ELECTRONIC SUPPORTING INFORMATION

for the **comment on**

"An unexpected formation of the novel 7-oxa-2-azabicyclo[2.2.1]hept-5-ene skeleton during the reaction of furfurylamine with maleimides and their bioprospection using a zebrafish embryo model" by C. E. Puerto Galvis and V. V. Kouznetsov, *Org. Biomol. Chem.*, 2013, *11*, 407.

by

Fedor I. Zubkov, Elizaveta A. Kvyatkovskaya, Eugenia E. Nikitina, Addy Amoyaw, Vladimir V. Kouznetsov, Vladimir A. Lazarenko, Victor N. Khrustalev

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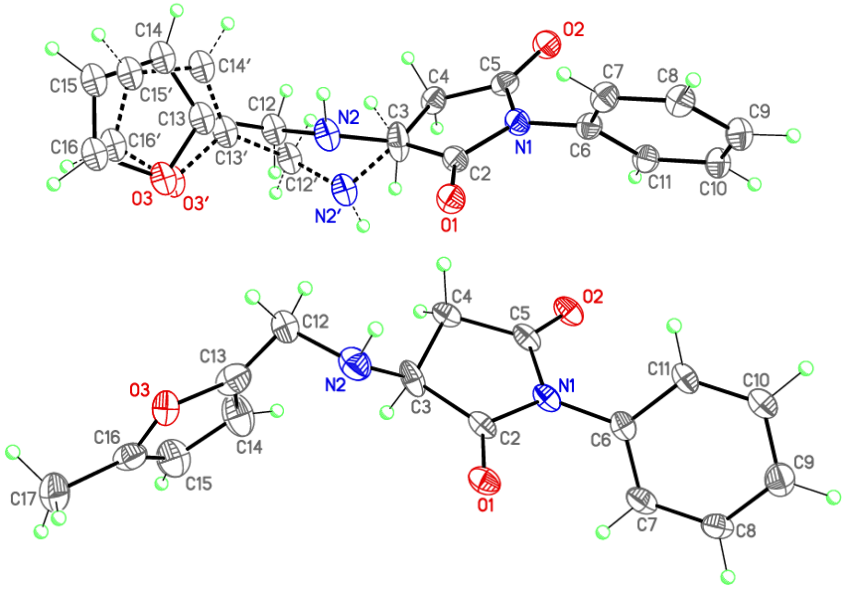
Contents

1. X-Ray description of compounds 6c and 6h

Compounds of **6c** and **6h** were characterized by single-crystal X-ray diffraction study, and their structures are shown in Figure 1 along with the atomic numbering schemes.

Figure 1



Molecular structures of **6c** (top) and **6h** (bottom). Displacement ellipsoids are shown at the 50% probability level. The alternative position of the disordered fragment in **6c** is depicted by dashed lines.

Despite the presence of different substituents in 5-position of the furyl group – H and Me, the compounds **6c** and **6h** are isostructural and crystallize in the orthorhombic space group *P*ca2$_1$. The central pyrrolidine-2,5-dione cycle is almost planar (rms deviation is 0.043 and 0.060 Å for **6c** and **6h**, respectively). The phenyl ring is twisted by 62.24(18) and 61.32(16)° for **6c** and **6h**, respectively, relative to the pyrrolidine-2,5-dione cycle. The N2 nitrogen atom has a trigonal-pyramidal configuration (the sum of bond angles is 333.1/329.6 and 329.1° for **6c** and **6h**, respectively).

The molecules of **6c** and **6h** are substantially distinguished by only conformation of the C3─N2─C12─C13 chain (the corresponding torsion angle is -96.6(14)/-177.1(10) and 79.7(9)° for **6c** and **6h**, respectively).

The molecules of **6c** and **6h** possess an asymmetric center at the C3 carbon atom; the crystals are racemic and consist of the enantiomeric pairs.

In the crystals, molecules of **6c** and **6h** form layers parallel to (100) by the intermolecular N─H···O and C─H···O hydrogen bonds (see Supplementary materials).

X-ray crystal structure determination. X-ray diffraction data were collected on the 'Belok' beamline (λ = 0.96990 Å) of the National Research Center 'Kurchatov Institute' (Moscow, Russian Federation) using a Rayonix SX165 CCD detector. A total of 360 images for each compound were collected using an oscillation range of 1.0° and φ scan mode, and corrected for absorption using the *Scala* program.[1] The data were indexed, integrated and scaled using the utility *iMOSFLM* in CCP4 program.[2] For details, see Table 1. The structures were determined by direct methods and refined by full-matrix least squares technique on F^2 with anisotropic displacement parameters for non-hydrogen atoms. In **6c**, the different isomers occupy the same positions with the equal occupancies. The hydrogen atoms were placed in calculated positions and refined within riding model with fixed isotropic displacement parameters [U_{iso}(H) = 1.5U_{eq}(N), 1.5U_{eq}(C) for the CH_3-groups and 1.2U_{eq}(C) for the other groups]. All calculations were carried out using the SHELXTL program.[3]

Crystallographic data for **6c** and **6h** have been deposited with the Cambridge Crystallographic Data Center, CCDC 1547011 and CCDC 1547012. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk).

Table 1. Crystallographic Data for **6c** and **6h**.

compound	**6c**	**6h**
empirical formula	$C_{15}H_{14}N_2O_3$	$C_{16}H_{16}N_2O_3$
fw	270.28	284.31
T, K	100(2)	100(2)
crystal size, mm	0.10×0.10×0.08	0.03×0.03×0.03
crystal system	orthorhombic	orthorhombic
space group	$Pca2_1$	$Pca2_1$
a, Å	17.132(3)	17.231(3)
b, Å	13.827(3)	14.729(3)
c, Å	5.5861(11)	5.6114(11)
α, deg.	90	90
β, deg.	90	90
γ, deg.	90	90
V, Å^3	1323.3(5)	1424.1(5)
Z	4	4
d_c, g · cm^{-3}	1.357	1.326

$F(000)$	568	600
μ, mm^{-1}	0.222	0.195
$2\theta_{max}$, deg.	76.59	76.89
index range	$-21 <= h <= 21$	$-21 <= h <= 21$
	$-17 <= k <= 17$	$-18 <= k <= 18$
	$-6 <= l <= 6$	$-6 <= l <= 6$
no. of rflns collected	11370	20771
no. of unique rflns	2694 (R_{int} = 0.0986)	3004 (R_{int} = 0.0717)
no. of rflns with $I > 2\sigma(I)$	1631	1676
data/restraints/parameters	2694 / 25 / 167	3004 / 1 / 192
R_1; wR_2 ($I > 2\sigma(I)$)	0.0890; 0.2070	0.0792; 0.1694
R_1; wR_2 (all data)	0.1270; 0.2300	0.1411; 0.1934
GOF on F^2	1.038	1.008
Extinction coefficient	0.043(4)	0.008(1)
T_{max}; T_{min}	0.980; 0.960	0.987; 0.987
ρ_{max} / ρ_{min}, ēÅ^3	0.314 / -0.298	-0.525 / 0.302

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1. P. R. Evans, *Acta Cryst.* 2005, **D62**, 72-82.

2. T. G. G. Battye, L. Kontogiannis, O. Johnson, H. R. Powell, A. G. W. Leslie, *Acta Cryst.* 2011, **D67**, 271-281.

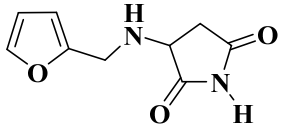
3. G. M. Sheldrick, *Acta Cryst.* 2015, **C71**, 3-8.

2. Experimental section

All commercially available reagents and solvents were used without further purification. Melting points were determined for recrystallized simples with SMP 30 apparatus within 0.5 °C accuracy and are uncorrected. IR spectra were obtained in thin film (for oils) or KBr pellets (for crystals) using an IR-Fourier spectrometer Infralum FT-801. High-resolution mass spectra (HRMS) were taken on a mass-spectrometer using an MALDI-TOF mass spectrometer Bruker autoflex speed (solid-state UV-laser with λ = 355 nm), operated in positive reflectron mode (2,5-dihydroxybenzoic acid was used as matrix). NMR spectra were run in deuterated (> 99.5%) solvents on Jeol JNM-ECA 600 (600.1 MHz for ^{1}H and 150.9 MHz for ^{13}C) spectrometer for solutions in $CDCl_3$ or DMSO-d_6 at 20-23 °C using TMS as internal standard. Assignments of ^{1}H and ^{13}C signals were made with the aid of 2D COSY, NOESY and HMBC NMR spectra where necessary or by analogy with the data of Supplementary materials of the paper *Org. Biomol. Chem*. 2013, **11**, 407.

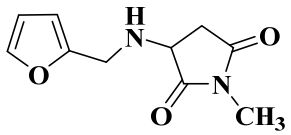
Microanalyses were performed for C, H, N on an elemental analysis system Eurovector EA 3000 (CHNS) and were within ±0.4 % of theoretical values.

General procedure for the preparation of the Michael adducts 6. Selected maleimide **1** (5 mmol) was added to a solution of the appropriate furfuryl amine **2** (5 mmol) in acetonitrile (15 mL). The resulting solution was boiled at reflux for 1 h. Then the reaction mixture was concentrated and recrystallization or flash chromatography purification on silica gel (CH_2Cl_2) was performed to yield an analytical simple of amide **6**.

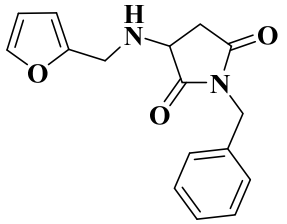


3-[(Furan-2-ylmethyl)amino]pyrrolidine-2,5-dione (6a). Purification by flash chromatography afforded compound **6a** as a light yellow oil (0.71 g, 3.61 mmol, 73 % yield). IR-FT (liquid film, cm^{-1}): 3316 (NH), 1770 and 1665 (C=O). ^{1}H NMR δ (600 MHz, $CDCl_3$): 8.62 (1H, br. s, NH), 7.39 (1H, dd, J = 1.0, 2.0 Hz, H_{Furyl}-5), 6.33 (1H, dd, J = 2.0, 3.0 Hz, H_{Furyl}-4), 6.24 (1H, br. dd, J = 1.0, 3.0 Hz, H_{Furyl}-3), 3.95 (1H, d, J = 14.6 Hz, NCH_2-A), 3.87 (1H, d, J = 14.6 Hz, NCH_2-B), 3.80 (1H, dd, J = 5.0, 8.1 Hz, H-3), 2.91 (1H, dd, J = 8.1, 18.2 Hz, H-4A), 2.56 (1H, dd, J = 5.0, 18.2 Hz, H-4B), 2.10 (1H, br. s, NH) ppm.

^{13}C NMR δ (150 MHz, $CDCl_3$): 178.9 and 176.3 (C-2 and C-5), 152.2 (C_{Furyl}-2), 142.6 (C_{Furyl}-5), 110.4 and 108.2 (C_{Furyl}-3 and C_{Furyl}-4), 56.2 (C-3), 43.9 (NH-CH_2), 37.2 (C-4) ppm. MALDI-TOF HRMS: found 195.0760. $C_9H_{11}N_2O_3$ requires for $(M+H)^+$ 195.0754; found 217.0582. Requires for $C_9H_{10}N_2O_3Na$ $(M+Na)^+$ 217.0571. Found: C, 55.32; H, 5.51; N, 14.27. $C_9H_{10}N_2O_3$ requires C, 55.67; H, 5.19; N, 14.43.

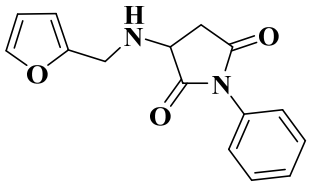


3-[(Furan-2-ylmethyl)amino]-1-methylpyrrolidine-2,5-dione (6b). Purification by flash chromatography afforded compound **6b** as a light yellow oil (0.89 g, 4.32 mmol, 86 % yield). IR-FT (liquid film, cm^{-1}): 3323 (NH), 1780 and 1704 (C=O). ^{1}H NMR δ (600 MHz, $CDCl_3$): 7.39 (1H, dd, J = 1.5, 2.0 Hz, H_{Furyl}-5), 6.33 (1H, dd, J = 2.0, 3.0 Hz, H_{Furyl}-4), 6.24 (1H, br. d, J = 3.0 Hz, H_{Furyl}-3), 3.95 (1H, d, J = 14.6 Hz, NCH_2-A), 3.87 (1H, d, J = 14.6 Hz, H-1B), 3.76 (1H, dd, J = 4.8, 8.0 Hz, H-3), 2.99 (3H, s, N-CH_3), 2.88 (1H, dd, J = 8.0, 17.7 Hz, H-4A), 2.49 (1H, dd, J = 7.8, 17.7 Hz, H-4B), 2.24 (1H, br. s, NH) ppm. ^{13}C NMR δ (150 MHz, $CDCl_3$): 177.9 and 175.3 (C-2 and C-5), 152.4 (C_{Furyl}-2), 142.5 (C_{Furyl}-5), 110.4 and 108.1 (C_{Furyl}-3 and C_{Furyl}-4), 55.1 (C-3), 44.1 (NH-CH_2), 36.2 (C-4), 24.8 (N-CH_3) ppm. MALDI-TOF HRMS: found 231.0736. $C_{10}H_{12}N_2O_3Na$ requires for $(M+Na)^+$ 195.075231.0740.

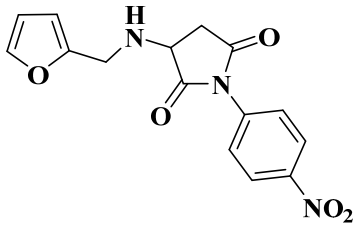


1-Benzyl-3-[(furan-2-ylmethyl)amino]pyrrolidine-2,5-dione (6c). Purification by flash chromatography afforded compound **6c** as a light brown oil (1.08 g, 3.84 mmol, 76 % yield). IR-FT (liquid film, cm^{-1}): 3322 (NH), 1777 and 1709 (C=O). ^{1}H NMR δ (600 MHz, $CDCl_3$): 7.36 (2H, dd, J = 1.0, 7.5 Hz, H_{Ph}-2,6), 7.30 (3H, m, H_{Ph}-3,4,5), 6.31 (1H, dd, J = 1.8, 3.4 Hz, H_{Furyl}-4), 6.20 (1H, br. d, J = 3.4 Hz, H_{Furyl}-3), 4.64 (1H, d, J = 14.7 Hz, N-C$\underline{H}_2$-Ph), 4.61 (1H, d, J = 14.7 Hz, N-C$\underline{H}_2$-Ph), 3.91 (1H, d, J = 14.6 Hz, N-C$\underline{H}_2$-Furyl), 3.84 (1H, d, J = 14.6 Hz, N-C$\underline{H}_2$-Furyl), 3.73 (1H, dd, J = 5.0, 8.3 Hz, H-3), 2.87 (1H, dd, J = 8.3, 17.9 Hz, H-4A), 2.49 (1H, dd, J = 5.0, 17.9 Hz, H-4B), 2.23 (1H, br. s, NH) ppm.

^{13}C NMR δ (150 MHz, $CDCl_3$): 177.5 and 174.9 (C-2 and C-5), 152.3 (C_{Furyl}-2), 142.5 (C_{Furyl}-5), 135.6 (C_{Ph}-1), 128.9 (2C, C_{Ph}-3,5), 128.8 (2C, C_{Ph}-2,6), 128.1 (C_{Ph}-4), 110.4 and 108.1 (C_{Furyl}-3 and C_{Furyl}-4), 55.1 (C-3), 44.2 and 42.5 (NH-<u>C</u>H_2-Ph and NH-<u>C</u>H_2-Furyl), 36.2 (C-4) ppm. MALDI-TOF HRMS: found 285.1222. $C_{16}H_{17}N_2O_3$ requires for $(M+H)^+$ 285.1234; found 307.1063. Requires for $C_{16}H_{16}N_2O_3Na$ $(M+Na)^+$ 307.1053. Found: C, 67.33; H, 5.85; N, 9.63. $C_{16}H_{15}N_2O_3$ requires C, 67.59; H, 5.67; N, 9.85.

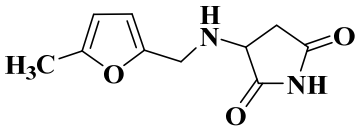


3-[(Furan-2-ylmethyl)amino]-1-phenylpyrrolidine-2,5-dione (6d). The crystals obtained after solvent evaporation were recrystallized from an hexane/EtOAc mixture (15 ml) to give compound **6d** as colorless needles (0.81 g, 3.02 mmol, 75 % yield). M.p 84.8 – 86.6 °C. IR-FT (KBr, cm^{-1}): 3293 (NH), 1770 and 1703 (C=O). ^{1}H NMR δ (600 MHz, $CDCl_3$): ^{1}H NMR δ (600 MHz, $CDCl_3$): 7.47 (2H, t, J = 7.3 Hz, H_{Ph}-3,5), 7.39 (1H, t, J = 7.3 Hz, H_{Ph}-4), 7.26 (2H, br. d, J = 7.3 Hz, H_{Ph}-2,6), 6.34 (1H, d, J = 3.2 Hz, H_{Furyl}-3), 6.25 (1H, d, J = 2.7 Hz, H_{Furyl}-4), 3.99 (1H, d, J = 14.7 Hz, NCH_2-A), 3.92 (2H, m, H-3, NCH_2-B), 3.03 (1H, dd, J = 8.7, 18.3 Hz, H-4A), 2.67 (1H, dd, J = 5.5, 17.9 Hz, H-4B) ppm. ^{13}C NMR δ (150 MHz, $CDCl_3$): 176.8 and 174.2 (C-2 and C-5), 152.4 (C_{Furyl}-2), 142.6 (C_{Furyl}-5), 131.7 (C_{Ph}-1), 129.3 (2C, C_{Ph}-3,5), 128.8 (C_{Ph}-4), 126.4 (2C, C_{Ph}-2,6), 110.5 and 108.2 (C_{Furyl}-3 and C_{Furyl}-4), 55.2 (C-3), 44.2 ($NH-CH_2$), 36.5 (C-4) ppm. MALDI-TOF HRMS: found 271.1086. $C_{15}H_{15}N_2O_3$ requires for $(M+H)^+$ 271.1077. Found: C, 66.91; H, 5.60; N, 10.71. $C_{15}H_{14}N_2O_3$ requires C, 66.66; H, 5.22; N, 10.36.

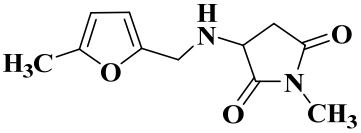


3-[(Furan-2-ylmethyl)amino]-1-(4-nitrophenyl)pyrrolidine-2,5-dione (6e). The crystals obtained after solvent evaporation were recrystallized from EtOH (~ 15 ml) to give compound **6e** as white powder (0.95 g, 3.01 mmol, 60 % yield). M.p 88.9 – 89.8 °C. IR-FT (KBr, cm^{-1}): 3236 (NH), 1789 and 1718 (C=O), 1524 and 1394 (NO_2). ^{1}H NMR δ (600

MHz, $CDCl_3$): 8.34 (2H, br. d, J ~ 9.1 Hz, H_{Ph}-3,5), 7.59 (2H, br. d, J ~ 9.1 Hz, H_{Ph}-2,6), 7.41 (1H, dd, J = 0.7, 1.9 Hz, H_{Furyl}-5), 6.36 (1H, dd, J = 1.9, 3.1 Hz, H_{Furyl}-4), 6.28 (1H, dd, J = 0.7, 3.1 Hz, H_{Furyl}-3), 4.02 (1H, d, J = 14.9 Hz, NC$\underline{H}_2$-A), 3.97 (1H, dd, J = 5.0, 8.1 Hz, H-3), 3.91 (1H, d, J = 14.9 Hz, NC$\underline{H}_2$-B), 3.12 (1H, dd, J = 8.1, 18.2 Hz, H-4A), 2.74 (1H, dd, J = 5.0, 18.2 Hz, H-4B), 2.23 (1H, br. s, NH) ppm. ^{13}C NMR δ (150 MHz, $CDCl_3$): 175.9 and 173.3 (C-2 and C-5), 152.0 (C_{Furyl}-2), 147.0 (C_{Ph}-4), 142.6 (C_{Furyl}-5), 137.1 (C_{Ph}-1), 126.8 (2C, C_{Ph}-2,6), 124.4 (2C, C_{Ph}-3,5), 110.4 and 108.3 (C_{Furyl}-3 and C_{Furyl}-4), 55.0 (C-3), 44.0 (NH-$\underline{C}H_2$), 36.3 (C-4) ppm. MALDI-TOF HRMS: found 316.0935. $C_{15}H_{14}N_3O_5$ requires for $(M+H)^+$ 316.0928.

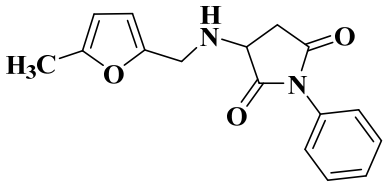


3-{[(5-Methylfuran-2-yl)methyl]amino}pyrrolidine-2,5-dione (6f): Purification by flash chromatography afforded compound **6f** as a yellow oil (0.63 g, 3.00 mmol, 61 % yield). IR-FT (liquid film, cm^{-1}): 3222 (2 × NH), 1784 and 1714 (C=O). ^{1}H NMR δ (600 MHz, $CDCl_3$): 8.65 (1H, br. s, NH), 6.10 (1H, d, J = 3.0 Hz, H_{Furyl}-3), 5.89 (1H, dq, J = 1.0, 3.0 Hz, H_{Furyl}-4), 3.88 (1H, d, J = 14.6 Hz, NCH_2-A), 3.81 (1H, d, J = 14.6 Hz, NCH_2-B), 3.79 (1H, dd, J = 5.3, 8.3 Hz, H-3), 2.91 (1H, dd, J = 8.3, 17.9 Hz, H-4A), 2.56 (1H, dd, J = 5.3, 17.9 Hz, H-4B), 3.66 (3H, s, CH_3), 2.24 (1H, br. s, NH) ppm. ^{13}C NMR δ (150 MHz, $CDCl_3$): 178.7 and 175.9 (C-2 and C-5), 152.3 and 150.1 (C_{Furyl}-2 and C_{Furyl}-5), 109.0 and 106.2 (C_{Furyl}-3 and C_{Furyl}-4), 55.1 (C-3), 44.1 (NH-CH_2), 37.2 (C-4), 13.6 (CH_3) ppm. MALDI-TOF HRMS: found 231.0732. Requires for $C_{10}H_{12}N_2O_3Na$ $(M+Na)^+$ 231.0740. Found: C, 57.21; H, 5.47; N, 13.09. $C_{10}H_{12}N_2O_3$ requires C, 57.69; H, 5.81; N, 13.45.

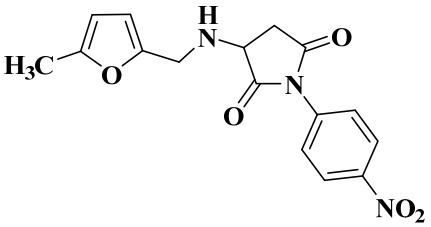


1-Methyl-3-{[(5-methylfuran-2-yl)methyl]amino}pyrrolidine-2,5-dione (6g). Purification by flash chromatography afforded compound **6g** as a light yellow oil (0.71 g, 3.21 mmol, 64 % yield). IR-FT (liquid film, cm^{-1}): 3323 (NH), 1778 and 1704 (C=O). ^{1}H NMR δ (600 MHz, $CDCl_3$): 6.09 (1H, br. d, J = 3.1 Hz, H_{Furyl}-3), 5.89 (1H, dq, J = 1.0, 3.1 Hz, H_{Furyl}-4), 3.88 (1H, d, J = 14.6 Hz, NCH_2-A), 3.80 (1H, d, J = 14.6 Hz, NCH_2-B), 3.76 (1H, dd, J = 5.0, 8.1 Hz, H-3), 2.98 (3H, s, N-CH_3), 2.89 (1H, dd, J = 8.1, 17.7 Hz, H-4A),

2.50 (1H, dd, J = 5.0, 17.7 Hz, H-4B), 2.77 (3H, s, CH_3), 2.19 (1H, br. s, NH) ppm. ^{13}C NMR δ (150 MHz, $CDCl_3$): 177.9 and 175.4 (C-2 and C-5), 152.2 and 150.3 (C_{Furyl}-2 and C_{Furyl}-5), 108.9 and 106.1 (C_{Furyl}-3 and C_{Furyl}-4), 55.0 (C-3), 44.3 (NH-CH_2), 36.2 (C-4), 24.8 (N-CH_3), 13.6 (CH_3) ppm. MALDI-TOF HRMS: found 223.1085. $C_{11}H_{15}N_2O_3$ requires for $(M+H)^+$ 223.1077; found 245.0882. Requires for $C_{11}H_{14}N_2O_3Na$ $(M+Na)^+$ 245.0897.



3-{[(5-Methylfuran-2-yl)methyl]amino}-1-phenylpyrrolidine-2,5-dione (6h). The crystals obtained after solvent evaporation were recrystallized from EtOH (~ 15 mL) to give compound **6h** as light-yellow crystals (0.99 g, 3.52 mmol, 70 % yield). M.p 73.4 – 74.8 °C. IR-FT (KBr, cm^{-1}): 3279 (NH), 1774 and 1700 (C=O). ^1H NMR δ (600 MHz, $CDCl_3$): 7.47 (2H, br. t, J = 7.6 Hz, H_{Ph}-3,5), 7.40 (1H, br. t, H_{Ph}-4), 7.28 (2H, m, H_{Ph}-2,6), 6.14 (1H, br. d, J = 3.0 Hz, H_{Furyl}-3), 5.91 (1H, dq, J = 3.0, 1.0 Hz, H_{Furyl}-4), 3.95 (1H, d, J = 14.1 Hz, NCH_2-A), 3.92 (1H, dd, J = 5.0, 8.6 Hz, H-3), 3.86 (1H, d, J = 14.1 Hz, NCH_2-B), 3.07 (1H, dd, J = 8.6, 18.0 Hz, H-4A), 2.70 (1H, dd, J = 5.0, 18.0 Hz, H-4B), 2.29 (3H, s, CH_3), 1.58 (1H, br. s, NH) ppm. ^{13}C NMR δ (150 MHz, $CDCl_3$): 176.9 and 174.3 (C-2 and C-5), 152.4 and 150.3 (C_{Furyl}-2 and C_{Furyl}-5), 131.7 (C_{Ph}-1), 129.3 (2C, C_{Ph}-3,5), 128.8 (C_{Ph}-4), 126.4 (2C, C_{Ph}-2,6), 109.1 and 106.3 (C_{Furyl}-3 and C_{Furyl}-4), 55.2 (C-3), 44.3 (CH_2-Furyl), 36.5 (C-4), 13.7 (CH_3) ppm. MALDI-TOF HRMS: found 285.1221. $C_{16}H_{17}N_2O_3$ requires for $(M+H)^+$ 285.1234.



3-{[(5-Methylfuran-2-yl)methyl]amino}-1-(4-nitrophenyl)pyrrolidine-2,5-dione (6i): The crystals obtained after solvent evaporation were recrystallized from EtOH (~ 15 mL) to give compound **6i** as white powder (1.23 g, 3.74 mmol, 75 % yield). M.p 64.7 – 66.2 °C. IR-FT (KBr, cm^{-1}): 3228 (NH), 1784 and 1715 (C=O), 1528 and 1354 (NO_2). ^1H NMR

δ (600 MHz, $CDCl_3$): 8.34 (2H, br. d, J = 9.1 Hz, H_{Ph}-3,5), 7.52 (2H, br. d, J = 9.1 Hz, H_{Ph}-2,6), 6.14 (1H, d, J = 3.0 Hz, H_{Furyl}-3), 5.91 (1H, dq, J = 3.0, 1.0 Hz, H_{Furyl}-4), 3.99 (1H, dd, J = 5.5, 8.6 Hz, H-3), 3.93 (1H, d, J = 14.6 Hz, NCH_2-A), 3.84(1H, d, J = 14.6 Hz, NCH_2-B), 3.12 (1H, dd, J = 8.6, 18.2 Hz, H-4A), 2.73 (1H, dd, J = 5.0, 18.2 Hz, H-4B), 3.71 (3H, s, CH_3) ppm. ^{13}C NMR δ (150 MHz, $CDCl_3$): 176.2 and 174.4 (C-2 and C-5), 152.5 and 150.1 (C_{Furyl}-2 and C_{Furyl}-5), 147.1 (C_{Ph}-4), 131.2 (C_{Ph}-1), 126.8 (2C, C_{Ph}-3,5), 124.5 (2C, C_{Ph}-2,6), 109.3 and 106.3 (C_{Furyl}-3 and C_{Furyl}-4), 55.1 (C-3), 44.3 (CH_2-Furyl), 36.5 (C-4), 13.7 (CH_3) ppm. MALDI-TOF HRMS: found 330.1071. $C_{16}H_{16}N_3O_5$ requires for $(M+H)^+$ 330.1084; found 352.0911. Requires for $C_{16}H_{15}N_3O_5Na$ $(M+Na)^+$ 352.0904.

3. Copies of ^{1}H and ^{13}C NMR spectra of the Michael adducts 6

Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 09:59:40				
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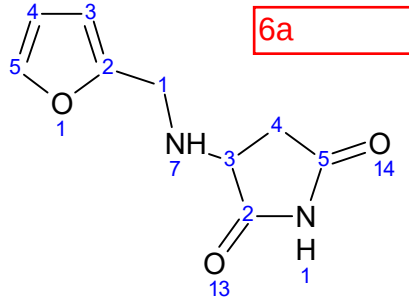
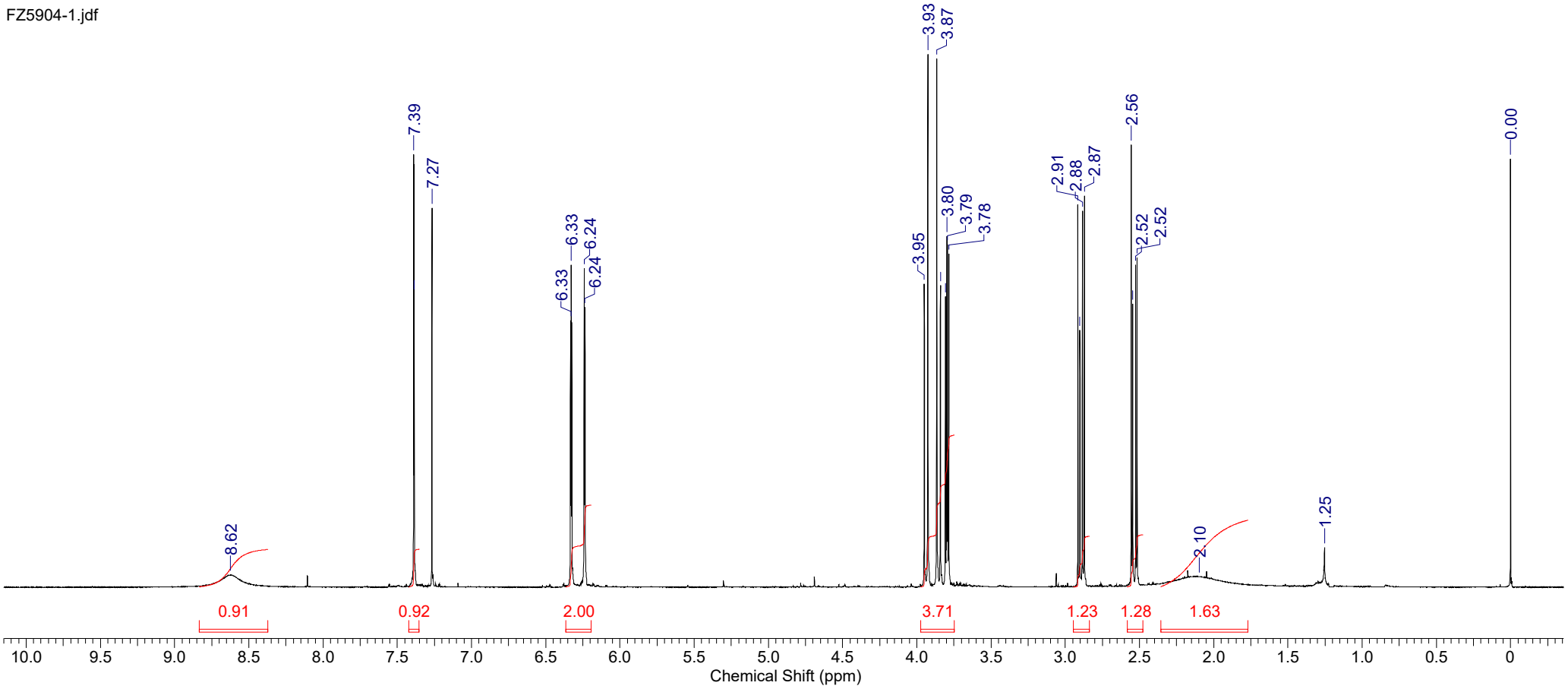
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5412.1411	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	21.800				





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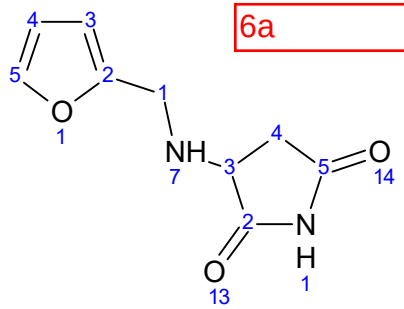
Spectrum Offset (Hz)	5412.1411	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	21.800				



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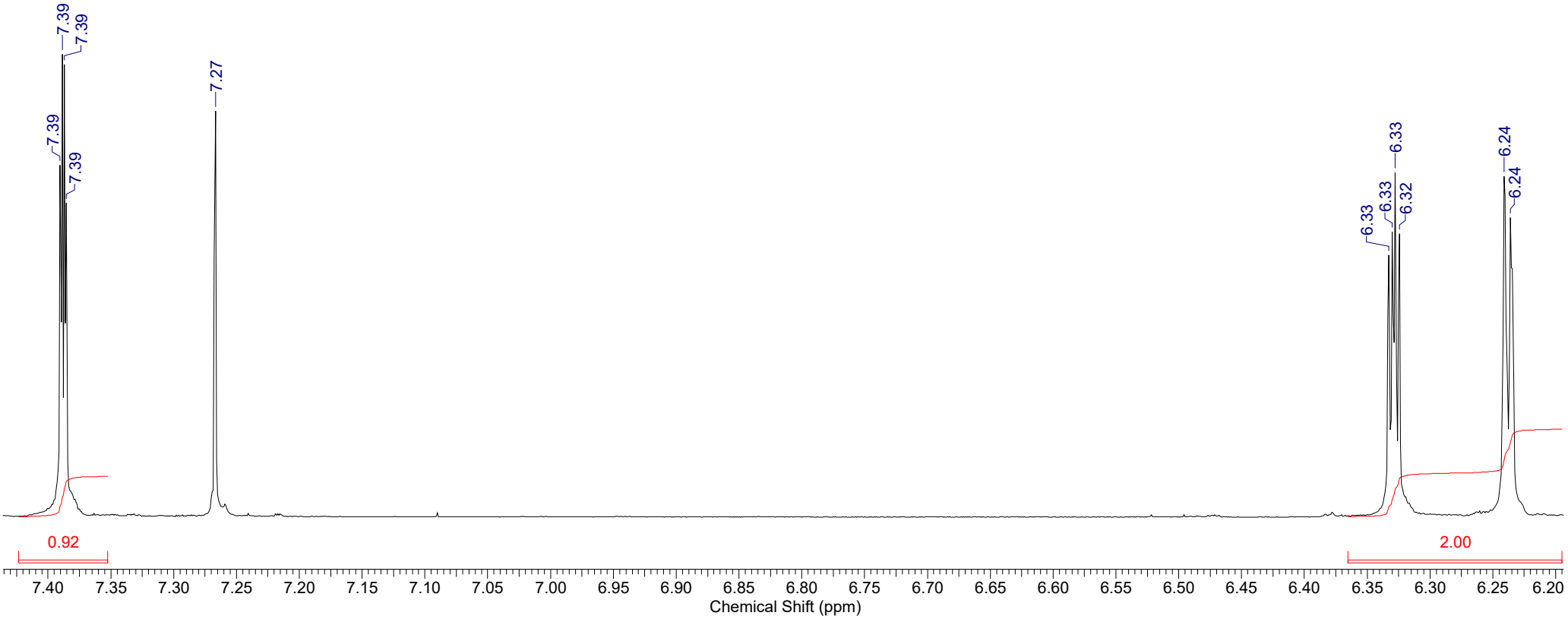

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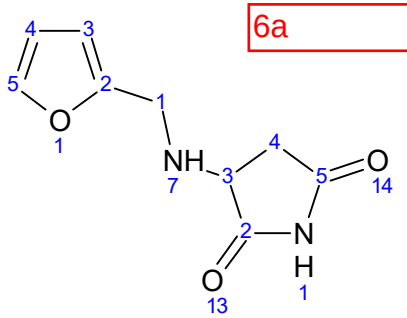
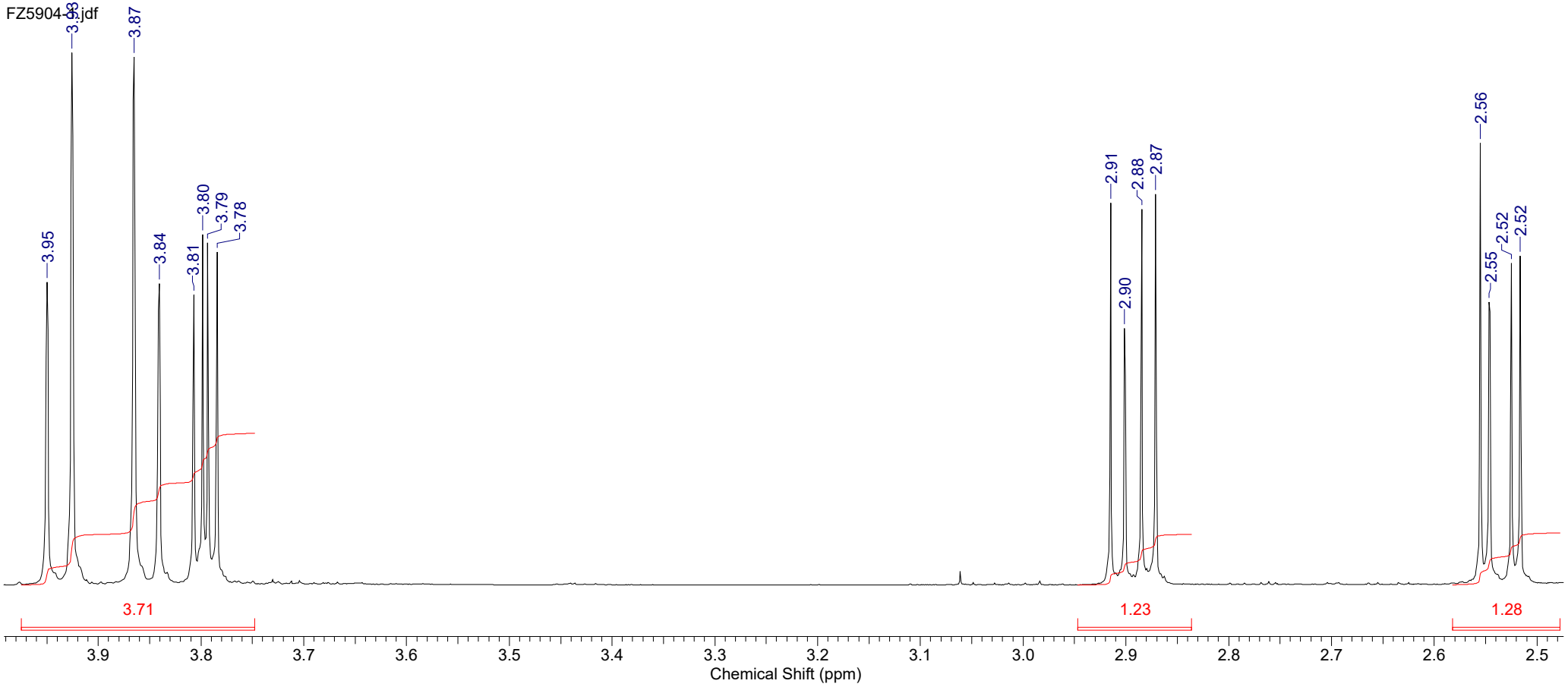
Spectrum Offset (Hz)	5412.1411	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	21.800				





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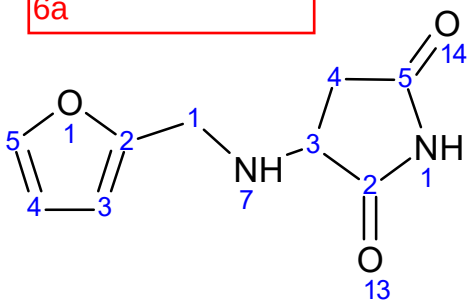
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.200				

6a



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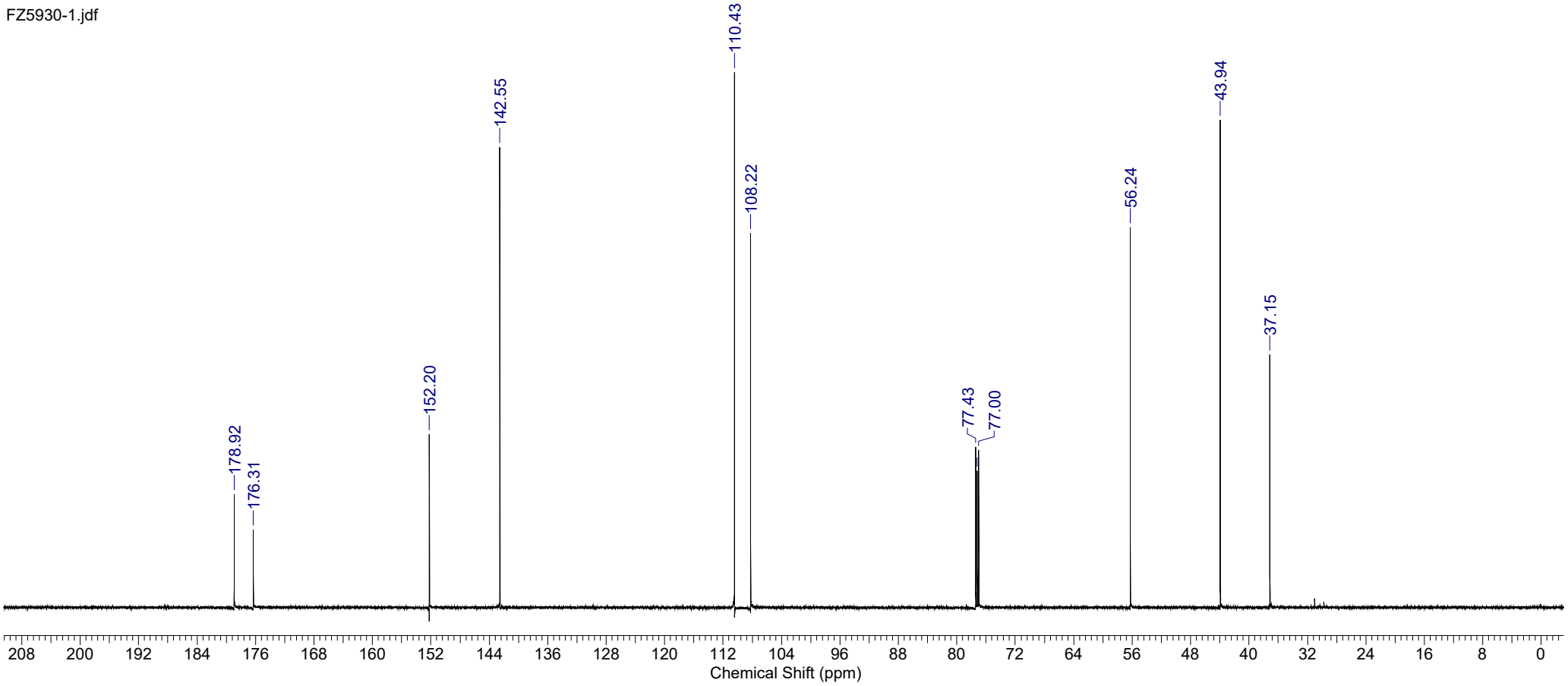

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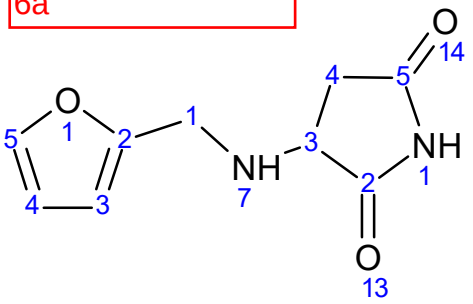
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.200				

6a



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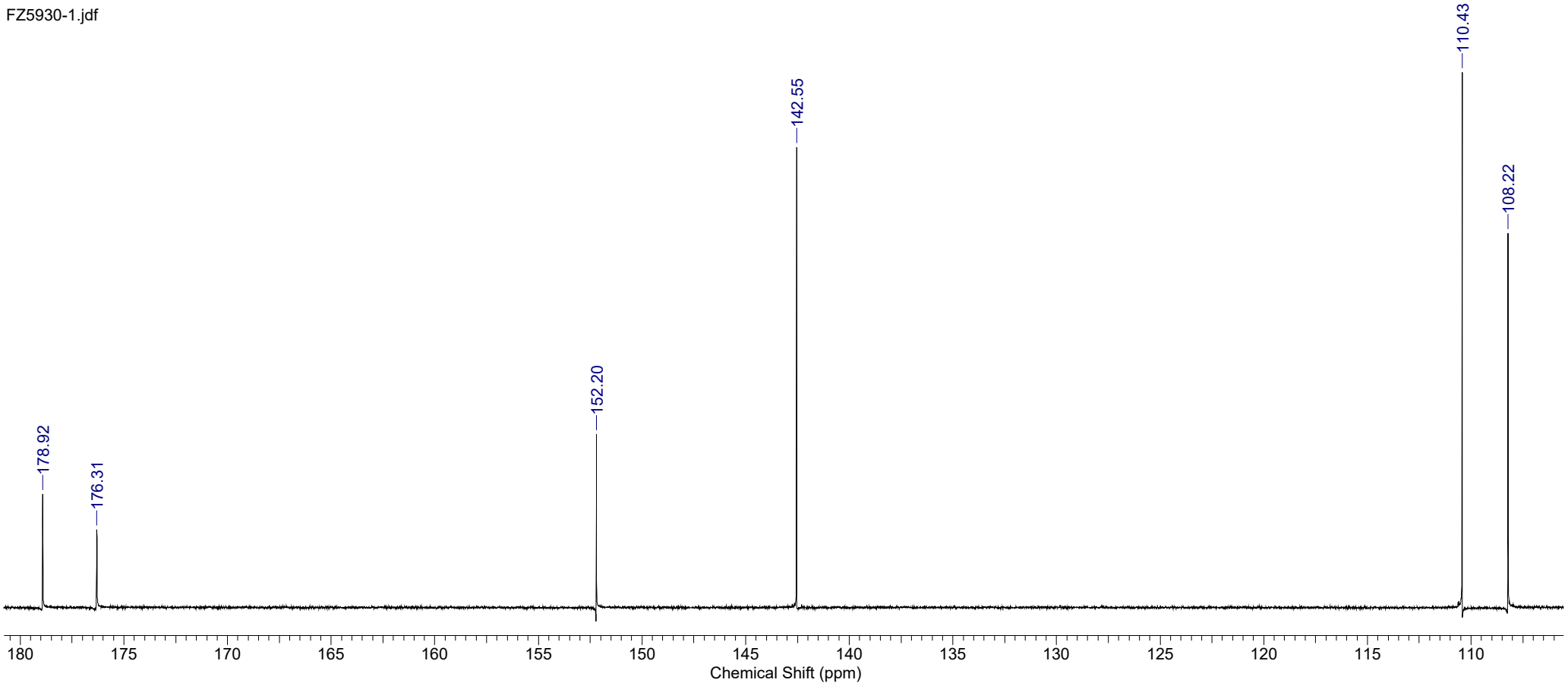

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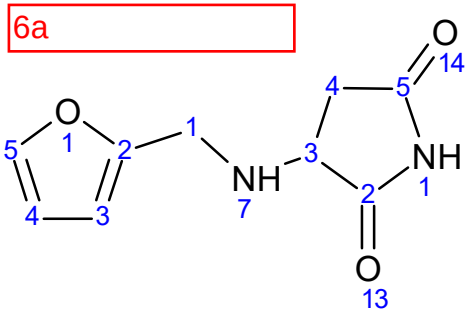
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.200				

6a



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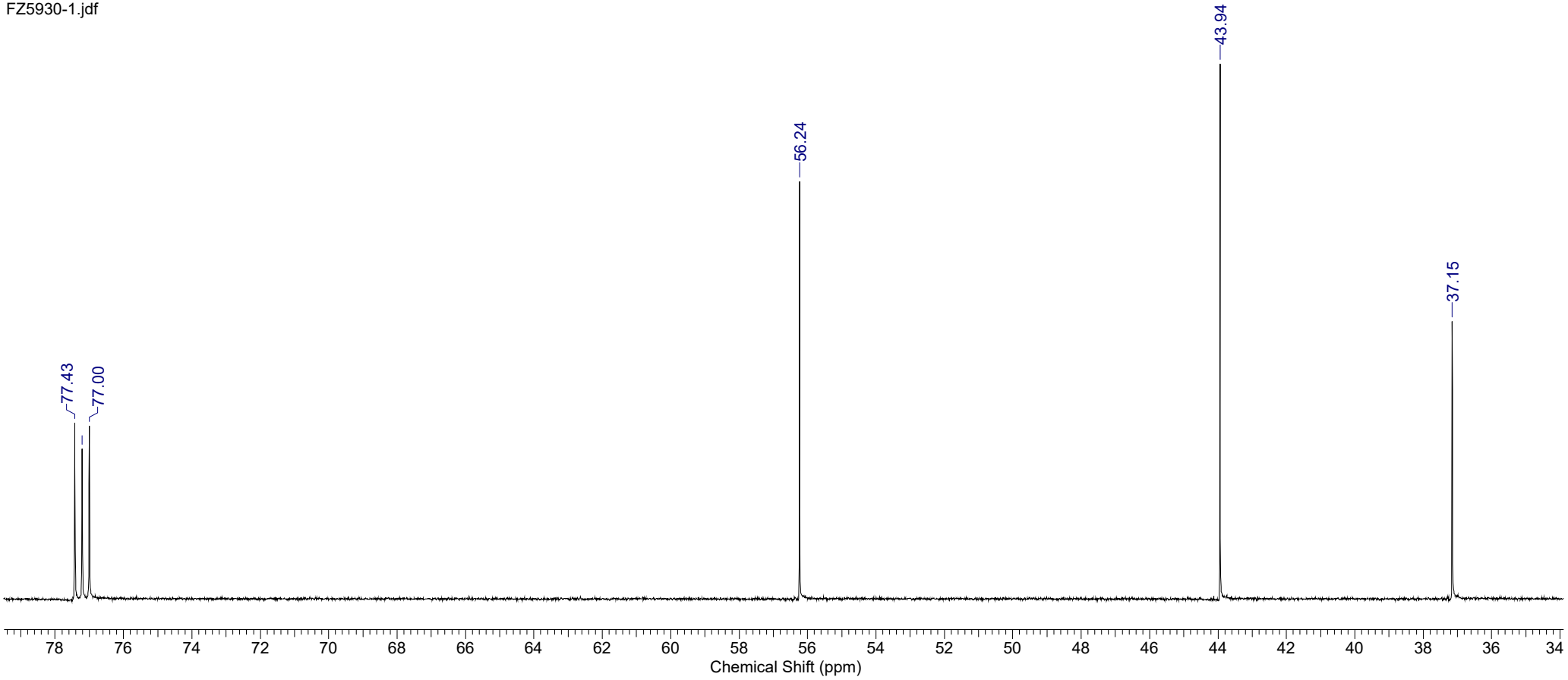

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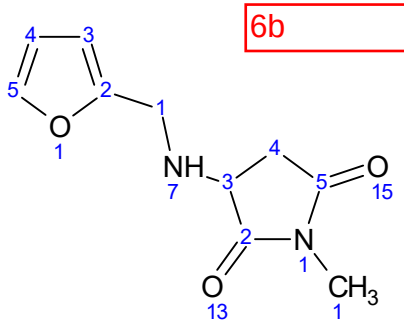
6b



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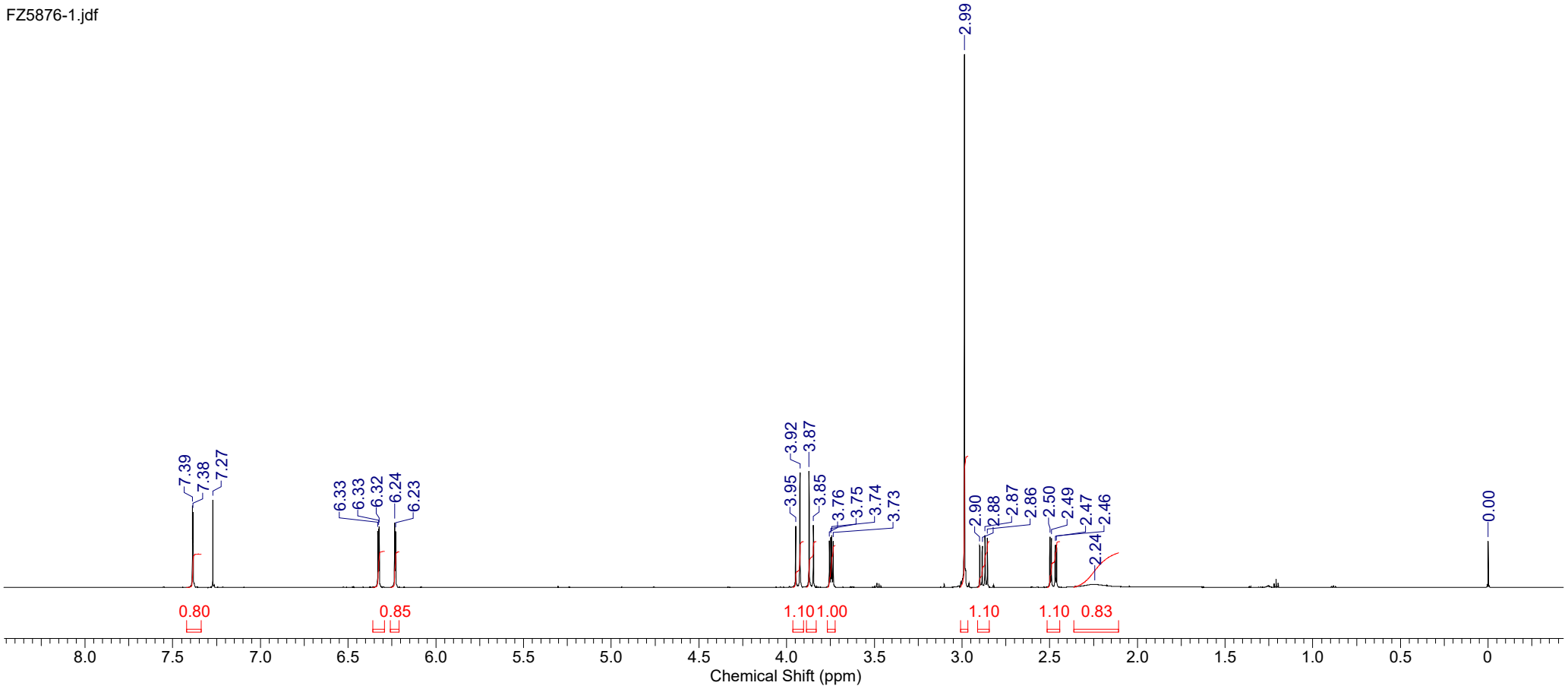

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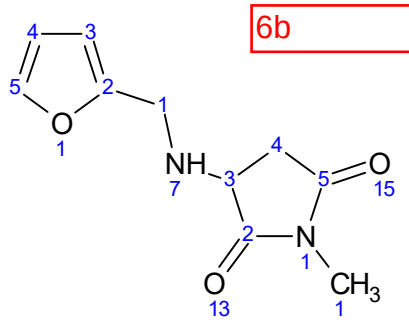

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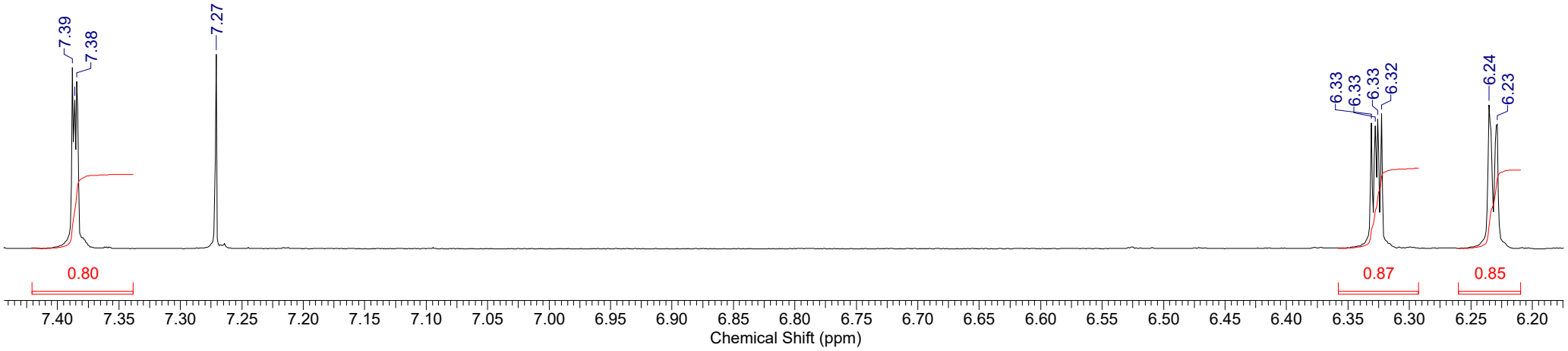

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Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	38.00	***Solvent***	CHLOROFORM-d
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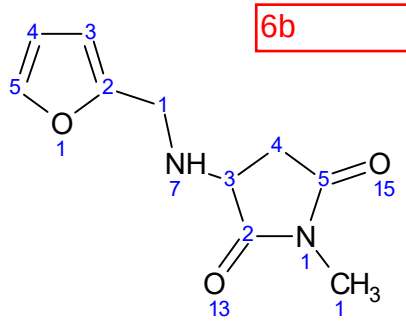
6b



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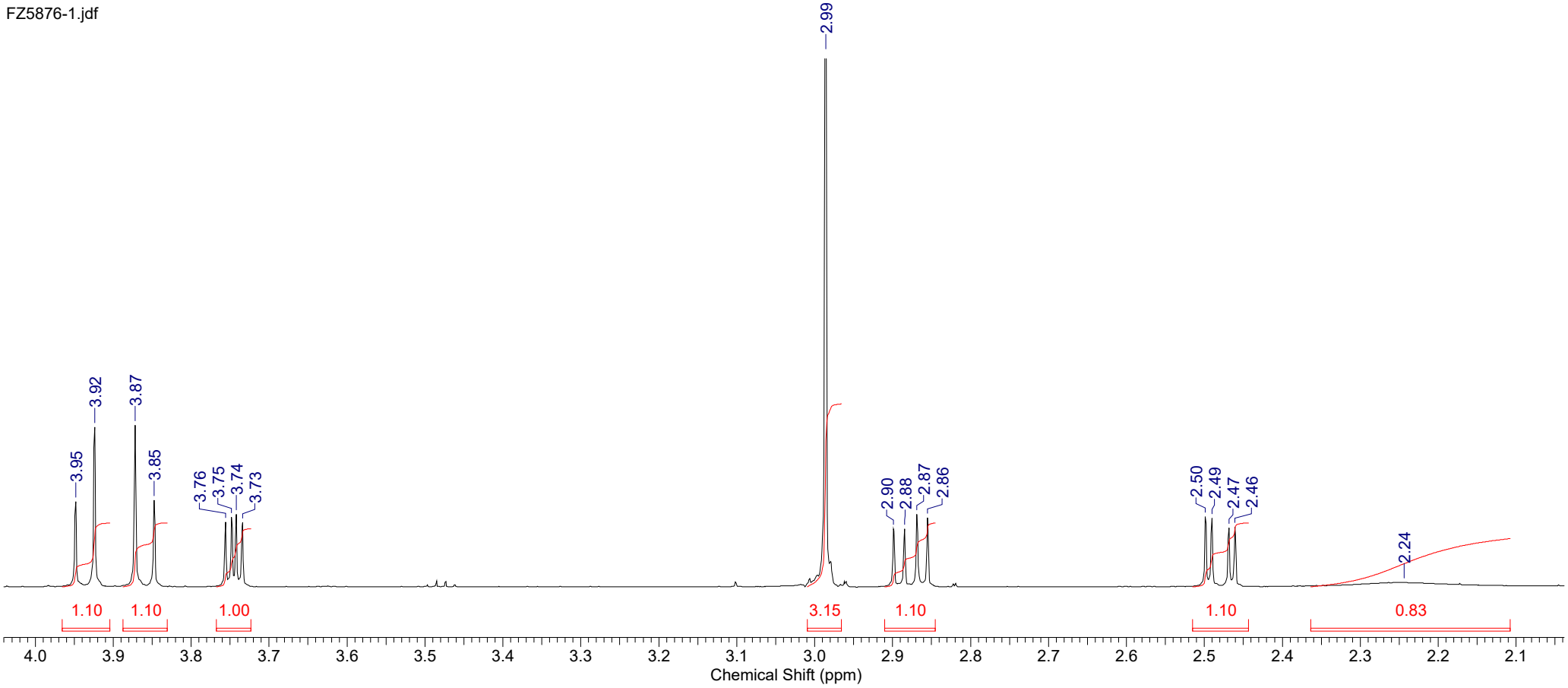

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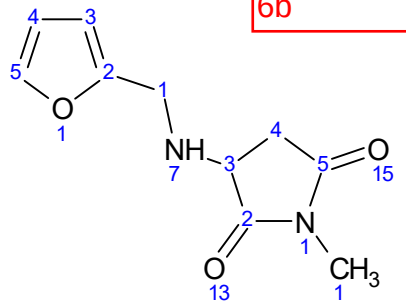
Receiver Gain	54.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.300				

6b



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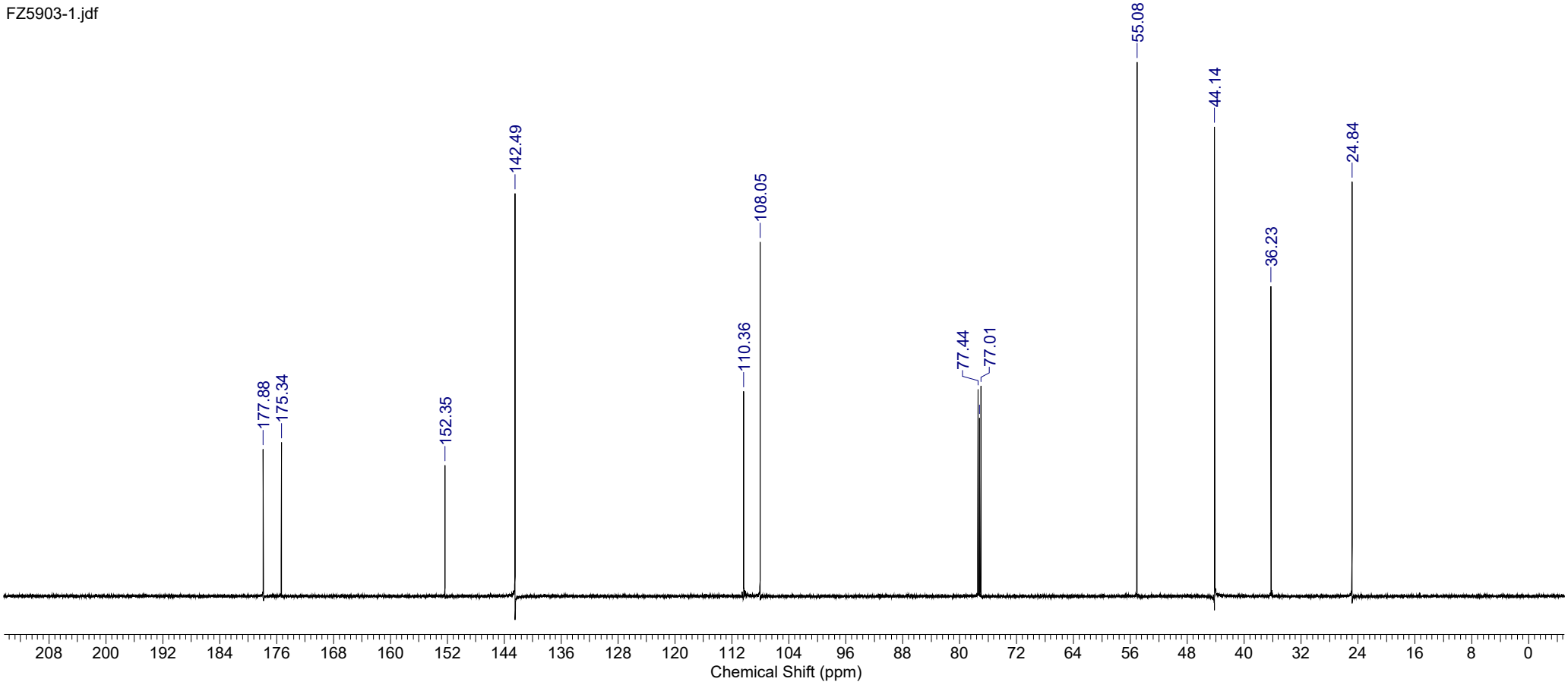

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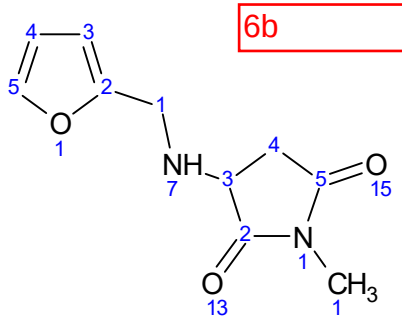
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.300				

6b



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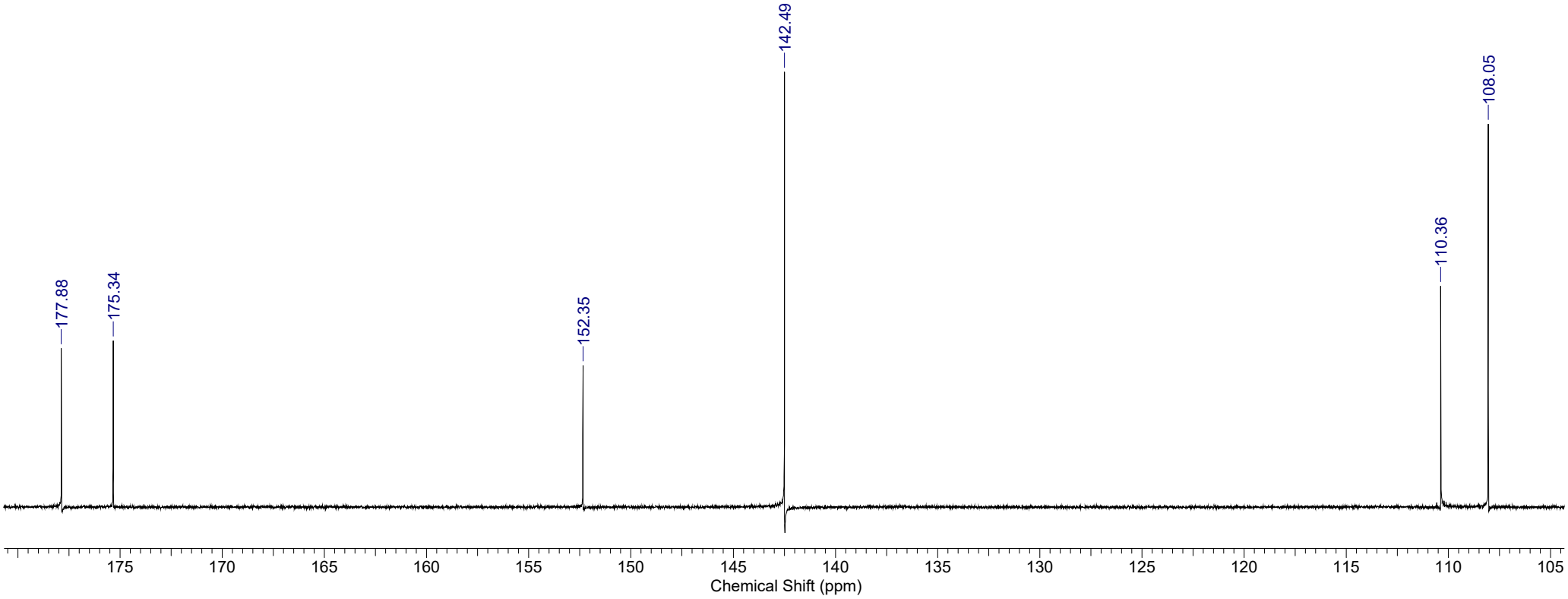

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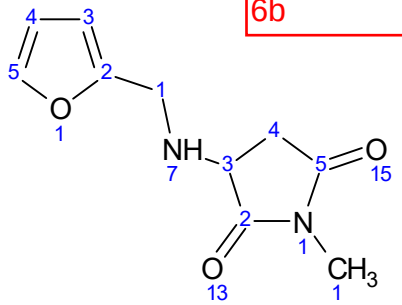
Receiver Gain	54.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.300				

6b



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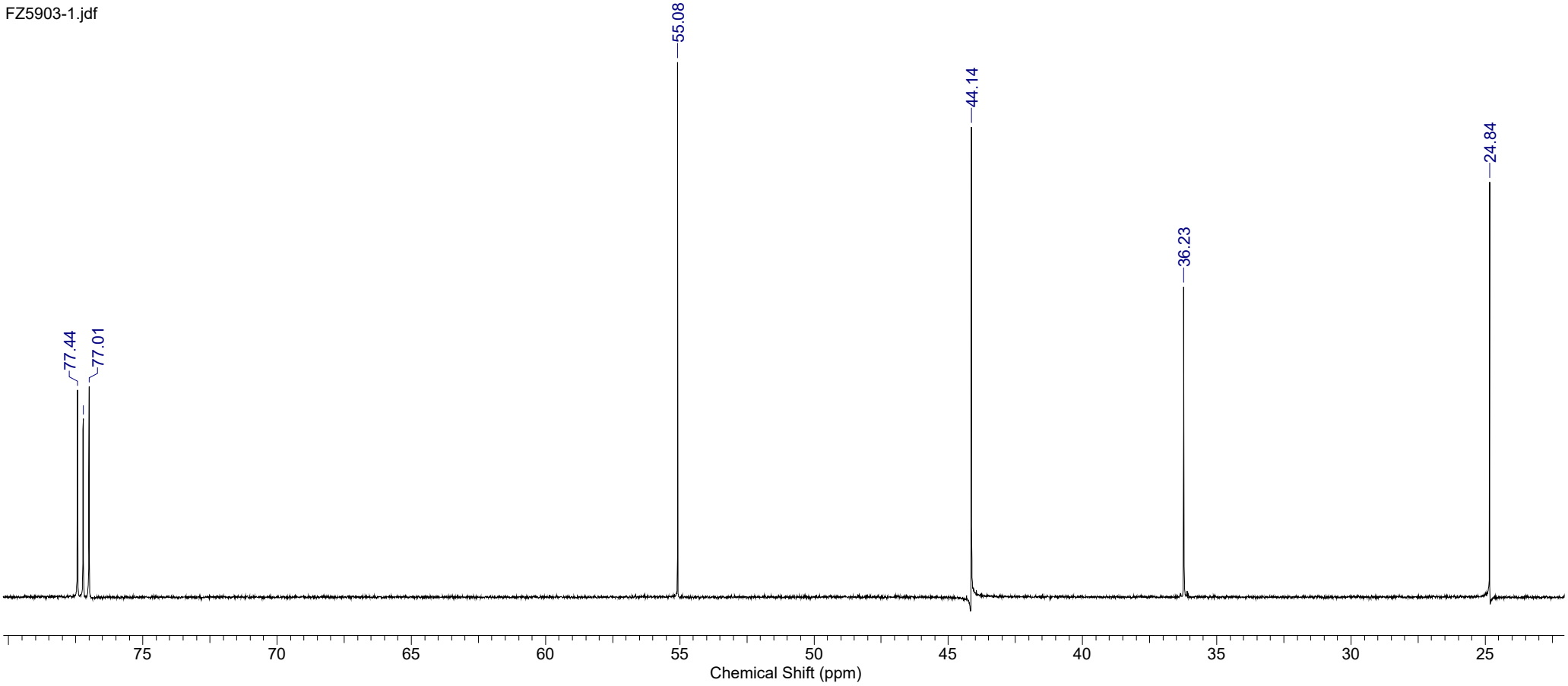

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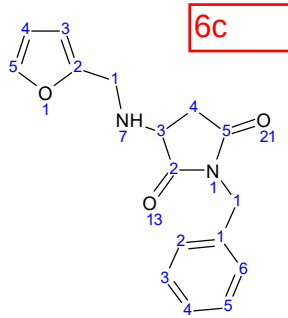
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5408.1045	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.200				

6c



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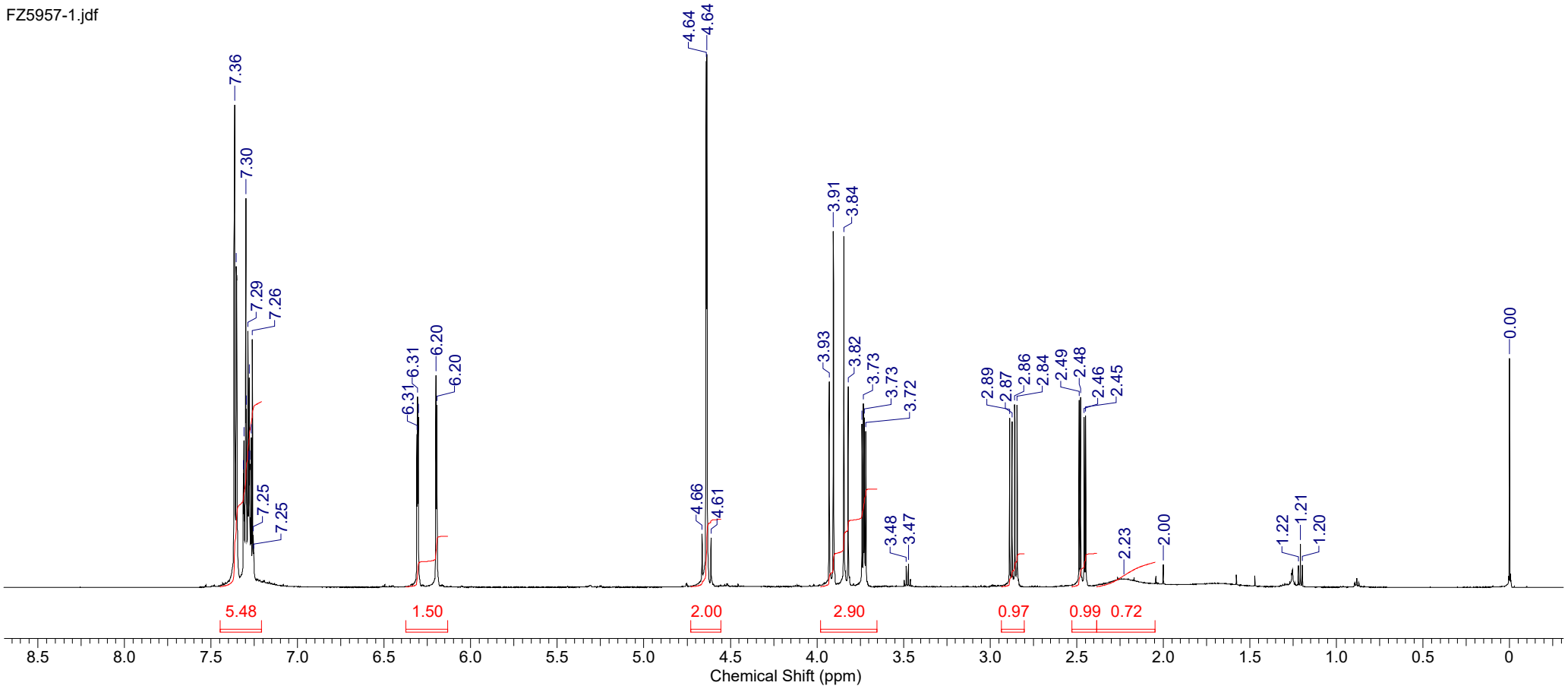

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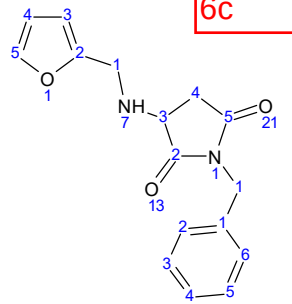
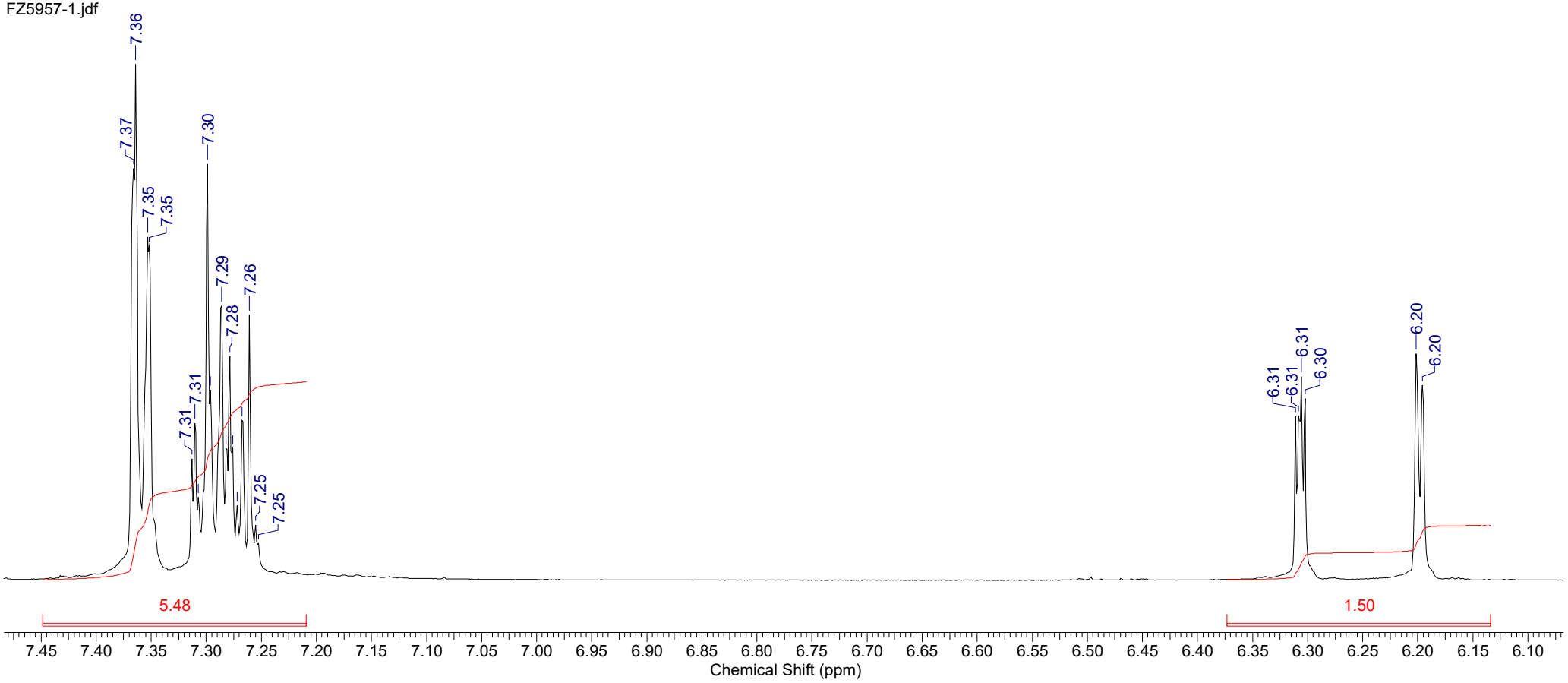
Spectrum Offset (Hz)	5408.1045	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.200				

6c

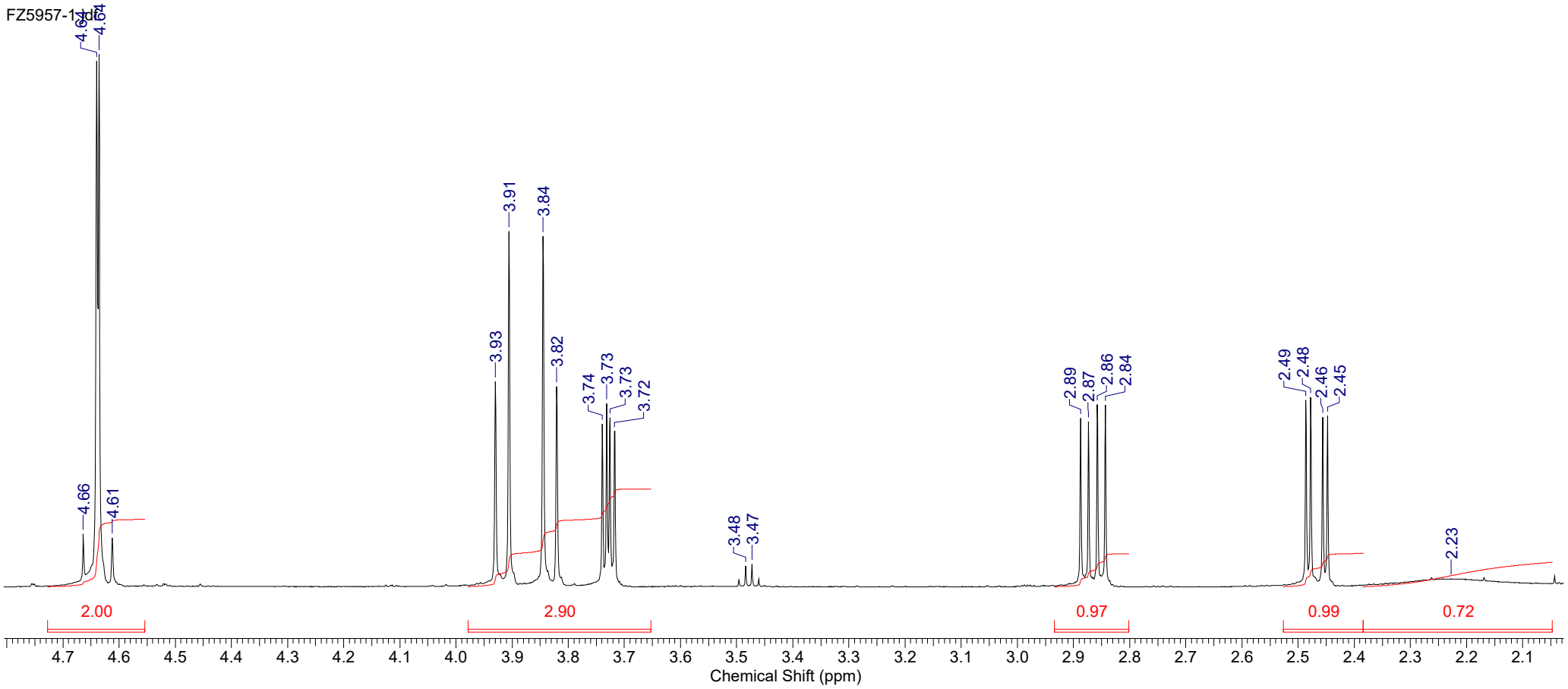


FZ5957-1.jdf

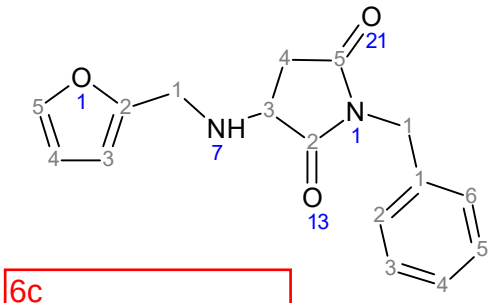


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:44:19				
Date Stamp	23 Mar 2017 10:05:32			***File Name***	C:\Users\Fedor\Desktop\21.03.17\FZ5957-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5408.1045	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.200				

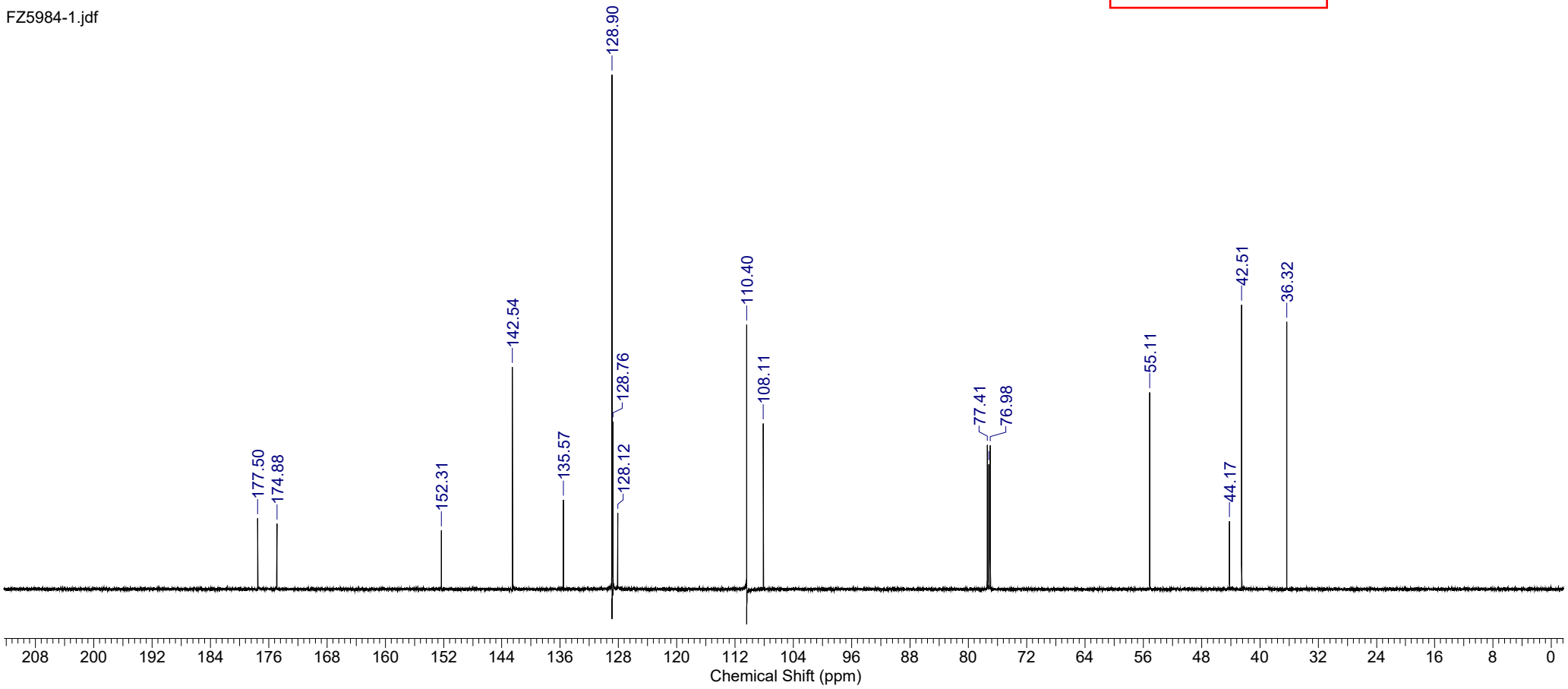
6c



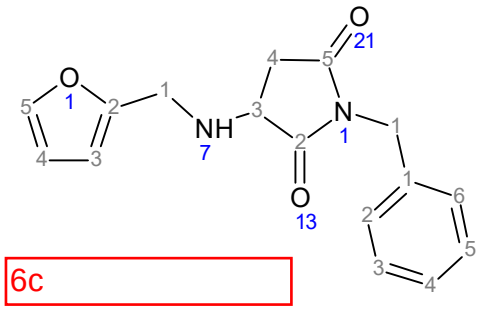
Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:38:38
Date Stamp	30 Mar 2017 08:28:56			***File Name***	C:\Users\Fedor\Desktop\28.03.17\FZ5984-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	278	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.000				



6c

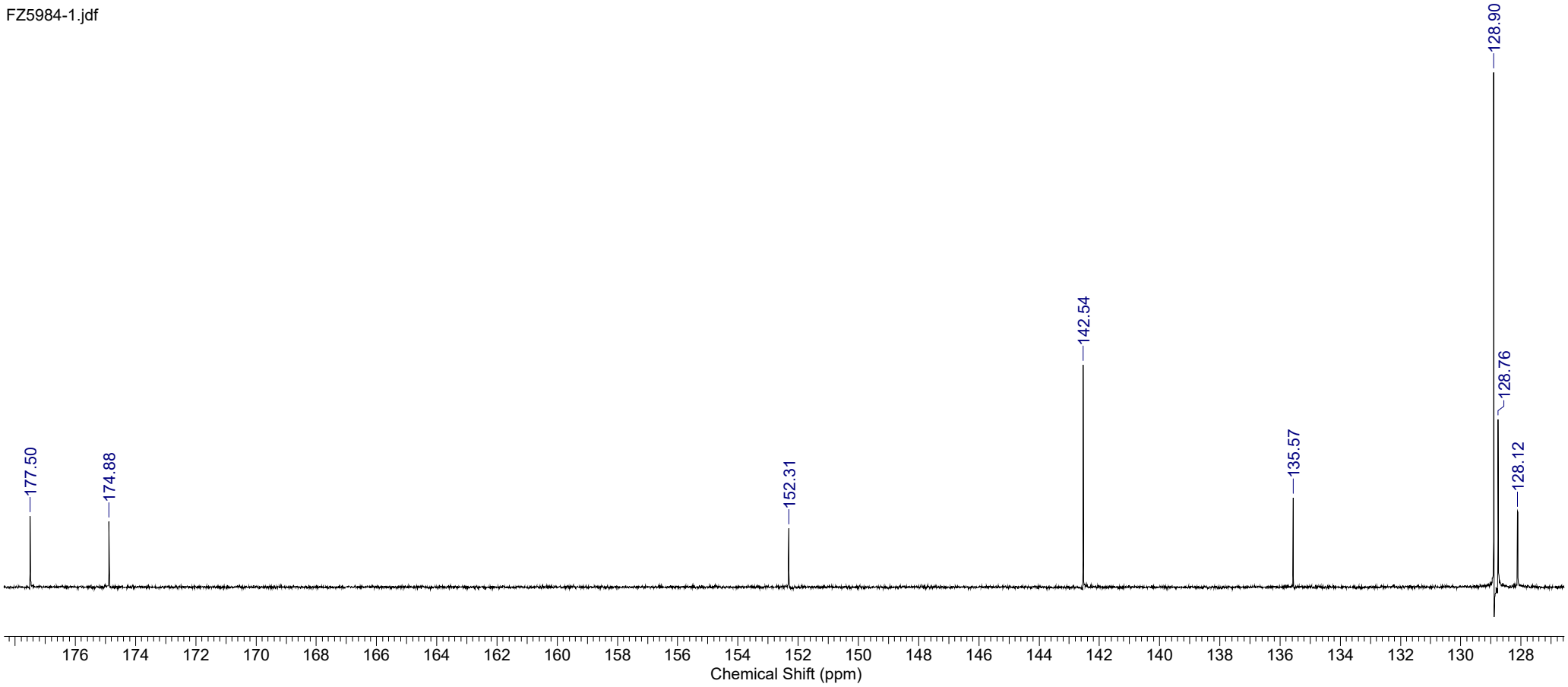


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:38:38
Date Stamp	30 Mar 2017 08:28:56			***File Name***	C:\Users\Fedor\Desktop\28.03.17\FZ5984-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	278	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.000				

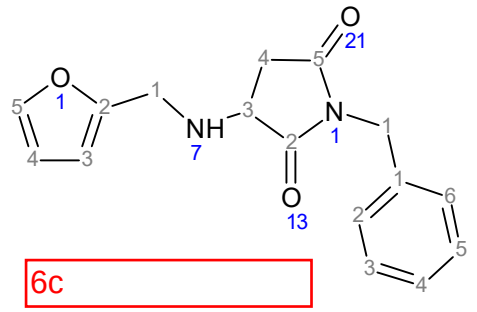


6c

FZ5984-1.jdf

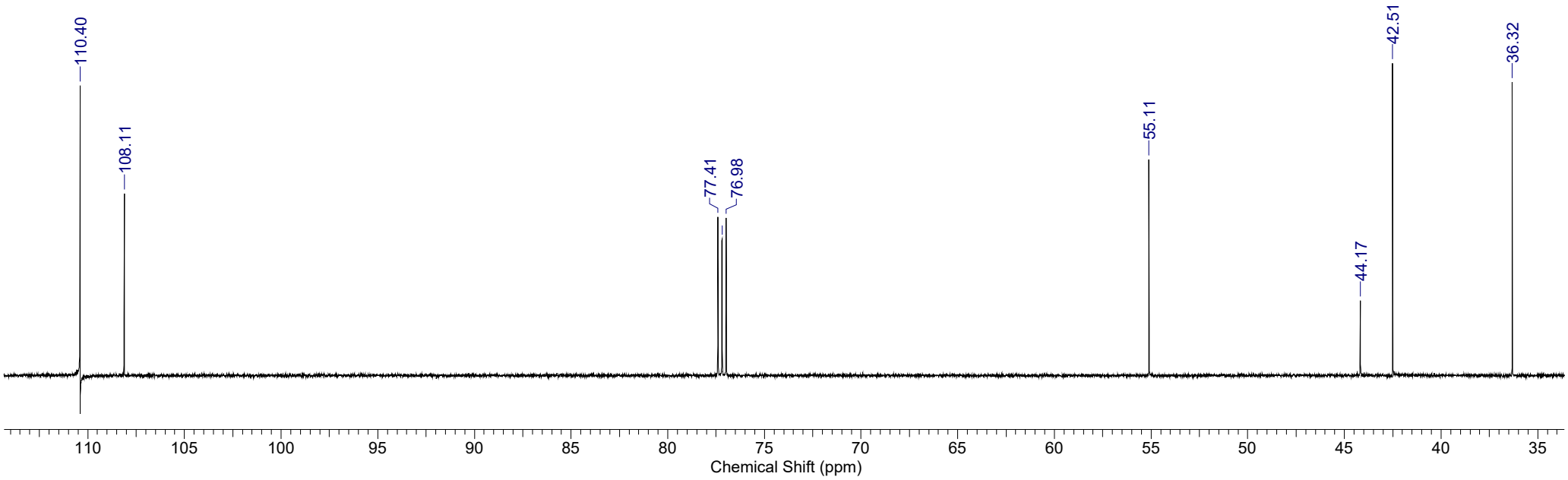


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:38:38
Date Stamp	30 Mar 2017 08:28:56			***File Name***	C:\Users\Fedor\Desktop\28.03.17\FZ5984-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	278	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.000				



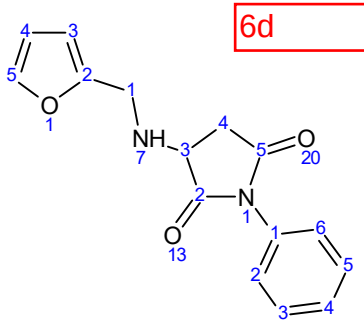
6c

FZ5984-1.jdf

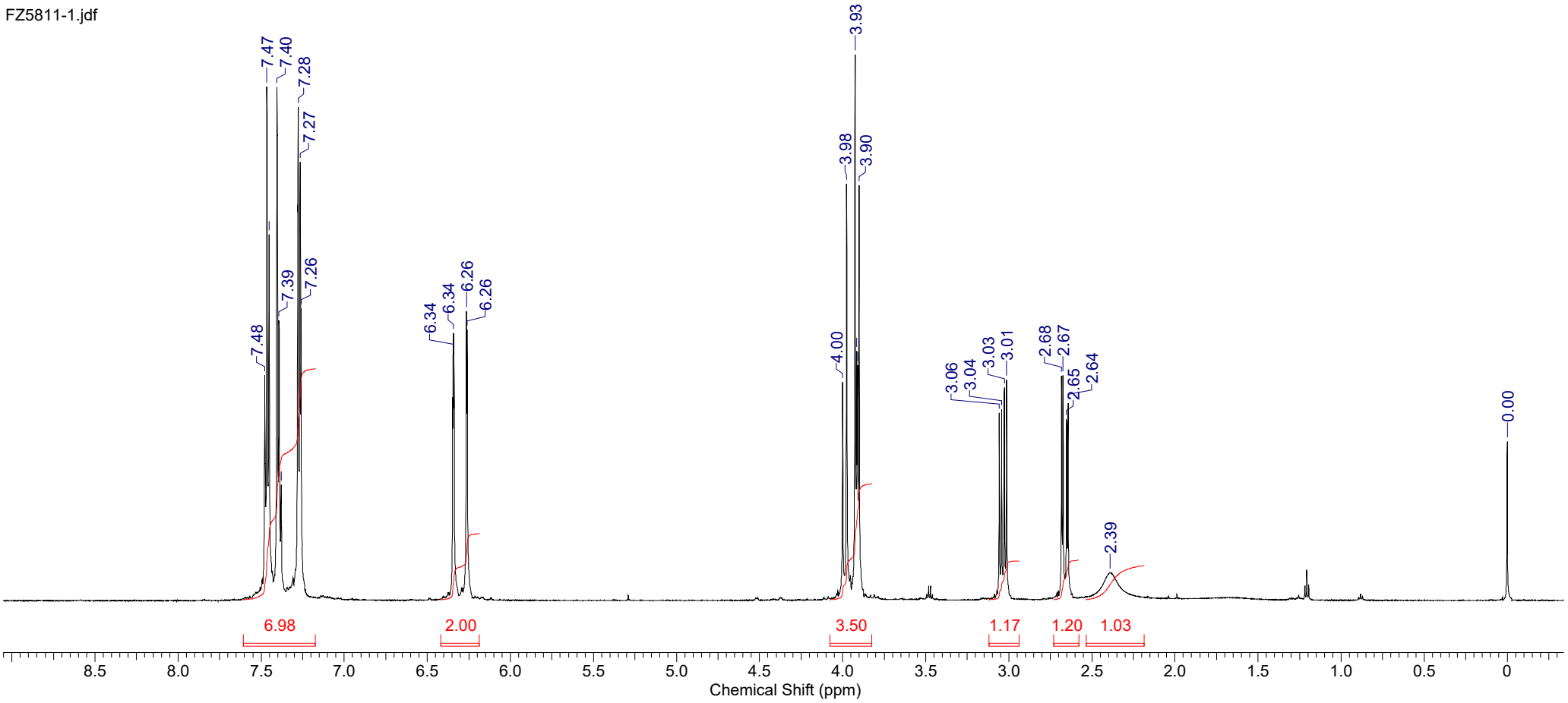


Acquisition Time (sec)	2.1810	***Comment***	single_pulse	***Date***	30 Aug 2016 10:29:17				
Date Stamp	15 Feb 2017 11:22:50			***File Name***	C:\Users\Fedor\Desktop\FZ5811-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	36.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	4807.2612	***Sweep Width (Hz)***	15024.04	***Temperature (degree C)***	25.000				

6d

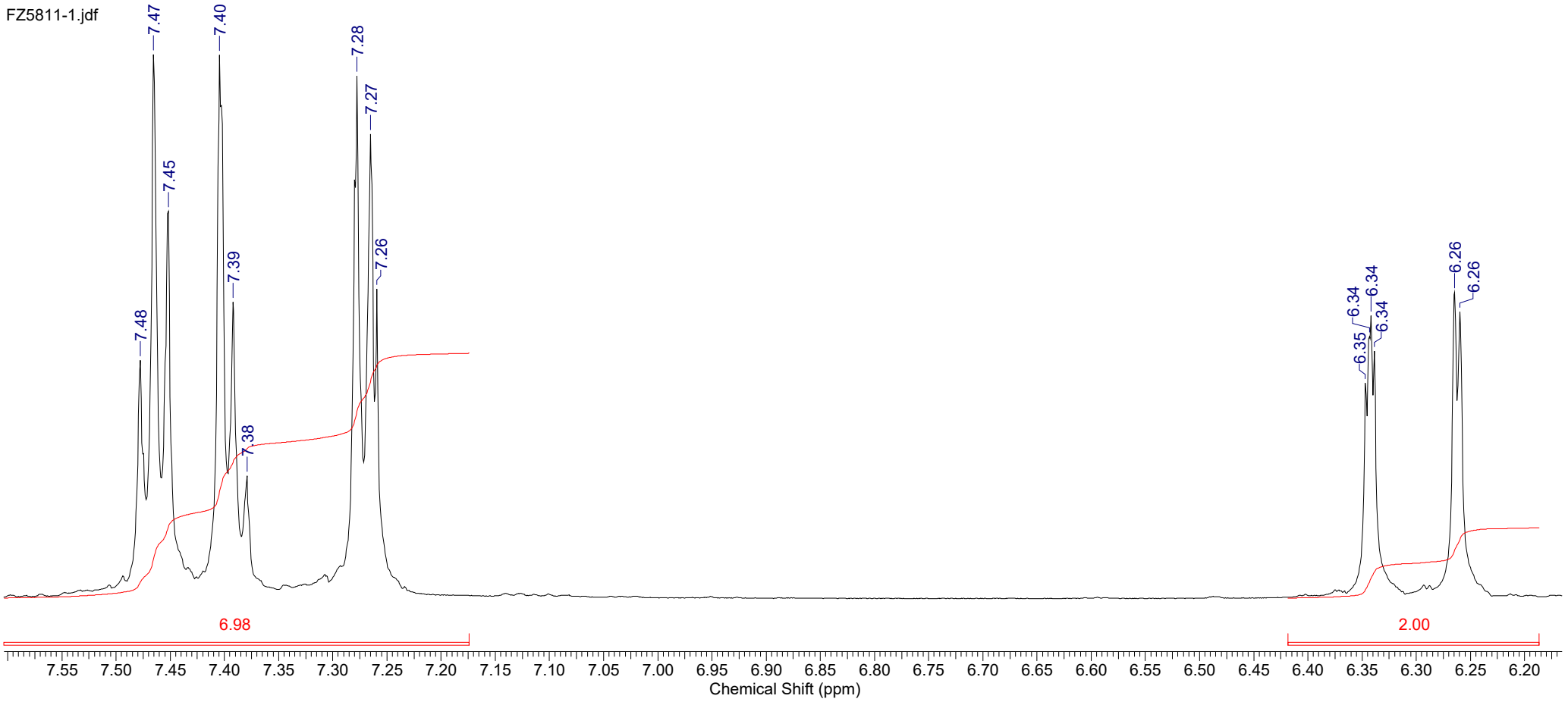


FZ5811-1.jdf



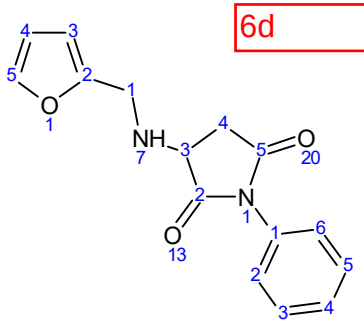
Acquisition Time (sec)	2.1810	***Comment***	single_pulse	***Date***	30 Aug 2016 10:29:17				
Date Stamp	15 Feb 2017 11:22:50			***File Name***	C:\Users\Fedor\Desktop\FZ5811-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	36.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	4807.2612	***Sweep Width (Hz)***	15024.04	***Temperature (degree C)***	25.000				

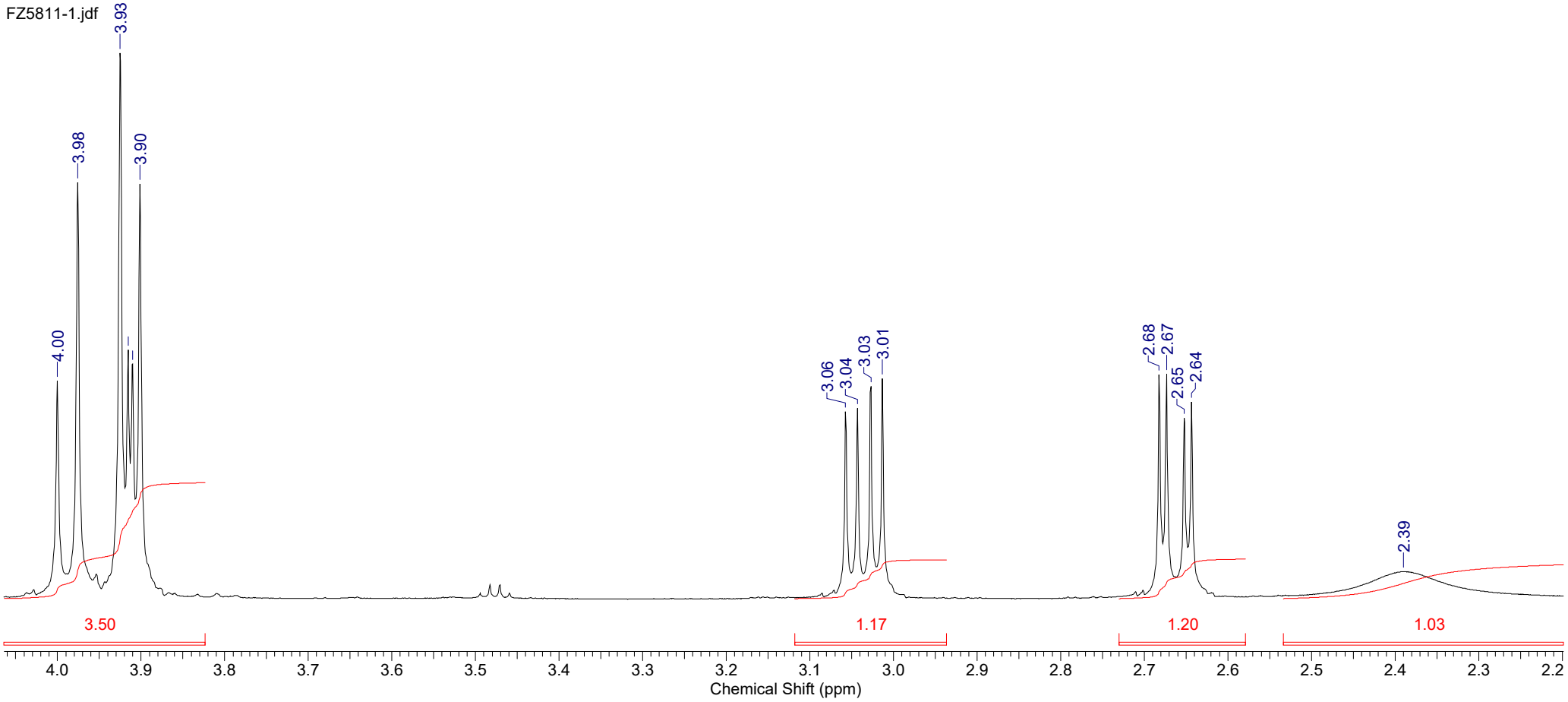
6d



Acquisition Time (sec)	2.1810	***Comment***	single_pulse	***Date***	30 Aug 2016 10:29:17				
Date Stamp	15 Feb 2017 11:22:50			***File Name***	C:\Users\Fedor\Desktop\FZ5811-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	36.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	4807.2612	***Sweep Width (Hz)***	15024.04	***Temperature (degree C)***	25.000				

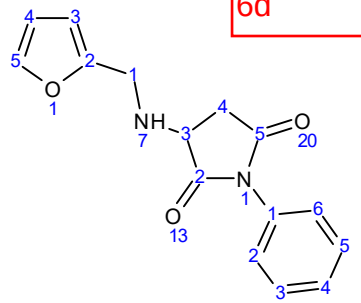
6d



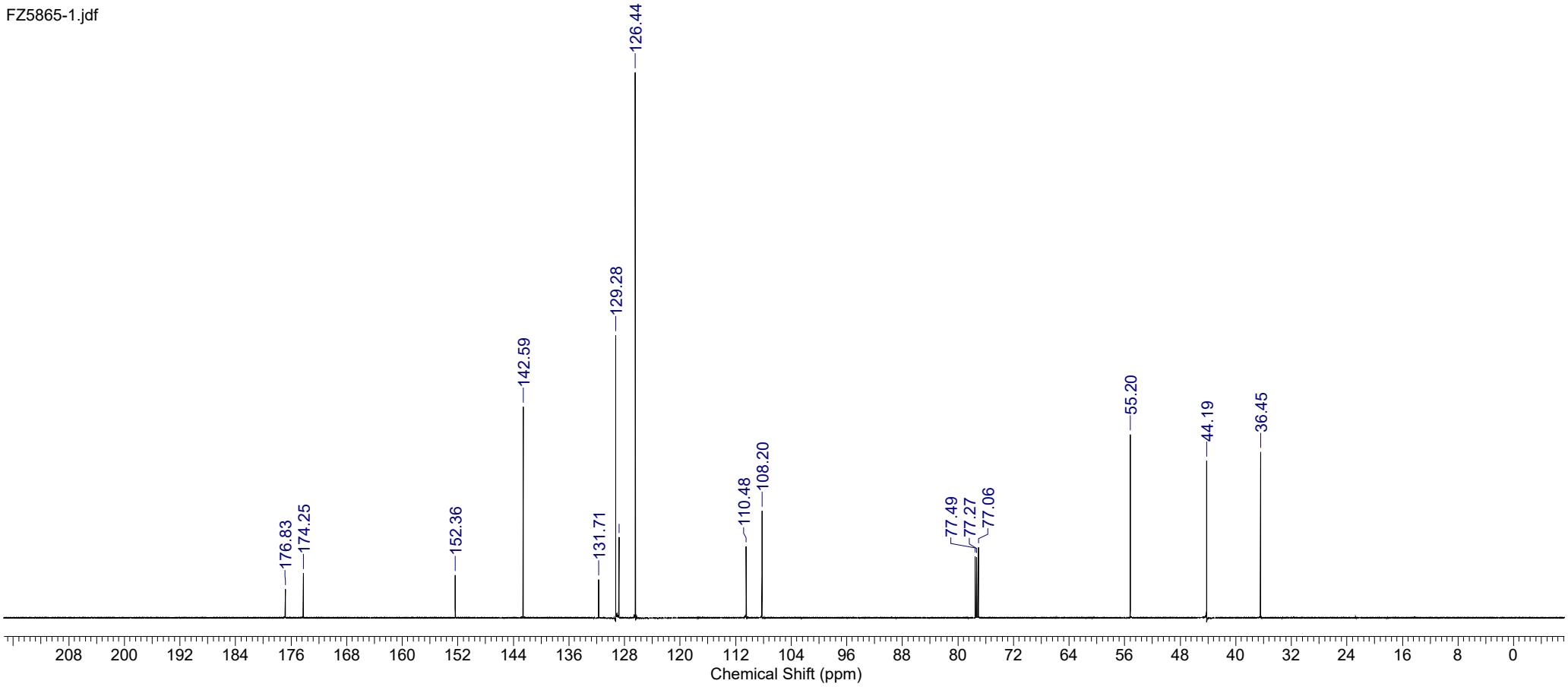


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:22:12
Date Stamp	21 Feb 2017 17:19:57			***File Name***	C:\Users\Fedor\Desktop\21.02.17\FZ5865-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	54.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.200				

6d

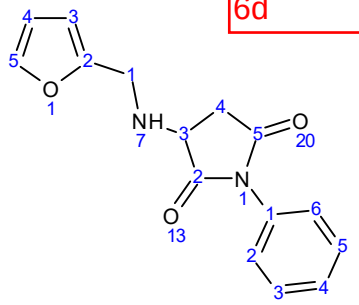


FZ5865-1.jdf

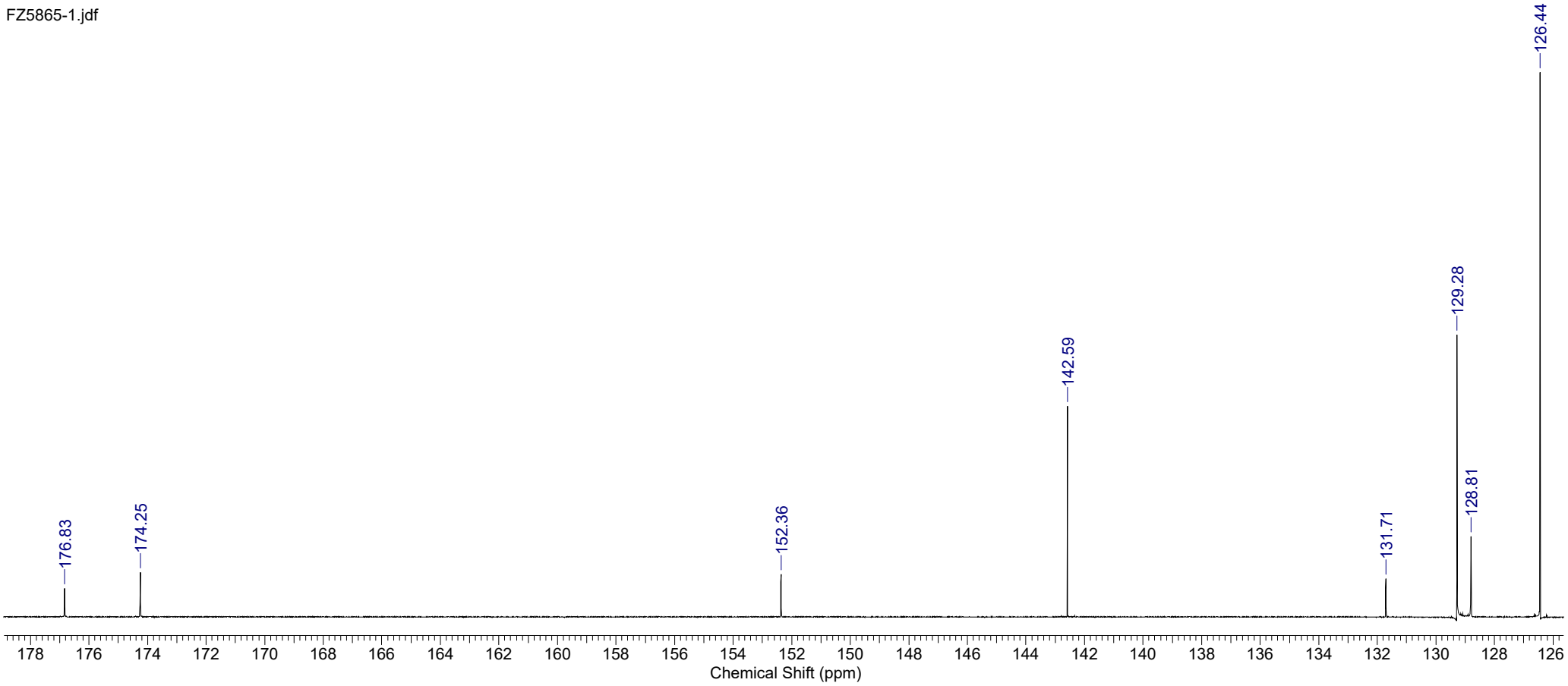


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:22:12
Date Stamp	21 Feb 2017 17:19:57			***File Name***	C:\Users\Fedor\Desktop\21.02.17\FZ5865-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	54.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.200				

6d

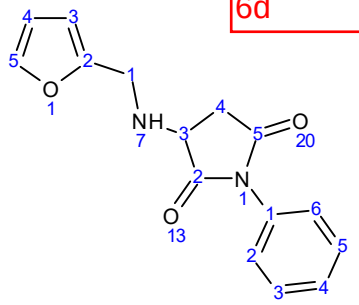


FZ5865-1.jdf

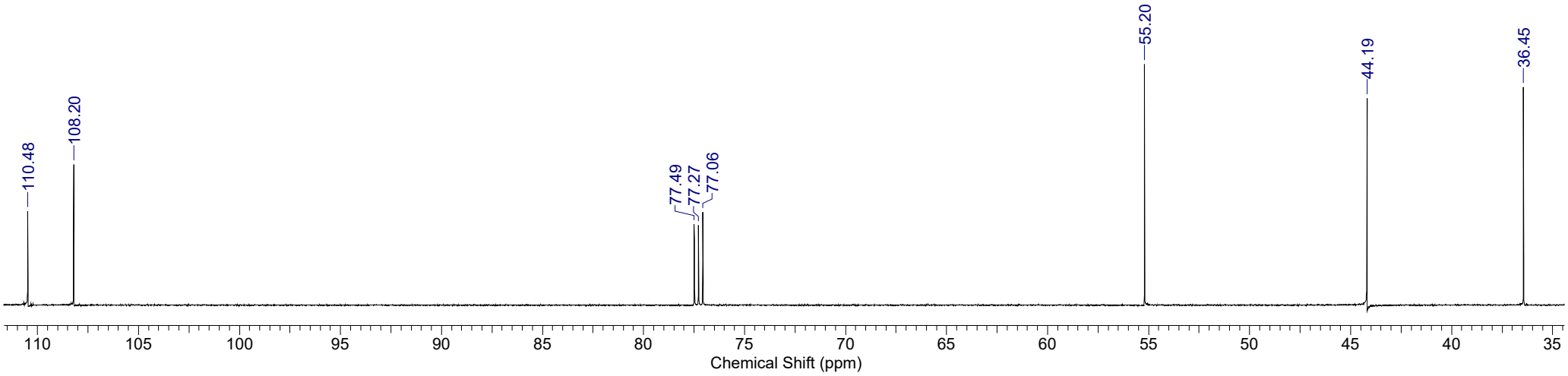


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:22:12
Date Stamp	21 Feb 2017 17:19:57			***File Name***	C:\Users\Fedor\Desktop\21.02.17\FZ5865-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	54.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.200				

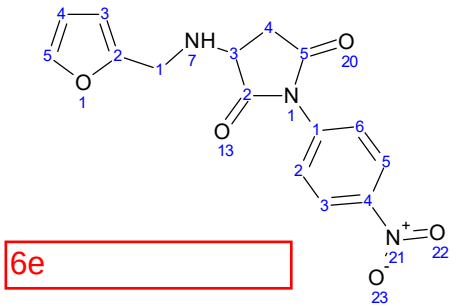
6d

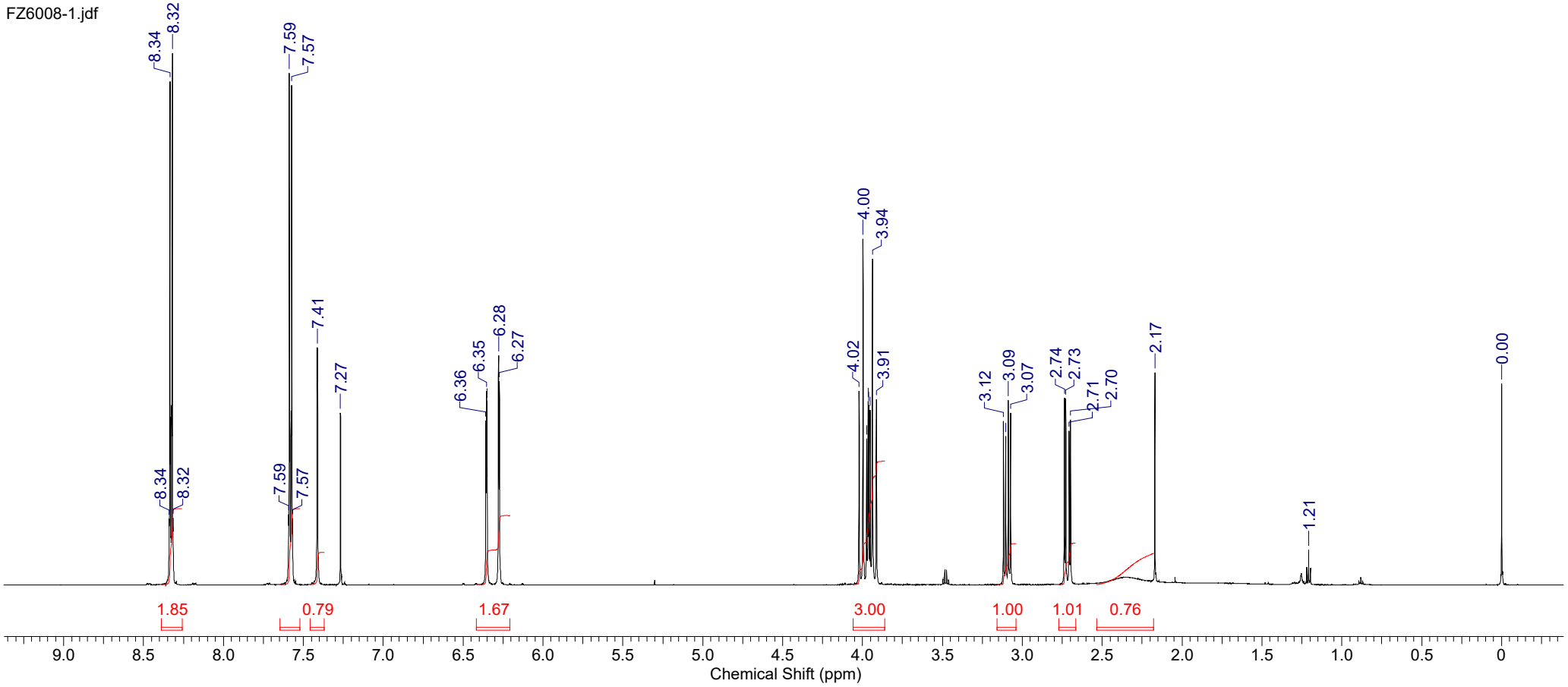


FZ5865-1.jdf

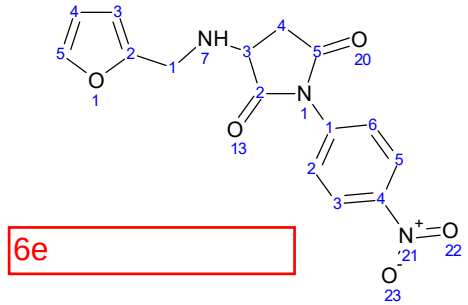


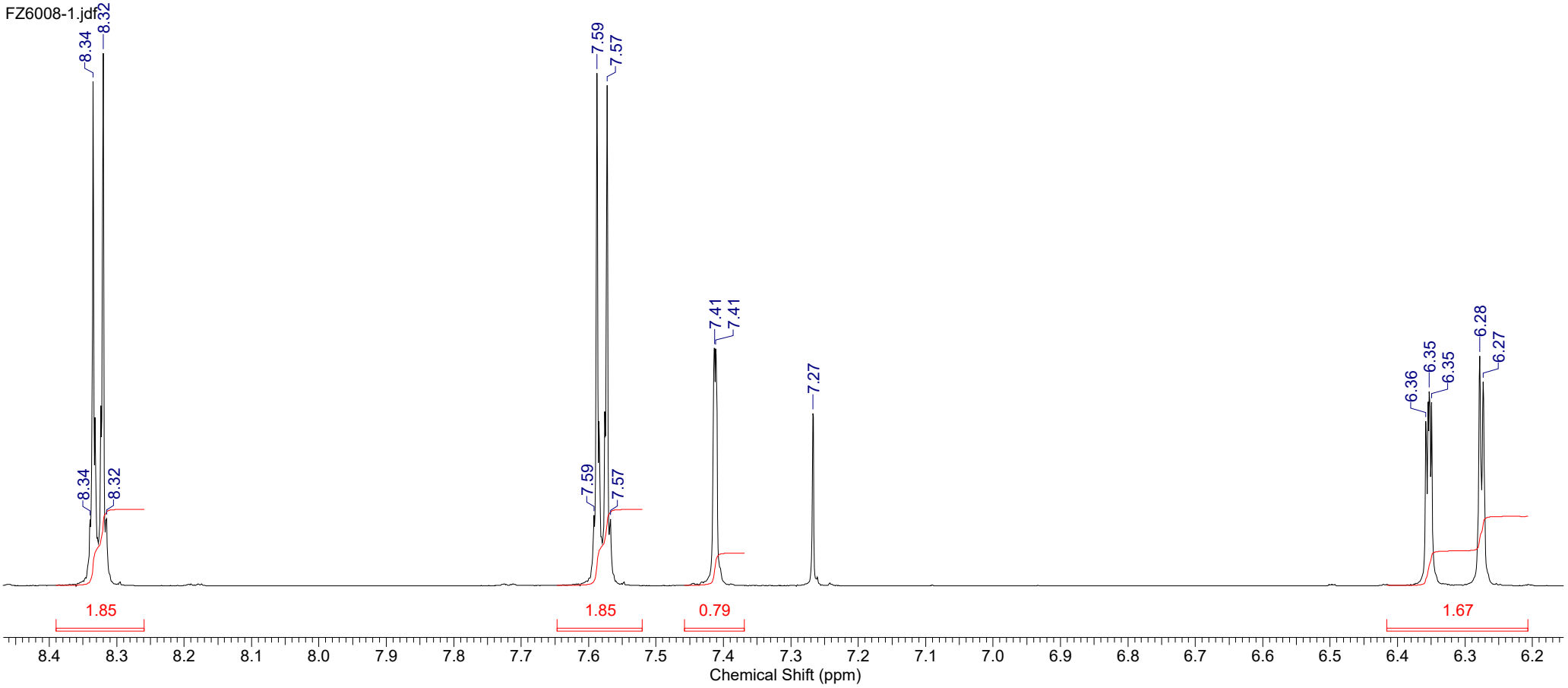
Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:18:29				
Date Stamp	05 Apr 2017 12:41:56			***File Name***	C:\Users\Fedor\Desktop\04.04.17\FZ6008-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5412.1411	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	21.600				



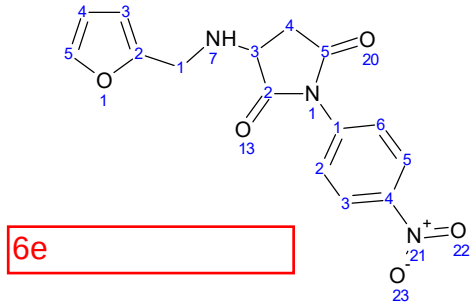


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:18:29				
Date Stamp	05 Apr 2017 12:41:56			***File Name***	C:\Users\Fedor\Desktop\04.04.17\FZ6008-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5412.1411	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	21.600				

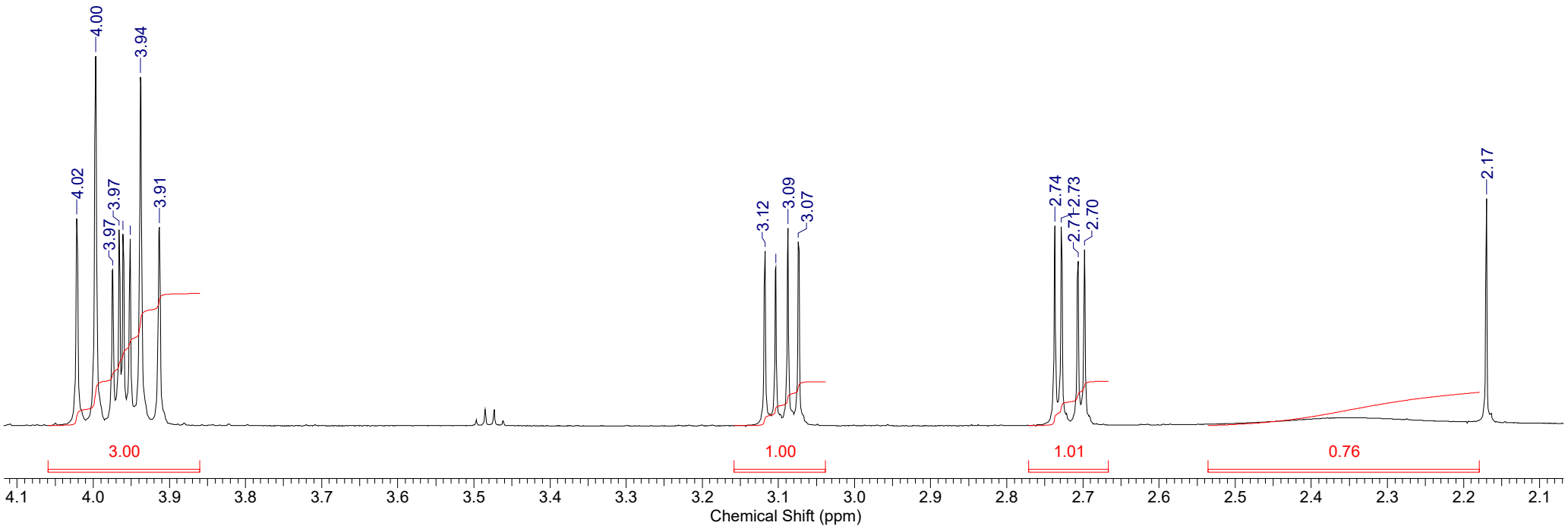




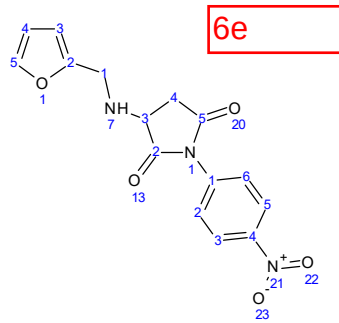
Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:18:29				
Date Stamp	05 Apr 2017 12:41:56			***File Name***	C:\Users\Fedor\Desktop\04.04.17\FZ6008-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5412.1411	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	21.600				

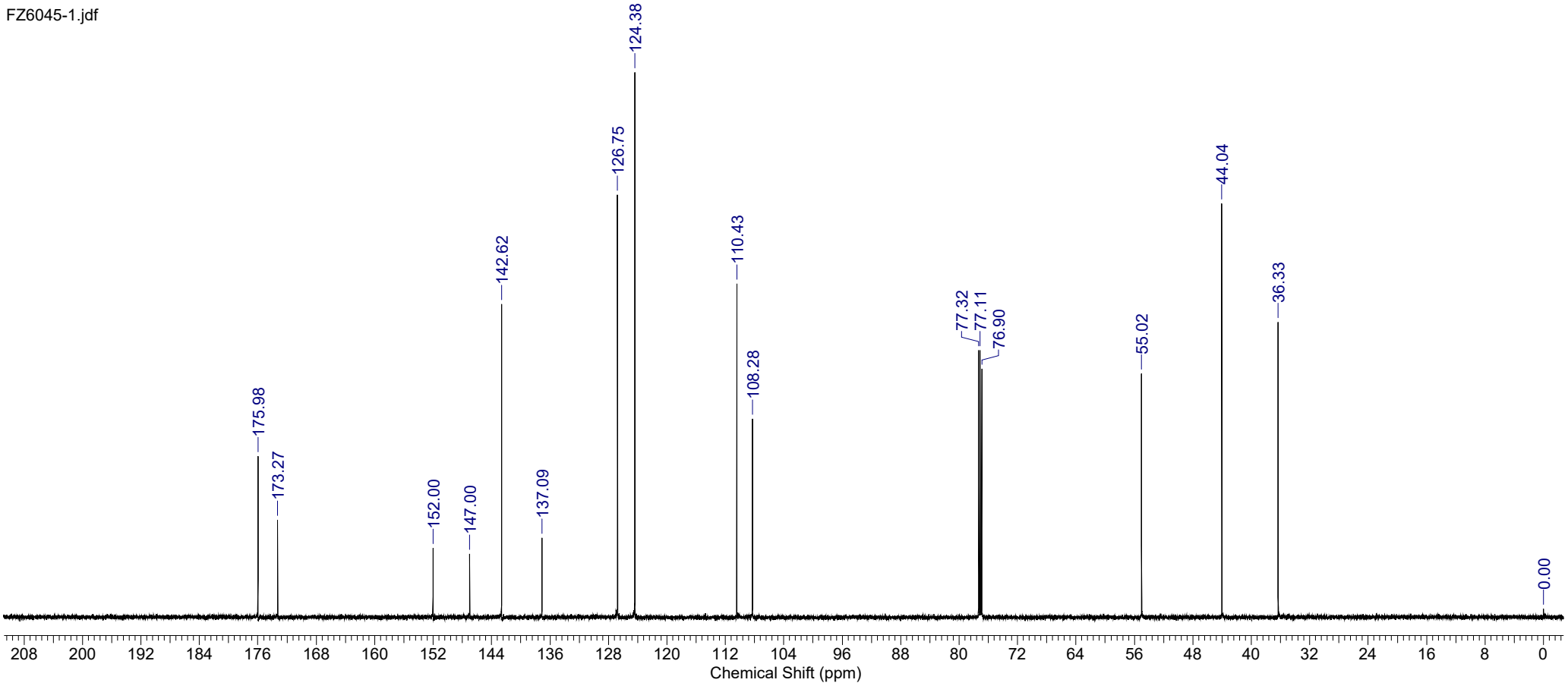


FZ6008-1.jdf



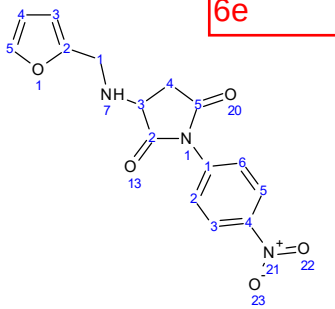
Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:19:31
Date Stamp	13 Apr 2017 04:22:29			***File Name***	C:\Users\Fedor\Desktop\11.04.17\FZ6045-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	500	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15079.3525
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.400				



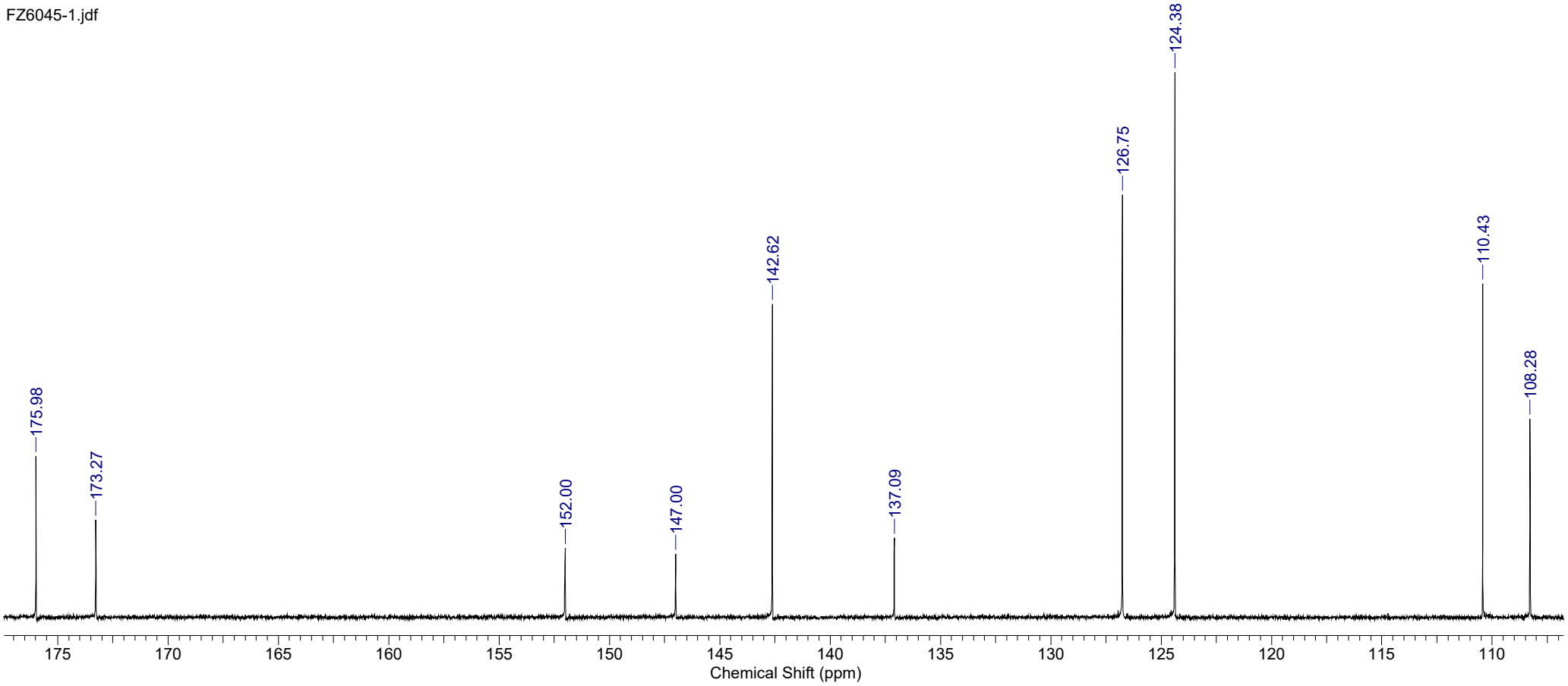


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:19:31
Date Stamp	13 Apr 2017 04:22:29			***File Name***	C:\Users\Fedor\Desktop\11.04.17\FZ6045-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	500	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15079.3525
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.400				

6e

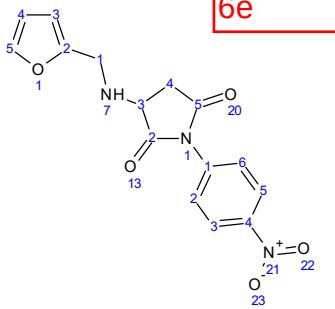


FZ6045-1.jdf

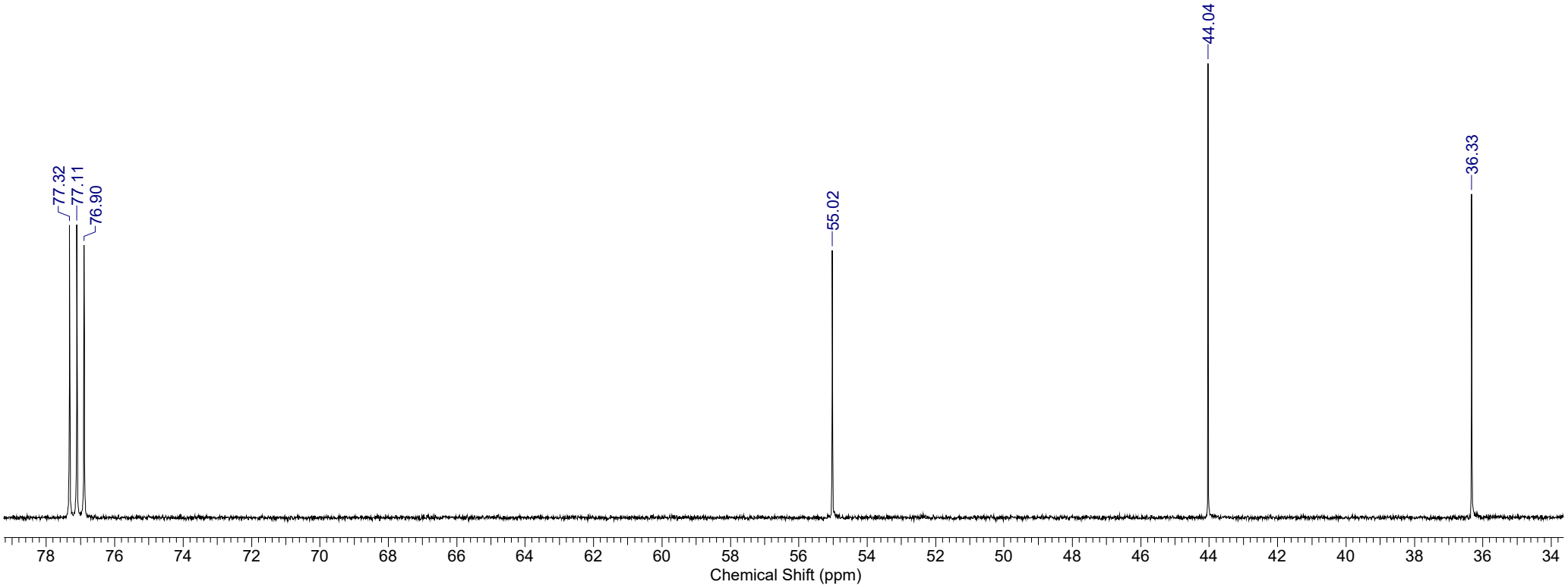


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:19:31
Date Stamp	13 Apr 2017 04:22:29			***File Name***	C:\Users\Fedor\Desktop\11.04.17\FZ6045-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	500	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15079.3525
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.400				

6e

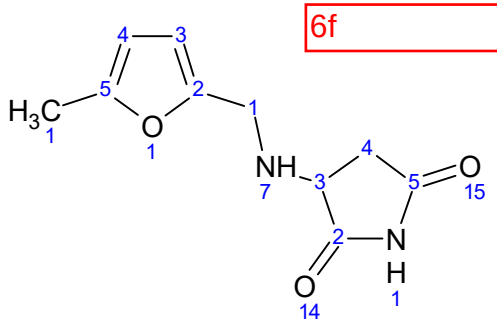


FZ6045-1.jdf

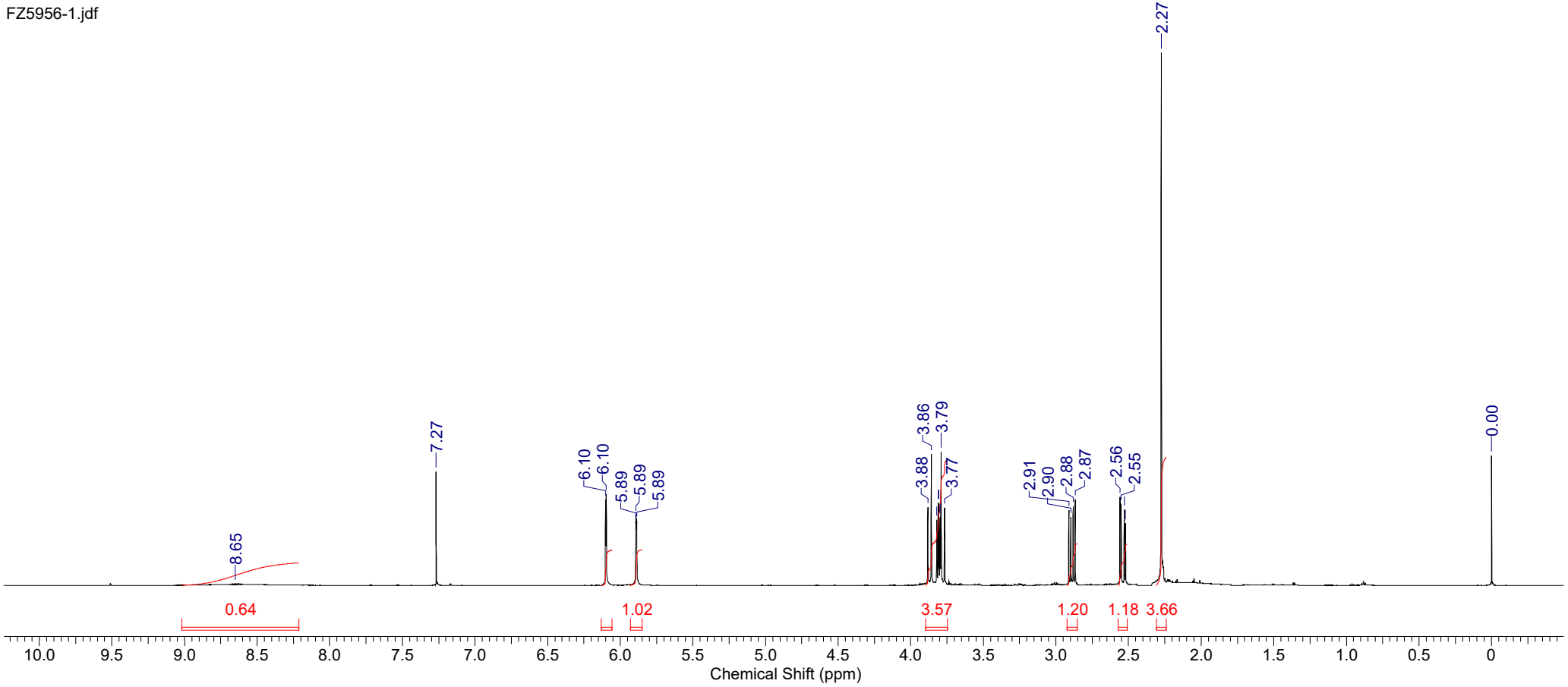


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:39:18				
Date Stamp	23 Mar 2017 10:00:31			***File Name***	C:\Users\Fedor\Desktop\21.03.17\FZ5956-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5412.6455	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.200				

6f

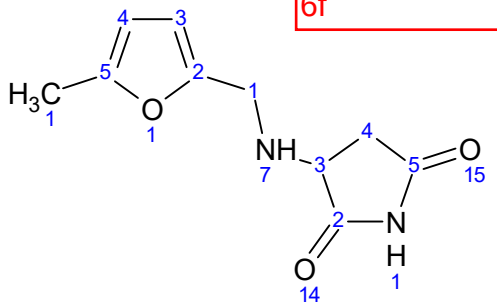


FZ5956-1.jdf

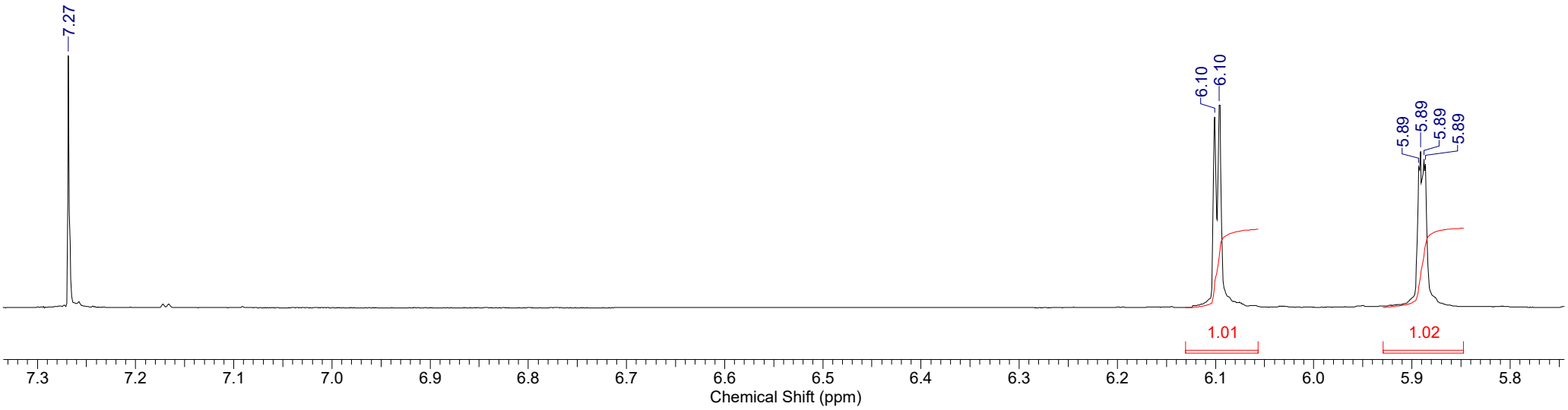


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:39:18				
Date Stamp	23 Mar 2017 10:00:31			***File Name***	C:\Users\Fedor\Desktop\21.03.17\FZ5956-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5412.6455	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.200				

6f

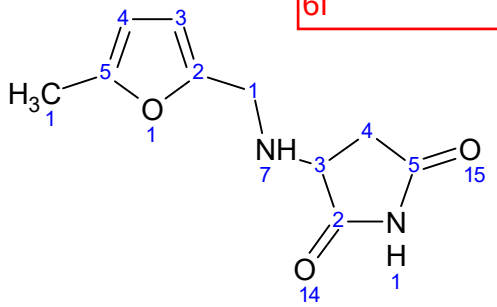


FZ5956-1.jdf

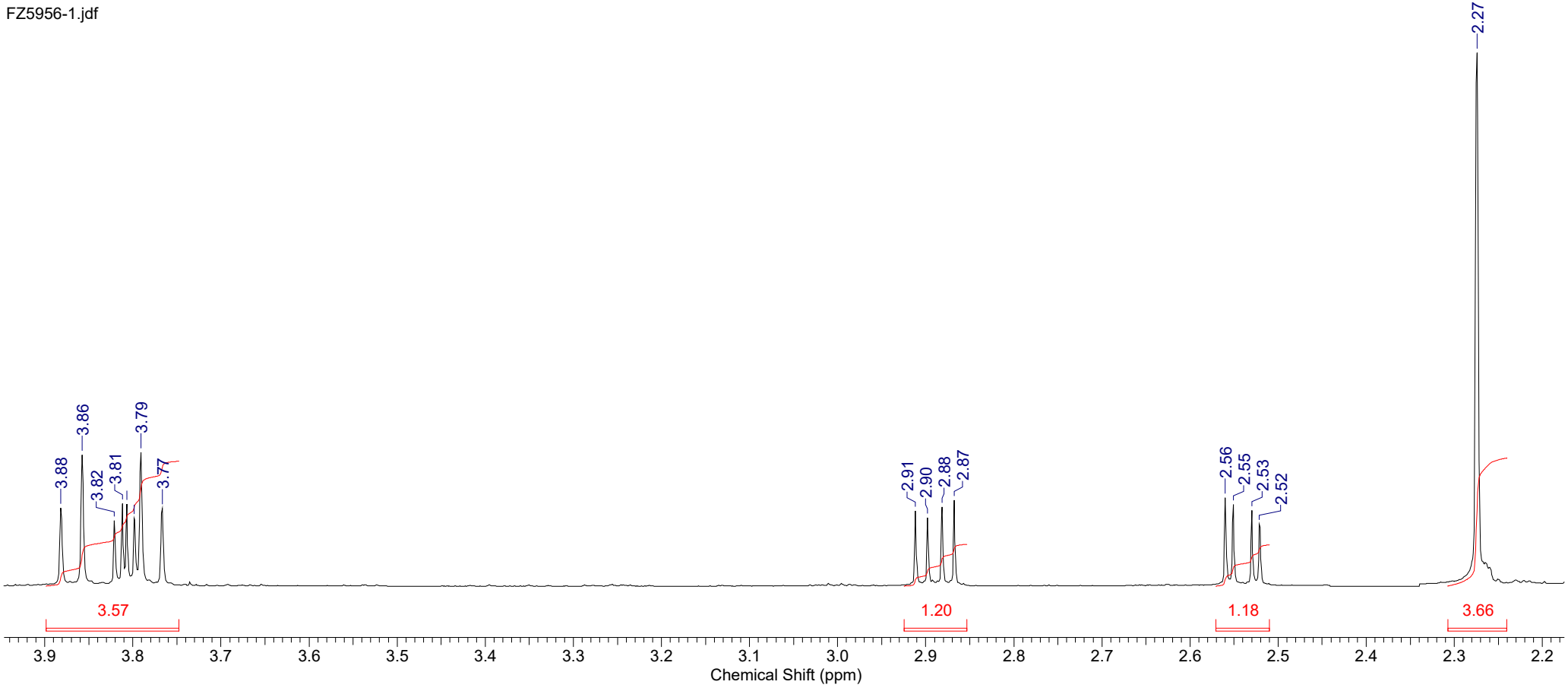


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:39:18				
Date Stamp	23 Mar 2017 10:00:31			***File Name***	C:\Users\Fedor\Desktop\21.03.17\FZ5956-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5412.6455	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.200				

6f

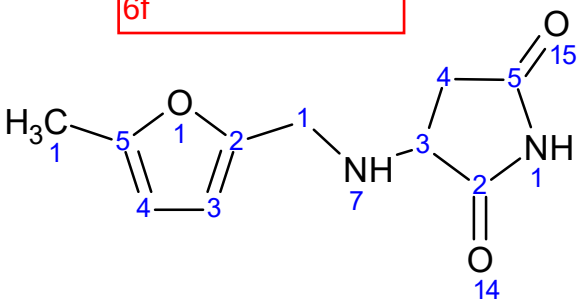


FZ5956-1.jdf

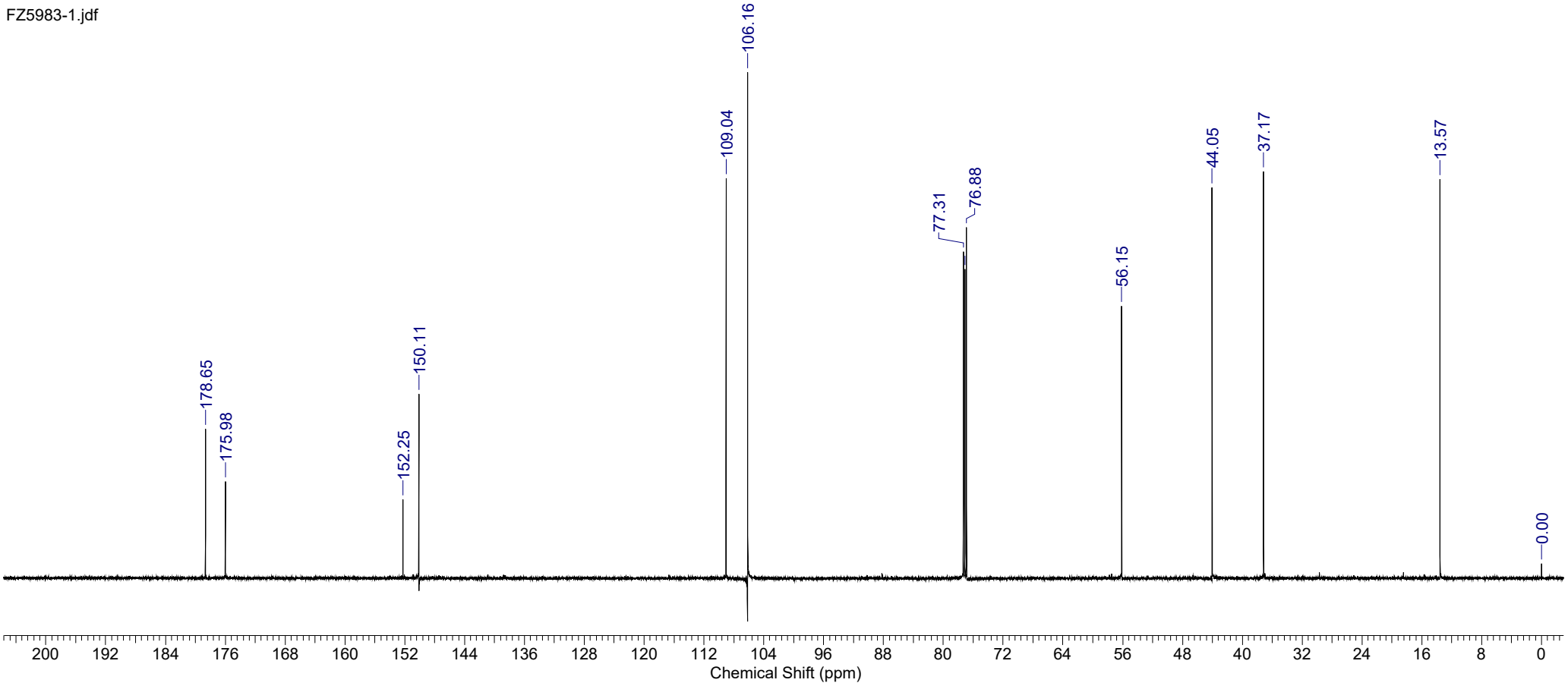


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:25:49
Date Stamp	29 Mar 2017 16:36:44			***File Name***	C:\Users\Fedor\Desktop\28.03.17\FZ5983-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	2000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15080.7979
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.500				

6f

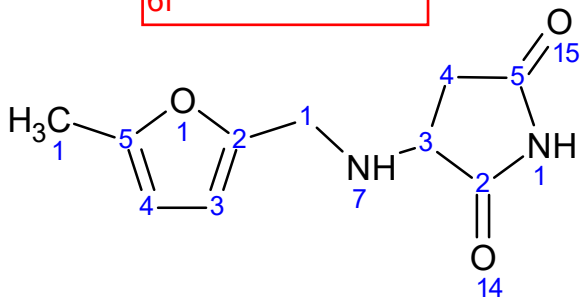


FZ5983-1.jdf

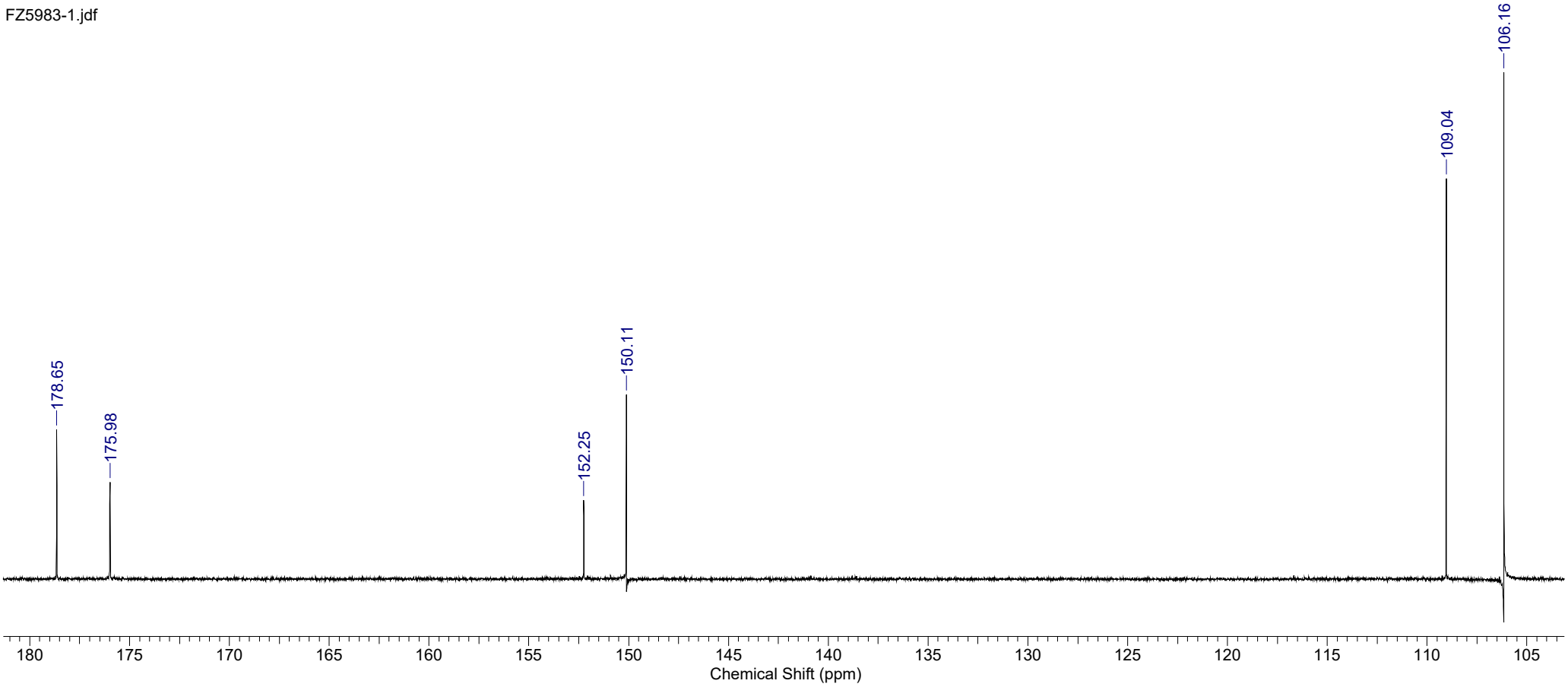


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:25:49
Date Stamp	29 Mar 2017 16:36:44			***File Name***	C:\Users\Fedor\Desktop\28.03.17\FZ5983-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	2000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15080.7979
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.500				

6f

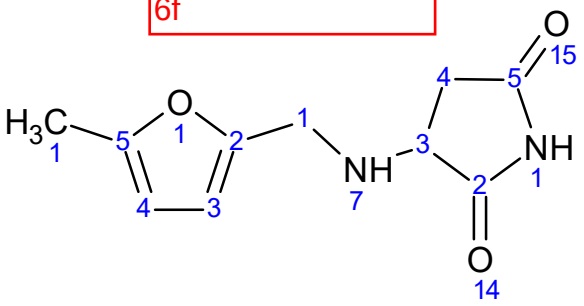


FZ5983-1.jdf

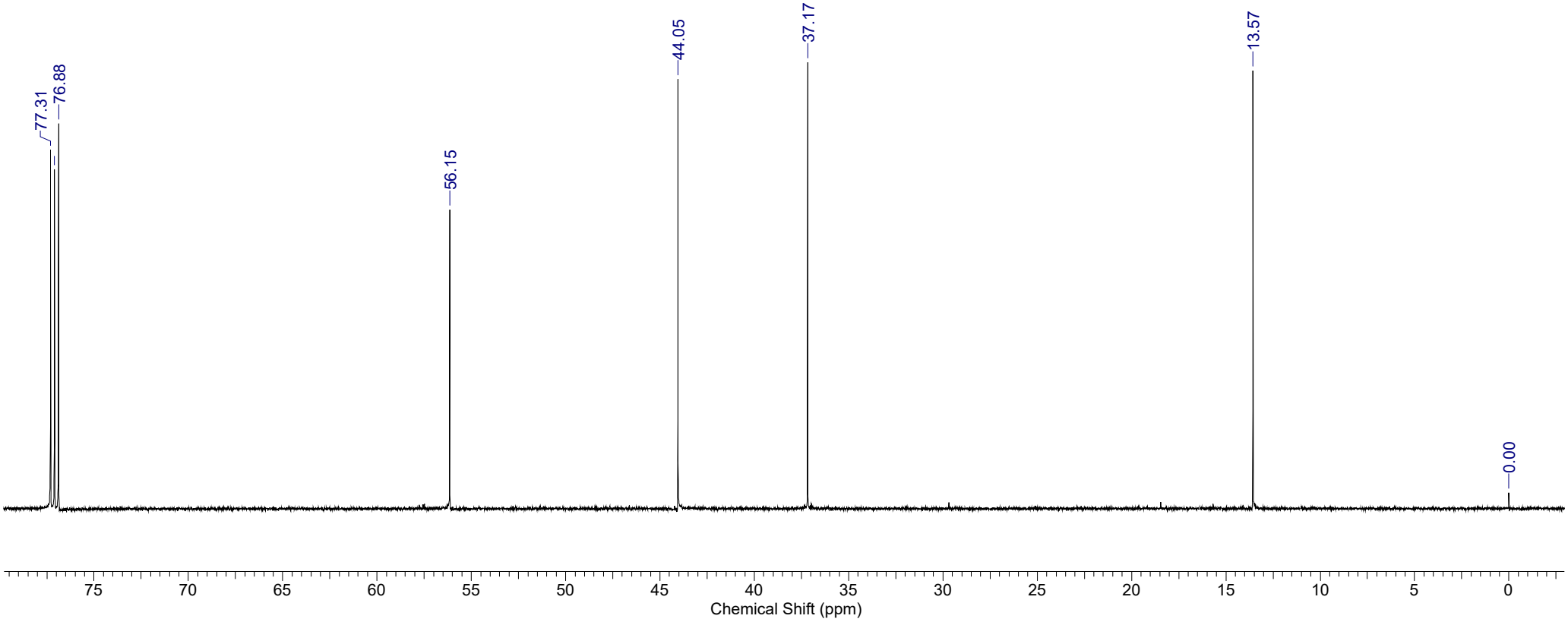


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:25:49
Date Stamp	29 Mar 2017 16:36:44			***File Name***	C:\Users\Fedor\Desktop\28.03.17\FZ5983-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	2000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15080.7979
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.500				

6f

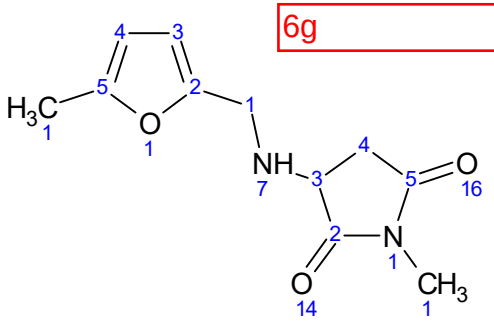


FZ5983-1.jdf

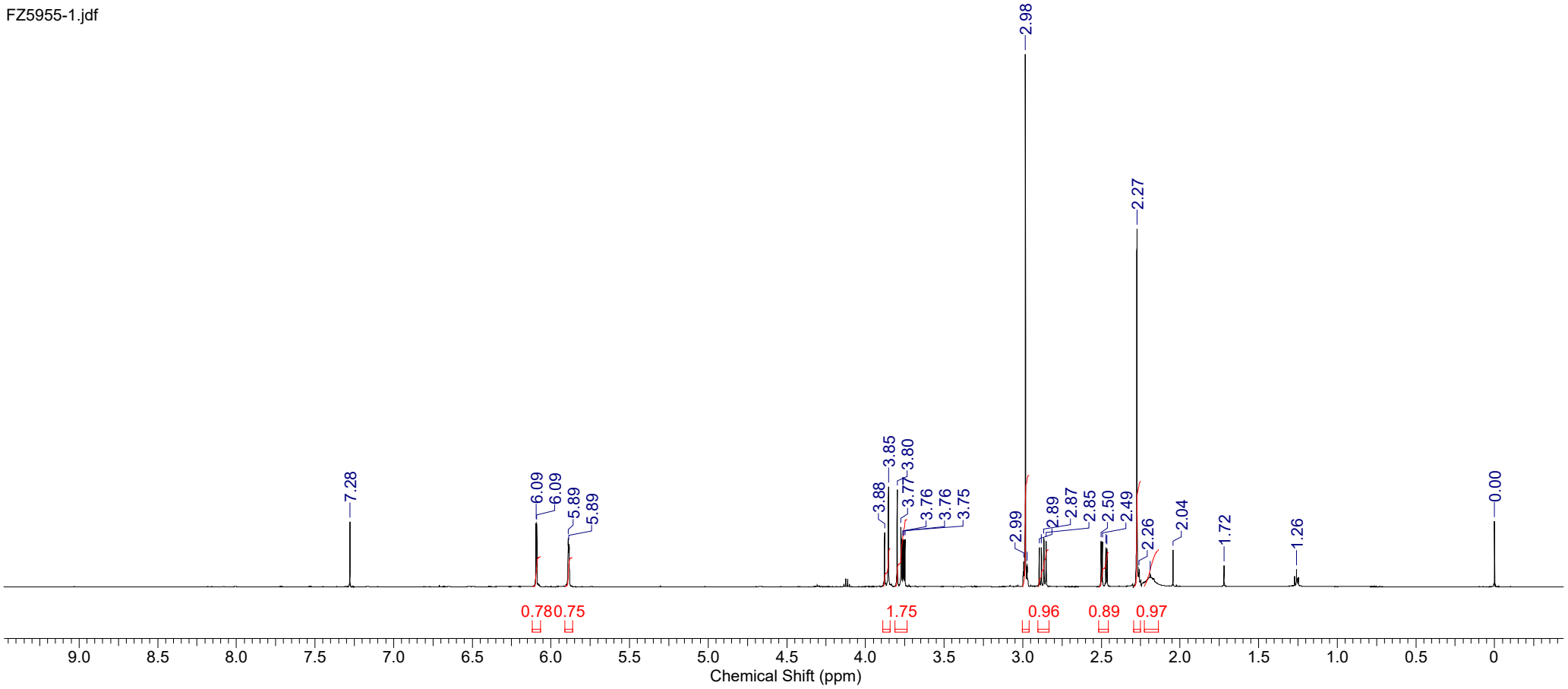


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:04:16				
Date Stamp	23 Mar 2017 10:10:59			***File Name***	C:\Users\Fedor\Desktop\21.03.17\FZ5955-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	30.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5418.7012	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.000				

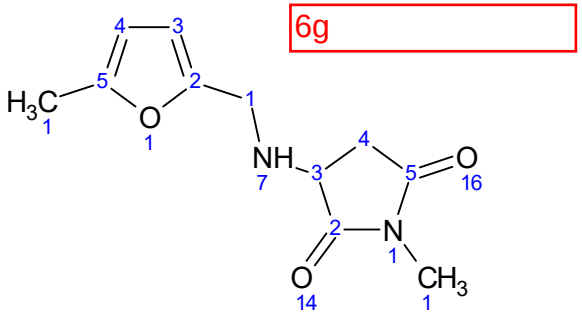
6g



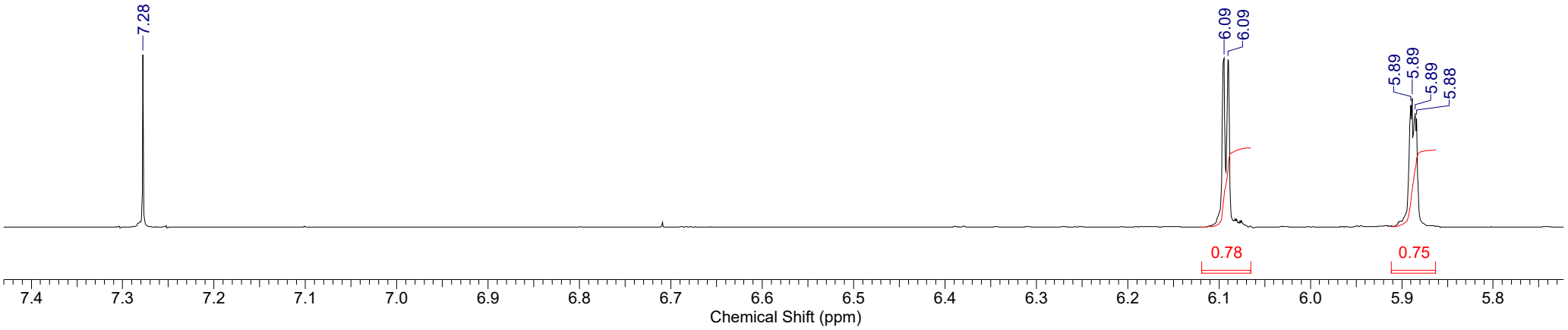
FZ5955-1.jdf



Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:04:16				
Date Stamp	23 Mar 2017 10:10:59			***File Name***	C:\Users\Fedor\Desktop\21.03.17\FZ5955-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	30.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5418.7012	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.000				

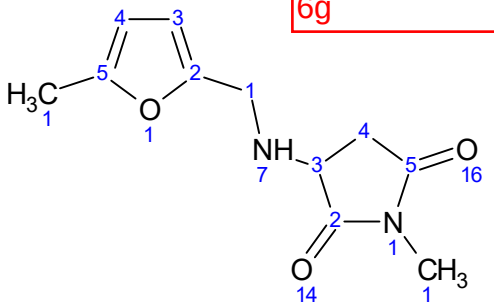


FZ5955-1.jdf

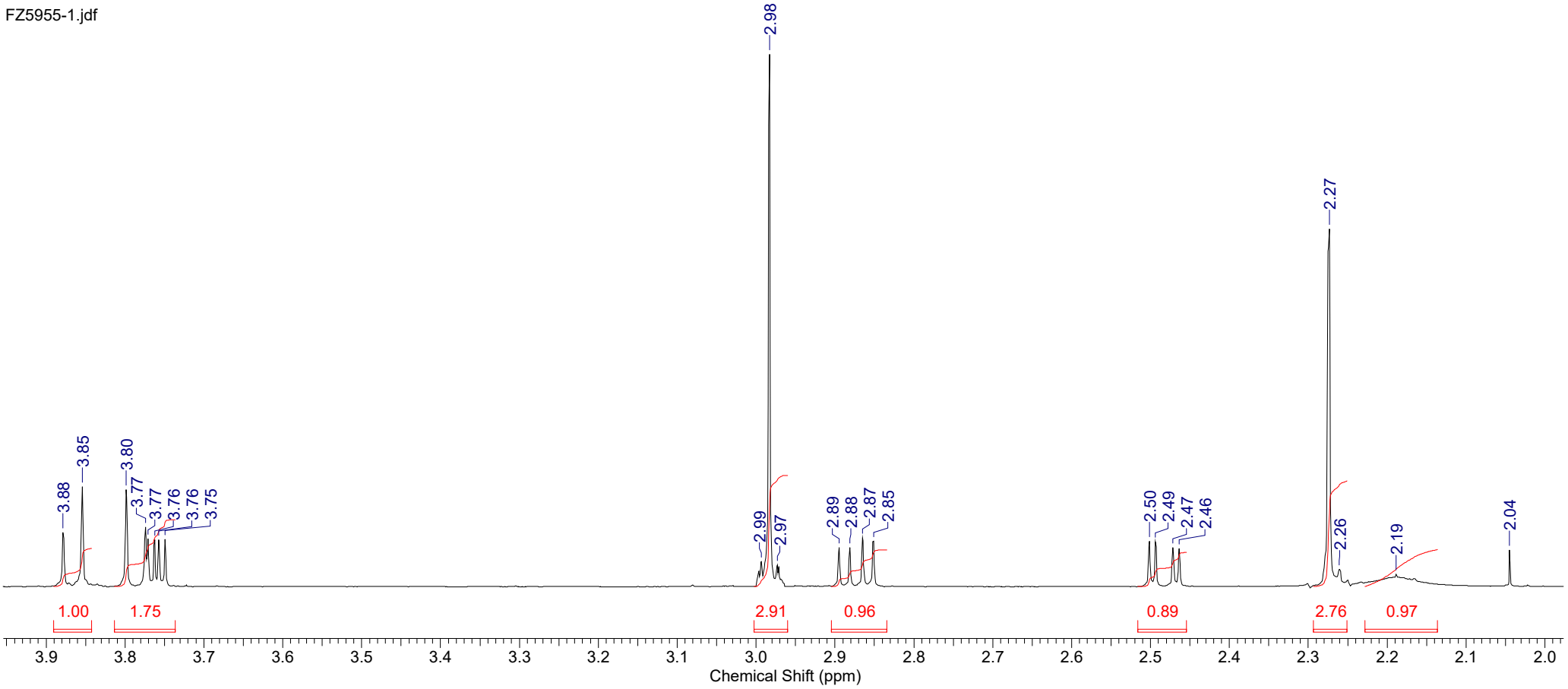


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:04:16				
Date Stamp	23 Mar 2017 10:10:59			***File Name***	C:\Users\Fedor\Desktop\21.03.17\FZ5955-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	30.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5418.7012	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.000				

6g

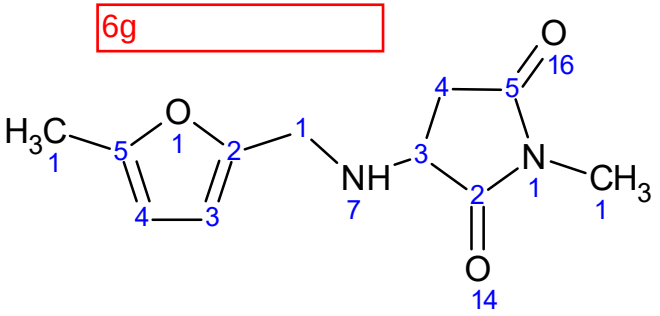


FZ5955-1.jdf

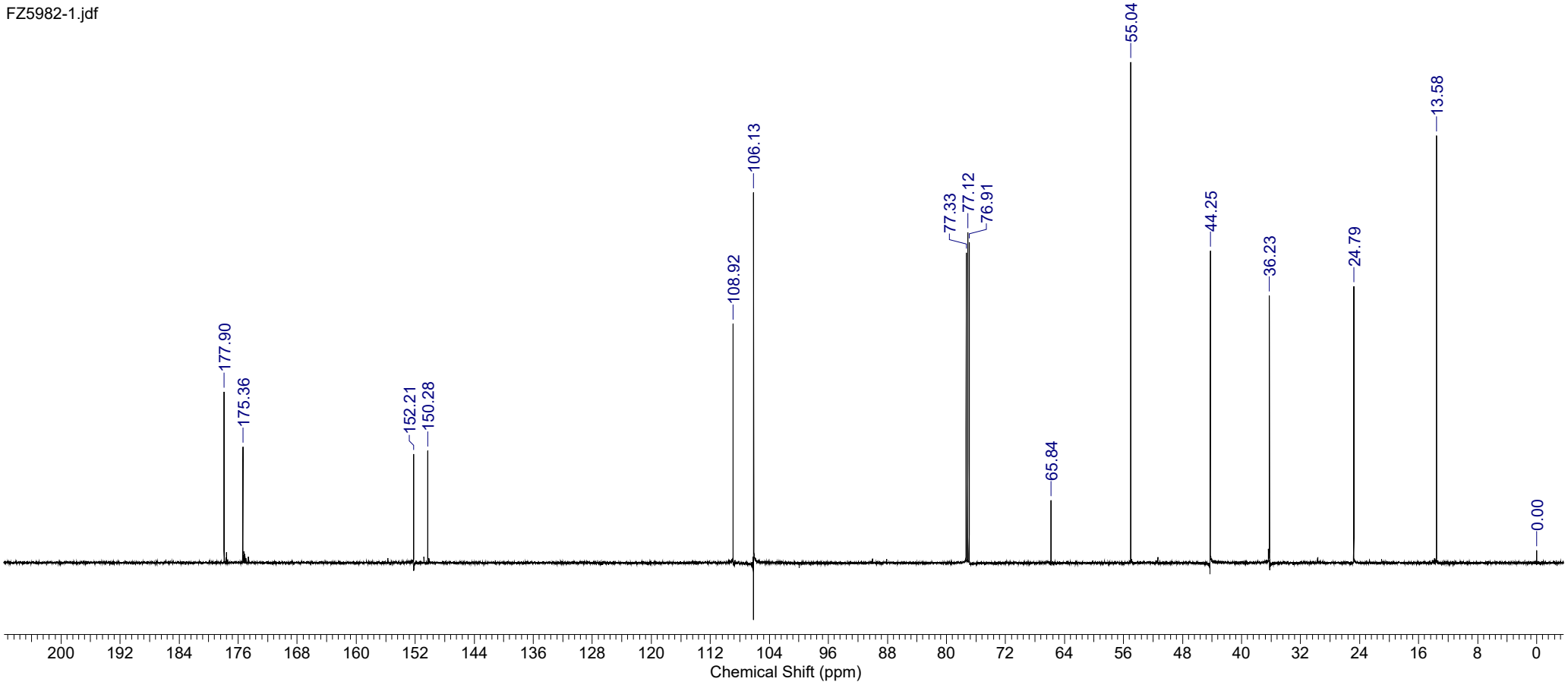


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:07:16
Date Stamp	29 Mar 2017 17:49:12			***File Name***	C:\Users\Fedor\Desktop\28.03.17\FZ5982-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	2000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15083.6875
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.400				

6g

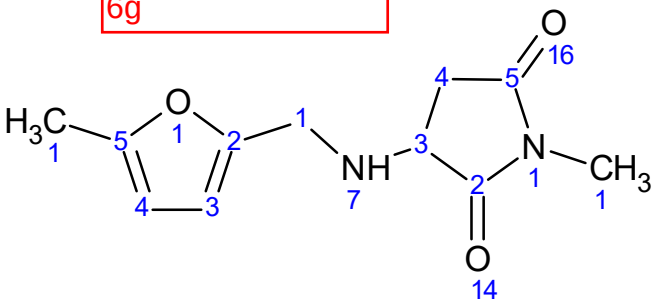


FZ5982-1.jdf

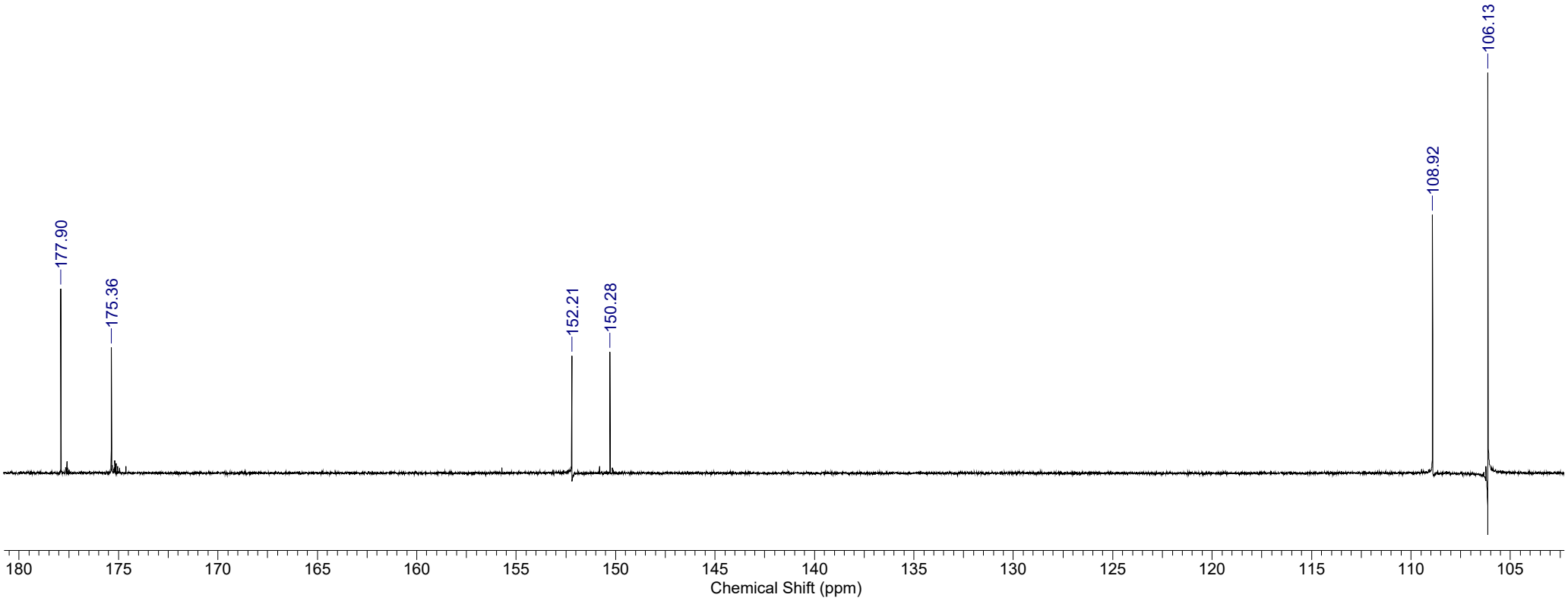


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:07:16
Date Stamp	29 Mar 2017 17:49:12			***File Name***	C:\Users\Fedor\Desktop\28.03.17\FZ5982-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	2000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15083.6875
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.400				

6g

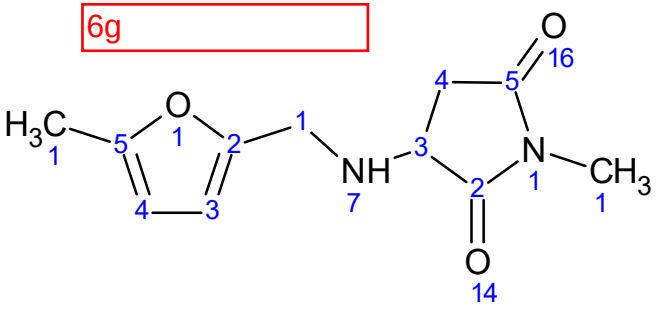


FZ5982-1.jdf

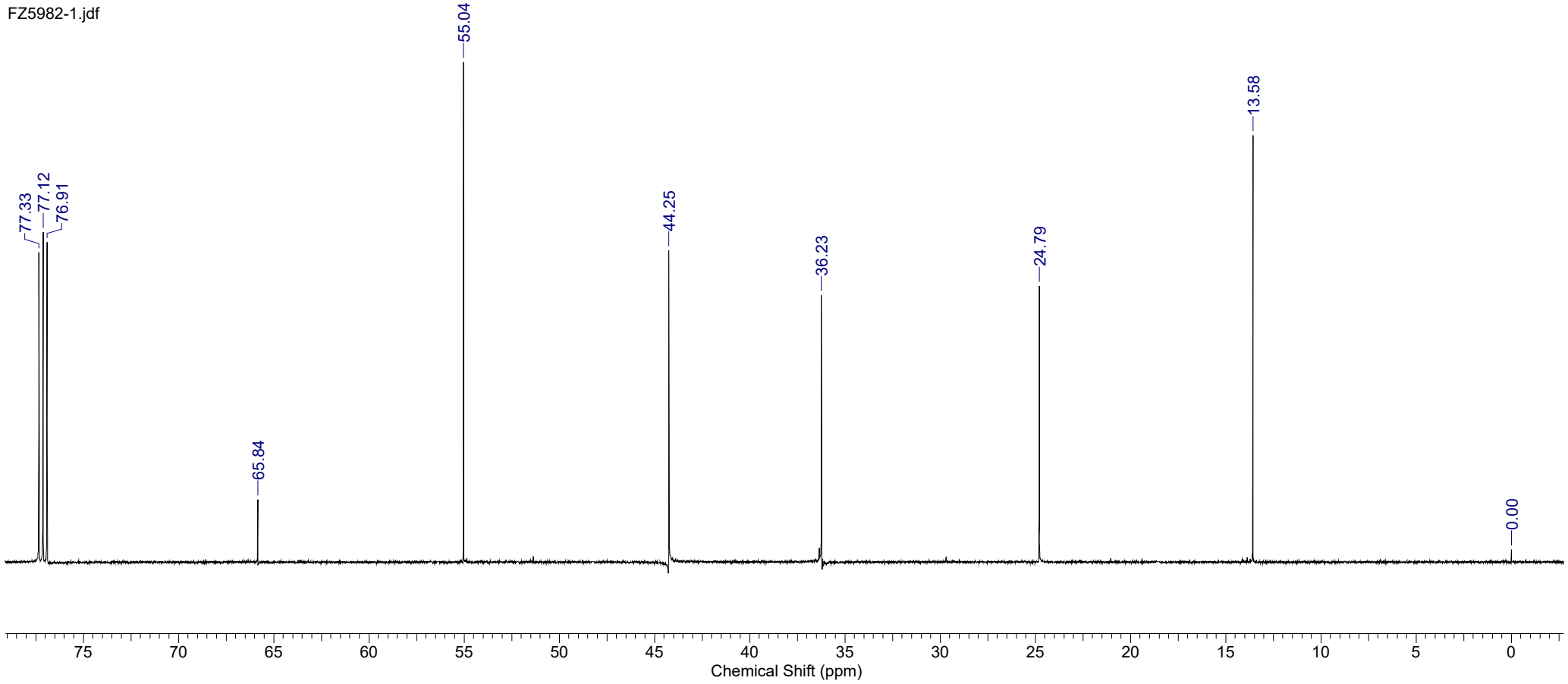


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:07:16
Date Stamp	29 Mar 2017 17:49:12			***File Name***	C:\Users\Fedor\Desktop\28.03.17\FZ5982-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	2000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15083.6875
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.400				

6g

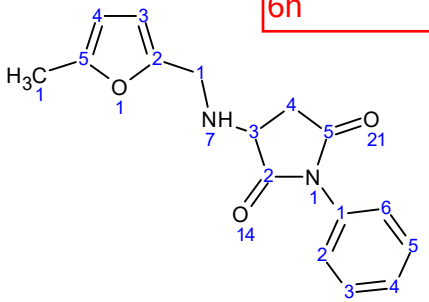


FZ5982-1.jdf

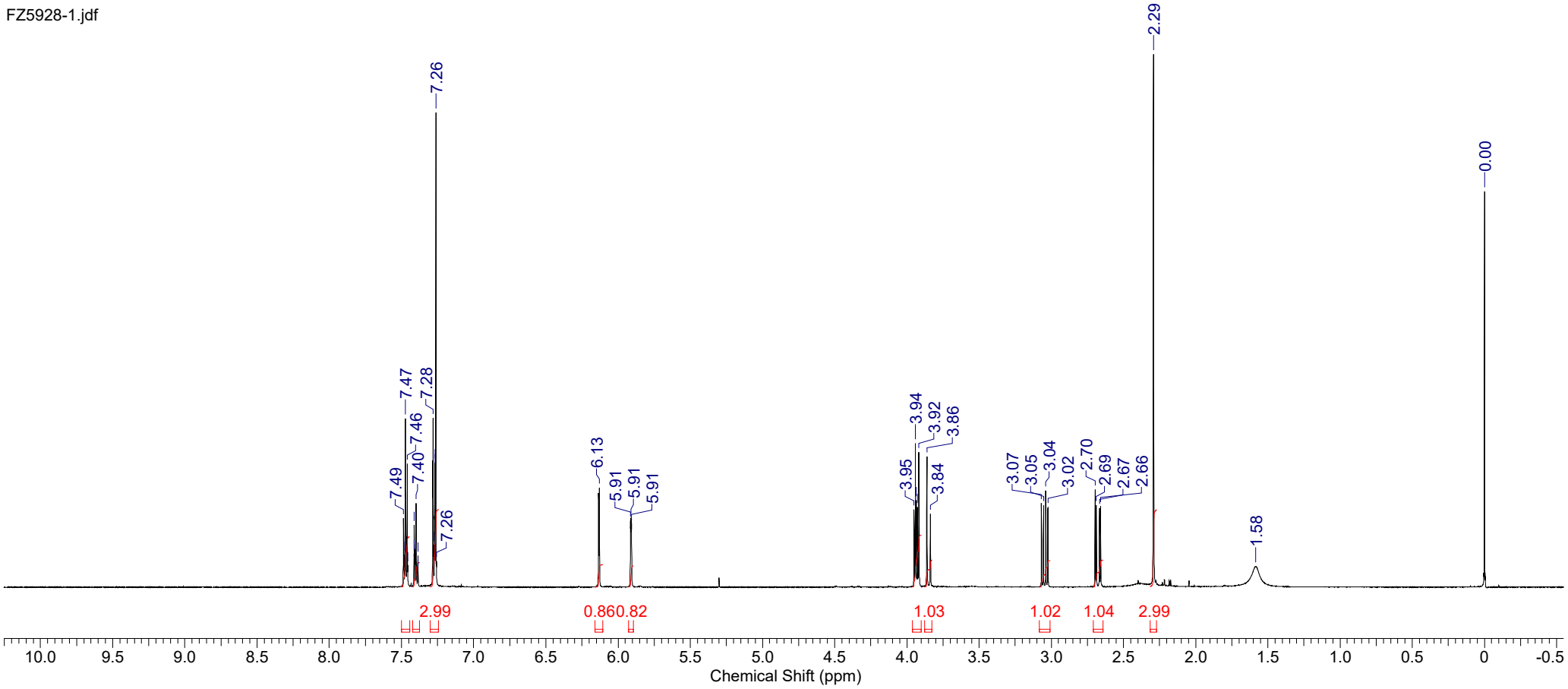


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:22:40				
Date Stamp	09 Mar 2017 10:29:47			***File Name***	C:\Users\Fedor\Desktop\07.03.17\FZ5928-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	46.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5409.1133	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.000				

6h

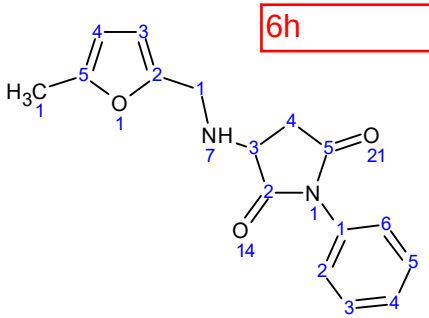


FZ5928-1.jdf

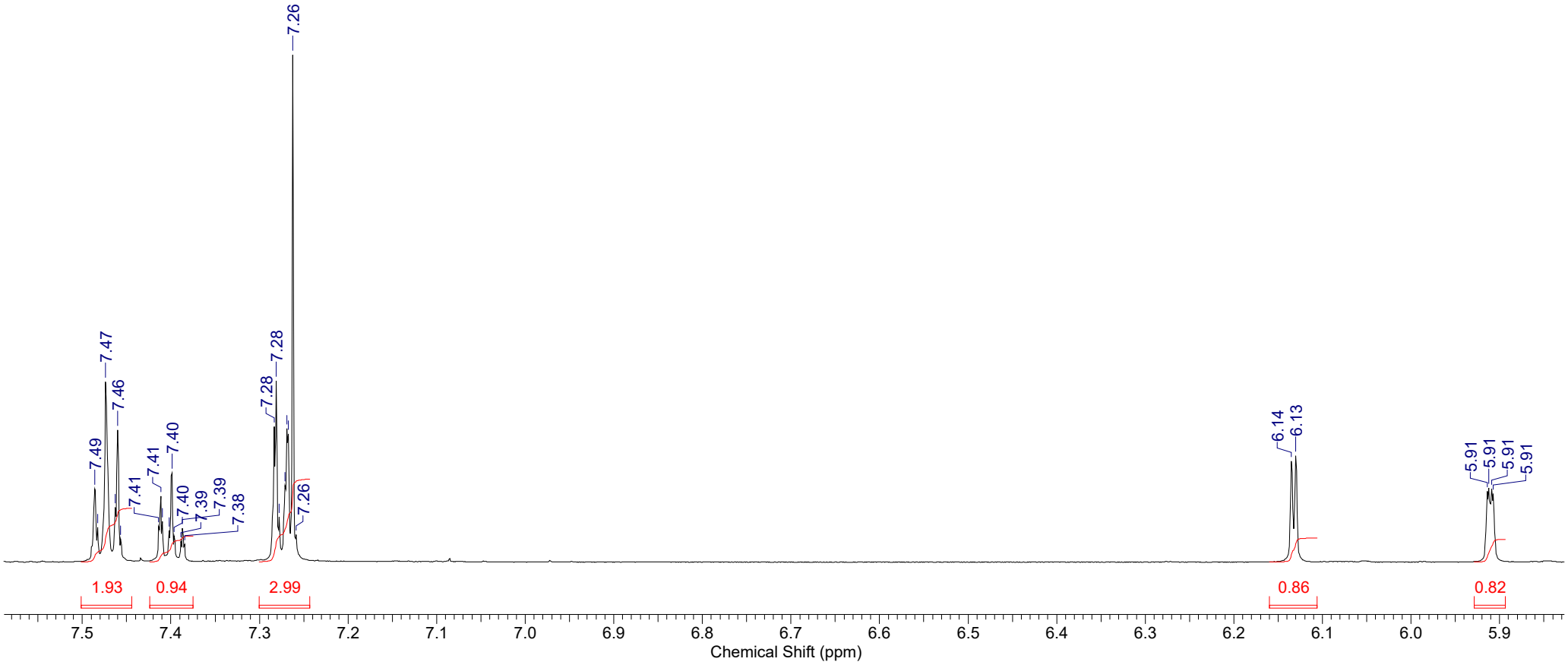


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:22:40				
Date Stamp	09 Mar 2017 10:29:47			***File Name***	C:\Users\Fedor\Desktop\07.03.17\FZ5928-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	46.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5409.1133	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.000				

6h

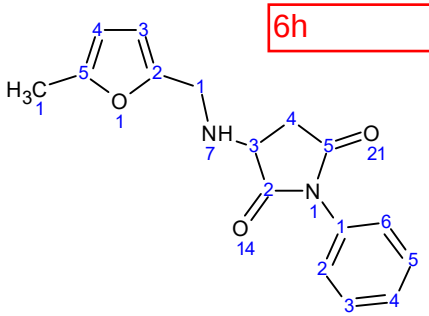


FZ5928-1.jdf

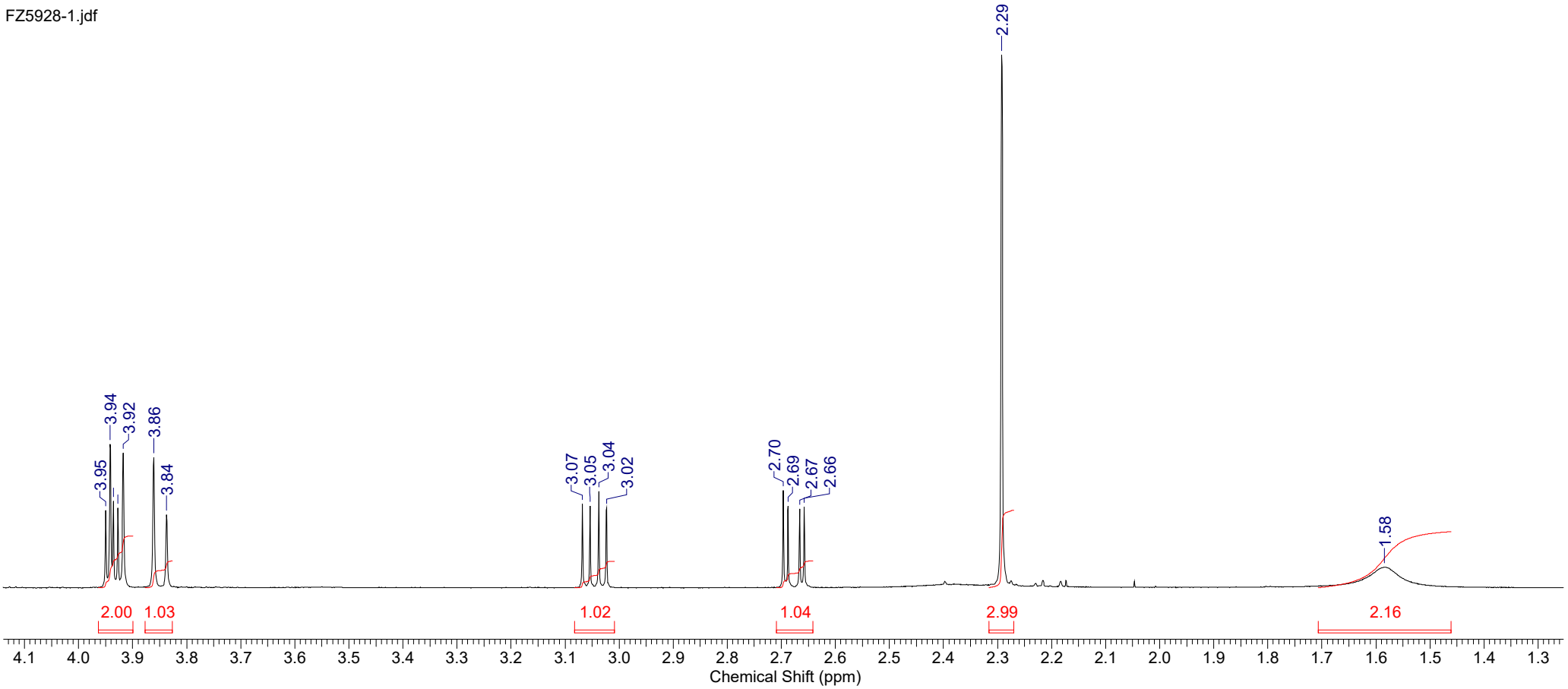


Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:22:40				
Date Stamp	09 Mar 2017 10:29:47			***File Name***	C:\Users\Fedor\Desktop\07.03.17\FZ5928-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	46.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5409.1133	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.000				

6h

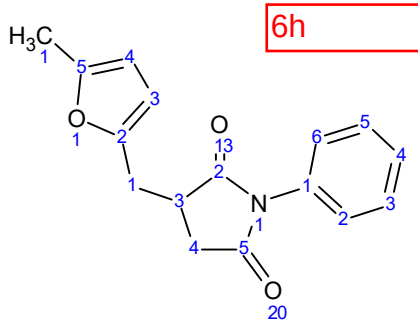


FZ5928-1.jdf

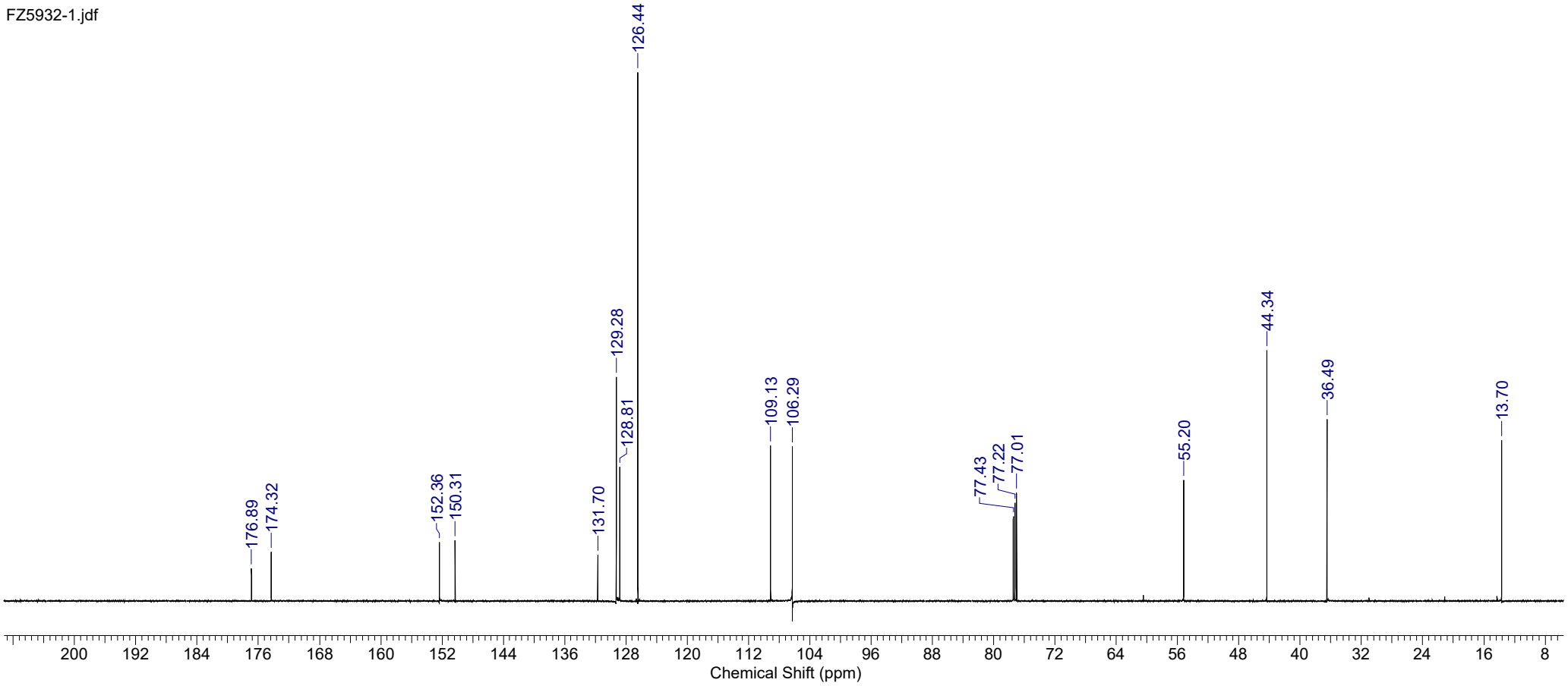


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:13:15
Date Stamp	15 Mar 2017 15:39:02			***File Name***	C:\Users\Fedor\Desktop\14.03.17\FZ5932-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.400				

6h

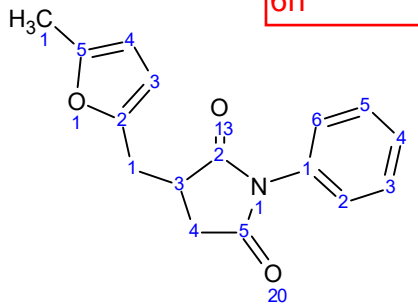


FZ5932-1.jdf

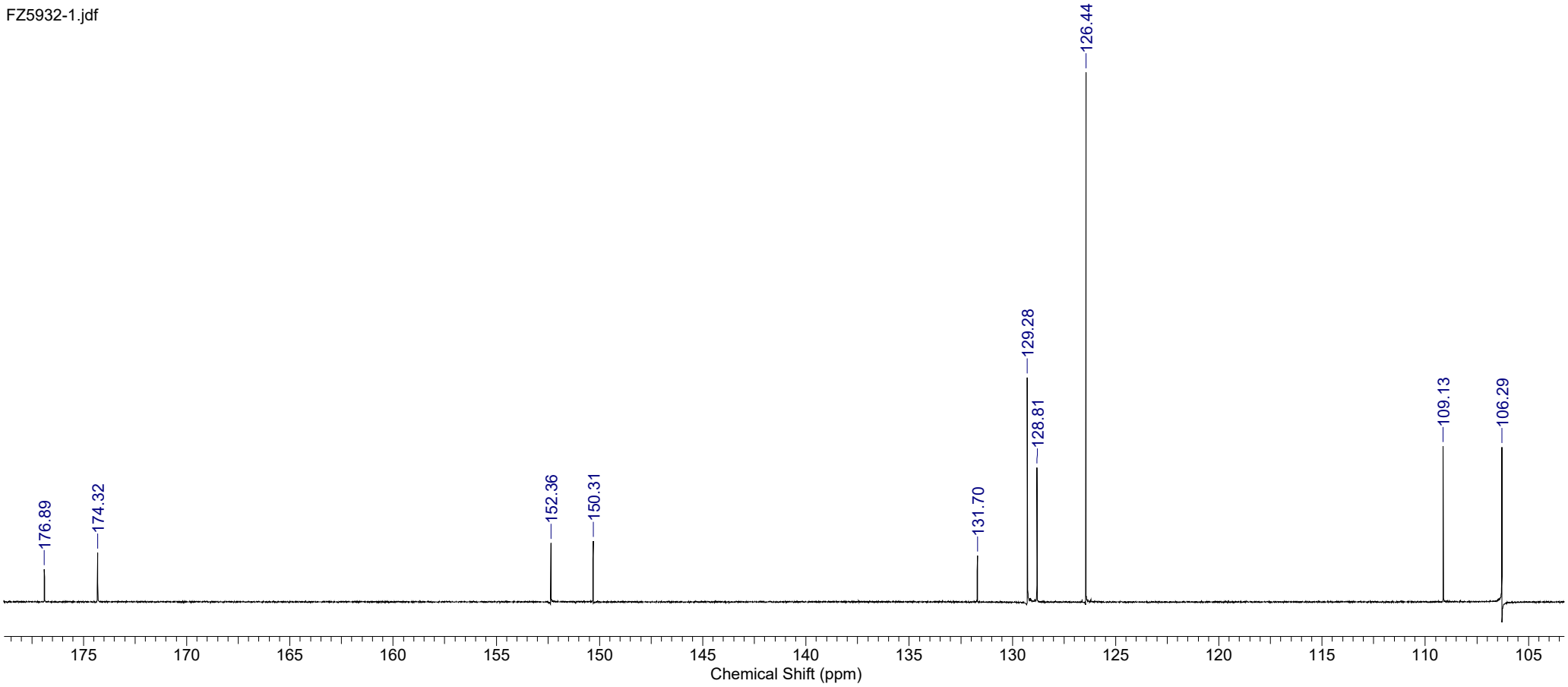


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:13:15
Date Stamp	15 Mar 2017 15:39:02			***File Name***	C:\Users\Fedor\Desktop\14.03.17\FZ5932-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.400				

6h

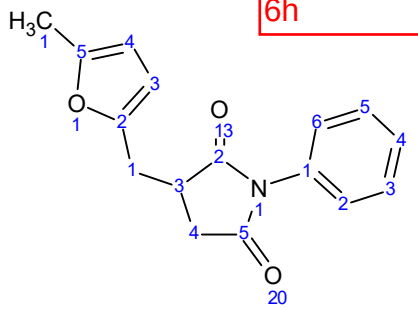


FZ5932-1.jdf

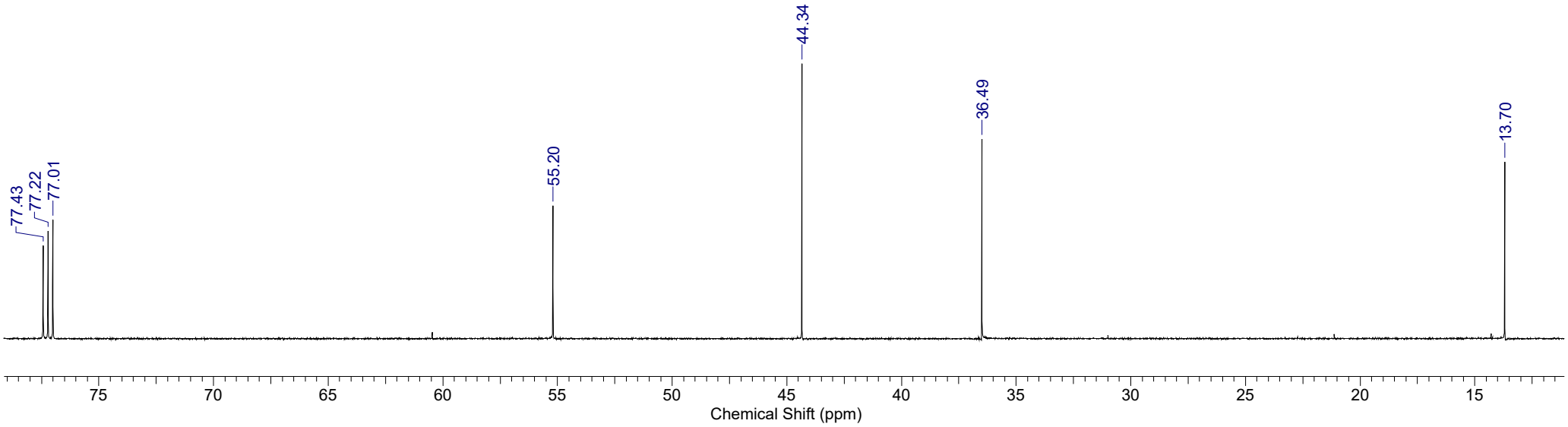


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:13:15
Date Stamp	15 Mar 2017 15:39:02			***File Name***	C:\Users\Fedor\Desktop\14.03.17\FZ5932-1.jdf		
Frequency (MHz)	150.91	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	ECA 600
Original Points Count	32768	***Owner***	delta	***Points Count***	32768	***Pulse Sequence***	single_pulse_dec
Receiver Gain	52.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	15091.3428
Sweep Width (Hz)	47348.49	***Temperature (degree C)***	23.400				

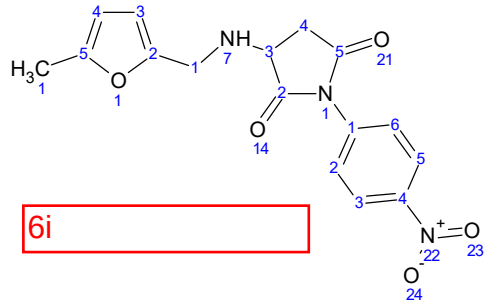
6h



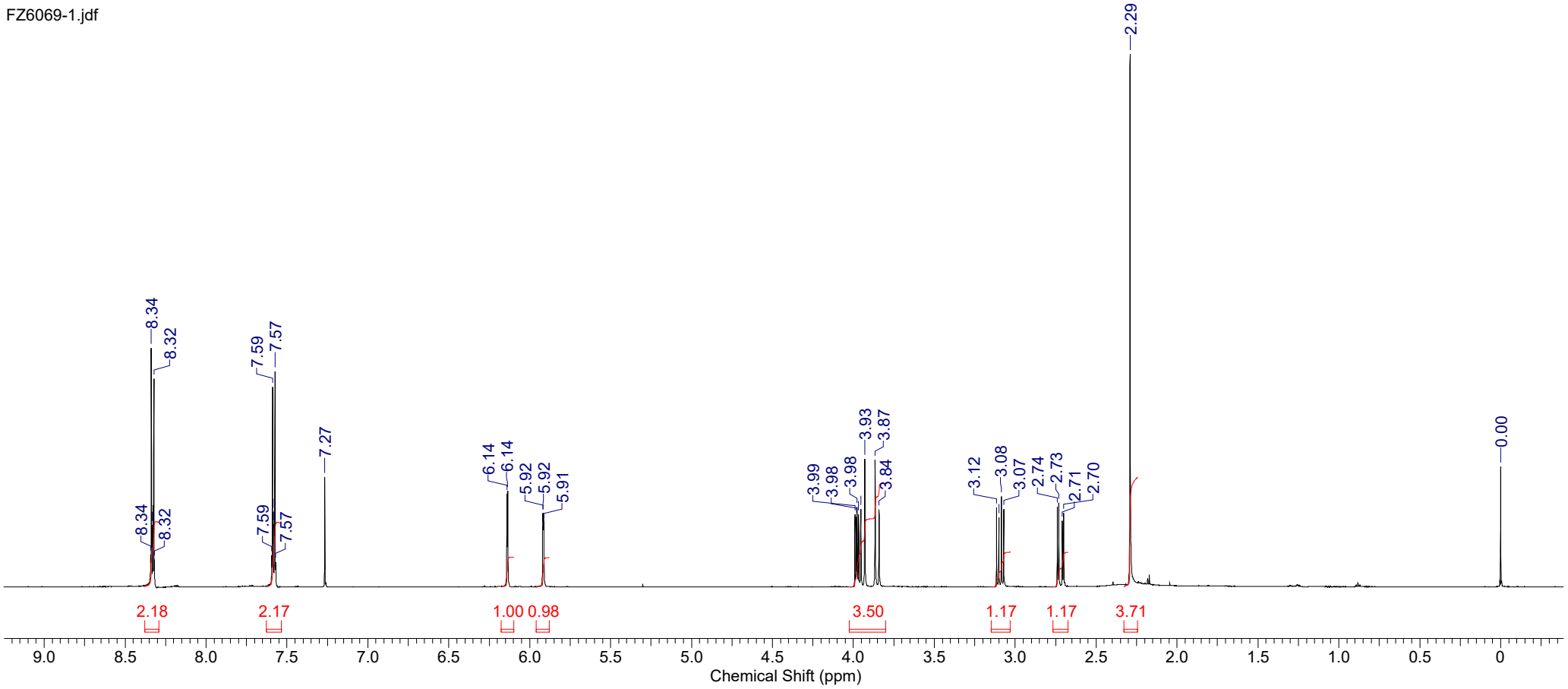
FZ5932-1.jdf



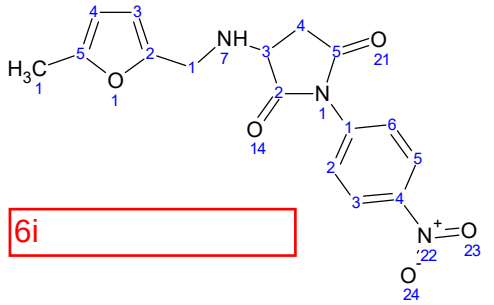
Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:15:19				
Date Stamp	19 Apr 2017 09:36:57			***File Name***	C:\Users\Fedor\Desktop\18.04.17\FZ6069-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5411.6367	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.700				



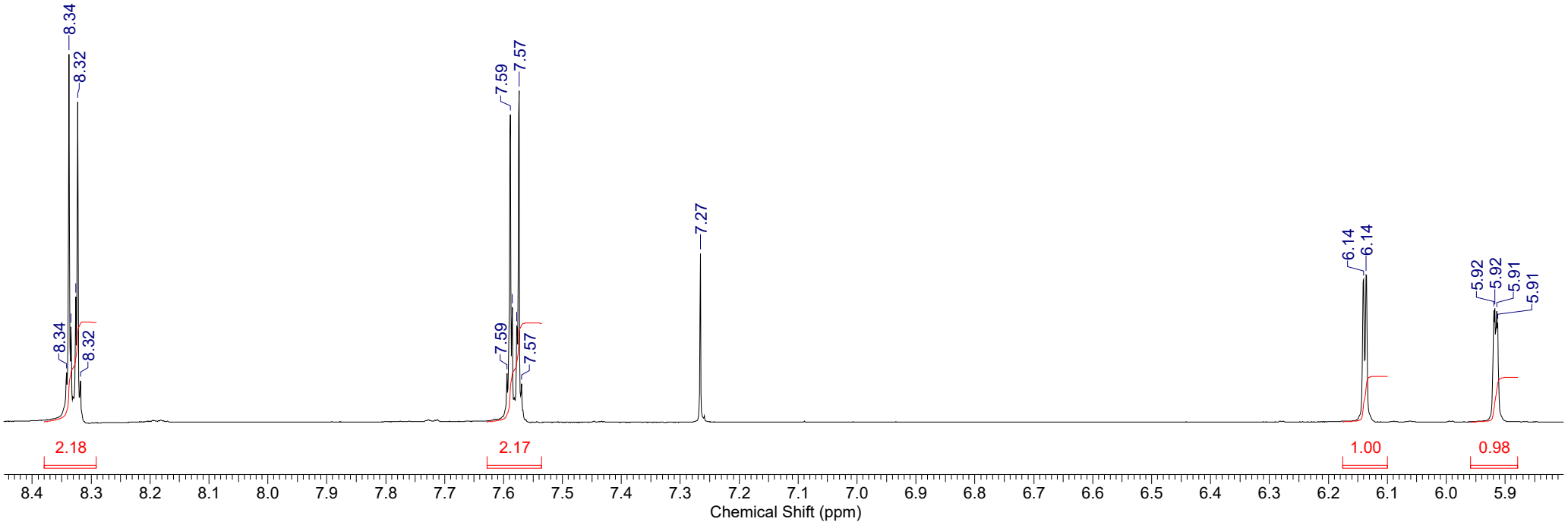
FZ6069-1.jdf



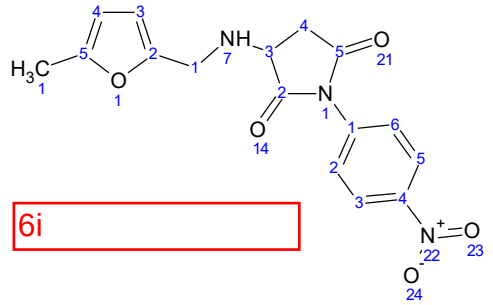
Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:15:19				
Date Stamp	19 Apr 2017 09:36:57			***File Name***	C:\Users\Fedor\Desktop\18.04.17\FZ6069-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5411.6367	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.700				



FZ6069-1.jdf



Acquisition Time (sec)	1.9818	***Comment***	single_pulse	***Date***	30 Aug 2016 10:15:19				
Date Stamp	19 Apr 2017 09:36:57			***File Name***	C:\Users\Fedor\Desktop\18.04.17\FZ6069-1.jdf			***Frequency (MHz)***	600.17
Nucleus	1H	***Number of Transients***	8	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse.ex2			***Receiver Gain***	40.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	5411.6367	***Sweep Width (Hz)***	16534.39	***Temperature (degree C)***	22.700				



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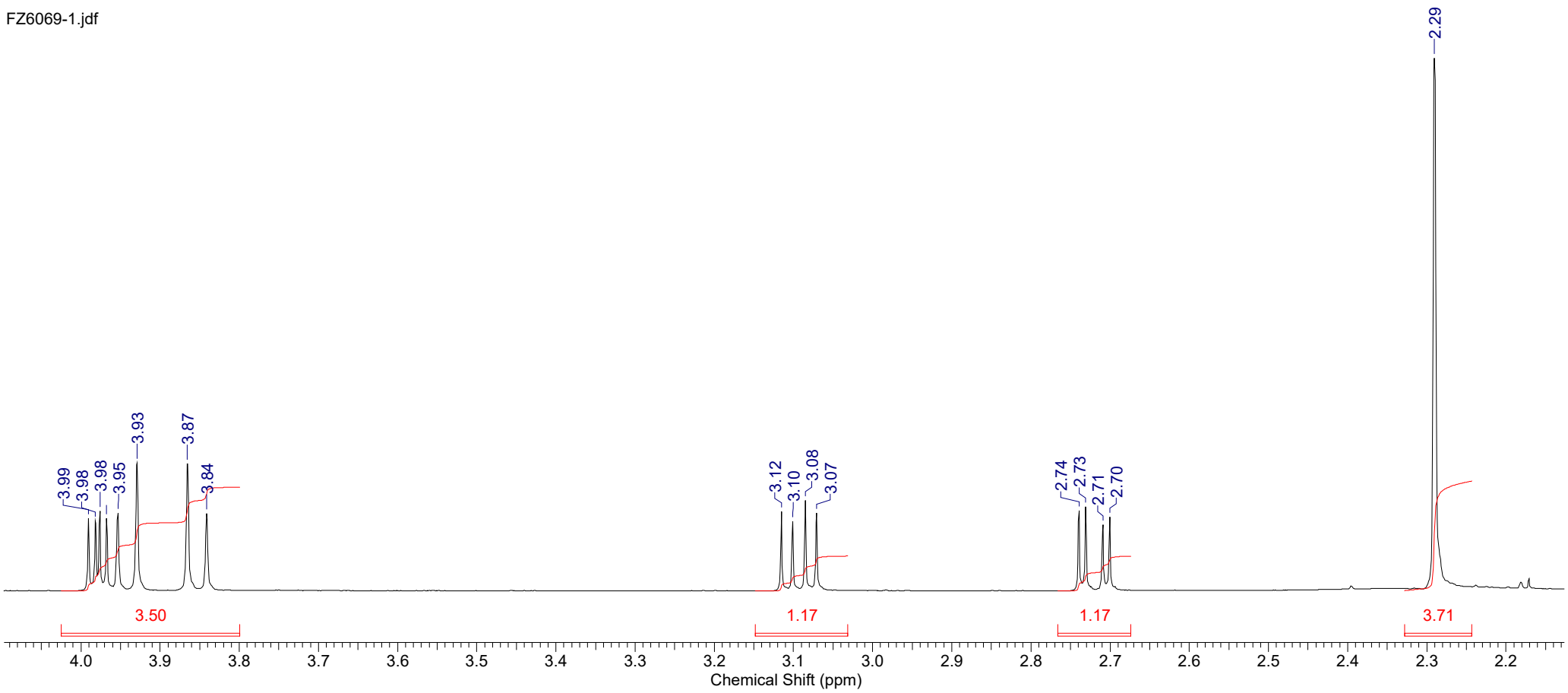
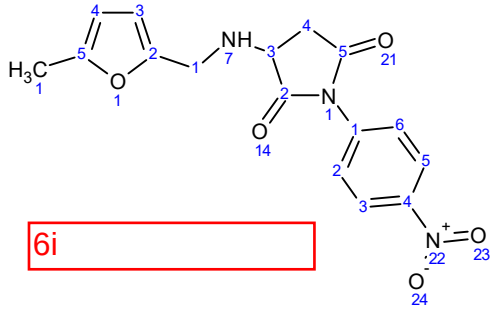
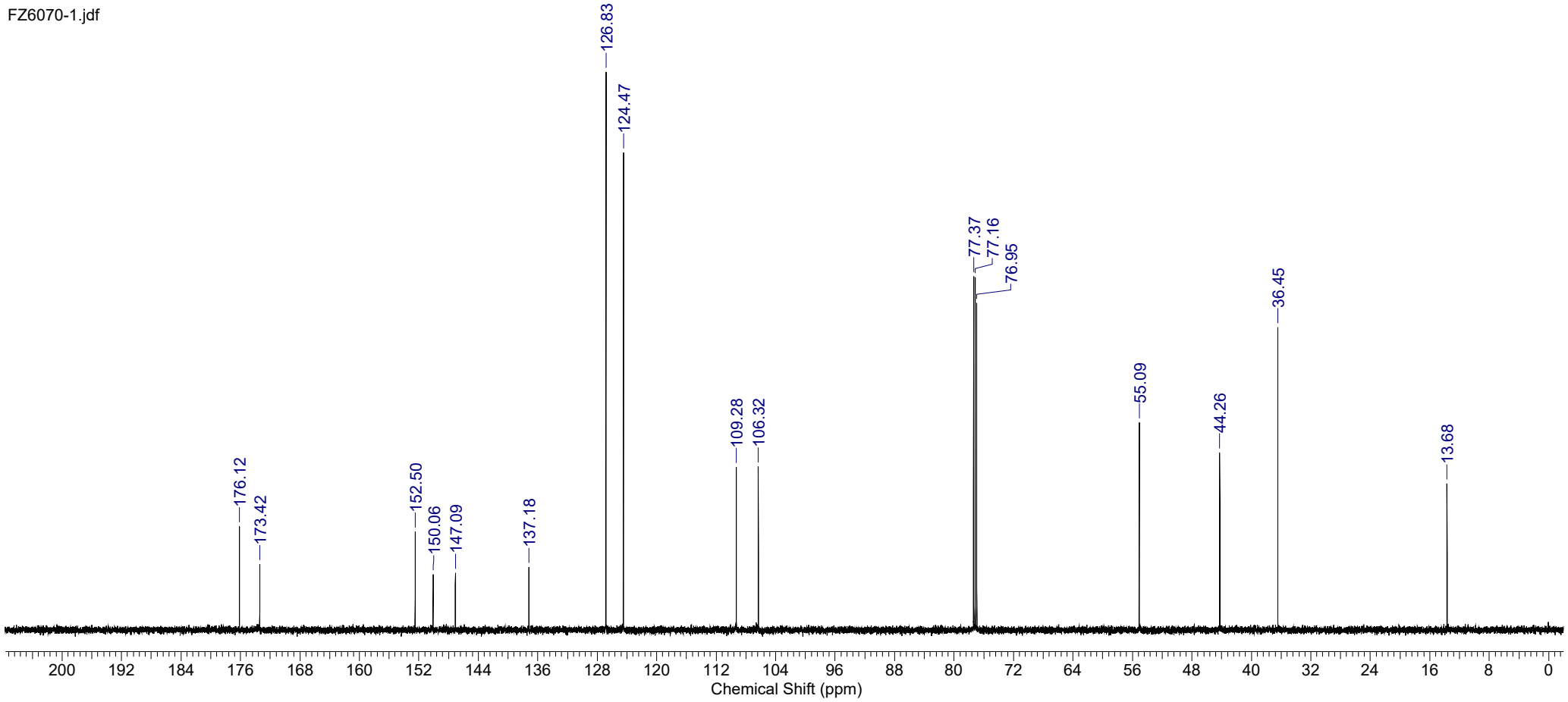


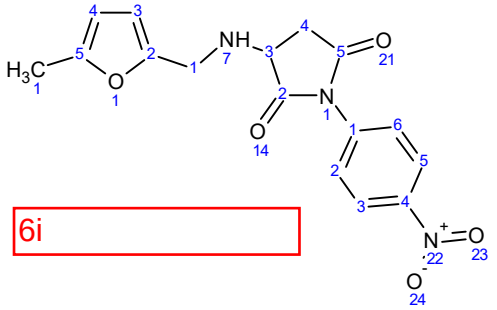
Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:02:07		
Date Stamp	20 Apr 2017 12:25:49			***File Name***	C:\Users\Fedor\Desktop\18.04.17\FZ6070-1.jdf			***Frequency (MHz)***	150.91
Nucleus	13C	***Number of Transients***	200	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse_dec			***Receiver Gain***	52.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	15091.3428	***Sweep Width (Hz)***	47348.49						



FZ6070-1.jdf



Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:02:07		
Date Stamp	20 Apr 2017 12:25:49			***File Name***	C:\Users\Fedor\Desktop\18.04.17\FZ6070-1.jdf			***Frequency (MHz)***	150.91
Nucleus	13C	***Number of Transients***	200	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse_dec			***Receiver Gain***	52.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	15091.3428	***Sweep Width (Hz)***	47348.49						



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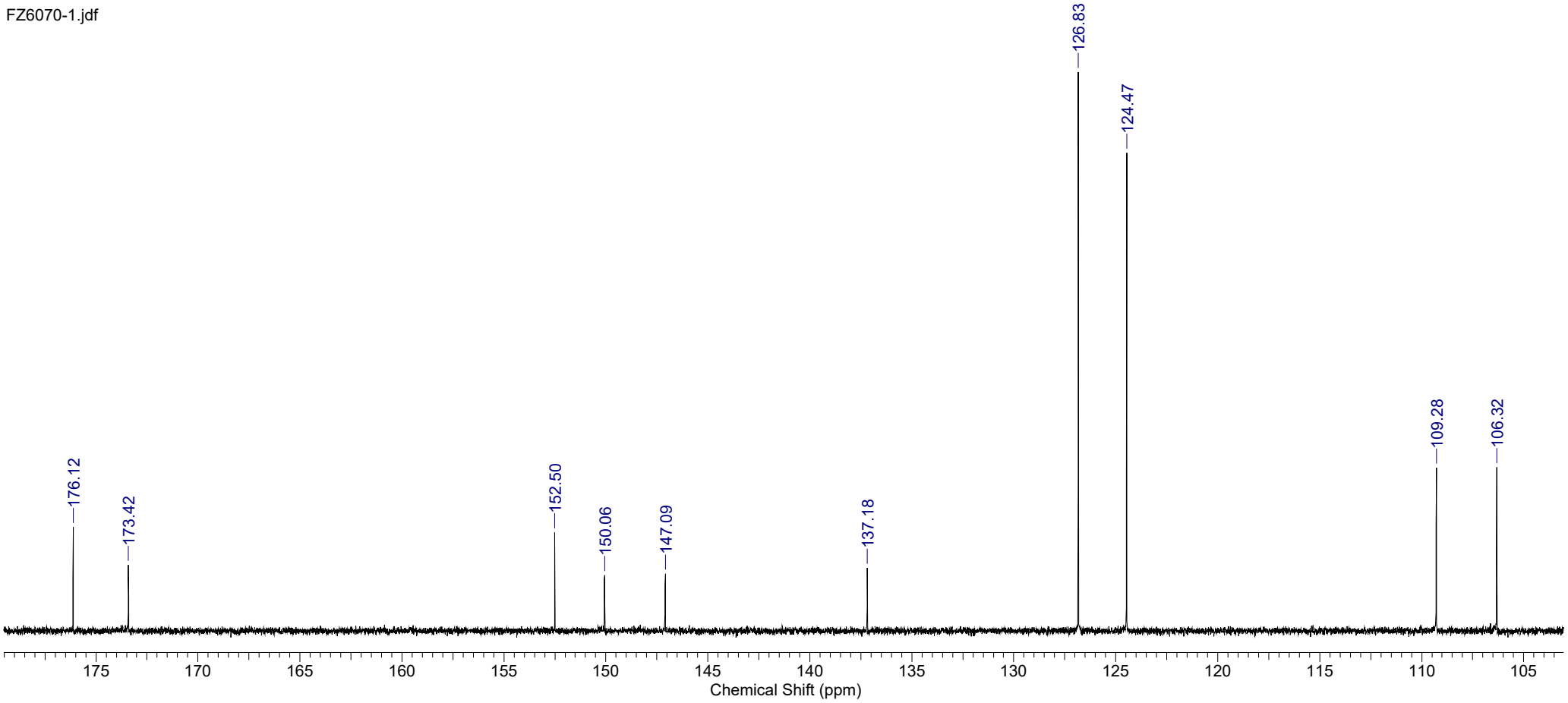
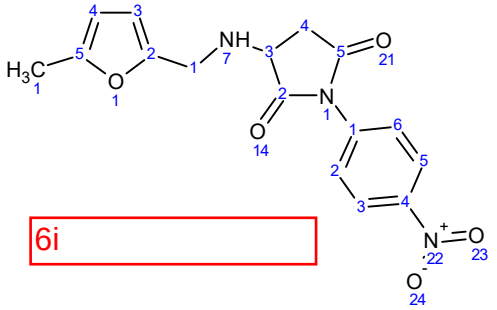


Acquisition Time (sec)	0.6921	***Comment***	single pulse decoupled gated NOE			***Date***	30 Aug 2016 10:02:07		
Date Stamp	20 Apr 2017 12:25:49			***File Name***	C:\Users\Fedor\Desktop\18.04.17\FZ6070-1.jdf			***Frequency (MHz)***	150.91
Nucleus	13C	***Number of Transients***	200	***Origin***	ECA 600	***Original Points Count***	32768	***Owner***	delta
Points Count	32768	***Pulse Sequence***	single_pulse_dec			***Receiver Gain***	52.00	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	15091.3428	***Sweep Width (Hz)***	47348.49						



FZ6070-1.jdf