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Reaction of CF_3-ynones with azides. An efficient regioselective and metal-free route to 4-trifluoroacetyl-1,2,3-triazoles

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General remarks. ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on Bruker AVANCE 400 MHz spectrometer in $CDCl_3$ at 400, 100 and 376 MHz respectively. Chemical shifts (δ) in ppm are reported with the use of the residual chloroform signal (7.25 for ^{1}H and 77.0 for ^{13}C) as internal reference. The ^{19}F chemical shifts were referenced to C_6F_6, (-162.9 ppm). The coupling constants (J) are given in Hertz (Hz). ESI-MS spectra were measured with Orbitrap Elite instrument. The silica gel used for column chromatography was 230-400 Mesh. TLC analysis was performed on "Silufol UV-254" plates. All reagents were of reagent grade and were used as such or distilled prior to use. CF_3-ynones **1** were prepared as reported previously. [V. M. Muzalevskiy, A. Yu. Rulev, A. R. Romanov, E. V. Kondrashov, I. A. Ushakov, V. A. Chertkov and V. G. Nenajdenko. *J. Org. Chem.*, 2017, **82**, 7200.]

Synthesis of 1,2,3-triazoles 2,3 (general procedure). A 3 ml vial with a screw cup was charged with the corresponding azide (1.1 mmol), DMSO (2 ml, or another solvent), the corresponding CF_3-ynone (1 mmol), and was heated at 80-90 °C for 5-7 h. The mixture was poured into 0.1 *M* HCl (30 ml) and extracted with CH_2Cl_2 (3×10 ml). The combined extracts were dried over Na_2SO_4, the volatiles were evaporated, and the residue was purified by column chromatography on silica gel using mixture of CH_2Cl_2 and MeOH (30:1) as an eluent. Minor isomers were not isolated in pure form. For minor regioisomeric triazoles **3**, the characteristic signals are given.

Ethyl [5-phenyl-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2a). Colourless oil, yield 300 mg (92%), isolated as 96:4 mixture with isomeric triazole **3a**. IR (ν, cm^{-1}): 1725 ($COCF_3$), 1753 (CO_2Et). ^1H NMR ($CDCl_3$): δ 1.23 (t, 3H, $\underline{CH_3}CH_2$, *J* = 7.1), 4.21 (q, 2H, $CH_3\underline{CH_2}$, *J* = 7.1), 5.05 (s, 2H, CH_2), 7.36-7.40 (m, 2H, Ar), 7.48-7.60 (m, 3H, Ar). ^{13}C NMR ($CDCl_3$): δ 13.9, 49.2, 62.7, 116.1 (q, CF_3, *J* = 290.4), 123.9, 129.1, 129.2, 131.1, 137.8, 144.8, 165.5, 174.1 (q, $\underline{CO}CF_3$, *J* = 37.6). ^{19}F NMR ($CDCl_3$): δ -75.3. **Ethyl [4-phenyl-5-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (3a).** ^1H NMR ($CDCl_3$): δ 1.30 (t, 3H, $\underline{CH_3}CH_2$, *J* = 7.1), 4.27 (q, 2H, $CH_3\underline{CH_2}$, *J* = 7.1), 5.47 (s, 2H, CH_2). ^{19}F NMR ($CDCl_3$): δ -73.8. ESI-MS (m/z): calcd $C_{14}H_{13}F_3N_3O_3$ [$M+H^+$] 328.0904, found 328.0907.

Ethyl [5-(4-methylphenyl)-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2b). Colourless oil, yield 178 mg (52%). IR (ν, cm^{-1}): 1723 ($COCF_3$), 1752 (CO_2Et). ^1H NMR ($CDCl_3$): δ 1.24 (t, 3H, $CH_2\underline{CH_3}$, *J* = 7.1), 2.43 (c, 3H, CH_3), 4.21 (q, 2H, $CH_3\underline{CH_2}$, *J* = 7.1), 5.05 (s, 2H, CH_2), 7.27 (d, 2H, Ar, *J* = 8.0), 7.33 (d, 2H, Ar, *J* = 8.0). ^{13}C NMR ($CDCl_3$): δ 13.8, 21.4, 49.1, 62.6, 116.0 (q, CF_3, *J* = 290.4), 120.7, 129.0, 129.8, 137.6, 141.6, 145.0, 165.6, 174.0 (q, $\underline{CO}CF_3$, *J* = 37.2). ^{19}F NMR ($CDCl_3$): δ -75.31. ESI-MS (m/z): calcd for $C_{15}H_{15}F_3N_3O_3$ [$M+H^+$] 342.1060, found 342.1056.

Ethyl [5-(4-bromophenyl)-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2c). Pale brown oil, yield 263 mg (65%). IR (ν, cm^{-1}): 1725 ($COCF_3$), 1752 (CO_2Et). ^1H NMR ($CDCl_3$): δ 1.27 (t, 3H, $CH_2\underline{CH_3}$, *J* = 7.1), 4.24 (q, 2H, $CH_3\underline{CH_2}$, *J* = 7.1), 5.05 (s, 2H, CH_2) 7.28 (d, 2H, Ar, *J* = 8.6), 7.69 (d, 2H, Ar, *J* = 8.5). ^{13}C NMR ($CDCl_3$): δ 14.0, 49.2, 62.9, 116.0 (q, CF_3, *J* = 290.8), 120.3, 122.9, 126.1, 130.8, 132.5, 138.0, 143.8, 165.4, 174.2 (q, $\underline{CO}CF_3$, *J* = 37.4). ^{19}F NMR ($CDCl_3$): δ -75.36. ESI-MS (m/z): calcd for $C_{14}H_{12}BrF_3N_3O_3$ [$M+H^+$] 406.0009, found 406.0009.

Ethyl [5-(4-chlorophenyl)-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2d). Colourless oil, yield 159 mg (44%). IR (ν, cm^{-1}): 1725 ($COCF_3$), 1752 (CO_2Et). ^1H NMR ($CDCl_3$): δ 1.24 (t, 3H, $CH_2\underline{CH_3}$, *J* = 7.2), 4.22 (q, 2H, $CH_3\underline{CH_2}$, *J* = 7.2), 5.03 (s, 2H, CH_2), 7.33 (d, 2H, Ar, *J* = 8.6), 7.51 (d, 2H, Ar, *J* = 8.6^{13}C NMR ($CDCl_3$): δ 13.8, 26.6, 49.1, 62.8, 115.9 (q, CF_3, *J* = 290.6), 122.2, 128.1, 129.4, 129.4, 130.6, 137.6, 143.7, 165.5, 174.0 (q, $\underline{CO}CF_3$, *J* = 37.4). ^{19}F

NMR ($CDCl_3$): δ -75.4. ESI-MS (m/z): calcd for $C_{14}H_{12}ClF_3N_3O_3$ [$M+H^+$] 362.0514, found 362.0520.

Ethyl [5-(4-methoxyphenyl)-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2e). Brown oil, yield 201 mg (56%). IR (ν, cm^{-1}): 1721 ($COCF_3$), 1753 (CO_2Et). ^1H NMR ($CDCl_3$): δ 1.24 (t, 3H, $CH_2\underline{CH_3}$, J = 7.1), 3.86 (c, 3H, CH_3O), 4.21 (q, 2H, $CH_3\underline{CH_2}$, J = 7.1), 5.05 (s, 2H, CH_2), 7.02 (d, 2H, Ar, J = 8.4), 7.32 (d, 2H, Ar, J = 8.4). ^{13}C NMR ($CDCl_3$): δ 13.8, 49.1, 55.3, 62.6, 114.5, 116.1 (q, CF_3, J = 290.4), 130.8, 137.5, 144.9, 161.7, 165.7, 174.0 (q, $\underline{CO}CF_3$, J = 36.9). ^{19}F NMR ($CDCl_3$): δ -75.2. ESI-MS (m/z): calcd for $C_{15}H_{15}F_3N_3O_4$ [$M+H^+$] 358.1009, found 358.1012.

Ethyl [5-(4-methylthiophenyl)-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2f). Colorless oil, yield 216 mg (58 %), isolated as 98:2 mixture with isomeric triazole **3f**. ^1H NMR ($CDCl_3$): δ 1.22 (t, 3H, $CH_2\underline{CH_3}$, J = 7.1), 2.49 (s, 3H, SCH_3), 4.18 (q, 2H, $\underline{CH_2}CH_3$, J = 7.1), 5.04 (s, 2H, CH_2), 7.26 (d, 2H, Ar, J = 8.3), 7.31 (d, 2H, Ar, J = 8.3). ^{13}C NMR ($CDCl_3$): δ 13.8, 14.6, 49.0, 62.7, 116.0 (q, CF_3, J = 290.8), 125.6, 129.4, 137.5, 143.5,144.5, 149.6, 165.6, 173.9, (q, $\underline{CO}CF_3$, J = 37.2). ^{19}F NMR ($CDCl_3$): δ -75.2. **Ethyl [4-(4-methylthiophenyl)-5-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (3f)**. ^1H NMR ($CDCl_3$): δ 5.43 (s, 2H, CH_2). ^{19}F NMR ($CDCl_3$): δ -73.6. ESI-MS (m/z): calcd for $C_{15}H_{15}F_3N_3O_3S$ [$M+H^+$] 374.0781, found 374.0788.

Ethyl [5-(4-*tert*-butylphenyl)-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2g). Colourless oil, yield 158 mg (41%). IR (ν, cm^{-1}): 1723 ($COCF_3$), 1754 (CO_2Et). ^1H NMR ($CDCl_3$): δ 1.21 (t, 3H, $CH_2\underline{CH_3}$, J = 7.1), 1.34 (s, 9H, t-Bu), 4.19 (q, 2H, $CH_3\underline{CH_2}$, J = 7.1), 5.05 (s, 2H, CH_2) 7.31 (d, 2H, Ar, J = 8.3), 7.52 (d, 2H, Ar, J = 8.3). ^{13}C NMR ($CDCl_3$): δ 13.8, 31.0, 34.9, 49.1, 62.6, 116.1 (q, CF_3, J = 290.8), 120.7, 126.0, 129.0, 137.6, 145.0, 154.6, 165.6, 174.0 (q, $\underline{CO}CF_3$, J = 37.2). ^{19}F NMR ($CDCl_3$): δ -75.2. ESI-MS (m/z): calcd for $C_{18}H_{21}F_3N_3O_3$ [$M+H^+$] 384.1530, found 384.1523.

Ethyl [5-(3,4-dimethylphenyl)-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2h). Colourless oil, yield 219 mg (62 %), isolated as 96:4 mixture with isomeric triazole **3h**. IR (ν, cm^{-1}): 1724 ($COCF_3$), 1752 (CO_2Et). ^1H NMR ($CDCl_3$): δ 1.25 (t, 3H, $\underline{CH_3}CH_2$, J = 7.1), 2.30 (s, 3H, CH_3), 2.34 (s, 3H, CH_3), 4.22 (q, 2H, $CH_3\underline{CH_2}$, J = 7.1), 5.04 (s, 2H, CH_2), 7.09 (s, 1H, Ar), 7.12 (d, 1H, Ar, J = 8.3), 7.28 (d, 1H, Ar, J = 8.3). ^{13}C NMR ($CDCl_3$): δ 13.9, 19.7, 49.1, 62.6, 116.1 (q, CF_3, J = 290.8), 121.1, 126.5, 130.0, 130.3, 137.6, 137.7, 140.3, 145.1, 165.6, 174.0 (q, $\underline{CO}CF_3$, J = 37.0). ^{19}F NMR ($CDCl_3$): δ -75.2. **Ethyl [4-(3,4-dimethylphenyl)-5-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (3h)**. ^1H NMR ($CDCl_3$): δ 5.45 (s, 2H, CH_2). ^{19}F NMR ($CDCl_3$): δ -73.5. ESI-MS (m/z): calcd for $C_{16}H_{17}F_3N_3O_3$ [$M+H^+$] 356.1217, found 356.1222.

Ethyl [5-hexyl-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2i). Colourless oil, yield 127 mg (51 %). IR (ν, cm^{-1}): 1717($COCF_3$), 1755 (CO_2Et). ^1H NMR ($CDCl_3$): δ 0.83 (t, 3H, $CH_2\underline{CH_3}$, J = 6.7), 1.22-1.36 (m, 9H), 1.49-1.57 (m, 2H, CH_2), 2.91 (t, 2H, CH_2, J = 7.9), 4 .24 (q,

2H, $CH_3\underline{CH_2}$, *J* = 7.1), 5.13 (s, 2H, CH_2). ^{13}C NMR ($CDCl_3$): δ 13.7, 13.8, 22.2, 23.4, 27.4, 28.8, 31.1, 48.6, 62.8, 116.0 (q, CF_3, *J* = 290.4), 137.7, 147.2, 165.3, 174.7 (q, $\underline{CO}CF_3$, *J* = 37.2). ^{19}F NMR ($CDCl_3$): δ -75.1. ESI-MS (m/z): calcd for $C_{14}H_{21}F_3N_3O_3$ [$M+H^+$] 336.1530, found 336.1536.

Ethyl [5-(4-methoxy-1-naphtyl)-4-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (2j). Brown oil, yield 274 mg (67%). IR (ν, cm^{-1}): 1724 ($COCF_3$), 1752 (CO_2Et). ^1H NMR ($CDCl_3$): δ 1.13 (t, 3H, $\underline{CH_3}CH_2$, *J* = 7.1), 4.06 (s, 3H, $OC\underline{H_3}$), 4.09 (q, 2H, $CH_3\underline{CH_2}$, *J* = 7.1), 4.80 (d, 1H, CH_2, *J* = 17.2), 5.10 (d, 1H, CH_2, *J* = 17.2), 6.92 (d, 1H, Ar, *J* = 8.1), 7.17 (d, 1H, Ar, *J* = 8.1), 7.40 (d, 1H, Ar, *J* = 8.0), 7.47-7.56 (m, 2H, Ar), 8.40 (d, 1H, Ar, *J* = 8.2). ^{13}C NMR ($CDCl_3$): δ 13.4, 48.7, 55.4 (MeO), 62.2, 102.9, 112.5,. 115.7 (q, CF_3, *J* = 290.4), 122.6, 123.0, 125.3, 125.8, 127.9, 128.9, 131.4, 138.9, 143.4, 157.7, 165.0, 173.3 (q, $\underline{CO}CF_3$, *J* = 37.6). ^{19}F NMR ($CDCl_3$): δ -75.4. ESI-MS (m/z): calcd for $C_{19}H_{17}F_3N_3O_4$ [$M+H^+$] 408.1166, found 408.1169.

1-(1-Benzyl-5-phenyl-1*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (2k). Colourless oil, yield 193 mg (58 %), isolated as 91:9 mixture with isomeric triazole **3k**. IR (ν, cm^{-1}): 1723 ($COCF_3$). ^1H NMR ($CDCl_3$): δ 5.48 (c, 2H, CH_2), 7.03-7.09 (m, 2H, Ar), 7.22-7.33 (m, 5H, Ar), 7.45-7.59 (m, 3H, Ar). ^{13}C NMR ($CDCl_3$): δ 52.1, 116.1 (q, CF_3, *J* = 290.8), 124.4, 127.6, 128.6, 128.8, 128.9, 129.3, 130.8, 133.9, 138.0, 143.9, 174.1 (q, $\underline{CO}CF_3$, *J* = 37.2). ^{19}F NMR ($CDCl_3$): δ -75.2. **1-(3-Benzyl-5-phenyl-3*H*-1,2,3-triazol-4-yl)-2,2,2-trifluoroethanone (3k)**. ^1H NMR ($CDCl_3$): δ 5.84 (s, 2H, CH_2). ^{19}F NMR ($CDCl_3$): δ -74.1. ESI-MS (m/z): calcd for $C_{17}H_{13}F_3N_3O$ [$M+H^+$] 332.1005, found 332.1008.

1-[1-(4-Chlorophenyl)-5-phenyl-1*H*-1,2,3-triazol-4-yl]-2,2,2-trifluoroethanone (2l). Colorless oil, (314 mg, 89 %), isolated as 80:20 mixture with isomeric triazole **3l**. ^1H NMR ($CDCl_3$): δ 7.24-7.29 (m, 2H, Ar), 7.32 (d, 2H, Ar, *J* = 7.7), 7.38-7.54 (m, 5H, Ar). ^{13}C NMR ($CDCl_3$): δ 116.1 (q, CF_3, *J* = 290.6), 123.9, 126.3, 128.8, 129.7, 129.9, 130.9, 133.6, 136.1, 137.1, 143.4, 174.1 (q, $\underline{CO}CF_3$, *J* = 37.8). ^{19}F NMR ($CDCl_3$): δ -74.8. **1-[3-(4-Chlorophenyl)-5-phenyl-3*H*-1,2,3-triazol-4-yl]-2,2,2-trifluoroethanone (4l)**. ^1H NMR ($CDCl_3$): δ 7.35 (d, 2H, Ar, *J* = 8.6), 7.67-7.69 (m, 2H, Ar). ^{19}F NMR ($CDCl_3$): δ -74.7. ESI-MS (m/z): calcd for $C_{16}H_{10}ClF_3N_3O$ [$M+H^+$] 352.0459, found 352.0465.

2,2,2-Trifluoro-1-[1-(4-methoxyphenyl)-5-phenyl-1*H*-1,2,3-triazol-4-yl]ethanone (2m). Colourless oil, yield 308 mg (89 %), isolated as 88:12 mixture with isomeric triazole **3m**. ^1H NMR ($CDCl_3$): δ 3.80 (s, 3H, CH_3O), 6.89 (d, 2H, Ar, *J* = 8.8), 7.20 (d, 2H, Ar, *J* = 8.8), 7.31 (d, 2H, Ar, *J* = 7.3), 7.36-7.49 (m, 3H, Ar). ^{13}C NMR ($CDCl_3$): δ 55.4, 114.6, 116.2 (q, CF_3, *J* = 290.8), 124.3, 126.5, 127.8, 128.6, 129.9, 130.6, 137.6, 143.3, 160.5, 174.2 (q, $\underline{CO}CF_3$, *J* = 36.9). ^{19}F NMR ($CDCl_3$): δ -74.9. **2,2,2-Trifluoro-1-[3-(4-methoxyphenyl)-5-phenyl-3*H*-1,2,3-triazol-4-yl]ethanone (4m).** ^1H NMR ($CDCl_3$): δ 3.87 (s, 3H, MeO), 7.05 (d, 2H, Ar, *J* = 8.6), 7.65-7.71 (m,

2H, Ar). ^{19}F NMR ($CDCl_3$): δ -75.1. ESI-MS (m/z): calcd for $C_{17}H_{13}F_3N_3O_2$ [M+H_3O^+] 348.0963, found 348.0963.

2,2,2-Trifluoro-1-[1-(4-nitrophenyl)-5-phenyl-1*H*-1,2,3-triazol-4-yl]ethanone (2n). Yellow oil, yield 250 mg (69 %). IR (ν, cm^{-1}): 1351, 1532 (NO_2); 1723 ($COCF_3$). ^{1}H NMR ($CDCl_3$): δ 7.30-7.36 (m, 2H, Ar), 7.44-7.58 (m, 5H, Ar), 8.25-8.31 (m, 2H, Ar). ^{13}C NMR ($CDCl_3$): δ 116.0 (q, CF_3, *J* = 290.6), 123.5, 125.0, 125.8, 129.2, 129.8, 131.4, 138.3, 139.8, 143.6, 148.1, 174.1 (q, $\underline{CO}CF_3$, *J* = 37.8). ^{19}F NMR ($CDCl_3$): δ -75.3. ESI-MS (m/z): calcd for $C_{16}H_{12}F_3N_4O_4$ [M+H_3O^+] 381.0805, found 381.0804.

Synthesis of 1,2,3-triazoles 2,3 by the reaction with azides obtained *in situ* (general procedure). A 3 ml vial with a screw cup was charged with the corresponding alkyl bromide (1.2 mmol), sodium azide (1.2 mmol), and DMSO (2 ml), and this was stirred overnight. The corresponding CF_3-ynone (1 ml) was added, and the mixture was heated at 85-90 ºC for 5-7 h. Thee mixture was poured into 0.1 *M* HCl (30 ml) and extracted with CH_2Cl_2 (3×10 ml). The combined extracts were dried over Na_2SO_4, the volatiles were evaporated and the residue was purified by column chromatography on silica gel using mixture of CH_2Cl_2 and MeOH (30:1) as an eluent.

2,2,2-Trifluoro-1-[1-(4-nitrobenzyl)-5-phenyl-1*H*-1,2,3-triazol-4-yl]ethanone (2o). Yellow oil, yield 128 mg (34 %). IR (ν, cm^{-1}): 1348, 1525 (NO_2); 1724 ($COCF_3$). ^{1}H NMR ($CDCl_3$): δ 5.59 (s, 2H, CH_2), 7.21-7.27 (m, 4H, Ar), 7.52-7.62 (t, 3H, Ar), 8.16 (d, 2H, Ar, *J* = 8.7). ^{13}C NMR ($CDCl_3$): δ 51.3, 118.9 (q, CF_3, *J* = 290.8), 124.0, 124.2, 128.6, 129.3, 131.3, 132.0, 138.2, 140.5, 144.0, 148.1, 174.1 (q, $\underline{CO}CF_3$, *J* = 37.2). ^{19}F NMR ($CDCl_3$): δ -74.3. ESI-MS (m/z): calcd for $C_{17}H_{12}F_3N_4O_3$ [M+H^+] 377.0856, found 377.0863.

2,2,2-Trifluoro-1-[5-phenyl-1-(2-phenylethyl)-1*H*-1,2,3-triazol-4-yl]ethanone (2p). Colorless oil, (104 mg, 30 %), isolated as 98:2 mixture with isomeric triazole **3p**. IR (ν, cm^{-1}): 1726 ($COCF_3$). ^{1}H NMR ($CDCl_3$): δ 3.20 (t, 2H, CH_2, *J* = 7.1), 4.48 (t, 2H, CH_2, *J* = 7.1), 7.21-7.25 (m, 3H, Ar), 7.40-7.47 (m, 4H, Ar), 7.49-7.55 (m, 3H, Ar). ^{13}C NMR ($CDCl_3$): δ 36.2, 49.6, 116.5 (q, CF_3, *J* = 290.8), 124.3, 127.3, 128.7, 128.7, 128.8, 128.9, 129.2, 130.7, 136.2, 144.2, 174.1 (q, $\underline{CO}CF_3$, *J* = 37.2). ^{19}F NMR ($CDCl_3$): δ -75.3. **2,2,2-Trifluoro-1-[5-phenyl-3-(2-phenylethyl)-3*H*-1,2,3-triazol-4-yl]ethanone (3p).** ^{19}F NMR ($CDCl_3$): δ -73.8. ESI-MS (m/z): calcd for $C_{18}H_{15}F_3N_3O$ [M+H^+] 346.1162, found 346.1168.

2,2,2-Trifluoro-1-[5-phenyl-1-(3-phenylpropyl)-1*H*-1,2,3-triazol-4-yl]ethanone (2q). Colourless oil, yield 150 mg (42 %), isolated as 96:4 mixture with isomeric triazole **3q**. IR (ν, cm^{-1}): 1722 ($COCF_3$). ^{1}H NMR ($CDCl_3$): δ 2.19 (t, 2H, CH_2, *J* = 7.2), 2.62 (t, 2H, CH_2, *J* = 7.2), 4.30 (t, 2H, CH_2, *J* = 7.2), 7.04-7.09 (m, 2H, Ar), 7.20-7.33 (m, 5H, Ar), 7.51-7.58 (m, 3H, Ar). ^{13}C NMR ($CDCl_3$): δ 31.0, 32.3, 47.7, 116.1 (q, CF_3, *J* = 290.6), 124.5, 126.3, 128.2, 128.5, 129.0, 129.2, 130.8, 137.8, 139.6, 143.7, 174.1 (q, $\underline{CO}CF_3$, *J* = 37.0). ^{19}F NMR ($CDCl_3$): δ -75.2. **2,2,2-**

Trifluoro-1-(5-phenyl-3-(3-phenylpropyl)-3H-1,2,3-triazol-4-yl)ethanone (**3q**). ^{1}H NMR ($CDCl_3$): δ 4.65 (t, 2H, CH_2 , J = 7.2). ^{19}F NMR ($CDCl_3$): δ -73.8. ESI-MS (m/z): calcd for $C_{19}H_{17}F_3N_3O$ [M+H$^+$] 360.1318, found 360.1328.

2,2,2-Trifluoro-1-(1-pentyl-5-phenyl-1*H*-1,2,3-triazol-4-yl)ethanone (2r). Colourless oil, yield 97 mg (31 %), isolated as 97:3 mixture with isomeric triazole **3r**. IR (ν, cm^{-1}): 1723 ($COCF_3$). ^{1}H NMR ($CDCl_3$): δ 0.84 (t, 3H, $CH_2\underline{CH_3}$, J = 6.8), 1.20-1.26 (m, 4H), 1.79-1.88 (m, 2H), 4.28 (t, 2H, CH_2 , J = 7.3), 7.35-7.40 (m, 2H, Ar), 7.55-7.60 (m, 3H, Ar). ^{13}C NMR ($CDCl_3$): δ 13.7, 21.8, 28.3, 29.5, 48.5, 116.2 (q, CF_3, J = 290.8), 124.7, 129.0, 129.3, 130.8, 137.8, 143.6, 174.2 (q, $\underline{CO}CF_3$, J = 37.2). ^{19}F NMR ($CDCl_3$): δ -75.2. **2,2,2-Trifluoro-1-(3-pentyl-5-phenyl-3*H*-1,2,3-triazol-4-yl)ethanone (3r).** ^{1}H NMR ($CDCl_3$): δ 4.62 (t, 2H, CH_2 , J = 7.4). ^{19}F NMR ($CDCl_3$): δ -73.9. ESI-MS (m/z): calcd for $C_{15}H_{17}F_3N_3O$ [M+H$^+$] 312.1318, found 312.1324.

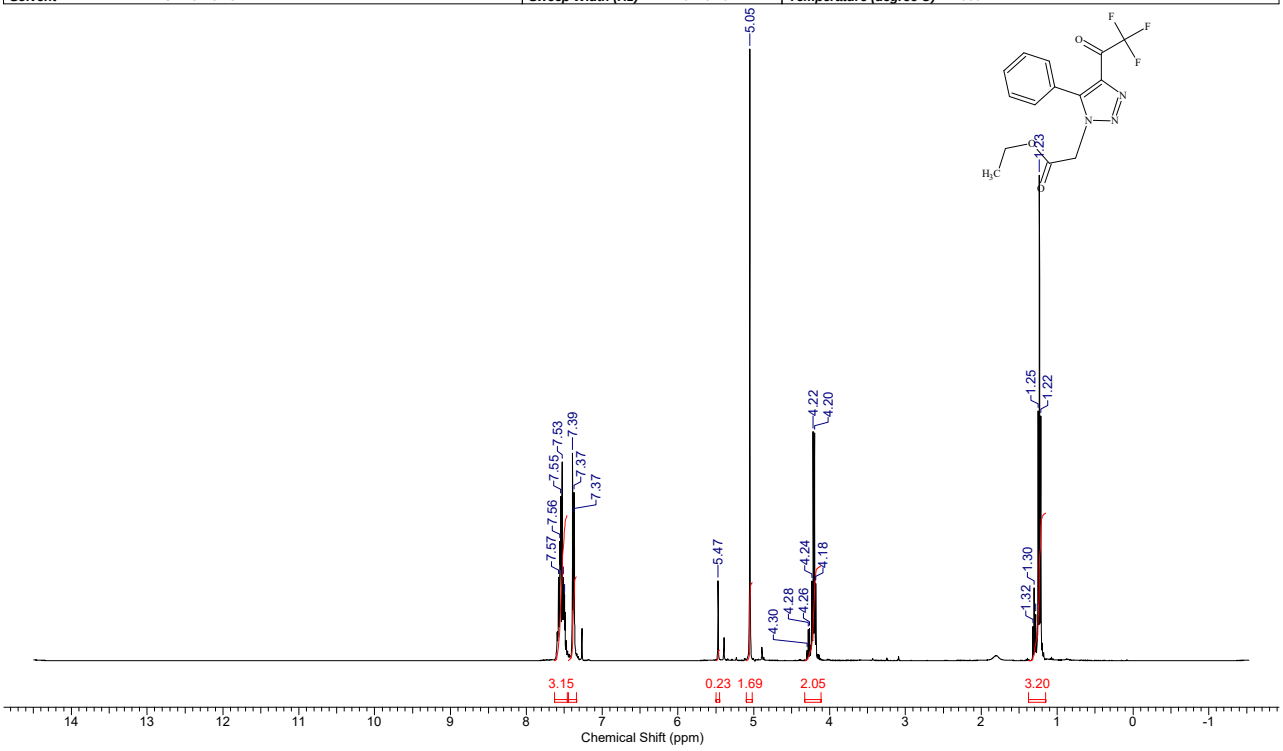
Table S1 ^{1}H and ^{19}F NMR data of minor isomers **3** obtained from spectra of the reaction mixtures.

Compound	^{1}H NMR ($CDCl_3$): δ	^{19}F NMR ($CDCl_3$): δ
Ethyl [4-(4-methylphenyl)-5-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (3b)	5.46 (s, 2H, CH_2)	-73.7.
Ethyl [4-(4-bromophenyl)-5-trifluoroacetyl)1*H*-1,2,3-triazol-1-yl]acetate (3c)	5.48 (s, 2H, CH_2)	-73.8
Ethyl [4-(4-chlorophenyl)-5-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (3d)	-	-73.7
Ethyl [4-(4-methoxyphenyl)-5-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (3e)	5.44 (s, 2H, CH_2)	-73.7
Ethyl [4-(4-*tert*-butylphenyl)-5-trifluoroacetyl-1*H*-1,2,3-triazol-1-yl]acetate (3g)	-	-73.6
2,2,2-Trifluoro-1-[3-(4-nitrophenyl)-5-phenyl-3*H*-1,2,3-triazol-4-yl]ethanone (3n)	-	-74.8
2,2,2-Trifluoro-1-[3-(4-nitrobenzyl)-5-phenyl-3*H*-1,2,3-triazol-4-yl]ethanone (3o)	5.80 (s, 2H, CH_2)	-73.8

1 Sep 2017

FW	327.2587	Formula	$C_{14}H_{12}F_3N_3O_3$

Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.	Date	12 Dec 2015 13:09:26
File Name	D:\BN\Docs (BN)\vasiliy\SPEC_BM_H,C\BM-863.H_001001r	Frequency (MHz)	400.13	Nucleus	1H
Number of Transients	4	Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000

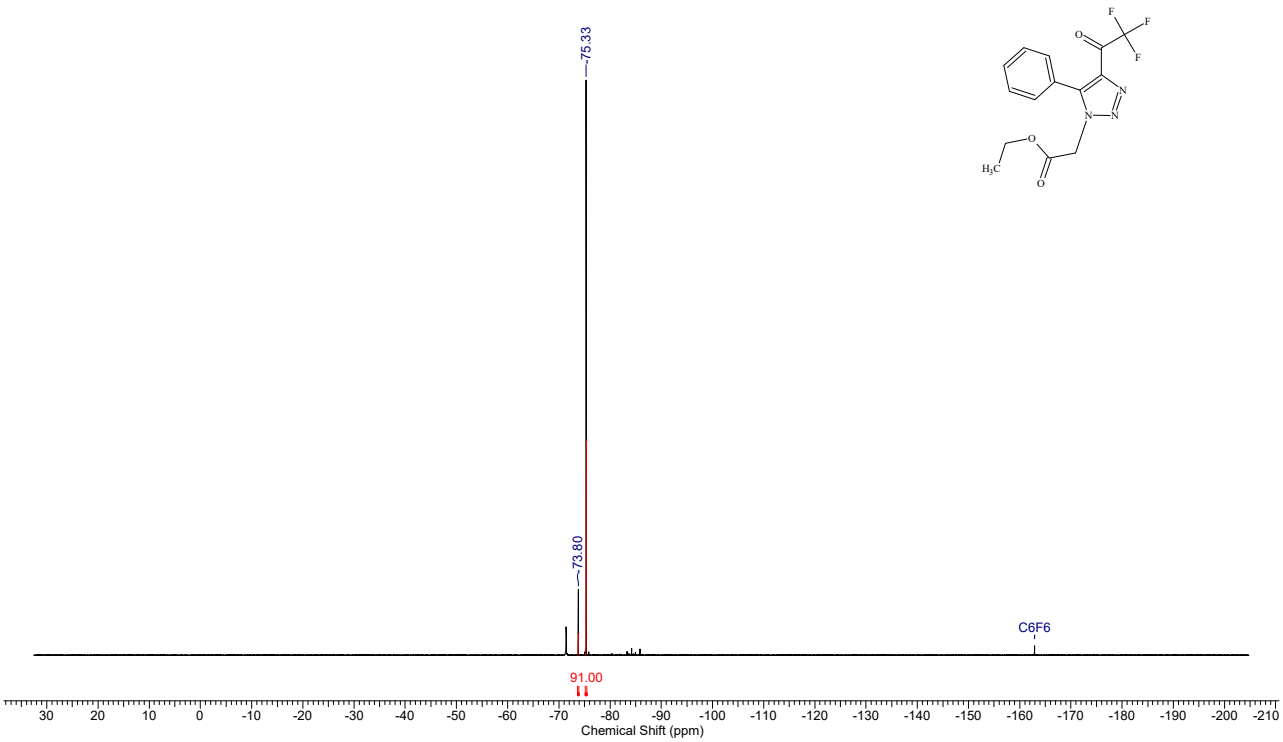


^{1}H NMR data of compound **3a**

1 Sep 2017

FW	327.2587	Formula	$C_{14}H_{12}F_3N_3O_3$

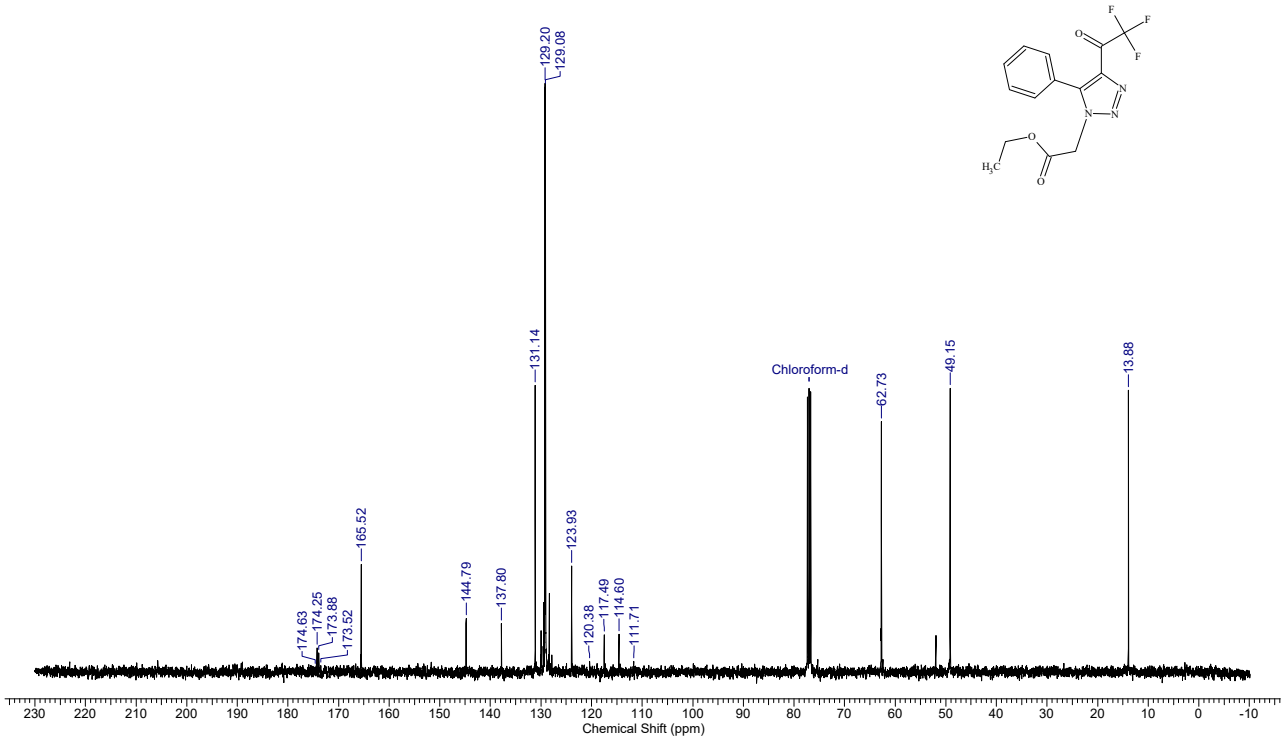
Acquisition Time (sec)	0.7500	Date	Dec 7 2015	File Name	D:\BN\Docs (BN)\vasiliy\SPEC_BM_F\BM-860_20151207_01\FLUORINE_01	
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	4	Original Points Count	66964
Points Count	131072	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D	
Sweep Width (Hz)	89285.71	Temperature (degree C)	20.000			



^{19}F NMR data of compound **3a**

1 Sep 2017

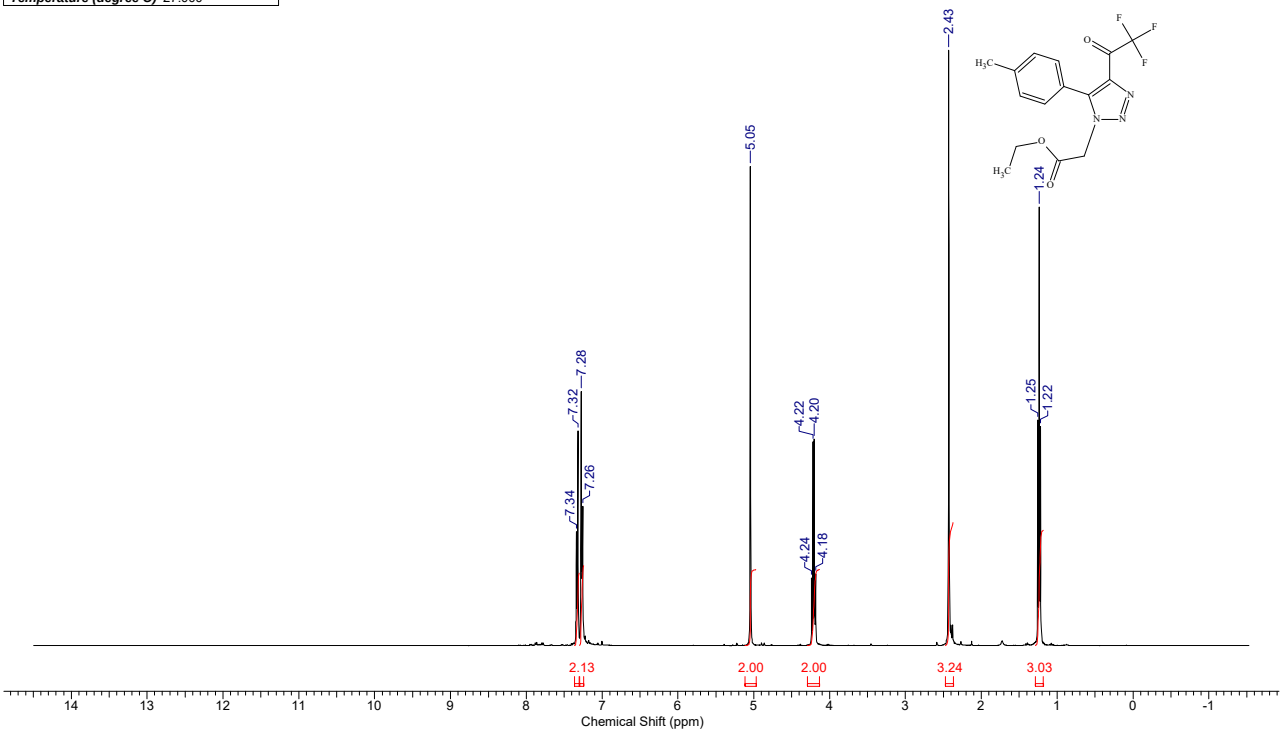
FW	327.2587	Formula	$C_{14}H_{12}F_3N_3O_3$				
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.			Date	12 Dec 2015 13:17:54
File Name	D:\BN\Docs (BN)\vasiliy\SPEC_BM_H,C\BM-863.C_002001r			Frequency (MHz)	100.61	Nucleus	13C
Number of Transients	244	Original Points Count	12076	Points Count	65536	Pulse Sequence	zgpg30
Solvent	DMSO-D6	Sweep Width (Hz)	24154.59	Temperature (degree C)	27.000		



^{13}C NMR data of compound **3a**

1 Sep 2017

FW	341.2853	Formula	$C_{15}H_{14}F_3N_3O_3$				
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.			Date	05 Apr 2016 15:25:44
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\MM-0074-1.H_001001r					Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	4	Original Points Count	16384	Points Count	65536
Pulse Sequence	zg30	Solvent	CHLOROFORM-D			Sweep Width (Hz)	6410.26
Temperature (degree C)	27.000						

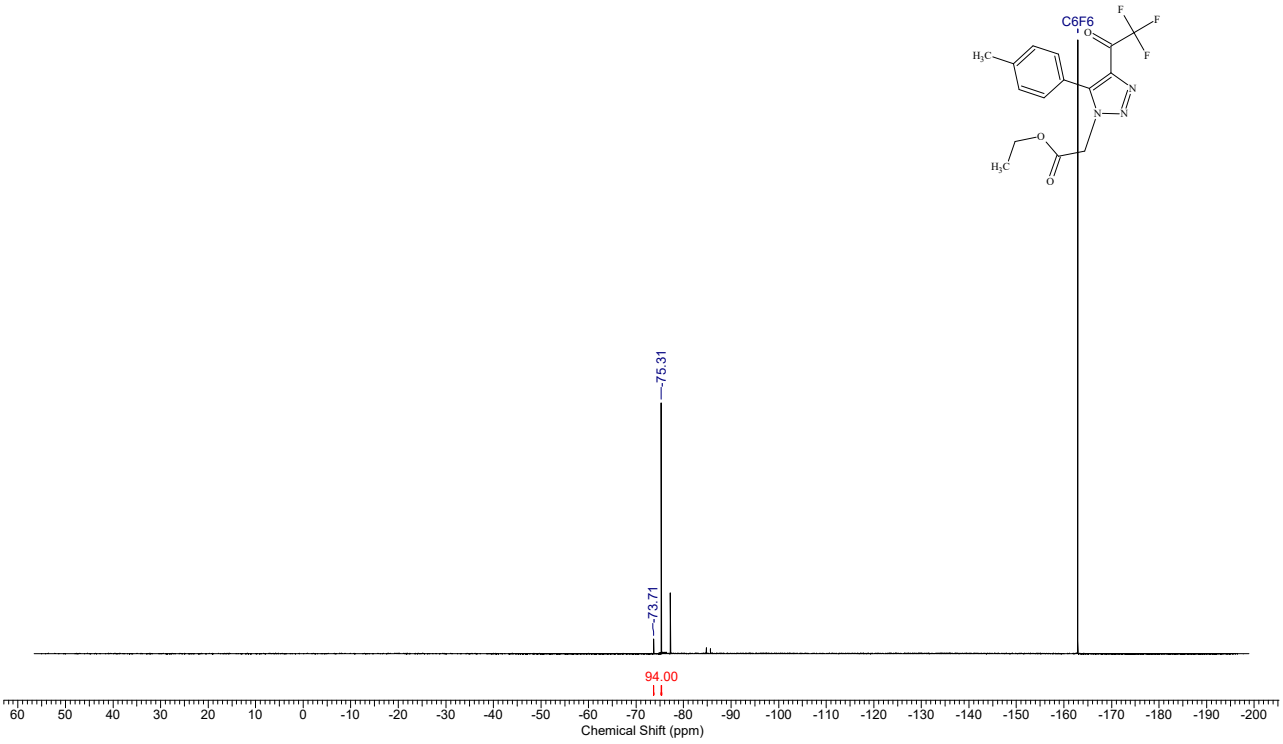


^{1}H NMR data of compound **3b**

1 Sep 2017

FW	341.2853	**Formula**	$C_{15}H_{14}F_3N_3O_3$

Acquisition Time (sec)	2.7263	**Date**	Mar 31 2016				
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\19F\MM-074-F_20160331_01\FLUORINE_01					**Frequency (MHz)**	376.31
Nucleus	19F	**Number of Transients**	8	**Original Points Count**	262144	**Points Count**	262144
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	96153.84	**Temperature (degree C)**	6.000

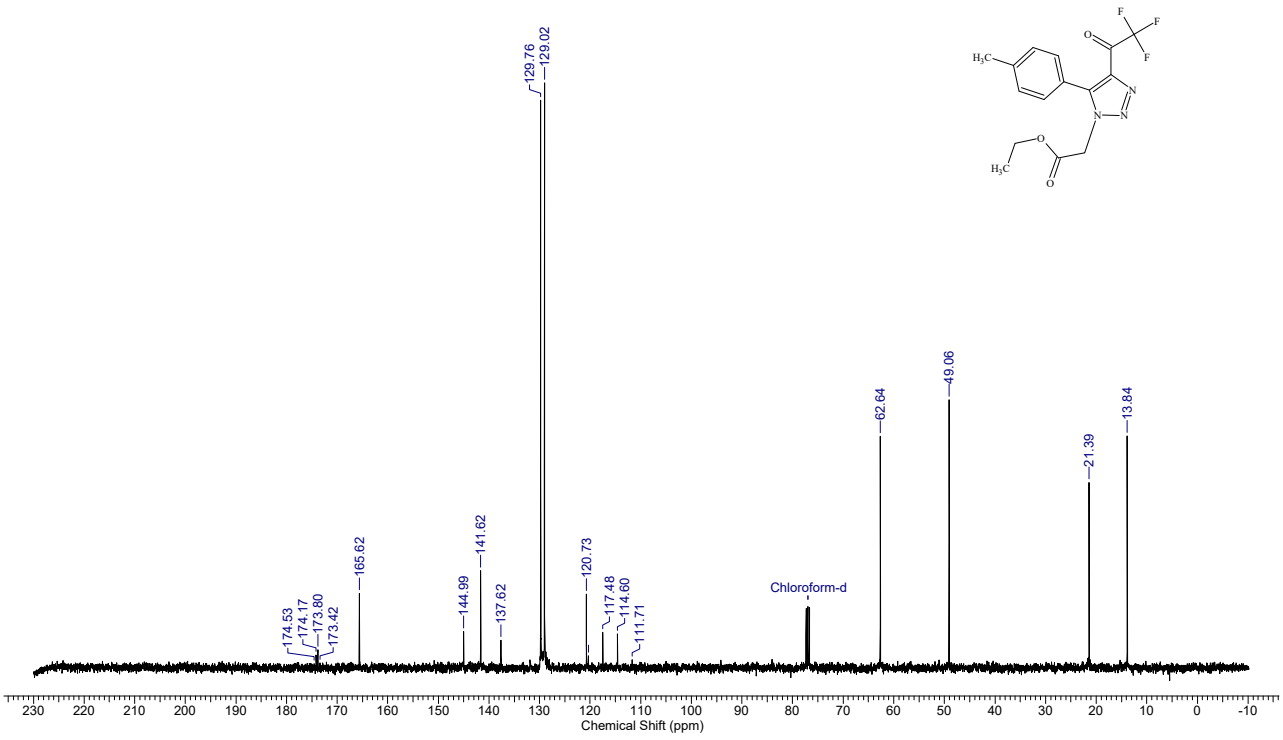


^{19}F NMR data of compound **3b**

1 Sep 2017

FW	341.2853	**Formula**	$C_{15}H_{14}F_3N_3O_3$

Acquisition Time (sec)	0.4999	**Comment**	Imported from UXNMR.			**Date**	23 Apr 2016 13:59:24
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\MM-074-1.C_002001r					**Frequency (MHz)**	100.61
Nucleus	13C	**Number of Transients**	65	**Original Points Count**	12076	**Points Count**	65536
Pulse Sequence	zgpg30	**Solvent**	DMSO-D6	**Sweep Width (Hz)**	24154.59	**Temperature (degree C)**	27.000

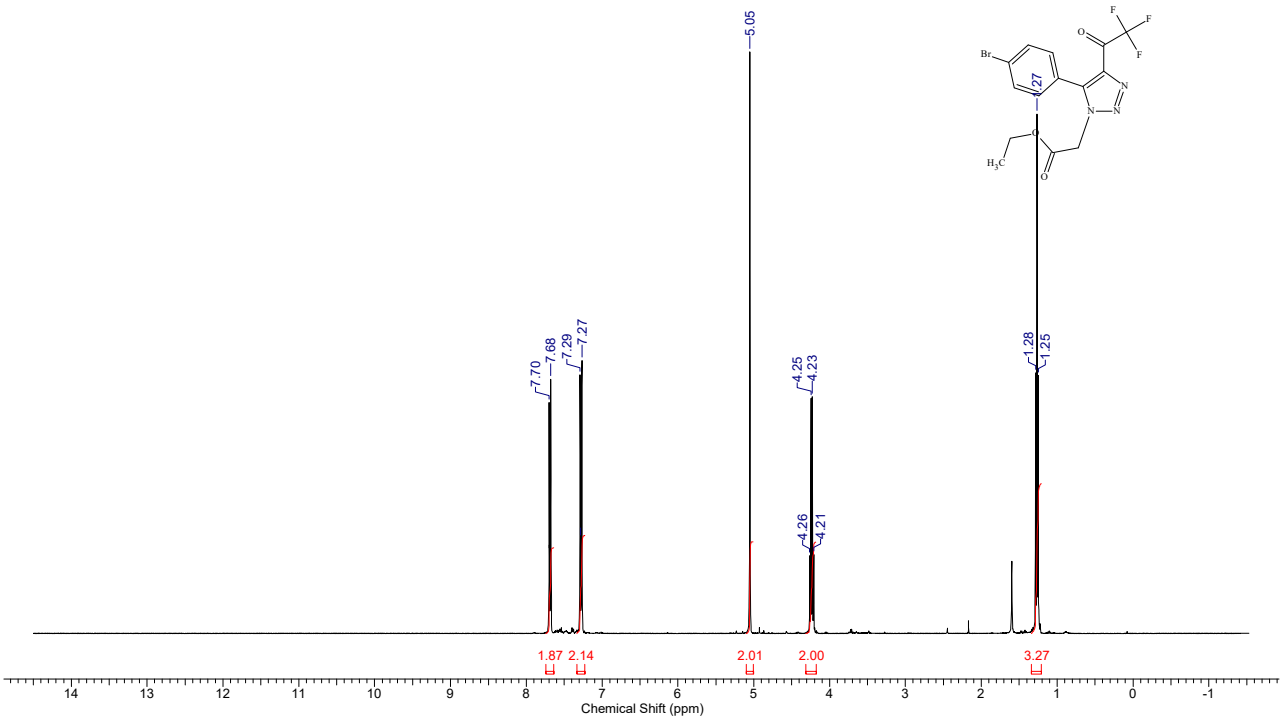


^{13}C NMR data of compound **3b**

1 Sep 2017

FW	406.1548	**Formula**	$C_{14}H_{11}BrF_3N_3O_3$

Acquisition Time (sec)	2.5559	**Comment**	Imported from UXNMR.			**Date**	16 Apr 2016 13:14:18
File Name	D:\BN\Docs (BN)\vasiliy\Максим_диссертация\Спектры_Максим\MM-093-1.H_001001r					**Frequency (MHz)**	400.13
Nucleus	1H	**Number of Transients**	4	**Original Points Count**	16384	**Points Count**	65536
Pulse Sequence	zg30	**Solvent**	CHLOROFORM-D			**Sweep Width (Hz)**	6410.26
Temperature (degree C)	27.000						

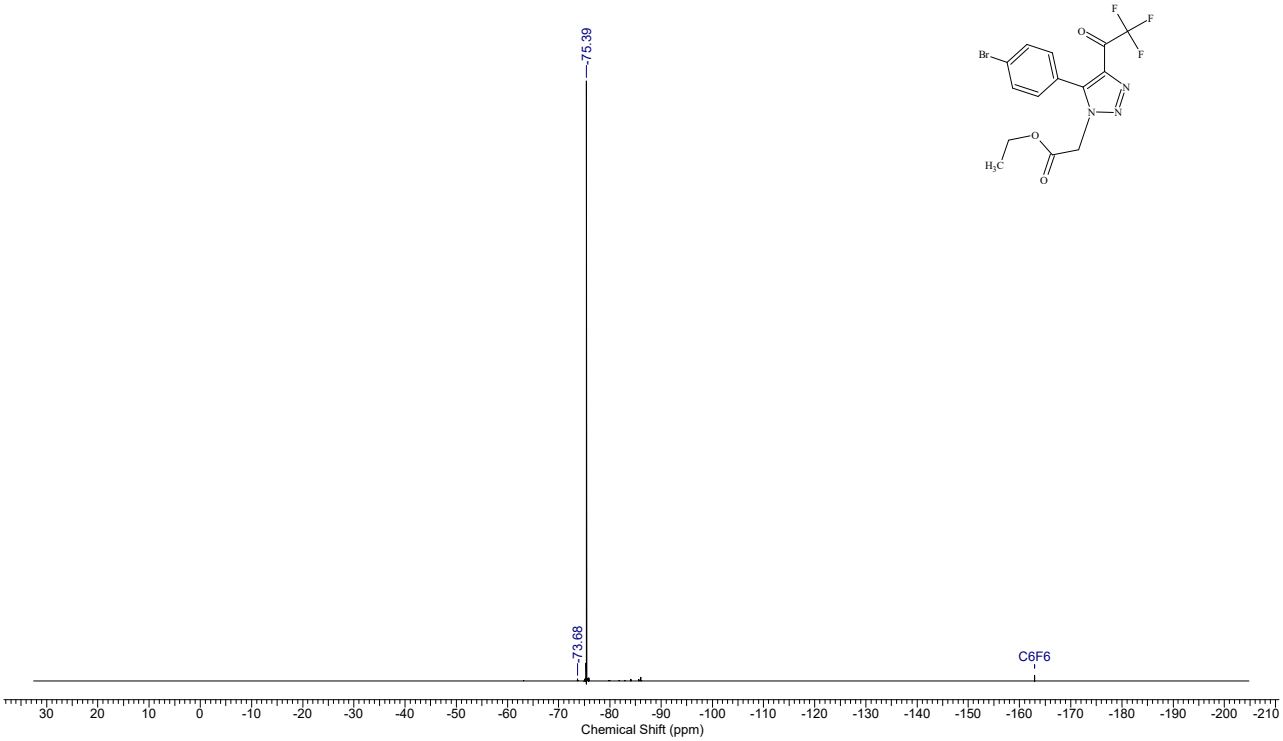


^{1}H NMR data of compound **3c**

1 Sep 2017

FW	406.1548	**Formula**	$C_{14}H_{11}BrF_3N_3O_3$

Acquisition Time (sec)	0.7340	**Date**	Apr 18 2016				
File Name	D:\BN\Docs (BN)\vasiliy\Максим_диссертация\Спектры_Максим\19F\MM-093-1_20160418_01\FLUORINE_01					**Frequency (MHz)**	376.31
Nucleus	19F	**Number of Transients**	4	**Original Points Count**	65536	**Points Count**	65536
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	89285.71	**Temperature (degree C)**	20.000

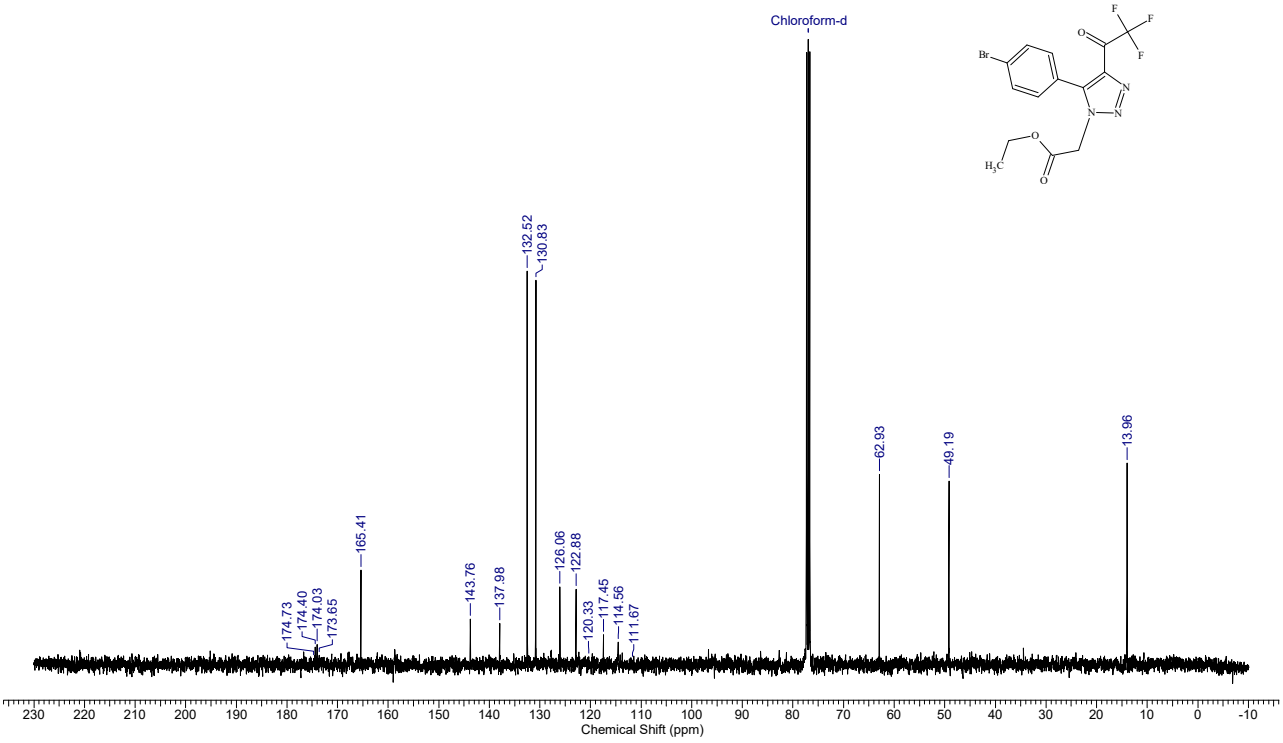


^{19}F NMR data of compound **3c**

1 Sep 2017

FW	406.1548	**Formula**	$C_{14}H_{11}BrF_3N_3O_3$

Acquisition Time (sec)	0.6783	**Comment**	Imported from UXNMR.			**Date**	18 Apr 2016 09:27:36
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\MM-093-1.C_002001r					**Frequency (MHz)**	100.61
Nucleus	13C	**Number of Transients**	257	**Original Points Count**	16384	**Points Count**	131072
Pulse Sequence	zgpg30	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	24154.59	**Temperature (degree C)**	27.000

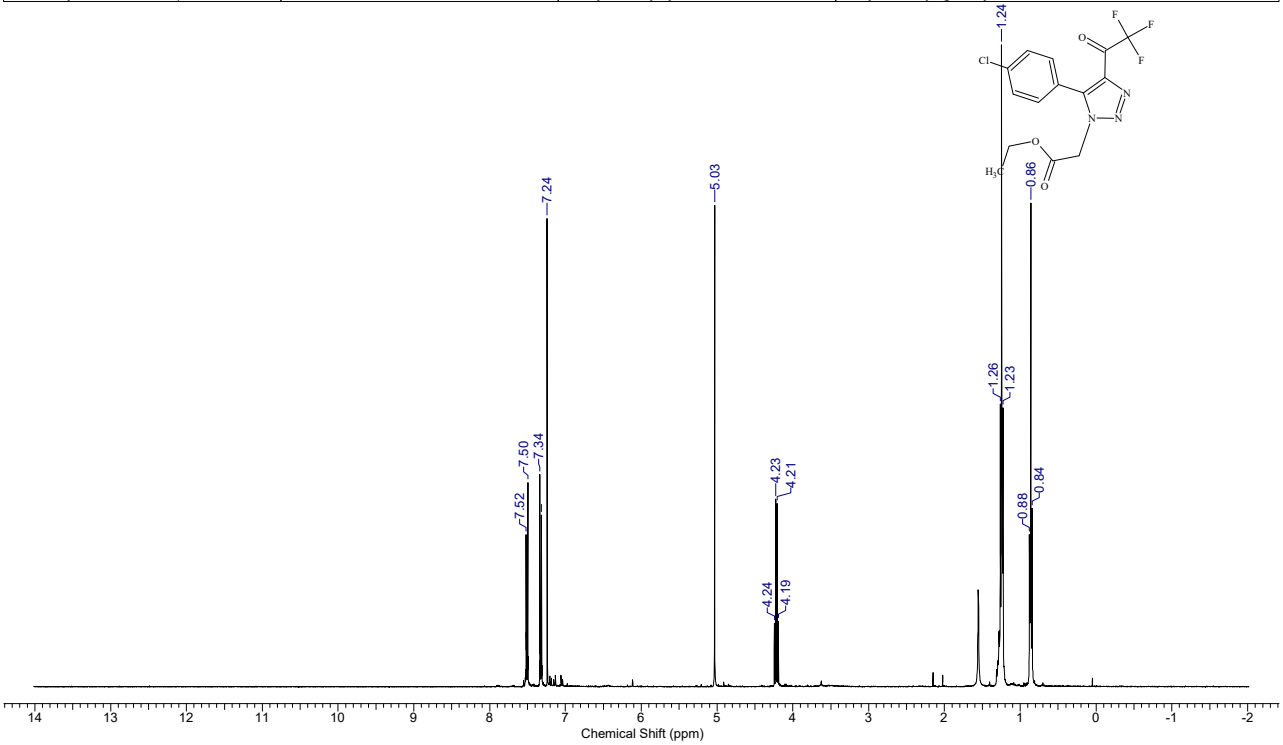


^{13}C NMR data of compound **3c**

1 Sep 2017

FW	361.7035	**Formula**	$C_{14}H_{11}ClF_3N_3O_3$

Acquisition Time (sec)	2.5559	**Date**	Apr 22 2016				
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\19F\MM-091-1_20160422_02\PROTON_01					**Frequency (MHz)**	399.96
Nucleus	1H	**Number of Transients**	8	**Original Points Count**	16384	**Points Count**	16384
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	6410.26	**Temperature (degree C)**	25.000

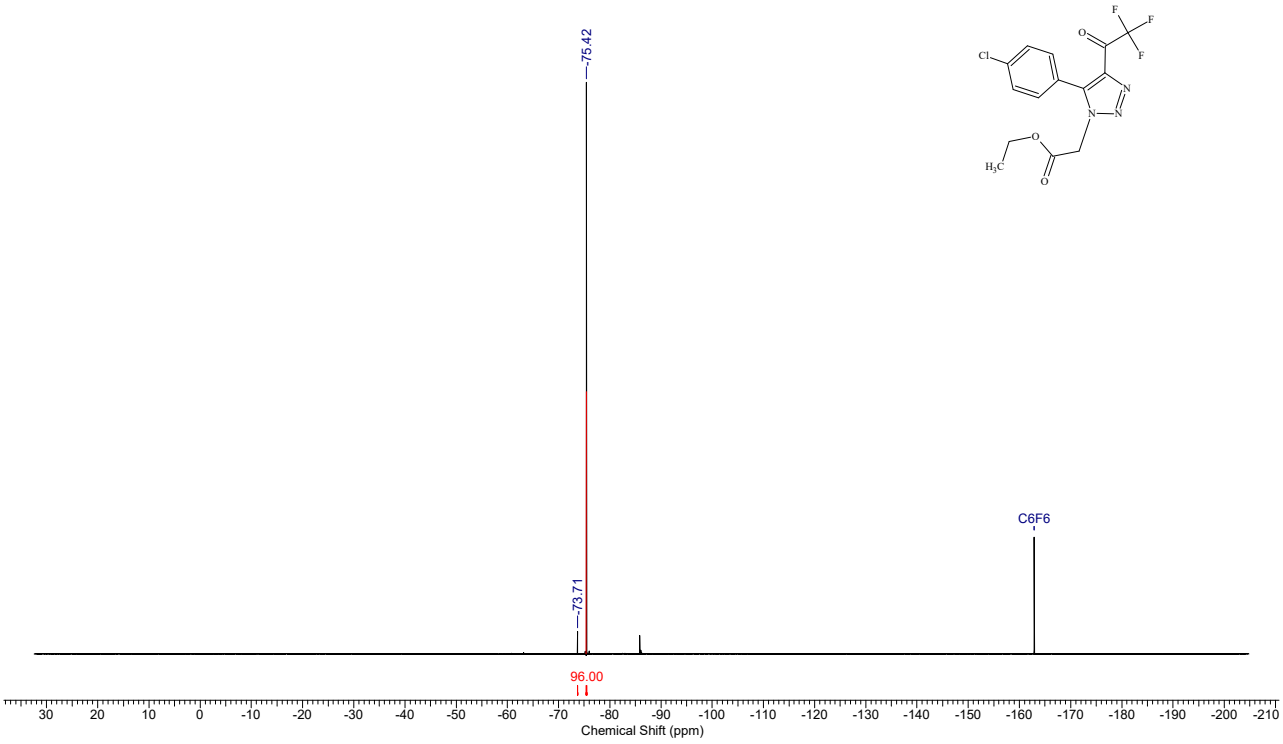


^{1}H NMR data of compound **3d**

1 Sep 2017

FW	361.7035	**Formula**	$C_{14}H_{11}ClF_3N_3O_3$

Acquisition Time (sec)	1.0000	**Date**	Apr 22 2016				
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\19F\MM-091-1_20160422_01\FLUORINE_01					**Frequency (MHz)**	376.31
Nucleus	19F	**Number of Transients**	16	**Original Points Count**	89286	**Points Count**	131072
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	89285.71	**Temperature (degree C)**	25.000

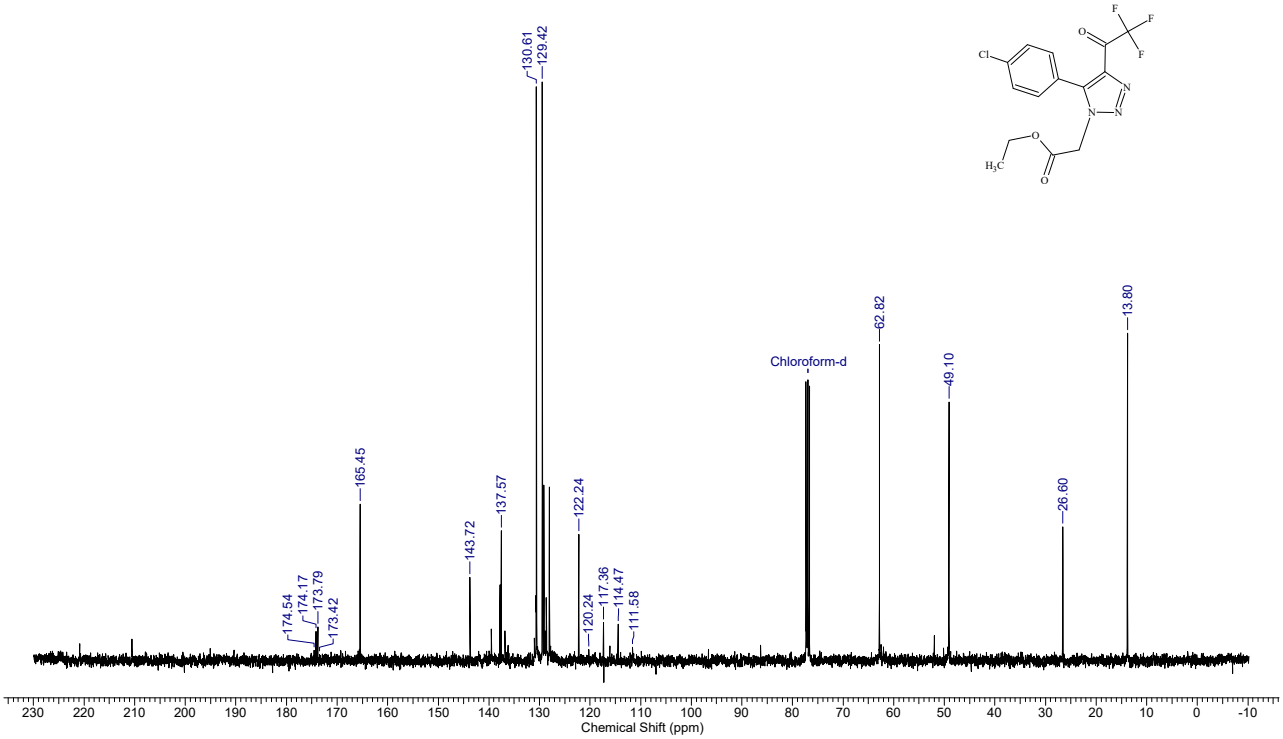


^{19}F NMR data of compound **3d**

1 Sep 2017

FW	361.7035	**Formula**	$C_{14}H_{11}ClF_3N_3O_3$

Acquisition Time (sec)	0.6783	**Comment**	Imported from UXNMR.			**Date**	01 Apr 2016 08:26:02
File Name	D:\BN\output\2016\04.апрель\BM-MM-073.C_002001r			**Frequency (MHz)**	100.61	**Nucleus**	13C
Number of Transients	101	**Original Points Count**	16384	**Points Count**	131072	**Pulse Sequence**	zgpg30
Solvent	CHLOROFORM-D			**Sweep Width (Hz)**	24154.59	**Temperature (degree C)**	27.000

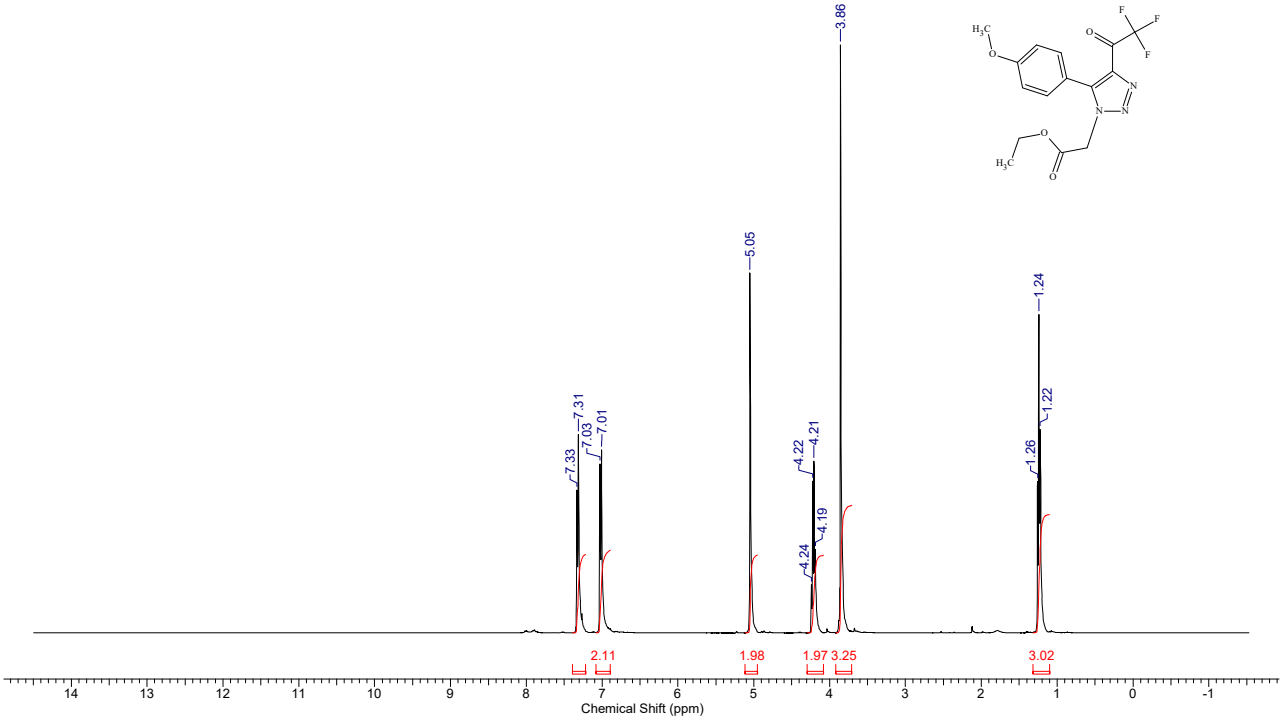


^{13}C NMR data of compound **3d**

1 Sep 2017

FW	357.2847	**Formula**	$C_{15}H_{14}F_3N_3O_4$

Acquisition Time (sec)	2.5559	**Comment**	Imported from UXNMR.			**Date**	07 Apr 2016 17:35:02
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\MM-084-1.H_001001r					**Frequency (MHz)**	400.13
Nucleus	1H	**Number of Transients**	10	**Original Points Count**	16384	**Points Count**	65536
Pulse Sequence	zg30	**Solvent**	CHLOROFORM-D			**Sweep Width (Hz)**	6410.26
Temperature (degree C)	27.000						

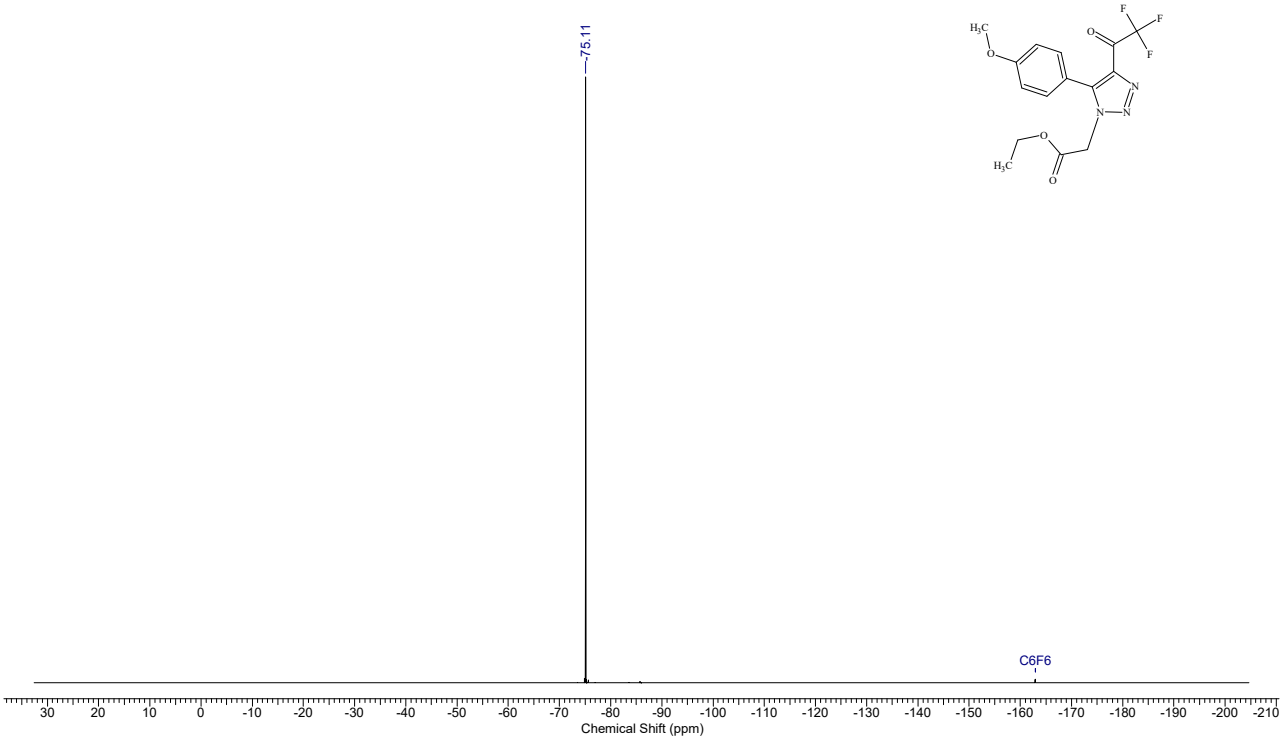


^{1}H NMR data of compound **3e**

1 Sep 2017

FW	357.2847	**Formula**	$C_{15}H_{14}F_3N_3O_4$

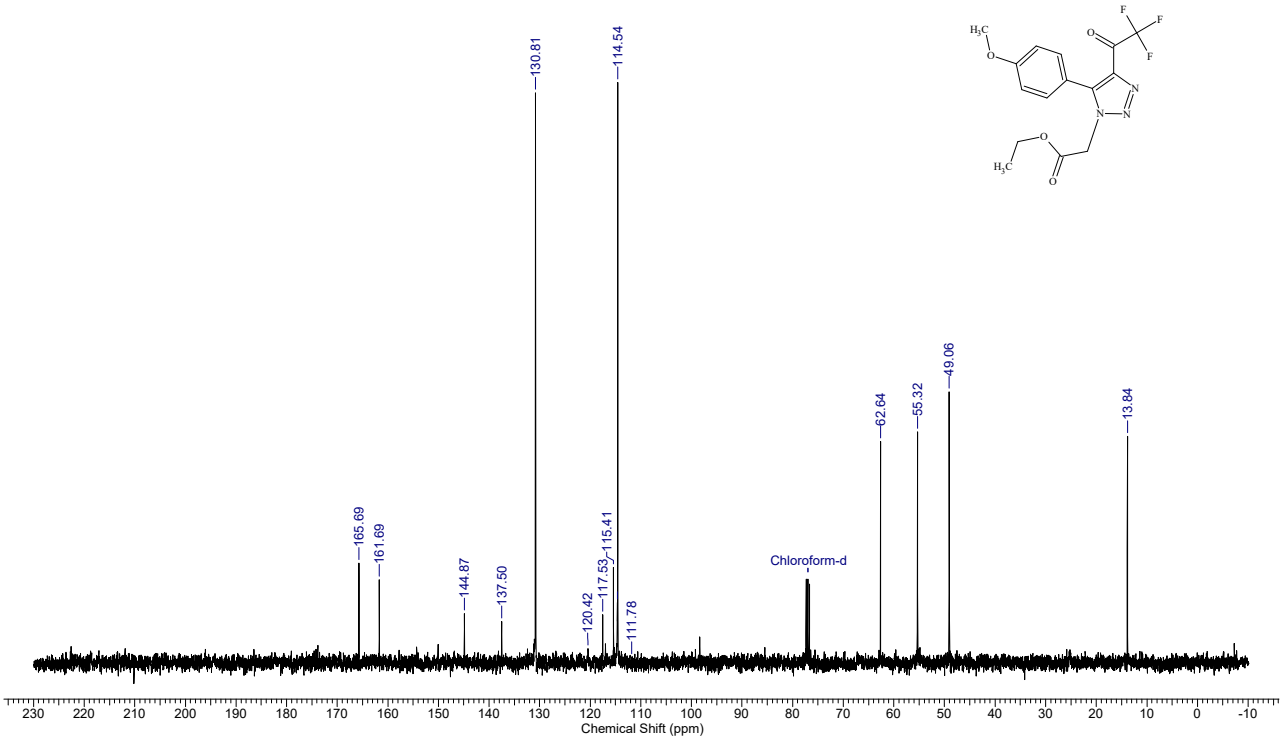
Acquisition Time (sec)	0.7340	**Date**	Apr 12 2016				
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\19F\mm084-2-f_20160412_01\FLUORINE_01					**Frequency (MHz)**	376.31
Nucleus	19F	**Number of Transients**	1000	**Original Points Count**	65536	**Points Count**	65536
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	89285.71	**Temperature (degree C)**	6.000



^{19}F NMR data of compound **3e**

1 Sep 2017

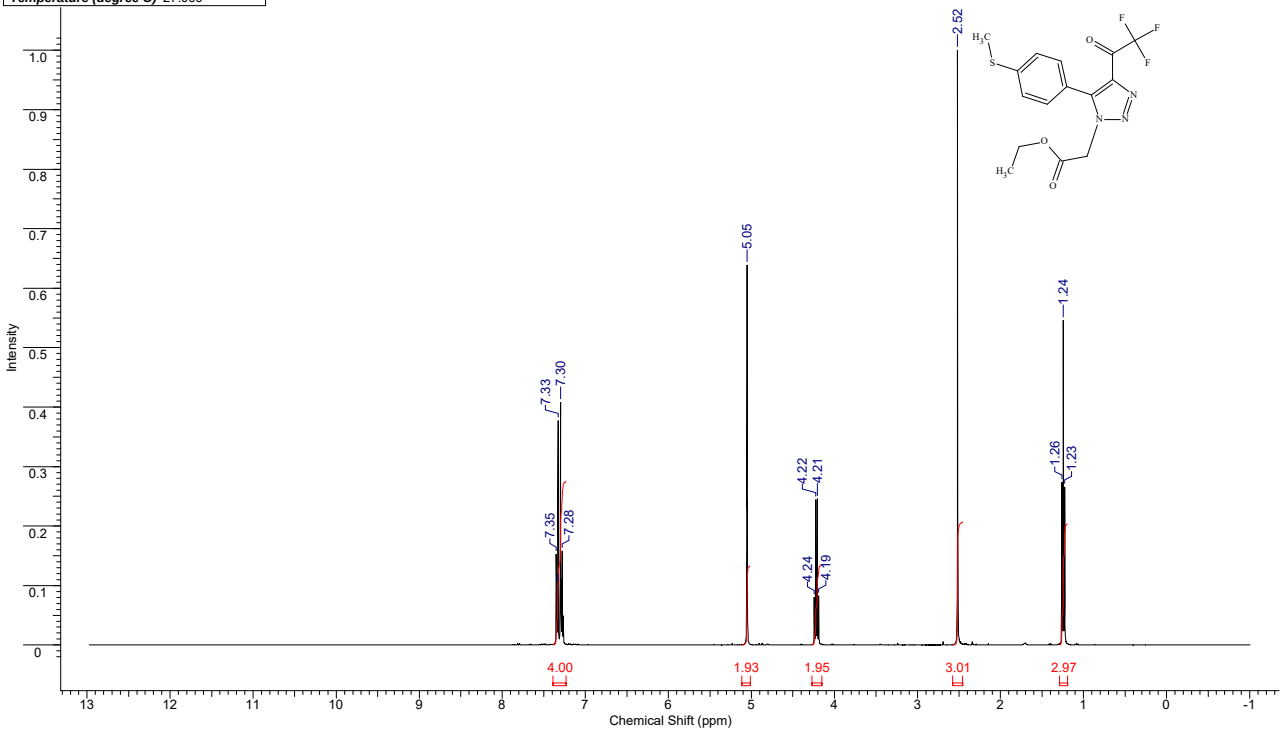
FW	357.2847	**Formula**	$C_{15}H_{14}F_3N_3O_4$				
Acquisition Time (sec)	0.4999	**Comment**	Imported from UXNMR.			**Date**	09 Apr 2016 14:09:48
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\MM-084-2.C_002001r					**Frequency (MHz)**	100.61
Nucleus	13C	**Number of Transients**	25	**Original Points Count**	12076	**Points Count**	65536
Pulse Sequence	zgpg30	**Solvent**	DMSO-D6	**Sweep Width (Hz)**	24154.59	**Temperature (degree C)**	27.000



^{13}C NMR data of compound **3e**

3 Nov 2017

FW	373.3513	**Formula**	$C_{15}H_{14}F_3N_3O_2S$				
Acquisition Time (sec)	2.9295	**Comment**	Imported from UXNMR.			**Date**	26 Oct 2017 19:36:36
File Name	D:\BN\output\2017\10.октябрь\BM-MM-077\BM-MM-077_001001r					**Frequency (MHz)**	400.13
Nucleus	1H	**Number of Transients**	8	**Original Points Count**	16384	**Points Count**	65536
Pulse Sequence	zg30	**Solvent**	CHLOROFORM-D			**Sweep Width (Hz)**	5592.84
Temperature (degree C)	27.000						

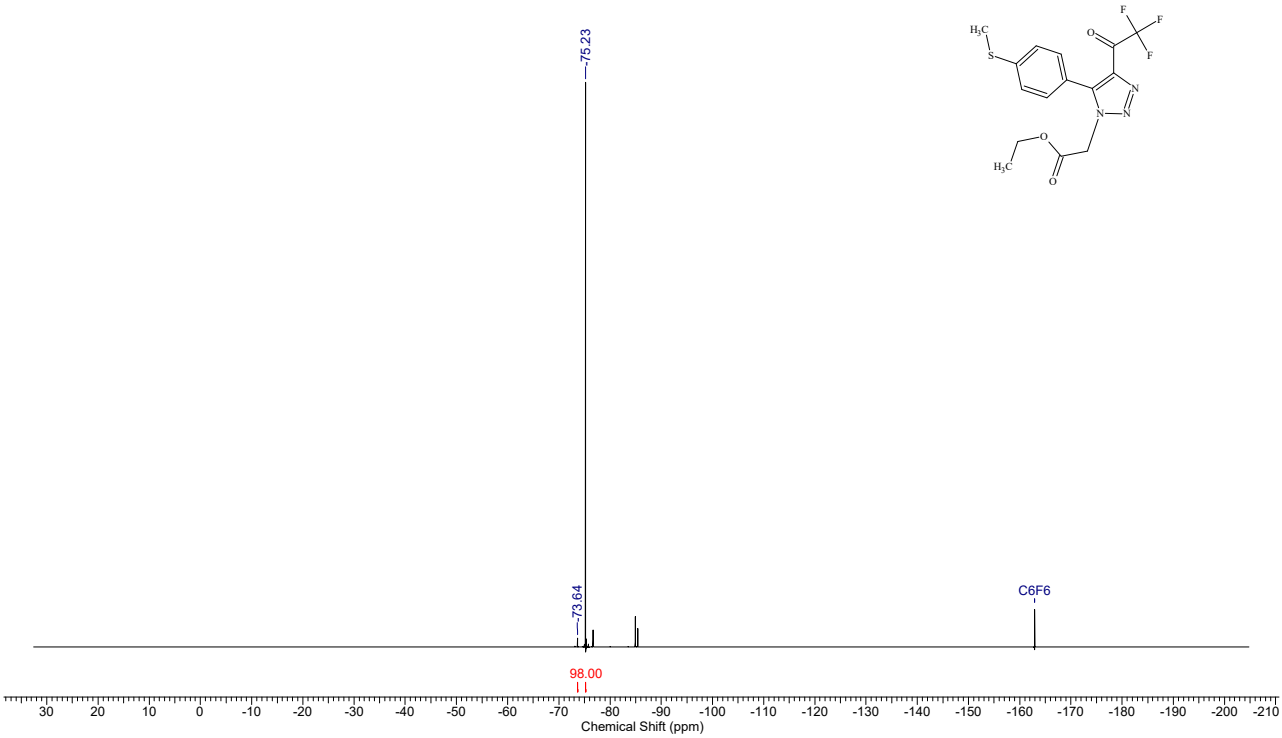


^{1}H NMR data of compound **3f**

1 Sep 2017

FW	373.3513	Formula	$C_{15}H_{14}F_3N_3O_3S$

Acquisition Time (sec)	1.0000	Date	May 20 2016	File Name	D:\BN\output\F19\2016.05.20\BM-MM077_20160520_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	8	Original Points Count	89286
Points Count	131072	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				

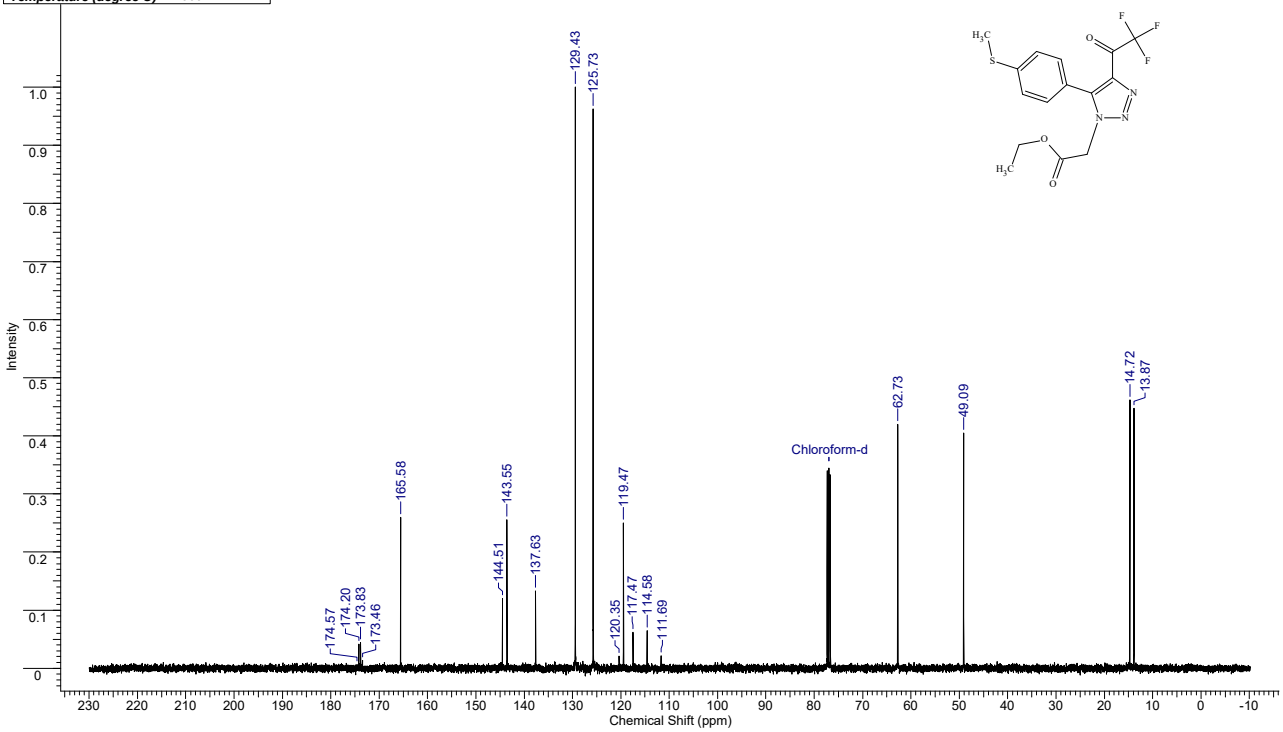


^{19}F NMR data of compound **3f**

3 Nov 2017

FW	373.3513	Formula	$C_{15}H_{14}F_3N_3O_3S$

Acquisition Time (sec)	0.6783	Comment	Imported from UXNMR.			Date	26 Oct 2017 19:46:00
File Name	D:\BN\output\2017\10.октябрь\BM-MM-077\BM-MM-077_002001r					Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	200	Original Points Count	16384	Points Count	131072
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D			Sweep Width (Hz)	24154.59
Temperature (degree C)	27.000						

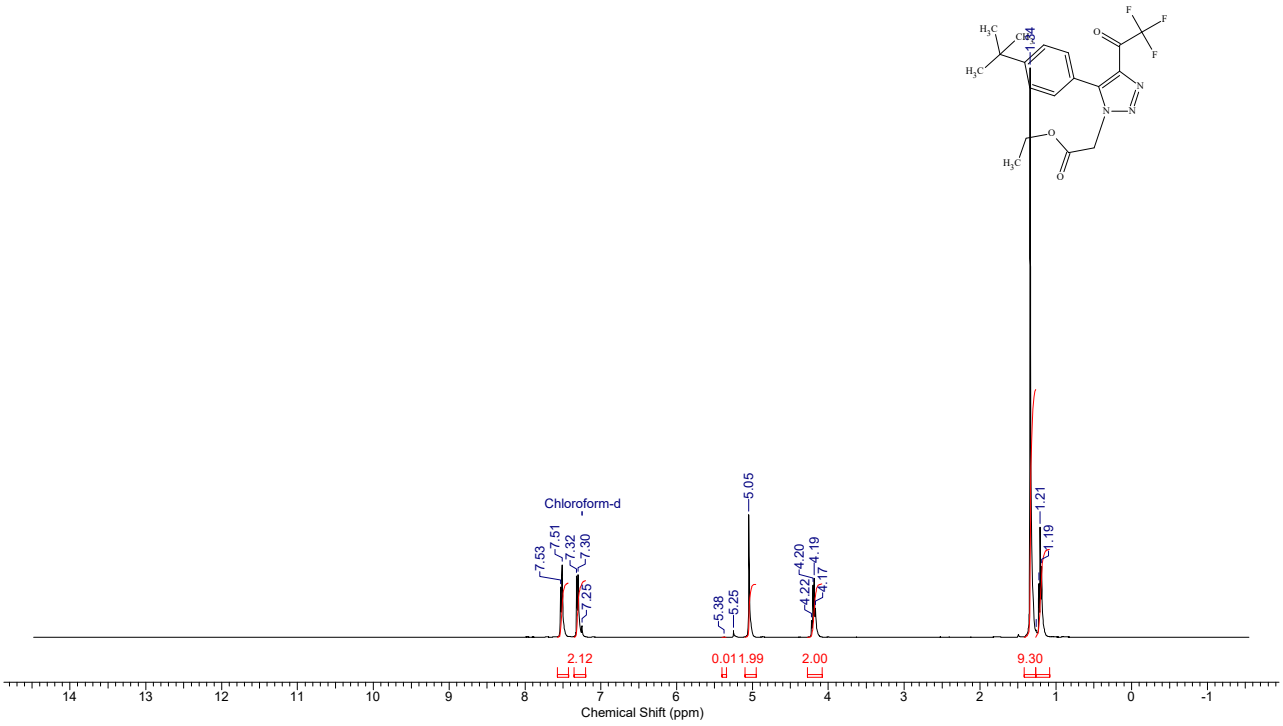


^{13}C NMR data of compound **3f**

1 Sep 2017

FW	383.3650	**Formula**	$C_{18}H_{20}F_3N_3O_3$

Acquisition Time (sec)	2.5559	**Comment**	Imported from UXNMR.			**Date**	07 Apr 2016 17:42:34
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\MM-076-1.H_001001r					**Frequency (MHz)**	400.13
Nucleus	1H	**Number of Transients**	5	**Original Points Count**	16384	**Points Count**	65536
Pulse Sequence	zg30	**Solvent**	CHLOROFORM-D			**Sweep Width (Hz)**	6410.26
Temperature (degree C)	27.000						

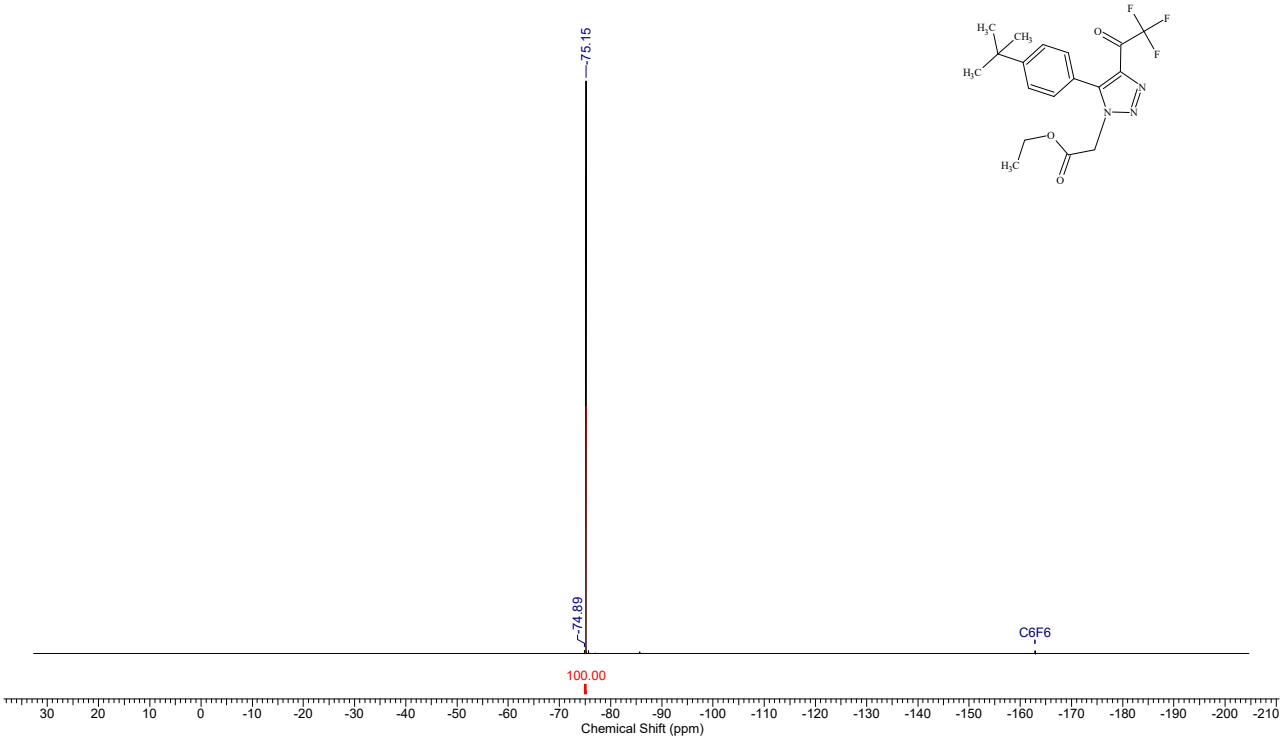


^{1}H NMR data of compound **3g**

1 Sep 2017

FW	383.3650	**Formula**	$C_{18}H_{20}F_3N_3O_3$

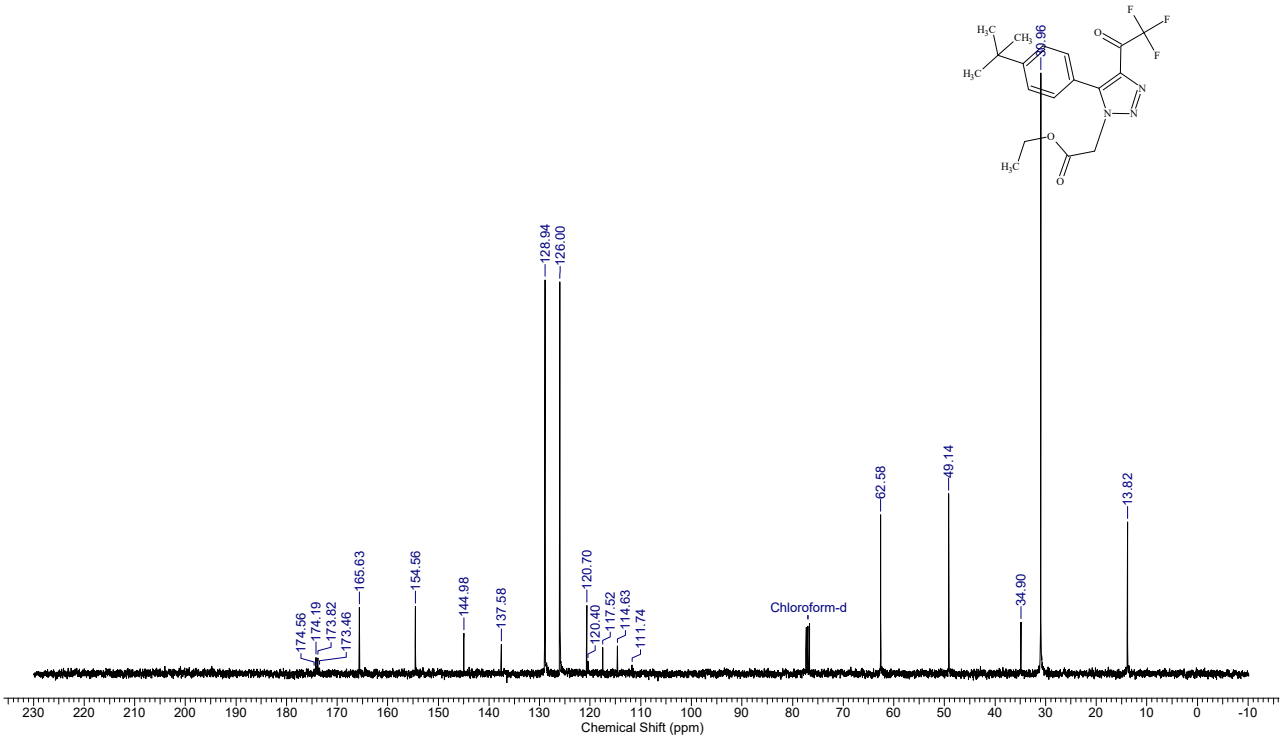
Acquisition Time (sec)	0.7340	**Date**	Apr 12 2016				
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\19F\mm076-2-f_20160412_01\FLUORINE_01					**Frequency (MHz)**	376.31
Nucleus	19F	**Number of Transients**	1000	**Original Points Count**	65536	**Points Count**	65536
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	89285.71	**Temperature (degree C)**	6.000



^{19}F NMR data of compound **3g**

1 Sep 2017

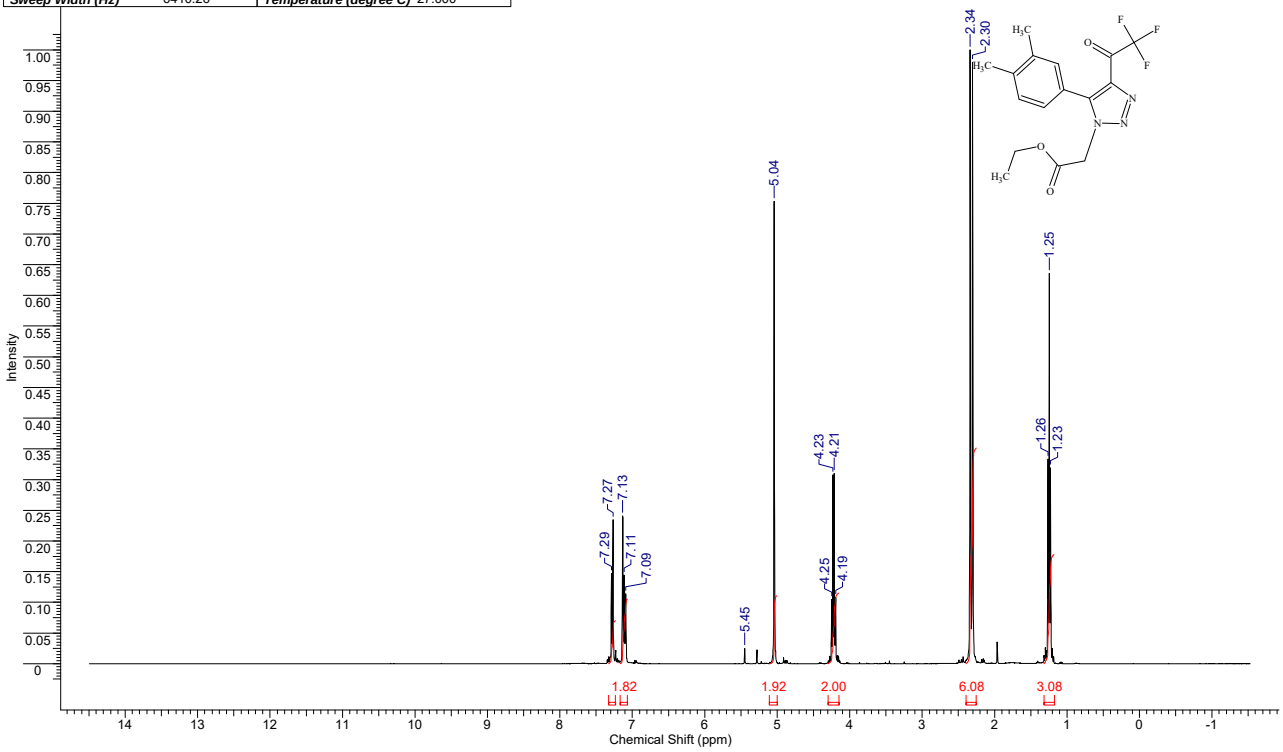
FW	383.3650	Formula	$C_{18}H_{20}F_3N_3O_3$				
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.			Date	09 Apr 2016 14:01:56
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\MM-076-2.C_002001r					Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	32	Original Points Count	12076	Points Count	65536
Pulse Sequence	zgpg30	Solvent	DMSO-D6	Sweep Width (Hz)	24154.59	Temperature (degree C)	27.000



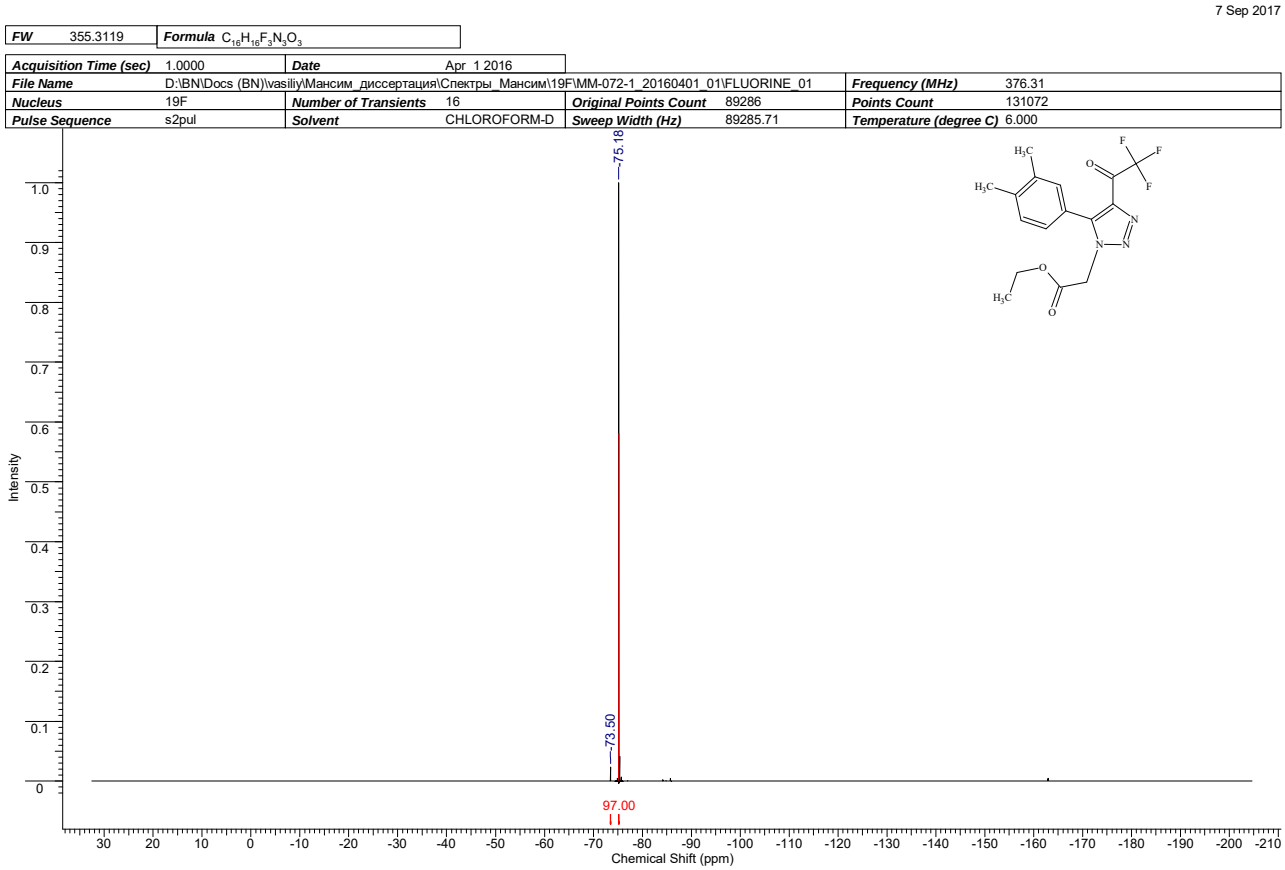
^{13}C NMR data of compound **3g**

7 Sep 2017

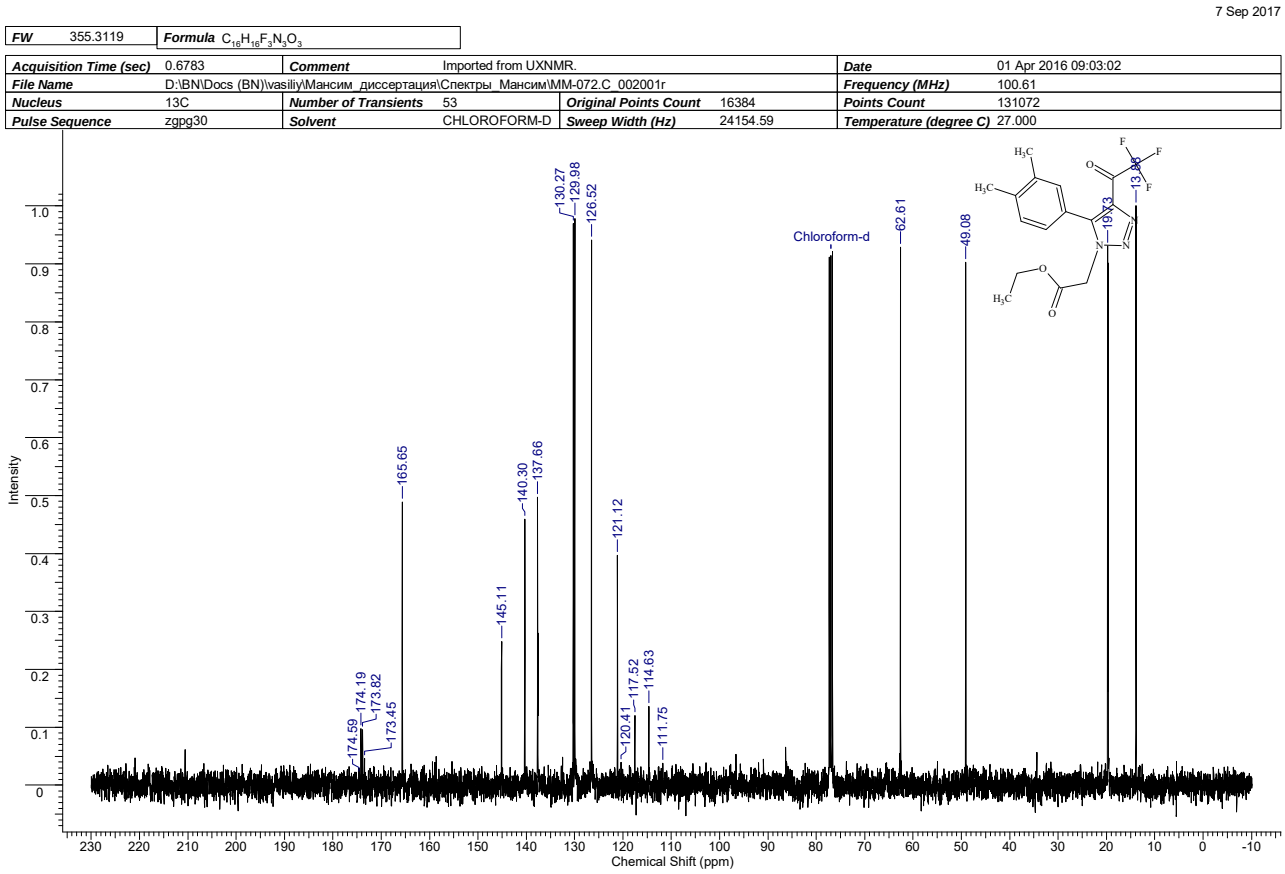
FW	355.3119	Formula	$C_{16}H_{16}F_3N_3O_3$				
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.			Date	01 Apr 2016 09:00:10
File Name	D:\BN\output\2016\04.апрель\MM-072.H_001001r			Frequency (MHz)	400.13	Nucleus	1H
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000				



^{1}H NMR data of compound **3h**



^{19}F NMR data of compound **3h**

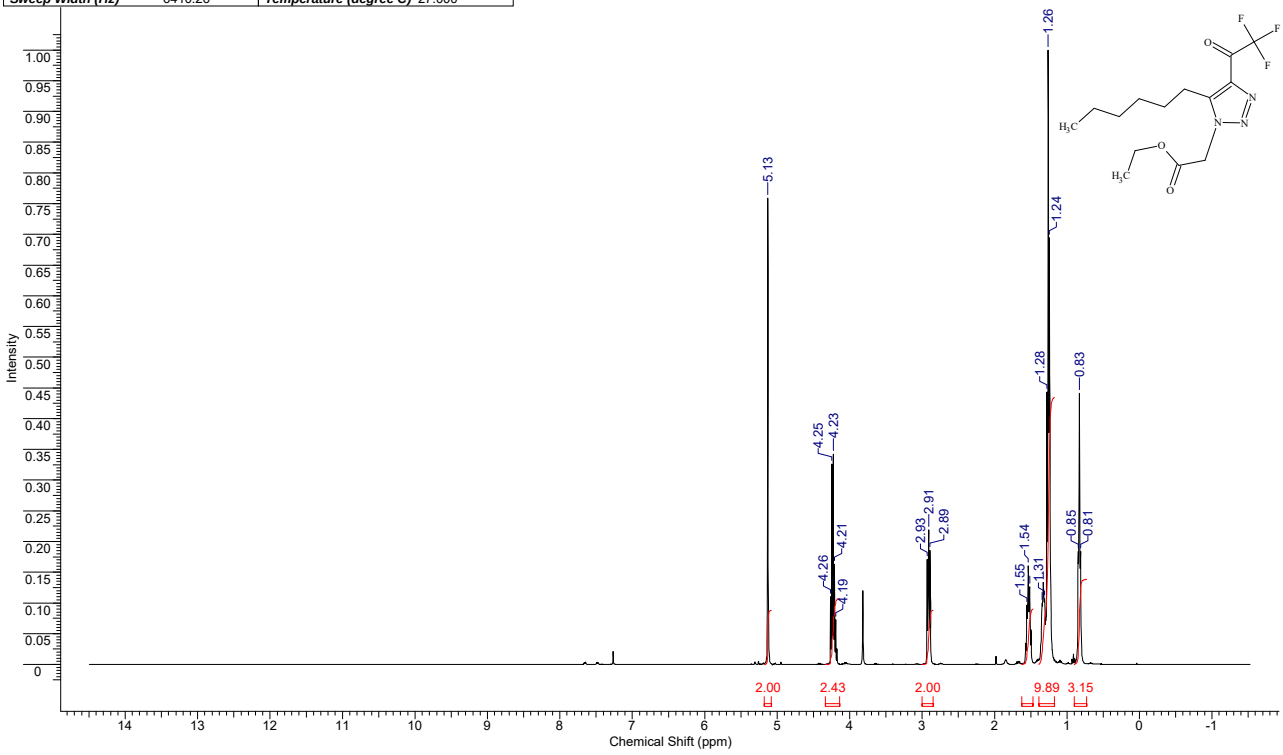


^{13}C NMR data of compound **3h**

7 Sep 2017

FW	335.3222	**Formula**	$C_{14}H_{20}F_3N_3O_3$

Acquisition Time (sec)	2.5559	**Comment**	Imported from UXNMR.			**Date**	15 Apr 2016 08:26:18
File Name	D:\BN\output\2016\04.апрель\MM-092-1.H_001001r			**Frequency (MHz)**	400.13	**Nucleus**	1H	**Number of Transients**	6
Original Points Count	16384	**Points Count**	65536	**Pulse Sequence**	zg30	**Solvent**	CHLOROFORM-D		
Sweep Width (Hz)	6410.26	**Temperature (degree C)**	27.000						

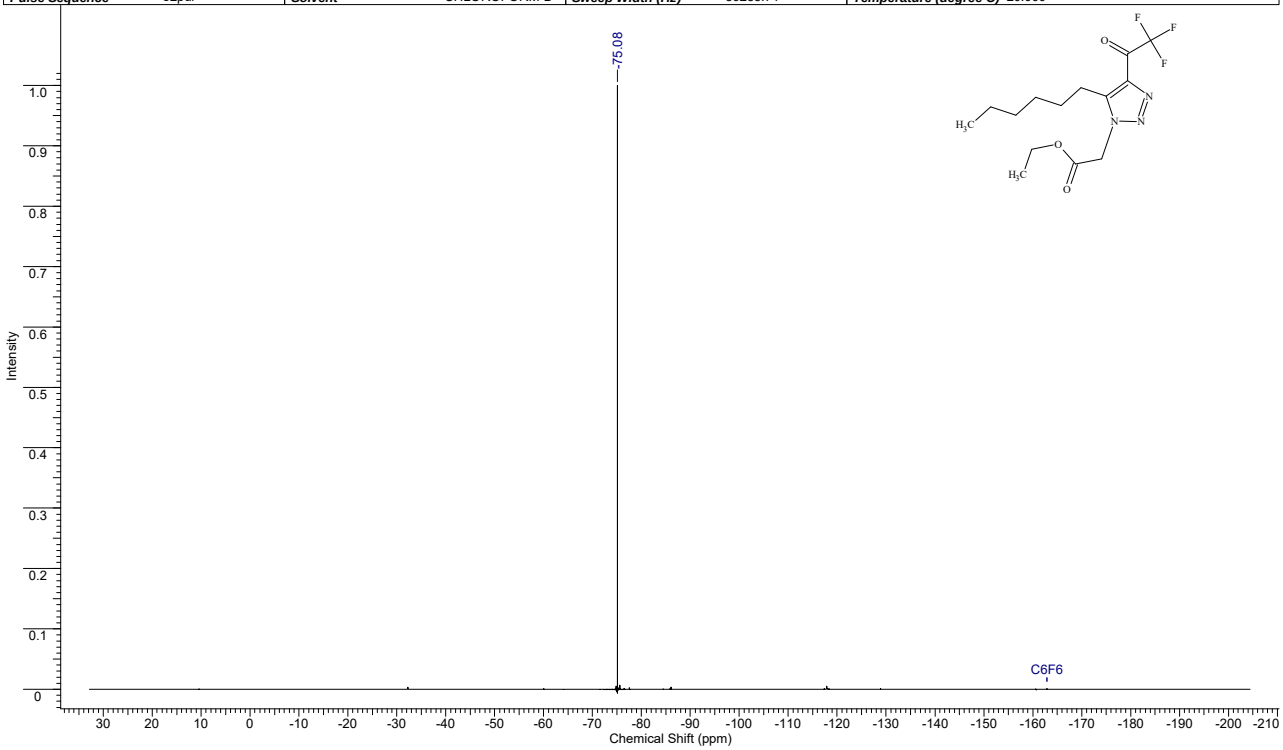


^{1}H NMR data of compound **3i**

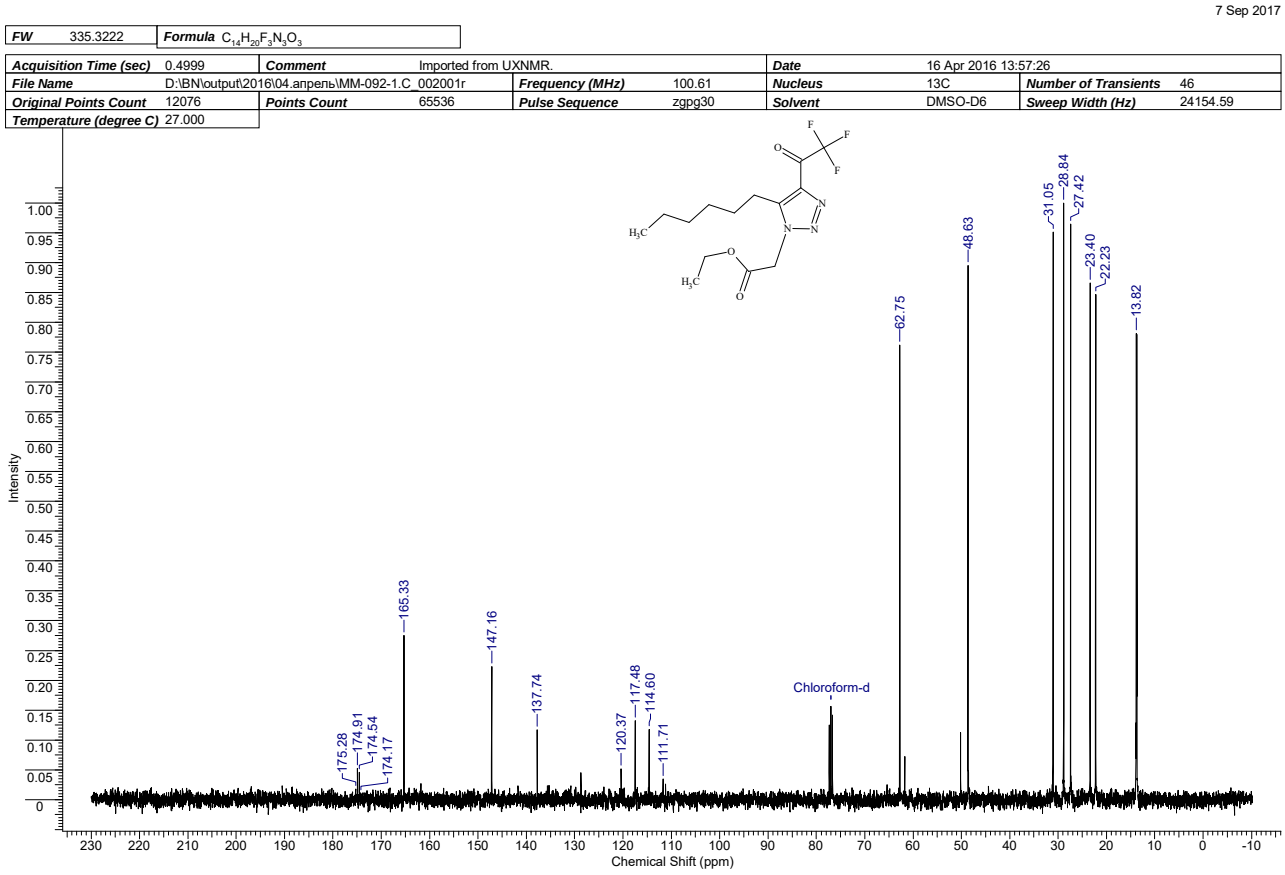
7 Sep 2017

FW	335.3222	**Formula**	$C_{14}H_{20}F_3N_3O_3$

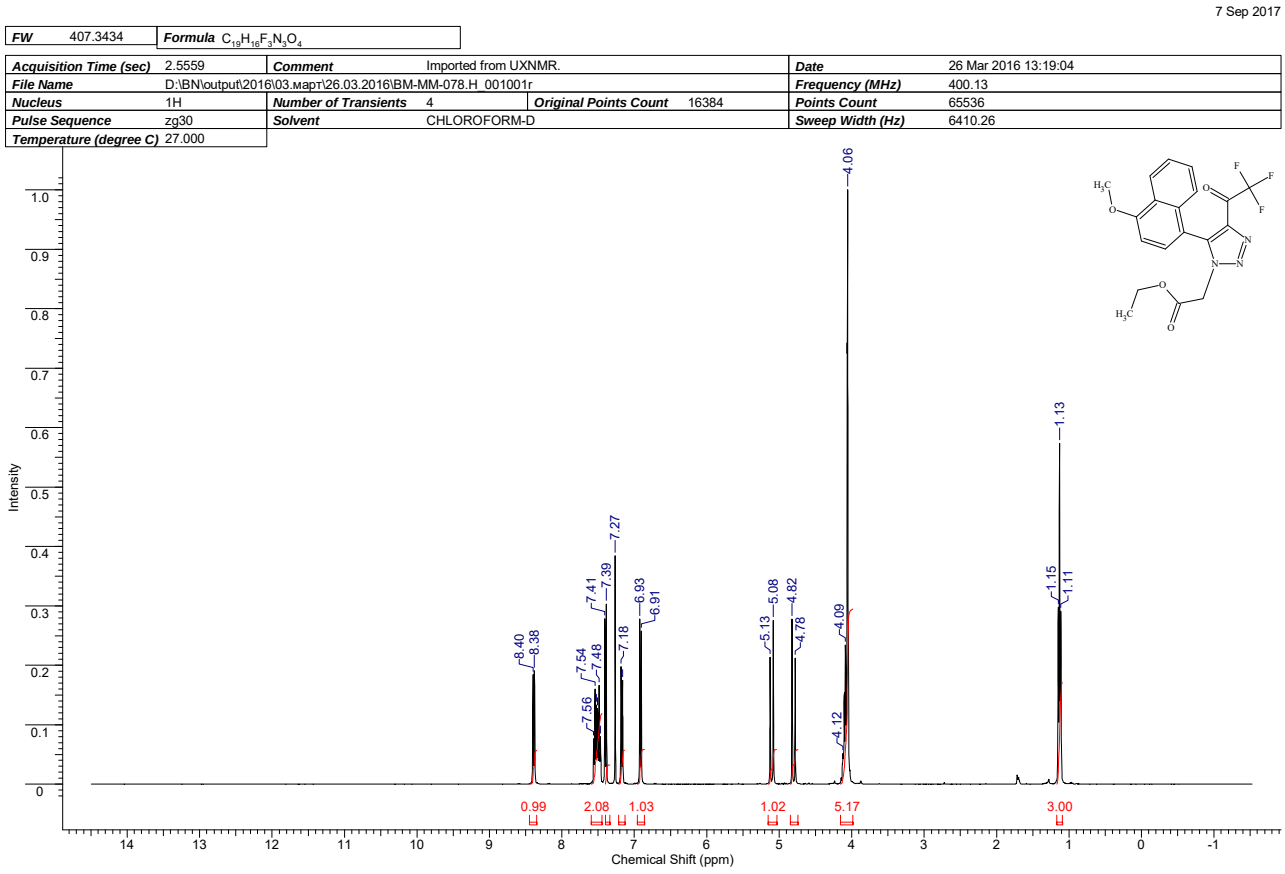
Acquisition Time (sec)	1.0000	**Date**	Apr 15 2016				
File Name	D:\BN\Docs (BN)\Vasiliy\Мансим_диссертация\Спектры_Мансим\19F\MM-092-1_20160415_01\FLUORINE_01					**Frequency (MHz)**	376.31
Nucleus	19F	**Number of Transients**	16	**Original Points Count**	89286	**Points Count**	131072
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	89285.71	**Temperature (degree C)**	20.000



^{19}F NMR data of compound **3i**



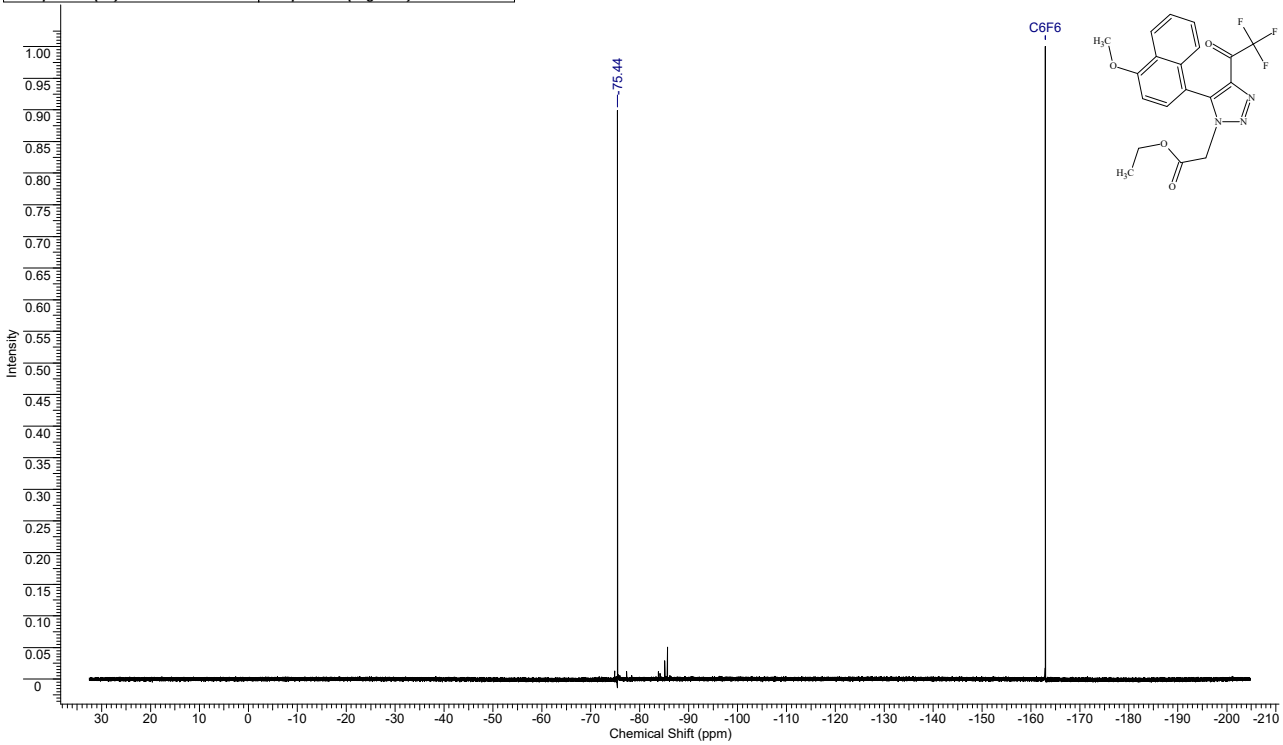
^{13}C NMR data of compound **3i**



^{1}H NMR data of compound **3j**

7 Sep 2017

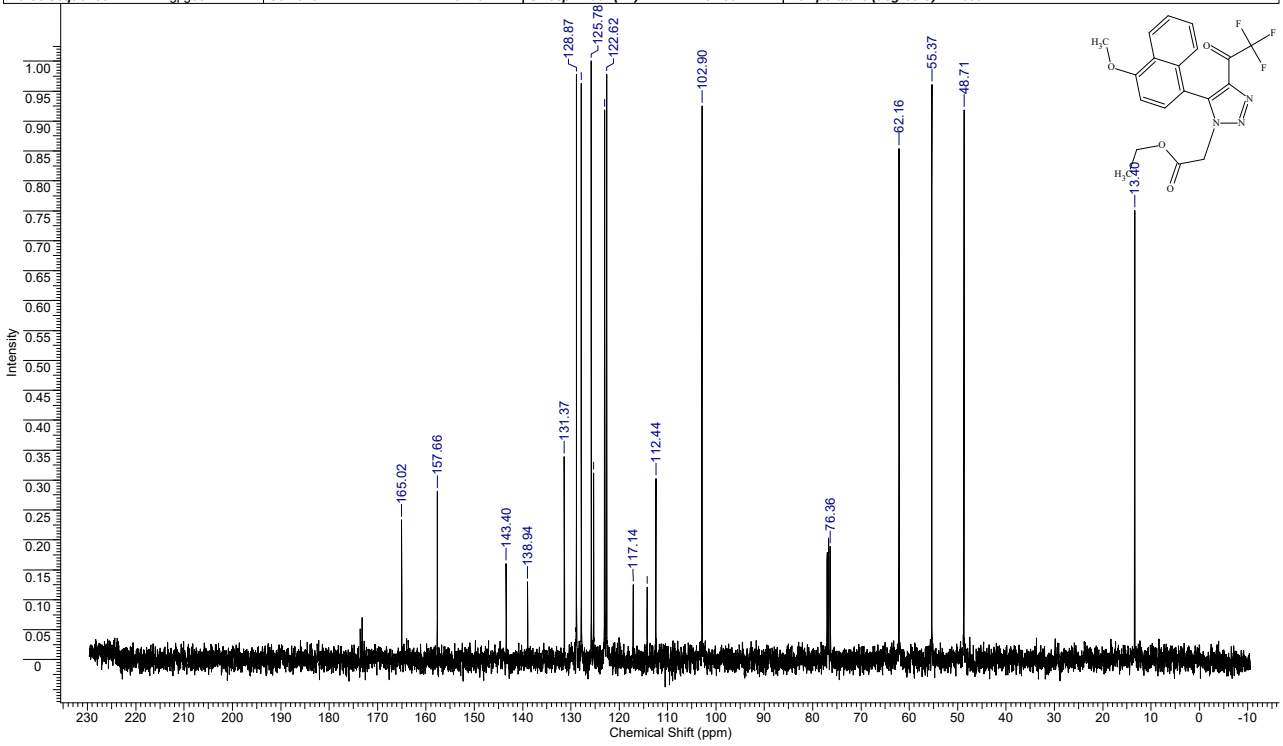
FW	407.3434	Formula	$C_{19}H_{16}F_3N_3O_4$				
Acquisition Time (sec)	1.0000	Date	Mar 25 2016	File Name	D:\BN\output\F19\2016.03.25\MM-078_20160325_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	4	Original Points Count	89286
Points Count	131072	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	20.000				



^{19}F NMR data of compound **3j**

7 Sep 2017

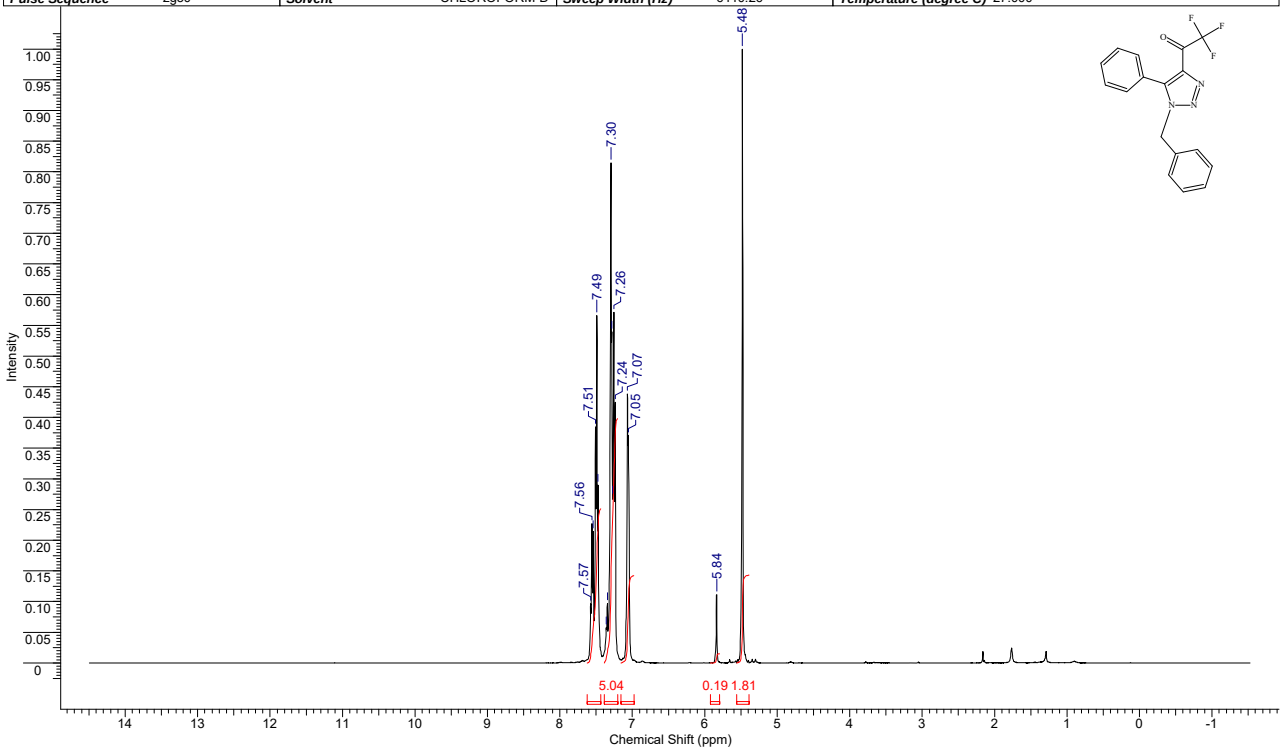
FW	407.3434	Formula	$C_{19}H_{16}F_3N_3O_4$				
Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.			Date	26 Mar 2016 13:20:54
File Name	D:\BN\output\2016\03.март\26.03.2016\BM-MM-078.C_002001r					Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	45	Original Points Count	12076	Points Count	65536
Pulse Sequence	zgpg30	Solvent	DMSO-D6	Sweep Width (Hz)	24154.59	Temperature (degree C)	27.000



^{13}C NMR data of compound **3j**

7 Sep 2017

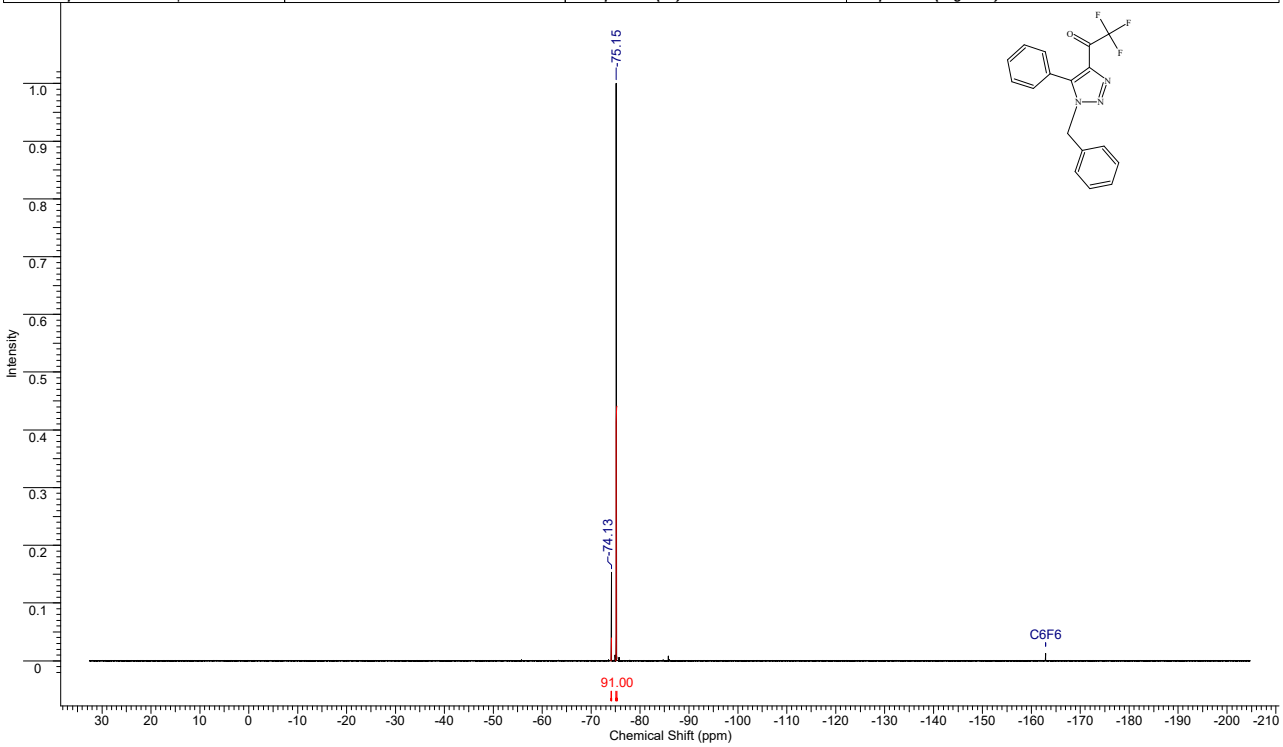
FW	331.2920	**Formula**	$C_{17}H_{12}F_3N_3O$				
Acquisition Time (sec)	2.5559	**Comment**	Imported from UXNMR.			**Date**	04 Apr 2016 09:30:26
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\BM-MM-086-3.H_001001r					**Frequency (MHz)**	400.13
Nucleus	1H	**Number of Transients**	5	**Original Points Count**	16384	**Points Count**	65536
Pulse Sequence	zg30	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	6410.26	**Temperature (degree C)**	27.000



^{1}H NMR data of compound **3k**

7 Sep 2017

FW	331.2920	**Formula**	$C_{17}H_{12}F_3N_3O$				
Acquisition Time (sec)	0.7340	**Date**	Apr 4 2016				
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\19F\BM-MM-086-3_20160404_01\FLUORINE_01					**Frequency (MHz)**	376.31
Nucleus	19F	**Number of Transients**	4	**Original Points Count**	65536	**Points Count**	65536
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	89285.71	**Temperature (degree C)**	6.000

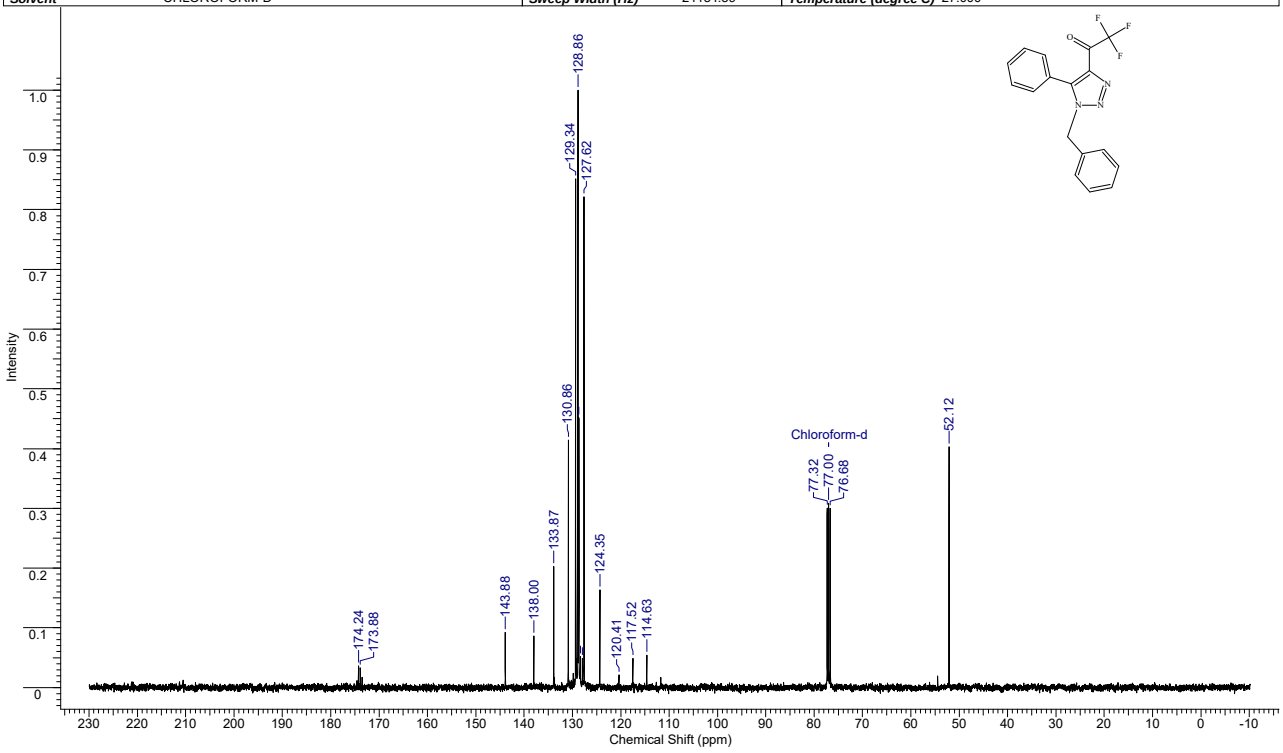


^{19}F NMR data of compound **3k**

7 Sep 2017

FW	331.2920	**Formula**	$C_{17}H_{12}F_3N_3O$

Acquisition Time (sec)	0.6783	**Comment**	Imported from UXNMR.			**Date**	22 Apr 2016 08:56:28
File Name	D:\BN\output\2016\04.апрель\MM-096-1.C_002001r			**Frequency (MHz)**	100.61	**Nucleus**	13C
Number of Transients	161	**Original Points Count**	16384	**Points Count**	131072	**Pulse Sequence**	zgpg30
Solvent	CHLOROFORM-D			**Sweep Width (Hz)**	24154.59	**Temperature (degree C)**	27.000

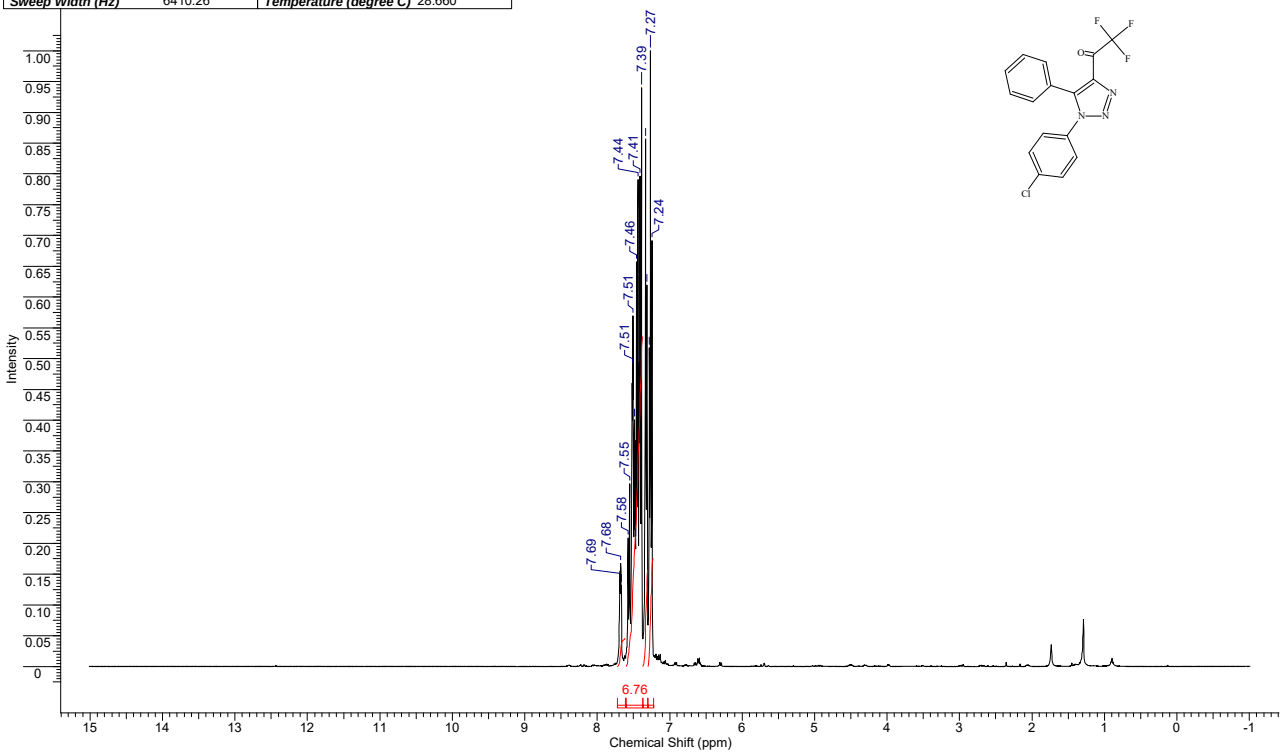


^{13}C NMR data of compound **3k**

7 Sep 2017

FW	351.7102	**Formula**	$C_{16}H_9ClF_3N_3O$

Acquisition Time (sec)	2.5559	**Comment**	Imported from UXNMR.			**Date**	02 Jul 2011 12:10:00		
File Name	D:\BN\output\2011\VG-000-11\VG026H11_001001r			**Frequency (MHz)**	400.13	**Nucleus**	1H	**Number of Transients**	4
Original Points Count	16384	**Points Count**	65536	**Pulse Sequence**	zg30	**Solvent**	CHLOROFORM-D		
Sweep Width (Hz)	6410.26	**Temperature (degree C)**	28.660						

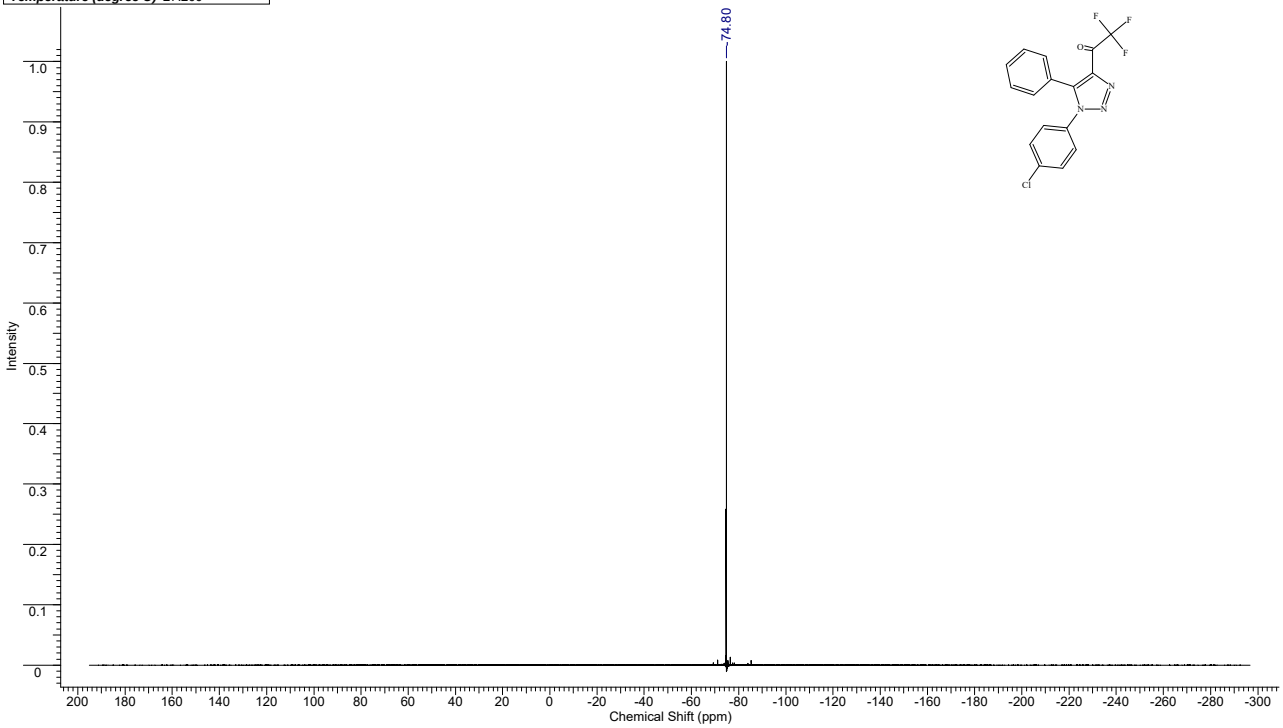


^{1}H NMR data of compound **3l**

7 Sep 2017

FW	351.7102	**Formula**	$C_{16}H_9ClF_3N_3O$

Acquisition Time (sec)	0.2449	**Comment**	19F with CPD	**Date**	05 Jul 2011 11:07:44		
File Name	D:\BN\output\F19\2011.07.05\BM-122\50541174.{19F}\50541174.{19F}_019000fid					**Frequency (MHz)**	282.39
Nucleus	19F	**Number of Transients**	1	**Original Points Count**	34018	**Points Count**	65536
Pulse Sequence	zg	**Solvent**	CHLOROFORM-D			**Sweep Width (Hz)**	138888.89
Temperature (degree C)	27.200						

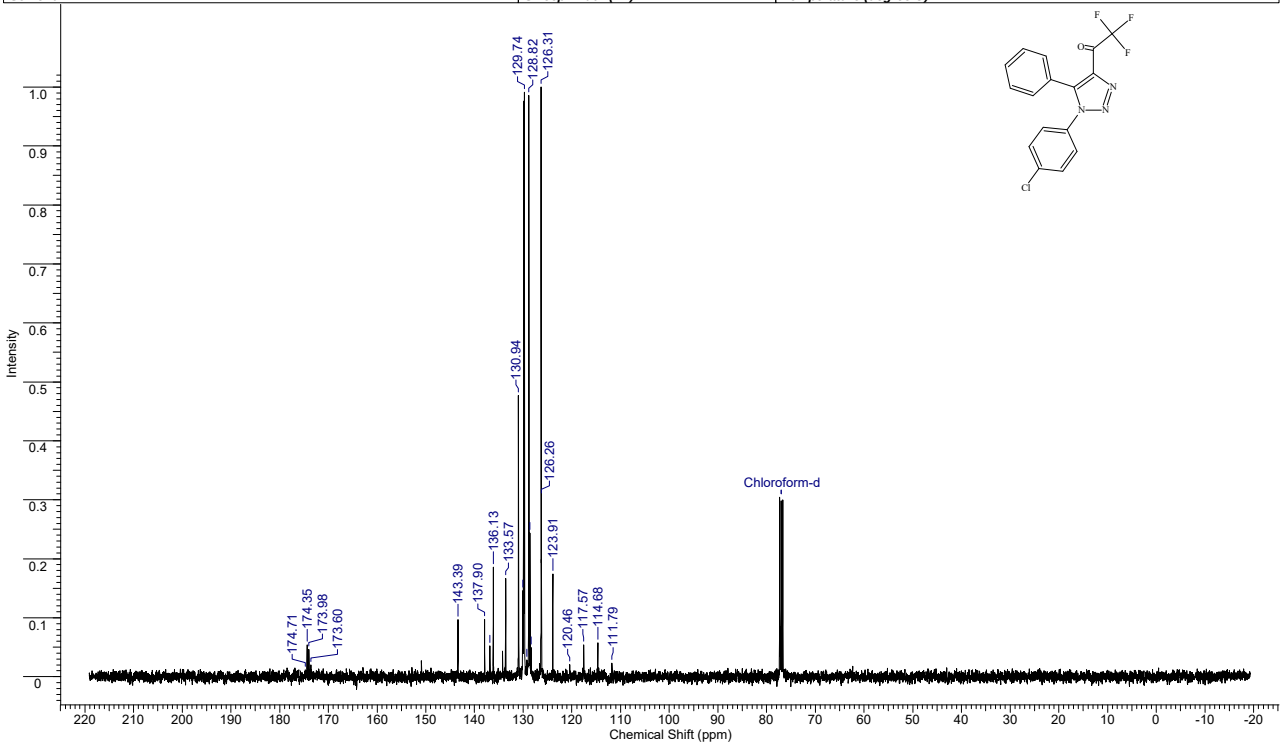


^{19}F NMR data of compound **3l**

7 Sep 2017

FW	351.7102	**Formula**	$C_{16}H_9ClF_3N_3O$

Acquisition Time (sec)	0.6832	**Comment**	Imported from UXNMR.			**Date**	02 Jul 2011 12:13:00
File Name	D:\BN\output\2011\VG-000-11\VG027C11_001001r			**Frequency (MHz)**	100.61	**Nucleus**	13C
Number of Transients	72	**Original Points Count**	16384	**Points Count**	65536	**Pulse Sequence**	zgpg30
Solvent	CHLOROFORM-D			**Sweep Width (Hz)**	23980.81	**Temperature (degree C)**	28.760

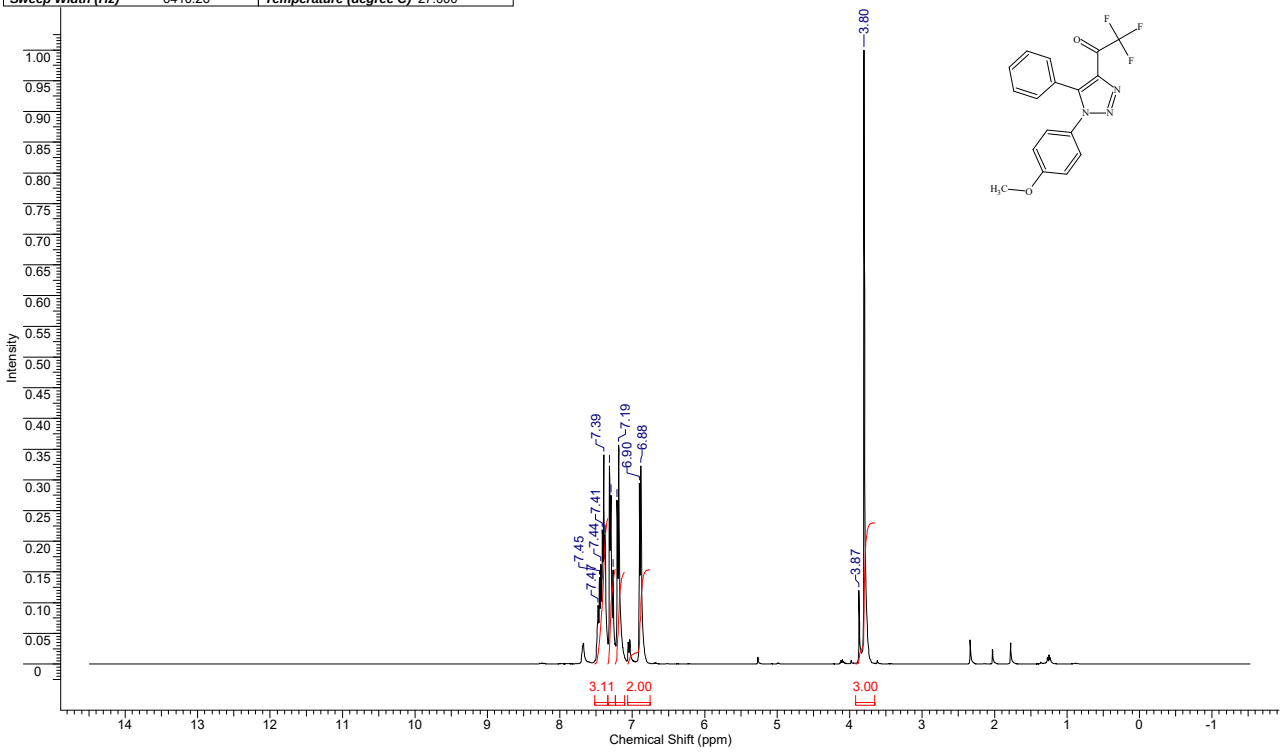


^{13}C NMR data of compound **3l**

7 Sep 2017

FW	347.2914	**Formula**	$C_{17}H_{12}F_3N_3O_2$

Acquisition Time (sec)	2.5559	**Comment**	Imported from UXNMR.			**Date**	07 Apr 2016 17:55:32
File Name	D:\BN\output\2016\04.апрель\MM-087-1.H_001001r			**Frequency (MHz)**	400.13	**Nucleus**	1H	**Number of Transients**	9
Original Points Count	16384	**Points Count**	65536	**Pulse Sequence**	zg30	**Solvent**	CHLOROFORM-D		
Sweep Width (Hz)	6410.26	**Temperature (degree C)**	27.000						

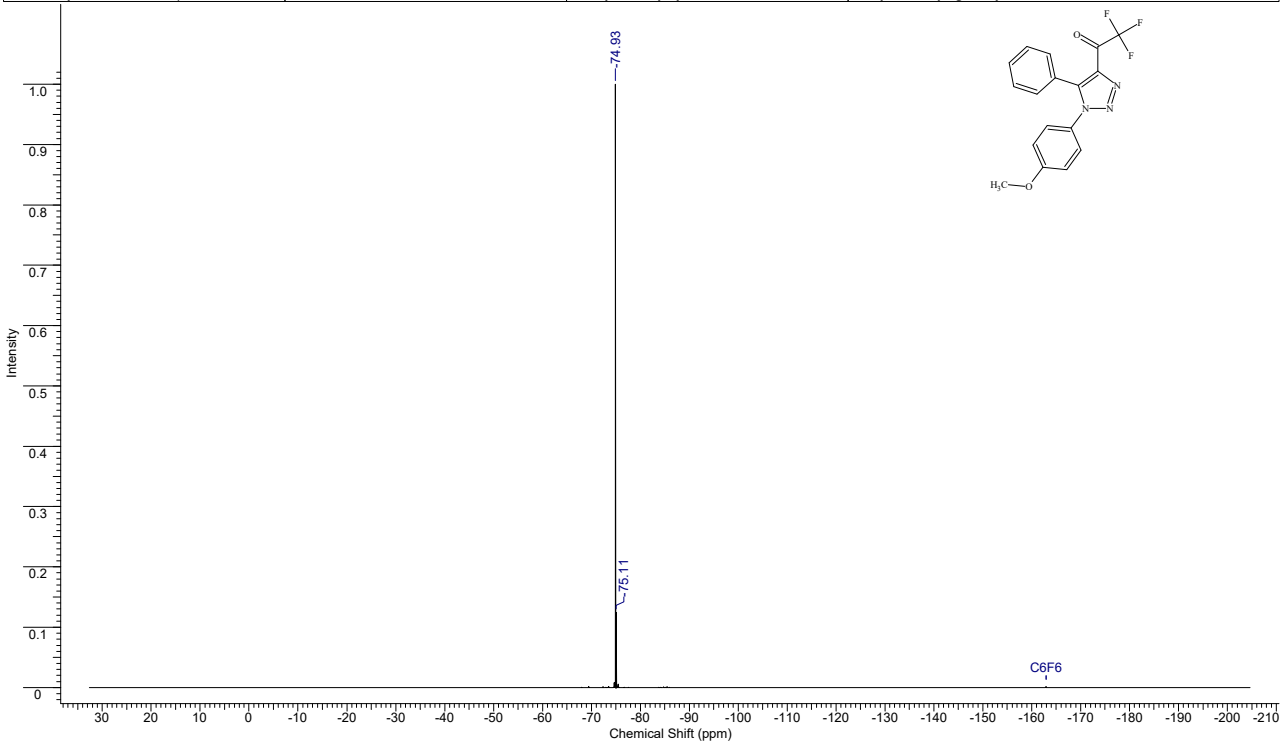


^{1}H NMR data of compound **3m**

7 Sep 2017

FW	347.2914	**Formula**	$C_{17}H_{12}F_3N_3O_2$

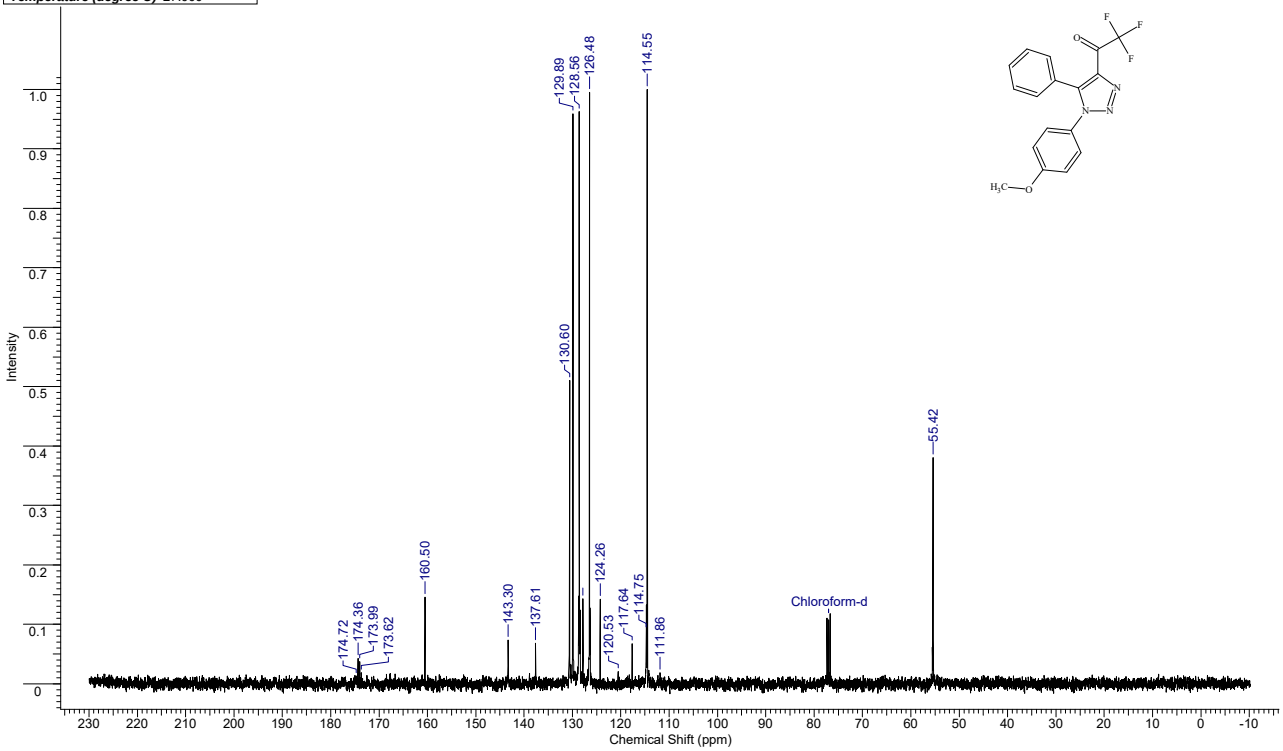
Acquisition Time (sec)	0.7340	**Date**	Apr 12 2016				
File Name	D:\BN\Docs (BN)\vasiliy\Мансим_диссертация\Спектры_Мансим\19F\mm087-2-f_20160412_01\FLUORINE_01					**Frequency (MHz)**	376.31
Nucleus	19F	**Number of Transients**	1000	**Original Points Count**	65536	**Points Count**	65536
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	89285.71	**Temperature (degree C)**	6.000



^{19}F NMR data of compound **3m**

7 Sep 2017

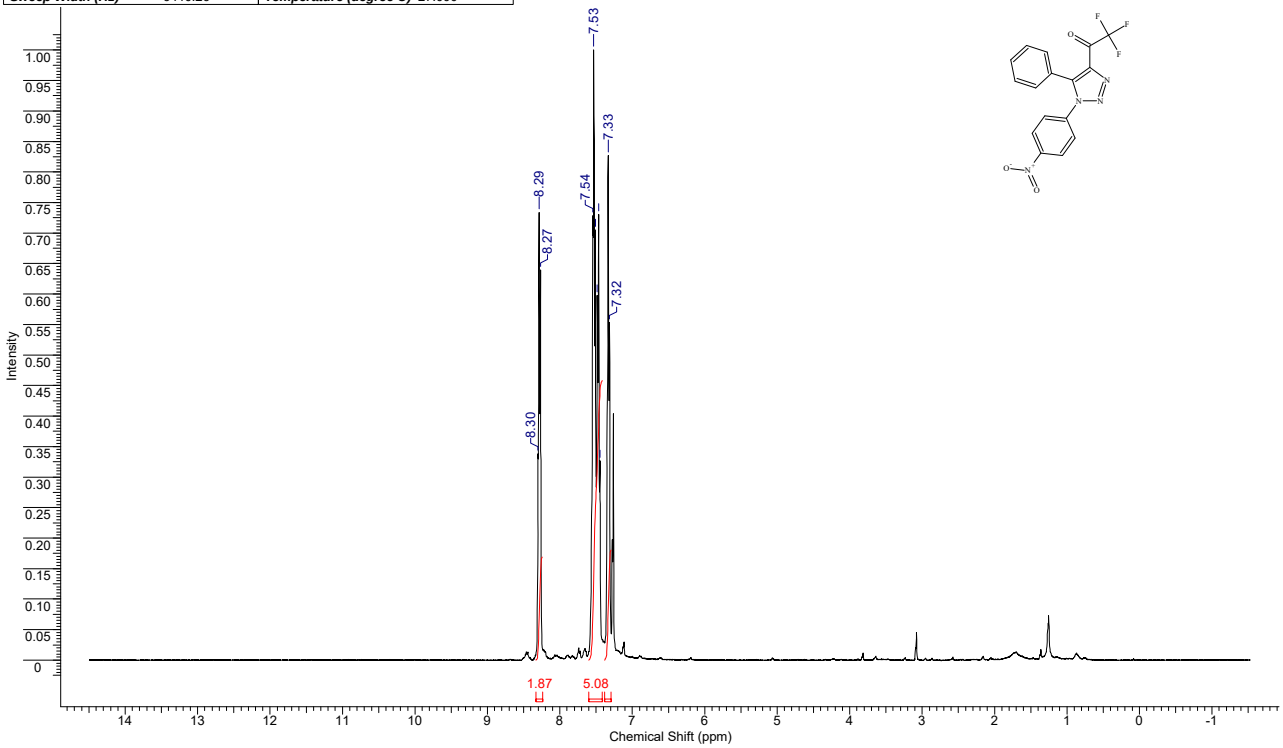
FW 347.2914	**Formula** $C_{17}H_{12}F_3N_3O_2$		
Acquisition Time (sec) 0.4999	**Comment** Imported from UXNMR.	**Date** 09 Apr 2016 13:59:22	
File Name D:\BN\output\2016\04.апрель\MM-087-2.C_002001r	**Frequency (MHz)** 100.61	**Nucleus** 13C	**Number of Transients** 32
Original Points Count 12076	**Points Count** 65536	**Pulse Sequence** zgpg30	**Solvent** DMSO-D6	**Sweep Width (Hz)** 24154.59
Temperature (degree C) 27.000			



^{13}C NMR data of compound **3m**

7 Sep 2017

FW 362.2630	**Formula** $C_{16}H_9F_3N_4O_3$				
Acquisition Time (sec) 2.5559	**Comment** Imported from UXNMR.		**Date** 09 Apr 2016 13:20:18		
File Name D:\BN\output\2016\04.апрель\MM-088-1.H_001001r		**Frequency (MHz)** 400.13	**Nucleus** 1H	**Number of Transients** 4	
Original Points Count 16384	**Points Count** 65536	**Pulse Sequence** zg30	**Solvent** CHLOROFORM-D		
Sweep Width (Hz) 6410.26	**Temperature (degree C)** 27.000				

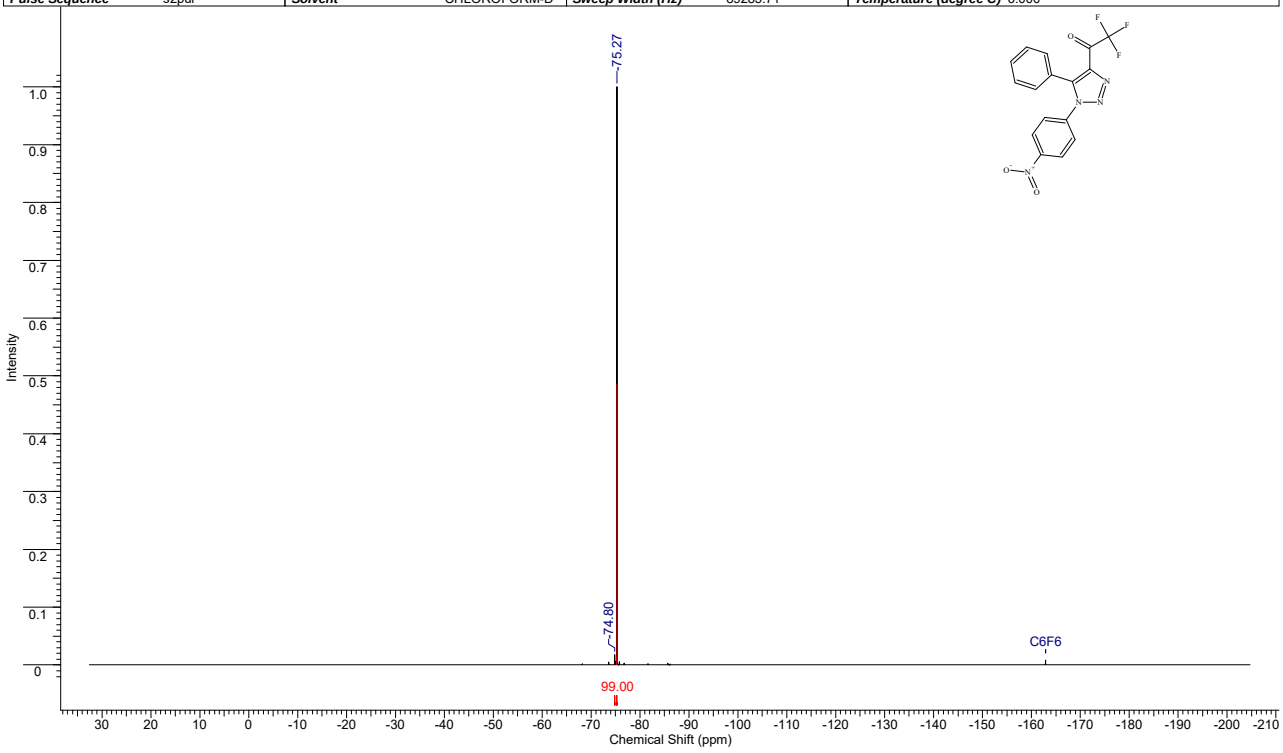


^{1}H NMR data of compound **3n**

7 Sep 2017

FW	362.2630	**Formula**	$C_{16}H_9F_3N_4O_3$

Acquisition Time (sec)	0.7340	**Date**	Apr 12 2016				
File Name	D:\BN\Docs (BN)\vasiliy\Максим_диссертация\Спектры_Максим\19F\mm088-3-f_20160412_01\FLUORINE_01					**Frequency (MHz)**	376.31
Nucleus	19F	**Number of Transients**	1000	**Original Points Count**	65536	**Points Count**	65536
Pulse Sequence	s2pul	**Solvent**	CHLOROFORM-D	**Sweep Width (Hz)**	89285.71	**Temperature (degree C)**	6.000

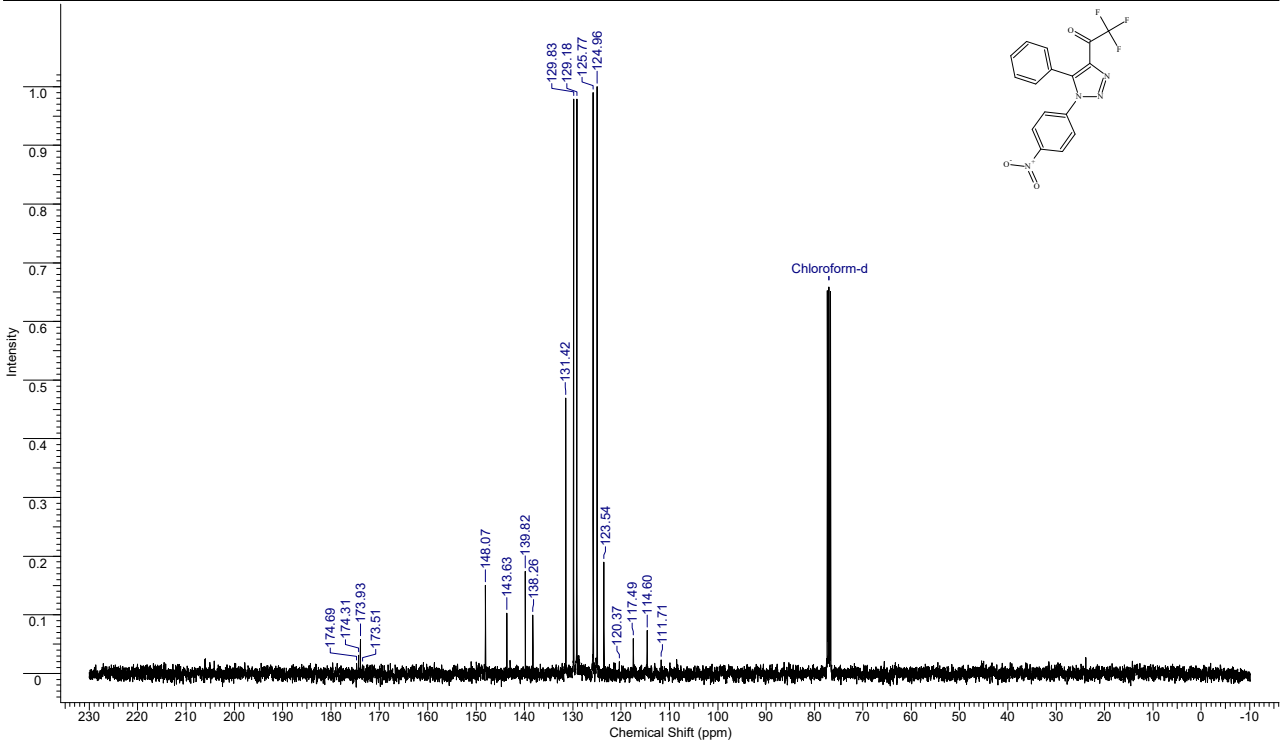


^{19}F NMR data of compound **3n**

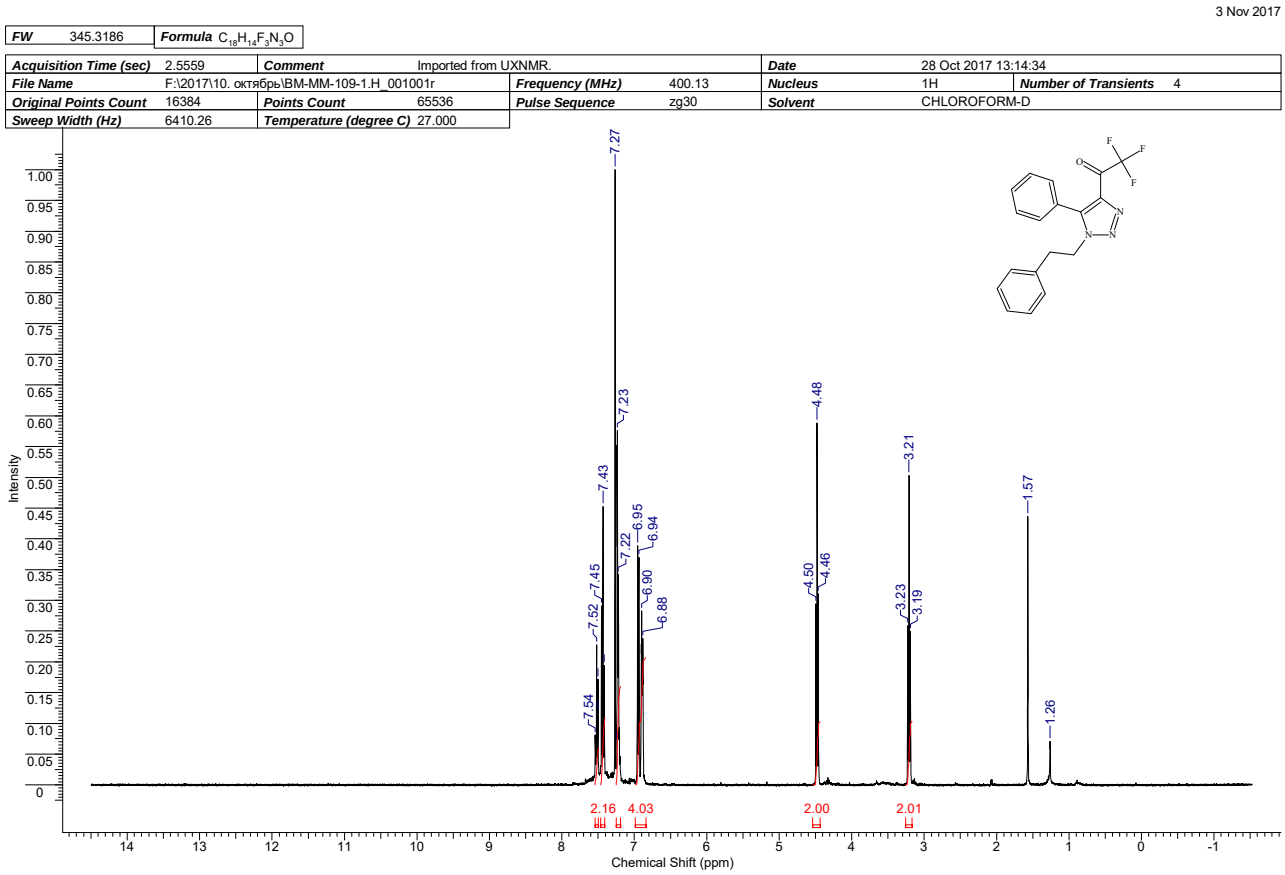
7 Sep 2017

FW	362.2630	**Formula**	$C_{16}H_9F_3N_4O_3$

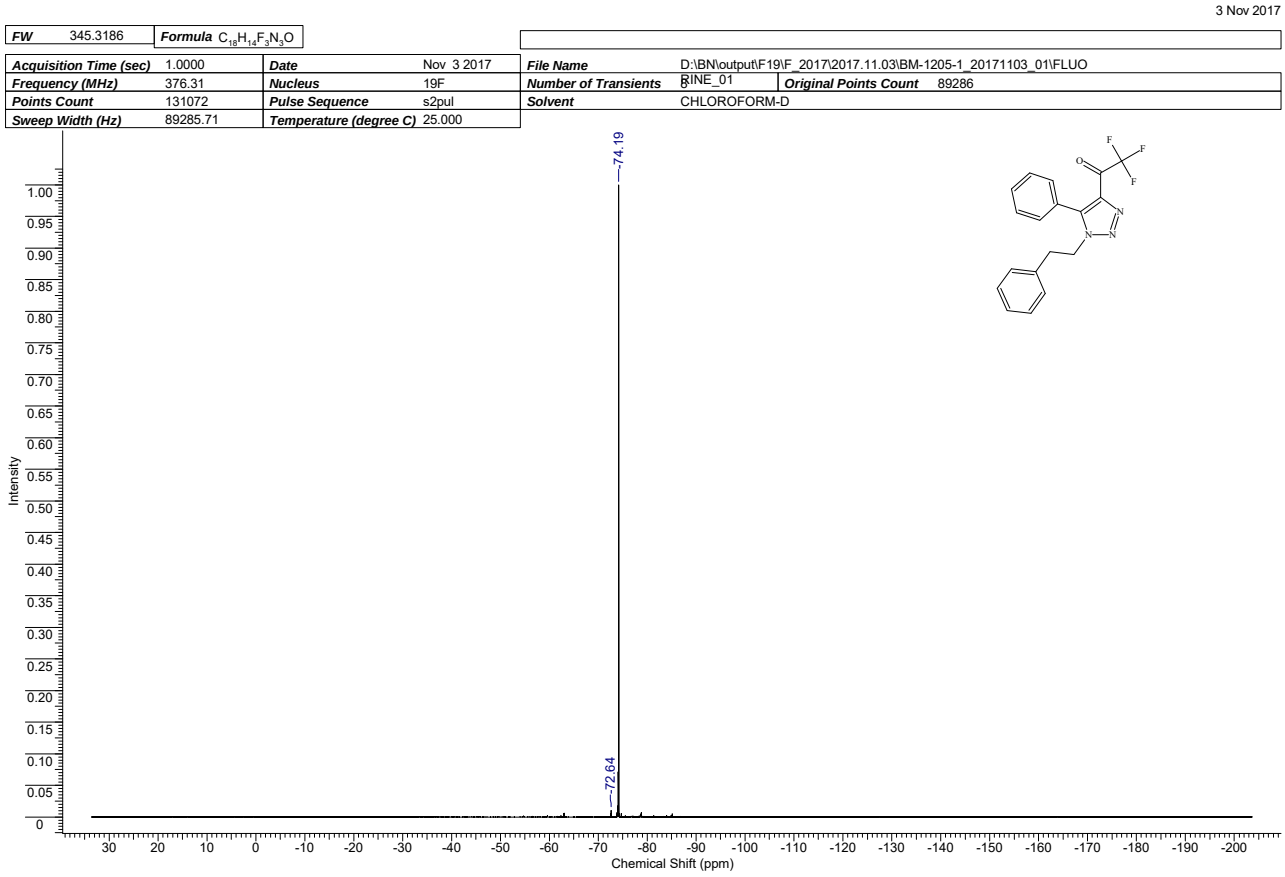
Acquisition Time (sec)	0.6783	**Comment**	Imported from UXNMR.			**Date**	15 Apr 2016 08:36:58
File Name	D:\BN\output\2016\04.апрель\MM-088-1.C_002001r			**Frequency (MHz)**	100.61	**Nucleus**	13C
Number of Transients	154	**Original Points Count**	16384	**Points Count**	131072	**Pulse Sequence**	zgpg30
Solvent	CHLOROFORM-D			**Sweep Width (Hz)**	24154.59	**Temperature (degree C)**	27.000



^{13}C NMR data of compound **3n**



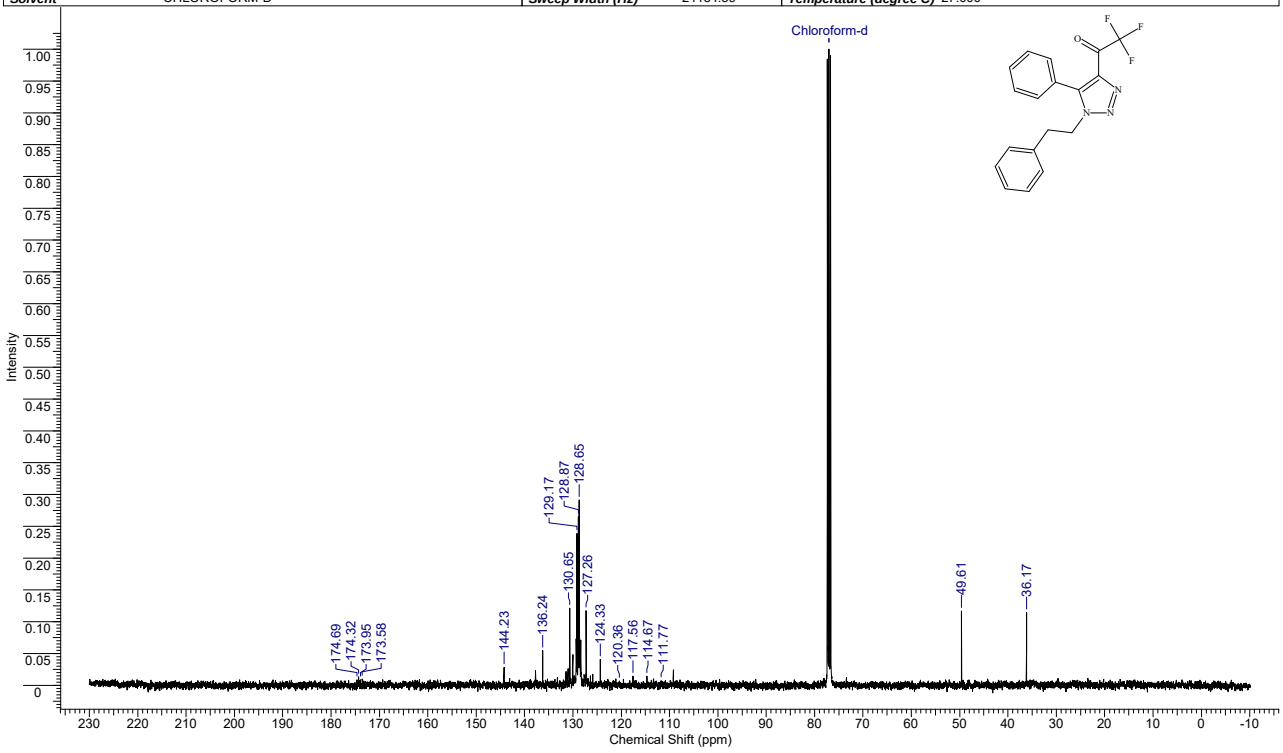
^{1}H NMR data of compound **3o**



^{19}F NMR data of compound **3o**

7 Sep 2017

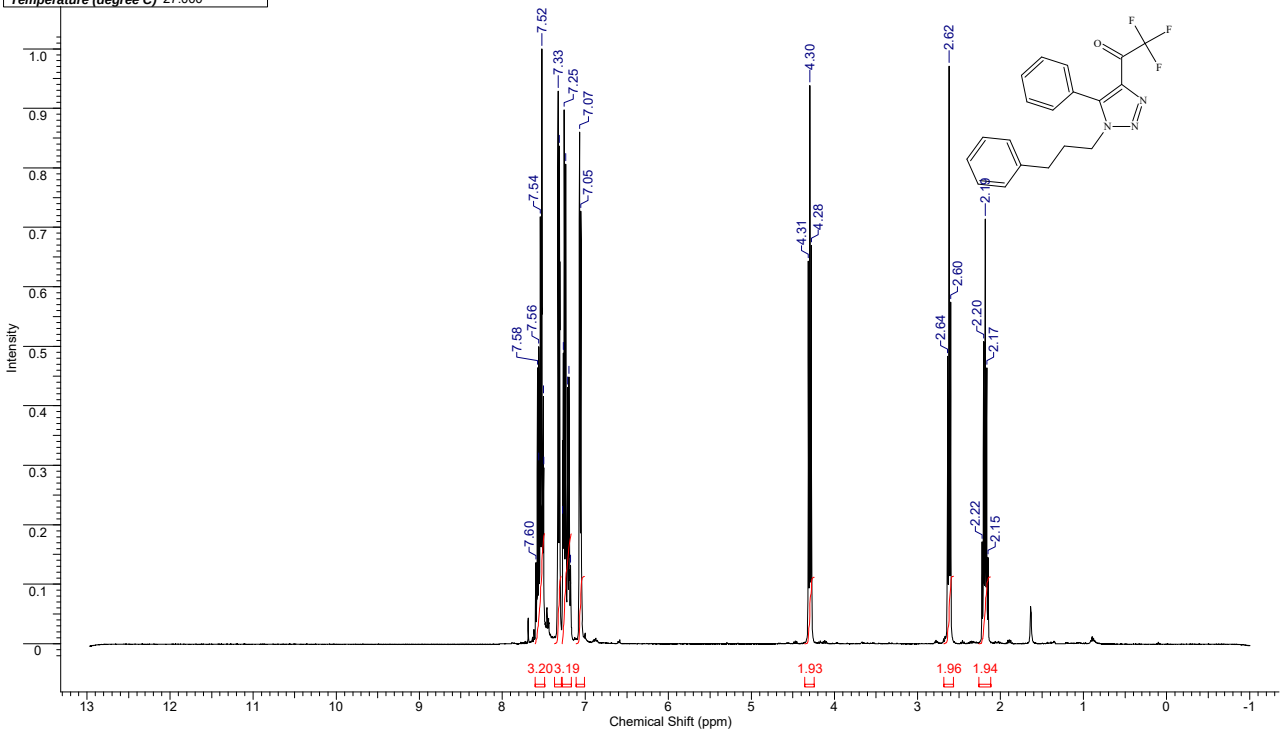
FW	345.3186	**Formula**	$C_{18}H_{14}F_3N_3O$				
Acquisition Time (sec)	0.6783	**Comment**	Imported from UXNMR.			**Date**	20 May 2016 07:46:40
File Name	D:\BN\output\2016\05.май\BM-MM109.C_002001r			**Frequency (MHz)**	100.61	**Nucleus**	13C
Number of Transients	1024	**Original Points Count**	16384	**Points Count**	131072	**Pulse Sequence**	zgpg30
Solvent	CHLOROFORM-D			**Sweep Width (Hz)**	24154.59	**Temperature (degree C)**	27.000



^{13}C NMR data of compound **3o**

3 Nov 2017

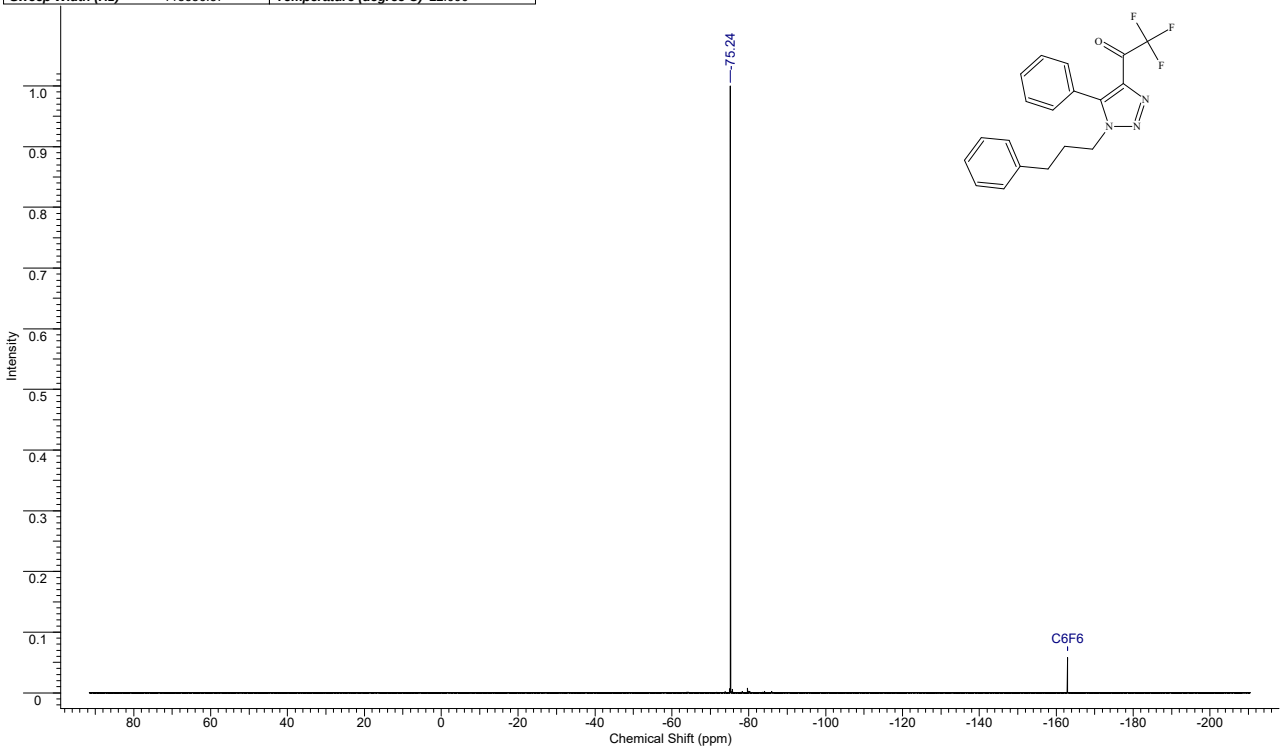
FW	359.3452	**Formula**	$C_{19}H_{16}F_3N_3O$				
Acquisition Time (sec)	2.9295	**Comment**	Imported from UXNMR.			**Date**	01 Nov 2017 22:05:50
File Name	D:\BN\output\2017\11.ноябрь\BM-MM-102-1\BM-MM-102-1_001001r					**Frequency (MHz)**	400.13
Nucleus	1H	**Number of Transients**	8	**Original Points Count**	16384	**Points Count**	65536
Pulse Sequence	zg30	**Solvent**	CHLOROFORM-D			**Sweep Width (Hz)**	5592.84
Temperature (degree C)	27.000						



^{1}H NMR data of compound **3p**

3 Nov 2017

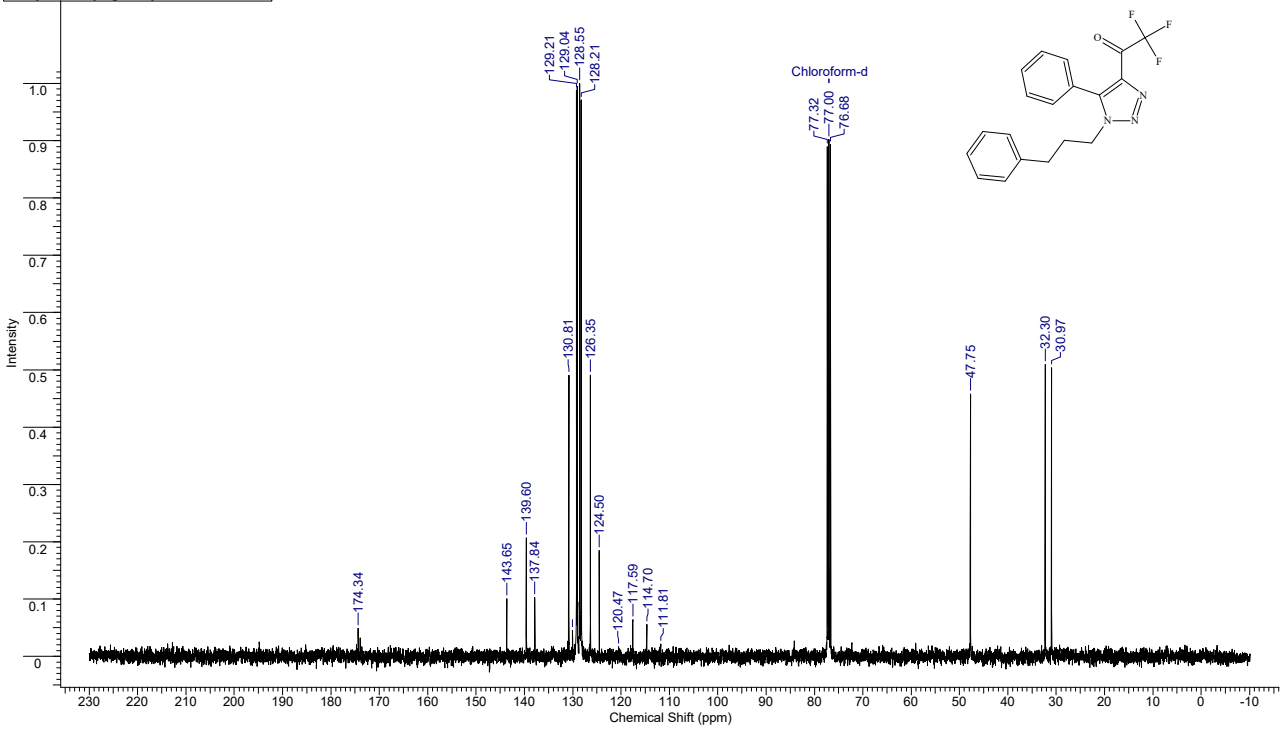
FW	359.3452	Formula	$C_{19}H_{16}F_3N_3O$				
Acquisition Time (sec)	1.5729	Date	Nov 2 2017	File Name	D:\BN\output\F19\F_2017\2017.11.02\BM-MM-102-1-F_20171102_01\FLUORINE_01		
Frequency (MHz)	376.32	Nucleus	19F	Number of Transients	8	Original Points Count	178735
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	113636.37	Temperature (degree C)	22.000				



^{19}F NMR data of compound **3p**

3 Nov 2017

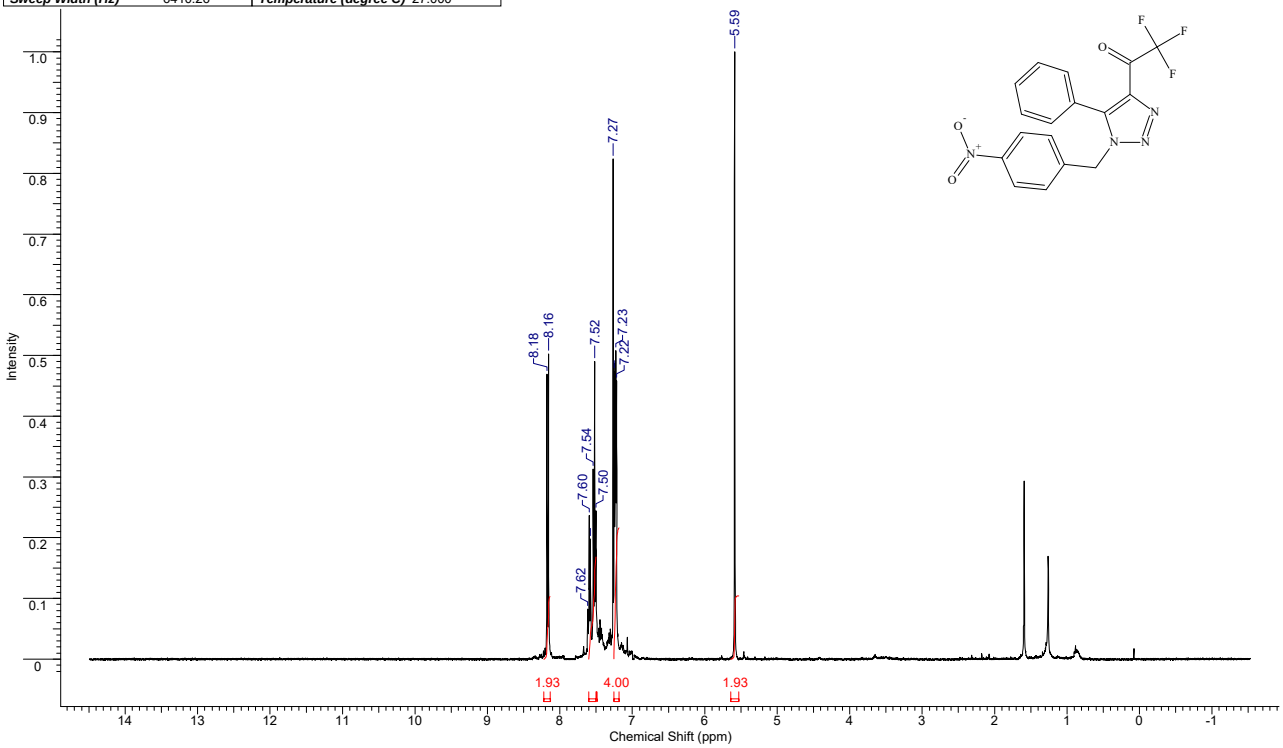
FW	359.3452	Formula	$C_{19}H_{16}F_3N_3O$						
Acquisition Time (sec)	0.6783	Comment	Imported from UXNMR.			Date	01 Nov 2017 22:17:18		
File Name	D:\BN\output\2017\11.ноябрь\BM-MM-102-1\BM-MM-102-1_002001r					Frequency (MHz)	100.61		
Nucleus	13C	Number of Transients	256	Original Points Count	16384	Points Count	131072		
Pulse Sequence	zgpg30	Solvent	CHLOROFORM-D			Sweep Width (Hz)	24154.59		
Temperature (degree C)	27.000								



^{13}C NMR data of compound **3p**

3 Nov 2017

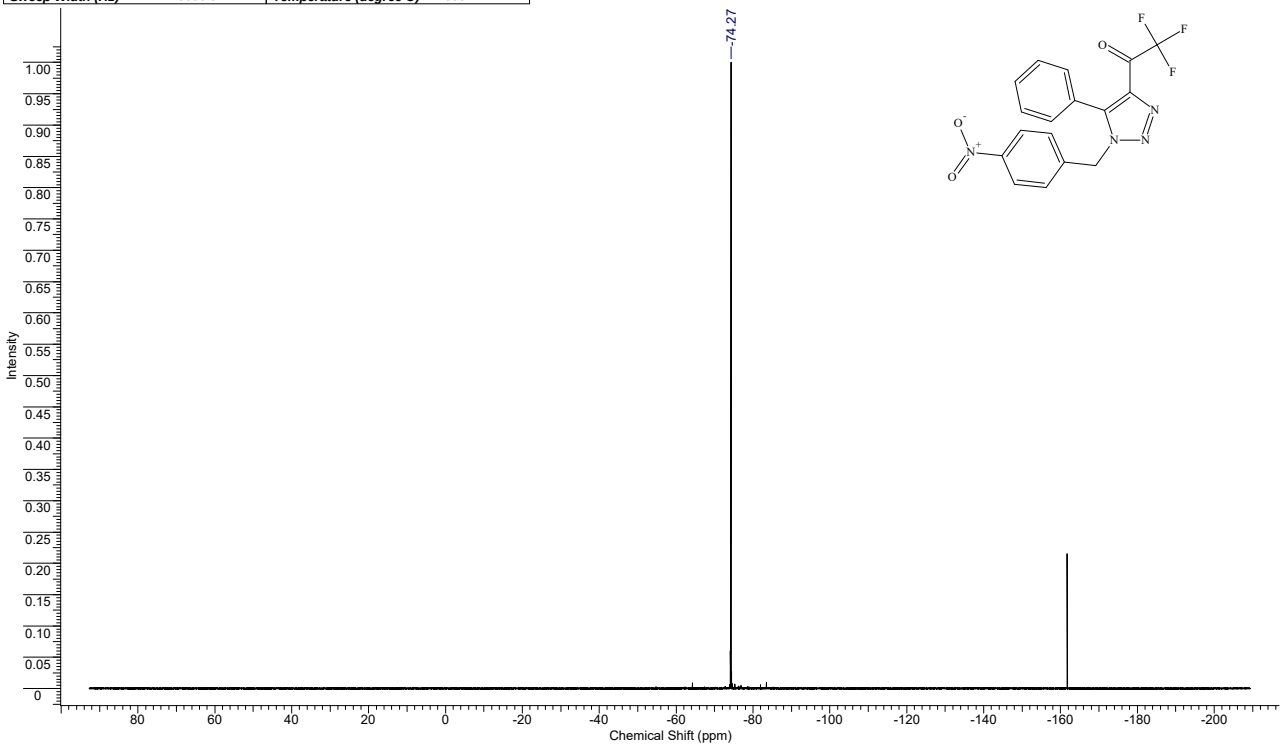
FW	376.2896	Formula	$C_{17}H_{11}F_3N_4O_3$				
Acquisition Time (sec)	2.5559	Comment	Imported from UXNMR.			Date	01 Nov 2017 17:11:26
File Name	F:\2017\11.ноябрь\BM-1201.H_001001r			Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	4
Original Points Count	16384	Points Count	65536	Pulse Sequence	zg30	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	6410.26	Temperature (degree C)	27.000						



^{1}H NMR data of compound **3q**

3 Nov 2017

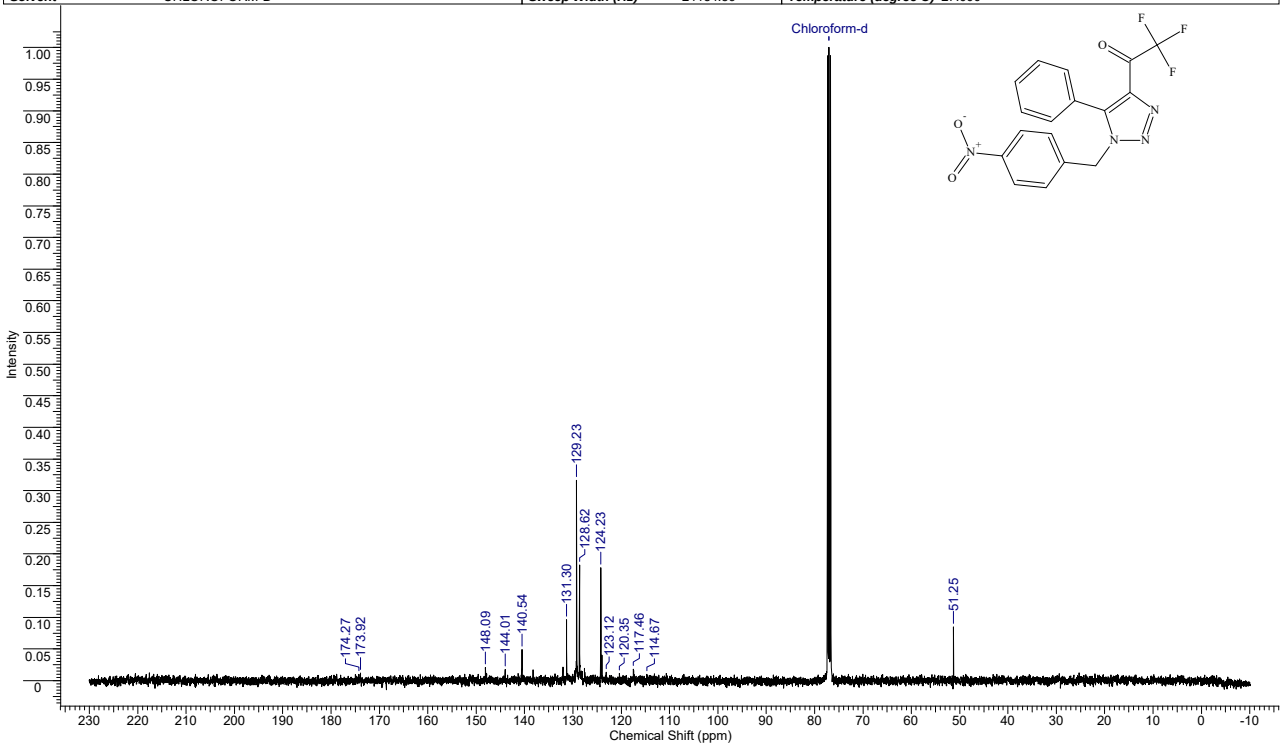
FW	376.2896	Formula	$C_{17}H_{11}F_3N_4O_3$				
Acquisition Time (sec)	1.5729	Date	Nov 2 2017	File Name	D:\BN\output\F19\F_2017\2017.11.02\BM-1201-F_20171102_01\FLUORINE_01		
Frequency (MHz)	376.32	Nucleus	19F	Number of Transients	8	Original Points Count	178735
Points Count	262144	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	113636.37	Temperature (degree C)	22.000				



^{19}F NMR data of compound **3q**

7 Sep 2017

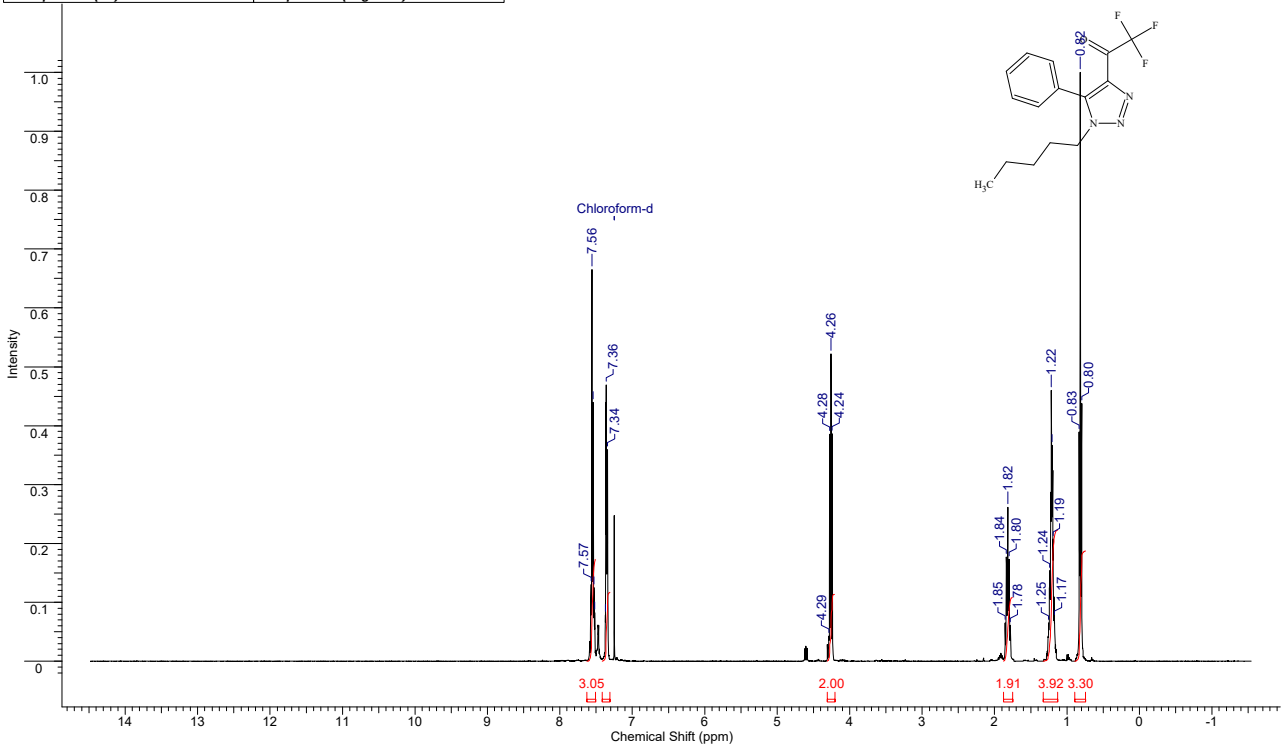
FW	376.2896	**Formula**	$C_{17}H_{11}F_3N_4O_3$				
Acquisition Time (sec)	0.6783	**Comment**	Imported from UXNMR.			**Date**	20 May 2016 08:44:40
File Name	D:\BN\output\2016\05.май\BM-MM108.C_002001r			**Frequency (MHz)**	100.61	**Nucleus**	13C
Number of Transients	1024	**Original Points Count**	16384	**Points Count**	131072	**Pulse Sequence**	zgpg30
Solvent	CHLOROFORM-D			**Sweep Width (Hz)**	24154.59	**Temperature (degree C)**	27.000



^{13}C NMR data of compound **3q**

3 Nov 2017

FW	311.3024	**Formula**	$C_{15}H_{16}F_3N_3O$				
Acquisition Time (sec)	2.5559	**Comment**	Imported from UXNMR.			**Date**	30 Oct 2017 15:19:22
File Name	F:\2017\10. октябрь\BM-1202-1.H_001001r			**Frequency (MHz)**	400.13	**Nucleus**	1H
Original Points Count	16384	**Points Count**	65536	**Pulse Sequence**	zg30	**Solvent**	CHLOROFORM-D
Sweep Width (Hz)	6410.26	**Temperature (degree C)**	27.000				

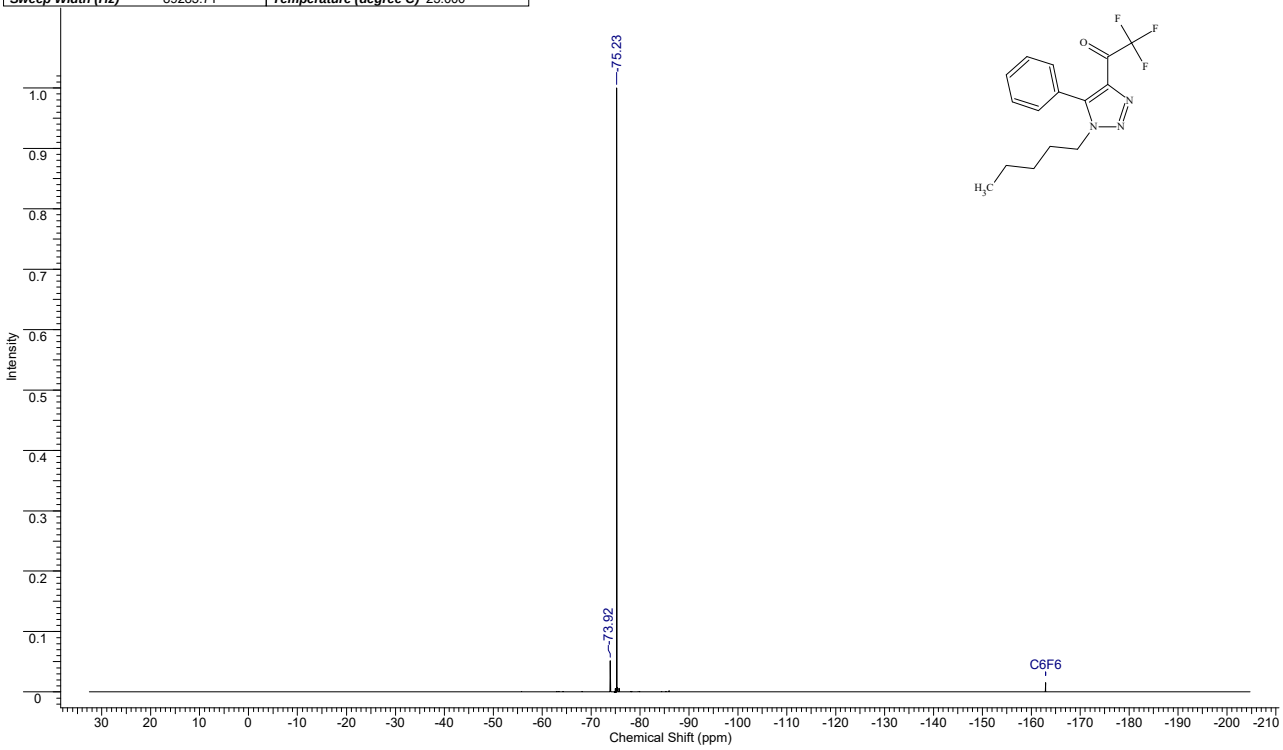


^{1}H NMR data of compound **3r**

3 Nov 2017

FW	311.3024	Formula	$C_{15}H_{16}F_3N_3O$

Acquisition Time (sec)	0.7340	Date	Oct 31 2017	File Name	D:\BN\output\F19\F_2017\2017.10.31\bm1202-1-f_20171031_01\FLUORINE_01		
Frequency (MHz)	376.31	Nucleus	19F	Number of Transients	160	Original Points Count	65536
Points Count	65536	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Sweep Width (Hz)	89285.71	Temperature (degree C)	25.000				

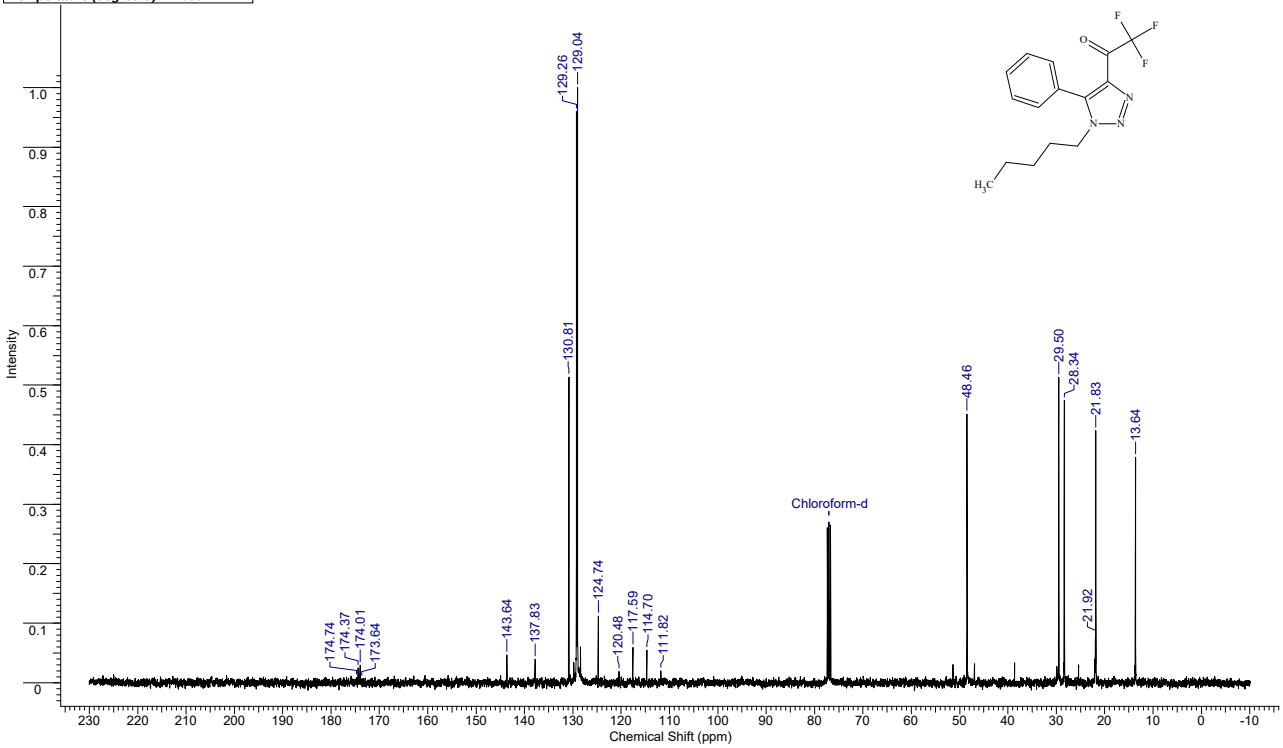


^{19}F NMR data of compound **3r**

3 Nov 2017

FW	311.3024	Formula	$C_{15}H_{16}F_3N_3O$

Acquisition Time (sec)	0.4999	Comment	Imported from UXNMR.			Date	01 Nov 2017 18:02:12		
File Name	F:\2017\11.ноябрь\BM-1202-1.C_002001r			Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	522
Original Points Count	12076	Points Count	65536	Pulse Sequence	zgpg30	Solvent	DMSO-D6	Sweep Width (Hz)	24154.59
Temperature (degree C)	27.000								



^{13}C NMR data of compound **3r**

*NMR spectral elucidation of compound **3g**.*

Technical details and spectra.

The ^{1}H and ^{13}C NMR spectra were recorded on Bruker AV-600 (600 and 150 MHz respectively) spectrometer in $CDCl_3$ (Aldrich) at 303 K, internal standard was TMS. Recording of ^{1}H and ^{13}C NMR spectra was carried out in FT mode. Two-dimensional COSY-90, HSQC, and HMBC NMR correlation spectra were recorded at optimal band frequencies with sizes of selected data 4K*1K (COSY-90) and 8K*1K (HSQC, HMBC) with relaxation delays from 1.5 to 2 sec using a TBI broad band pickup, fitted with a control system for impulse field gradients. The HSQC experiments were carried out with a 140 Hz BIRD filter. The HMBC experiments were carried out with three different values of the *J*-filter (4, 7, and 8 Hz). In the case of the COSY-90 experiments a two-dimensional Fourier conversion (4K*4K points) in magnitude representation of data mode was used after preliminary processing with QSIM digital filters at each coordinate. Processing of the HSQC and HMBC experiments was carried out in phase-sensitive mode for 8K*1K data stocks using a Lorentz filter (with parameter width 1 Hz for proton coordinates and 20-30 Hz for carbon coordinates). Assignment based on principles described in the main section.

^{1}H NMR, 2D NOESY, ^{13}C NMR, 2D COSY, HSQC and HMBC spectra for compound **3g** are presented in the figures S1-S6.

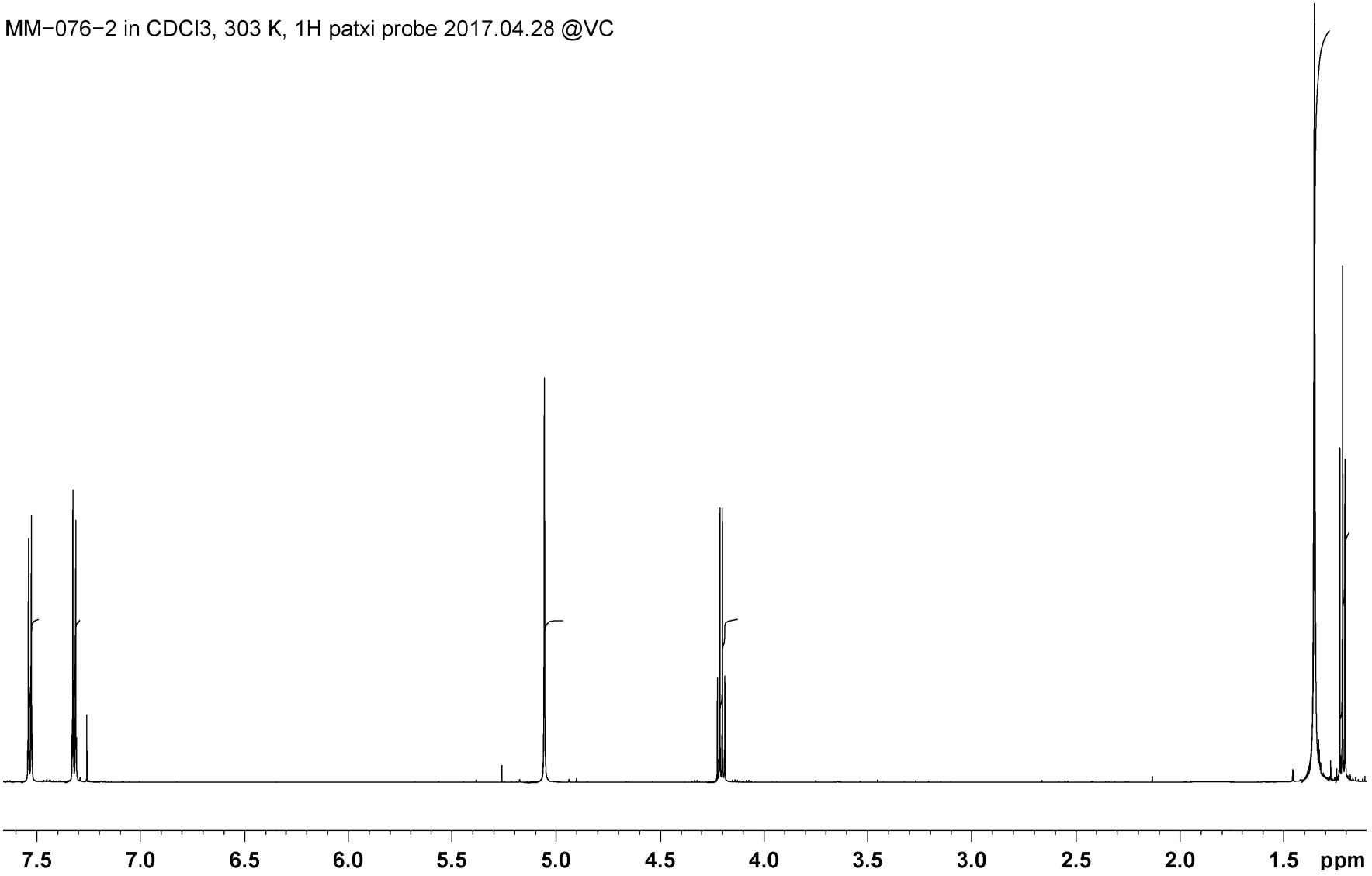


Figure S-1. Spectrum NMR ^{1}H (CDCL3, 303K, “Bruker-AV-600”).

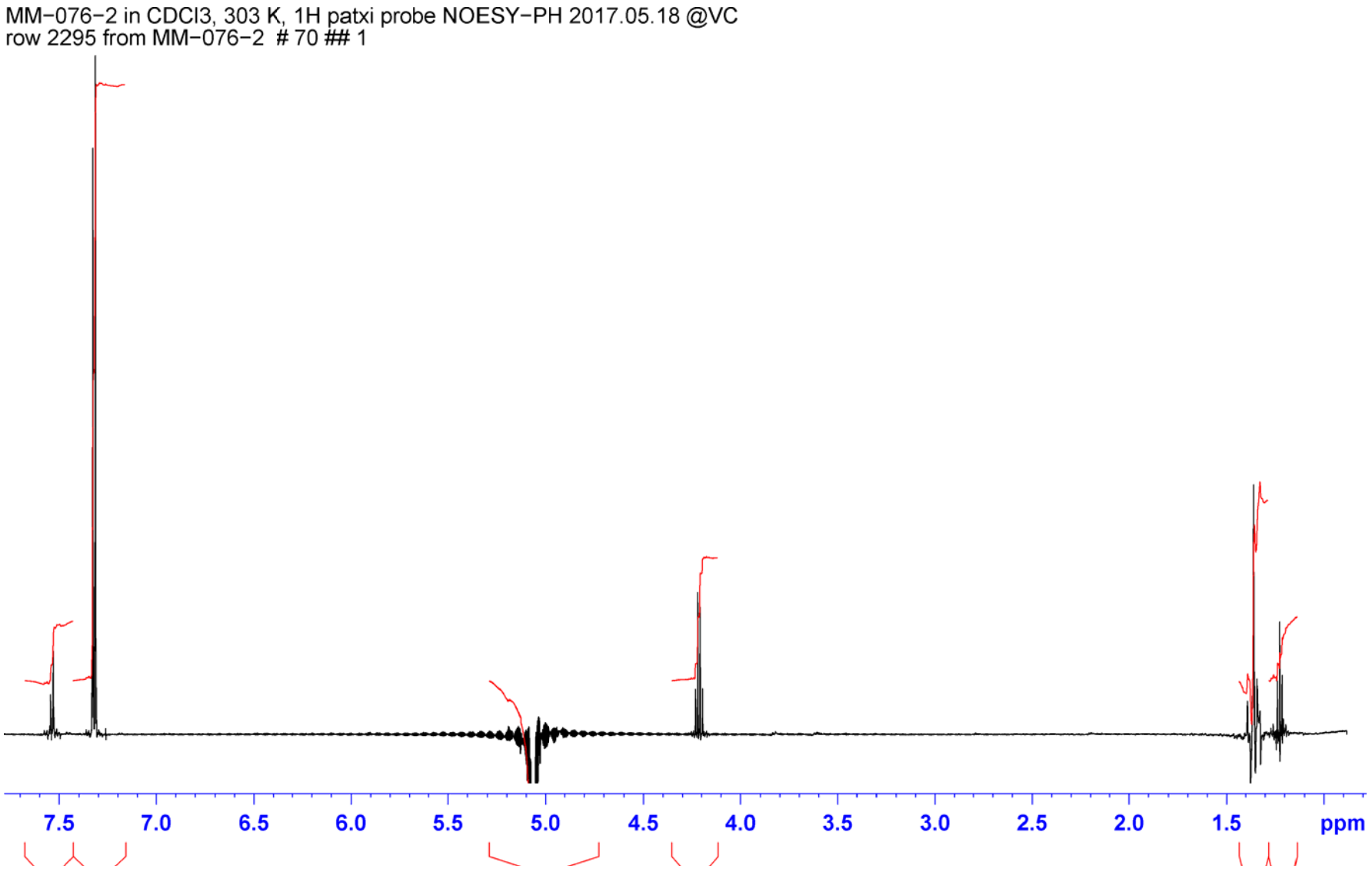


Figure S-2. Crossection of 2D spectrum -NOESY at resonance frequency of the CH_2-protons ($CDCL_3$, 303K, “Bruker-AV-600”).

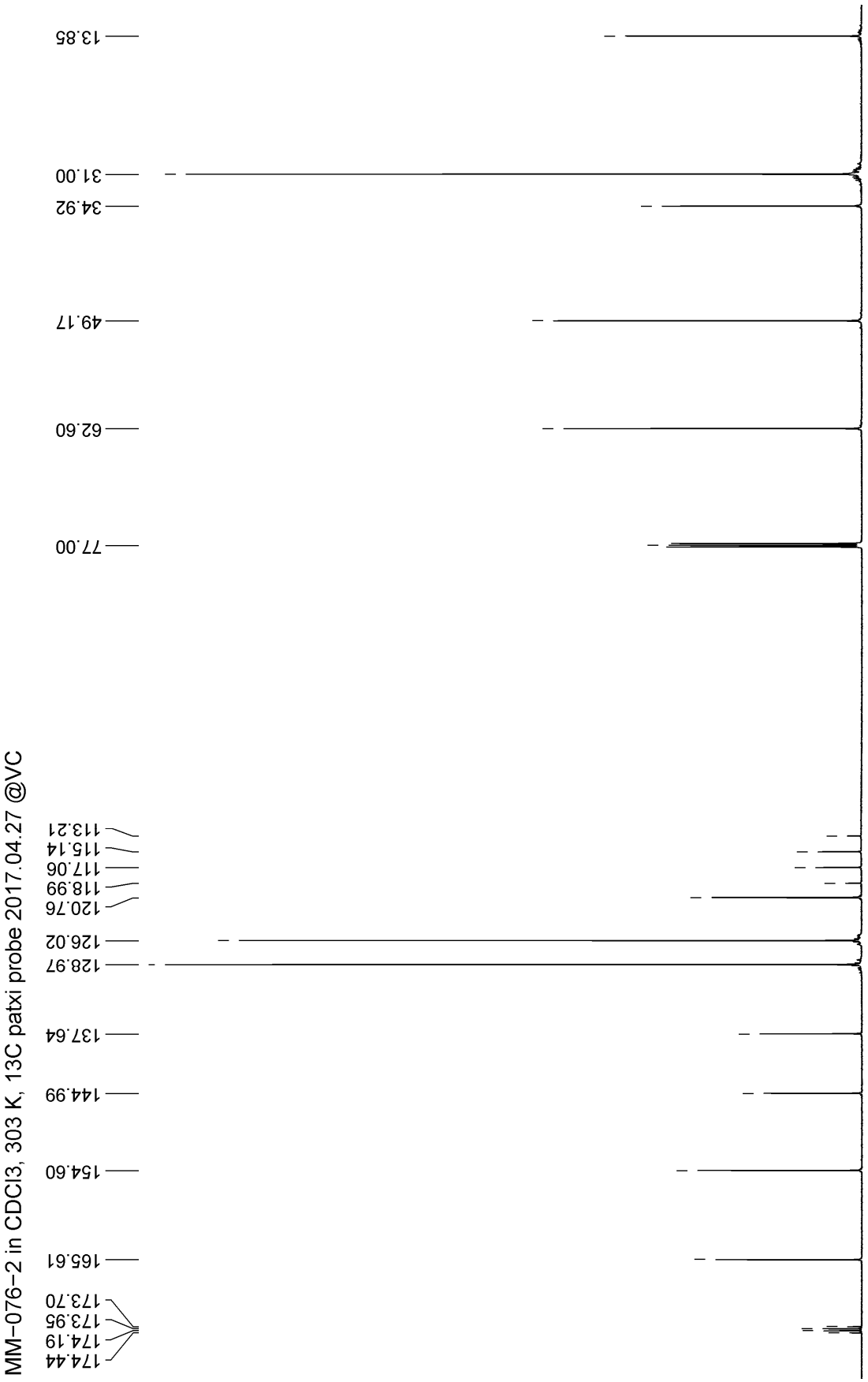


Figure S3. Spectrum NMR ^{13}C ($CDCL_3$, 303K, “Bruker-AV-600”).

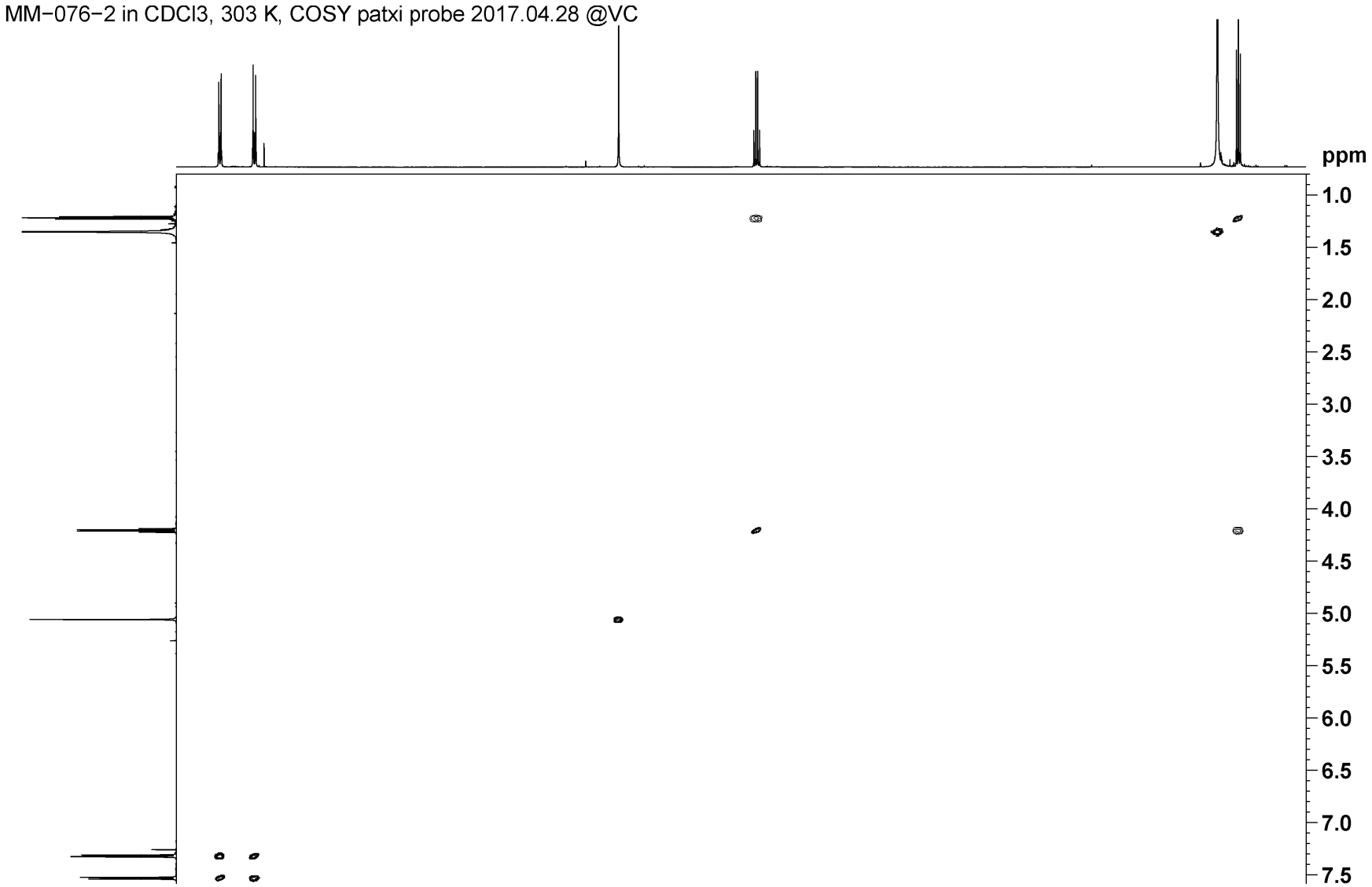


Figure S-4. 2D spectrum NMR ^{1}H-COSY ($CDCL_3$, 303K, “Bruker-AV-600”).

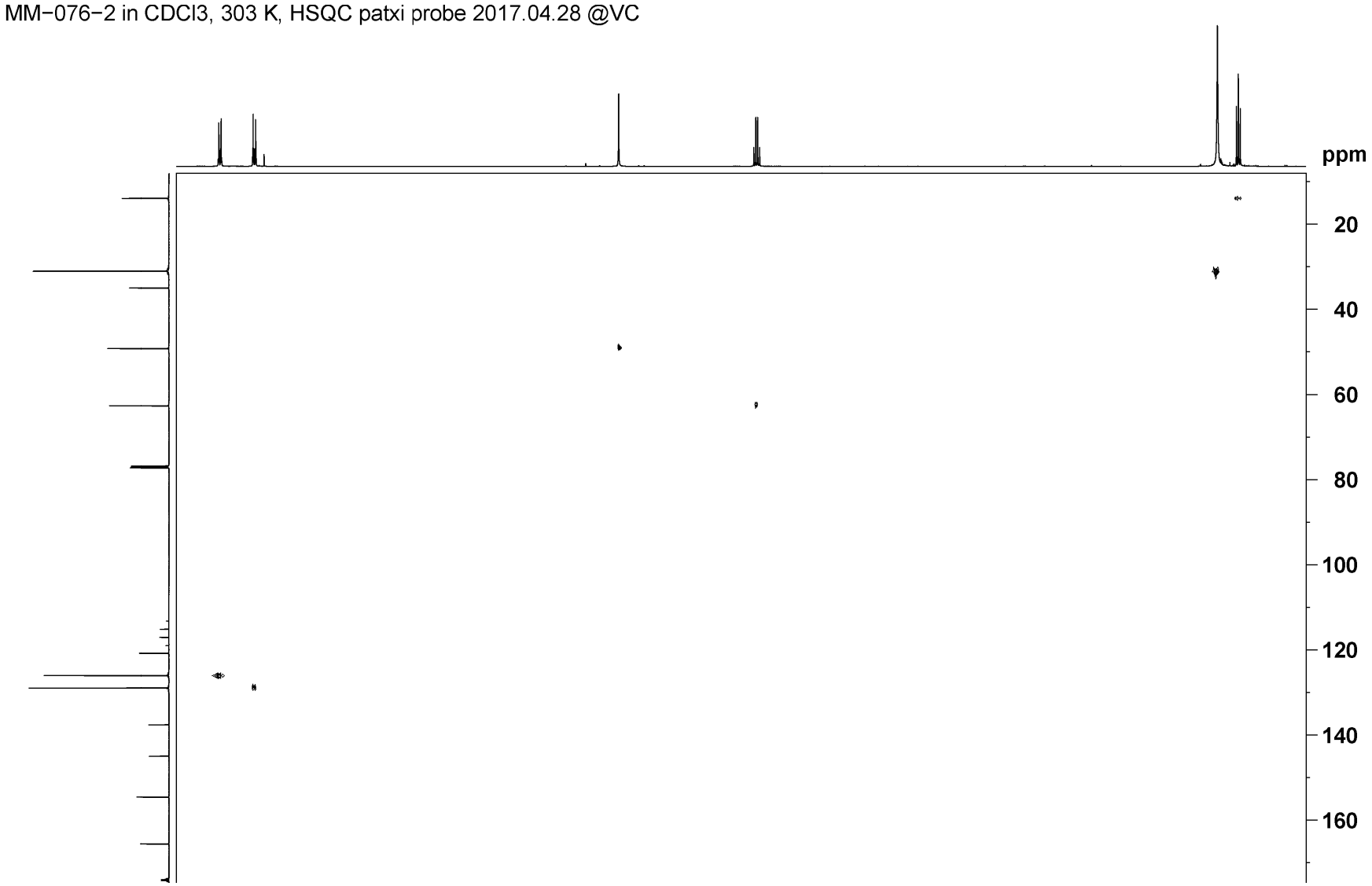


Figure S-5. 2D spectrum NMR HSQC ($CDCL_3$, 303K, “Bruker-AV-600”).

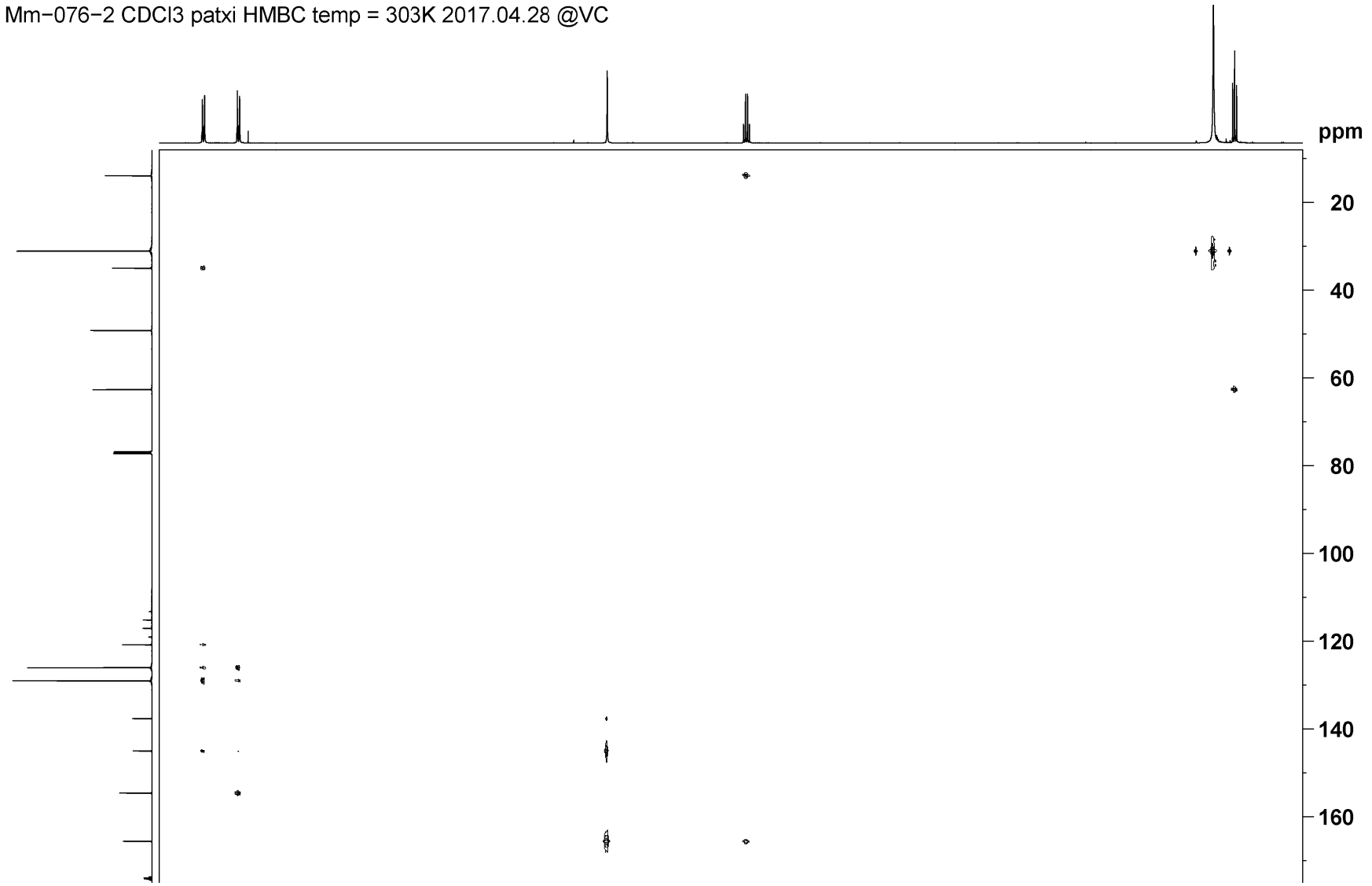


Figure S-6. 2D spectrum NMR HMBC ($CDCL_3$, 303K, “Bruker-AV-600”).