SUPPLEMENTARY

Kragujevac Journal of Science

Electronic Supplementary Information associated with the paper

CYTOTOXIC POTENTIAL OF NOVEL *N*-FORMYL PYRAZOLINES DERIVED FROM VANILLIN

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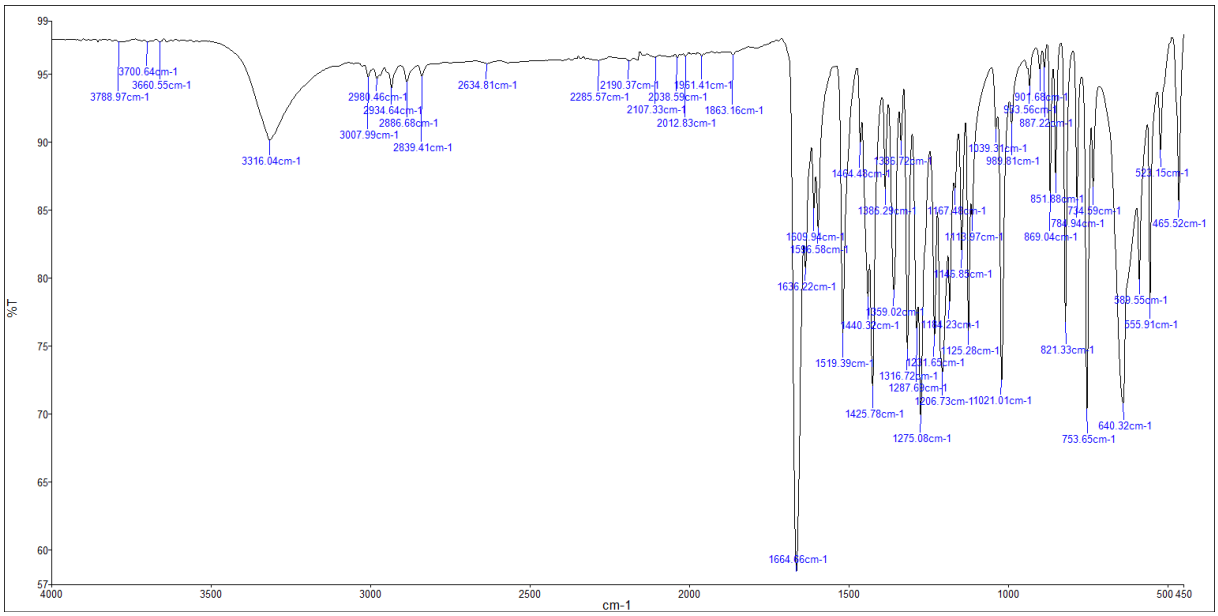
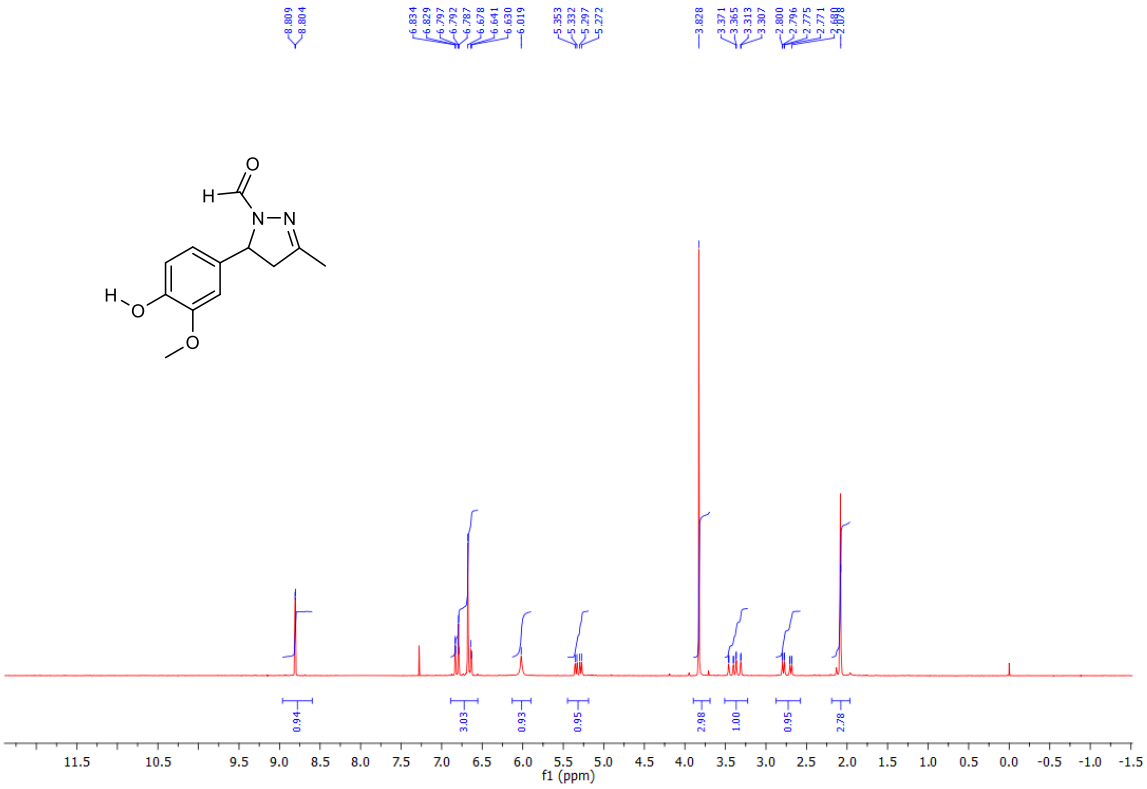
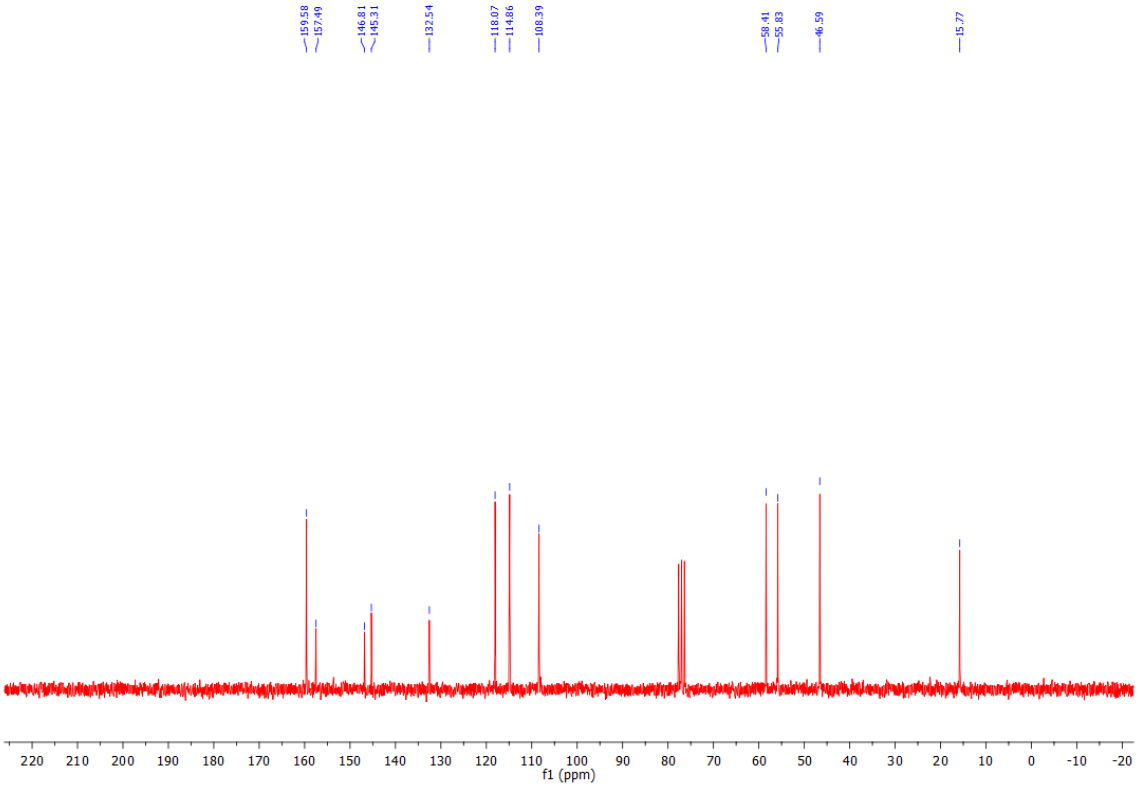
5-(4-Hydroxy-3-methoxyphenyl)-3-methyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde (**3a**)
Light beige powder; yield: 78%; m.p. 129-130°C; IR (KBr, cm^{-1}) ν: 3316, 1664, 1519, 1426, 1317, 1275, 1207, 1021, 821, 754; ^{1}HNMR (200 MHz, $CDCl_3$) δ: 2.08 (*s*, 3H, CH_3), 2.74 (*dd*, 1H, *J*=18.2, 5.0 Hz, $CH_{2pyrazoline}$), 3.38 (*ddq*, 1H, *J*=18.2, 11.5, 1.0 Hz, $CH_{2pyrazoline}$), 3.85 (*s*, 3H, OCH_3), 5.31 (*dd*, 1H, *J*=11.5, 5.0 Hz, $CH_{pyrazoline}$), 6.02 (*bs*, 1H, OH), 6.63-6.68 (*m*, 2H, Ar-H), 6.79-6.83 (*m*, 1H, Ar-H), 8.81 (*d*, 1H, *J*=1.0 Hz, CHO); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 15.8, 46.6, 55.8, 58.4, 108.4, 114.9, 118.1, 133.5, 145.3, 146.8, 157.5, 159.6.



The IR spectrum of compound **3a**



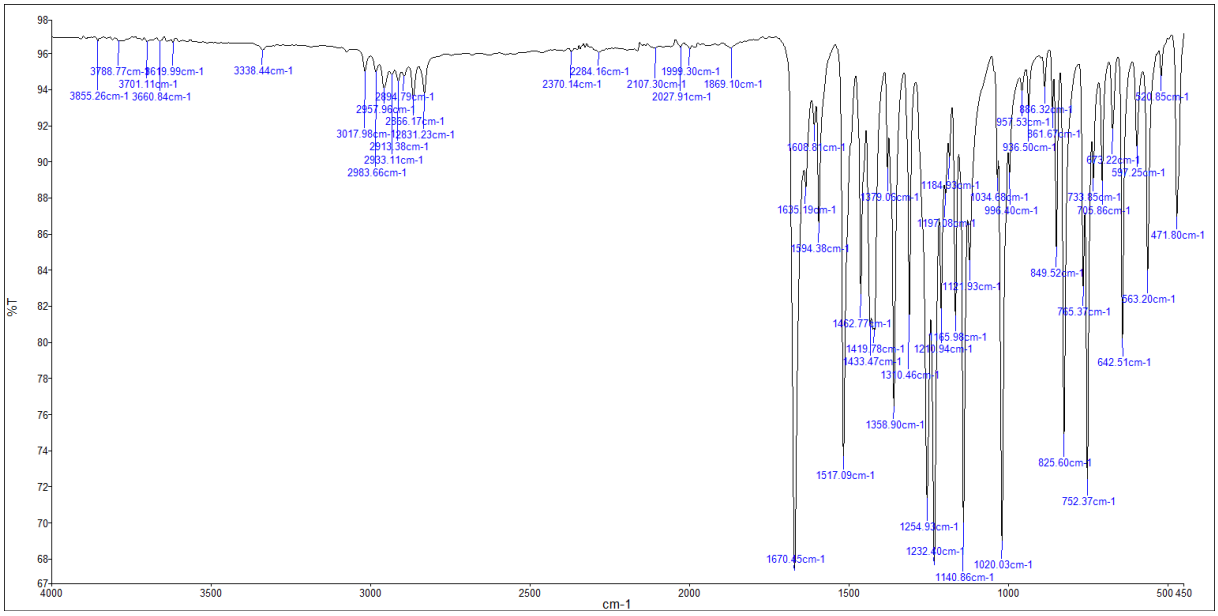
^{1}H NMR spectrum of compound **3a**



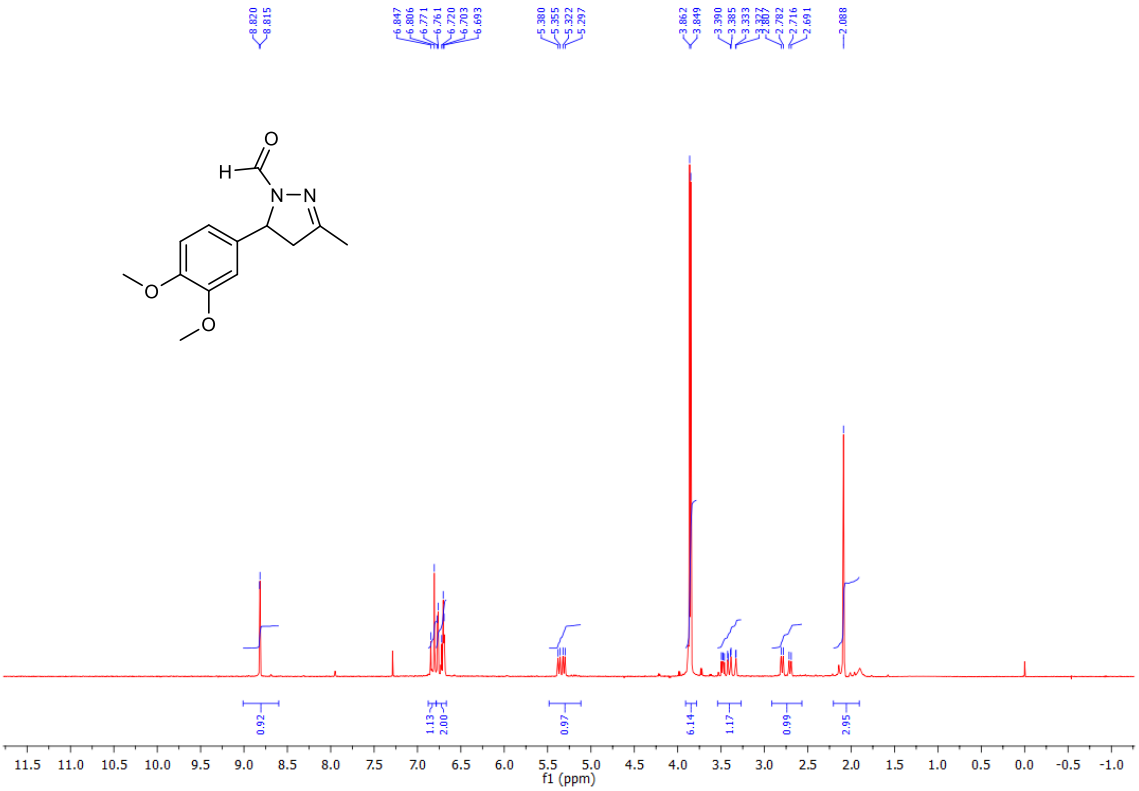
^{13}C NMR spectrum of compound **3a**

5-(3,4-Dimethoxyphenyl)-3-methyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde (**3b**)

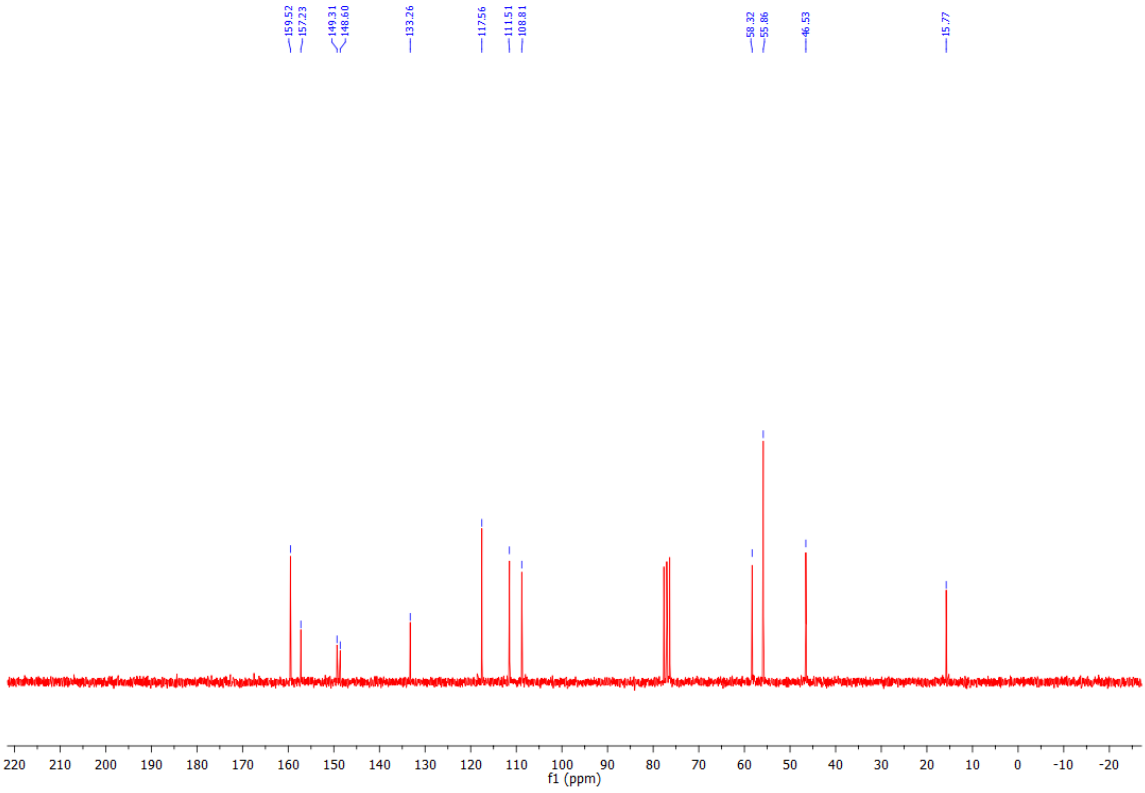
Beige powder; yield: 76%; m.p. 105-106°C; IR (KBr, cm^{-1}) ν: 2983, 1670, 1517, 1433, 1359, 1255, 1232, 1141, 1020, 826, 752; ^{1}HNMR (200 MHz, $CDCl_3$) δ: 2.09 (*s*, 3H, CH_3), 2.75 (*dd*, 1H, *J*=18.2, 5.0 Hz, $CH_{2pyrazoline}$), 3.40 (*dd*, 1H, *J*=18.2, 11.6 Hz, $CH_{2pyrazoline}$), 3.85 (*s*, 3H, OCH_3), 3.86 (*s*, 3H, OCH_3), 5.34 (*dd*, 1H, *J*=11.6, 5.0 Hz, $CH_{pyrazoline}$), 6.69-6.77 (*m*, 2H, Ar-H), 6.83 (*d*, 1H, *J*=8.2 Hz, Ar-H), 8.82 (*d*, 1H, *J*=1.0 Hz, CHO); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 15.8, 46.5, 55.9 (2C), 58.3, 108.8, 111.5, 117.6, 133.3, 148.2, 149.3, 157.2, 159.5.



The IR spectrum of compound **3b**

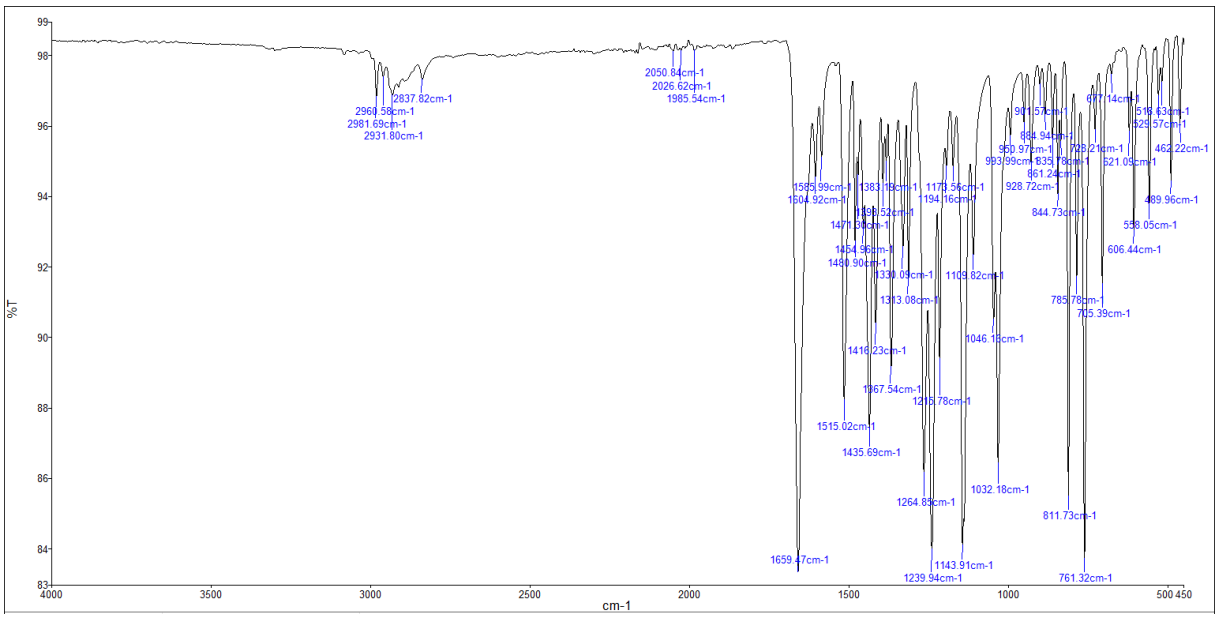


^{1}H NMR spectrum of compound **3b**

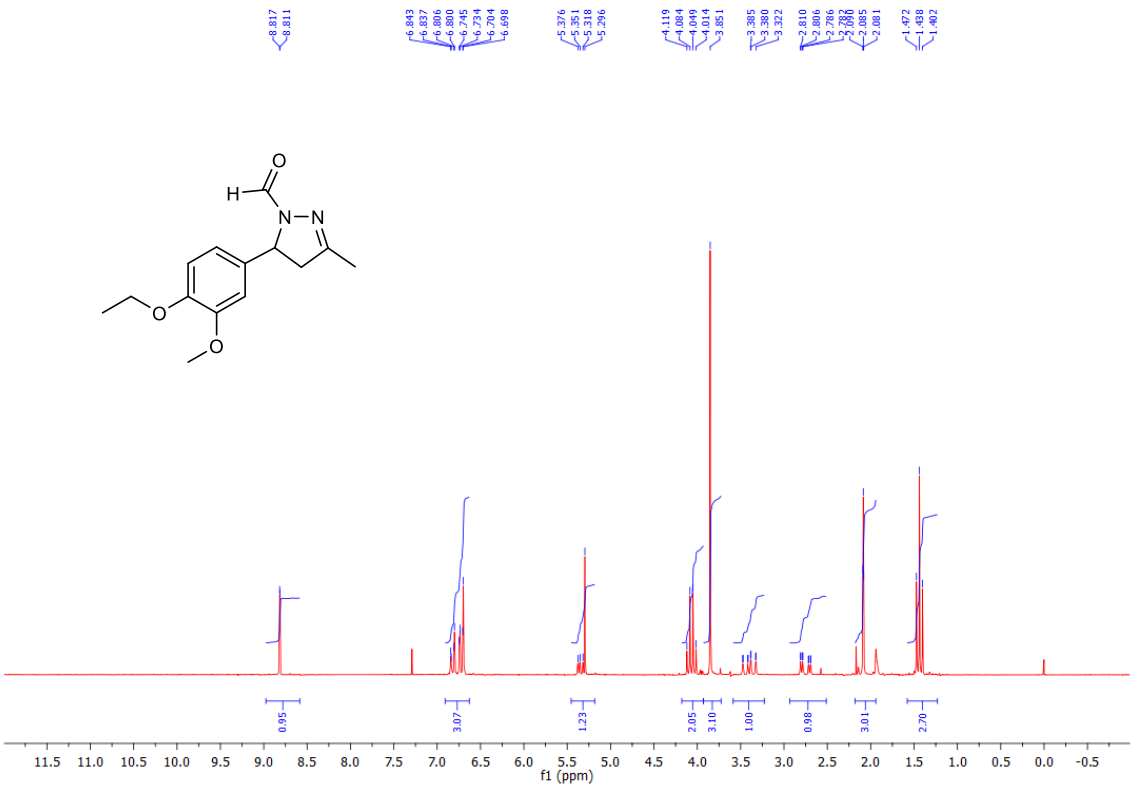


^{13}C NMR spectrum of compound **3b**

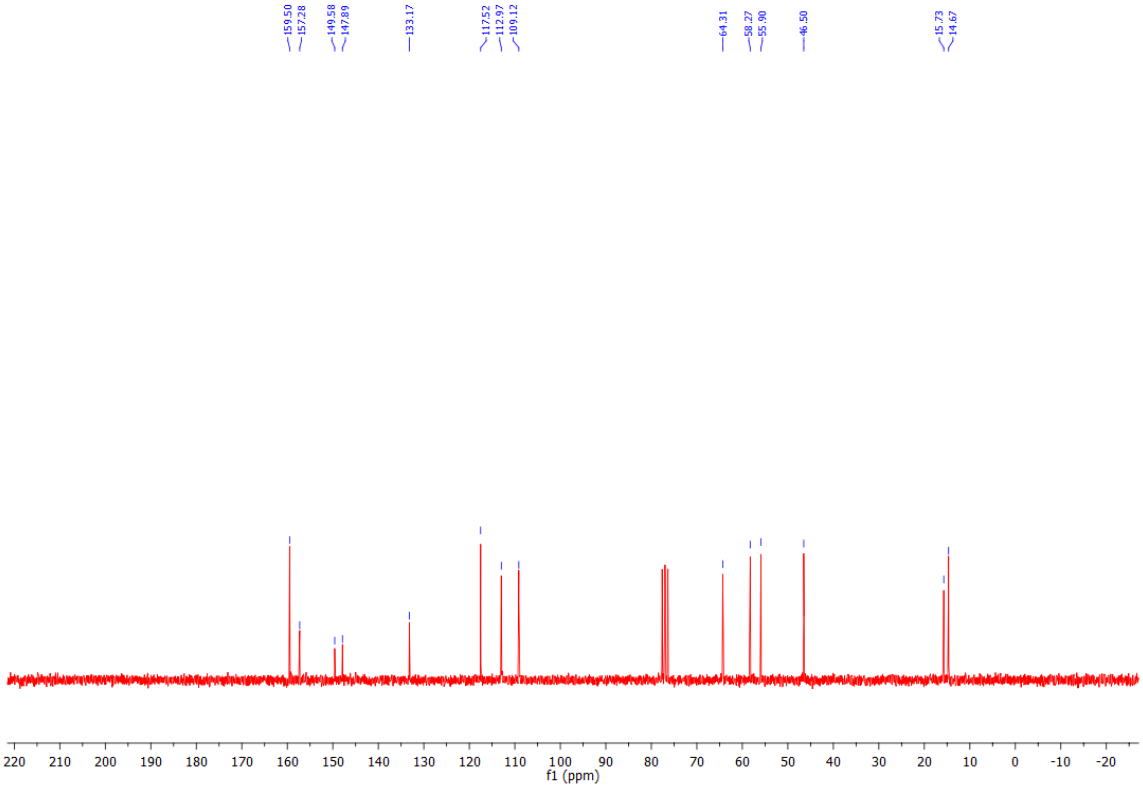
5-(4-Ethoxy-3-methoxyphenyl)-3-methyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde (**3c**)
Cream powder; yield: 82%; m.p. 73-74°C; IR (KBr, cm^{-1}) ν: 2931, 1659, 1515, 1435, 1265, 1239, 1143, 1032, 812, 761; ^{1}HNMR (200 MHz, $CDCl_3$) δ: 1.44 (*t*, 3H, *J*=7.0 Hz, CH_3), 2.08 (*t*, 3H, *J*=1.0 Hz, CH_3), 2.75 (*ddq*, 1H, *J*=18.2, 4.8, 1.0 Hz, $CH_{2pyrazoline}$), 3.40 (*ddq*, 1H, *J*=18.2, 11.6, 1.0 Hz, $CH_{2pyrazoline}$), 3.85 (*s*, 3H, OCH_3), 4.07 (*q*, 2H, *J*=7.0 Hz, CH_2), 5.34 (*ddd*, 1H, *J*=11.6, 4.8, 1.0 Hz, $CH_{pyrazoline}$), 6.69-6.84 (*m*, 3H, Ar-H), 8.81 (*d*, 1H, *J*=1.0 Hz, CHO); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 14.7, 15.7, 46.5, 55.9, 58.3, 64.3, 109.1, 112.9, 117.5, 133.2, 147.9, 149.6, 157.3, 159.5.



The IR spectrum of compound **3c**

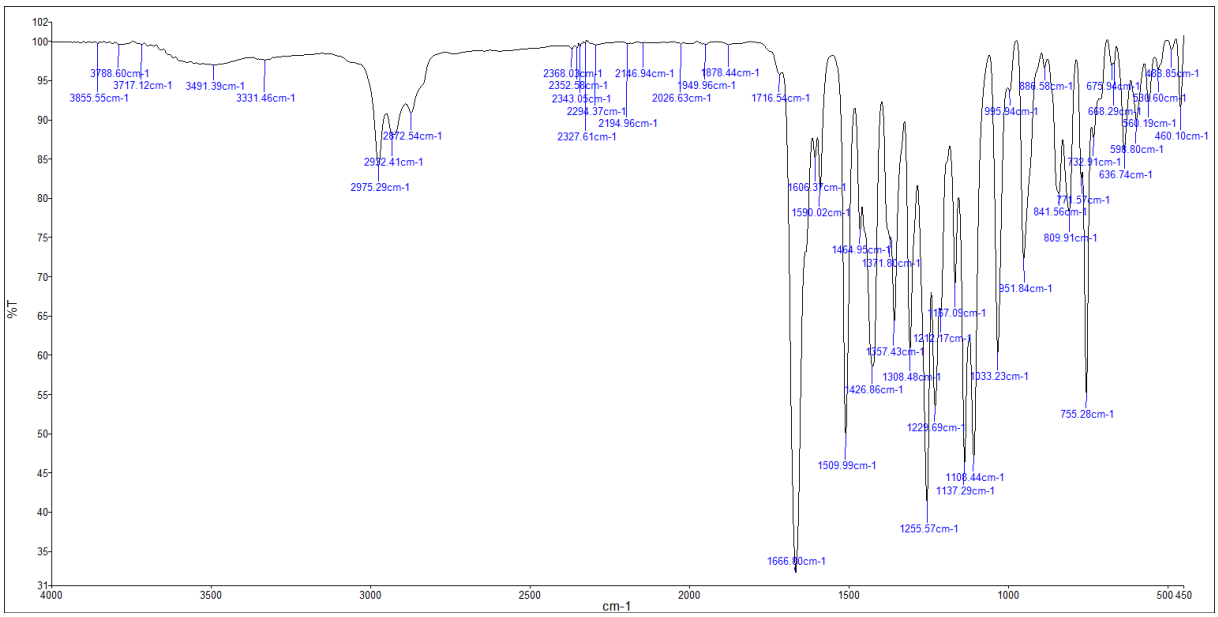


^{1}H NMR spectrum of compound **3c**

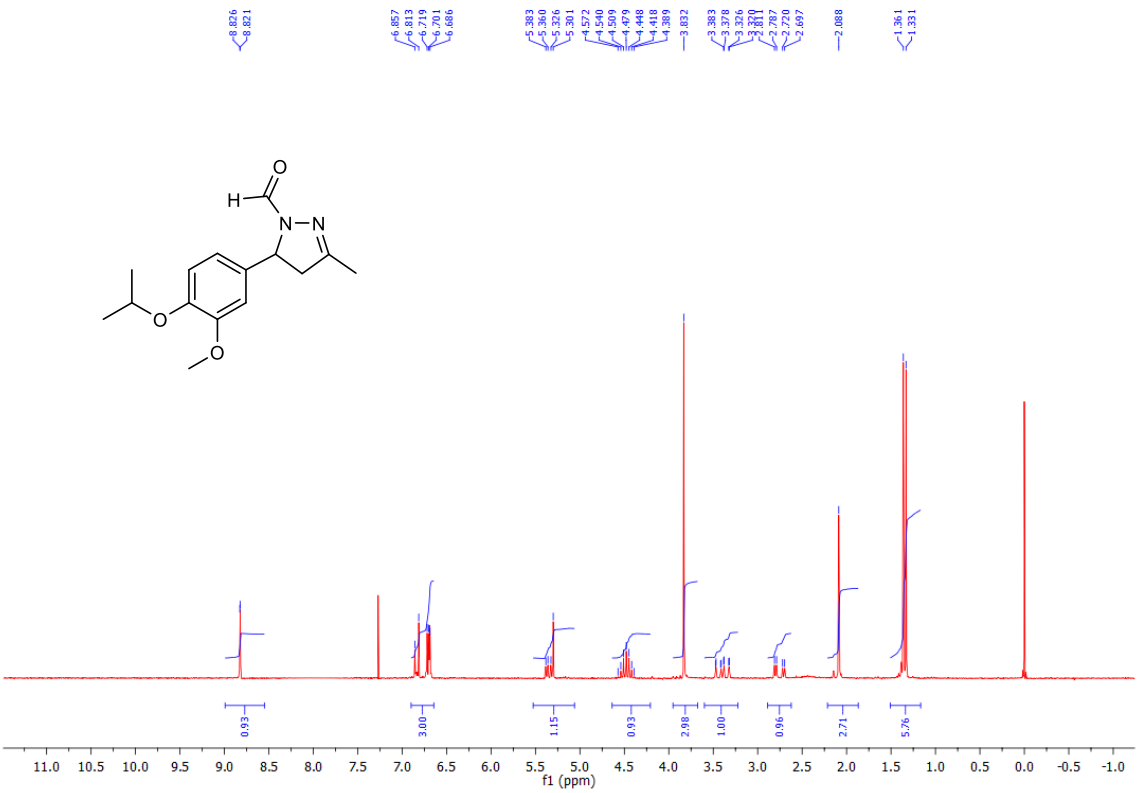


^{13}C NMR spectrum of compound **3c**

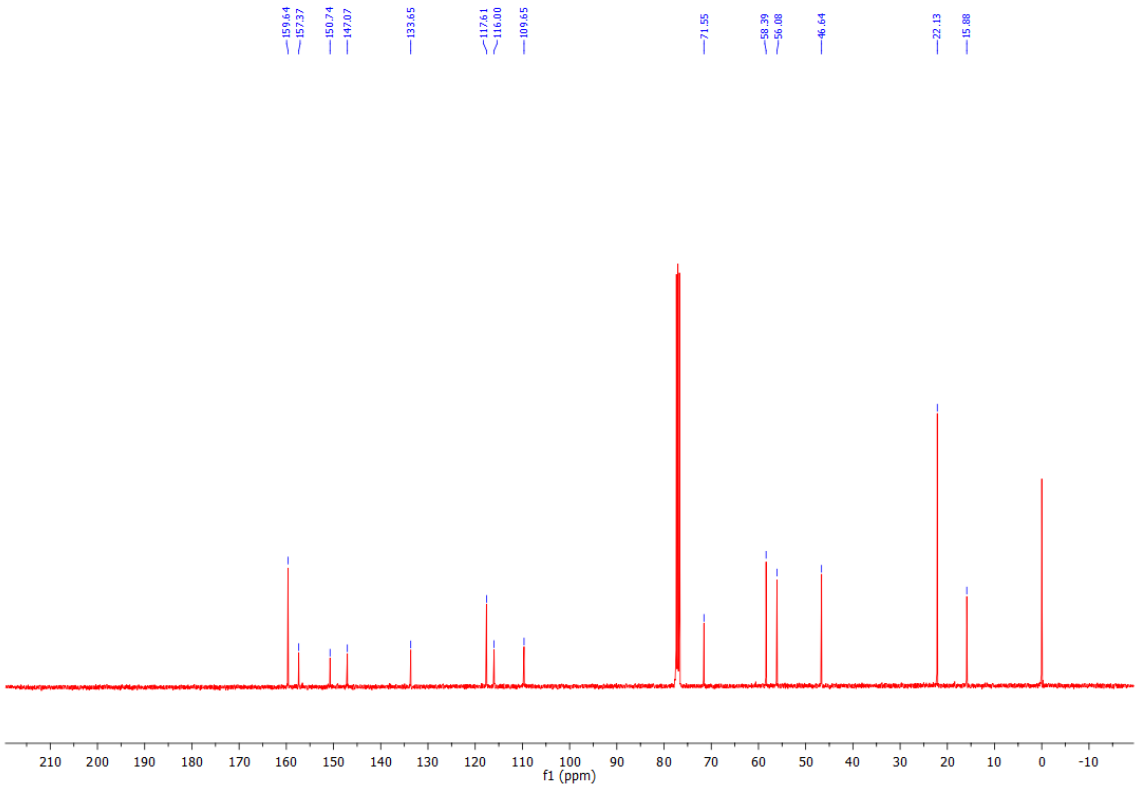
5-(4-Isopropoxy-3-methoxyphenyl)-3-methyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde (**3d**)
Red-orange oil; yield: 82%; IR (KBr, cm^{-1}) ν: 2975, 1666, 1510, 1427, 1309, 1229, 1256, 1137, 1108, 1033, 755; ^{1}HNMR (200 MHz, $CDCl_3$) δ: 1.34 (*d*, 6H, *J*=6.0 Hz, $CH(\underline{CH_3})_2$), 2.08 (*s*, 3H, CH_3), 2.75 (*dd*, 1H, *J*=18.4, 4.8 Hz, $CH_{2pyrazoline}$), 3.38 (*dd*, 1H, *J*=18.0, 11.6 Hz, $CH_{2pyrazoline}$), 3.83 (*s*, 3H, OCH_3), 4.48 (*sep*, 1H, *J*=6.2 Hz, $\underline{CH}(CH_3)_2$), 5.34 (*dd*, 1H, *J*=11.8, 5.0 Hz, $CH_{pyrazoline}$), 6.69-6.72 (*m*, 2H, Ar-H), 6.83 (*d*, 1H, *J*=8.8 Hz, Ar-H), 8.82 (*d*, 1H, *J*=1.0 Hz, CHO); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 15.9, 22.1, 46.6, 56.1, 58.4, 71.5, 109.6, 116, 117.6, 133.6, 147.1, 150.7, 157.4, 159.6.



The IR spectrum of compound **3d**

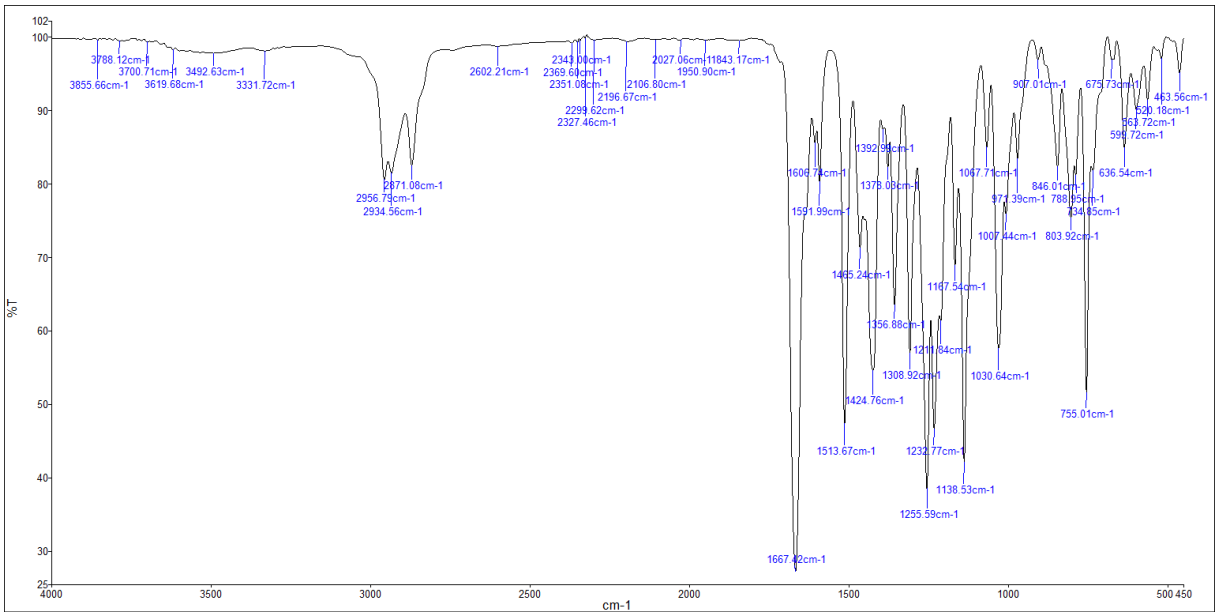


^{1}H NMR spectrum of compound **3d**

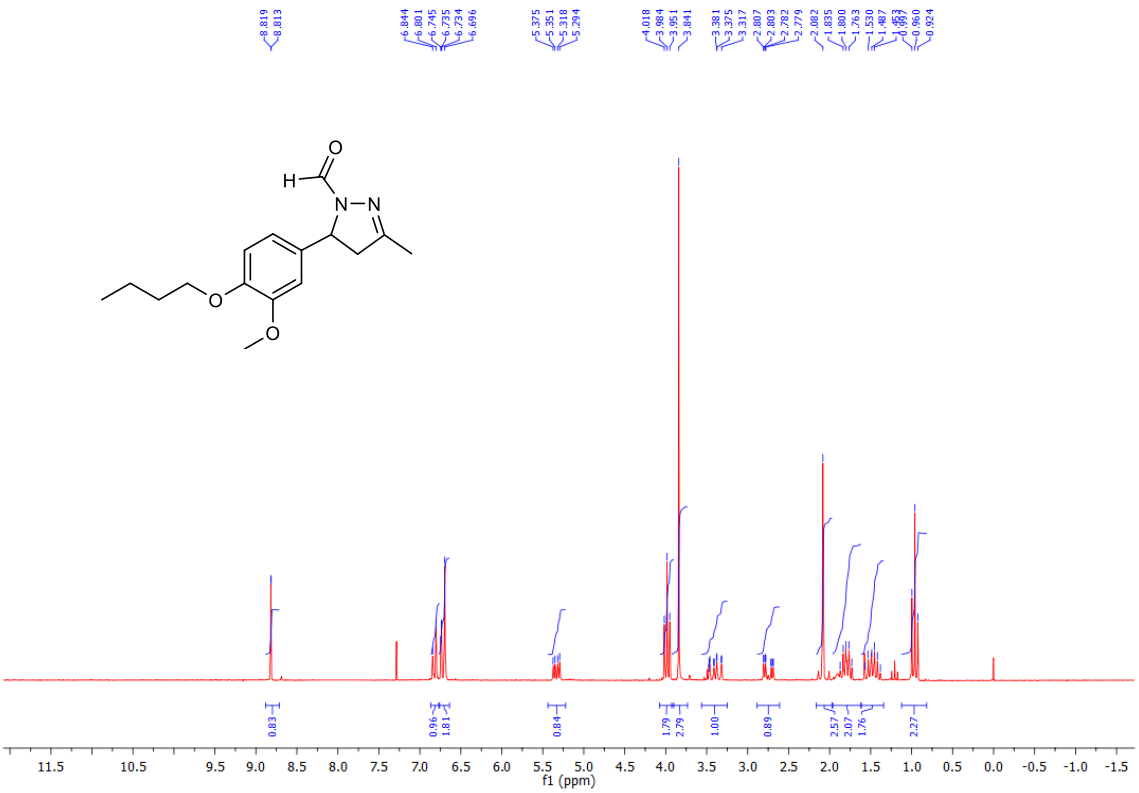


^{13}C NMR spectrum of compound **3d**

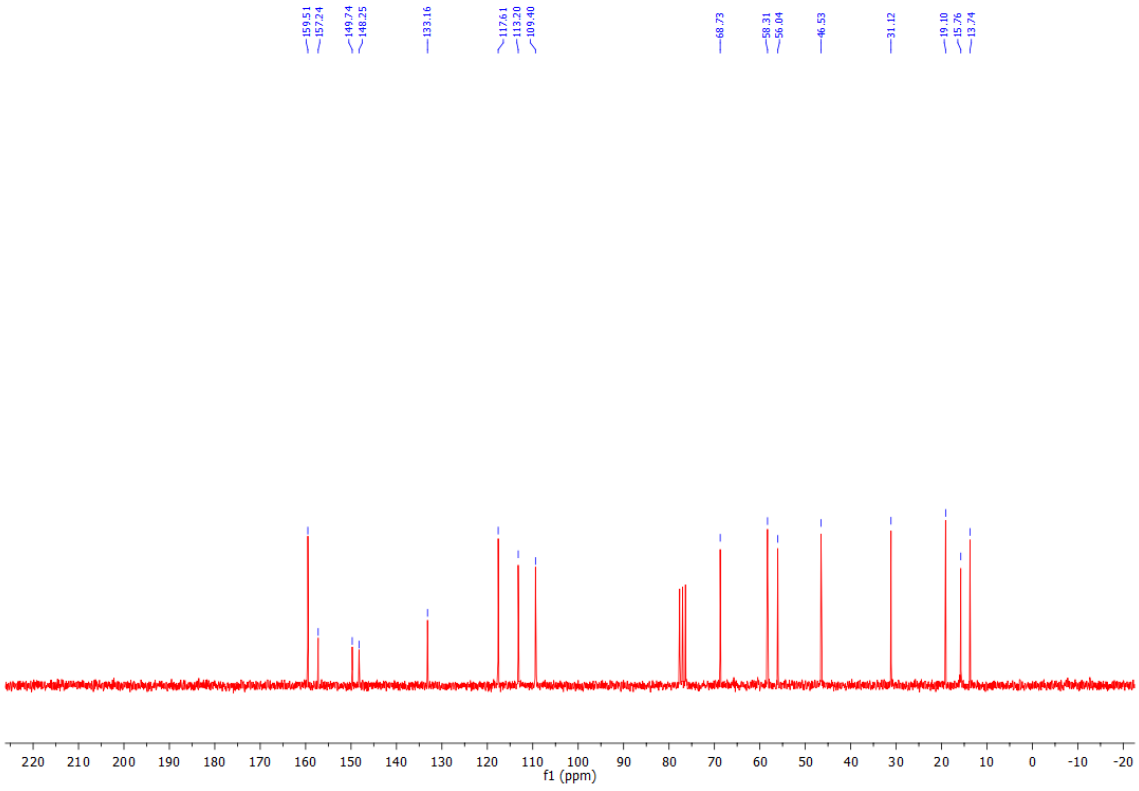
5-(4-Butoxy-3-methoxyphenyl)-3-methyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde **(3e)**
Red-orange oil; yield: 93%; IR (KBr, cm^{-1}) ν: 2934, 1667, 1514, 1425, 1309, 1233, 1256, 1138, 1030, 755; ^{1}HNMR (200 MHz, $CDCl_3$) δ: 0.96 (*t*, 3H, *J*=7.2 Hz, CH_3), 1.38-1.57 (*m,* 2H, CH_2), 1.73-1.87 (*m,* 2H, CH_2), 2.08 (*s*, 3H, CH_3), 2.75 (*dd*, 1H, *J*=18.2, 4.8 Hz, $CH_{2pyrazoline}$), 3.39 (*dd*, 1H, *J*=18.2, 11.5 Hz, $CH_{2pyrazoline}$), 3.84 (*s*, 3H, OCH_3), 3.98 (*t*, 2H, *J*=6.6 Hz, CH_2), 5.34 (*dd*, 1H, *J*=11.5, 4.8 Hz, $CH_{pyrazoline}$), 6.69-6.74 (*m*, 2H, Ar-H), 6.82 (*d*, 1H, *J*=8.6 Hz, Ar-H), 8.82 (*d*, 1H, *J*=1.0 Hz, CHO); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 13.7, 15.8, 19.1, 31.1, 46.5, 56.0, 58.3, 68.7, 109.4, 113.2, 117.6, 133.2, 148.2, 149.7, 157.2, 159.5.



The IR spectrum of compound **3e**



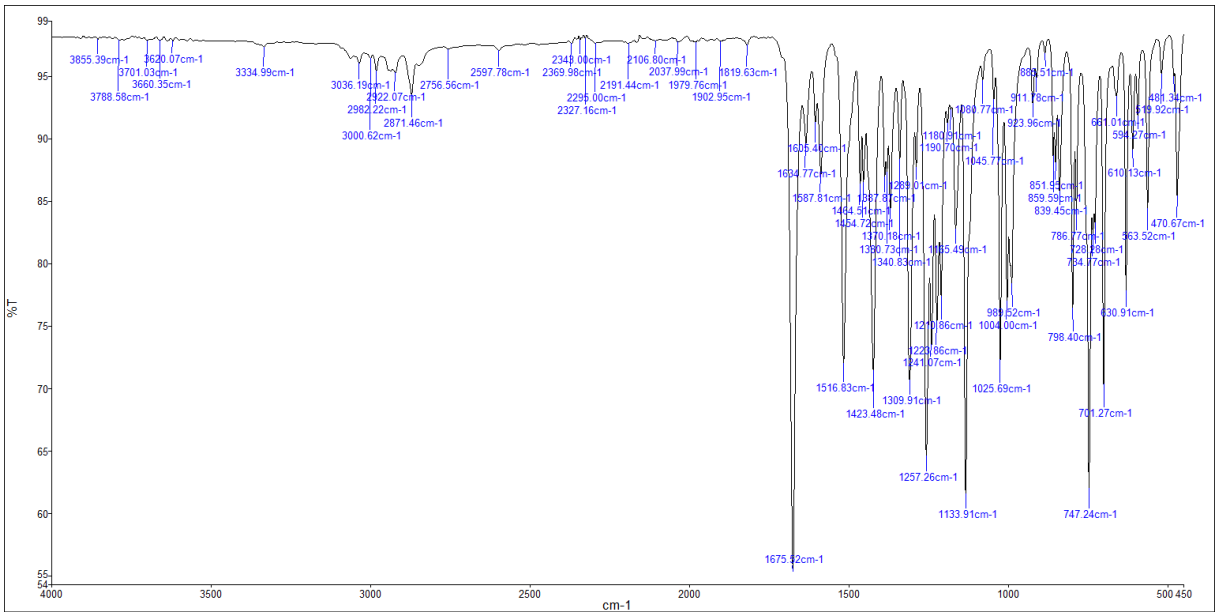
^{1}H NMR spectrum of compound **3e**



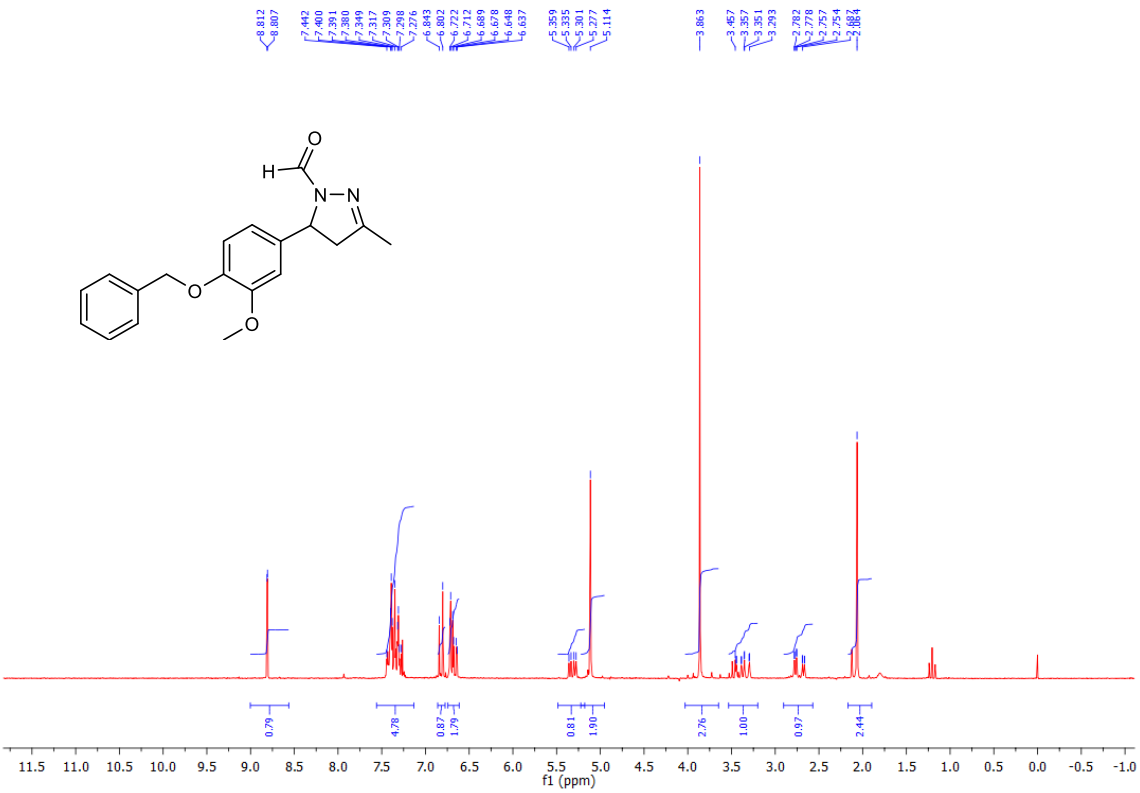
^{13}C NMR spectrum of compound **3e**

5-(4-(Benzyloxy)-3-methoxyphenyl)-3-methyl-4,5-dihydro-1*H*-pyrazole-1-carbaldehyde (3f)

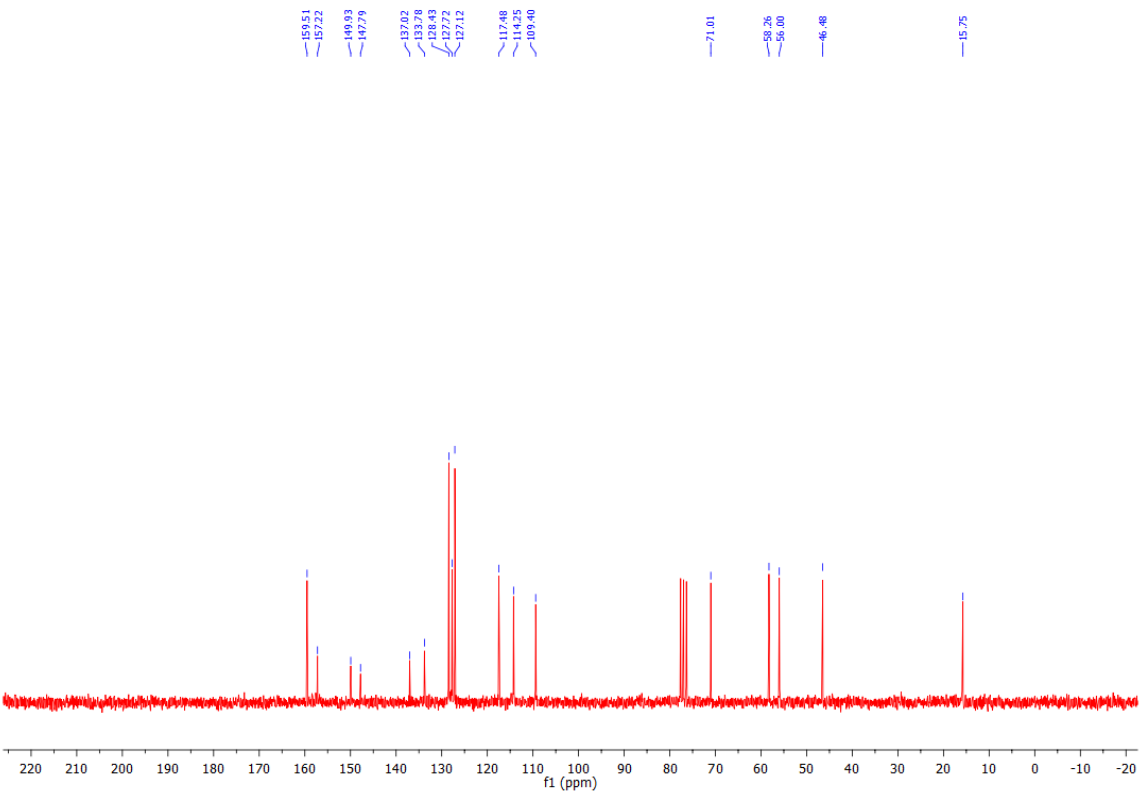
Cream powder; yield: 93%; m.p. 79-80°C; IR (KBr, cm^{-1}) ν: 3000, 2327, 1675, 1516, 1423, 1310, 1257, 1134, 1025, 798, 747; ^{1}HNMR (200 MHz, $CDCl_3$) δ: 2.06 (*s*, 3H, CH_3), 2.72 (*dd*, 1H, *J*=18.2, 4.8 Hz, $CH_{2pyrazoline}$), 3.37 (*dd*, 1H, *J*=18.2, 11.5 Hz, $CH_{2pyrazoline}$), 3.86 (*s*, 3H, OCH_3), 5.11 (*s*, 2H, CH_2), 5.32 (*dd*, 1H, *J*=11.5, 4.8 Hz, $CH_{pyrazoline}$), 6.64-6.72 (*m*, 2H, Ar-H), 6.82 (*d*, 1H, *J*=8.2 Hz, Ar-H), 7.28-7.44 (*m*, 5H, Ar-H), 8.81 (*d*, 1H, *J*=1.0 Hz, CHO); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 15.8, 46.5, 56.0, 58.3, 71.0, 109.4, 114.2, 117.5, 127.1 (2C), 127.7, 128.4 (2C), 133.8, 137.0, 147.8, 149.9, 157.2, 159.5.



The IR spectrum of compound **3f**



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



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