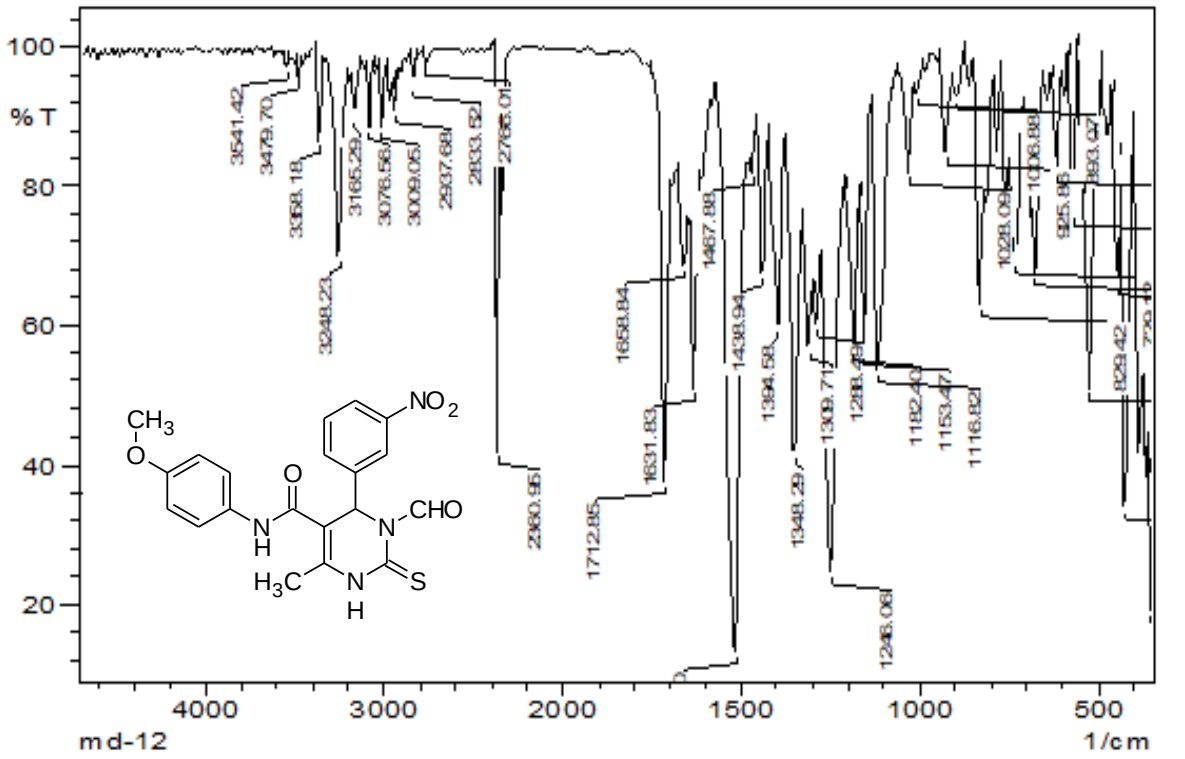
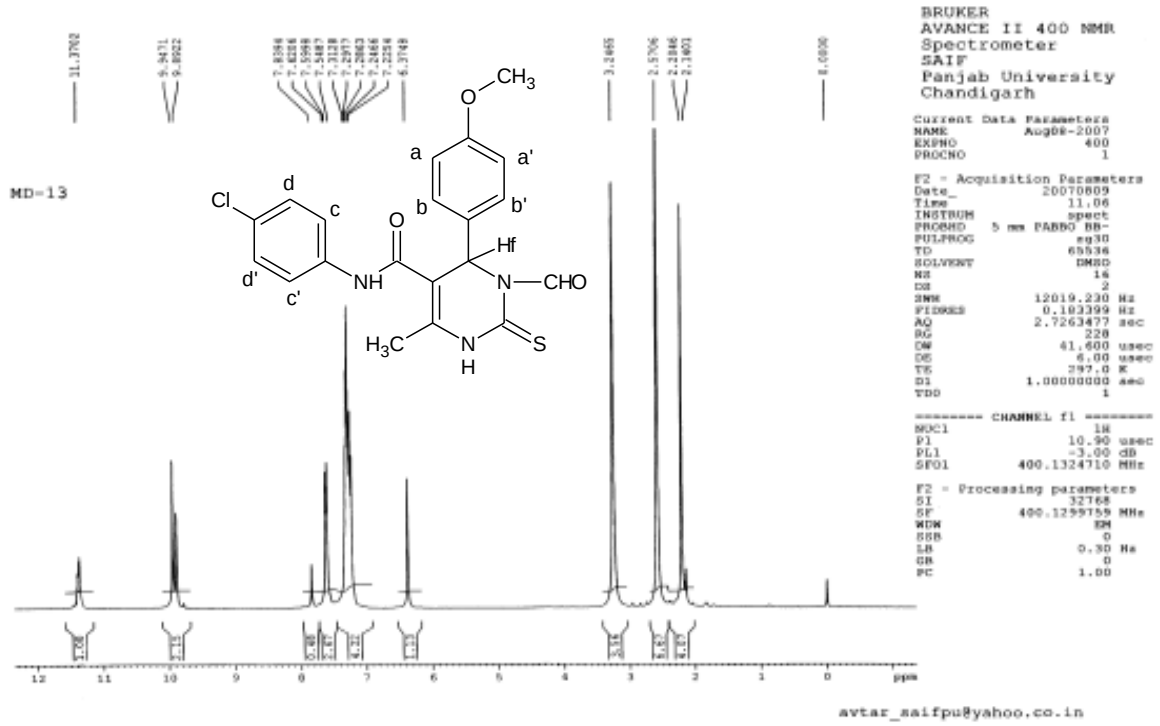
Supplementary Data

IR SPECRAL STUDY OF 3-FORMYL-*N*-(4-METHOXYPHENYL)-6-METHYL-4-(3-NITROPHENYL)-2-THIOXO-1,2,3,4-TETRAHYDROPYRIMIDINE-5-CARBOXAMIDE (4i)



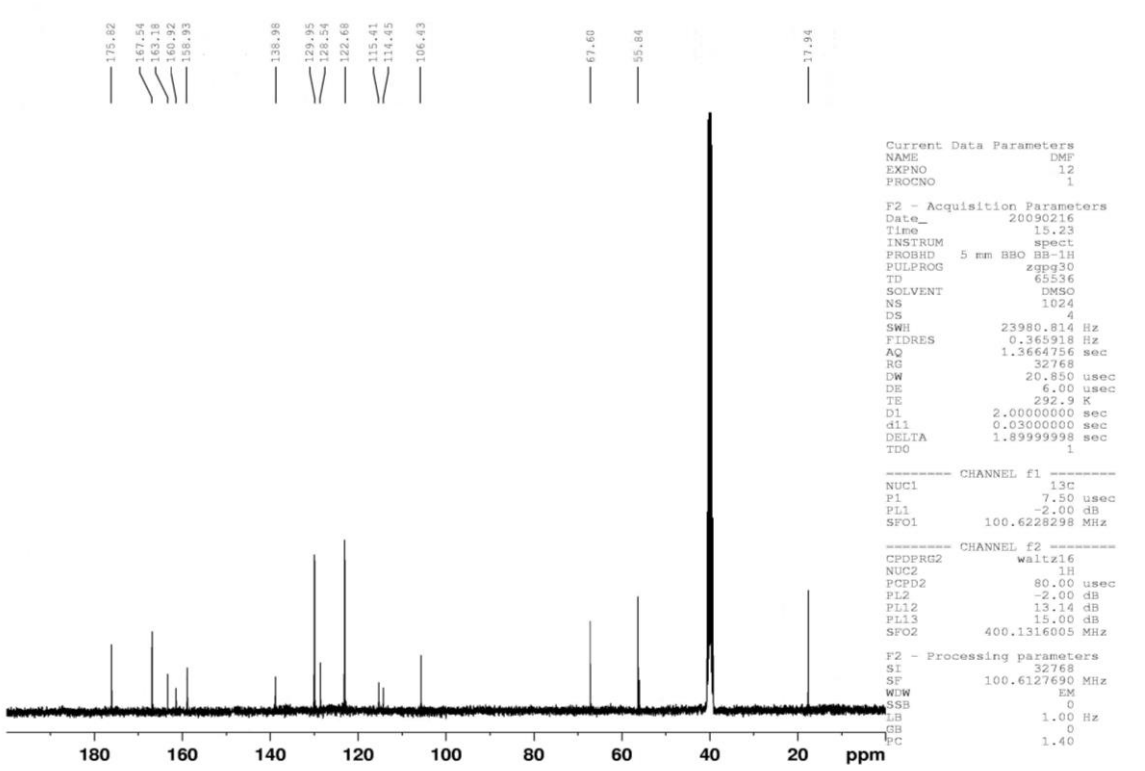
Type	Vibration Mode	Frequency in cm^{-1} Observed	Reported
Alkane	C-H str. (asym.)	2937	2975-2950
-CH_3	C-H str. (sym.)	2833	2880-2860
	C-H i.p. def. (asym.)	1438	1470-1435
	C-H o.o.p. def. (asym.)	1394	1390-1370
Aromatic	C-H str.	3076	3090-3030
	C=C str.	1467	1520-1480
	C-H i.p. (def).	1006	1070-1000
	C-H o.o.p. (def.)	829	835-810
	C-O-C str.	1246	1300-1000
	-N=O str. (sym.)	1348	1355-1315
Pyrimidine moity	C=C str.	1520	1580-1520
	C-H str.	3009	3080-3030
	C-H i.p. (def).	1116	1125-1090
Amine	-N-H i.p. (def.)	1631	1650-1580
	C-N- str.	1309	1360-1310
Carbonyl (ald.)	-C=O str.	1712	1715-1695
Amide	-C=O str.	1658	1690-1660

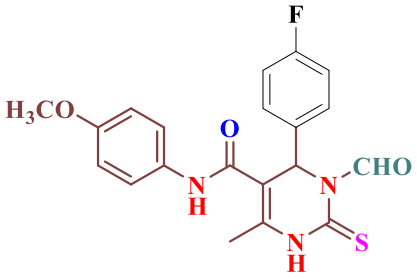
[1]H-NMR OF N-(4-CHLOROPHENYL)-3-FORMYL-4-(4-METHOXYPHENYL)-6-METHYL-2-THIOXO-1,2,3,4-TETRAHYDROPYRIMIDINE-5-CAR –BOXAMIDE (4d)



Signal No.	Signal Position (δ ppm)	Relative No. of protons	Multiplicity	Inference	J Value In Hz
1	2.14	1H	singlet	Pyrimidine-NH	-
2	2.20	3H	singlet	Pyrimidine-CH_3	-
3	3.24	3H	singlet	Ar-OCH_3	-
4	6.37	1H	singlet	Chiral-Hf	-
5	7.31-7.22	4H	multiplate	Ar-Ha,a',b,b'	J = 8.48 J = 4.56
6	7.62	2H	doublet	Ar-Hd,d'	J = 8.32
7	7.83	1H	singlet	-NH-CO-	-
8	9.94	2H	doublet	Ar-Hc,c'	-
9	11.37	1H	Singlet	-CHO	-

^{13}C-NMR OF N-(4-METHOXYPHENYL)-3-FORMYL-4-(4-FLOUROPHENYL)-6-METHYL-2-THIOXO-1,2,3,4-TETRAHYDROPYRIMIDINE-5-CARBOXAMIDE (4l)





The ^{13}C-NMR spectrum of compound **4l** showed signals at 175.82, 167.54, 163.18, 160.92, 158.93, 138.98, 129.94, 128.54, 122.68, 115.37, 114.45, 106.43, 67.60, 55.84 and 17.94 δ corresponding to twenty different type of carbon atoms present in the compound. The most downfield signal appeared at 175.82 δ can be assigned to the carbonyl carbon of C=S group in pyrimidine nucleus. The signals appeared at 167.54 δ and 163.18 δ can be assigned to carbonyl carbon of –CHO and –CONH– groups, respectively. The signals of carbon of –OCH_3 and –CH_3 group appeared at 55.84 δ and 17.94 δ, respectively. The rest of signals are corresponding to aromatic carbons of pyrimidine and phenyl nucleus.

MASS SPECTRAL STUDY OF 3-FORMYL-*N*-(4-METHOXYPHENYL)-6-METHYL 4-(3-NITROPHENYL)-2-THIOXO-1,2,3,4-TETRAHYDROPYRIMIDINE-5-CARBOX –AMIDE (4i)