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Synthesis of 1-aryl-3*H*-[1,2,5]triazepino[5,4-*a*]benzimidazol-4(5*H*)-ones and quantum chemical investigation of the rotamers of the Boc-protected hydrazide key intermediate

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Table of contents

Results and discussion of the computations for conformational and NPA analysis

The B3LYP/6-31G(d,p), the ωB97XD/6-31G(d,p) and the ωB97XD/6-311G++(2d,2p) methods and basis sets were used under the Gaussian09 program package. The role of the DMSO solvent was taken into account using an IEFPCM implicit solvent model or/and also one or two explicit molecules of DMSO forming significant H-bonding interactions with the rotamers and eliminating the intramolecular H-bonds. Moreover, a Natural Bond Orbital (NBO) population analysis was also performed. The main differences can be found in the conformational switch of the hydrazide and the carbazate groups. The geometries of the conformers were optimized, and the distribution of the conformers was determined by calculating the equilibrium constants k_A–k_D from the equation $k = e^{-\Delta G/RT}$ followed by dividing k_x with Σk (Table S1). It should be noted, that in the case of B3LYP/6-31G(d,p) basis set, the role of the explicit DMSO molecules was not significant in comparison to the implicit solvent model, while the ωB97XD/6-31G(d,p) computations showed the important role of the explicit solvent molecules. Finally, the ωB97XD/6-311G++(2d,2p) method considering the implicit DMSO solvent model together with two explicit DMSO molecules gave the nearest distribution values compared to the experimental values (Supplementary Table S2).

Table S1. Energetic data for the determination of the distribution of **4b** conformers[a]

Conformer	G (Hartree)	ΔG (kJ mol^{-1})[b]	k	Distribution (k/Σk)
4'b	−2438.999278	0.00	1.00	60.5%
4"b	−2438.998164	2.92	0.31	18.8%
4'"b	−2438.997628	4.33	0.18	10.7%
4""b	−2438.997568	4.49	0.17	10.0%

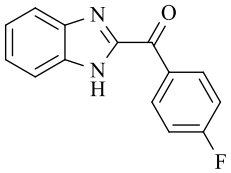
[a] computed with ωB97XD/6-311++G(2d,2p) method considering DMSO as the implicit solvent and two explicit DMSO molecules

[b] relatively to the lowest Gibbs Free Energy conformer **4'b**

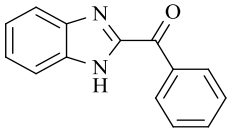
Experimental Section.

General. All melting points were determined on a Büchi B-540 capillary melting point apparatus and are uncorrected. IR spectra were obtained on a Bruker Alpha FT-IR spectrometer in KBr pellets. ^{1}H NMR and ^{13}C NMR spectra were recorded in DMSO-d_6 or $CDCl_3$ in 5 mm tubes at room temperature, on a Varian Unity Inova 500 (500 and 125 MHz for ^{1}H and ^{13}C NMR spectra, respectively), a Bruker Avance III HD 600 (600 and 150 MHz for ^{1}H and ^{13}C NMR spectra, respectively), or a Bruker Avance III 400 (400 and 100 MHz for ^{1}H and ^{13}C NMR spectra, respectively) spectrometer with the deuterium signal of the solvent as the lock and TMS as the internal standard. Chemical shifts (δ) and coupling constants (J) are given in ppm and in Hz, respectively. The following abbreviations were used to designate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Mass spectra were recorded on a Bruker O-TOF MAXIS Impact mass spectrometer coupled to a Dionex Ultimate 3000 RS HPLC system with a diode array detector. Reactions were monitored by thin-layer chromatography (TLC) carried out on silica gel plates (60 F_{254}) using UV light as visualizing agent. Purifications by flash column chromatography were carried out using Merck 107736 silica gel 60 H using a hexane–CH_2Cl_2 or CH_2Cl_2–MeOH solvent system. All reagents were purchased from commercial sources and used without further purification. Analytical samples of new compounds were obtained by recrystallization from the solvents or solvent mixtures given below in parentheses. Compounds **1a**–**e**, **2b** and **3b** are described in the literature, while other compounds are new.

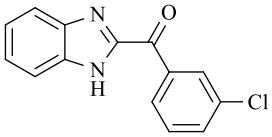
General procedure for the preparation of 2-aroylbenzimidazoles. Synthesis of compounds 1a–e. Benzimidazole (8.27 g, 0.07 mmol) was dissolved in a mixture of pyridine (9.8 ml) and triethylamine (29.2 ml). This solution was cooled to 0 °C, and the corresponding aroyl chloride (0.21 mol) was added dropwise. The mixture was stirred at room temperature for 3 h. Aqueous NaOH solution (40 w/w%, 14 ml) was slowly added, and the mixture was refluxed for 1 h. The reaction was quenched by pouring into cold water (140 ml), the precipitated solid was filtered, washed with water and dried.



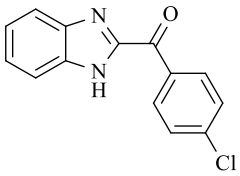
(1*H*-Benzimidazol-2-yl)(4-fluorophenyl)methanone (1a). Yield 12.53 g (75%). Pale yellow crystals. Mp 216–217 °C (EtOH) (lit.[S1] 213 °C). IR (KBr, cm^{-1}): 1657, 1599, 1318, 1157, 850, 745. ^{1}H NMR (500 MHz, DMSO-d_6): δ 13.58 (br s, 1H), 8.78–8.75 (m, 2H), 7.80 (br s, 2H), 7.50–7.46 (m, 2H), 7.42 (br s, 2H) ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ 182.0, 165.6 (d, J = 253.4 Hz), 148.0, 143.3, 134.2 (d, J = 9.3 Hz), 132.4 (d, J = 2.4 Hz), 125.5, 123.8, 121.4, 115.7 (d, J = 22.0 Hz), 113.1 ppm, one signal missing. (The rapid movement of the hydrogen atom between the two nitrogens causes the lack of imidazole NCHN signal in ^{13}C NMR spectrum.)



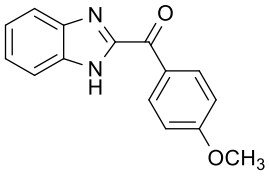
1*H*-Benzimidazol-2-yl(phenyl)methanone (1b). Yield 13.85 g (89%). Pale yellow crystals. Mp 220–221 °C (EtOH) (lit.[S2] 218–219 °C). IR (KBr, cm^{-1}): 1657, 1320, 920, 739, 696. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.56 (br s, 1H), 8.62–8.61 (m, 1H), 8.60–8.59 (m, 1H), 7.91 (br s, 1H), 7.78–7.73 (m, 1H), 7.66–7.64 (m, 2H), 7.63–7.62 (m, 1H), 7.44 (br s, 1H), 7.38 (br s, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 138.7, 148.1, 143.4, 135.8, 134.3, 133.8, 131.1, 128.6, 125.9, 123.4, 121.5, 113.0 ppm.



1*H*-Benzimidazol-2-yl(3-chlorophenyl)methanone (1c). Yield 16.20 g (90%). Pale yellow crystals. Mp 191–193 °C (EtOH) (lit.[S1] 185 °C). IR (KBr, cm^{-1}): 3312, 1634, 1325, 1248, 754. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.61 (br s, 1H), 8.64–8.63 (m, 1H), 8.53–8.50 (m, 1H), 7.83–7.80 (m, 1H), 7.78 (br s, 2H), 7.69–7.66 (m, 1H), 7.41 (br s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 182.2, 147.7, 143.1, 137.5, 134.5, 133.4, 133.3, 130.6, 129.6, 125.7, 124.2, 121.4, 113.2 ppm, one signal missing. (The rapid movement of the hydrogen atom between the two nitrogens causes the lack of imidazole NCHN signal in ^{13}C NMR spectrum.)

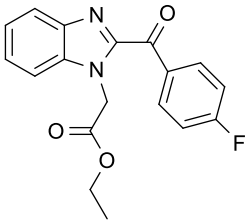


1*H*-Benzimidazol-2-yl(4-chlorophenyl)methanone (1d). Yield 11.95 g (67%). Pale yellow crystals. Mp 228–230 °C (EtOH) (lit.[S3] 224–226 °C). IR (KBr, cm^{-1}): 1656, 1319, 1262, 1089, 921, 745. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.58 (br s, 1H), 8.65–8.63 (m, 2H), 7.90 (br s, 1H), 7.73–7.71 (m, 2H), 7.65 (br s, 1H), 7.43 (br s, 1H), 7.38 (br s, 1H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 182.3, 147.9, 143.3, 138.9, 134.4, 132.9, 128.8, 126.1, 123.5, 121.5, 113.0 ppm, one signal missing. (The rapid movement of the hydrogen atom between the two nitrogens causes the lack of imidazole NCHN signal in ^{13}C NMR spectrum.)

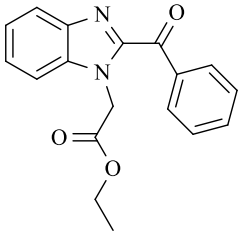


1*H*-Benzimidazol-2-yl(4-methoxyphenyl)methanone (1e). Yield 12.11 g (69%). Pale yellow crystals. Mp 195–197 °C (MeCN) (lit.[S1] 194 °C). IR (KBr, cm^{-1}): 3299, 1594, 1255, 1158, 749. ^{1}H NMR (400 MHz, DMSO-d_6): δ 13.45 (br s, 1H), 8.72–8.69 (m, 2H), 7.84 (br s, 1H), 7.70 (br s, 1H), 7.38 (br s, 2H), 7.19–7.16 (m, 2H), 3.91 (s, 3H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 181.7, 164.0, 148.5, 143.3, 134.0, 133.6, 128.4, 125.4, 123.3, 121.2, 114.0, 112.8, 55.8 ppm.

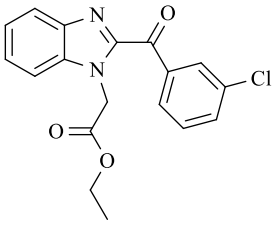
General procedure for the preparation of ethyl (2-aroyl-1*H*-benzimidazol-1-yl)acetates 2a–e. The appropriate 2-aroylbenzimidazole (**1**, 18 mmol) was dissolved in a mixture of MeCN (200 ml) and CH_2Cl_2 (200 ml). To this solution were added Cs_2CO_3 (7.04 g, 21.6 mmol) and ethyl bromoacetate (2.2 ml, 19.8 mmol). The mixture was stirred for 24 h at room temperature. The mixture was filtered, and the filtrate was concentrated. The residue was taken up in CH_2Cl_2 and it was washed with water twice. The organic phase was dried (Na_2SO_4), filtered, and concentrated to afford alkylated products **2**.



Ethyl [2-(4-fluorobenzoyl)-1*H*-benzimidazol-1-yl]acetate (2a). Yield: 5.77 g (98%). Pale yellow crystals. Mp 101–102 °C (EtOH). IR (KBr, cm^{-1}): 1743, 1638, 1482, 1279, 1225, 930, 747. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.48–8.46 (m, 2H), 7.96–7.95 (m, 1H), 7.50–7.47 (m, 1H), 7.42–7.40 (m, 2H), 7.22–7.19 (m, 2H), 5.36 (s, 2H), 4.23 (q, J = 7.1 Hz, 2H), 1.25 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.7, 167.7, 166.2 (d, J = 256.0 Hz), 146.1, 141.7, 135.9, 134.1 (d, J = 9.5 Hz), 132.8 (d, J = 2.9 Hz), 126.3, 124.0, 122.3, 115.5 (d, J = 21.8 Hz), 109.8, 62.0, 46.6, 14.1 ppm. HRMS calcd. for $C_{18}H_{16}FN_2O_3$ $[M+H]^+$ 327.1145; found 327.1144.

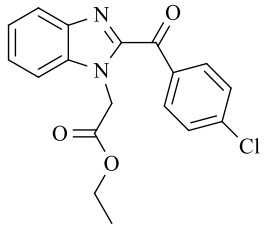


Ethyl (2-benzoyl-1*H*-benzimidazol-1-yl)acetate (2b).[S4] Yield 4.20 g (76%). Off-white crystals. Mp 85–87 °C (EtOH–hexane). IR (KBr, cm^{-1}): 1752, 1651, 1492, 1278, 1216, 1194, 769. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.38–8.36 (m, 2H), 7.96–7.95 (m, 1H), 7.64–7.60 (m, 1H), 7.53–7.50 (m, 2H), 7.47–7.44 (m, 1H), 7.40–7.37 (m, 2H), 5.35 (s, 2H), 4.21 (q, J = 7.1 Hz, 2H), 1.23 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ 186.4, 167.6, 146.3, 141.8, 136.5, 135.9, 133.5, 131.2, 128.3, 126.1, 123.9, 122.3, 109.7, 61.9, 46.5, 14.0 ppm.

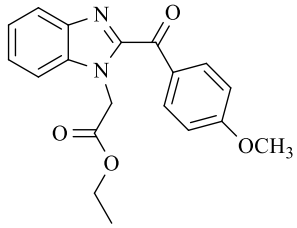


Ethyl [2-(3-chlorobenzoyl)-1*H*-benzimidazol-1-yl]acetate (2c). Yield: 4.44 g (72%). Pale yellow crystals. Mp 66–68 °C (EtOH). IR (KBr, cm^{-1}): 1742, 1642, 1484, 1225, 943, 744. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.36–8.35 (m, 1H), 8.31–8.29 (m, 1H), 7.98–7.96 (m, 1H), 7.61–7.59 (m, 1H), 7.51–7.46 (m, 2H), 7.43–7.41 (m, 2H), 5.36 (s, 2H), 4.23 (q, J = 7.1 Hz, 2H),

1.26 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ 185.0, 167.6, 145.8, 141.8, 138.0, 136.0, 134.5, 133.4, 131.0, 129.6, 129.4, 126.5, 124.1, 122.5, 109.8, 77.0, 62.1, 46.6, 14.1 ppm. HRMS calcd. for $C_{18}H_{16}ClN_2O_3$ $[M+H]^+$ 343.0849; found 343.0827.

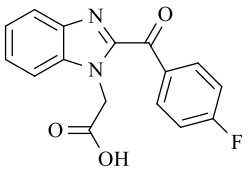


Ethyl [2-(4-chlorobenzoyl0-1*H*-benzimidazol-1-yl]acetate (2d). Yield: 5.70 g (92%). Pale yellow crystals. Mp 113–115 °C (EtOH). IR (KBr, cm^{-1}): 1743, 1634, 1480, 1279, 1221, 928, 743. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.37–8.36 (m, 1H), 8.36–8.35 (m, 1H), 7.96–7.95 (m, 1H), 7.52–7.50 (m, 2H), 7.49–7.47 (m, 1H), 7.42–7.40 (m, 2H), 5.36 (s, 2H), 4.23 (q, J = 7.1 Hz, 2H), 1.26 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ 185.1, 167.6, 146.0, 141.8, 140.2, 136.0, 134.8, 132.6, 128.7, 126.4, 124.1, 122.4, 109.8, 77.0, 62.0, 46.6, 14.1 ppm. HRMS calcd. for $C_{18}H_{16}ClN_2O_3$ $[M+H]^+$ 343.0849; found 343.0837.

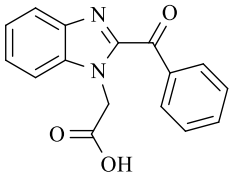


Ethyl [2-(4-methoxybenzoyl)-1*H*-benzimidazol-1-yl]acetate (2e). Yield 5.44 g (89%). White crystals. Mp 100–101 °C (EtOH). IR (KBr, cm^{-1}): 1742, 1626, 1597, 1484, 1032, 928, 738. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.43–8.42 (m, 2H), 7.96–7.94 (m, 1H), 7.47–7.45 (m, 1H), 7.41–7.38 (m, 2H), 7.02–7.01 (m, 2H), 5.35 (s, 2H), 4.21 (q, J = 7.1 Hz, 2H), 3.90 (s, 3H), 1.23 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ 184.7, 167.8, 164.1, 146.7, 141.7, 135.8, 133.8, 129.3, 125.9, 123.8, 122.2, 113.7, 109.7, 61.9, 55.5, 46.5, 14.0 ppm. HRMS calcd. for $C_{19}H_{19}N_2O_4$ $[M+H]^+$ 339.1340; found 339.1336.

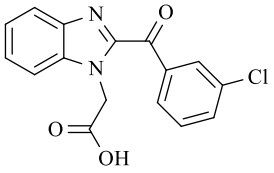
General procedure for the preparation of (2-aroyl-1*H*-benzimidazol-1-yl)acetic acids 3a–e. The appropriate ester (**2**, 10 mmol) was dissolved in a mixture of THF (45 ml) and EtOH (27 ml). Then an aqueous solution of NaOH (35 ml, 5 w/w%) was added. The resulting mixture was stirred at room temperature for 20 min, the organic solvents were evaporated under reduced pressure. To the remaining aqueous solution, 1 M HCl solution was added until a precipitation occurred. The product was filtered and dried under reduced pressure at 50 °C.



[2-(4-Fluorobenzoyl)-1*H*-benzimidazol-1-yl]acetic acid (3a). Yield: 2.77 g (93%). White crystals. Mp 248–249 °C (EtOH). IR (KBr, cm^{-1}): 2517, 1717, 1654, 1598, 1230, 748. ^{1}H NMR (600 MHz, DMSO-d_6): δ 13.23 (br s, 1H), 8.45–8.41 (m, 2H), 7.91–7.89 (m, 1H), 7.86–7.84 (m, 1H), 7.51–7.48 (m, 1H), 7.47–7.44 (m, 2H), 7.41–7.39 (m, 1H), 5.38 (s, 2H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6): δ 184.0, 169.8, 165.5 (d, J = 253.0 Hz), 146.2, 141.2, 136.4, 134.2 (d, J = 9.6 Hz), 133.0 (d, J = 2.7 Hz), 126.1, 123.9, 121.5, 115.7 (d, J = 21.9 Hz), 111.8, 47.0 ppm. HRMS calcd. for $C_{16}H_{12}FN_2O_3$ $[M+H]^+$ 299.0832; found 299.0828.

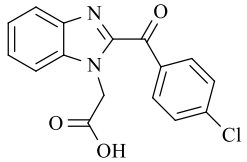


(2-Benzoyl-1*H*-benzimidazol-1-yl)acetic acid (3b).[S5] Yield: 2.30 g (82%). White crystals. Mp 241–243 °C (EtOH). IR (KBr, cm^{-1}): 2510, 1716, 1654, 1447, 1231, 729. ^{1}H NMR (500 MHz, DMSO-d_6): δ 13.20 (br s, 1H), 8.32–8.30 (m, 2H), 7.91–7.89 (m, 1H), 7.86–7.84 (m, 1H), 7.74–7.70 (m, 1H), 7.62–7.59 (m, 2H), 7.51–7.47 (m, 1H), 7.42–7.38 (m, 1H), 5.40 (s, 2H) ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ 185.7, 169.8, 146.4, 141.2, 136.4 (two signals: 136.44, 136.36), 133.7, 131.1, 128.5, 126.0, 123.8, 121.5, 111.7, 46.9 ppm.

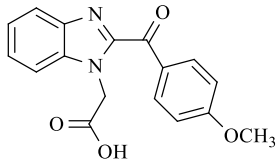


[2-(3-Chlorobenzoyl)-1*H*-benzimidazol-1-yl]acetic acid (3c). Yield: 1.89 g (60%). White crystals. Mp 207–210 °C (EtOH). IR (KBr, cm^{-1}): 2523, 1719, 1643, 1488, 1448, 1230, 734.

^{1}H NMR (600 MHz, DMSO-d_6): δ 13.27 (br s, 1H), 8.32–8.31 (m, 1H), 8.26–8.24 (m, 1H) 7.94–7.92 (m, 1H), 7.87–7.85 (m, 1H), 7.82–7.80 (m, 1H), 7.67–7.64 (m, 1H), 7.52–7.49 (m, 1H), 7.42–7.40 (m, 1H), 5.38 (s, 2H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6): δ 184.1, 169.8, 146.0, 141.2, 138.2, 136.4, 133.4, 133.2, 130.6 (two signals: 130.64, 130.60), 129.6, 126.3, 124.0, 121.7, 111.8, 47.0 ppm. HRMS calcd. for $C_{16}H_{12}ClN_2O_3$ $[M+H]^+$ 315.0536; found 315.0534.

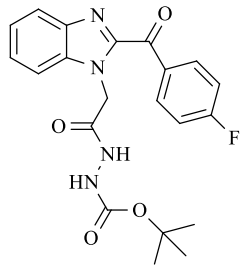


[2-(4-Chlorobenzoyl)-1*H*-benzimidazol-1-yl]acetic acid (3d). Yield: 2.99 g (95%). Pale yellow crystals. Mp 277–280 °C (EtOH). IR (KBr, cm^{-1}): 2515, 1719, 1645, 1447, 1229, 746. ^{1}H NMR (600 MHz, DMSO-d_6): δ 13.24 (br s, 1H), 8.36–8.34 (m, 2H), 7.91–7.89 (m, 1H), 7.87–7.85 (m, 1H), 7.71–7.68 (m, 2H), 7.51–7.48 (m, 1H), 7.42–7.39 (m, 1H), 5.39 (s, 2H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6): δ 184.3, 169.8, 146.1, 141.2, 138.9, 136.4, 135.1, 133.0, 128.7, 126.2, 124.0, 121.6, 111.8, 47.0 ppm. HRMS calcd. for $C_{16}H_{12}ClN_2O_3$ $[M+H]^+$ 315.0536; found 315.0529.

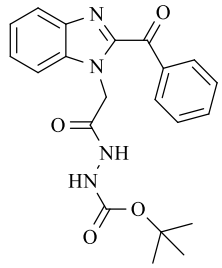


[2-(4-Methoxybenzoyl)-1*H*-benzimidazol-1-yl]acetic acid (3e). Yield: 2.92 g (94%). White crystals. Mp 256–258 °C (EtOH). IR (KBr, cm^{-1}): 2509, 1720, 1601, 1449, 1258, 744. ^{1}H NMR (600 MHz, DMSO-d_6): δ 13.17 (br s, 1H), 8.39–8.37 (m, 2H), 7.90–7.88 (m, 1H), 7.84–7.82 (m, 1H), 7.48–7.45 (m, 1H), 7.40–7.37 (m, 1H), 7.16–7.13 (m, 2H), 5.36 (s, 2H), 3.89 (s, 3H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6): δ 183.8, 169.8, 163.9, 146.7, 141.2, 136.3, 133.7, 129.0, 125.7, 123.7, 121.4, 114.0, 111.6, 55.9, 46.8 ppm. HRMS calcd. for $C_{17}H_{15}N_2O_4$ $[M+H]^+$ 311.1026; found 311.1021.

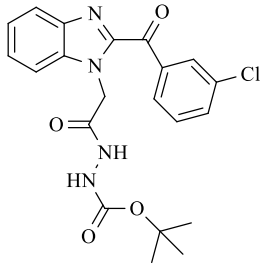
General procedure for the preparation of *tert*-butyl 2-[(2-aroyl-1*H*-benzimidazol-1-yl)acetyl]hydrazinecarboxylates 4a–e. The appropriate carboxylic acid (**3**, 8.6 mmol) was dissolved in THF (150 ml), then a solution of *tert*-butyl carbazate (1.36 g, 10.32 mmol) in THF (50 ml), the Hünig's base (3.0 ml, 17.2 mmol), and coupling reagent HATU (3.92 g, 10.32 mmol) were added. The mixture was stirred at room temperature for 2 h. The reaction was monitored by TLC (CH_2Cl_2–MeOH, 19:1). When the reaction was completed, the solvent was evaporated. The residue was dissolved in CH_2Cl_2 (30 ml), washed three times with water (15 ml), dried (Na_2SO_4), filtered, and concentrated. The crude product was purified by flash column chromatography (silica gel, CH_2Cl_2–MeOH) to afford the products as a mixture of rotamers.



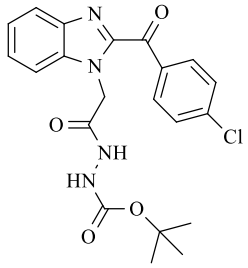
***tert*-Butyl 2-{[2-(4-fluorobenzoyl)-1*H*-benzimidazol-1-yl]acetyl}hydrazine-carboxylate (4a).** Yield 3.22 g (91%). White crystals. Mp 193–195 °C (EtOH). IR (KBr, cm^{-1}): 3373, 1731, 1679, 1644, 1161, 743. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.11/9.54/9.38 (br s, 1H), 8.92 (br s, 1H), 8.38 (dd, J_1 = 7.8 Hz, J_2 = 5.6 Hz, 2H), 7.90–7.89 (m, 1H), 7.71–7.69/5.52–7.50 (m, 1H), 7.45 (t, J = 8.9 Hz, 2H), 7.40–7.38 (m, 1H), 5.40/5.34 (s, 2H), 1.50/1.35/1.26 (s, 9H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 184.3/184.2, 166.7, 165.5 (d, J = 253.2 Hz), 155.2, 146.8, 141.3, 136.4/136.3, 134.2 (d, J = 9.6 Hz), 133.0 (d, J = 2.6 Hz), 125.9, 123.9, 121.6/121.5, 115.6 (d, J = 21.9 Hz), 111.6/111.0, 80.7/79.4, 46.0/45.5, 28.2 ppm. HRMS calcd. for $C_{21}H_{22}FN_4O_4$ $[M+H]^+$ 413.1620; found 413.1626.



***tert*-Butyl 2-[(2-benzoyl-1*H*-benzimidazol-1-yl)acetyl]hydrazinecarboxylate (4b).** Yield 2.85 g (84%). White crystals. Mp 107–109 °C (EtOH). IR (KBr, cm^{-1}): 3404, 3233, 1740, 1682, 1657, 1273, 1161. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.11/9.52 (br s, 1H), 8.91 (br s, 1H), 8.26–8.24 (m, 2H), 7.89–7.87 (m, 1H), 7.75–7.73 (m, 1H), 7.71–7.69 (m, 1H), 7.62–7.58 (m, 2H), 7.51–7.47 (m, 1H), 7.41–7.38 (m, 1H), 5.40/5.35 (s, 2H), 1.50/1.35/1.25 (s, 9H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 185.9, 166.6, 155.1, 146.9, 141.3, 136.5, 136.4, 133.7, 131.1, 128.4, 125.8, 123.8, 121.5, 111.5/111.0, 80.6/79.4, 45.9/45.4, 28.2 ppm. HRMS calcd. for $C_{21}H_{23}N_4O_4$ $[M+H]^+$ 395.1719; found 395.1726.

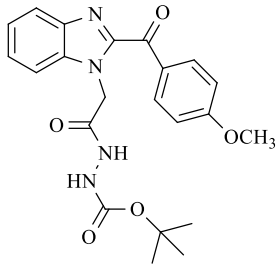


***tert*-Butyl 2-{2-[(3-chlorobenzoyl)-1*H*-benzimidazol-1-yl]acetyl}hydrazine-carboxylate (4c).** Yield 2.58 g (70%). Pale yellow crystals. Mp 101–103 °C (EtOH). IR (KBr, cm^{-1}): 3394, 3237, 1739, 1698, 1660, 1158, 746. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.12/9.56 (br s, 1H), 8.92 (br s, 1H), 8.26–8.24 (m, 1H), 8.22–8.19 (m, 1H), 7.93–7.91 (m, 1H), 7.82–7.79 (m, 1H), 7.72–7.70 (m, 1H), 7.67–7.63 (m, 1H), 7.53–7.49 (m, 1H), 7.43–7.39 (m, 1H), 5.39/5.35 (s, 2H), 1.50/1.35/1.26 (s, 9H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 184.42/184.37, 166.7, 155.2, 146.5, 141.3, 138.2, 136.43/136.38, 133.4, 133.2, 130.6 (two signals: 130.61, 130.56), 129.6, 126.2, 124.0, 121.7/121.6, 111.6/111.1, 80.7/79.5, 46.1/46.6, 28.2 ppm. HRMS calcd. for $C_{21}H_{22}ClN_4O_4$ $[M+H]^+$ 429.1330; found 429.1327.



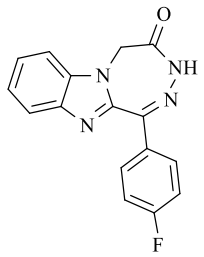
***tert*-Butyl 2-{[2-(4-chlorobenzoyl)-1*H*-benzimidazol-1-yl]acetyl}hydrazine-carboxylate (4d).** Yield 3.17 g (86%). Pale yellow crystals. Mp 192–194 °C (EtOH). IR (KBr, cm^{-1}): 3276, 1731, 1679, 1644, 1161, 743. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.11/9.54 (br s, 1H), 8.92 (br s, 1H), 8.31–8.29 (m, 2H), 7.90–7.88 (m, 1H), 7.70–7.68 (m, 3H), 7.52–7.48 (m, 1H), 7.42–7.38 (m, 1H), 5.39/5.35 (s, 2H), 1.50/1.36/1.26 (s, 9H) ppm. ^{13}C NMR (100 MHz,

DMSO-d_6): δ 184.5, 166.6, 155.2, 146.6, 141.3, 138.8, 136.4, 135.1, 132.9, 128.7, 126.0, 123.9, 121.5, 111.6, 79.4, 46.0, 28.2 ppm. HRMS calcd. for $C_{21}H_{22}ClN_4O_4$ $[M+H]^+$ 429.1330; found 429.1316.



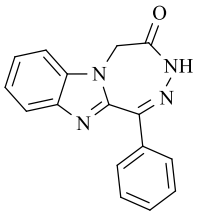
***tert*-Butyl 2-{[2-(4-methoxybenzoyl)-1*H*-benzimidazol-1-yl]acetyl}hydrazine-carboxylate (4e).** Yield 3.28 g (90%). White crystals. Mp 178–181 °C (EtOH). IR (KBr, cm^{-1}): 3248, 1715, 1679, 1636, 1597, 1256, 1174, 743. ^{1}H NMR (600 MHz, DMSO-d_6): δ 10.10 (br s, 1H), 9.51/9.38/8.91 (br s, 1H), 8.33–8.31 (m, 2H), 7.88–7.87 (m, 1H), 7.68–7.66 (m, 1H), 7.49–7.47 (m, 1H), 7.40–7.37 (m, 1H), 7.15–7.13 (m, 2H), 5.38/5.32 (s, 2H), 3.89 (s, 3H), 1.50/1.35/1.25 (s, 9H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6): δ 184.2/184.1, 166.7, 163.9, 155.2, 147.2, 141.31/141.27, 136.3/136.2, 133.7, 129.05/129.02, 125.6, 123.7/123.6, 121.43/121.36, 113.9, 111.5/110.9, 79.4, 55.9, 45.9, 28.2/27.9 ppm. HRMS calcd. for $C_{22}H_{25}N_4O_5$ $[M+H]^+$ 425.1819; found 425.1818.

General procedure for the preparation of 1-aryl-3*H*-[1,2,5]triazepino[5,4-*a*]-benzimidazol-4(5*H*)-ones 5a–e. To a solution of the appropriate hydrazide (**4**, 0.50 mmol) in EtOH (8 ml) was added pyridinium *p*-toluenesulfonate (PPTS, 0.10 g, 0.40 mmol). The reaction mixture was stirred at reflux temperature for 2 days, then cooled to room temperature and evaporated. The residue was dissolved in CH_2Cl_2 (10 ml) and washed three times with water (5 ml). The organic layer was dried (Na_2SO_4), filtered and concentrated under reduced pressure. The crude material was purified by flash column chromatography to afford the products.

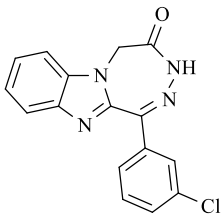


1-(4-Fluorophenyl)-3*H*-[1,2,5]triazepino[5,4-*a*]benzimidazo-4(5*H*)-one (5a). Yield 15 mg (10%). White crystals. Mp 223–225 °C (*i*-PrOH). IR (KBr, cm^{-1}): 3243, 1704, 1605, 1594, 1231, 851, 736. ^{1}H NMR (600 MHz, DMSO-d_6): δ 11.63 (br s, 1H), 8.00–7.99 (m, 1H), 7.98–

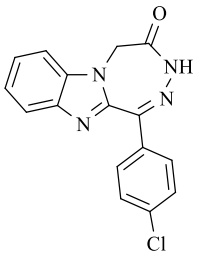
7.96 (m, 2H), 7.81–7.79 (m, 1H), 7.46–7.43 (m, 1H), 7.39–7.38 (m, 1H), 7.37–7.35 (m, 1H), 7.34–7.32 (m, 1H), 5.24 (s, 2H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6): δ 166.7, 163.5 (d, J = 247.8 Hz), 149.2, 145.0, 142.8, 133.5, 132.3 (d, J = 2.9 Hz), 131.4 (d, J = 8.8 Hz), 124.4, 123.7, 120.6, 115.3 (d, J = 21.8 Hz), 111.0, 46.9 ppm. HRMS calcd. for $C_{16}H_{12}FN_4O$ $[M+H]^+$ 295.0990; found 295.0990.



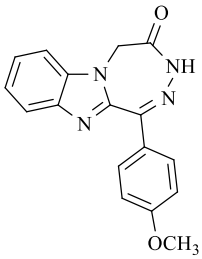
1-Phenyl-3*H*-[1,2,5]triazepino[5,4-*a*]benzimidazo-4(5*H*)-one (5b). Yield 23.5 mg (17%). White crystals. Mp 231–233 °C (EtOAc–hexane). IR (KBr, cm^{-1}): 3196, 1673, 1374, 753. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.62 (br s, 1H), 7.99–7.97 (m, 1H), 7.92–7.91 (m, 1H), 7.90–7.89 (m, 1H), 7.81–7.78 (m, 1H), 7.53–7.50 (m, 2H), 7.49–7.48 (m, 1H), 7.45–7.42 (m, 1H), 7.40–7.35 (m, 1H), 5.25 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.7, 150.3, 145.1, 142.8, 135.8, 133.4, 130.3, 129.1, 128.3, 124.3, 123.6, 120.5, 110.9, 46.9 ppm. HRMS calcd. for $C_{16}H_{13}N_4O$ $[M+H]^+$ 277.1084; found 277.1087.



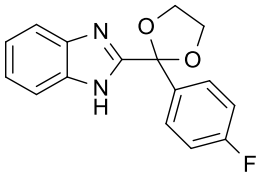
1-(3-Chlorophenyl)-3*H*-[1,2,5]triazepino[5,4-*a*]benzimidazo-4(5*H*)-one (5c). Yield 15.5 mg (10%). White crystals. Mp 201–203 °C (EtOAc–hexane). IR (KBr, cm^{-1}): 3114, 1693, 1343, 1201, 747. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.72 (br s, 1H), 7.99–7.97 (m, 1H), 7.93–7.92 (m, 1H), 7.91–7.89 (m, 1H), 7.83–7.81 (m, 1H), 7.61–7.58 (m, 1H), 7.56–7.52 (m, 1H), 7.47–7.43 (m, 1H), 7.40–7.36 (m, 1H), 5.26 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.6, 148.4, 144.8, 142.8, 137.9, 133.5, 132.9, 130.2, 130.0, 128.8, 127.6, 124.5, 123.7, 120.6, 110.9, 49.9 ppm. HRMS calcd. for $C_{16}H_{12}ClN_4O$ $[M+H]^+$ 311.0694; found 311.0696.



1-(4-Chlorophenyl)-3*H*-[1,2,5]triazepino[5,4-*a*]benzimidazo-4(5*H*)-one (5d). Yield: 14 mg (9%). White crystals. Mp 225–228 °C (EtOAc–hexane). IR (KBr, cm^{-1}): 3217, 3113, 1674, 1594, 1357, 1092, 743, 736. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.69 (br s, 1H), 7.99–7.97 (m, 1H), 7.96–7.94 (m, 2H), 7.81–7.79 (m, 1H), 7.58–7.56 (m, 2H), 7.46–7.42 (m, 1H), 7.40–7.36 (m, 1H), 5.25 (s, 2H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 166.6, 148.9, 144.8, 142.8, 135.1, 134.6, 133.4, 130.8, 128.4, 124.4, 123.7, 120.5, 110.9, 46.9 ppm HRMS calcd. for $C_{16}H_{12}ClN_4O$ $[M+H]^+$ 311.0694; found 311.0694.

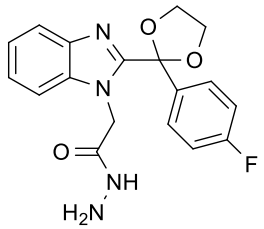


1-(4-Methoxyphenyl)-3*H*-[1,2,5]triazepino[5,4-*a*]benzimidazo-4(5*H*)-one (5e). Yield: 49 mg (32%). White crystals. Mp 253–255 °C (decomp., *i*-PrOH). IR (KBr, cm^{-1}): 3219, 1667, 1606, 1252, 1174, 751. ^{1}H NMR (600 MHz, DMSO-d_6): δ 11.48 (br s, 1H), 7.98–7.96 (m, 1H), 7.89–7.87 (m, 2H), 7.80–7.79 (m, 1H), 7.45–7.42 (m, 1H), 7.38–7.36 (m, 1H), 7.06–7.04 (m, 2H), 5.20 (s, 2H), 3.83 (s, 3H) ppm. ^{13}C NMR (150 MHz, DMSO-d_6): δ 166.8, 161.2, 150.4, 145.1, 142.7, 133.4, 130.7, 128.0, 124.3, 123.6, 120.5, 113.8, 110.9, 55.6, 46.9 ppm. HRMS calcd. for $C_{17}H_{15}N_4O_2$ $[M+H]^+$ 307.1190; found 307.1192.



2-[2-(4-Fluorophenyl)-1,3-dioxolan-2-yl]-1*H*-benzimidazole (6). (1*H*-Benzimidazol-2-yl)(4-fluorophenyl)methanone (**1a**, 2.80 g, 11.66 mmol) was dissolved in ethylene glycol (40 ml). *p*-Toluenesulfonic acid monohydrate (2.44 g, 12.88 mmol) was added, and the reaction mixture was heated to 120 °C for 7 hours. The cooled to room temperature mixture was then poured into an aqueous solution of Na_2CO_3 (100 ml, 5 w/w%). The mixture was extracted with $CHCl_3$ (2 × 40 ml). The organic layer was washed with water (40 mL) and brine (40 ml), dried ($MgSO_4$), filetered and evaporated under reduced pressure to give product **6**. Yield 3.11

g (94%). White crystals. Mp 255–256 °C (MeCN). IR (KBr, cm^{-1}): 3442, 3049, 1421, 1229, 1090, 835. ^{1}H NMR (500 MHz, DMSO-d_6): δ 12.61 (br s, 1H), 7.60–7.57 (m, 2H), 7.56–7.48 (m, 2H), 7.24–7.20 (m, 2H), 7.19–7.16 (m, 2H), 4.16–4.12 (m, 2H), 4.11–4.07 (m, 2H) ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.4 (d, J = 244.6 Hz), 153.4, 143.1, 136.2 (d, J = 2.9 Hz), 134.1, 128.5 (d, J = 8.8 Hz), 122.8, 121.6, 119.4, 115.0 (d, J = 21.5 Hz), 111.9, 105.0, 65.5 ppm. HRMS calcd. for $C_{16}H_{14}FN_2O_2$ $[M+H]^+$ 285.1034; found 285.1034.



2-{2-[2-(4-Fluorophenyl)-1,3-dioxolan-2-yl]-1*H*-benzimidazol-1-yl}acetohydrazide (7).

Step 1. Ethyl {2-[2-(4-fluorophenyl)-1,3-dioxolan-2-yl]-1H-benzimidazol-1-yl}acetate. Precursor 2-[2-(4-fluorophenyl)-1,3-dioxolan-2-yl]-1*H*-benzimidazole **6** (3.11 g, 10.94 mmol) was dissolved in a mixture of MeCN (200 ml) and CH_2Cl_2 (50 ml). To this solution were added Cs_2CO_3 (4.63 g, 14.21 mmol) and ethyl bromoacetate (1.45 ml, 2.18 g, 13.05 mmol). The mixture was stirred overnight at room temperature, filtered and concentrated *in vacuo*. The residue was dissolved in CH_2Cl_2 (30 ml), washed with water (2 × 15 mlL), dried ($MgSO_4$), filtered and concentrated under reduced pressure to give alkylated product **7**. Yield 3.73 g (92%). Pale yellow oil. IR (film, cm^{-1}): 2983, 2902, 1753, 1604, 1508, 1208, 839, 767. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89–7.87 (m, 1H), 7.56–7.53 (m, 2H), 7.32–7.29 (m, 2H), 7.21–7.19 (m, 1H), 7.05–7.01 (m, 2H), 4.23–4.20 (m, 2H), 4.19–4.17 (m, 2H), 4.79 (s, 2H), 4.10 (q, J = 7.1 Hz, 2H), 1.20 (t, J = 7.1 Hz, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 163.3 (d, J = 248.6 Hz), 151.6, 141.6, 136.2, 133.7 (d, J = 3.1 Hz), 128.3 (d, J = 8.6 Hz), 123.7, 122.6, 120.8, 115.4 (d, J = 21.6 Hz), 109.1, 105.4, 65.7, 61.6, 45.6, 14.1 ppm. HRMS calcd. for $C_{16}H_{14}FN_2O_2$ $[M+H]^+$ 371.1390; found 371.1400.

Step 2. Compound 7. Ethyl {2-[2-(4-fluorophenyl)-1,3-dioxolan-2-yl]-1*H*-benzimidazol-1-yl}acetate (3.96 g, 10.69 mmol) from Step 1 was dissolved in EtOH (50 ml). Hydrazine monohydrate (3.50 ml, 3.69 g, 72.8 mmol) was added and the solution was stirred at reflux temperature for 48 h until TLC showed complete consumption of the starting material. After cooling to room temperature, the reaction mixture was evaporated and the residue was purified by flash column chromatography to afford product **8**. Yield 1.88 g (49%). White foam. IR (KBr, cm^{-1}): 3728, 2851, 1684, 1603, 1508, 1223, 746. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87–7.86 (m, 1H), 7.57–7.55 (m, 2H), 7.35–7.33 (m, 2H), 7.31–7.28 (m, 1H), 7.10–7.05 (m, 2H), 6.63 (s, 1H), 4.84 (s, 2H), 4.25–4.23 (m, 2H), 4.22–4.20 (m, 2H), 3.63 (br

s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 163.3 (d, J = 249.2 Hz), 151.3, 141.6, 135.7, 133.7 (d, J = 3.2 Hz), 128.2 (d, J = 8.4 Hz), 124.4, 123.3, 121.1, 115.7 (d, J = 21.9 Hz), 109.9, 105.8, 65.8, 47.0 ppm. HRMS calcd. for $C_{18}H_{18}FN_4O_3$ $[M+H]^+$ 357.1357; found 357.1632.

References

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Table S2. Distribution (%) of **4b** conformers calculated using various quantum chemical methods

Conformer	Distr. A	Distr. B	Distr. C	Distr. D	Distr. E	Distr. F	Distr. G	Distr. H
4'b	73.5	73.5	79.5	70.5	39.6	26.0	2.6	60.5
4"b	0.6	0.7	0.0	1.0	27.7	17.7	4.1	18.8
4'"b	3.4	3.6	0.5	0.4	4.2	55.1	93.0	10.7
4""b	22.5	22.2	20.0	28.1	28.5	1.2	0.3	10.0

A: B3LYP/6-31G(d,p) (gas phase)
B: B3LYP/6-31G(d,p) (DMSO)
C: B3LYP/6-31G(d,p) (DMSO), one DMSO molecule
D: B3LYP/6-31G(d,p) (DMSO), two DMSO molecules
E: ωB97XD/6-31G(d,p) (DMSO)
F: ωB97XD/6-31G(d,p) (DMSO), one DMSO molecule
G: ωB97XD/6-31G(d,p) (DMSO), two DMSO molecules
H: ωB97XD/6-311++G(2d,2p) (DMSO), two DMSO molecules

Cartesian coordinates for computed structures

4'b_A

C	1.72482400	2.41829400	0.23282500
C	2.88789100	2.26708000	-0.56040800
C	3.50571300	3.39579500	-1.12661800
C	2.93936900	4.63609900	-0.87267100
C	1.77596100	4.76802000	-0.07739900
C	1.14557800	3.66727300	0.48949200
C	2.32466600	0.29245100	0.07189800
H	4.39631400	3.28838300	-1.73699600
H	3.39192900	5.52856100	-1.29313000
H	1.36054900	5.75727200	0.08736400
H	0.23973100	3.76813500	1.07689500
N	3.23646600	0.93706800	-0.63855200
N	1.37690800	1.14141800	0.62885000
C	2.23083700	-1.18673900	0.16456700
O	1.12266200	-1.71249200	0.33982600
C	3.44820800	-2.02353100	0.02041000
C	4.75100000	-1.53091000	0.21346700
C	3.26312100	-3.38801400	-0.27068800
C	5.84342400	-2.39000800	0.10820800
H	4.90386800	-0.48504200	0.44499200
C	4.35717900	-4.23797300	-0.38572000
H	2.25417800	-3.76008400	-0.40939400
C	5.65057000	-3.73963500	-0.19524700
H	6.84626100	-2.00562500	0.26515700
H	4.20639000	-5.28659900	-0.62189300
H	6.50543200	-4.40358200	-0.28148000
C	0.28713400	0.84358900	1.55630800
H	0.28300100	1.59776000	2.34451600
H	0.45847800	-0.13606200	1.99977000
C	-1.08946700	0.89358500	0.87034200
O	-1.88664600	1.80265200	1.06593300
N	-1.30894300	-0.14940900	0.02392000
H	-0.61520000	-0.88966600	-0.06138900
N	-2.48379000	-0.26264500	-0.68946900
H	-2.60785600	0.40710300	-1.43980000

C	-3.63422000	-0.64446500	-0.00711200
O	-3.63192600	-1.17967000	1.08587200
O	-4.69133900	-0.36700100	-0.78634900
C	-6.06751800	-0.75050900	-0.39276800
C	-6.89783400	-0.26116700	-1.58026700
H	-6.78763600	0.81909000	-1.71077000
H	-6.58416400	-0.75780600	-2.50283900
H	-7.95485800	-0.48314200	-1.40952800
C	-6.16112400	-2.27164000	-0.25098500
H	-5.56280900	-2.62951400	0.58747400
H	-7.20430400	-2.55574500	-0.08313600
H	-5.81903300	-2.76143600	-1.16777200
C	-6.46053700	-0.01373900	0.88994900
H	-7.51366600	-0.21025700	1.11266600
H	-5.85655400	-0.34359100	1.73555900
H	-6.33520100	1.06579200	0.76273800

4"b_A

C	-1.94054200	-2.35925100	0.18502800
C	-2.88391400	-1.77736700	-0.69580900
C	-3.75702500	-2.59230000	-1.43600900
C	-3.66118400	-3.96522000	-1.26278500
C	-2.71608700	-4.53073500	-0.37550000
C	-1.83929800	-3.74454500	0.36278200
C	-1.80944700	-0.14370700	0.19685600
H	-4.48014400	-2.15034200	-2.11346300
H	-4.32205200	-4.62410500	-1.81691800
H	-2.67123600	-5.61019700	-0.27103700
H	-1.11309100	-4.19203400	1.03261000
N	-2.77755500	-0.40388700	-0.66313400
N	-1.24633800	-1.29617800	0.74011000
C	-1.27513300	1.21038500	0.50595500
O	-0.13472200	1.30318400	0.96678800
C	-2.09908600	2.42310900	0.24391700
C	-3.50051300	2.40359800	0.13617400
C	-1.42154900	3.65358600	0.16620000
C	-4.20284500	3.59309800	-0.05303600
H	-4.03347100	1.46443600	0.20242600
C	-2.12548700	4.83578200	-0.03576400
H	-0.34141000	3.66167600	0.26079100
C	-3.51977900	4.80763100	-0.14457700
H	-5.28561600	3.57110400	-0.12713100
H	-1.59216400	5.77864400	-0.10648300
H	-4.07105600	5.73059700	-0.29751500
C	-0.25223100	-1.41306500	1.80008100
H	-0.29076900	-0.53412500	2.43923500
H	-0.50588500	-2.28354800	2.41198200
C	1.20640400	-1.58397200	1.36615700
O	2.09840400	-1.56780100	2.20360900
N	1.43078600	-1.81808500	0.04142400
H	0.69620200	-1.76113200	-0.64852600
N	2.70681900	-2.07689400	-0.42582300
H	3.08567700	-2.97120400	-0.13476100
C	3.68141800	-1.07974000	-0.46696900
O	4.86583900	-1.37077300	-0.49837200
O	3.13232400	0.13293600	-0.53942100
C	3.96691700	1.36028700	-0.56057700
C	2.91587000	2.46873700	-0.63077400
H	2.33544900	2.39106900	-1.55479000
H	2.22722100	2.40358800	0.21542200
H	3.40740600	3.44548900	-0.61334300
C	4.77171300	1.44612200	0.73808900
H	5.51442900	0.64953500	0.79600800
H	5.28786700	2.40970700	0.78294900
H	4.10514400	1.37395900	1.60270700
C	4.85304200	1.36817100	-1.80812800
H	5.36594300	2.33219500	-1.87897100
H	5.59942300	0.57480200	-1.76961600
H	4.24392600	1.24121500	-2.70831500

4"'b_A

C	-1.98589100	-2.42627300	0.19231200
C	-2.94297800	-1.97855200	-0.75013100
C	-3.65375600	-2.90526100	-1.53151000
C	-3.38721000	-4.25247800	-1.33733000
C	-2.43108400	-4.68404900	-0.38861100
C	-1.71314800	-3.78536100	0.39142300
C	-2.15038800	-0.21247500	0.18488500
H	-4.38680700	-2.56593400	-2.25585900
H	-3.91995900	-4.99531000	-1.92241400
H	-2.24999700	-5.74754800	-0.26890200
H	-0.97611400	-4.12953800	1.10880700
N	-3.02094200	-0.60331400	-0.72837600
N	-1.47438800	-1.27815000	0.77580600
C	-1.82082600	1.20076000	0.51372100
O	-0.74863400	1.44070000	1.07332000
C	-2.75826900	2.30202900	0.15447600
C	-4.12892800	2.11454200	-0.09428400
C	-2.22750300	3.60474900	0.12904200
C	-4.94443100	3.21163300	-0.36947100
H	-4.54899200	1.11789500	-0.07150500
C	-3.04252000	4.69427100	-0.15792400
H	-1.17121600	3.74055700	0.33316200
C	-4.40513300	4.49925100	-0.40672700
H	-6.00356800	3.06027800	-0.55320900
H	-2.62066500	5.69409000	-0.18627300
H	-5.04390900	5.34941300	-0.62675000
C	-0.52800000	-1.25808900	1.88494100
H	-0.65231600	-2.18325000	2.45456600
H	-0.75339900	-0.42624700	2.54834200
C	0.95683600	-1.14845700	1.52593200
O	1.79021500	-0.99735900	2.40831500
N	1.27883800	-1.29844300	0.20882000
H	0.57471000	-1.38691200	-0.50893400
N	2.59271700	-1.29274800	-0.20873300
H	3.14423700	-2.08767100	0.09289200
C	3.26300100	-0.07432400	-0.28300700
O	2.70904900	1.00771100	-0.32154600
O	4.57762900	-0.33121300	-0.36161400
C	5.56883400	0.75091500	-0.57328800
C	6.88959500	-0.01838600	-0.62211600
H	7.05815300	-0.55744200	0.31444400
H	6.88733800	-0.73989200	-1.44405900
H	7.71886700	0.67774700	-0.77482300
C	5.29249500	1.45006700	-1.90627500
H	4.34297100	1.98561100	-1.88264000
H	6.09353900	2.16631100	-2.11233700
H	5.27028300	0.72073600	-2.72170800
C	5.54000200	1.71458600	0.61523500
H	6.34974300	2.44313400	0.51097200
H	4.59185900	2.25028300	0.66653800
H	5.69140800	1.16897900	1.55150400

4""b_A

C	-1.68441800	2.40280400	-0.32499100
C	-2.95634400	2.20150300	0.26372400
C	-3.76122800	3.30516900	0.59554000
C	-3.26535100	4.57079400	0.31948000
C	-1.99140500	4.75277400	-0.26966800
C	-1.17637500	3.67791500	-0.60280100
C	-2.12133300	0.24843900	-0.05749500
H	-4.73632900	3.15967800	1.04861400
H	-3.86155600	5.44492800	0.56136500
H	-1.63855700	5.76166300	-0.45930400
H	-0.19068000	3.82123200	-1.03149600
N	-3.19956600	0.85395300	0.41337900
N	-1.16236400	1.13893700	-0.52200200

C	-1.88369100	-1.21559100	0.02063800
O	-0.72121200	-1.63380500	0.11428100
C	-3.02860600	-2.15958600	0.01290000
C	-4.30189700	-1.82178400	-0.47895800
C	-2.79129800	-3.46866000	0.47179700
C	-5.31590500	-2.77762200	-0.50198900
H	-4.49222600	-0.82014000	-0.84162400
C	-3.80978200	-4.41476600	0.45734800
H	-1.80374500	-3.72154300	0.84122700
C	-5.07474200	-4.07032200	-0.03130100
H	-6.29473100	-2.51361100	-0.88963000
H	-3.62202600	-5.41909600	0.82364100
H	-5.86958800	-4.80995400	-0.04661100
C	0.09687000	0.87547300	-1.21431200
H	0.09333800	-0.15235400	-1.57452300
H	0.17705900	1.55162400	-2.06664200
C	1.32202800	1.12528900	-0.31813900
O	2.09224400	2.05882000	-0.50753200
N	1.44700100	0.22358600	0.69388300
H	0.81780200	-0.57541800	0.74367600
N	2.49647100	0.29197500	1.59128700
H	2.43142800	1.03454900	2.27793800
C	3.80548000	0.02878300	1.19942400
O	4.74880800	0.40418600	1.87688100
O	3.83963000	-0.70408300	0.08327700
C	5.12411600	-1.10883300	-0.53673000
C	4.66154400	-1.88058300	-1.77341800
H	4.04684900	-2.73857900	-1.48687500
H	4.07498200	-1.23698100	-2.43512400
H	5.53023700	-2.24663900	-2.32761100
C	5.91660600	0.13812000	-0.93575800
H	6.25024100	0.69281800	-0.05839100
H	6.79439200	-0.16027300	-1.51664600
H	5.30108300	0.79456500	-1.55817100
C	5.89718900	-2.02046200	0.41894500
H	6.78692100	-2.40488600	-0.08888700
H	6.21014400	-1.48100000	1.31316500
H	5.27964800	-2.87380300	0.71542200

4'b_B

C	1.72431000	2.41810200	0.23277800
C	2.88674500	2.26684700	-0.56138700
C	3.50398400	3.39551600	-1.12833100
C	2.93773100	4.63583000	-0.87414900
C	1.77501000	4.76780300	-0.07788400
C	1.14521800	3.66708500	0.48974900
C	2.32424900	0.29232800	0.07188700
H	4.39410300	3.28814800	-1.73942500
H	3.38987100	5.52824400	-1.29515200
H	1.35969200	5.75705000	0.08712700
H	0.23998900	3.76806800	1.07808300
N	3.23541900	0.93683300	-0.63949100
N	1.37686100	1.14126600	0.62934600
C	2.23084100	-1.18685500	0.16485400
O	1.12287200	-1.71301200	0.34023400
C	3.44850700	-2.02304200	0.02023100
C	4.75093900	-1.53016800	0.21511700
C	3.26419400	-3.38713300	-0.27316800
C	5.84381200	-2.38864100	0.10935100
H	4.90326800	-0.48469300	0.44882500
C	4.35871400	-4.23644400	-0.38877800
H	2.25553500	-3.75945000	-0.41329800
C	5.65174900	-3.73785800	-0.19650200
H	6.84635800	-2.00412800	0.26780600
H	4.20856100	-5.28473700	-0.62680400
H	6.50695700	-4.40129200	-0.28317400
C	0.28765400	0.84344300	1.55745100
H	0.28382500	1.59771700	2.34554700
H	0.45941300	-0.13606000	2.00108900
C	-1.08929200	0.89297400	0.87216800
O	-1.88694400	1.80151600	1.06861500
N	-1.30870500	-0.14985500	0.02560000
H	-0.61451100	-0.88961900	-0.06048400
N	-2.48336000	-0.26302100	-0.68810600
H	-2.60679600	0.40591100	-1.43928000
C	-3.63410900	-0.64445600	-0.00628000
O	-3.63247900	-1.17896100	1.08712800
O	-4.69077900	-0.36743800	-0.78618500
C	-6.06722700	-0.75085100	-0.39327200
C	-6.89675700	-0.26282000	-1.58184100
H	-6.78679700	0.81735400	-1.71323800
H	-6.58225900	-0.76023200	-2.50371500
H	-7.95383000	-0.48495900	-1.41167300
C	-6.16051100	-2.27186400	-0.25009000
H	-5.56231100	-2.62873900	0.58889000
H	-7.20365500	-2.55607500	-0.08226500
H	-5.81800700	-2.76244400	-1.16629900
C	-6.46134900	-0.01291600	0.88843400
H	-7.51461300	-0.20939100	1.11050300
H	-5.85801400	-0.34187500	1.73486100
H	-6.33613600	1.06652300	0.76028600

4"b_B

C	-1.94265000	-2.35839200	0.18328500
C	-2.88328600	-1.77429000	-0.69904100
C	-3.75603600	-2.58723300	-1.44188800
C	-3.66261400	-3.96045100	-1.26973200
C	-2.72026800	-4.52818400	-0.38090900
C	-1.84388900	-3.74401500	0.35999600
C	-1.80843100	-0.14306800	0.19755100
H	-4.47708000	-2.14361800	-2.12047500
H	-4.32326300	-4.61784200	-1.82589200
H	-2.67724900	-5.60780500	-0.27733900
H	-1.11982200	-4.19323800	1.03097300
N	-2.77505900	-0.40099600	-0.66481500
N	-1.24804100	-1.29680800	0.74073000
C	-1.27318800	1.21000600	0.50902100
O	-0.13355600	1.30136200	0.97218700
C	-2.09551100	2.42363500	0.24624500
C	-3.49698100	2.40559700	0.13867800
C	-1.41662800	3.65332200	0.16781100
C	-4.19805000	3.59574700	-0.05114600
H	-4.03103200	1.46711100	0.20585400
C	-2.11929900	4.83616800	-0.03487000
H	-0.33646600	3.66040400	0.26227300
C	-3.51363700	4.80947000	-0.14356100
H	-5.28085600	3.57491900	-0.12501400
H	-1.58495500	5.77839700	-0.10624400
H	-4.06391100	5.73293700	-0.29705500
C	-0.25621600	-1.41555200	1.80261300
H	-0.29677700	-0.53824200	2.44390300
H	-0.51067700	-2.28763500	2.41186600
C	1.20341000	-1.58432600	1.37137400
O	2.09417300	-1.56446200	2.21020700
N	1.43049100	-1.82034200	0.04753000
H	0.69663100	-1.76869000	-0.64362700
N	2.70746800	-2.07967500	-0.41668700
H	3.08659200	-2.97289700	-0.12264700
C	3.68113500	-1.08202000	-0.46111100
O	4.86587500	-1.37221000	-0.49106600
O	3.13127700	0.13003300	-0.53807800
C	3.96513200	1.35784800	-0.56690300
C	2.91326300	2.46526000	-0.64066600
H	2.33080100	2.38237900	-1.56293100
H	2.22665300	2.40430800	0.20754400
H	3.40429100	3.44234400	-0.62946900

C	4.77232900	1.45081200	0.72976800
H	5.51483800	0.65427100	0.79092600
H	5.28897100	2.41441300	0.76807000
H	4.10737900	1.38415700	1.59608600
C	4.84887700	1.35997900	-1.81613700
H	5.36047400	2.32421100	-1.89310700
H	5.59634400	0.56776200	-1.77483300
H	4.23818700	1.22745900	-2.71444800

4"'b_B

C	-1.98396200	-2.42665000	0.19245000
C	-2.94094600	-1.97992200	-0.75058600
C	-3.65073900	-2.90741200	-1.53194700
C	-3.38339000	-4.25437500	-1.33710300
C	-2.42744200	-4.68494000	-0.38773500
C	-1.71045700	-3.78548800	0.39229200
C	-2.14997100	-0.21301100	0.18415100
H	-4.38368100	-2.56888600	-2.25678300
H	-3.91535000	-4.99780200	-1.92214700
H	-2.24573600	-5.74827300	-0.26750100
H	-0.97357600	-4.12889700	1.11019800
N	-3.01993200	-0.60470800	-0.72935000
N	-1.47345700	-1.27791000	0.77564300
C	-1.82148400	1.20060800	0.51208900
O	-0.74875300	1.44217200	1.07003400
C	-2.76081900	2.30040300	0.15352700
C	-4.13206300	2.11095000	-0.09050200
C	-2.23152600	3.60361500	0.12404200
C	-4.94963700	3.20662500	-0.36517300
H	-4.55106900	1.11393400	-0.06422300
C	-3.04861500	4.69171500	-0.16248800
H	-1.17475800	3.74100300	0.32463200
C	-4.41179700	4.49473600	-0.40664300
H	-6.00919900	3.05381900	-0.54518500
H	-2.62795300	5.69193400	-0.19408800
H	-5.05216500	5.34379000	-0.62629700
C	-0.52777600	-1.25619800	1.88533500
H	-0.65102400	-2.18148500	2.45499500
H	-0.75483600	-0.42468200	2.54858800
C	0.95701000	-1.14427200	1.52697800
O	1.78947300	-0.98778500	2.40935700
N	1.28021800	-1.29804700	0.21063700
H	0.57677100	-1.39220800	-0.50708500
N	2.59437900	-1.29227300	-0.20592900
H	3.14615100	-2.08663000	0.09675400
C	3.26399300	-0.07379300	-0.28244100
O	2.70947500	1.00796200	-0.32370200
O	4.57877300	-0.33000800	-0.35959300
C	5.56965600	0.75221800	-0.57304900
C	6.89069100	-0.01670100	-0.62009100
H	7.05913400	-0.55404300	0.31747200
H	6.88893800	-0.73962200	-1.44078400
H	7.71975300	0.67946400	-0.77374900
C	5.29349400	1.44882600	-1.90737300
H	4.34381800	1.98414700	-1.88506500
H	6.09442400	2.16490500	-2.11443500
H	5.27178100	0.71800300	-2.72148000
C	5.54006600	1.71794700	0.61377300
H	6.34946000	2.44672800	0.50844600
H	4.59166000	2.25329900	0.66389500
H	5.69152900	1.17405800	1.55103200

4""b_B

C	-1.68425400	2.40264900	-0.32474300
C	-2.95607500	2.20138400	0.26422500
C	-3.76088400	3.30506100	0.59620200
C	-3.26504800	4.57070000	0.32004300
C	-1.99123900	4.75265800	-0.26940500
C	-1.17630200	3.67776400	-0.60271200
C	-2.12109800	0.24831300	-0.05712800
H	-4.73592400	3.15962600	1.04943700
H	-3.86121200	5.44483400	0.56201400
H	-1.63845500	5.76153300	-0.45922300
H	-0.19077200	3.82110200	-1.03178800
N	-3.19927600	0.85380900	0.41392500
N	-1.16223300	1.13877200	-0.52177900
C	-1.88357500	-1.21574900	0.02108100
O	-0.72123400	-1.63415000	0.11546700
C	-3.02875700	-2.15936600	0.01287400
C	-4.30123700	-1.82139200	-0.48096600
C	-2.79266700	-3.46811500	0.47335400
C	-5.31571100	-2.77673500	-0.50439900
H	-4.49048700	-0.82003400	-0.84502400
C	-3.81163600	-4.41370800	0.45853800
H	-1.80575000	-3.72118700	0.84435600
C	-5.07580200	-4.06909500	-0.03209400
H	-6.29387200	-2.51264000	-0.89365000
H	-3.62487800	-5.41777000	0.82606400
H	-5.87099300	-4.80833900	-0.04771200
C	0.09693400	0.87525100	-1.21419700
H	0.09334100	-0.15253000	-1.57454300
H	0.17707800	1.55138700	-2.06652900
C	1.32212600	1.12485100	-0.31805400
O	2.09264200	2.05822300	-0.50747400
N	1.44711000	0.22316900	0.69390000
H	0.81776100	-0.57571300	0.74389200
N	2.49661100	0.29163200	1.59128100
H	2.43135100	1.03406000	2.27808700
C	3.80559000	0.02879200	1.19917000
O	4.74899600	0.40452500	1.87645200
O	3.83979700	-0.70413800	0.08313300
C	5.12421900	-1.10899900	-0.53708600
C	4.66142800	-1.88121500	-1.77339300
H	4.04715300	-2.73936000	-1.48640300
H	4.07441900	-1.23797300	-2.43505700
H	5.53006600	-2.24709200	-2.32777300
C	5.91642400	0.13793600	-0.93673600
H	6.25002600	0.69316900	-0.05966900
H	6.79427600	-0.16058400	-1.51743200
H	5.30083900	0.79393100	-1.55958000
C	5.89765000	-2.02018400	0.41869900
H	6.78721200	-2.40470400	-0.08933200
H	6.21092300	-1.48041500	1.31262800
H	5.28028700	-2.87347600	0.71567900

4'b_C

C	-1.70068400	2.76972400	-0.85647600
C	-2.93026000	3.04050900	-0.20565600
C	-3.45425200	4.34521100	-0.19666800
C	-2.73176900	5.33623400	-0.84341700
C	-1.50539800	5.04985200	-1.48957700
C	-0.96779200	3.76927100	-1.50960500
C	-2.55665900	0.94187900	0.04810700
H	-4.39485900	4.55648900	0.30152500
H	-3.10772000	6.35441800	-0.85599700
H	-0.96711500	5.85579600	-1.97864300
H	-0.02022300	3.56561000	-1.99611200
N	-3.43730200	1.88526900	0.34440300
N	-1.48256800	1.41817000	-0.68866500
C	-2.62300800	-0.46032100	0.53157600
O	-1.57822900	-1.11470900	0.59939300
C	-3.92391200	-1.04678200	0.95705100
C	-5.16800700	-0.58468400	0.49485200
C	-3.87936100	-2.15802100	1.81787900
C	-6.34146200	-1.22384600	0.89295100
H	-5.21233800	0.26624700	-0.17230400
C	-5.05357500	-2.78283200	2.22464900

H	-2.91469300	-2.51202100	2.16459600
C	-6.28815300	-2.31722800	1.76025500
H	-7.29863300	-0.86782700	0.52486300
H	-5.01006000	-3.63161200	2.90001400
H	-7.20538600	-2.80719600	2.07297800
C	-0.34140700	0.68698000	-1.21261500
H	0.02076400	1.22007400	-2.09700400
H	-0.63866700	-0.31154100	-1.53018100
C	0.80648800	0.61262500	-0.19643500
O	0.97185100	1.44865800	0.68386800
N	1.63630800	-0.44277300	-0.41511300
H	1.39922200	-1.19204300	-1.08132900
N	2.74087300	-0.63930400	0.39424800
H	2.53668200	-0.82671100	1.36971700
C	3.86972100	0.13737200	0.16031800
O	4.08706400	0.73650000	-0.87694900
O	4.66592300	0.05091300	1.23992000
C	6.00552600	0.68106600	1.26832900
C	6.51963800	0.29959500	2.65735100
H	5.86000000	0.69393600	3.43555200
H	6.57449900	-0.78744500	2.76491900
H	7.52032600	0.71341700	2.80970300
C	6.88638400	0.07401200	0.17360500
H	6.50892800	0.32135800	-0.81903900
H	7.90422800	0.46417400	0.26874600
H	6.92842400	-1.01450400	0.27772100
C	5.86478100	2.19961200	1.13596400
H	6.84353000	2.66860600	1.27520400
H	5.48030800	2.47593200	0.15393600
H	5.18908800	2.58746900	1.90428500
S	0.32342400	-3.80706900	-1.92298100
O	0.66841700	-2.33952700	-2.24270500
C	1.86584500	-4.75482700	-2.12691600
H	1.68920500	-5.78724000	-1.81717800
H	2.12484400	-4.72445400	-3.18625500
H	2.65671300	-4.29703600	-1.52857800
C	0.18118400	-3.94462700	-0.11194700
H	-0.63157500	-3.28390900	0.19502300
H	-0.05199800	-4.98175300	0.13957400
H	1.11714100	-3.63400300	0.35819100

4"b_C

C	1.86680100	-2.11724000	-1.21125400
C	2.94686900	-1.61116100	-0.44898500
C	3.94543900	-2.47852800	0.02499700
C	3.83357600	-3.82521200	-0.28944900
C	2.75215100	-4.31385300	-1.05910400
C	1.75099100	-3.47462200	-1.53400000
C	1.70951400	0.07535500	-0.93816500
H	4.77388300	-2.09595600	0.61213800
H	4.58868000	-4.52278000	0.05887500
H	2.70060500	-5.37507800	-1.28156300
H	0.92183500	-3.86270300	-2.11572800
N	2.82136400	-0.24743900	-0.29977800
N	1.07750100	-1.02204800	-1.51049600
C	1.11103800	1.43582300	-0.97108000
O	-0.09449100	1.55060000	-1.20350500
C	1.95542500	2.63377500	-0.69860800
C	3.34965700	2.65915100	-0.87526600
C	1.29061800	3.80980300	-0.30607500
C	4.05923500	3.83921500	-0.65661500
H	3.87001500	1.76194100	-1.18346300
C	2.00499400	4.98059800	-0.07422500
H	0.21324300	3.78381500	-0.18503700
C	3.39229300	4.99759300	-0.25153600
H	5.13463600	3.85424600	-0.80390000
H	1.48454100	5.87974700	0.24052400
H	3.95070300	5.91229100	-0.07639000
C	-0.08218400	-1.05914100	-2.39143400
H	-0.20547300	-0.08807100	-2.86708700
H	0.10468500	-1.79518100	-3.17763200
C	-1.43090000	-1.42464700	-1.76450500
O	-2.39837000	-1.60075700	-2.49882200
N	-1.47778600	-1.55374600	-0.41303200
H	-0.70955900	-1.32573300	0.22092400
N	-2.66941100	-1.91393800	0.19851200
H	-2.93528200	-2.88368800	0.07001400
C	-3.77079400	-1.06499800	0.20680500
O	-4.89526700	-1.50080900	0.40120100
O	-3.40569700	0.21076100	0.05493500
C	-4.40957800	1.29891300	-0.01217100
C	-3.53757400	2.53717000	-0.22625700
H	-2.85701500	2.67995200	0.61808600
H	-2.94059700	2.43875100	-1.13657700
H	-4.17012200	3.42477900	-0.31496500
C	-5.33383300	1.06643500	-1.20963000
H	-5.95539900	0.18263800	-1.06263800
H	-5.98498600	1.93567700	-1.34147000
H	-4.74448800	0.93797300	-2.12248000
C	-5.16975700	1.39083300	1.31287500
H	-5.82175200	2.26958200	1.29496900
H	-5.78027100	0.50359800	1.48064400
H	-4.46969700	1.50444400	2.14626100
S	1.19928300	-0.81836900	2.88206100
O	0.17072900	-1.23622500	1.82881500
C	0.59467400	-1.49532100	4.46437800
H	0.65097300	-2.58235400	4.38948400
H	1.24062100	-1.14516600	5.27264300
H	-0.43876800	-1.18053900	4.62536100
C	0.89900400	0.94200700	3.25608200
H	1.51341400	1.23158200	4.11164400
H	1.19613700	1.51720000	2.37825000
H	-0.16195600	1.09287600	3.46803300

4"'b_C

C	2.04892300	-2.43771400	-0.62885400
C	3.01329800	-1.91890700	0.26820200
C	3.78119600	-2.78724100	1.06229500
C	3.56187100	-4.15012300	0.92647600
C	2.59645600	-4.65329300	0.02315100
C	1.82345800	-3.81255700	-0.76861800
C	2.12651800	-0.22524600	-0.71323100
H	4.52124200	-2.39340400	1.75132400
H	4.13931100	-4.84956700	1.52269200
H	2.45267100	-5.72672100	-0.05049900
H	1.07897400	-4.21097500	-1.44928100
N	3.03790100	-0.54426000	0.19132100
N	1.48356200	-1.33619900	-1.24429400
C	1.73345700	1.15918900	-1.08872400
O	0.63364000	1.33880400	-1.61722100
C	2.64323100	2.30687500	-0.81064100
C	4.02918300	2.17708700	-0.61648100
C	2.06650400	3.59002300	-0.80708600
C	4.81496600	3.31151200	-0.41572300
H	4.48442000	1.19564000	-0.62340400
C	2.85240200	4.71741800	-0.59401300
H	0.99813700	3.68088400	-0.96905300
C	4.23067700	4.57981300	-0.39885600
H	5.88593000	3.20443100	-0.27411800
H	2.39556500	5.70210300	-0.58159900
H	4.84651100	5.45938100	-0.23664700
C	0.51853000	-1.39494200	-2.33396200
H	0.66486500	-2.34102500	-2.86256500
H	0.71258100	-0.59064700	-3.04029400
C	-0.96722600	-1.31152900	-1.97417000
O	-1.79178800	-1.23430600	-2.88151100

N	-1.30494500	-1.42577600	-0.66324900
H	-0.66000100	-1.34710700	0.13950000
N	-2.65103000	-1.42430900	-0.32442600
H	-3.19658700	-2.14088900	-0.78829200
C	-3.29166100	-0.20626000	-0.14849200
O	-2.71454300	0.83869900	0.10694900
O	-4.61586200	-0.40809500	-0.23567400
C	-5.59252100	0.67936800	0.00905200
C	-6.93164000	-0.03553900	-0.17813700
H	-7.01083800	-0.45049600	-1.18691600
H	-7.03971700	-0.85050300	0.54327600
H	-7.75311300	0.67041500	-0.02867100
C	-5.44717800	1.20026500	1.44054100
H	-4.49892800	1.72037800	1.57865700
H	-6.26204600	1.89822000	1.65561800
H	-5.50954800	0.37448200	2.15574500
C	-5.40691600	1.77901800	-1.03899900
H	-6.20015200	2.52453500	-0.92809800
H	-4.44264300	2.27480200	-0.92343500
H	-5.47260600	1.35910500	-2.04720800
S	0.15201700	0.38478200	2.17904000
O	-0.02795700	-1.09236600	1.77741300
C	1.49569800	0.39510800	3.40609600
H	2.40836100	0.13788900	2.86674000
H	1.58074500	1.39676700	3.83306800
H	1.28345100	-0.34440700	4.18120600
C	-1.22883400	0.78358000	3.29640700
H	-1.06123500	1.77204900	3.73034900
H	-2.12819700	0.79362700	2.67948300
H	-1.29813400	0.02100800	4.07527100

4""b_C

C	-0.73777700	2.79909200	-0.73062300
C	-1.97399300	3.36886200	-0.33630800
C	-2.18102500	4.75553500	-0.44425300
C	-1.14449000	5.52626800	-0.94783900
C	0.08456000	4.94220000	-1.33793600
C	0.31227500	3.57582000	-1.23768800
C	-2.14113100	1.25570300	0.00564800
H	-3.12603900	5.19546000	-0.14264200
H	-1.27101400	6.59988000	-1.04548000
H	0.87347400	5.58194400	-1.72109000
H	1.26348500	3.14228200	-1.52636400
N	-2.82387900	2.38527300	0.11466000
N	-0.86731900	1.44363800	-0.51069700
C	-2.62063600	-0.07192200	0.46456000
O	-1.79072800	-0.95157800	0.71677500
C	-4.07779400	-0.32405900	0.64271900
C	-5.07781700	0.39543700	-0.03359100
C	-4.44741000	-1.38362500	1.49074800
C	-6.41946600	0.05930400	0.14249700
H	-4.80354700	1.20905600	-0.69217400
C	-5.78799700	-1.70555100	1.67490900
H	-3.66871600	-1.93784200	2.00311200
C	-6.77749400	-0.98477800	0.99819300
H	-7.18630400	0.61320800	-0.39002000
H	-6.06403300	-2.51637600	2.34183700
H	-7.82425300	-1.23815100	1.13705900
C	0.16345800	0.45635300	-0.78406000
H	-0.28075700	-0.47824800	-1.12216800
H	0.78723700	0.84037100	-1.59737300
C	1.06753200	0.22122200	0.43399900
O	1.25851800	1.07378800	1.29358300
N	1.67234400	-0.99581100	0.41466500
H	1.41873900	-1.72231800	-0.27243600
N	2.58997800	-1.33578400	1.39598100
H	2.19973500	-1.49589900	2.31816400
C	3.84265600	-0.73696500	1.45081300
O	4.51186200	-0.77487800	2.47218400
O	4.18811000	-0.21371300	0.26990600
C	5.47987300	0.48796100	0.08526900
C	5.40605900	0.92837400	-1.37771500
H	5.30226400	0.06247200	-2.03776600
H	4.55266500	1.59326200	-1.53906200
H	6.31909200	1.46444700	-1.65085700
C	5.54481200	1.70069700	1.01689900
H	5.59282100	1.39473000	2.06224800
H	6.43531700	2.29155300	0.78226100
H	4.66532500	2.33556200	0.87293800
C	6.63810900	-0.48841800	0.30330900
H	7.58074000	0.00443100	0.04660600
H	6.68607400	-0.81815800	1.34122100
H	6.52495700	-1.36370500	-0.34358600
S	0.08801800	-4.11146500	-0.88950600
O	0.71461000	-2.82935600	-1.47741300
C	-1.71579800	-3.92640900	-1.04736000
H	-2.19305200	-4.85845700	-0.73585200
H	-2.00652200	-3.11045800	-0.38288800
H	-1.96741400	-3.68614200	-2.08294800
C	0.32650000	-5.40017600	-2.15312200
H	1.39745700	-5.59866700	-2.21328700
H	-0.20268800	-6.30324300	-1.84133000
H	-0.04821300	-5.03842000	-3.11299300

4'b_D

C	1.80379800	-2.72002900	-1.45559800
C	2.96315600	-3.14167600	-0.75808600
C	3.39160500	-4.47845400	-0.83960500
C	2.64780200	-5.34880700	-1.62160100
C	1.49281400	-4.91202300	-2.31365700
C	1.04923100	-3.59762200	-2.24521700
C	2.72362500	-1.05107700	-0.33323100
H	4.27820500	-4.80515500	-0.30593700
H	2.95098200	-6.38753600	-1.70730200
H	0.93451100	-5.62691400	-2.91009800
H	0.15409800	-3.27923300	-2.76795000
N	3.51248400	-2.08231200	-0.07246200
N	1.67053900	-1.37618400	-1.17497300
C	2.86385900	0.29559700	0.27518300
O	1.86950500	1.02525900	0.34411700
C	4.17852800	0.73969200	0.81520000
C	5.40877400	0.21823900	0.37965000
C	4.16852500	1.77784100	1.76412700
C	6.60233300	0.72800200	0.88913700
H	5.42729100	-0.57745900	-0.35357000
C	5.36140800	2.27296000	2.28052100
H	3.21484500	2.17773700	2.09075900
C	6.58197400	1.74964600	1.84120100
H	7.54944600	0.32741600	0.54139900
H	5.34346600	3.06552600	3.02210700
H	7.51410100	2.13881600	2.23980400
C	0.62326100	-0.51684500	-1.70169000
H	0.32269600	-0.91495000	-2.67590700
H	1.00156700	0.49186900	-1.85921000
C	-0.61525600	-0.49762800	-0.79382900
O	-0.90168300	-1.43697600	-0.05373300
N	-1.36238300	0.62099500	-0.94518600
H	-1.02507500	1.42335700	-1.49786600
N	-2.55579200	0.77317100	-0.25559500
H	-2.46331900	0.83475000	0.77161800
C	-3.66966400	0.14074100	-0.77057100
O	-3.75445600	-0.31715300	-1.89901900
O	-4.64055500	0.16470300	0.16754500
C	-5.99523200	-0.35361100	-0.10843800
C	-6.72369300	-0.09807800	1.21282700
H	-6.23823100	-0.63577400	2.03245700

H	-6.72851500	0.96928700	1.45174200
H	-7.75942700	-0.44133400	1.13984700
C	-6.63828300	0.44544100	-1.24551300
H	-6.11425300	0.28139900	-2.18740800
H	-7.68110100	0.13580800	-1.36477300
H	-6.62557800	1.51483500	-1.01320200
C	-5.92885300	-1.85334200	-0.41005900
H	-6.94369900	-2.25418900	-0.49493000
H	-5.39671500	-2.04313800	-1.34224400
H	-5.42113500	-2.38183700	0.40266900
S	0.00726400	4.00910300	-1.50743000
O	-0.18090600	2.74179500	-2.36762100
C	1.78862000	4.14002800	-1.15816200
H	1.97677000	5.08456200	-0.64248800
H	2.04230900	3.29775100	-0.51160900
H	2.34844800	4.08887000	-2.09483600
C	-0.13580600	5.41424100	-2.65628500
H	-1.16921900	5.44050600	-3.00481600
H	0.09872600	6.33512700	-2.11781700
H	0.54582700	5.26710900	-3.49689300
S	-2.08276400	-0.58799200	3.10594500
O	-2.03409600	0.83797100	2.52643600
C	-2.42358800	-0.38309400	4.88399600
H	-3.43382800	0.01898000	4.97367300
H	-2.36747000	-1.35913500	5.37126600
H	-1.69962400	0.31123400	5.31608800
C	-0.35815300	-1.15536300	3.24378800
H	-0.33851800	-2.10209600	3.78889200
H	-0.00491700	-1.30128900	2.22238800
H	0.23421100	-0.39584500	3.75908900

4"b_D

C	1.47719800	-2.42033000	-1.30324700
C	2.51101200	-2.86015900	-0.44157000
C	2.62503100	-4.22127200	-0.11286800
C	1.70282200	-5.09965100	-0.66465900
C	0.68094900	-4.64531600	-1.53084400
C	0.54850000	-3.30260700	-1.86801800
C	2.74985200	-0.73613800	-0.63761600
H	3.41374600	-4.56350200	0.54924500
H	1.76332000	-6.15819300	-0.43218800
H	-0.02063500	-5.36461400	-1.94171400
H	-0.24406300	-2.96471500	-2.52698700
N	3.28712200	-1.79150900	-0.05165800
N	1.64013100	-1.05266400	-1.41267900
C	3.17533900	0.67069400	-0.41120900
O	2.36007200	1.57525800	-0.60597000
C	4.55333300	0.97245400	0.06966400
C	5.63938100	0.09304600	-0.07892900
C	4.76724500	2.23736400	0.64618400
C	6.91028200	0.47494700	0.34945200
H	5.48680700	-0.88020400	-0.52651100
C	6.03400300	2.60905300	1.08368000
H	3.92469700	2.91271700	0.74618200
C	7.10960900	1.72725000	0.93463400
H	7.74635400	-0.20619900	0.22485400
H	6.18657700	3.58309200	1.53809700
H	8.10021000	2.01749300	1.27190300
C	0.88779300	-0.20866100	-2.33258500
H	1.48027600	0.67287500	-2.57184700
H	0.72399900	-0.76467300	-3.25910100
C	-0.48828300	0.28936100	-1.87573400
O	-1.23719000	0.79343100	-2.70943300
N	-0.78749400	0.16067100	-0.56037600
H	-0.16150500	-0.23319400	0.15597500
N	-2.02332100	0.58174900	-0.08967400
H	-2.80713800	-0.07336400	-0.22754100
C	-2.37112500	1.91265900	-0.04364300
O	-3.54028300	2.25760000	0.10528400
O	-1.30385000	2.71837100	-0.11635400
C	-1.44178300	4.19049900	-0.13062500
C	0.01017900	4.65449200	-0.26155500
H	0.60598500	4.30077300	0.58462800
H	0.45738200	4.27143300	-1.18298100
H	0.05141100	5.74707400	-0.28254300
C	-2.26187600	4.61945600	-1.35015100
H	-3.29949500	4.29609200	-1.26273700
H	-2.24009000	5.70973200	-1.43983100
H	-1.83318800	4.19170500	-2.26146600
C	-2.04920000	4.67266900	1.18928000
H	-2.04219000	5.76674100	1.21381800
H	-3.07597600	4.32417000	1.30020000
H	-1.45714100	4.31021500	2.03532500
S	-0.30038200	-1.73416300	2.71460700
O	0.49716400	-0.91240200	1.68909400
C	-1.43392400	-2.83077900	1.79620300
H	-0.81272300	-3.48627300	1.18321400
H	-1.98829200	-3.42710400	2.52522600
H	-2.12004300	-2.25565400	1.16884400
C	-1.55826700	-0.61907900	3.42012100
H	-2.23201100	-1.19922800	4.05467400
H	-1.03021600	0.12303700	4.02087600
H	-2.10006800	-0.13322600	2.60548200
S	-5.40226500	-0.87769900	0.39711900
O	-4.10350700	-1.33420800	-0.30083700
C	-6.56804900	-2.26463500	0.21432800
H	-6.18126400	-3.09234200	0.81046700
H	-7.54504200	-1.95729800	0.59395400
H	-6.62894600	-2.54976300	-0.83816800
C	-6.21180900	0.29155500	-0.73915900
H	-7.19752600	0.54601400	-0.34290100
H	-5.57161600	1.17475200	-0.76486200
H	-6.29283100	-0.16194000	-1.72957600

4"'b_D

C	-1.87728900	2.75644700	0.01274800
C	-3.06762700	2.44216700	0.71178700
C	-3.58005500	3.33035300	1.67226900
C	-2.88587900	4.51019300	1.89630800
C	-1.70006100	4.81193900	1.18657300
C	-1.17329100	3.94611400	0.23554700
C	-2.70377500	0.80536100	-0.63171200
H	-4.49114800	3.09249500	2.21163600
H	-3.25495000	5.21992700	2.62994100
H	-1.18426600	5.74427000	1.39415100
H	-0.25668000	4.18429800	-0.29312700
N	-3.55733000	1.22692300	0.28728600
N	-1.65445400	1.69061000	-0.83931600
C	-2.76709100	-0.51039100	-1.32232000
O	-1.73440300	-0.97318200	-1.81233400
C	-4.05191900	-1.26219300	-1.39491600
C	-5.31546400	-0.65863800	-1.27582500
C	-3.97105700	-2.64121200	-1.65997600
C	-6.47129700	-1.42639500	-1.41427900
H	-5.38921700	0.40272500	-1.07862100
C	-5.12650600	-3.40545200	-1.78323200
H	-2.99140100	-3.09517500	-1.76160300
C	-6.38063300	-2.79782100	-1.66203000
H	-7.44419700	-0.95225500	-1.32978600
H	-5.05348000	-4.47131100	-1.97580500
H	-7.28382000	-3.39218100	-1.76295300
C	-0.60560000	1.63597600	-1.84908900
H	-0.37503400	2.66163200	-2.15050600
H	-0.97199800	1.10983200	-2.72787600
C	0.72629000	0.97854200	-1.47034100
O	1.56922800	0.84212300	-2.35572600

N	0.91828000	0.66505400	-0.16617200
H	0.17195200	0.63291900	0.54528800
N	2.13184000	0.13320600	0.23863800
H	2.94179800	0.76829400	0.20118500
C	2.30376500	-1.22610900	0.22988000
O	1.40414300	-2.04431500	0.08826200
O	3.61027500	-1.49735400	0.44969300
C	4.10128000	-2.88425100	0.58685300
C	5.58918700	-2.68305900	0.88253900
H	6.08150100	-2.15472800	0.06090300
H	5.72641100	-2.10469800	1.80069700
H	6.07745500	-3.65341500	1.00841200
C	3.40955700	-3.57917000	1.76319100
H	2.35503400	-3.75682300	1.55238700
H	3.89549200	-4.54117600	1.95269700
H	3.49641700	-2.97141100	2.66923900
C	3.90399800	-3.63556300	-0.73246100
H	4.35937700	-4.62807400	-0.65977800
H	2.84448400	-3.75233500	-0.96207600
H	4.38853200	-3.09852000	-1.55362900
S	-1.38708700	-1.14453000	2.08935500
O	-0.70485900	0.23594100	2.06221500
C	-2.87465400	-0.93819400	3.11813900
H	-3.54882600	-0.29002400	2.55612600
H	-3.33617400	-1.91536900	3.27679800
H	-2.59859900	-0.47664700	4.06883600
C	-0.41788700	-2.17175500	3.23848700
H	-0.94190200	-3.11637800	3.40134400
H	0.54142300	-2.35693500	2.75432600
H	-0.27972000	-1.63399600	4.17909900
S	5.11086900	2.25966800	-1.08587900
O	4.09937800	2.14484300	0.06753600
C	4.91506200	0.77230700	-2.11948900
H	3.88868800	0.78605500	-2.49119300
H	5.63290900	0.82038900	-2.94135800
H	5.07309400	-0.11851100	-1.50756800
C	6.74620500	1.85800300	-0.38701000
H	7.47842100	1.82763900	-1.19735700
H	7.00346200	2.65234000	0.31534800
H	6.69448000	0.89675900	0.12915000
4""b_D			
C	1.90773200	3.07491600	-0.08788000
C	3.10310300	3.14367700	-0.84634000
C	3.55632500	4.37837100	-1.34400300
C	2.79983200	5.50543900	-1.06235300
C	1.60795200	5.42073500	-0.30323400
C	1.14004400	4.21225800	0.19619700
C	2.83715200	1.08069000	-0.31461700
H	4.47059100	4.43437800	-1.92586300
H	3.12116100	6.47469600	-1.43048700
H	1.04072100	6.32617200	-0.11104200
H	0.21767700	4.15916200	0.76400200
N	3.65661300	1.89015900	-0.96857700
N	1.75865000	1.74612700	0.24970700
C	2.97918700	-0.39536900	-0.25150600
O	1.98416300	-1.08243600	0.00043400
C	4.29861500	-1.03377900	-0.51849400
C	5.52855900	-0.38106300	-0.32854600
C	4.29005300	-2.38131400	-0.92115600
C	6.72315400	-1.06746400	-0.54303000
H	5.54570800	0.65367000	-0.01225100
C	5.48421400	-3.05729800	-1.14925100
H	3.33635200	-2.87900500	-1.05856700
C	6.70444500	-2.40085500	-0.95804500
H	7.66991900	-0.56036600	-0.38509300
H	5.46733100	-4.09317700	-1.47346900
H	7.63756500	-2.92872000	-1.13085400
C	0.66665200	1.20901600	1.04439500
H	1.01495400	0.38240700	1.66115500
H	0.32115500	2.00143500	1.71577900
C	-0.52036800	0.77602400	0.16939300
O	-0.75448700	1.28265000	-0.92239000
N	-1.29350400	-0.16413100	0.76980700
H	-1.00443200	-0.61972300	1.64779700
N	-2.45173400	-0.62433200	0.16222900
H	-2.33161700	-1.26301800	-0.63896600
C	-3.59271900	0.14120800	0.11792400
O	-4.53162900	-0.15830900	-0.61569400
O	-3.55249200	1.16716000	0.98098500
C	-4.67942000	2.11548100	1.10967900
C	-4.16321900	3.09719500	2.16379700
H	-3.94439700	2.57823600	3.10138800
H	-3.25034700	3.59085300	1.81824000
H	-4.91818900	3.86348500	2.36030400
C	-4.91656600	2.82737900	-0.22488700
H	-5.28487000	2.13456200	-0.98158900
H	-5.65419100	3.62375600	-0.08674000
H	-3.98705800	3.28140600	-0.58178400
C	-5.92401800	1.38094700	1.61499000
H	-6.71870200	2.10635700	1.81480800
H	-6.28245100	0.66155800	0.87852300
H	-5.70231800	0.85436900	2.54841900
S	-0.00270400	-2.89118700	2.93620000
O	-0.23864800	-1.37377800	3.08614600
C	1.79629500	-3.12419000	2.78613200
H	2.01450300	-4.19464400	2.79821600
H	2.08895600	-2.68757400	1.82931200
H	2.29853600	-2.61446700	3.61163500
C	-0.21499300	-3.59292700	4.60314500
H	-1.26644400	-3.47693700	4.86971700
H	0.04716800	-4.65290400	4.57577600
H	0.41867000	-3.05074600	5.30819600
S	-3.54101600	-2.78695100	-2.66149700
O	-2.17906900	-2.35013600	-2.09122500
C	-4.12702900	-1.42796800	-3.72219600
H	-5.02280800	-1.75434900	-4.25563900
H	-4.36567000	-0.60477900	-3.04770800
H	-3.33712700	-1.14482800	-4.42168200
C	-3.15432000	-3.98495200	-3.97863000
H	-2.72819700	-4.86667900	-3.49776300
H	-4.07726500	-4.25376300	-4.49724600
H	-2.43221300	-3.54354200	-4.66888100
4'b_E			
C	1.59371900	2.38964600	0.25501200
C	2.72751500	2.31650400	-0.57255000
C	3.26752500	3.48568400	-1.12729100
C	2.64707000	4.68409300	-0.82643300
C	1.50620000	4.73654300	0.00466200
C	0.95608600	3.59538400	0.56125700
C	2.28386600	0.31348900	0.02445300
H	4.14187800	3.44071300	-1.76728500
H	3.03929700	5.60764400	-1.23873800
H	1.04477300	5.69779600	0.20455200
H	0.06657800	3.63017600	1.18056800
N	3.13790500	1.00619800	-0.69564900
N	1.32393300	1.09246300	0.63035300
C	2.25644800	-1.17455700	0.08388000
O	1.17314100	-1.74507200	0.18881500
C	3.52078300	-1.94095000	-0.00674000
C	4.77592700	-1.36468600	0.22514600
C	3.42703500	-3.31105700	-0.28684300
C	5.91997400	-2.15273700	0.16884200
H	4.85621100	-0.30781700	0.44534300
C	4.57246000	-4.09089300	-0.34993800

H	2.44922200	-3.74801400	-0.45579100
C	5.82046500	-3.51119900	-0.12151600
H	6.89046600	-1.70466400	0.35215000
H	4.49505500	-5.14929000	-0.57389000
H	6.71696600	-4.12102500	-0.16787600
C	0.26533900	0.72426000	1.55482400
H	0.25249000	1.43858400	2.37876200
H	0.46079400	-0.27116300	1.95139200
C	-1.10670500	0.77454600	0.87745000
O	-1.95265100	1.60300000	1.17050300
N	-1.26430300	-0.16472300	-0.09042900
H	-0.56071000	-0.88652500	-0.21921600
N	-2.44526200	-0.27066300	-0.78151000
H	-2.60843900	0.44369900	-1.47844000
C	-3.55785100	-0.72527200	-0.09169400
O	-3.50130100	-1.32761200	0.95959200
O	-4.64259200	-0.42709500	-0.80590400
C	-5.98461300	-0.79713500	-0.34625000
C	-6.87976100	-0.25330900	-1.45470600
H	-6.74970100	0.82705700	-1.55907100
H	-6.64240400	-0.72908800	-2.40994300
H	-7.92696100	-0.45653100	-1.21705200
C	-6.10591900	-2.31555300	-0.24987200
H	-5.47348400	-2.71260600	0.54428500
H	-7.14594300	-2.57774200	-0.03701700
H	-5.82334300	-2.77936700	-1.19911200
C	-6.28260500	-0.10304600	0.98025200
H	-7.32603000	-0.28267000	1.25318500
H	-5.63998700	-0.48233200	1.77513400
H	-6.13316600	0.97595900	0.88299100

4"b_E

C	-1.97206900	-2.29485600	0.18360300
C	-2.75414200	-1.63858400	-0.78356900
C	-3.58278900	-2.37768400	-1.63974600
C	-3.59607700	-3.75179700	-1.49197700
C	-2.80234300	-4.39487600	-0.51738200
C	-1.97569500	-3.68496700	0.33562800
C	-1.68046400	-0.11022600	0.25568700
H	-4.18846900	-1.87709100	-2.38706200
H	-4.22628100	-4.35506500	-2.13652100
H	-2.83958300	-5.47602000	-0.43698500
H	-1.36070100	-4.18886200	1.07300700
N	-2.55325600	-0.27766500	-0.71080100
N	-1.28092000	-1.29565800	0.83941200
C	-1.08360600	1.19646400	0.65263400
O	0.00116900	1.19776200	1.21993700
C	-1.79464100	2.46398900	0.33845000
C	-3.17745700	2.53521300	0.13083900
C	-1.03253000	3.63939000	0.32064500
C	-3.78153200	3.76662800	-0.09829000
H	-3.77569500	1.63350100	0.15136400
C	-1.63748300	4.86405300	0.07680200
H	0.03552600	3.57794800	0.49580700
C	-3.01477400	4.92873000	-0.13129000
H	-4.85424900	3.81918600	-0.25046100
H	-1.03939600	5.76875500	0.05297700
H	-3.49056500	5.88658000	-0.31503100
C	-0.35517600	-1.49979400	1.93641900
H	-0.41572800	-0.67431500	2.64108600
H	-0.64539500	-2.41203700	2.46436900
C	1.10756100	-1.64563800	1.53184300
O	1.99888600	-1.52529800	2.35364800
N	1.33285500	-1.99962500	0.23703400
H	0.59741000	-2.02971400	-0.45164000
N	2.61147300	-2.22313600	-0.21447400
H	3.05103000	-3.05990900	0.14561000
C	3.50030300	-1.17499800	-0.40109500
O	4.69814800	-1.37685000	-0.45574200
O	2.85890200	-0.02666200	-0.56509600
C	3.58703500	1.23204700	-0.75740800
C	2.46148800	2.25471400	-0.86371800
H	1.80919000	2.02386800	-1.71051400
H	1.86121600	2.24809100	0.04887000
H	2.88280500	3.25271600	-1.00910200
C	4.45541800	1.51243500	0.46580100
H	5.26363900	0.78547800	0.55049200
H	4.88979900	2.51190400	0.37767800
H	3.84722000	1.47797900	1.37422100
C	4.39505500	1.17695600	-2.05075200
H	4.83589500	2.15981800	-2.23867900
H	5.19439300	0.43886700	-1.98571200
H	3.74352300	0.92610400	-2.89270100

4"'b_E

C	-2.05768500	-2.38138300	0.18729000
C	-2.95110400	-1.86569700	-0.76837000
C	-3.68270700	-2.73350000	-1.59137500
C	-3.48956200	-4.09176900	-1.42336200
C	-2.58506900	-4.59270600	-0.46191600
C	-1.85224700	-3.75361300	0.35902700
C	-2.09351800	-0.17636800	0.22198200
H	-4.37464700	-2.34172600	-2.32870200
H	-4.04070900	-4.79192000	-2.04190700
H	-2.45809400	-5.66570300	-0.36599200
H	-1.15147600	-4.14724100	1.08686000
N	-2.95073900	-0.48881300	-0.72193600
N	-1.50908300	-1.27969300	0.81297000
C	-1.67987600	1.21091700	0.57534200
O	-0.61224400	1.37942200	1.14819700
C	-2.54462700	2.36069200	0.19822400
C	-3.92708100	2.25039700	0.00951100
C	-1.92888100	3.61382100	0.09008100
C	-4.67735500	3.38236300	-0.29059000
H	-4.41042300	1.28602300	0.09886500
C	-2.67940800	4.73801000	-0.22500200
H	-0.85869800	3.68949600	0.24863500
C	-4.05615200	4.62255800	-0.41454000
H	-5.74952800	3.29403300	-0.42936100
H	-2.19474700	5.70357100	-0.32195200
H	-4.64448300	5.50164800	-0.65738700
C	-0.57025700	-1.33041800	1.91681900
H	-0.71639500	-2.27586900	2.44494000
H	-0.76981200	-0.52485200	2.61958800
C	0.90217400	-1.24475900	1.53343000
O	1.75756900	-1.09669000	2.38829300
N	1.18867300	-1.42312000	0.21525500
H	0.46986300	-1.47674100	-0.48918800
N	2.48759600	-1.40574600	-0.22472900
H	3.04778800	-2.20189200	0.04900800
C	3.14090400	-0.18511300	-0.29542400
O	2.57462700	0.88639200	-0.31423400
O	4.44934800	-0.42073300	-0.39055500
C	5.40891400	0.67194700	-0.57949300
C	6.74388500	-0.06226900	-0.64632200
H	6.93077600	-0.60515600	0.28396700
H	6.75175000	-0.77361500	-1.47629200
H	7.55200000	0.65806500	-0.79653800
C	5.12114800	1.39282600	-1.89361500
H	4.16334700	1.91220900	-1.85592500
H	5.91079200	2.12507000	-2.08289500
H	5.10944600	0.67815700	-2.72133300
C	5.36797200	1.61063200	0.62329100
H	6.16701900	2.35119700	0.52913900
H	4.41210200	2.13108900	0.68392600
H	5.52777900	1.04919900	1.54809000

4""b_E

C	-1.58099400	2.39947900	-0.33639600
C	-2.84311300	2.22253500	0.25678500
C	-3.63253900	3.33792000	0.57134700
C	-3.12230900	4.58837400	0.27464600
C	-1.85159600	4.74565800	-0.32129000
C	-1.05601500	3.65885800	-0.63965000
C	-2.02614100	0.26899900	-0.02188300
H	-4.60635800	3.21284600	1.03170200
H	-3.70516700	5.47354900	0.50616800
H	-1.48708700	5.74636700	-0.52766100
H	-0.07268000	3.77923200	-1.08103600
N	-3.09589900	0.87902900	0.43700300
N	-1.07076800	1.13205200	-0.50857700
C	-1.78501900	-1.19318800	0.11761700
O	-0.63918600	-1.59039100	0.31551900
C	-2.92594800	-2.13380300	0.05373400
C	-4.13793000	-1.80634000	-0.56622000
C	-2.74368800	-3.41382000	0.59356300
C	-5.15366800	-2.75252600	-0.64077100
H	-4.28156400	-0.82128700	-0.99254800
C	-3.76581200	-4.34932900	0.52929100
H	-1.79795400	-3.65559500	1.06580100
C	-4.97121200	-4.01894900	-0.09023800
H	-6.08883700	-2.50156800	-1.12939300
H	-3.62614000	-5.33495900	0.95980100
H	-5.76877900	-4.75273200	-0.14476200
C	0.18473900	0.85249800	-1.18175600
H	0.20130800	-0.19082700	-1.49768300
H	0.26329100	1.48770000	-2.06489800
C	1.39846300	1.14001000	-0.29560100
O	2.26375100	1.93827900	-0.61232400
N	1.40482600	0.42457700	0.86199500
H	0.77346000	-0.36798500	0.95124100
N	2.50390900	0.45739200	1.69096000
H	2.54505600	1.24142700	2.32749200
C	3.74319400	0.04108000	1.23230500
O	4.76951200	0.36734600	1.79688500
O	3.61076900	-0.76881800	0.18860300
C	4.77036100	-1.21292300	-0.58866500
C	4.12170400	-1.98060900	-1.73572200
H	3.52887700	-2.81548600	-1.35282700
H	3.46878800	-1.32299200	-2.31604300
H	4.89413000	-2.37740400	-2.39931900
C	5.53233000	0.00106400	-1.11307400
H	6.02548700	0.53774300	-0.30197900
H	6.28979700	-0.33037700	-1.82836200
H	4.84453600	0.68079600	-1.62352300
C	5.64289100	-2.13142700	0.26078400
H	6.44355000	-2.54296800	-0.36010700
H	6.08710400	-1.58671500	1.09407800
H	5.04973000	-2.96280900	0.65190300

4'b_F

C	-1.62449600	2.86521000	-0.69201400
C	-2.82639700	3.12511900	-0.00701200
C	-3.32481700	4.43345300	0.07139600
C	-2.59914900	5.43582600	-0.54444000
C	-1.39405100	5.15806900	-1.22652900
C	-0.88401900	3.87491700	-1.31443900
C	-2.48634400	1.02458200	0.14254700
H	-4.25090200	4.63915100	0.59711800
H	-2.95658200	6.45934600	-0.50351800
H	-0.85160000	5.97573600	-1.68950700
H	0.05059700	3.67200500	-1.82519600
N	-3.34430700	1.95349200	0.50208300
N	-1.42847300	1.50758700	-0.58901800
C	-2.54403100	-0.39859500	0.57836700
O	-1.48753700	-0.99542300	0.74455100
C	-3.85567000	-1.04854700	0.82119500
C	-5.05304200	-0.55433100	0.29100300
C	-3.86393100	-2.23565400	1.56490800
C	-6.24300100	-1.23917400	0.51099000
H	-5.05249300	0.36028500	-0.28843600
C	-5.05536300	-2.90997400	1.79071700
H	-2.92892900	-2.61353100	1.96423100
C	-6.24640300	-2.41160400	1.26258200
H	-7.16832700	-0.85643700	0.09407000
H	-5.05885500	-3.82419900	2.37461500
H	-7.17865200	-2.93926300	1.43632000
C	-0.33782500	0.76419800	-1.17923500
H	0.00392000	1.30566300	-2.06576400
H	-0.67821700	-0.21924800	-1.50615300
C	0.83874600	0.63411800	-0.21568700
O	1.10087800	1.47304400	0.63160700
N	1.57453600	-0.48048000	-0.43975100
H	1.24931800	-1.21985700	-1.07657600
N	2.69286300	-0.73293200	0.32135000
H	2.51927100	-0.87311100	1.30900400
C	3.84063400	-0.01544600	0.01941100
O	4.02973600	0.54918700	-1.03716500
O	4.67670900	-0.10971800	1.05427800
C	5.99716900	0.52582800	1.02944500
C	6.56148500	0.17877500	2.40305000
H	5.91957500	0.57712500	3.19324900
H	6.63927300	-0.90463300	2.52664000
H	7.55825600	0.61344700	2.51313300
C	6.84965100	-0.08756900	-0.07786400
H	6.43461000	0.13423500	-1.06125900
H	7.86099900	0.32443600	-0.02112800
H	6.91339800	-1.17196700	0.04888300
C	5.84180100	2.03694200	0.87696100
H	6.81781000	2.51358200	1.00262300
H	5.44781000	2.29601500	-0.10573800
H	5.16775000	2.42586900	1.64546900
S	0.05169900	-3.74173900	-1.49747000
O	0.31159500	-2.34812300	-2.07077100
C	1.48221200	-4.74127000	-1.95410900
H	1.40535100	-5.71536700	-1.46724300
H	1.46353400	-4.86688100	-3.03706900
H	2.39484400	-4.22489500	-1.64856500
C	0.37159900	-3.64897600	0.27543100
H	-0.34591500	-2.93745400	0.68763200
H	0.22140500	-4.63947300	0.70942100
H	1.39362700	-3.30353500	0.45058700

4"b_F

C	2.12311900	-2.31721300	-0.53961500
C	2.99514700	-1.47050800	0.16525400
C	3.94362600	-2.00715600	1.04731700
C	3.98215700	-3.38189900	1.18736300
C	3.09998200	-4.21916300	0.46995100
C	2.15557200	-3.70812300	-0.40333300
C	1.73591500	-0.20023900	-1.00922300
H	4.61512100	-1.35718500	1.59756900
H	4.70127900	-3.83227800	1.86323500
H	3.16222200	-5.29283100	0.61243400
H	1.47493000	-4.35779400	-0.94223000
N	2.73113800	-0.15818400	-0.15174100
N	1.32669900	-1.48483900	-1.29605600
C	1.01725000	1.00082300	-1.51971100
O	-0.02424400	0.86537400	-2.14531200
C	1.54256300	2.35861500	-1.20171500
C	2.90193600	2.65208500	-1.05158200
C	0.59696500	3.38286200	-1.07815500
C	3.30167500	3.95288900	-0.76331600

H	3.64010800	1.86756100	-1.15303300
C	0.99871100	4.67633600	-0.77154700
H	-0.45278600	3.14805500	-1.21287000
C	2.35360500	4.96198500	-0.61199200
H	4.35726600	4.17698900	-0.65201200
H	0.25764600	5.46072200	-0.65979000
H	2.67037100	5.97277700	-0.37573800
C	0.29868800	-1.95886900	-2.20207300
H	0.12490500	-1.21695800	-2.97701100
H	0.65536700	-2.87398800	-2.68064100
C	-1.04871200	-2.28804800	-1.56720700
O	-1.91424300	-2.82699200	-2.24040800
N	-1.18028400	-2.01944800	-0.24154100
H	-0.61791200	-1.31048500	0.24782300
N	-2.39228600	-2.28666600	0.36532300
H	-2.63718800	-3.26341500	0.43619000
C	-3.46002900	-1.41827900	0.27992100
O	-4.57754000	-1.74466600	0.63893700
O	-3.06688000	-0.23378600	-0.16999200
C	-3.88583900	0.96582900	-0.00792000
C	-2.92964900	2.07031700	-0.44543200
H	-2.03336200	2.04466900	0.18076400
H	-2.62666800	1.92538400	-1.48594900
H	-3.41395700	3.04568100	-0.34992600
C	-5.10531800	0.88578400	-0.92024200
H	-5.77281700	0.08202600	-0.60657400
H	-5.65007100	1.83341700	-0.88233700
H	-4.79412000	0.70887800	-1.95357900
C	-4.26899100	1.14639900	1.45904000
H	-4.75188600	2.11914300	1.58558000
H	-4.95697300	0.36825400	1.79020000
H	-3.37349300	1.12343000	2.08636100
S	0.53140600	0.30976900	2.45671500
O	-0.25735100	0.20680600	1.15368900
C	-0.64045600	0.93942200	3.67549800
H	-1.39986000	0.17045500	3.82281500
H	-0.11902500	1.13053200	4.61538800
H	-1.09895400	1.85389000	3.29211300
C	1.55701000	1.78480700	2.31412300
H	2.01312500	1.99304200	3.28403300
H	2.32139700	1.56002800	1.56891100
H	0.93847500	2.62183800	1.98123300

4"'b_F

C	2.22677400	-2.45870100	-0.34791300
C	3.12770500	-1.69618300	0.41522000
C	3.94960200	-2.31521000	1.36775000
C	3.83537100	-3.68372000	1.51918800
C	2.92385100	-4.43578600	0.74527500
C	2.10349900	-3.84350400	-0.19820300
C	2.09967300	-0.31995500	-0.85821500
H	4.64219000	-1.72891300	1.96161100
H	4.45346800	-4.19742800	2.24774400
H	2.86071400	-5.50764400	0.90032300
H	1.39858000	-4.42829300	-0.77846500
N	3.02580000	-0.36958400	0.07428500
N	1.57847900	-1.55924600	-1.16579700
C	1.56388400	0.94022600	-1.44197500
O	0.57403700	0.90402300	-2.15907900
C	2.18909800	2.24034900	-1.06750200
C	3.55664400	2.40444100	-0.82495400
C	1.33300000	3.34522000	-0.98541900
C	4.05496300	3.66140800	-0.49839700
H	4.22464000	1.55543800	-0.89037600
C	1.83161400	4.59341300	-0.63737100
H	0.27508800	3.20459500	-1.17961900
C	3.19524800	4.75251200	-0.39526600
H	5.11749100	3.78875300	-0.32085600
H	1.15957500	5.44124900	-0.55758700
H	3.58871200	5.72797300	-0.12807500
C	0.58457300	-1.91709500	-2.15853700
H	0.78072800	-2.94330200	-2.47903600
H	0.67768300	-1.27190300	-3.02796000
C	-0.87025300	-1.85486000	-1.70638700
O	-1.76270900	-1.98465200	-2.53067600
N	-1.09019300	-1.74488700	-0.37138600
H	-0.39343300	-1.44571900	0.32586300
N	-2.39070700	-1.68582600	0.07908100
H	-2.92912000	-2.53450400	-0.02420100
C	-3.07303400	-0.49414500	-0.02936300
O	-2.53446900	0.58212800	-0.20869500
O	-4.37269800	-0.72499900	0.15681700
C	-5.34532500	0.37149300	0.17838300
C	-6.65674200	-0.35080800	0.46839500
H	-6.86640900	-1.09318700	-0.30607800
H	-6.61185200	-0.85611600	1.43677300
H	-7.47682800	0.37117600	0.48990800
C	-5.01111000	1.35323700	1.29897800
H	-4.10049300	1.91017400	1.07708400
H	-5.83530300	2.06286300	1.41222100
H	-4.88572900	0.82090300	2.24646100
C	-5.38711800	1.04606600	-1.18995400
H	-6.18628300	1.79220000	-1.20014900
H	-4.44116500	1.54221300	-1.40933600
H	-5.59456700	0.30806400	-1.96976500
S	0.19266700	0.87015500	1.60811300
O	0.20388800	-0.64532500	1.81376900
C	1.63046900	1.50939600	2.48442700
H	2.50398400	1.10907500	1.96666600
H	1.62379300	2.59947400	2.41502100
H	1.61018800	1.18223900	3.52600000
C	-1.09106400	1.51976600	2.69171500
H	-1.03153400	2.61006000	2.69923400
H	-2.04574900	1.20503100	2.27014100
H	-0.95701700	1.11510900	3.69700700

4""b_F

C	-0.18749200	2.75644800	-0.52991200
C	-1.30895700	3.51747200	-0.15027800
C	-1.28145100	4.91539400	-0.26081400
C	-0.12905600	5.49883800	-0.75304400
C	0.98777400	4.71987000	-1.12835900
C	0.98247700	3.34035500	-1.02485200
C	-1.81982100	1.47451300	0.18932200
H	-2.14181200	5.50798400	0.03085300
H	-0.07352300	6.57759400	-0.85359700
H	1.87591700	5.21803000	-1.50271300
H	1.84970900	2.74975300	-1.29817800
N	-2.31687300	2.68720600	0.29247000
N	-0.54033600	1.44563500	-0.30920500
C	-2.49198300	0.23326100	0.66351300
O	-1.79457600	-0.66936500	1.11286400
C	-3.96830800	0.10800200	0.58393400
C	-4.75224100	0.92040000	-0.24372000
C	-4.57370200	-0.91661200	1.32365000
C	-6.12383000	0.70744800	-0.32551400
H	-4.29052600	1.71287500	-0.81931200
C	-5.94362300	-1.12079900	1.24407500
H	-3.95635500	-1.54162100	1.95970800
C	-6.71982400	-0.30897500	0.41693700
H	-6.72833900	1.33469300	-0.97172500
H	-6.40839000	-1.91172000	1.82286100
H	-7.79074800	-0.47093400	0.34988500
C	0.28365600	0.29334200	-0.59459200
H	-0.32851700	-0.56054900	-0.88502400
H	0.92668200	0.53550600	-1.44640800

C	1.19057500	-0.05262900	0.58071200
O	1.60451200	0.78920100	1.36313300
N	1.53994400	-1.36109200	0.61577800
H	1.17030700	-2.03302100	-0.06894900
N	2.54668900	-1.77727600	1.46274000
H	2.27409800	-1.88869800	2.43094000
C	3.81604200	-1.23500700	1.32736000
O	4.61185900	-1.24395800	2.24707200
O	4.01537000	-0.79918300	0.08817200
C	5.17031000	0.03174700	-0.25448500
C	4.90767400	0.37280200	-1.71776100
H	4.87229200	-0.53628000	-2.32411700
H	3.95604000	0.90061400	-1.82346800
H	5.70631700	1.01464700	-2.09802200
C	5.15738600	1.29224300	0.60568700
H	5.35577800	1.05670100	1.65221400
H	5.92640000	1.98320500	0.25002100
H	4.18259900	1.78242900	0.53188400
C	6.46159700	-0.76800300	-0.10838900
H	7.29551500	-0.18082900	-0.50313700
H	6.65876400	-1.00489900	0.93696600
H	6.39693600	-1.69879100	-0.67910500
S	-0.71942200	-3.99887900	-0.69578100
O	0.17631200	-2.90168500	-1.27538100
C	-2.40223500	-3.35511600	-0.73228900
H	-3.09649700	-4.15617800	-0.47083300
H	-2.45095900	-2.55790800	0.01102500
H	-2.61698600	-2.96243300	-1.72861500
C	-0.89143200	-5.23044100	-2.00125200
H	0.08473500	-5.69408800	-2.14589800
H	-1.61564500	-5.98274900	-1.68327400
H	-1.21803900	-4.74000100	-2.92043400

4'b_G

C	-1.45341800	2.78098000	-1.54798500
C	-2.46426600	3.28386100	-0.70763400
C	-2.77261300	4.65272900	-0.71428800
C	-2.05251600	5.46875700	-1.56519800
C	-1.03862500	4.94829200	-2.40060800
C	-0.71937200	3.60273800	-2.40966400
C	-2.35717100	1.18485200	-0.33877500
H	-3.54967400	5.04477700	-0.06716100
H	-2.26236200	6.53270100	-1.59560000
H	-0.49019400	5.62488100	-3.04753400
H	0.07037000	3.21494100	-3.04307400
N	-3.01281300	2.26293600	0.03486100
N	-1.40910400	1.42869900	-1.30515400
C	-2.51260000	-0.15548900	0.28410400
O	-1.56326800	-0.93074100	0.25485200
C	-3.78261500	-0.52512900	0.95816200
C	-5.01011400	0.07619200	0.65773900
C	-3.73020400	-1.56705500	1.89310600
C	-6.16804300	-0.36175300	1.29091200
H	-5.05614900	0.87765600	-0.06862200
C	-4.88661000	-1.99208300	2.53158900
H	-2.77318800	-2.02829600	2.11219300
C	-6.10739200	-1.38963000	2.22895800
H	-7.11961800	0.10089800	1.05219700
H	-4.83965400	-2.79057300	3.26418100
H	-7.01311200	-1.72377900	2.72459800
C	-0.47416400	0.50171500	-1.90564800
H	-0.17981100	0.89995100	-2.88028600
H	-0.94220100	-0.46909300	-2.06917700
C	0.77334200	0.36483800	-1.03433700
O	1.16532100	1.27793300	-0.31673600
N	1.40221600	-0.81968200	-1.17293600
H	0.94753100	-1.60018700	-1.66321400
N	2.50434000	-1.10042000	-0.38796100
H	2.28501600	-1.15576800	0.61908000
C	3.67254900	-0.44426100	-0.71283200
O	3.90916700	0.07348900	-1.78662900
O	4.49775000	-0.52221800	0.34018400
C	5.78702900	0.16263600	0.35040800
C	6.31752400	-0.14199400	1.74822600
H	5.63385600	0.24383900	2.50955700
H	6.42882600	-1.22006000	1.89186600
H	7.29411100	0.32939300	1.88584700
C	6.70741000	-0.42528100	-0.71647800
H	6.31995300	-0.22948600	-1.71644500
H	7.69966000	0.02563600	-0.62539300
H	6.80757700	-1.50539800	-0.57643700
C	5.57800900	1.66533400	0.17424100
H	6.52978600	2.18277500	0.32281600
H	5.20354900	1.89652600	-0.82298800
H	4.86458100	2.03457900	0.91688800
S	-0.57168700	-3.96131500	-1.70561700
O	-0.17983700	-2.71175700	-2.49623300
C	-2.29800700	-3.75123900	-1.23296700
H	-2.66381800	-4.68396300	-0.79885500
H	-2.32523800	-2.95244900	-0.49048500
H	-2.88249200	-3.47607200	-2.11368900
C	-0.80115300	-5.25715300	-2.93860100
H	0.17337200	-5.45838100	-3.38427800
H	-1.17697900	-6.15609400	-2.44640200
H	-1.50143900	-4.91047300	-3.70135100
S	1.65605500	0.36093500	2.81797900
O	1.58634200	-1.06260800	2.26999900
C	1.67500400	0.17828500	4.61316400
H	2.61723200	-0.30090200	4.88117300
H	1.61720900	1.16529000	5.07609400
H	0.83384600	-0.44499000	4.92405700
C	0.00215300	1.06342400	2.65793300
H	-0.04196300	2.00128100	3.21562000
H	-0.14711300	1.25337100	1.59496300
H	-0.73243700	0.34863600	3.03572400

4"b_G

C	1.15793800	-2.37809000	-1.34993500
C	2.05589300	-2.90520800	-0.40489300
C	1.95680500	-4.24762200	-0.01386700
C	0.96114100	-5.01426500	-0.59324500
C	0.07251100	-4.46942000	-1.54569200
C	0.15213300	-3.14533100	-1.94318400
C	2.58015400	-0.85229700	-0.65308400
H	2.64240800	-4.66018100	0.71822800
H	0.85423900	-6.05672300	-0.31296300
H	-0.69773200	-5.10444100	-1.97025700
H	-0.54293900	-2.72883600	-2.66379700
N	2.93859400	-1.93101000	0.00339400
N	1.51073600	-1.05609200	-1.49862400
C	3.14240200	0.50487200	-0.40913900
O	2.45488500	1.48476200	-0.66298900
C	4.50130100	0.64864600	0.17882100
C	5.48955100	-0.33614700	0.07015700
C	4.79679600	1.85895300	0.81797100
C	6.75418600	-0.11021100	0.60319500
H	5.26845700	-1.27227100	-0.42695300
C	6.05559100	2.07445800	1.36138600
H	4.02528800	2.61818600	0.88571600
C	7.03633300	1.08900100	1.25293000
H	7.52033100	-0.87276600	0.51229800
H	6.27458200	3.00909400	1.86667100
H	8.02155200	1.25685000	1.67596000
C	0.90099400	-0.15692500	-2.45825700
H	1.56895900	0.68148200	-2.64516000
H	0.75665000	-0.69058000	-3.40059600

C	-0.45610700	0.41215800	-2.05647800
O	-1.15482900	0.96003600	-2.89745400
N	-0.79951100	0.25725900	-0.75812500
H	-0.16085800	-0.07297300	-0.01988200
N	-2.00435300	0.75104300	-0.30917100
H	-2.81552300	0.13449400	-0.43552100
C	-2.23378500	2.09307100	-0.17055600
O	-3.35588300	2.53424100	0.03382700
O	-1.10391900	2.79218300	-0.23385500
C	-1.10119700	4.25347900	-0.20857000
C	0.37935500	4.58424900	-0.36924500
H	0.95948400	4.15346600	0.45096500
H	0.76255600	4.18342300	-1.31119000
H	0.51934100	5.66825800	-0.36593100
C	-1.90497600	4.78999000	-1.39029000
H	-2.96758100	4.57528300	-1.27386600
H	-1.76913300	5.87271600	-1.45980300
H	-1.54890000	4.33714100	-2.31996200
C	-1.62493400	4.75737000	1.13356600
H	-1.48564700	5.84049600	1.19268700
H	-2.68427300	4.52984000	1.25177400
H	-1.06715000	4.29554200	1.95341200
S	-0.36721700	-1.44865100	2.44557300
O	0.49336200	-0.57689100	1.53512200
C	-1.31638200	-2.56529400	1.39288300
H	-0.60296000	-3.20783200	0.87455800
H	-1.95540600	-3.17409000	2.03686000
H	-1.92458600	-2.00550200	0.67646800
C	-1.74163000	-0.41193200	2.98918100
H	-2.46590300	-1.02839700	3.52520400
H	-1.33688300	0.34945600	3.65685800
H	-2.19462000	0.05489200	2.11121900
S	-4.98750600	-1.05479800	0.71444000
O	-3.98938600	-1.23029500	-0.43327200
C	-6.24324700	-2.32465900	0.47203400
H	-5.76622600	-3.29169900	0.63389000
H	-7.03980100	-2.17749900	1.20398000
H	-6.63261200	-2.25866400	-0.54584700
C	-5.97862000	0.38834400	0.28653100
H	-6.74619400	0.53565400	1.04902100
H	-5.28915300	1.23627300	0.26641400
H	-6.42952800	0.24125200	-0.69733200
4"'b_G			
C	-1.81152400	2.88938100	-0.14285300
C	-2.96776800	2.55355800	0.58255400
C	-3.44718700	3.40858100	1.58520900
C	-2.74389800	4.57350300	1.82457100
C	-1.58072700	4.89420700	1.08960700
C	-1.09153100	4.06388900	0.09700600
C	-2.63534300	0.95585000	-0.79958600
H	-4.33925700	3.15305800	2.14664600
H	-3.08485600	5.25945000	2.59260300
H	-1.05480500	5.81635700	1.31325200
H	-0.18964400	4.31225700	-0.45138700
N	-3.45793100	1.34523600	0.15041300
N	-1.61635700	1.85521900	-1.03153100
C	-2.70013000	-0.37223600	-1.46917000
O	-1.77137700	-0.74473200	-2.17217600
C	-3.85811000	-1.26786200	-1.18946300
C	-5.15907700	-0.80586400	-0.96501000
C	-3.59870800	-2.64342300	-1.17513500
C	-6.18279400	-1.71524300	-0.72134500
H	-5.36605700	0.25633900	-0.97962600
C	-4.61950600	-3.54633100	-0.90947000
H	-2.58631100	-2.98888200	-1.35528200
C	-5.91420900	-3.08135400	-0.68282400
H	-7.19251600	-1.35452700	-0.55636200
H	-4.40875700	-4.61002000	-0.87949400
H	-6.71388400	-3.78564400	-0.47739400
C	-0.55505600	1.81124800	-2.01827200
H	-0.31955500	2.83784800	-2.30934800
H	-0.89631900	1.28248900	-2.90421400
C	0.75130600	1.15928700	-1.57652700
O	1.64956600	1.02820100	-2.39762100
N	0.84888800	0.82522000	-0.27018500
H	0.06033600	0.78278600	0.38943400
N	2.01100500	0.25753200	0.19851900
H	2.80825700	0.89745000	0.32790700
C	2.17910300	-1.08818000	0.07848500
O	1.30797700	-1.87169000	-0.26109500
O	3.43772300	-1.40434400	0.43065200
C	3.90218400	-2.79250800	0.41767000
C	5.33789900	-2.67295900	0.91838000
H	5.93522400	-2.05637900	0.24059200
H	5.36234000	-2.22527600	1.91578700
H	5.79573900	-3.66378000	0.97158000
C	3.06996300	-3.64193800	1.37601000
H	2.06310100	-3.79751500	0.98880700
H	3.55078800	-4.61549900	1.50493200
H	3.00936400	-3.15811900	2.35539300
C	3.87353300	-3.33454700	-1.00905700
H	4.32315900	-4.33127300	-1.02559700
H	2.85167900	-3.40357300	-1.38262500
H	4.45471100	-2.68816900	-1.67338600
S	-1.46388500	-1.17268900	1.50441000
O	-0.82726700	0.17622600	1.83749900
C	-3.05551400	-1.20146300	2.34754600
H	-3.66053400	-0.42308600	1.87861000
H	-3.51833200	-2.17820500	2.18944600
H	-2.91659700	-1.00036200	3.41168800
C	-0.60799200	-2.40267200	2.50268300
H	-1.12575700	-3.35940800	2.40830200
H	0.39966800	-2.48763500	2.09599000
H	-0.58184700	-2.07508100	3.54400700
S	5.22467800	2.05594600	-0.44861600
O	3.93053700	2.25566500	0.33639500
C	4.90591500	0.77649700	-1.68368600
H	4.01479100	1.08069000	-2.23610900
H	5.77363400	0.70574700	-2.34226700
H	4.71012800	-0.17542300	-1.18608200
C	6.30941100	1.08802600	0.61971900
H	7.17952600	0.75875400	0.04803200
H	6.62620700	1.72841100	1.44338200
H	5.74572900	0.23237300	0.99807600
4""b_G			
C	-0.96054900	3.04218100	-0.41394600
C	-2.01126000	3.54051600	0.37870600
C	-2.09176300	4.91203500	0.66085800
C	-1.11428800	5.73537700	0.13462800
C	-0.06510300	5.21792000	-0.65730100
C	0.03401300	3.86867000	-0.94577100
C	-2.30877700	1.43334200	0.23285000
H	-2.89833400	5.30185800	1.27231400
H	-1.14696900	6.80158400	0.33235900
H	0.68724800	5.89820700	-1.04255700
H	0.85242200	3.47538500	-1.53832400
N	-2.84174000	2.51084600	0.76598300
N	-1.17669500	1.68728000	-0.50219400
C	-2.77944100	0.04266400	0.47855900
O	-1.95056100	-0.86027700	0.49178800
C	-4.22041600	-0.22158600	0.71381000
C	-5.22551900	0.66543500	0.31136900
C	-4.56878000	-1.44032600	1.31037800
C	-6.56139100	0.33471700	0.50996000

H	-4.96256100	1.60698900	-0.15447400
C	-5.90303100	-1.76137500	1.51607800
H	-3.78223500	-2.12217700	1.61514100
C	-6.90063900	-0.87311800	1.11467600
H	-7.33807600	1.02172400	0.19181200
H	-6.16724200	-2.70140700	1.98834500
H	-7.94455600	-1.12326400	1.27373200
C	-0.35615200	0.75117600	-1.23655300
H	-0.95788900	-0.07295800	-1.61961900
H	0.07243600	1.27299500	-2.09758100
C	0.79827100	0.23853200	-0.38212800
O	1.30488000	0.91822400	0.50109700
N	1.23146400	-0.98437000	-0.75445700
H	0.75679700	-1.51251400	-1.49713500
N	2.38417600	-1.50987000	-0.20376100
H	2.27519600	-1.94456400	0.72311400
C	3.56658000	-0.81998600	-0.34967800
O	4.50405800	-0.98925200	0.41447800
O	3.54793900	-0.02953200	-1.42096400
C	4.55690300	1.00983400	-1.61689000
C	4.04416900	1.73891500	-2.85481800
H	3.97139800	1.05110600	-3.70157700
H	3.05596100	2.16783900	-2.66630000
H	4.73016900	2.54700300	-3.12124100
C	4.56935300	1.94332100	-0.40880300
H	4.96199200	1.43886800	0.47511300
H	5.19962400	2.80986900	-0.62719900
H	3.55373600	2.28844800	-0.19686700
C	5.92016900	0.37854700	-1.88546900
H	6.63377000	1.15985200	-2.16222300
H	6.28900200	-0.14154200	-1.00165000
H	5.85132900	-0.33217800	-2.71409800
S	-1.06541800	-3.50341400	-2.20859600
O	-0.43428000	-2.18416300	-2.65807100
C	-2.77300600	-3.13127700	-1.76768100
H	-3.30020300	-4.06795600	-1.57562400
H	-2.74091000	-2.52401000	-0.86158200
H	-3.24563600	-2.57916700	-2.58305800
C	-1.39169800	-4.42582900	-3.72334500
H	-0.42766700	-4.66672100	-4.17206500
H	-1.92360400	-5.34551600	-3.47228900
H	-1.98197600	-3.80830400	-4.40324700
S	3.22385200	-1.83196200	3.29735900
O	2.17895000	-2.55047800	2.44465300
C	2.75200400	-0.09187400	3.31336300
H	3.46651200	0.46505900	3.92285300
H	2.77092200	0.25840600	2.27975500
H	1.74058800	0.01053400	3.71287200
C	2.79971400	-2.21261400	5.00973400
H	3.00299300	-3.27131900	5.17440000
H	3.42496300	-1.60890600	5.67100900
H	1.74136400	-2.00176200	5.17733000
4'b_H			
C	-1.70106000	2.96028200	-1.15820100
C	-2.79775400	3.24533500	-0.32524900
C	-3.25167000	4.56287100	-0.17934800
C	-2.58907900	5.55078400	-0.88263400
C	-1.49118700	5.24782600	-1.71796600
C	-1.02717600	3.95425100	-1.87262500
C	-2.48646800	1.13661700	-0.22451500
H	-4.09348300	4.78948900	0.46336800
H	-2.91174300	6.58097300	-0.79281900
H	-0.99594100	6.05346500	-2.24651500
H	-0.17674800	3.73305800	-2.50473200
N	-3.27141400	2.08230600	0.24021200
N	-1.51945900	1.60024400	-1.07935500
C	-2.53964500	-0.28728200	0.20605300
O	-1.50308600	-0.92880900	0.23833900
C	-3.83803500	-0.88843100	0.59840500
C	-5.05735000	-0.41950000	0.10050300
C	-3.81388700	-2.00873100	1.43700300
C	-6.23880800	-1.06956600	0.43839000
H	-5.08194400	0.43858700	-0.55770700
C	-4.99688200	-2.64322100	1.78659200
H	-2.86336600	-2.36850500	1.81232400
C	-6.21057800	-2.17505800	1.28389600
H	-7.18053800	-0.71179800	0.04087200
H	-4.97619400	-3.50131600	2.44708500
H	-7.13445400	-2.67448900	1.55035700
C	-0.51268400	0.84023400	-1.78534400
H	-0.26243500	1.37376800	-2.70449500
H	-0.90730300	-0.13490700	-2.06672100
C	0.76078200	0.69788500	-0.95518000
O	1.14320300	1.57793400	-0.19994300
N	1.41982900	-0.45602400	-1.17627300
H	0.96280400	-1.23398200	-1.66701800
N	2.54919700	-0.75434200	-0.44736500
H	2.38568200	-0.85706300	0.56221900
C	3.73696200	-0.19167800	-0.84534900
O	3.93569200	0.31553100	-1.92923400
O	4.62236200	-0.34015800	0.14156400
C	6.00767700	0.11549000	0.02002900
C	6.60362500	-0.27660900	1.36834900
H	6.07594700	0.22467800	2.18307800
H	6.53501500	-1.35634400	1.51878600
H	7.65578100	0.01341200	1.40554900
C	6.71167300	-0.62833500	-1.11125800
H	6.32394600	-0.33426300	-2.08568600
H	7.77985600	-0.40098200	-1.07637500
H	6.58796800	-1.70692300	-0.98755500
C	6.04700900	1.62986000	-0.16294500
H	7.08484600	1.96791500	-0.11102200
H	5.63079800	1.92651700	-1.12501900
H	5.48704800	2.12229400	0.63596600
S	-0.41589300	-3.56903100	-1.35058200
O	0.00843700	-2.55480500	-2.40872100
C	-2.19160000	-3.76510100	-1.55002300
H	-2.52982700	-4.57028700	-0.89641100
H	-2.64812000	-2.82475200	-1.24544900
H	-2.40733000	-3.98449100	-2.59622700
C	0.09375900	-5.16966100	-1.99340300
H	1.18297200	-5.16961100	-2.01268800
H	-0.26695700	-5.94653900	-1.31785000
H	-0.31199700	-5.29889100	-2.99736200
S	1.61872700	0.38167200	2.94603400
O	1.71818500	-0.97153400	2.25264000
C	1.62947400	0.00962200	4.70628100
H	2.61748700	-0.38476200	4.94079500
H	1.45373700	0.93311600	5.25939800
H	0.85770600	-0.73131300	4.91825400
C	-0.09915700	0.89602400	2.80364600
H	-0.24537800	1.78765800	3.41498200
H	-0.26182600	1.13036000	1.75243400
H	-0.74442400	0.07968400	3.13061500
4"b_H			
C	-1.00185400	-2.62989100	0.98265500
C	-1.79461600	-2.95711500	-0.13032600
C	-1.57421600	-4.15360400	-0.82390800
C	-0.56756400	-4.98517600	-0.36696000
C	0.21467700	-4.64436400	0.75761600
C	0.01471500	-3.46400400	1.45211500
C	-2.48901300	-1.06627000	0.57596600
H	-2.17602000	-4.41179600	-1.68654000
H	-0.37057800	-5.91894400	-0.87914800

H	0.99536700	-5.32226800	1.08026200
H	0.62717300	-3.20362700	2.30622800
N	-2.72115500	-1.96410600	-0.35220800
N	-1.46011500	-1.40933200	1.42141800
C	-3.16300400	0.25929400	0.63950000
O	-2.60038900	1.19056300	1.18783700
C	-4.49080800	0.42826900	-0.00731000
C	-5.43282400	-0.60226200	-0.06569100
C	-4.80884600	1.69034400	-0.51898100
C	-6.68279700	-0.36730200	-0.62714700
H	-5.19605100	-1.57776100	0.33763200
C	-6.04863800	1.91413900	-1.10135100
H	-4.07272000	2.48331100	-0.46632500
C	-6.98807000	0.88568400	-1.15231400
H	-7.41726600	-1.16257400	-0.65739800
H	-6.28352900	2.88730000	-1.51467800
H	-7.95809800	1.06098500	-1.60199800
C	-0.99778700	-0.75087400	2.62500800
H	-1.76458100	-0.07352200	2.99167100
H	-0.82960200	-1.50799100	3.39312800
C	0.29613700	0.04793200	2.50321700
O	0.81264300	0.49558600	3.51509300
N	0.79717100	0.17460600	1.25985200
H	0.27715200	-0.07819900	0.41118700
N	1.97669200	0.84790400	1.04552800
H	2.80543600	0.26502200	0.89421600
C	2.00581500	2.10963800	0.52318600
O	3.03850200	2.58550500	0.08081700
O	0.82227300	2.70141200	0.58567200
C	0.56792300	3.99889500	-0.04710700
C	-0.91325800	4.22202900	0.23758400
H	-1.50969400	3.40392200	-0.17165300
H	-1.09402500	4.27899000	1.31324800
H	-1.23769400	5.15884300	-0.22012700
C	1.41142800	5.08562900	0.61204200
H	2.47137900	4.95157900	0.40081300
H	1.09607200	6.05936300	0.22923900
H	1.25880000	5.07793000	1.69402900
C	0.81274100	3.89404500	-1.54925600
H	0.50034000	4.82519800	-2.02748400
H	1.86631400	3.72539400	-1.77123200
H	0.22083900	3.07725200	-1.96956100
S	0.68719600	-0.75462500	-2.41268300
O	-0.17048200	-0.11293000	-1.33266800
C	1.62828000	-2.05586800	-1.60434600
H	0.91524400	-2.82670600	-1.31219600
H	2.33995300	-2.46049400	-2.32603400
H	2.14661800	-1.64986200	-0.73254300
C	2.04044400	0.39339200	-2.71401200
H	2.75349100	-0.07569400	-3.39329400
H	1.60886700	1.27888800	-3.17870500
H	2.51223400	0.65094100	-1.76438600
S	5.08463400	-0.70197600	-0.55722400
O	4.10943600	-0.96757600	0.58482000
C	6.40961500	-1.89625900	-0.34372200
H	5.98138500	-2.88082400	-0.52710800
H	7.18806600	-1.68298100	-1.07743200
H	6.79424100	-1.82245900	0.67403900
C	5.97782100	0.78872500	-0.10082000
H	6.74110500	0.98215200	-0.85573600
H	5.23703500	1.58969900	-0.08795700
H	6.42161500	0.65042000	0.88584600
4"'b_H			
C	-1.88204000	2.75288200	-0.10144300
C	-3.03566400	2.41644200	0.62619800
C	-3.52435300	3.27786500	1.61621700
C	-2.83523700	4.45497700	1.83833400
C	-1.67795400	4.77994000	1.09719700
C	-1.17930700	3.93989800	0.11733200
C	-2.67938500	0.80410300	-0.72841500
H	-4.41169000	3.02149200	2.18193600
H	-3.18375500	5.14683700	2.59532700
H	-1.16514100	5.71123300	1.30472700
H	-0.28308200	4.19244300	-0.43521200
N	-3.51266400	1.19724000	0.20852600
N	-1.66808400	1.70450500	-0.96655500
C	-2.73737100	-0.53107000	-1.38041400
O	-1.75310200	-0.97118400	-1.94763500
C	-3.98991800	-1.32671100	-1.27361900
C	-5.25692000	-0.74230700	-1.34428100
C	-3.86889900	-2.71438500	-1.15630700
C	-6.39182700	-1.54469200	-1.30795100
H	-5.35594700	0.33046900	-1.44316100
C	-5.00534200	-3.50988400	-1.09215100
H	-2.88221200	-3.15854200	-1.10319700
C	-6.26769900	-2.92518200	-1.17348400
H	-7.37243900	-1.09102600	-1.38229100
H	-4.90718900	-4.58277800	-0.98168500
H	-7.15489200	-3.54605500	-1.13343500
C	-0.63936300	1.66586100	-1.98379800
H	-0.43072100	2.69071100	-2.29717000
H	-0.99953600	1.12522700	-2.85466400
C	0.69414100	1.04350000	-1.58885000
O	1.54957400	0.89201800	-2.44892100
N	0.87125600	0.75673900	-0.28403400
H	0.12175500	0.76566200	0.41769900
N	2.06466100	0.23496200	0.15035600
H	2.86707100	0.87458600	0.18042600
C	2.24714500	-1.11536200	0.14251100
O	1.37023700	-1.93001900	-0.06617800
O	3.52407900	-1.38169000	0.43780300
C	4.02021600	-2.75636200	0.53797200
C	5.49406800	-2.55440700	0.87385600
H	6.00439500	-2.02046100	0.06843500
H	5.60475300	-1.98848400	1.80163800
H	5.97833900	-3.52469900	0.99993100
C	3.30931600	-3.49221600	1.66974300
H	2.26363300	-3.67993300	1.42864300
H	3.80358700	-4.45221200	1.83640100
H	3.36682000	-2.91379100	2.59521900
C	3.87216700	-3.46763600	-0.80402200
H	4.38557200	-4.43084500	-0.75403700
H	2.82547900	-3.64223400	-1.04868600
H	4.33175800	-2.87728800	-1.60077300
S	-1.41469500	-0.99314900	1.88429400
O	-0.74529400	0.37413000	1.94825100
C	-2.87189200	-0.86249100	2.92672100
H	-3.55465900	-0.18762800	2.41027300
H	-3.32107300	-1.85139700	3.02709000
H	-2.57844200	-0.45965600	3.89689800
C	-0.42395700	-2.06769500	2.92934300
H	-0.92699900	-3.03123400	3.02186700
H	0.53199200	-2.19213000	2.42183700
H	-0.29422100	-1.59362800	3.90291000
S	5.26972300	2.06449400	-0.83709400
O	4.11642600	2.16353500	0.15425800
C	4.88255500	0.68630300	-1.92711300
H	3.94013200	0.92872900	-2.41951300
H	5.68939000	0.59038800	-2.65465900
H	4.77089700	-0.22150400	-1.33260300
C	6.62125800	1.29394100	0.06799000
H	7.41742300	1.04602500	-0.63530600
H	6.97682200	2.01903400	0.79870700
H	6.23776500	0.40084500	0.56316100

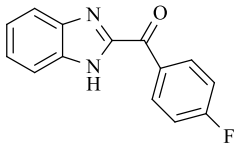
4""b_H

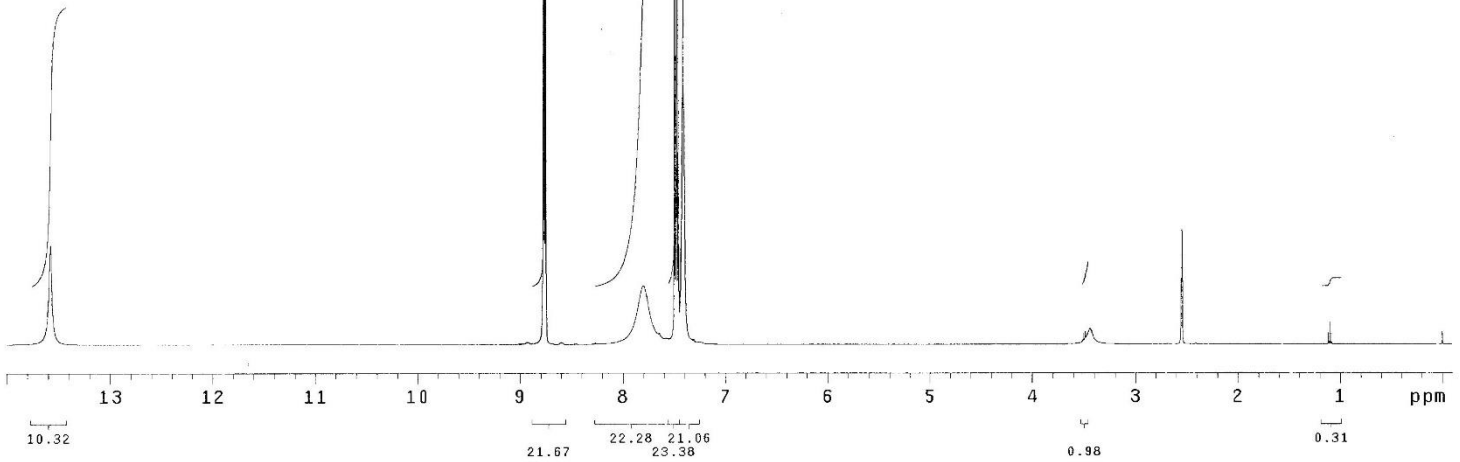
C	-0.89168900	3.13530600	-0.85519200
C	-2.06547900	3.56575600	-0.21127700
C	-2.30670500	4.93263300	-0.01972900
C	-1.35885600	5.82278900	-0.48690500
C	-0.18502300	5.37499600	-1.13239600
C	0.07122900	4.03035500	-1.32907600
C	-2.14407200	1.43362100	-0.26139400
H	-3.20811300	5.27016900	0.47672800
H	-1.51200100	6.88686100	-0.35480700
H	0.53669900	6.10553700	-1.47712900
H	0.98055400	3.69642700	-1.81215600
N	-2.83127600	2.47803300	0.14339800
N	-0.96493100	1.76321600	-0.88023700
C	-2.52235900	0.02044700	0.00909700
O	-1.63831700	-0.81153900	0.12685000
C	-3.95318800	-0.34972000	0.14615600
C	-4.97963000	0.37585800	-0.46602100
C	-4.25569700	-1.51627600	0.85820400
C	-6.29407700	-0.06611700	-0.36616700
H	-4.75166800	1.27377800	-1.02440000
C	-5.57043500	-1.94364500	0.97059100
H	-3.45173700	-2.07443800	1.32260400
C	-6.59073200	-1.21971300	0.35458300
H	-7.08694900	0.48995900	-0.85098000
H	-5.80172400	-2.84067800	1.53168100
H	-7.61723900	-1.55666700	0.43725400
C	0.02795800	0.87555000	-1.44077500
H	-0.45144400	0.01595000	-1.90648800
H	0.56942800	1.41467400	-2.22081600
C	1.03344300	0.43301700	-0.38159300
O	1.36938300	1.16724900	0.53577600
N	1.53370400	-0.79741000	-0.59431700
H	1.09678800	-1.43206800	-1.27353800
N	2.42641400	-1.35341300	0.29648400
H	2.01761600	-1.62727700	1.19885600
C	3.73256100	-0.93674500	0.33725600
O	4.45864700	-1.22708500	1.27009300
O	4.07084200	-0.25184600	-0.74791000
C	5.39800500	0.34480800	-0.90754100
C	5.28457300	1.03905200	-2.26114500
H	5.06202000	0.31368600	-3.04689000
H	4.49232000	1.79079700	-2.24189000
H	6.22795800	1.53385400	-2.50085800
C	5.64589700	1.36654600	0.19816100
H	5.74157500	0.88655400	1.17137600
H	6.57226200	1.90470800	-0.01655900
H	4.82909800	2.09139400	0.23444900
C	6.46703100	-0.74281500	-0.95164200
H	7.42218500	-0.29035500	-1.22904600
H	6.57967600	-1.23106700	0.01547500
H	6.21241700	-1.49304800	-1.70405500
S	-0.65669600	-3.49963900	-1.47502200
O	0.12096300	-2.50232300	-2.32910900
C	-2.37504000	-3.34585900	-1.97969900
H	-2.95039300	-4.12929700	-1.48429000
H	-2.71597300	-2.36755800	-1.64511800
H	-2.43733600	-3.43610700	-3.06470300
C	-0.32418100	-5.11037700	-2.20272100
H	0.72714000	-5.32930800	-2.02036900
H	-0.95249000	-5.85233600	-1.70818800
H	-0.53051600	-5.06627500	-3.27272800
S	0.78987900	-1.02789900	3.76370300
O	1.01129700	-2.04654000	2.65201100
C	2.16339500	0.13158800	3.66099100
H	2.00524100	0.91353600	4.40547200
H	3.06800000	-0.42936800	3.89277300
H	2.20294100	0.54308700	2.65039300
C	-0.50960500	0.07735500	3.18806100
H	-1.41945500	-0.51602400	3.10445700
H	-0.64268700	0.86223000	3.93449300
H	-0.21896500	0.49250000	2.22213

1a

STANDARD 1H
67808
MM382
Milen Matyas
2007.02.21. (BB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 11999.4 Hz
16 repetitions
OBSERVE H1, 499.5268107 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes

INDEX	FREQUENCY	PPM	HEIGHT
1	6783.169	13.579	17.2
2	4387.354	8.783	11.8
3	4384.607	8.778	77.4
4	4382.410	8.773	33.0
5	4378.748	8.766	87.4
6	4375.636	8.760	82.8
7	4371.974	8.752	34.6
8	4369.960	8.748	74.6
9	4367.030	8.742	9.4
10	3896.656	7.801	10.1
11	3829.276	7.666	2.0
12	3819.755	7.647	1.9
13	3747.798	7.503	12.8
14	3745.052	7.497	83.1
15	3742.855	7.493	28.9
16	3736.080	7.479	156.6
17	3729.306	7.466	31.9
18	3727.292	7.462	80.0
19	3724.362	7.456	12.7
20	3704.954	7.417	44.4
21	1749.302	3.502	1.9
22	1742.345	3.488	2.2
23	1735.387	3.474	1.8
24	1719.457	3.442	2.7
25	1274.717	2.552	15.0
26	1273.069	2.549	13.9
27	1271.238	2.545	14.4
28	557.345	1.116	1.9
29	550.388	1.102	3.8
30	543.430	1.088	1.8
31	-0.000	-0.000	2.1



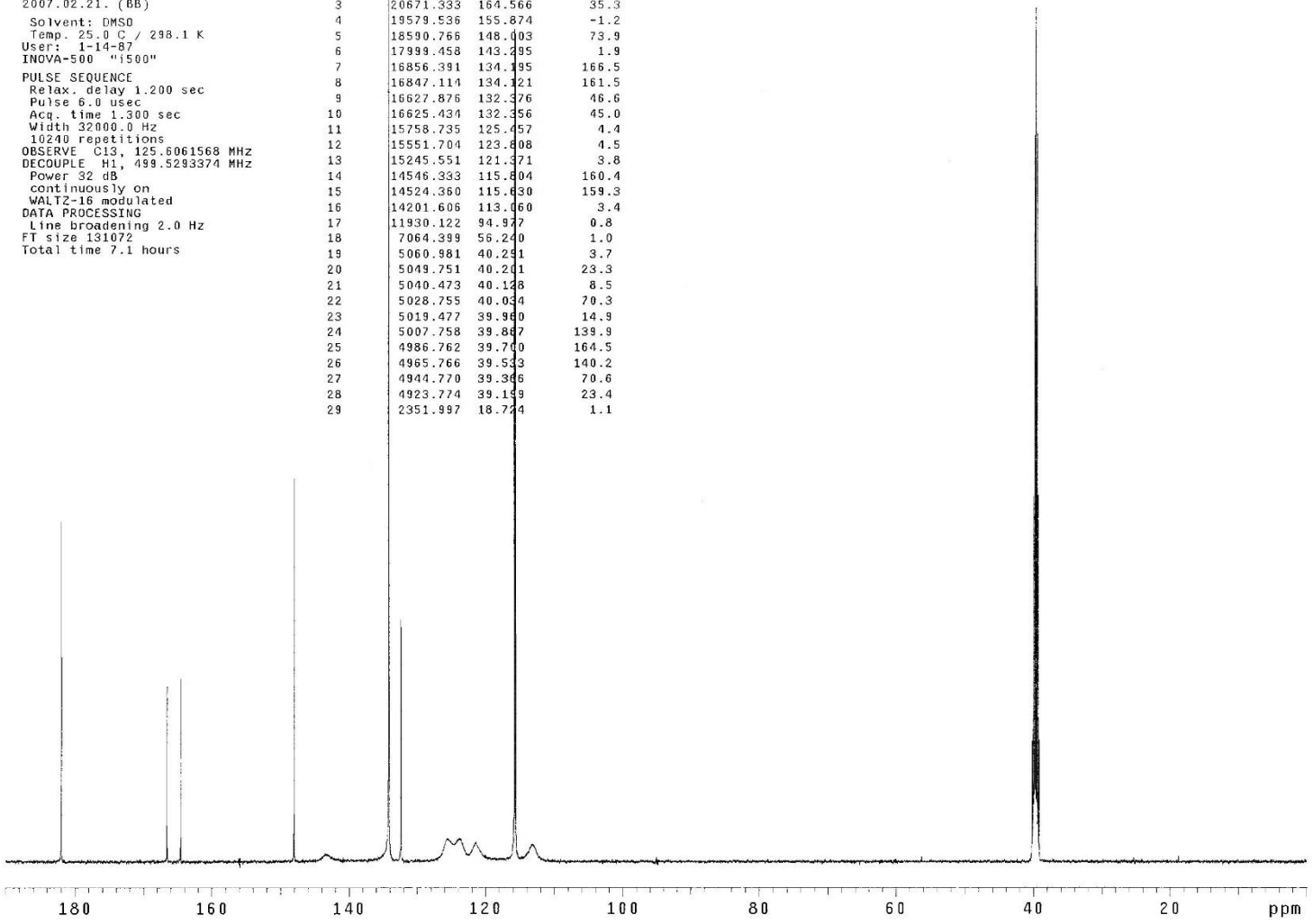


1a

STANDARD 13C
67808
MM382
Milen Matyas
2007.02.21. (BB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"

PULSE SEQUENCE
Relax. delay 1.200 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
10240 repetitions
OBSERVE C13, 125.6061568 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 7.1 hours

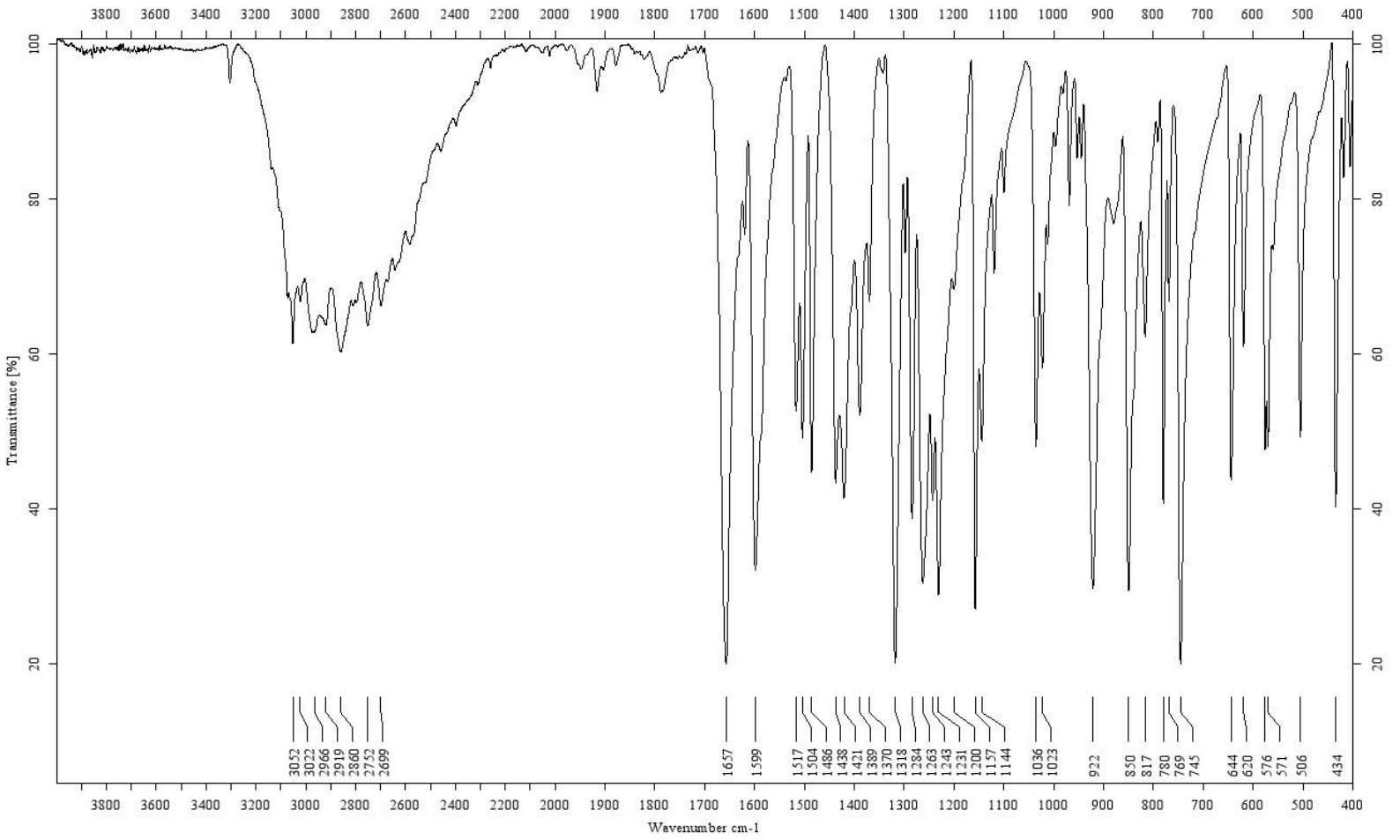
INDEX	FREQUENCY	PPM	HEIGHT
1	22855.415	181.954	65.5
2	20921.751	166.584	33.7
3	20671.333	164.566	35.3
4	19579.536	155.874	-1.2
5	18590.766	148.003	73.9
6	17999.458	143.295	1.9
7	16856.391	134.195	166.5
8	16847.114	134.121	161.5
9	16627.876	132.376	46.6
10	16625.434	132.356	45.0
11	15758.735	125.457	4.4
12	15551.704	123.808	4.5
13	15245.551	121.371	3.8
14	14546.333	115.804	160.4
15	14524.360	115.630	159.3
16	14201.606	113.060	3.4
17	11930.122	94.977	0.8
18	7064.399	56.240	1.0
19	5060.981	40.291	3.7
20	5049.751	40.201	23.3
21	5040.473	40.128	8.5
22	5028.755	40.034	70.3
23	5019.477	39.960	14.9
24	5007.758	39.867	139.9
25	4986.762	39.700	164.5
26	4965.766	39.533	140.2
27	4944.770	39.366	70.6
28	4923.774	39.199	23.4
29	2351.997	18.724	1.1



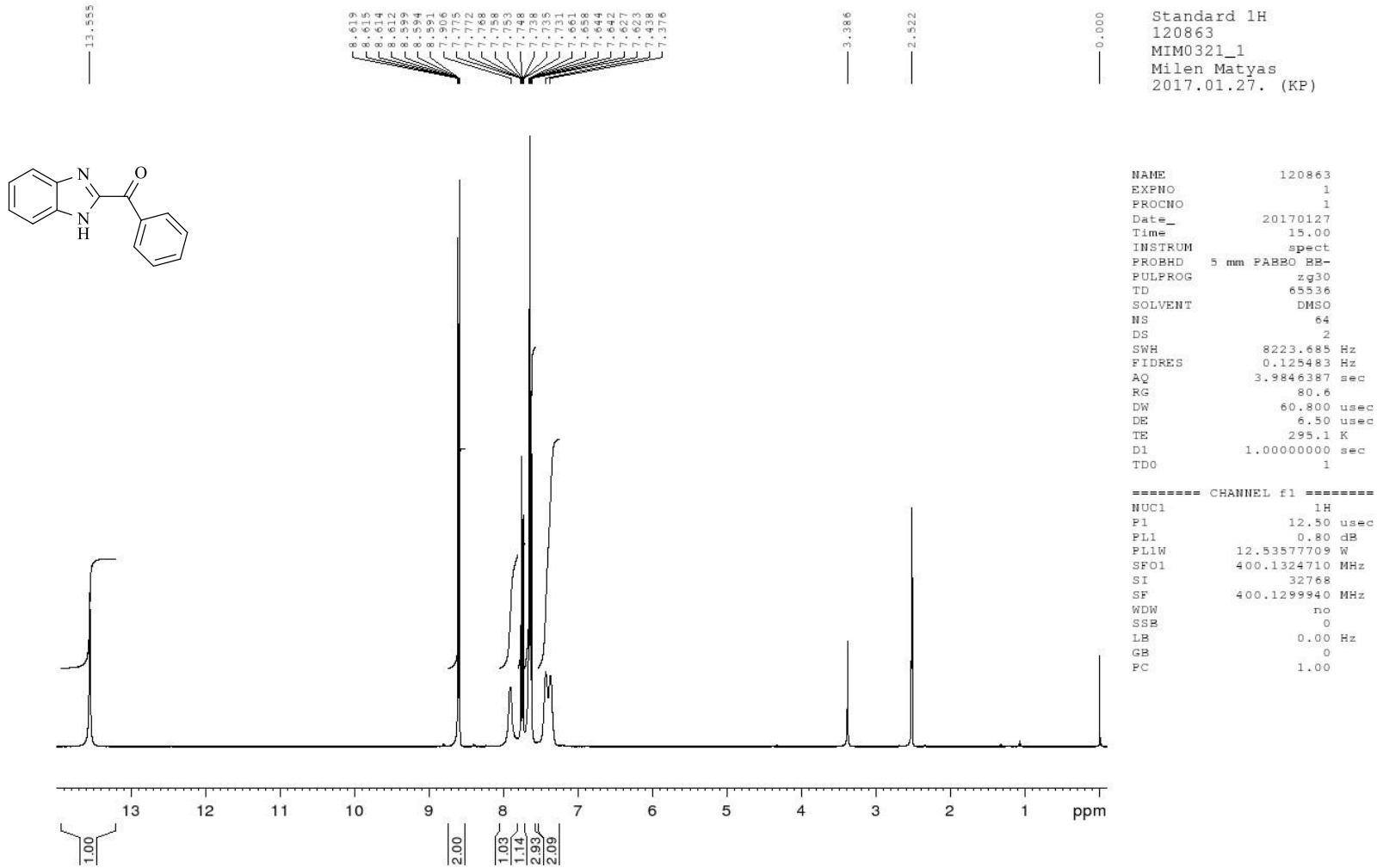
1a

120864	Milen Matyas	KP
MIM0322_1	KBr	27/01/2017

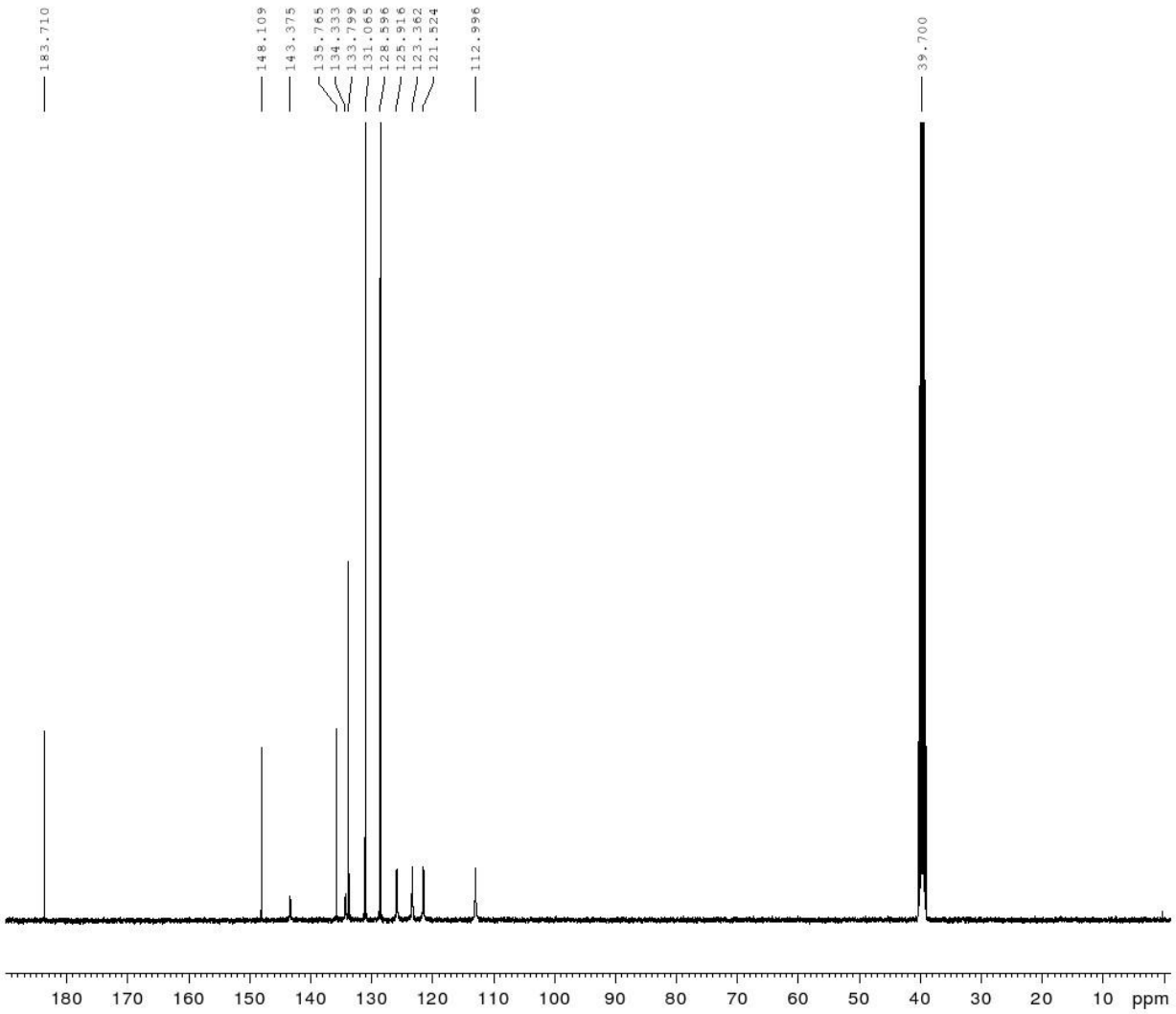
BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



1b


13.555
8.619
8.615
8.614
8.612
8.599
8.594
8.591
7.906
7.775
7.772
7.768
7.758
7.753
7.748
7.738
7.735
7.731
7.661
7.658
7.644
7.642
7.627
7.623
7.438
7.376
3.386
2.522
0.000
Standard 1H
120863
MIM0321_1
Milen Matyas
2017.01.27. (KP)
N
O
N
H
NAME 120863
EXPNO 1
PROCNO 1
Date_ 20170127
Time 15.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 80.6
DW 60.800 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 0.80 dB
PL1W 12.53577709 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1299940 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.00
1.03
1.14
2.93
2.09

1b



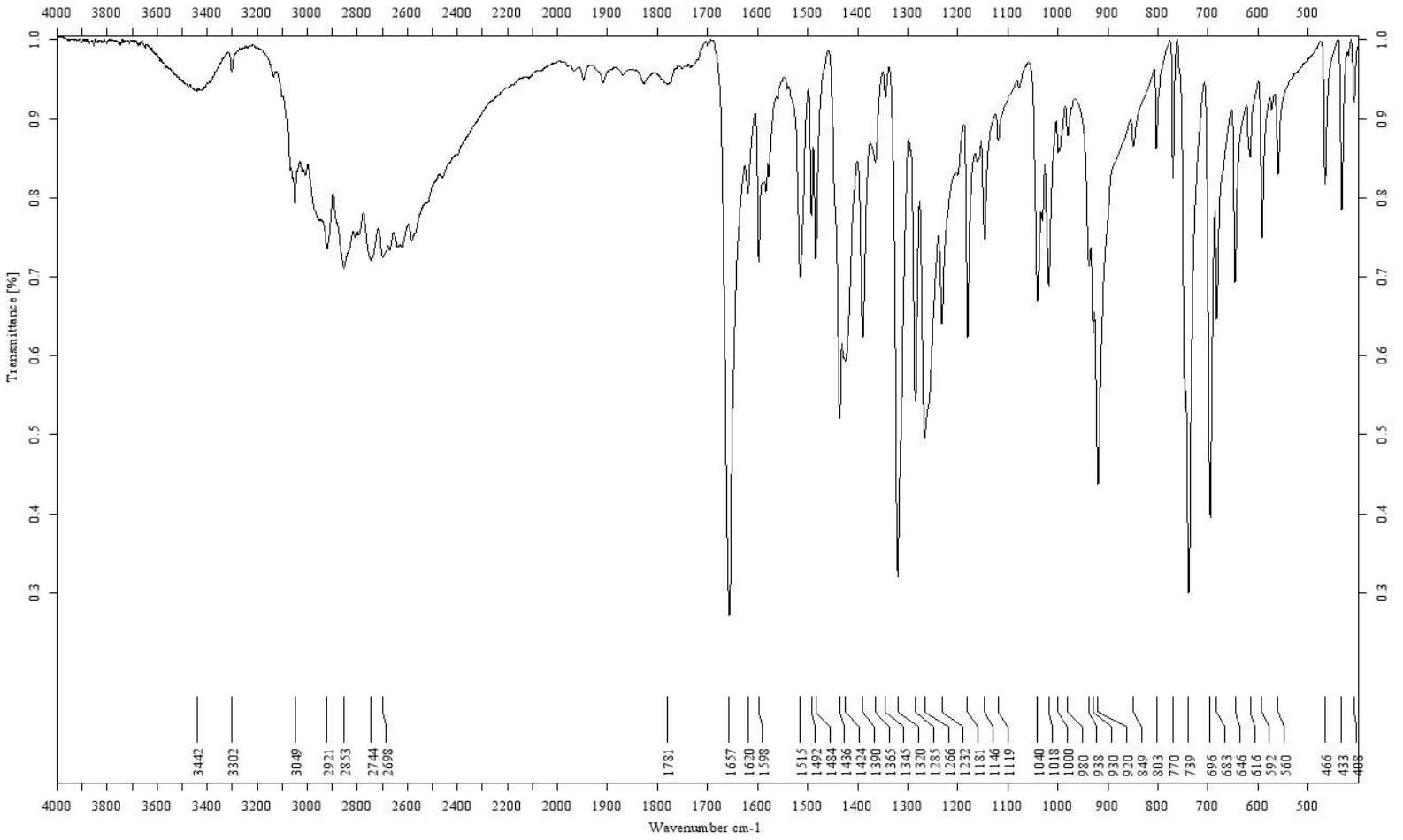
Standard 13C
120863
MIM0321_1
Milen Matyas
2017.01.27. (KP)

NAME	120863
EXPNO	2
PROCNO	1
Date_	20170127
Time	16.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	3296
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	296.7 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.44 dB
PL1W	43.99363327 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.80 dB
PL12	18.30 dB
PL13	18.40 dB
PL2W	12.53577709 W
PL12W	0.22292118 W
PL13W	0.21784686 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127984 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

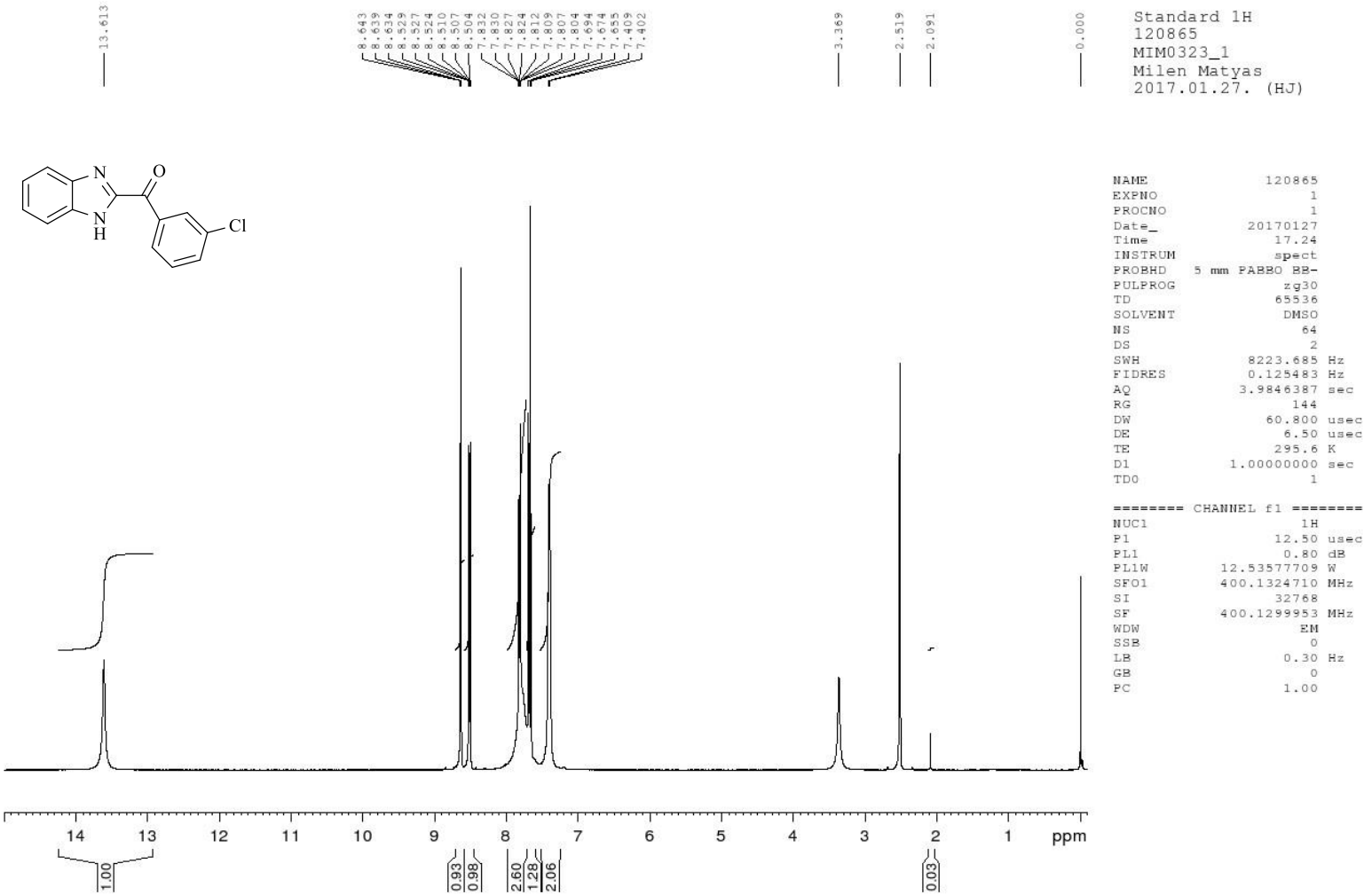
1b

77805	Milen Mátyás	BB
E1874	KBr	16/12/2008

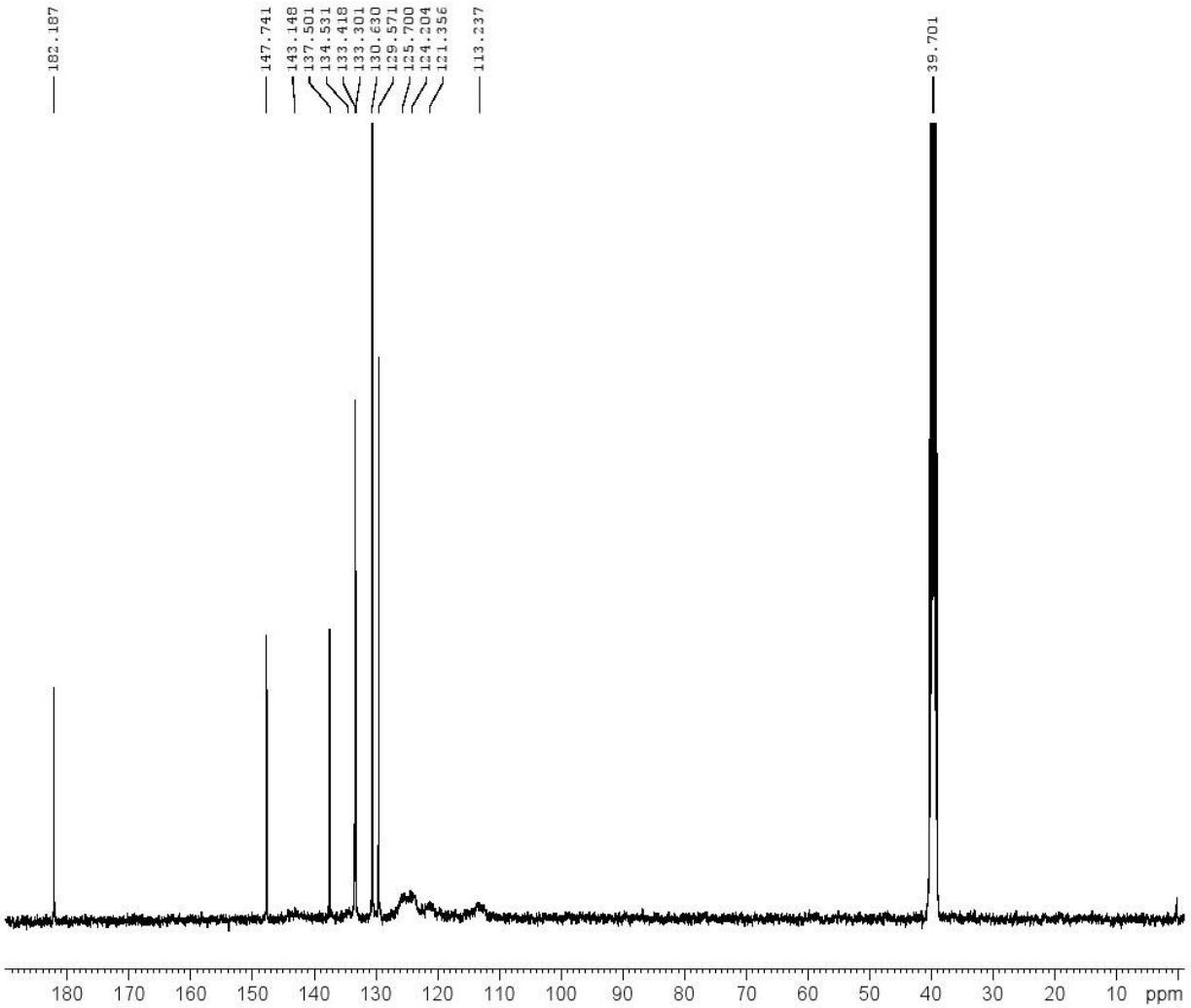
BRUKER VECTOR22
Resolution: 2 cm-1
Number of Scans: 8



1c


13.613
8.643
8.639
8.634
8.529
8.527
8.524
8.510
8.507
8.504
7.832
7.830
7.827
7.824
7.812
7.809
7.807
7.804
7.694
7.674
7.655
7.409
7.402
3.369
2.519
2.091
0.000
Standard 1H
120865
MIM0323_1
Milen Matyas
2017.01.27. (HJ)
N
O
N
H
Cl
NAME 120865
EXPNO 1
PROCNO 1
Date_ 20170127
Time 17.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 0.80 dB
PL1W 12.53577709 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1299953 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.93
0.98
2.60
1.28
2.06
0.03

1c

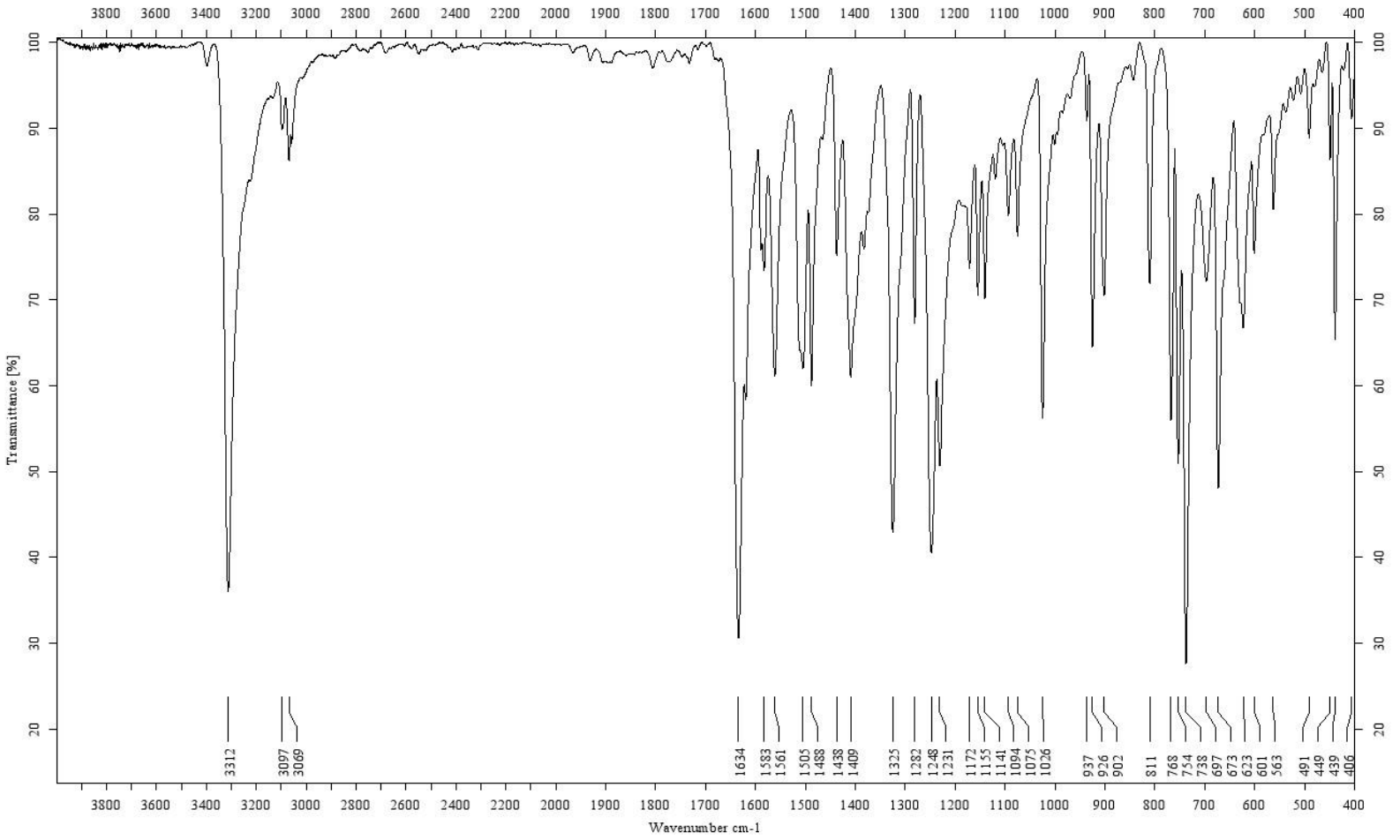



```
Standard 13C
120865
MIM0323_1
Milen Matyas
2017.01.27.  (HJ)

Current Data Parameters
NAME                  120865
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170127
Time                  17.32
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    2786
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    2050
DW                  20.800 usec
DE                   6.50 usec
TE                  296.6 K
D1               1.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.50 usec
PL1                   1.44 dB
PL1W           43.99363327 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                90.00 usec
PL2                   0.80 dB
PL12                 18.30 dB
PL13                 18.40 dB
PL2W           12.53577709 W
PL12W           0.22292118 W
PL13W           0.21784686 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6127983 MHz
WDW                      EM
SSB       0
LB                    3.00 Hz
GB        0
PC                    1.40
```

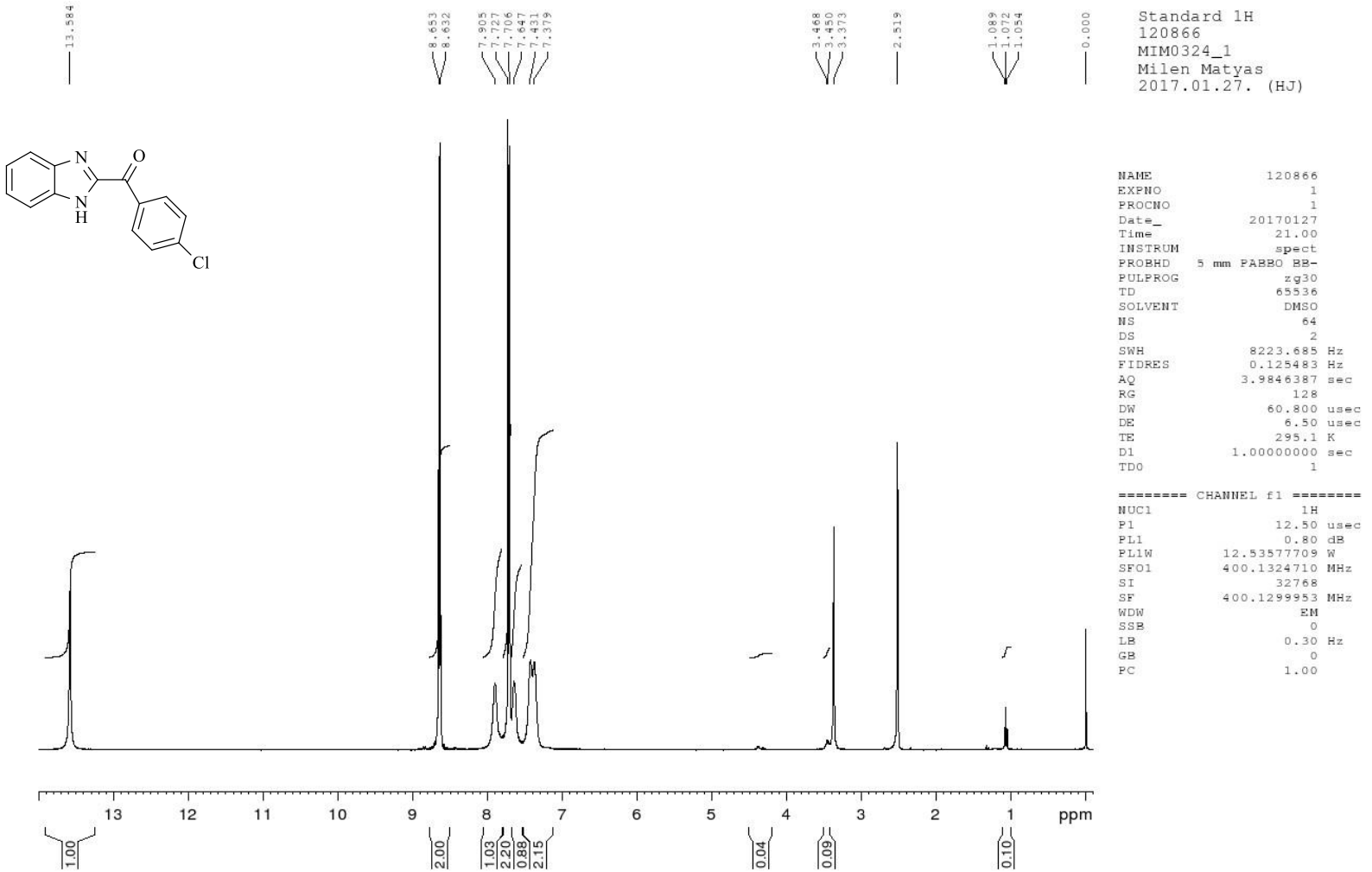
1c

120865	Milen Matyas	KP
MIM0323_1	KBr	27/01/2017

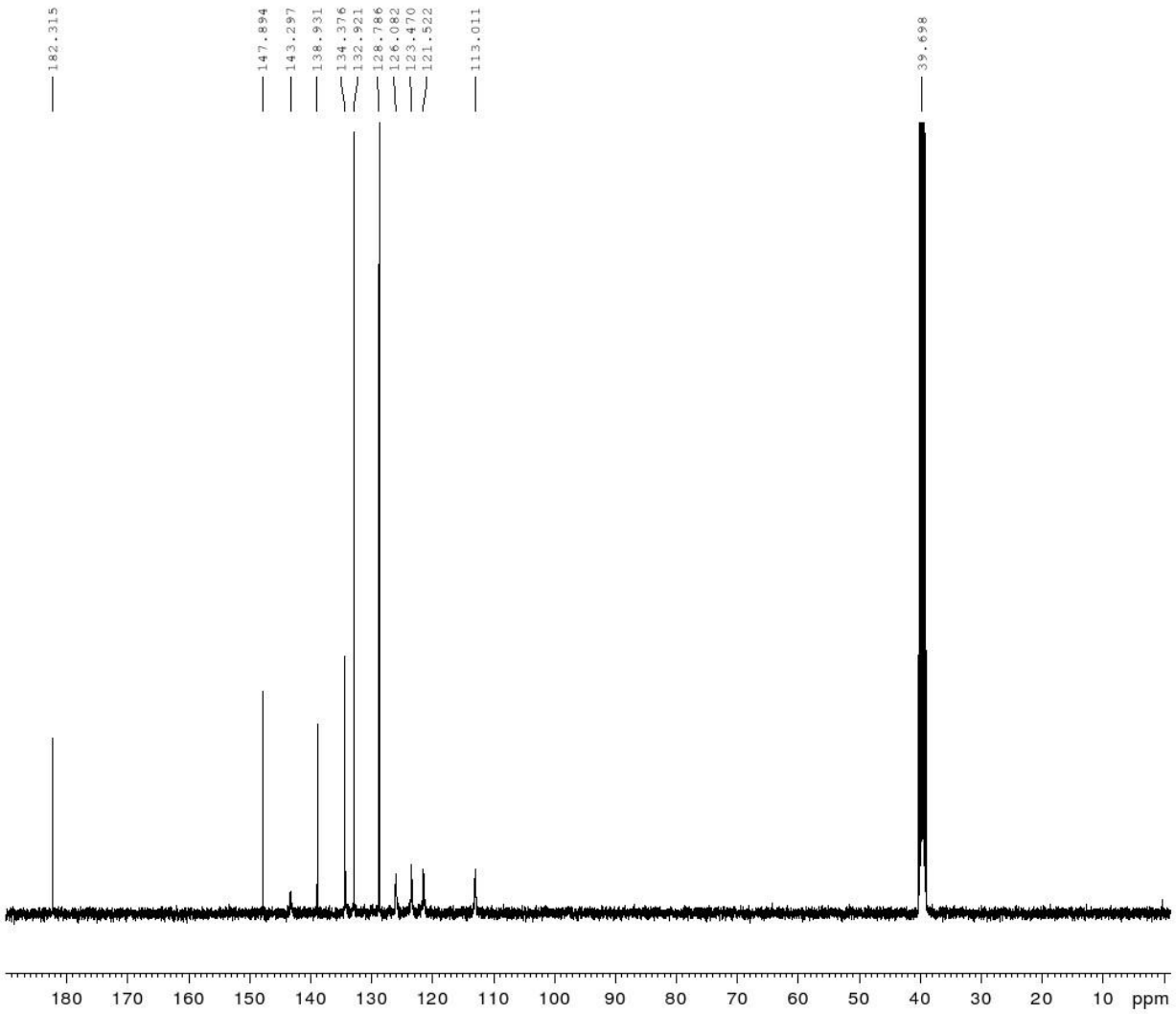
BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



1d


13.584
8.653
8.632
7.905
7.727
7.706
7.647
7.431
7.379
3.468
3.450
3.373
2.519
1.089
1.072
1.054
0.000
Standard 1H
120866
MIM0324_1
Milen Matyas
2017.01.27. (HJ)
N
O
N
H
Cl
NAME 120866
EXPNO 1
PROCNO 1
Date_ 20170127
Time 21.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 0.80 dB
PL1W 12.53577709 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1299953 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.00
1.03
2.20
0.88
2.15
0.04
0.09
0.10

1d



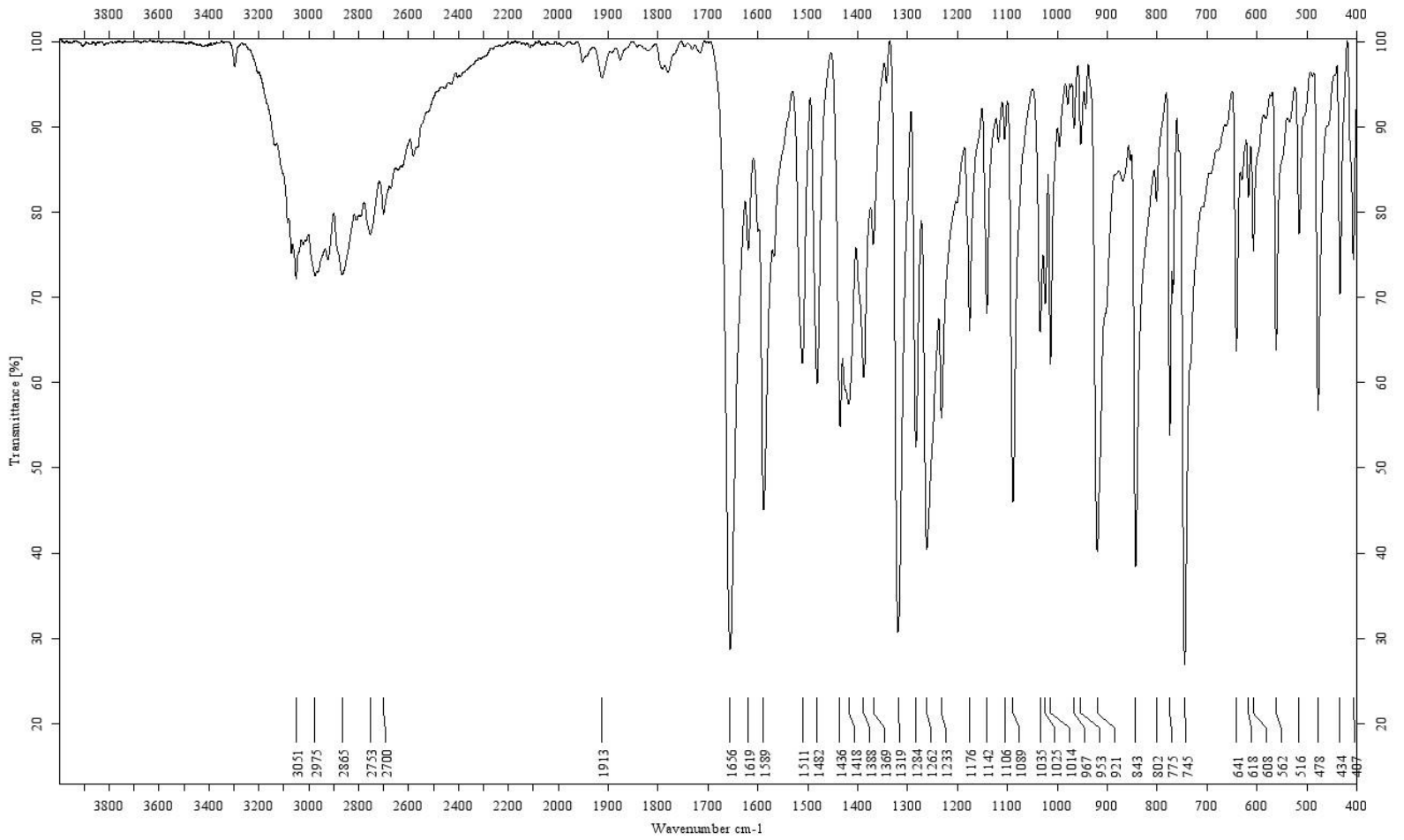
Standard 13C
120866
MIM0324_1
Milen Matyas
2017.01.27. (HJ)

NAME	120866
EXPNO	2
PROCNO	1
Date_	20170127
Time	21.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1152
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	296.5 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.44 dB
PL1W	43.99363327 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.80 dB
PL12	18.30 dB
PL13	18.40 dB
PL2W	12.53577709 W
PL12W	0.22292118 W
PL13W	0.21784686 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127984 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

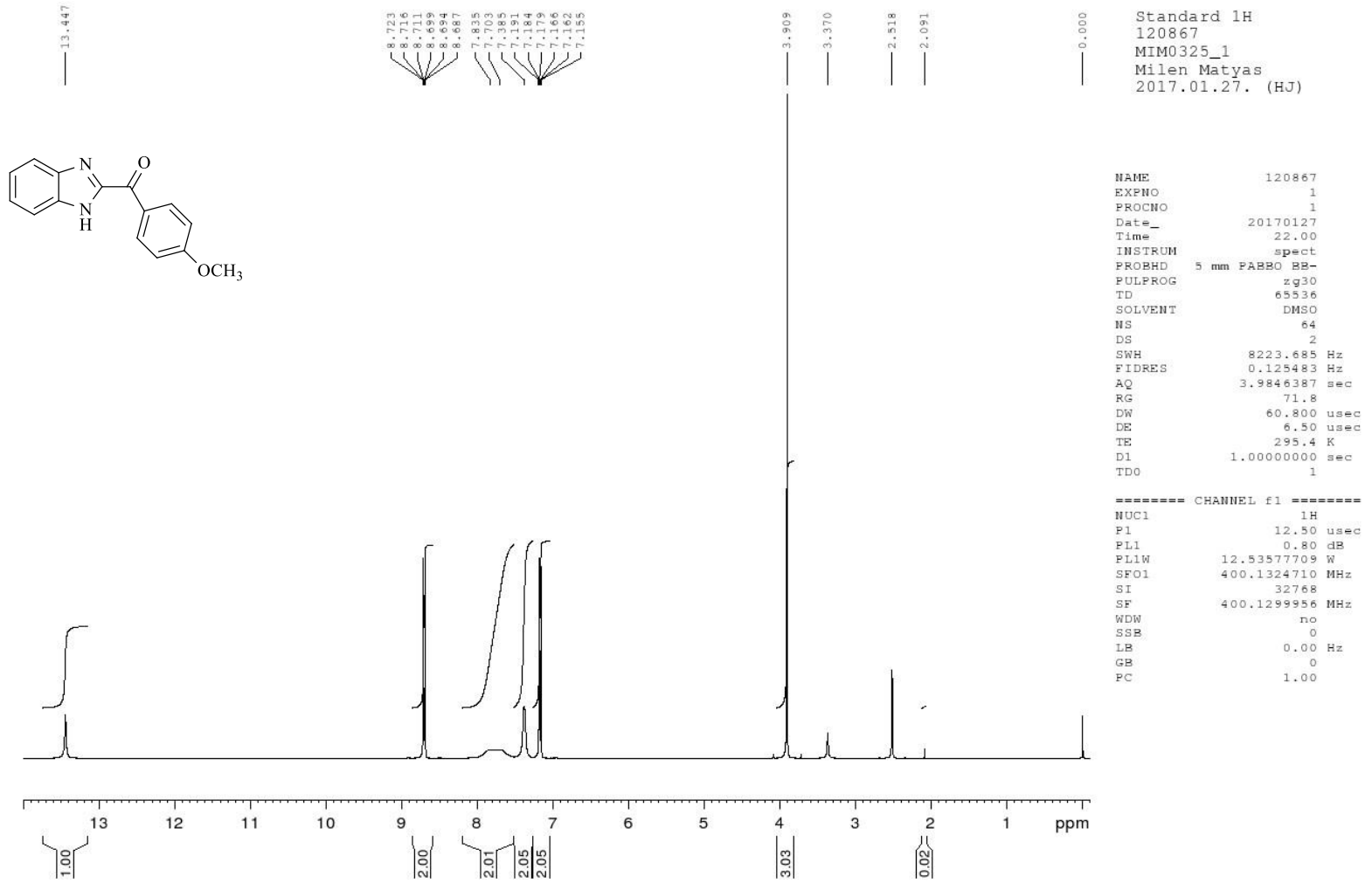
1d

120866	Milen Matyas	KP
MIM0324_1	KBr	27/01/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



1e

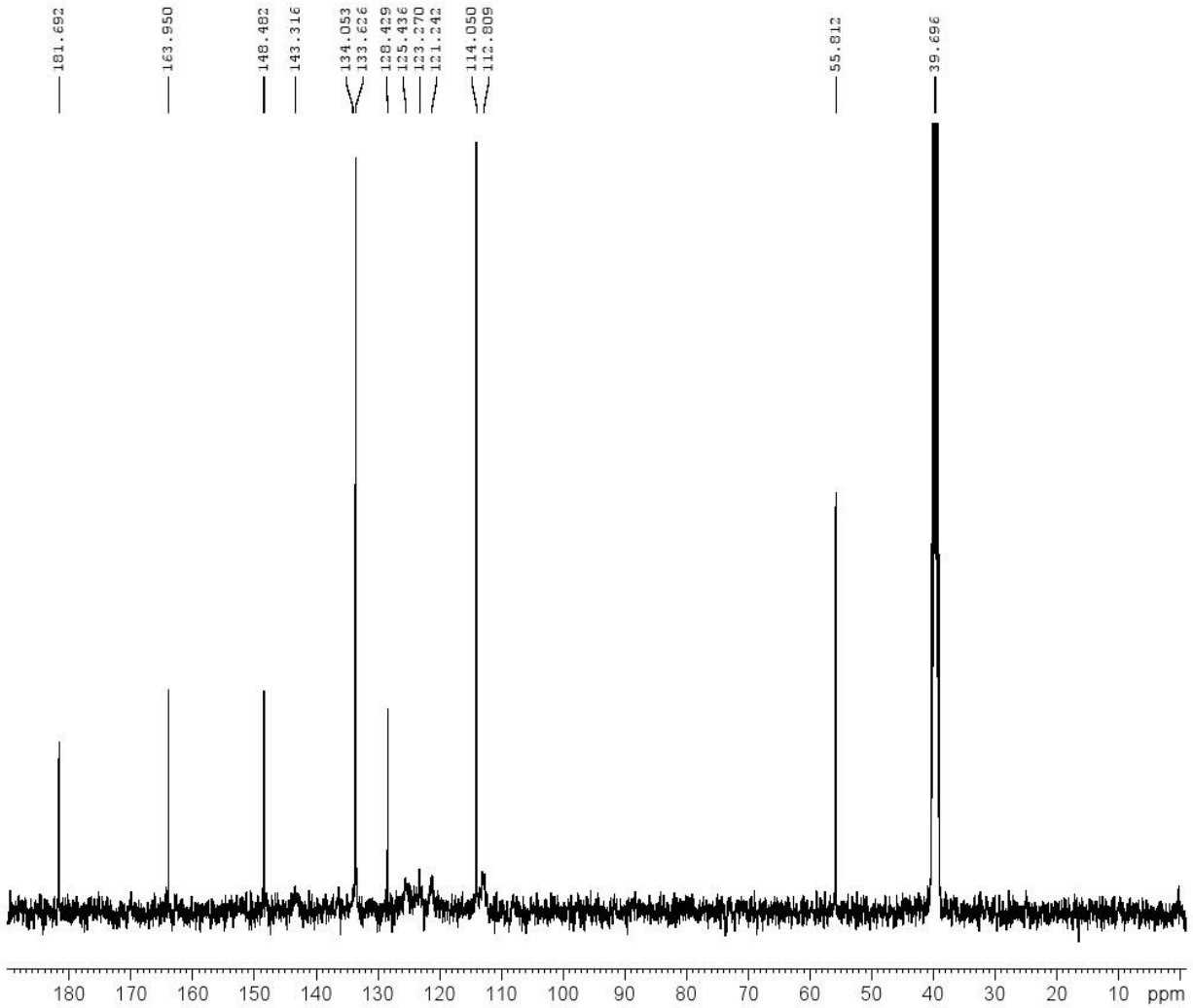


Standard 1H
120867
MIM0325_1
Milen Matyas
2017.01.27. (HJ)

NAME	120867
EXPNO	1
PROCNO	1
Date_	20170127
Time	22.00
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	71.8
DW	60.800 usec
DE	6.50 usec
TE	295.4 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	12.50 usec
PL1	0.80 dB
PL1W	12.53577709 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1299956 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1e

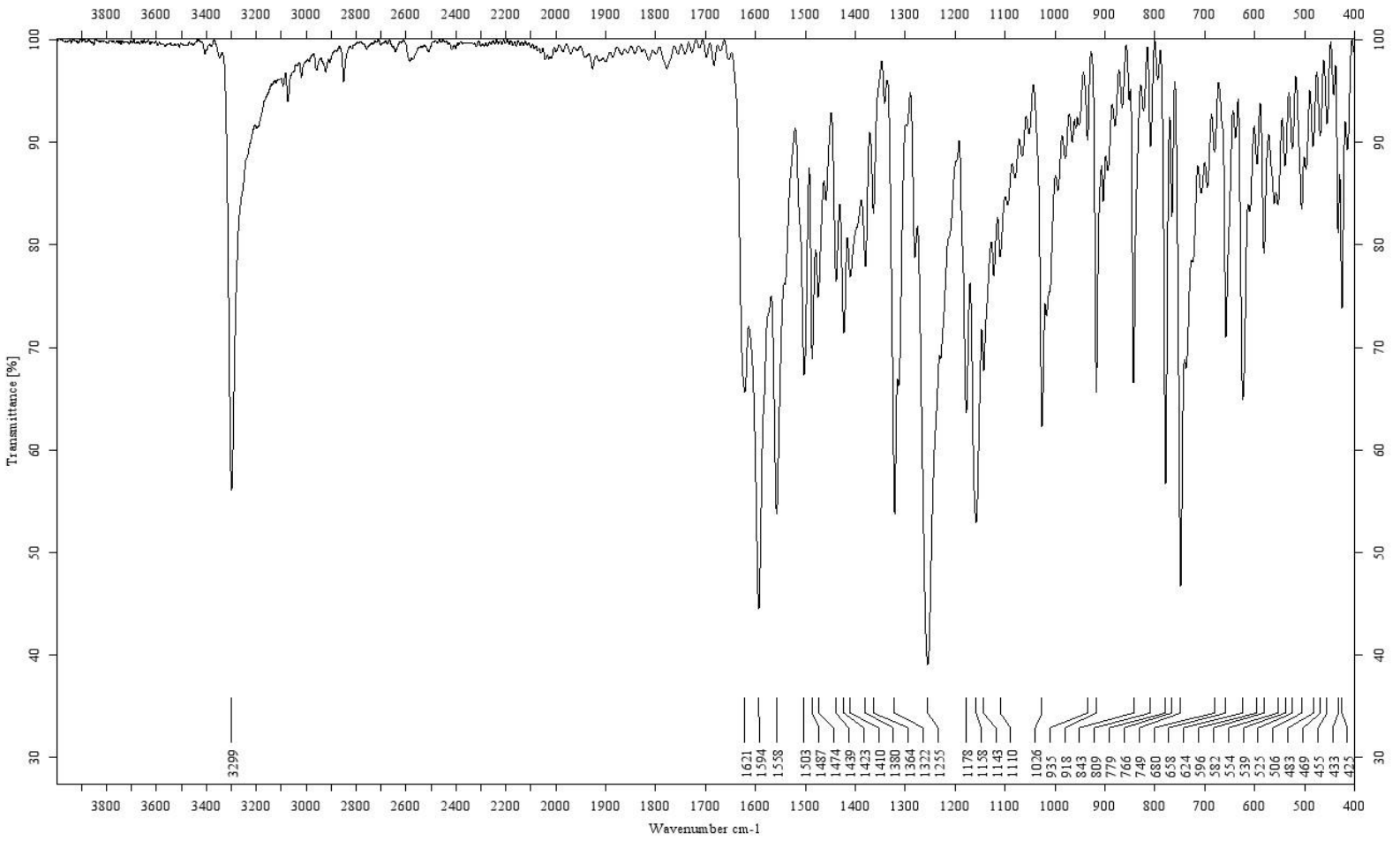



```
Standard 13C
120867
MIM0325_1
Milen Matyas
2017.01.27.  (HJ)

Current Data Parameters
NAME                  120867
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170127
Time                   22.09
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     8192
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                      2050
DW                   20.800 usec
DE                    6.50 usec
TE                   296.3 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      9.50 usec
PL1                     1.44 dB
PL1W             43.99363327 W
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                     1H
PCPD2                  90.00 usec
PL2                     0.80 dB
PL12                   18.30 dB
PL13                   18.40 dB
PL2W             12.53577709 W
PL12W             0.22292118 W
PL13W             0.21784686 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF              100.6127980 MHz
WDW                         EM
SSB          0
LB                      4.00 Hz
GB           0
PC                      1.40
```

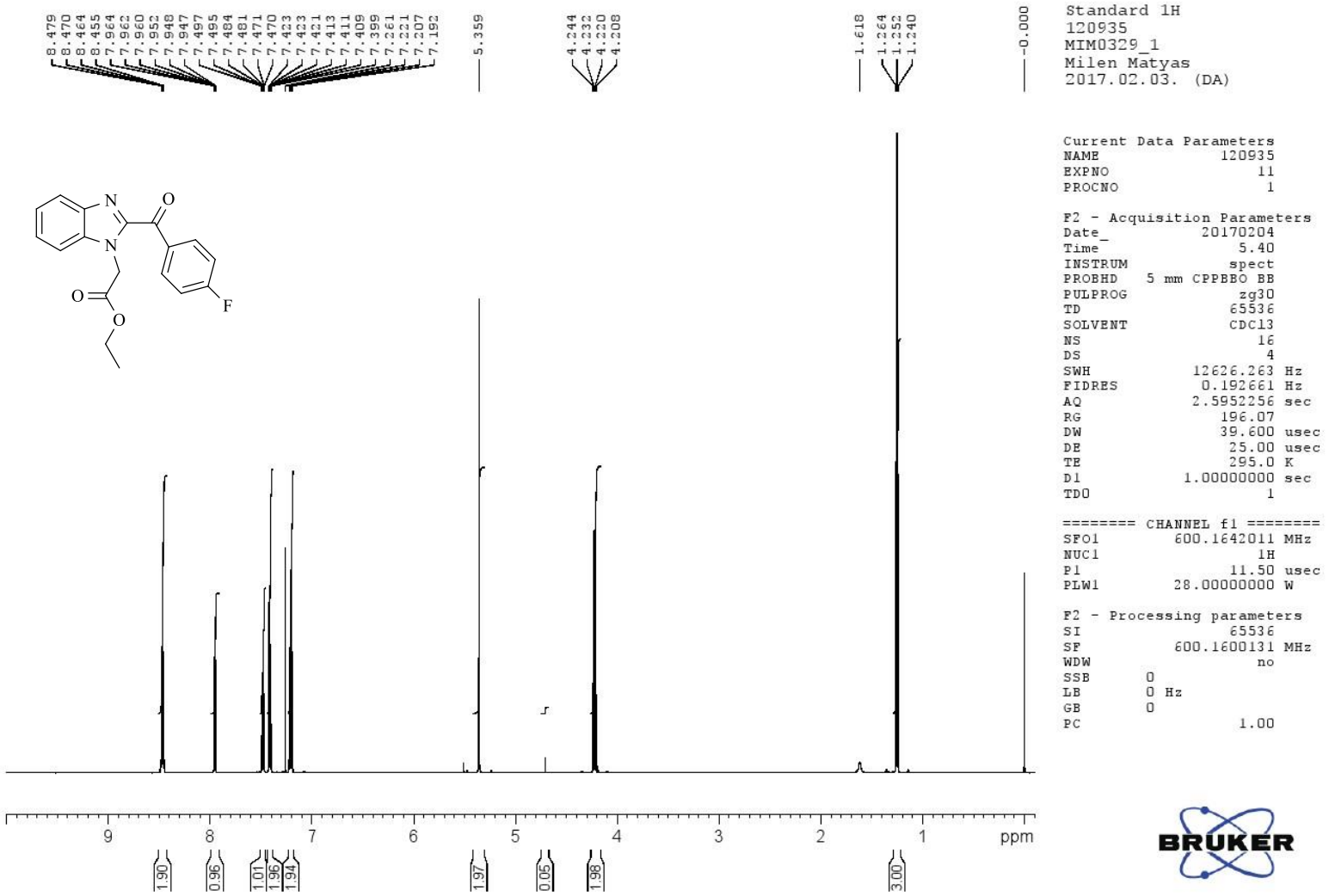
1e

120867	Milen Matyas	KP
MIM0325_1	KBr	27/01/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

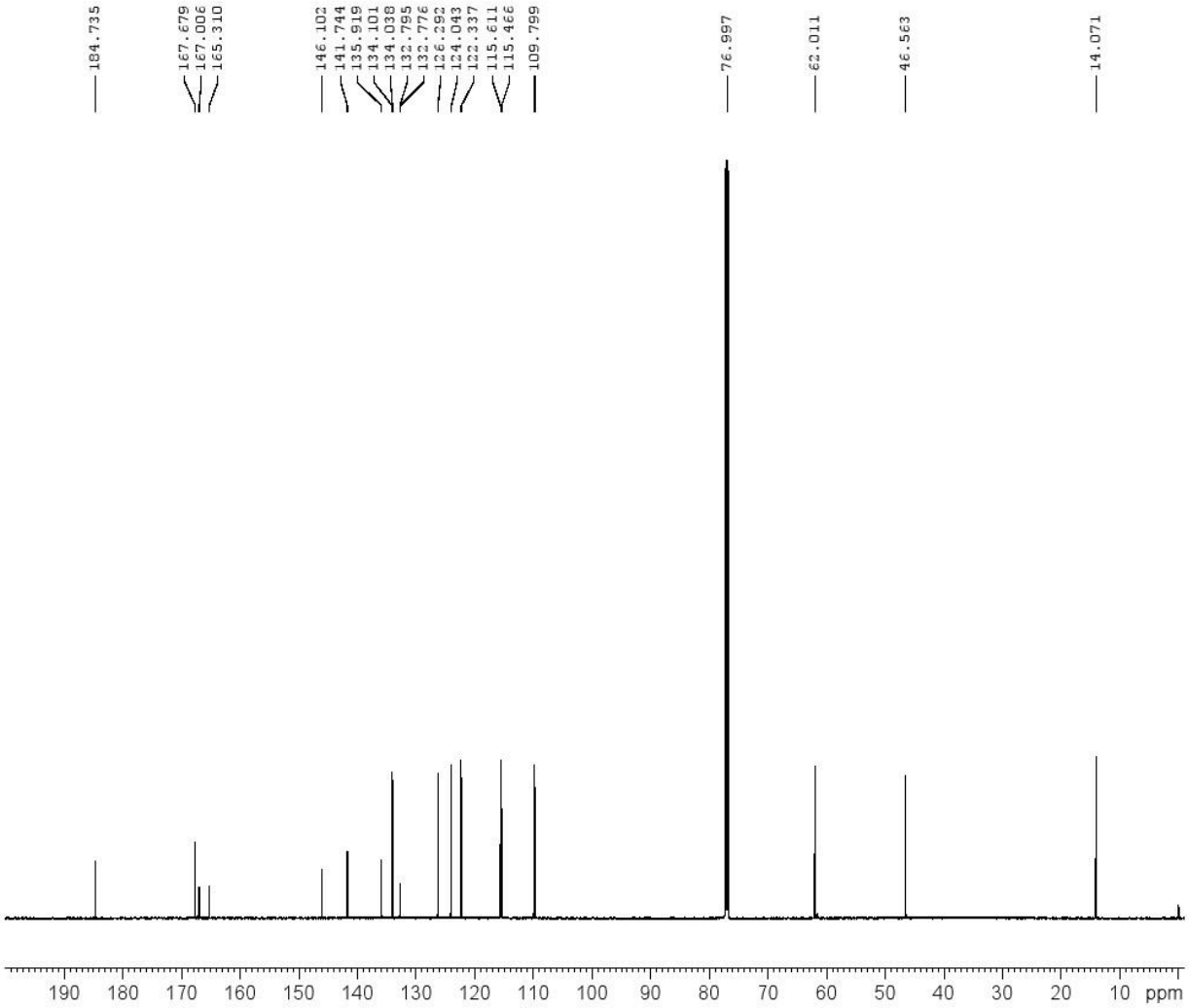


2a




```
Standard 1H
120935
MIM0329_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME                  120935
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   5.40
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        4
SWH               12626.263 Hz
FIDRES             0.192661 Hz
AQ                 2.5952256 sec
RG                    196.07
DW                    39.600 usec
DE                    25.00 usec
TE                    295.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            600.1642011 MHz
NUC1                      1H
P1                     11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                    65536
SF              600.1600131 MHz
WDW                      no
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```

2a



Standard 13C
120935
MIM0329_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME 120935
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170204
Time 6.23
INSTRUM spect
PROBHD 5 mm CPPBB0 BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 196.07
DW 13.867 usec
DE 18.00 usec
TE 295.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SF01 150.9254424 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W

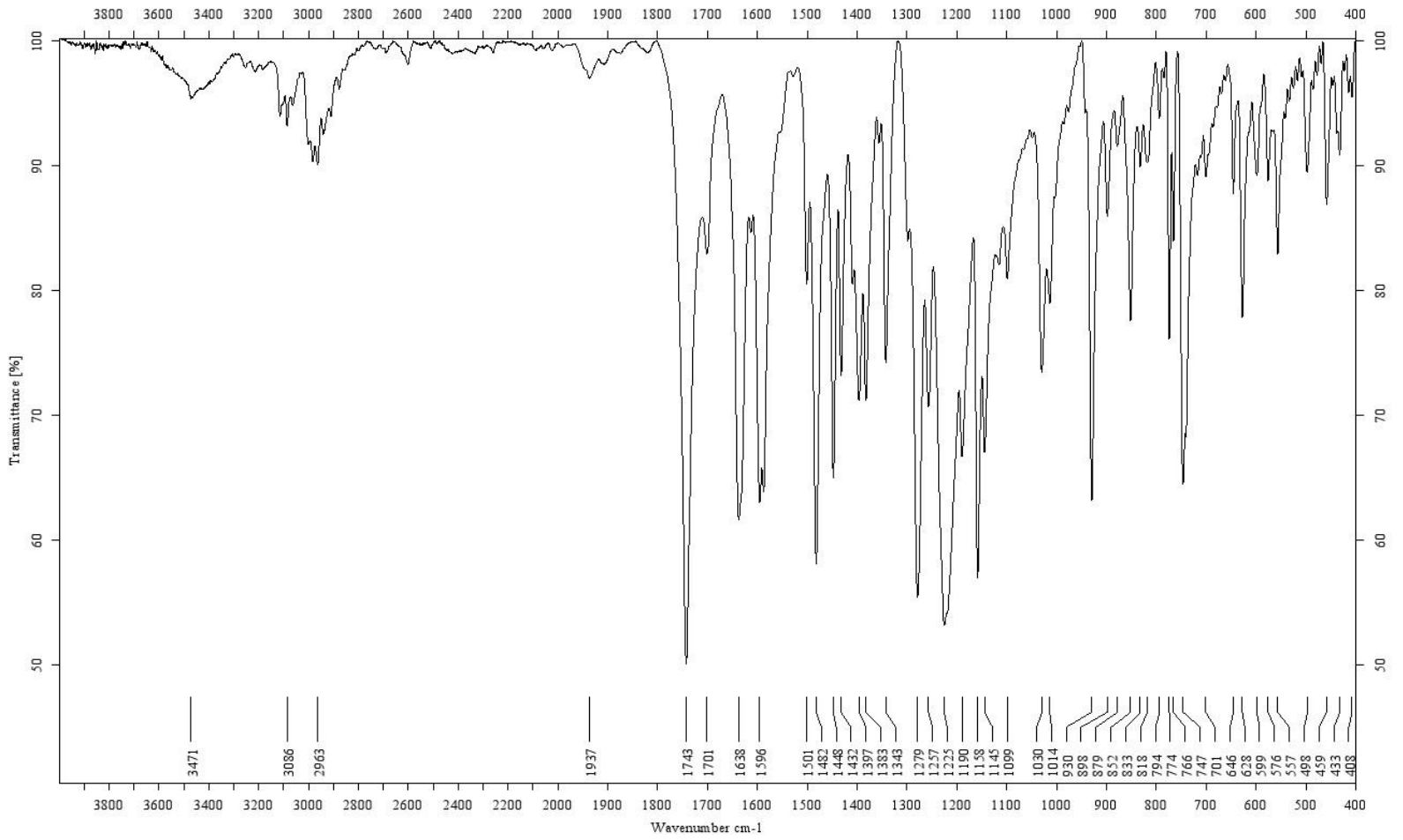
======== CHANNEL f2 ========
SF02 600.1624006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 28.00000000 W
PLW12 0.75571001 W
PLW13 0.37029999 W

F2 - Processing parameters
SI 65536
SF 150.9103595 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2a

120935	Milen Matyas	KP
MIM0329_1	KBr	02/02/2017

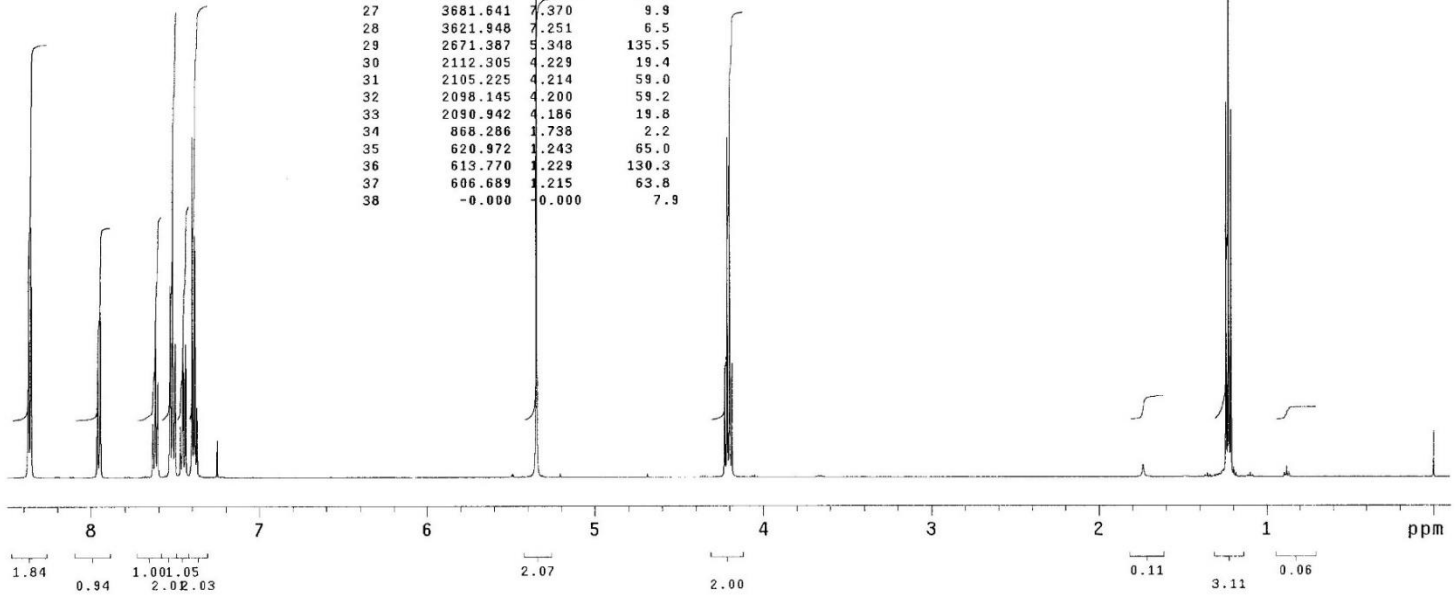
BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



2b

STANDARD 1H
60522
MM63
Milen Matyas
2005.11.14. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5244752 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

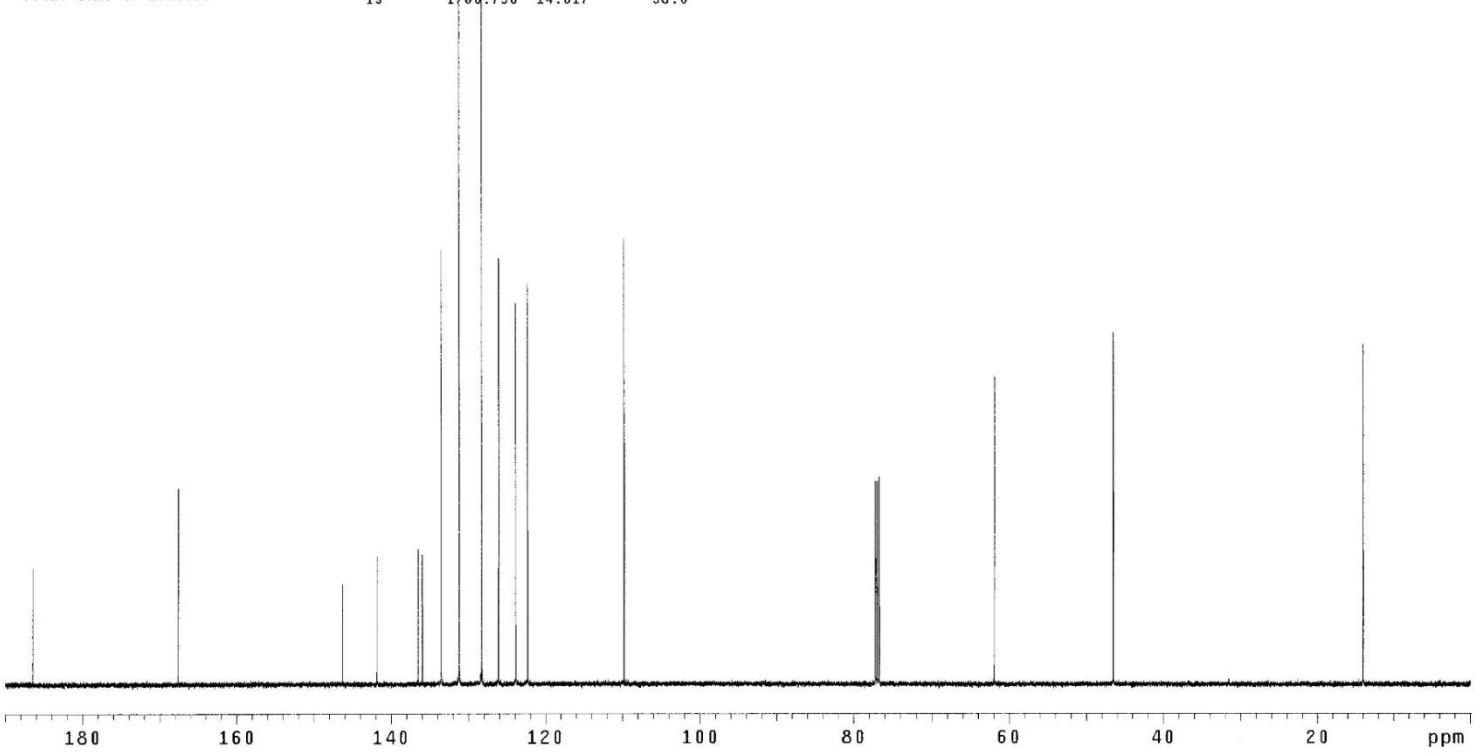
INDEX	FREQUENCY	PPM	HEIGHT
1	4183.594	8.375	37.8
2	4182.617	8.373	38.7
3	4175.415	8.359	43.5
4	4174.072	8.356	33.1
5	3978.271	7.964	18.3
6	3977.051	7.962	22.0
7	3969.238	7.946	28.8
8	3814.575	7.636	6.3
9	3813.354	7.634	9.4
10	3812.256	7.632	5.5
11	3806.030	7.619	24.3
12	3799.805	7.607	11.6
13	3798.584	7.604	16.6
14	3797.485	7.602	8.8
15	3762.695	7.533	33.3
16	3754.883	7.517	49.5
17	3747.192	7.502	23.3
18	3731.812	7.471	9.0
19	3730.957	7.469	8.4
20	3723.999	7.455	20.0
21	3722.656	7.452	18.3
22	3716.675	7.440	23.2
23	3715.698	7.438	19.4
24	3697.266	7.402	59.2
25	3689.575	7.386	42.1
26	3682.739	7.372	12.2
27	3681.641	7.370	9.9
28	3621.948	7.251	6.5
29	2671.387	5.348	135.5
30	2112.305	4.229	19.4
31	2105.225	4.214	59.0
32	2098.145	4.200	59.2
33	2090.942	4.186	19.8
34	868.286	1.738	2.2
35	620.972	1.243	65.0
36	613.770	1.229	130.3
37	606.689	1.215	63.8
38	-0.000	-0.000	7.9



2b

STANDARD 13C
60522
MM63
Milen Matyas
2005.11.14. (BT)
Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.200 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
1126 repetitions
OBSERVE C13, 125.6055367 MHz
DECOUPLE H1, 499.5269647 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 46 minutes

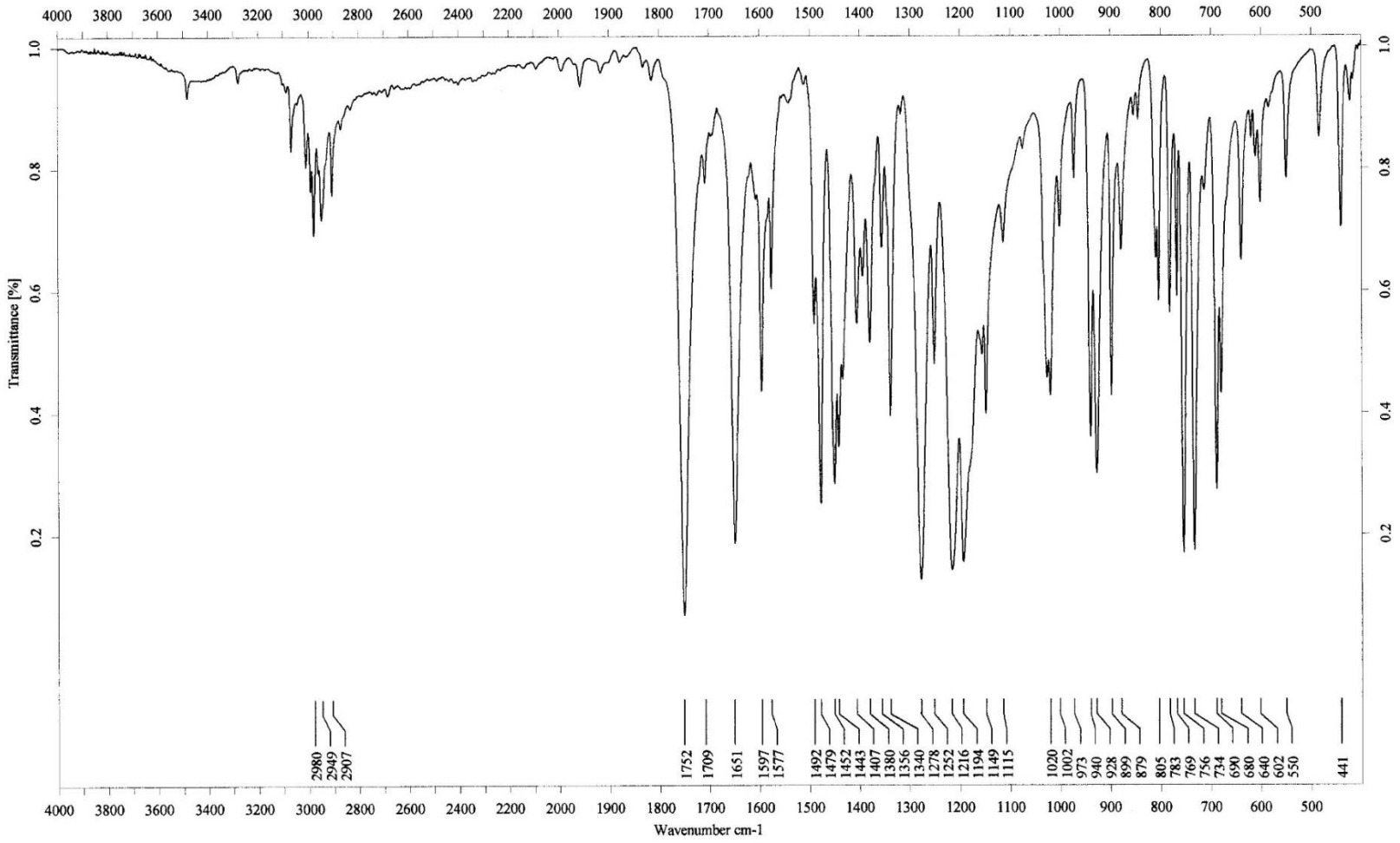
INDEX	FREQUENCY	PPM	HEIGHT
1	23417.977	186.426	19.8
2	21055.672	167.620	33.5
3	18373.543	146.268	17.1
4	17808.602	141.771	21.8
5	17143.074	136.473	23.0
6	17073.250	135.917	22.1
7	16768.563	133.491	74.2
8	16476.082	131.163	161.6
9	16112.801	128.271	138.9
10	15841.316	126.110	72.8
11	15559.578	123.867	65.0
12	15364.266	122.312	68.5
13	13785.652	109.745	76.1
14	9704.598	77.257	34.7
15	9672.371	77.000	34.7
16	9640.633	76.747	35.4
17	7774.422	61.891	52.7
18	5841.805	46.506	60.1
19	1760.750	14.017	58.0



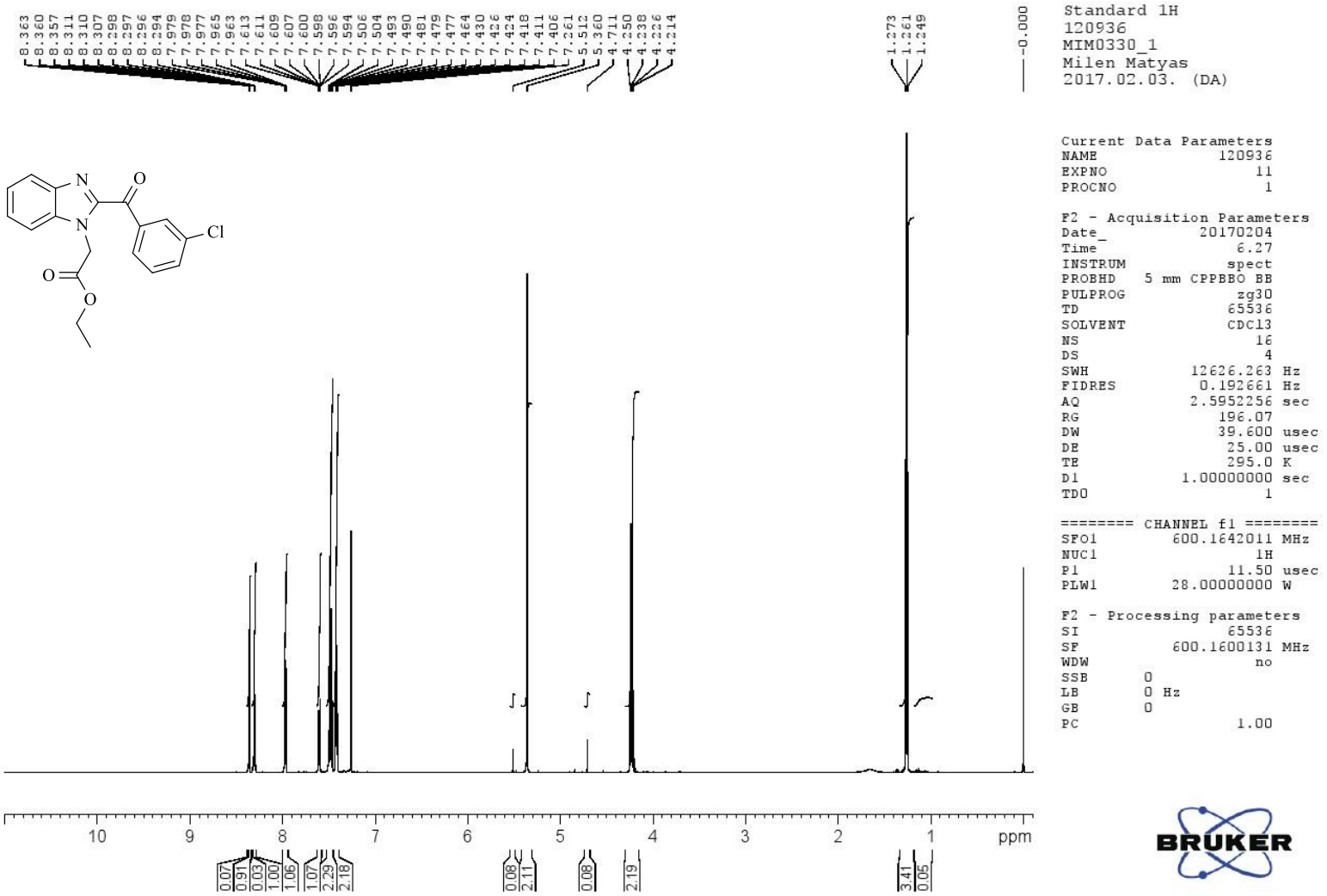
2b

60522	Milen Mátyás	CzB
MM63	KBr	14/11/2005

BRUKER VECTOR22
Resolution: 2 cm-1
Number of Scans: 8

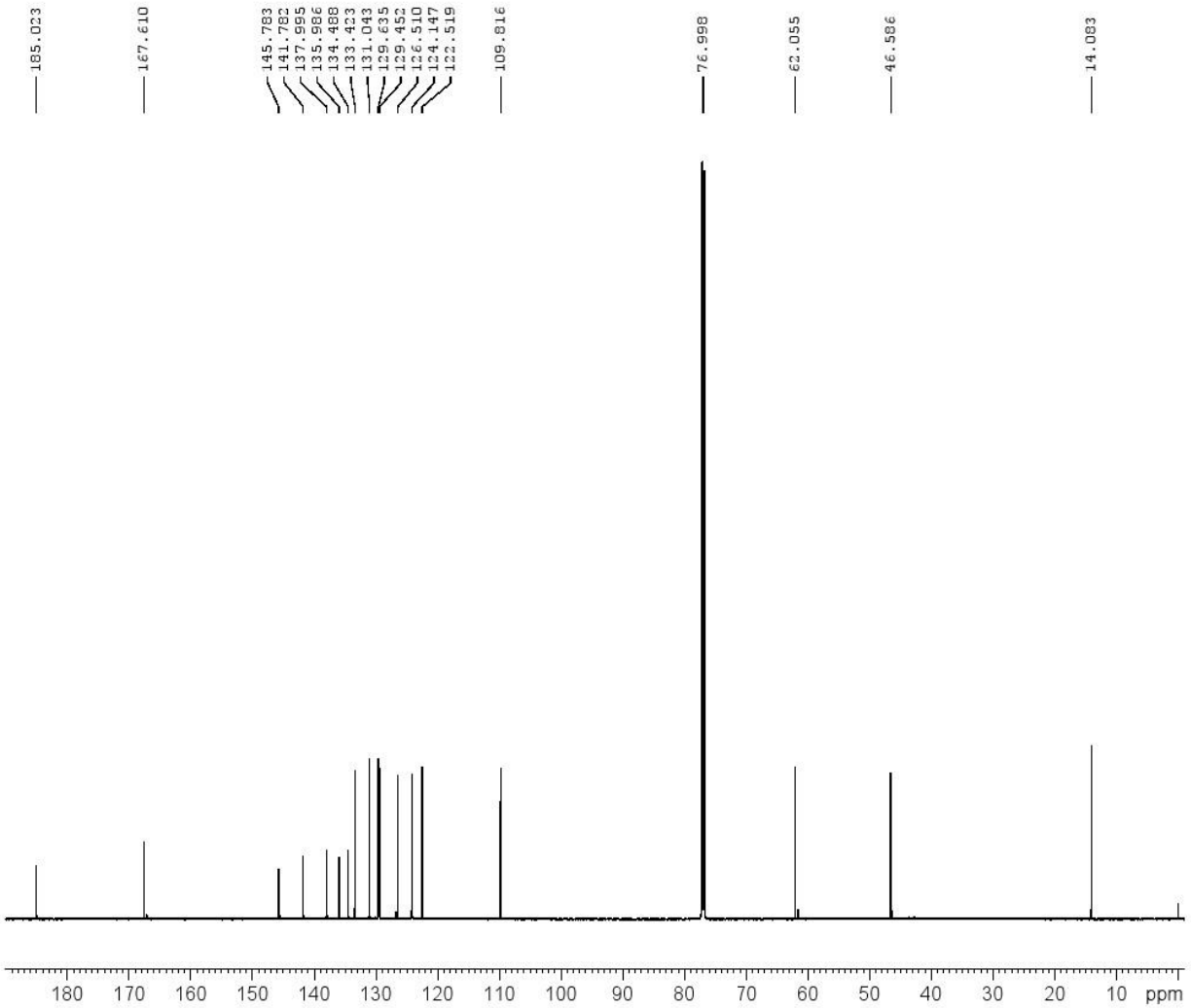


2c




```
Standard 1H
120936
MIM0330_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME                  120936
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   6.27
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        4
SWH               12626.263 Hz
FIDRES             0.192661 Hz
AQ                2.5952256 sec
RG                   196.07
DW                   39.600 usec
DE                   25.00 usec
TE                   295.0 K
D1               1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            600.1642011 MHz
NUC1                    1H
P1                   11.50 usec
PLW1            28.00000000 W

F2 - Processing parameters
SI                    65536
SF              600.1600131 MHz
WDW                      no
SSB       0
LB        0 Hz
GB        0
PC                    1.00
```

2c

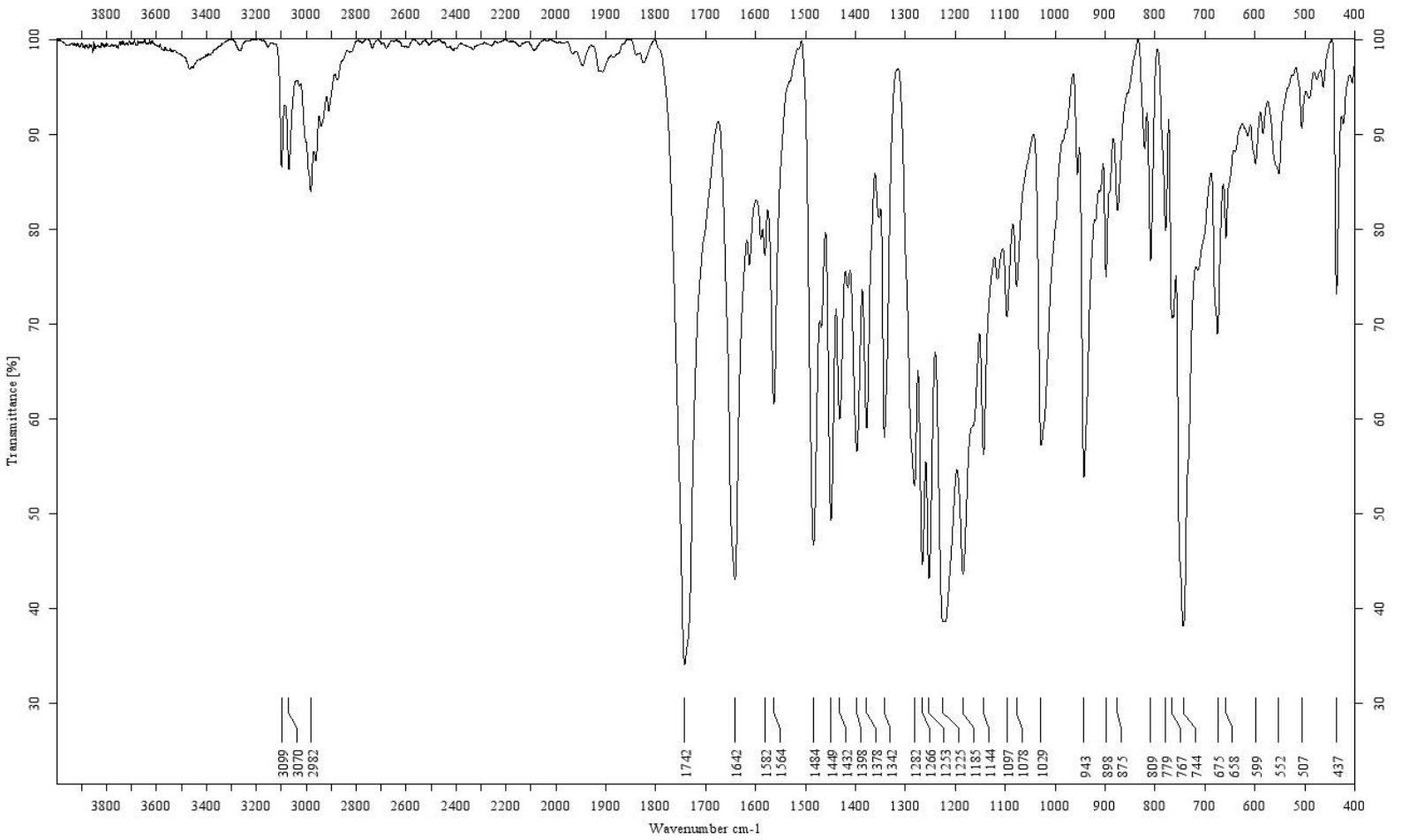



```
Standard 13C
120936
MIM0330_1
Milen Matyas
2017.02.03.  (DA)

Current Data Parameters
NAME                  120936
EXPNO                     12
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   7.11
INSTRUM               spect
PROBHD    5 mm CPPBB0 BB
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              36057.691 Hz
FIDRES            0.550197 Hz
AQ                0.9087659 sec
RG                   196.07
DW                  13.867 usec
DE                  18.00 usec
TE                  295.0 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SF01           150.9254424 MHz
NUC1                    13C
P1                   10.00 usec
PLW1           65.00000000 W

======== CHANNEL f2 ========
SF02           600.1624006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                70.00 usec
PLW2           28.00000000 W
PLW12           0.75571001 W
PLW13           0.37029999 W

F2 - Processing parameters
SI                   65536
SF             150.9103596 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

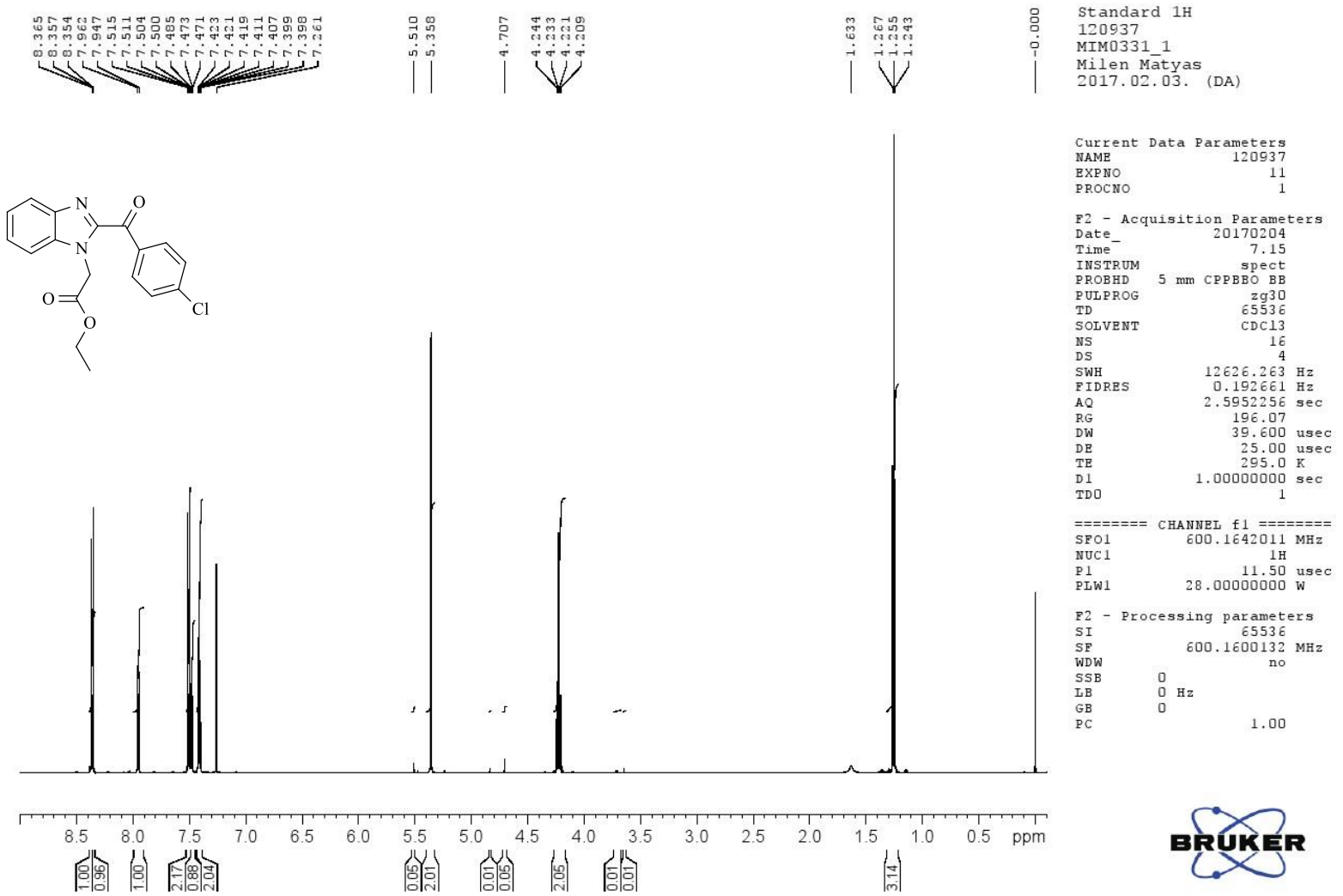
2c

120936	Milen Matyas	KP
MIM0330_1	KBr	02/02/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

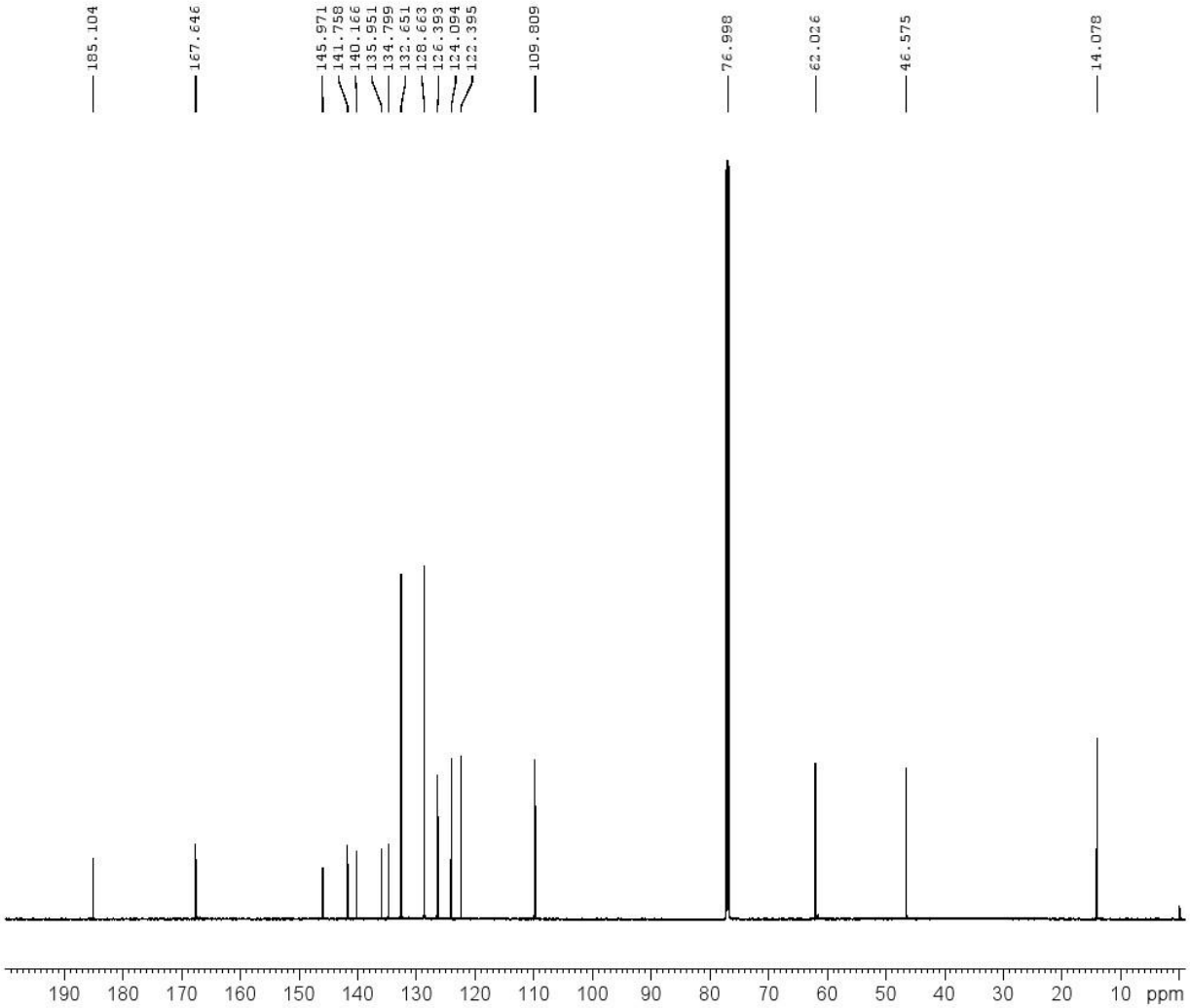


2d




```
Standard 1H
120937
MIM0331_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME                  120937
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   7.15
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        4
SWH               12626.263 Hz
FIDRES             0.192661 Hz
AQ                2.5952256 sec
RG                    196.07
DW                   39.600 usec
DE                   25.00 usec
TE                   295.0 K
D1               1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            600.1642011 MHz
NUC1                      1H
P1                     11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                    65536
SF              600.1600132 MHz
WDW                      no
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```

2d



Standard 13C
120937
MIM0331_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME 120937
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170204
Time 7.58
INSTRUM spect
PROBHD 5 mm CPPBB0 BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 196.07
DW 13.867 usec
DE 18.00 usec
TE 295.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SF01 150.9254424 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W

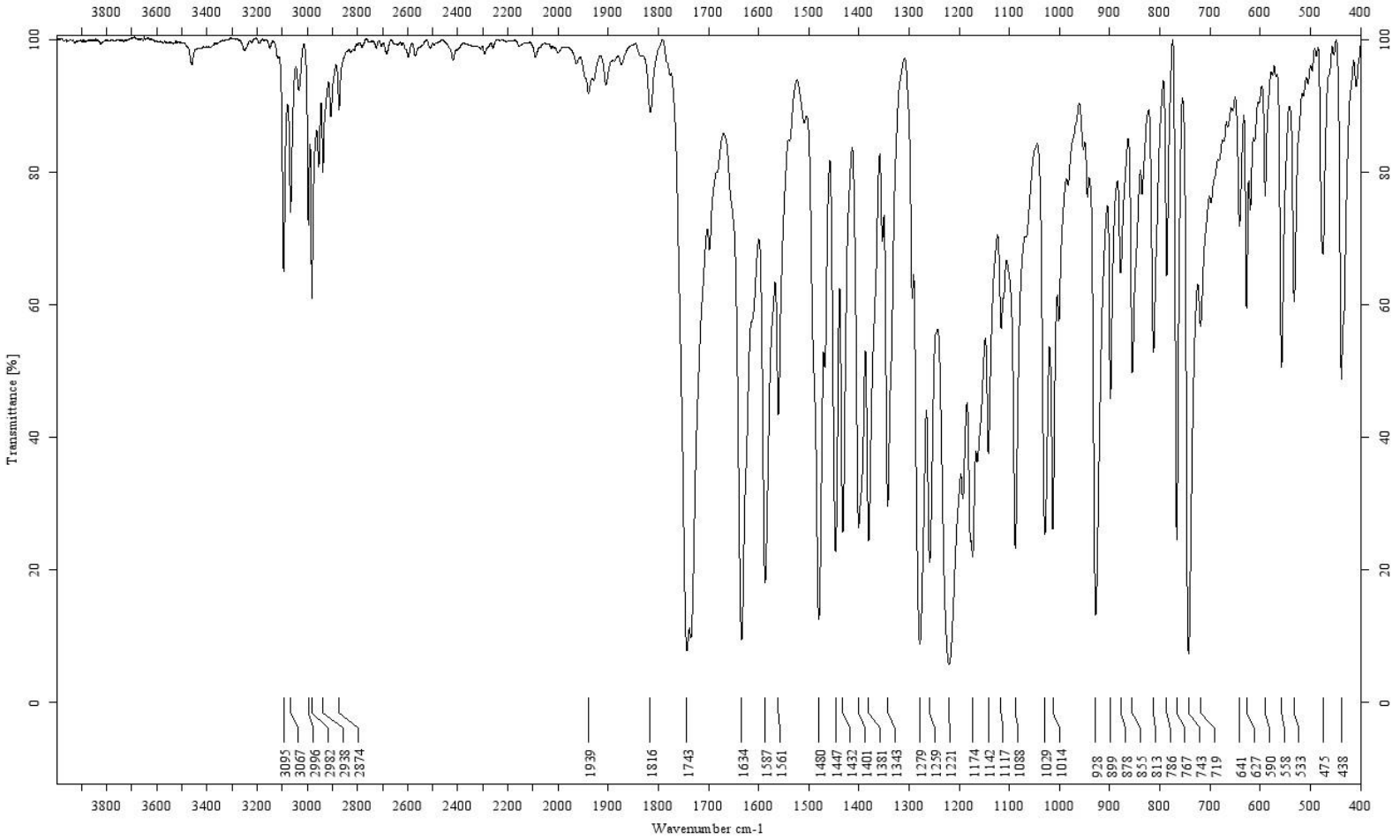
======== CHANNEL f2 ========
SF02 600.1624006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 28.00000000 W
PLW12 0.75571001 W
PLW13 0.37029999 W

F2 - Processing parameters
SI 65536
SF 150.9103601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

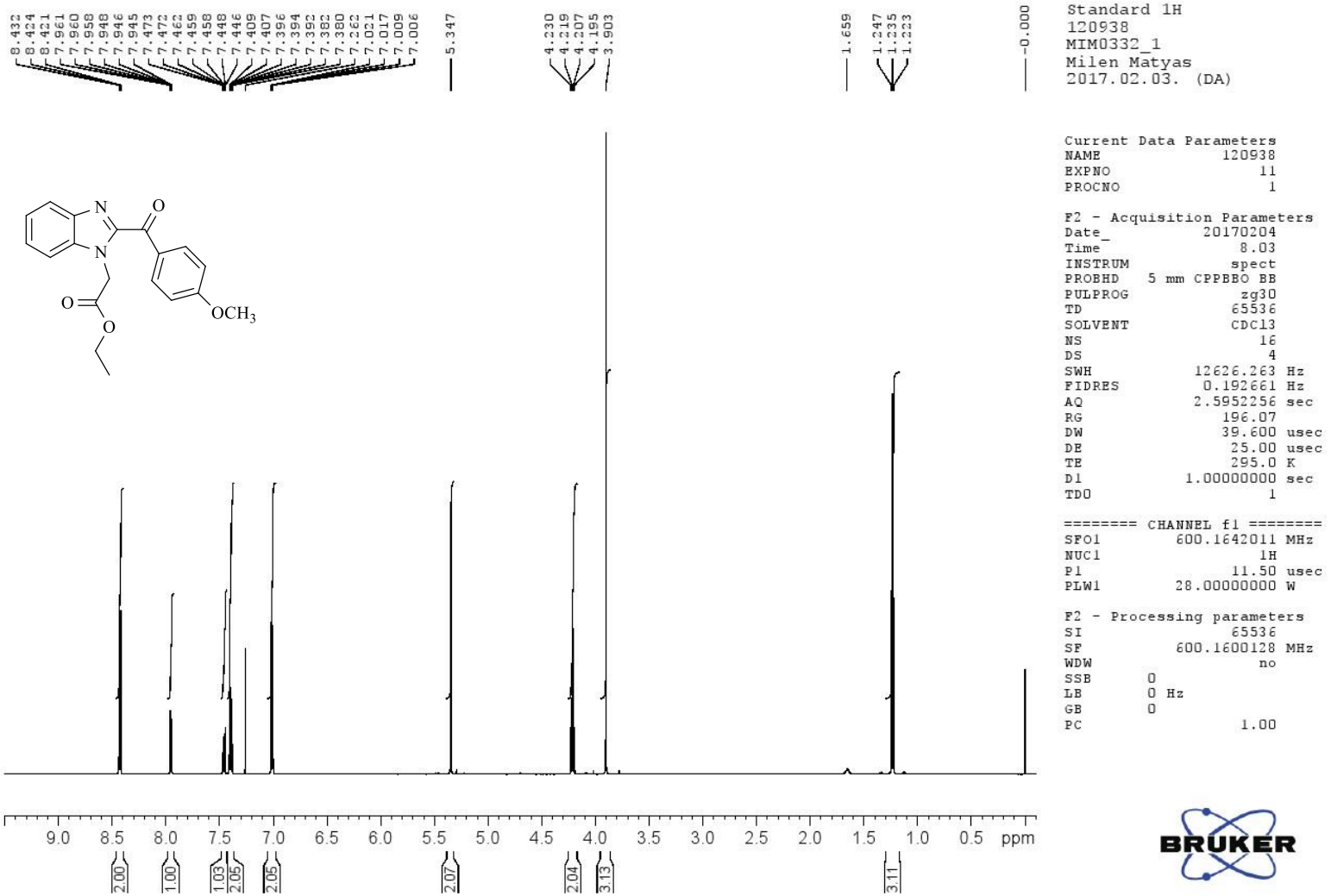
2d

120937	Milen Matyas	KP
MIM0331_1	KBr	02/02/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

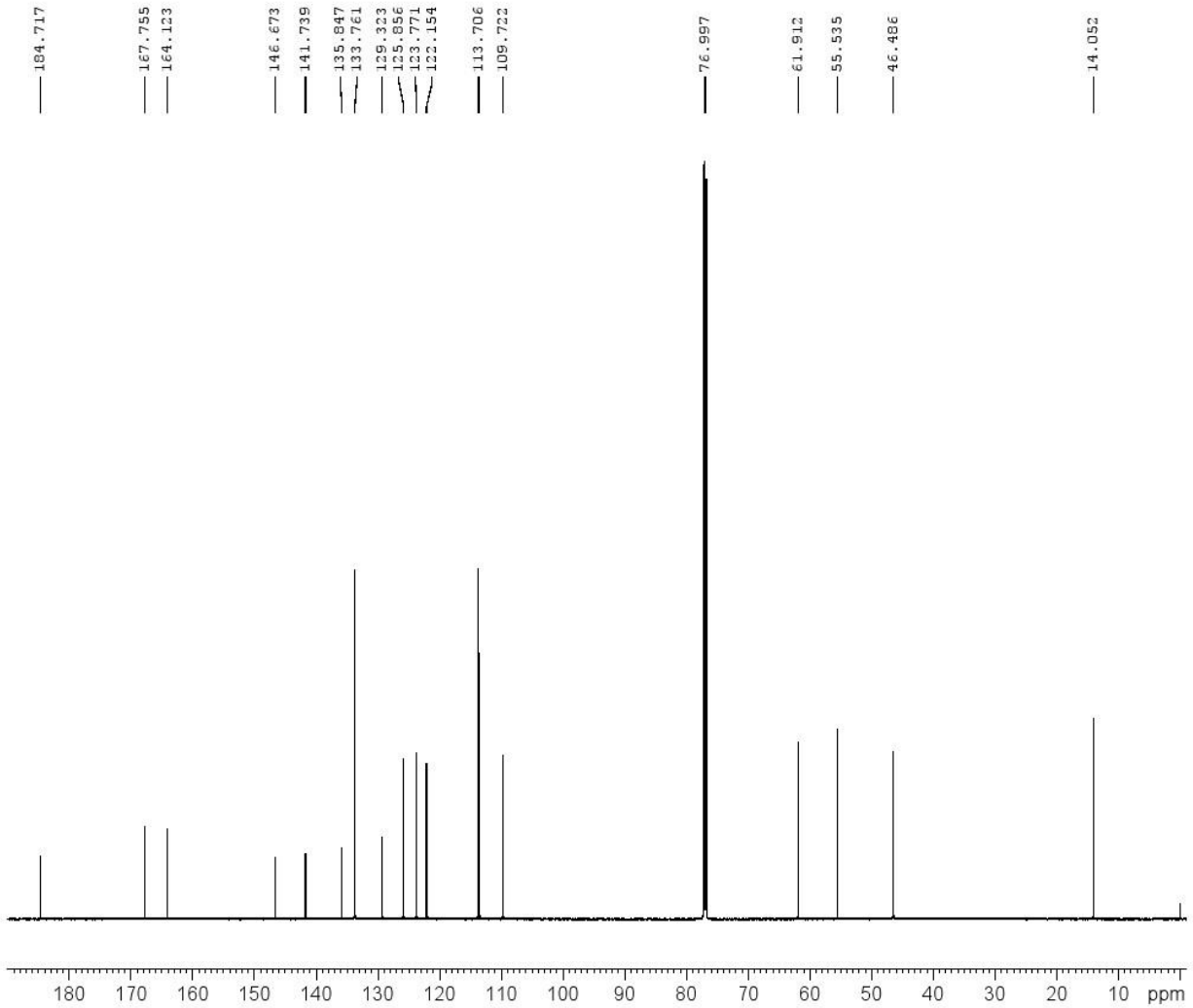


2e




```
Standard 1H
120938
MIM0332_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME                  120938
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   8.03
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        4
SWH               12626.263 Hz
FIDRES             0.192661 Hz
AQ                 2.5952256 sec
RG                    196.07
DW                    39.600 usec
DE                    25.00 usec
TE                    295.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            600.1642011 MHz
NUC1                      1H
P1                     11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                    65536
SF              600.1600128 MHz
WDW                      no
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```

2e

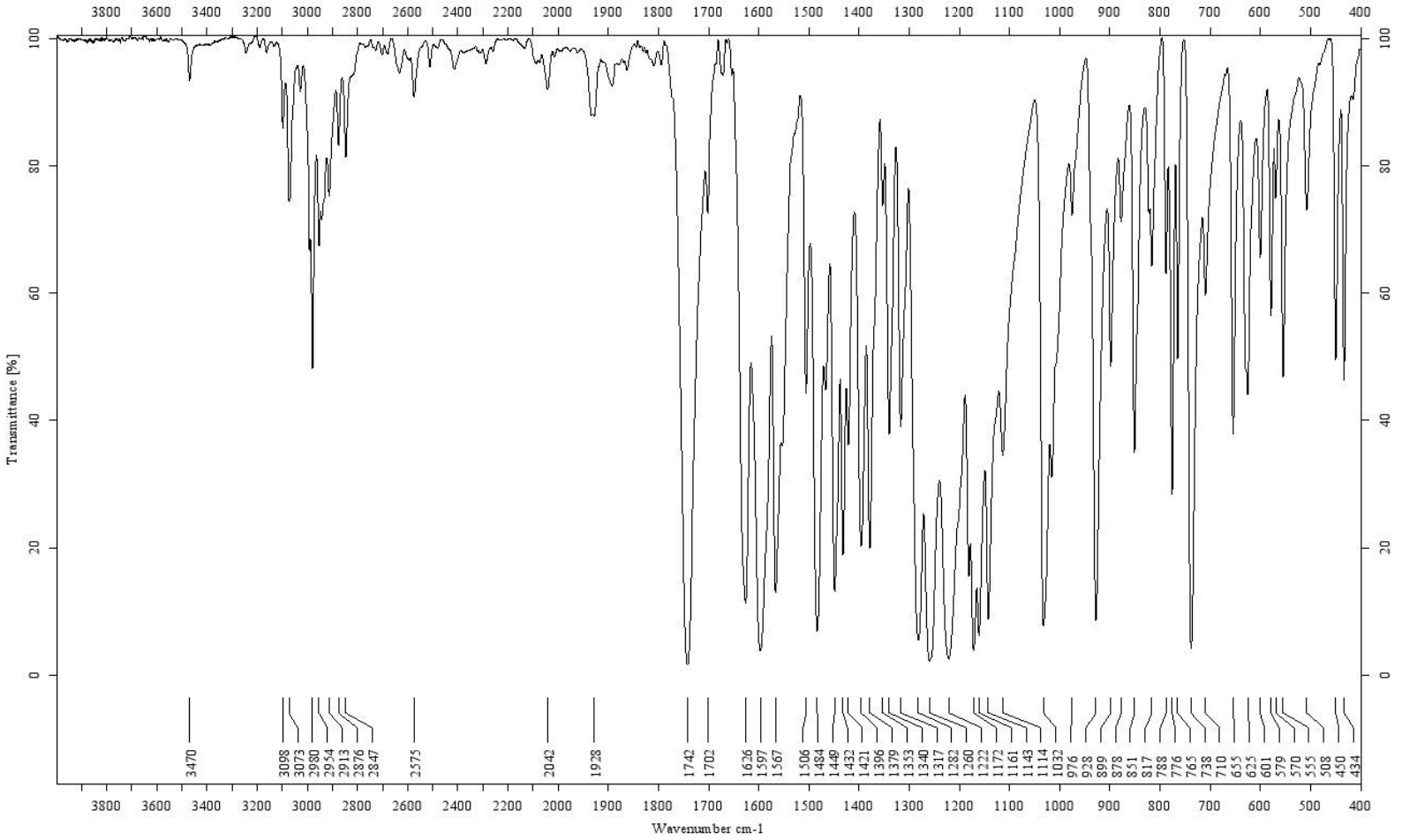



```
Standard 13C
120938
MIM0332_1
Milen Matyas
2017.02.03.  (DA)

Current Data Parameters
NAME                  120938
EXPNO                     12
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   8.46
INSTRUM               spect
PROBHD    5 mm CPPBB0 BB
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               36057.691 Hz
FIDRES             0.550197 Hz
AQ                 0.9087659 sec
RG                    196.07
DW                   13.867 usec
DE                   18.00 usec
TE                   295.0 K
D1                1.50000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SF01           150.9254424 MHz
NUC1                    13C
P1                   10.00 usec
PLW1           65.00000000 W

======== CHANNEL f2 ========
SF02           600.1624006 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                70.00 usec
PLW2           28.00000000 W
PLW12           0.75571001 W
PLW13           0.37029999 W

F2 - Processing parameters
SI                    65536
SF             150.9103604 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

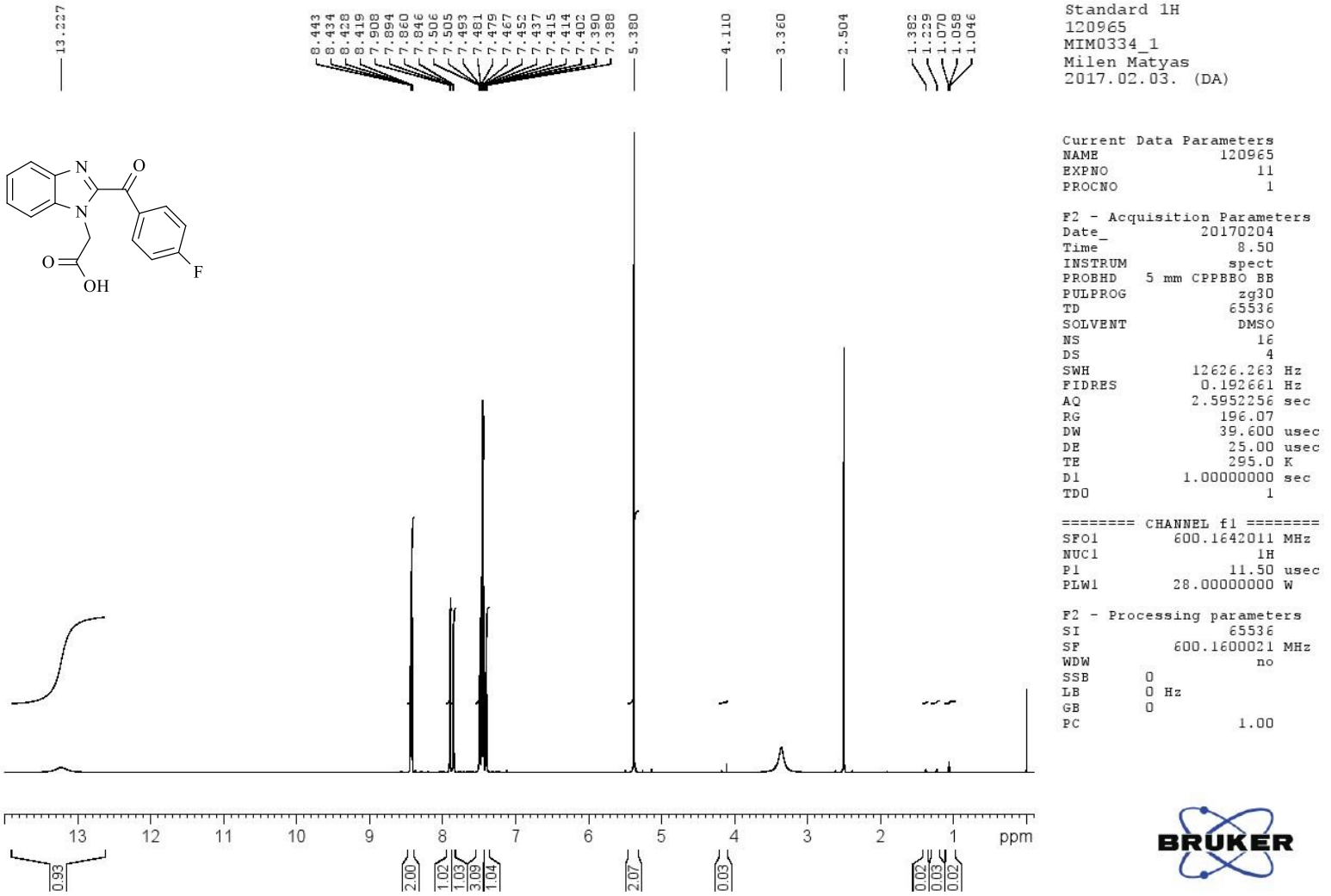
2e

120938	Milen Matyas	KP
MIM0332_1	KBr	02/02/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

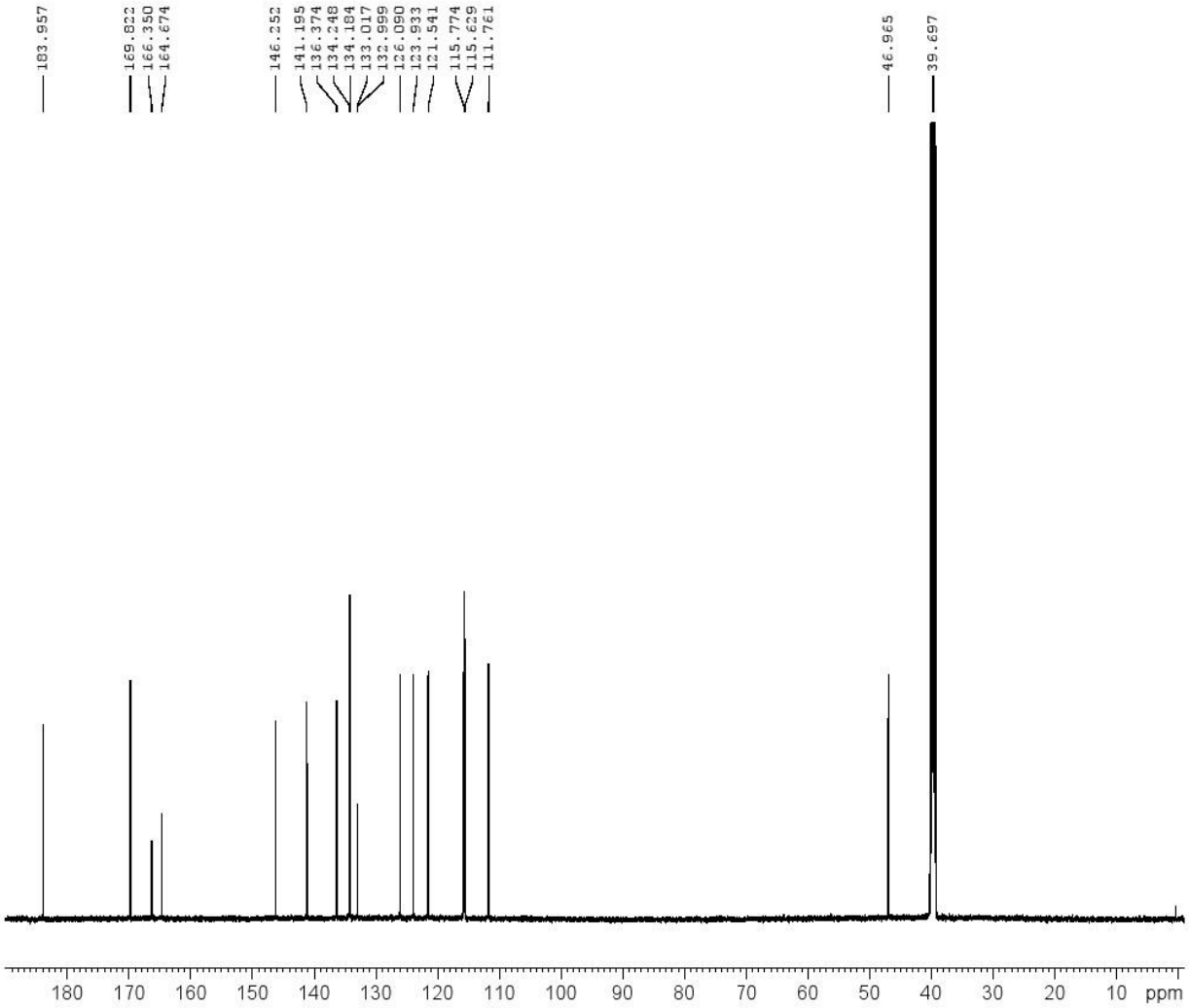


3a




```
Standard 1H
120965
MIM0334_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME                  120965
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   8.50
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         4
SWH               12626.263 Hz
FIDRES             0.192661 Hz
AQ                 2.5952256 sec
RG                    196.07
DW                    39.600 usec
DE                    25.00 usec
TE                    295.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            600.1642011 MHz
NUC1                      1H
P1                     11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                    65536
SF              600.1600021 MHz
WDW                      no
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```

3a

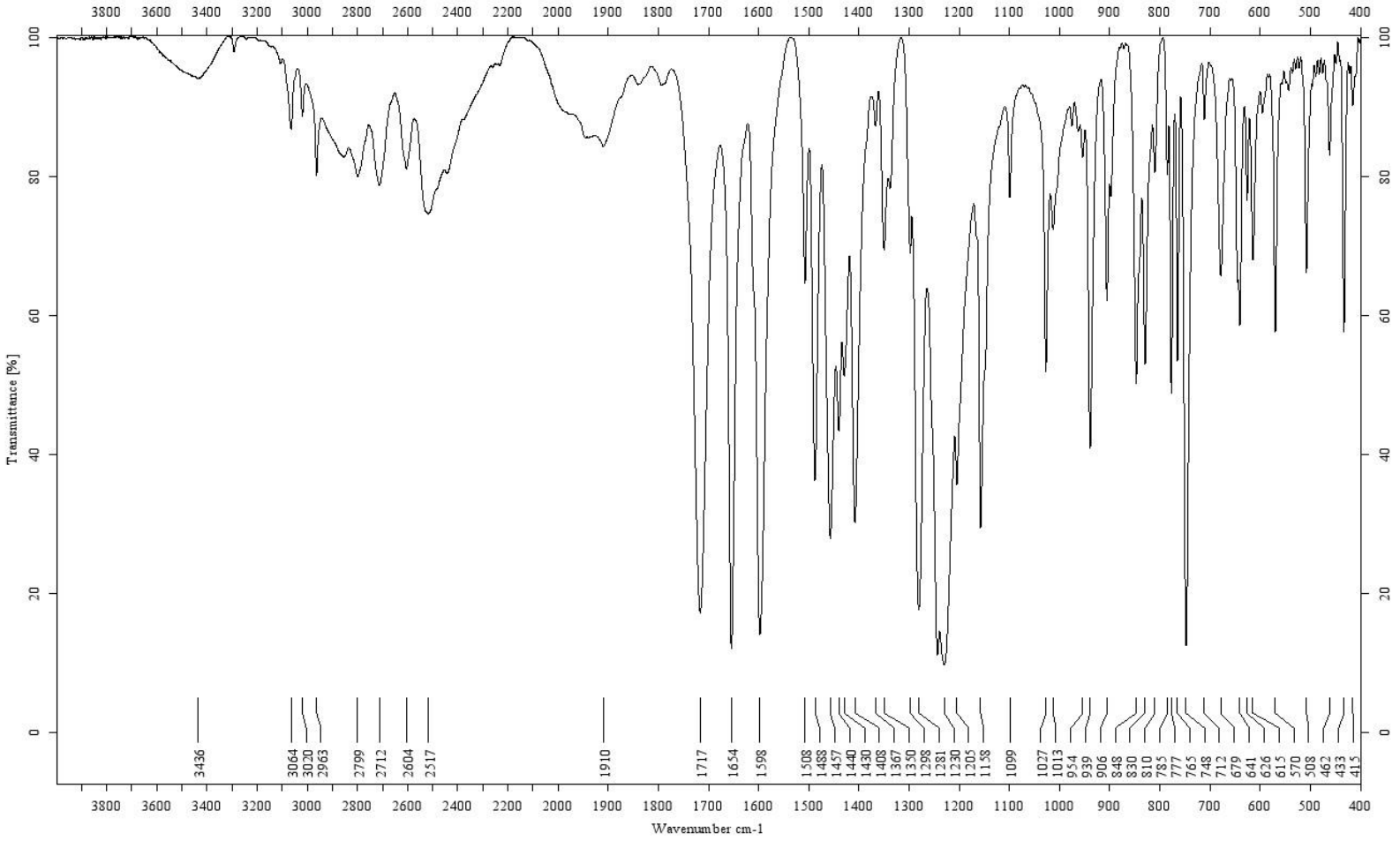



```
Standard 13C
120965
MIM0334_1
Milen Matyas
2017.02.03.  (DA)

Current Data Parameters
NAME                  120965
EXPNO                     12
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   9.34
INSTRUM               spect
PROBHD    5 mm CPPBB0 BB
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH               36057.691 Hz
FIDRES             0.550197 Hz
AQ                0.9087659 sec
RG                   196.07
DW                   13.867 usec
DE                    18.00 usec
TE                    295.0 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SF01           150.9254424 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           65.00000000 W

======== CHANNEL f2 ========
SF02           600.1624006 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 70.00 usec
PLW2           28.00000000 W
PLW12           0.75571001 W
PLW13           0.37029999 W

F2 - Processing parameters
SI                    65536
SF             150.9103912 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

3a

120965	Milen Matyas	KP
MIM0334_1	KBr	07/02/2017

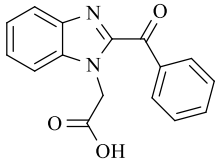
BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

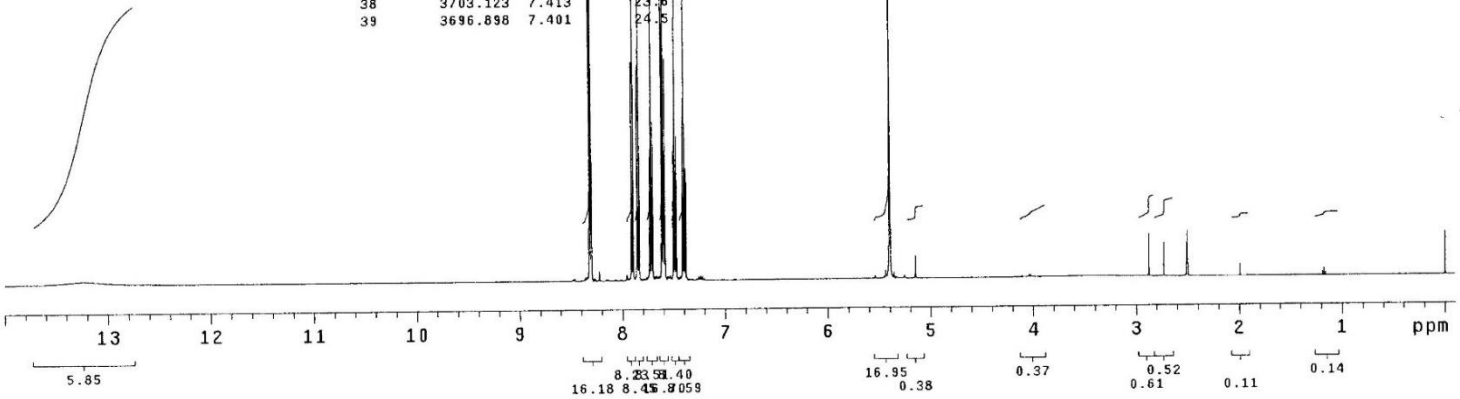


3b

STANDARD 1H
62974
MM152
Milen Matyas
2006.04.10. (CzB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 11999.4 Hz
16 repetitions
OBSERVE H1, 499.5268332 MHz
DATA PROCESSING
FT size 131072
Total time 1 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	4158.300	8.324	9.3	40	3695.982	7.399	38.6
2	4156.653	8.321	55.1	41	3694.884	7.397	24.6
3	4156.103	8.320	48.8	42	3688.841	7.385	19.3
4	4155.371	8.319	63.3	43	3687.743	7.382	17.0
5	4150.244	8.308	18.2	44	2717.332	5.440	1.4
6	4148.230	8.304	67.2	45	2697.192	5.399	154.0
7	4146.948	8.302	57.2	46	2676.868	5.359	1.1
8	4108.498	8.225	1.7	47	2571.405	5.148	3.9
9	3974.289	7.956	0.9	48	1436.207	2.875	7.3
10	3951.585	7.911	37.7	49	1363.152	2.729	5.8
11	3943.345	7.894	41.0	50	1362.603	2.728	4.8
12	3923.937	7.855	36.3	51	1253.844	2.510	2.6
13	3915.698	7.839	39.6	52	1252.013	2.506	5.8
14	3865.346	7.738	9.3	53	1250.182	2.503	7.8
15	3864.065	7.735	16.6	54	1248.351	2.499	5.5
16	3862.783	7.733	9.1	55	1246.520	2.495	2.4
17	3858.389	7.724	13.2	56	994.030	1.990	2.0
18	3856.741	7.721	37.7	57	585.542	1.172	1.2
19	3854.910	7.717	12.2	58	0.000	0.000	7.4
20	3850.515	7.708	15.9				
21	3849.234	7.706	27.2				
22	3847.952	7.703	13.5				
23	3805.291	7.618	49.2				
24	3803.643	7.614	18.1				
25	3797.601	7.602	70.0				
26	3797.234	7.602	67.7				
27	3791.375	7.590	14.6				
28	3789.728	7.587	38.2				
29	3749.629	7.506	18.8				
30	3748.531	7.504	18.0				
31	3742.489	7.492	28.5				
32	3741.390	7.490	36.6				
33	3740.292	7.488	18.6				
34	3734.249	7.476	24.8				
35	3733.151	7.473	21.8				
36	3707.883	7.423	0.9				
37	3704.038	7.415	25.4				
38	3703.123	7.413	23.6				
39	3696.898	7.401	24.5				





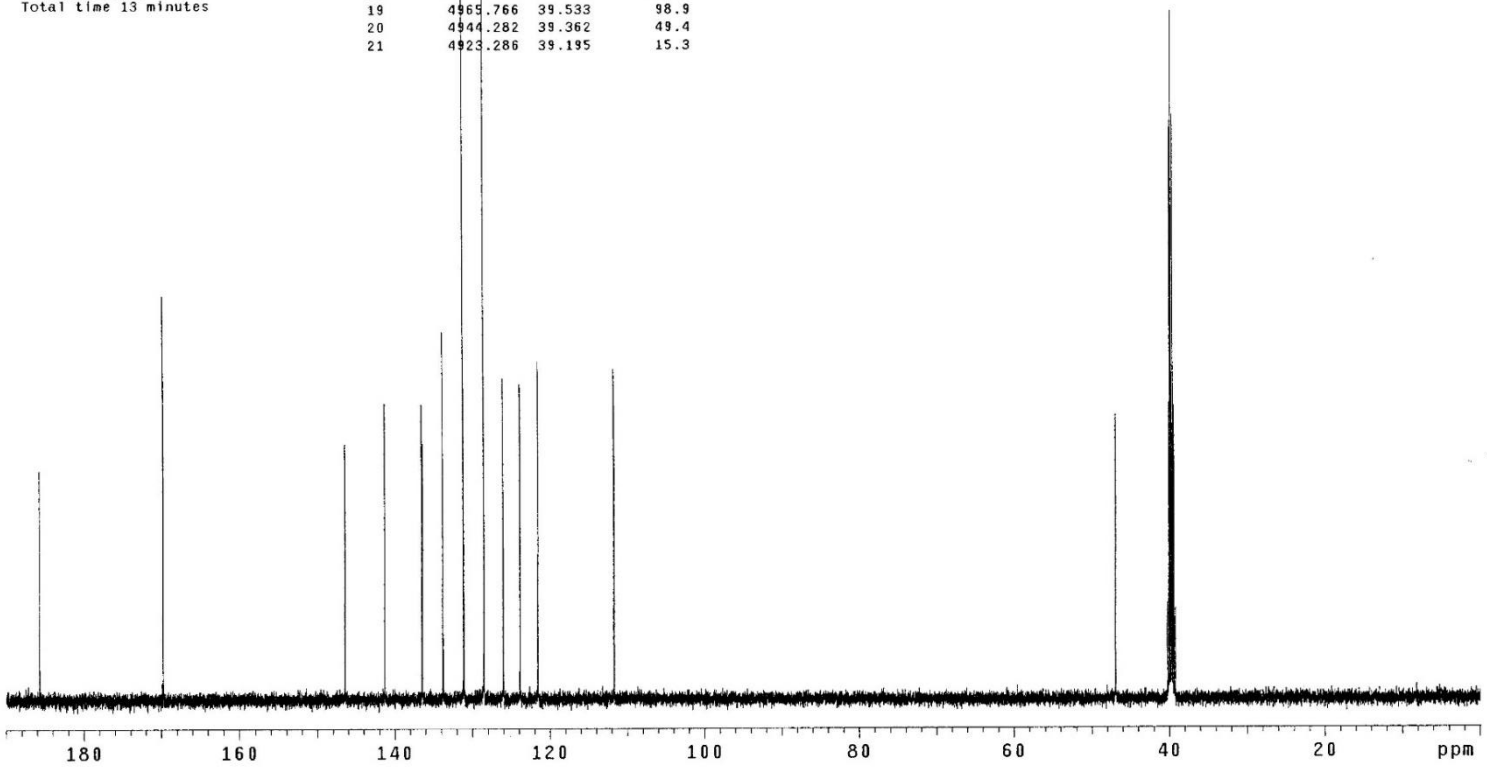
3b

STANDARD 13C
62974
MM152
Milen Matyas
2006.04.10. (CzB)

Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"

PULSE SEQUENCE
Relax. delay 1.200 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
320 repetitions
OBSERVE C13, 125.6061568 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 13 minutes

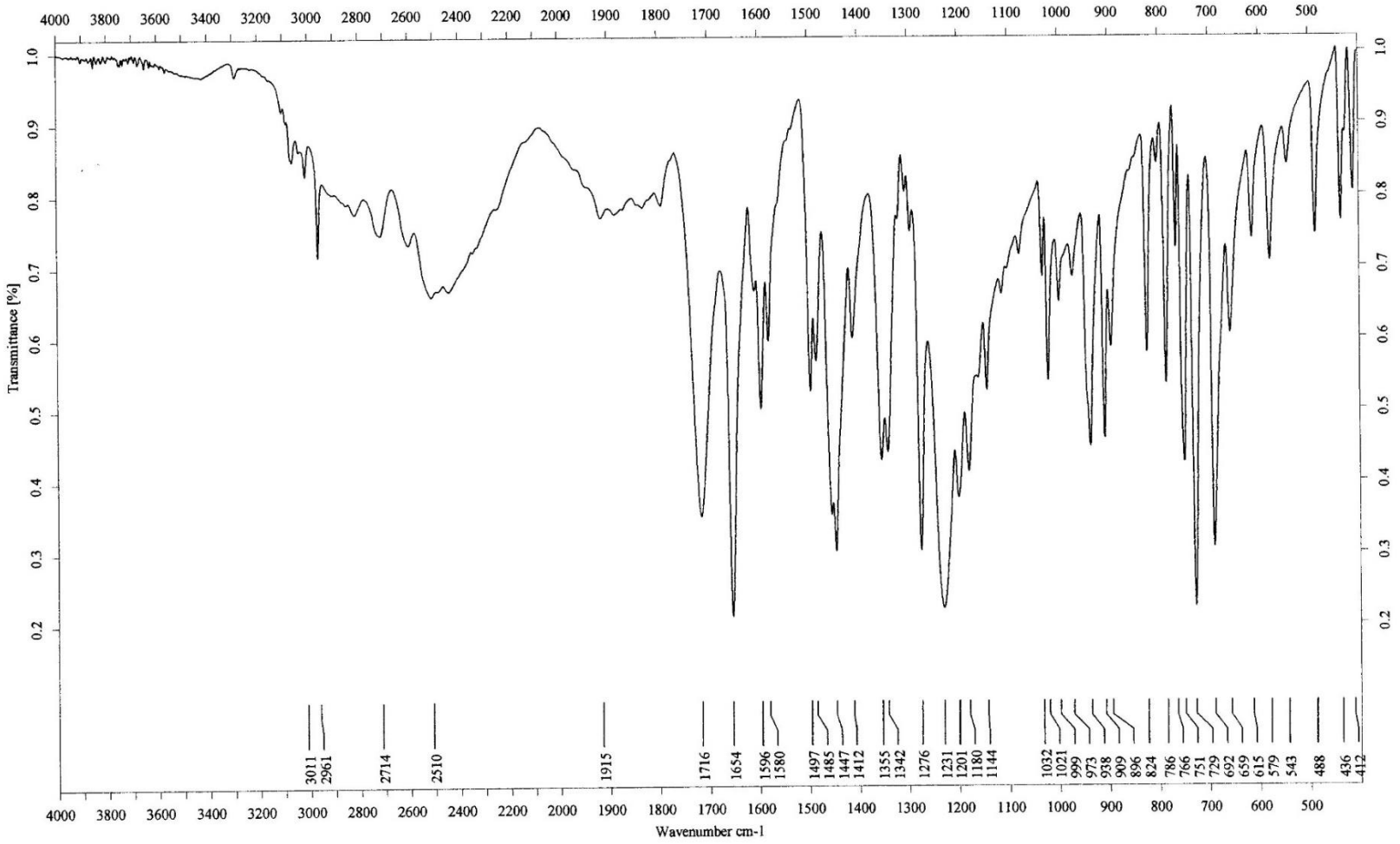
INDEX	FREQUENCY	PPM	HEIGHT
1	23325.141	185.693	38.9
2	21326.606	169.783	68.5
3	18391.548	146.417	43.2
4	17743.110	141.254	50.1
5	17138.130	136.438	49.9
6	17128.852	136.364	43.2
7	16798.774	133.736	62.1
8	16466.743	131.093	161.4
9	16135.106	128.485	156.6
10	15826.606	125.997	54.4
11	15556.098	123.843	53.4
12	15266.548	121.538	57.1
13	14026.755	111.684	55.9
14	5892.036	46.907	48.0
15	5049.751	40.201	16.2
16	5028.755	40.034	49.9
17	5007.758	39.867	98.0
18	4986.762	39.700	116.5
19	4965.766	39.533	98.9
20	4944.282	39.362	49.4
21	4923.286	39.195	15.3



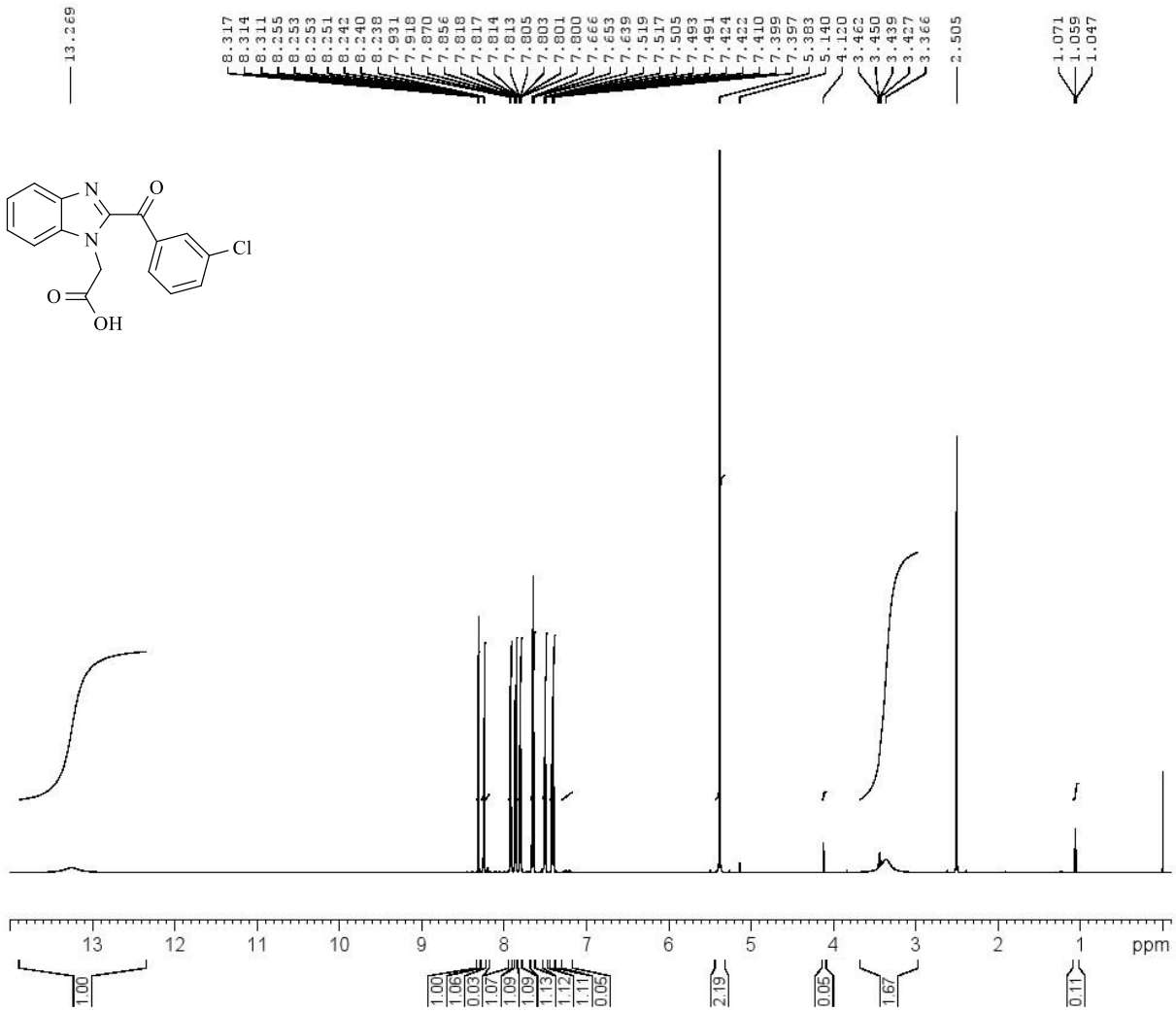
3b

62974	Milen Mátyás	SzA
MM152	KBr	12/04/2006

BRUKER VECTOR22
Resolution: 2 cm-1
Number of Scans: 8

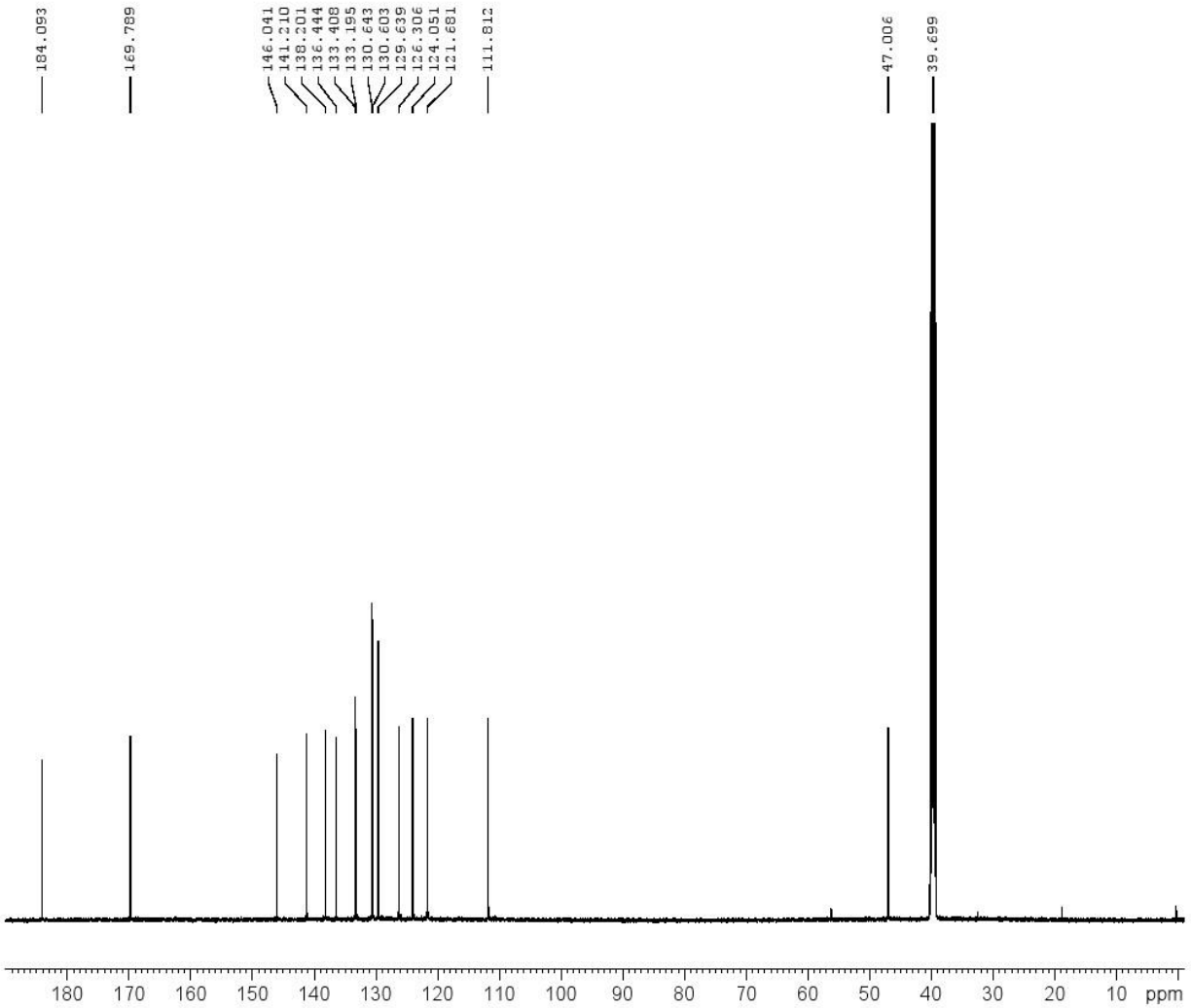


3c




```
Standard 1H
120967
MIM0336_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME                  120967
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   10.25
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         4
SWH               12626.263 Hz
FIDRES             0.192661 Hz
AQ                 2.5952256 sec
RG                    196.07
DW                   39.600 usec
DE                   25.00 usec
TE                   295.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            600.1642011 MHz
NUC1                      1H
P1                     11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                    65536
SF              600.1600019 MHz
WDW                      no
SSB       0
LB        0 Hz
GB        0
PC                     1.00
```

3c



Standard 13C
120967
MIM0336_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME 120967
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170204
Time 11.08
INSTRUM spect
PROBHD 5 mm CPPBB0 BB
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 196.07
DW 13.867 usec
DE 18.00 usec
TE 295.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SF01 150.9254424 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W

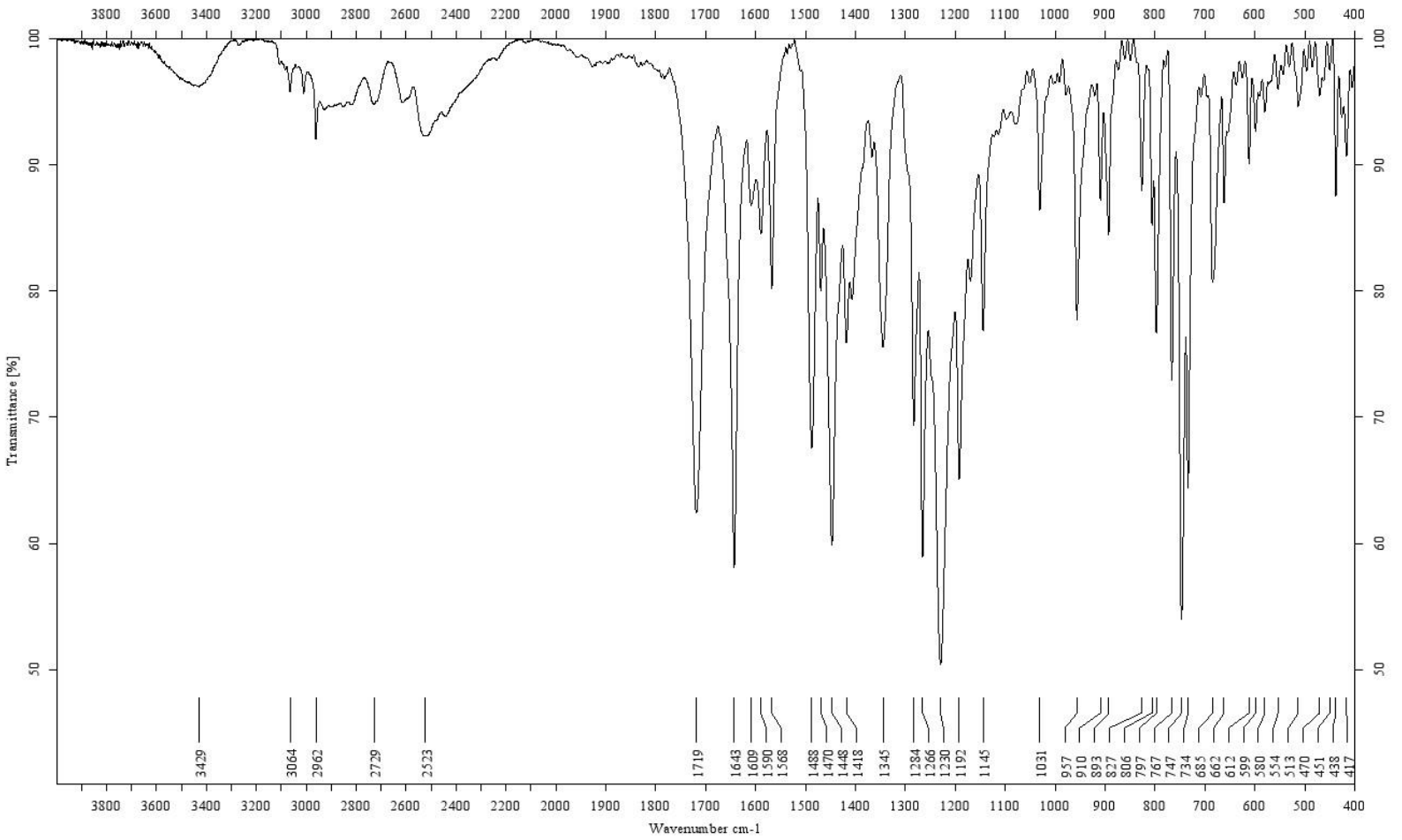
======== CHANNEL f2 ========
SF02 600.1624006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 28.00000000 W
PLW12 0.75571001 W
PLW13 0.37029999 W

F2 - Processing parameters
SI 65536
SF 150.9103911 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

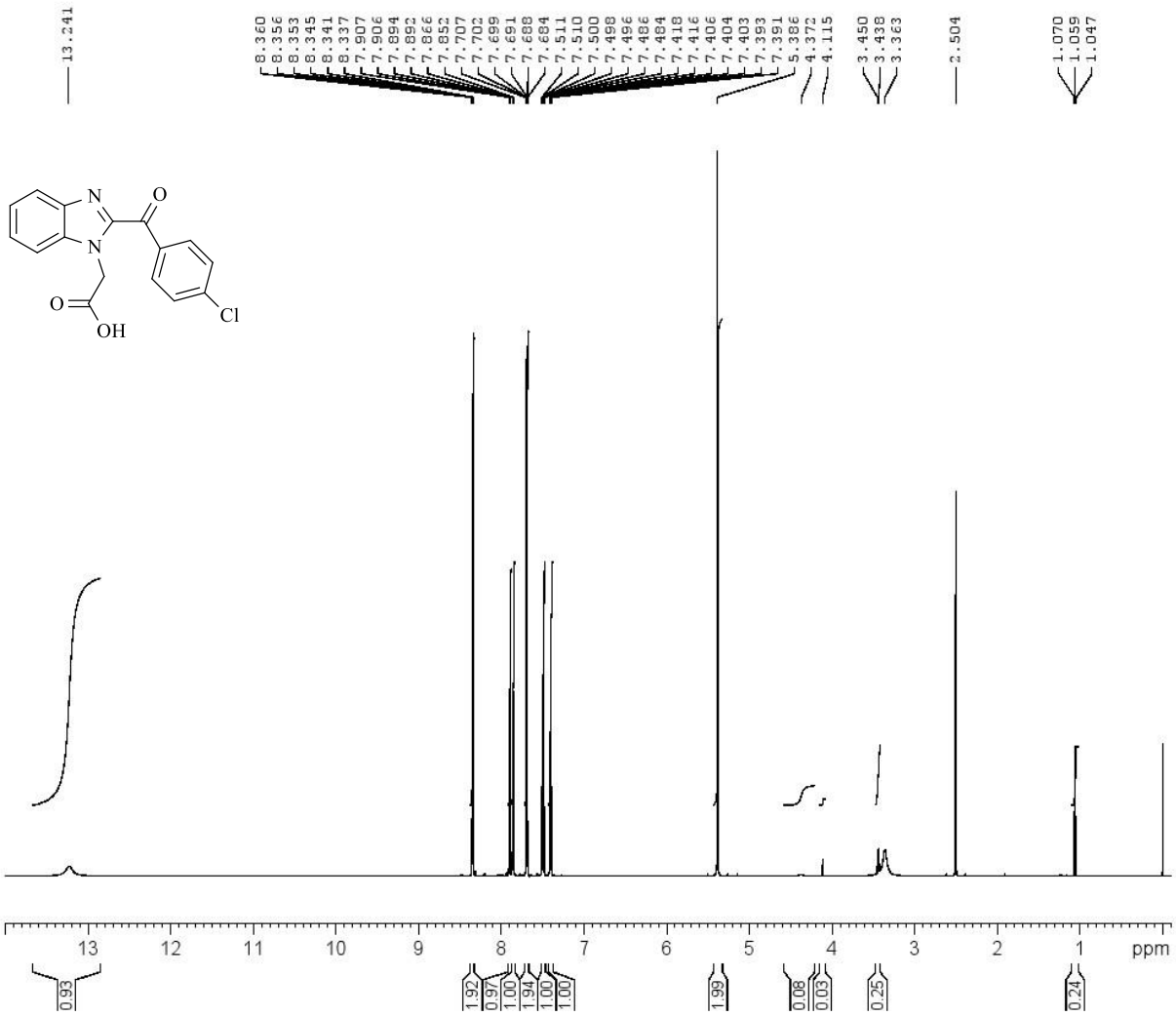
3c

120967	Milen Matyas	KP
MIM0336_1	KBr	06/02/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

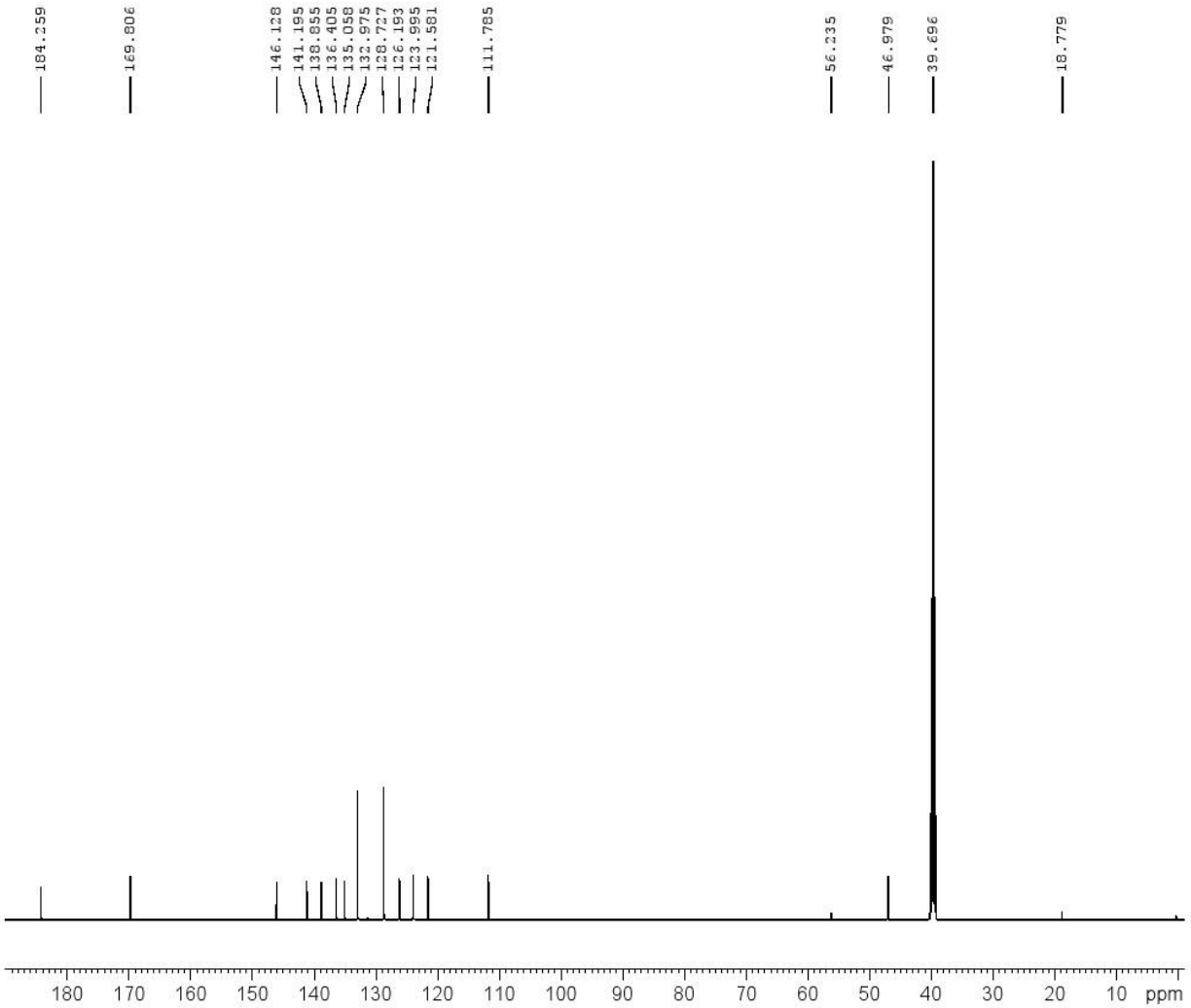


3d




```
Standard 1H
120966
MIM0335_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME                  120966
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                   9.38
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         4
SWH               12626.263 Hz
FIDRES             0.192661 Hz
AQ                 2.5952256 sec
RG                    196.07
DW                    39.600 usec
DE                    25.00 usec
TE                    295.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            600.1642011 MHz
NUC1                      1H
P1                     11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                    65536
SF              600.1600021 MHz
WDW                      no
SSB       0
LB        0 Hz
GB        0
PC                     1.00
```

3d



Standard 13C
120966
MIM0335_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME 120966
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170204
Time 10.21
INSTRUM spect
PROBHD 5 mm CPPBB0 BB
PULPROG zgpg30
TD 65536
SOLVENT DMS0
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 196.07
DW 13.867 usec
DE 18.00 usec
TE 295.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SF01 150.9254424 MHz
NUC1 13C
P1 10.00 usec
PLW1 65.00000000 W

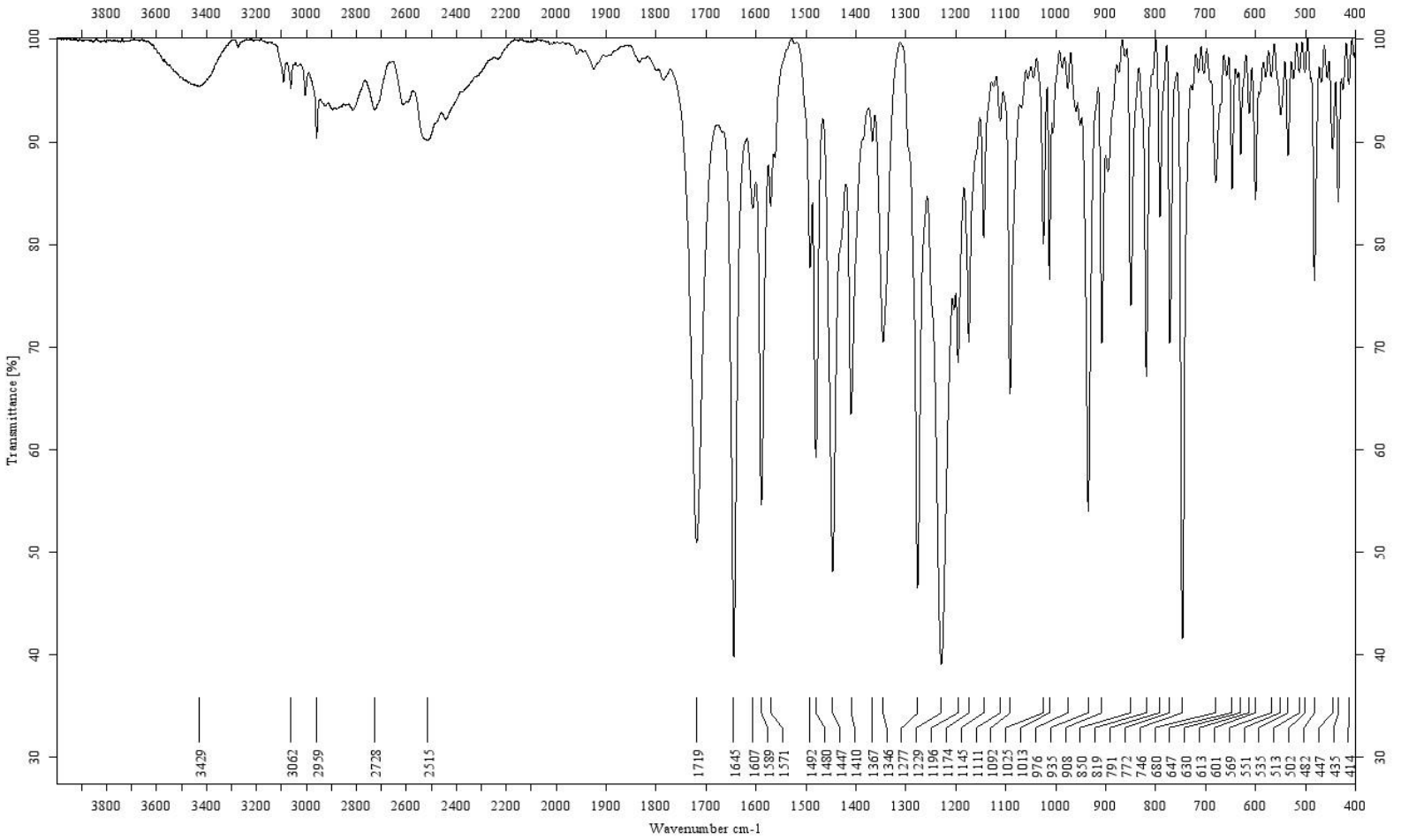
======== CHANNEL f2 ========
SF02 600.1624006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 28.00000000 W
PLW12 0.75571001 W
PLW13 0.37029999 W

F2 - Processing parameters
SI 65536
SF 150.9103916 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

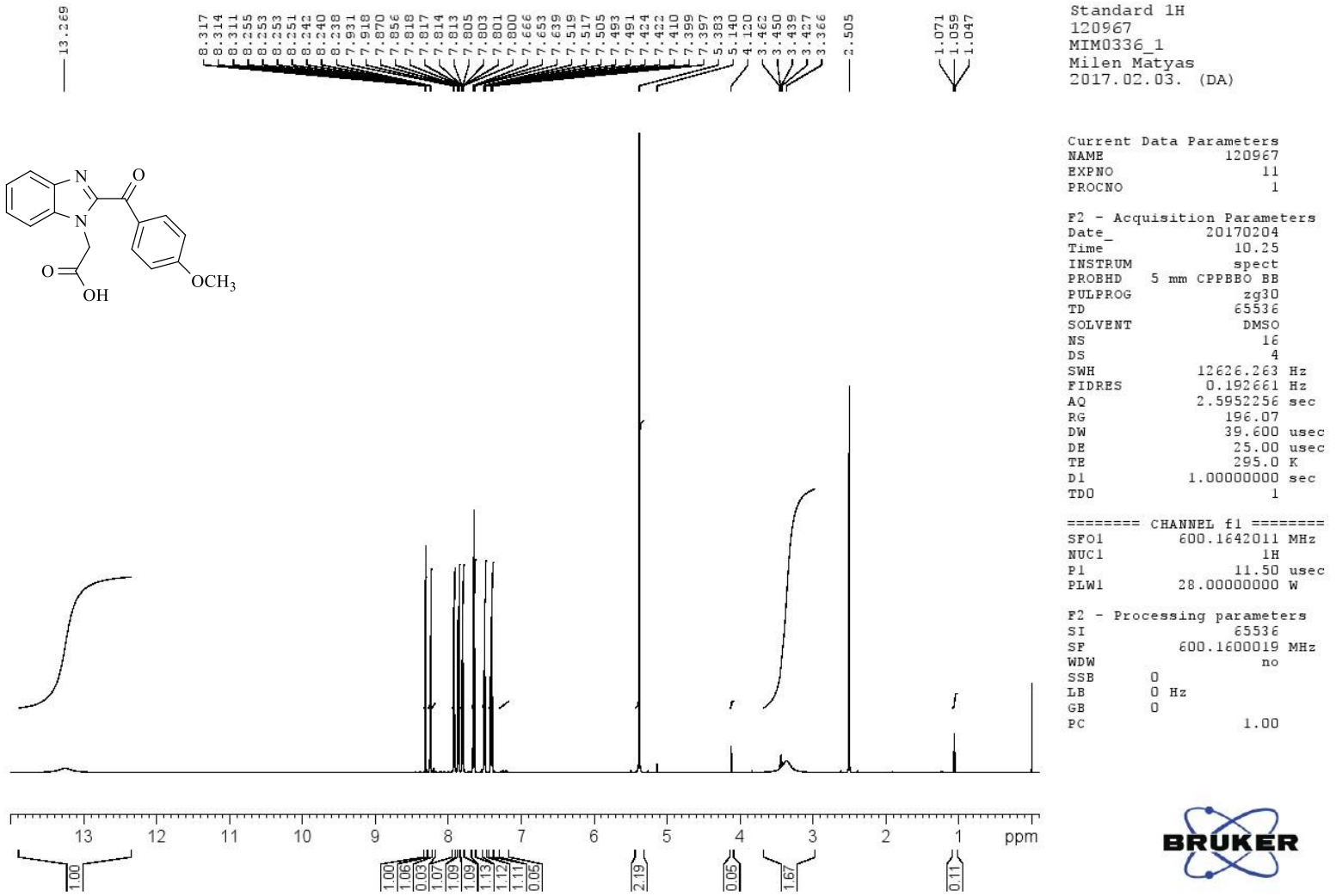
3d

120966	Milen Matyas	KP
MIM0335_1	KBr	07/02/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

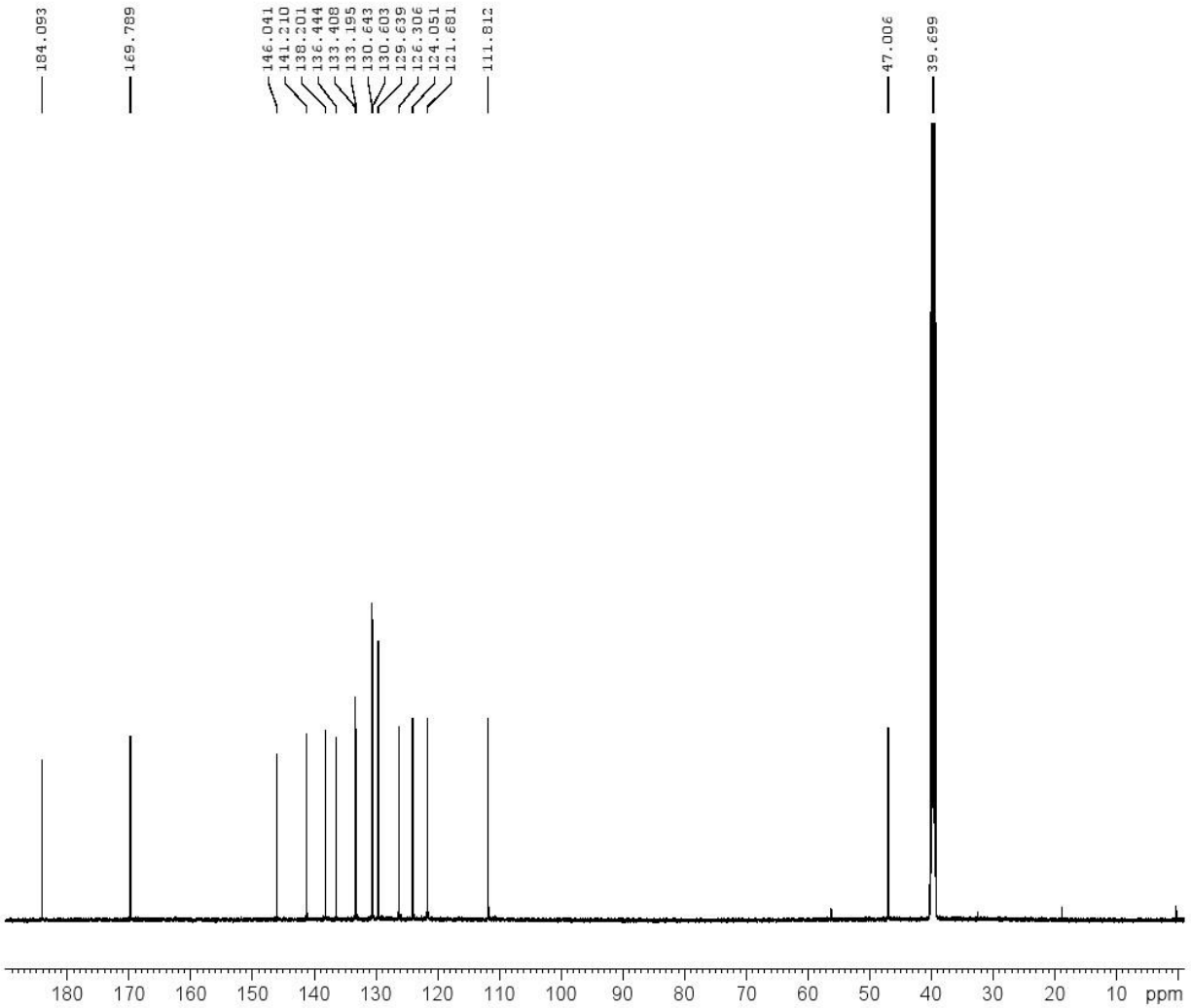


3e




```
Standard 1H
120967
MIM0336_1
Milen Matyas
2017.02.03. (DA)

Current Data Parameters
NAME                  120967
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                  10.25
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         4
SWH               12626.263 Hz
FIDRES             0.192661 Hz
AQ                 2.5952256 sec
RG                    196.07
DW                    39.600 usec
DE                    25.00 usec
TE                    295.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            600.1642011 MHz
NUC1                      1H
P1                    11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                    65536
SF              600.1600019 MHz
WDW                      no
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```

3e

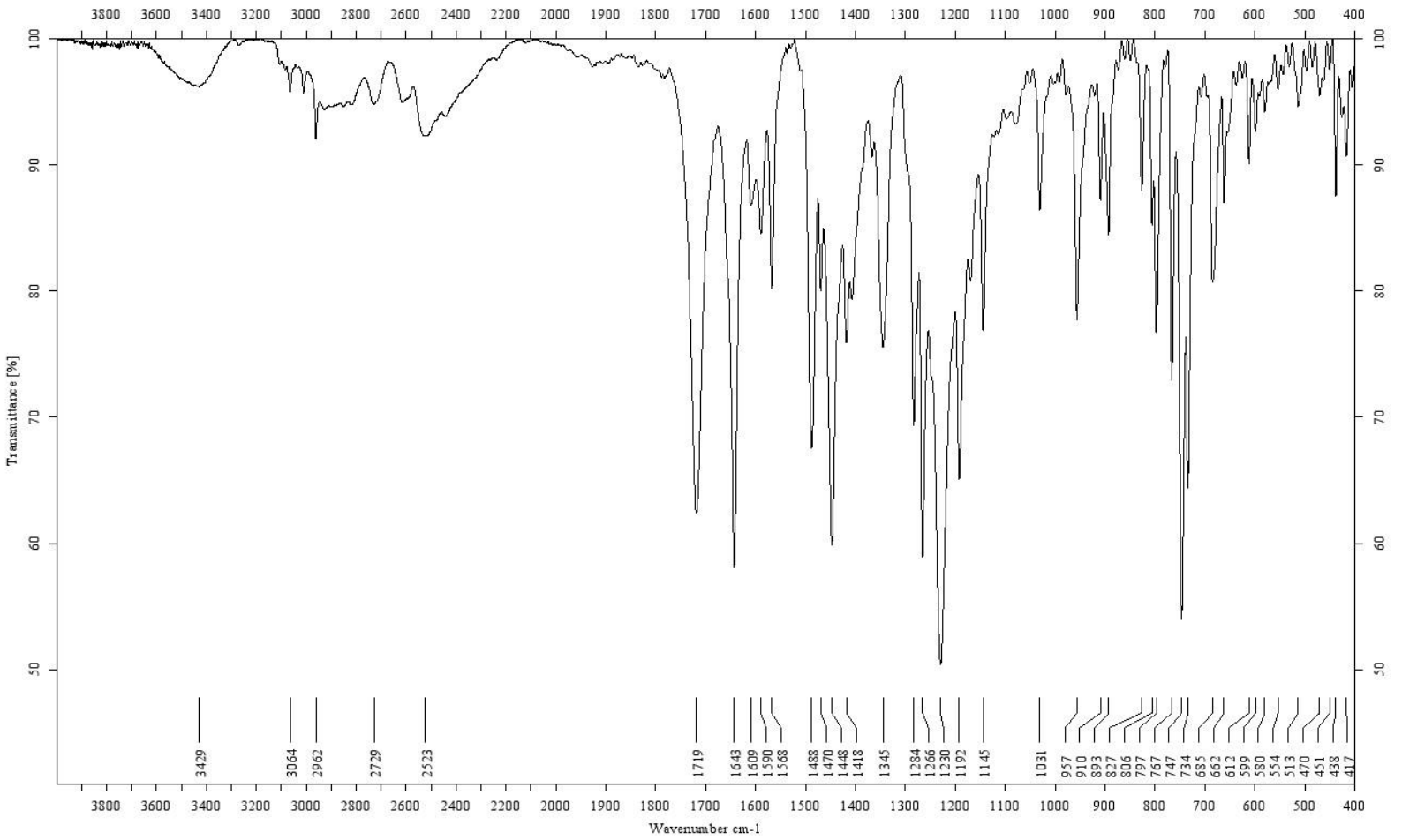



```
Standard 13C
120967
MIM0336_1
Milen Matyas
2017.02.03.  (DA)

Current Data Parameters
NAME                  120967
EXPNO                     12
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170204
Time                  11.08
INSTRUM               spect
PROBHD    5 mm CPPBB0 BB
PULPROG               zgpg30
TD                    65536
SOLVENT                DMSO
NS                      1024
DS                         4
SWH               36057.691 Hz
FIDRES             0.550197 Hz
AQ                0.9087659 sec
RG                   196.07
DW                   13.867 usec
DE                   18.00 usec
TE                   295.0 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SF01            150.9254424 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           65.00000000 W

======== CHANNEL f2 ========
SF02            600.1624006 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 70.00 usec
PLW2           28.00000000 W
PLW12           0.75571001 W
PLW13           0.37029999 W

F2 - Processing parameters
SI                    65536
SF              150.9103911 MHz
WDW                     EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

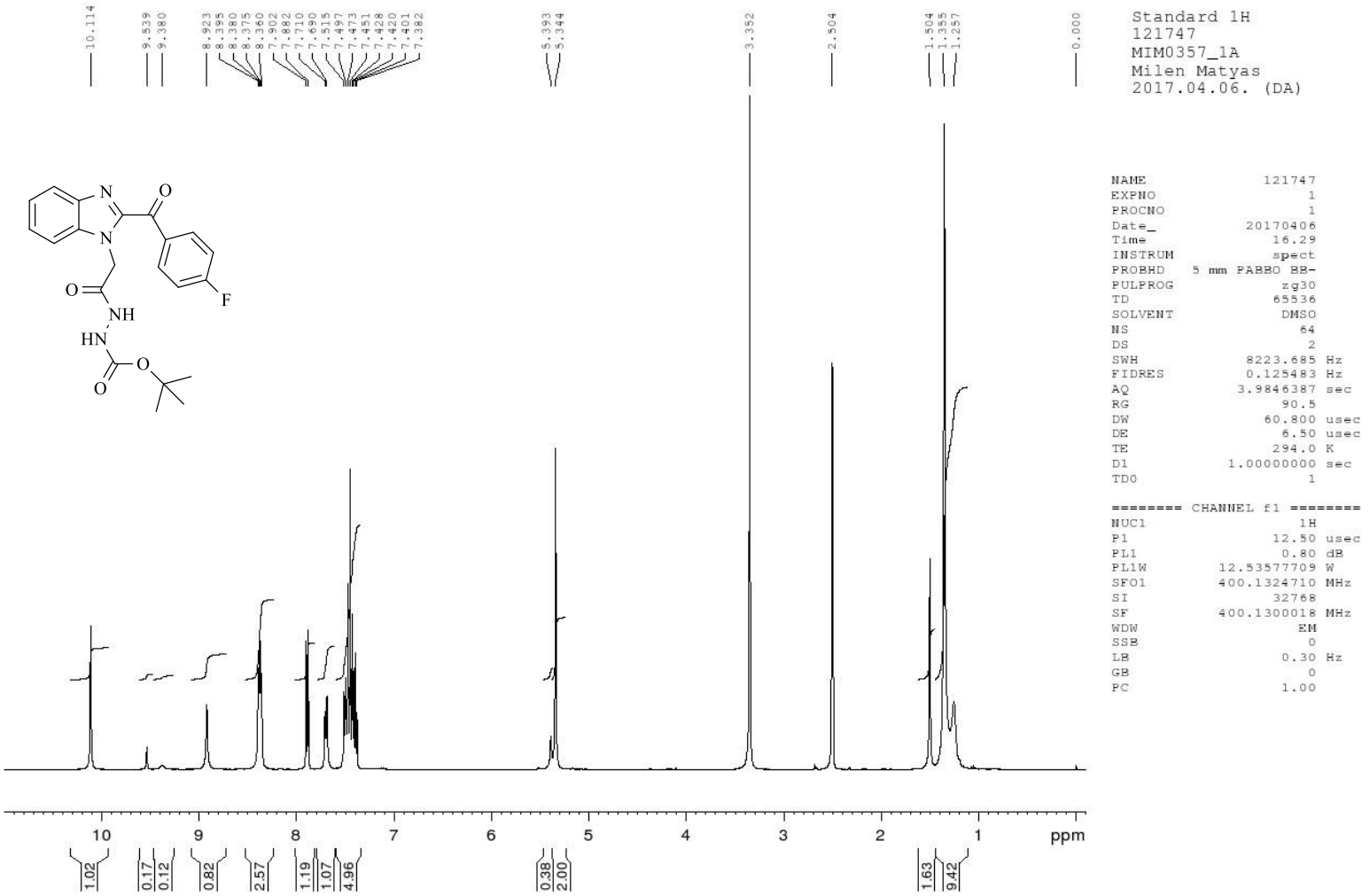
3e

120967	Milen Matyas	KP
MIM0336_1	KBr	06/02/2017

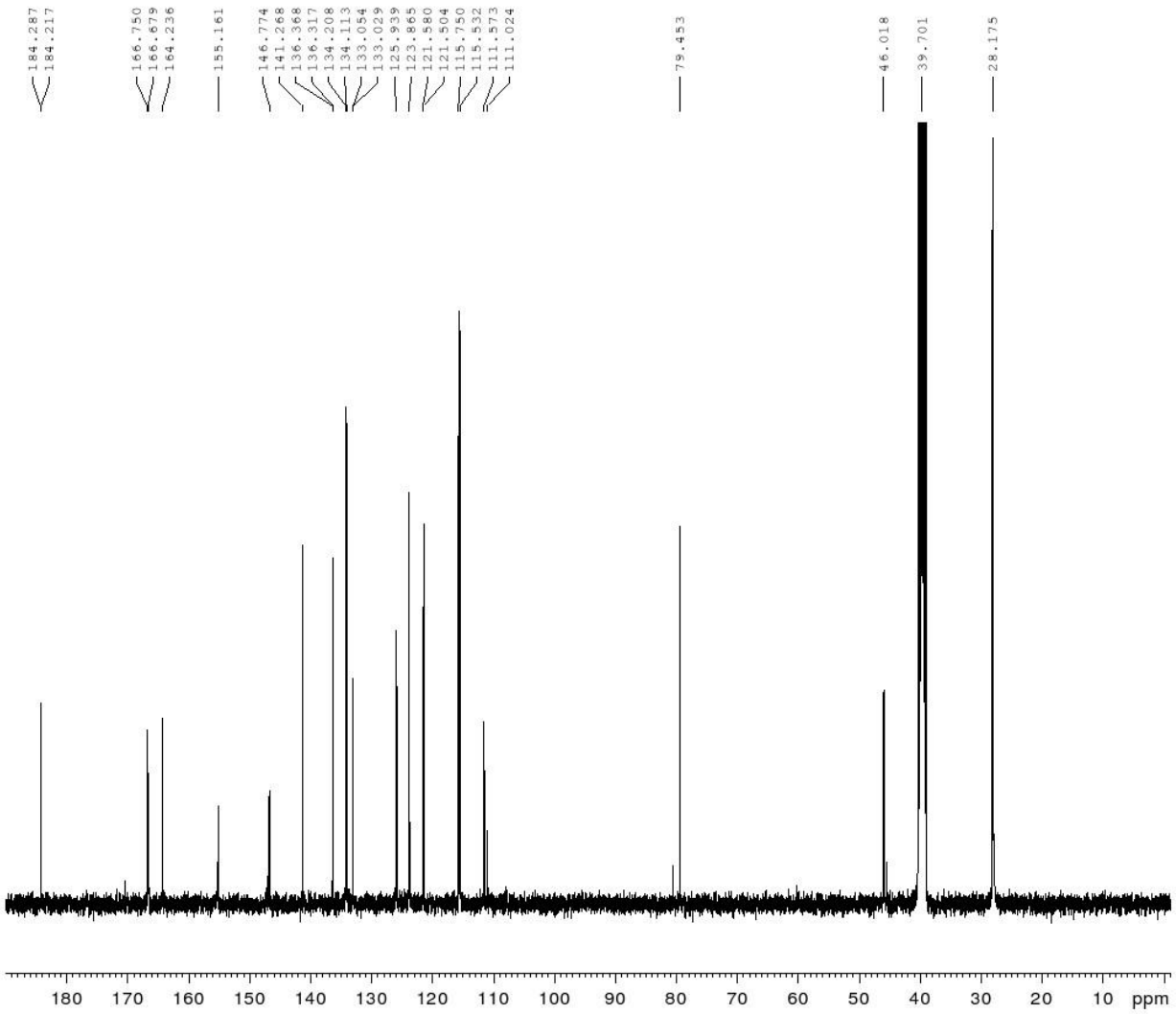
BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



4a


10.114
9.539
9.380
8.923
8.395
8.380
8.375
8.360
7.902
7.882
7.710
7.690
7.515
7.497
7.473
7.451
7.428
7.420
7.401
7.382
5.393
5.344
3.352
2.504
1.504
1.355
1.257
0.000
Standard 1H
121747
MIM0357_1A
Milen Matyas
2017.04.06. (DA)
NAME 121747
EXPNO 1
PROCNO 1
Date_ 20170406
Time 16.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 90.5
DW 60.800 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 0.80 dB
PL1W 12.53577709 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300018 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.02
0.17
0.12
0.82
2.57
1.19
1.07
4.96
0.38
2.00
1.63
9.42

4a



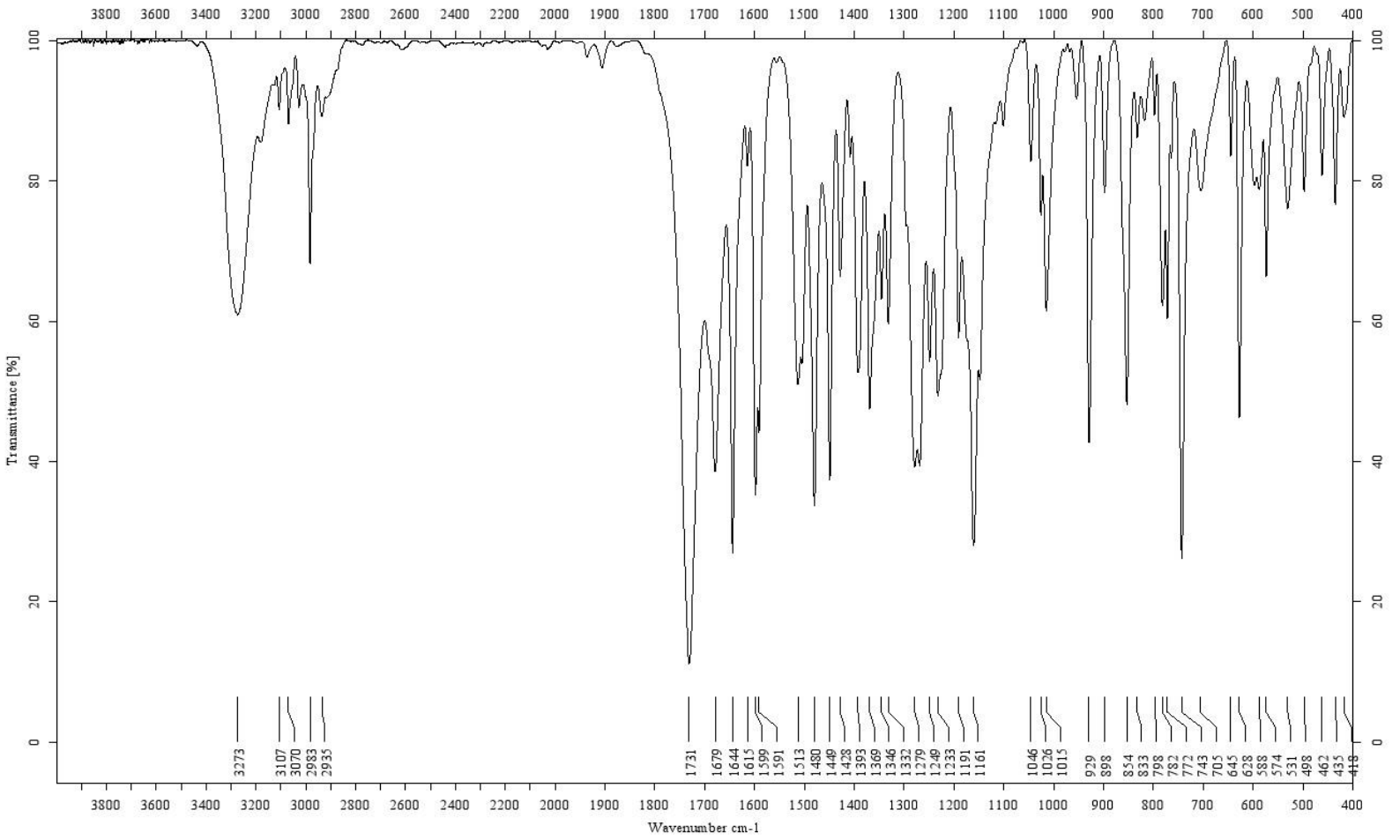
Standard 13C
121747
MIM0357_1A
Milen Matyas
2017.04.06. (DA)

NAME	121747
EXPNO	2
PROCNO	1
Date_	20170406
Time	22.01
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	8192
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	295.5 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.44 dB
PL1W	43.99363327 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.80 dB
PL12	18.30 dB
PL13	18.40 dB
PL2W	12.53577709 W
PL12W	0.22292118 W
PL13W	0.21784686 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127968 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

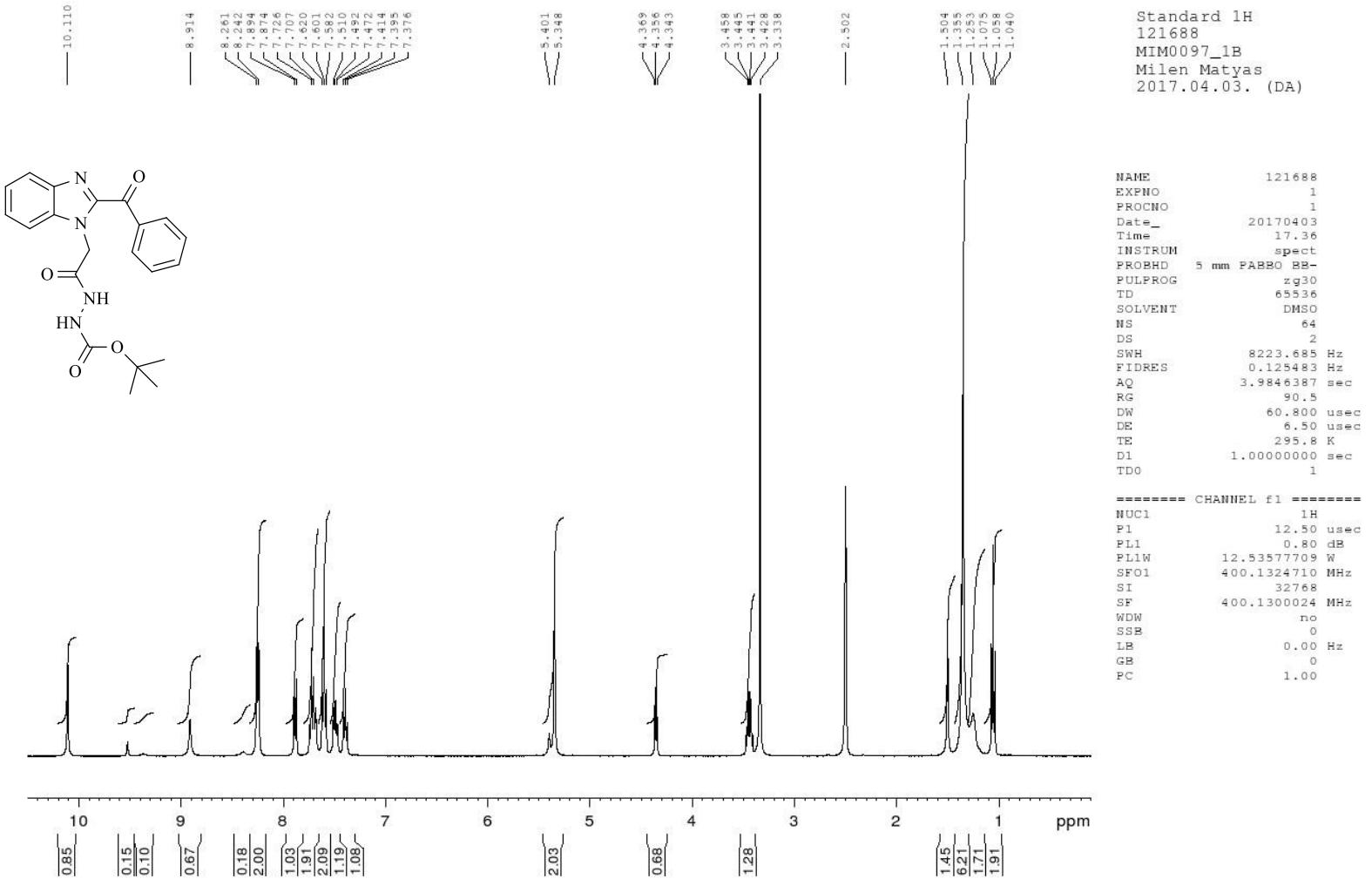
4a

121747	Milen Matyas	KP
MIM0357_1A	KBr	06/04/2017

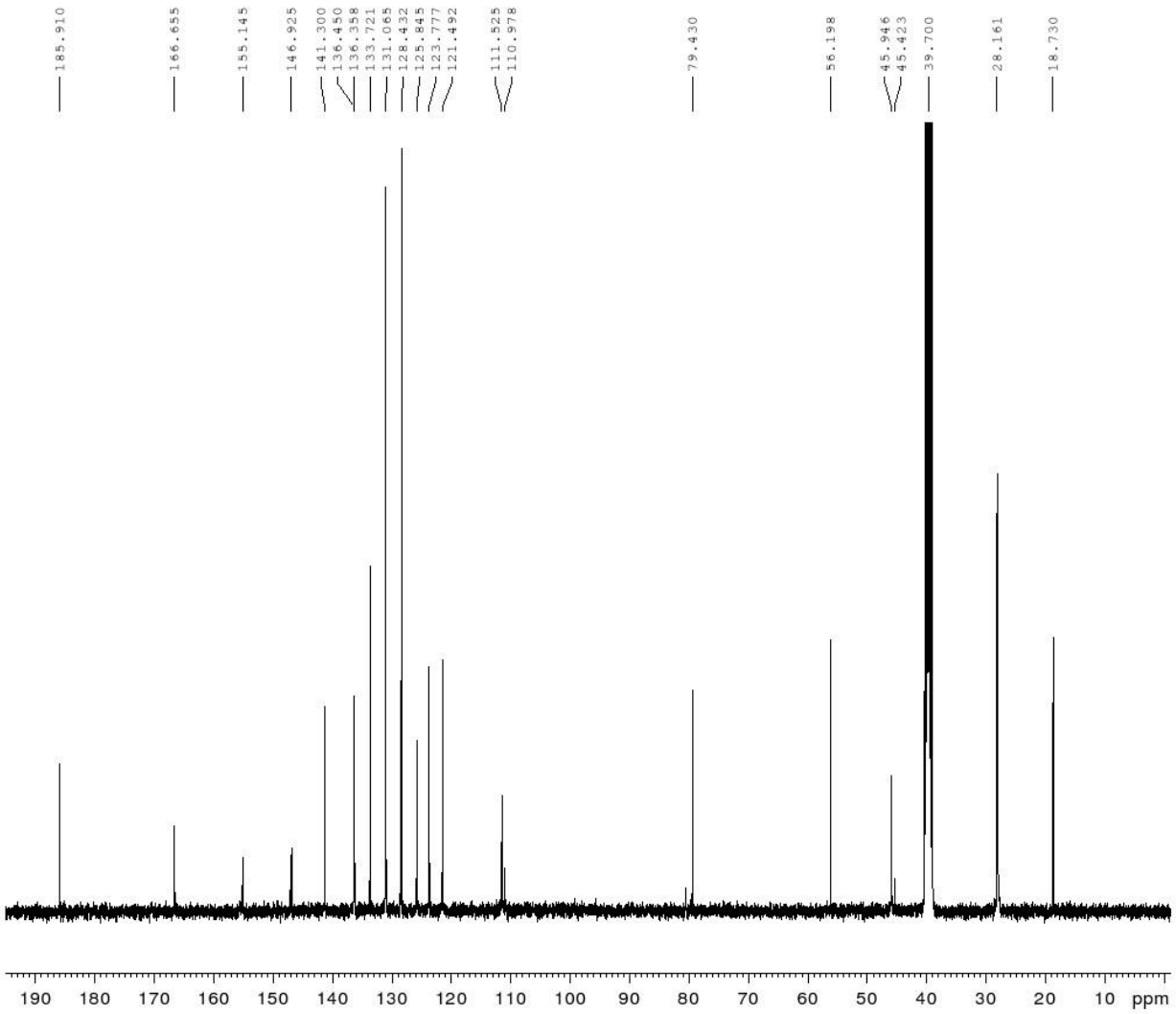
BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



4b


10.110
8.914
8.261
8.242
7.894
7.874
7.726
7.707
7.620
7.601
7.582
7.510
7.492
7.472
7.414
7.395
7.376
5.401
5.348
4.369
4.356
4.343
3.458
3.445
3.441
3.428
3.338
2.502
1.504
1.355
1.253
1.075
1.058
1.040
Standard 1H
121688
MIM0097_1B
Milen Matyas
2017.04.03. (DA)
NAME 121688
EXPNO 1
PROCNO 1
Date_ 20170403
Time 17.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 90.5
DW 60.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 0.80 dB
PL1W 12.53577709 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300024 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
0.85
0.15
0.10
0.67
0.18
2.00
1.03
1.91
2.09
1.19
1.08
2.03
0.68
1.28
1.45
6.21
1.71
1.91

4b



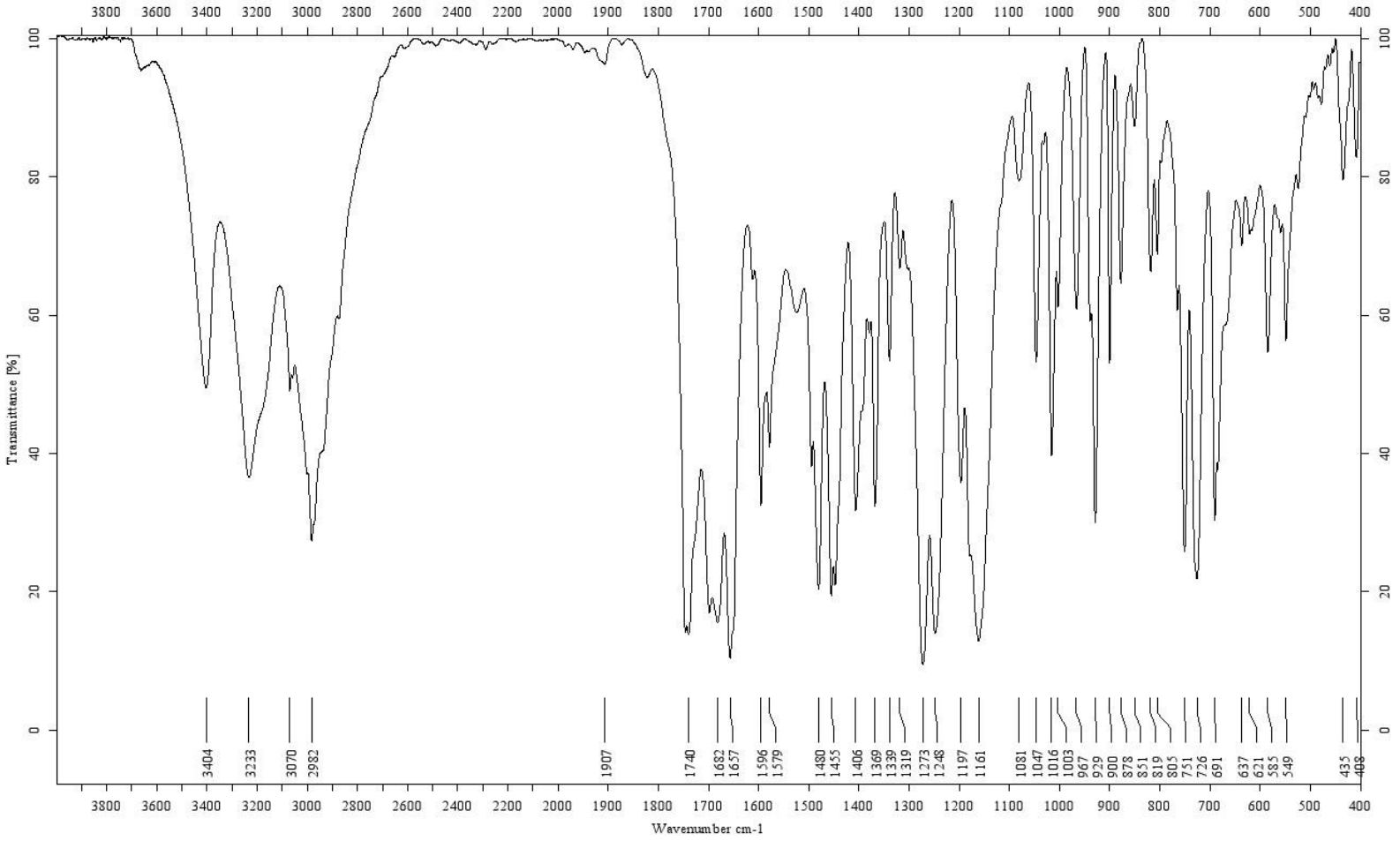
Standard 13C
121688
MIM0097_1B
Milen Matyas
2017.04.03. (DA)

NAME	121688
EXPNO	2
PROCNO	1
Date_	20170403
Time	23.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	8192
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	296.6 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.44 dB
PL1W	43.99363327 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.80 dB
PL12	18.30 dB
PL13	18.40 dB
PL2W	12.53577709 W
PL12W	0.22292118 W
PL13W	0.21784686 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127986 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

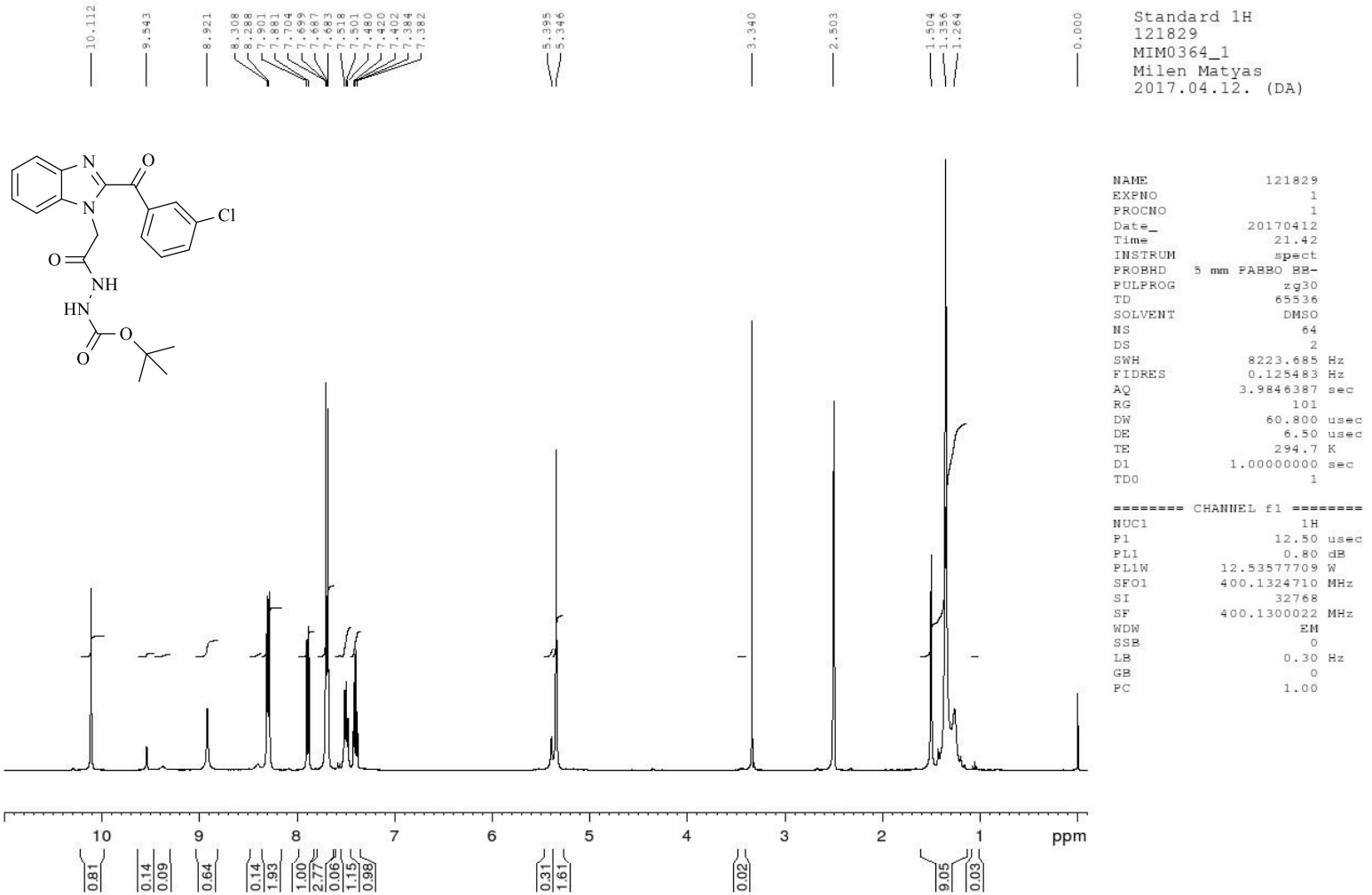
4b

121688	Milen Matyas	KP
MIM0097_1B	KBr	05/04/2017

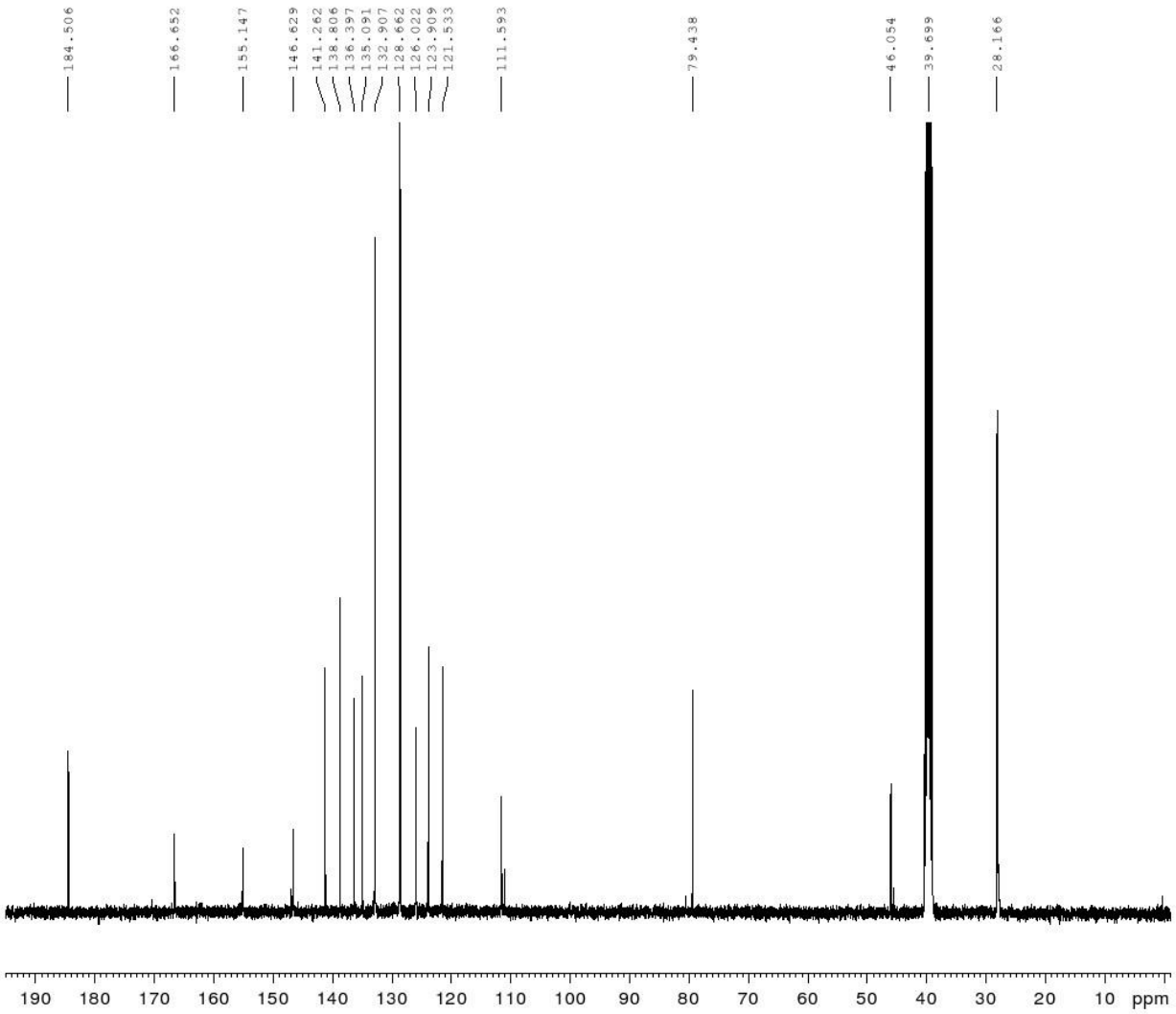
BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



4c


10.112
9.543
8.921
8.308
8.288
7.901
7.881
7.704
7.699
7.687
7.683
7.518
7.501
7.480
7.420
7.402
7.384
7.382
5.395
5.346
3.340
2.503
1.504
1.356
1.264
0.000
Standard 1H
121829
MIM0364_1
Milen Matyas
2017.04.12. (DA)
Cl
O
N
N
O
NH
HN
O
O
NAME 121829
EXPNO 1
PROCNO 1
Date_ 20170412
Time 21.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 101
DW 60.800 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 0.80 dB
PL1W 12.53577709 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
0.81
0.14
0.09
0.64
0.14
1.93
1.00
2.77
0.06
1.15
0.98
0.31
1.61
0.02
9.05
0.03

4c



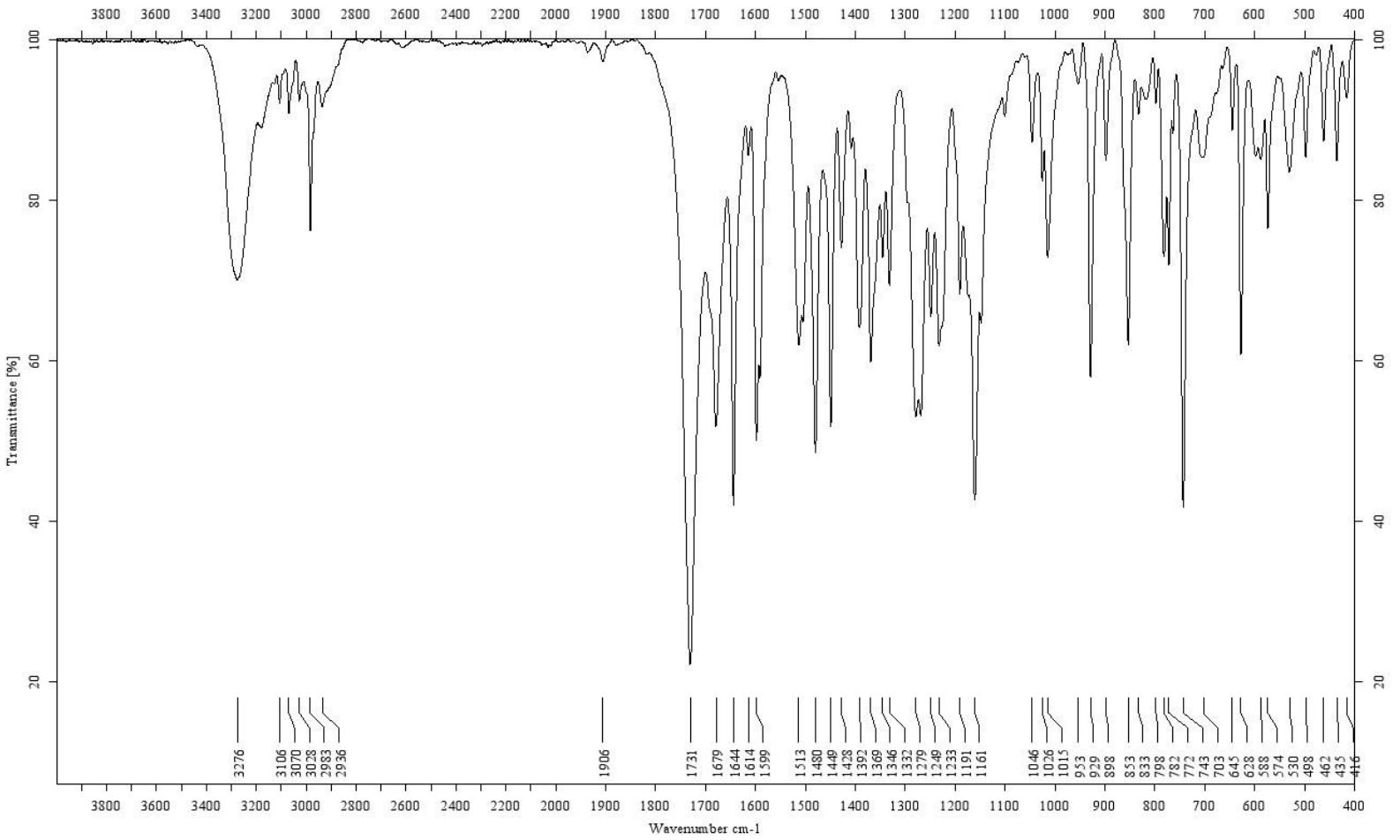
Standard 13C
121829
MIM0364_1
Milen Matyas
2017.04.12. (DA)

NAME	121829
EXPNO	2
PROCNO	1
Date_	20170413
Time	1.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	6144
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	295.8 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.44 dB
PL1W	43.99363327 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.80 dB
PL12	18.30 dB
PL13	18.40 dB
PL2W	12.53577709 W
PL12W	0.22292118 W
PL13W	0.21784686 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127981 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

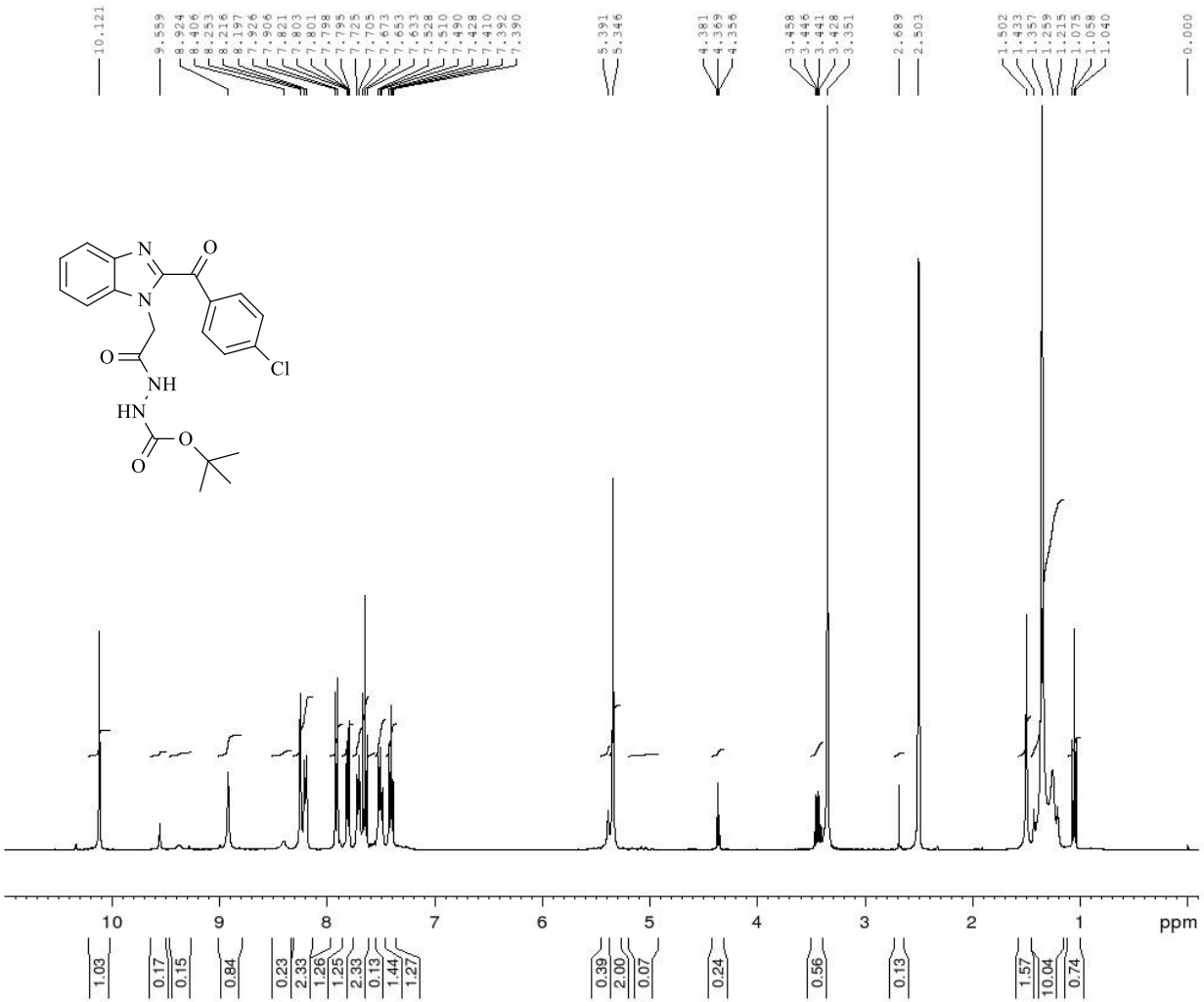
4c

121829	Milen Matyas	KP
MIM0364_1	KBr	12/05/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



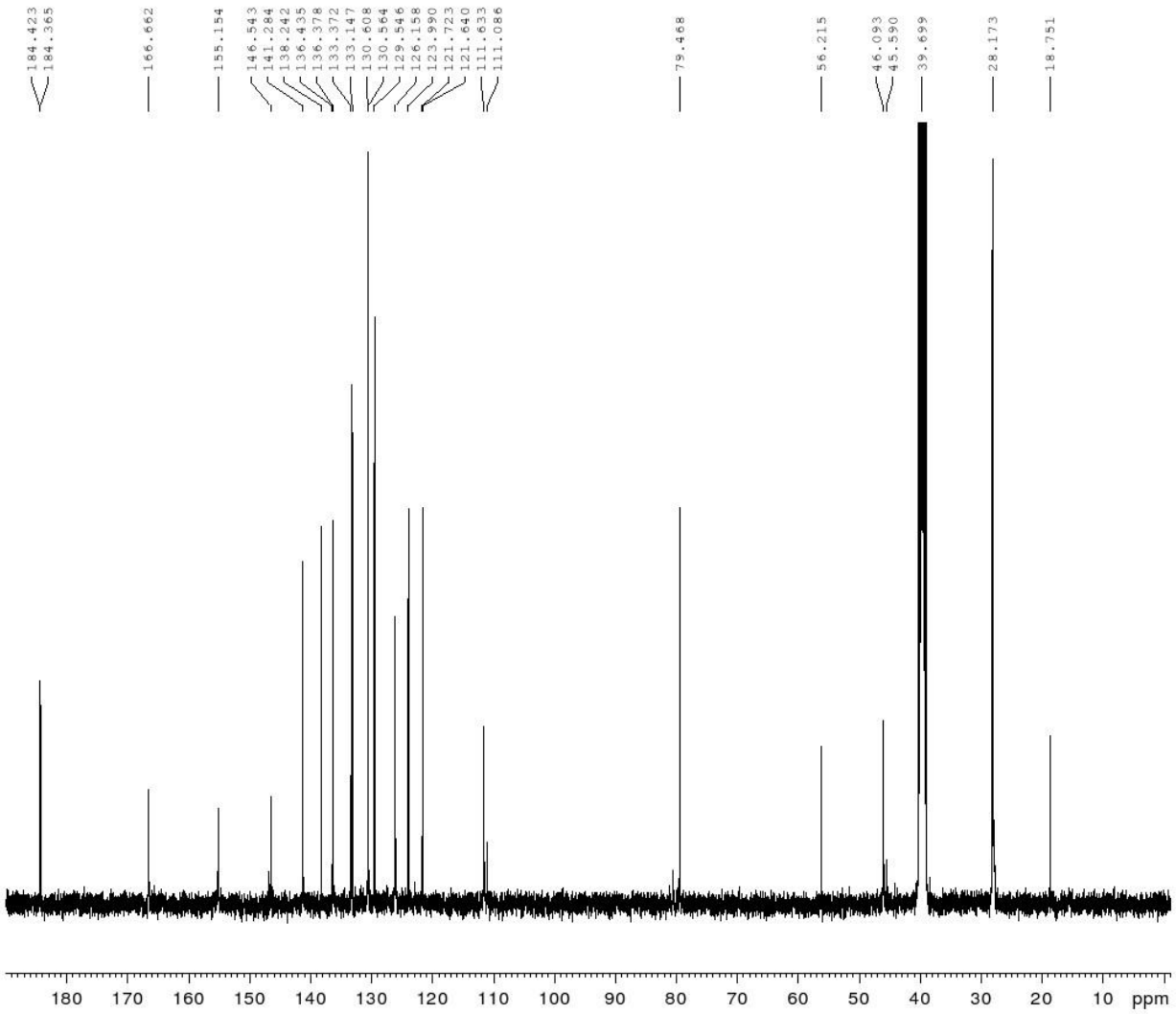
4d



NAME	121748
EXPNO	1
PROCNO	1
Date_	20170407
Time	1.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	90.5
DW	60.800 usec
DE	6.50 usec
TE	293.8 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	12.50 usec
PL1	0.80 dB
PL1W	12.53577709 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300018 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

4d



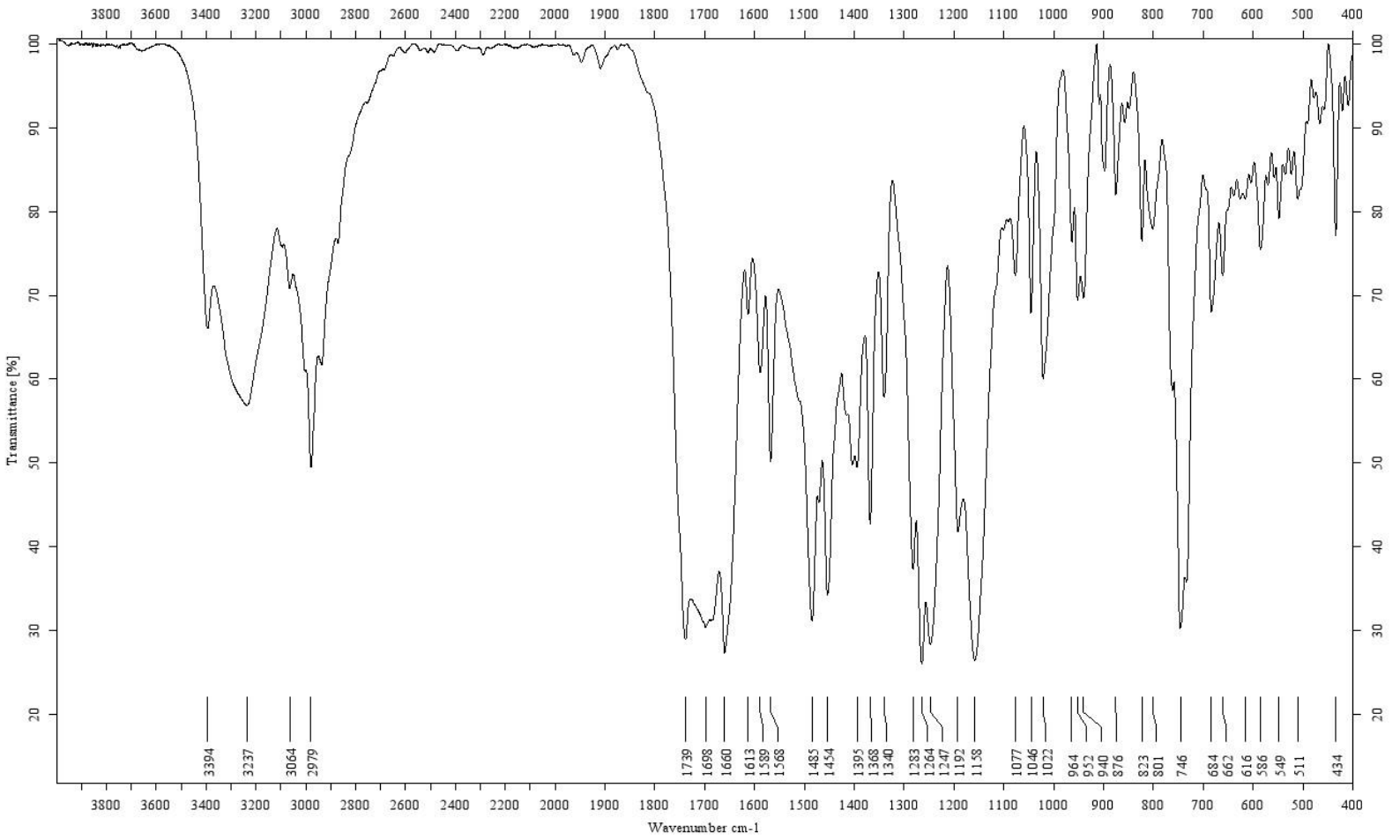
Standard 13C
121748
MIM0362_1
Milen Matyas
2017.04.06. (DA)

NAME	121748
EXPNO	2
PROCNO	1
Date_	20170407
Time	7.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	8192
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	295.1 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.44 dB
PL1W	43.99363327 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.80 dB
PL12	18.30 dB
PL13	18.40 dB
PL2W	12.53577709 W
PL12W	0.22292118 W
PL13W	0.21784686 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127968 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

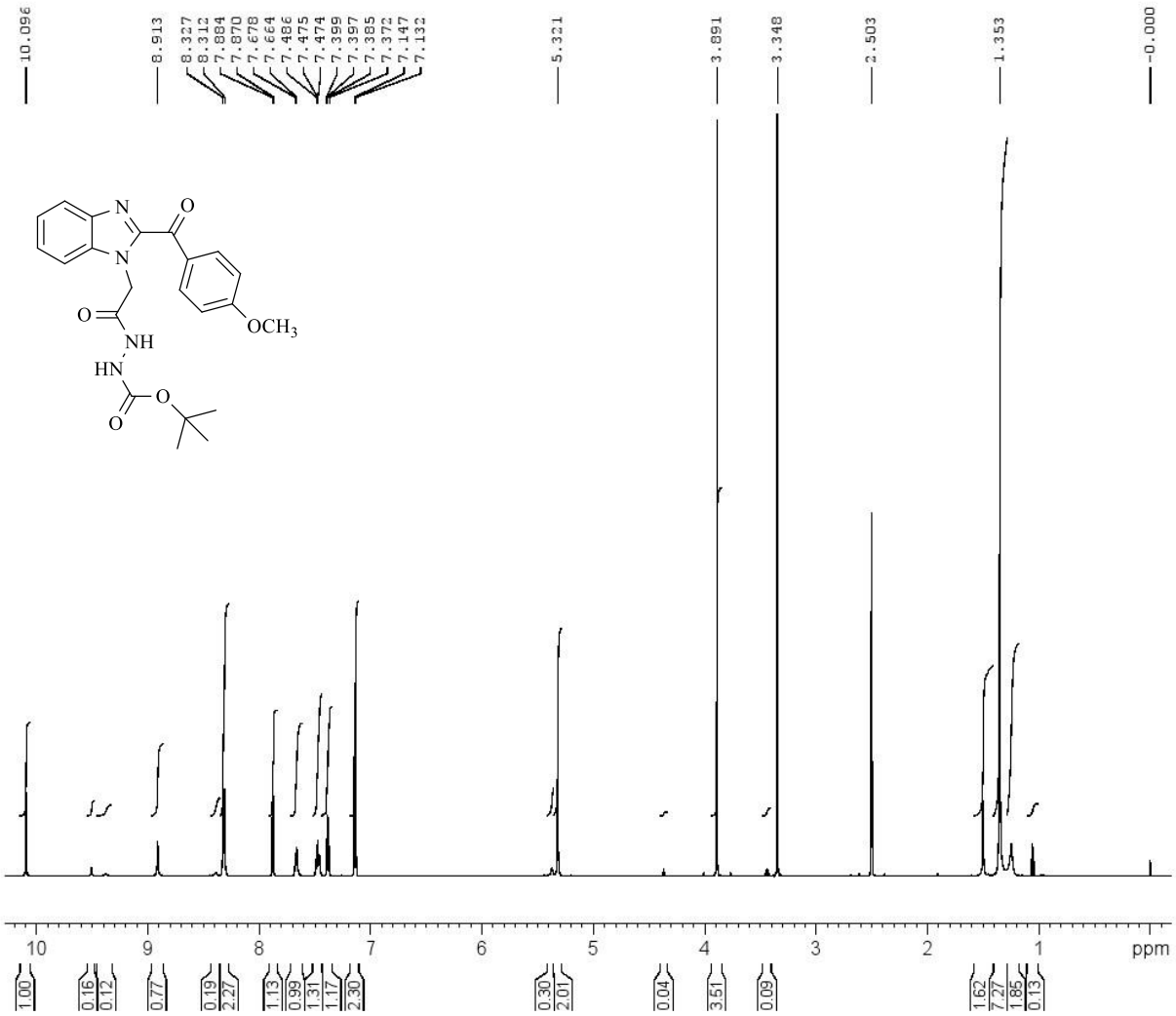
4d

121748	Milen Matyas	KP
MIM0362_1	KBr	06/04/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

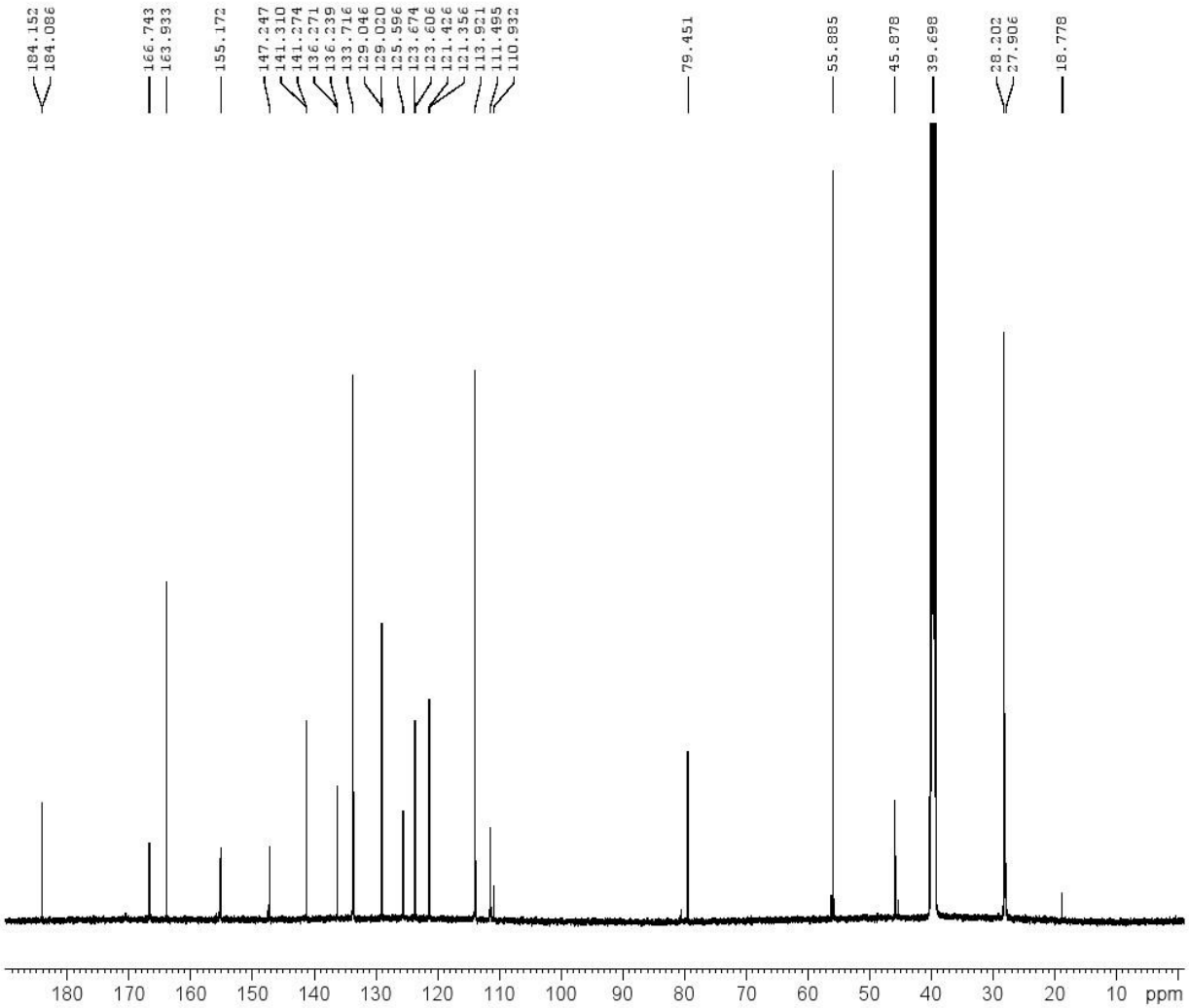


4e




```
Standard 1H
125250
MIM0446_1
Milen Matyas
2018.03.21. (DA)

Current Data Parameters
NAME                  125250
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_               20180322
Time                    6.14 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         4
SWH               12626.263 Hz
FIDRES             0.385323 Hz
AQ                2.5952256 sec
RG                   155.77
DW                   39.600 usec
DE                   25.00 usec
TE                   295.0 K
D1              1.00000000 sec
TD0                        1
SFO1            600.1642011 MHz
NUC1                      1H
P1                   11.50 usec
PLW1           28.00000000 W

F2 - Processing parameters
SI                    65536
SF              600.1600032 MHz
WDW                      no
SSB         0
LB          0 Hz
GB          0
PC                     1.00
```

4e



Standard 13C
125250
MIM0446_1
Milen Matyas
2018.03.21. (DA)

Current Data Parameters
NAME 125250
EXPNO 12
PROCNO 1

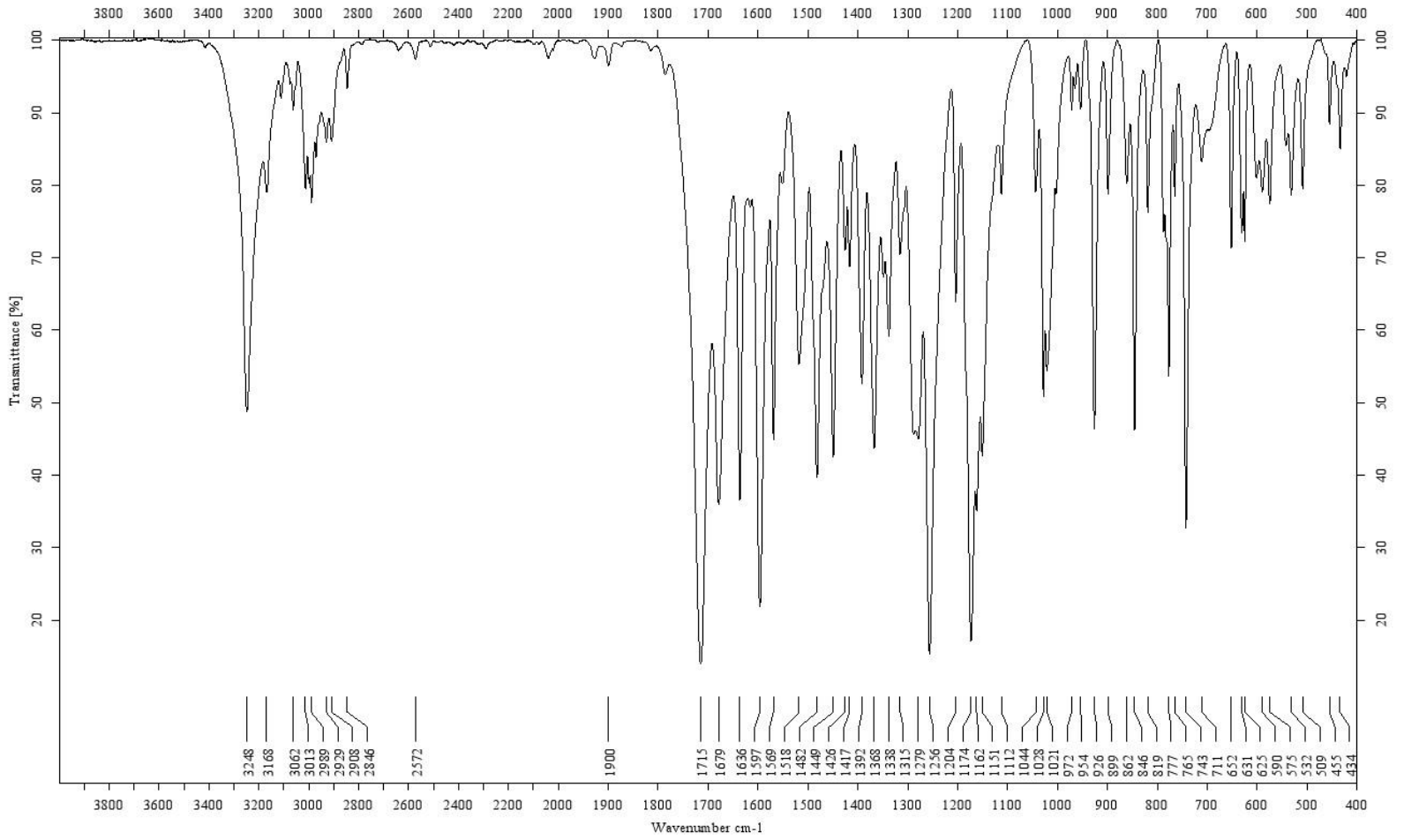
F2 - Acquisition Parameters
Date_ 20180322
Time 9.04 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.9087659 sec
RG 196.07
DW 13.867 usec
DE 18.00 usec
TE 295.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9254424 MHz
NUC1 13C
P1 10.00 usec
PLW1 60.36299896 W
SFO2 600.1624006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 26.42600060 W
PLW12 0.59460002 W
PLW13 0.29861000 W

F2 - Processing parameters
SI 65536
SF 150.9103917 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

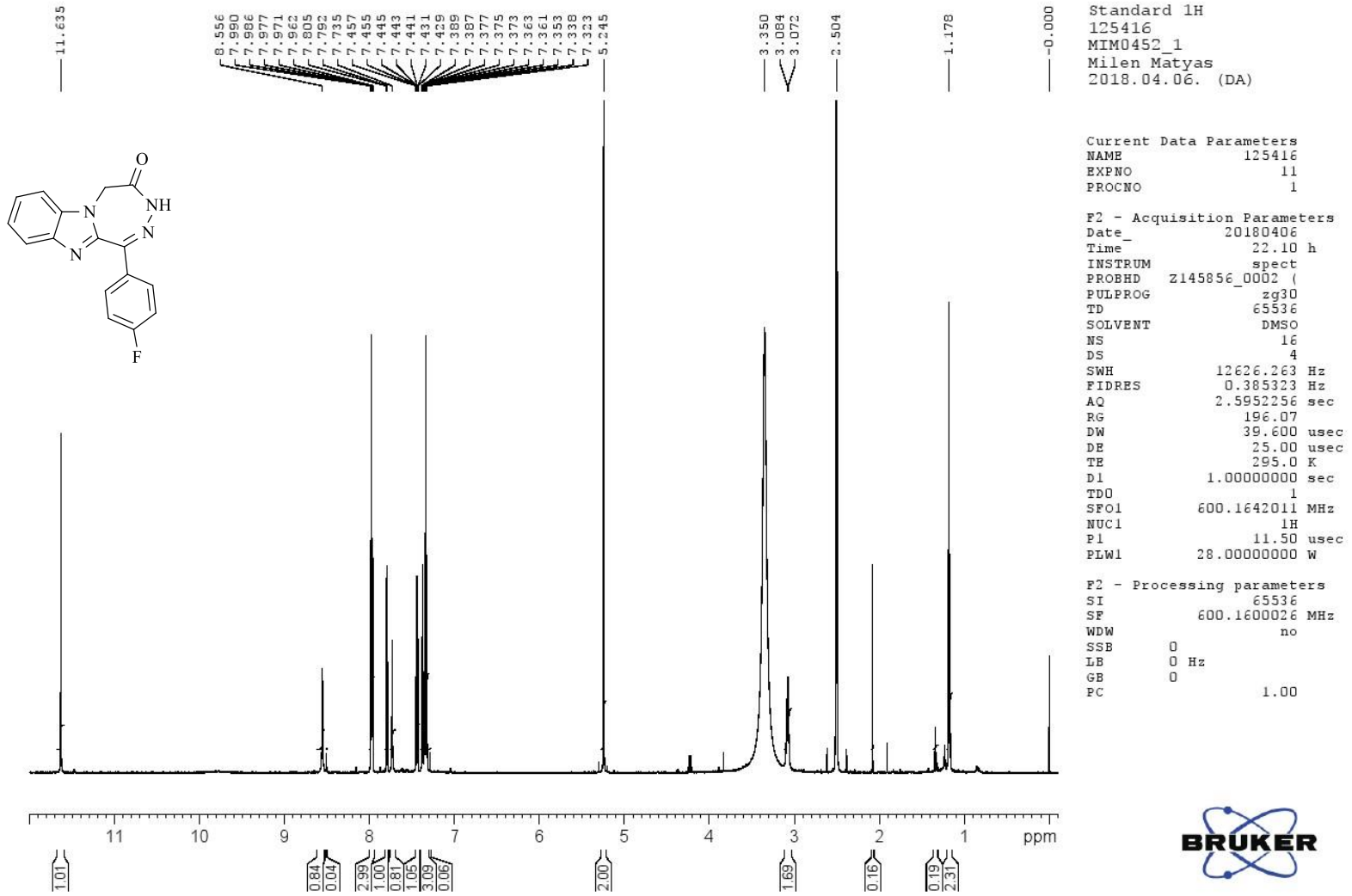
4e

125250	Milen Matyas	KP
MIM0446_1	KBr	2018.03.21.

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

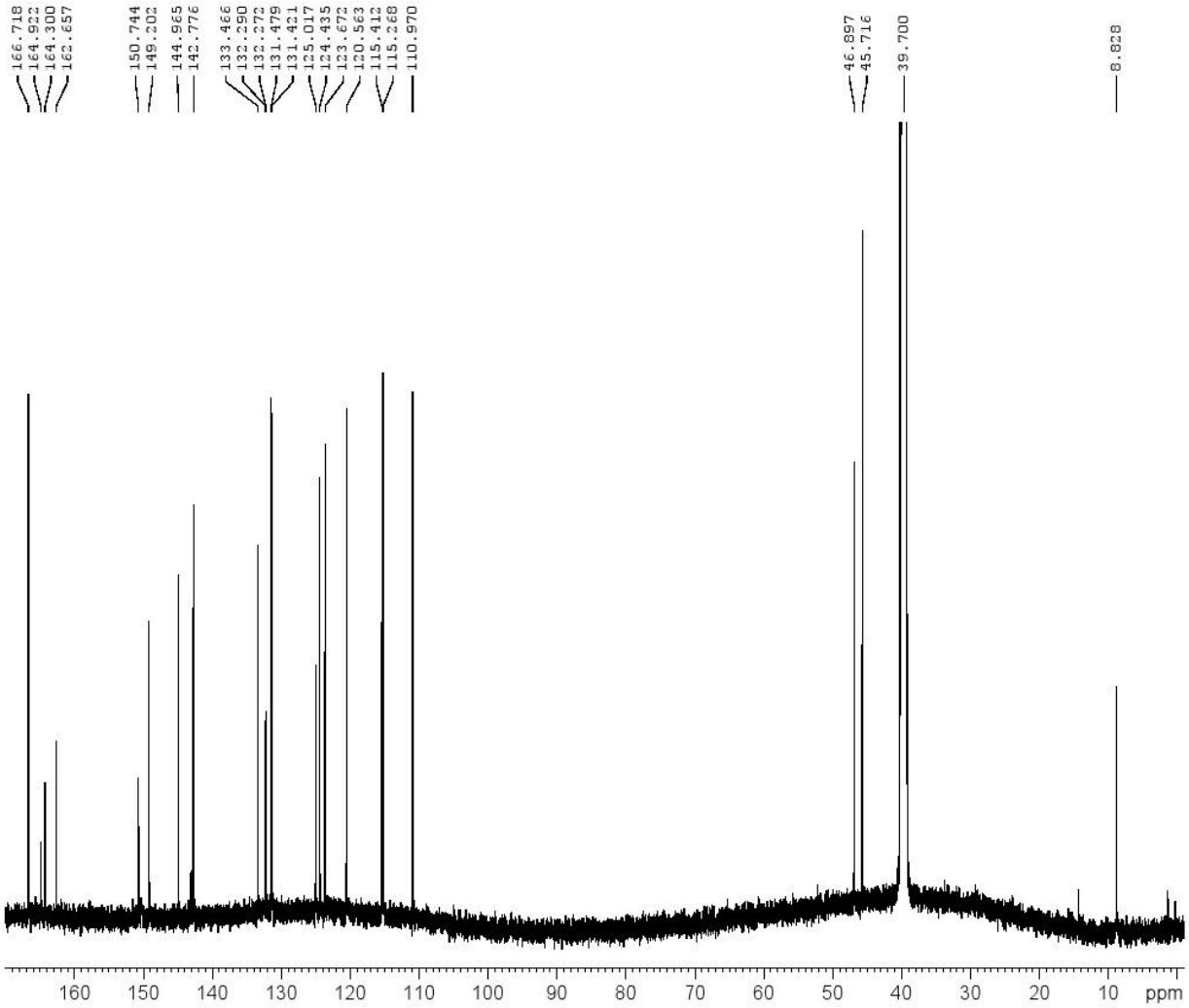


5a




```
Standard 1H
125416
MIM0452_1
Milen Matyas
2018.04.06. (DA)

Current Data Parameters
NAME                  125416
EXPNO                     11
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180406
Time                   22.10 h
INSTRUM                spect
PROBHD     Z145856_0002 (
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         4
SWH               12626.263 Hz
FIDRES             0.385323 Hz
AQ                 2.5952256 sec
RG                    196.07
DW                    39.600 usec
DE                    25.00 usec
TE                    295.0 K
D1                 1.00000000 sec
TD0                        1
SFO1              600.1642011 MHz
NUC1                      1H
P1                    11.50 usec
PLW1              28.00000000 W

F2 - Processing parameters
SI                    65536
SF                600.1600026 MHz
WDW                       no
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```

5a

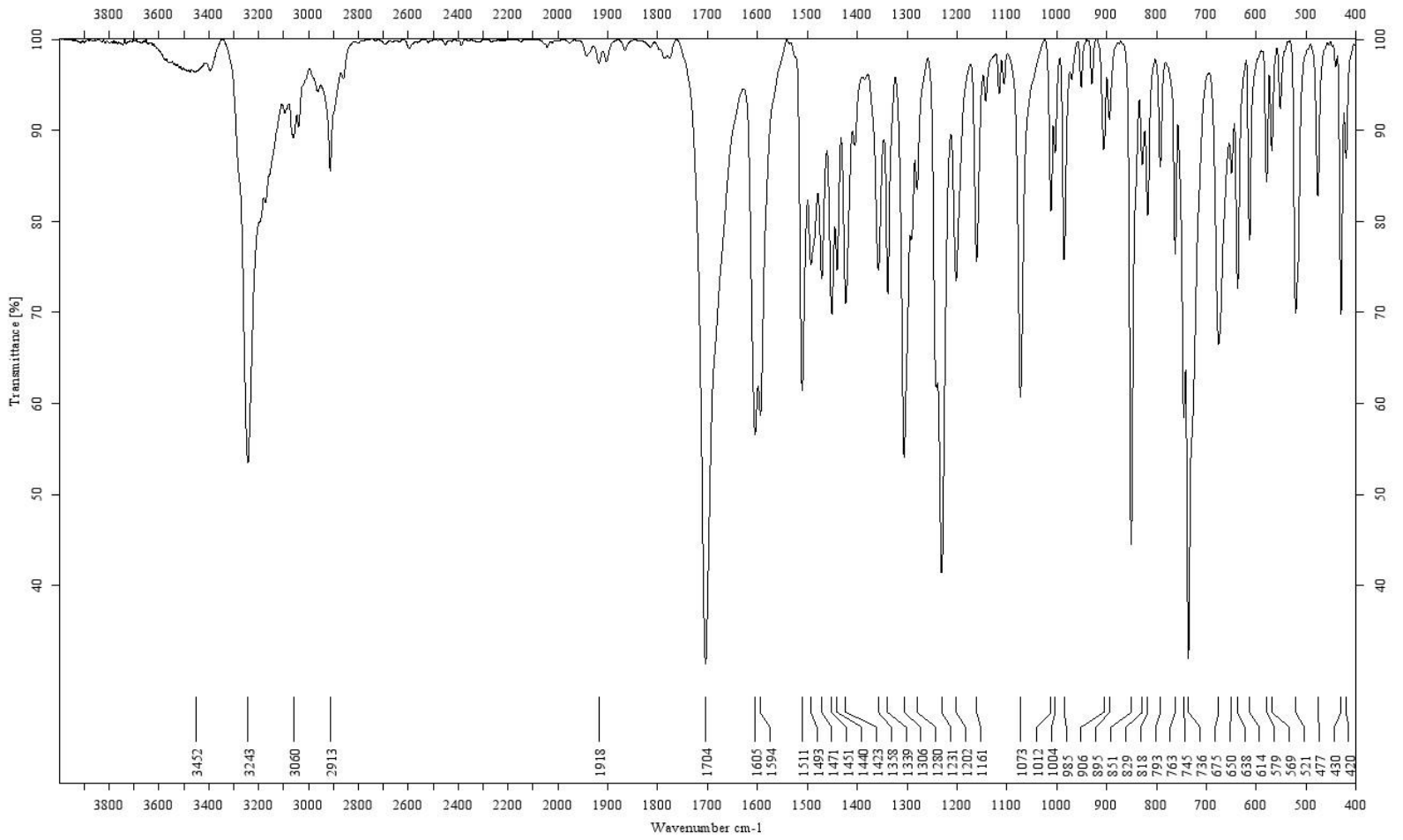



```
Standard 13C
125416
MIM0452_1
Milen Matyas
2018.04.06. (DA)

Current Data Parameters
NAME                  125416
EXPNO                     12
PROCNO                     1

F2 - Acquisition Parameters
Date_               20180407
Time                    3.48 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       8192
DS                          4
SWH                 36057.691 Hz
FIDRES               1.100393 Hz
AQ                   0.9087659 sec
RG                      196.07
DW                      13.867 usec
DE                       18.00 usec
TE                       295.0 K
D1                1.50000000 sec
D11               0.03000000 sec
TD0                         1
SFO1              150.9254424 MHz
NUC1                      13C
P1                       10.00 usec
PLW1              60.36299896 W
SFO2              600.1624006 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                    80.00 usec
PLW2              26.42600060 W
PLW12              0.59460002 W
PLW13              0.29861000 W

F2 - Processing parameters
SI                      65536
SF                150.9103913 MHz
WDW                        EM
SSB       0
LB                       1.00 Hz
GB        0
PC                       1.40
```

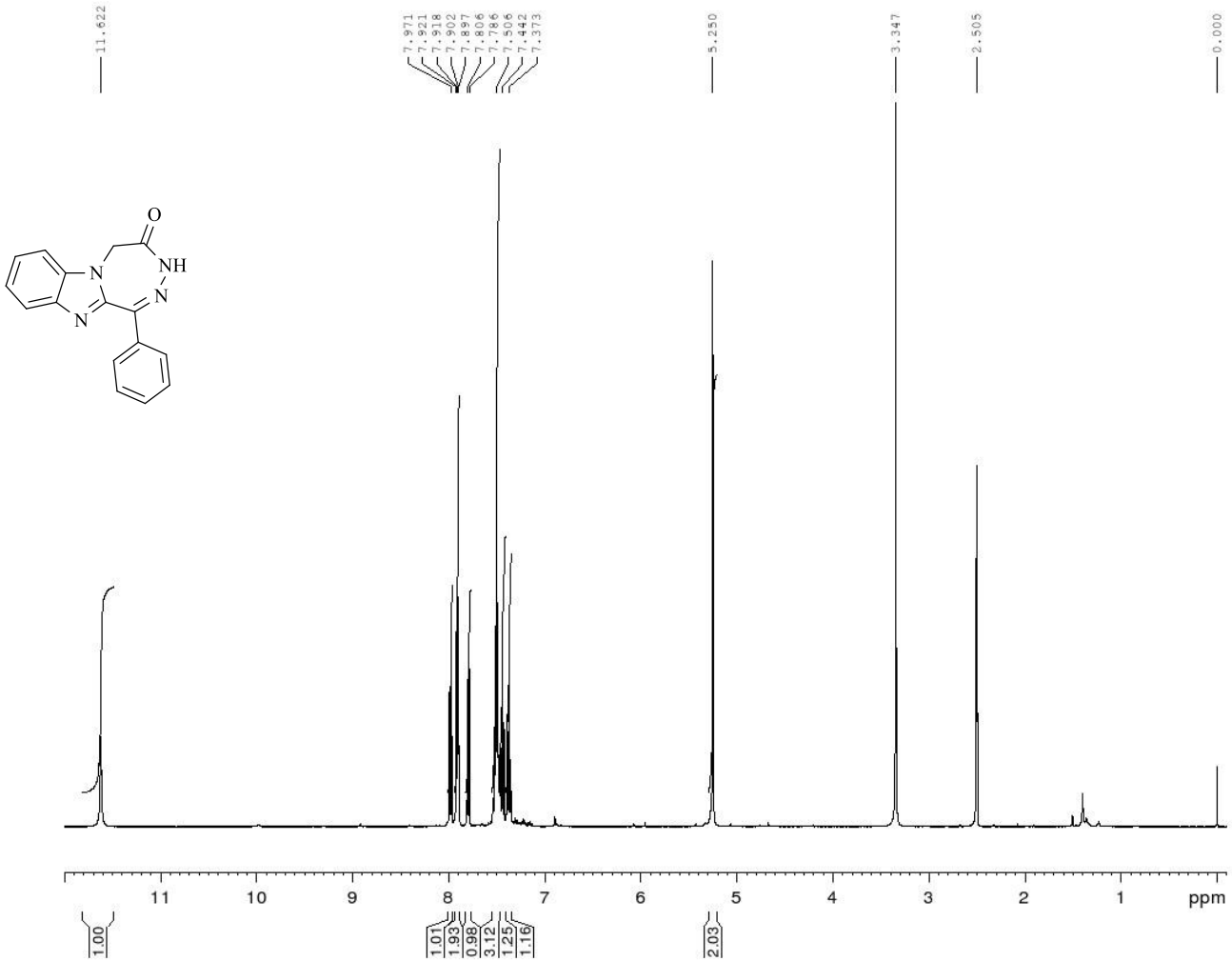
5a

125416	Milen Matyas	KP
MIM0452_1	KBr	2018.04.09.

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



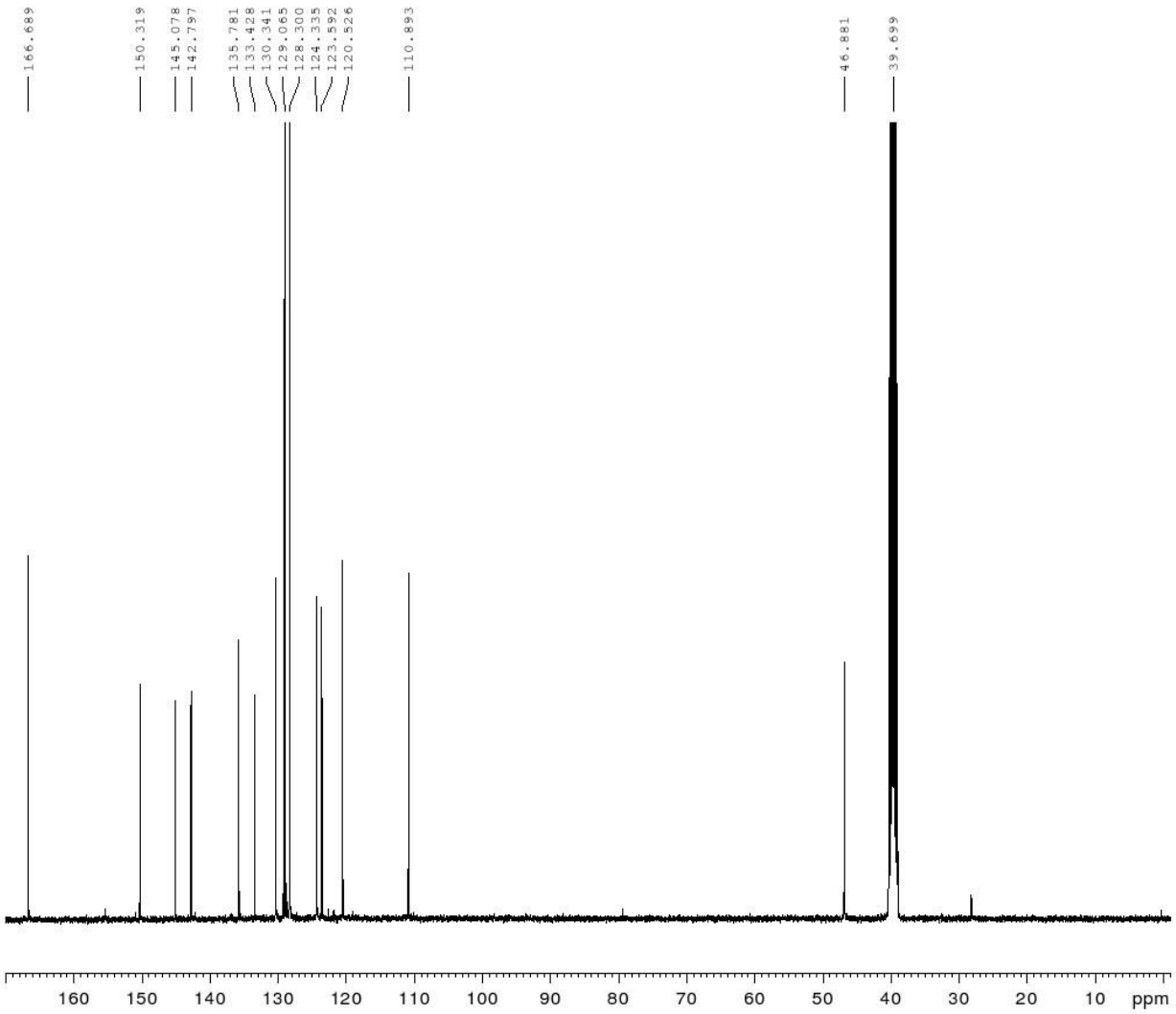
5b



Standard 1H
121975
MIM0371_1
Milen Matyas
2017.04.28. (DA)

NAME	121975
EXPNO	11
PROCNO	1
Date_	20170428
Time	16.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	101
DW	60.800 usec
DE	6.50 usec
TE	295.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.50 usec
PL1	0.80 dB
PL1W	12.53577709 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300011 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

5b

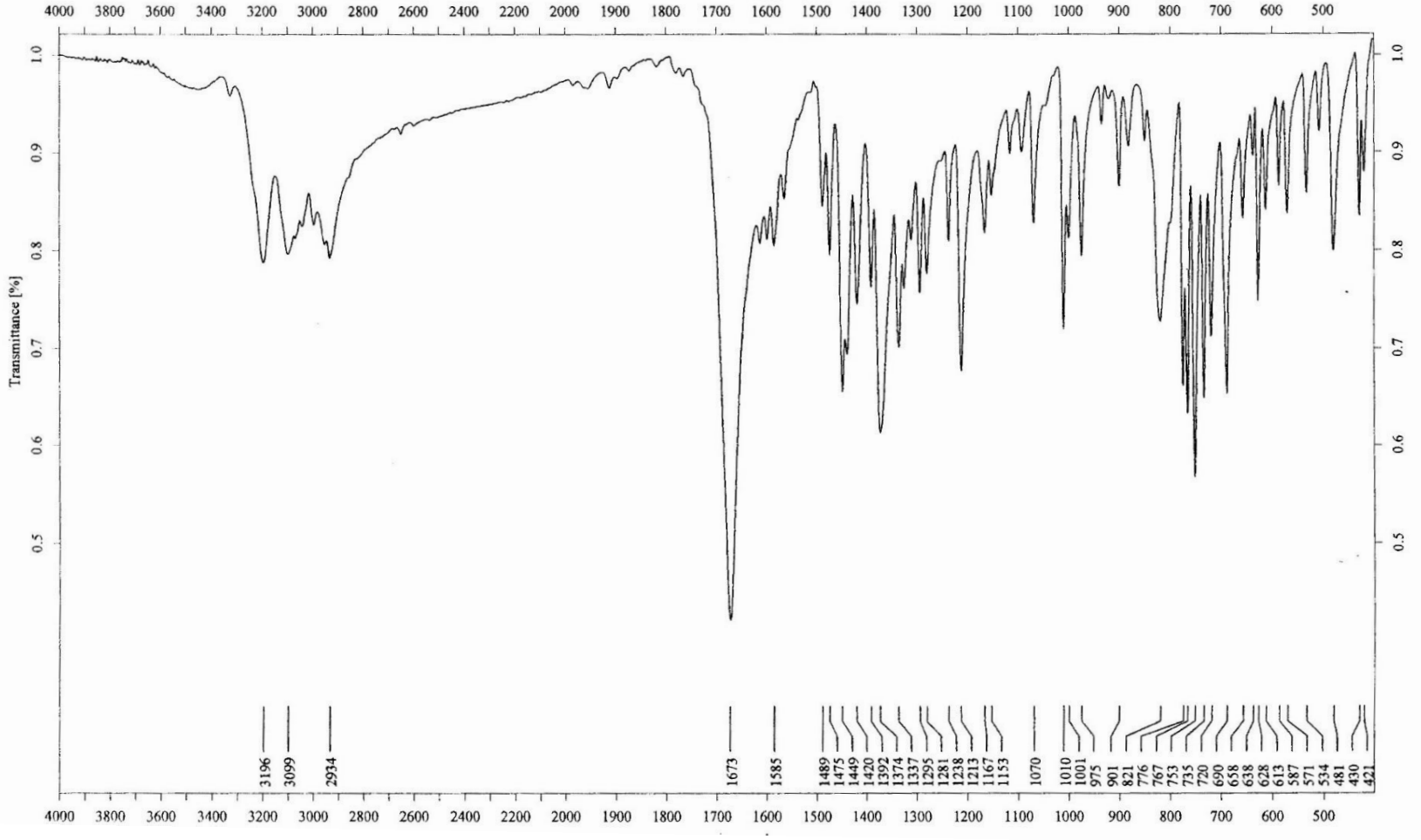



```
Standard 13C
121975
MIM0371_1
Milen Matyas
2017.04.28. (DA)

NAME                121975
EXPNO                   12
PROCNO                   1
Date_             20170429
Time                 4.01
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                   16384
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    2050
DW                 20.800 usec
DE                  6.50 usec
TE                 295.8 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.50 usec
PL1                 1.44 dB
PL1W         43.99363327 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                 0.80 dB
PL12               18.30 dB
PL13               18.40 dB
PL2W         12.53577709 W
PL12W         0.22292118 W
PL13W         0.21784686 W
SFO2        400.1316005 MHz
SI                 32768
SF          100.6127980 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

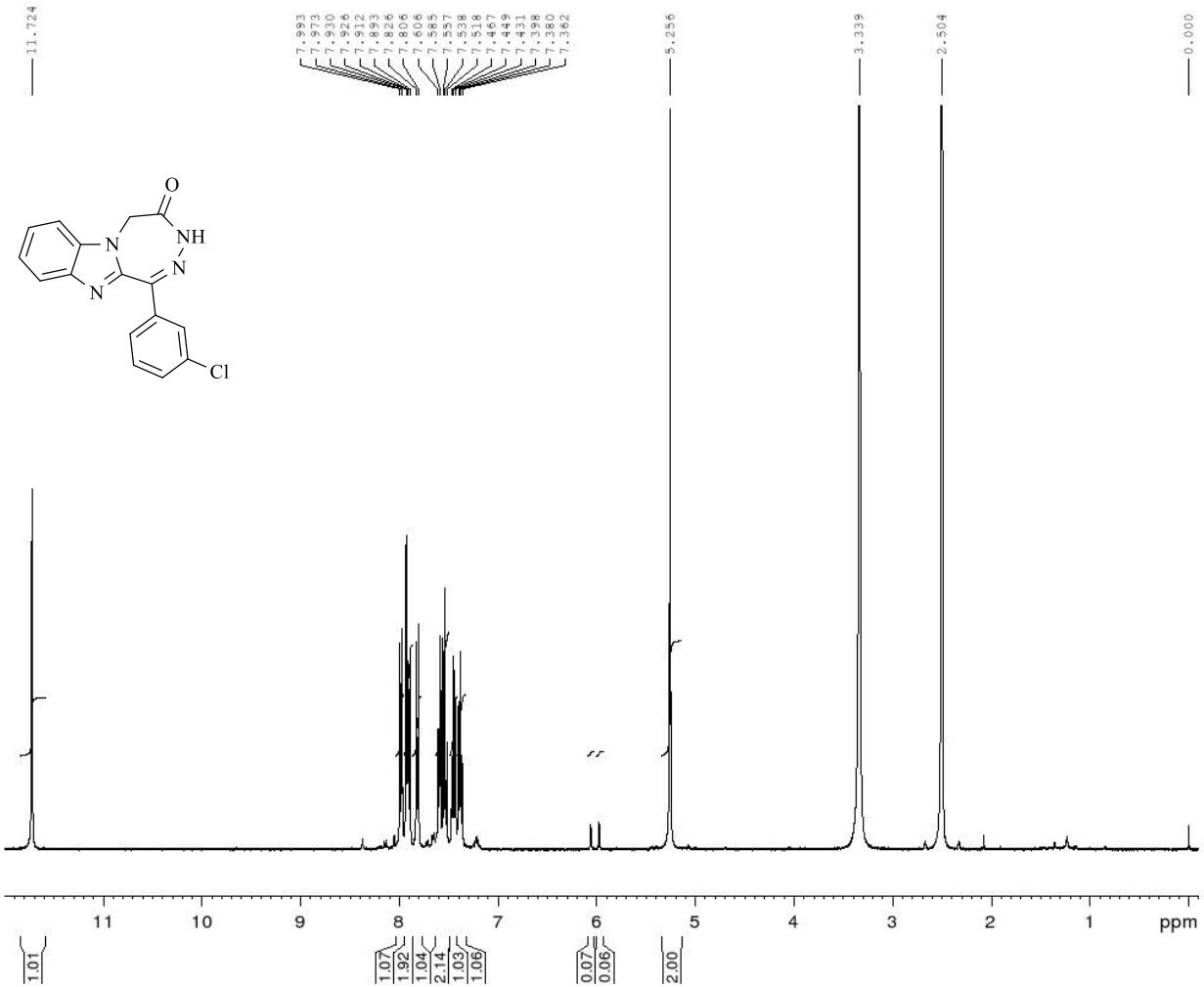
5b

62647	Milen Mátyás	CzB
MM158	KBr	23/03/2006

BRUKER VECTOR22
Resolution: 2 cm-1
Number of Scans: 8



5c

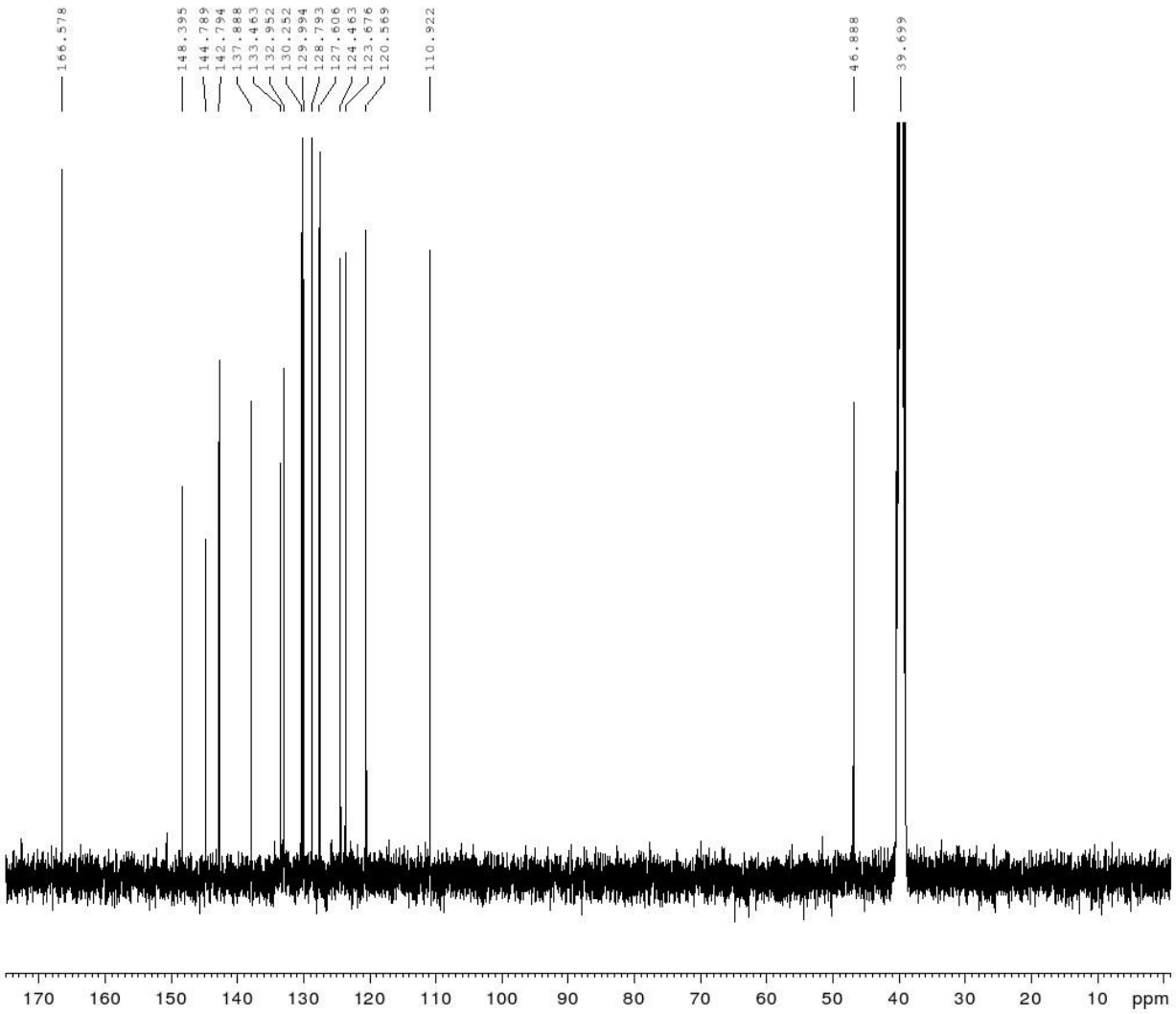


Standard 1H
122107
MIM0373_1
Milen Matyas
2017.05.16. (DA)

NAME	122107
EXPNO	1
PROCNO	1
Date_	20170516
Time	16.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	228
DW	60.800 usec
DE	6.50 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	12.50 usec
PL1	0.80 dB
PL1W	12.53577709 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300017 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

5c



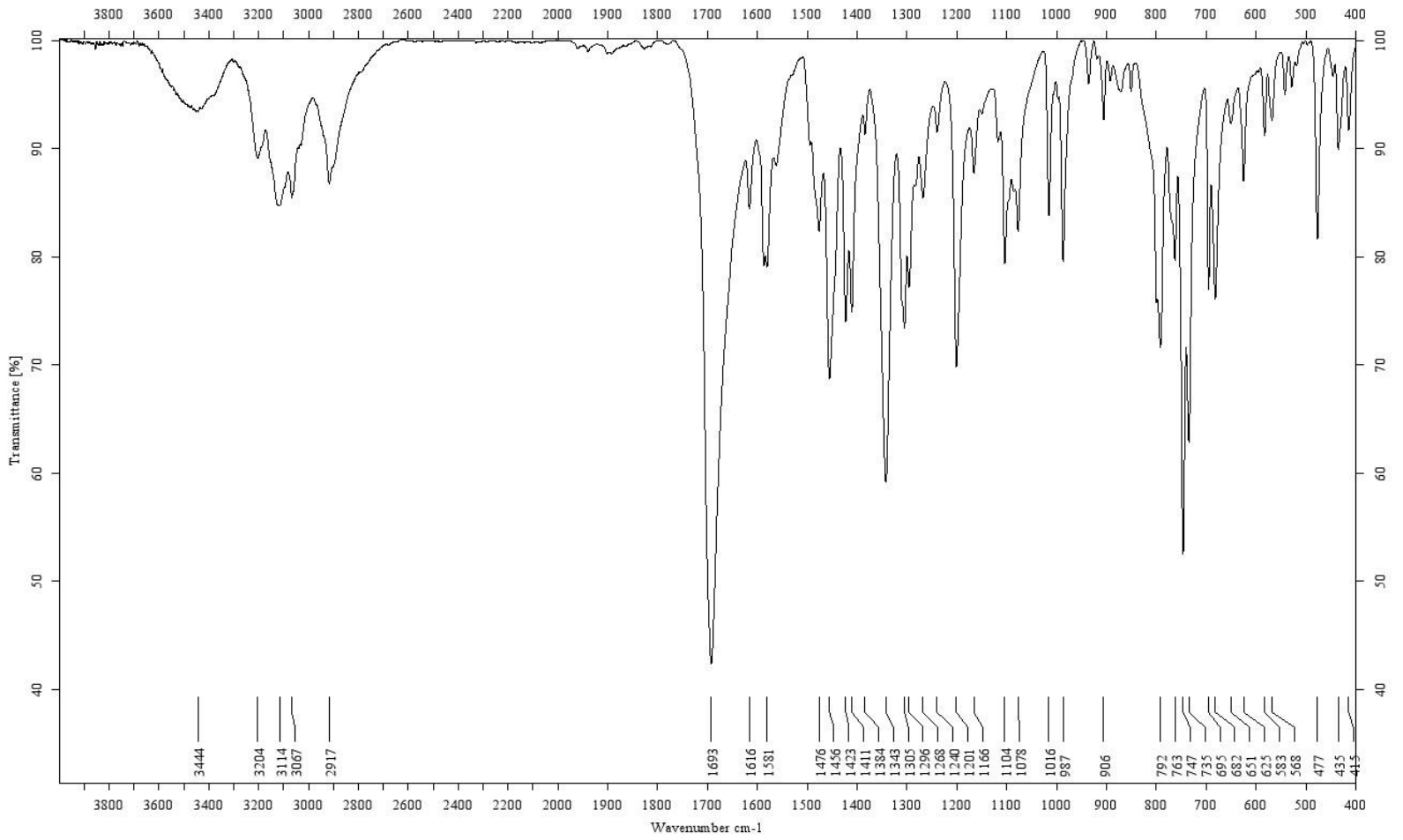
Standard 13C
122107
MIM0373_1
Milen Matyas
2017.05.16. (DA)

NAME	122107
EXPNO	2
PROCNO	1
Date_	20170516
Time	22.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	8192
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	297.2 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.44 dB
PL1W	43.99363327 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.80 dB
PL12	18.30 dB
PL13	18.40 dB
PL2W	12.53577709 W
PL12W	0.22292118 W
PL13W	0.21784686 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127988 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

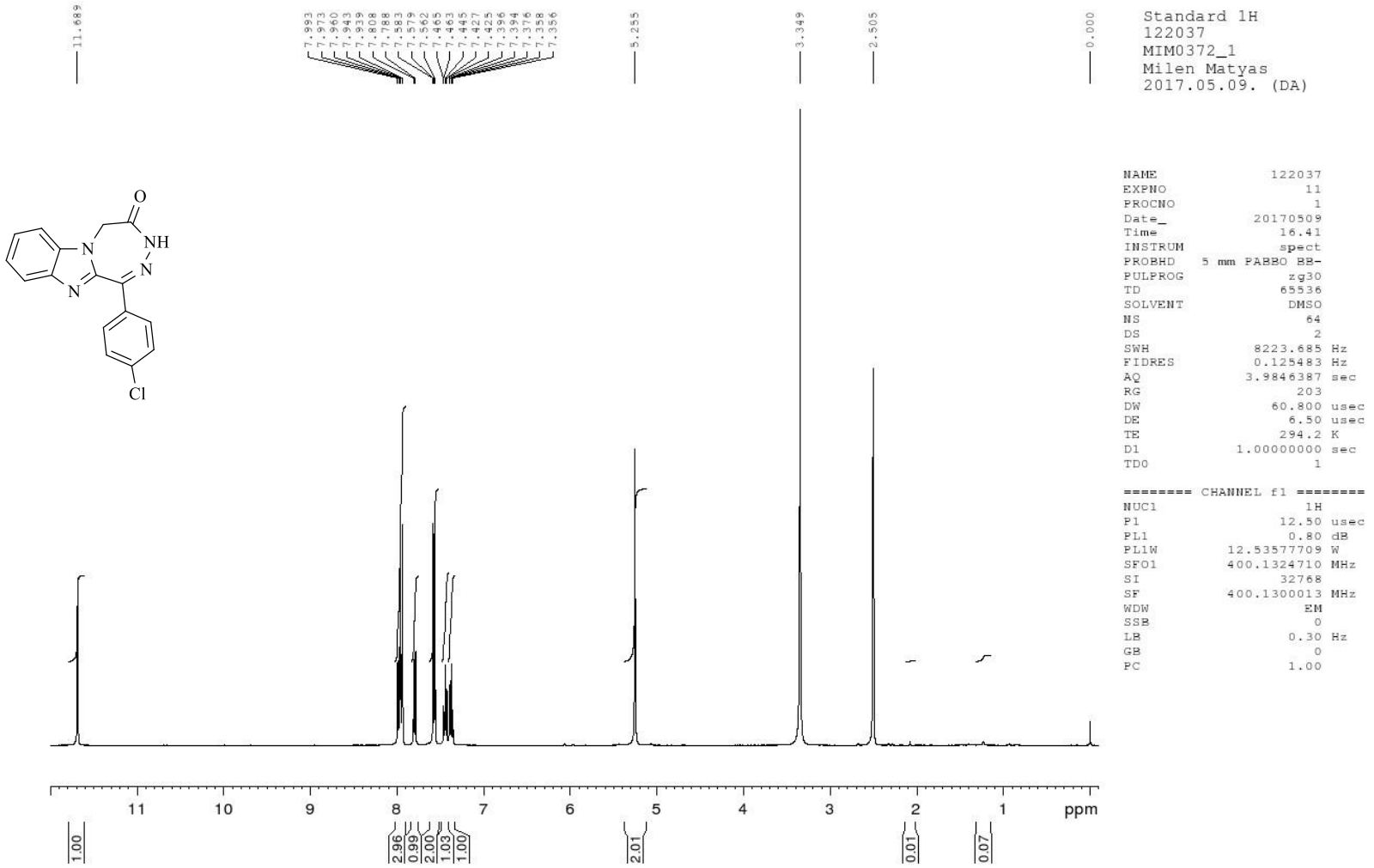
5c

122107	Milen Matyas	KP
MIM0373_1	KBr	16/05/2017

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



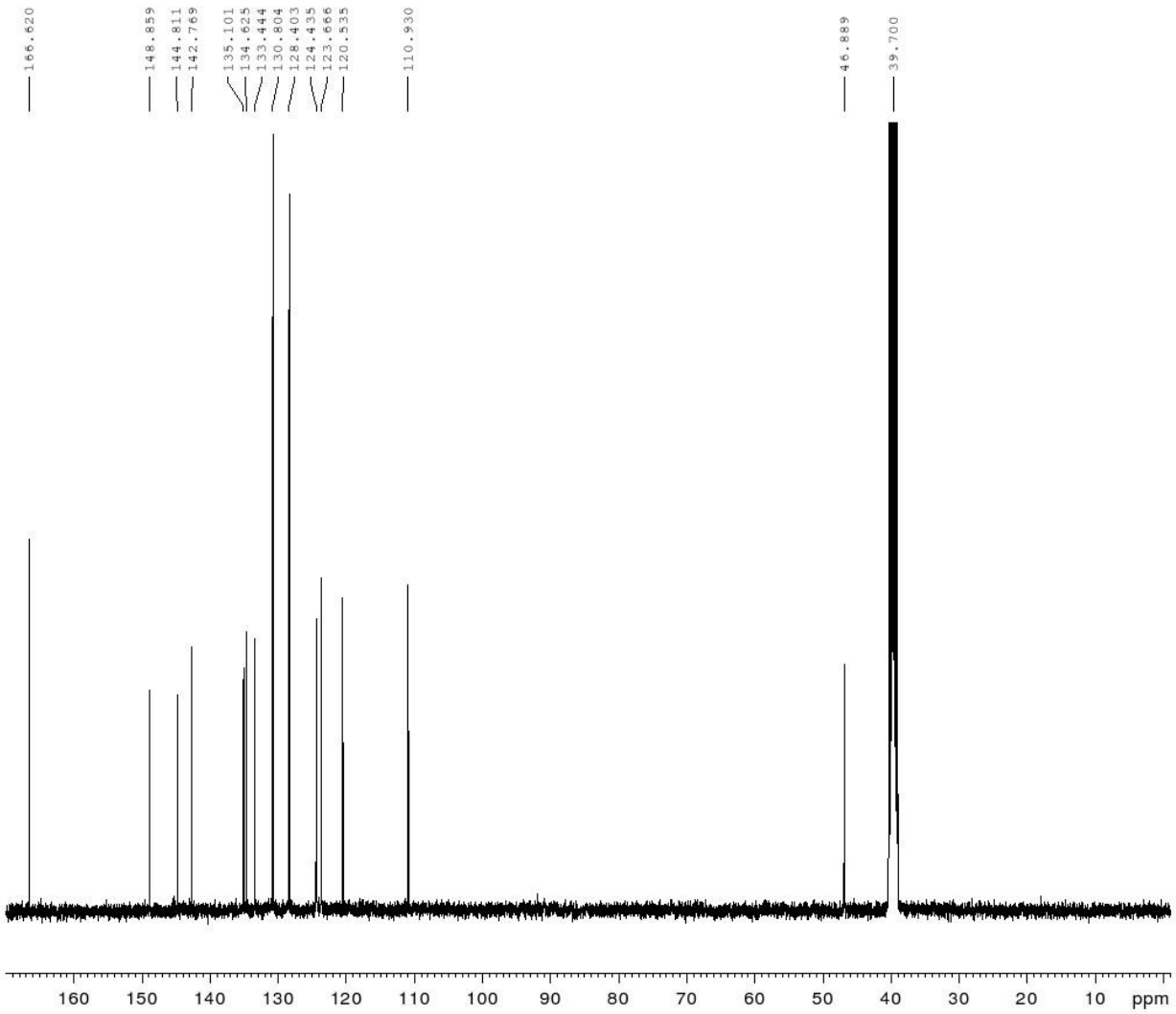
5d



Standard 1H
122037
MIM0372_1
Milen Matyas
2017.05.09. (DA)

NAME	122037
EXPNO	11
PROCNO	1
Date_	20170509
Time	16.41
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	294.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	12.50 usec
PL1	0.80 dB
PL1W	12.53577709 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300013 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

5d



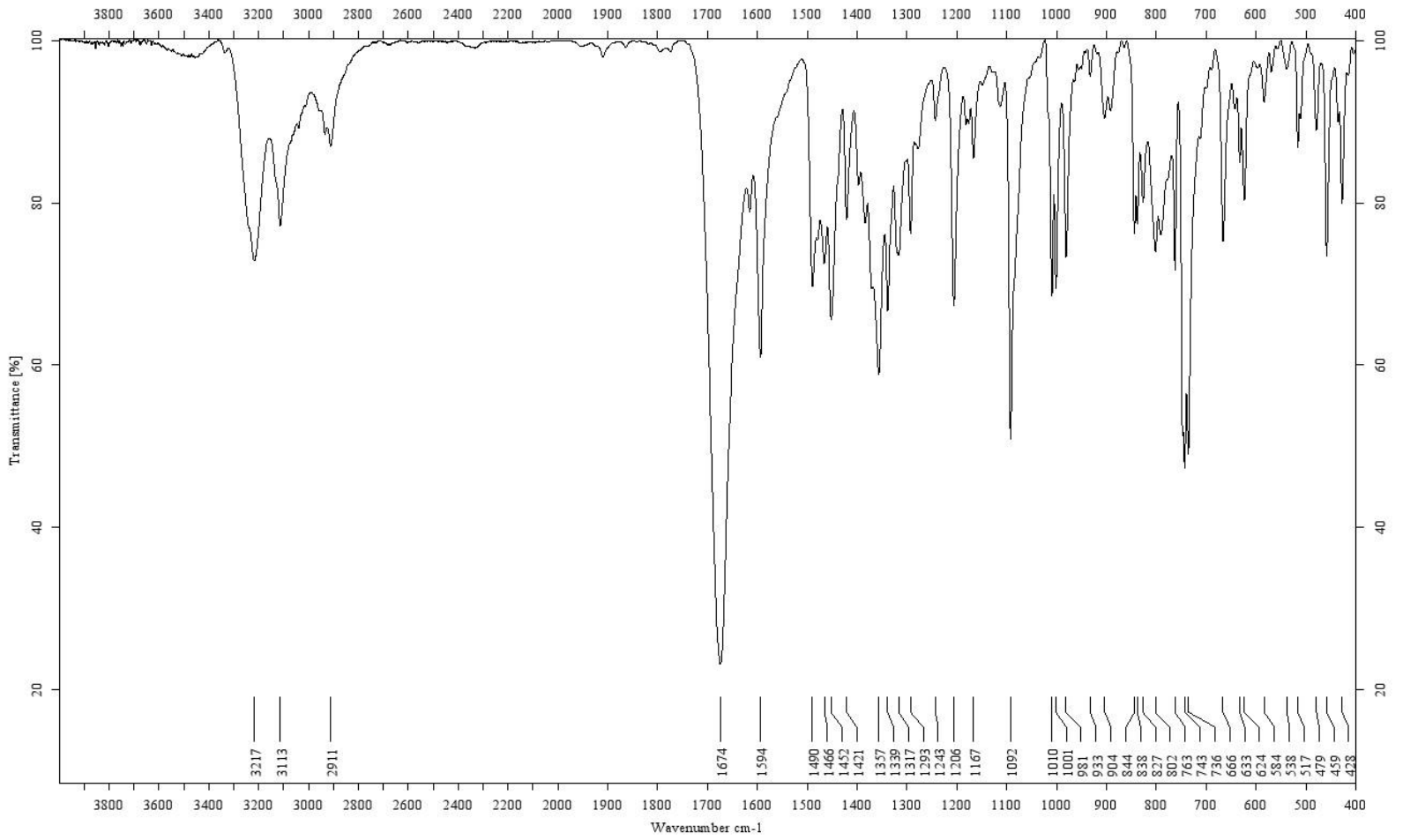
Standard 13C
122037
MIM0372_1
Milen Matyas
2017.05.09. (DA)

NAME	122037
EXPNO	12
PROCNO	1
Date_	20170509
Time	22.13
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	8192
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	295.5 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	1.44 dB
PL1W	43.99363327 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	0.80 dB
PL12	18.30 dB
PL13	18.40 dB
PL2W	12.53577709 W
PL12W	0.22292118 W
PL13W	0.21784686 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127976 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

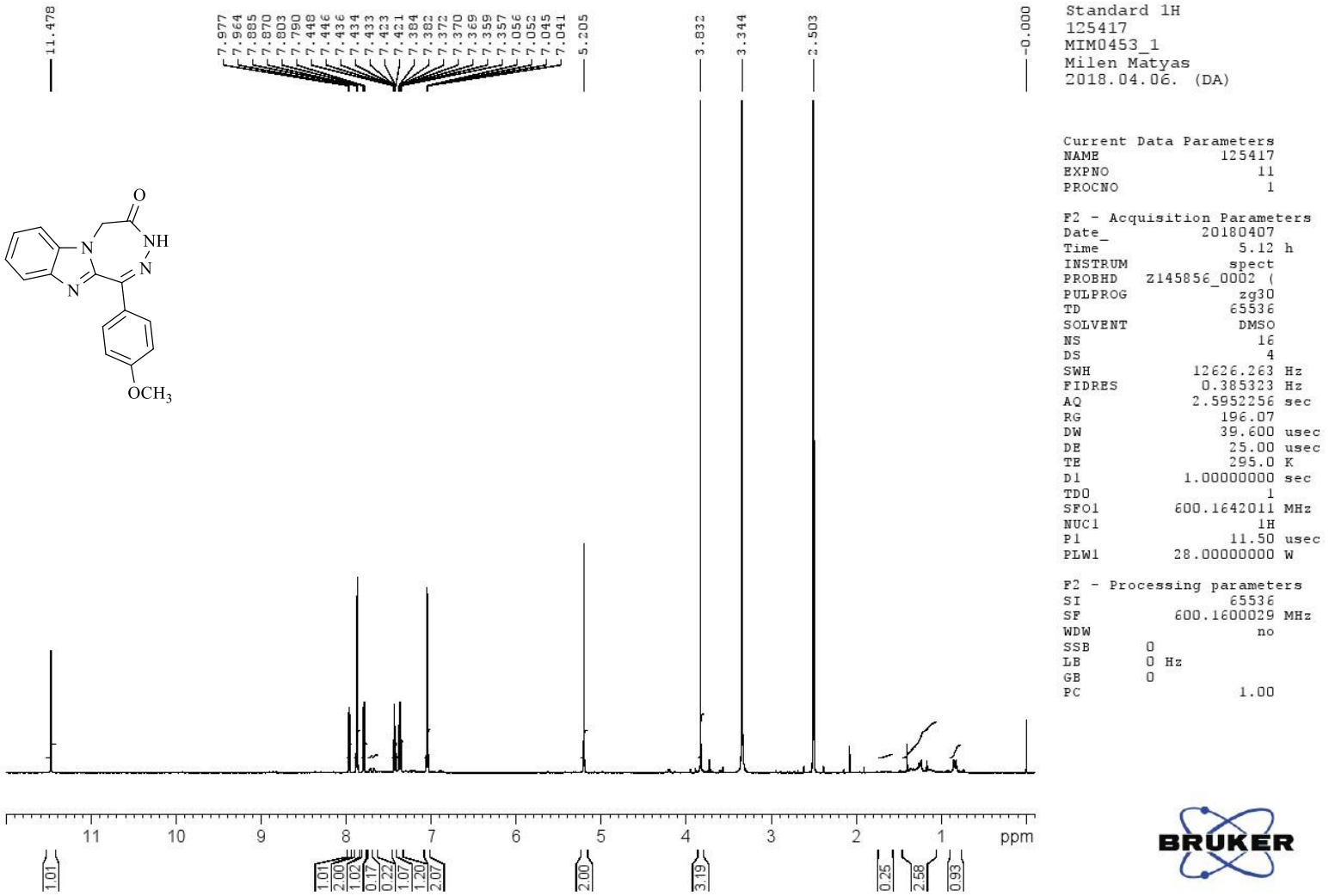
5d

122037	Milen Matyas	KP
MIM0372_1	KBr	09/05/2017

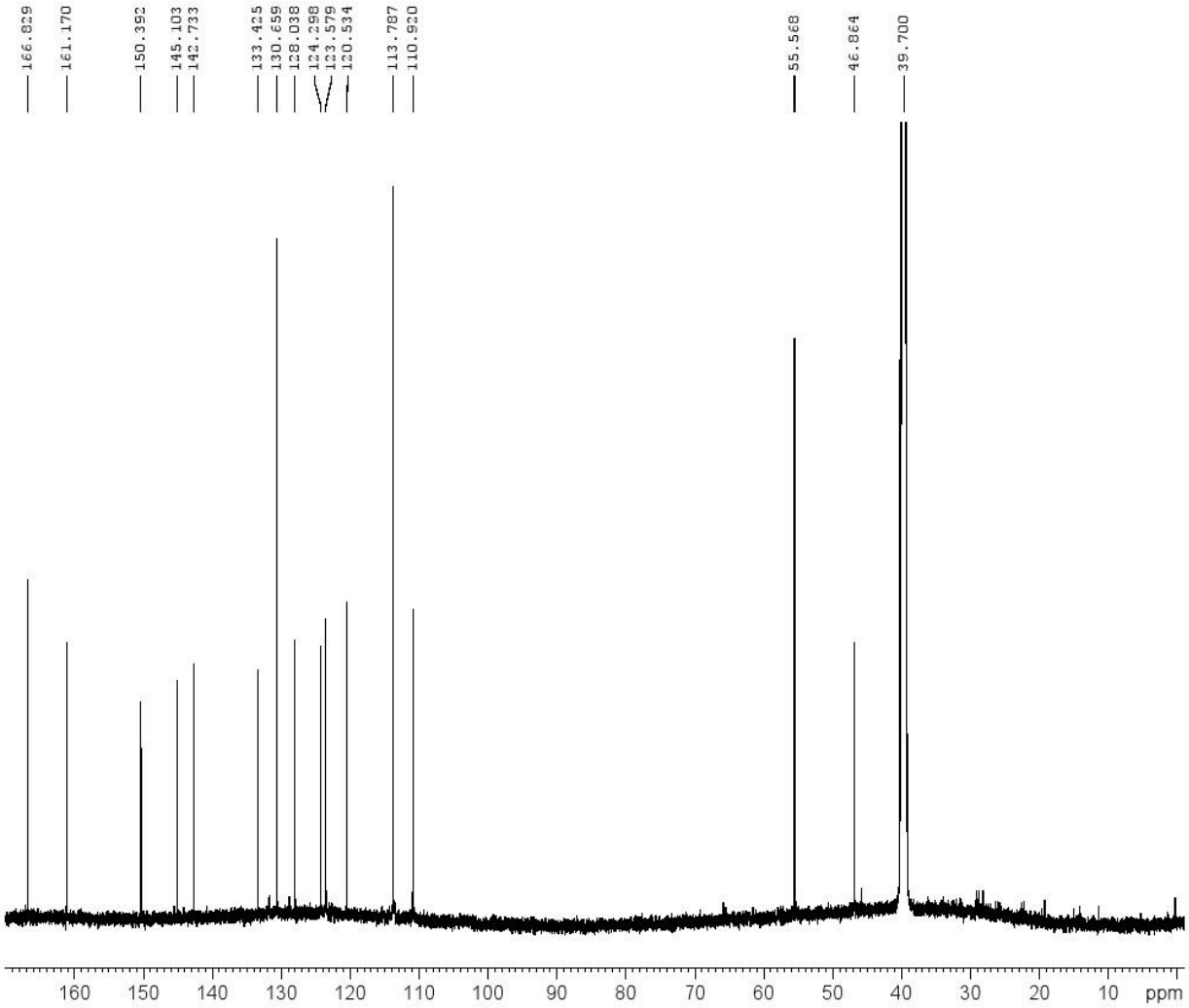
BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16



5e


11.478
7.977
7.964
7.885
7.870
7.803
7.790
7.448
7.446
7.436
7.434
7.433
7.423
7.421
7.384
7.382
7.372
7.370
7.369
7.359
7.357
7.056
7.052
7.045
7.041
5.205
3.832
3.344
2.503
-0.000
O
NH
N
N
N
OCH3
11
10
9
8
7
6
5
4
3
2
1
ppm
1.01
1.01
2.00
1.02
0.17
0.22
1.07
1.20
2.07
2.00
3.19
0.25
2.58
0.93
Standard 1H
125417
MIM0453_1
Milen Matyas
2018.04.06. (DA)
Current Data Parameters
NAME 125417
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180407
Time 5.12 h
INSTRUM spect
PROBHD Z145856_0002 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 4
SWH 12626.263 Hz
FIDRES 0.385323 Hz
AQ 2.5952256 sec
RG 196.07
DW 39.600 usec
DE 25.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.1642011 MHz
NUC1 1H
P1 11.50 usec
PLW1 28.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1600029 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
BRUKER

5e

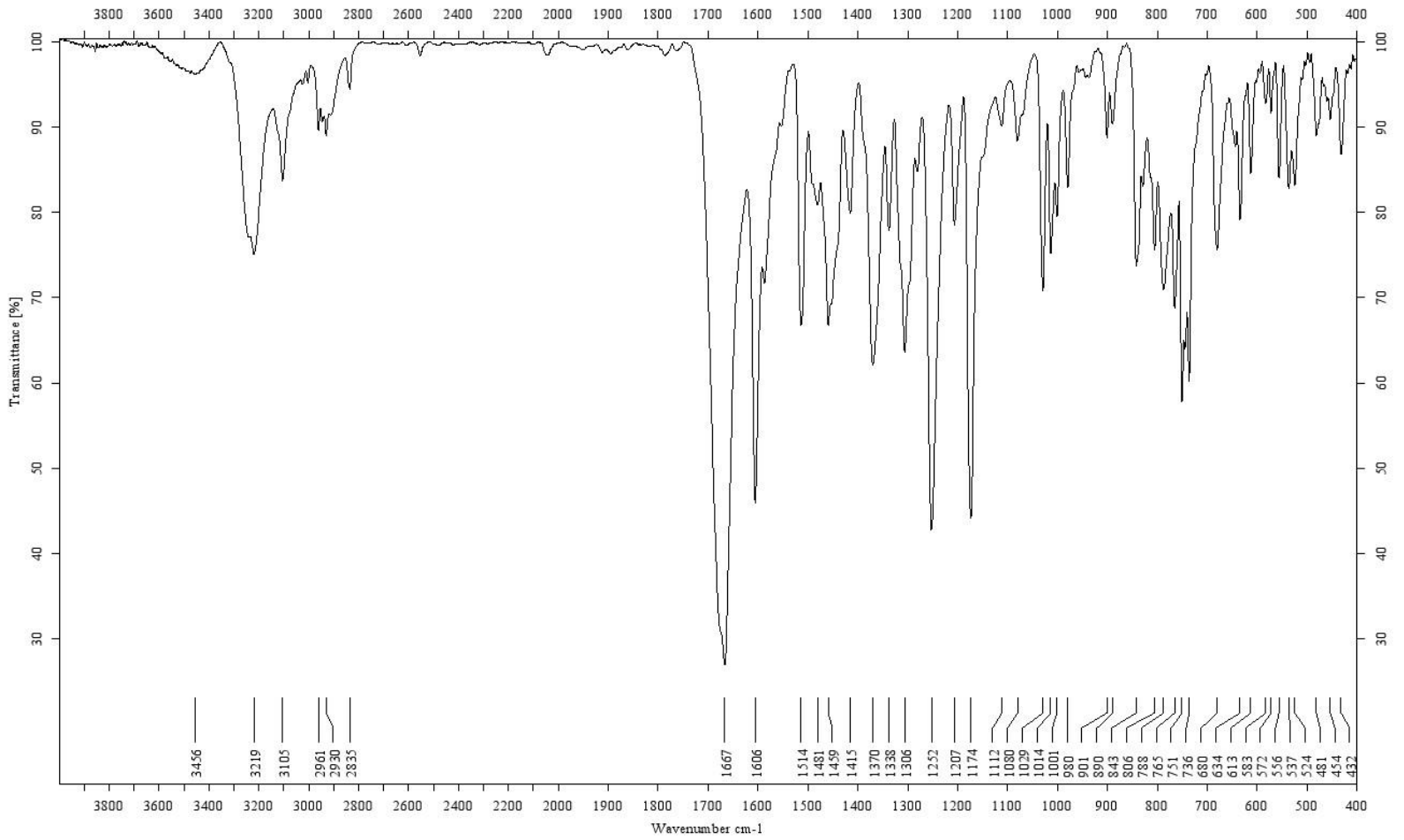



```
Standard 13C
125417
MIM0453_1
Milen Matyas
2018.04.06. (DA)

Current Data Parameters
NAME                  125417
EXPNO                     12
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180407
Time                  10.51 h
INSTRUM                spect
PROBHD    Z145856_0002 (
PULPROG               zgpg30
TD                     65536
SOLVENT                DMSO
NS                      8192
DS                         4
SWH               36057.691 Hz
FIDRES             1.100393 Hz
AQ                0.9087659 sec
RG                    196.07
DW                    13.867 usec
DE                     18.00 usec
TE                     295.0 K
D1               1.50000000 sec
D11              0.03000000 sec
TD0                        1
SFO1            150.9254424 MHz
NUC1                    13C
P1                     10.00 usec
PLW1            60.36299896 W
SFO2            600.1624006 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                  80.00 usec
PLW2            26.42600060 W
PLW12            0.59460002 W
PLW13            0.29861000 W

F2 - Processing parameters
SI                     65536
SF              150.9103915 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

5e

125417	Milen Matyas	KP
MIM0453_1	KBr	2018.04.09.

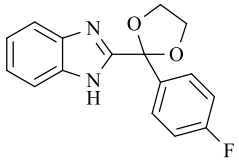
BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16

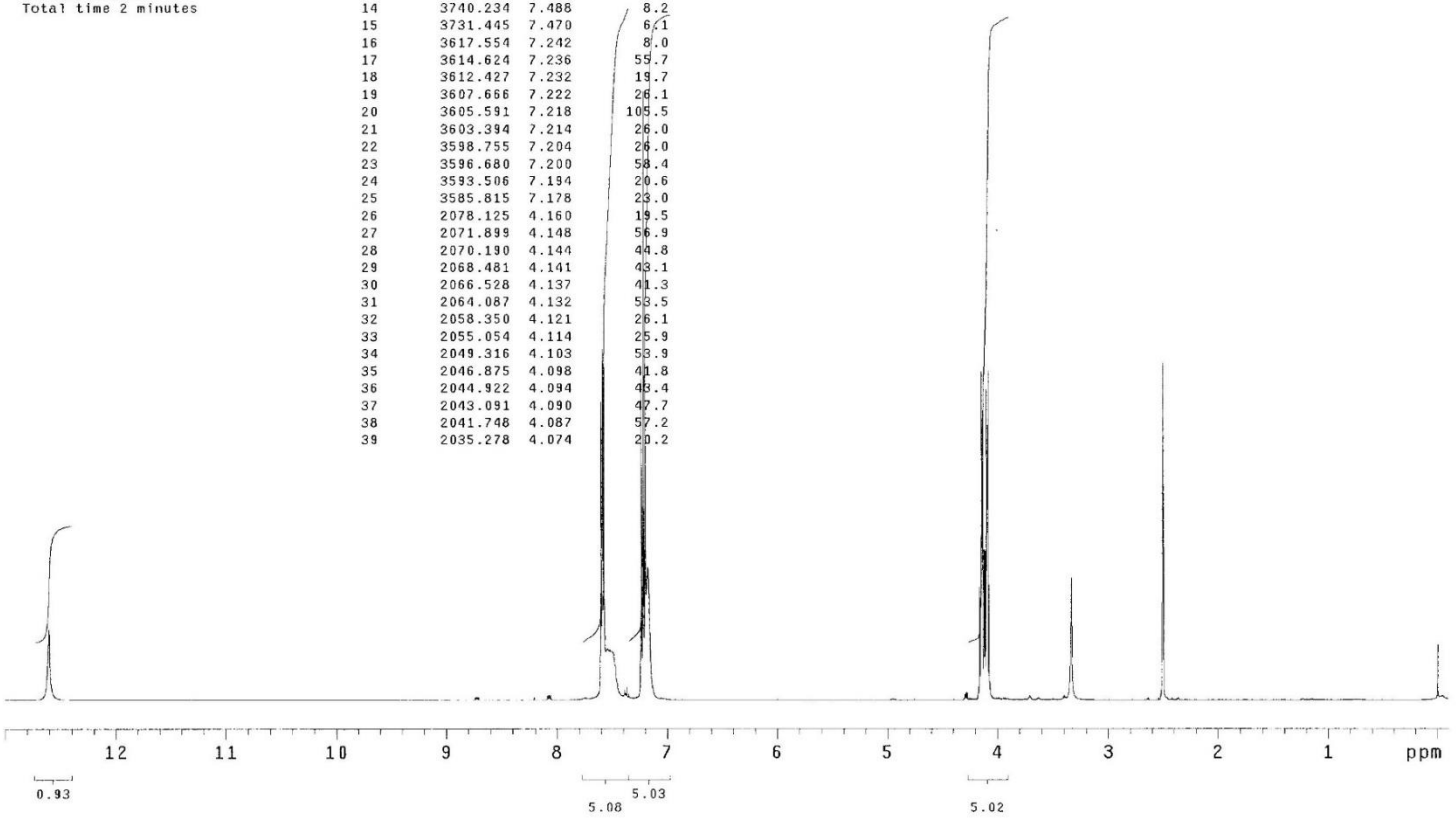


6

STANDARD 1H
72332
MM543
Milen Matyas
2008.01.08. (BB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "i500"
PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 6.4 usec
Acq. time 5.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.5268340 MHz
DATA PROCESSING
FT size 131072
Total time 2 minutes

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	6297.974	12.608	12.3	40	1667.480	3.338	21.1
2	3800.781	7.609	7.8	41	1254.028	2.510	21.5
3	3797.852	7.603	51.7	42	1252.319	2.507	43.8
4	3795.654	7.598	23.9	43	1250.610	2.504	58.5
5	3792.236	7.592	58.8	44	1248.779	2.500	42.6
6	3788.940	7.585	60.9	45	1247.070	2.497	20.5
7	3785.522	7.578	28.6	46	-0.000	-0.000	9.6
8	3783.447	7.574	57.7				
9	3780.396	7.568	13.1				
10	3769.653	7.546	8.8				
11	3766.958	7.541	9.0				
12	3757.812	7.523	8.7				
13	3748.779	7.505	8.5				
14	3740.234	7.488	8.2				
15	3731.445	7.470	6.1				
16	3617.554	7.242	8.0				
17	3614.624	7.236	55.7				
18	3612.427	7.232	19.7				
19	3607.666	7.222	26.1				
20	3605.591	7.218	105.5				
21	3603.394	7.214	26.0				
22	3598.755	7.204	26.0				
23	3596.680	7.200	58.4				
24	3593.506	7.194	20.6				
25	3585.815	7.178	23.0				
26	2078.125	4.160	19.5				
27	2071.899	4.148	56.9				
28	2070.190	4.144	44.8				
29	2068.481	4.141	43.1				
30	2066.528	4.137	41.3				
31	2064.087	4.132	53.5				
32	2058.350	4.121	26.1				
33	2055.054	4.114	25.9				
34	2049.316	4.103	53.9				
35	2046.875	4.098	41.8				
36	2044.922	4.094	43.4				
37	2043.091	4.090	47.7				
38	2041.748	4.087	57.2				
39	2035.278	4.074	20.2				



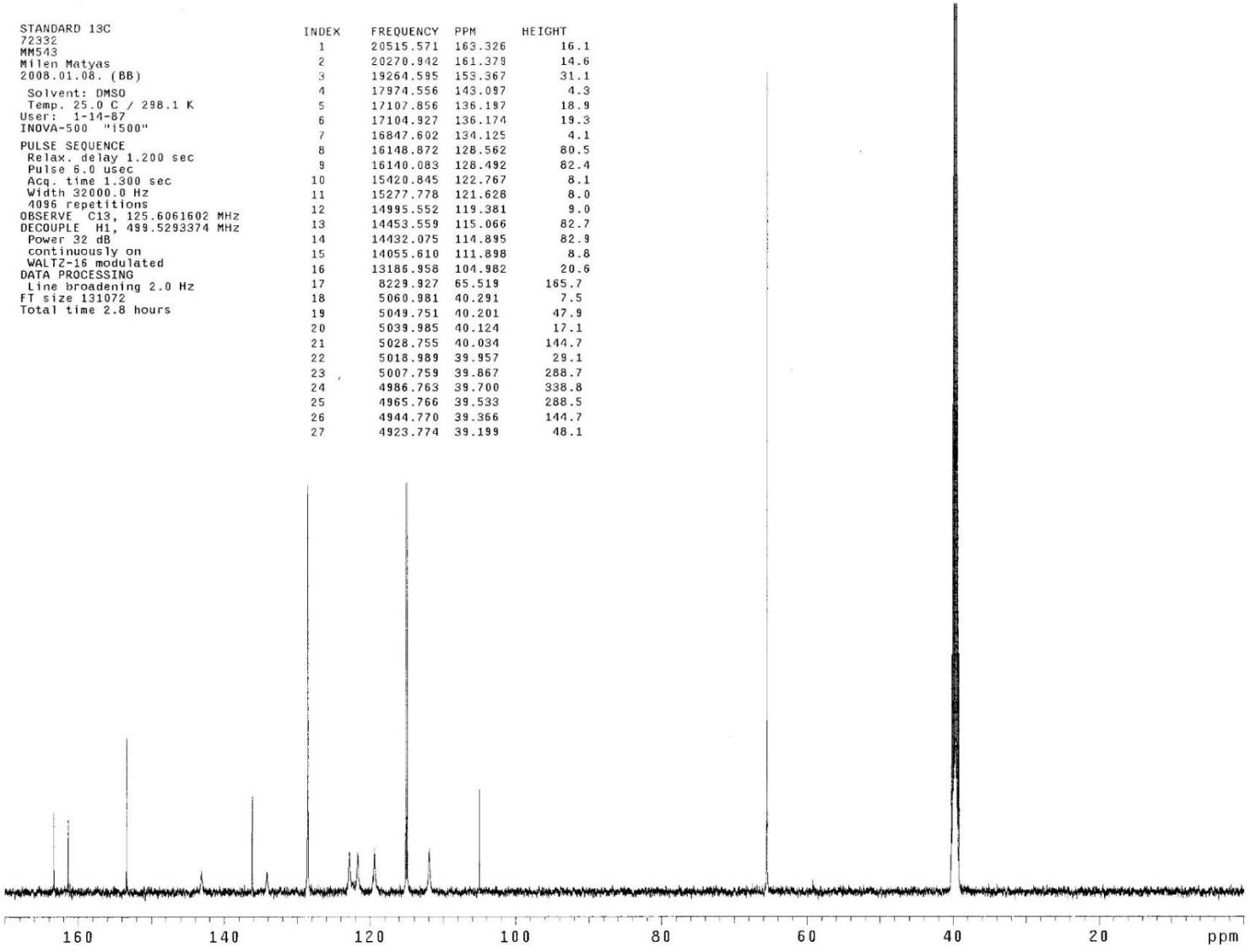


6

STANDARD 13C
72332
MM543
Milen Matyas
2008.01.08. (BB)
Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "i500"

PULSE SEQUENCE
Relax. delay 1.200 sec
Pulse 6.0 usec
Acq. time 1.300 sec
Width 32000.0 Hz
4096 repetitions
OBSERVE C13, 125.6061602 MHz
DECOUPLE H1, 499.5293374 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 2.8 hours

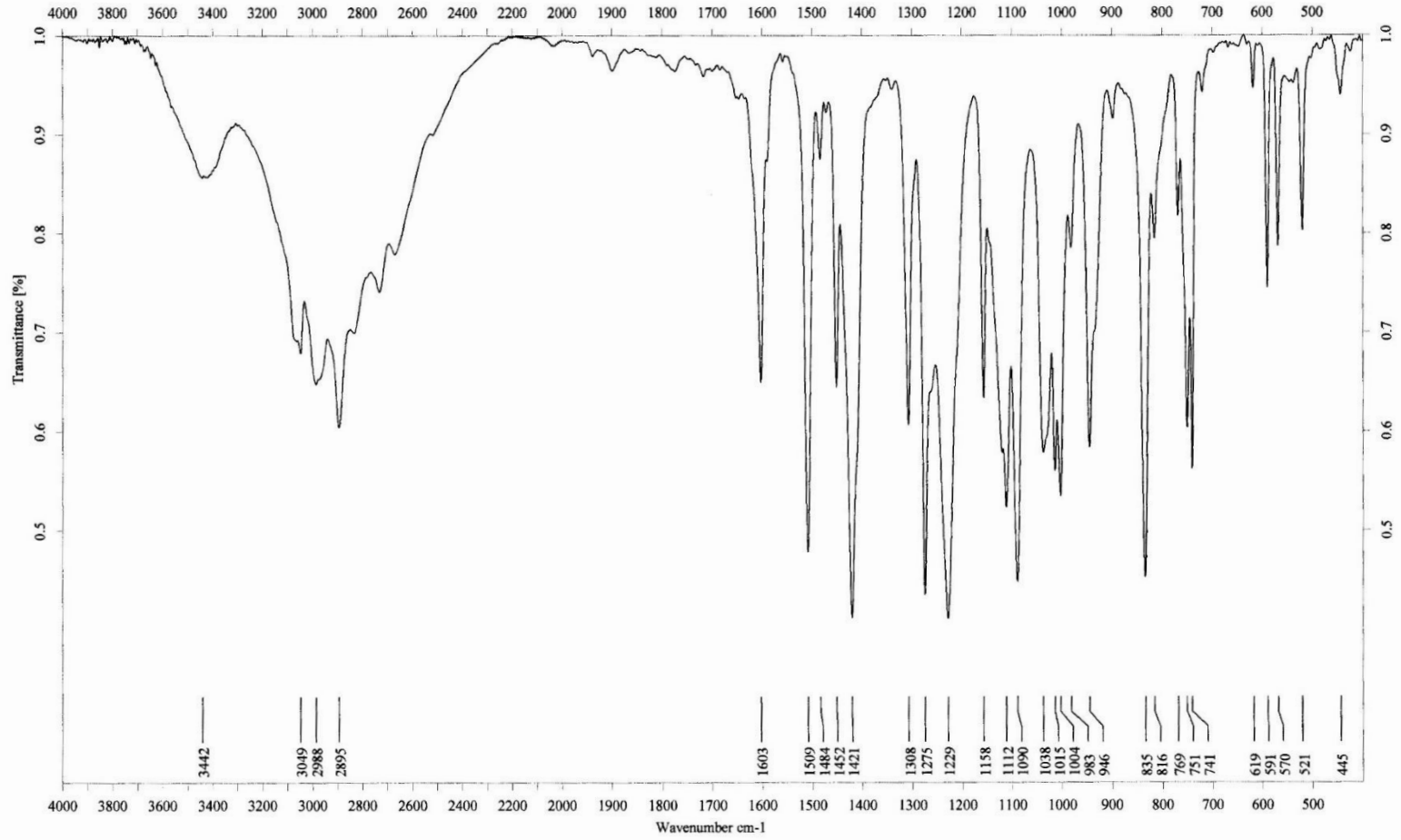
INDEX	FREQUENCY	PPM	HEIGHT
1	20515.571	163.326	16.1
2	20270.942	161.378	14.6
3	19264.595	153.367	31.1
4	17974.556	143.097	4.3
5	17107.856	136.197	18.9
6	17104.927	136.174	19.3
7	16847.602	134.125	4.1
8	16148.872	128.562	80.5
9	16140.083	128.492	82.4
10	15420.845	122.767	8.1
11	15277.778	121.628	8.0
12	14995.552	119.381	9.0
13	14453.559	115.066	82.7
14	14432.075	114.895	82.9
15	14055.610	111.898	8.8
16	13186.958	104.982	20.6
17	8229.927	65.519	165.7
18	5060.981	40.291	7.5
19	5049.751	40.201	47.9
20	5039.985	40.124	17.1
21	5028.755	40.034	144.7
22	5018.989	39.957	29.1
23	5007.759	39.867	288.7
24	4986.763	39.700	338.8
25	4965.766	39.533	288.5
26	4944.770	39.366	144.7
27	4923.774	39.199	48.1

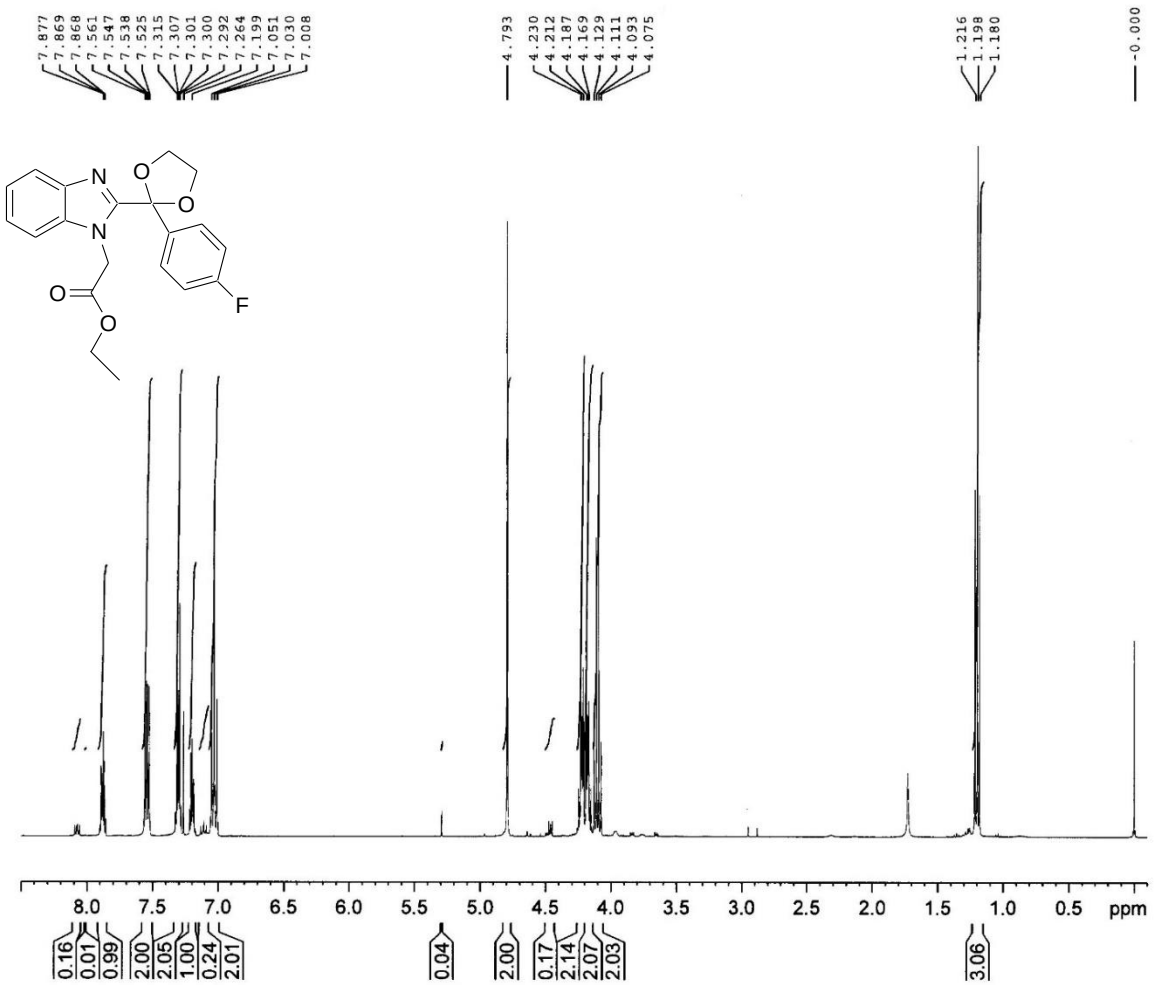


6

72332	Milen Mátyás	BB
MM543	KBr	08/01/2008

BRUKER VECTOR22
Resolution: 2 cm-1
Number of Scans: 8





Standard 1H
125632
MIM0455_1
Milen Matyas
2018.04.25. (DA)

Current Data Parameters

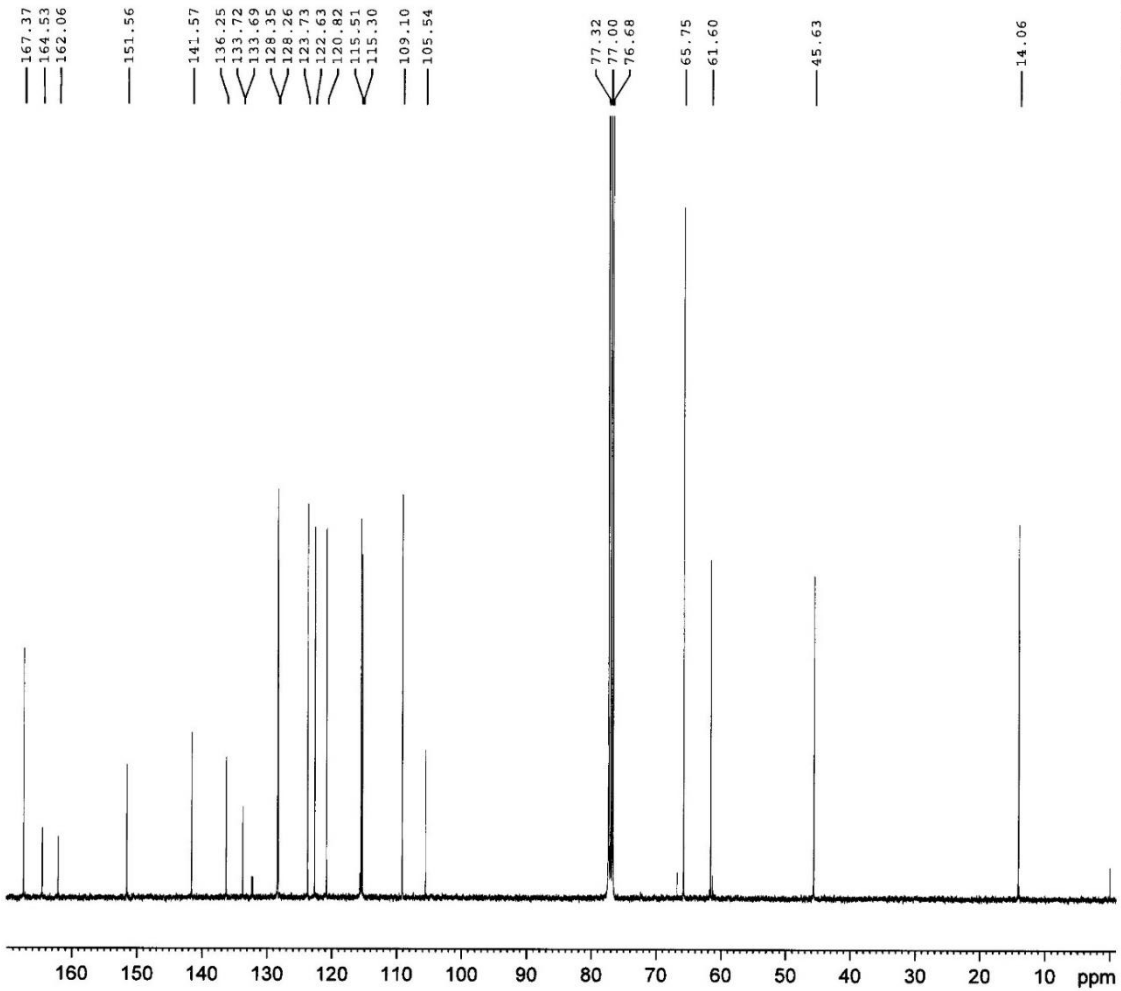
NAME	125632
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20180425
Time	16.51 h
INSTRUM	spect
PROBHD	Z105190_0010 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	3.9845889 sec
RG	161
DW	60.800 usec
DE	6.50 usec
TE	295.6 K
D1	1.00000000 sec
TD0	1
SFO1	400.1324710 MHz
NUC1	1H
P1	12.70 usec
PLW1	11.39999962 W

F2 - Processing parameters

SI	32768
SF	400.1300083 MHz
WDW	no
SSB	0
LB	0 Hz
GB	0
PC	1.00



Standard 13C
125632
MIM0455_1
Milen Matyas
2018.04.25. (DA)

Current Data Parameters

NAME	125632
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

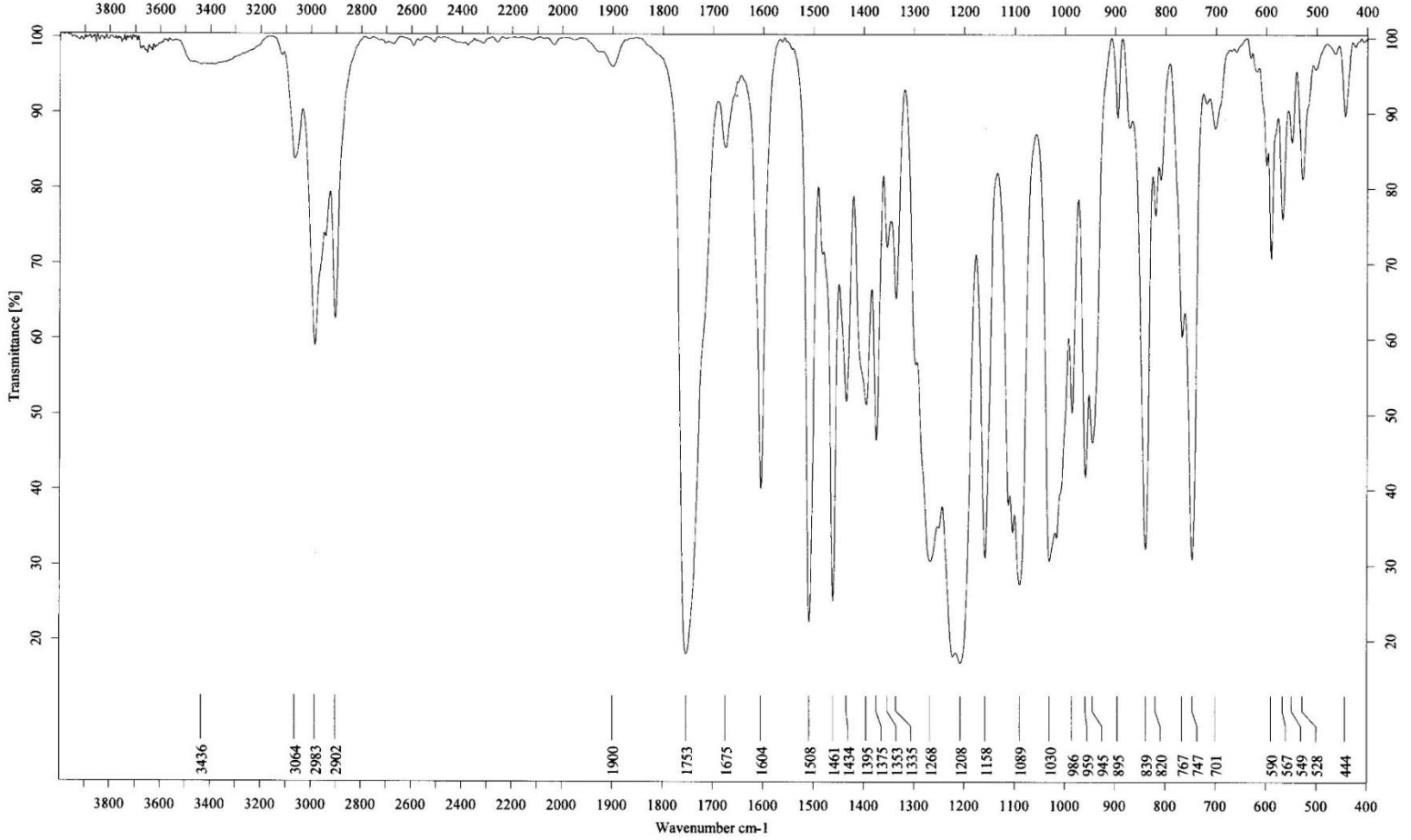
Date_	20180425
Time	22.23 h
INSTRUM	spect
PROBHD	Z105190_0010 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	8192
DS	4
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	1.3631488 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	296.5 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P1	8.80 usec
PLW1	46.20000076 W
SFO2	400.1316005 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	90.00 usec
PLW2	11.39999962 W
PLW12	0.22700000 W
PLW13	0.11418000 W

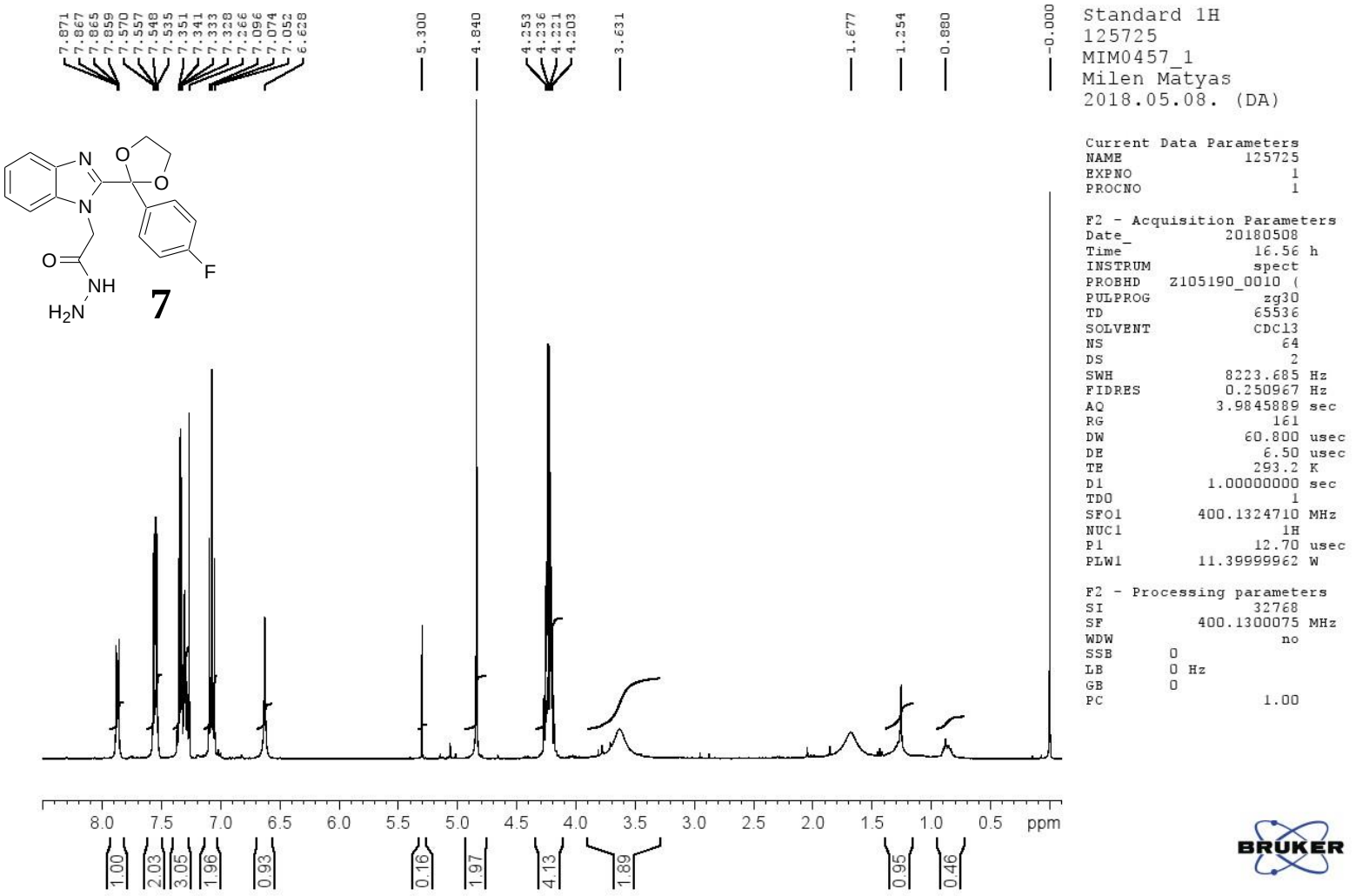
F2 - Processing parameters

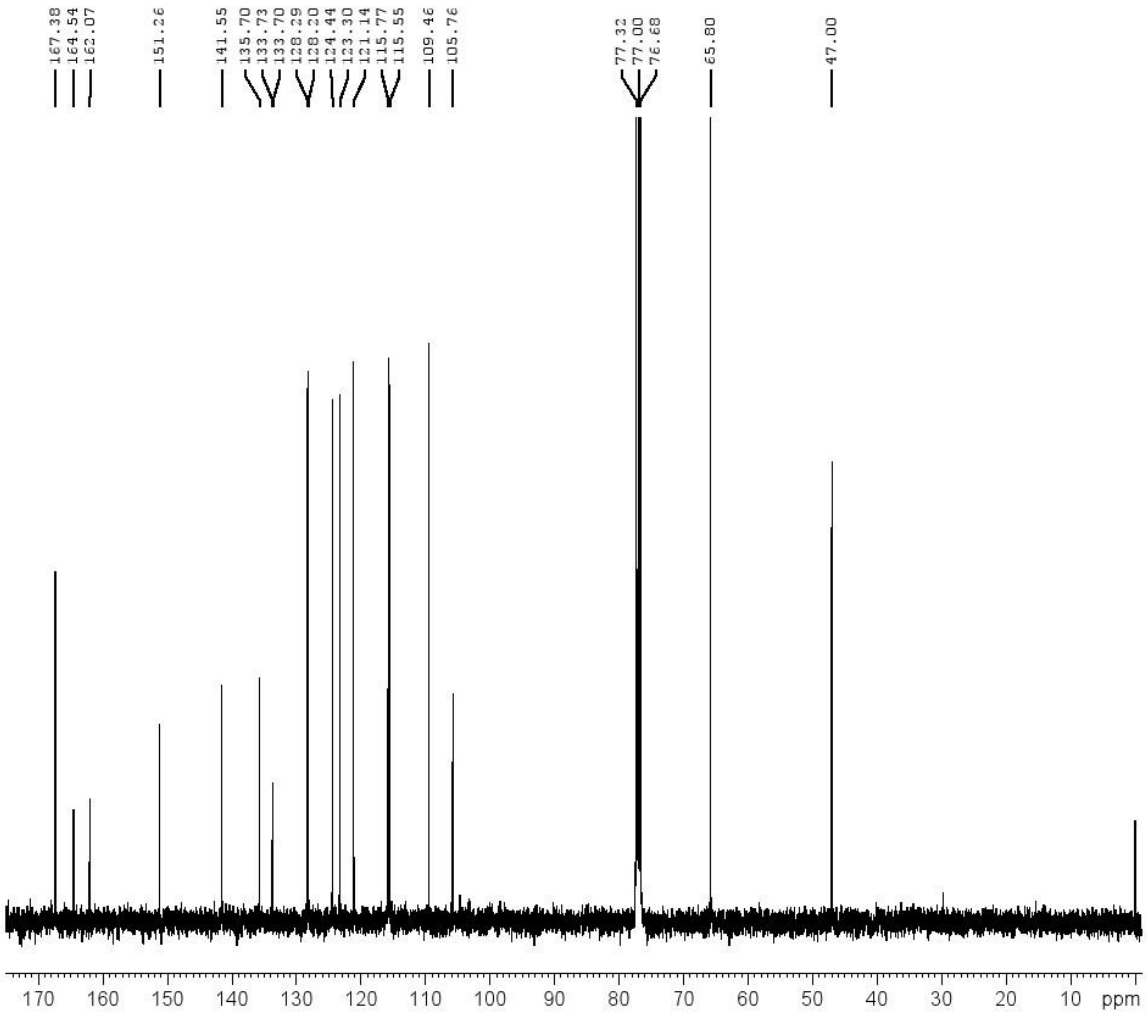
SI	32768
SF	100.6127725 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

125632	Milen Matyas	KP
MIM0455_1	Film	2018.04.25.

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16




7.871
7.867
7.865
7.859
7.570
7.557
7.548
7.535
7.351
7.341
7.333
7.328
7.266
7.096
7.074
7.052
6.628
5.300
4.840
4.253
4.236
4.221
4.203
3.631
1.677
1.254
0.880
-0.000
Standard 1H
125725
MIM0457_1
Milen Matyas
2018.05.08. (DA)
Current Data Parameters
NAME 125725
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180508
Time 16.56 h
INSTRUM spect
PROBHD Z105190_0010 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 3.9845889 sec
RG 161
DW 60.800 usec
DE 6.50 usec
TE 293.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1324710 MHz
NUC1 1H
P1 12.70 usec
PLW1 11.39999962 W
F2 - Processing parameters
SI 32768
SF 400.1300075 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
N
O
O
N
O
NH
H2N
F
7
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
2.03
3.05
1.96
0.93
0.16
1.97
4.13
1.89
0.95
0.46
BRUKER



Standard 13C
125725
MIM0457_1
Milen Matyas
2018.05.08. (DA)

Current Data Parameters

NAME	125725
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20180508	
Time	19.44	h
INSTRUM	spect	
PROBHD	Z105190_0010 (	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	4096	
DS	4	
SWH	24038.461	Hz
FIDRES	0.733596	Hz
AQ	1.3631488	sec
RG	2050	
DW	20.800	usec
DE	6.50	usec
TE	294.6	K
D1	1.00000000	sec
D11	0.03000000	sec
TD0	1	
SFO1	100.6228298	MHz
NUC1	13C	
P1	8.80	usec
PLW1	46.20000076	W
SFO2	400.1316005	MHz
NUC2	1H	
CPDPRG[2	waltz16	
PCPD2	90.00	usec
PLW2	11.39999962	W
PLW12	0.22700000	W
PLW13	0.11418000	W

F2 - Processing parameters

SI	32768	
SF	100.6127724	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

125725	Milen Matyas	KP
MIM0457_1	KBr	2018.05.08.

BRUKER Alpha
Resolution: 2 cm-1
Number of Scans: 16