (m, 2H), 2.47 (s, 3H), 2.43 (s, 3H), 2.06-2.34 (m, 4H), 1.77-2.00 (m, 6H), 0.59 (s, 2H); $^{13}$C{$^{1}$H} NMR (100 MHz, $CD_2Cl_2$) δ 156.5, 143.3, 139.5, 139.2, 137.6, 134.0, 133.8, 133.70, 133.68, 130.5, 127.0, 126.6, 121.8, 117.9, 33.3, 30.0, 25.0, 23.8, 22.4, 21.3; HRMS (EI$^+$) Calcd for $C_{27}H_{30}BN$ ($M^+$) 379.2471, Found 379.2471; mp. 242-246 °C.

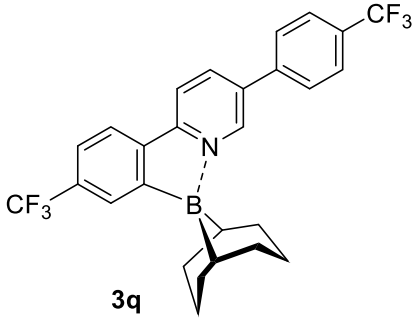
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-4-fluorophenyl]-5-(4-fluorophenyl)pyridine (3p).**



**3p**

The typical procedure of **3a** was applied to 2,5-di(4-fluorophenyl)pyridine (**3p**, 133 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 83% yield as a white crystal (161 mg, 0.415 mmol). $^{1}$H NMR (400 MHz, $CD_2Cl_2$) δ 9.21 (d, $J$ = 1.8 Hz, 1H), 8.17 (dd, $J$ = 8.2, 1.8 Hz, 1H), 8.07 (d, $J$ = 8.4 Hz, 1H), 7.93 (dd, $J$ = 8.2, 5.2 Hz, 1H), 7.67 (dd, $J$ = 10.4, 2.4 Hz, 1H), 7.62 (dd, $J$ = 9.6, 5.2 Hz, 2H), 7.24 (t, $J$ = 12.2 Hz, 2H), 7.03 (td, $J$ = 8.4, 2.4 Hz, 1H), 2.05-2.43 (m, 6H), 1.78-2.01 (m, 6H), 0.61 (s, 2H); $^{13}$C{$^{1}$H} NMR (100 MHz, $CD_2Cl_2$) δ 174.4, 165.1 ($J_{FC}$ = 44.0 Hz), 162.6 ($J_{FC}$ = 43.0 Hz), 155.8, 143.4, 138.0, 133.0 ($J_{FC}$ = 3.8 Hz), 132.1, 129.2 ($J_{FC}$ = 8.7 Hz), 123.8 ($J_{FC}$ = 8.6 Hz), 119.1 ($J_{FC}$ = 20.2 Hz), 118.1, 116.9 ($J_{FC}$ = 22.1 Hz), 112.0 ($J_{FC}$ = 24 Hz), 33.1, 29.8, 24.7, 23.6; HRMS (EI$^+$) Calcd for $C_{25}H_{24}BF_2N$ ($M^+$) 387.1970, Found 387.1970; mp. 228-229 °C.

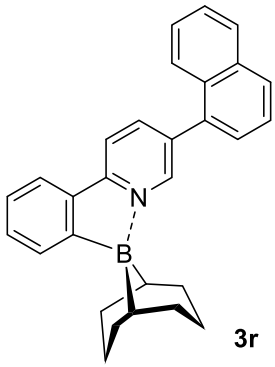
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-4-trifluoromethylphenyl]-5-(4-trifluoromethylphenyl)pyridine (3q).**



**3q**

The typical procedure of **3a** was applied to 2,5-bis(4-trifluoromethylphenyl)pyridine (**1q**, 184 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 86% yield as a white crystal (210 mg, 0.430 mmol). $^{1}$H NMR (400 MHz, $CD_2Cl_2$) δ 9.26 (s, 1H), 8.23 (d, $J$ = 7.2 Hz, 1H), 8.13 (d, $J$ = 8.8 Hz, 1H), 8.02 (d, $J$ = 8.4 Hz, 1H), 7.86 (s, 1H), 7.69 (d, $J$ = 8.4 Hz, 2H), 7.43 (d, $J$ = 8.0 Hz, 2H), 7.23 (d, $J$ = 8.0 Hz, 1H), 1.66-2.52 (m, 12H), 0.67 (s, 2H); $^{13}$C{$^{1}$H} NMR (100 MHz, $CD_2Cl_2$) δ 155.4, 149.8 ($J_{FC}$ = 13.0 Hz), 143.3, 137.8, 135.2, 134.1, 132.9, 128.7, 124.5, 123.0, 122.0, 119.3 ($J_{FC}$ = 20.0 Hz), 118.3, 117.8, 32.8, 29.5, 24.3, 23.2 [Solubility of **3q** was too low to observe all carbon signals.]; HRMS (EI$^+$) Calcd for $C_{27}H_{24}BF_6N$ ($M^+$) 487.1906, Found 487.1903; mp. 208-212 °C.

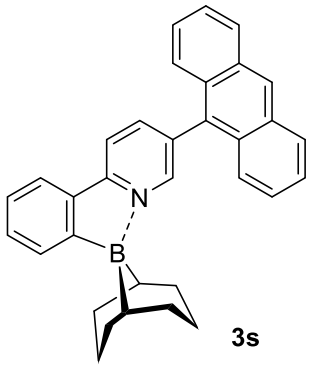
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-phenyl]-5-(1-naphthyl)pyridine (3r).**



3r

The typical procedure of **3a** was applied to 5-(1-naphthyl)-2-phenylpyridine (**1r**, 141 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 81% yield as a white crystal (163 mg, 0.405 mmol). $^{1}$H NMR (500 MHz, $CDCl_3$) δ 9.10 (s 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 8.03 (dd, *J* = 8.0, 1.7 Hz, 1H), 8.01 (d, *J* = 7.5 Hz, 1H), 7.91 (d, *J* = 7.5 Hz, 2H),7.84 (d, *J* = 7.5 Hz, 1H), 7.81 (d, *J* = 8 Hz 1H), 7.41-7.60 (m, 4H), 7.38 (t, *J* = 7.0 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 1H), 2.37-2.44 (m, 2H), 1.97-2.14 (m, 4H), 1.62-1.81 (m, 6H), 0.63 (s, 2H); $^{13}$C{$^{1}$H} NMR (125 MHz, $CDCl_3$) δ 156.8, 145.6, 140.5, 135.7, 135.0, 134.1, 133.3, 132.9, 131.4, 129.4, 129.3, 128.9, 127.8, 127.2, 126.6, 125.7, 125.3, 124.8, 121.7, 117.4, 33.1, 29.7, 24.7, 23.4; HRMS ($EI^+$) Calcd for $C_{29}H_{28}BN$ ($M^+$) 401.2315, Found 401.2312; mp. 244-249 °C.

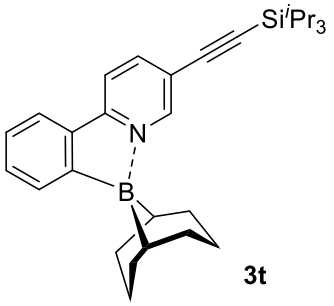
**2-[1-(9-Borabicyclo[3.3.1]-9-nonyl)-phenyl]-5-anthrylpyridine (3s).**



3s

The typical procedure of **3a** was applied to 5-(9-anthryl)-2-phenylpyridine (**1s**, 166 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 72% yield as a white crystal (163 mg, 0.360 mmol). $^{1}$H NMR (400 MHz, $CDCl_3$) δ 9.15 (s, 1H), 8.64 (s, 1H), 8.27 (d, *J* = 8.7 Hz, 1H), 7.85-8.14 (m, 5H), 7.70 (dd, *J* = 33.8, 8.7 Hz, 2H), 7.38-7.56 (m, 6H), 2.46-2.52 (m, 2H), 2.06-2.14 (m, 4H), 1.71-1.90 (m, 5H), 1.48-1.54 (m, 1H), 0.77 (s, 2H); $^{13}$C{$^{1}$H} NMR (100 MHz, $CDCl_3$) δ 166.7, 157.2, 146.8, 142.1, 135.9, 133.0, 131.5, 131.3, 130.9, 130.7, 129.5, 129.0, 128.6, 126.8, 125.7, 125.5, 125.4, 121.8, 117.7, 33.1, 29.7, 24.7, 24.5, 23.3; HRMS ($EI^+$) Calcd for $C_{33}H_{30}BN$ ($M^+$) 451.2471, Found 451.2471; mp. 310-315 °C (decomp.)

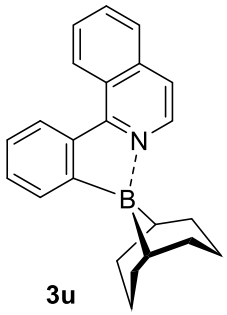
**2-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-phenyl]-5-(triisopropylsilylethynyl)pyridine (3t).**



**3t**

The typical procedure of **3a** was applied to 5-(triisopropylsilylethynyl)-2-phenylpyridine (**1t**, 168 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 83% yield as a yellow crystal (189 mg, 0.415 mmol). $^1$H NMR (400 MHz, $CDCl_3$) δ 9.14 (s, 1H), 8.04 (d, $J$ = 6.8 Hz, 1H), 7.94-7.99 (m, 2H), 7.89 (d, $J$ = 7.7 Hz, 1H), 7.43 (t, $J$ = 7.2 Hz, 1H), 7.33 (t, $J$ = 7.7 Hz, 1H), 2.40-2.43 (m, 2H), 2.08-2.21 (m, 4H), 1.82-1.88 (m, 6H), 1.14-1.20 (m, 21H), 0.61 (s, 2H); $^{13}$C{$^1$H} NMR (100 MHz, $CDCl_3$) δ 156.9, 148.2, 141.2, 135.5, 132.9, 129.6, 125.4, 122.0, 117.4, 117.1, 102.5, 96.9, 33.0, 29.6, 24.7, 23.5, 18.8, 11.4; HRMS (EI$^+$) Calcd for $C_{30}H_{42}BNSi$ ($M^+$) 455.3180, Found 455.3184; mp. 117-121 °C.

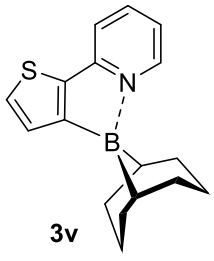
**1-[2-(9-Borabicyclo[3.3.1]-9-nonyl)-phenyl]-isoquinoline (3u).**



**3u**

The typical procedure of **3a** was applied to 1-phenylisoquinoline (**1u**, 103 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 69% yield as a white crystal (112 mg, 0.345 mmol). $^1$H NMR (400 MHz, $CDCl_3$) δ 9.18 (d, $J$ = 8.5 Hz, 1H), 9.00 (d, $J$ = 6.5 Hz, 1H), 8.64 (d, $J$ = 8.0 Hz, 1H), 8.22 (d, $J$ = 7.0 Hz, 1H), 7.96 (d, $J$ = 8.0 Hz, 1H), 7.84 (td, $J$ = 7.5, 1.0 Hz, 1H), 7.79 (td, $J$ = 8.5, 1.3 Hz, 1H), 7.64 (d, $J$ = 6.5 Hz, 1H), 7.50 (td, $J$ = 7.5, 1.0 Hz, 1H), 7.43 (td, $J$ = 7.5, 1.0 Hz, 1H), 2.51-2.60 (m, 2H), 2.11-2.43 (m, 4H), 1.69-2.04 (m, 6H), 0.66 (s, 2H); $^{13}$C{$^1$H} NMR (100 MHz, $CDCl_3$) δ 157.1, 137.6, 137.2, 136.9, 132.8, 131.8, 128.7, 128.6, 127.7, 126.9, 126.5, 126.0, 125.3, 118.4, 33.7, 30.1, 24.7, 23.6; HRMS (EI$^+$) Calcd for $C_{23}H_{24}BN$ ($M^+$) 325.2002, Found 325.2002; mp. 214-217 °C.

**2-[3-(9-Borabicyclo[3.3.1]-9-nonyl)-2-thiophenyl]-pyridine (3v).**



**3v**

The typical procedure of **3a** was applied to 2-(2-thiophenyl)pyridine (**1v**, 81.0 mg, 0.500 mmol) and 9-BBN dimer (**2**, 85.4 mg, 0.350 mmol). The desired product was obtained in 79% yield as a white crystal (111 mg, 0.395 mmol). $^1$H NMR (500 MHz, $CDCl_3$) δ 8.90 (d, $J$ = 6.0 Hz, 1H), 7.85 (t, $J$ = 8.0 Hz, 1H), 7.59 (d, $J$ = 8.0 Hz, 1H), 7.52

(d, $J$ = 4.5 Hz, 1H), 7.44 (d, $J$ = 4.5 Hz, 1H), 7.15 (t, $J$ = 6.0 Hz, 1H), 2.02-2.37 (m, 6H), 1.78-1.93 (m, 6H), 0.59 (s, 2H); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) δ 154.2, 145.1, 139.0, 134.8, 131.8, 130.3, 117.7, 117.5, 34.1, 29.3, 25.1, 23.7; HRMS ($EI^+$) Calcd for $C_{17}H_{20}BNS$ ($M^+$) 281.1410, Found 281.1411; mp. 201-210 °C (decomp.)

**Plausible Mechanism**

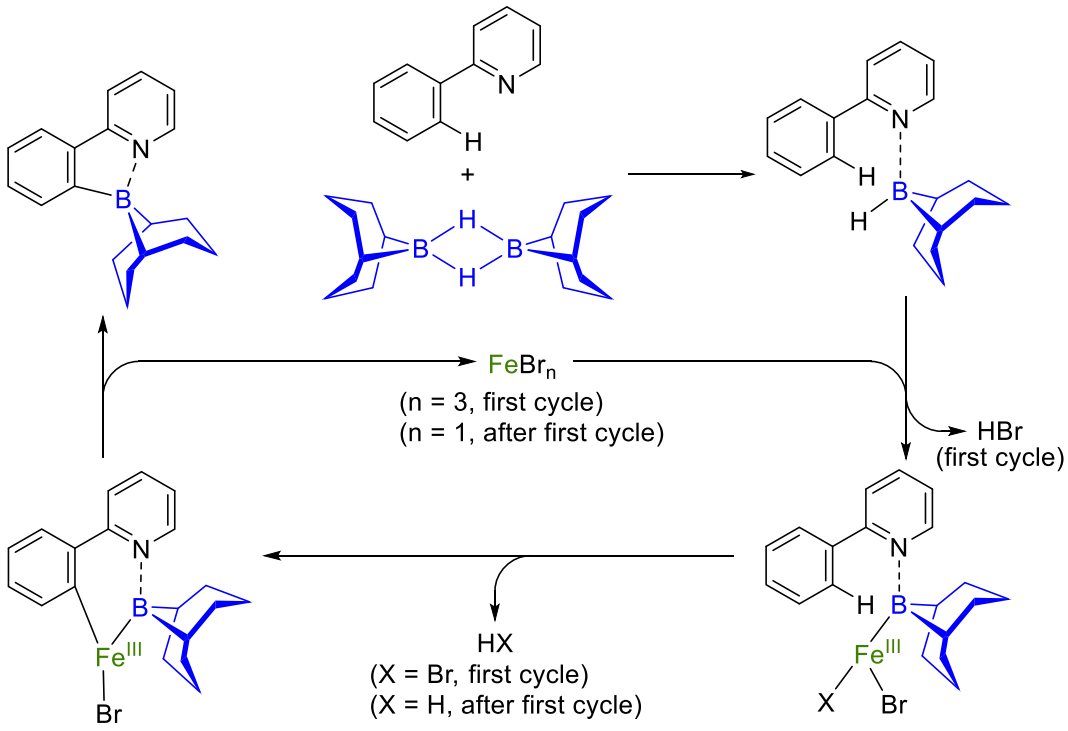



**Figure S1**. Lewis acid-base interaction mechanism.

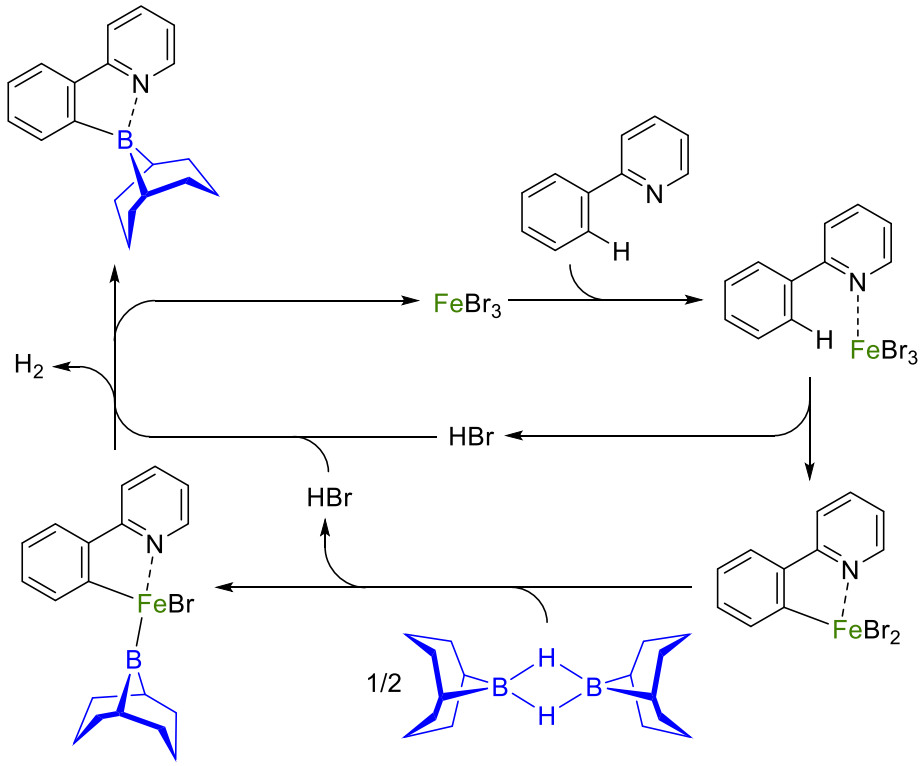



**Figure S2**. C−H activation by $FeBr_3$.

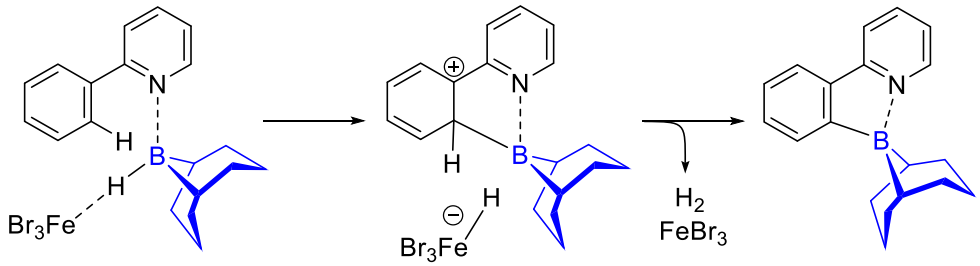



**Figure S3**. Hetero-Friedel-Crafts reaction.

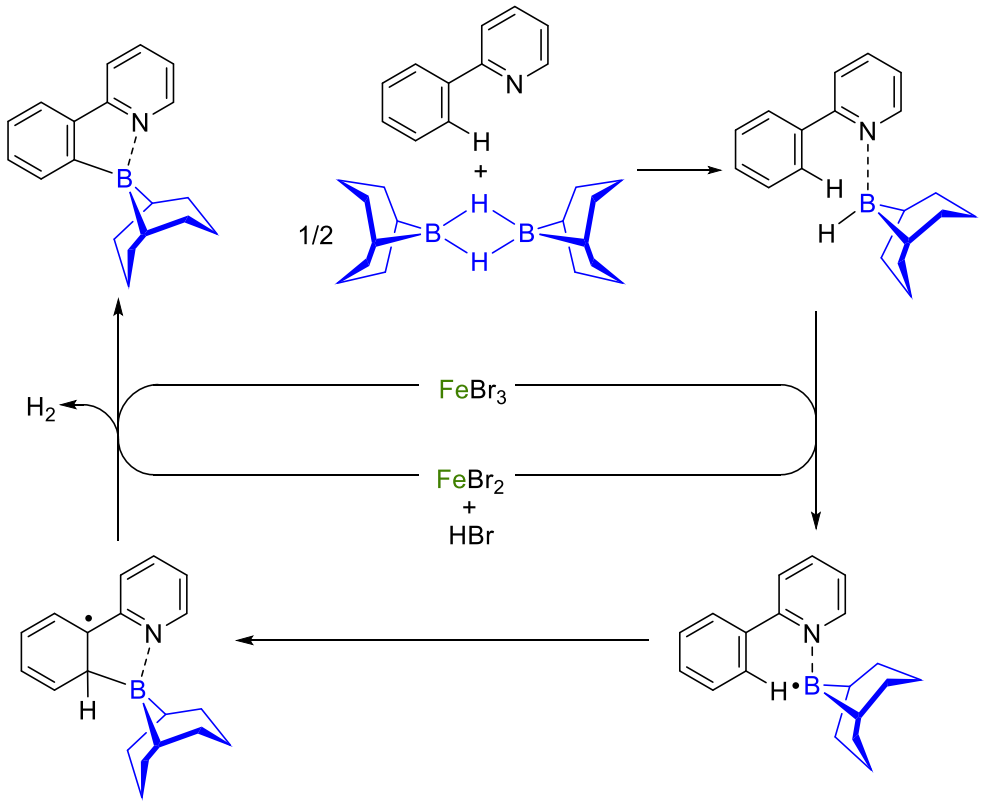



**Figure S4**. Radical process.

**DFT calculations**

All DFT calculations were carried out using Jaguar 8.0.[3] Initial structure for calculation of **3a** was employed its reported crystal stracture.[1,2] Imput structure of **1m** was obtained by conformational searches using Merk Molecular Force Field (MMFFs, Maestro 10.6.014)[4]. Frontier orbitals and potential map of **3a** in the ground state were calculated in M06-2X/aug-cc-pVTZ(-f) level.[5,6]

DFT calculation revealed natural atomic charges of each atoms of **1m** (B97D/6-31G+(d, p)).[7,8] Atomic charges of two carbons at 1- and 3-positions of the naphthalene ring were -0.196 and -0.078, respectively. The less electron density of the 3-position was consistent with the reaction site (3-position).

**Table S1.** Cartesian coordinates of the optimized structure of **3a**

| | | | |
|---|---|---|---|
| N1 | 2.83000 | 1.05230 | 9.03330 |
| C2 | 2.95400 | 0.88480 | 10.35520 |
| C3 | 2.21680 | 1.61430 | 11.26050 |
| C4 | 1.31160 | 2.55500 | 10.78450 |
| C5 | 1.17660 | 2.73170 | 9.42490 |
| C6 | 1.95100 | 1.96560 | 8.56150 |
| C7 | 1.96820 | 1.99530 | 7.10990 |
| C8 | 1.18430 | 2.81350 | 6.30370 |
| C9 | 1.32310 | 2.71610 | 4.93360 |
| C10 | 2.23800 | 1.81070 | 4.40220 |
| C11 | 3.01220 | 1.00430 | 5.22430 |
| C12 | 2.89830 | 1.07080 | 6.61490 |
| C13 | 5.22340 | 0.49150 | 7.93430 |
| C14 | 5.84840 | -0.09620 | 6.65820 |
| C15 | 5.46650 | -1.55610 | 6.35790 |
| C16 | 3.98690 | -1.90840 | 6.59020 |
| C17 | 3.36560 | -1.31190 | 7.86400 |
| C18 | 3.93100 | -1.96390 | 9.13360 |
| C19 | 5.39000 | -1.60280 | 9.47460 |
| C20 | 5.81220 | -0.14540 | 9.20140 |

| | | | |
|---|---|---|---|
| B21 | 3.61890 | 0.28880 | 7.82690 |
| H22 | 3.66180 | 0.14680 | 10.68380 |
| H23 | 2.35230 | 1.44500 | 12.31650 |
| H24 | 0.72090 | 3.14070 | 11.47420 |
| H25 | 0.48420 | 3.45240 | 9.01940 |
| H26 | 0.47880 | 3.51230 | 6.73200 |
| H27 | 0.72880 | 3.33560 | 4.27760 |
| H28 | 2.34590 | 1.73670 | 3.32880 |
| H29 | 3.70720 | 0.32290 | 4.75710 |
| H30 | 5.48430 | 1.55510 | 7.95510 |
| H31 | 5.56040 | 0.53500 | 5.81780 |
| H32 | 6.93960 | -0.02950 | 6.71760 |
| H33 | 5.72420 | -1.78200 | 5.32010 |
| H34 | 6.09010 | -2.21850 | 6.95490 |
| H35 | 3.39670 | -1.57460 | 5.73690 |
| H36 | 3.88920 | -2.99880 | 6.60850 |
| H37 | 2.29480 | -1.54020 | 7.83210 |
| H38 | 3.86240 | -3.05310 | 9.04590 |
| H39 | 3.28090 | -1.71650 | 9.97480 |
| H40 | 5.57730 | -1.83610 | 10.52600 |
| H41 | 6.04930 | -2.26490 | 8.91850 |
| H42 | 6.90550 | -0.11260 | 9.15120 |
| H43 | 5.55990 | 0.48140 | 10.05860 |

**Table S2.** Electrostatic Potential at the Nuclei (EPN) of **3a**

| Atom | EPN (au) | EPN (kcal/mol) |
|---|---|---|
| N1 | -18.309 | -11489.28 |
| C2 | -14.687 | -9216.51 |
| C3 | -14.723 | -9239.12 |
| C4 | -14.711 | -9231.08 |
| C5 | -14.723 | -9239.08 |
| C6 | -14.685 | -9214.92 |

| | | |
|---|---|---|
| C7 | -14.754 | -9258.07 |
| C8 | -14.752 | -9256.74 |
| C9 | -14.758 | -9260.93 |
| C10 | -14.758 | -9260.58 |
| C11 | -14.765 | -9265.47 |
| C12 | -14.785 | -9277.51 |
| C13 | -14.801 | -9287.71 |
| C14 | -14.785 | -9277.78 |
| C15 | -14.783 | -9276.20 |
| C16 | -14.785 | -9277.76 |
| C17 | -14.801 | -9287.82 |
| C18 | -14.778 | -9273.53 |
| C19 | -14.776 | -9271.94 |
| C20 | -14.778 | -9273.47 |
| B21 | -11.498 | -7215.14 |
| H22 | -1.070 | -671.61 |
| H23 | -1.071 | -671.94 |
| H24 | -1.068 | -670.36 |
| H25 | -1.070 | -671.54 |
| H26 | -1.098 | -688.77 |
| H27 | -1.108 | -695.34 |
| H28 | -1.112 | -697.56 |
| H29 | -1.122 | -704.37 |
| H30 | -1.166 | -731.45 |
| H31 | -1.159 | -727.06 |
| H32 | -1.157 | -726.25 |
| H33 | -1.153 | -723.52 |
| H34 | -1.156 | -725.64 |
| H35 | -1.159 | -727.13 |
| H36 | -1.157 | -726.25 |
| H37 | -1.166 | -731.53 |
| H38 | -1.152 | -722.68 |
| H39 | -1.149 | -721.03 |

| | | |
|---|---|---|
| H40 | -1.146 | -719.09 |
| H41 | -1.151 | -722.28 |
| H42 | -1.152 | -722.66 |
| H43 | -1.149 | -720.97 |

**Table S3.** Cartesian coordinates of the optimized structure of **1m**

| | | | |
|---|---|---|---|
| C1 | 0.01160 | 0.00810 | 0.00070 |
| C2 | -0.69460 | -1.1946 | -0.05010 |
| C3 | 1.50140 | 0.00490 | 0.00010 |
| N4 | 2.11430 | -1.10210 | -0.49050 |
| C5 | 3.45620 | -1.13720 | -0.50250 |
| C6 | 4.27480 | -0.09220 | -0.04000 |
| C7 | 3.64450 | 1.04800 | 0.48060 |
| C8 | 2.24550 | 1.09830 | 0.50610 |
| C9 | -0.72650 | 1.23510 | 0.05380 |
| C10 | -2.11070 | 1.23840 | 0.06440 |
| C11 | -2.84920 | 0.01810 | 0.02660 |
| C12 | -2.11670 | -1.22500 | -0.03480 |
| C13 | -4.27480 | -0.01710 | 0.04060 |
| C14 | -4.95350 | -1.22750 | -0.00180 |
| C15 | -4.23280 | -2.45510 | -0.06110 |
| C16 | -2.84550 | -2.45320 | -0.07720 |
| H17 | -0.14020 | -2.13160 | -0.1007018 |
| H18 | 3.90400 | -2.04930 | -0.90750 |
| H19 | 5.36100 | -0.17680 | -0.08200 |
| H20 | 4.23110 | 1.88190 | 0.86970 |
| H21 | 1.73790 | 1.96170 | 0.93370 |
| H22 | -0.19410 | 2.18610 | 0.05550 |
| H23 | -2.65680 | 2.18360 | 0.09150 |
| H24 | -4.82390 | 0.92580 | 0.08530 |
| H25 | -6.04440 | -1.24280 | 0.01010 |
| H26 | -4.77840 | -3.39930 | -0.09460 |

| | | | |
|---|---|---|---|
| H27 | -2.28840 | 3.39090 | -0.12370 |

**Table S4.** Atomic charges of the optimized **1m** calculated from electrostatic potential

| | |
|---|---|
| C1 | -0.19609 |
| C2 | -0.19289 |
| C3 | 0.71762 |
| N4 | -0.61447 |
| C5 | 0.36032 |
| C6 | -0.43612 |
| C7 | 0.18788 |
| C8 | -0.5435 |
| C9 | -0.07803 |
| C10 | -0.30052 |
| C11 | 0.2293 |
| C12 | 0.22764 |
| C13 | -0.28695 |
| C14 | -0.09656 |
| C15 | -0.09502 |
| C16 | -0.30308 |
| H17 | 0.1176 |
| H18 | 0.03732 |
| H19 | 0.16845 |
| H20 | 0.08356 |
| H21 | 0.18833 |
| H22 | 0.11308 |
| H23 | 0.15398 |
| H24 | 0.15228 |
| H25 | 0.12018 |
| H26 | 0.11895 |
| H27 | 0.16674 |

**Absorption and Fluorescent Spectra**

Absorption spectrum was recorded on JASCO V-650 spectrophotometer. Solution fluorescent spectrum was measured on a JASCO FP-6500. Solid-state fluorescent spectrum was measured on a Hitachi F-7000. Fluorescence quantum yield was measured on Hamamatsu Photonics Quantaurus-Tau. The solution for the spectra was prepared as a dichloromethane solusion ($CH_2Cl_2$: spectroscopic grade, 100 μM). The summery of the experimental results was listed below.

**Table S5.** Summery of spectroscopic data.

| Compound | $\lambda_{abs}$ (nm) | $\varepsilon_{max}$ ($\times 10^4$ $M^{-1}\cdot cm^{-1}$) | $\lambda_{em,\ solution}$[a] (nm) | $\lambda_{em,\ solid}$[b] (nm) | $\Phi_{F,\ solid}$ | $\tau_{solid}$ ($\tau_1$, $\tau_2$) (ns) |
|---|---|---|---|---|---|---|
| **3a** | 308 | 1.77 | 479 | 460, 575 | 0.81 | 6.07 (3.04, 6.21) |

[a] $\lambda_{ex}$ = 308 nm. [b] $\lambda_{ex}$ = 370 nm.

**References**


(1) Kuninobu, Y.; Iwanaga, T.; Omura, T.; Takai, K. *Angew. Chem. Int. Ed.* **2013**, *52*, 4431.

(2) Crystallographic structure of **3a** (CCDC 926839) has been reported in ref 1.

(3) DFT calculations were conducted by Jaguar 8.0, released by Schrödinger, LLC, New York, NY, 2016. See also: Bochevarov, A. D.; Harder, E.; Hughes, T. F.; Greenwood, J. R.; Braden, D. A.; Philipp, D. M.; Rinaldo, D.; Halls, M. D.; Zhang, J.; Friesner, R. A. *Int. J. Quantum Chem.* **2013**, *113*, 2110.

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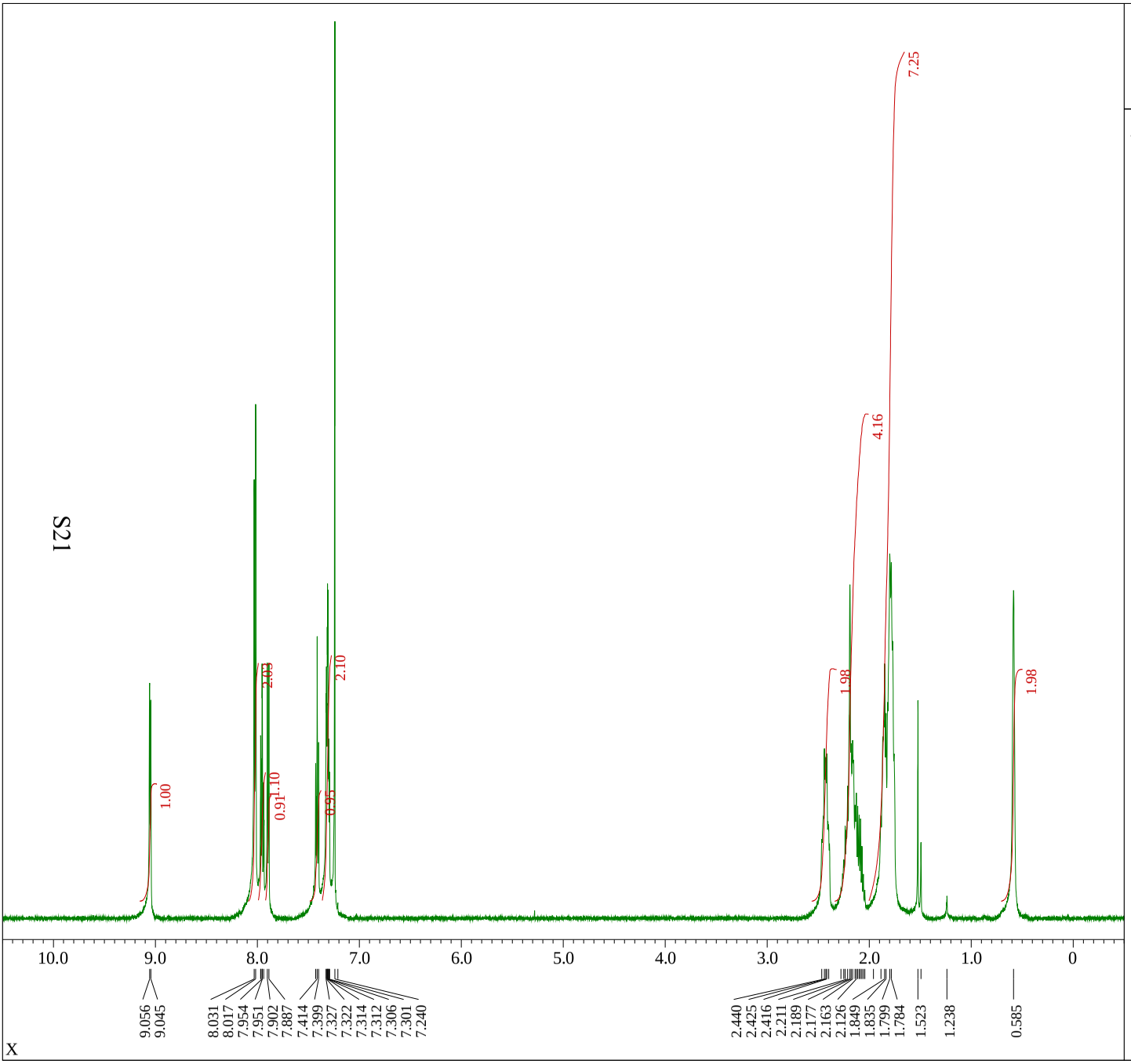


JEOL
Solutions for Innovation

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Scans             = 8

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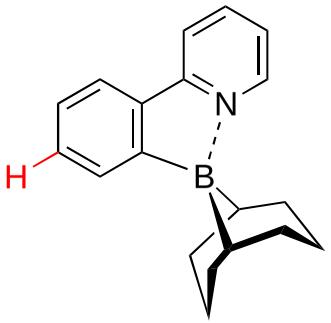
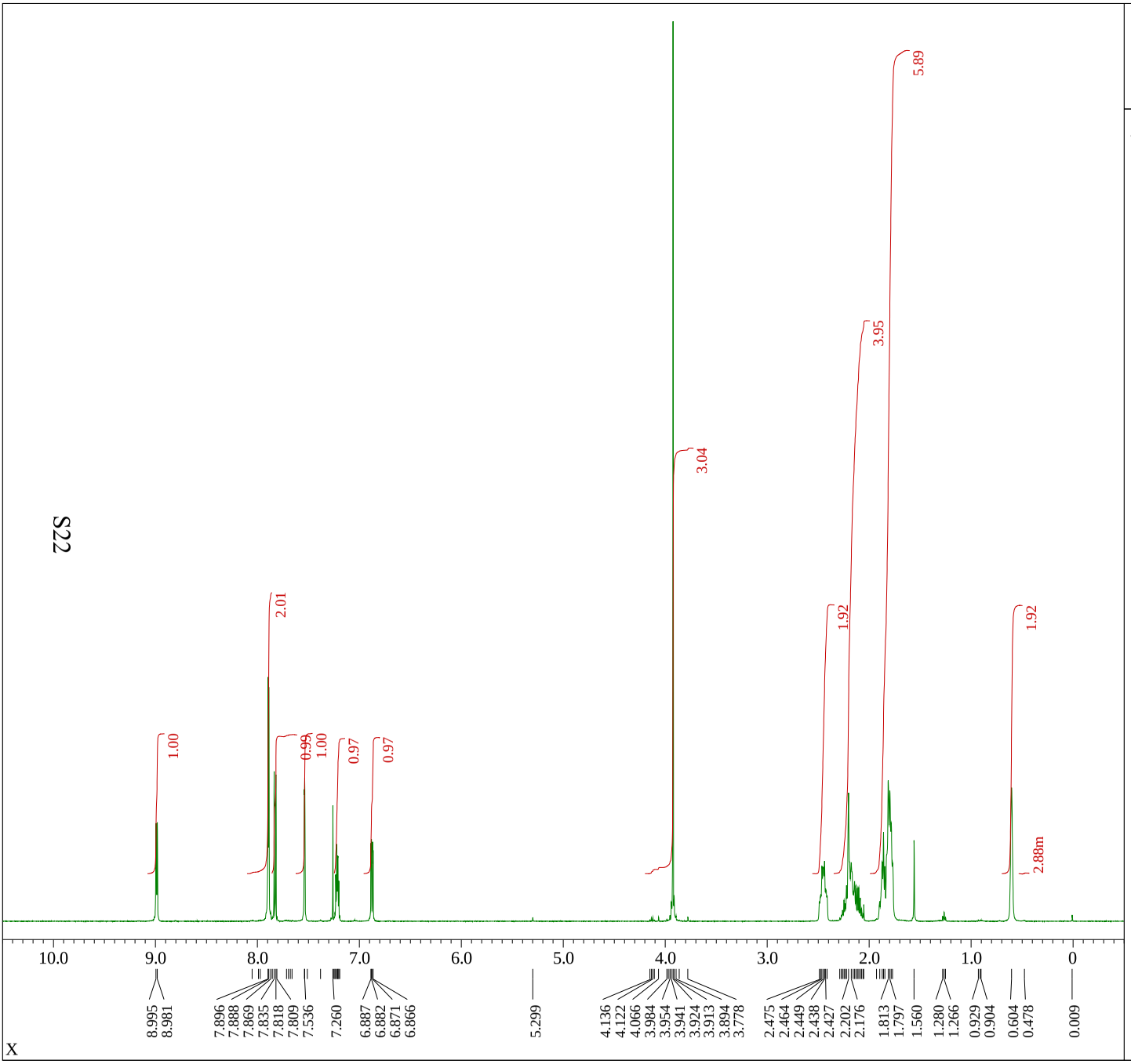



**3a**




JEOL
Solutions for Innovation

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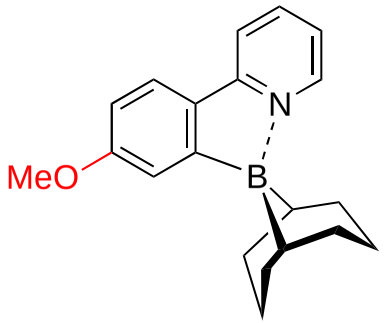


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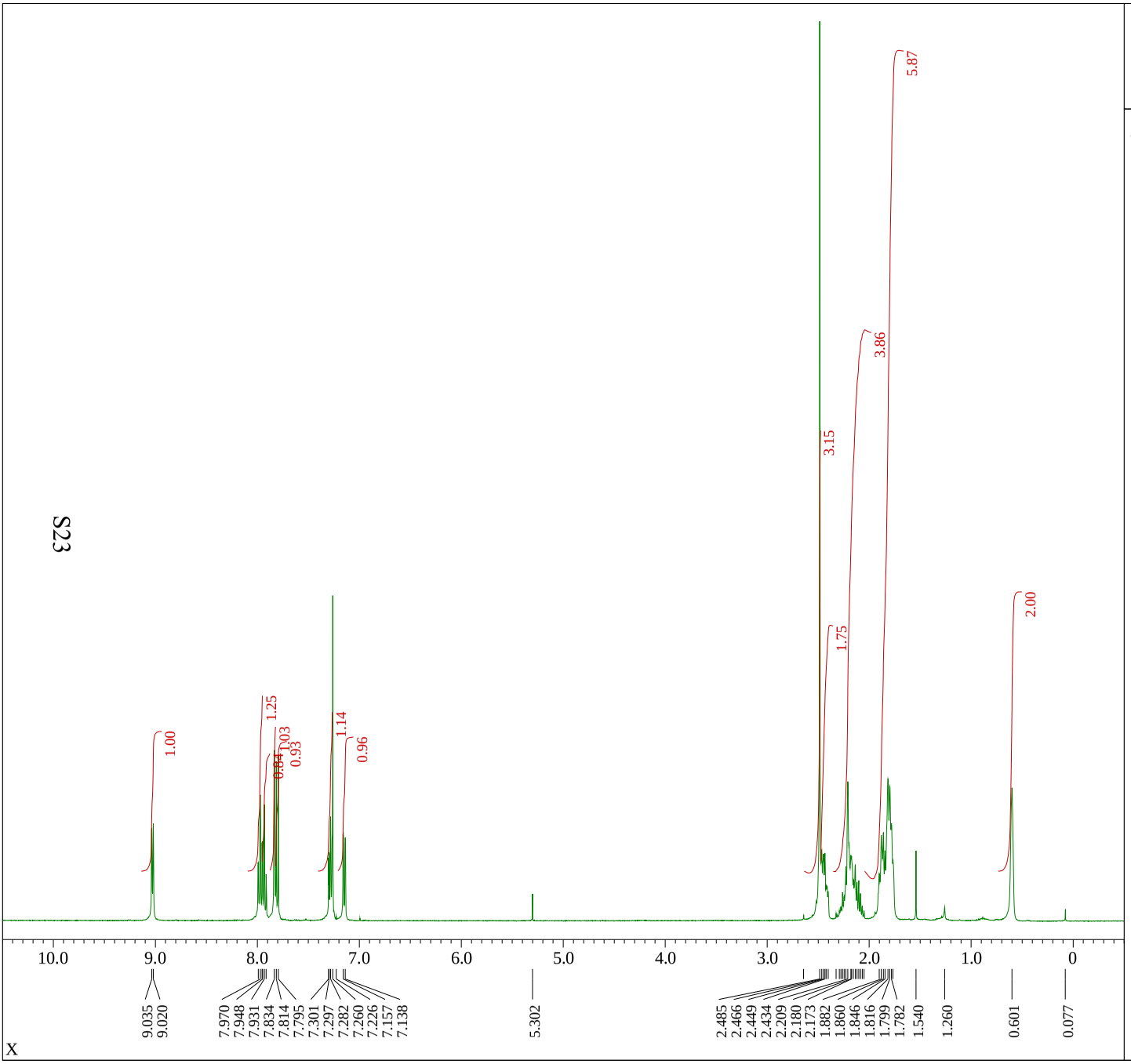


JEOL
Solutions for Innovation

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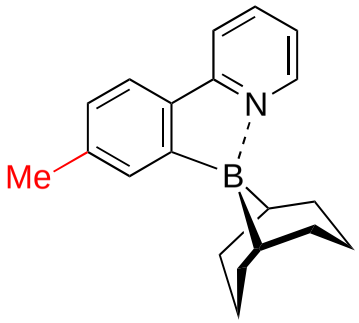


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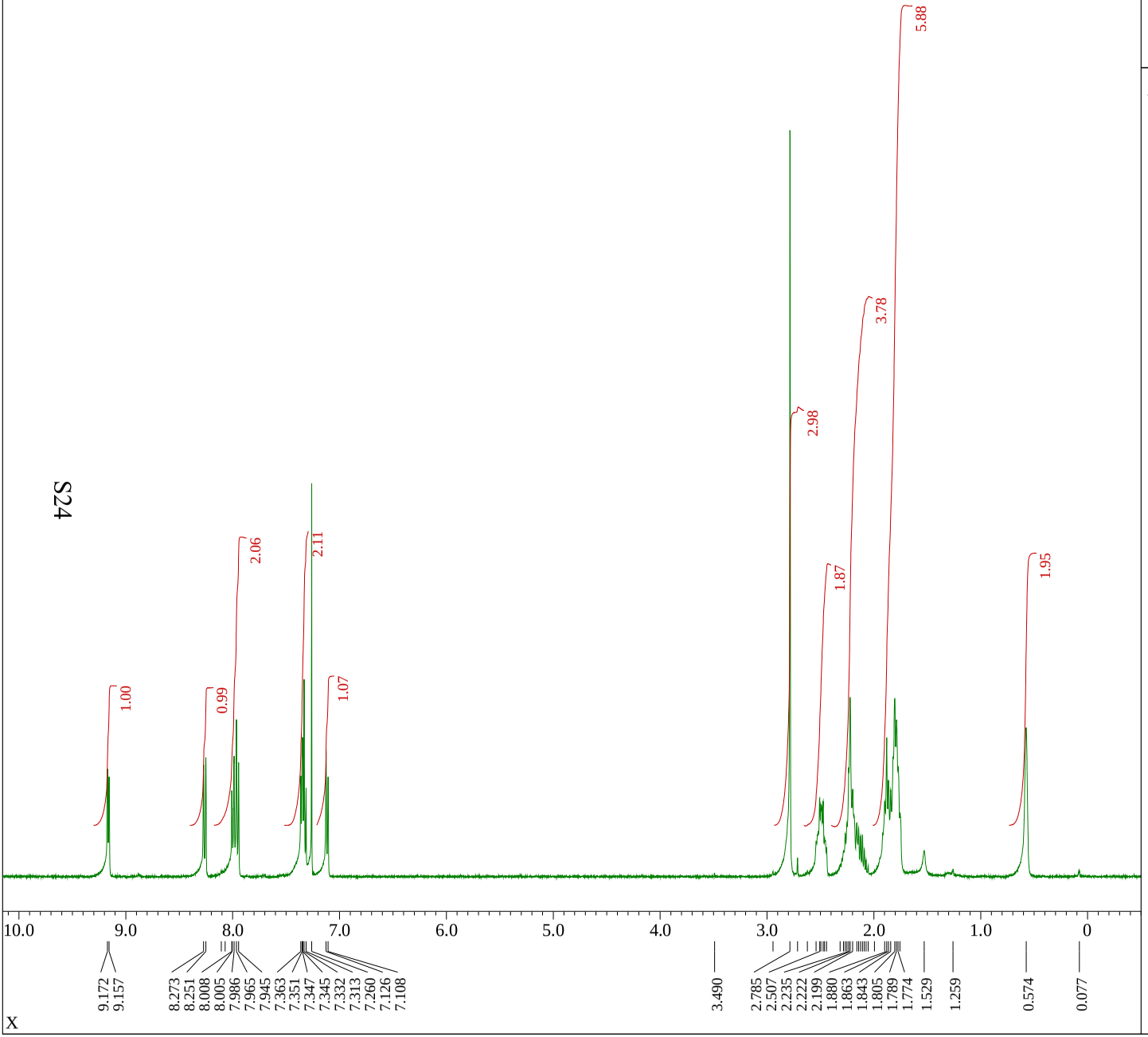


JEOL
Solutions for Innovation

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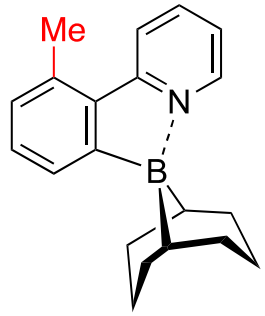


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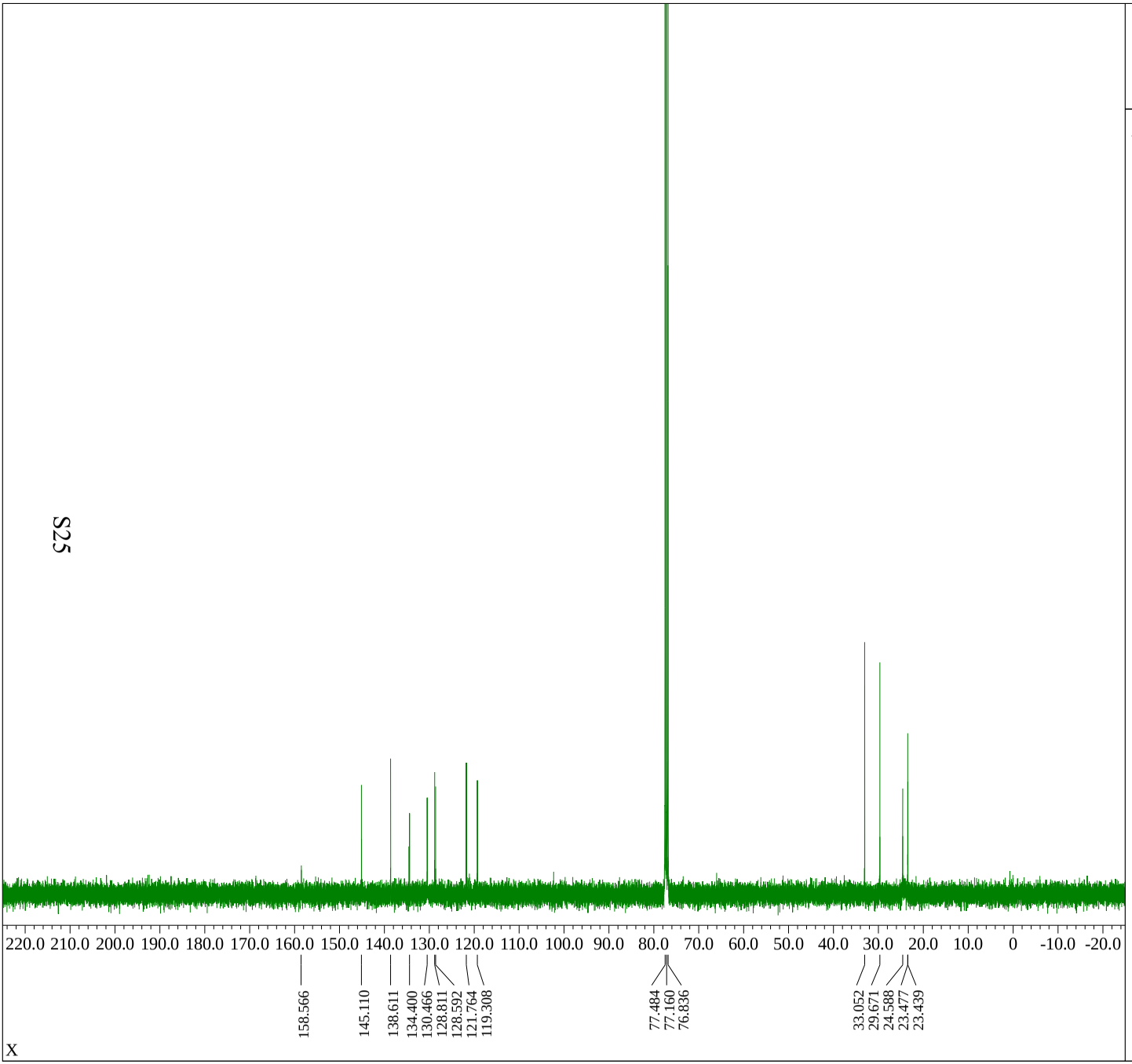


JEOL
Solutions for Innovation

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Current_Time      = 25-APR-2017 16:20:31

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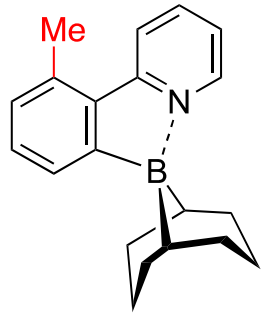


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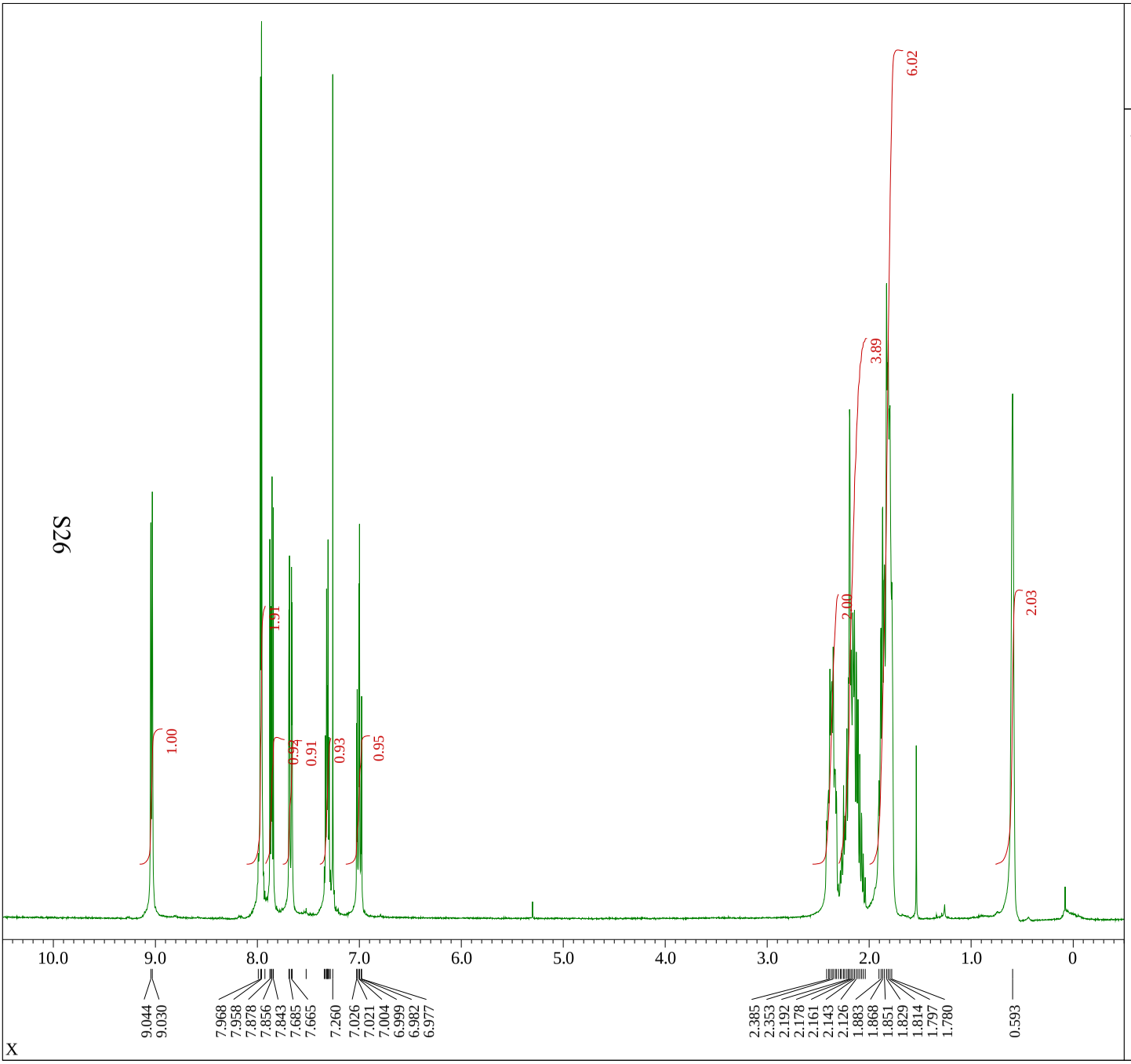


JEOL
Solutions for Innovation

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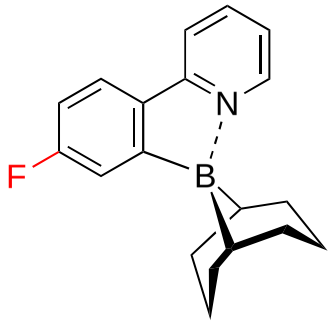


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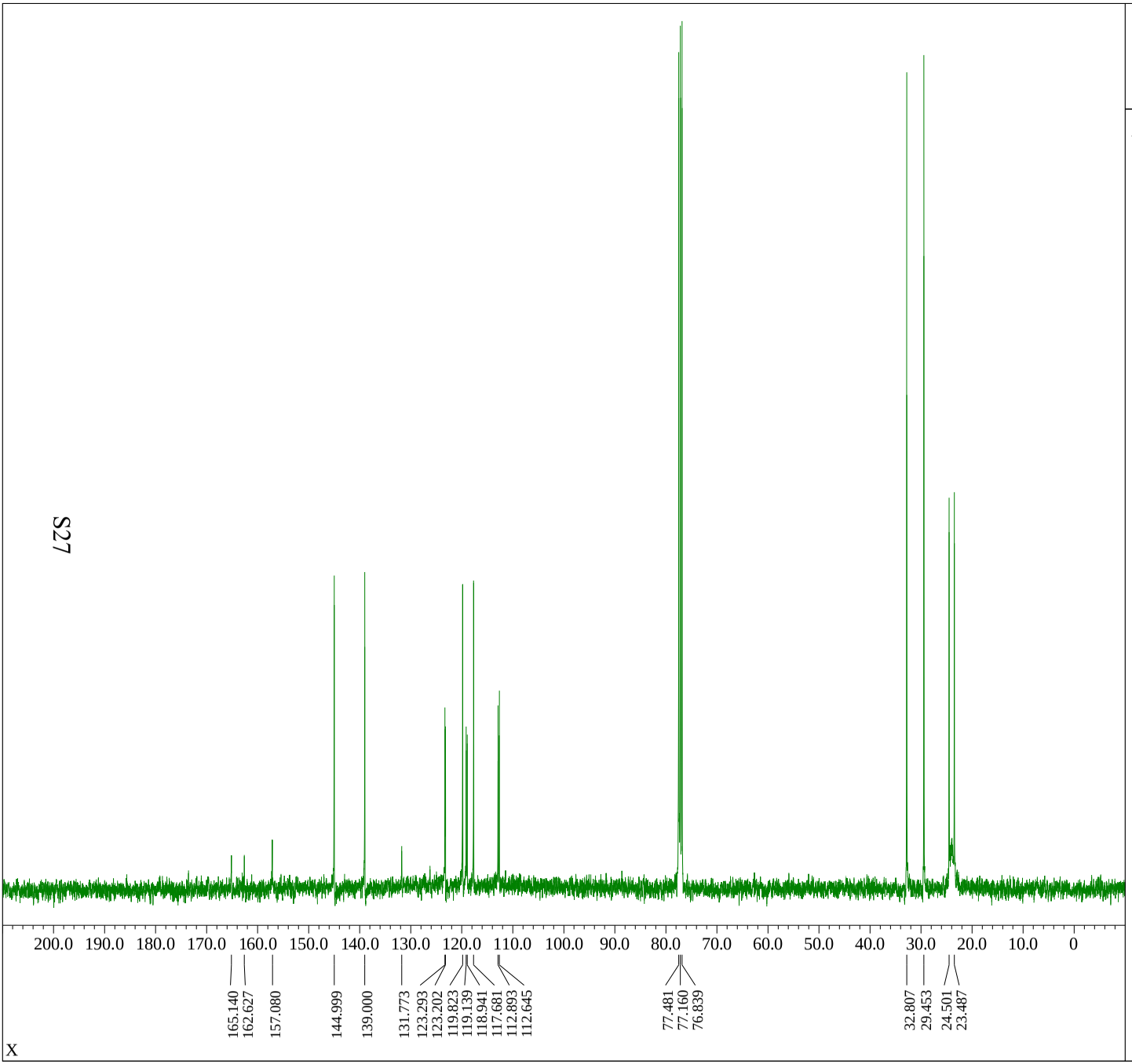


JEOL
Solutions for Innovation

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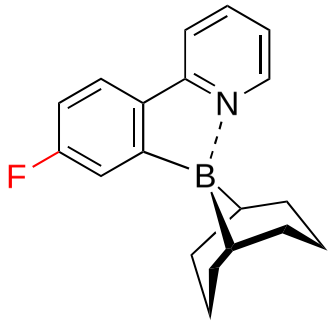


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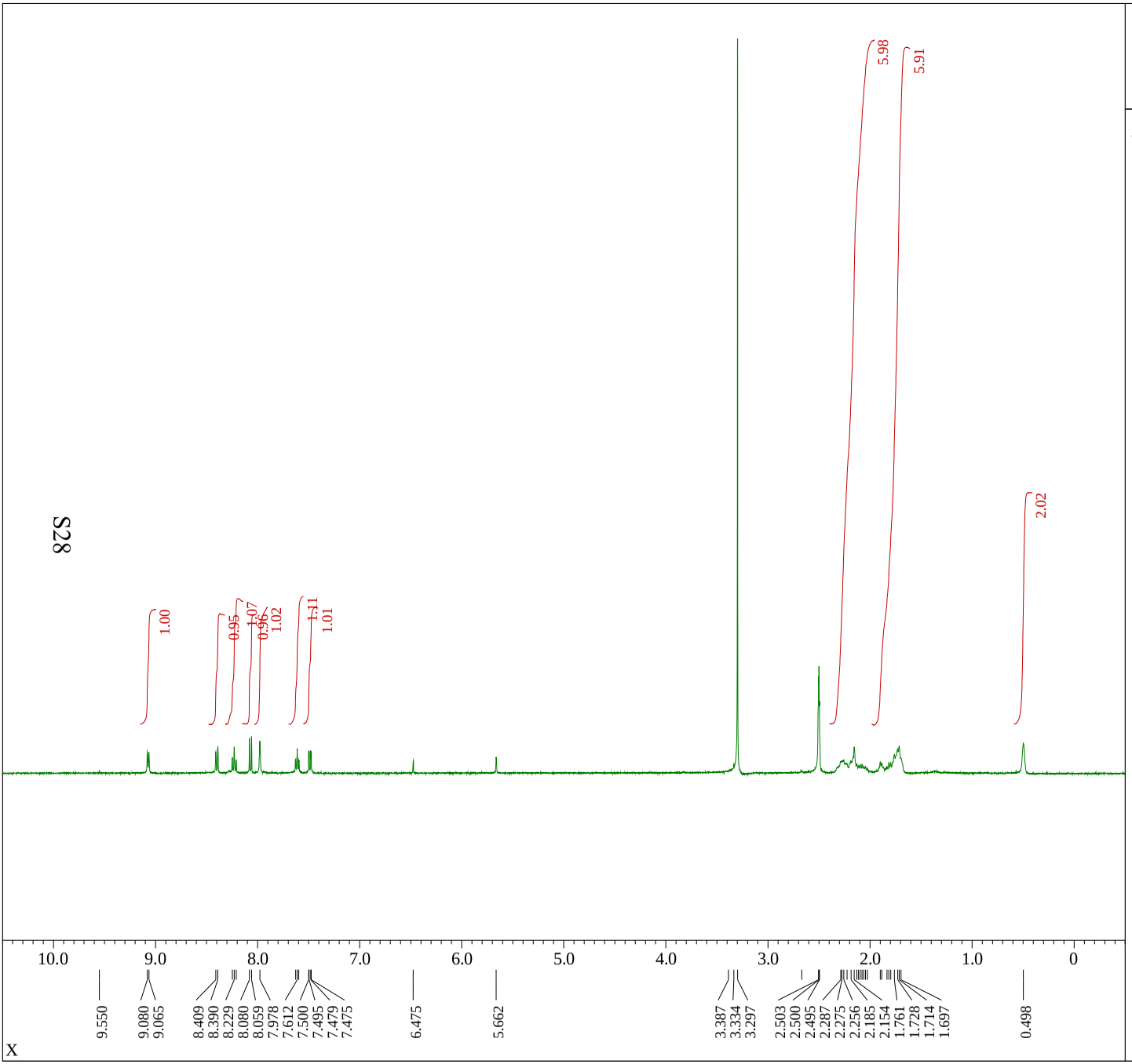


JEOL
Solutions for Innovation

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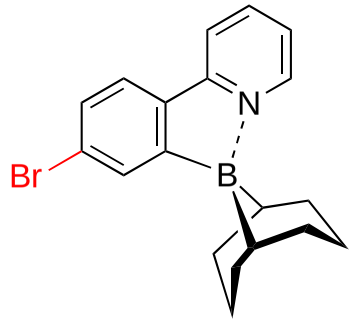


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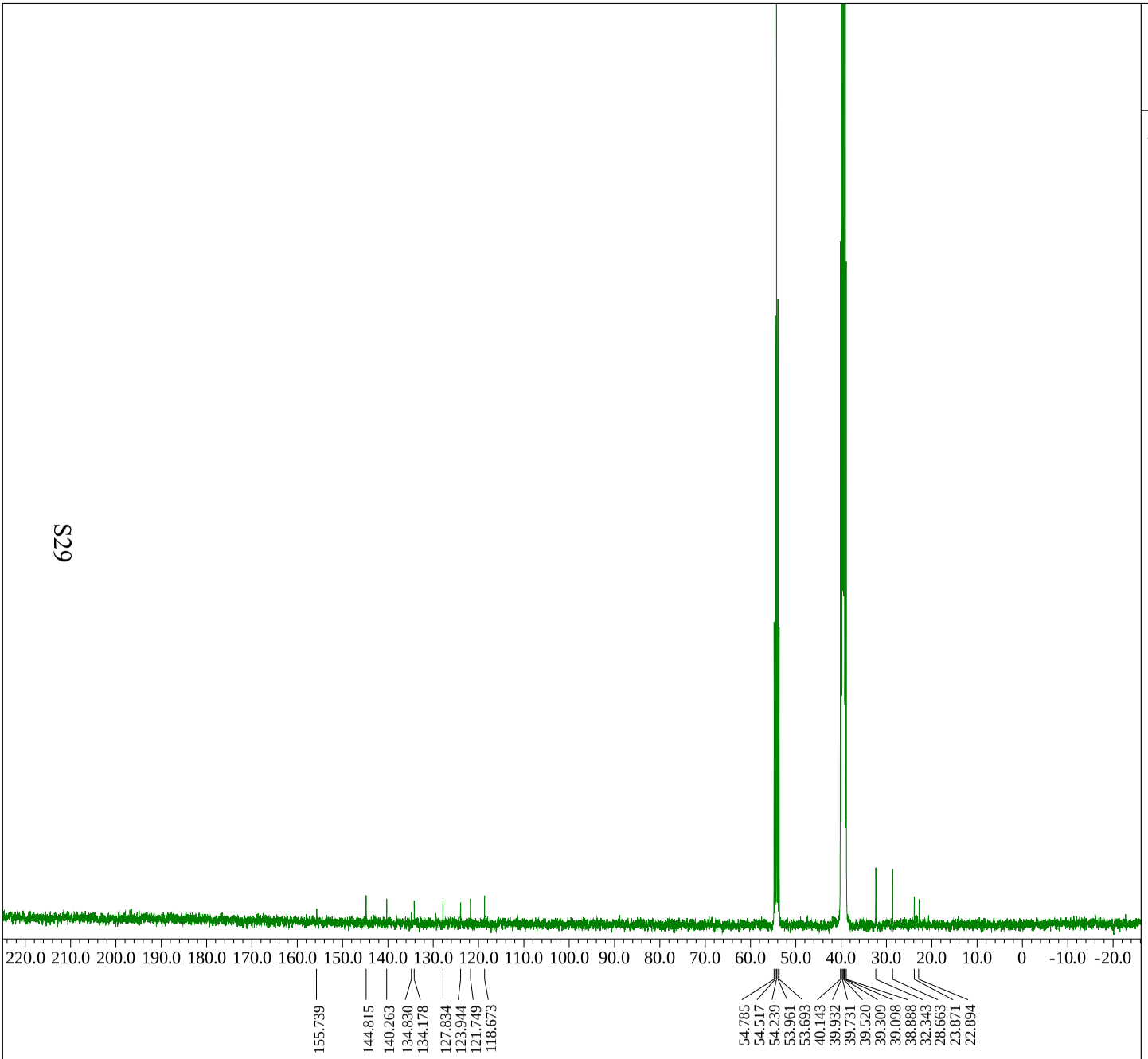


JEOL
Solutions for Innovation

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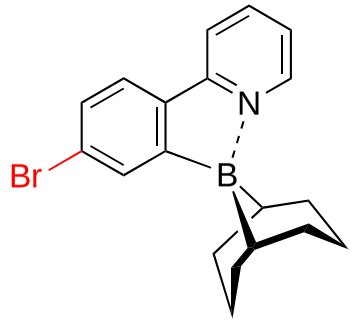


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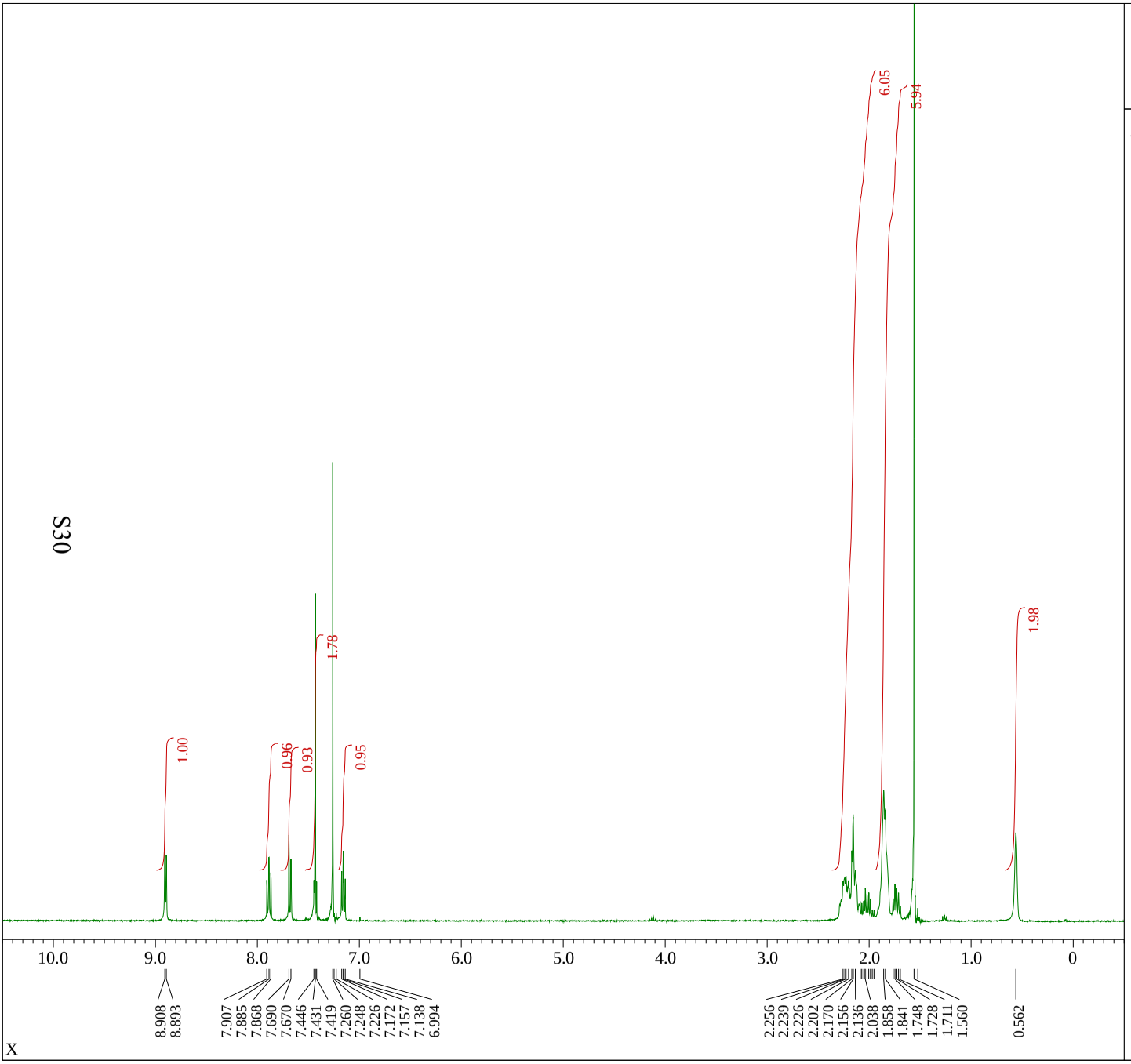


JEOL
Solutions for Innovation

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X_Points          = 8192
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X_Sweep           = 7.91765625[kHz]
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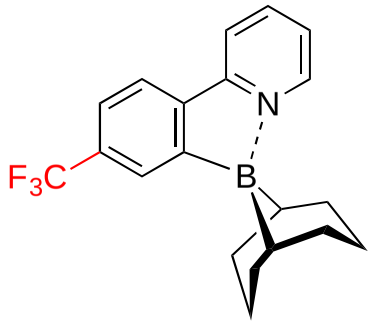


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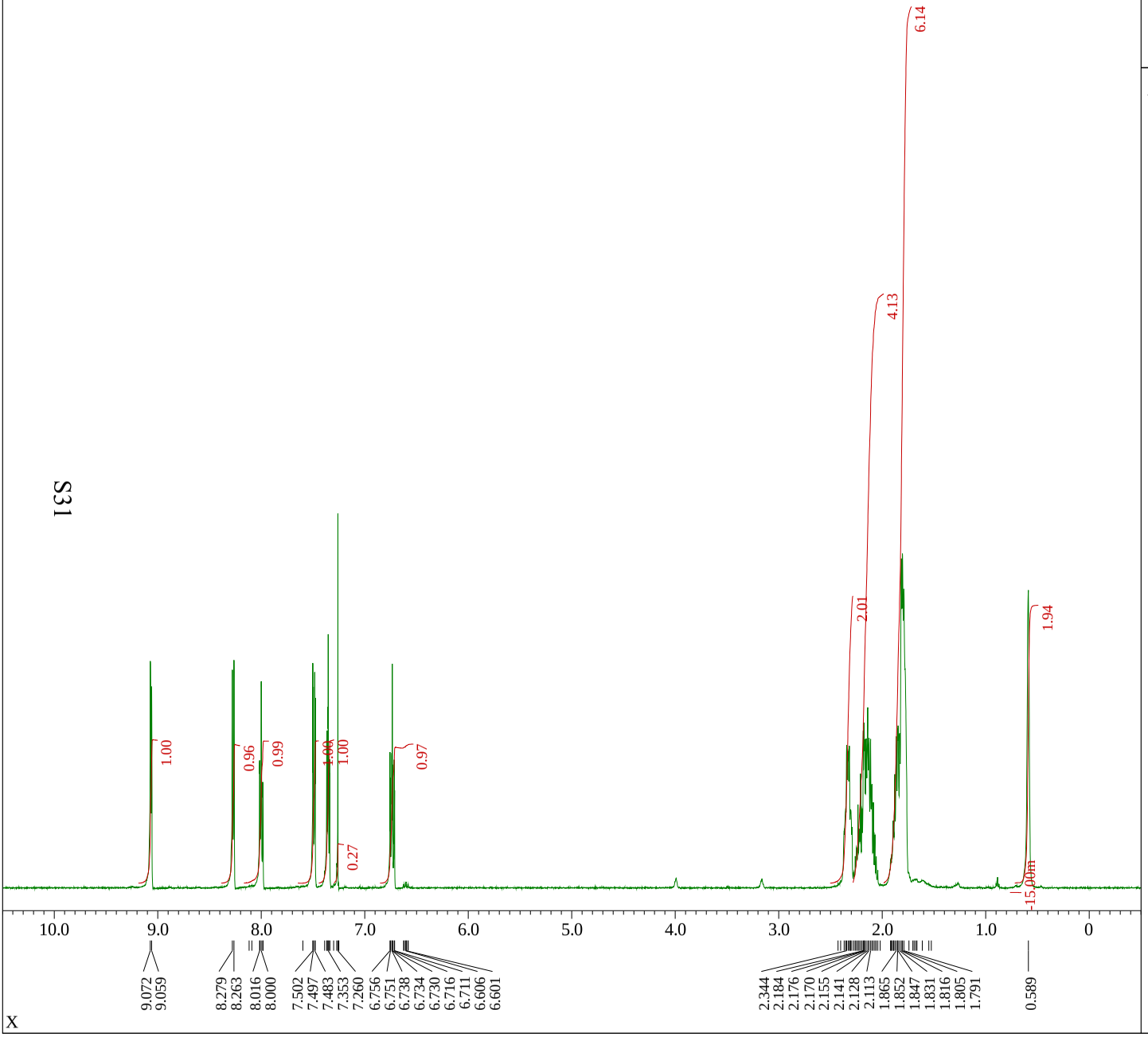


JEOL
Solutions for Innovation

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Spectrometer      = ALICE_NMR

X_Domain          = 1H
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X_Points          = 13107
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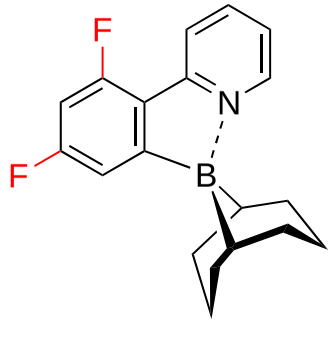


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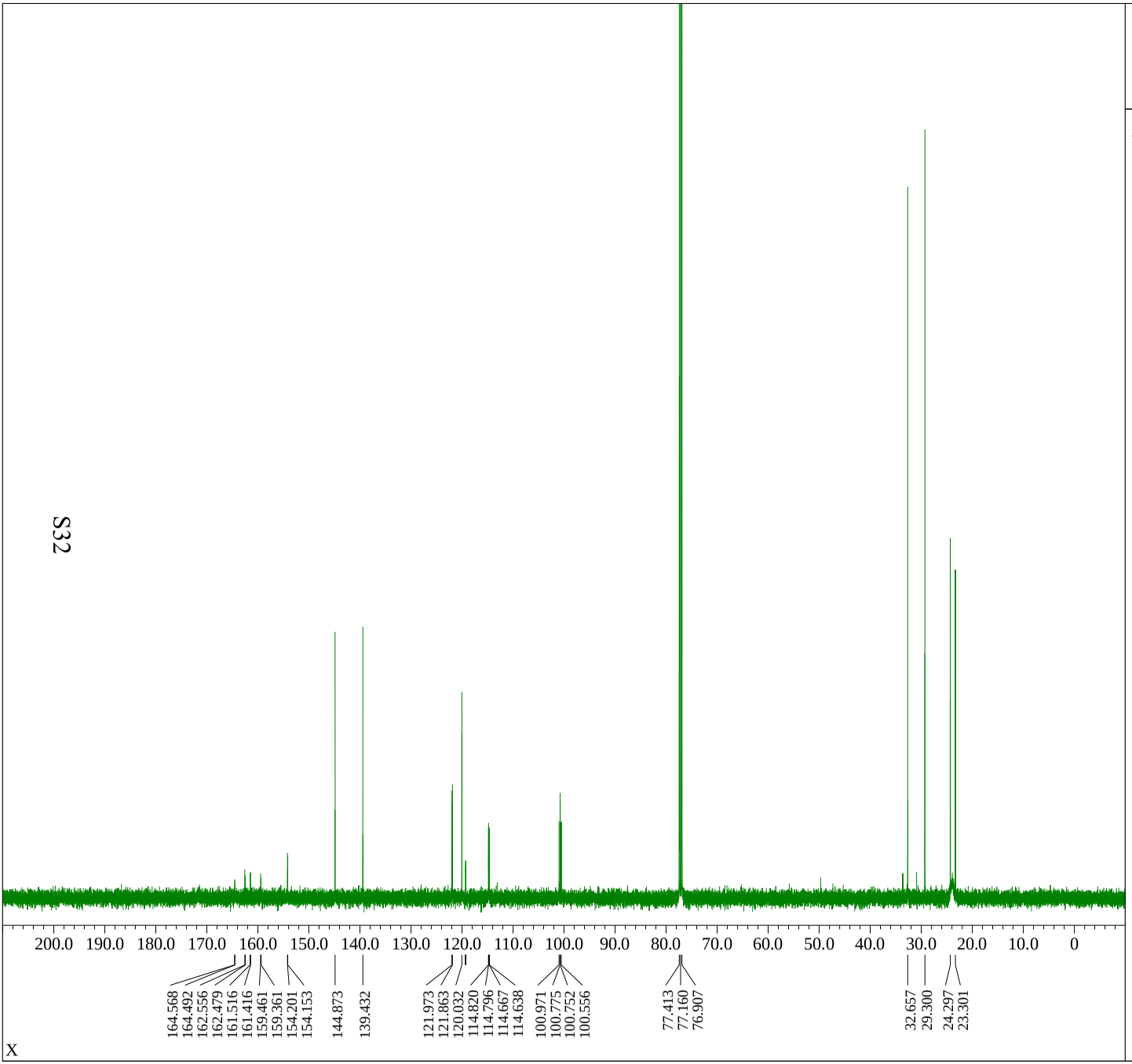


JEOL
Solutions for Innovation

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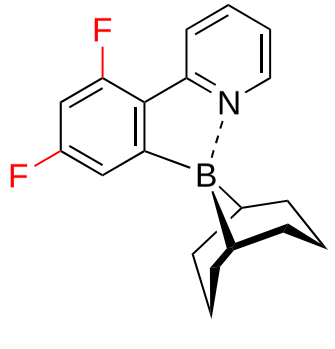


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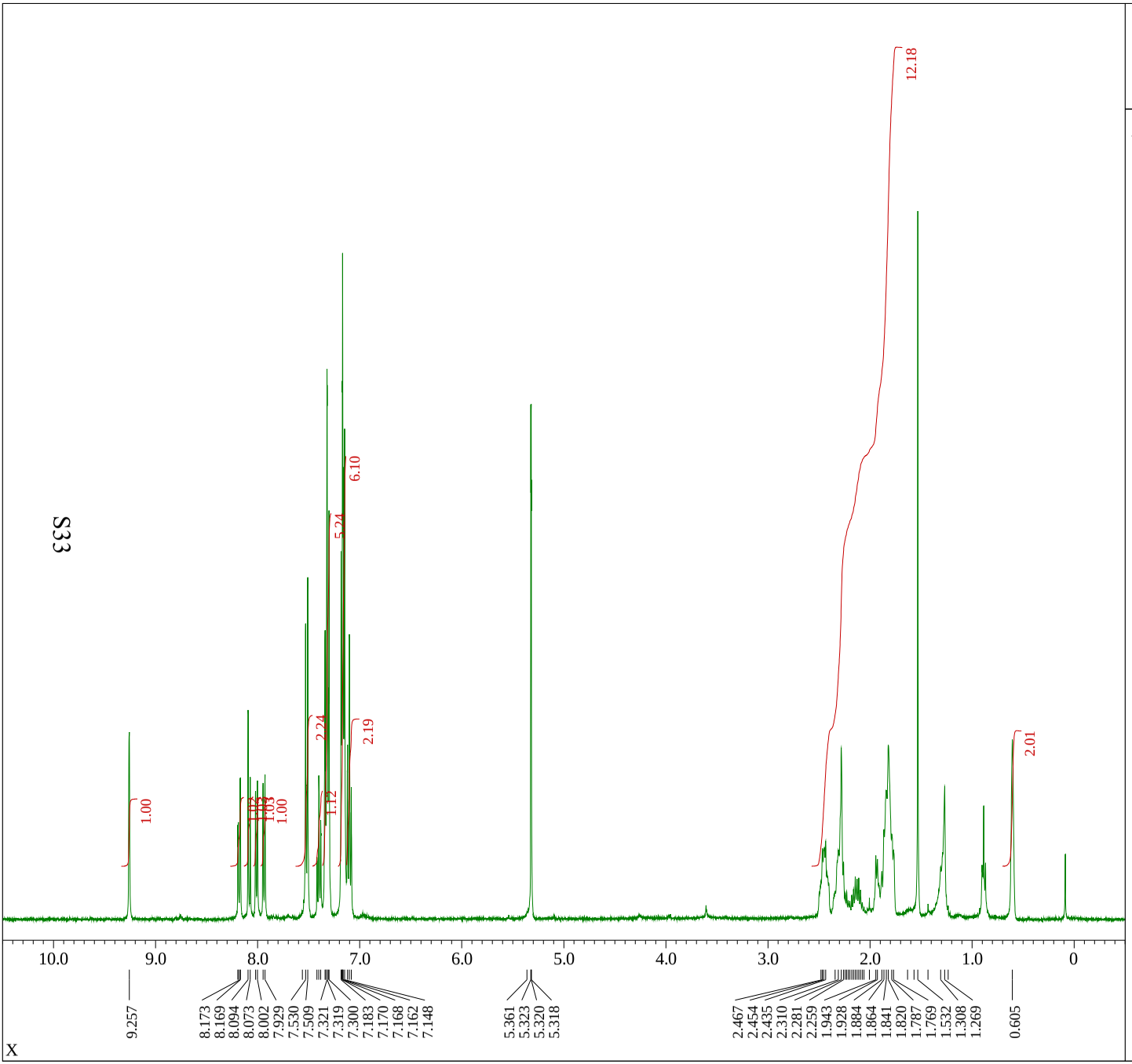


JEOL
Solutions for Innovation

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| Revision_Time | = 25-APR-2017 22:35:51 |
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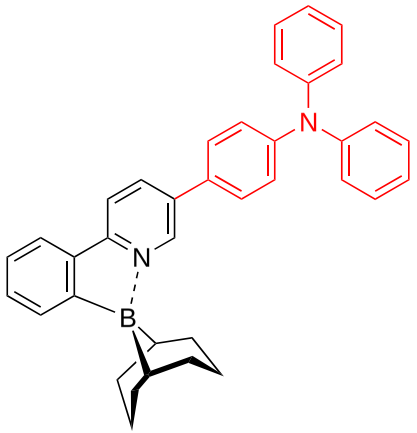
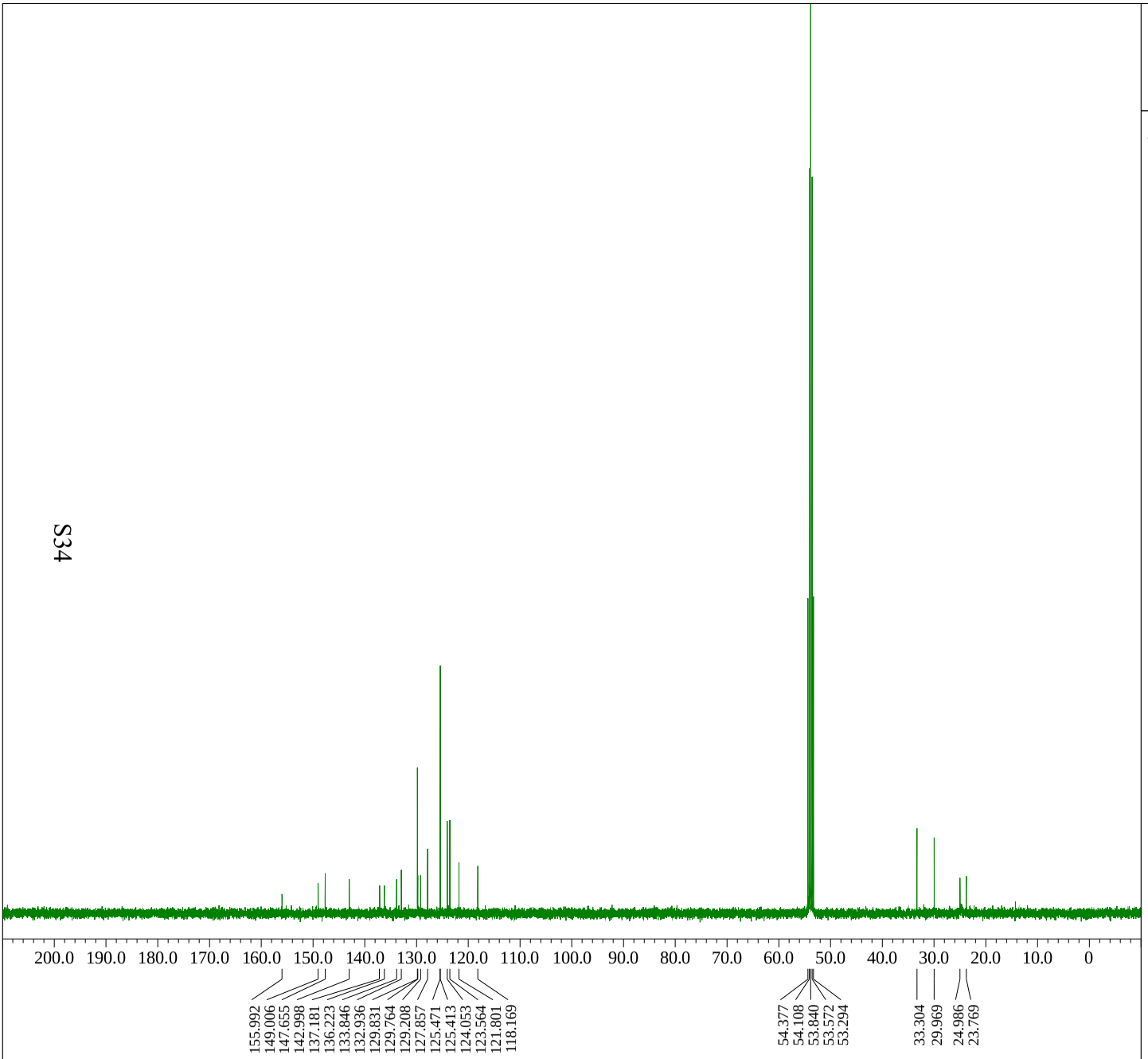
| Site | = JNM-ECZ400S |
| Spectrometer | = JNM-ECZ400S/L1 |

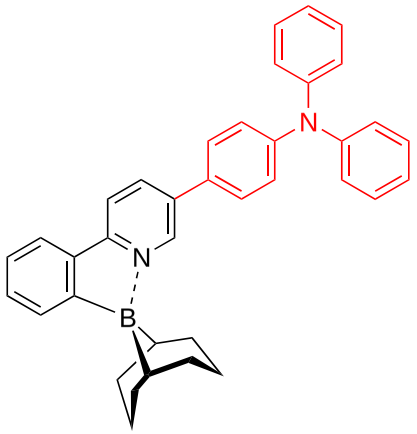



**3i**

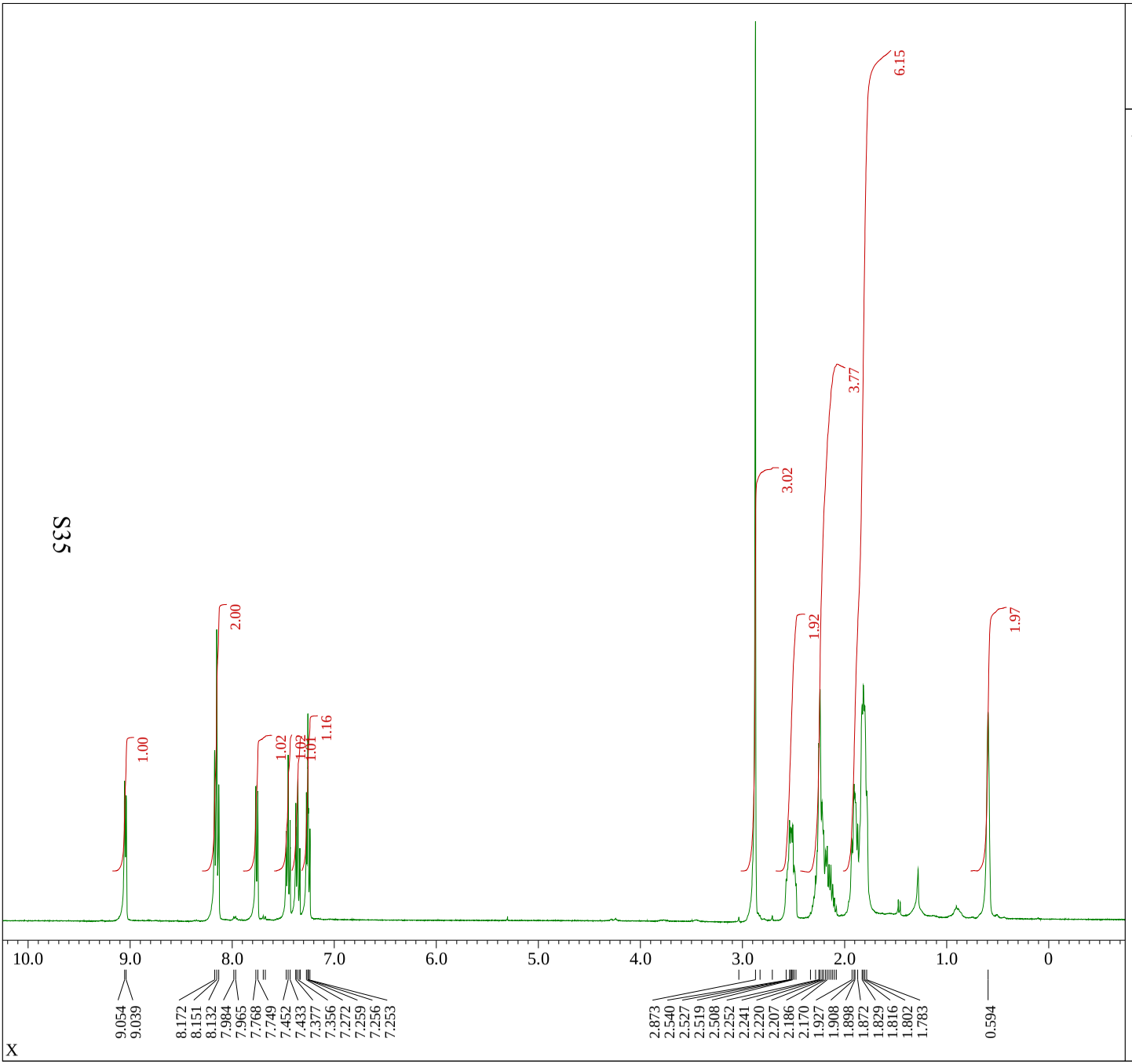



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-N000025_Carbon |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = kyy-N000025 |
| Solvent | = METHYLENE-CHLORIDE |
| Creation_Time | = 24-APR-2017 17:18: |
| Revision_Time | = 25-APR-2017 22:43: |
| Current_Time | = 25-APR-2017 22:45: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECZ400S |
| Spectrometer | = JNM-ECZ400S/L1 |

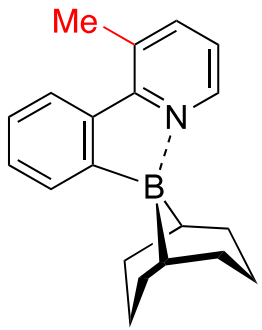



**3i**

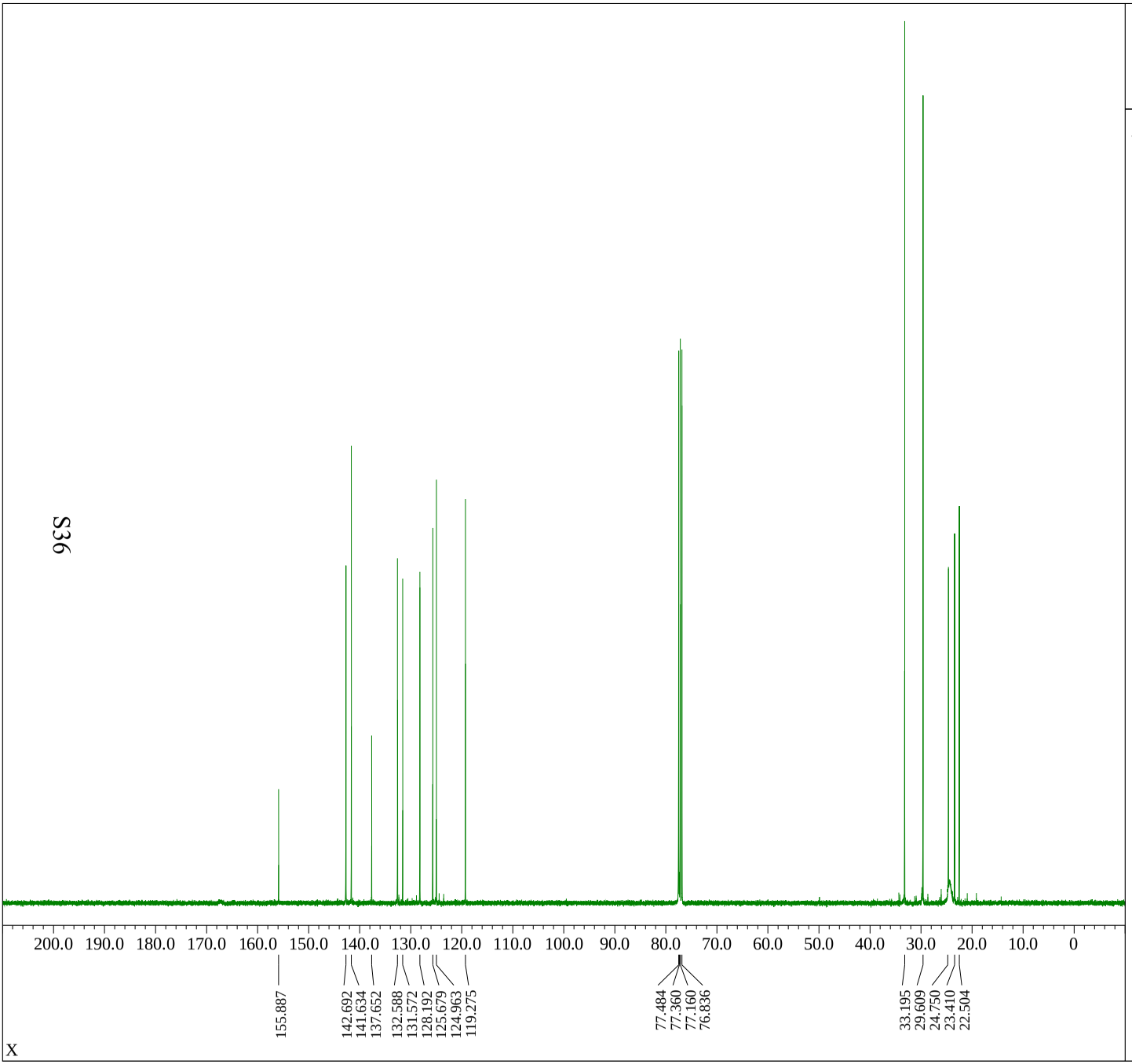



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = yoshigoe_2-Ph-3-MePy_boryl |
| Author | = yossy12g |
| Experiment | = proton.jxp |
| Solvent | = CDCL3 |
| Creation_Time | = 12-APR-2017 17:45:53 |
| Revision_Time | = 12-APR-2017 18:01:45 |
| Current_Time | = 12-APR-2017 18:02:13 |
| Comment | = yoshigoe_2-Ph-3-MePy_boryl |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = 1H |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = ALICE_NMR |
| X_Domain | = 1H |
| X_Freq | = 391.78851212[MHz] |
| X_Offset | = 0[Hz] |
| X_Points | = 13107 |
| X_Prescans | = 1 |
| X_Sweep | = 5.88235303[kHz] |
| Scans | = 8 |
| Relaxation_Delay | = 5 |
| Recvr_Gain | = 28 |
| Temp_Get | = 19.89999962[dC] |

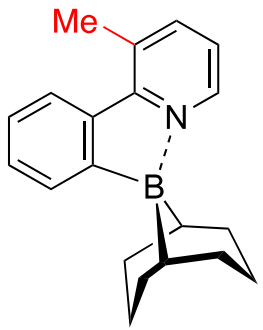



**3j**

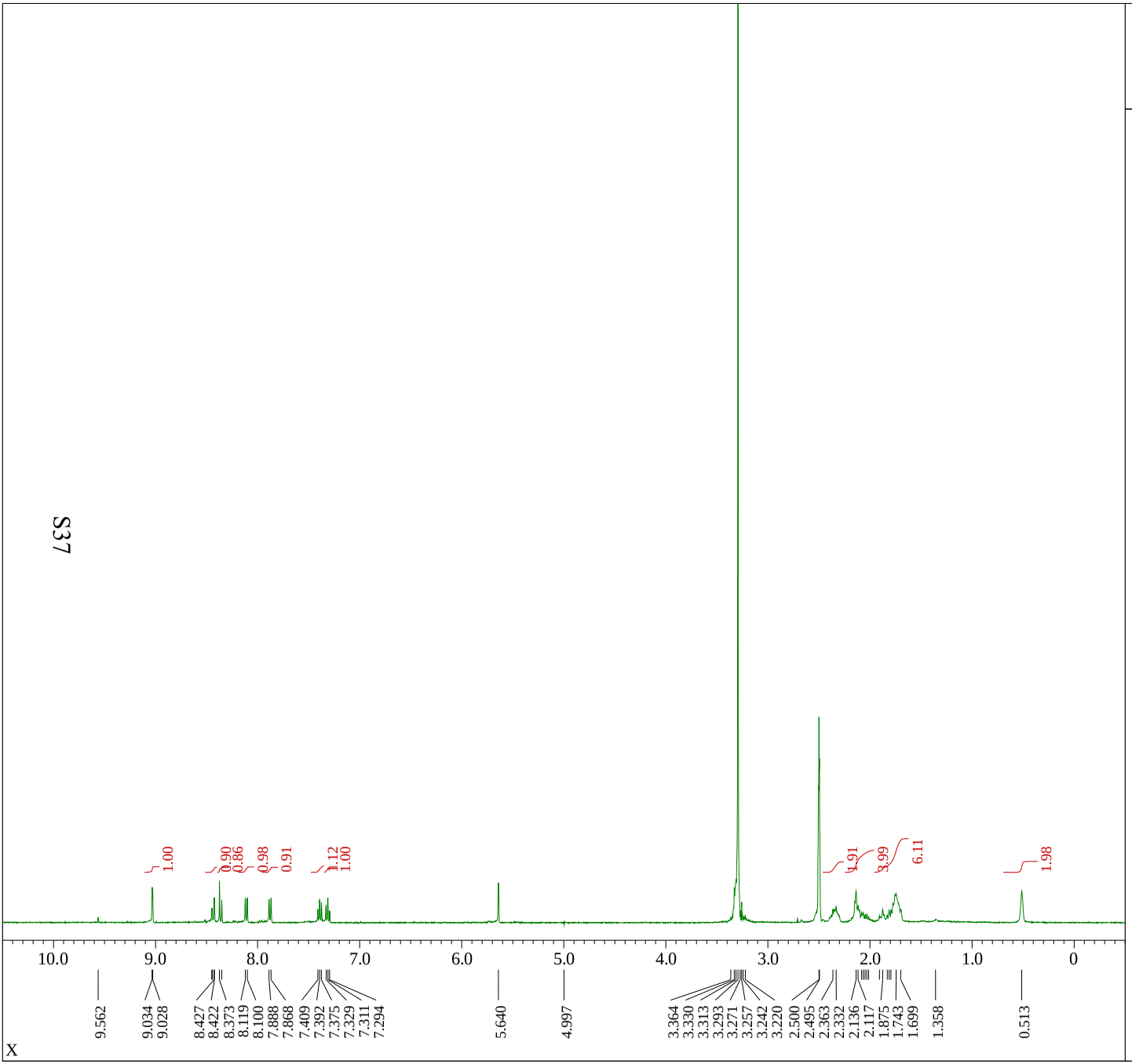



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = yoshigoe_2-Ph-3-MePy_boryl |
| Author | = yossy12g |
| Experiment | = carbon.jxp |
| Solvent | = CDCL3 |
| Creation_Time | = 12-APR-2017 18:37:25 |
| Revision_Time | = 12-APR-2017 18:38:58 |
| Current_Time | = 12-APR-2017 18:39:41 |
| Comment | = yoshigoe_2-Ph-3-MePy_boryl |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 52428 |
| Dim_Title | = 13C |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = ALICE_NMR |
| X_Domain | = 13C |
| X_Freq | = 98.52464538[MHz] |
| X_Offset | = 0[Hz] |
| X_Points | = 52428 |
| X_Prescans | = 1 |
| X_Sweep | = 24.63054297[kHz] |
| Scans | = 10147 |
| Relaxation_Delay | = 2 |
| Recvr_Gain | = 60 |
| Temp_Get | = 19.39999962[dC] |

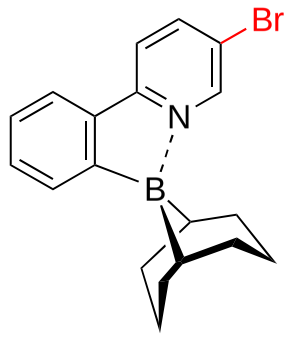



**3j**

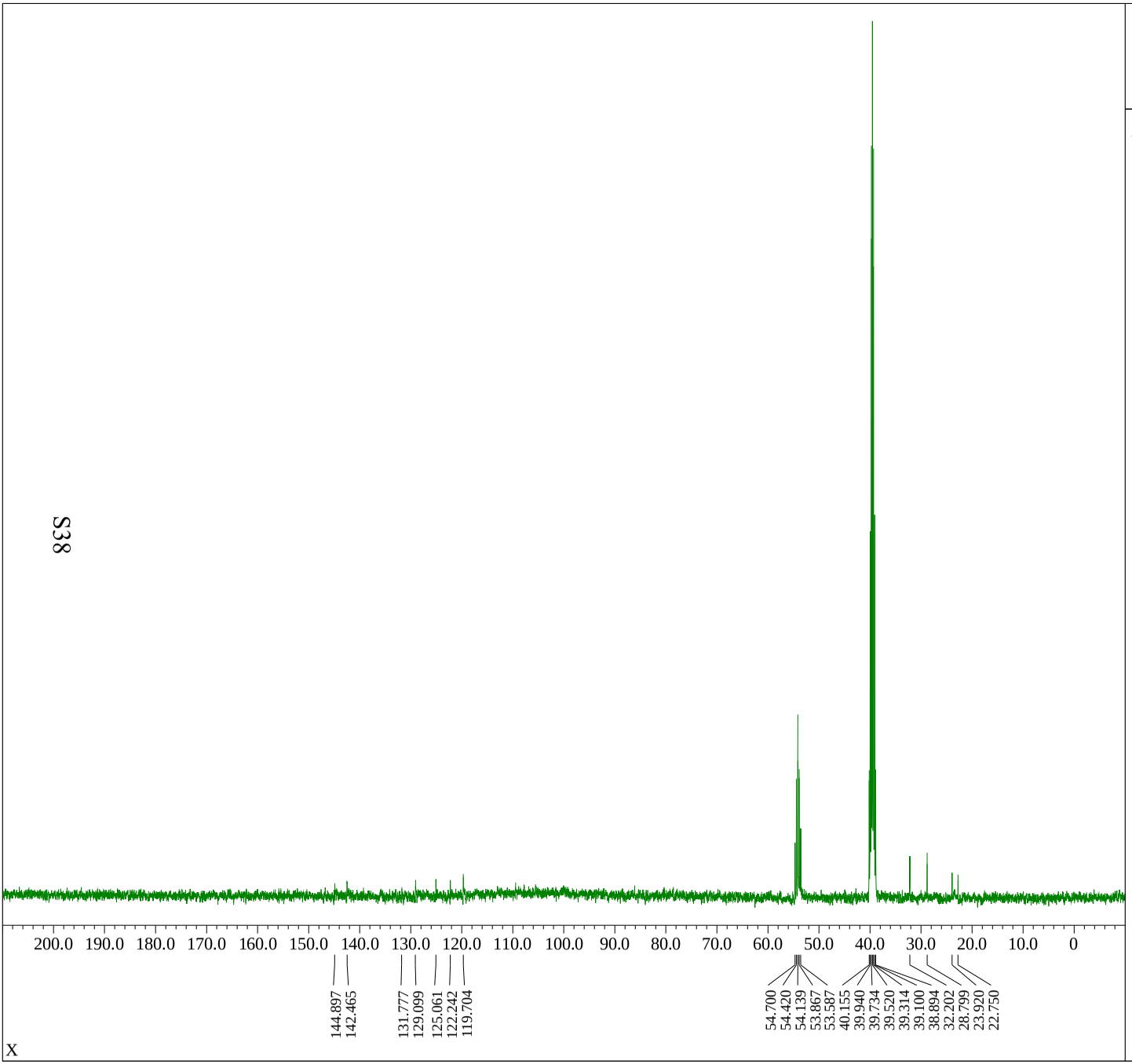



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-N0000191non_E2-7.jdf |
| Author | = yossy12g |
| Experiment | = non |
| Solvent | = DMSO |
| Creation_Time | = 22-APR-2017 17:39:26 |
| Revision_Time | = 22-APR-2017 17:45:28 |
| Current_Time | = 22-APR-2017 17:45:51 |
| Comment | = 002-3j |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 8192 |
| Dim_Title | = 1H |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = ALICE_NMR |
| X_Domain | = 1H |
| X_Freq | = 395.884498[MHz] |
| X_Offset | = 0[Hz] |
| X_Points | = 8192 |
| X_Prescans | = 0 |
| X_Sweep | = 7.91765625[kHz] |
| Scans | = 16 |
| Relaxation_Delay | = 5.96540022 |
| Recvr_Gain | = 22 |
| Temp_Get | = 0[dC] |

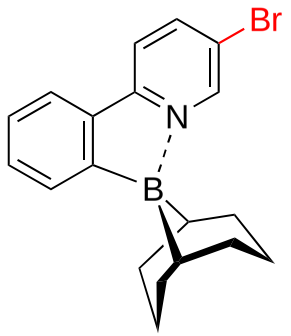



**3k**

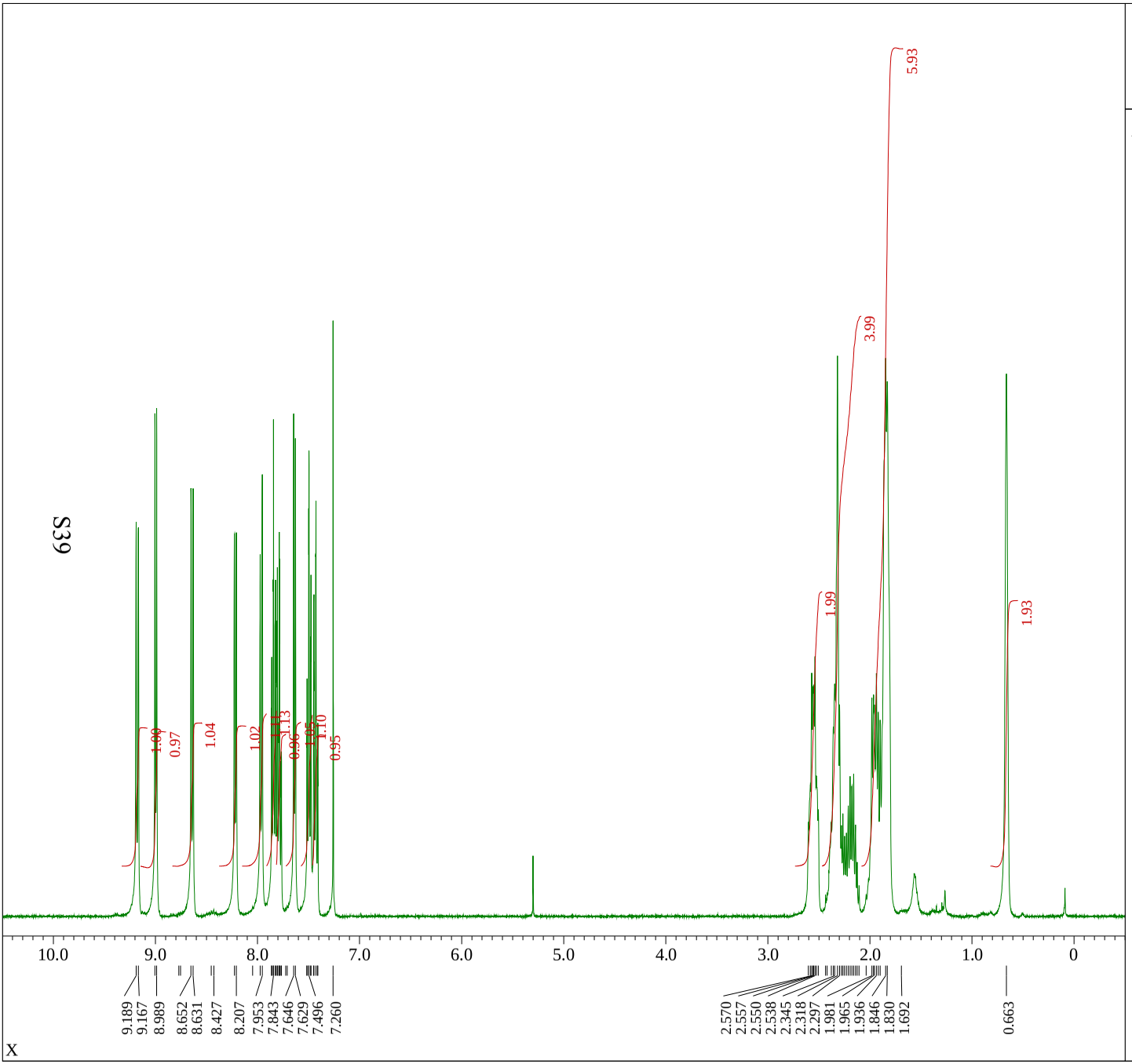



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-N0000192bcm_E2-3.jdf |
| Author | = yossy12g |
| Experiment | = bcm |
| Solvent | = DMSO |
| Creation_Time | = 22-APR-2017 17:48:45 |
| Revision_Time | = 22-APR-2017 17:56:29 |
| Current_Time | = 22-APR-2017 17:56:58 |
| Comment | = 002-3j |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 32768 |
| Dim_Title | = 13C |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = ALICE_NMR |
| X_Domain | = 13C |
| X_Freq | = 99.55474695[MHz] |
| X_Offset | = 0[Hz] |
| X_Points | = 32768 |
| X_Prescans | = 1 |
| X_Sweep | = 26.8817207[kHz] |
| Scans | = 1792 |
| Relaxation_Delay | = 1.78100002 |
| Recvr_Gain | = 22 |
| Temp_Get | = 0[dC] |

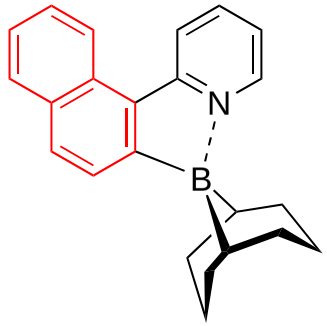



**3k**

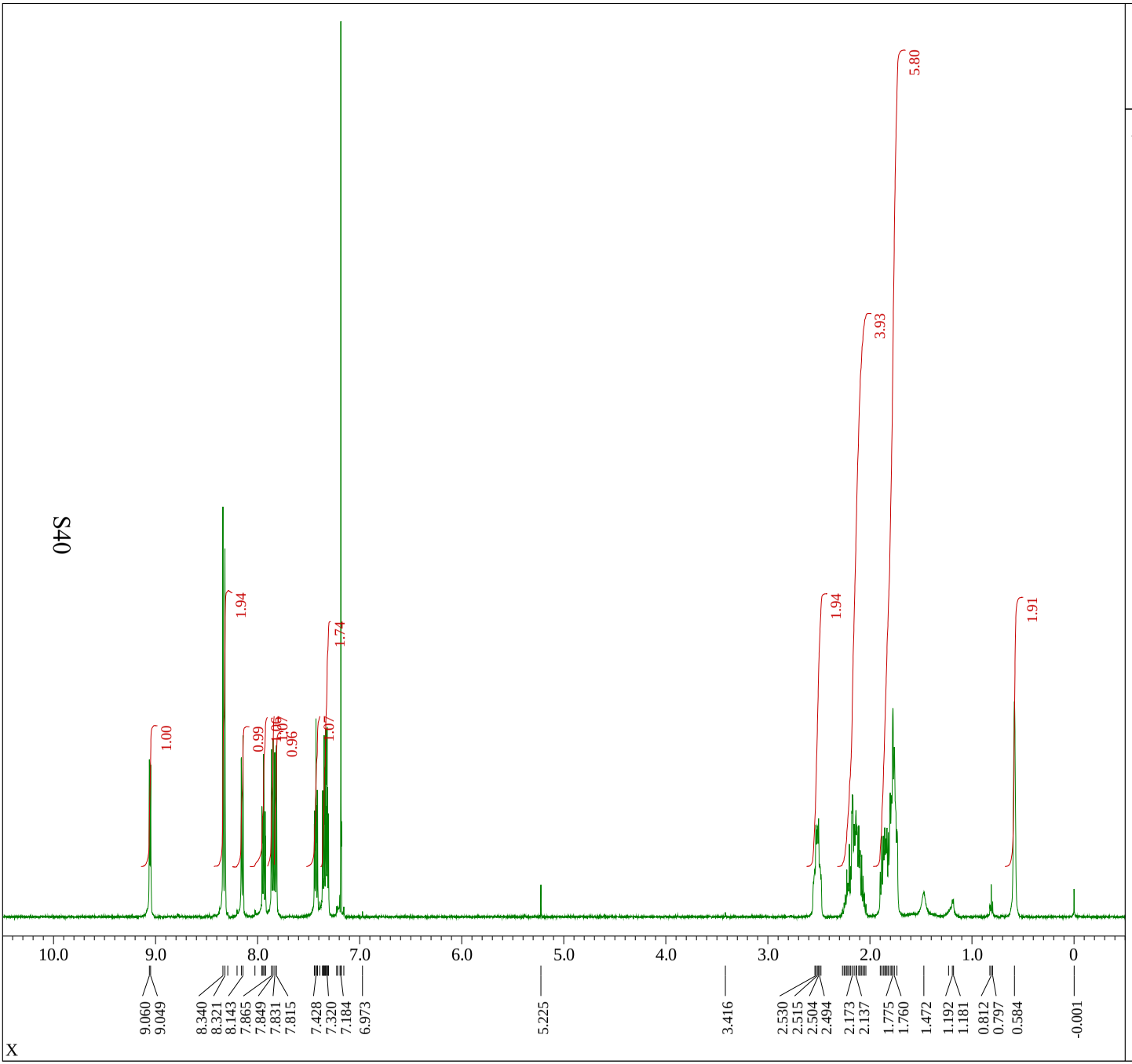



JEOL
Solutions for Innovation

```
Filename          = 002-160613-08-0101-1-1-9.j
Author            = yossy12g
Experiment        = proton.jxp
Solvent           = CDCL3
Creation_Time     = 12-APR-2017 10:32:12
Revision_Time     = 12-APR-2017 10:35:02
Current_Time      = 12-APR-2017 10:35:17

Comment           = 002-160613-08-0101
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 1H
X_Freq            = 391.78851212[MHz]
X_Offset          = 0[Hz]
X_Points          = 13107
X_Prescans        = 1
X_Sweep           = 5.88235303[kHz]
Scans             = 8

Relaxation_Delay = 5
Recvr_Gain        = 34
Temp_Get          = 20[dC]
```

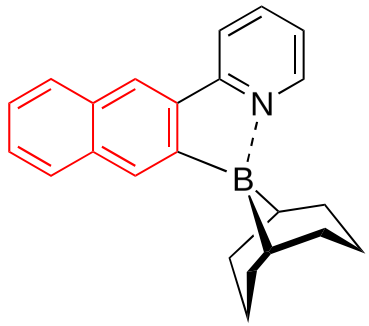



**3l**

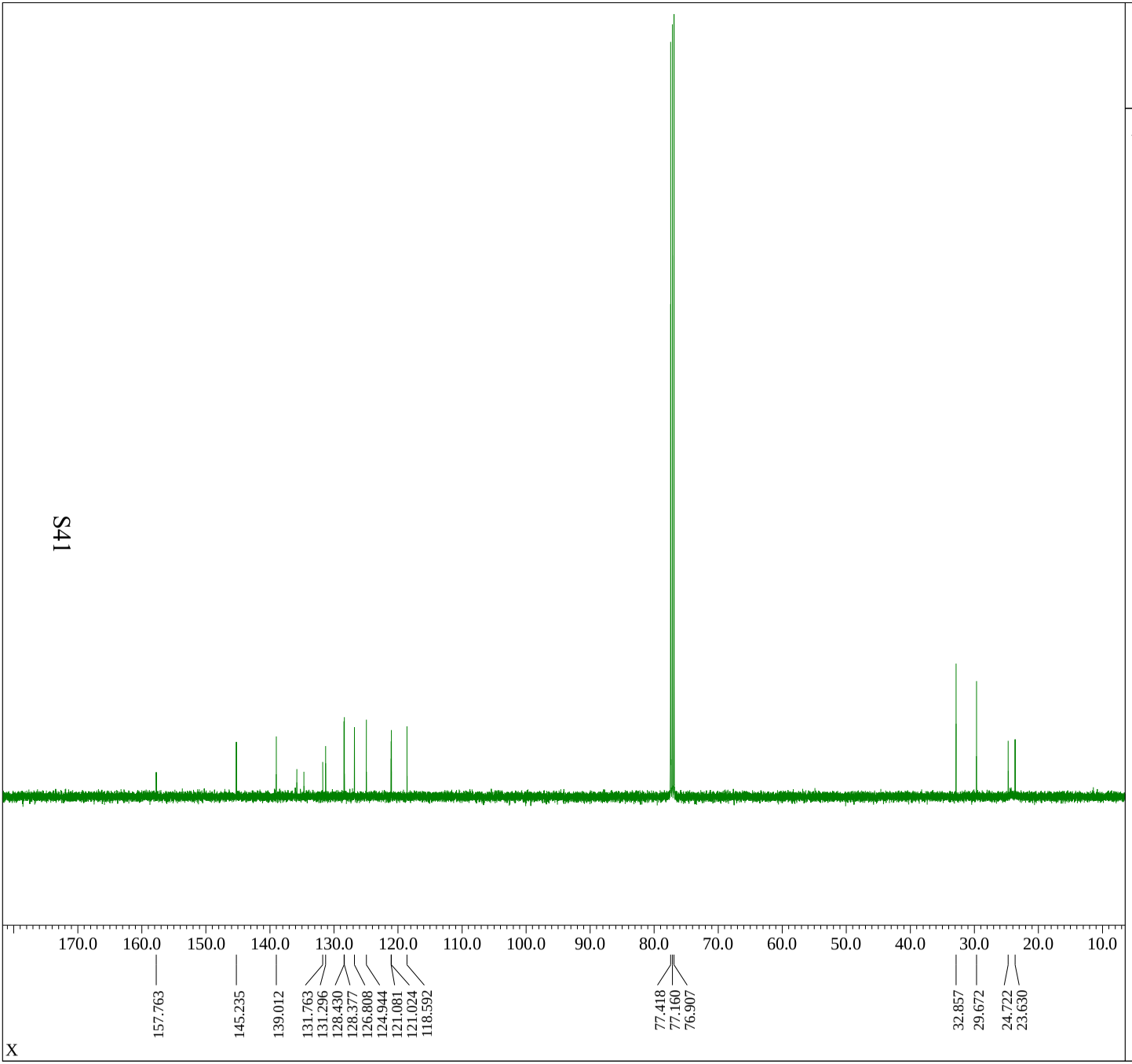



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = 002-160708-03-0101-1-1-4.j |
| Author | = yossy12g |
| Experiment | = proton.jxp |
| Solvent | = CDCL3 |
| Creation_Time | = 12-APR-2017 01:08:14 |
| Revision_Time | = 12-APR-2017 01:10:54 |
| Current_Time | = 12-APR-2017 01:13:38 |
| Comment | = 002-160708-03-0101 |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = 1H |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = ALICE_NMR |
| X_Domain | = 1H |
| X_Freq | = 500.16241967[MHz] |
| X_Offset | = 0[Hz] |
| X_Points | = 13107 |
| X_Prescans | = 1 |
| X_Sweep | = 7.50750781[kHz] |
| Scans | = 8 |
| Relaxation_Delay | = 5 |
| Recvr_Gain | = 30 |
| Temp_Get | = 21.29999924[dC] |

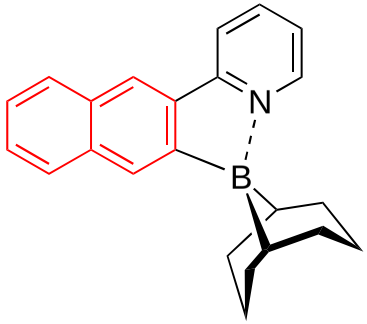



**3m**

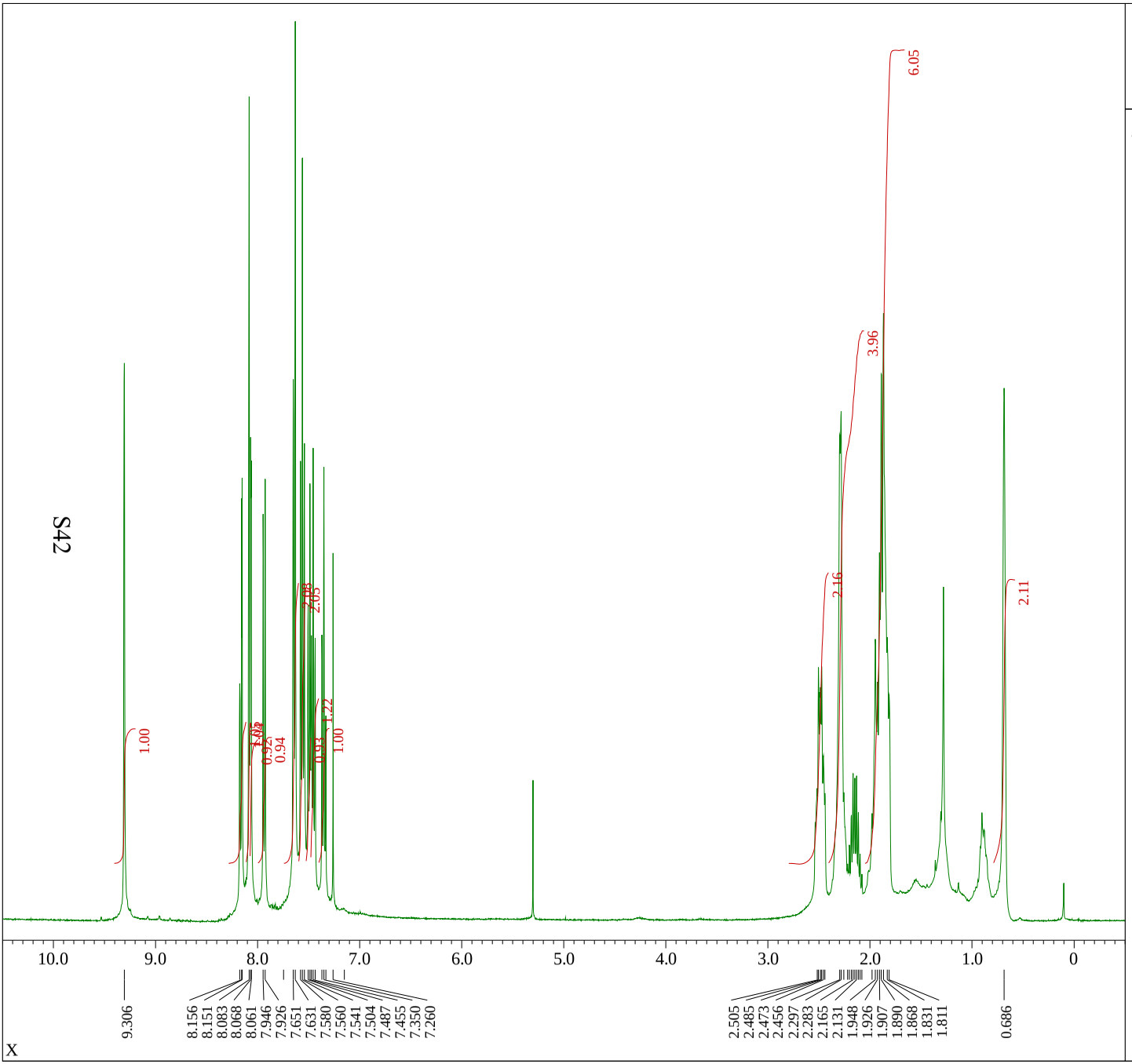



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = 002-160708-03-1301-1-1-4.j |
| Author | = yossy12g |
| Experiment | = carbon.jxp |
| Solvent | = CDCL3 |
| Creation_Time | = 12-APR-2017 01:05:27 |
| Revision_Time | = 12-APR-2017 01:05:54 |
| Current_Time | = 12-APR-2017 01:06:16 |
| Comment | = 002-160708-03-1301 |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 52428 |
| Dim_Title | = 13C |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = ALICE_NMR |
| X_Domain | = 13C |
| X_Freq | = 125.77787086[MHz] |
| X_Offset | = 0[Hz] |
| X_Points | = 52428 |
| X_Prescans | = 1 |
| X_Sweep | = 31.44654102[kHz] |
| Scans | = 857 |
| Relaxation_Delay | = 2 |
| Recvr_Gain | = 60 |
| Temp_Get | = 21.20000076[dC] |

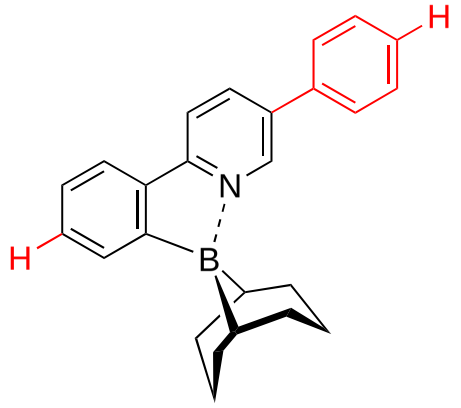



**3m**

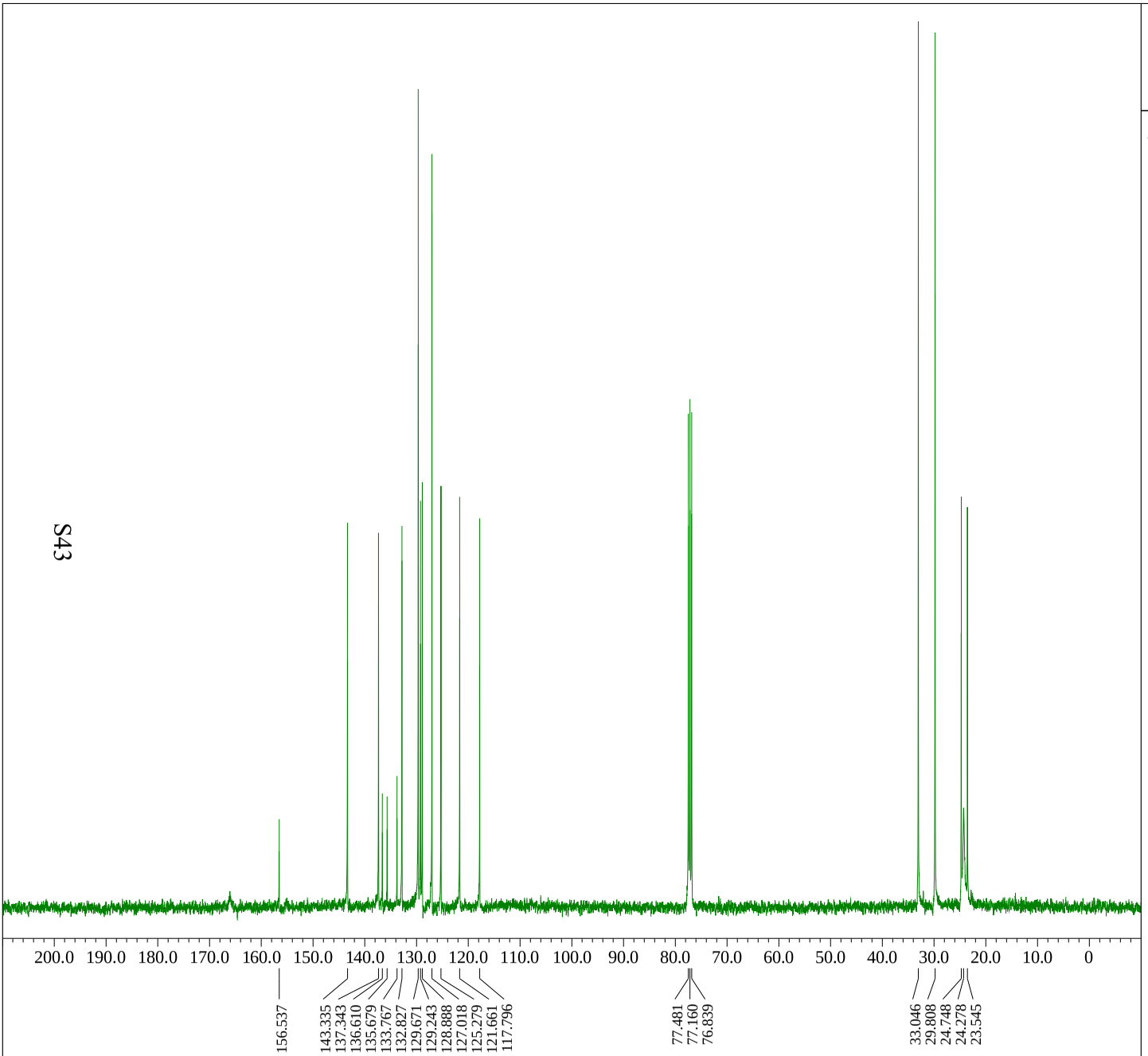



JEOL
Solutions for Innovation

```
Filename          = kyy-00000081non_E5-23.jdf
Author            = yossy12g
Experiment        = non
Solvent           = CDCL3
Creation_Time     = 12-APR-2017 19:33:06
Revision_Time     = 13-APR-2017 00:36:36
Current_Time      = 13-APR-2017 00:58:31

Comment           = 002-161115-03
Data_Format       = 1D COMPLEX
Dim_Size          = 8192
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 1H
X_Freq            = 395.884498[MHz]
X_Offset          = 0[Hz]
X_Points          = 8192
X_Prescans        = 0
X_Sweep           = 7.91765625[kHz]
Scans             = 8

Relaxation_Delay = 5.96540022
Recvr_Gain        = 13
Temp_Get          = 0[dC]
```

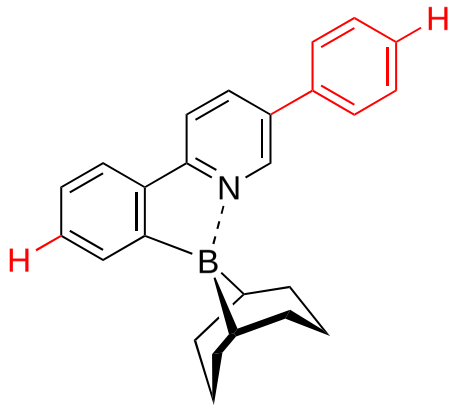



**3n**

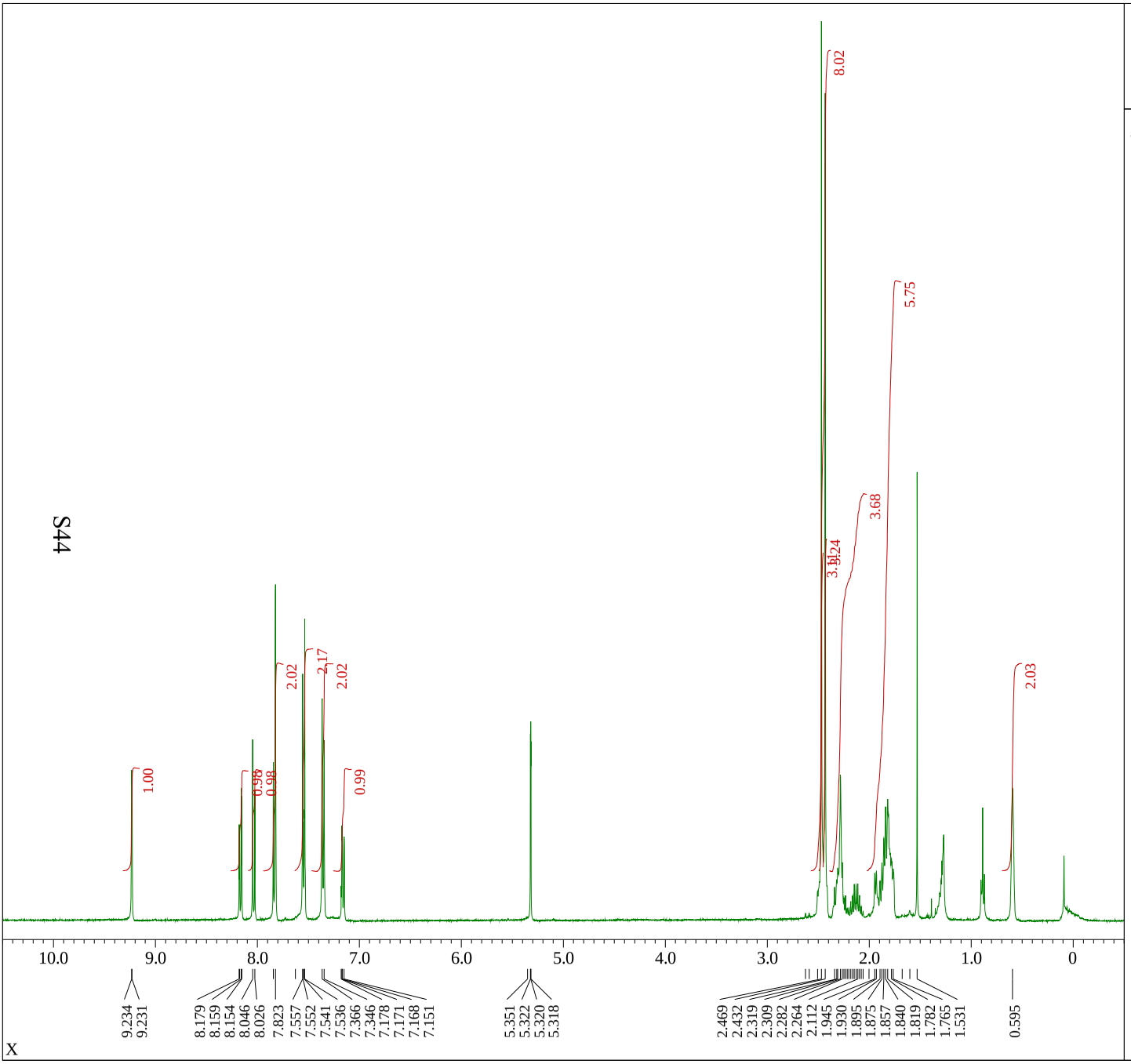



JEOL
Solutions for Innovation

```
Filename          = kyy-00000082bcm_E5-4.jdf
Author            = yossy12g
Experiment        = bcm
Solvent           = CDCL3
Creation_Time     = 13-APR-2017 00:49:18
Revision_Time     = 13-APR-2017 00:50:20
Current_Time      = 13-APR-2017 00:56:36

Comment           = 002-161115-03
Data_Format       = 1D COMPLEX
Dim_Size          = 32768
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 13C
X_Freq            = 99.55474695[MHz]
X_Offset          = 0[Hz]
X_Points          = 32768
X_Prescans        = 1
X_Sweep           = 26.8817207[kHz]
Scans             = 1024

Relaxation_Delay = 1.78100002
Recvr_Gain        = 23
Temp_Get          = 0[dC]
```

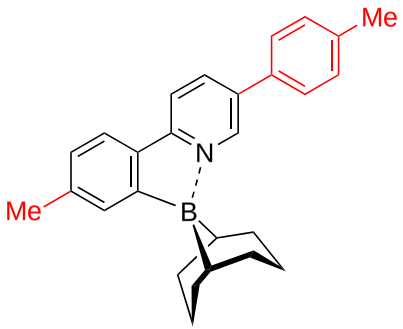



**3n**

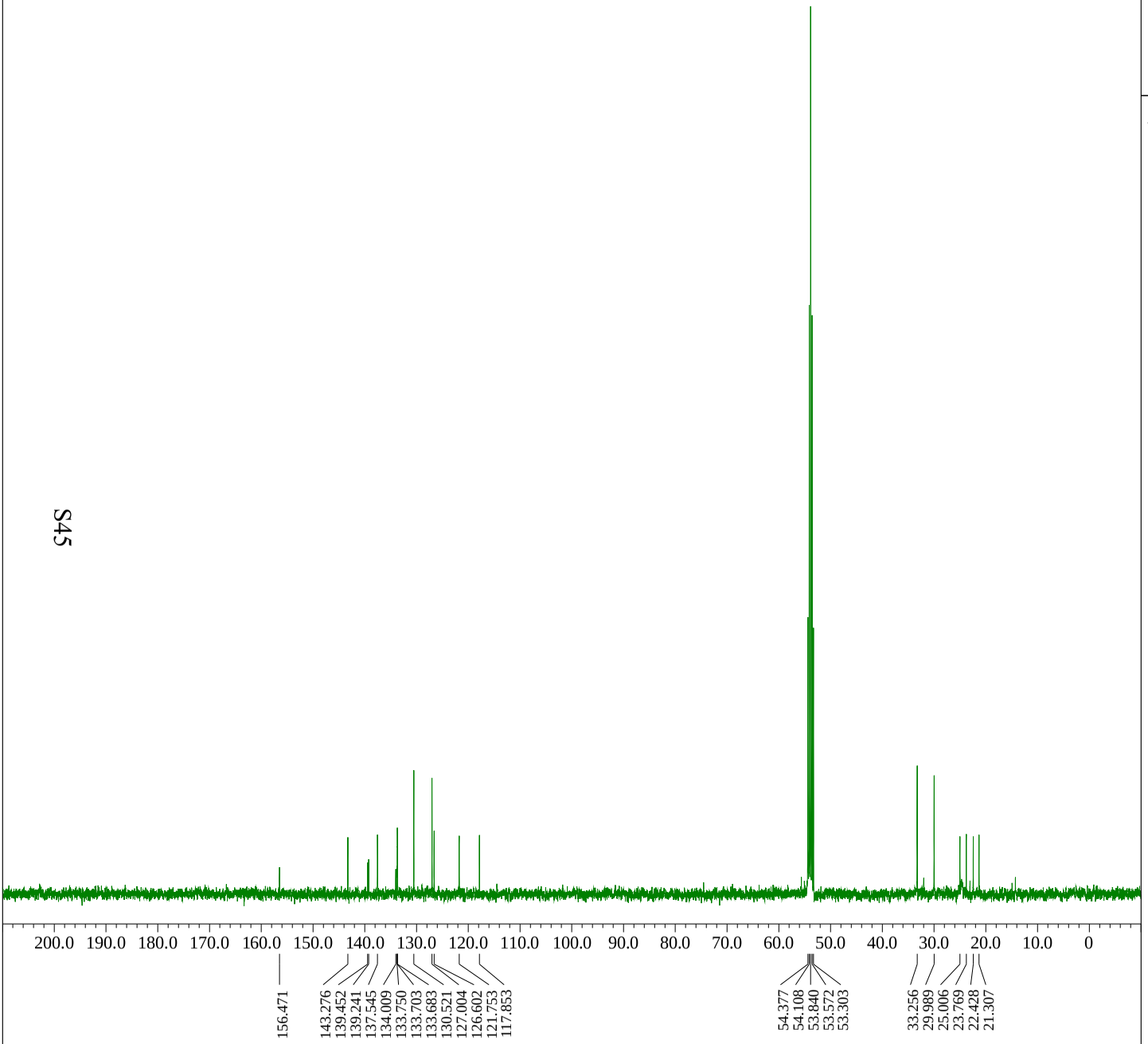



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-N000029_Proton-1- |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = kyy-N000029 |
| Solvent | = METHYLENE-CHLORIDE-D2 |
| Creation_Time | = 24-APR-2017 22:27:28 |
| Revision_Time | = 25-APR-2017 16:33:13 |
| Current_Time | = 25-APR-2017 16:44:26 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECZ400S |
| Spectrometer | = JNM-ECZ400S/L1 |

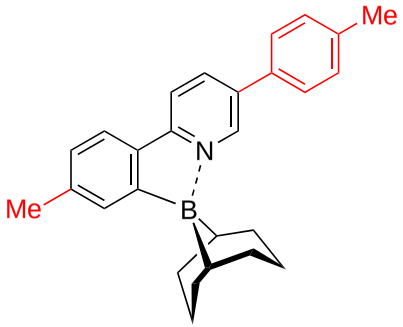



**3o**

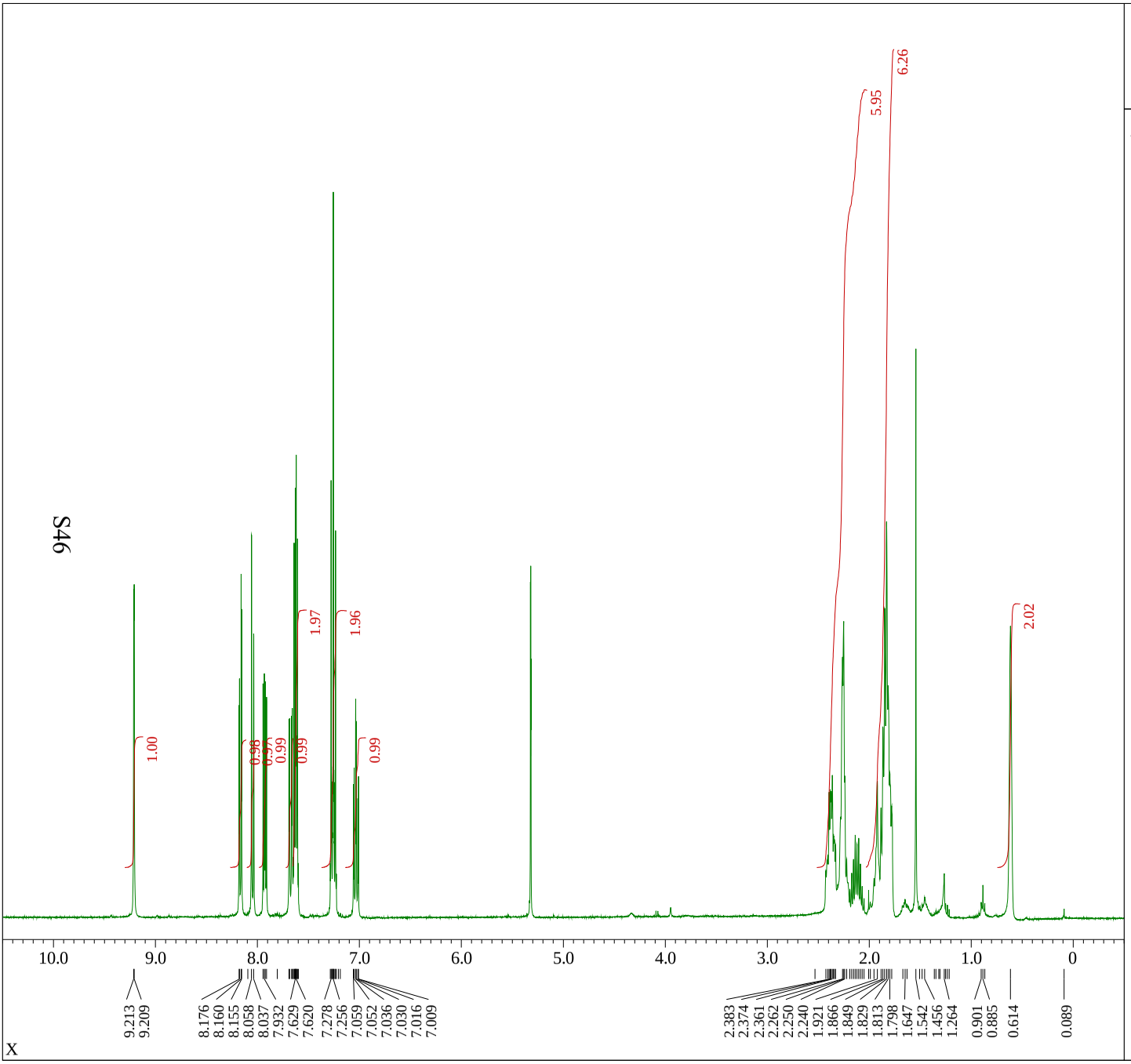



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-N000029_Carbon |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = kyy-N000029 |
| Solvent | = METHYLENE-CHLORIDE |
| Creation_Time | = 24-APR-2017 22:30: |
| Revision_Time | = 25-APR-2017 16:48: |
| Current_Time | = 25-APR-2017 16:52: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECZ400S |
| Spectrometer | = JNM-ECZ400S/L1 |

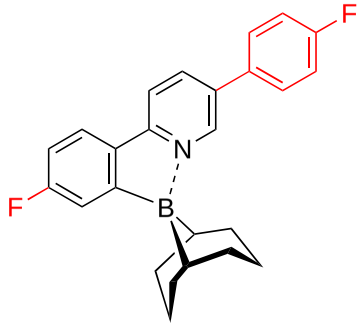



**3o**

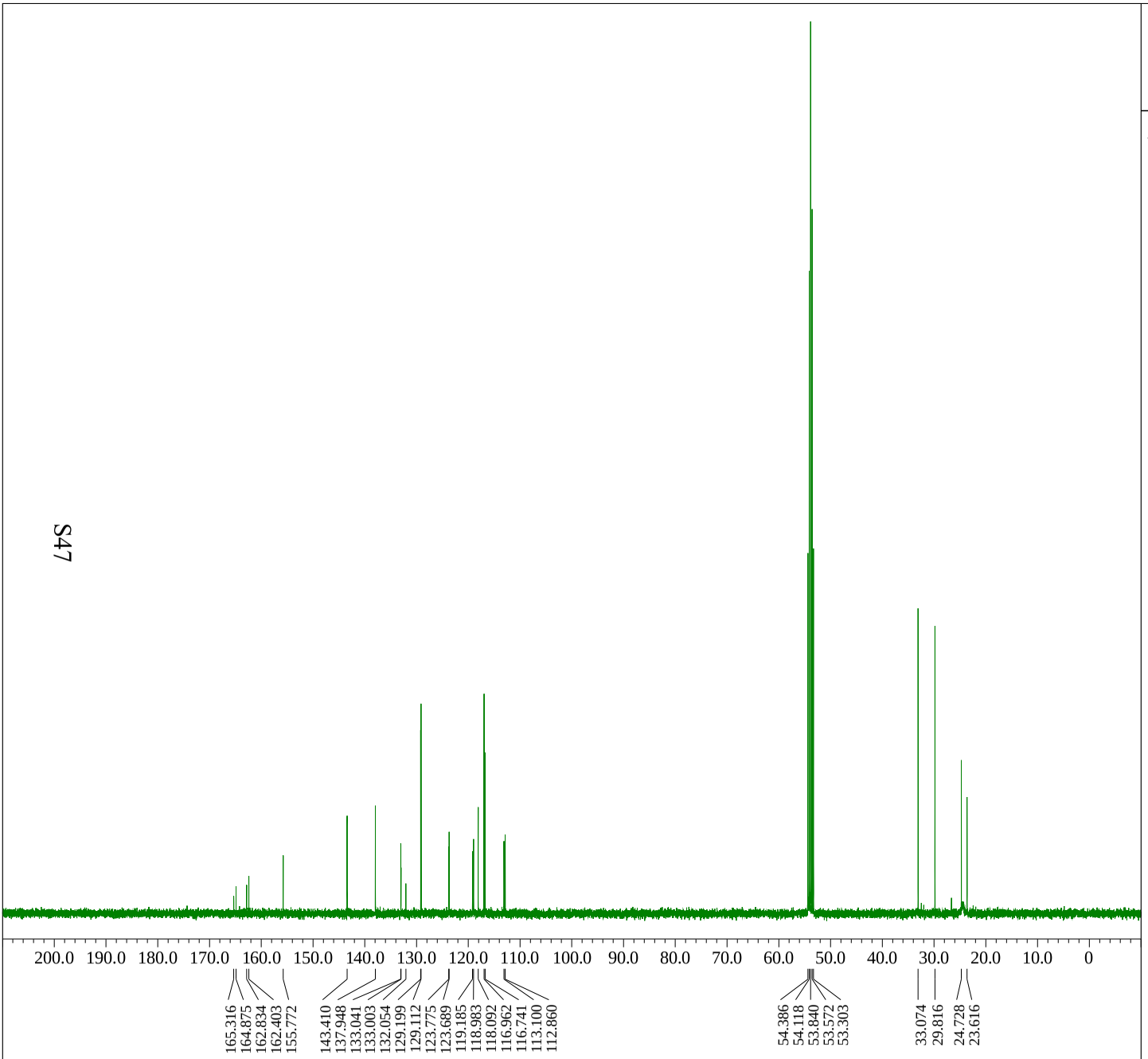



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-N000020_Proton-1- |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = kyy-N000020 |
| Solvent | = METHYLENE-CHLORIDE-D2 |
| Creation_Time | = 21-APR-2017 20:20:58 |
| Revision_Time | = 25-APR-2017 21:56:16 |
| Current_Time | = 25-APR-2017 21:56:29 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECZ400S |
| Spectrometer | = JNM-ECZ400S/L1 |

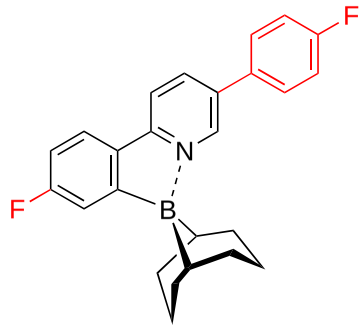



**3p**

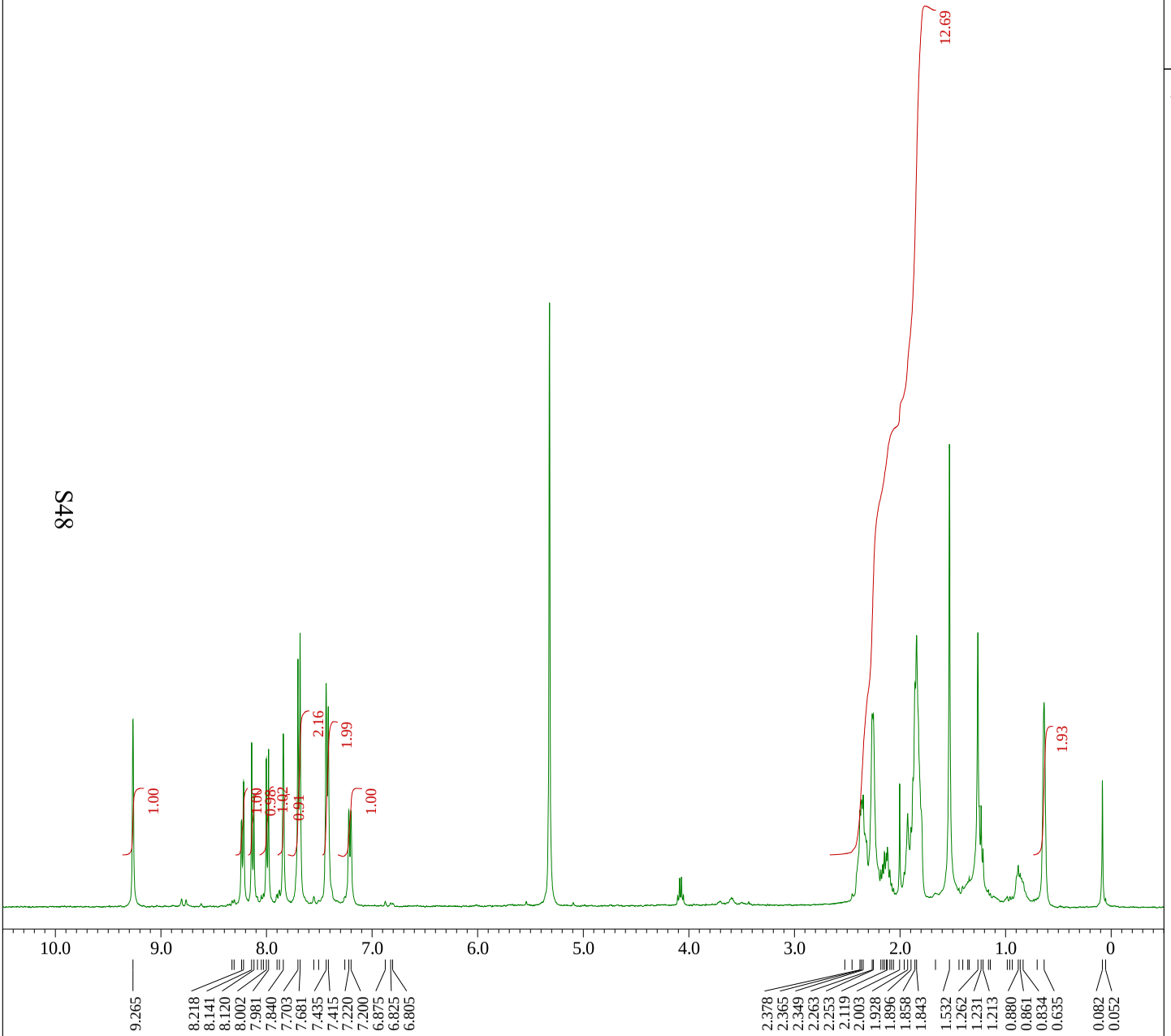



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-N000020_Carbon |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = kyy-N000020 |
| Solvent | = METHYLENE-CHLORIDE |
| Creation_Time | = 21-APR-2017 20:36: |
| Revision_Time | = 25-APR-2017 22:08: |
| Current_Time | = 25-APR-2017 22:08: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECZ400S |
| Spectrometer | = JNM-ECZ400S/L1 |

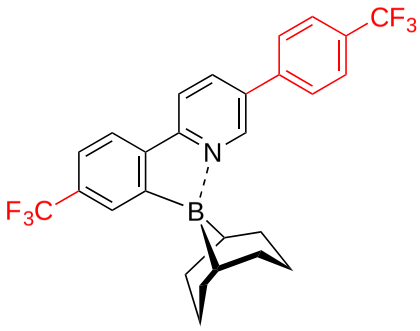



**3p**

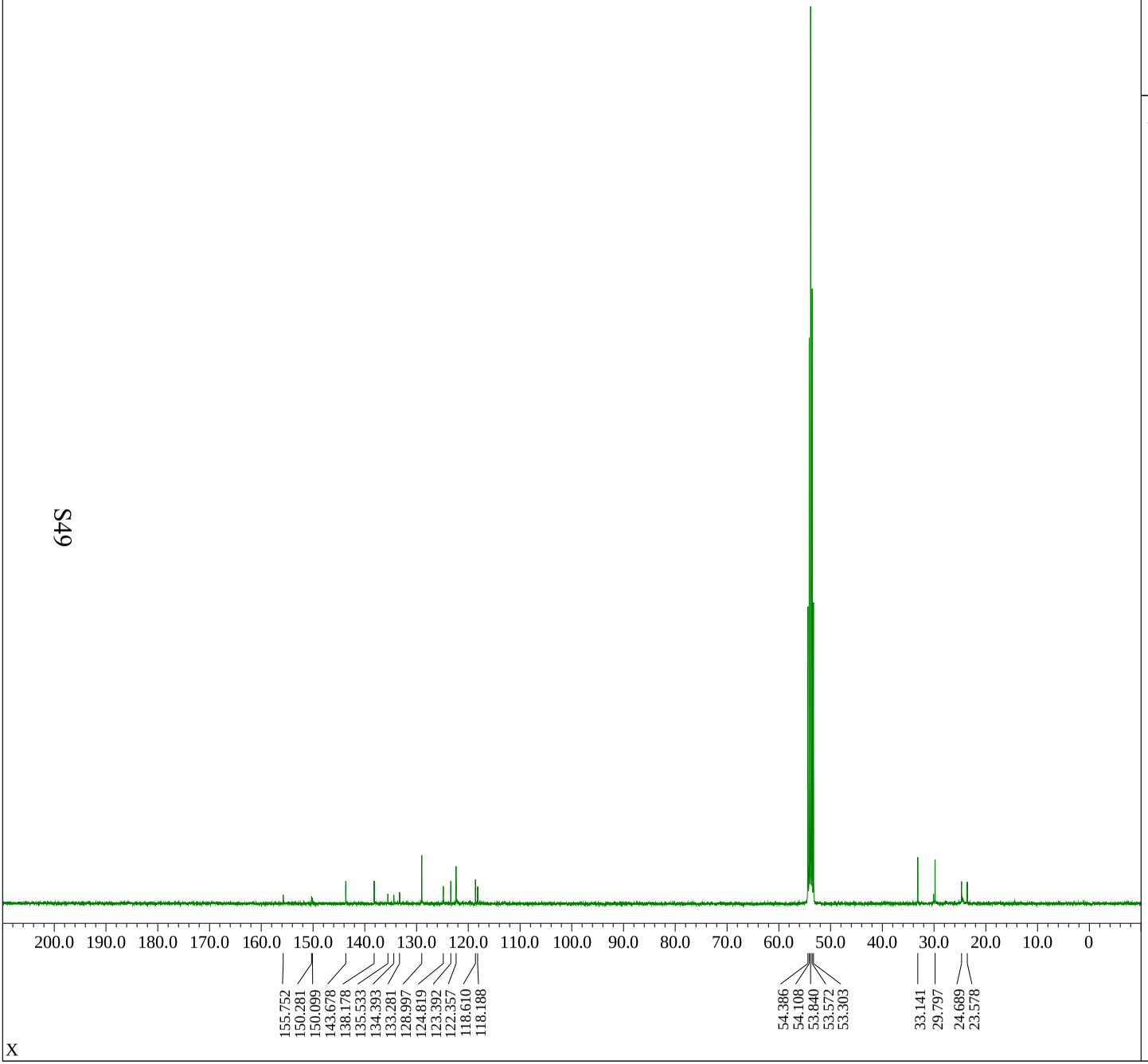



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-N000028_Proton-1- |
| Author | = delta |
| Experiment | = proton.jxp |
| Sample_Id | = kyy-N000028 |
| Solvent | = METHYLENE-CHLORIDE-D2 |
| Creation_Time | = 24-APR-2017 15:33:39 |
| Revision_Time | = 25-APR-2017 17:14:11 |
| Current_Time | = 25-APR-2017 17:14:52 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECZ400S |
| Spectrometer | = JNM-ECZ400S/L1 |

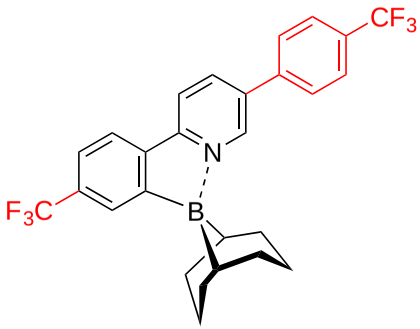



**3q**

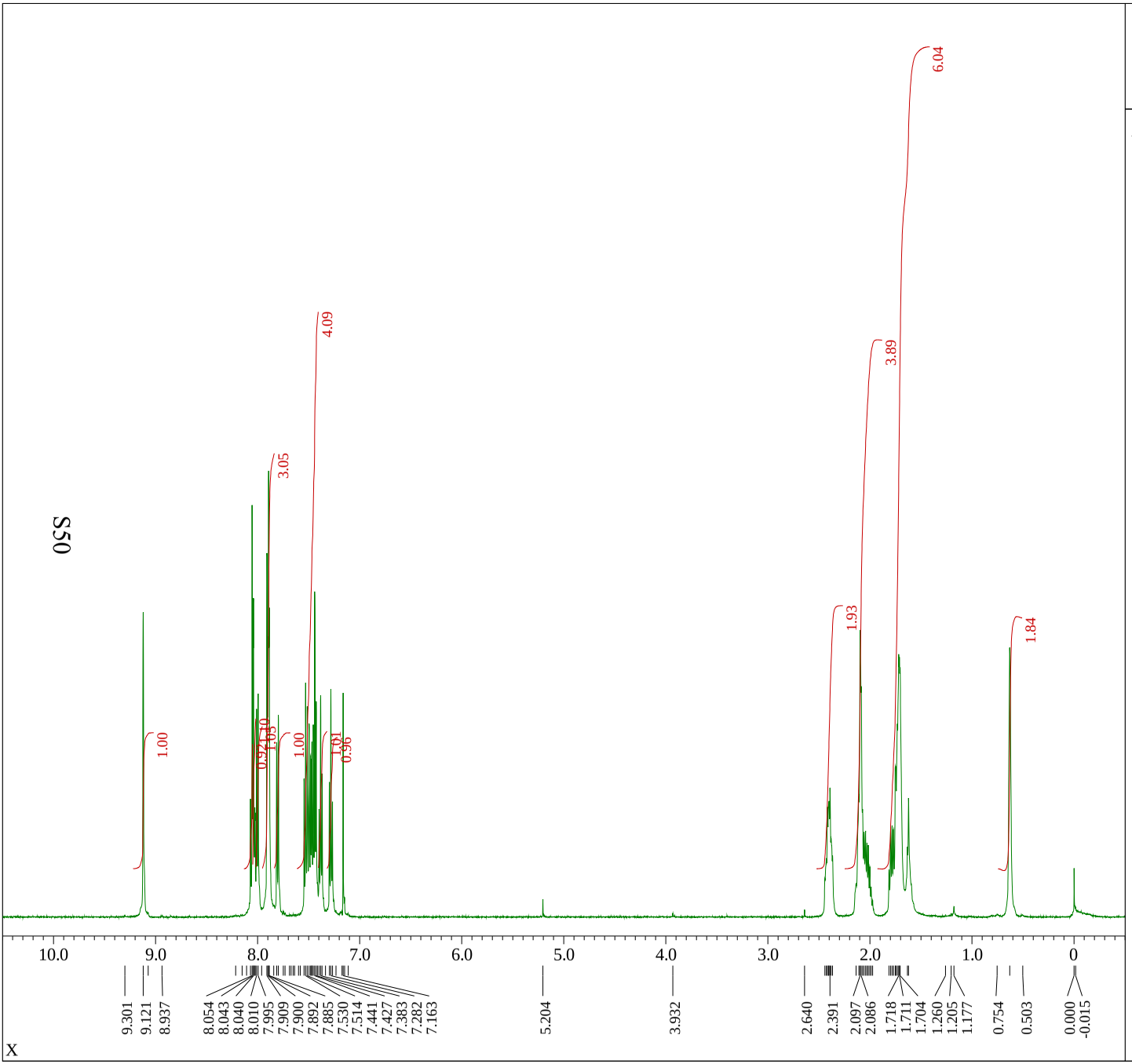



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-N000028_Carbon |
| Author | = delta |
| Experiment | = carbon.jxp |
| Sample_Id | = kyy-N000028 |
| Solvent | = METHYLENE-CHLORIDE |
| Creation_Time | = 24-APR-2017 22:49: |
| Revision_Time | = 25-APR-2017 16:58: |
| Current_Time | = 25-APR-2017 16:58: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = JNM-ECZ400S |
| Spectrometer | = JNM-ECZ400S/L1 |

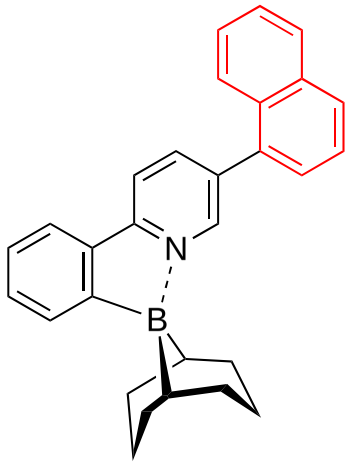



**3q**

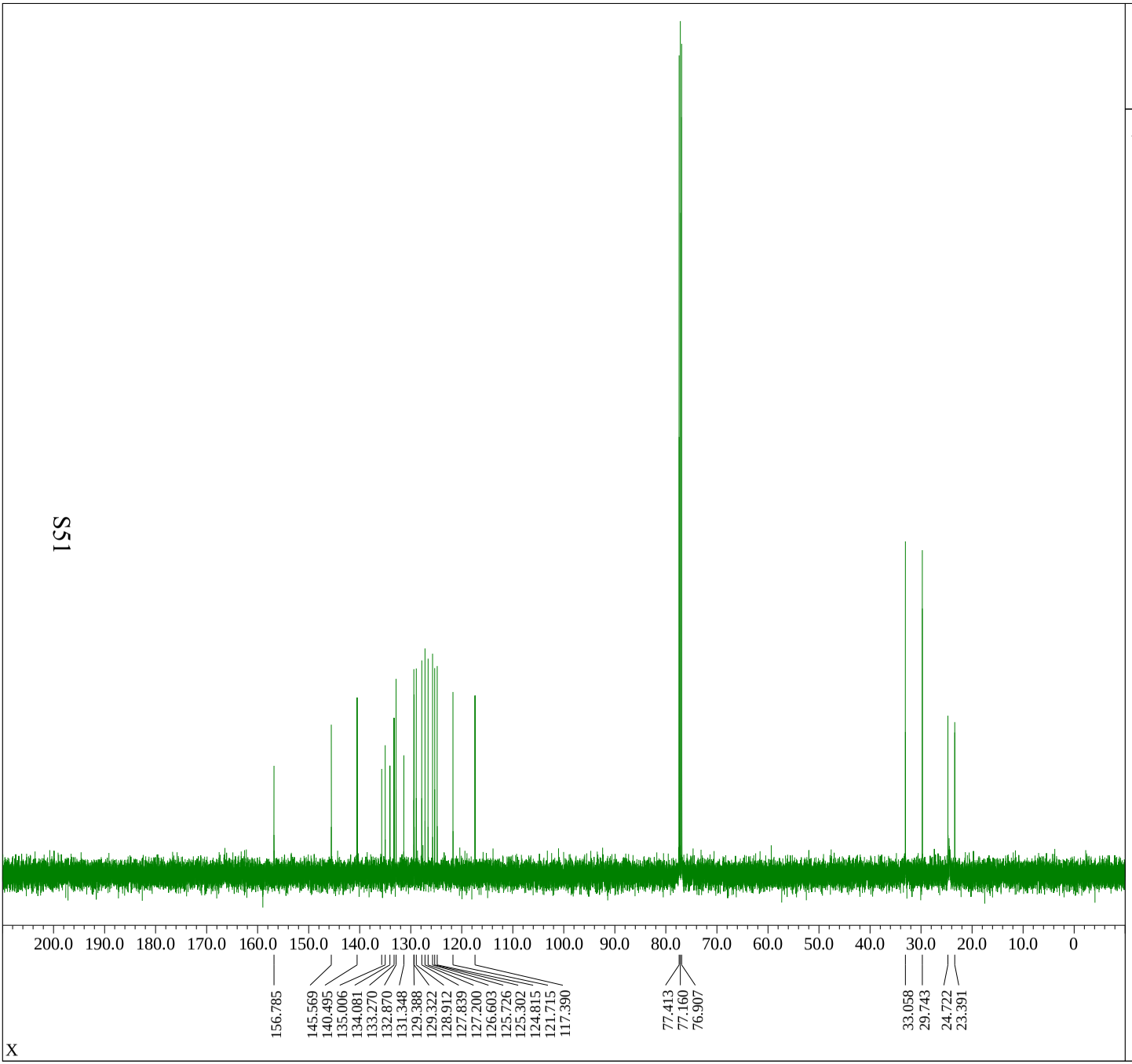



JEOL
Solutions for Innovation

```
Filename          = 002-160722-04-0101-1-1-4.j
Author            = yossy12g
Experiment        = proton.jxp
Solvent           = CDCL3
Creation_Time     = 13-APR-2017 10:58:23
Revision_Time     = 13-APR-2017 11:02:03
Current_Time      = 13-APR-2017 11:02:38

Comment           = 002-160722-04-0101
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 1H
X_Freq            = 500.16241967[MHz]
X_Offset          = 0[Hz]
X_Points          = 13107
X_Prescans        = 1
X_Sweep           = 7.50750781[kHz]
Scans             = 8

Relaxation_Delay  = 5
Recvr_Gain        = 30
Temp_Get          = 21[dC]
```

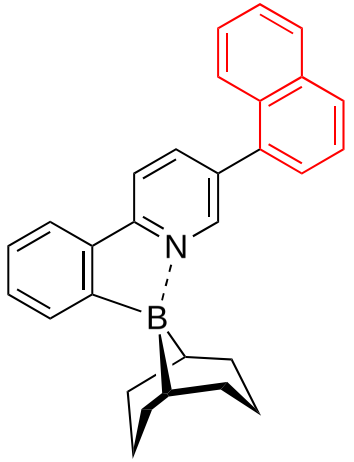



**3r**

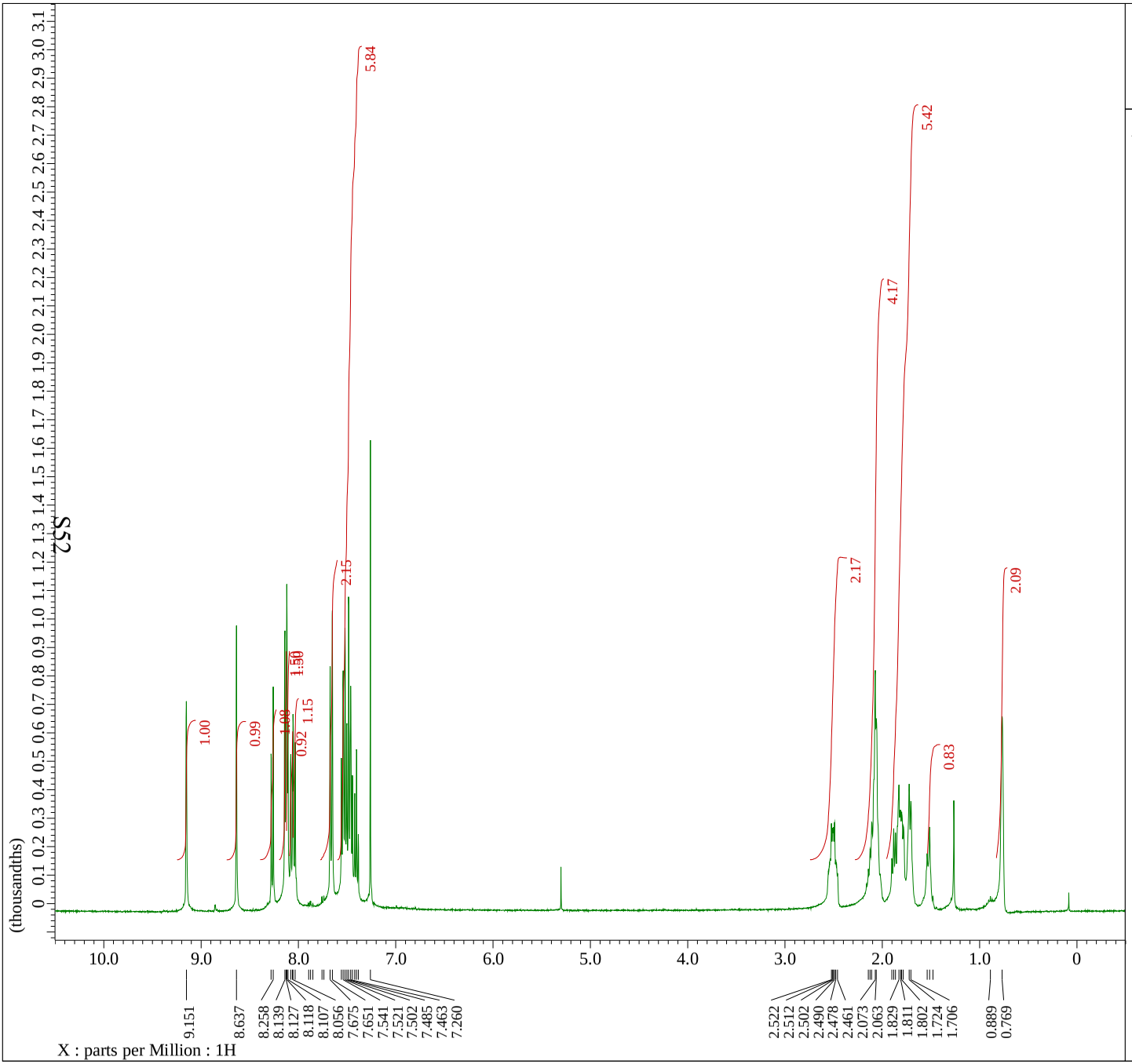



JEOL
Solutions for Innovation

```
Filename          = 002-160722-04-1301-1-1-3.j
Author            = yossy12g
Experiment        = carbon.jxp
Solvent           = CDCL3
Creation_Time     = 13-APR-2017 11:14:55
Revision_Time     = 13-APR-2017 11:15:35
Current_Time      = 13-APR-2017 11:18:39

Comment           = 002-160722-04-0101
Data_Format       = 1D COMPLEX
Dim_Size          = 52428
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 13C
X_Freq            = 125.77787086[MHz]
X_Offset          = 0[Hz]
X_Points          = 52428
X_Prescans        = 1
X_Sweep           = 31.44654102[kHz]
Scans             = 125

Relaxation_Delay = 2
Recvr_Gain        = 60
Temp_Get          = 21.5[dC]
```

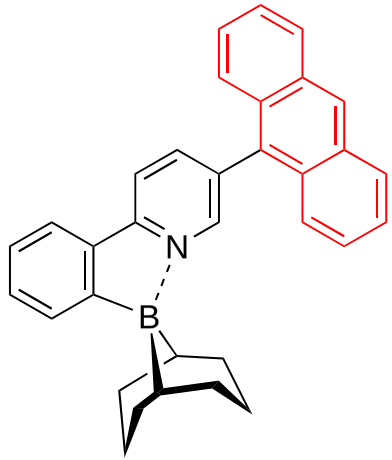



**3r**

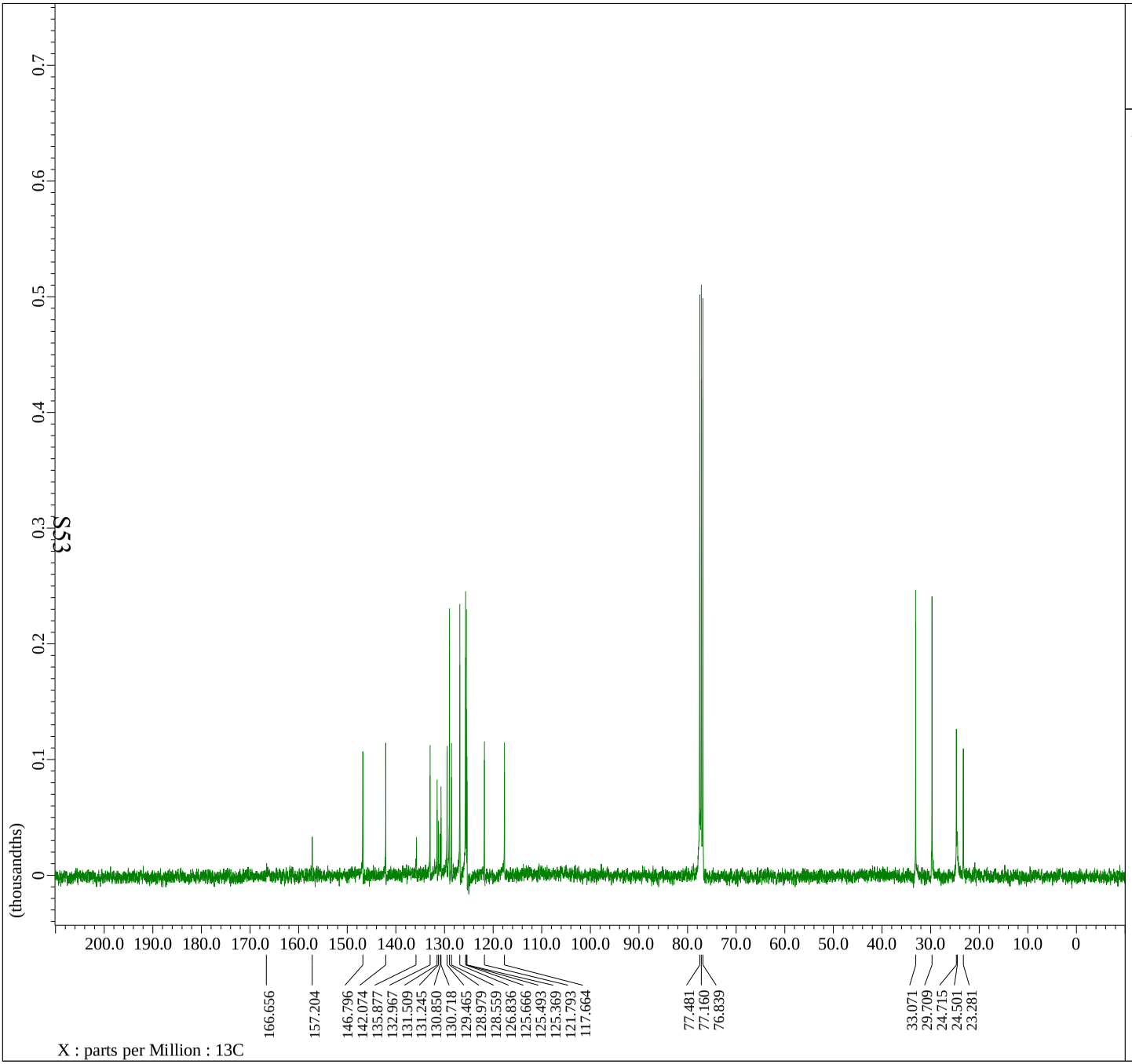



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-00000061non_E3-7.jdf |
| Author | = yossy12g |
| Experiment | = non |
| Solvent | = CDCL3 |
| Creation_Time | = 6-APR-2017 13:51:39 |
| Revision_Time | = 6-APR-2017 14:03:18 |
| Current_Time | = 6-APR-2017 14:03:27 |
| Comment | = 002-0000006 |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 8192 |
| Dim_Title | = 1H |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = ALICE_NMR |
| X_Domain | = 1H |
| X_Freq | = 395.884498[MHz] |
| X_Offset | = 0[Hz] |
| X_Points | = 8192 |
| X_Prescans | = 0 |
| X_Sweep | = 7.91765625[kHz] |
| Scans | = 8 |
| Relaxation_Delay | = 5.96540022 |
| Recvr_Gain | = 16 |
| Temp_Get | = 0[dC] |

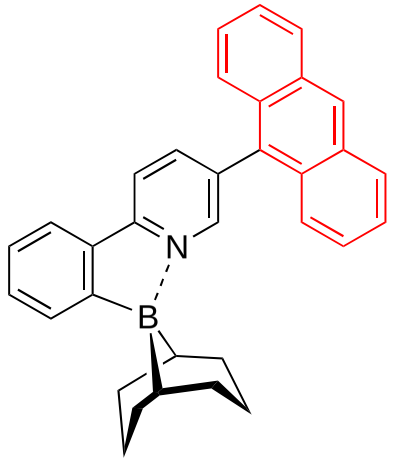



**3s**

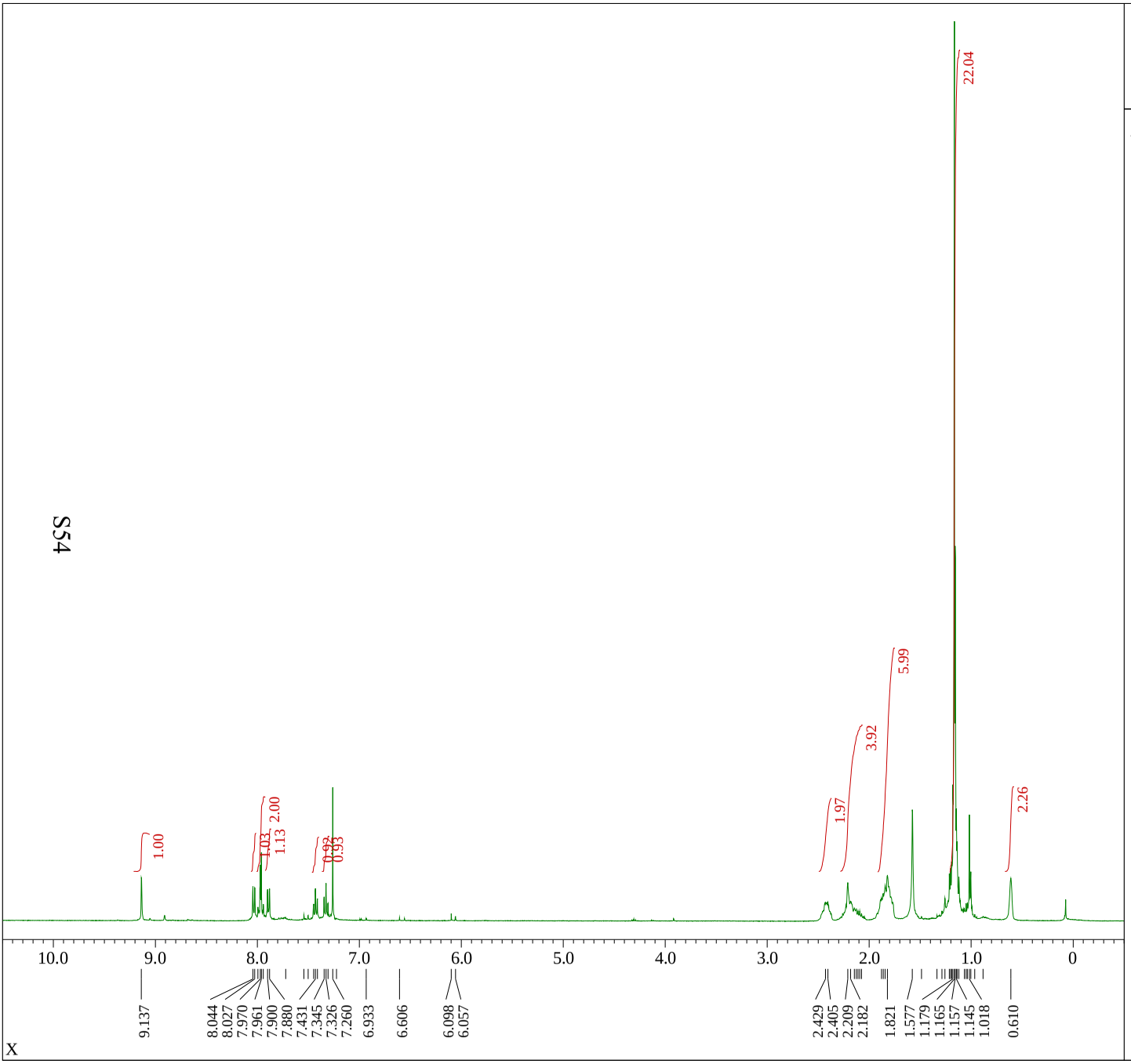



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = kyy-00000062bcm_E3-10.jdf |
| Author | = yossy12g |
| Experiment | = bcm |
| Solvent | = CDCL3 |
| Creation_Time | = 6-APR-2017 10:00:00 |
| Revision_Time | = 6-APR-2017 13:34:05 |
| Current_Time | = 6-APR-2017 13:34:05 |
| Comment | = 002-0000006 |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 32768 |
| Dim_Title | = 13C |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = ALICE_NMR |
| X_Domain | = 13C |
| X_Freq | = 99.55474695[MHz] |
| X_Offset | = 0[Hz] |
| X_Points | = 32768 |
| X_Prescans | = 1 |
| X_Sweep | = 26.8817207[kHz] |
| Scans | = 1024 |
| Relaxation_Delay | = 1.78100002 |
| Recvr_Gain | = 24 |
| Temp_Get | = 0[dC] |

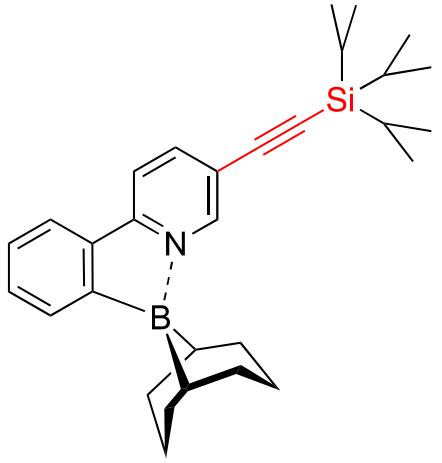



**3s**

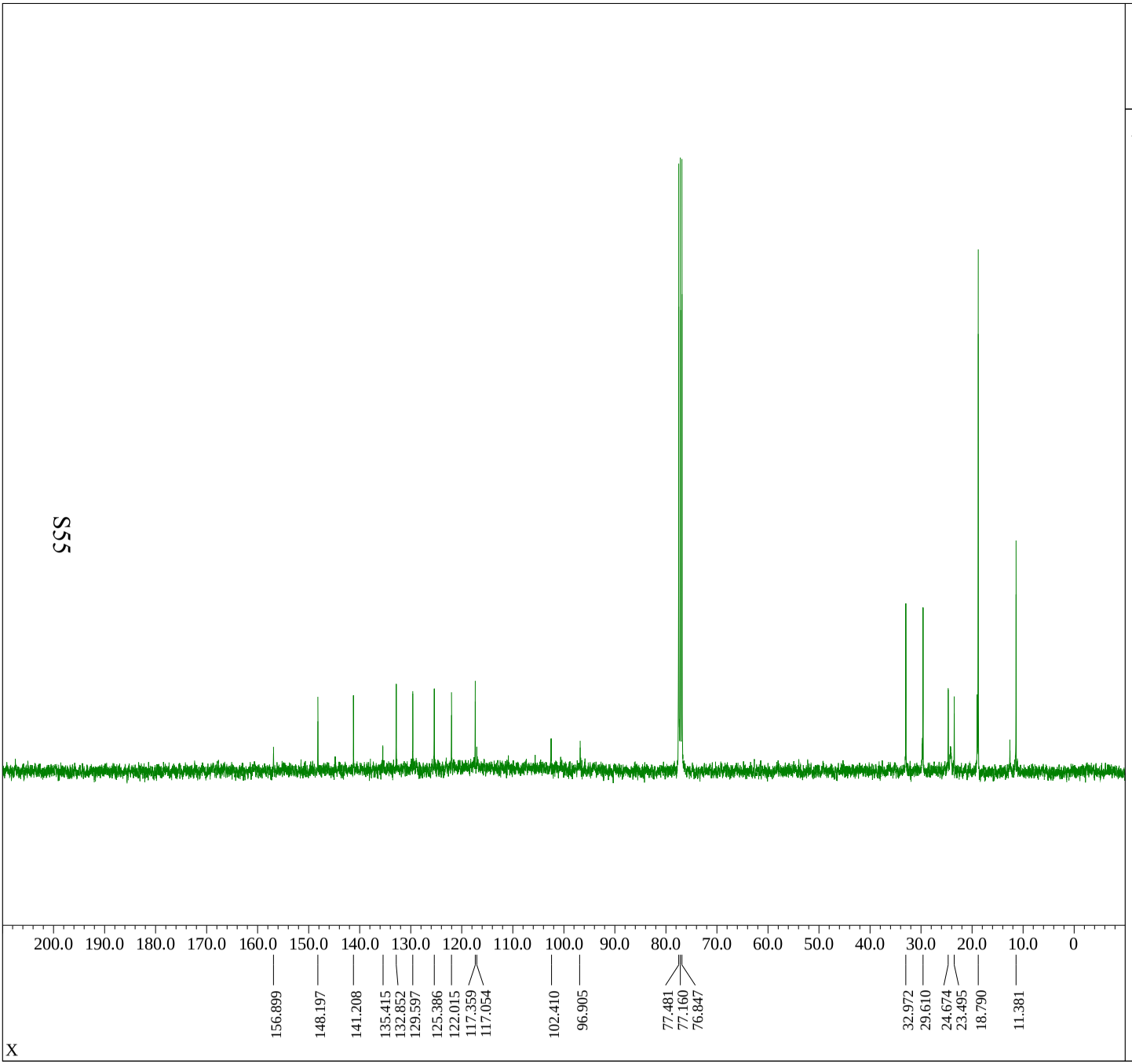



JEOL
Solutions for Innovation

```
Filename          = kyy-N0000071non_E1-5.jdf
Author            = yossy12g
Experiment        = non
Solvent           = CDCL3
Creation_Time     = 14-APR-2017 14:49:03
Revision_Time     = 14-APR-2017 14:59:00
Current_Time      = 14-APR-2017 14:59:09

Comment           = 3u
Data_Format       = 1D COMPLEX
Dim_Size          = 8192
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 1H
X_Freq            = 395.884498[MHz]
X_Offset          = 0[Hz]
X_Points          = 8192
X_Prescans        = 0
X_Sweep           = 7.91765625[kHz]
Scans             = 8

Relaxation_Delay = 5.96540022
Recvr_Gain        = 17
Temp_Get          = 0[dC]
```

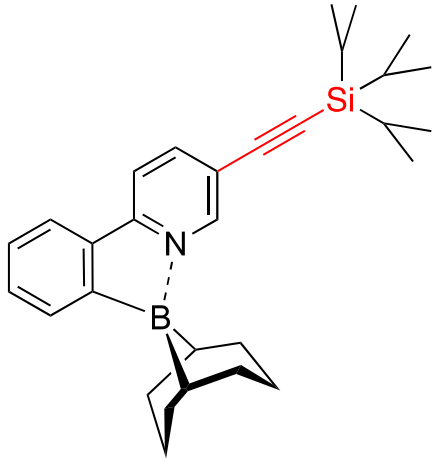



**3t**

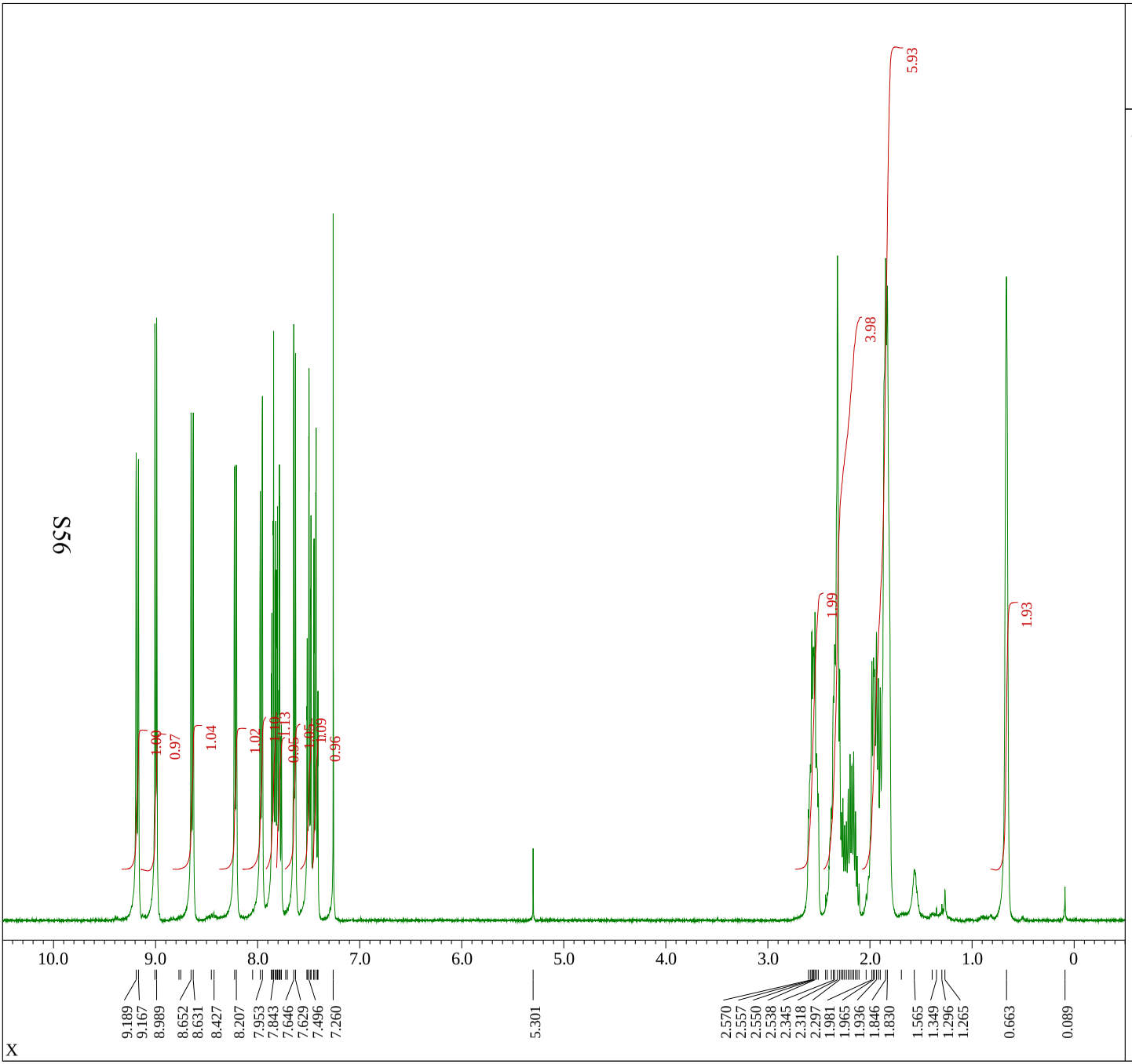



JEOL
Solutions for Innovation

```
Filename          = kyy-N0000072bcm_E1-6.jdf
Author            = yossy12g
Experiment        = bcm
Solvent           = CDCL3
Creation_Time     = 14-APR-2017 14:26:25
Revision_Time     = 14-APR-2017 14:33:01
Current_Time      = 14-APR-2017 14:34:50

Comment           = 3u
Data_Format       = 1D COMPLEX
Dim_Size          = 32768
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 13C
X_Freq            = 99.55474695[MHz]
X_Offset          = 0[Hz]
X_Points          = 32768
X_Prescans        = 1
X_Sweep           = 26.8817207[kHz]
Scans             = 1024

Relaxation_Delay = 1.78100002
Recvr_Gain        = 24
Temp_Get          = 0[dC]
```

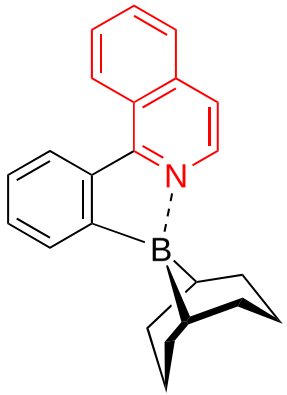



**3t**

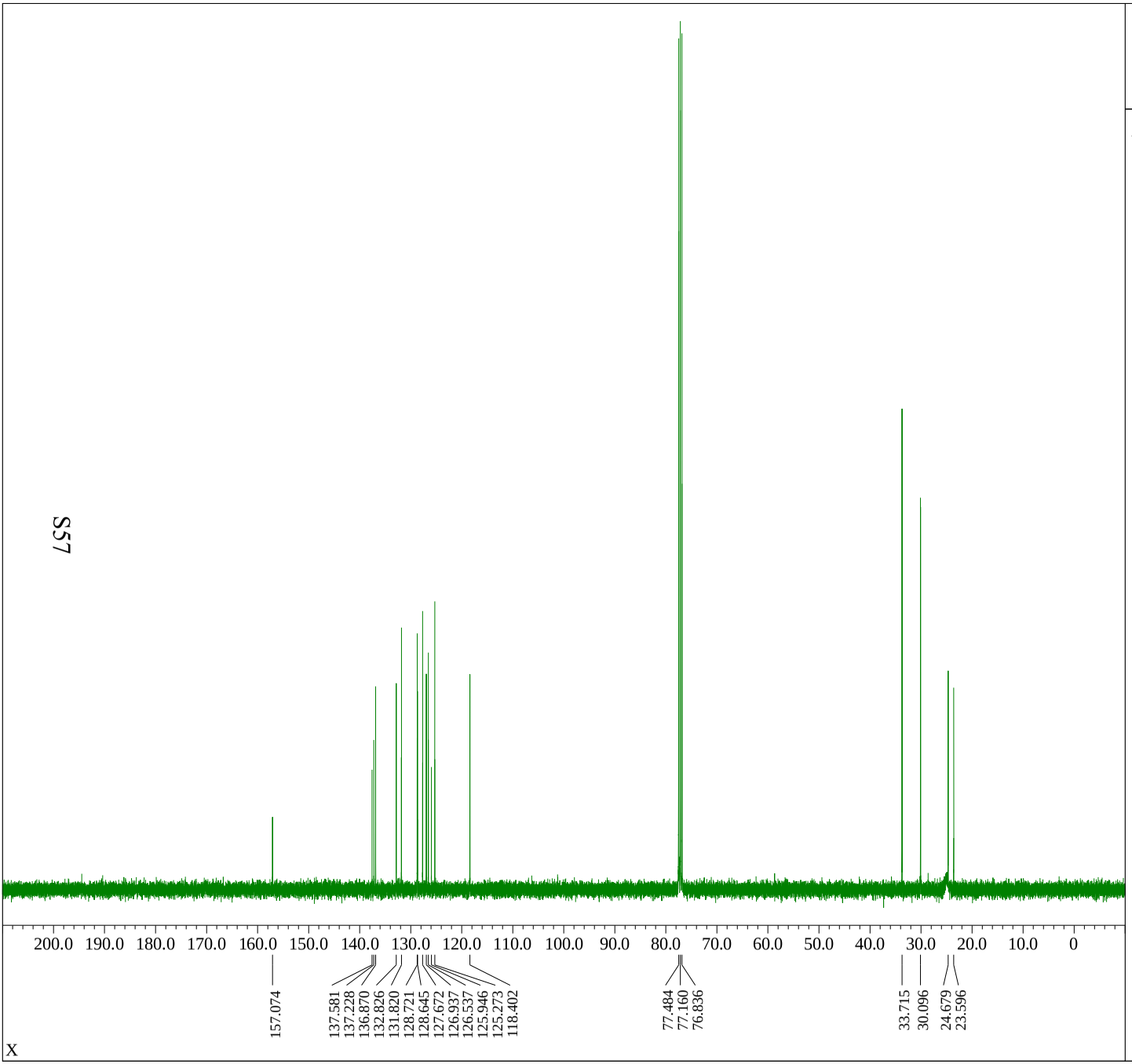



JEOL
Solutions for Innovation

| | |
|---|---|
| Filename | = 002-160613-08-0101-1-1-15. |
| Author | = yossy12g |
| Experiment | = proton.jxp |
| Solvent | = CDCL3 |
| Creation_Time | = 12-APR-2017 11:58:18 |
| Revision_Time | = 12-APR-2017 12:57:07 |
| Current_Time | = 12-APR-2017 12:57:33 |
| Comment | = 002-160613-08-0101 |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| Dim_Title | = 1H |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = ALICE_NMR |
| X_Domain | = 1H |
| X_Freq | = 391.78851212[MHz] |
| X_Offset | = 0[Hz] |
| X_Points | = 13107 |
| X_Prescans | = 1 |
| X_Sweep | = 5.88235303[kHz] |
| Scans | = 8 |
| Relaxation_Delay | = 5 |
| Recvr_Gain | = 34 |
| Temp_Get | = 20[dC] |

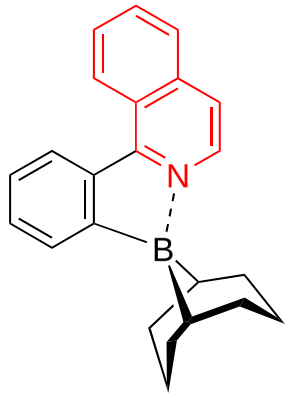



**3u**

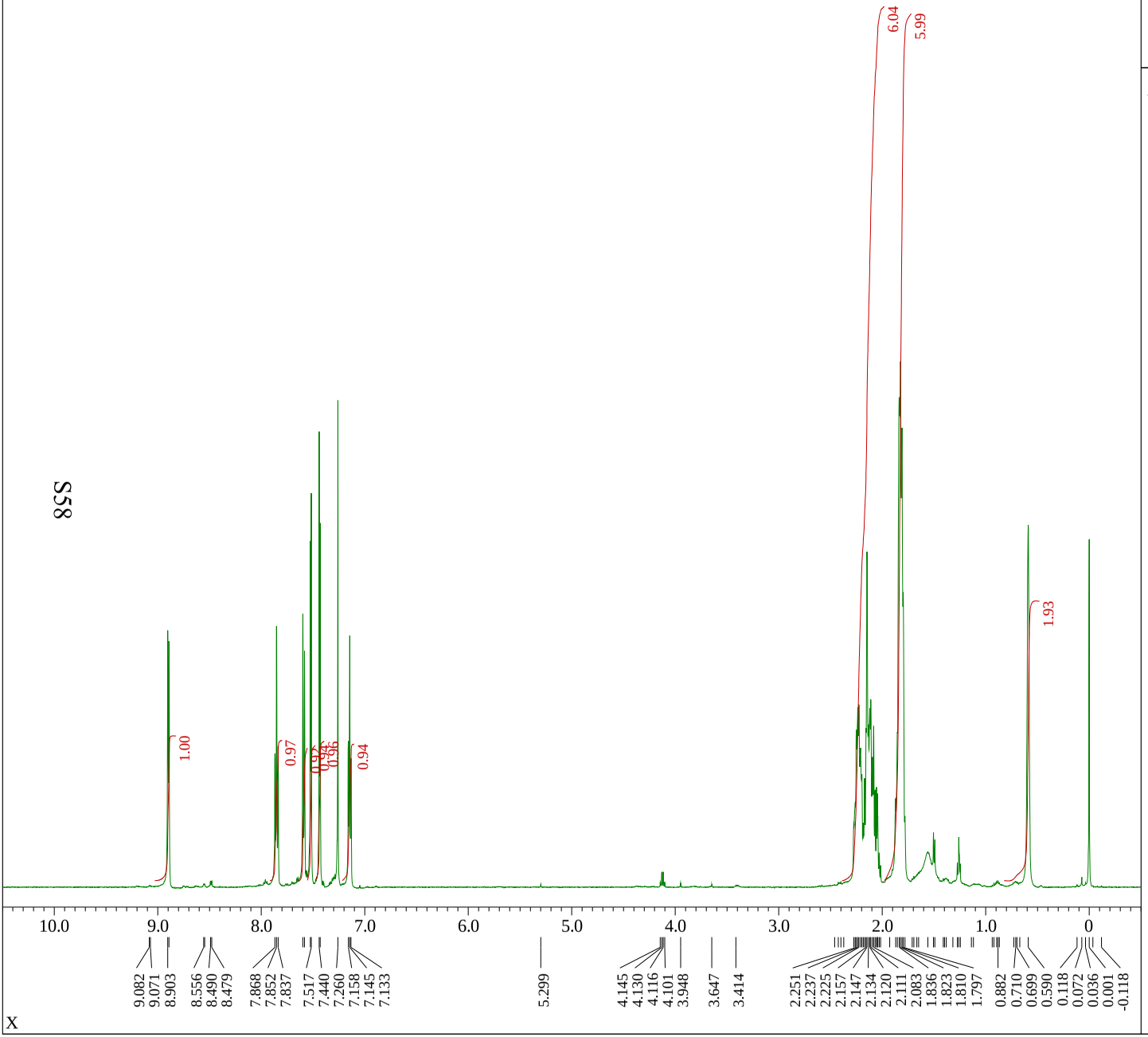



JEOL
Solutions for Innovation

```
Filename          = 002-160613-08-1301-1-1-7.j
Author            = yossy12g
Experiment        = carbon.jxp
Solvent           = CDCL3
Creation_Time     = 12-APR-2017 13:26:19
Revision_Time     = 12-APR-2017 13:26:43
Current_Time      = 12-APR-2017 13:27:11

Comment           = 002-160613-08-1301
Data_Format       = 1D COMPLEX
Dim_Size          = 52428
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 13C
X_Freq            = 98.52464538[MHz]
X_Offset          = 0[Hz]
X_Points          = 52428
X_Prescans        = 1
X_Sweep           = 24.63054297[kHz]
Scans             = 608

Relaxation_Delay = 2
Recvr_Gain        = 60
Temp_Get          = 20.39999962[dC]
```

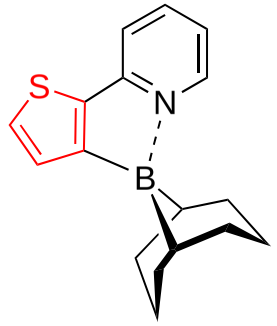



**3u**

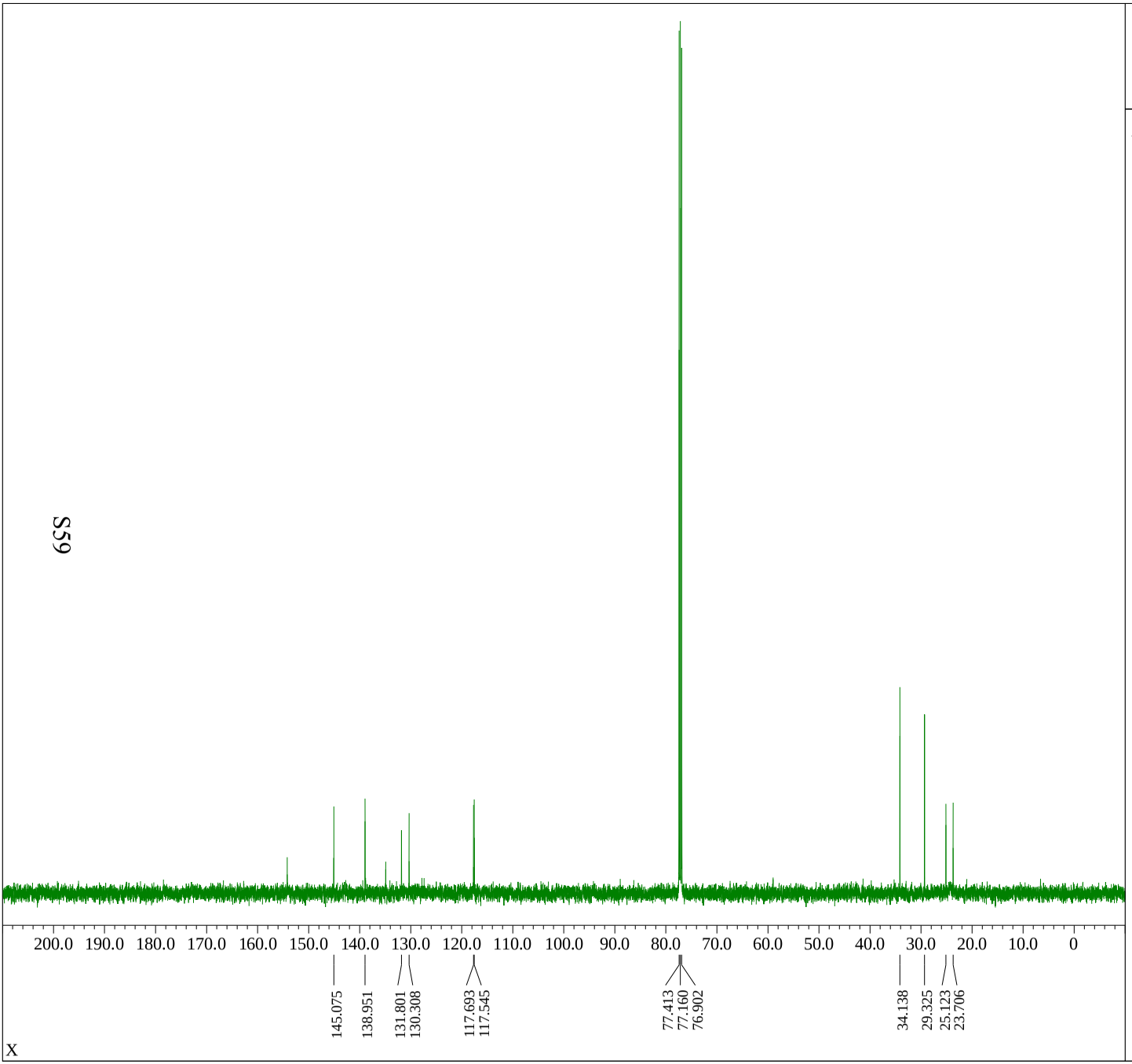



JEOL
Solutions for Innovation

```
Filename          = 002-160613-04-0101-1-1-10.
Author            = yossy12g
Experiment        = proton.jxp
Solvent           = CDCL3
Creation_Time     = 12-APR-2017 16:40:55
Revision_Time     = 12-APR-2017 16:49:14
Current_Time      = 12-APR-2017 16:49:41

Comment           = 002-160613-04-0101
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = 1H
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 1H
X_Freq            = 500.16241967[MHz]
X_Offset          = 0[Hz]
X_Points          = 13107
X_Prescans        = 1
X_Sweep           = 7.50750781[kHz]
Scans             = 8

Relaxation_Delay  = 5
Recvr_Gain        = 30
Temp_Get          = 21[dC]
```

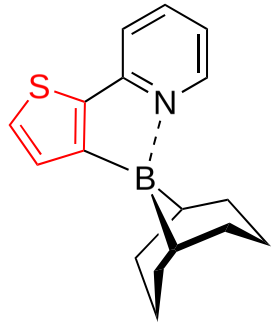



**3v**




JEOL
Solutions for Innovation

```
Filename          = 002-160613-04-1301-1-1-5.j
Author            = yossy12g
Experiment        = carbon.jxp
Solvent           = CDCL3
Creation_Time     = 12-APR-2017 17:09:05
Revision_Time     = 12-APR-2017 17:09:43
Current_Time      = 12-APR-2017 17:10:00

Comment           = 002-160613-04-1301
Data_Format       = 1D COMPLEX
Dim_Size          = 52428
Dim_Title         = 13C
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = ALICE_NMR

X_Domain          = 13C
X_Freq            = 125.77787086[MHz]
X_Offset          = 0[Hz]
X_Points          = 52428
X_Prescans        = 1
X_Sweep           = 31.44654102[kHz]
Scans             = 124

Relaxation_Delay = 2
Recvr_Gain        = 60
Temp_Get          = 21.60000038[dC]
```




**3v**