

Potential anti-bacterial agents: Montmorillonite Clay catalyzed synthesis of novel 2-(3, 5-substituted-1*H*-pyrazol-1-yl)-3-substituted quinolones and their in-silico molecular docking studies

Pasupala Pavan, R. Subashini*, K. R. Ethiraj and Fazlur-Rahman Nawaz Khan*

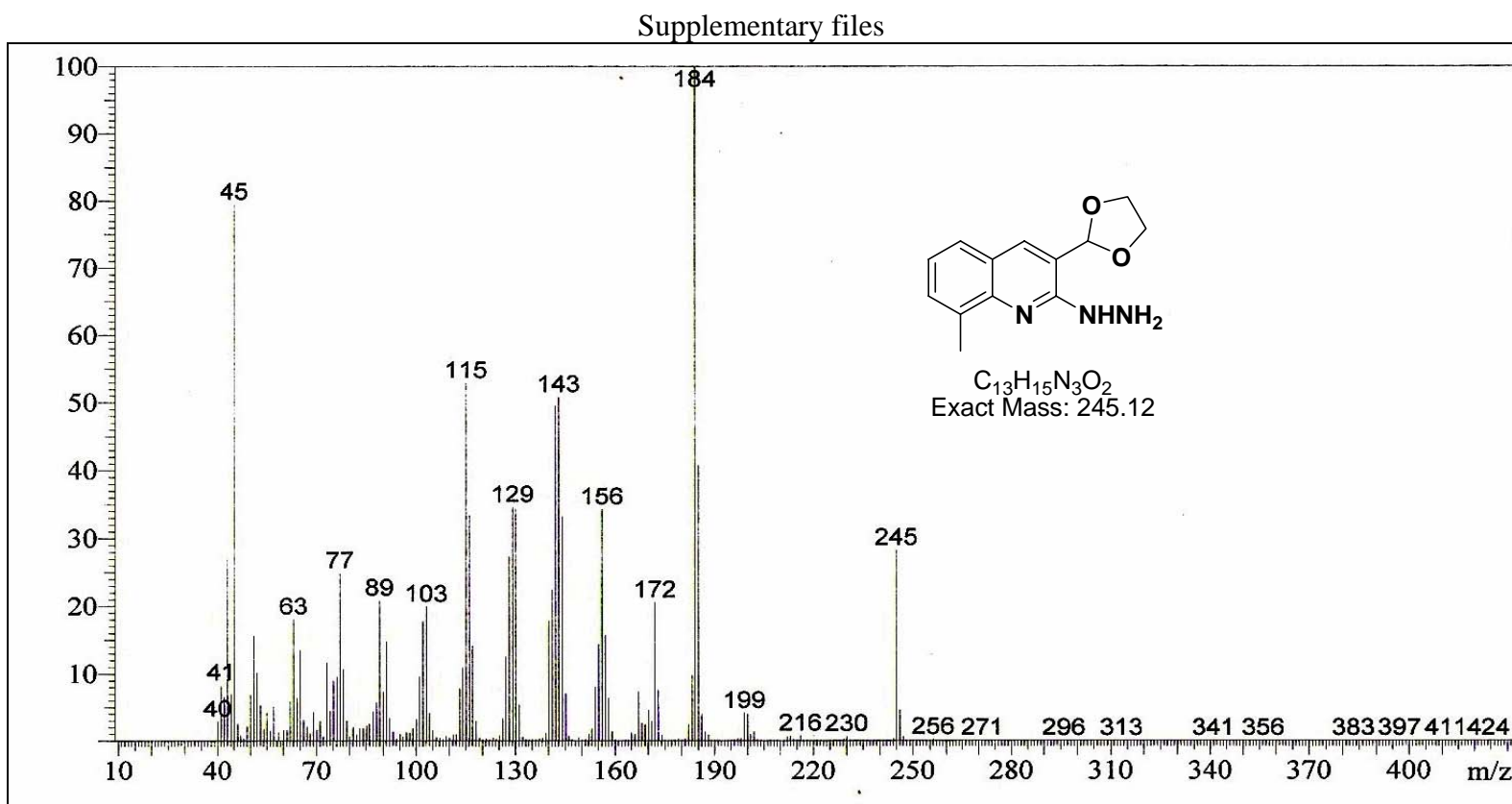
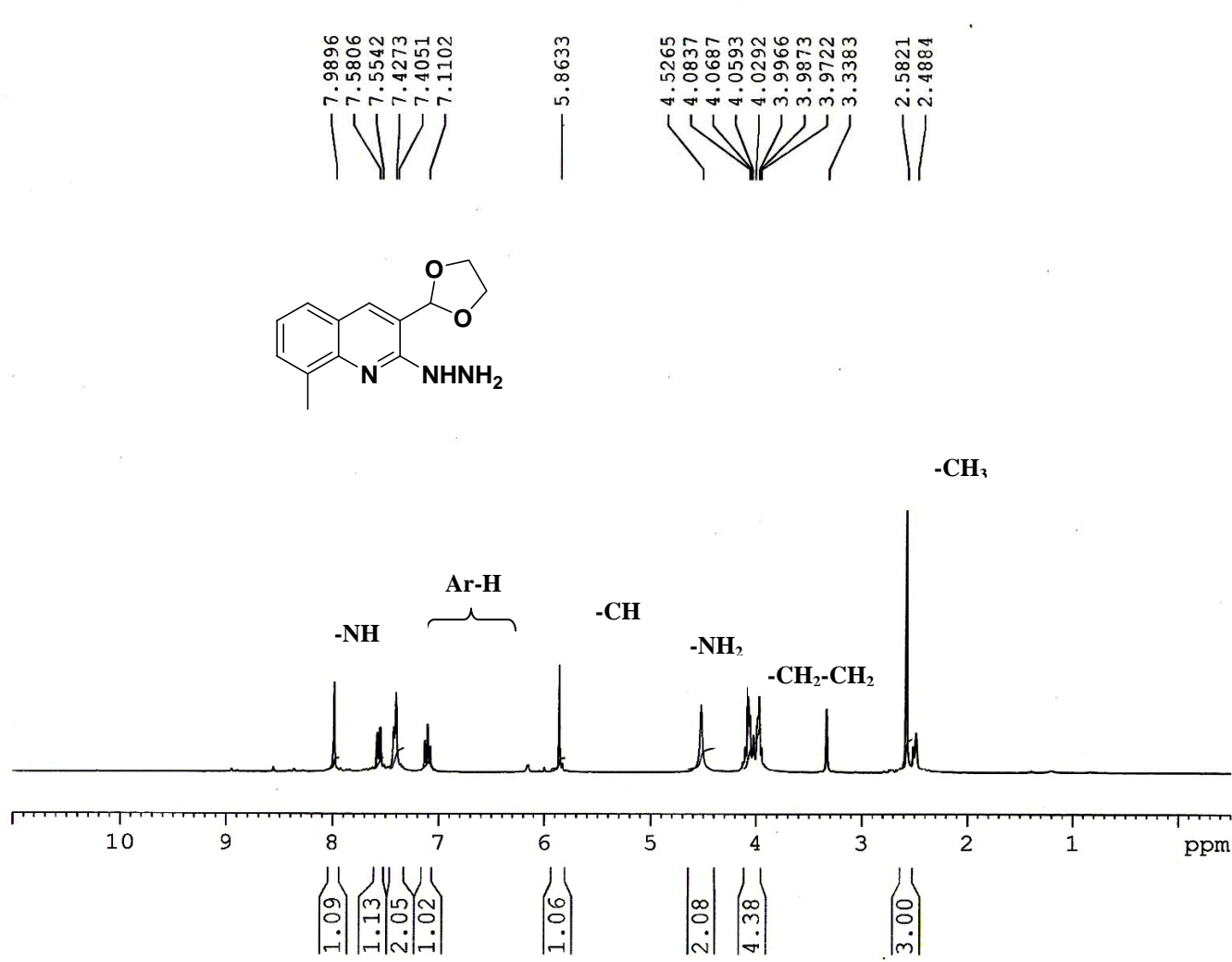


Fig. 1: GC-MS spectrum of 1-(3-(1,3-dioxolan-2-yl)-8-methylquinolin-2-yl)hydrazine, **2e**



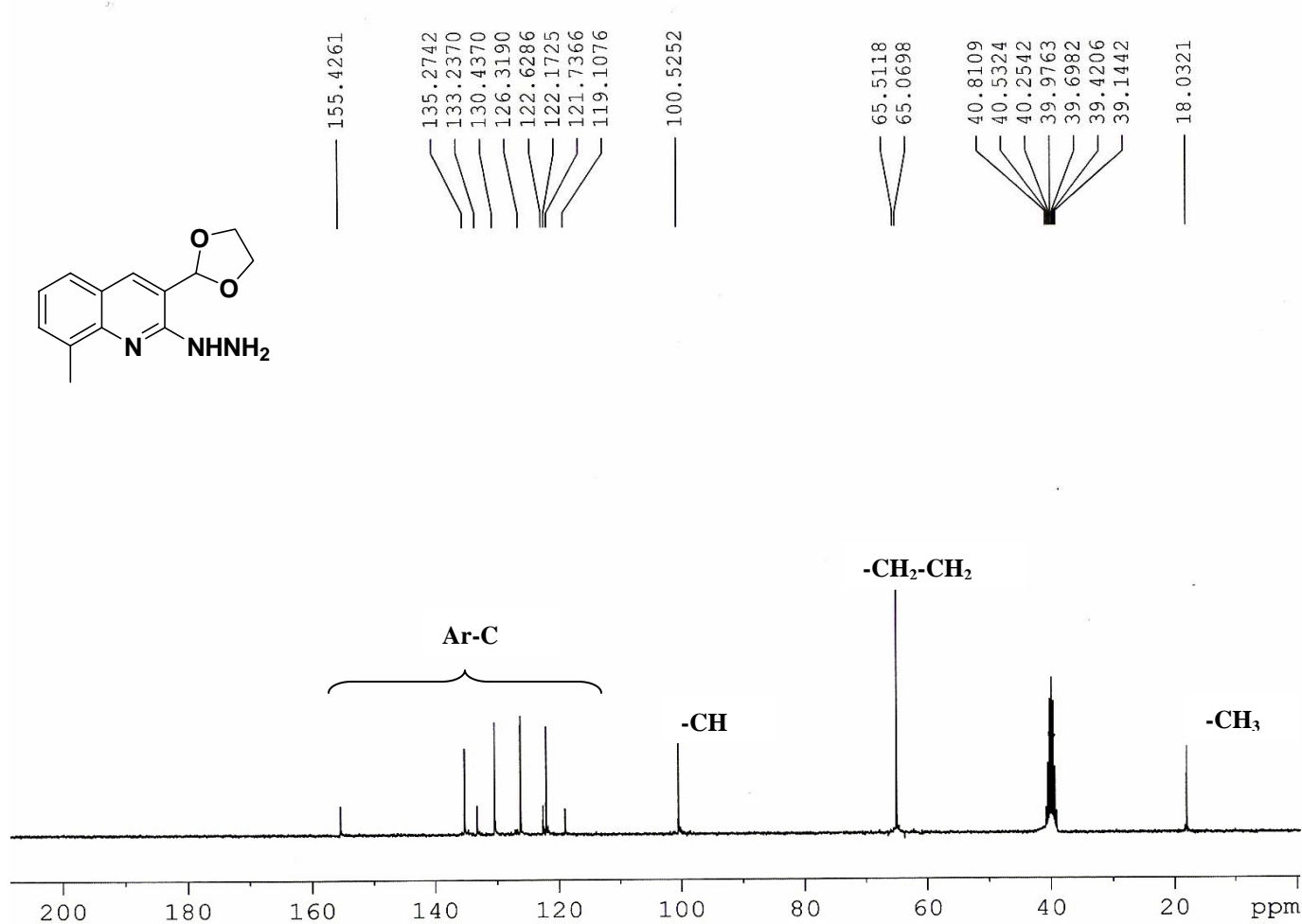
Current Data Parameters
 NAME GI821553-8107010
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080528
 Time_ 20.46
 INSTRUM spect
 PROBHD 5 mm DUL BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.219235 Hz
 AQ 2.2807028 sec
 RG 362
 DW 69.600 usec
 DE 6.00 usec
 TE 0.0 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL1 0.00 dB
 SFO1 300.1327012 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300044 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40

Fig. 2: ¹H NMR spectrum of 1-(3-(1,3-dioxolan-2-yl)-8-methylquinolin-2-yl)hydrazine, **2e**



Current Data Parameters
 NAME GI821553-8107010
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080528
 Time 22.03
 INSTRUM spect
 PROBHD 5 mm DUL BB-1H
 PULPROG zgpg
 TD 32768
 SOLVENT DMSO
 NS 2000
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 90.5
 DW 27.600 usec
 DE 6.00 usec
 TE 0.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.75 usec
 PL1 0.00 dB
 SFO1 75.4752958 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 17.81 dB
 PL13 18.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 131072
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 2.00

Fig. 3: ¹³C NMR spectrum of 1-(3-(1,3-dioxolan-2-yl)-8-methylquinolin-2-yl)hydrazine, **2e**

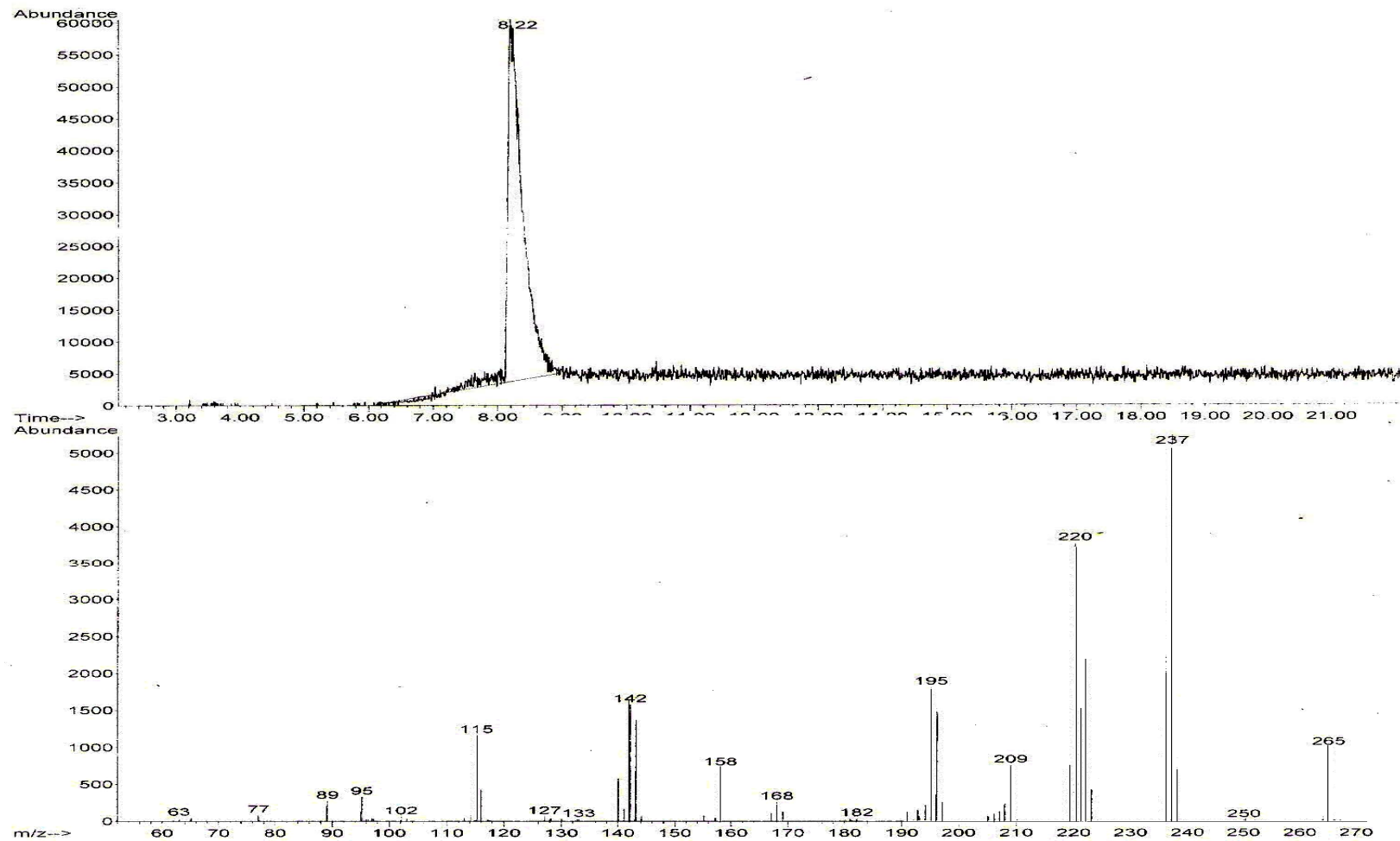
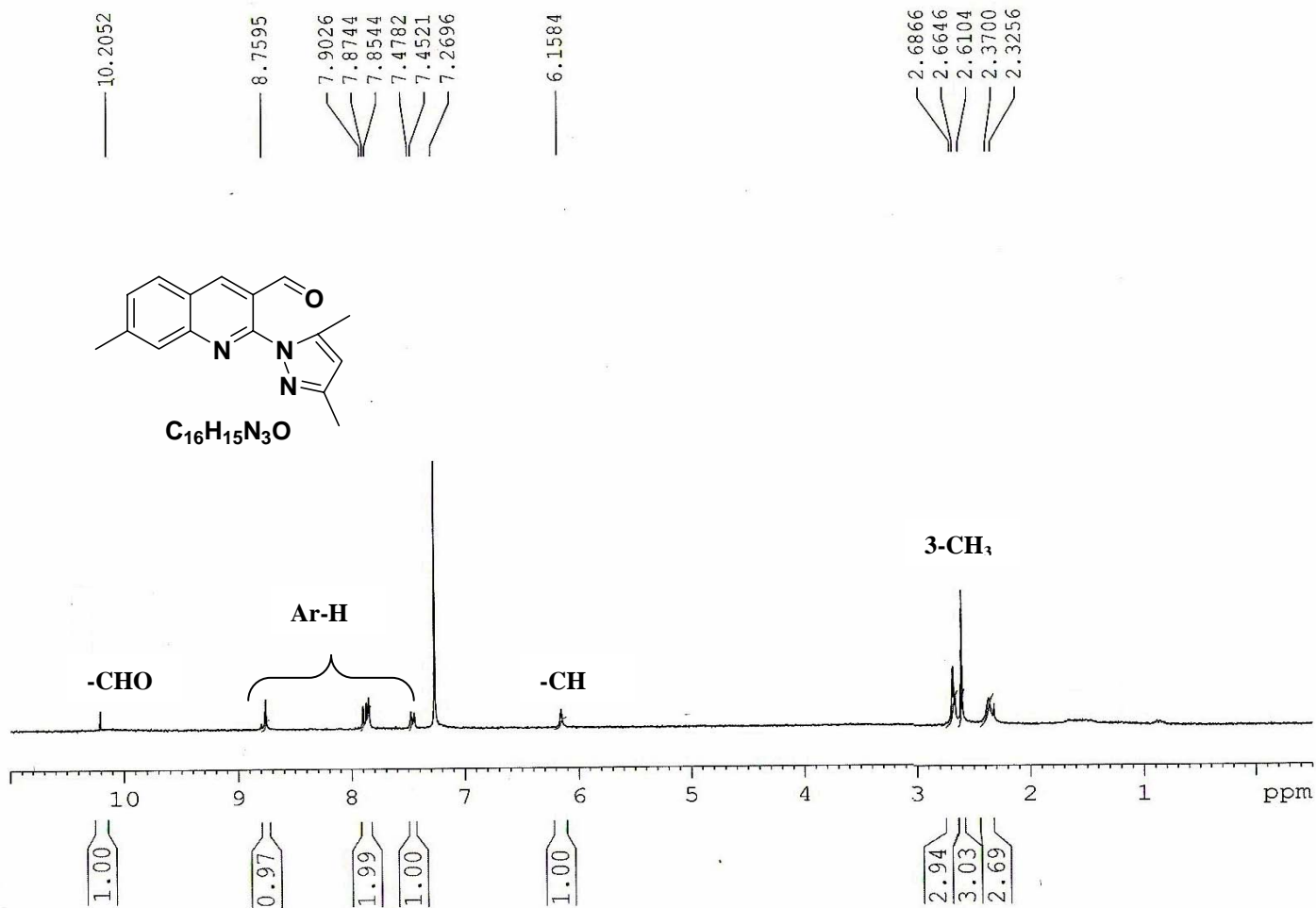


Fig. 4: GC-MS spectrum of 2-pyrazoloquinoline-3-carbaldehyde, 4



Current Data Parameters
 NAME GI800234-8038742
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080225
 Time 21.00
 INSTRUM spect
 PROBHD 5 mm DUL BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.219235 Hz
 AQ 2.2807028 sec
 RG 812.7
 DW 69.600 usec
 DE 6.00 usec
 TE 0.0 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL1 0.00 dB
 SFO1 300.1327012 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1298168 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.40

Fig. 5: ¹H-NMR spectrum of 2-pyrazoloquinoline-3-carbaldehyde, 4

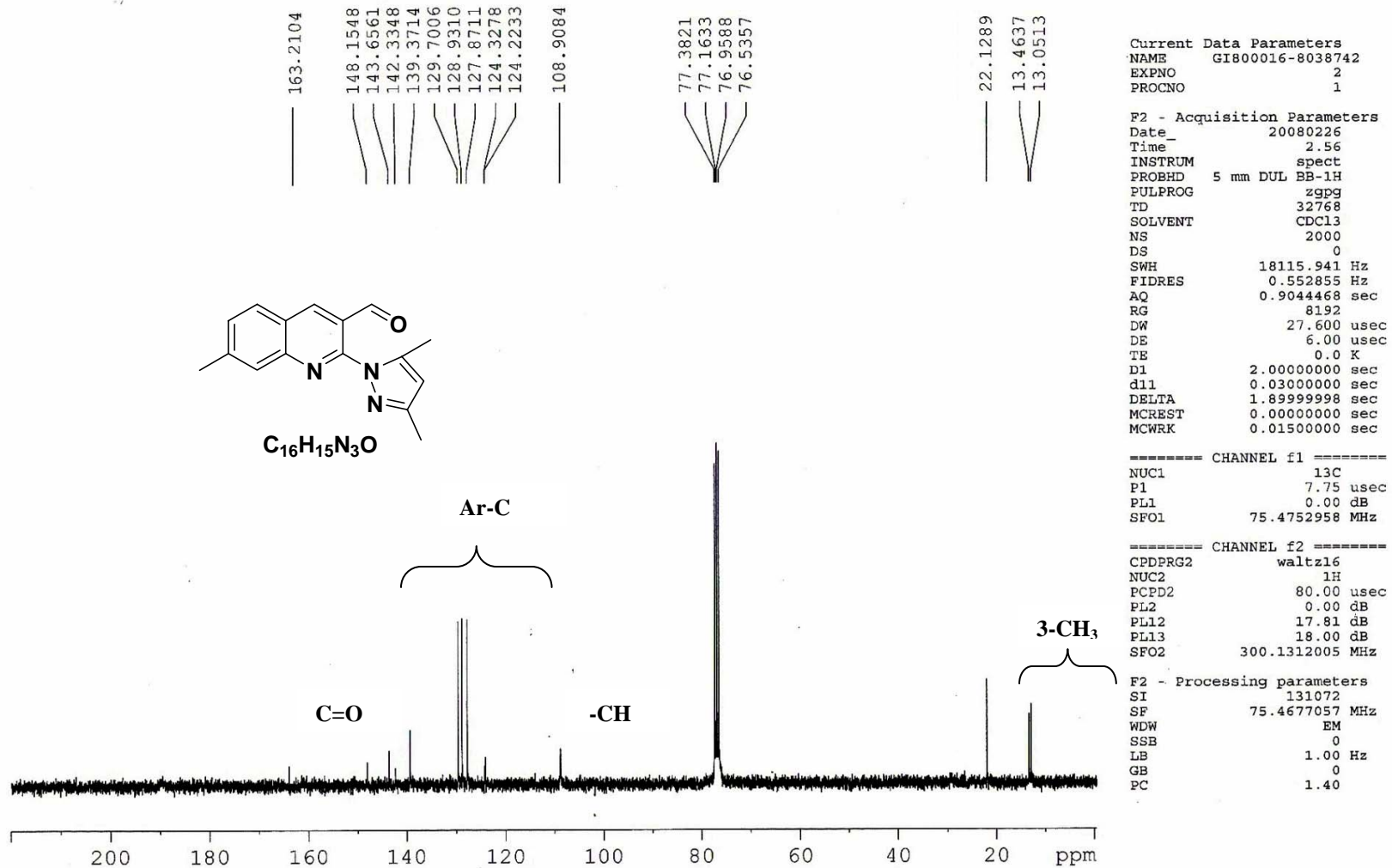
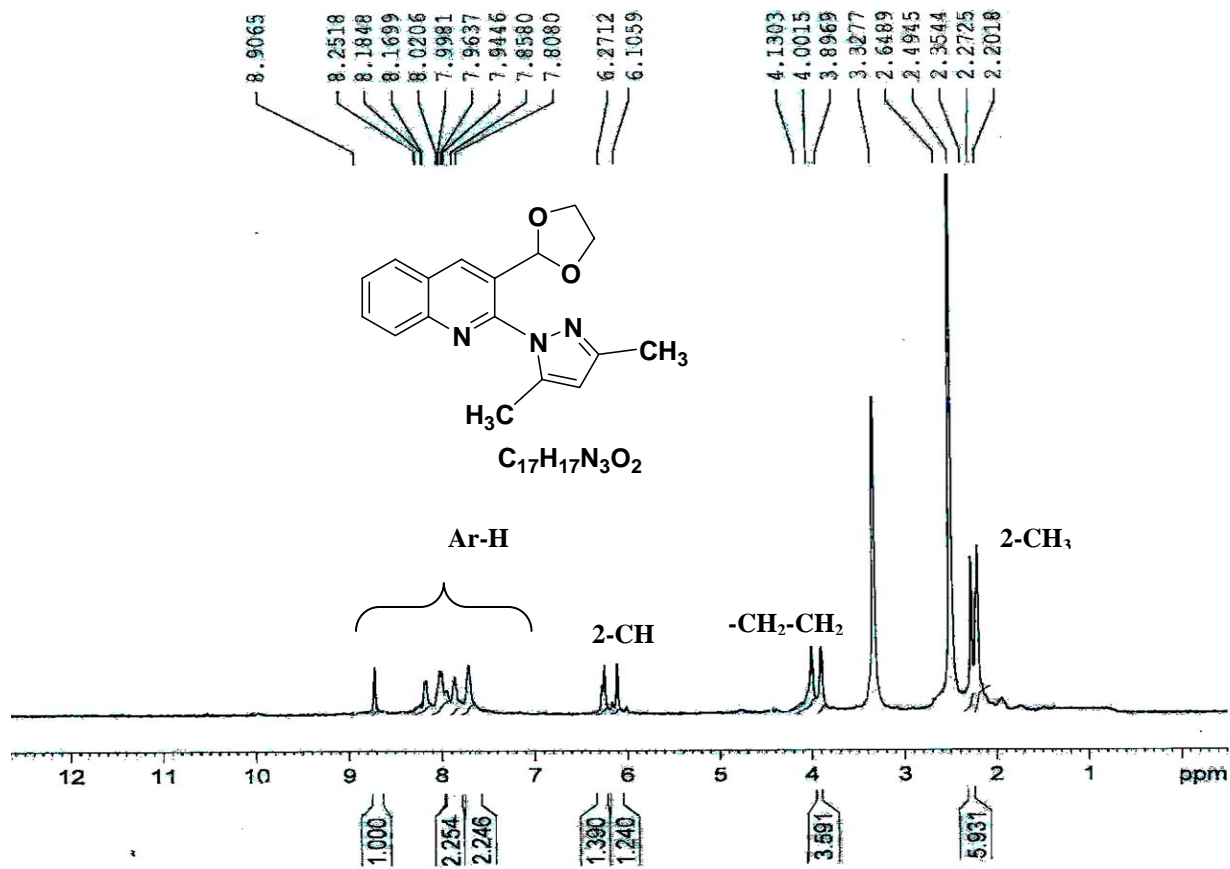


Fig. 6: ¹³C-NMR spectrum of 2-pyrazoloquinoline-3-carbaldehyde, **4**



Current Data Parameters
 NAME SS081_GI929792-9151065-3
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090619
 Time 20.23
 INSTRUM spect
 PROBRD 5 mm PABBO RB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 9615.385 Hz
 FIDRES 0.293438 Hz
 AQ 1.7039869 sec
 RG 645
 DW 52.000 usec
 DE 6.00 usec
 TE 295.2 K
 EI 2.00000000 sec
 TD0 1

CHANNEL f1
 NOC1 1R
 P1 14.00 usec
 PL1 0.00 dB
 SFO1 400.1534013 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1500000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Fig. 7: 1H -NMR- spectrum 2-(3,5-dimethyl-1H-pyrazol-1-yl)-3-(1,3-dioxolan-2-yl)quinoline.

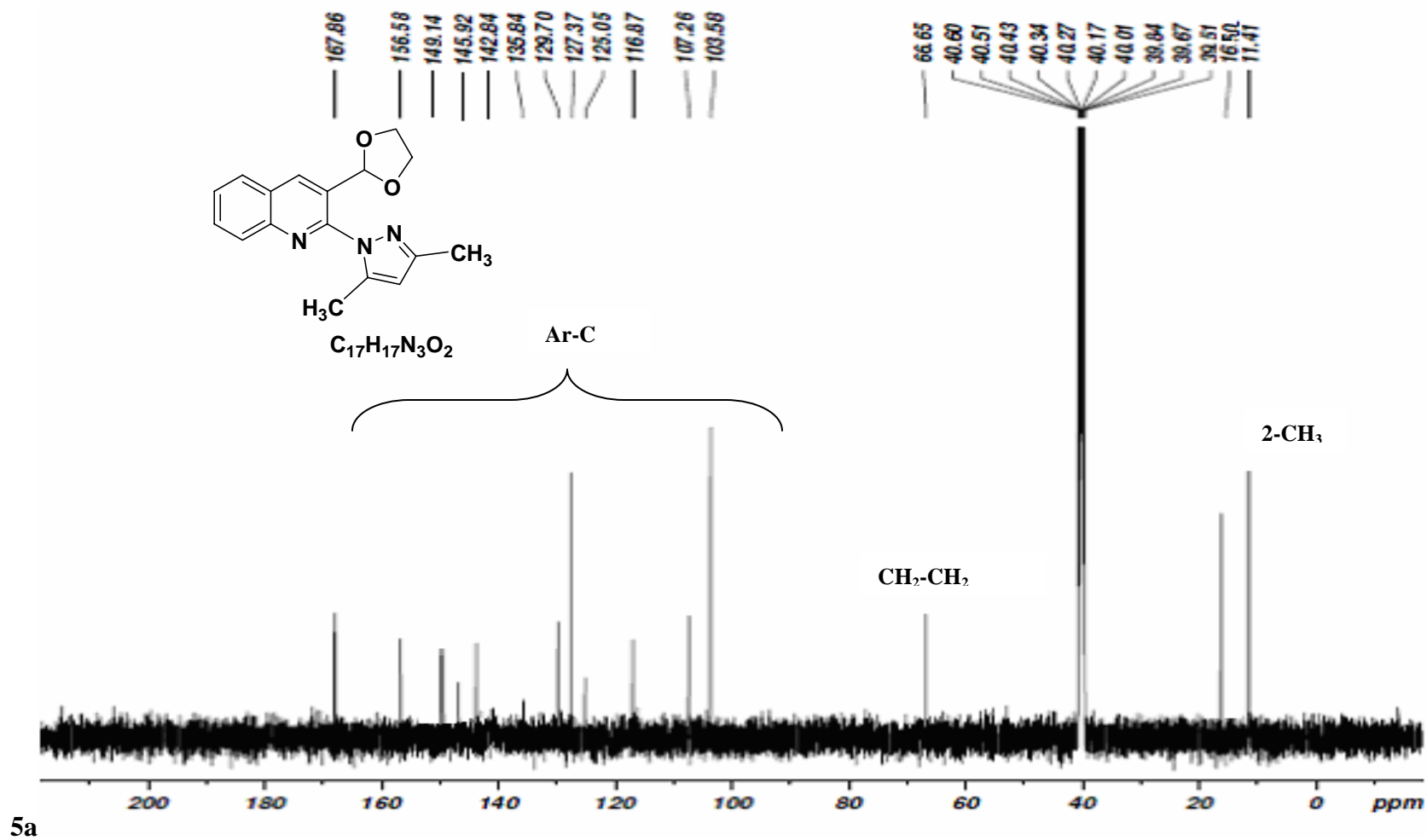


Fig. 8: ¹³C-NMR- spectrum 2-(3,5-dimethyl-1H-pyrazol-1-yl)-3-(1,3-dioxolan-2-yl)quinoline, 5a

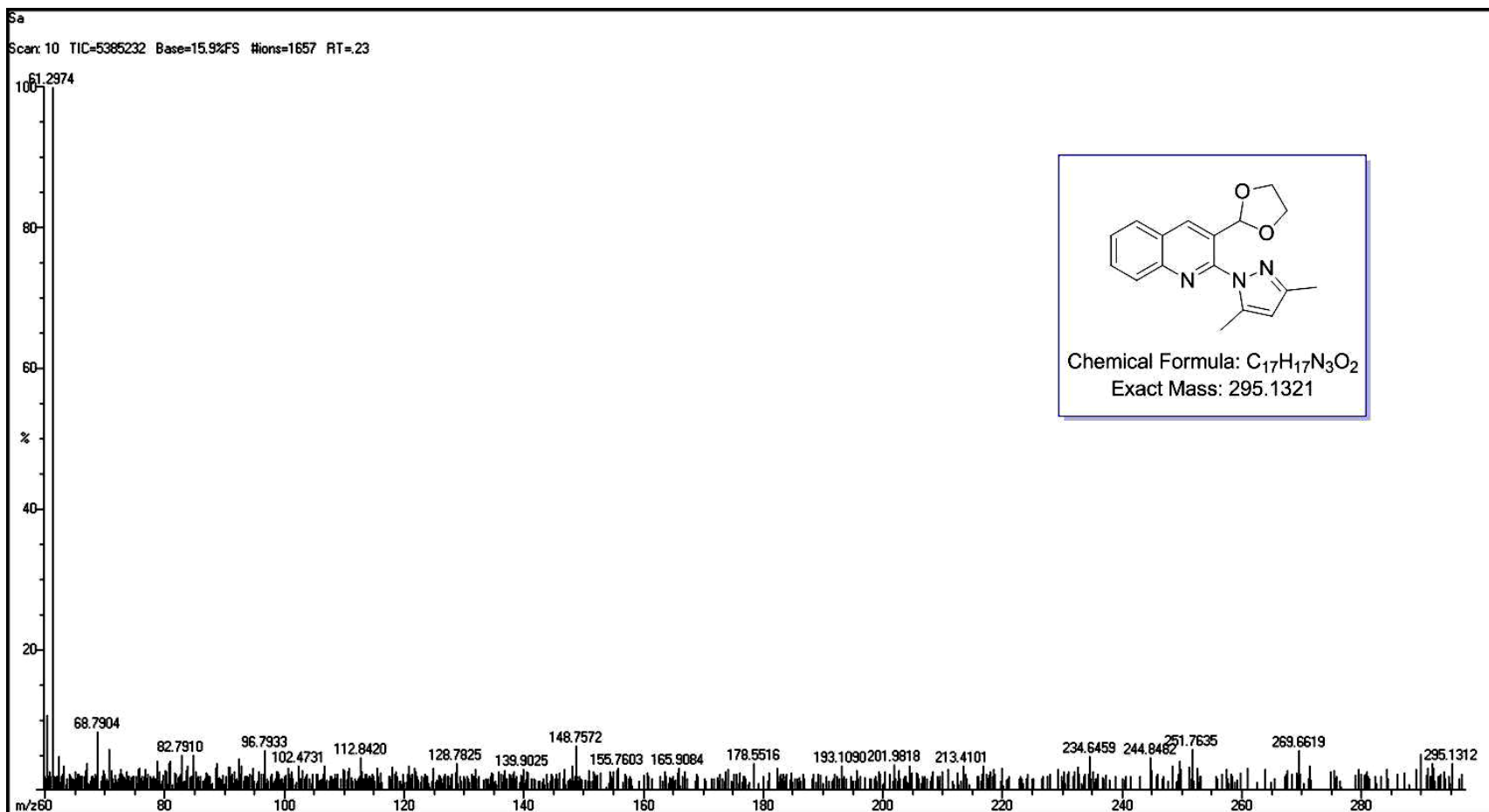


Fig. 9: HRMS-spectrum 2-(3,5-dimethyl-1H-pyrazol-1-yl)-3-(1,3-dioxolan-2-yl)quinoline, **5a**

Signature SIF VIT VELLORE
5B

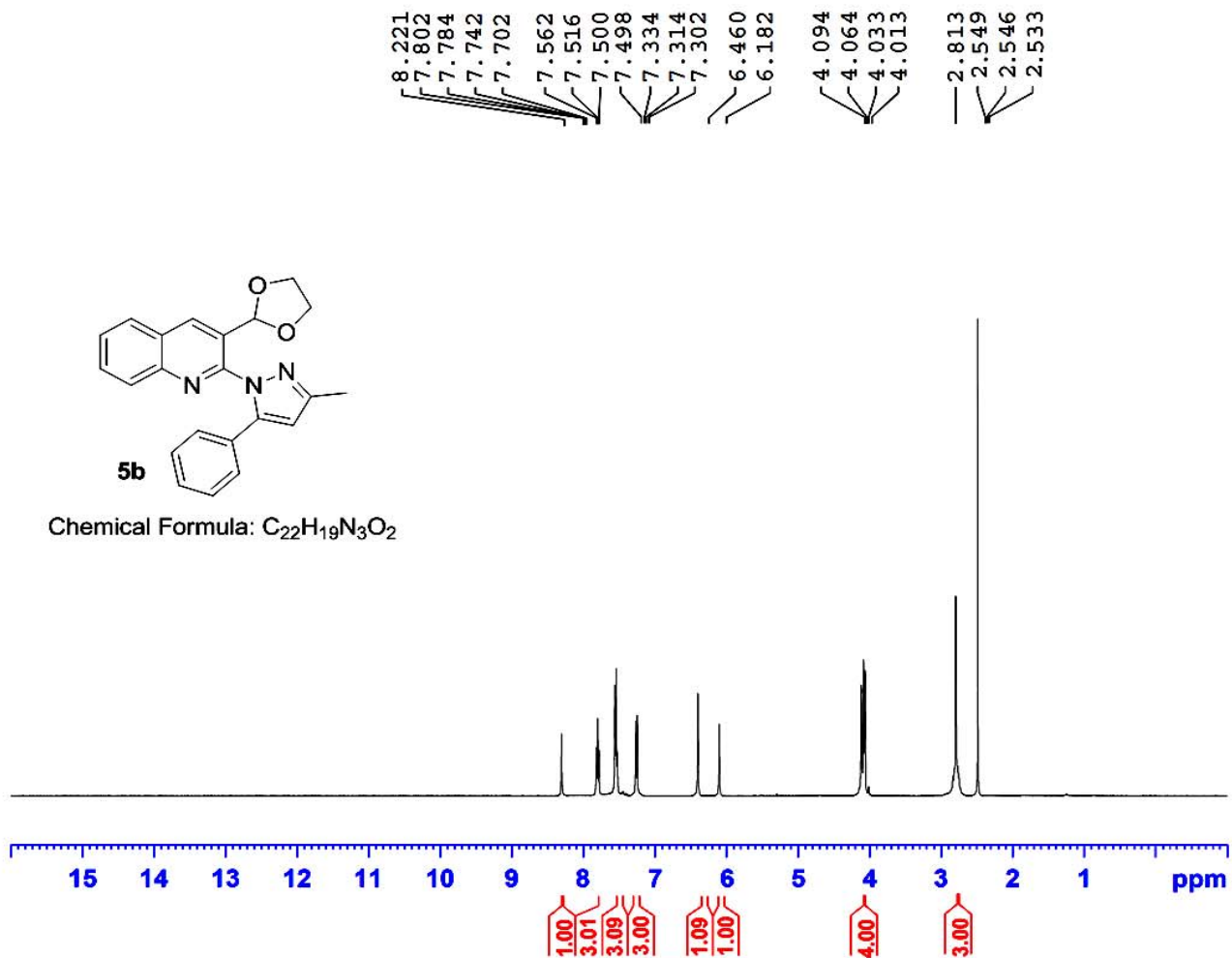


Fig. 10: 1H -NMR- spectrum of 3-(1,3-dioxolan-2-yl)-2-(3-methyl-5-phenyl-1H-pyrazol-1-yl)quinolone, **5b**

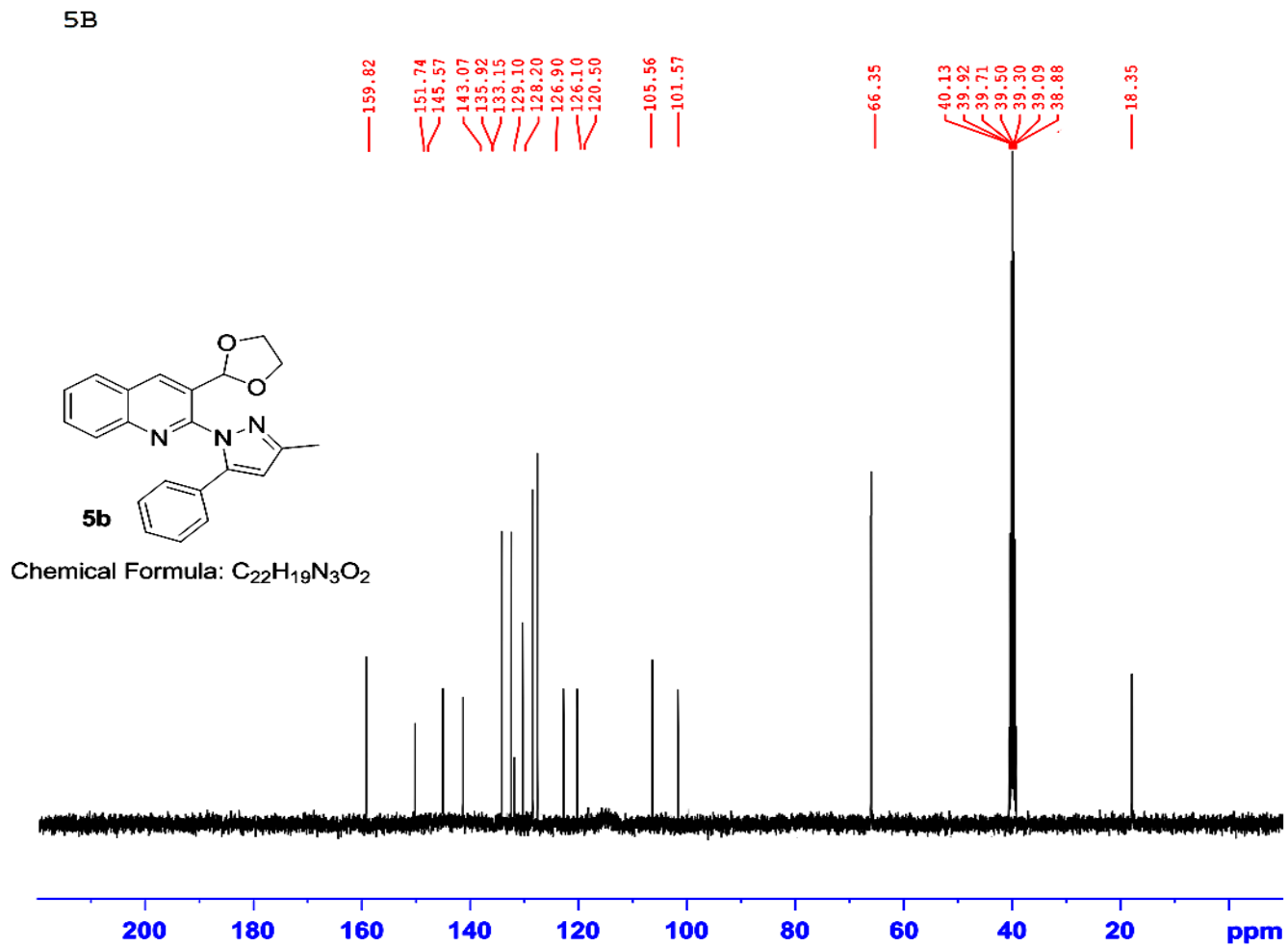


Fig. 11: ^{13}C -NMR- spectrum of 3-(1,3-dioxolan-2-yl)-2-(3-methyl-5-phenyl-1H-pyrazol-1-yl)quinolone, **5b**

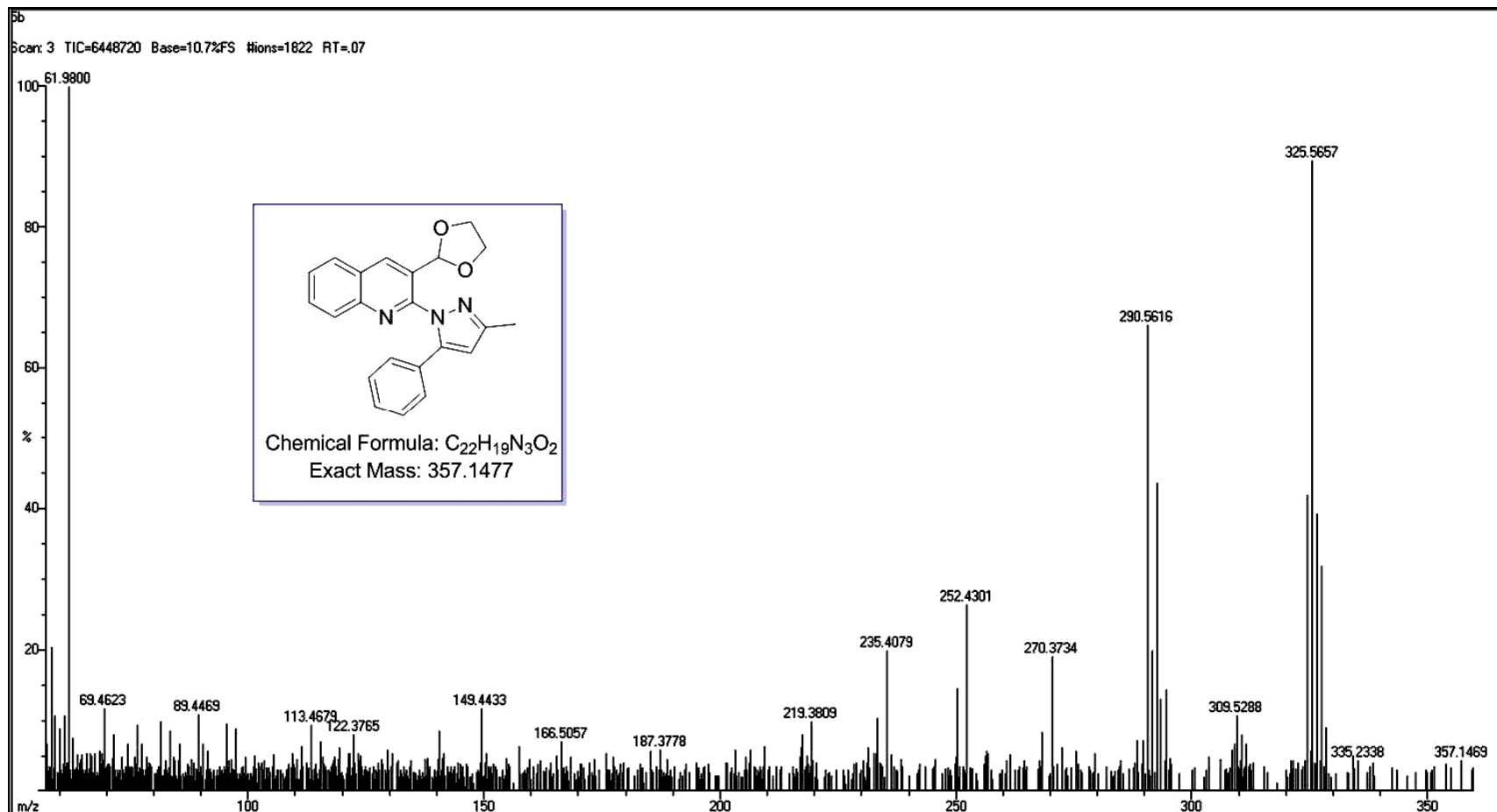


Fig. 12: HRMS-spectrum 3-(1,3-dioxolan-2-yl)-2-(3-methyl-5-phenyl-1H-pyrazol-1-yl)quinoline, **5b**

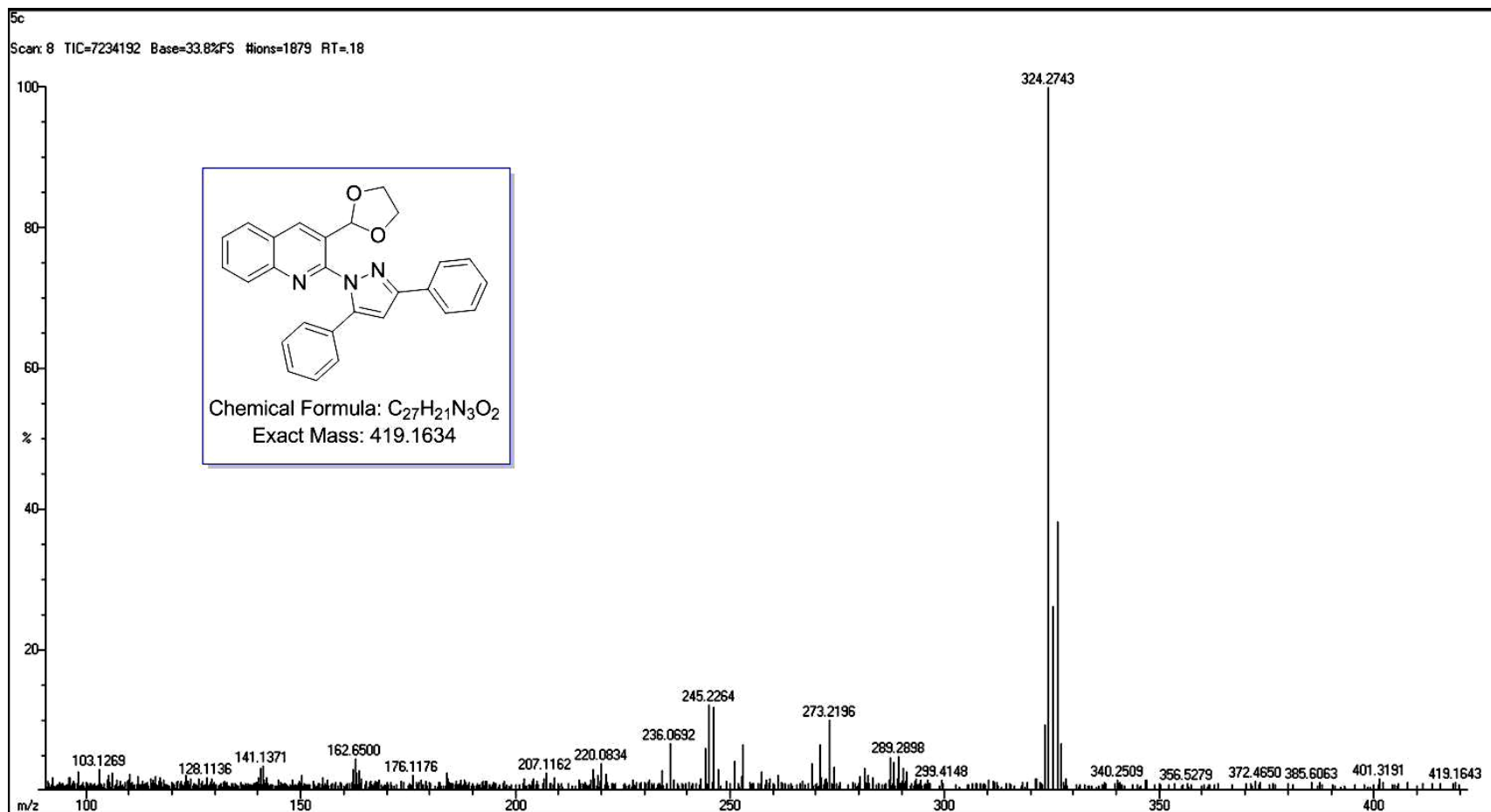


Fig. 13: HRMS-spectrum 3-(1, 3-dioxolan-2-yl)-2-(3,5-diphenyl-1H-pyrazol-1-yl)quinoline, **5c**

5D

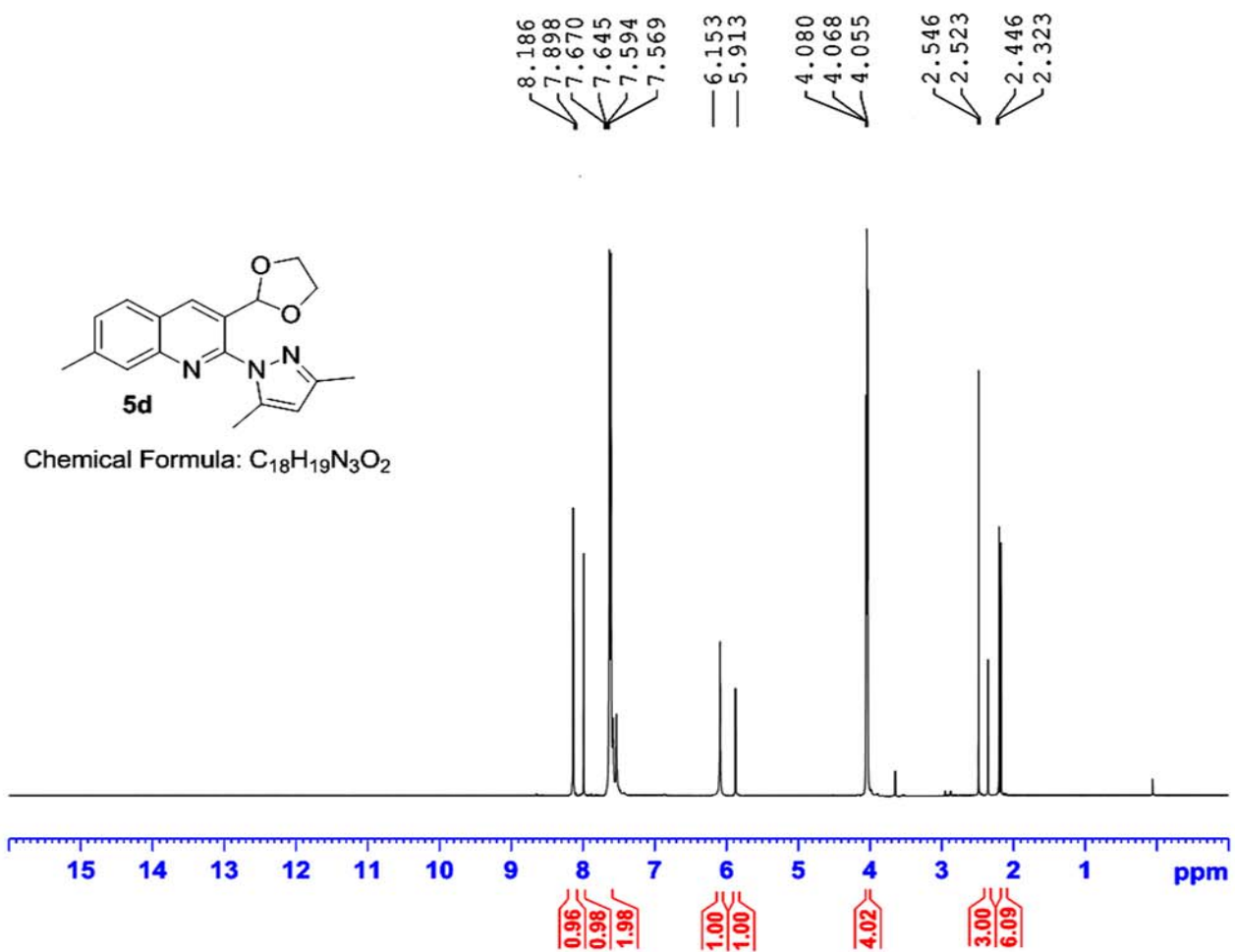


Fig. 14: 1H -NMR- spectrum of 2-(3,5-dimethyl-1H-pyrazol-1-yl)-3-(1,3-dioxolan-2-yl)-7-methylquinoline, **5d**

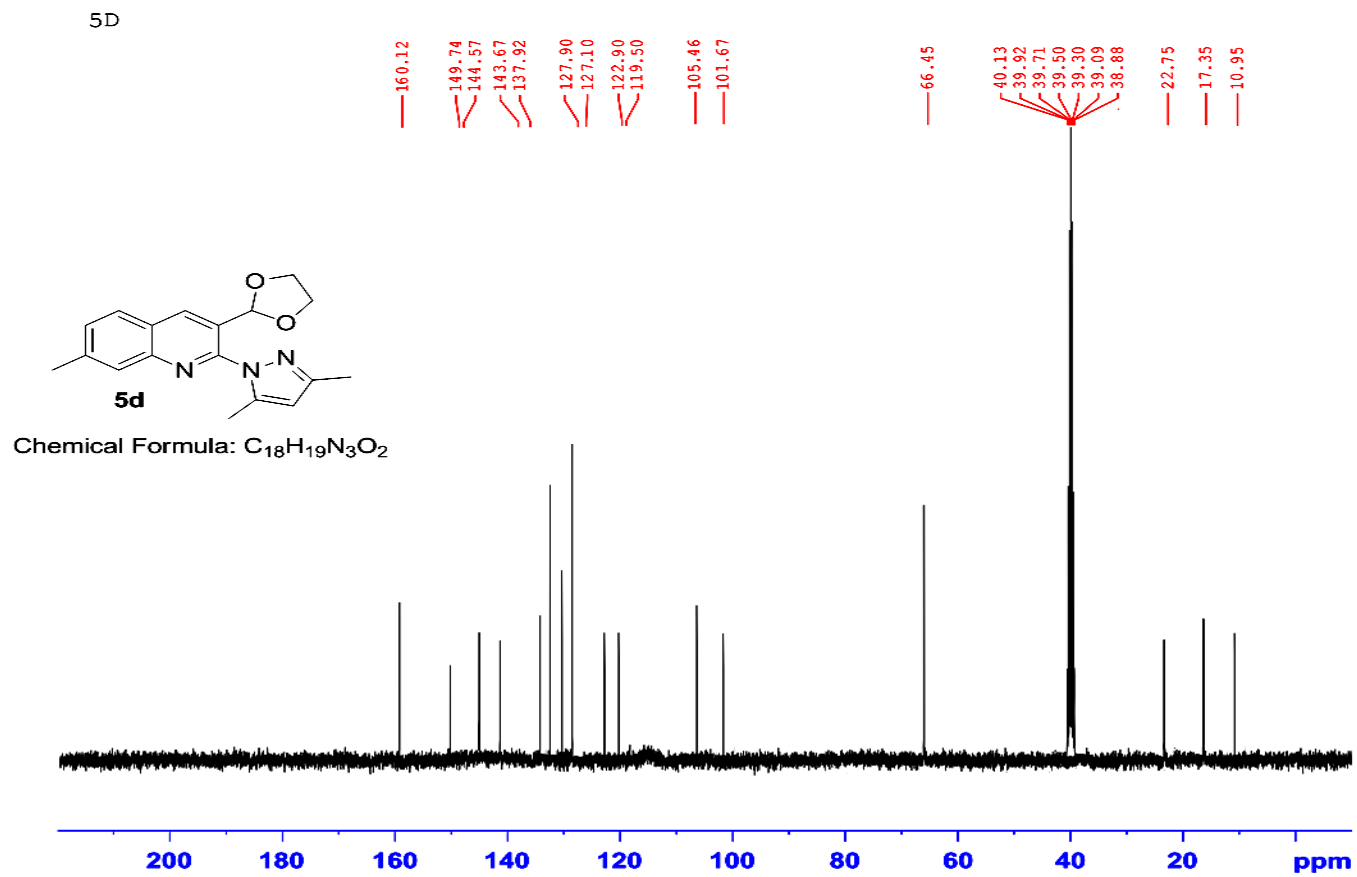


Fig. 15: ¹³C-NMR- spectrum of 2-(3,5-dimethyl-1H-pyrazol-1-yl)-3-(1,3-dioxolan-2-yl)-7-methylquinoline, **5d**

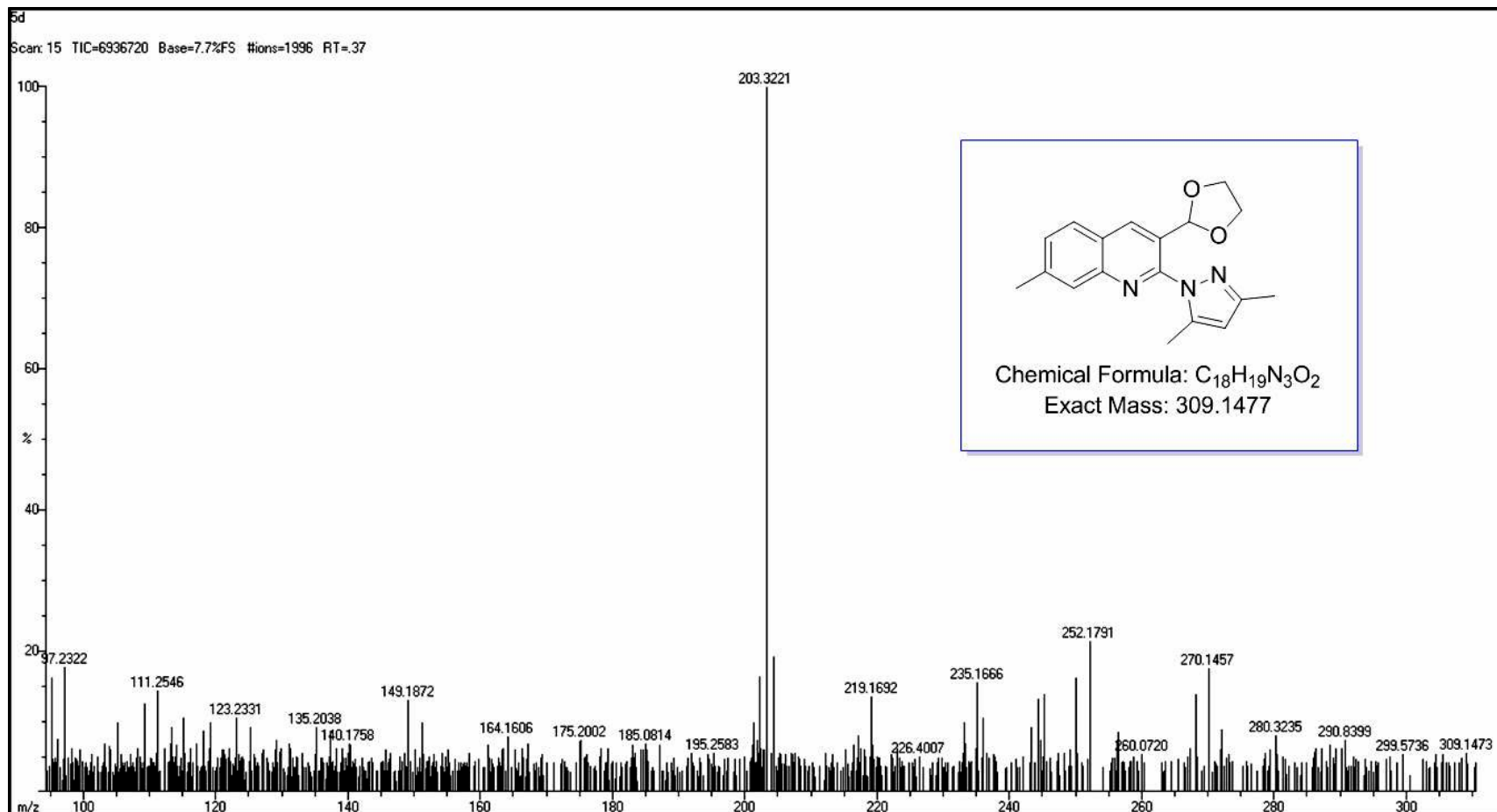


Fig. 16: HRMS-spectrum 2-(3, 5-dimethyl-1H-pyrazol-1-yl)-3-(1, 3-dioxolan-2-yl)-7-methyl quinoline, **5d**

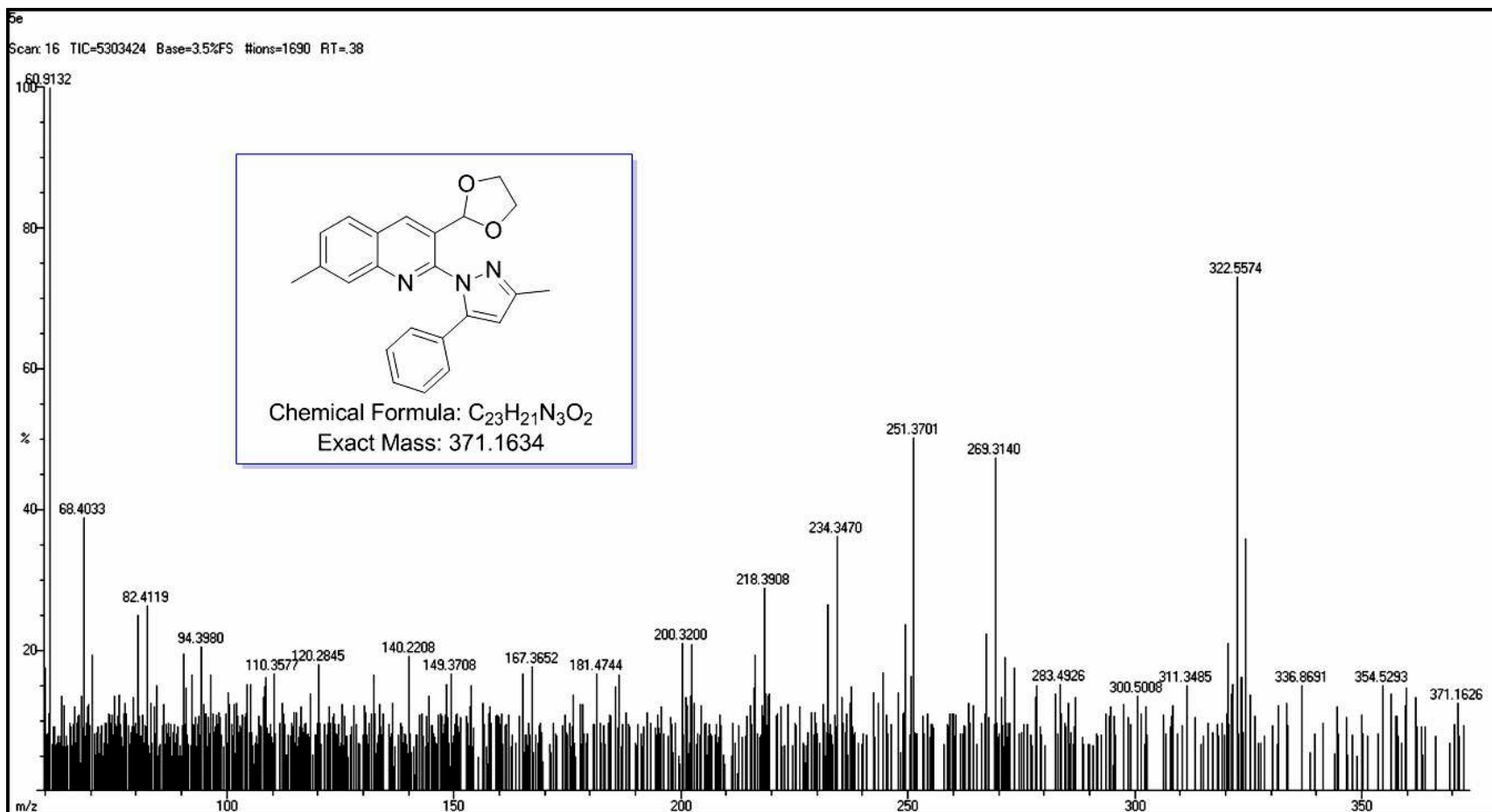


Fig. 17: HRMS-spectrum 3-(1,3-dioxolan-2-yl)-7-methyl-2-(3-methyl-5-phenyl-1H-pyrazol-1-yl)quinoline, **5e**

5F

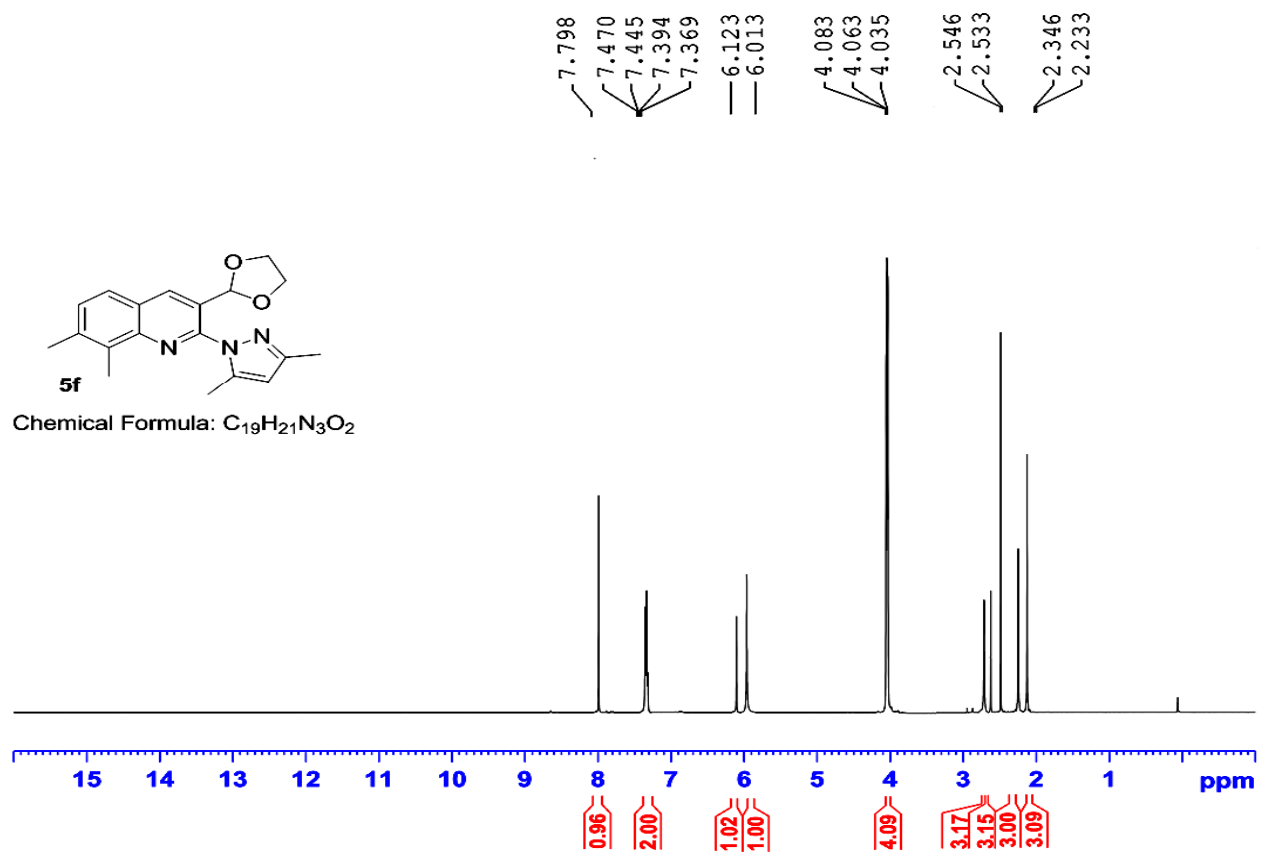


Fig. 18: ¹H-NMR- spectrum of 2-(3,5-dimethyl-1H-pyrazol-1-yl)-3-(1,3-dioxolan-2-yl)-7,8-dimethylquinoline, **5f**

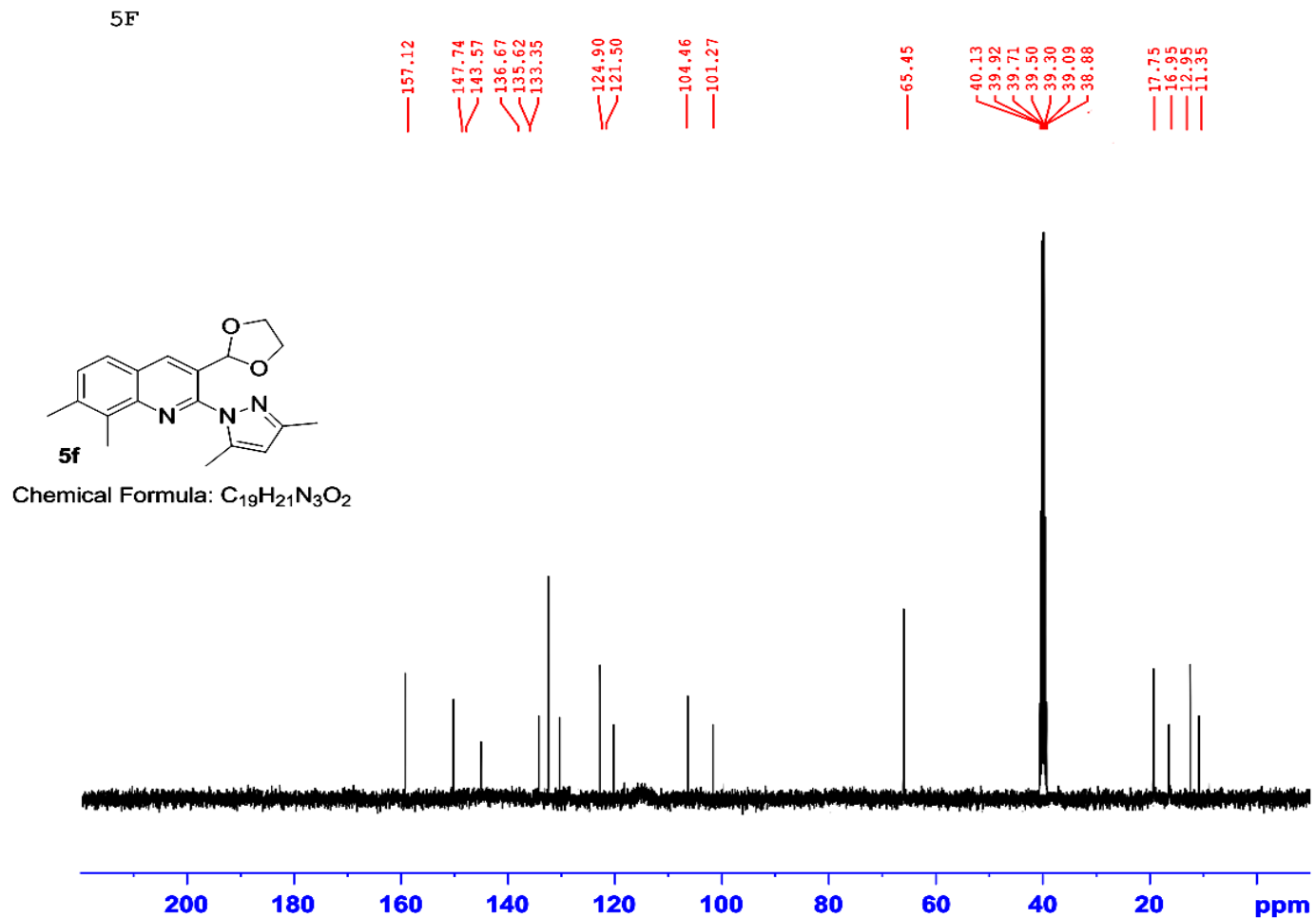


Fig. 19: ¹³C-NMR- spectrum of 2-(3,5-dimethyl-1H-pyrazol-1-yl)-3-(1,3-dioxolan-2-yl)-7,8-dimethylquinoline, **5f**

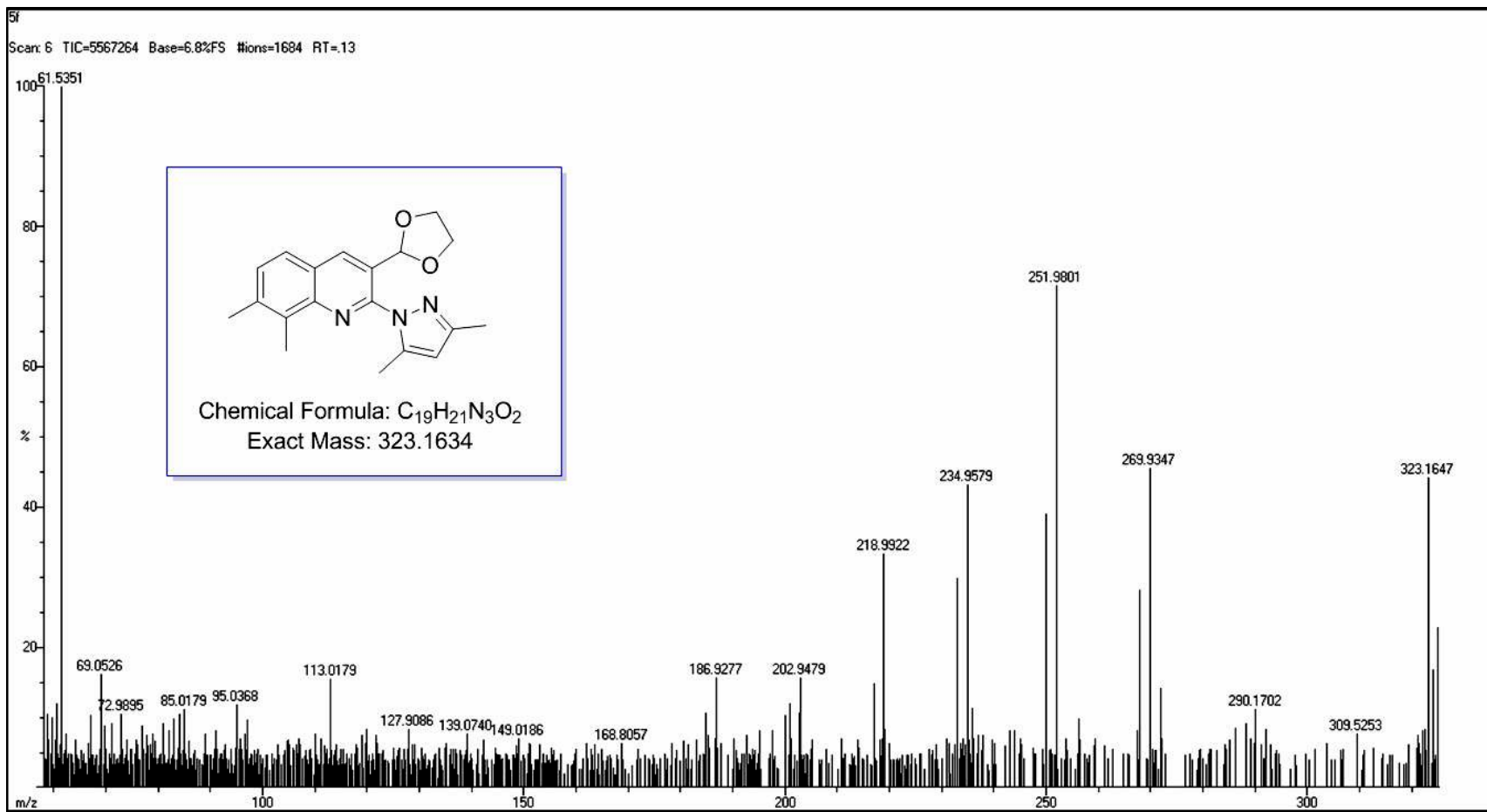


Fig. 20: HRMS-spectrum2-(3,5-dimethyl-1H-pyrazol-1-yl)-3-(1,3-dioxolan-2-yl)-7,8-dimethylquinoline, **5f**

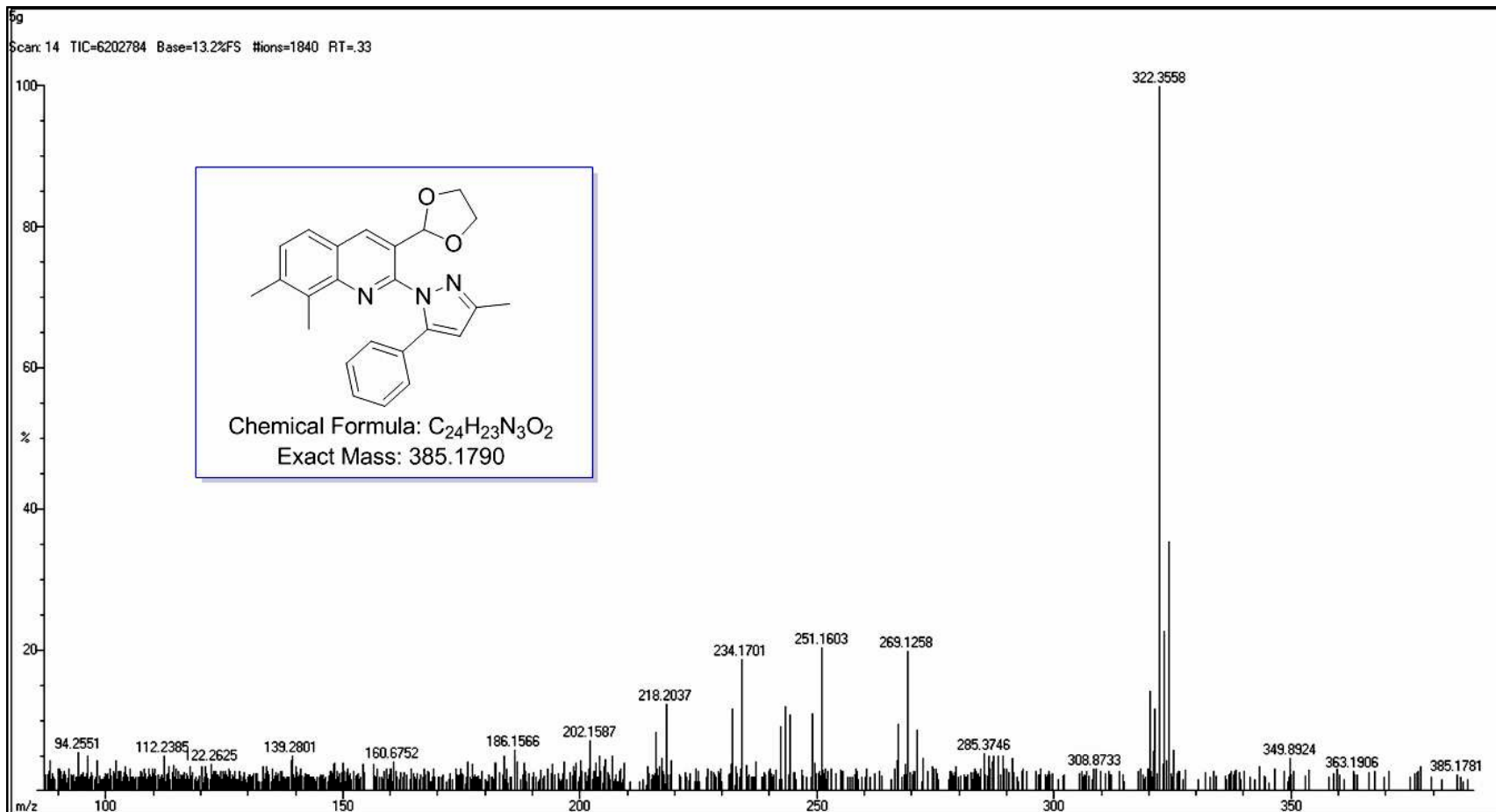


Fig. 21: HRMS-spectrum 3-(1,3-dioxolan-2-yl)-7,8-dimethyl-2-(3-methyl-5-phenyl-1H-pyrazol-1-yl)quinoline, **5g**