Electronic Supplementary Material (ESI) for Green Chemistry.

Electronic Supplementary Information

Synthesis of pyrrolidinone derivatives from aniline, an aldehyde and diethyl acetylenedicarboxylate in an ethanolic citric acid solution under ultrasound irradiation

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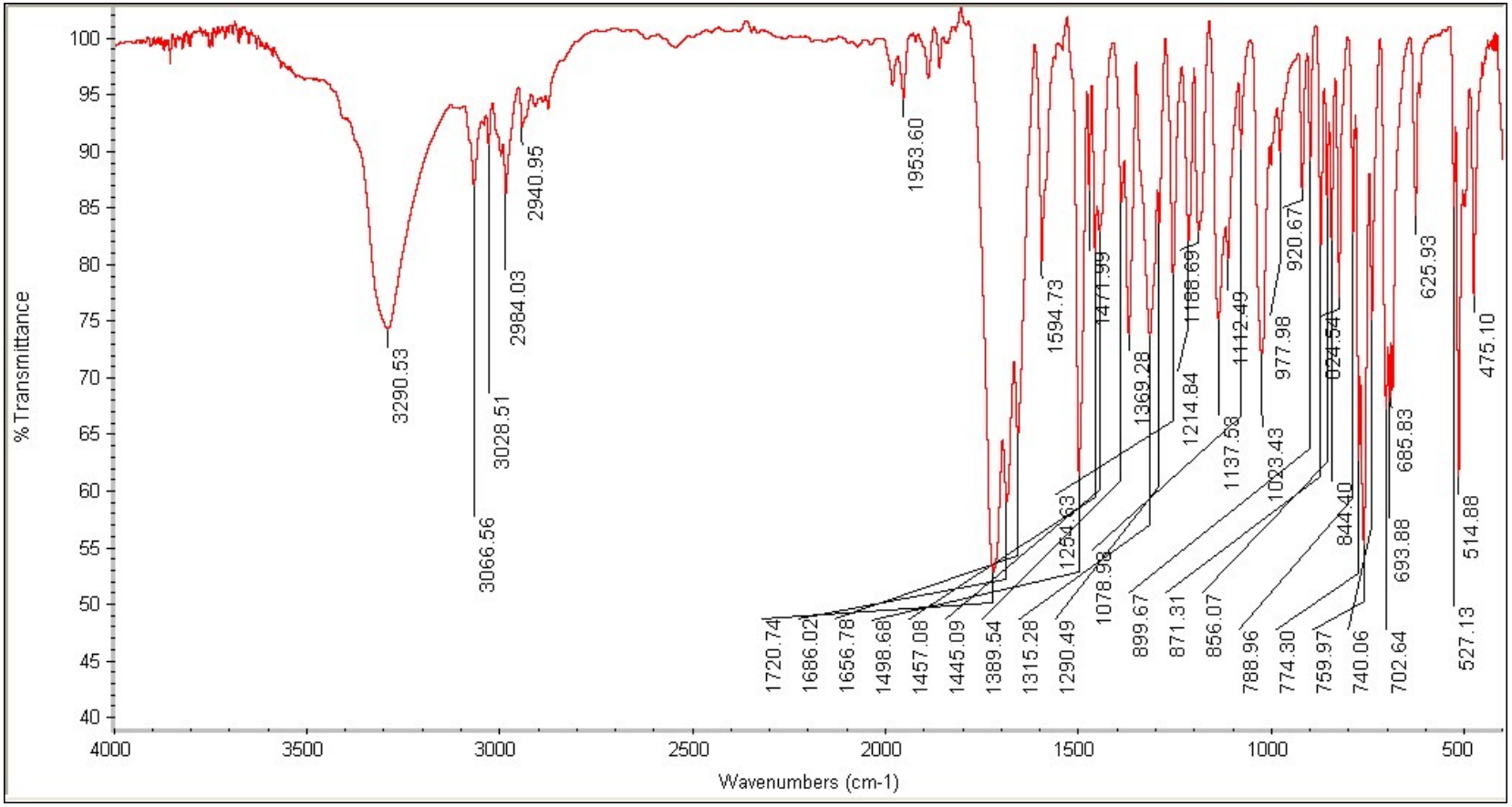

Fig. 1 FT-IR spectrum of Ethyl 4-hydroxy-5-oxo-1,2-diphenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4a).**

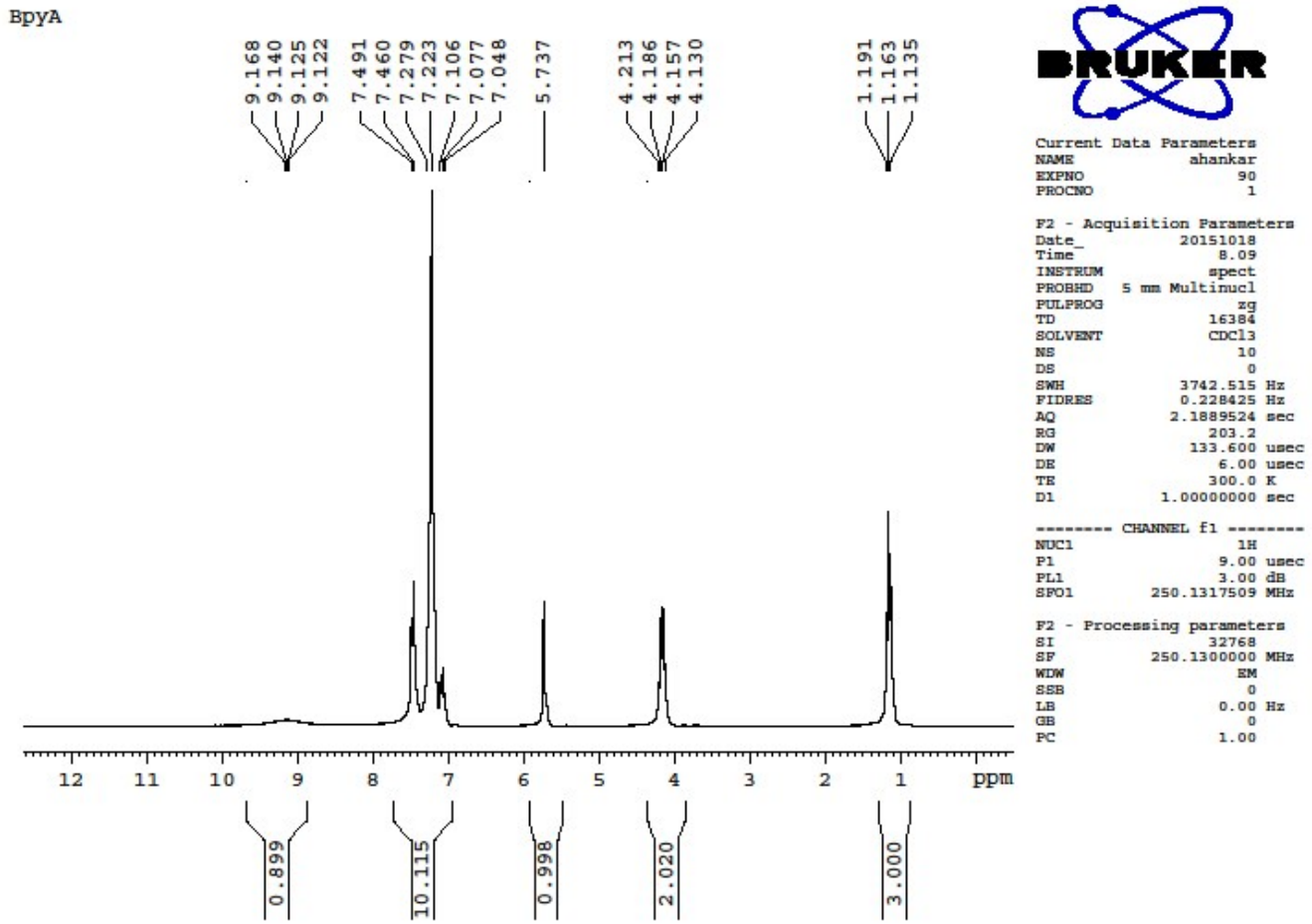

Fig. 2 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-5-oxo-1,2-diphenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4a).**

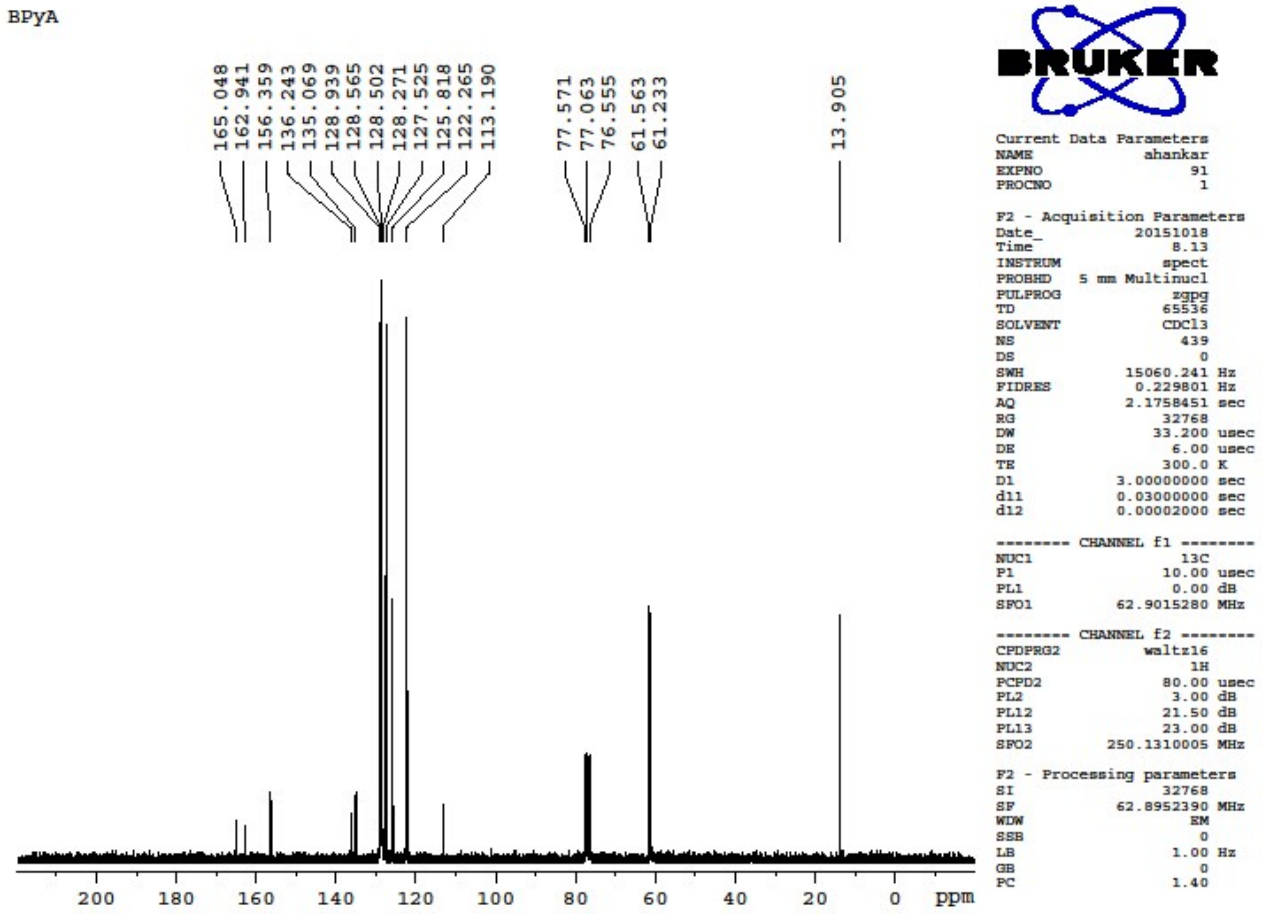

Fig. 3 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-5-oxo-1,2-diphenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4a).**

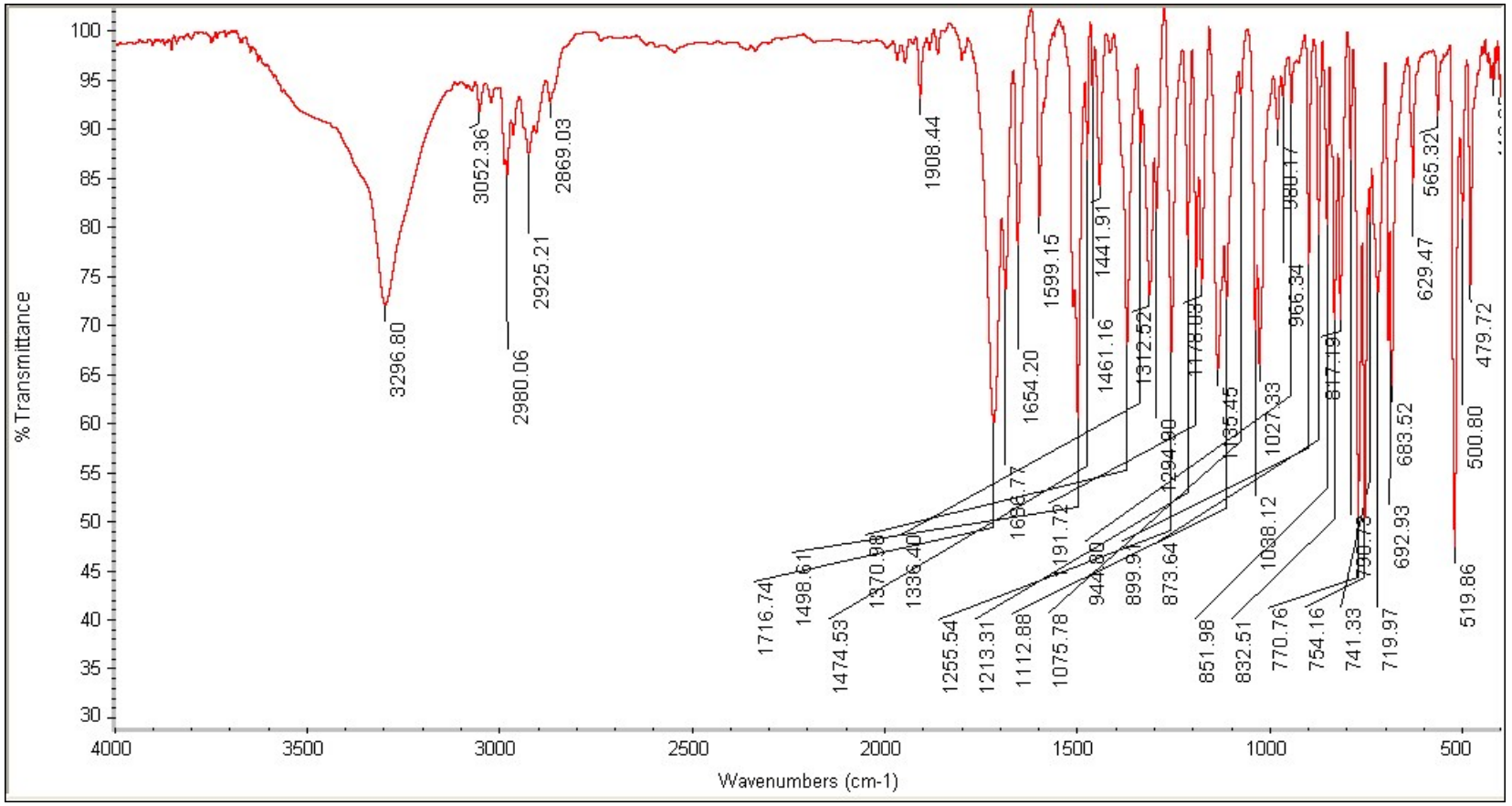

Fig. 4 FT-IR spectrum of Ethyl 4-hydroxy-5-oxo-1-phenyl-2-(p-tolyl)-2,5-dihydro-1H-pyrrole-3-carboxylate **(4b).**

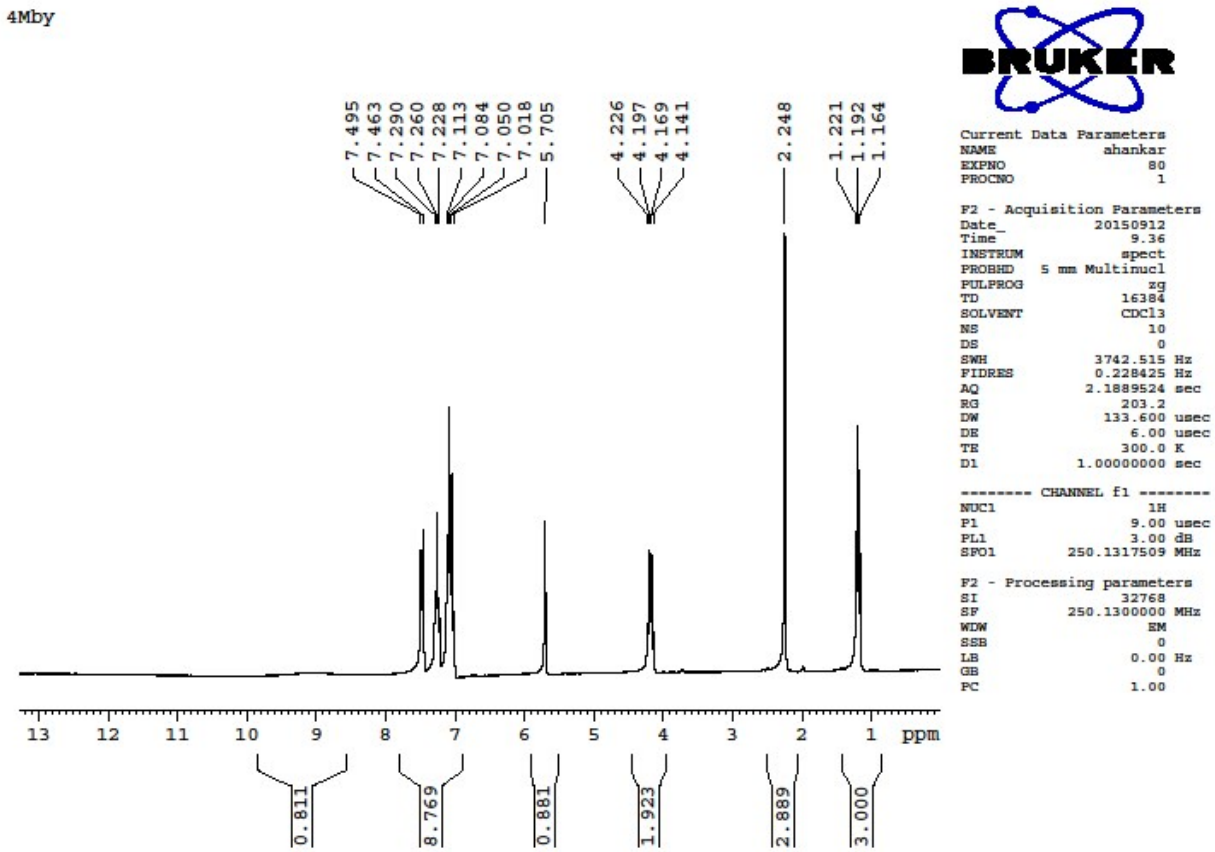

Fig. 5 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-5-oxo-1-phenyl-2-(p-tolyl)-2, 5-dihydro-1H-pyrrole-3-carboxylate **(4b)**

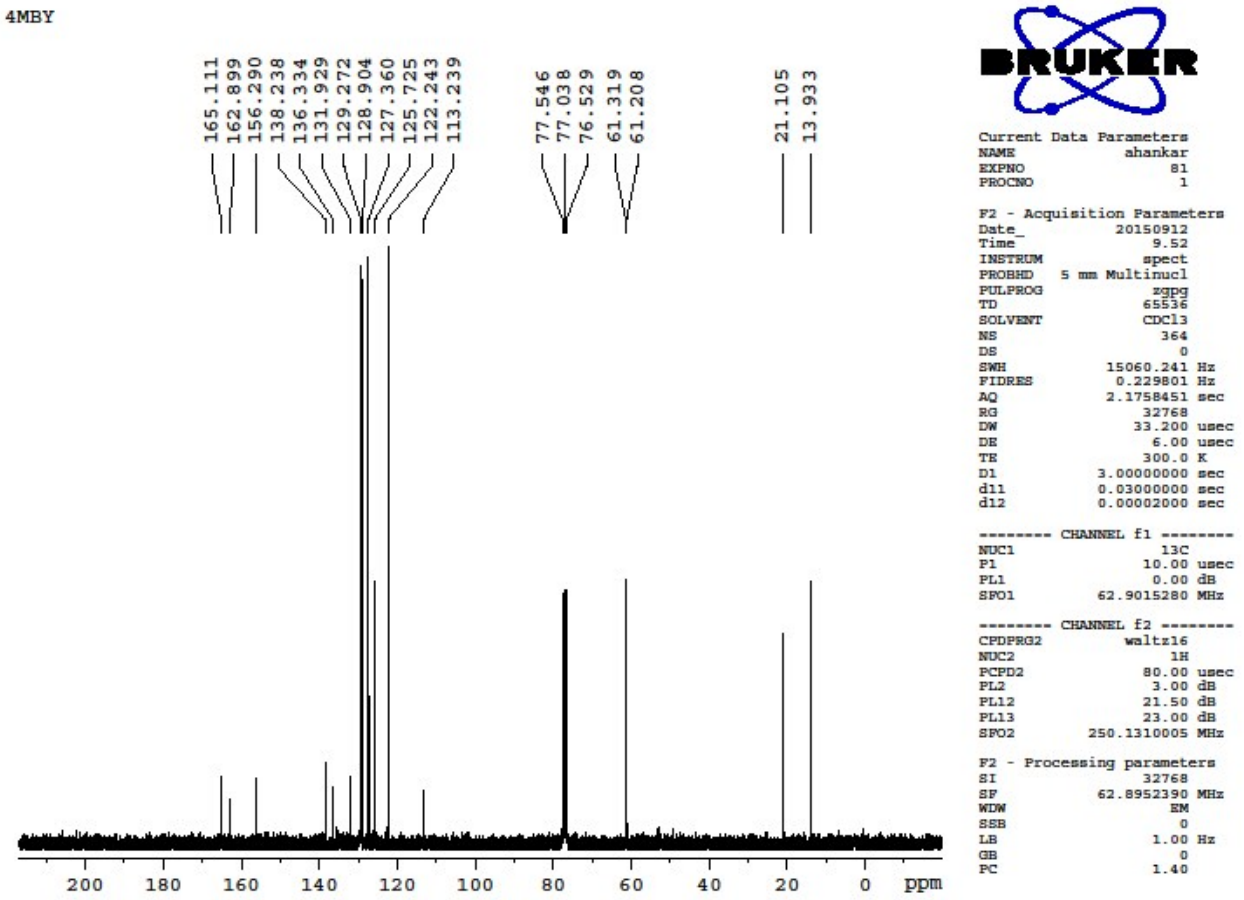

Fig. 6 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-5-oxo-1-phenyl-2-(p-tolyl)-2,5-dihydro-1H-pyrrole-3-carboxylate **(4b).**

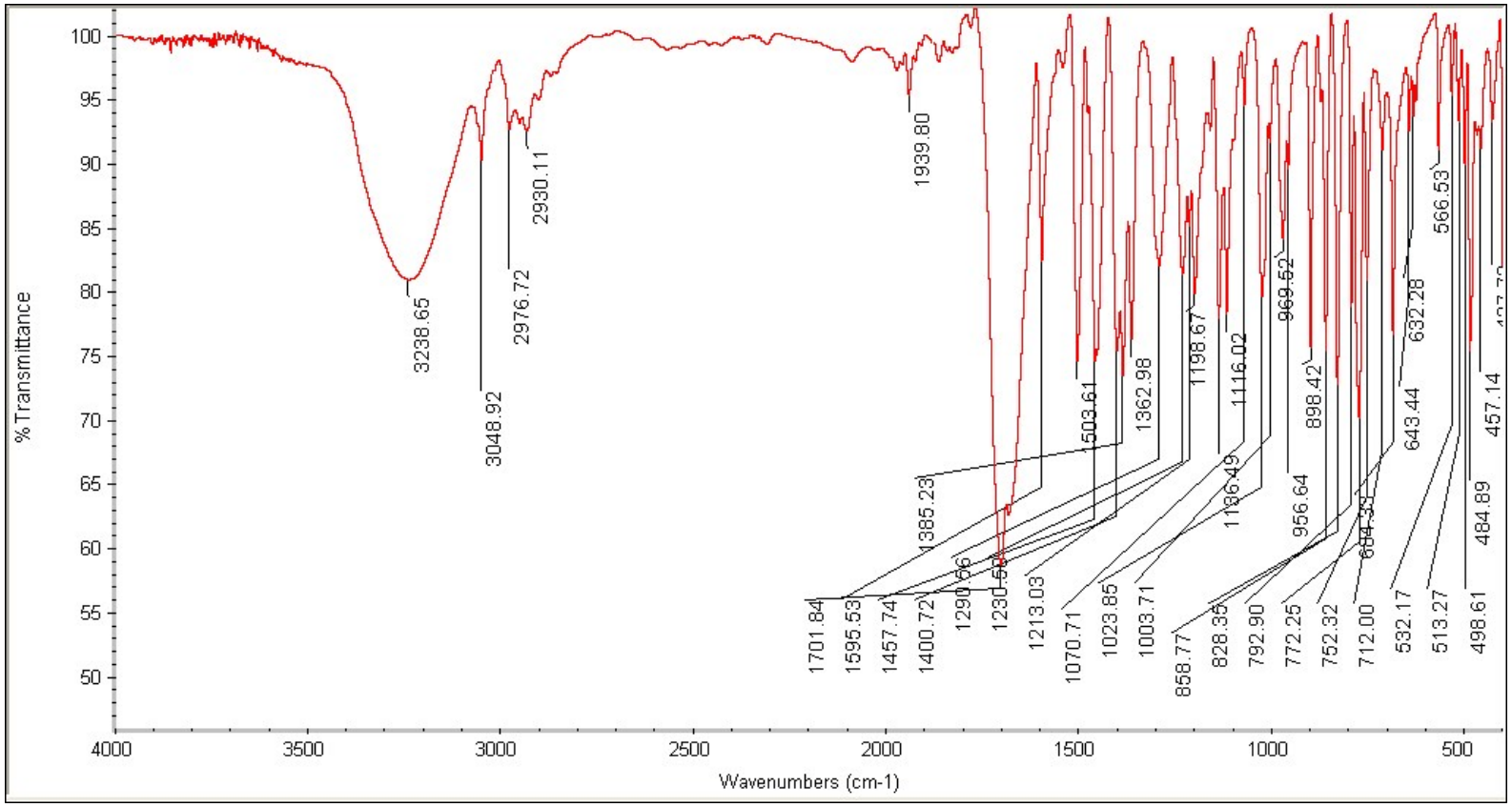

Fig .7 FT-IR spectrum of Ethyl 4-hydroxy-2-(naphthalen-2-yl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4c).**

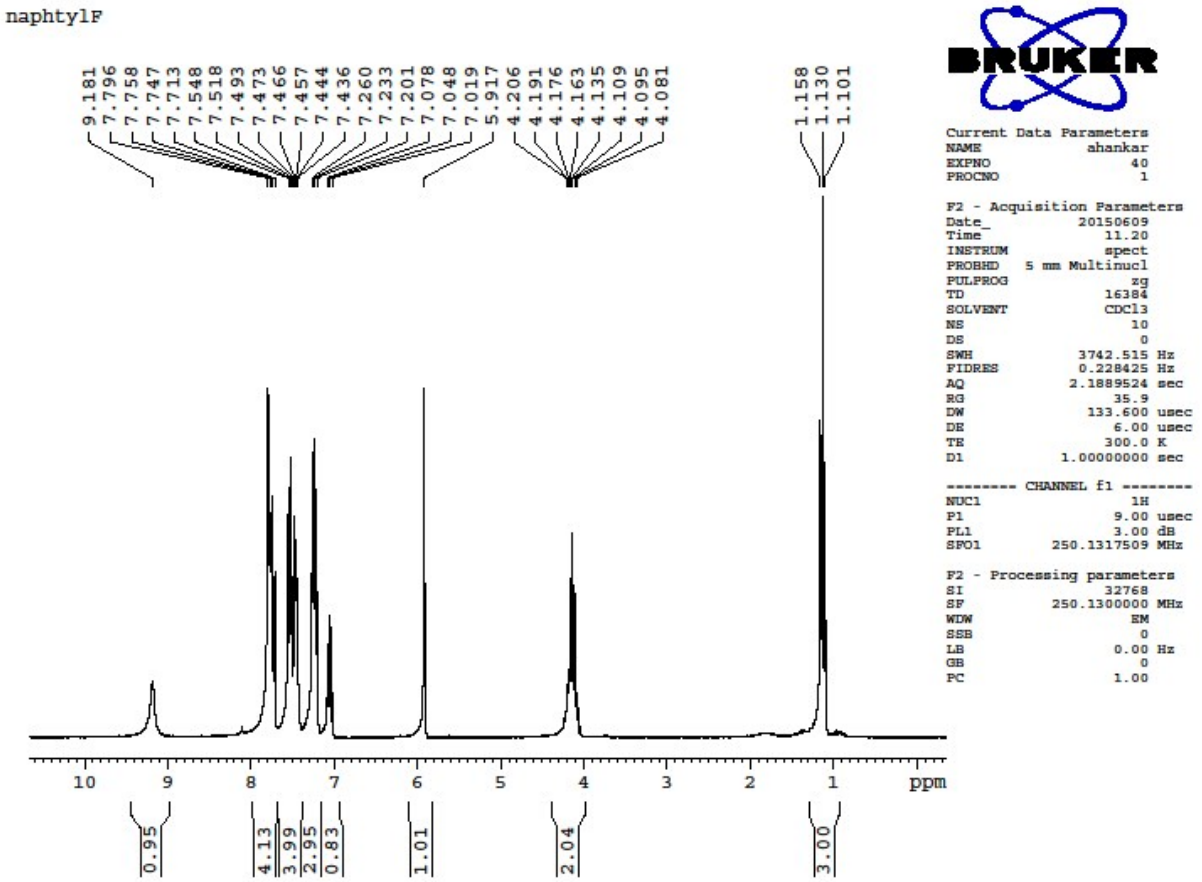

Fig. 8 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-2-(naphthalen-2-yl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4c).**

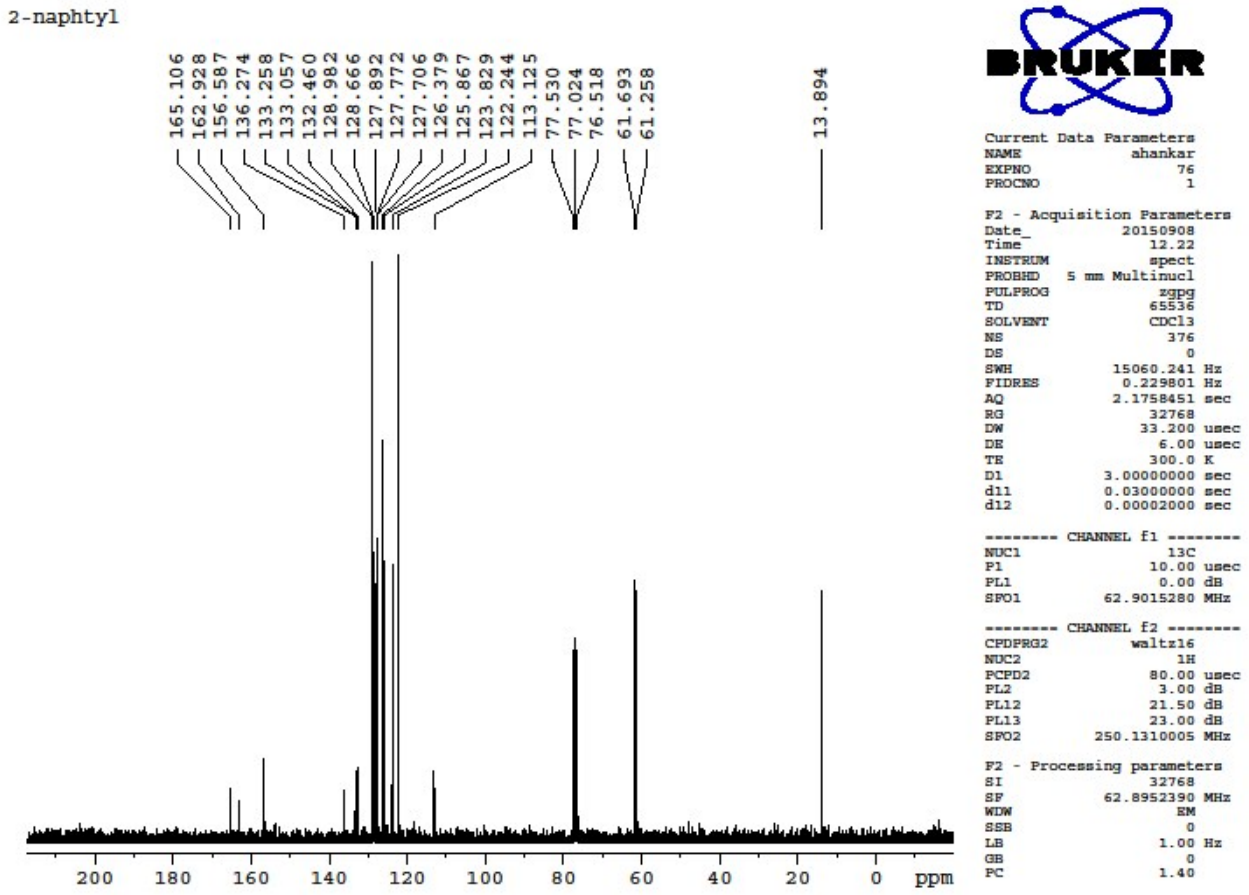

Fig. 9 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-2-(naphthalen-2-yl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4c).**

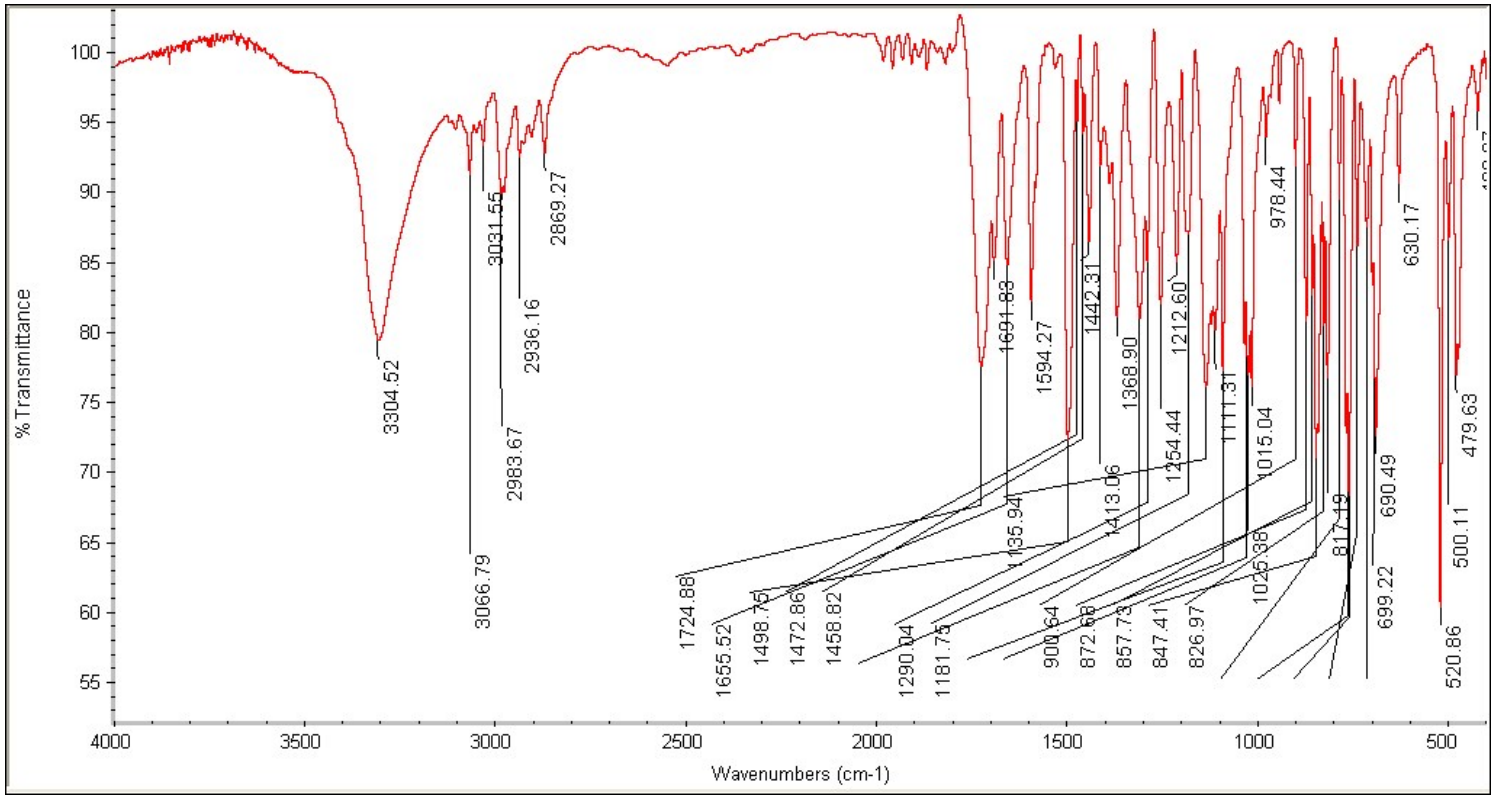

Fig. 10 FT-IR spectrum of Ethyl 2-(4-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4d).**

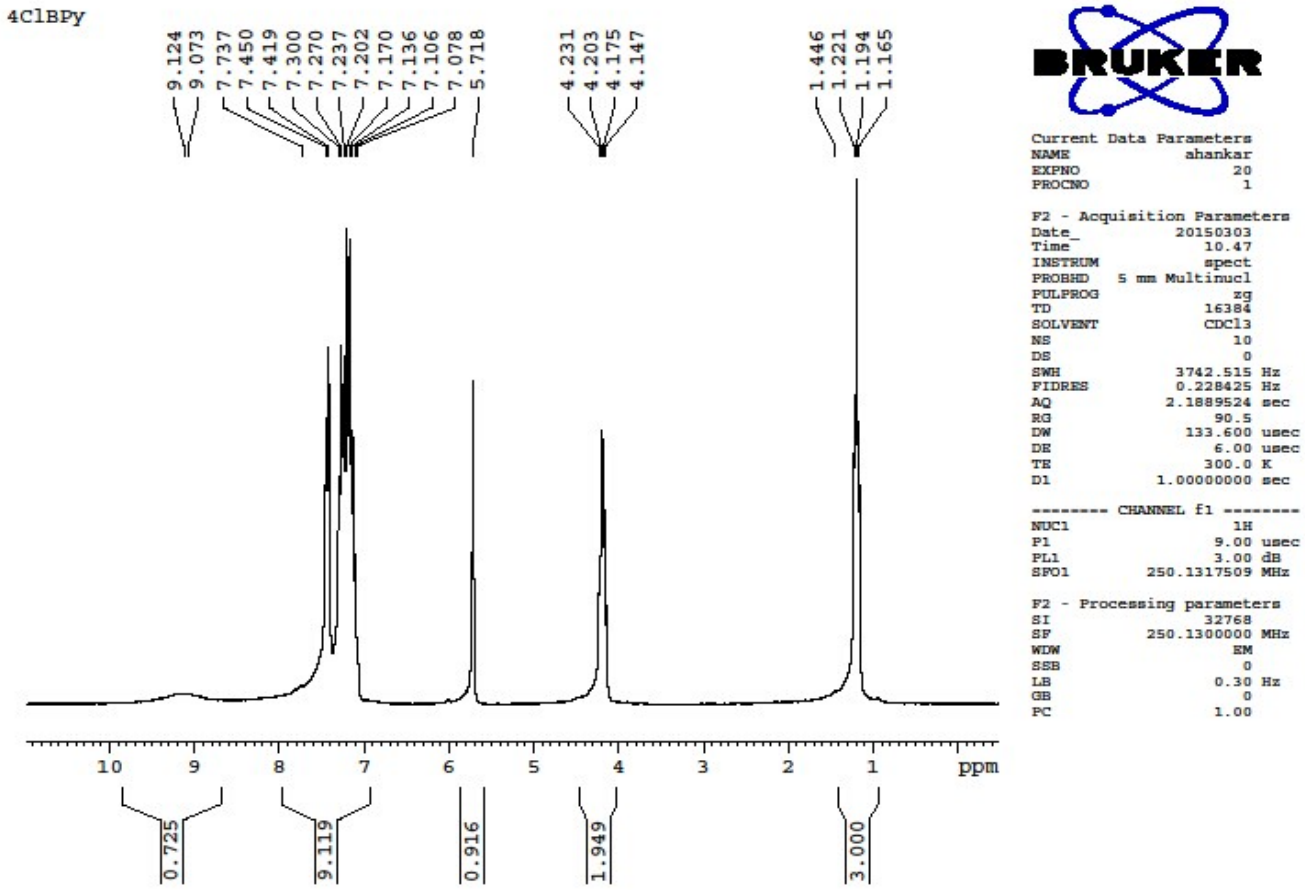

Fig. 11 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 2-(4-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4d).**

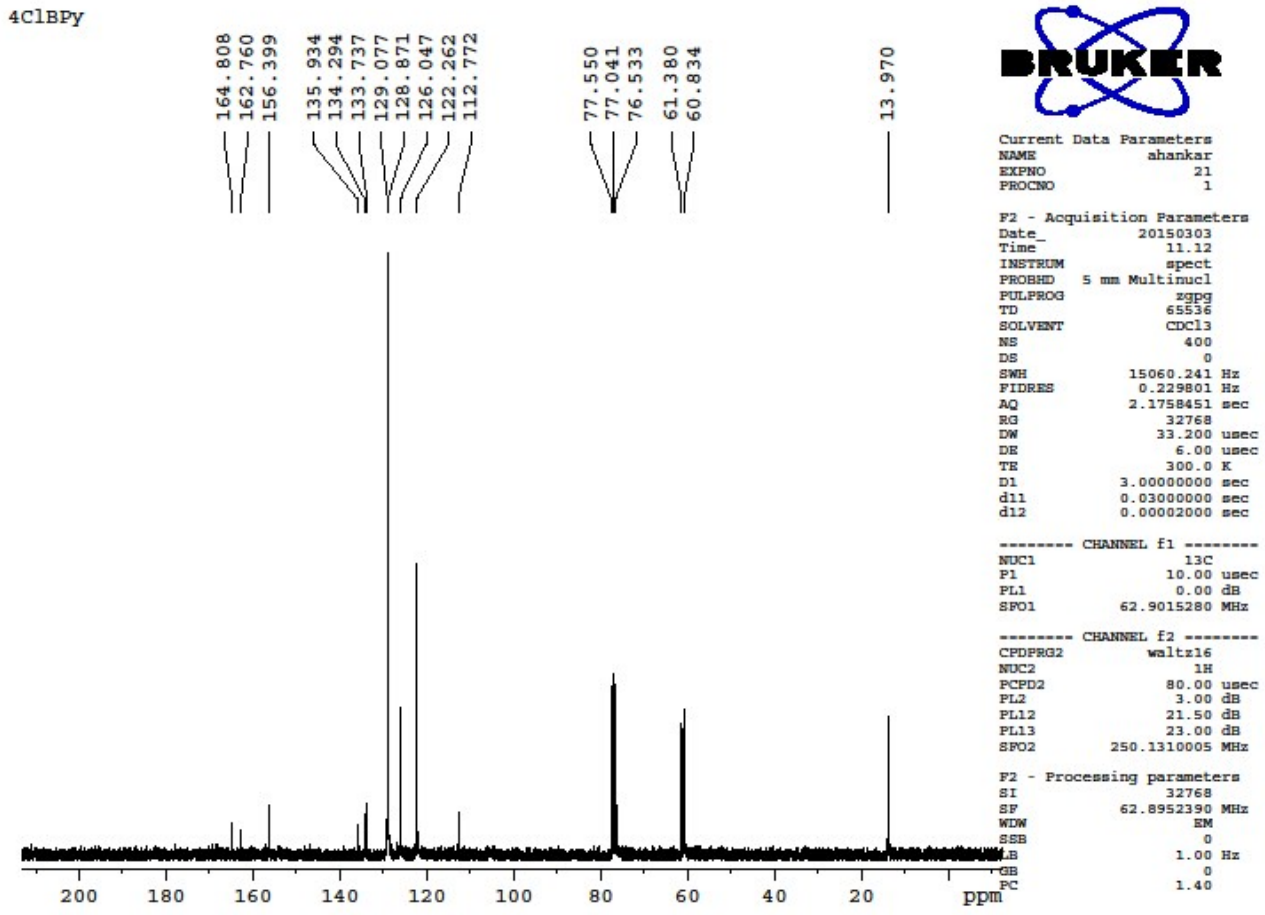

Fig. 12 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 2-(4-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4d).**

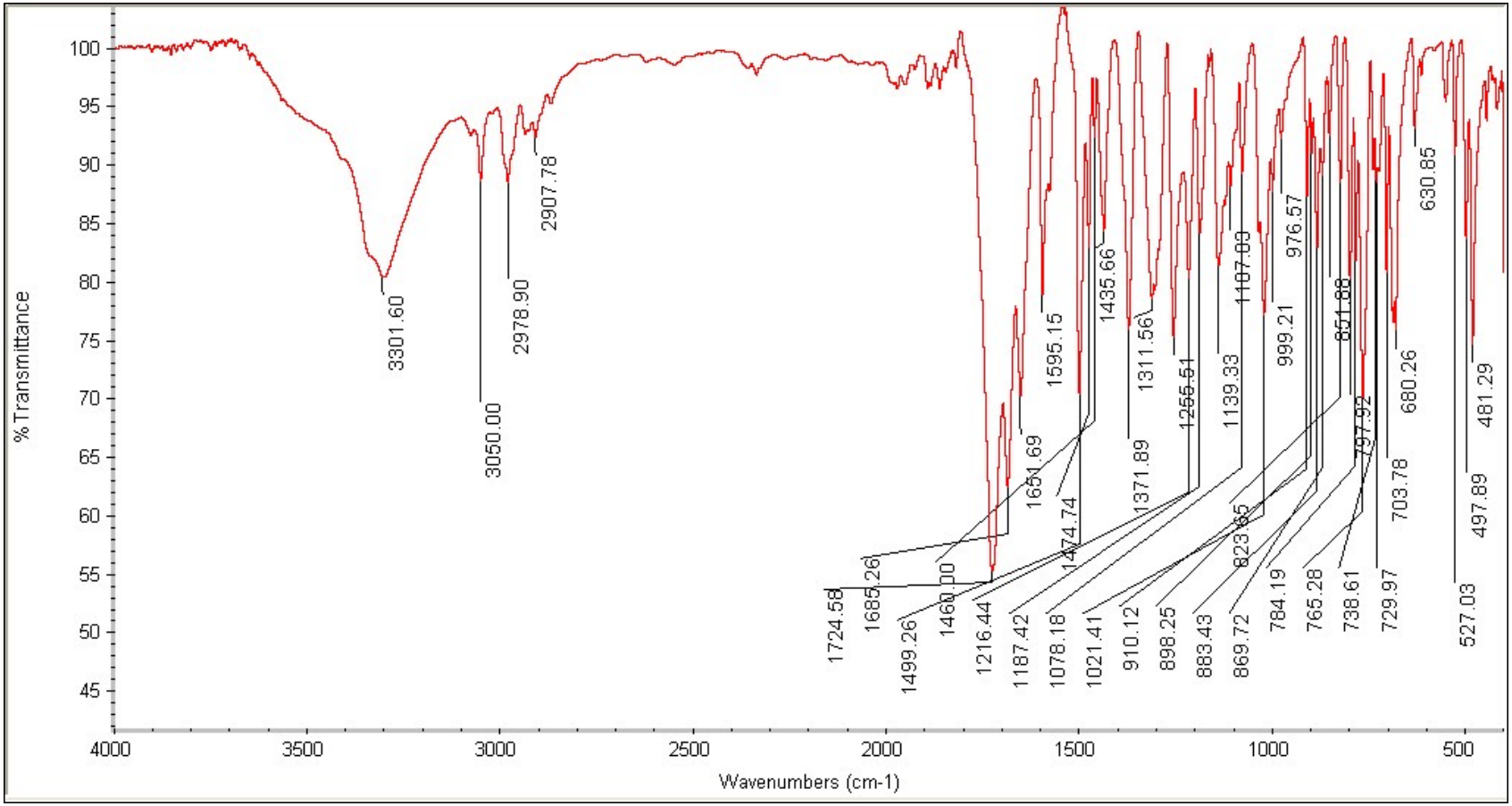

Fig. 13 FT-IR spectrum of Ethyl 2-(3-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4e).**

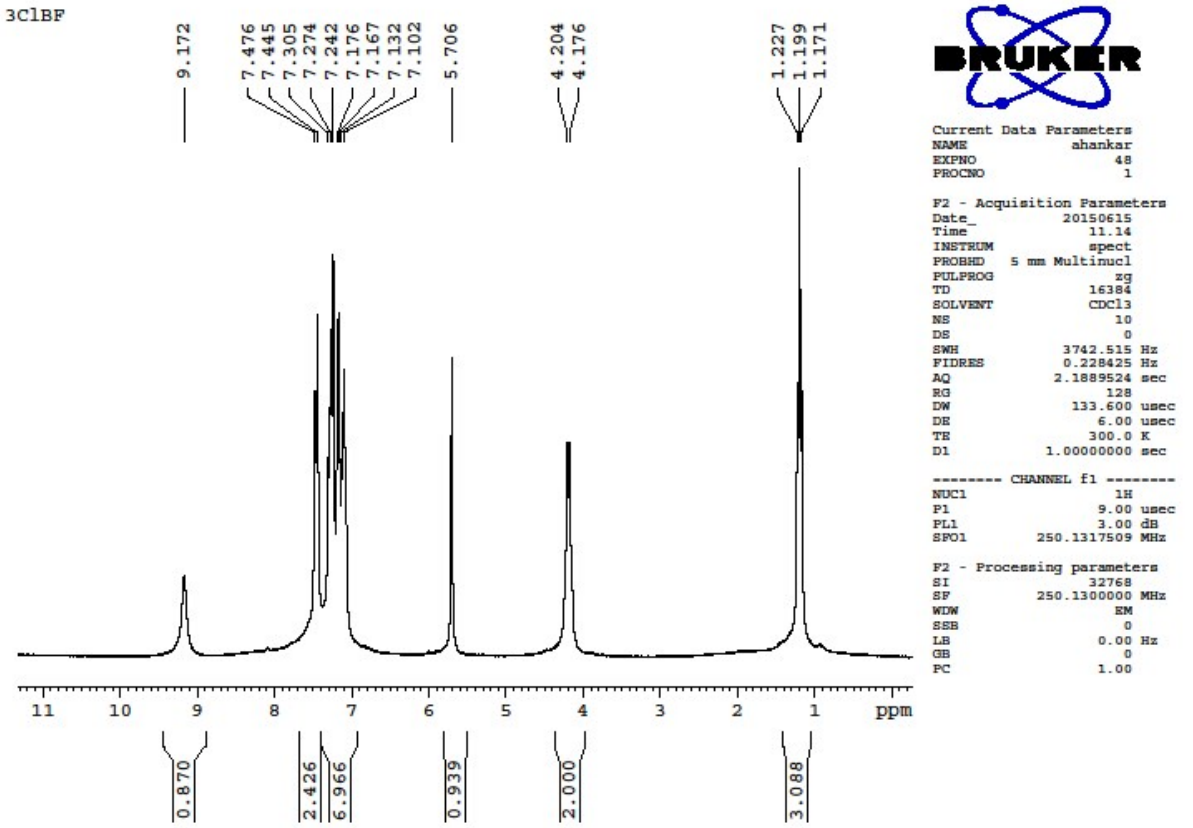

Fig. 14 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 2-(3-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4e).**

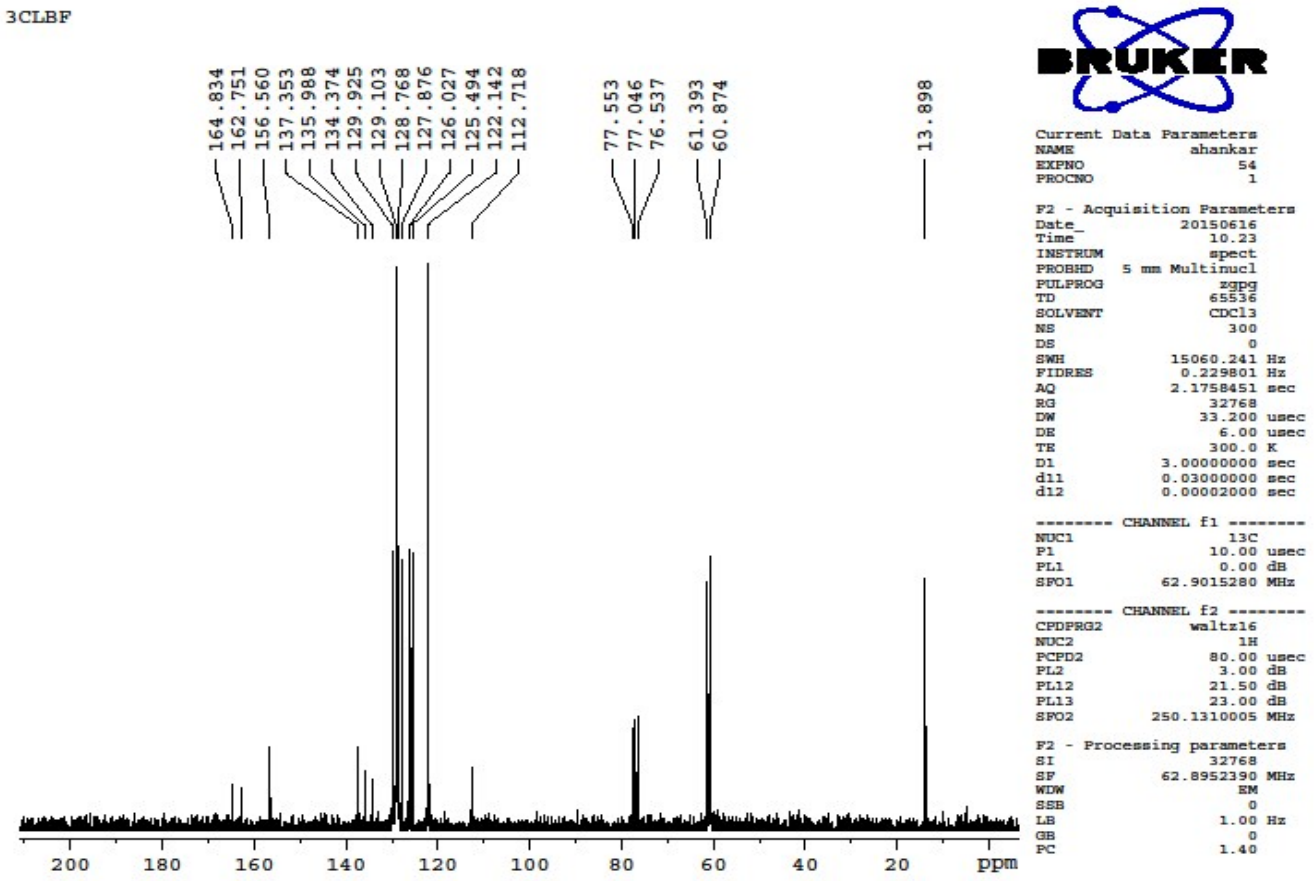

Fig. 15 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 2-(3-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4e).**

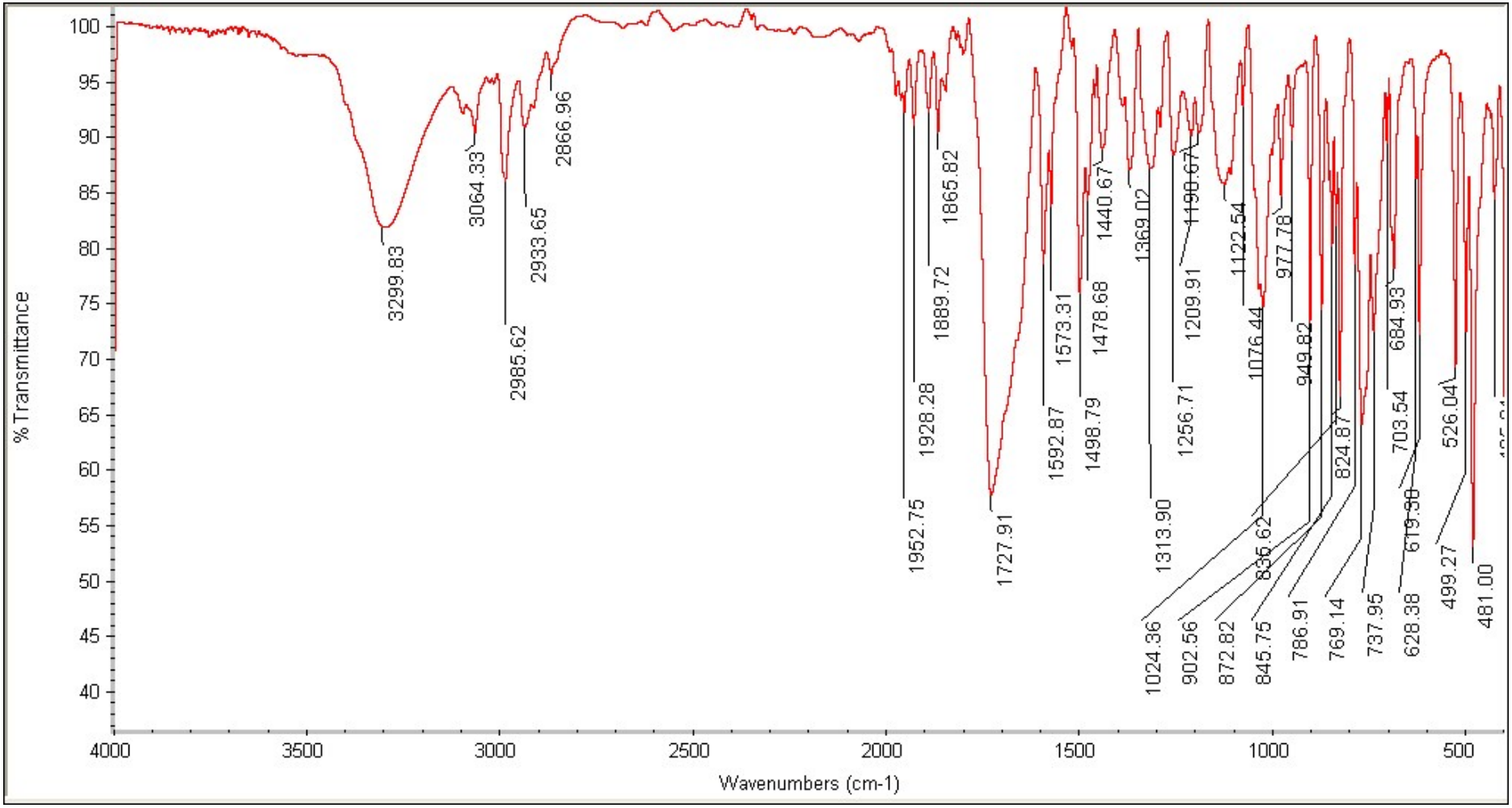

Fig. 16 FT-IR spectrum of Ethyl 2-(2-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4f).**

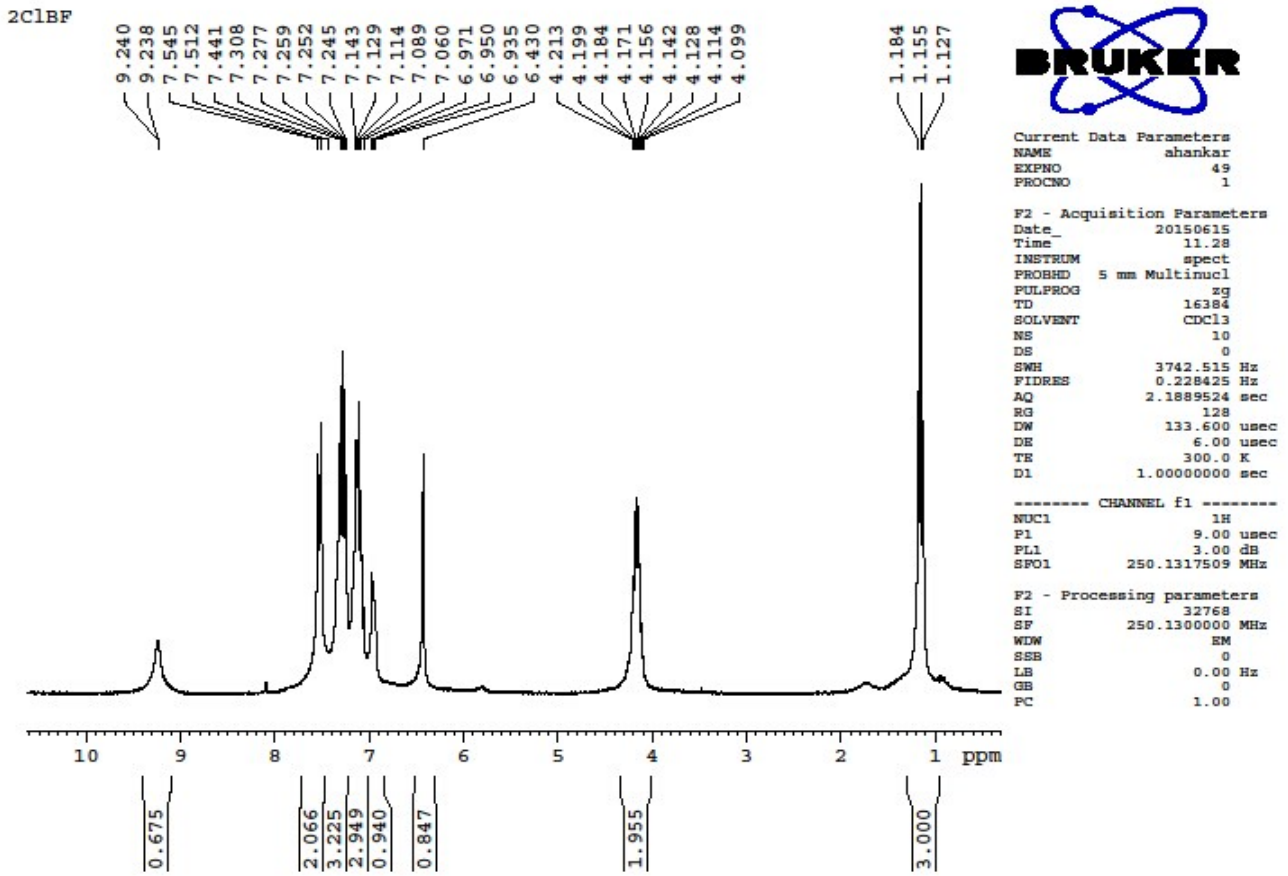

Fig. 17 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 2-(2-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4f).**

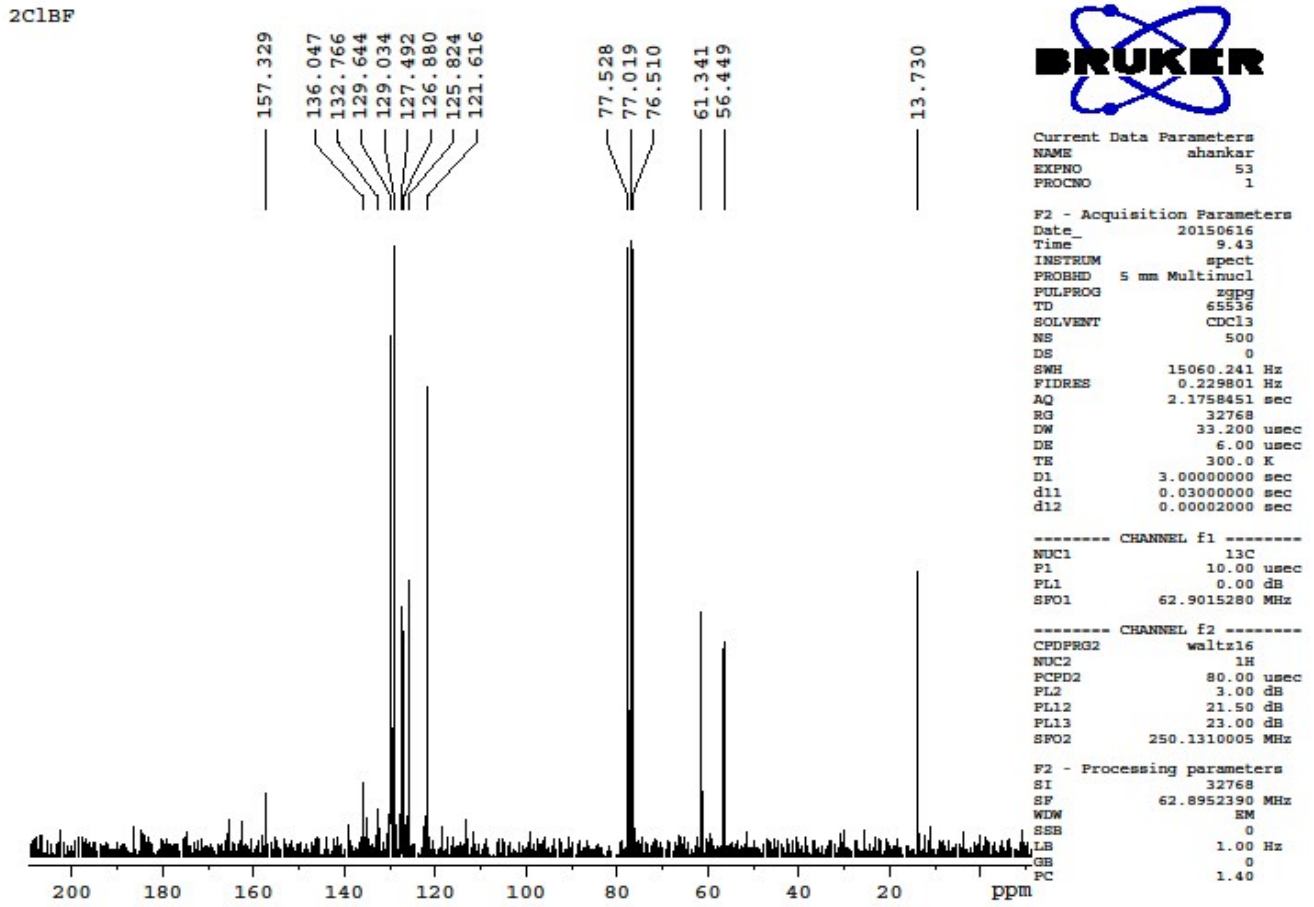

Fig. 18 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 2-(2-chlorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4f).**

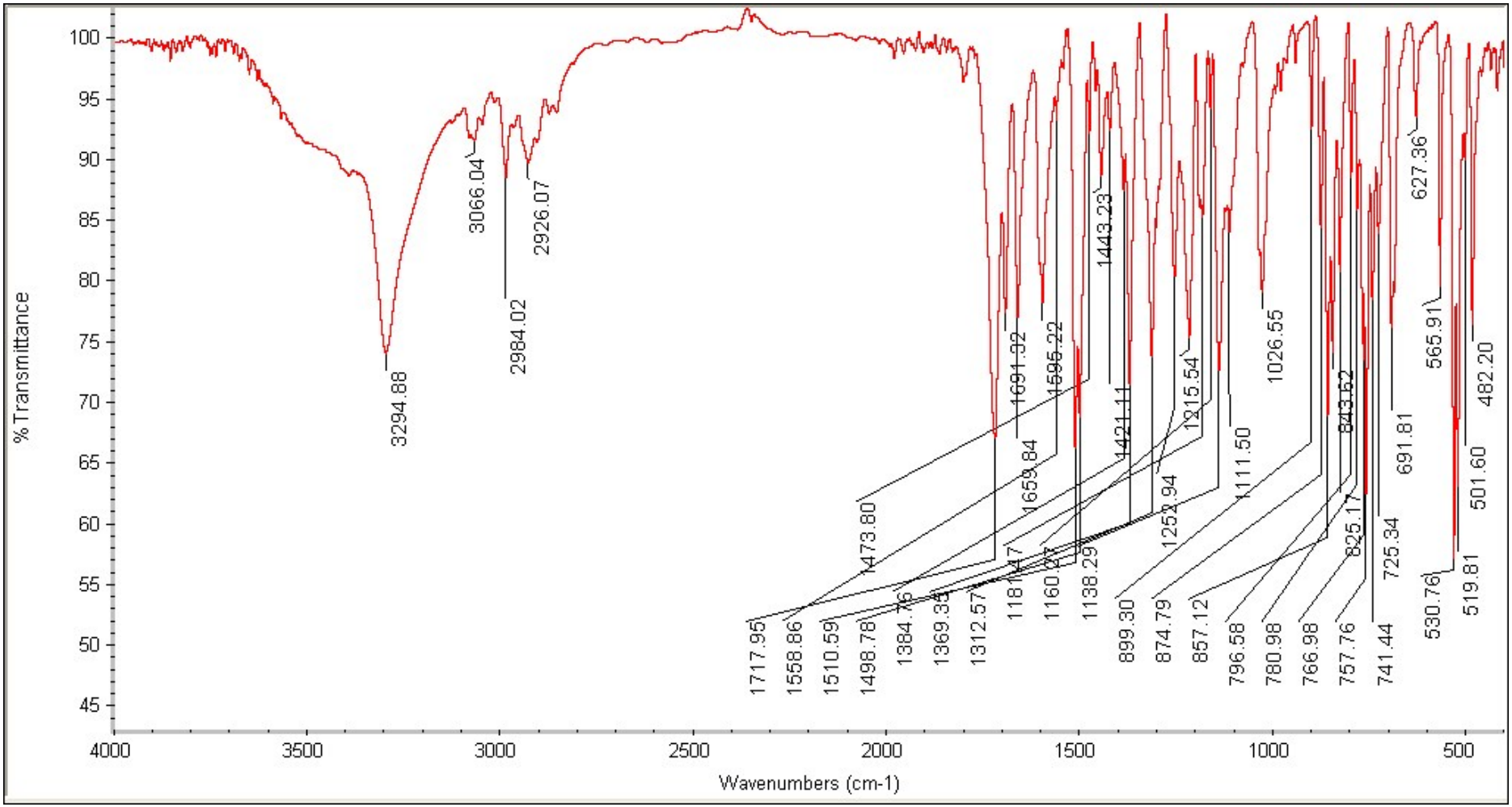

Fig. 19 FT-IR spectrum of Ethyl 2-(4-fluorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4g).**

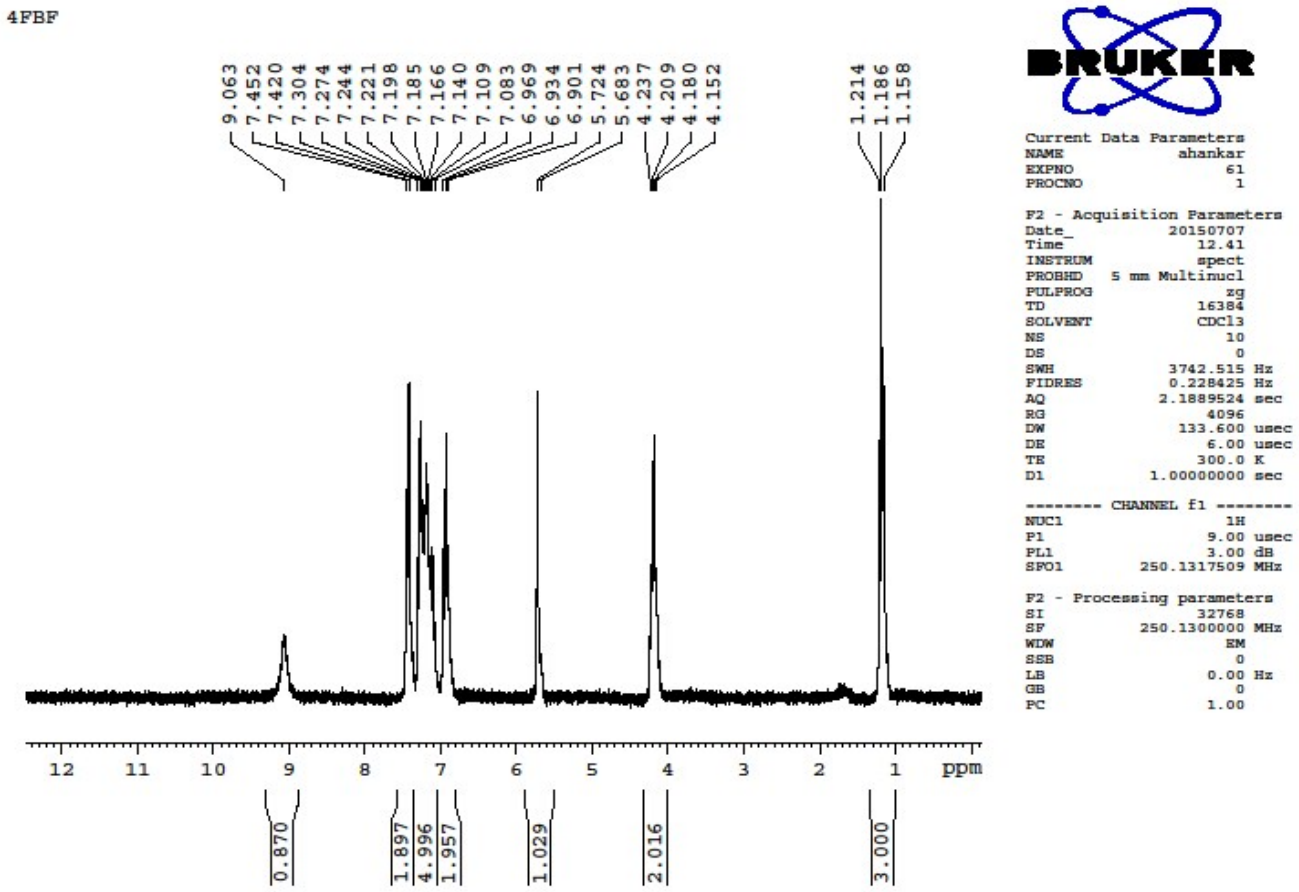

Fig. 20 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 2-(4-fluorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4g).**

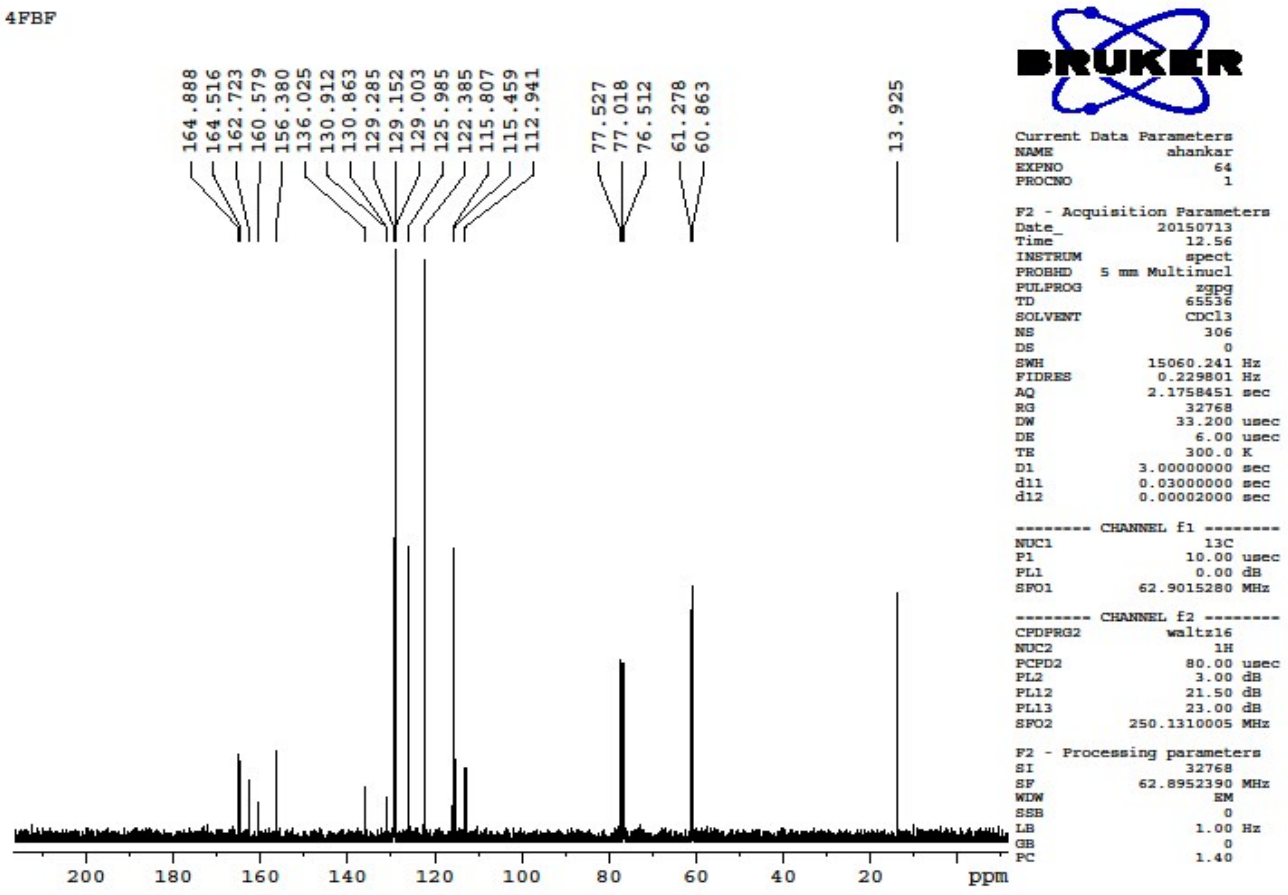

Fig. 21 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 2-(4-fluorophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4g).**

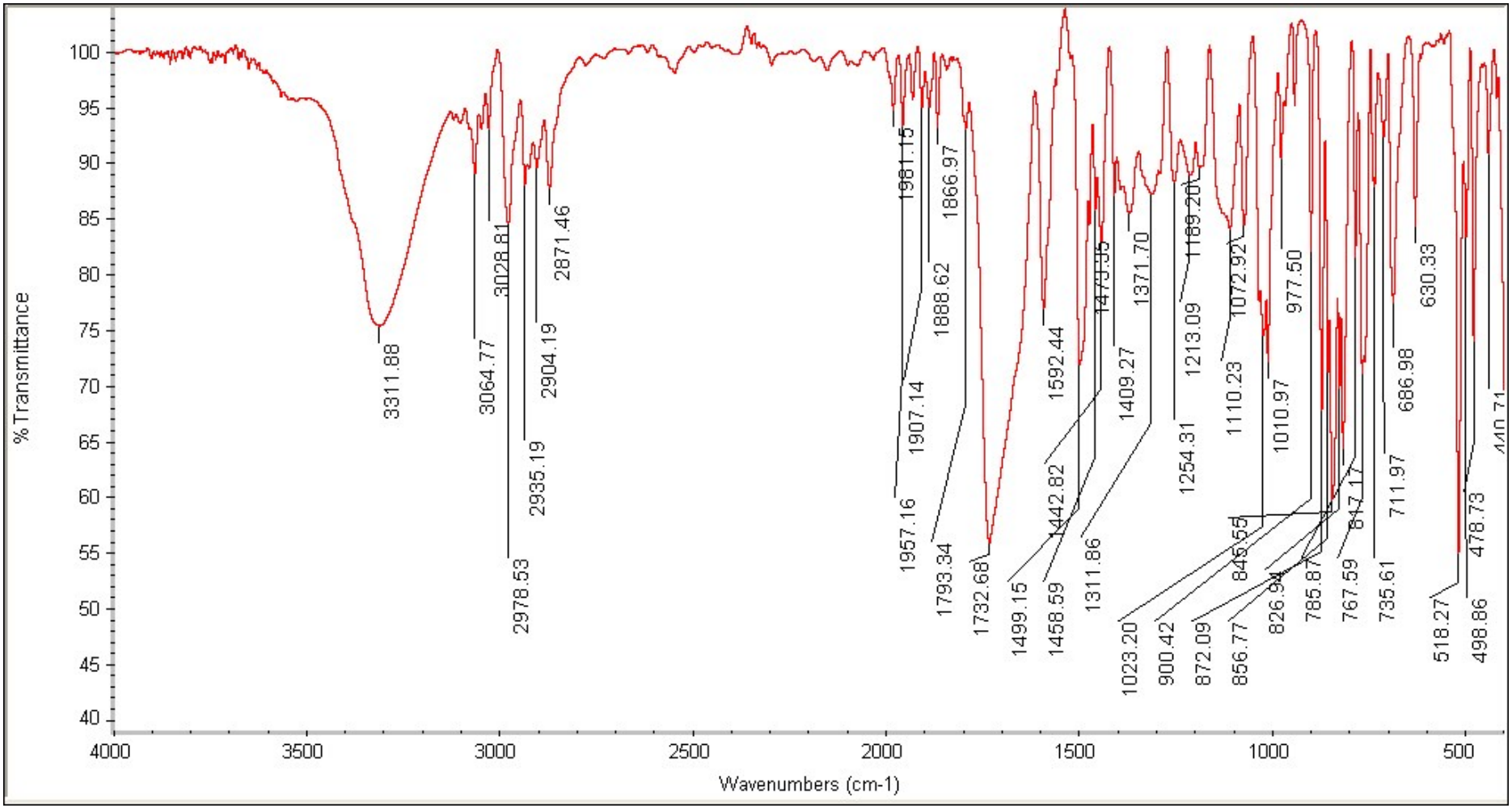

Fig. 22 FT-IR spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4h).**

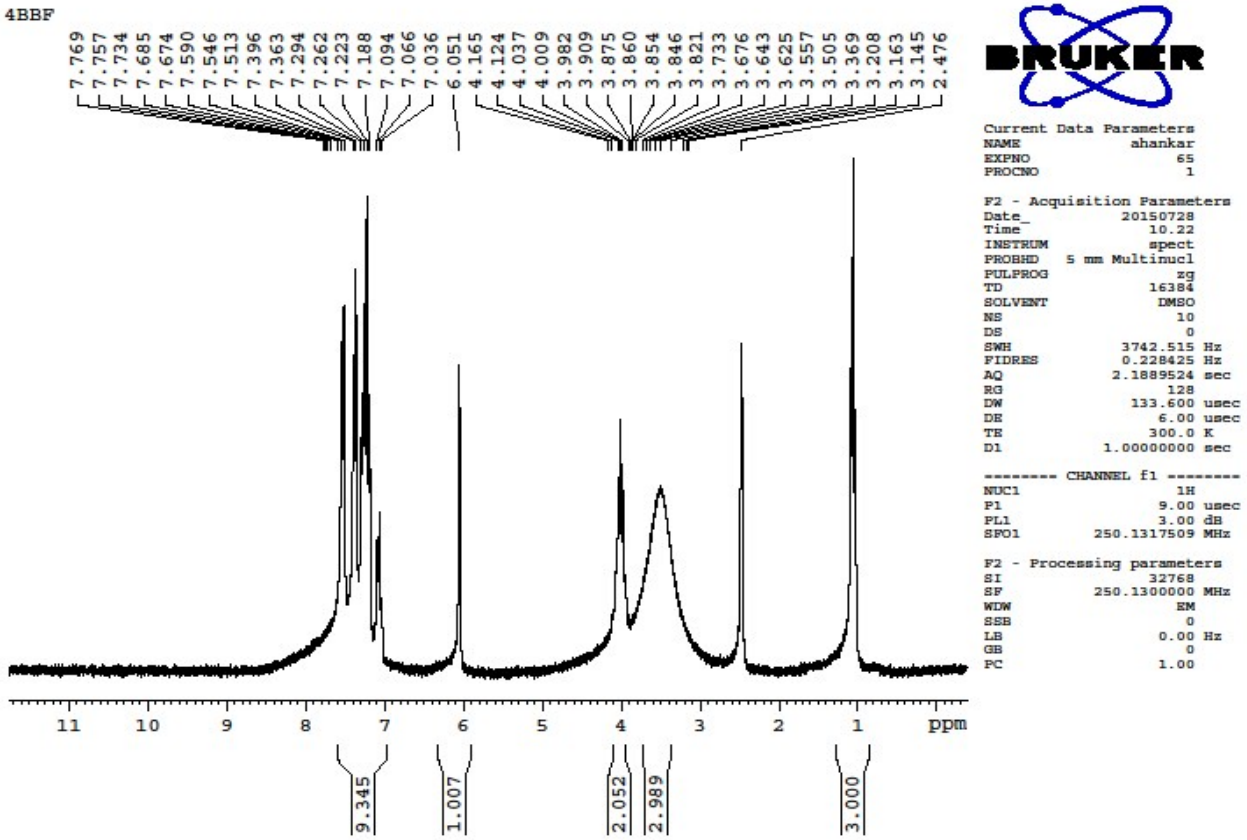

Fig. 23 ^{1}H NMR (250.13 MHz, DMSO-d_6) spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4h).**

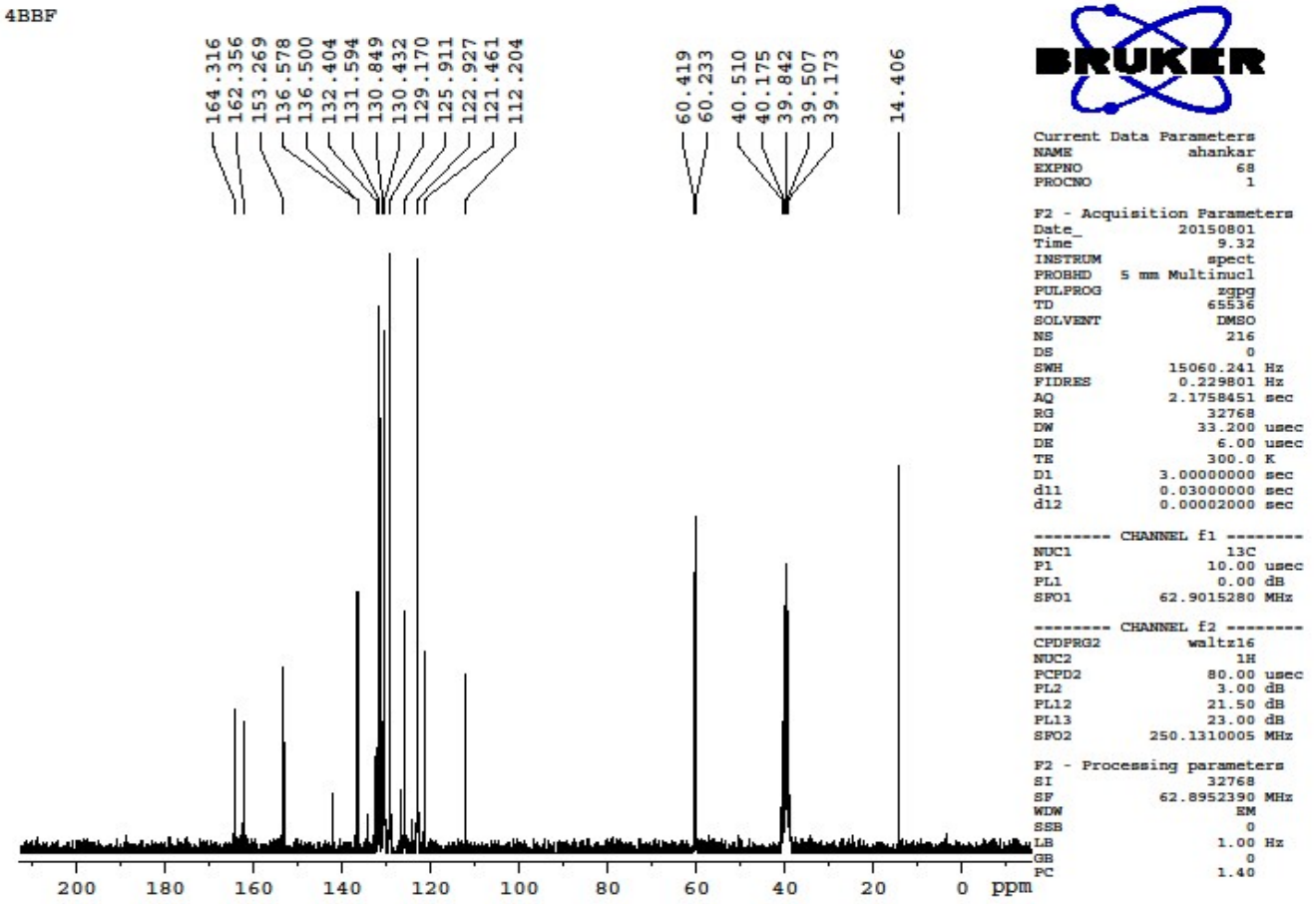

Fig. 24 ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4h).**

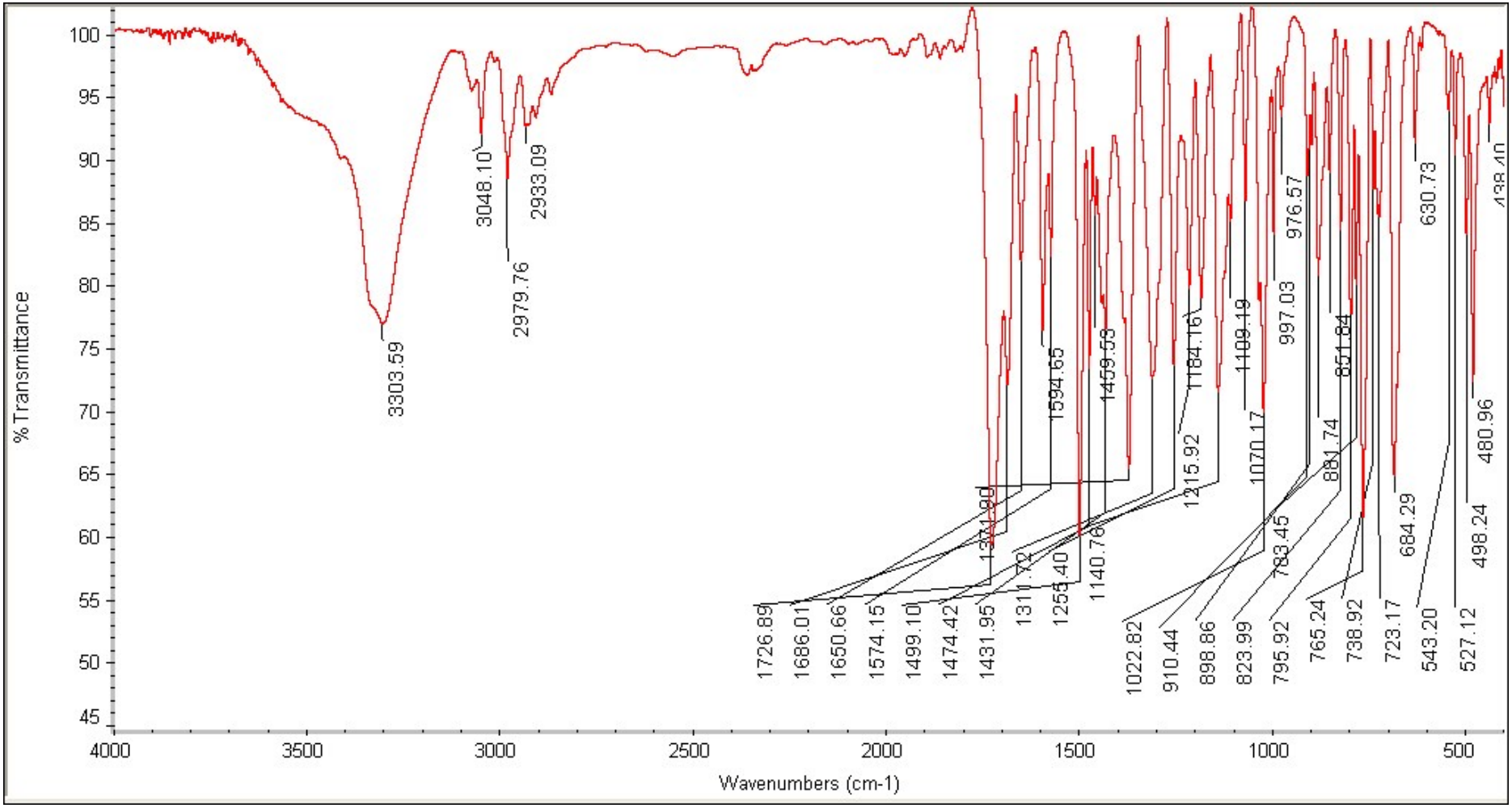

Fig. 25 FT-IR spectrum of Ethyl 2-(3-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4i).**

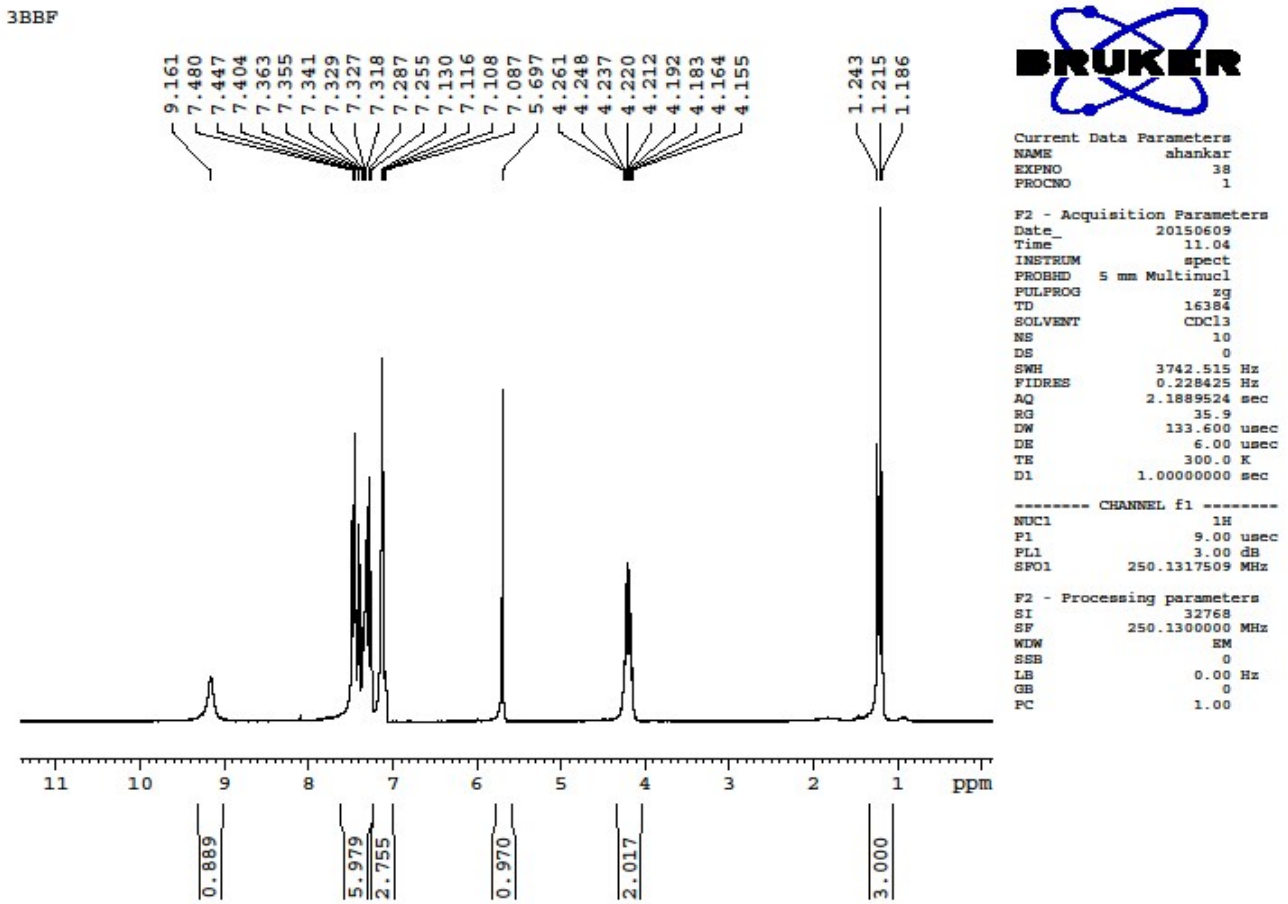

Fig. 26 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 2-(3-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4i).**

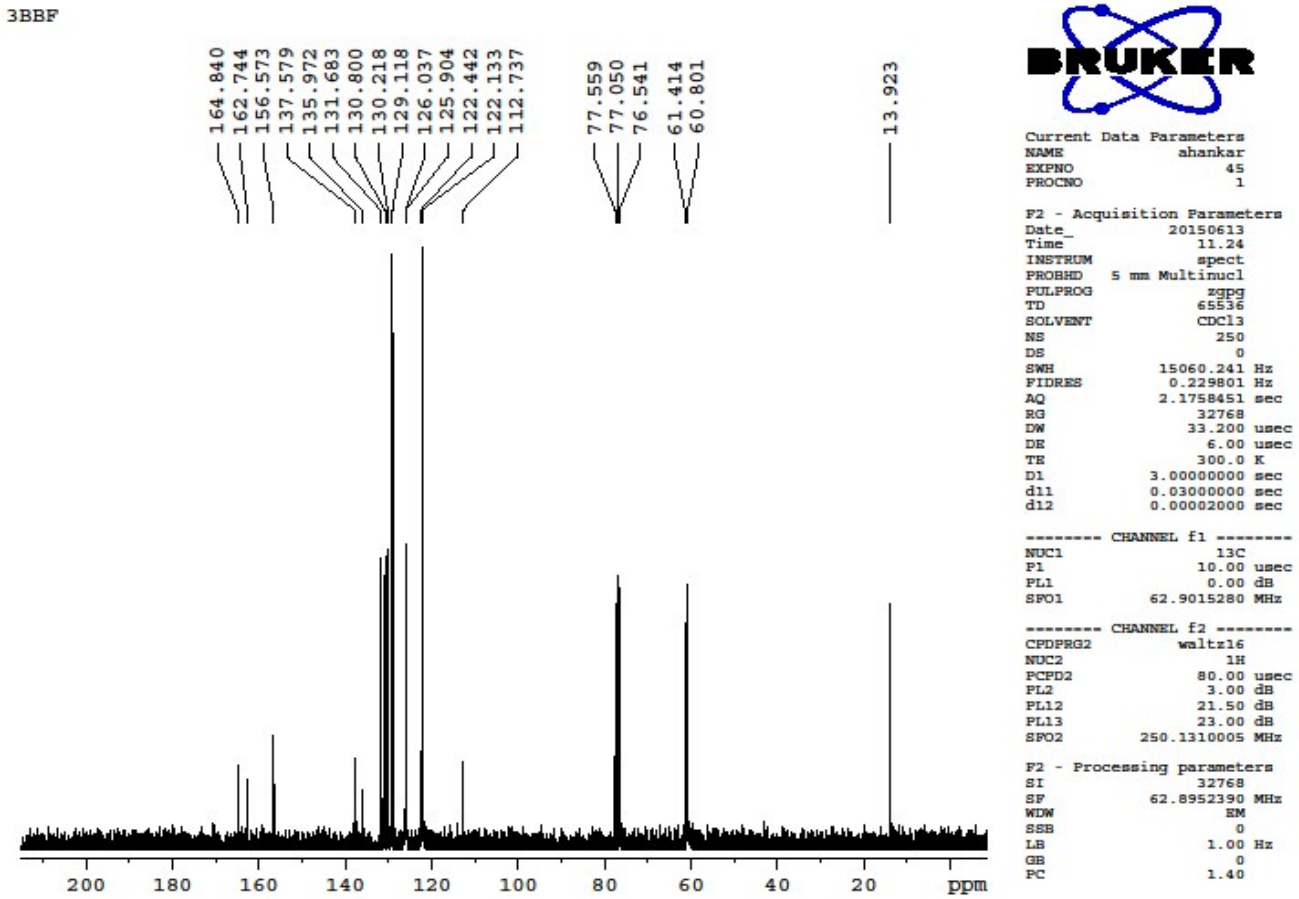

Fig. 27 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 2-(4-bromophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4i).**

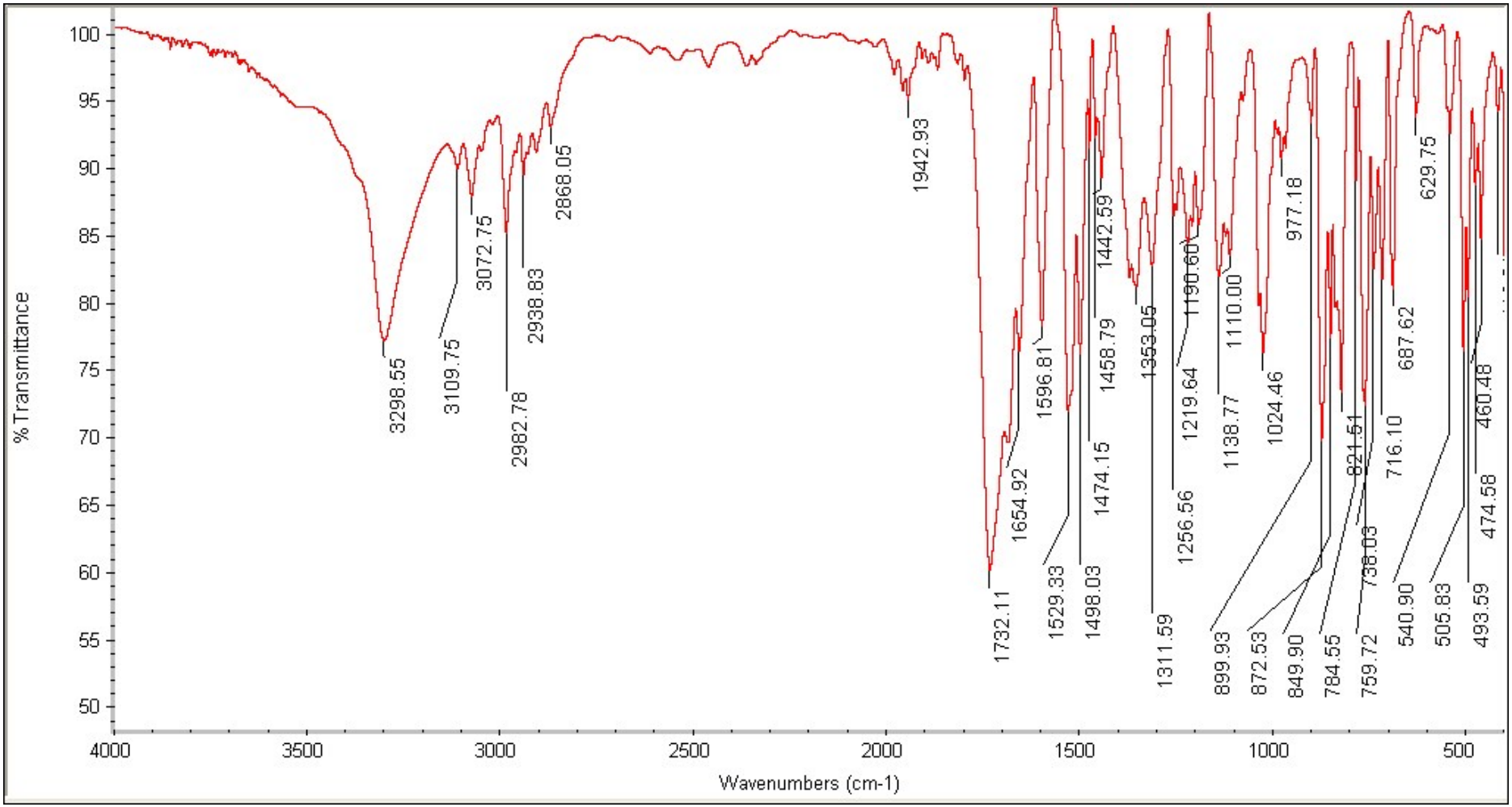

Fig. 28 FT-IR spectrum of Ethyl 2-(4-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4j).**

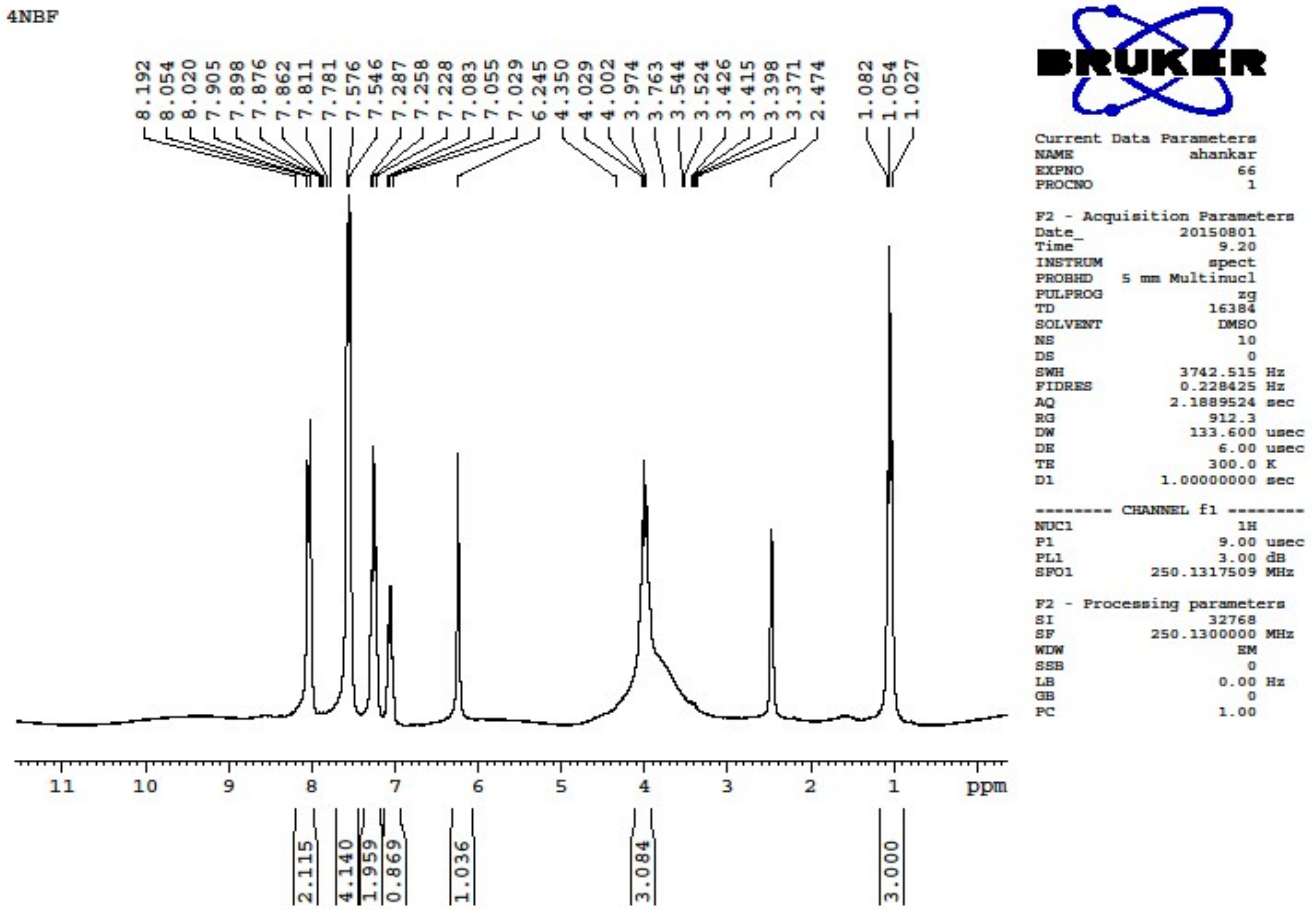

Fig. 29 ^{1}H NMR (250.13 MHz, DMSO-d_6) spectrum of Ethyl 2-(4-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4j).**

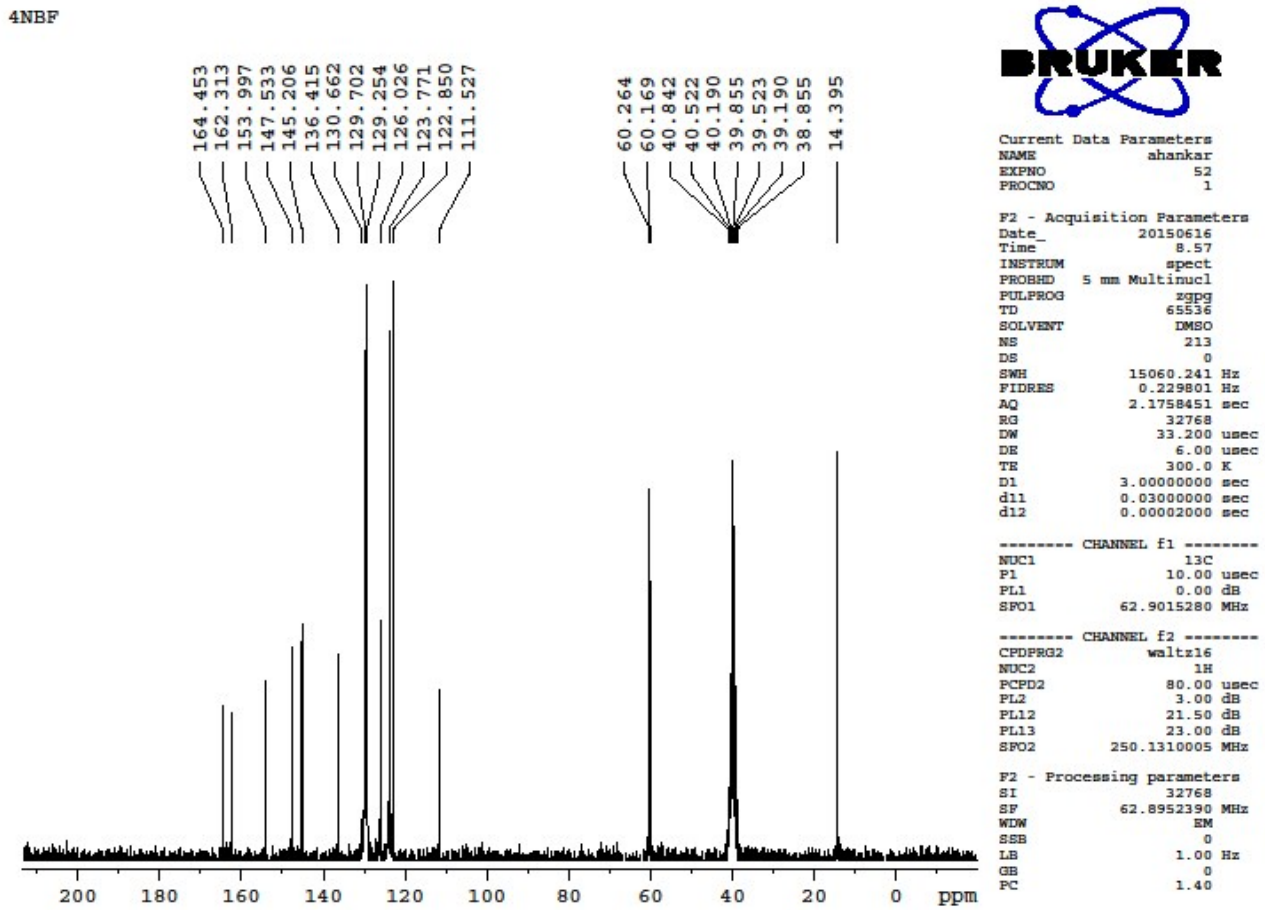

Fig. 30 ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(4-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4j).**

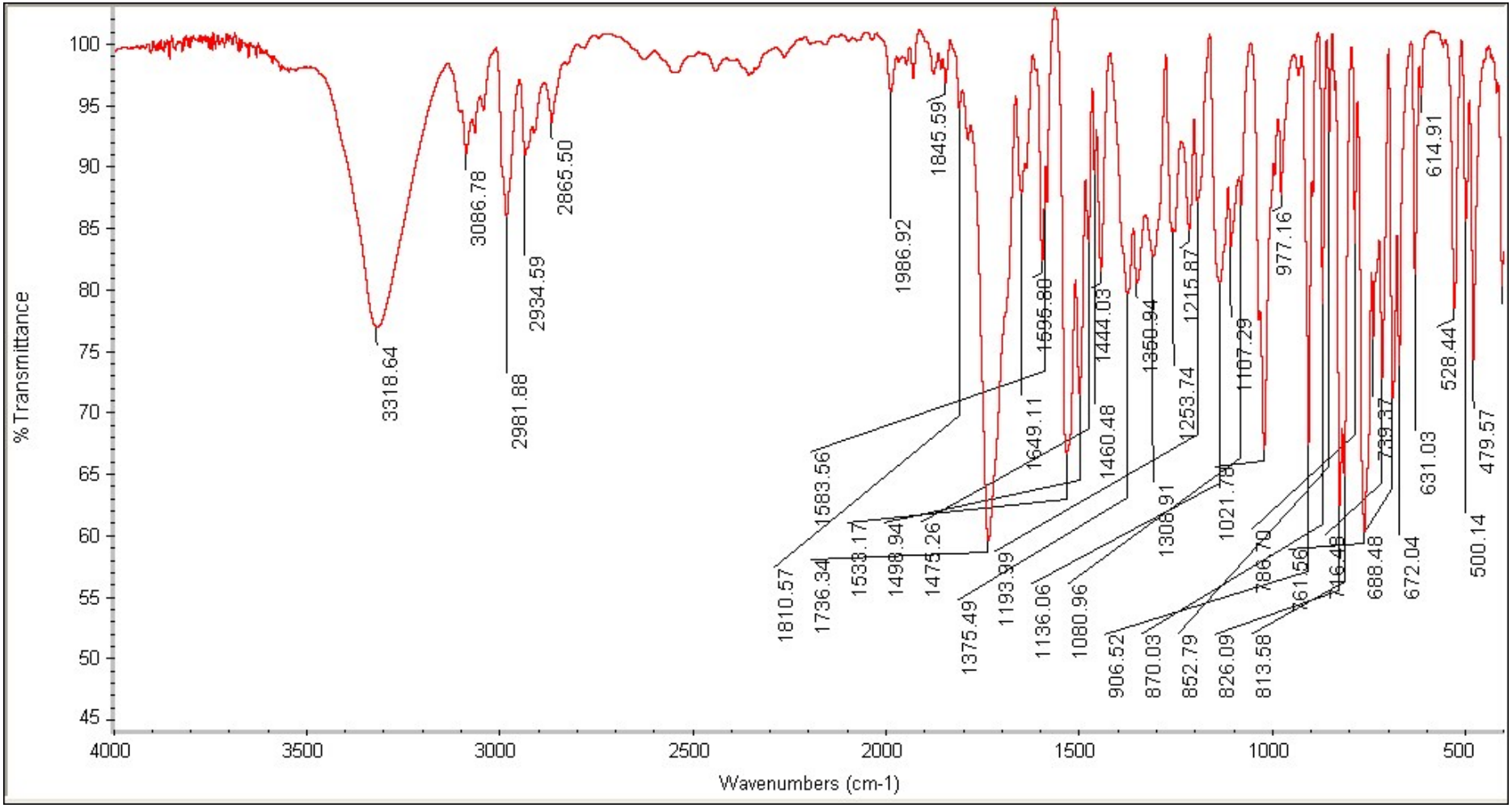

Fig. 31 FT-IR spectrum of Ethyl 2-(3-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4k).**

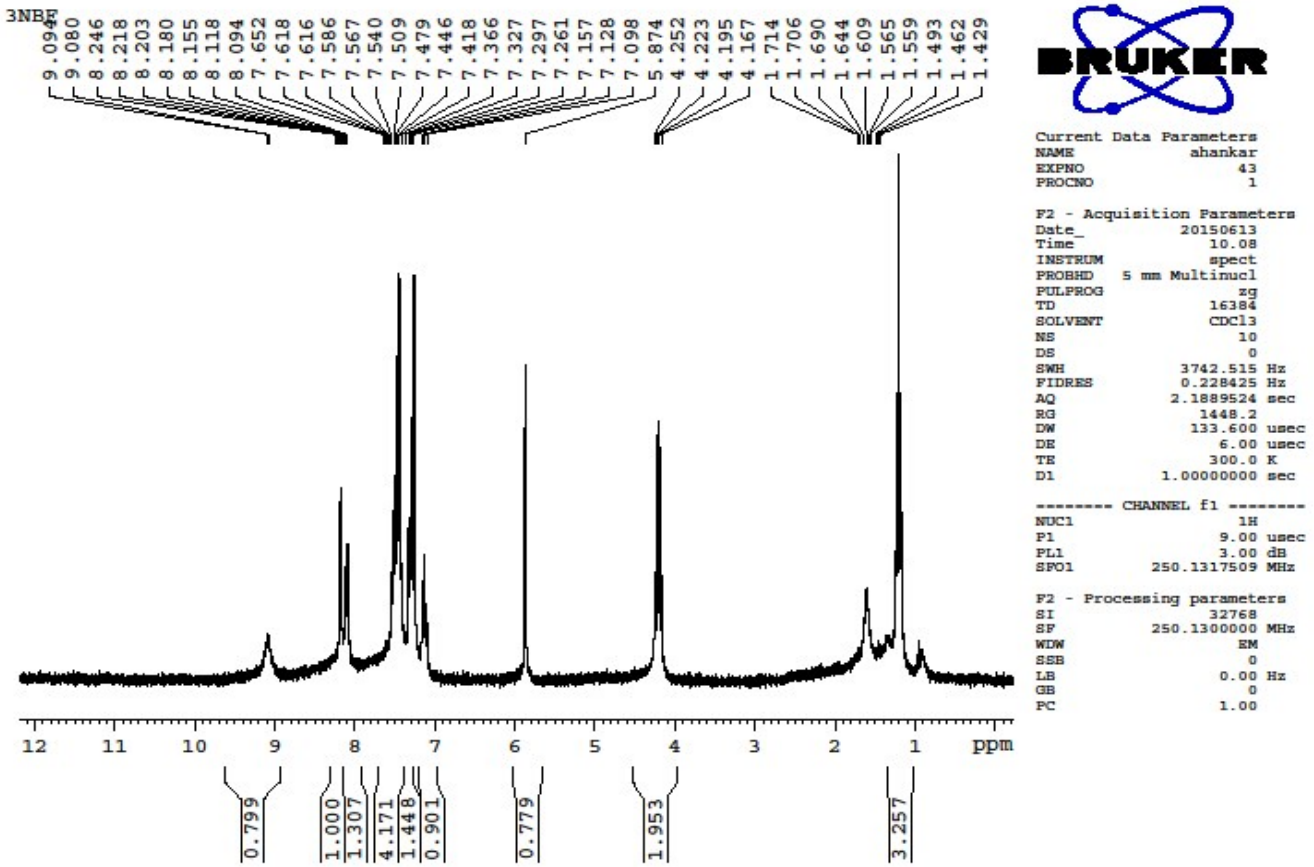

Fig. 32 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 2-(3-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4k).**

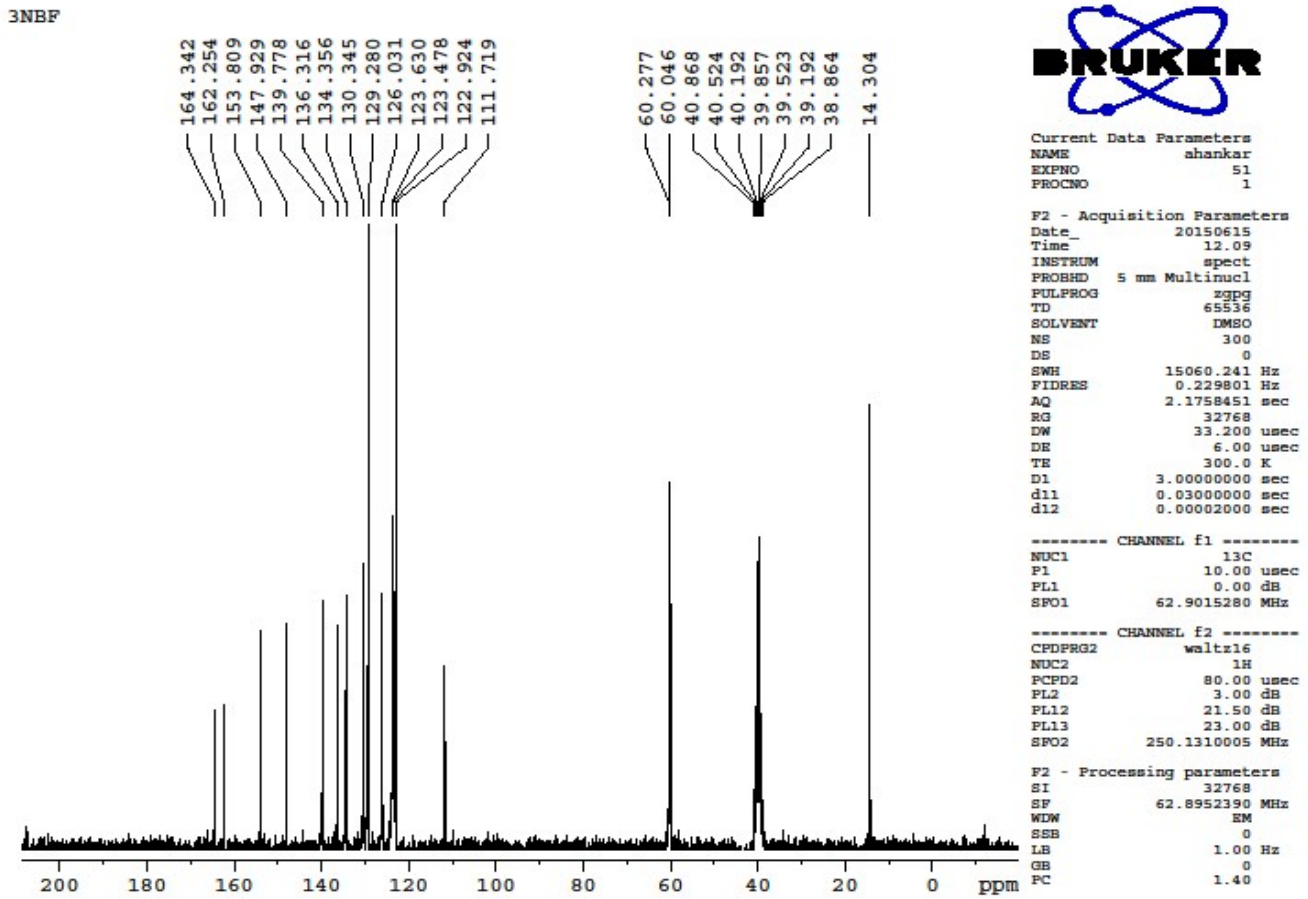

Fig. 33 ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(3-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4k).**

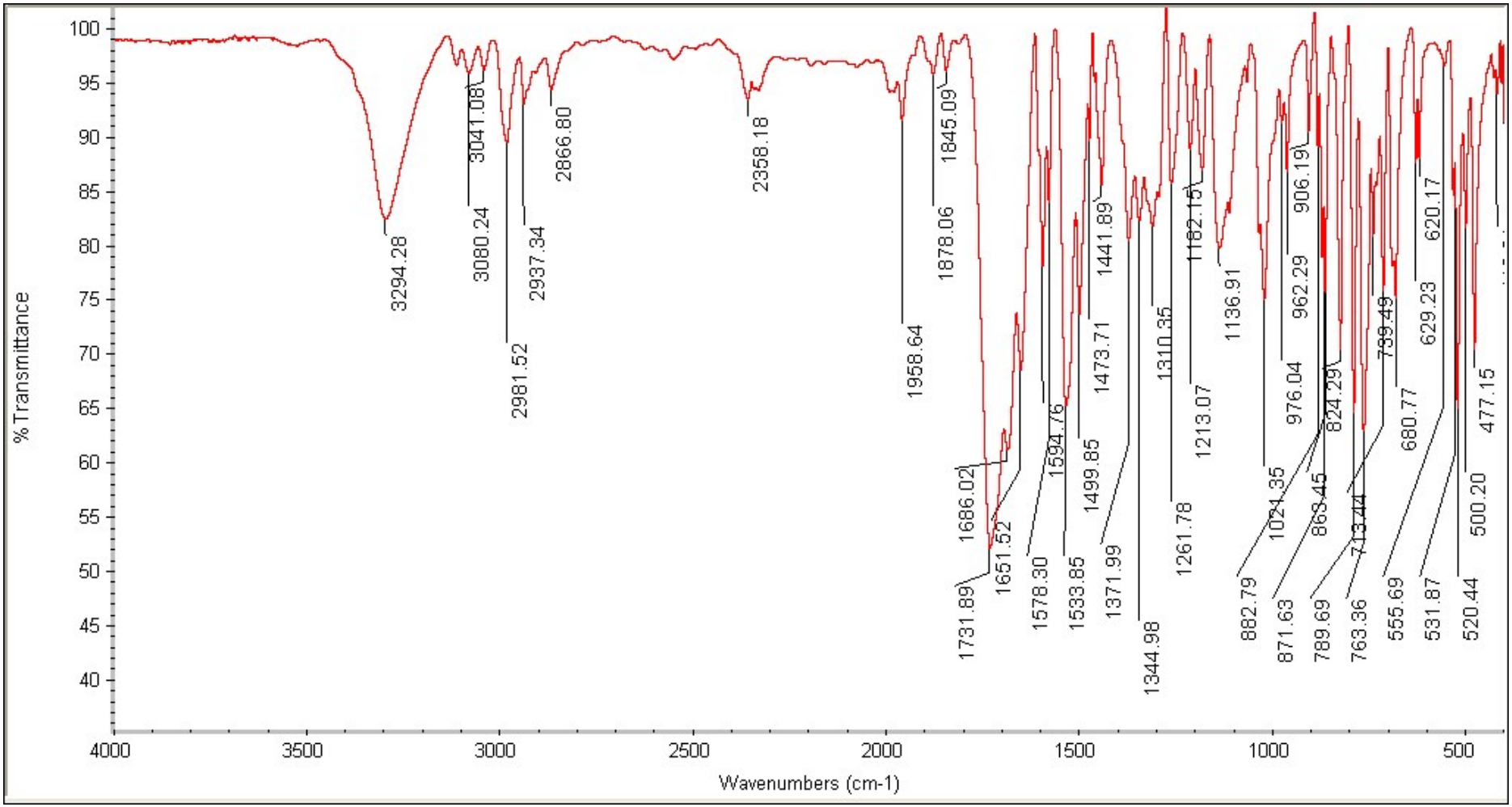

Fig. 34 FT-IR spectrum of Ethyl 2-(2-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4l).**

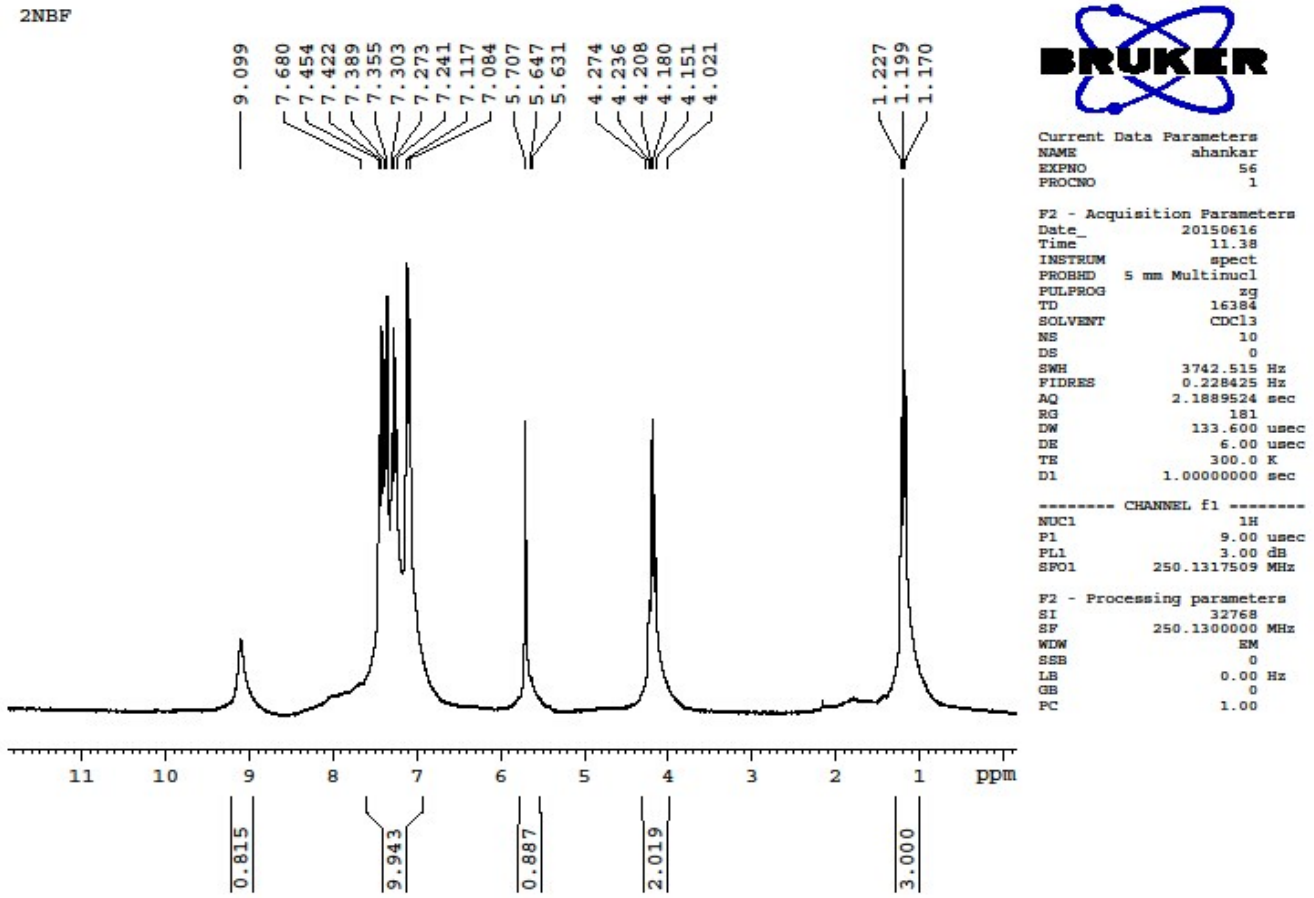

Fig. 35 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 2-(2-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4l).**

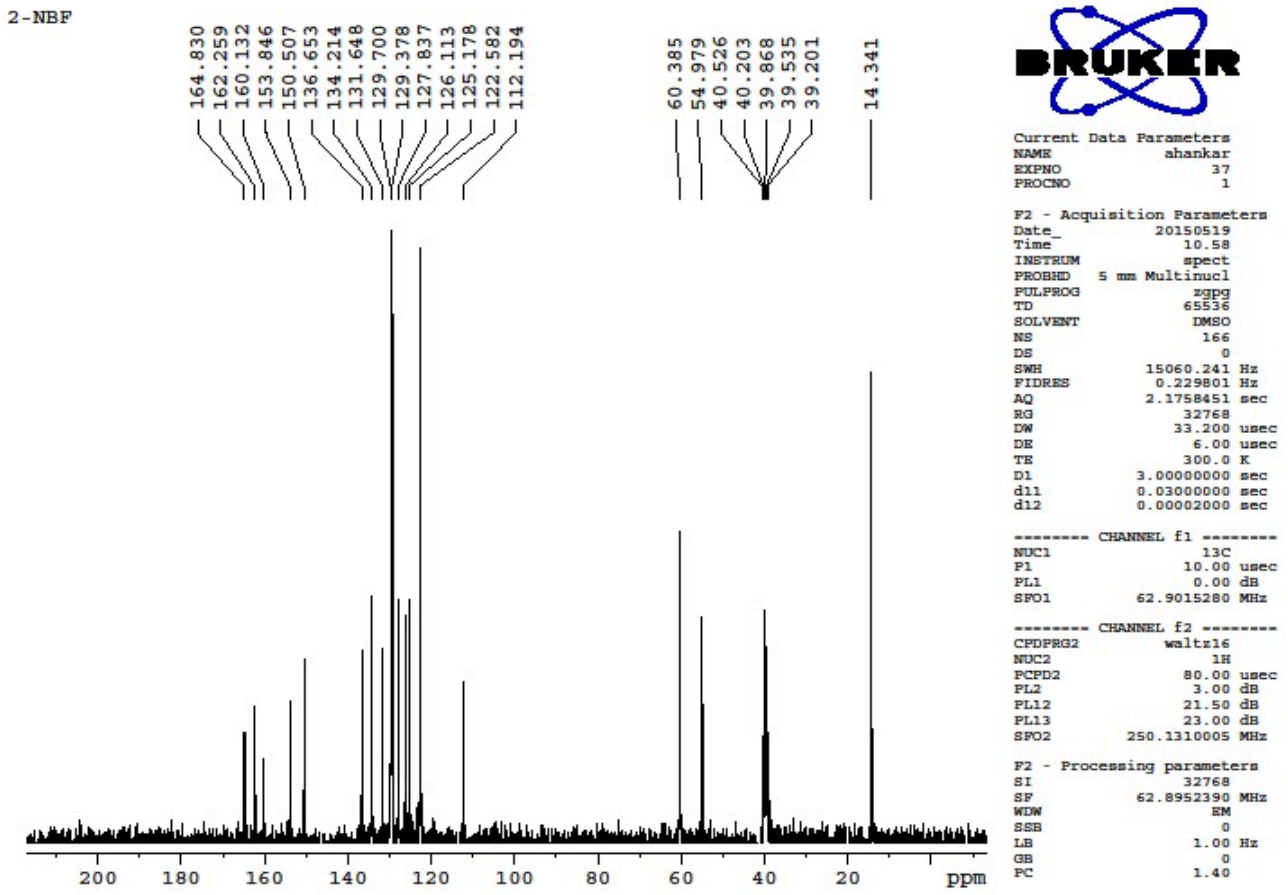

Fig. 36 ^{13}C NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 2-(2-nitrophenyl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4l).**

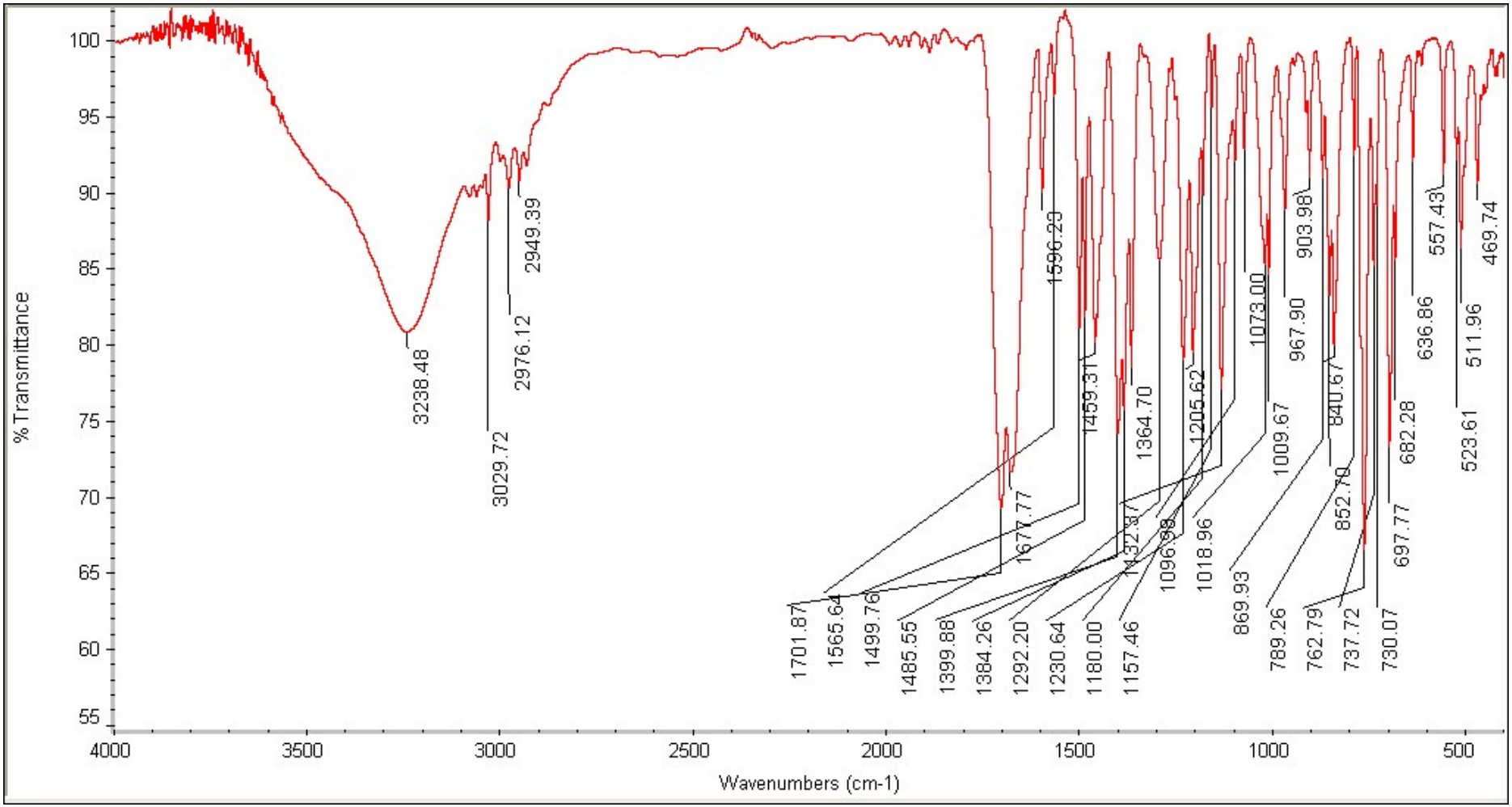

Fig. 37 FT-IR spectrum of Ethyl 2-([1,1'-biphenyl]-4-yl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4m).**

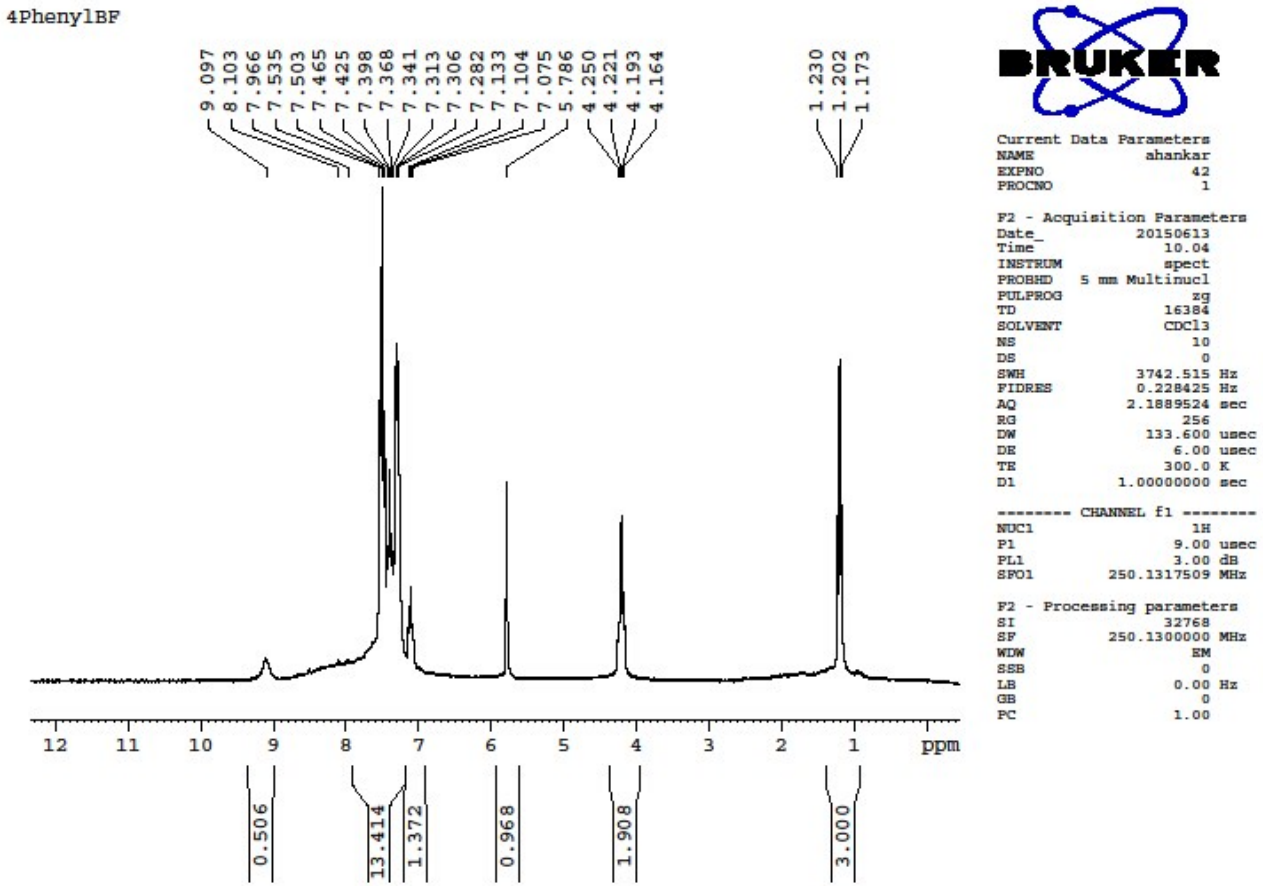

Fig. 38 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 2-([1,1'-biphenyl]-4-yl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4m).**

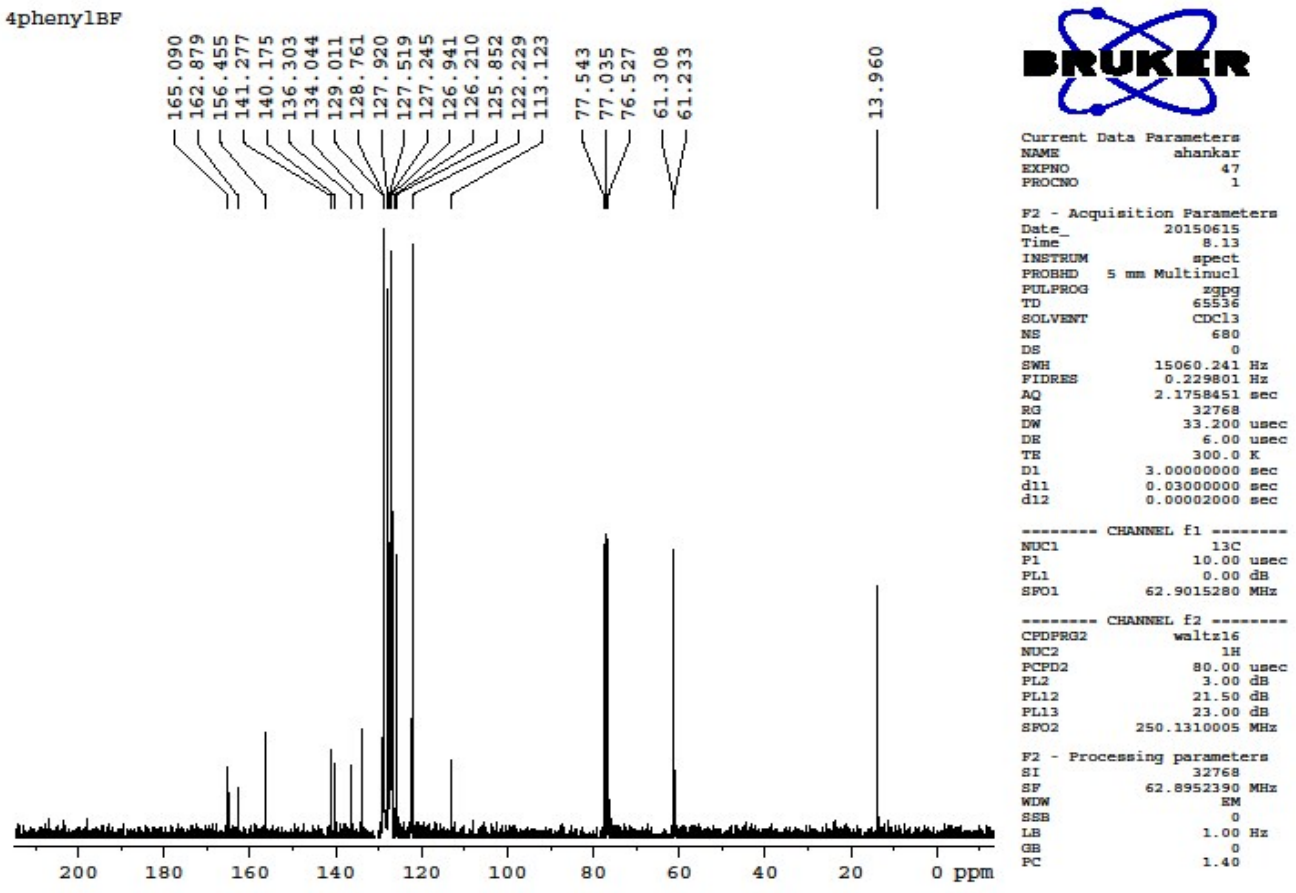

Fig. 39 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 2-([1,1'-biphenyl]-4-yl)-4-hydroxy-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4m).**

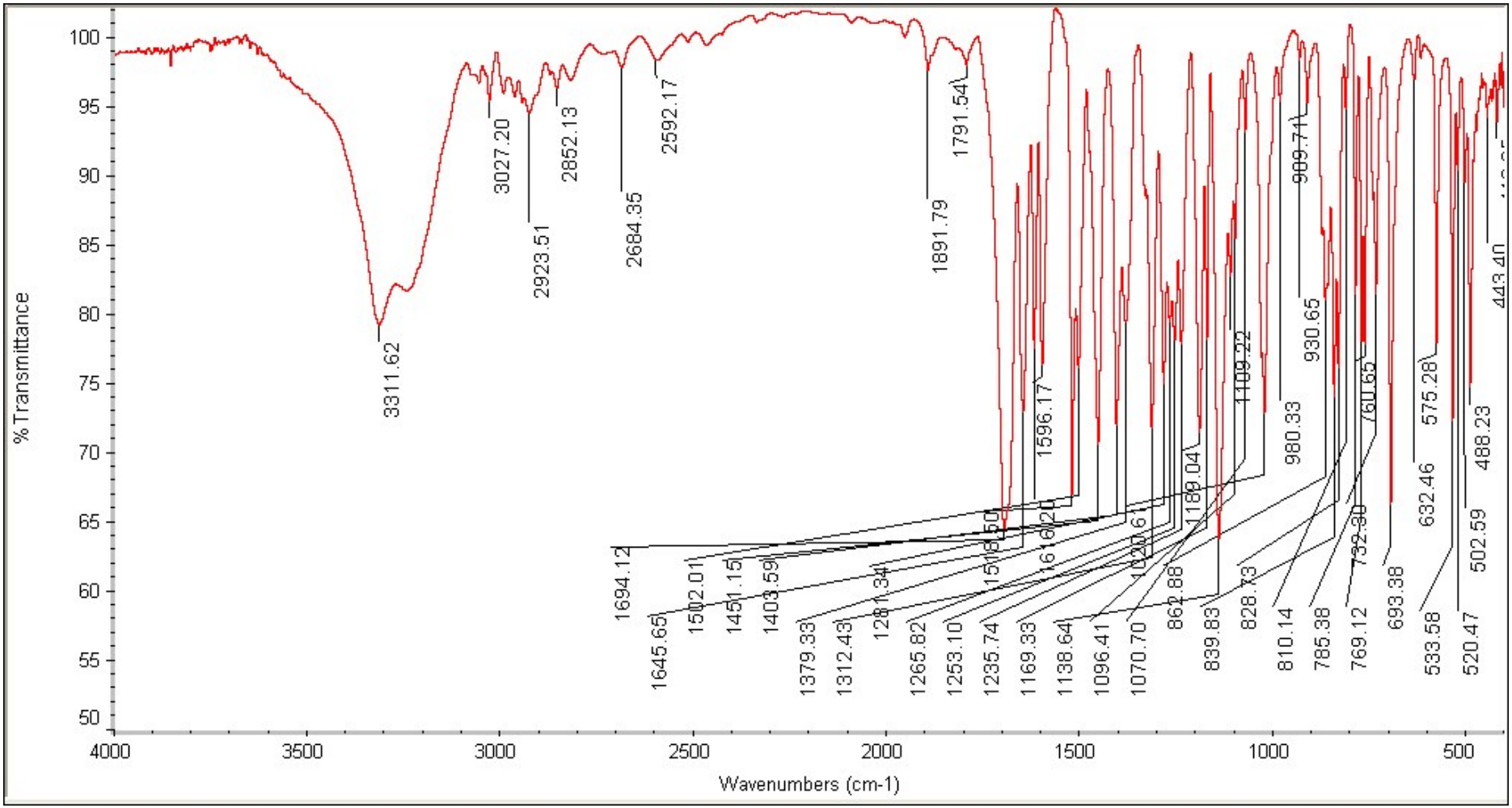

Fig. 40 FT-IR spectrum of Ethyl 4-hydroxy-2-(4-hydroxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4n).**

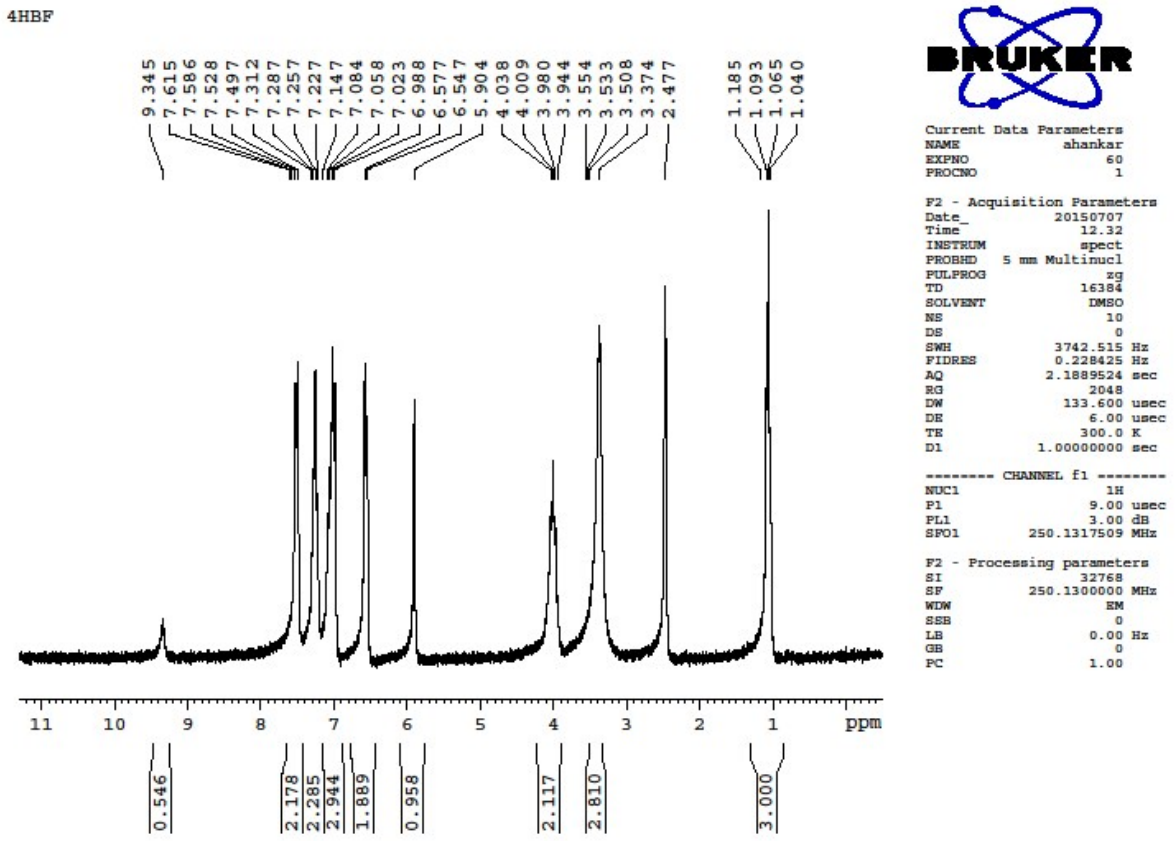

Fig. 41 ^{1}H NMR (250.13 MHz, DMSO-d_6) spectrum of Ethyl 4-hydroxy-2-(4-hydroxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4n).**

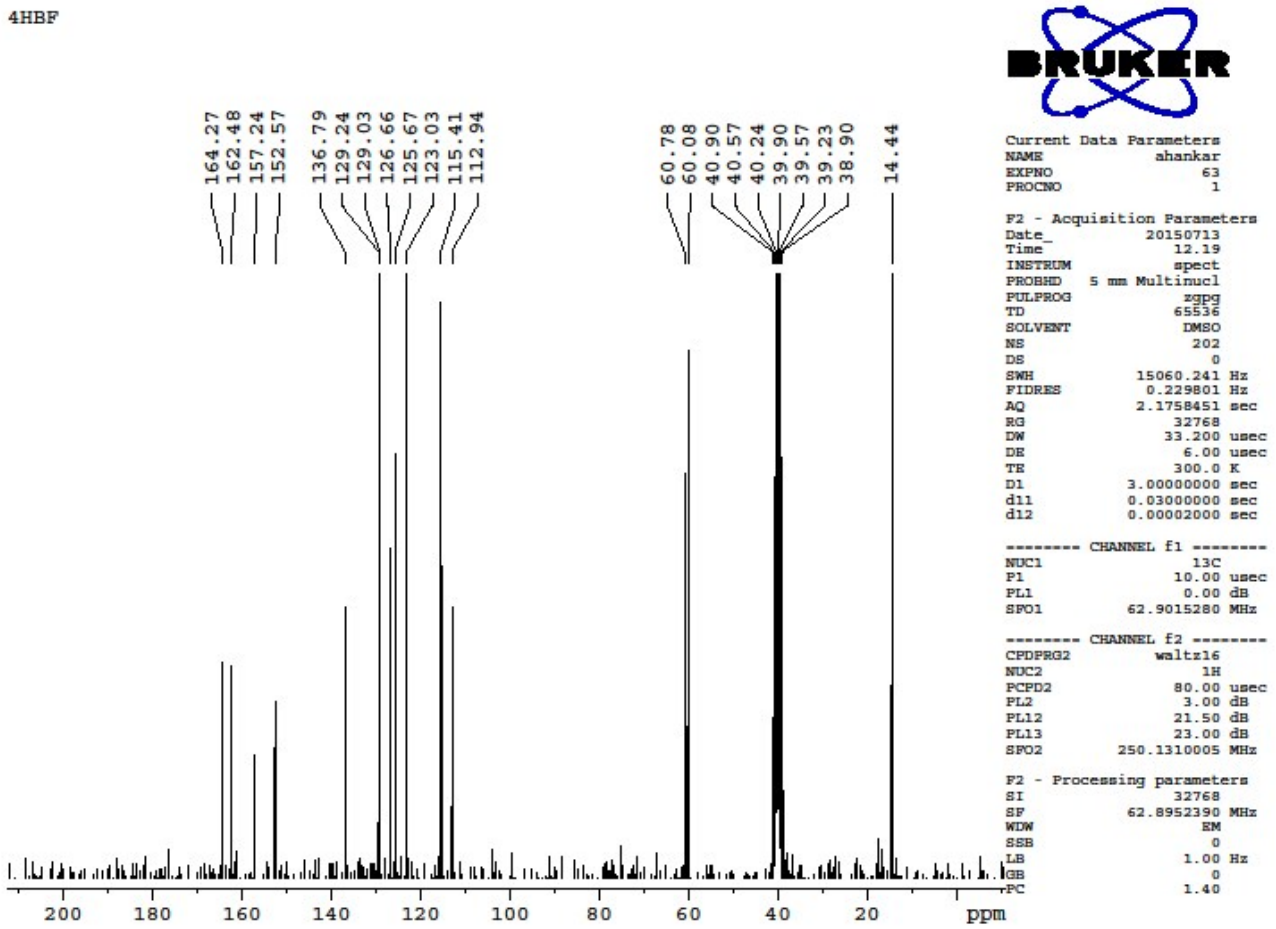

Fig. 42 ^{1}H NMR (62.90 MHz, DMSO-d_6) spectrum of Ethyl 4-hydroxy-2-(4-hydroxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate **(4n).**

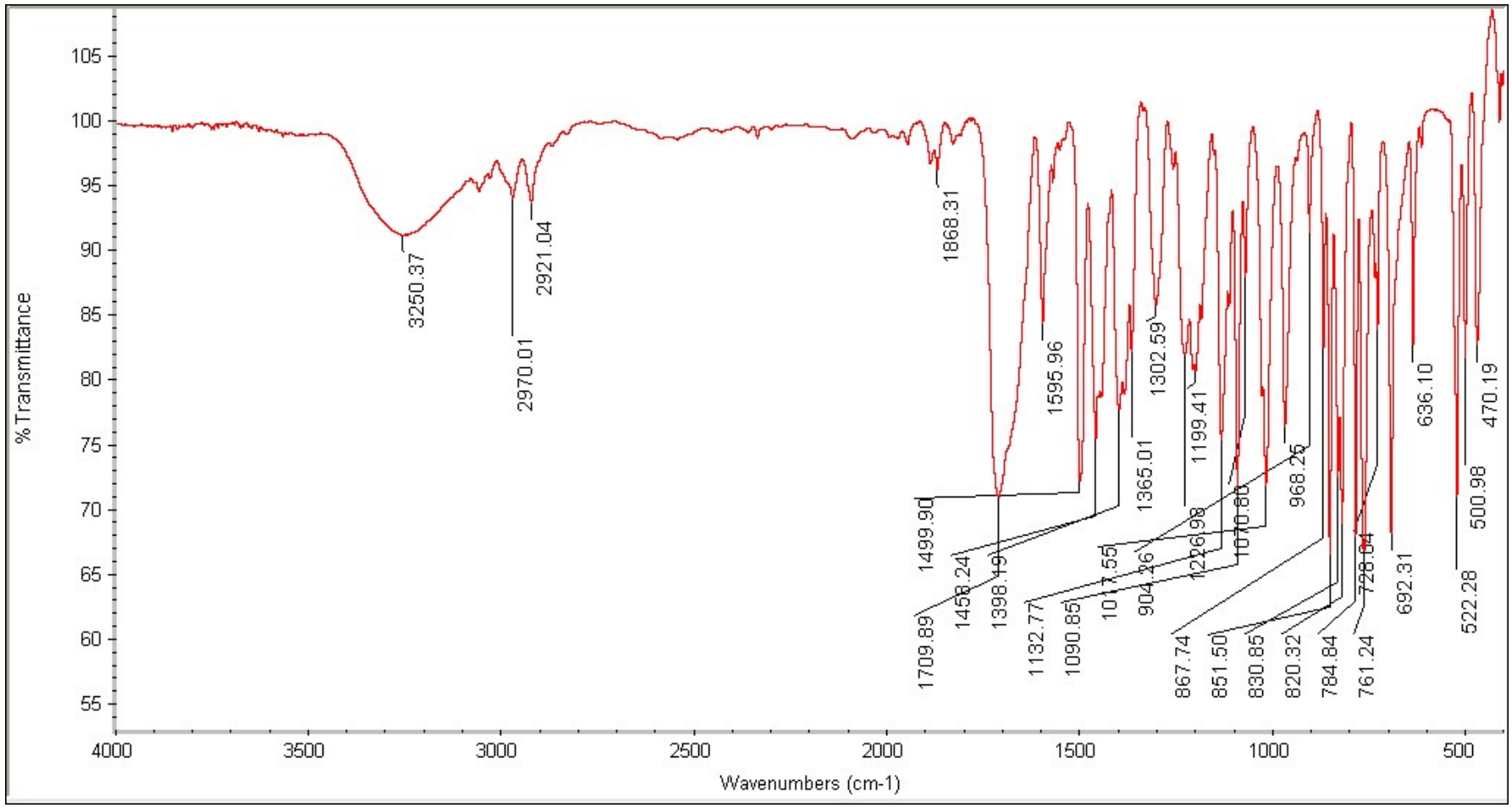

Fig. 43 FT-IR spectrum of Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4o**).

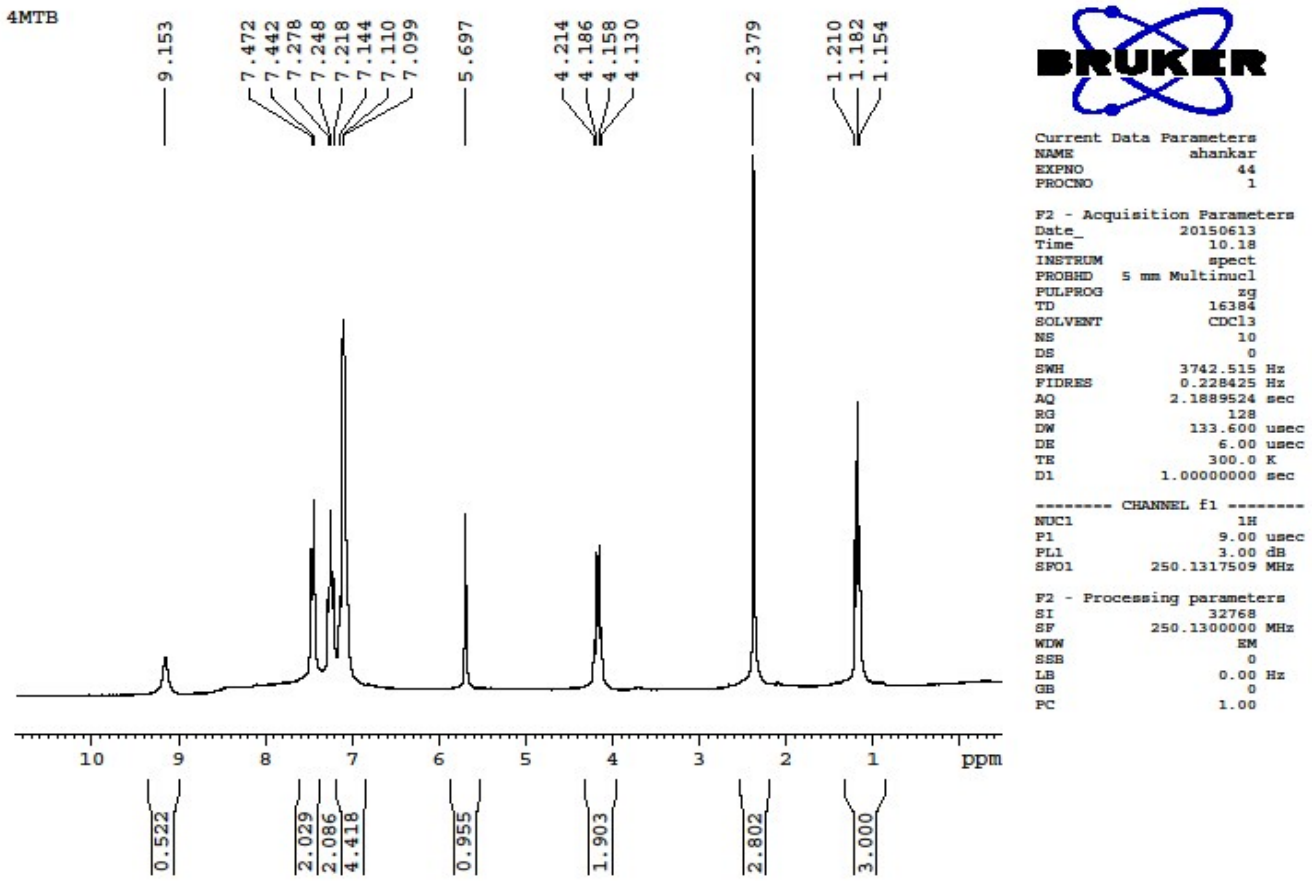

Fig. 44 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4o**).

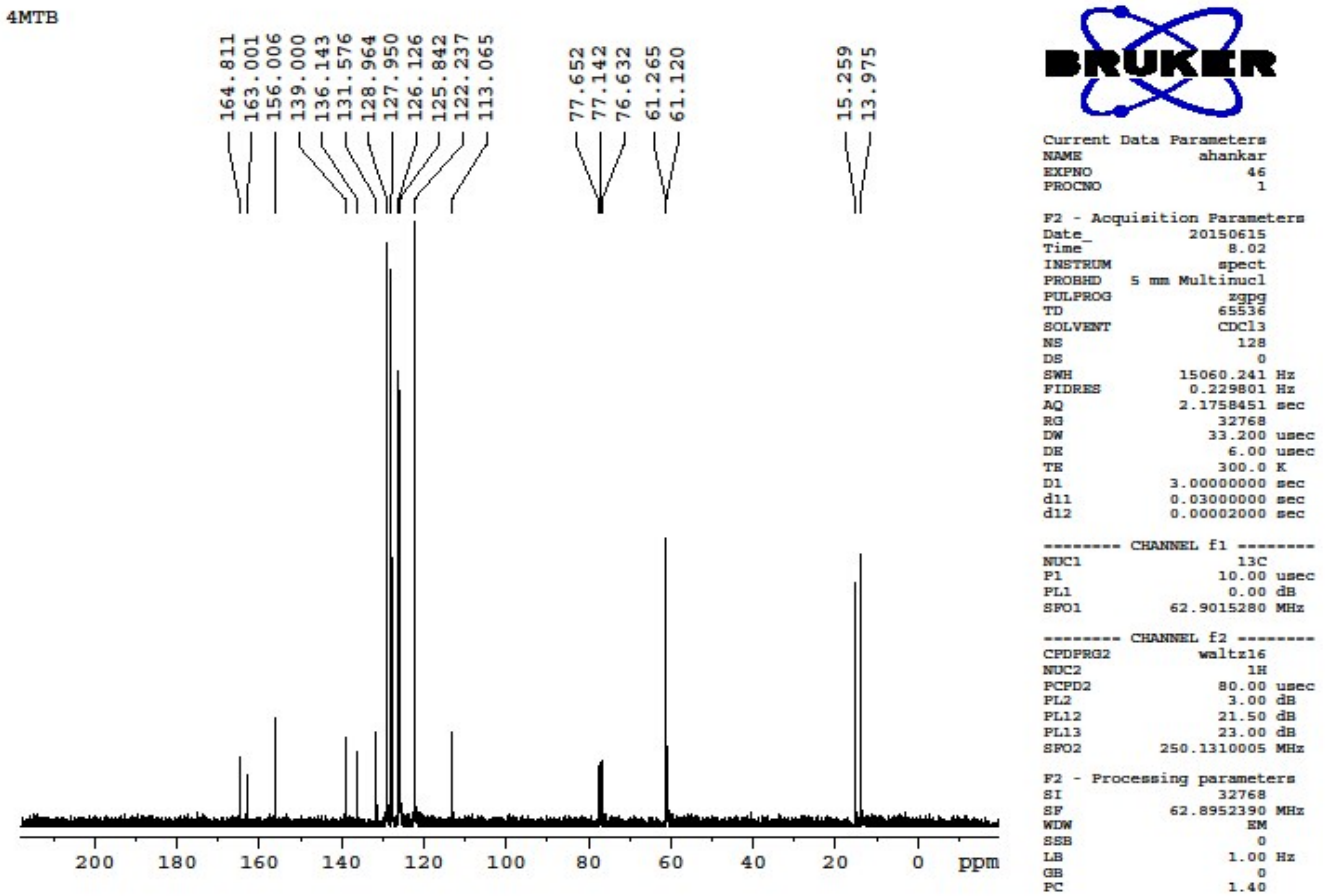

Fig. 45 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-2-(4-(methylthio)phenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4o**)

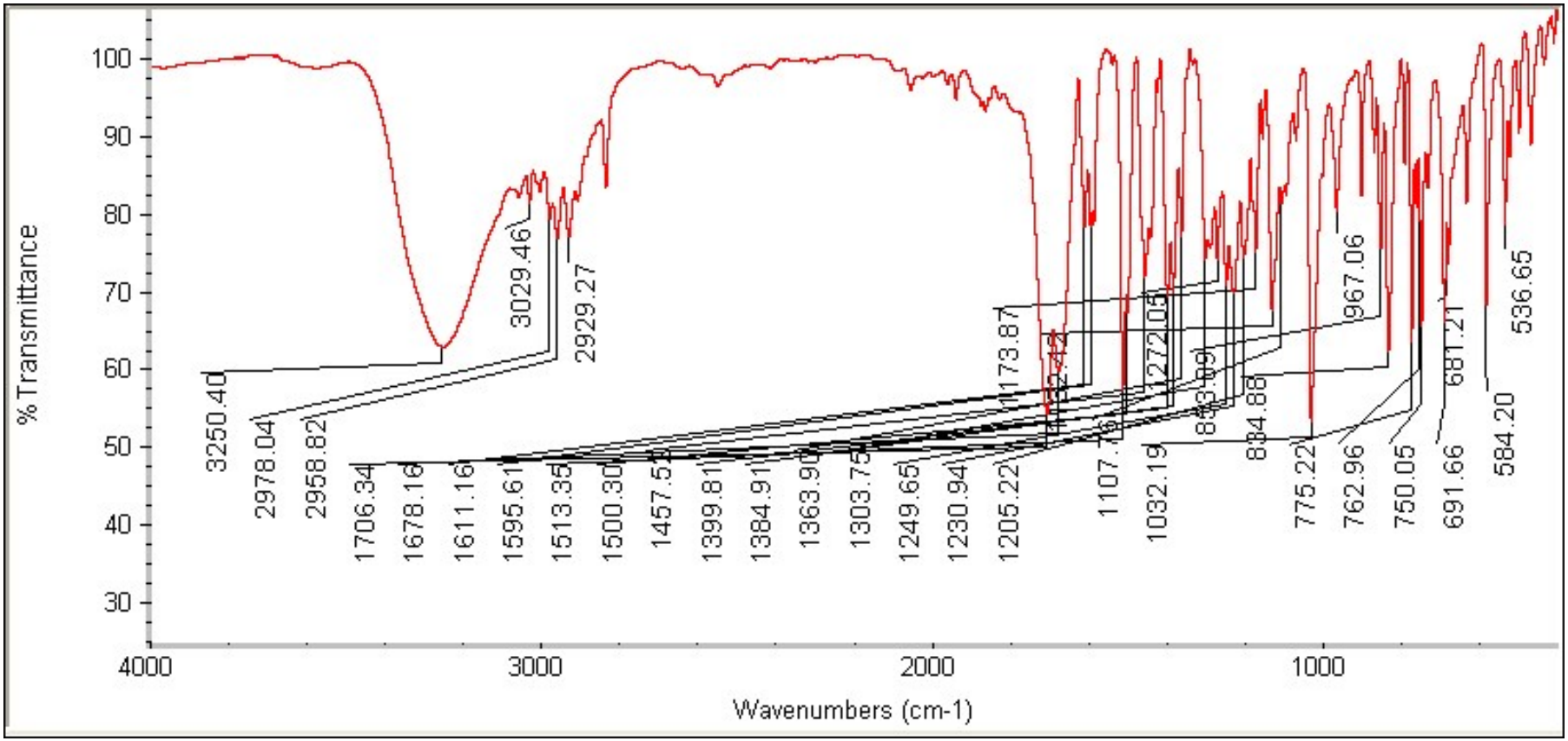

Fig. 46 FT-IR spectrum of Ethyl 4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4p**).

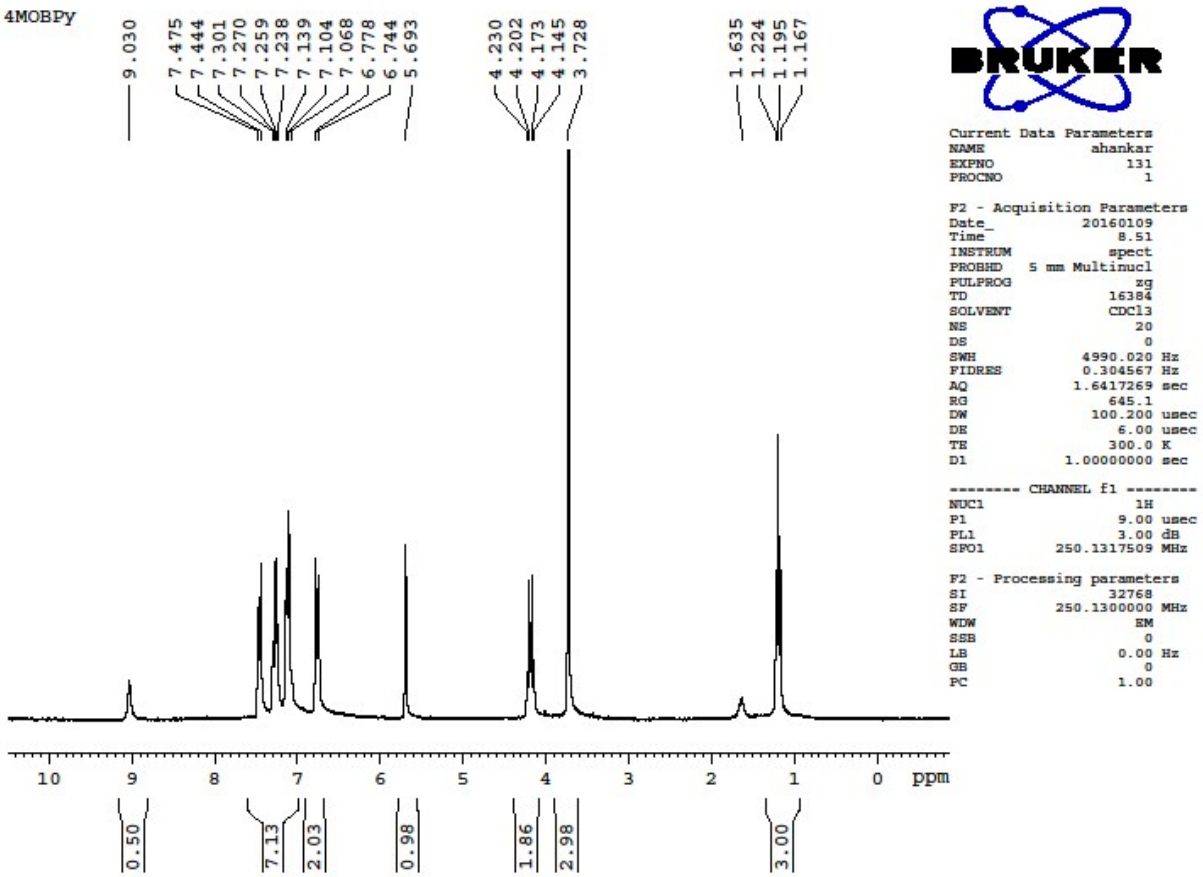

Fig. 47 ^{1}H NMR (250.13 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4p**)

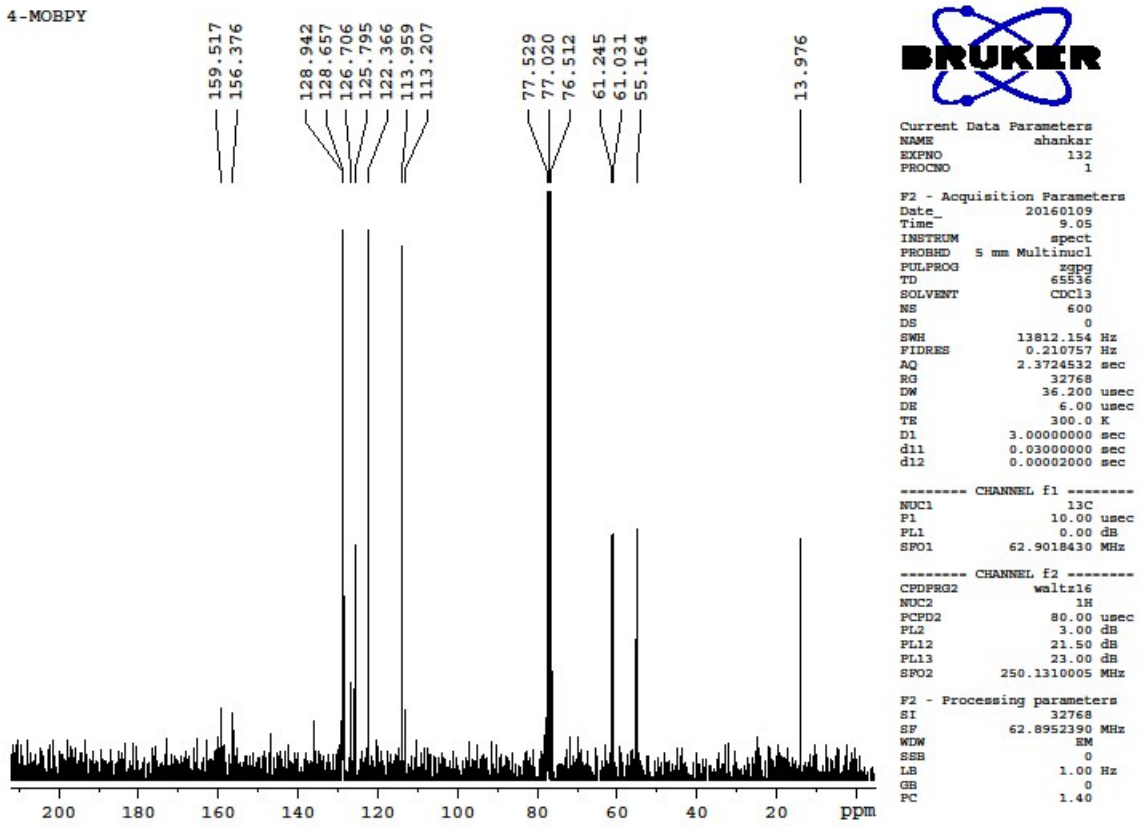

Fig. 48 ^{13}C NMR (62.90 MHz, $CDCl_3$) spectrum of Ethyl 4-hydroxy-2-(4-methoxyphenyl)-5-oxo-1-phenyl-2,5-dihydro-1H-pyrrole-3-carboxylate (**4p**)

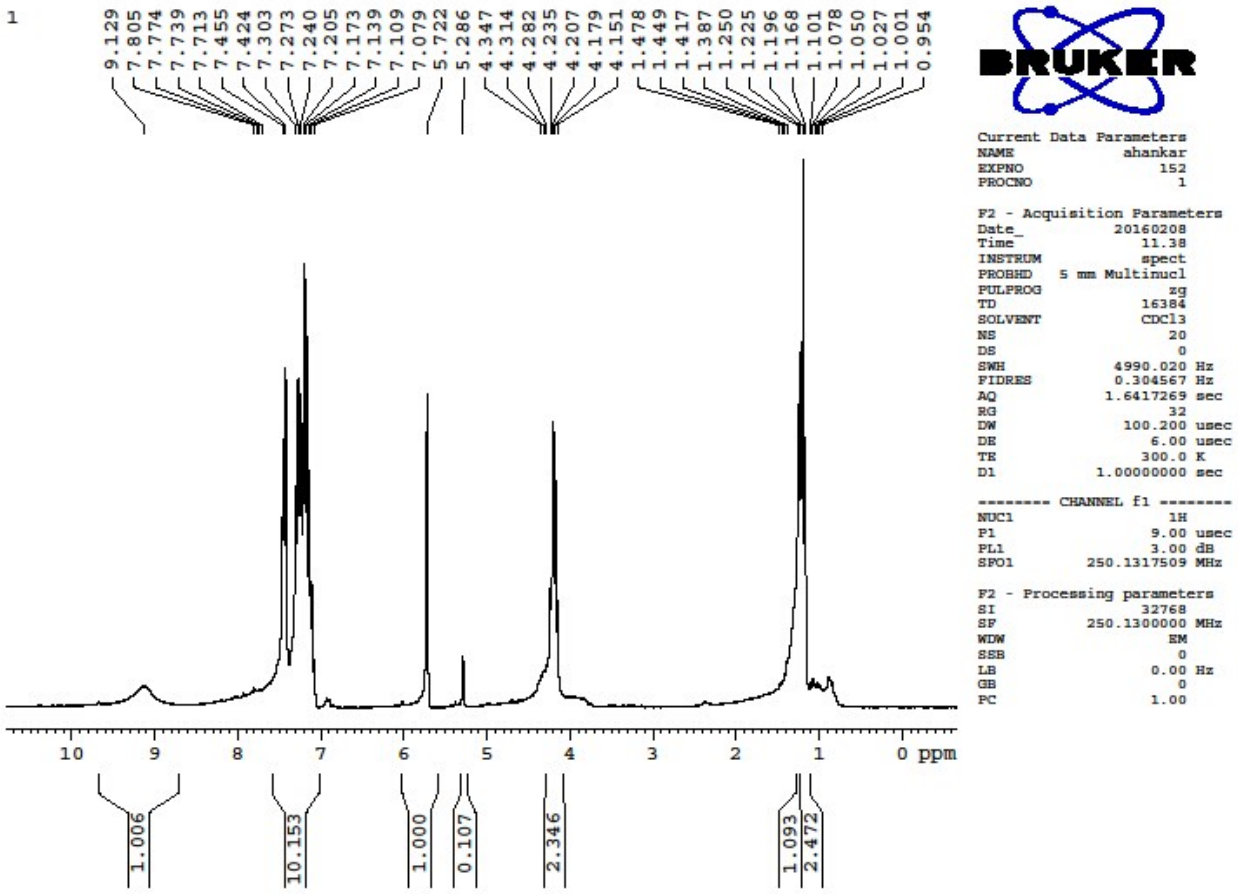

Fig. 49 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained under ultrasound irradiation conditions.

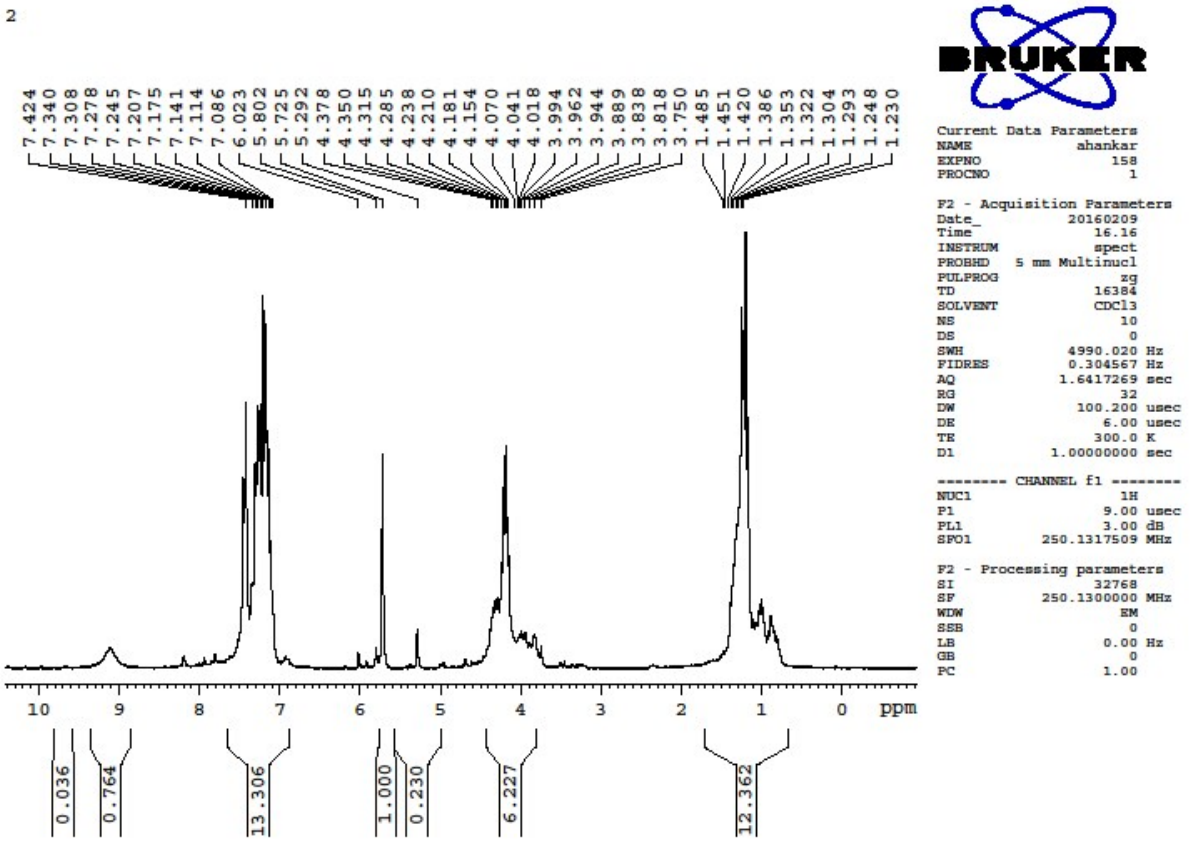

Fig. 50 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained at room temperature conditions.

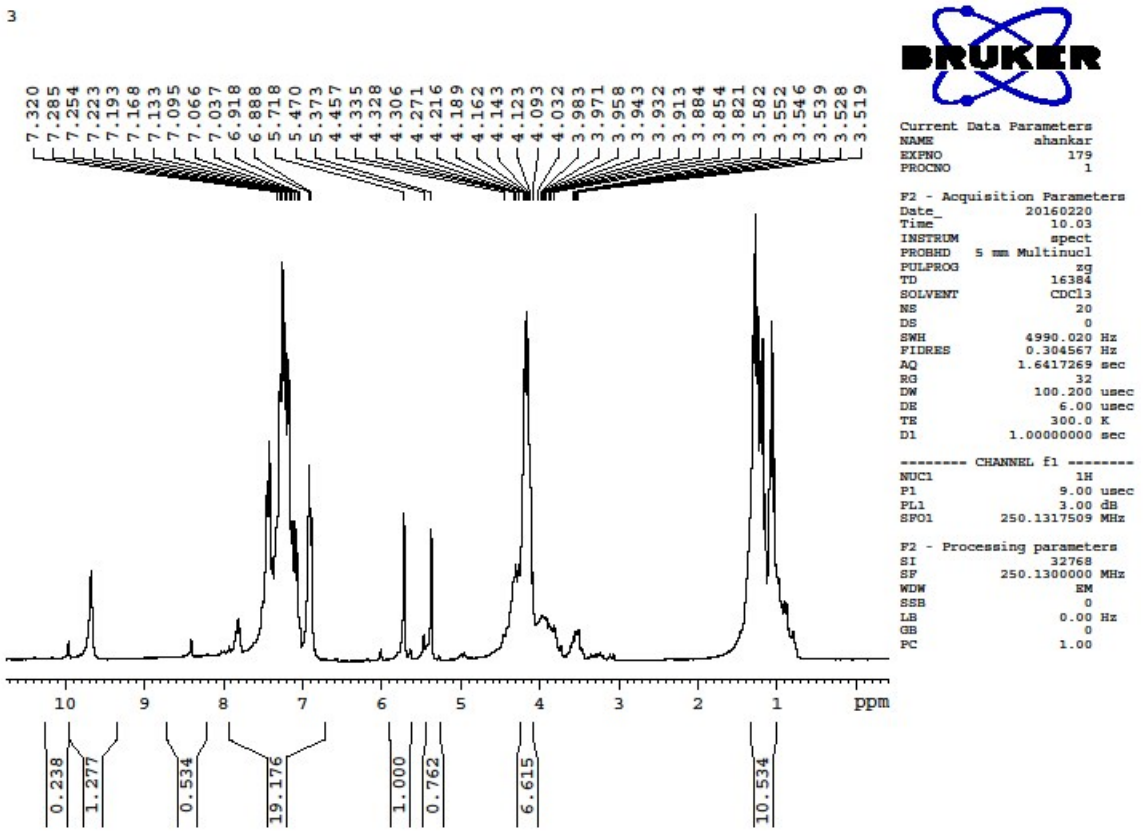

Fig. 51 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained at 40 ^{o}C for 15 min.

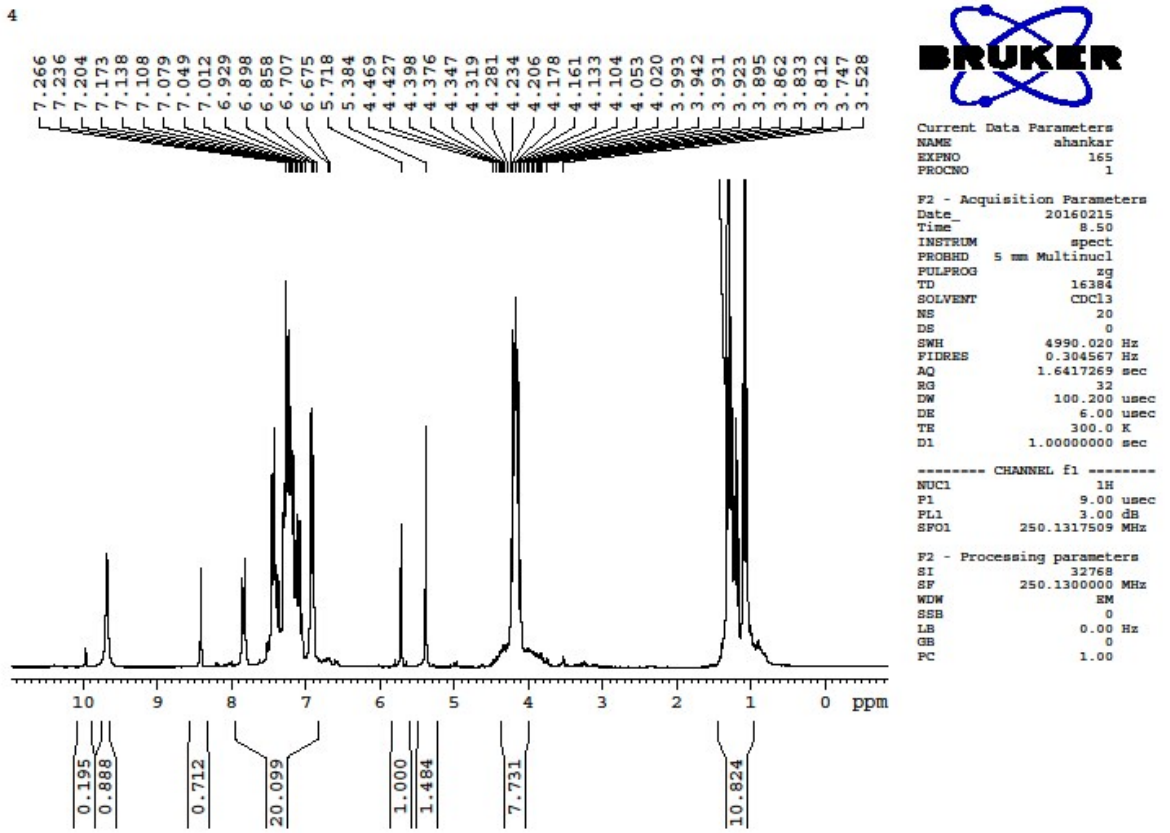

Fig. 52 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained at 40 ^{o}C for 30 min.

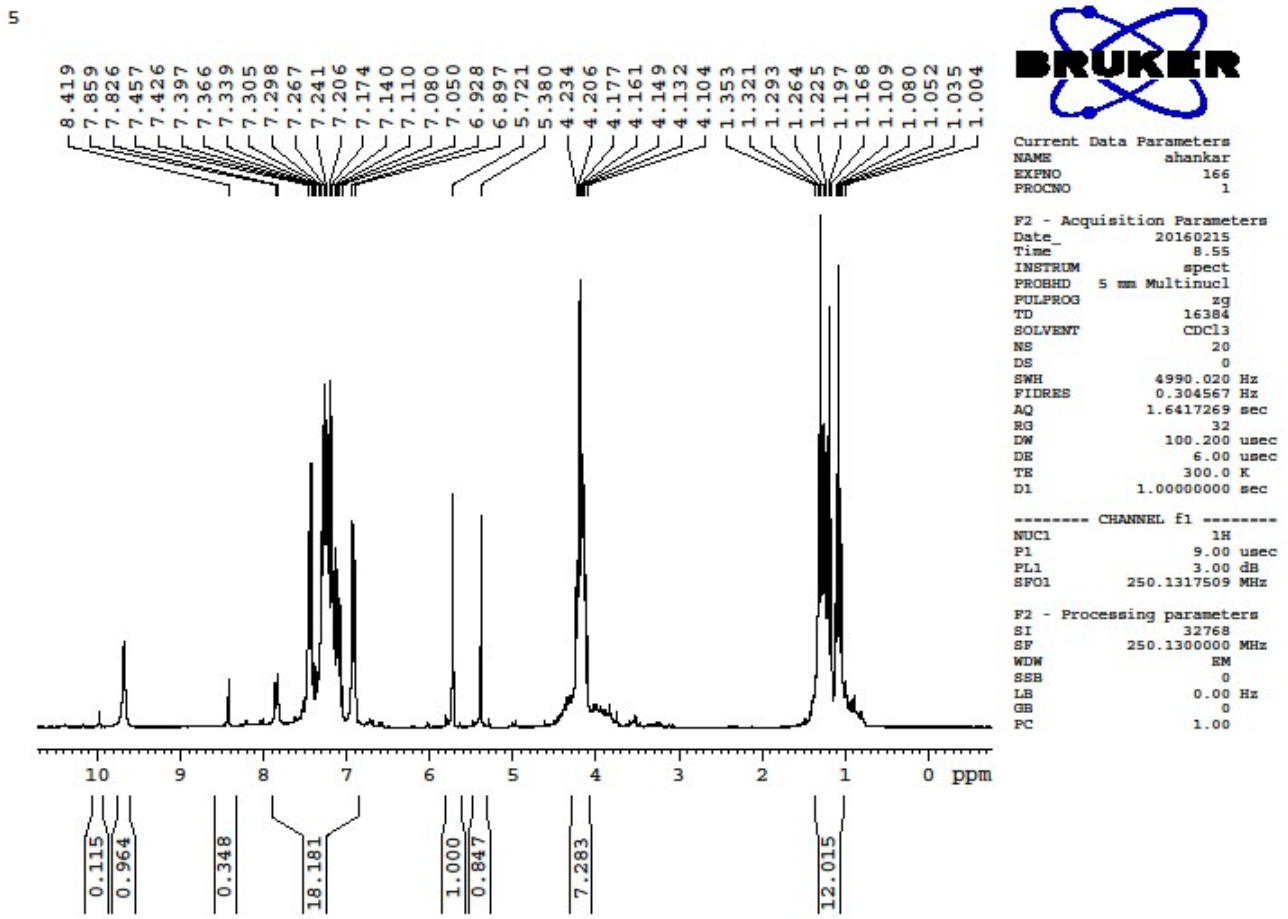

Fig. 53 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained at 40 ^{o}C for 60 min.

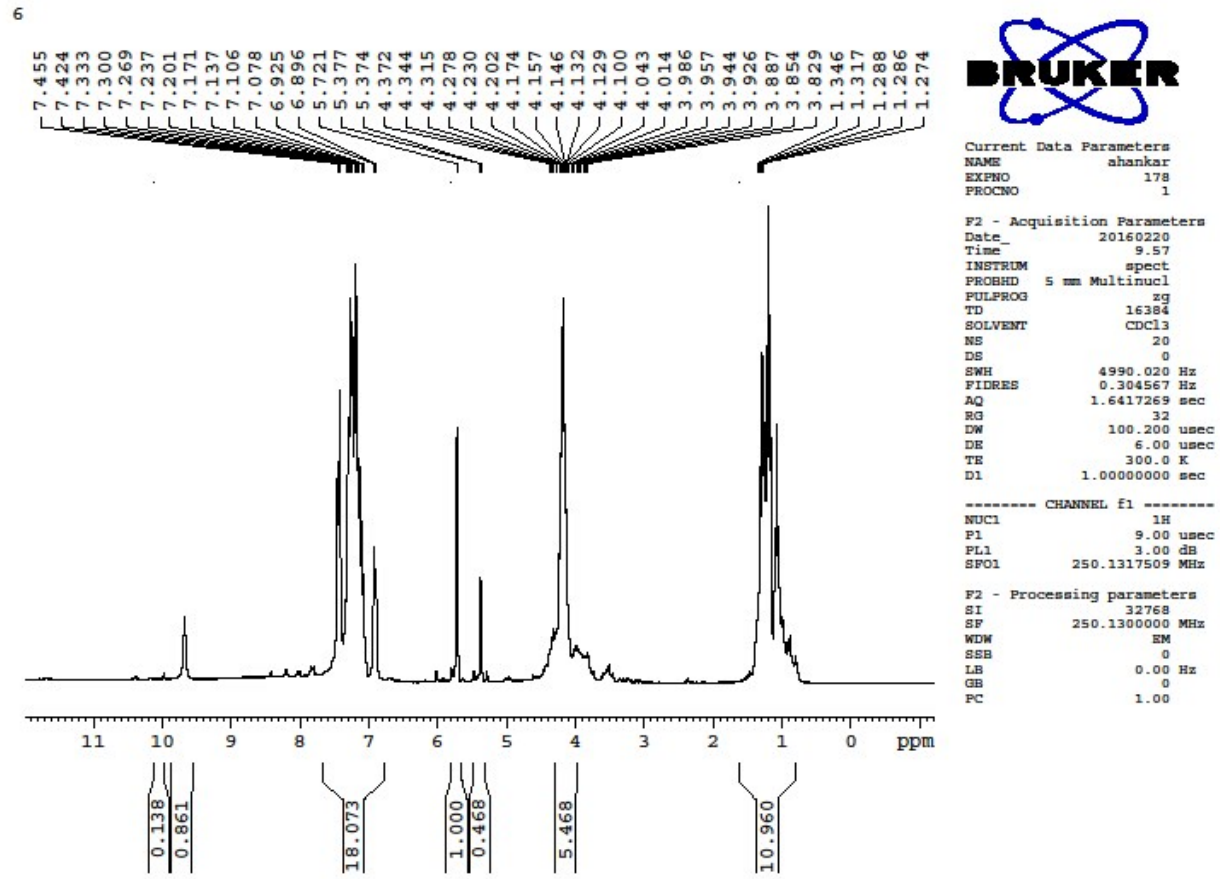

Fig. 54 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained in reflux conditions for 15 min.

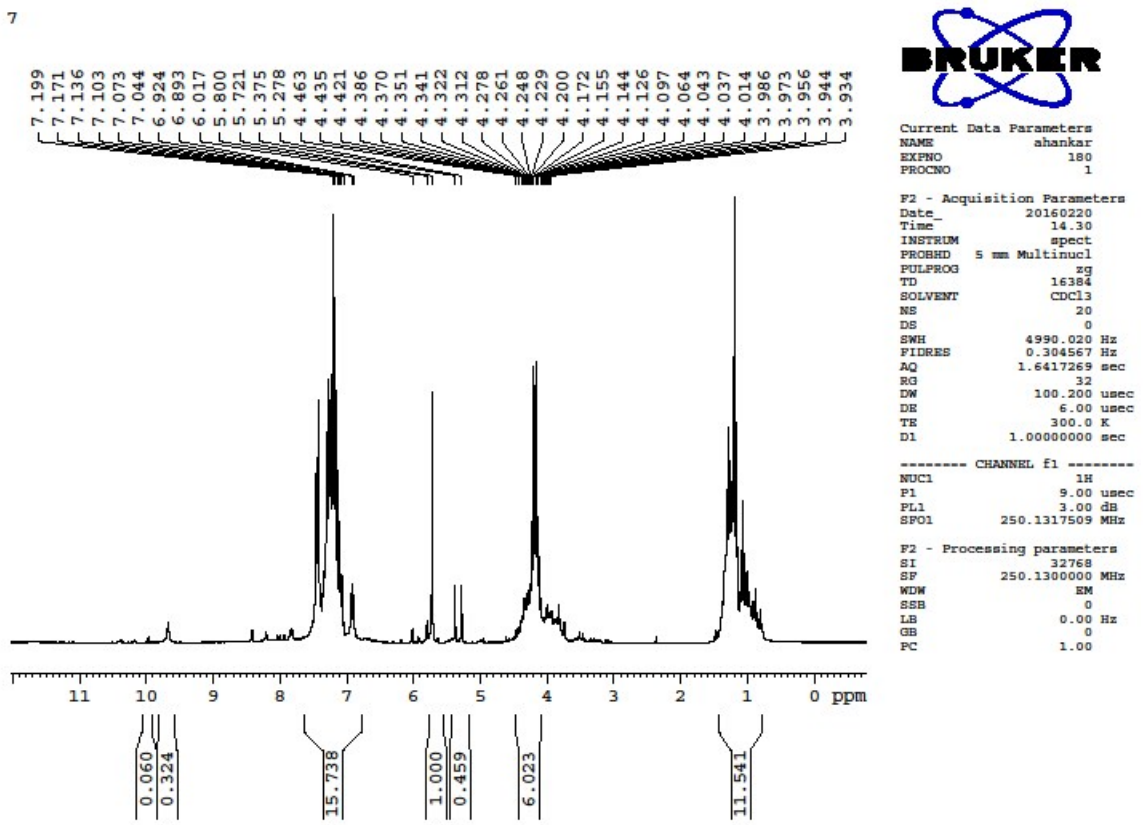

Fig. 55 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained in reflux conditions for 30 min.

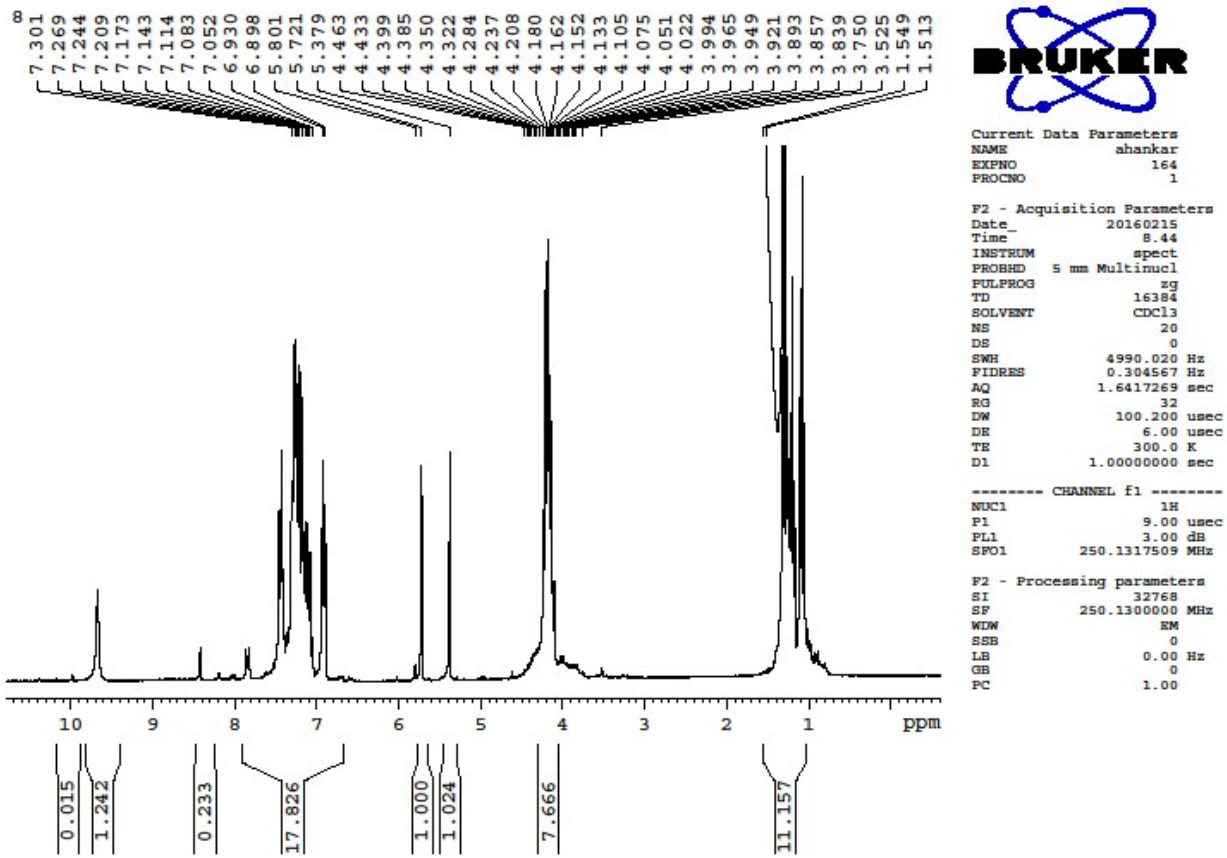

Fig. 56 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained in reflux conditions for 90 min.

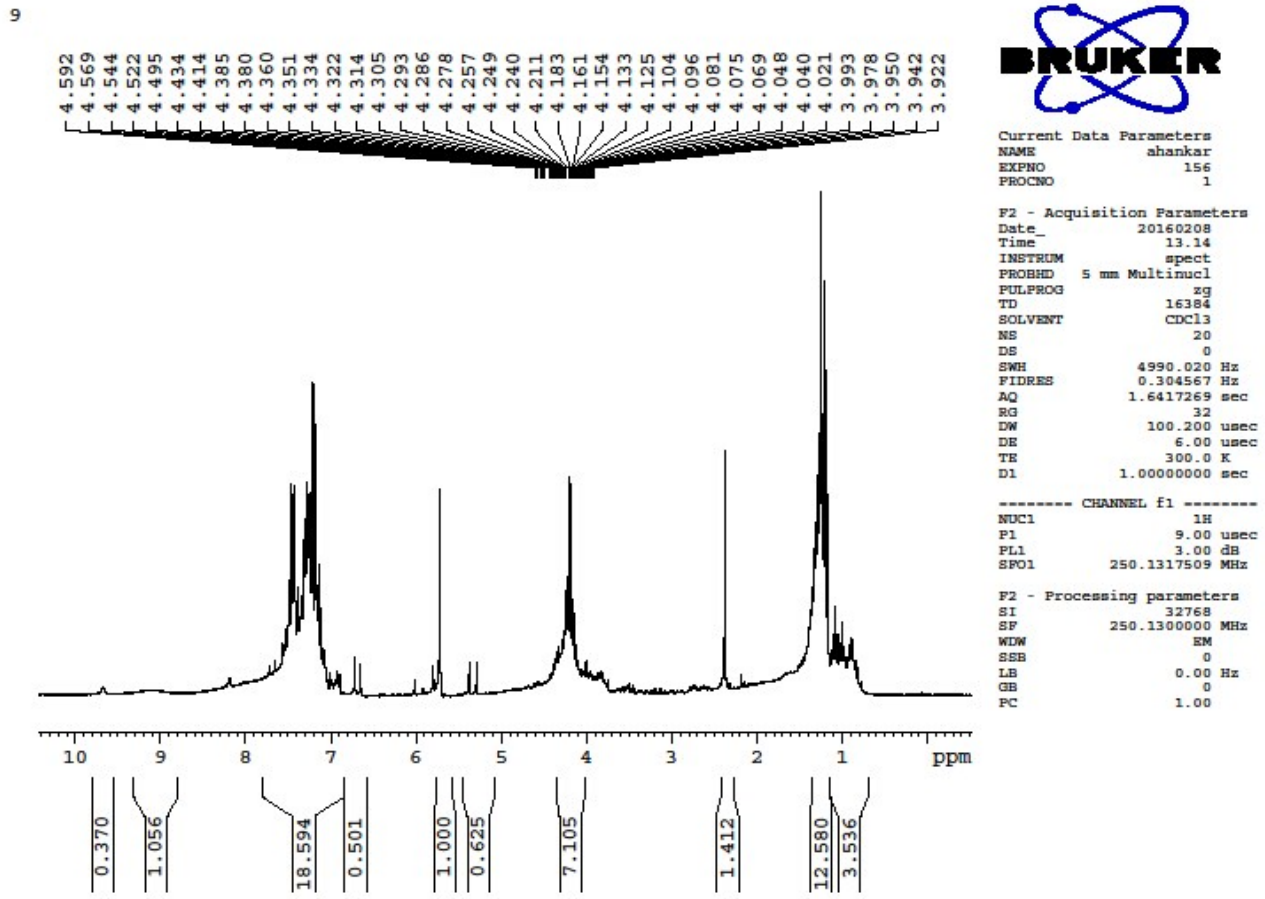

Fig. 57 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained in reflux conditions for 180 min.

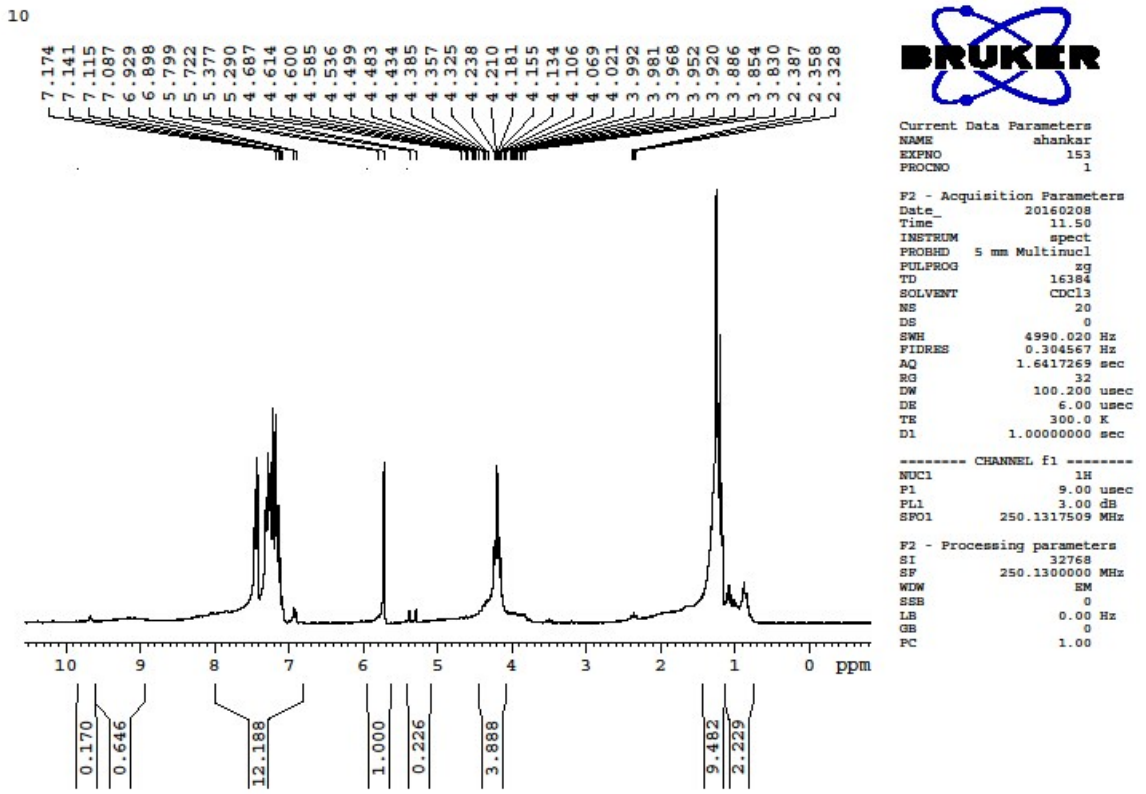

Fig. 58 ^{1}H NMR (250.13 MHz, $CDCl_3$) of the crude product **4d** that obtained in reflux conditions for 360 min.

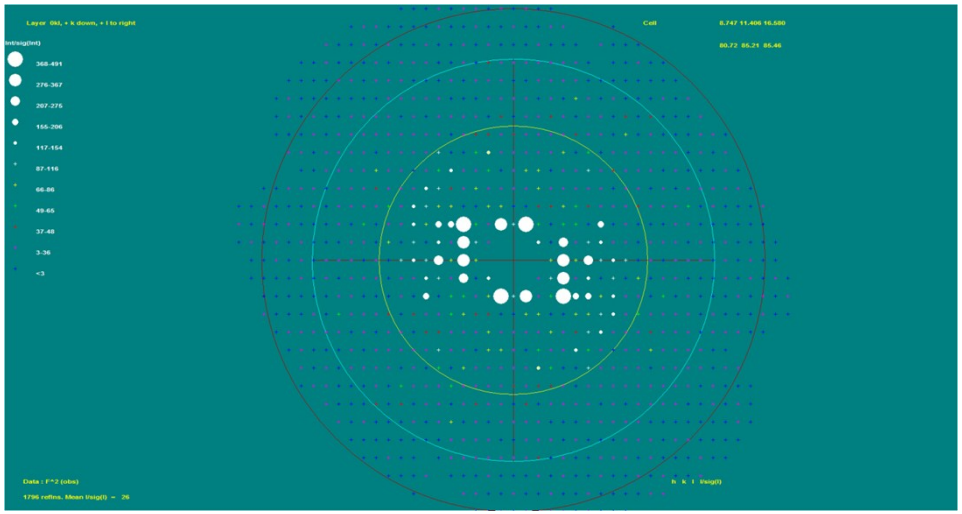

Fig. 59 Symmetry of diffraction pattern **0*kl***.

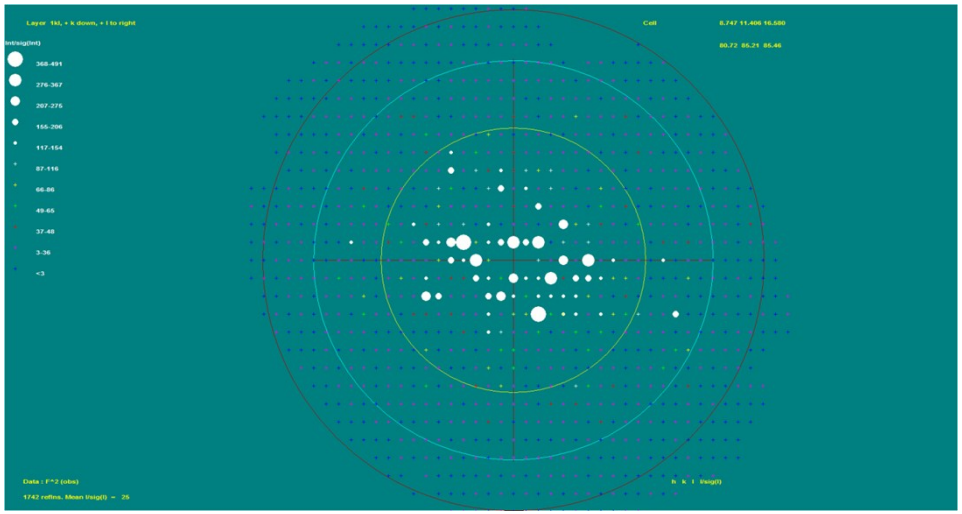

Fig. 60 Symmetry of diffraction pattern **1*kl***.

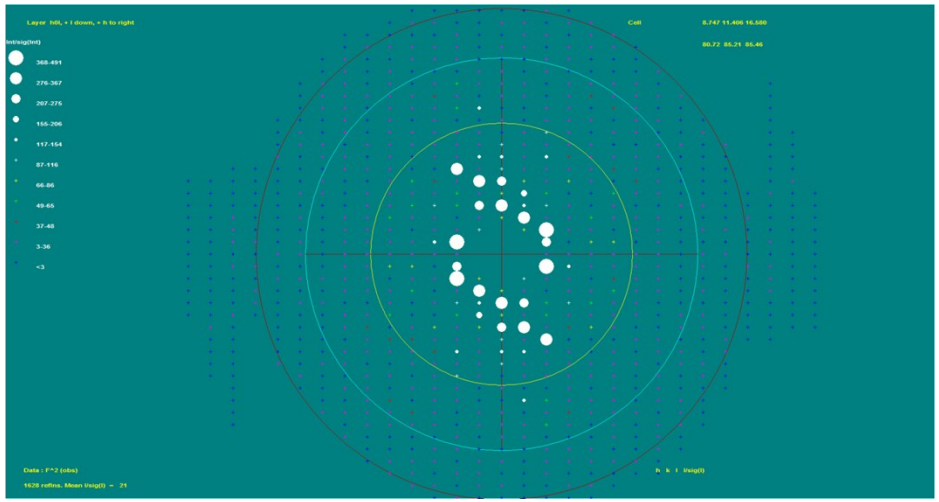

Fig. 61 Symmetry of diffraction pattern ***h0l***.

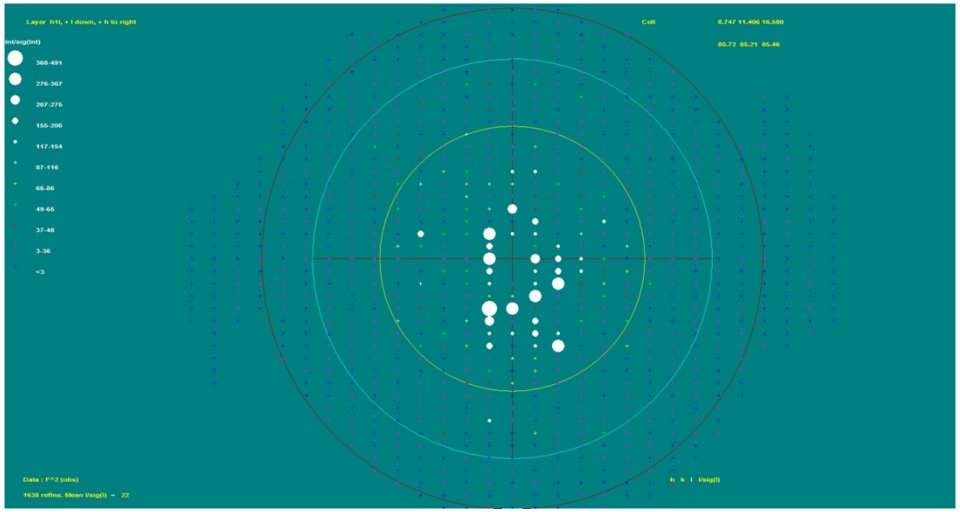

Fig. 62 Symmetry of diffraction pattern ***h1l***.

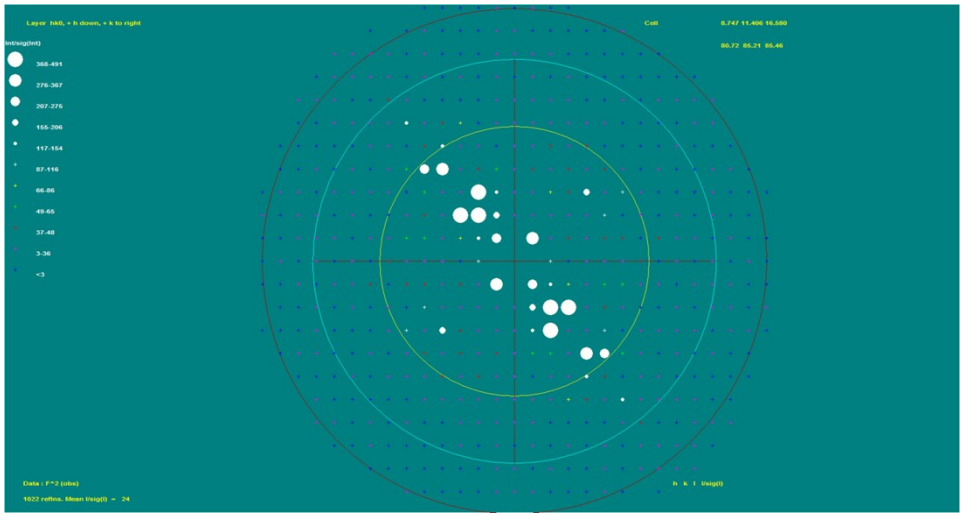

Fig. 63 Symmetry of diffraction pattern ***hk*0**.

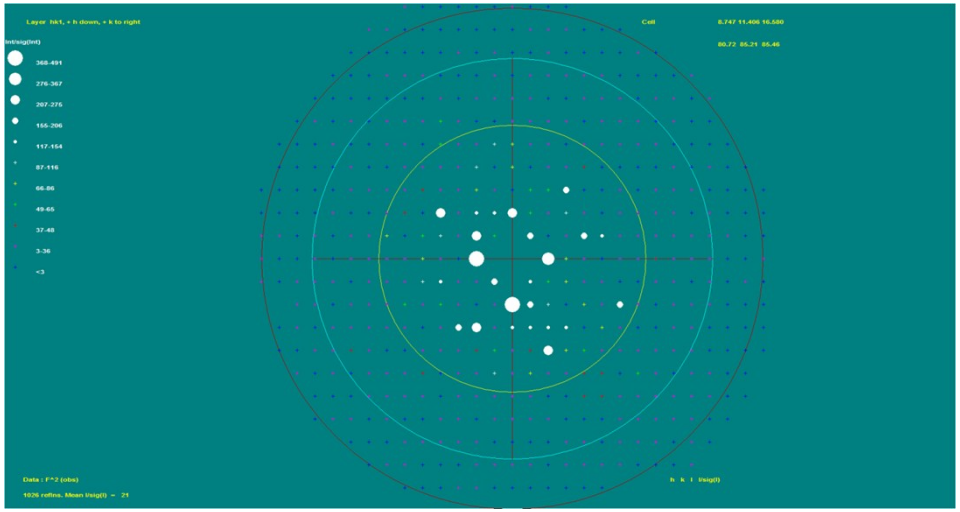

Fig. 64 Symmetry of diffraction pattern ***hk1***.

Table S1 Selected geometric parameters (Å, º) for **4g**

Molecule A		**Molecule B**	
F1—C17	1.367(3)	F2—C36	1.370(3)
O1—C7	1.216(3)	O5—C26	1.218(3)
O2—C8	1.337(3)	O6—C27	1.331(3)
N1—C7	1.380(3)	N2—C26	1.375(3)
N1—C6	1.433(3)	N2—C25	1.421(3)
N1—C13	1.476(3)	N2—C32	1.484(3)
C7—N1—C6—C1	−16.0(4)	C26—N2—C25—C20	−19.4(4)
C11—O4—C10—C9	178.9(2)	C30—O8—C29—C28	−177.8(2)
C8—C9—C10—O4	−172.6(2)	C27—C28—C29—O8	−177.0 (2)
C10—O4—C11—C12	−173.5(2)	C29—O8—C30—C31	−175.9(2)
C7—N1—C13—C14	119.5(2)	C26—N2—C32—C33	124.4(2)
N1—C13—C14—C15	136.4(2)	N2—C32—C33—C38	137.7(2)
C9—C13—C14—C15	−108.1(2)	C28—C32—C33—C38	−105.8(3)