

**Exploration of 6,7-dimethoxyquinazoline derivatives as dual acting  $\alpha_1$ - and AT<sub>1</sub>- receptors antagonists: Synthesis, evaluation, pharmacophore & 3D-QSAR modeling and receptor docking studies**

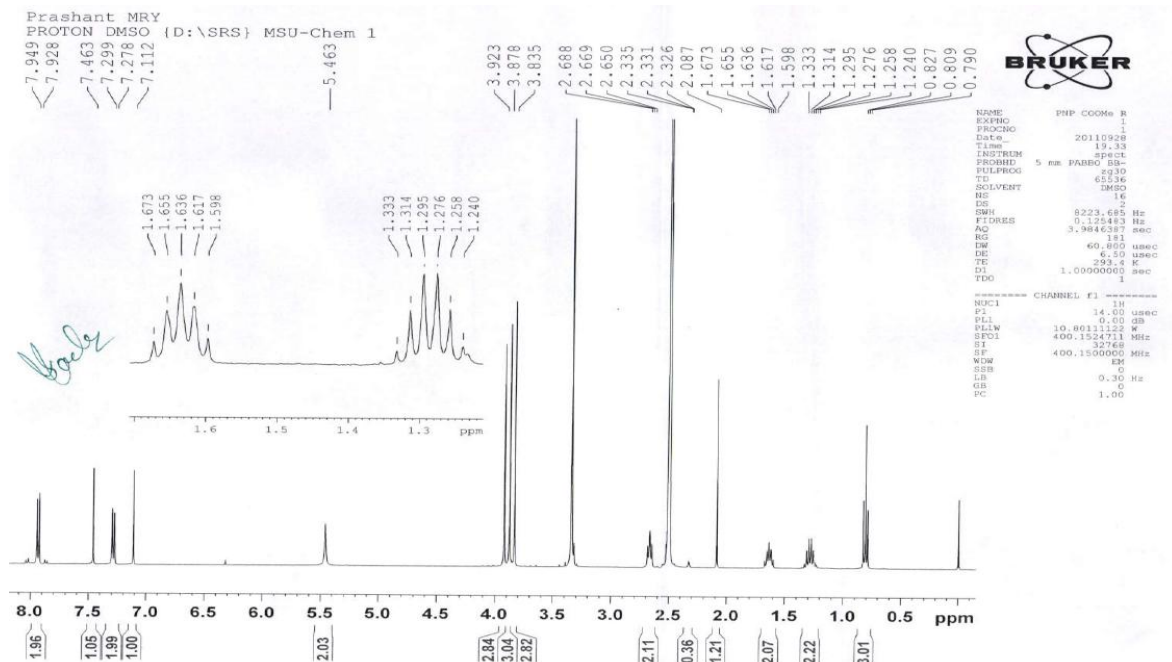
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*Faculty of Pharmacy, Kalabhavan campus  
The M.S. University of Baroda  
Vadodara – 390 001, India*

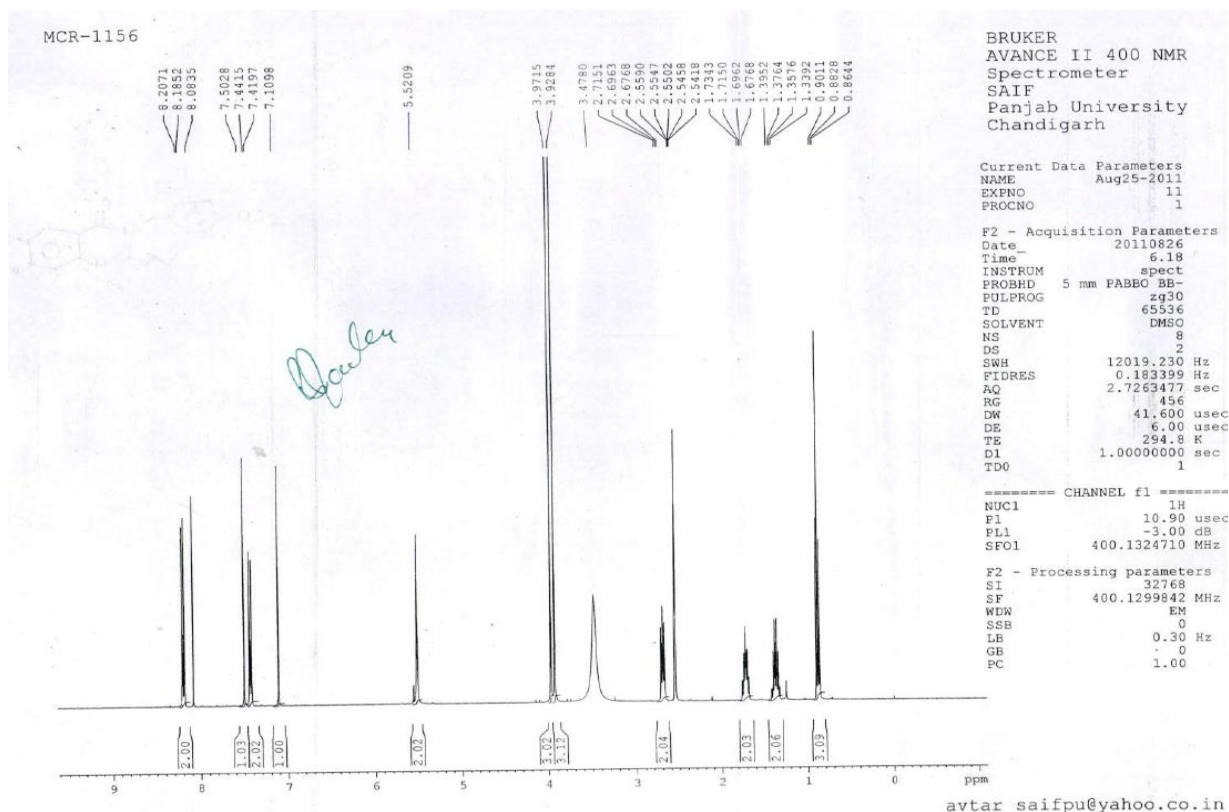
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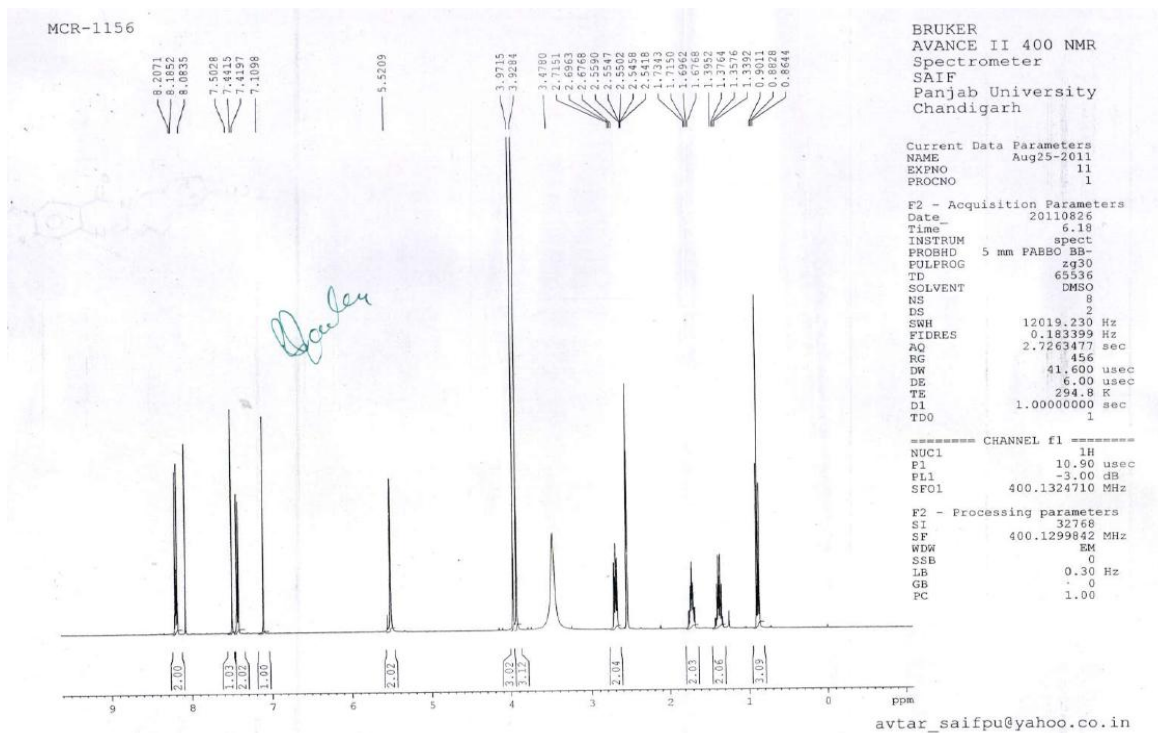
### Methyl 4-[(2-butyl-6,7-dimethoxy-4-oxoquinazolin-3(3H)-yl)methyl]benzoate (11)



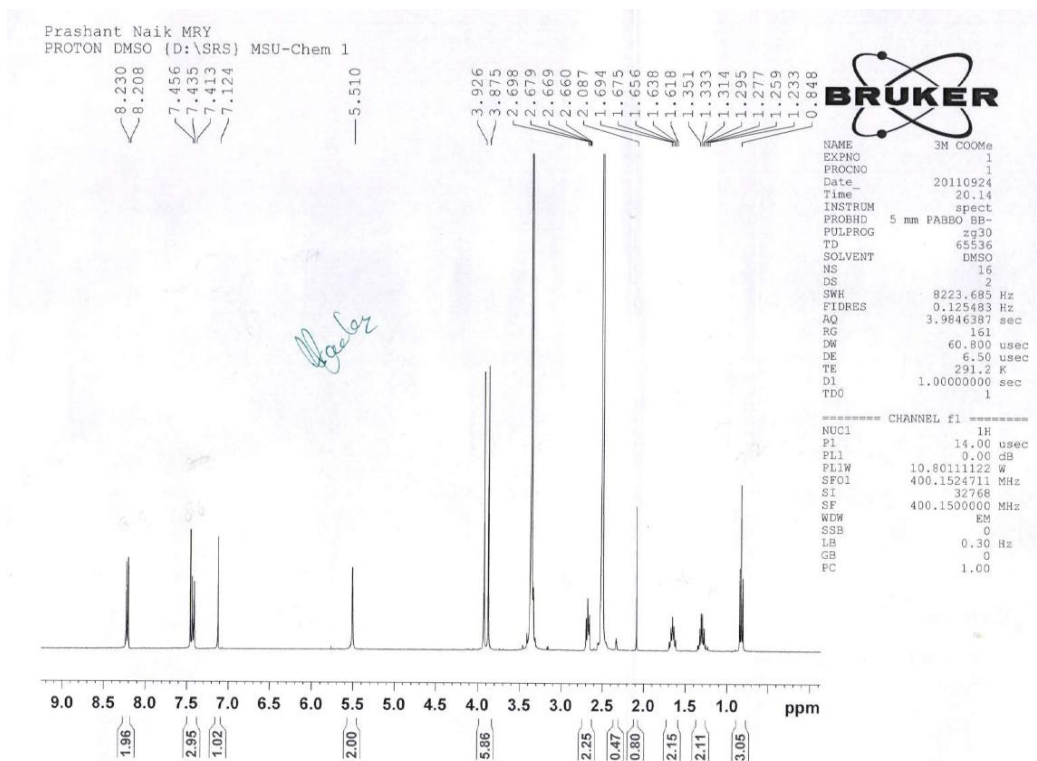
### 4-[(2-Butyl-6,7-dimethoxy-4-oxoquinazolin-3(3H)-yl)methyl]benzotrile (12)



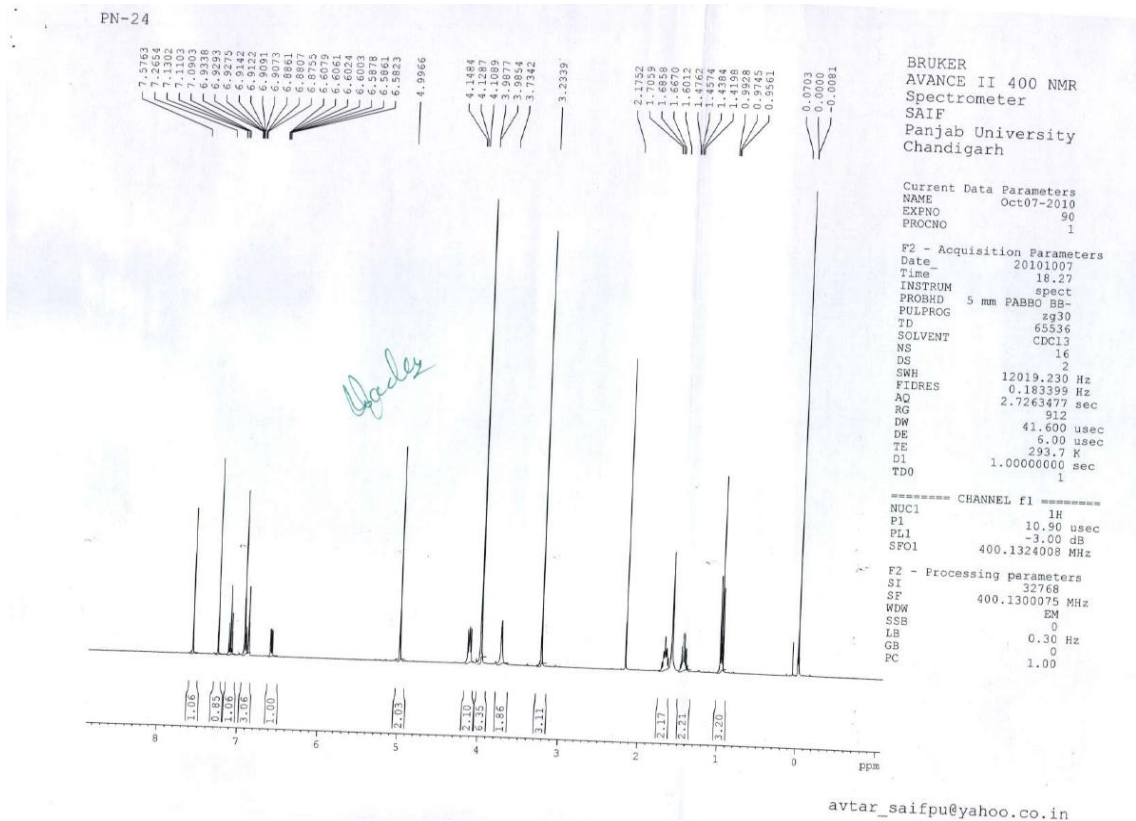
**2-Butyl-6,7-dimethoxy-3-(4-nitrobenzyl)quinazolin-4(3H)-one (14)**



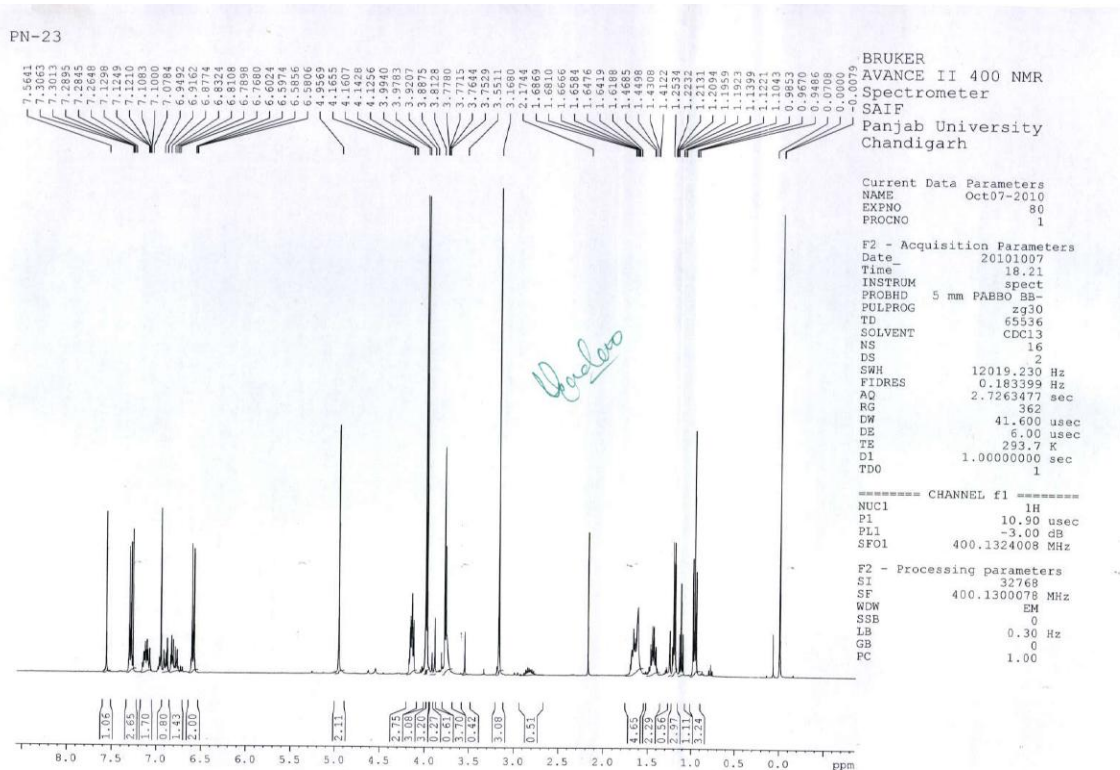
**4-[(2-Butyl-6,7-dimethoxy-4-oxoquinazolin-3(3H)-yl)methyl]benzoic acid (15)**



**N-{3-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazolin-2yl)methylamino]phenyl}methanesulfonamide (24)**



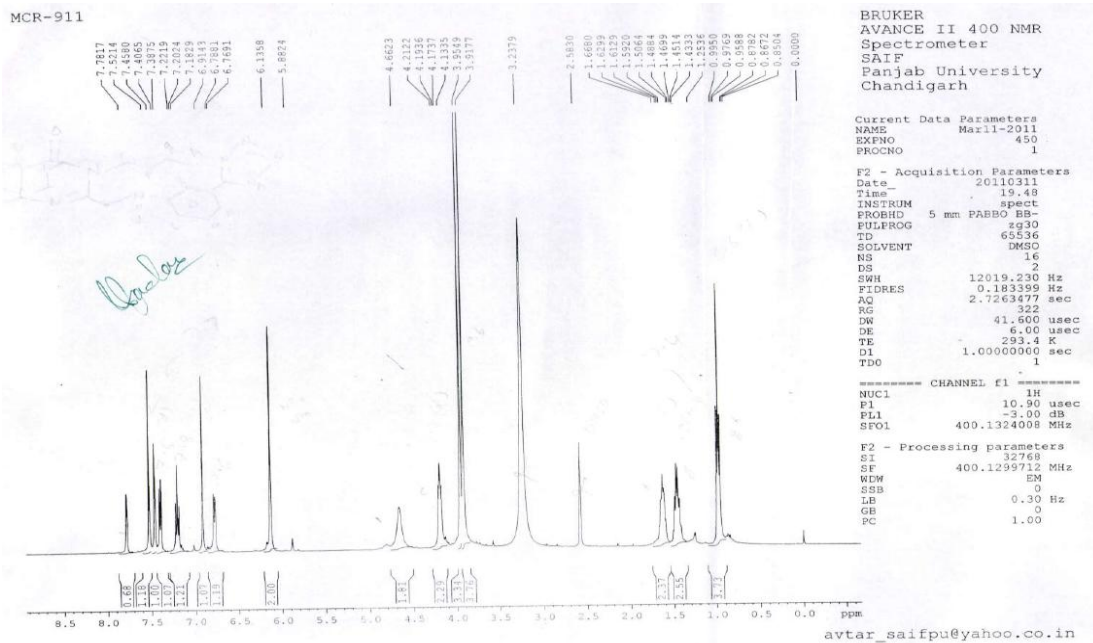
**N-{4-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazoline-2yl)methylamino]phenyl}methanesulfonamide (25)**



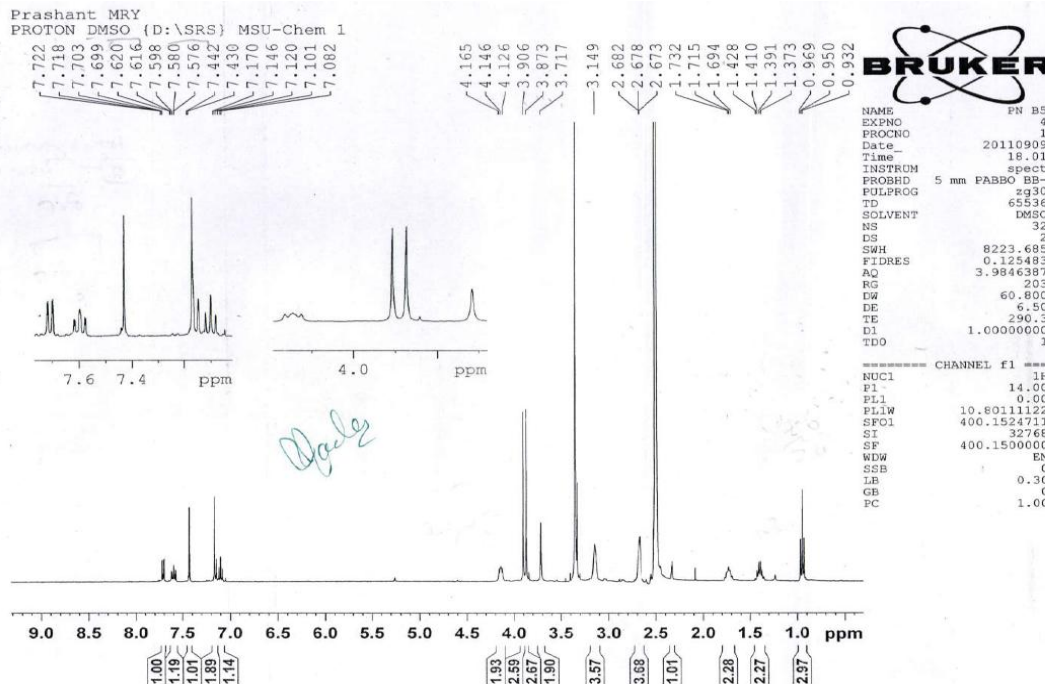




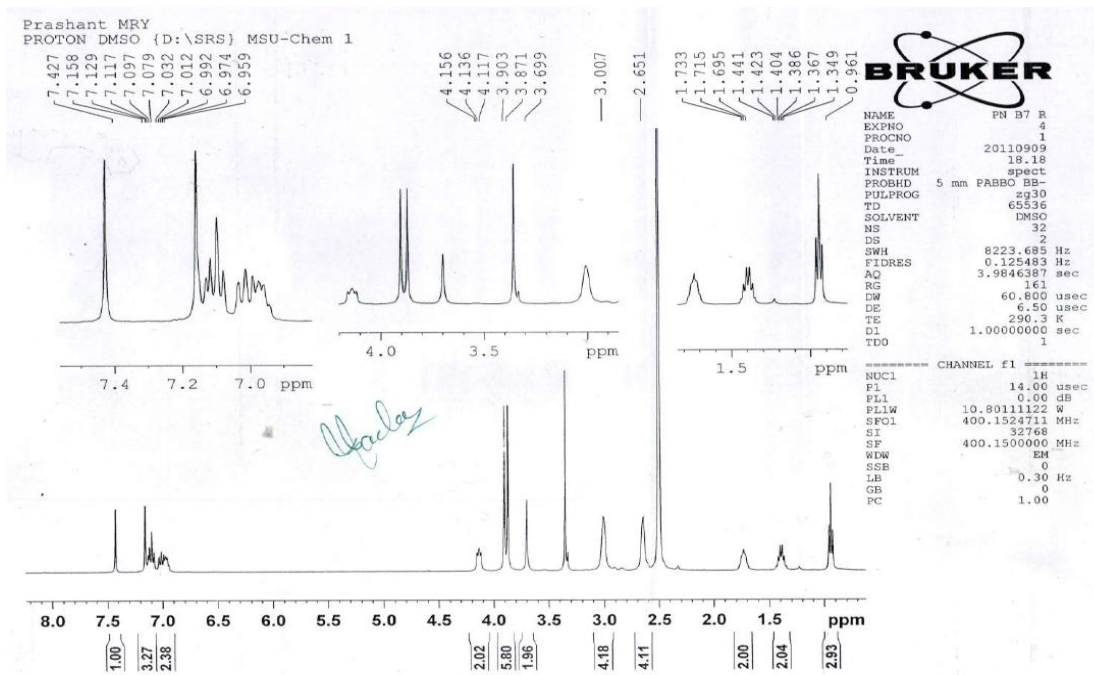
**5-{3-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazolin-2-yl)methylamino]phenyl}-1H-tetrazole (28)**



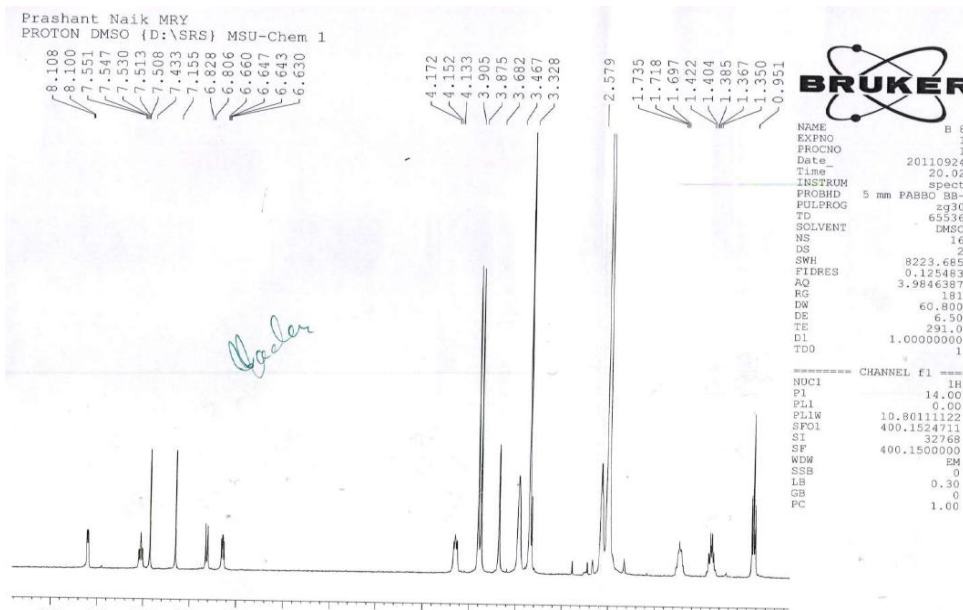
**2-{4-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazolin-2-yl)methyl]piperazin-1-yl}benzotrile (33)**



**3-Butyl-2-[[4-(2-fluorophenyl)piperazin-1-yl]methyl]-6,7-dimethoxyquinazolin-4(3H)-one (34)**



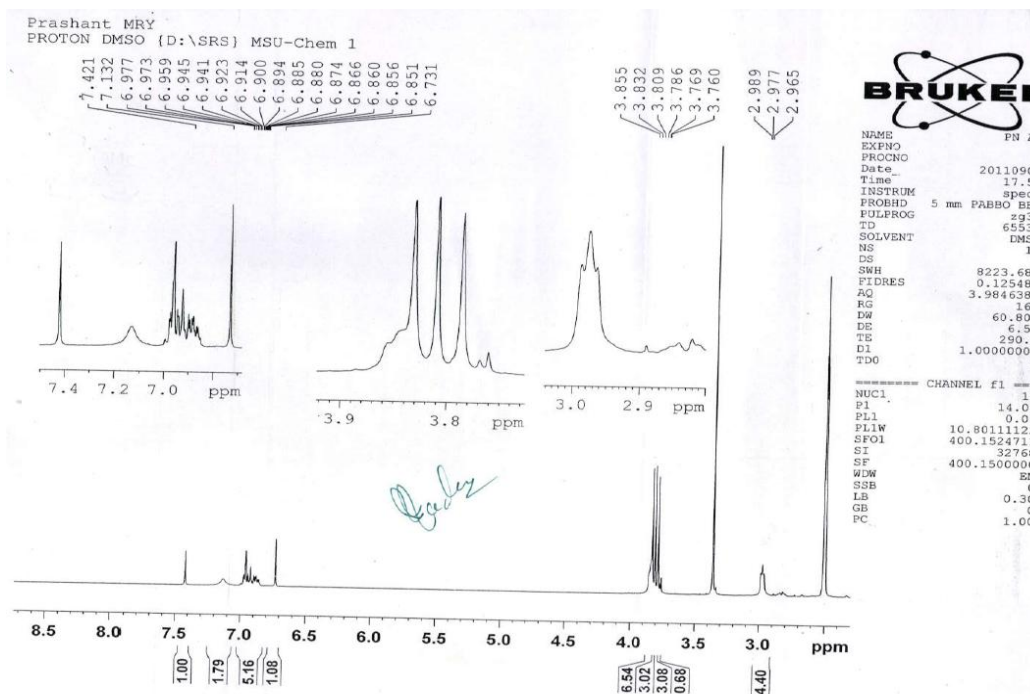
**3-Butyl-6,7-dimethoxy-2-[(4-(pyridin-2-yl)piperazin-1-yl)methyl]quinazolin-4(3H)-one (35)**



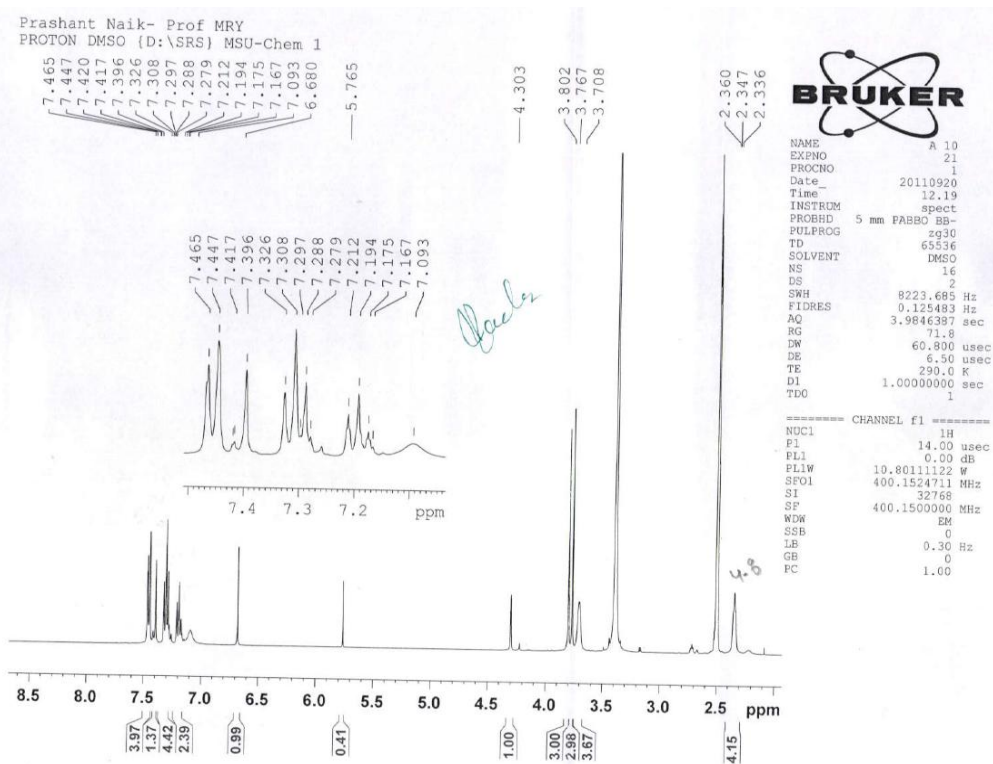




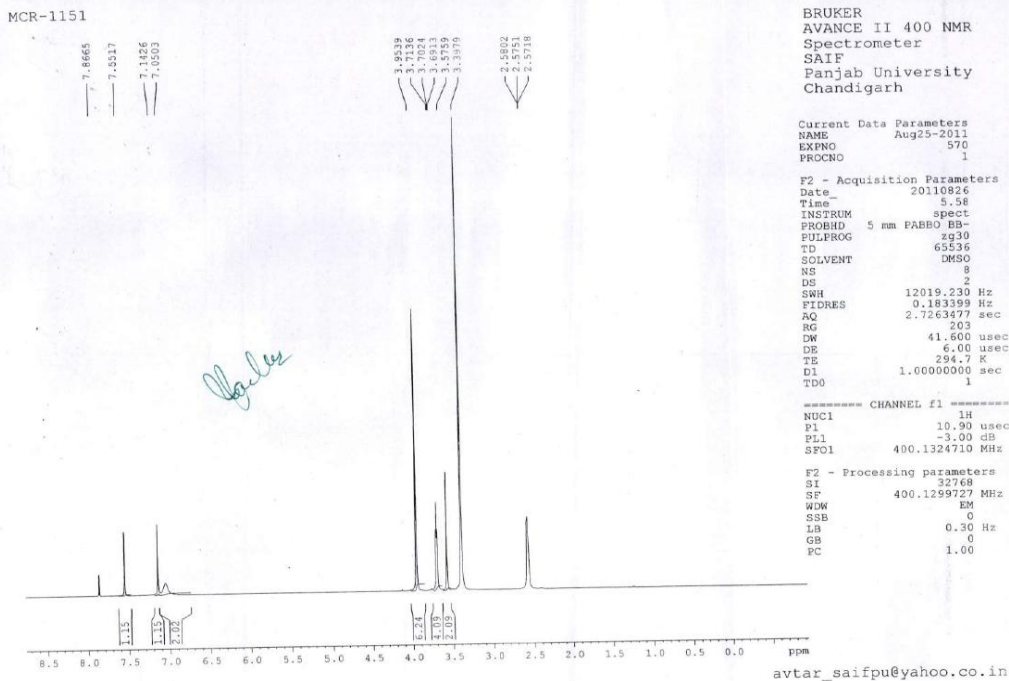
**6,7-Dimethoxy-2-[4-(2-methoxyphenyl)piperazin-1-yl]quinazolin-4-ylamine (43)**



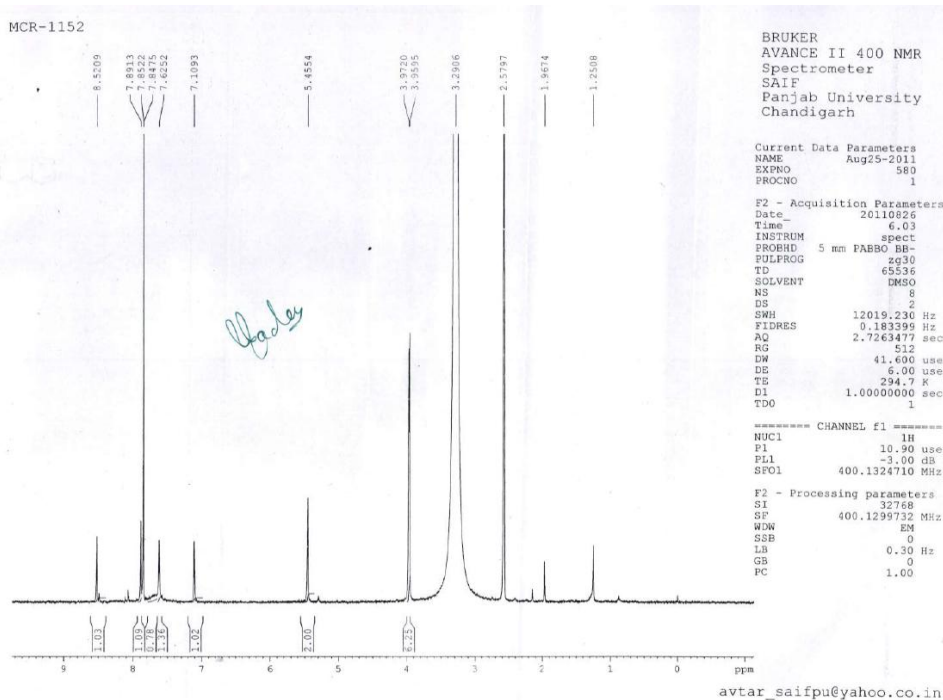
**2-(4-Benzhydrylpiperazin-1-yl)-6,7-dimethoxyquinazolin-4-ylamine (44)**



**6,7-Dimethoxy-2-(4-morpholinomethyl)quinazolin-4-ylamine (50)**

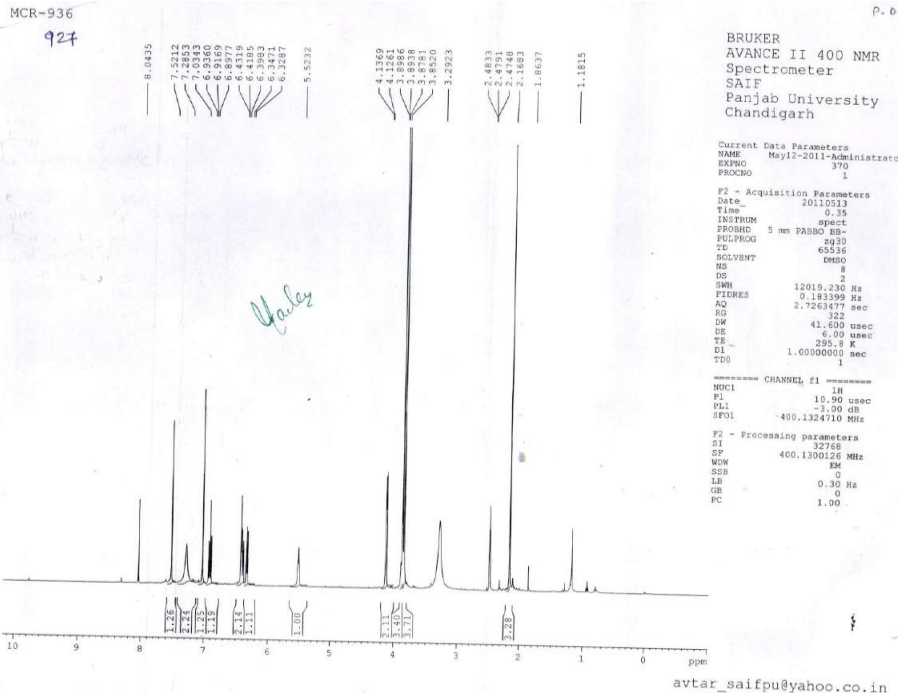


**6,7-Dimethoxy-2-[(1H-1,2,4-triazol-1-yl)methyl]quinazolin-4-ylamine (53)**

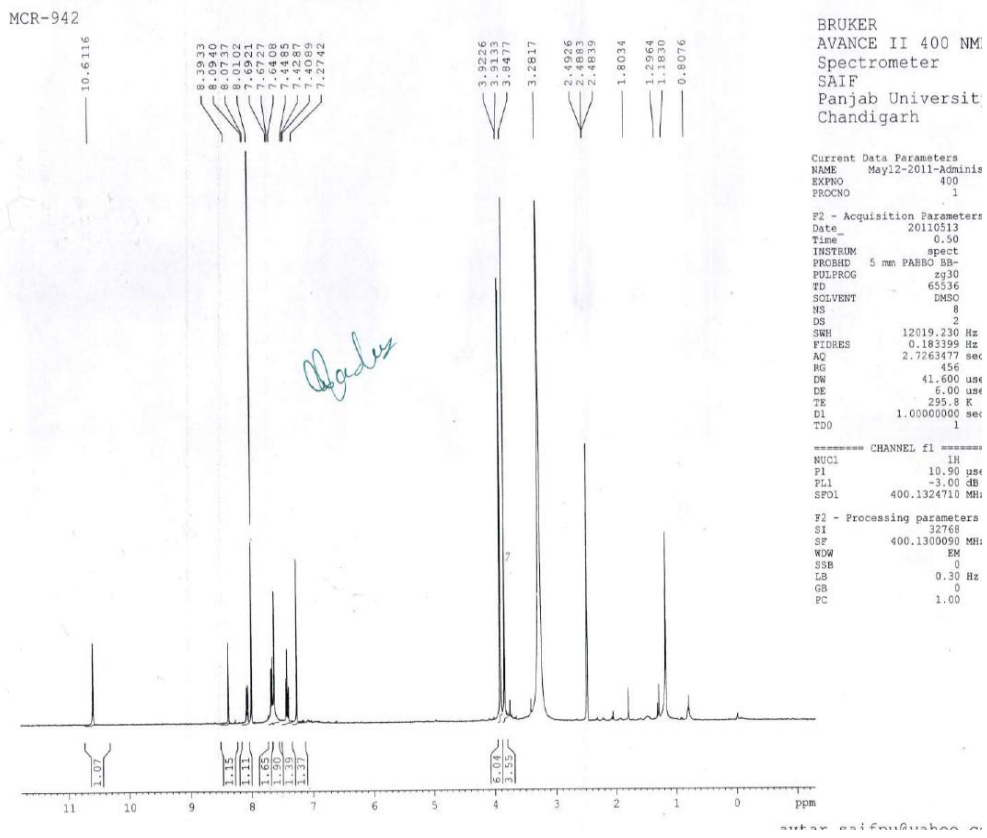




**2-[(3-Toluidino)methyl]-6,7-dimethoxyquinazolin-4-ylamine (63)**



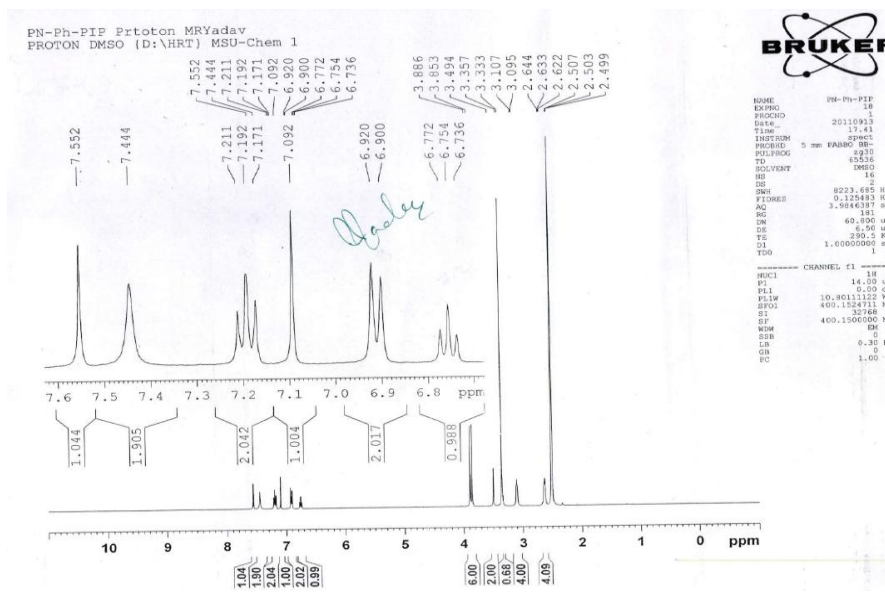
**2-[(3-Chlorophenylamino)methyl]-6,7-dimethoxyquinazolin-4-ylamine (65)**



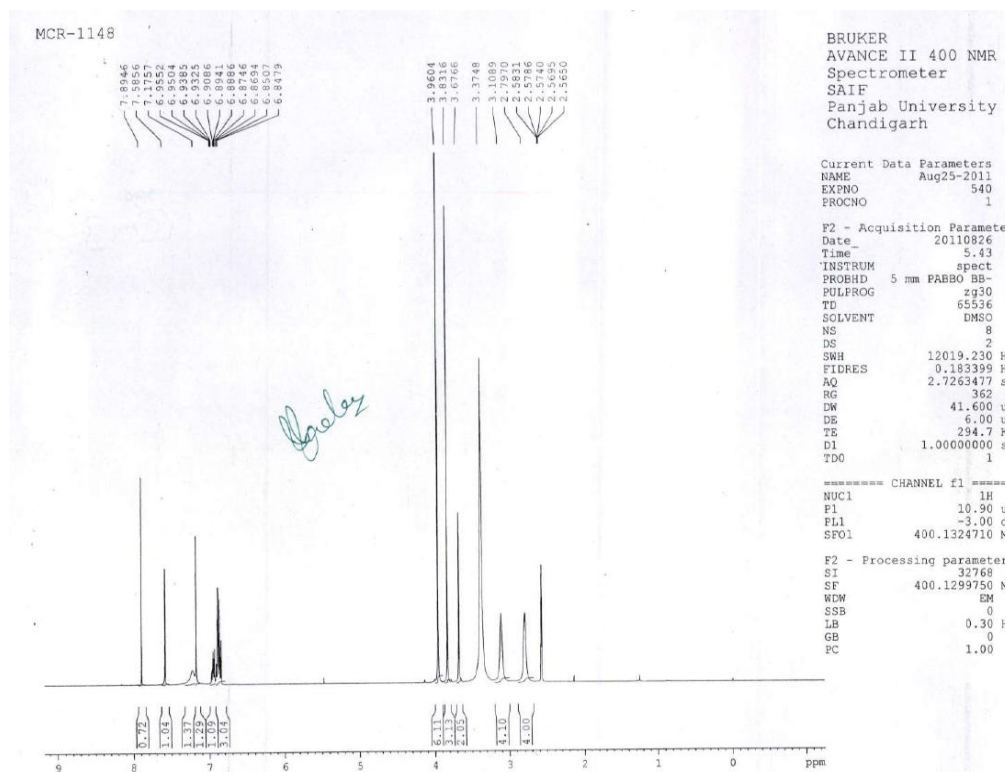




### 6,7-Dimethoxy-2-[(4-phenylpiperazin-1-yl)methyl]quinazolin-4-ylamine (96)

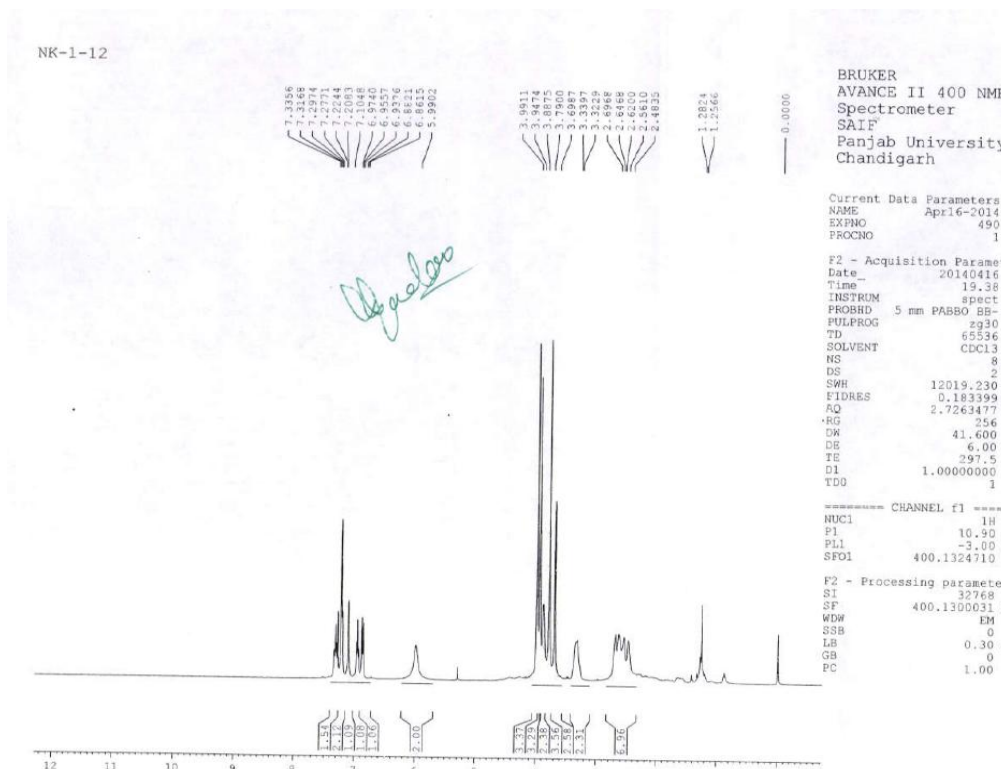


### 6,7-Dimethoxy-2-[(4-(2-methoxyphenyl)piperazin-1-yl)methyl]quinazolin-4-ylamine (97)

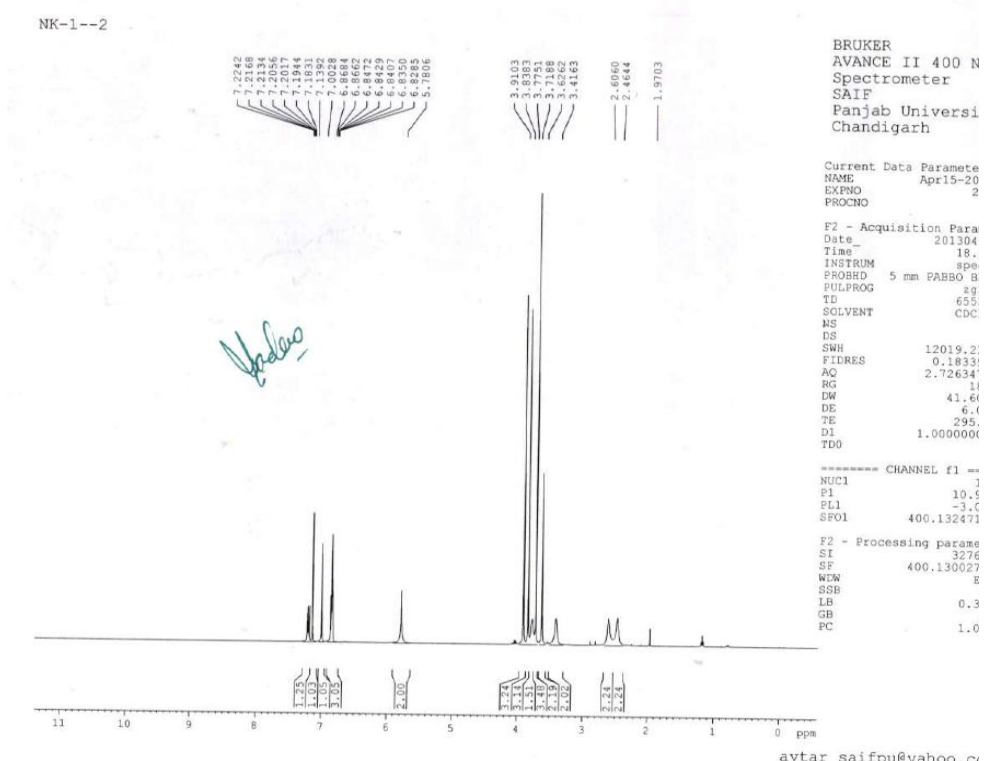




**4-Amino-2-[4-(2-methoxybenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (100)**



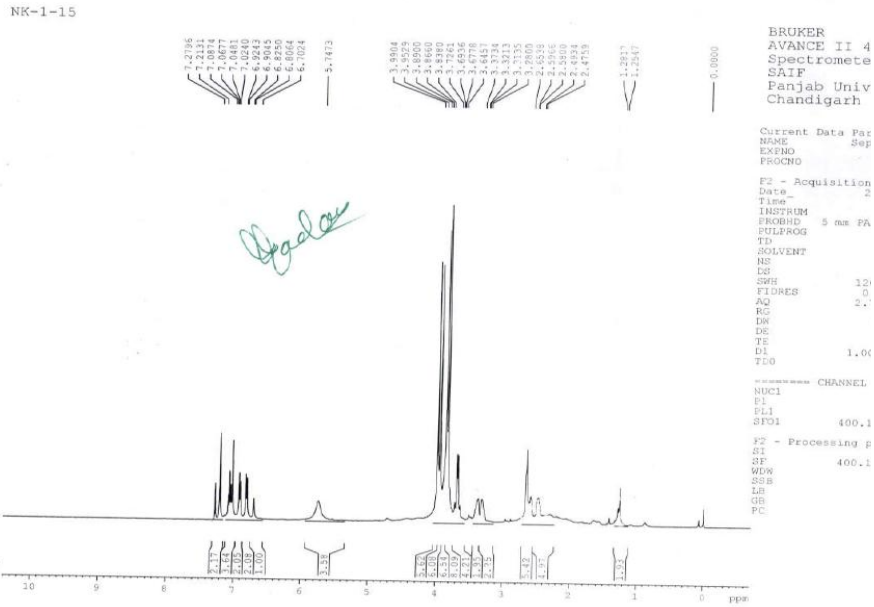
**4-Amino-2-[4-(3-methoxybenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (101)**



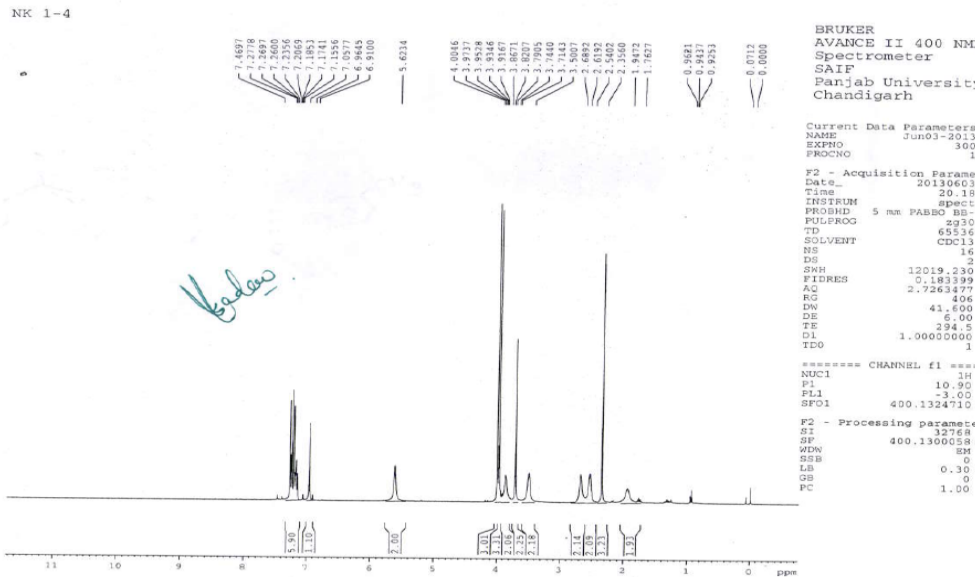




**4-Amino-2-[4-(2,3-dimethoxybenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (104)**

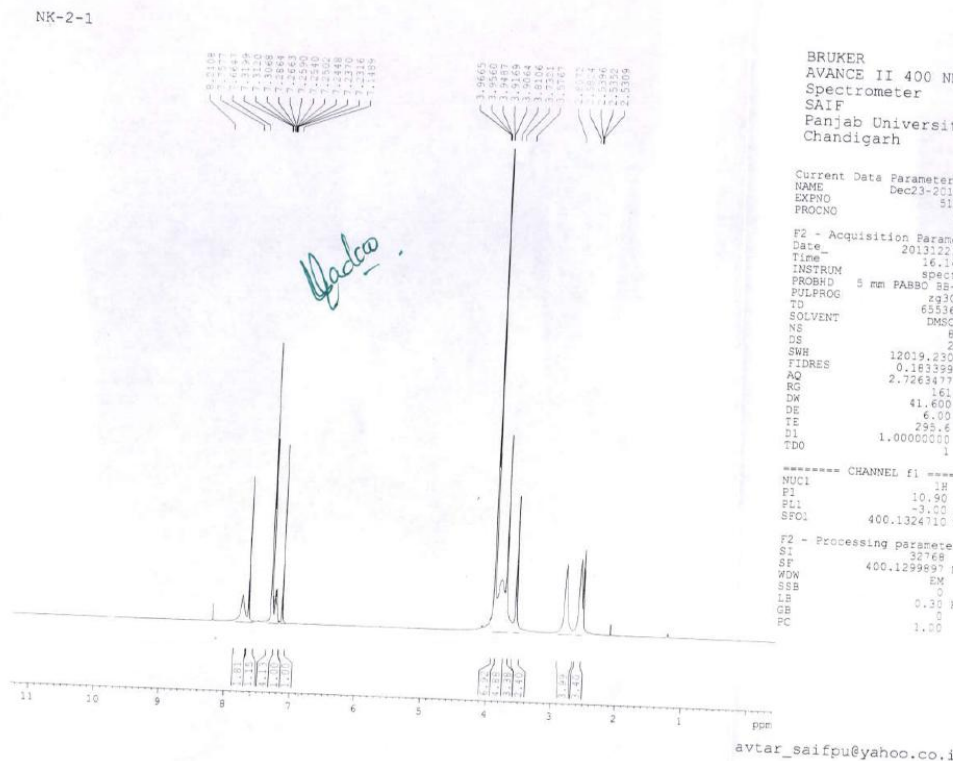


**4-Amino-2-[4-(3-methylbenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (105)**

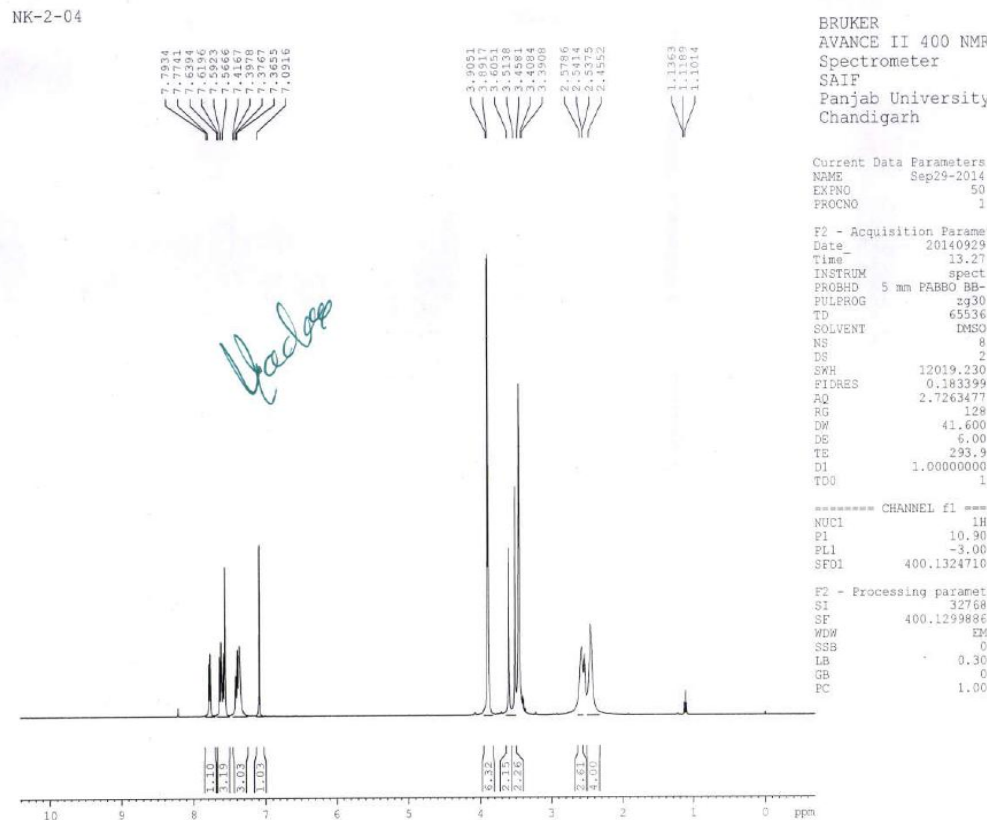




**4-Amino-2-[(4-benzylpiperazin-1-yl)methyl]-6,7-dimethoxyquinazoline (108)**

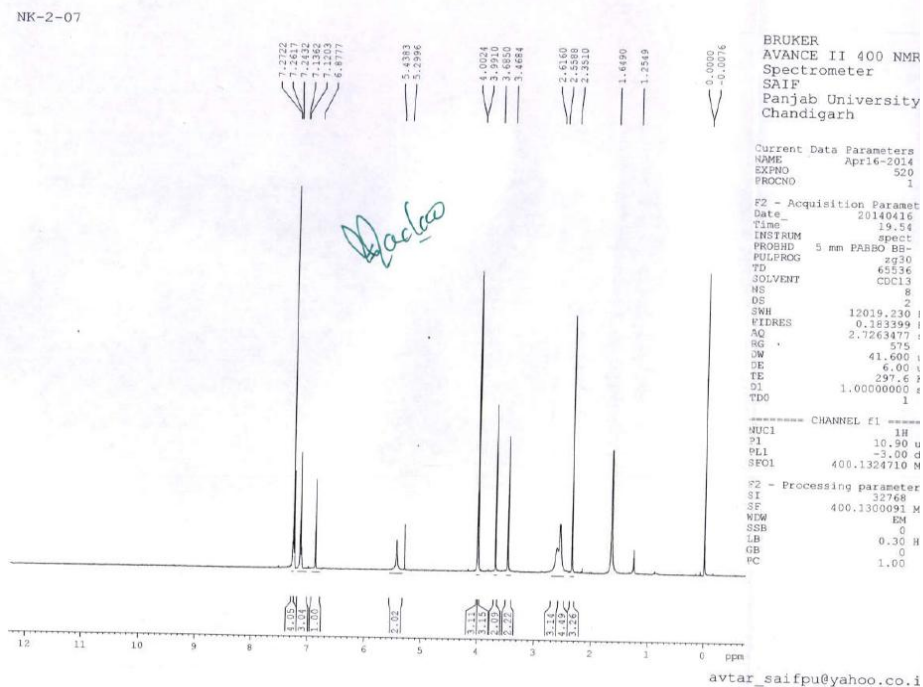


**4-Amino-2-[4-(2-trifluoromethylbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (109)**





### 4-Amino-2-[4-(2-methylbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (110)

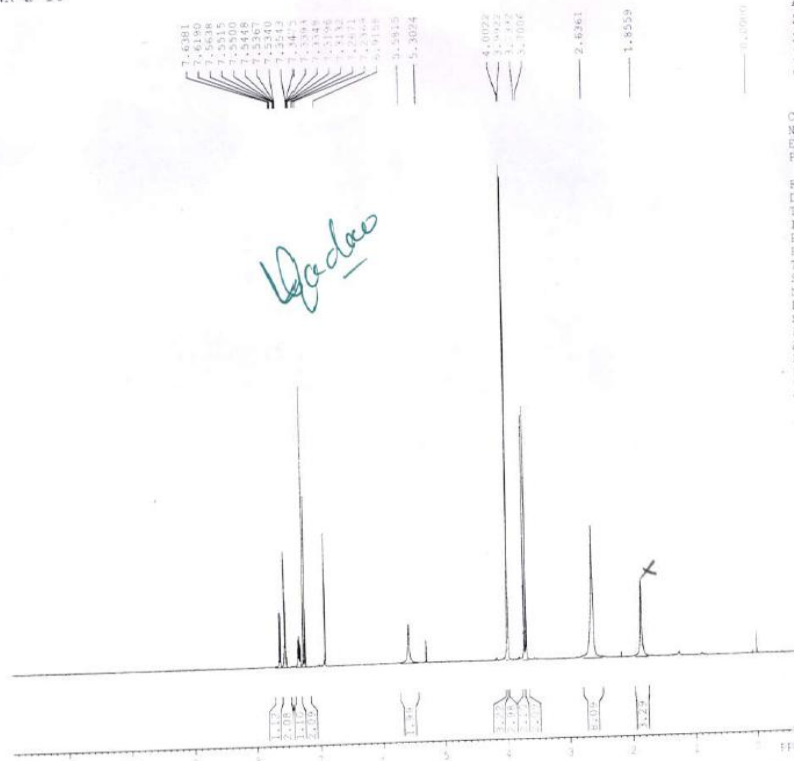


### 4-Amino-2-[4-(2-bromobenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (111)



### 4-Amino-2-[4-(2-cyanobenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (112)

NK-2-10



BRUKER  
AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

Current Data Parameters  
NAME Feb19-2014  
EXPNO 330  
PROCNO 1

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### 4-Amino-2-[4-(4-bromobenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (113)

NK-2-02



BRUKER  
AVANCE II 400 N  
Spectrometer  
SAIF  
Panjab Universi  
Chandigarh

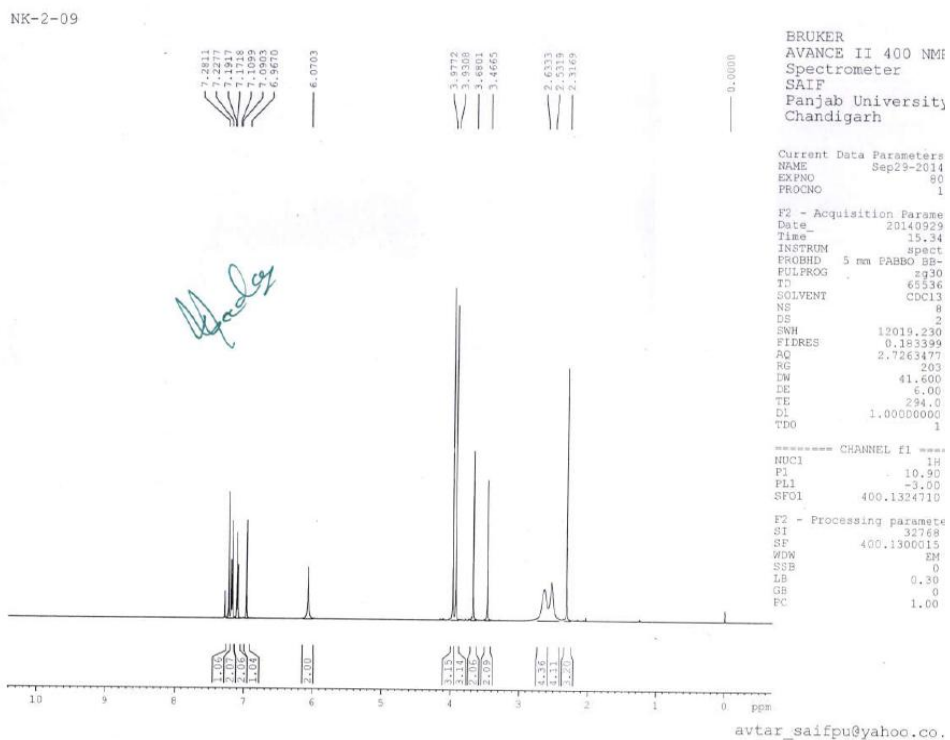
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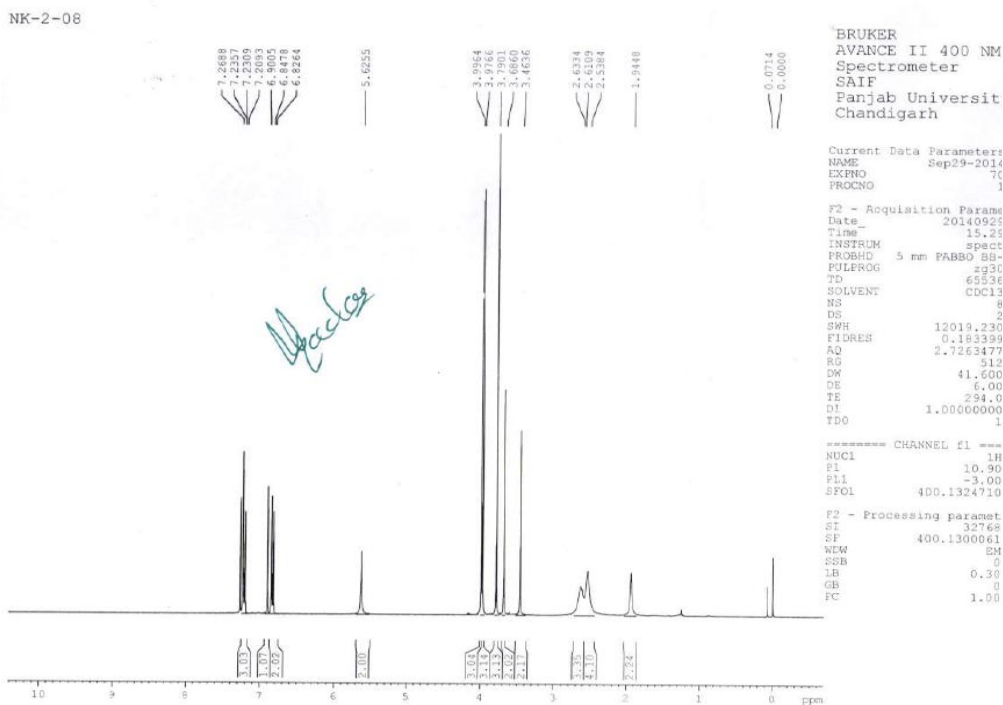
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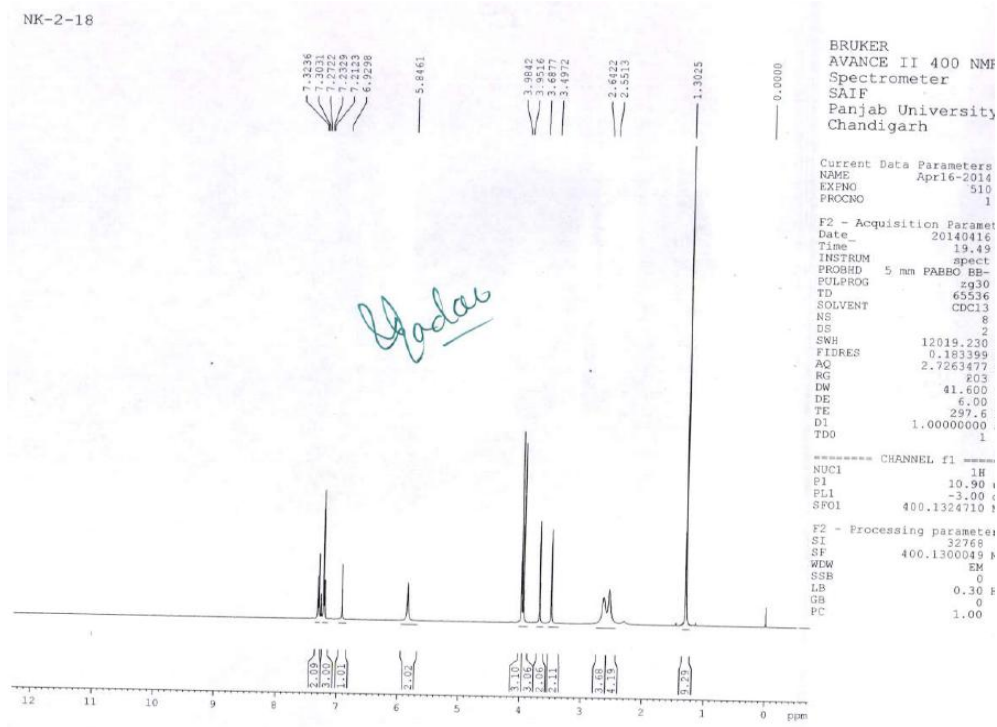
### 4-Amino-2-[4-(4-methylbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (114)



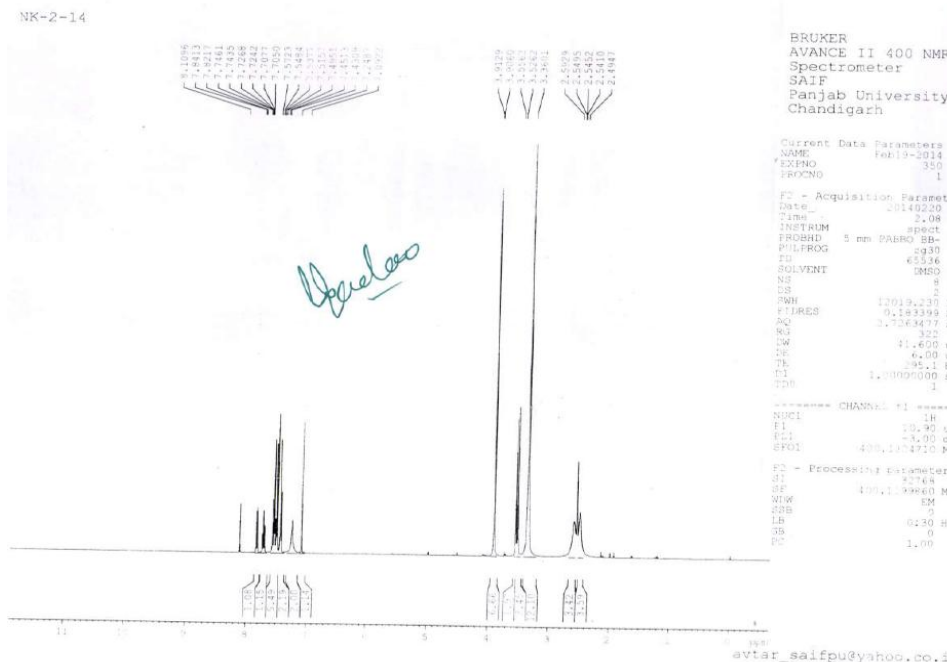
### 4-Amino-2-[4-(4-methoxybenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (115)



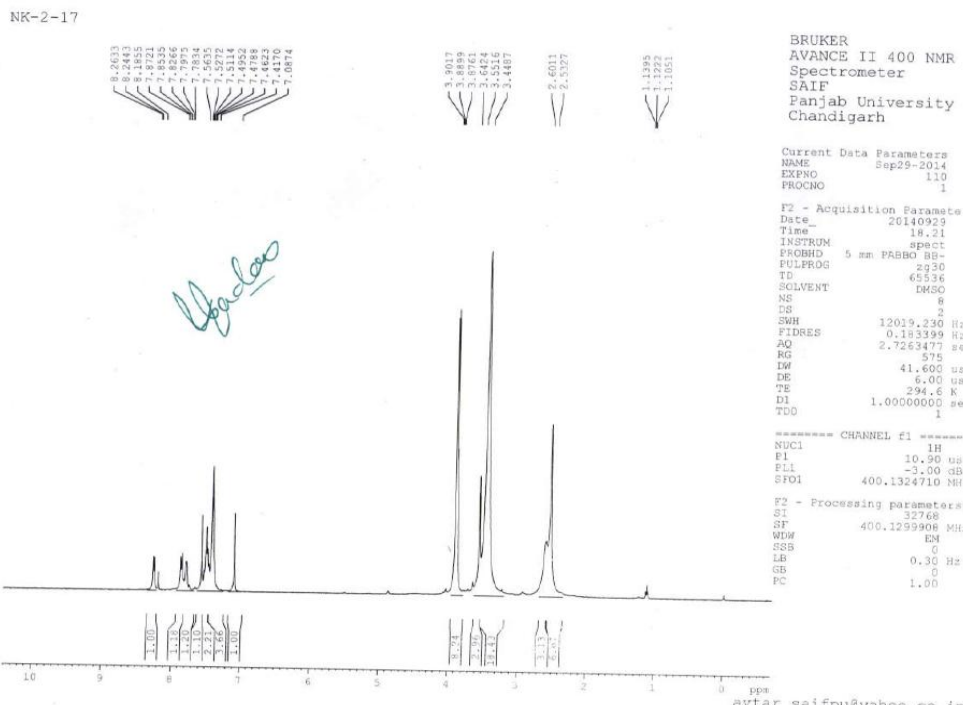
### 4-Amino-2-[4-(4-*t*-butylbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (116)



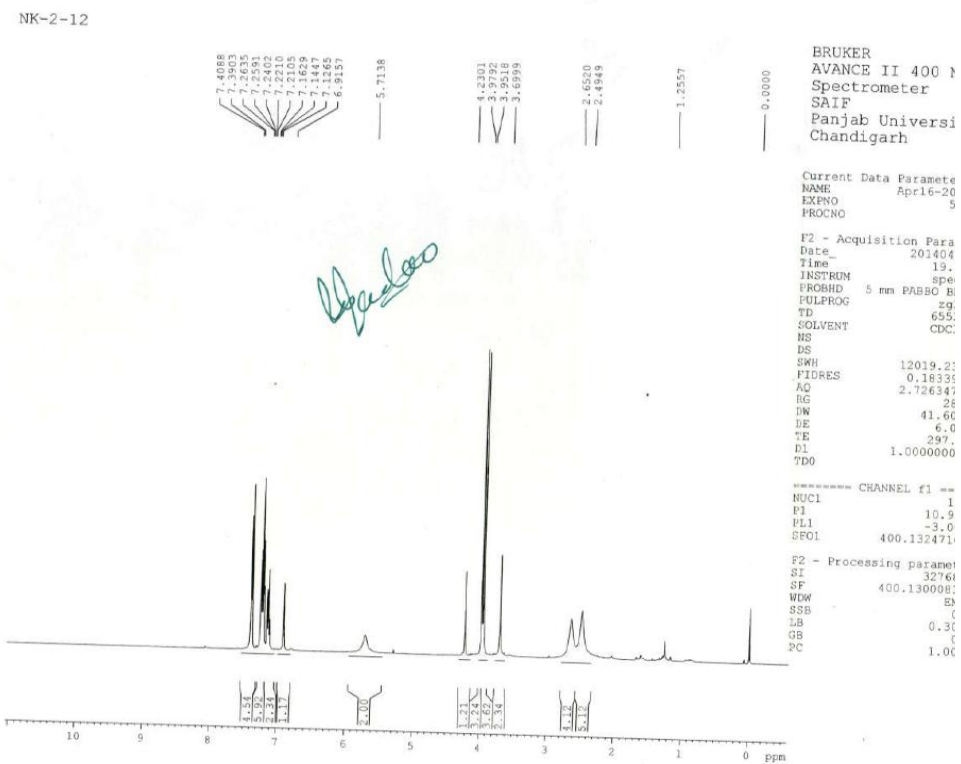
### 4-Amino-2-{4-[4-(2-cyanophenyl)benzyl]piperazin-1-ylmethyl}-6,7-dimethoxyquinazoline (117)



### 4-Amino-2-[4-(1-naphthylmethyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (118)

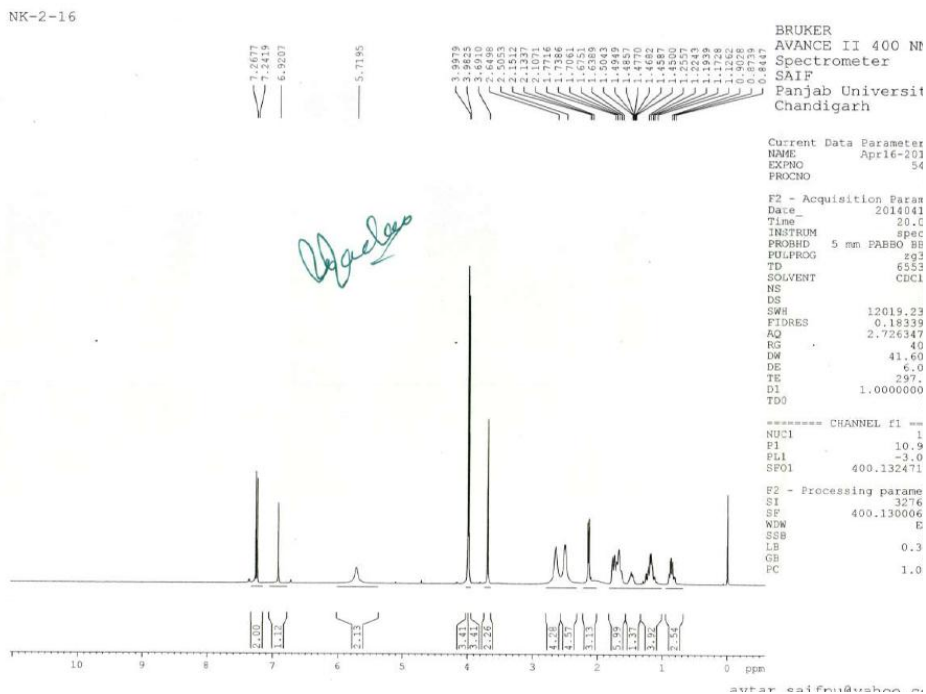


### 4-Amino-2-[(4-benzhydryl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (119)

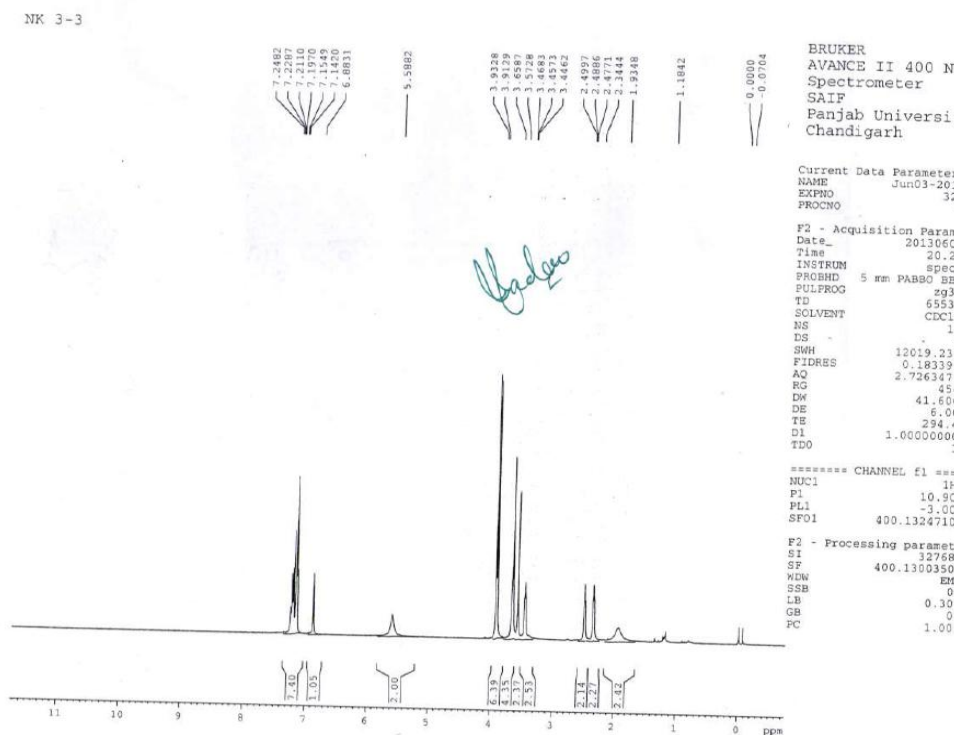




### 4-Amino-2-[4-(cyclohexylmethyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (120)

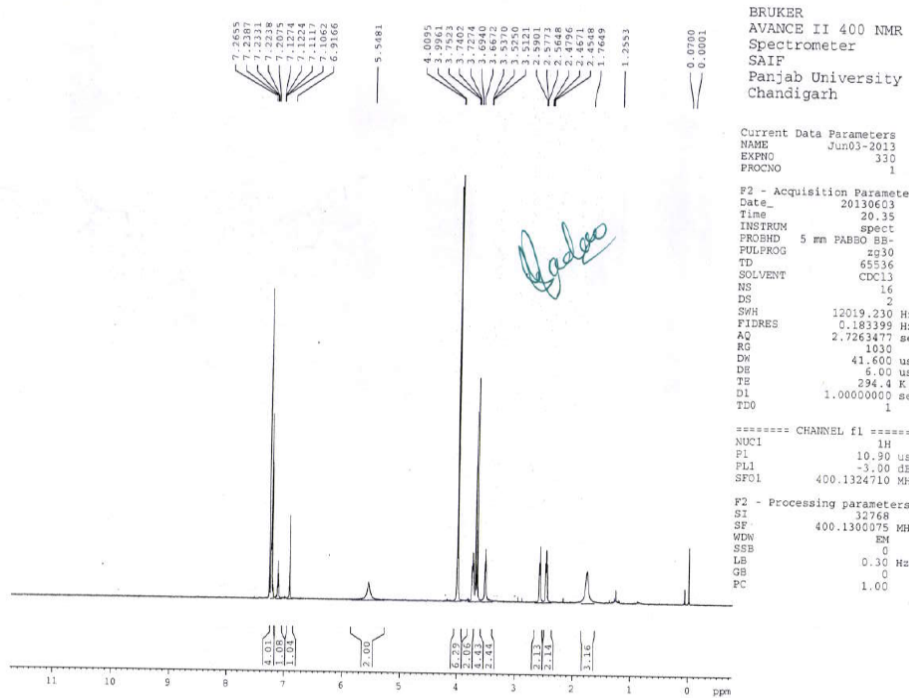


### 1-[4-(4-Amino-6,7-dimethoxyquinazolin-2-yl)methylpiperazin-1-yl]-2-phenylethanone (121)



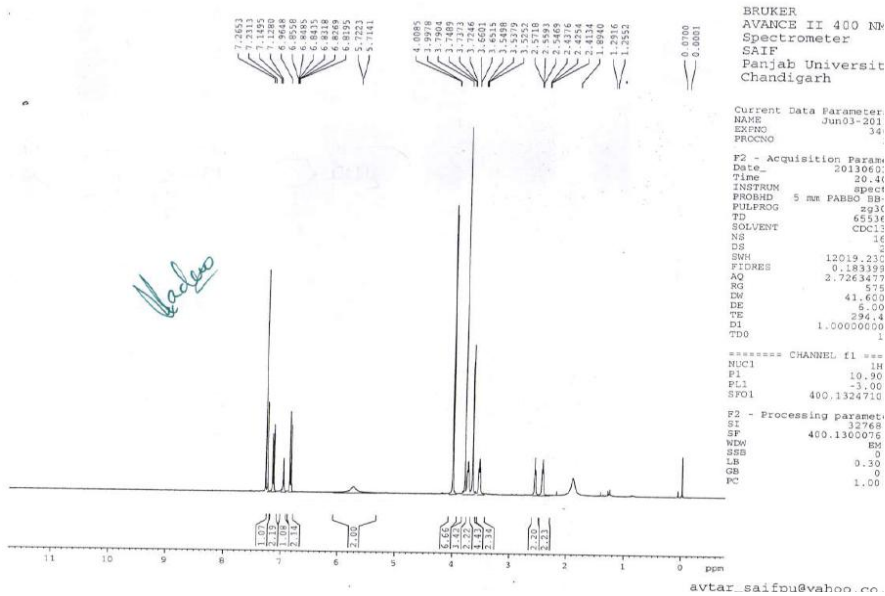
**1-[4-(4-Amino-6,7-dimethoxyquinazolin-2-yl)methylpiperazin-1-yl]-2-(3-chlorophenyl) ethanone (122)**

NK 3-4

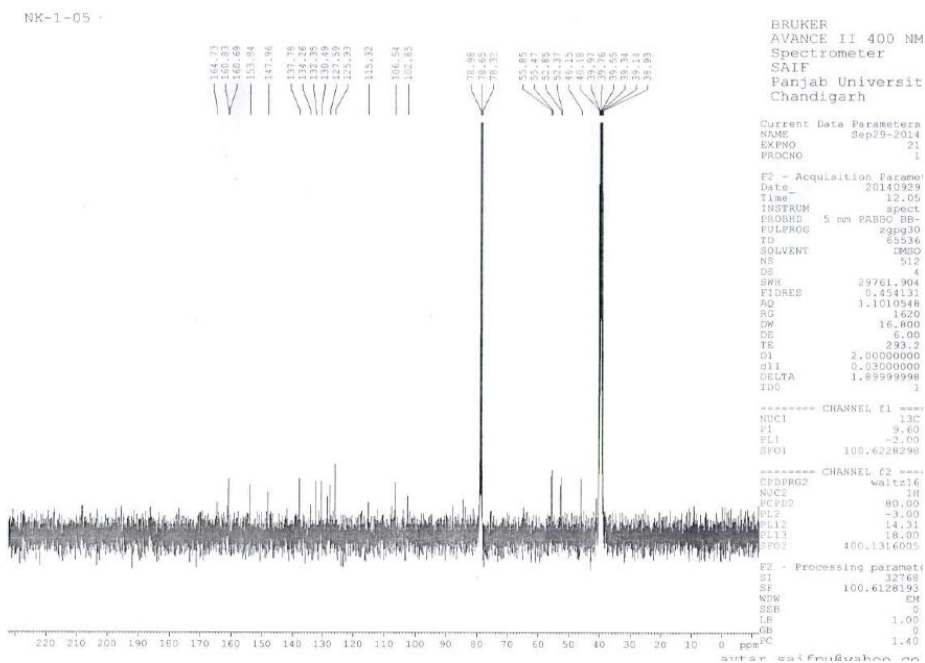


**1-[4-(4-Amino-6,7-dimethoxyquinazolin-2-yl)methylpiperazin-1-yl]-2-(4-methoxyphenyl) ethanone (123)**

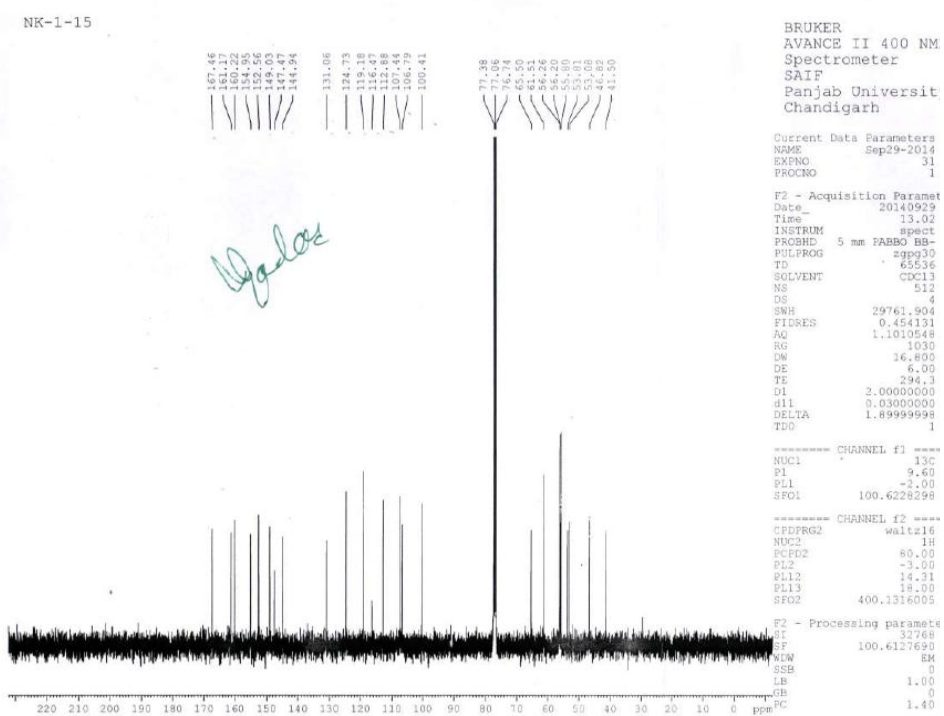
NK 3-5



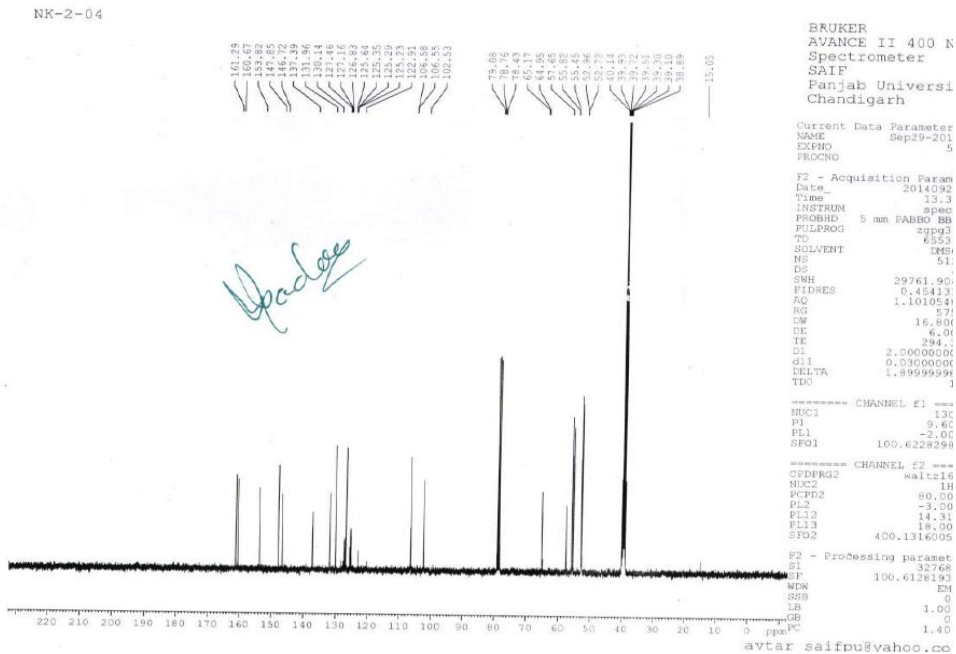
### 4-Amino-2-[4-(2,3-dichlorobenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (103)



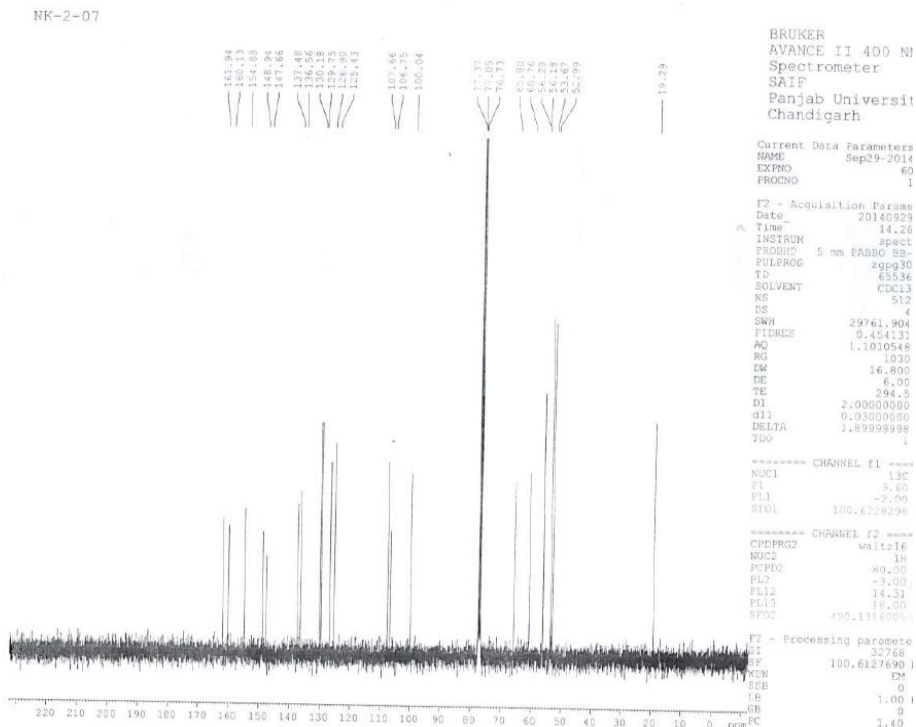
### 4-Amino-2-[4-(2,3-dimethoxybenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (104)



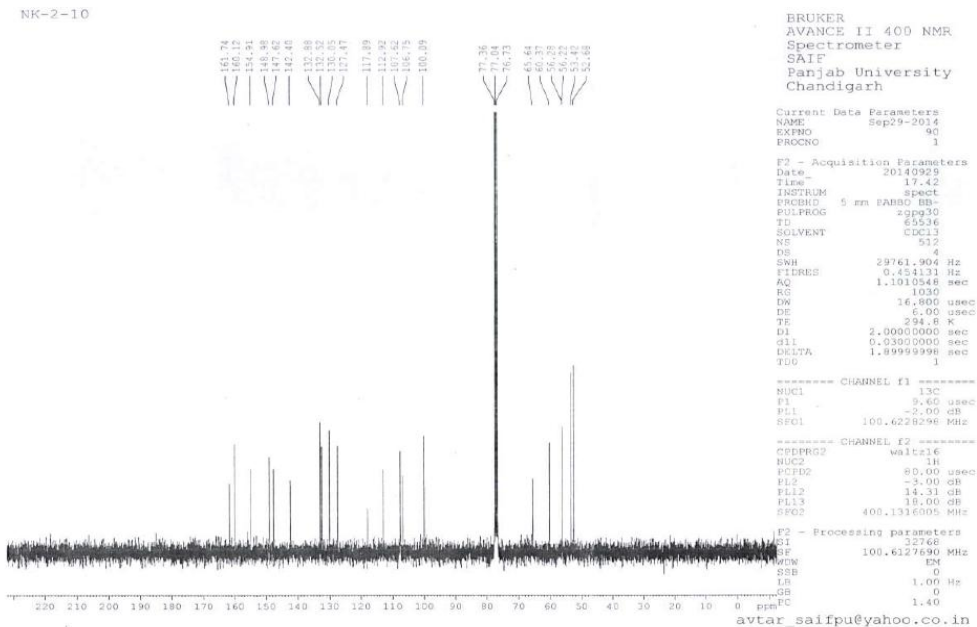
**4-Amino-2-[4-(2-trifluoromethylbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (109)**



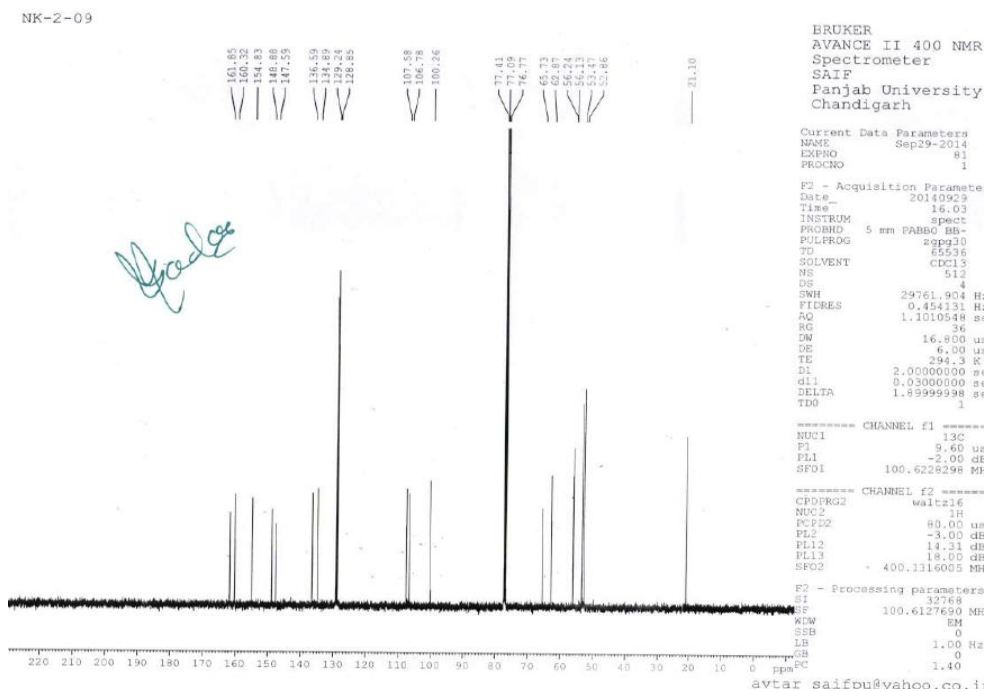
**4-Amino-2-[4-(2-methylbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (110)**



### 4-Amino-2-[4-(2-cyanobenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (112)



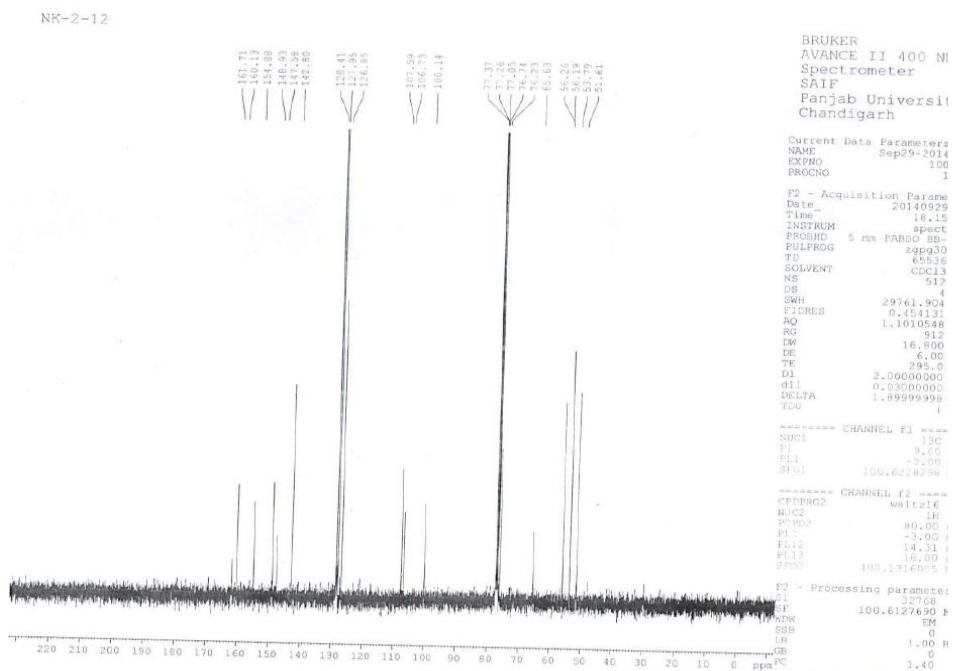
### 4-Amino-2-[4-(4-methylbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (114)



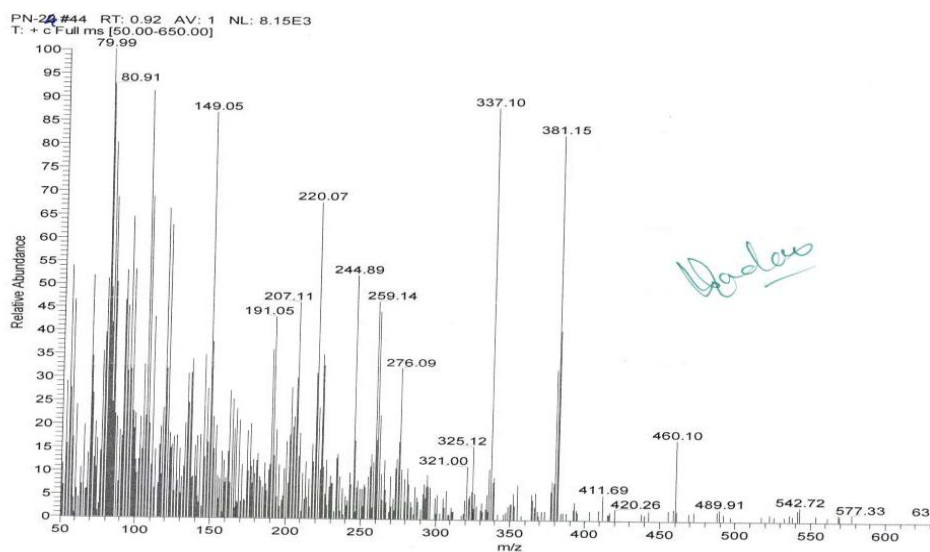




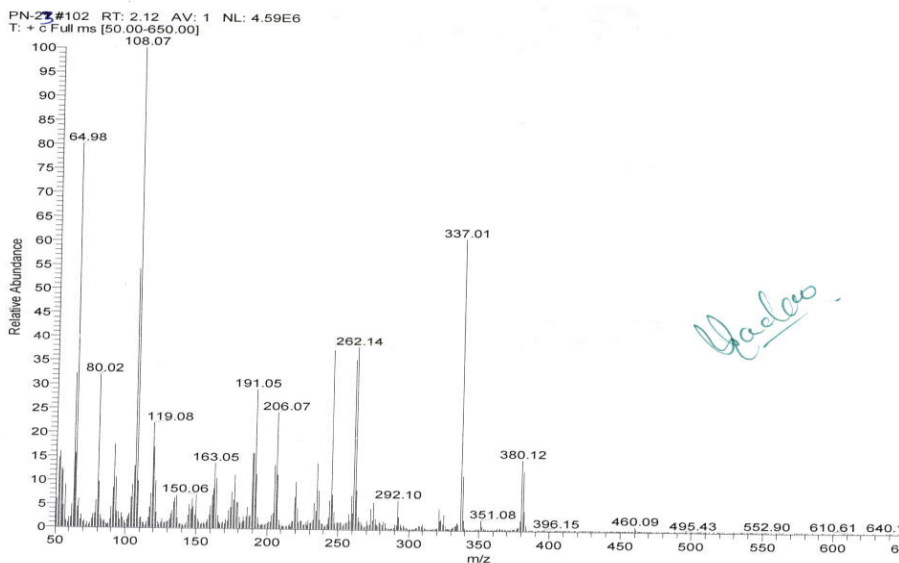
# 4-Amino-2-[(4-benzhydryl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (119)



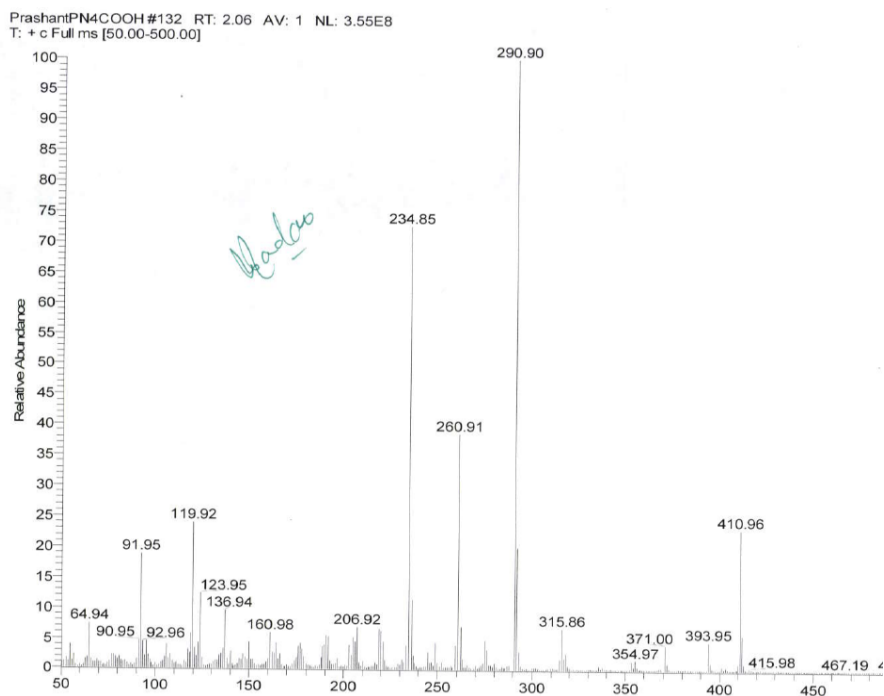
***N*-{3-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazolin-2yl)methylamino]phenyl}methanesulfonamide (24)**



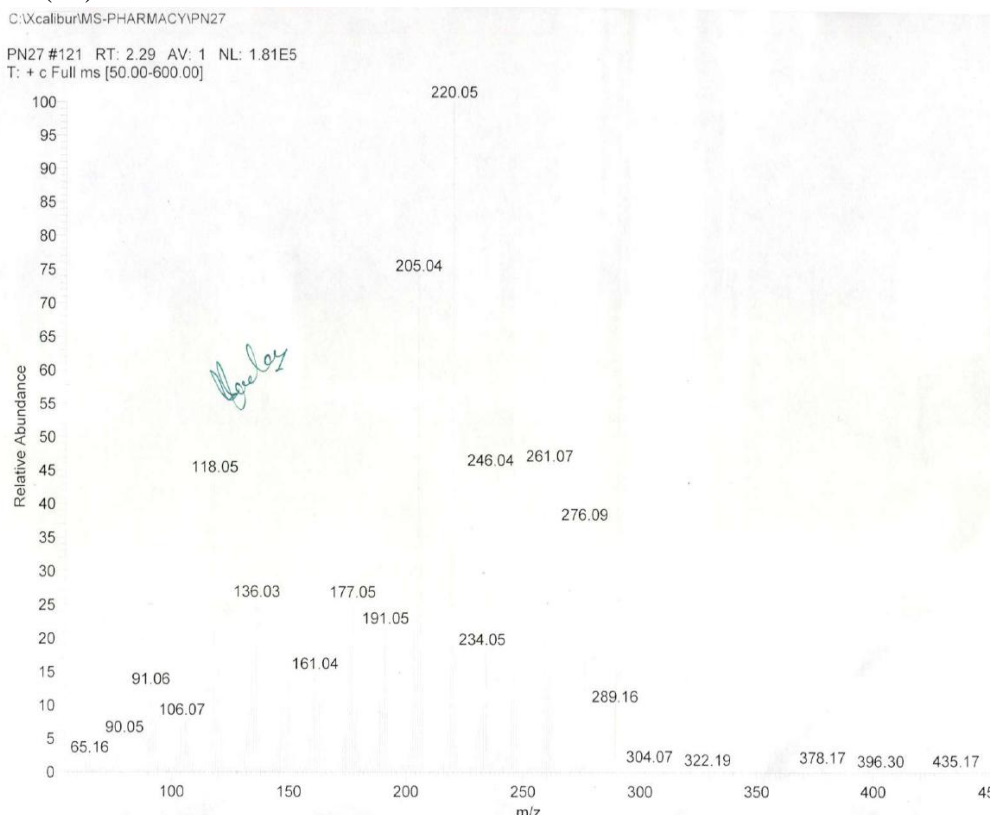
***N*-{4-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazoline-2yl)methylamino]phenyl}methanesulfonamide (25)**



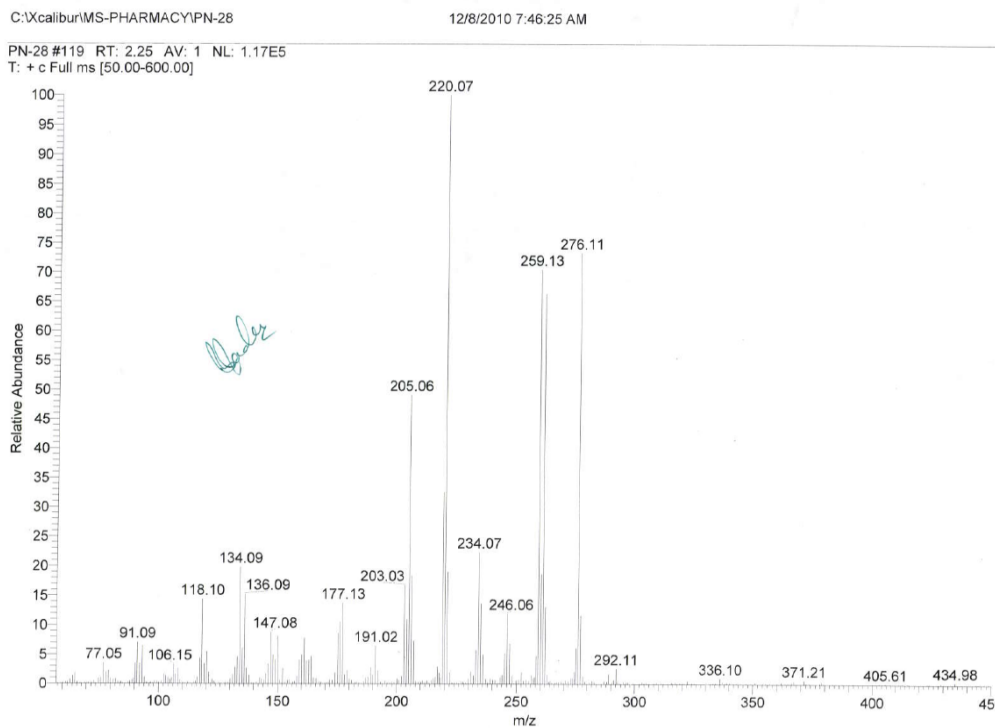
### 4-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazolin-2-yl)methylamino]benzoic acid (26)



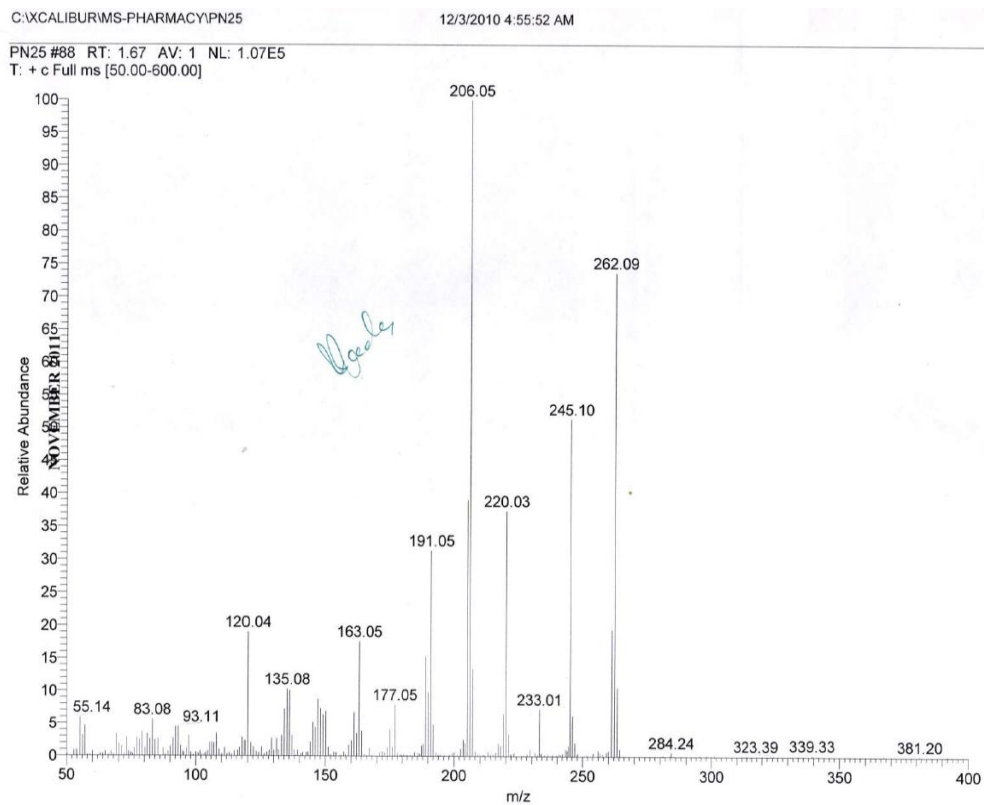
### 5-{4-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazolin-2-yl)methylamino]phenyl}-1H-tetrazole (27)



## 5-{3-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazolin-2yl)methylamino]phenyl}-1H-tetrazole (28)

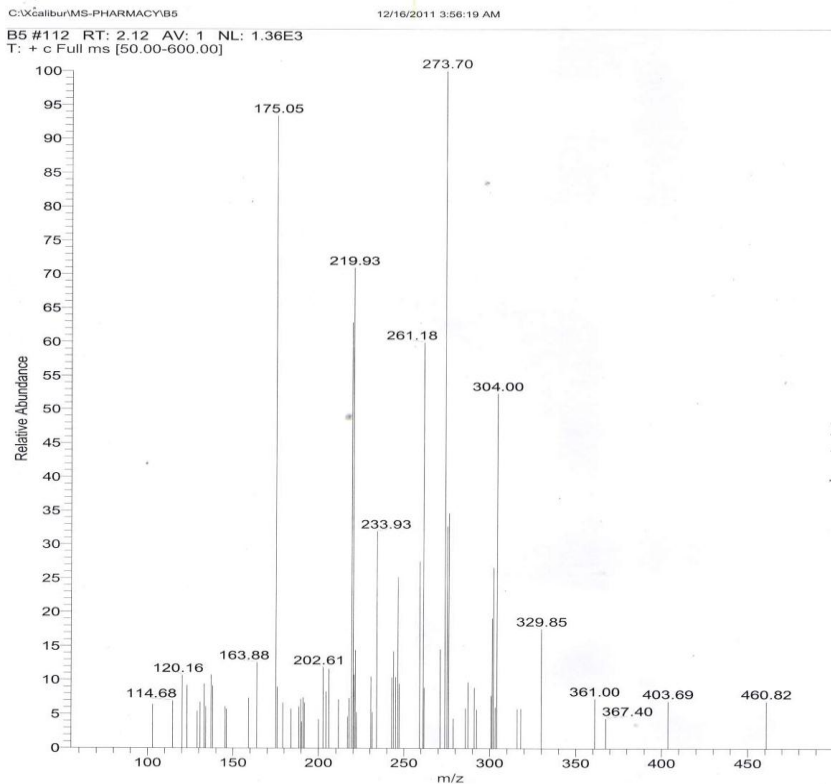


## 2-[(4-Aminophenyl)aminomethyl]-3-butyl-6,7-dimethoxyquinazolin-4(3H)-one (29)

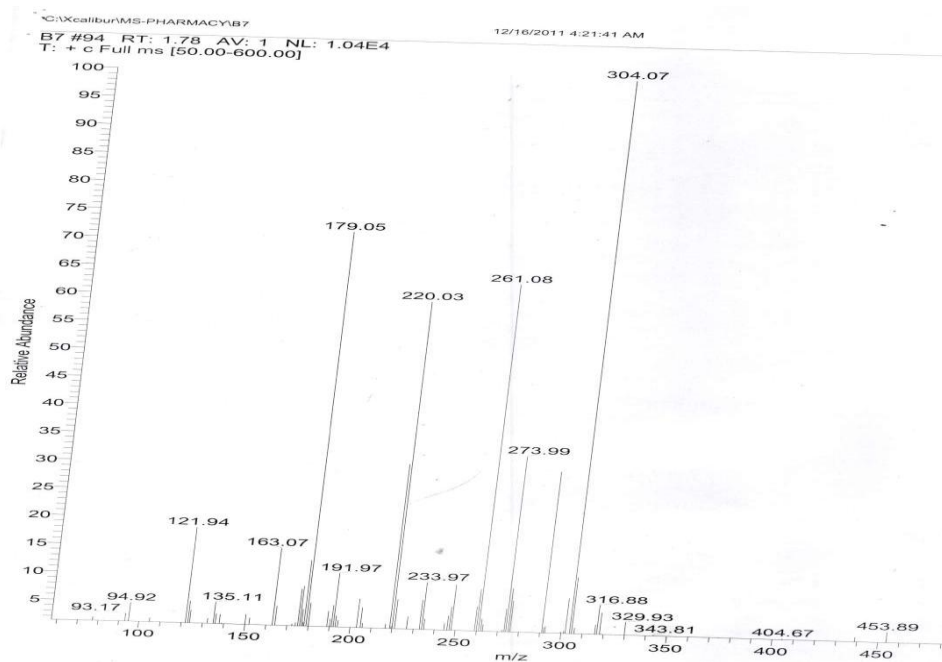




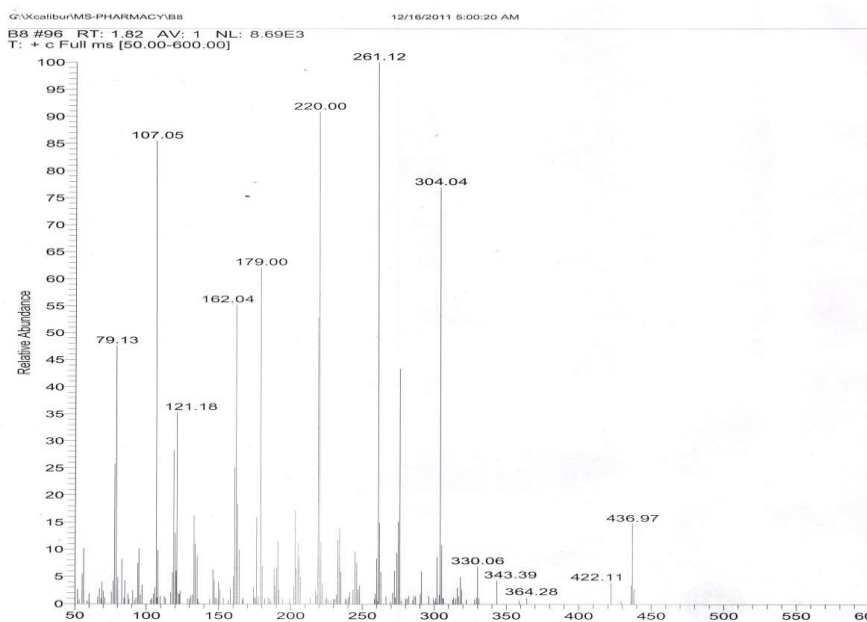
**2-[4-[(3-Butyl-3,4-dihydro-6,7-dimethoxy-4-oxoquinazolin-2-yl)methyl]piperazin-1-yl]benzonitrile (33)**



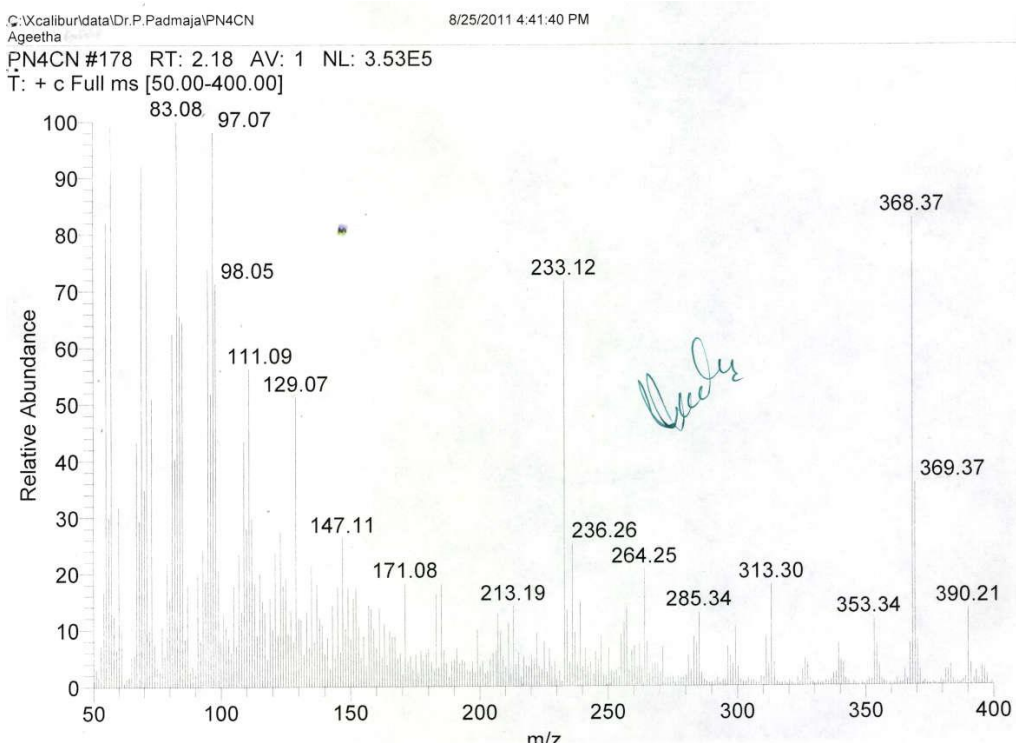
**3-Butyl-2-[[4-(2-fluorophenyl)piperazin-1-yl]methyl]-6,7-dimethoxyquinazolin-4(3H)-one (34)**



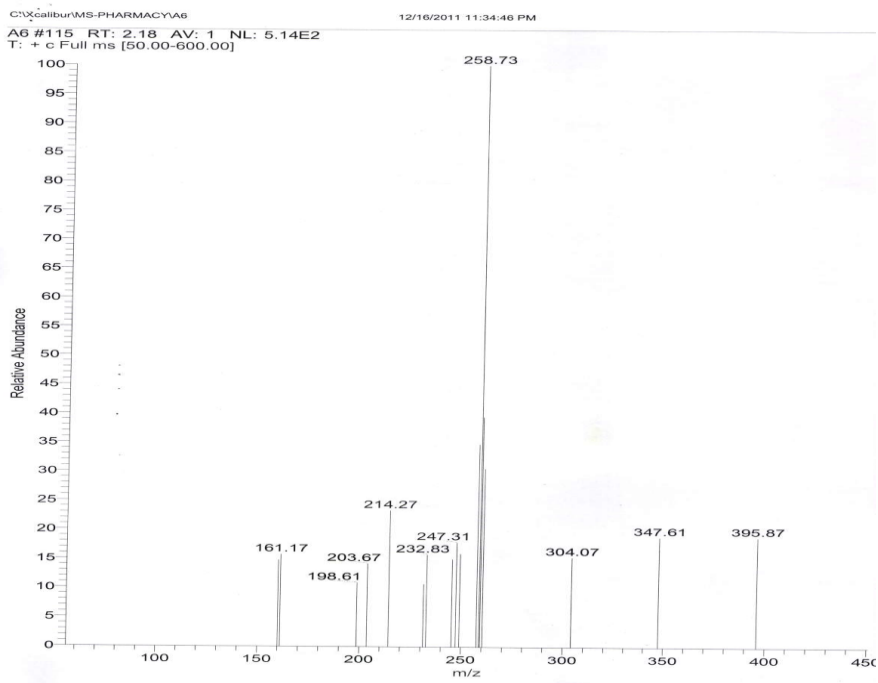
### 3-Butyl-6,7-dimethoxy-2-[(4-(pyridin-2-yl)piperazin-1-yl)methyl]quinazolin-4(3H)-one (35)



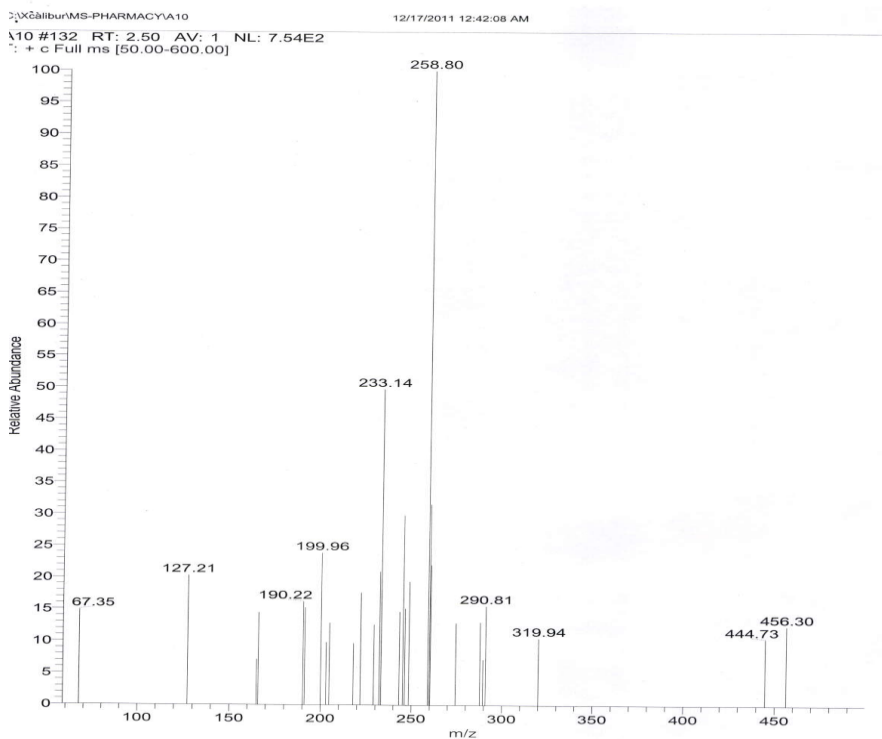
### 2-[4-(4-Amino-6,7-dimethoxyquinazolin-2-yl)piperazin-1-yl]benzotrile (42)



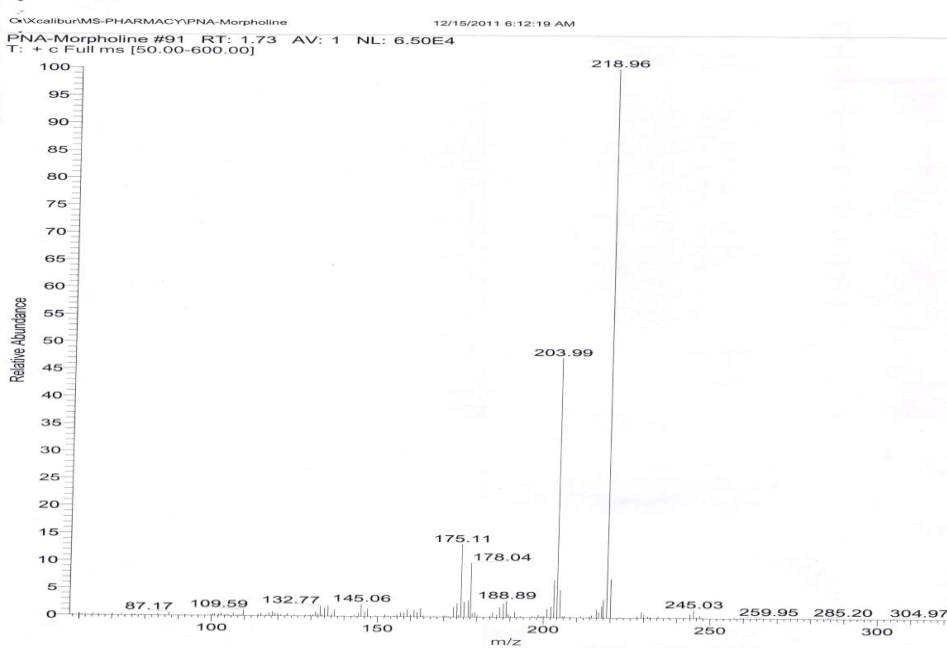
### 6,7-Dimethoxy-2-[4-(2-methoxyphenyl)piperazin-1-yl]quinazolin-4-ylamine (43)



### 2-(4-Benzhydrylpiperazin-1-yl)-6,7-dimethoxyquinazolin-4-ylamine (44)

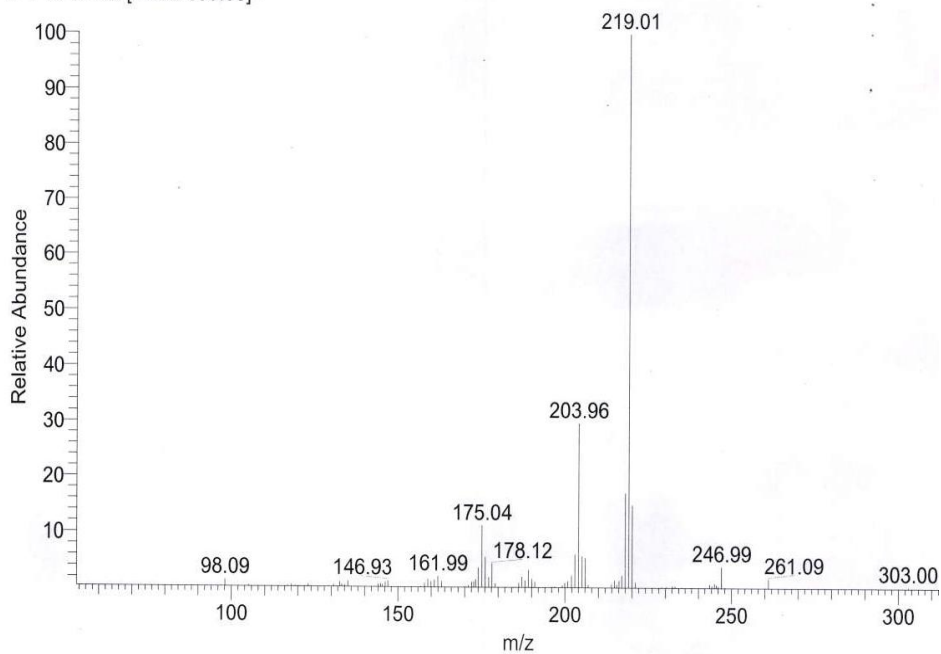


### 6,7-Dimethoxy-2-(4-morpholinomethyl)quinazolin-4-ylamine (50)

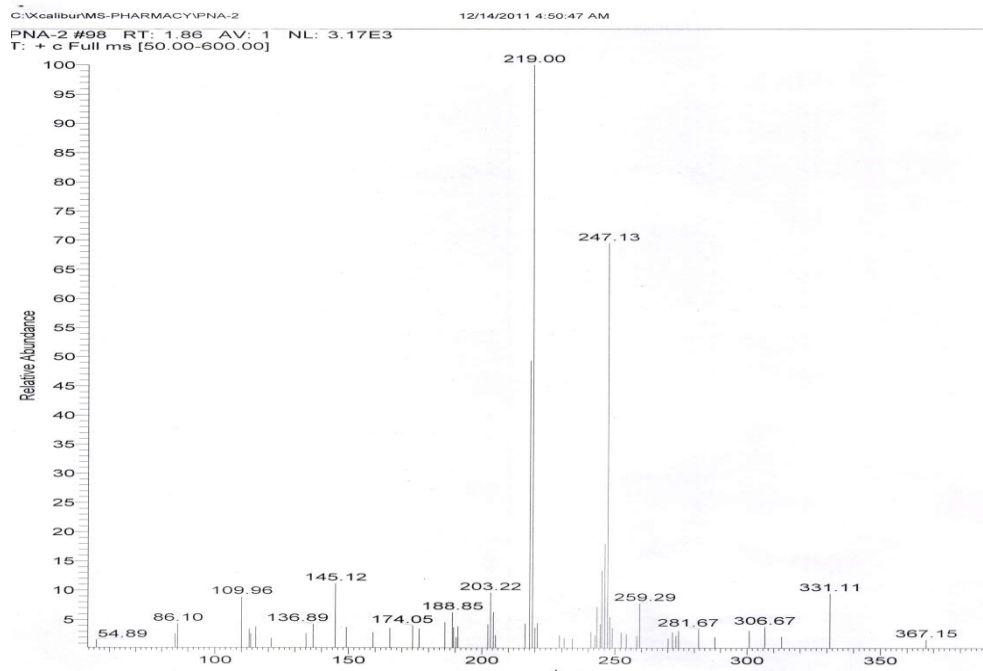


### 6,7-Dimethoxy-2-[(piperidin-1-yl)methyl]quinazolin-4-ylamine (51)

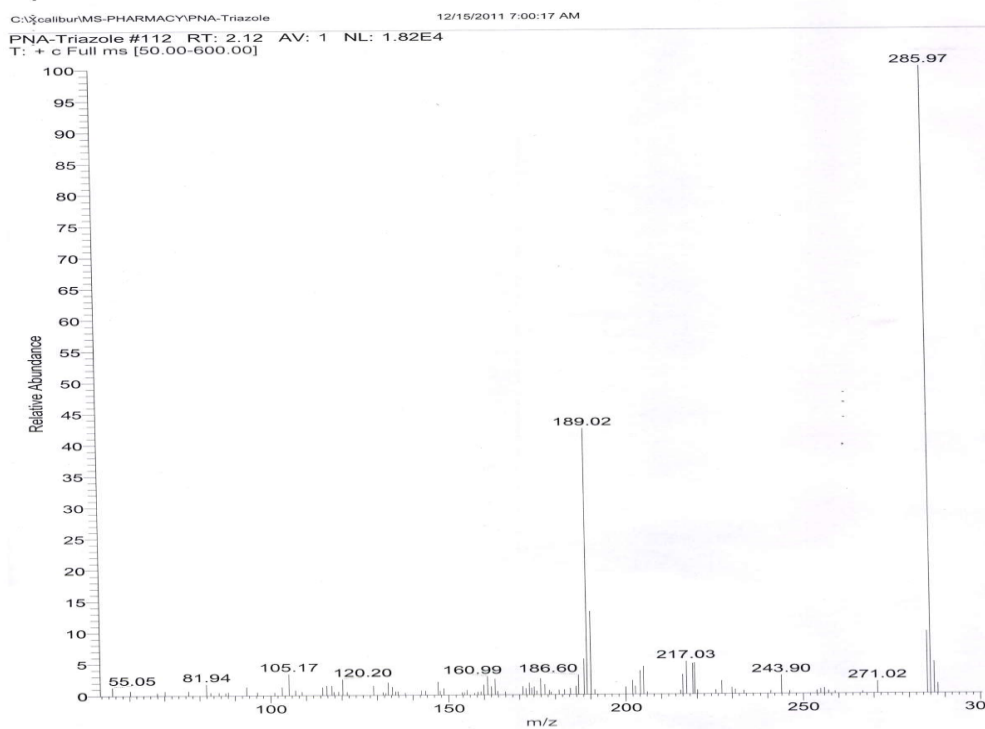
PNA-Piperidine #106 RT: 2.01 AV: 1 NL: 2.33E5  
T: + c Full ms [50.00-600.00]



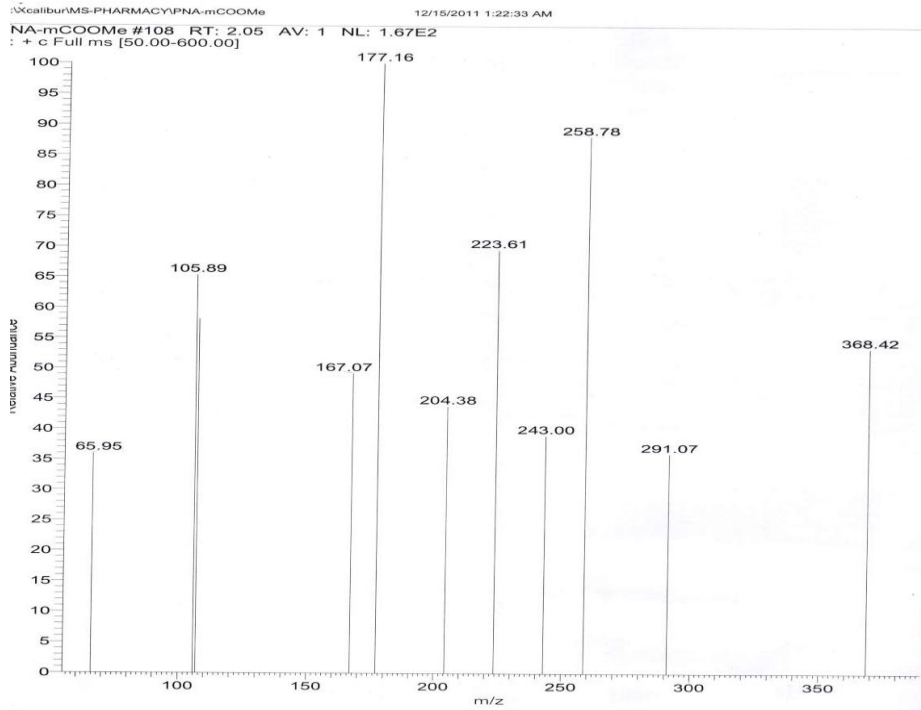
## 2-[(4-Ethylpiperazin-1-yl)methyl]-6,7-dimethoxyquinazolin-4-ylamine (52)



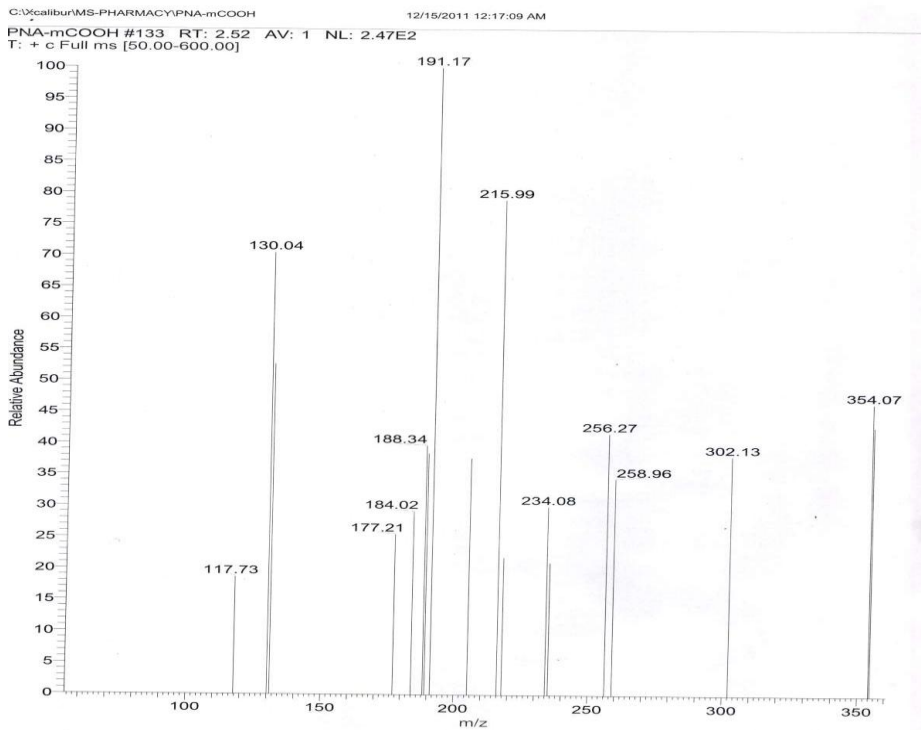
## 6,7-Dimethoxy-2-[(1H-1,2,4-triazol-1-yl)methyl]quinazolin-4-ylamine (53)



### Methyl 3-[(4-amino-6,7-dimethoxyquinazolin-2-yl)methylamino]benzoate (61)

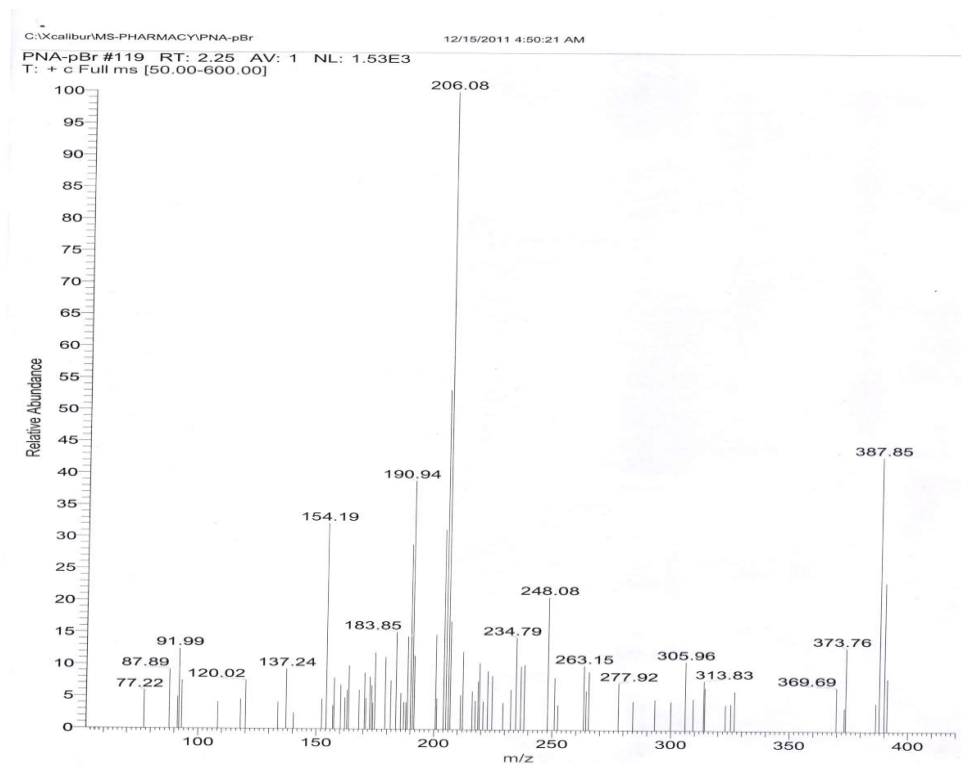


### 3-[(4-Amino-6,7-dimethoxyquinazolin-2-yl)methylamino]benzoic acid (62)

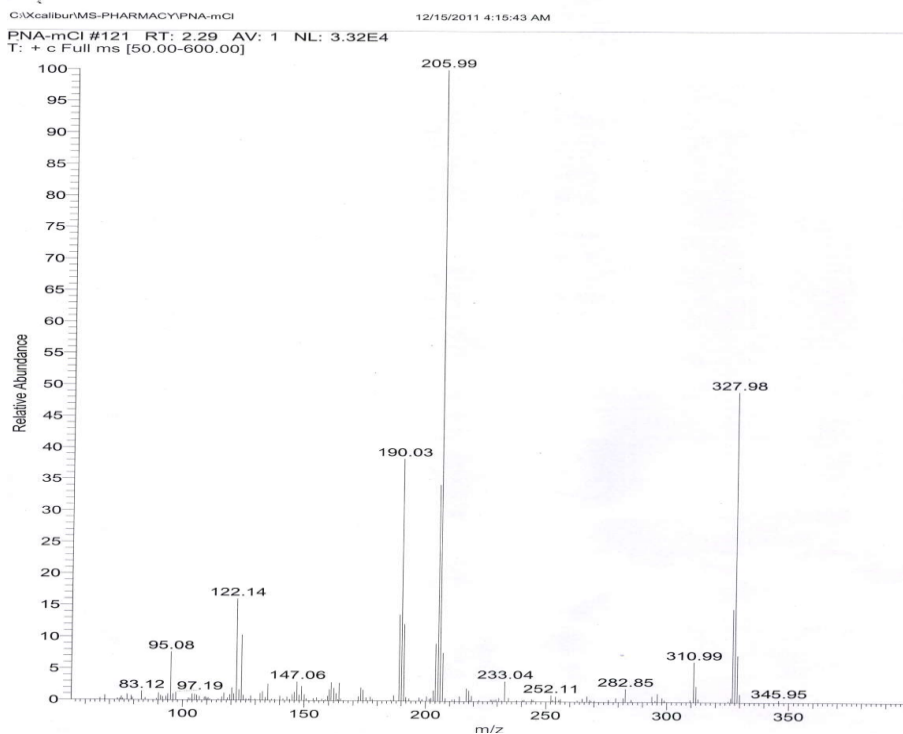




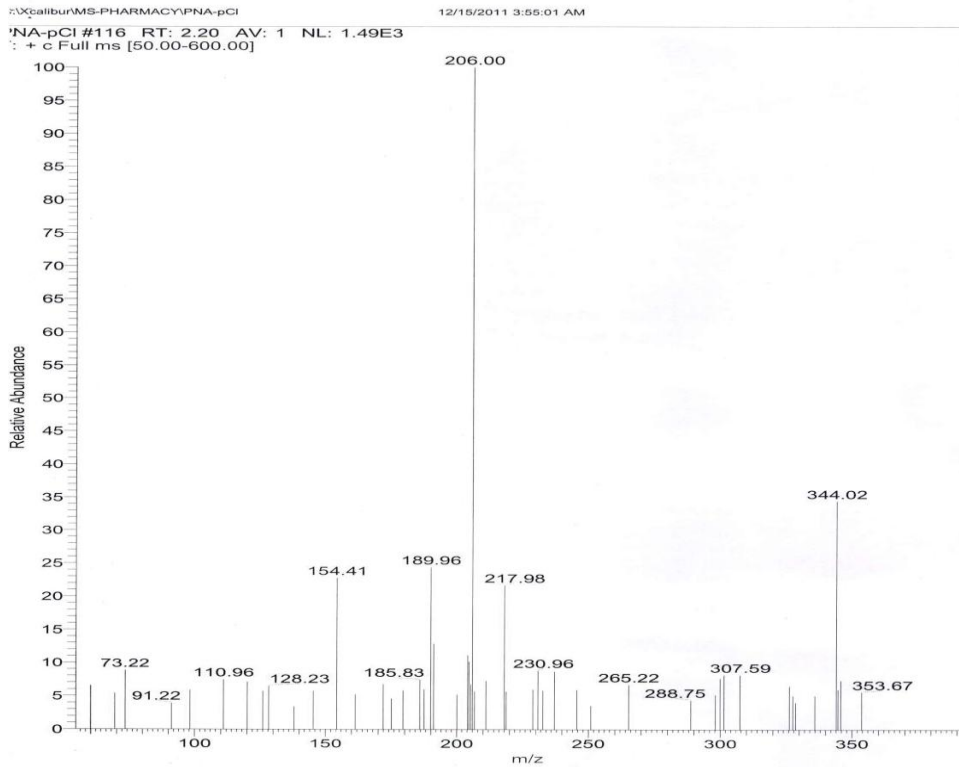
### 4-[(4-Amino-6,7-dimethoxyquinazolin-2-yl)methylamino]bromobenzene (64)



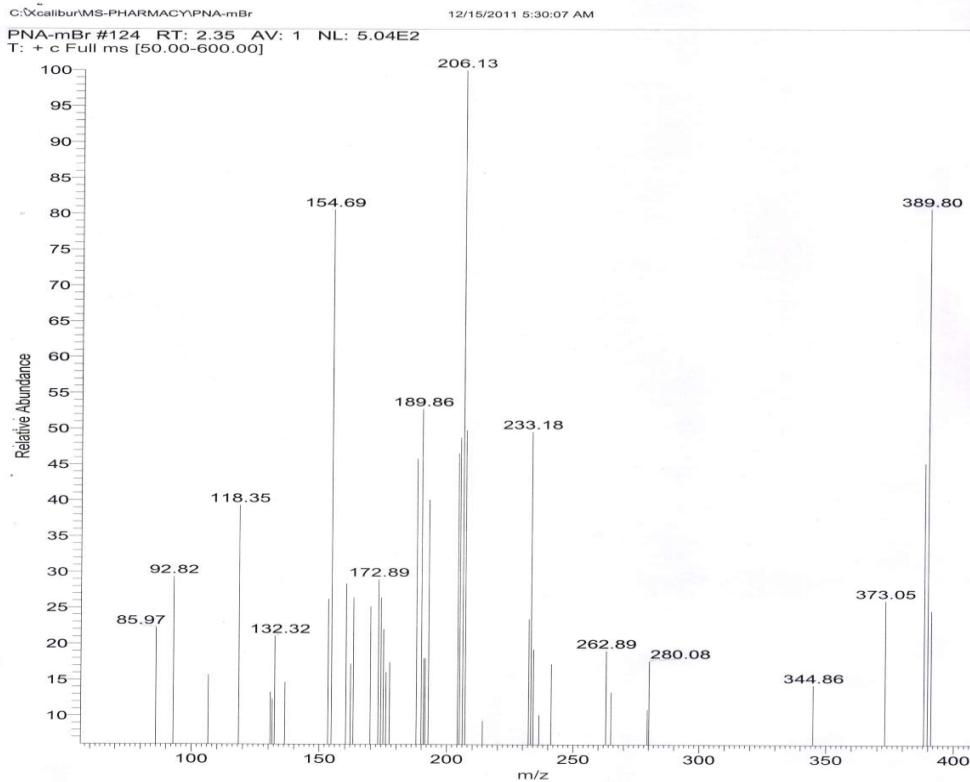
### 2-[(3-Chlorophenylamino)methyl]-6,7-dimethoxyquinazolin-4-ylamine (65)



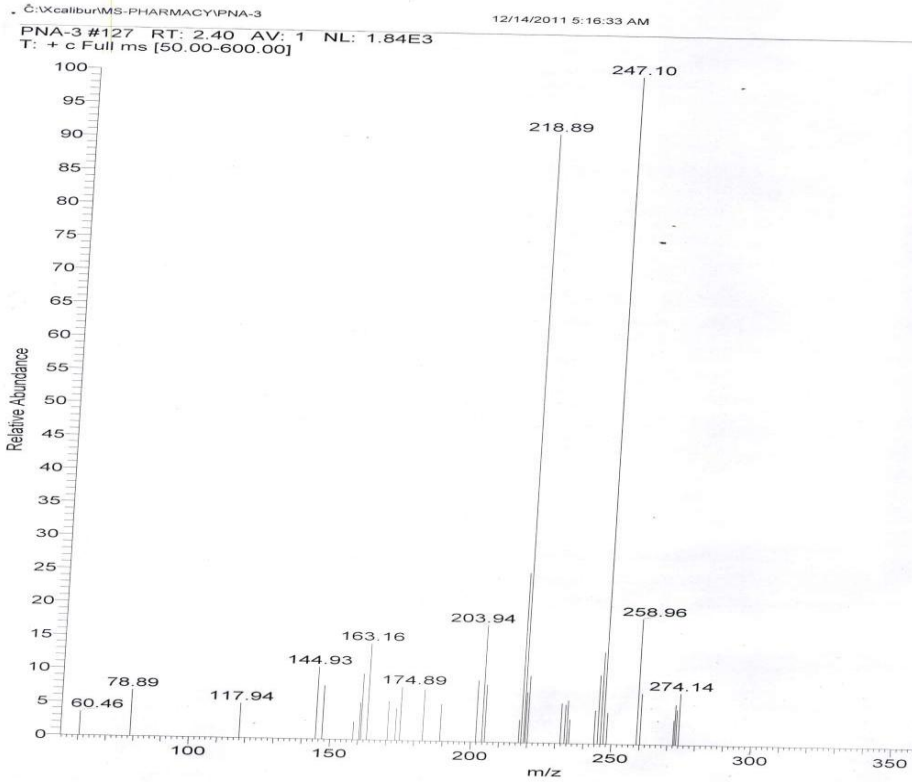
## 2-[(4-Chlorophenylamino)methyl]-6,7-dimethoxyquinazolin-4-ylamine (66)



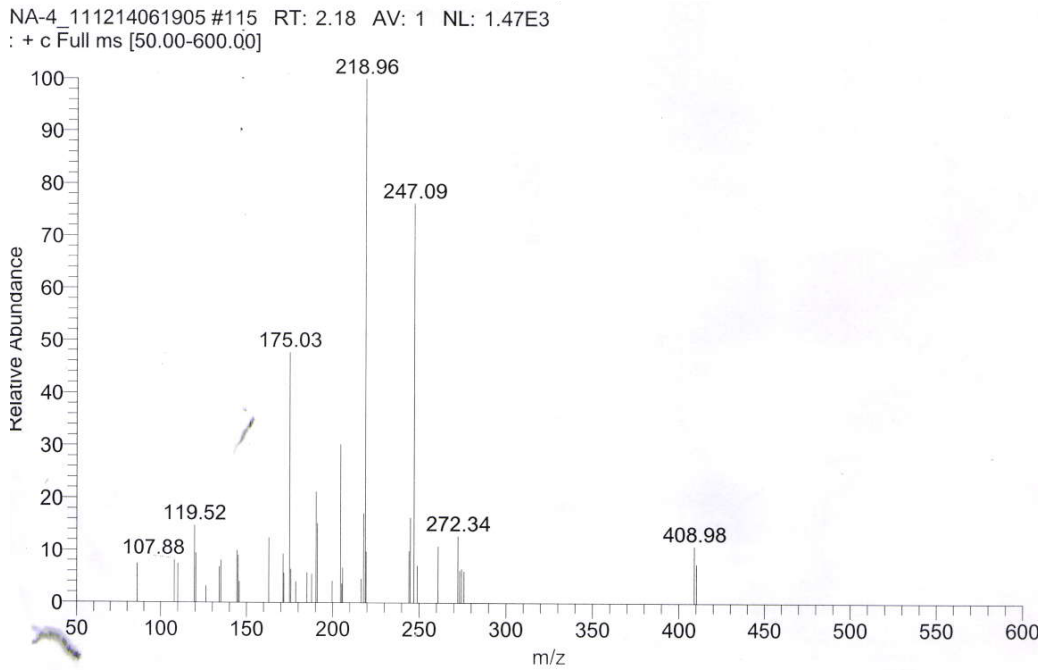
## 3-[(4-Amino-6,7-dimethoxyquinazolin-2-yl)methylamino]bromobenzene (67)



**6,7-Dimethoxy-2-[(4-phenylpiperazin-1-yl)methyl]quinazolin-4-ylamine (96)**



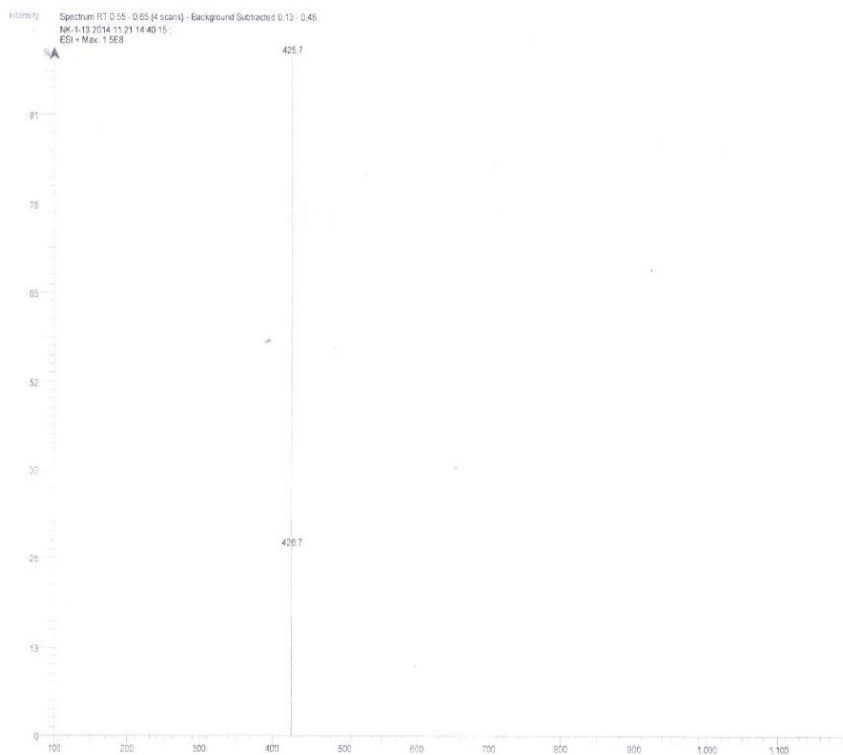
**6,7-Dimethoxy-2-[(4-(2-methoxyphenyl)piperazin-1-yl)methyl]quinazolin-4-ylamine (97)**



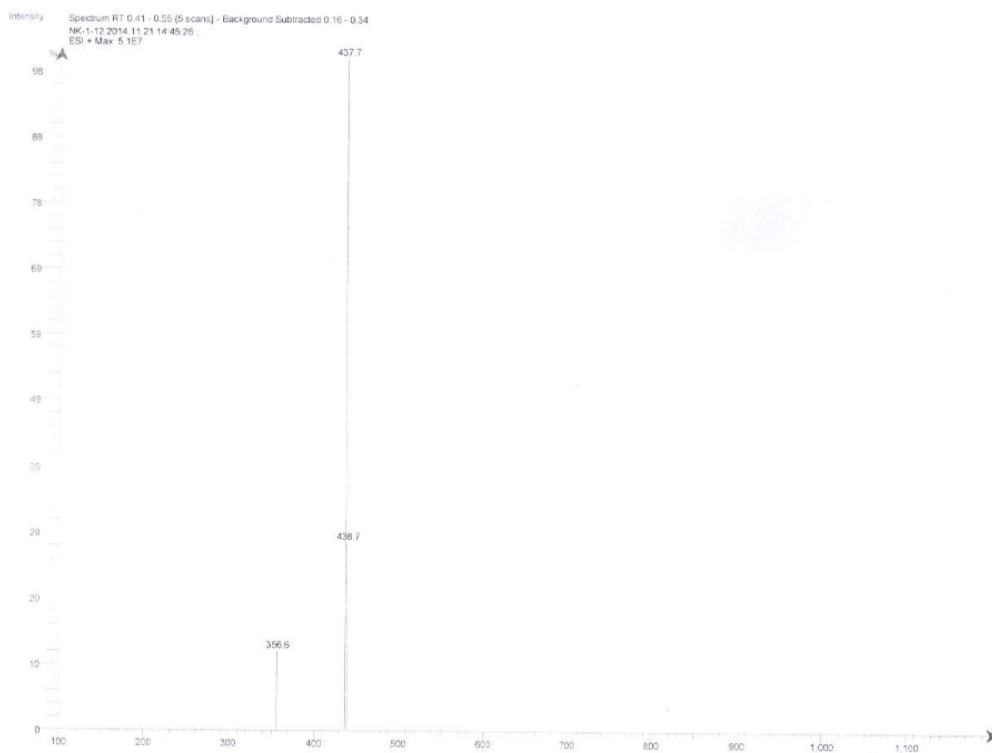
### 4-Amino-2-[4-(benzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (98)



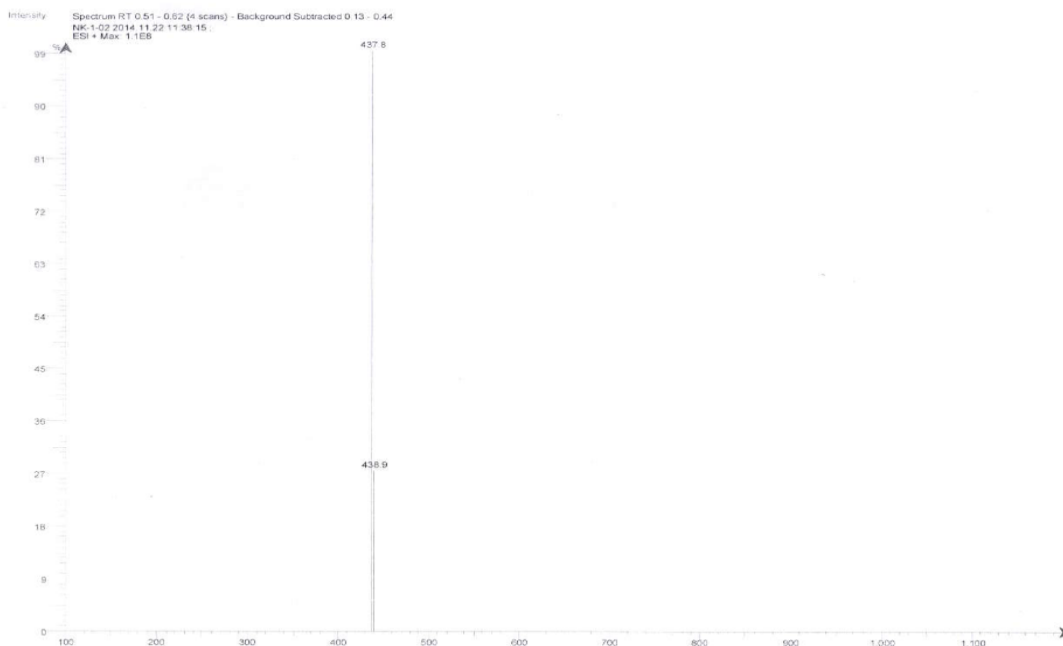
### 4-Amino-2-[4-(2-fluorobenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (99)



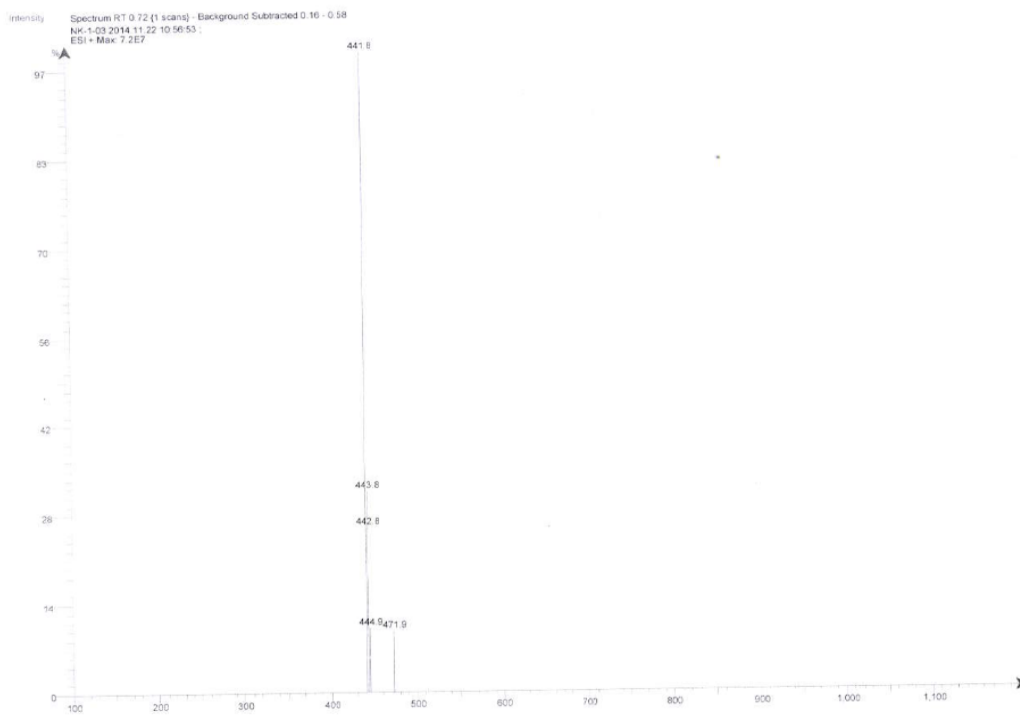
### 4-Amino-2-[4-(2-methoxybenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (100)



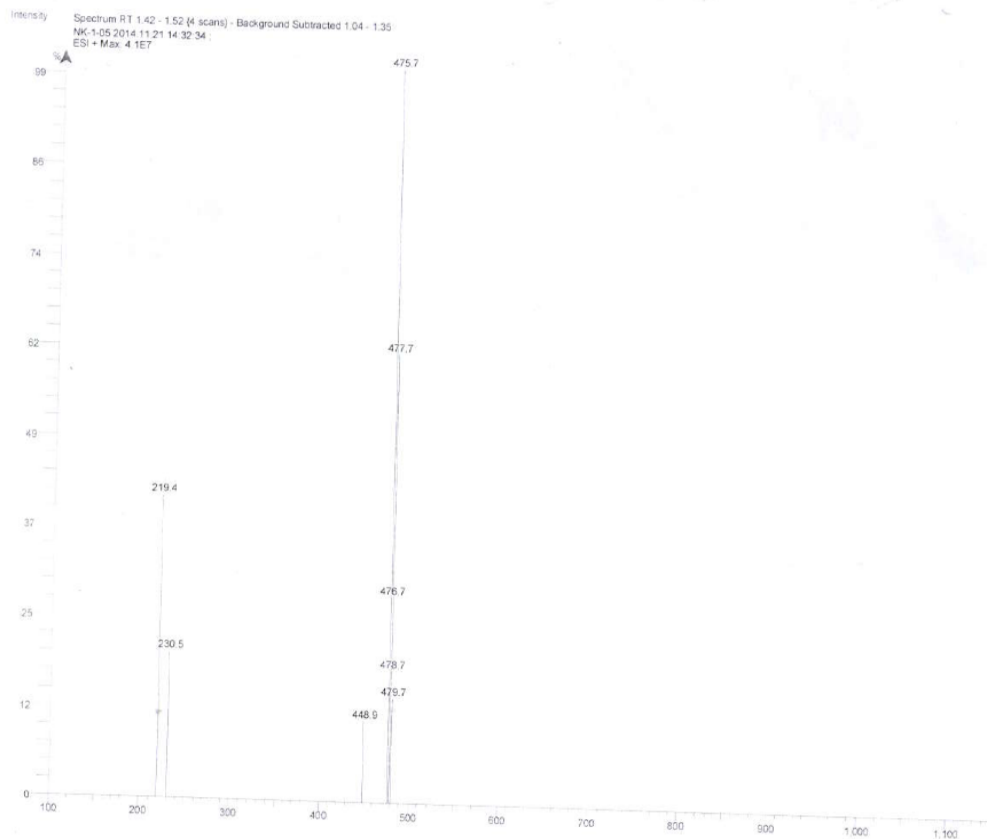
### 4-Amino-2-[4-(3-methoxybenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (101)



### 4-Amino-2-[4-(3-chlorobenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (102)

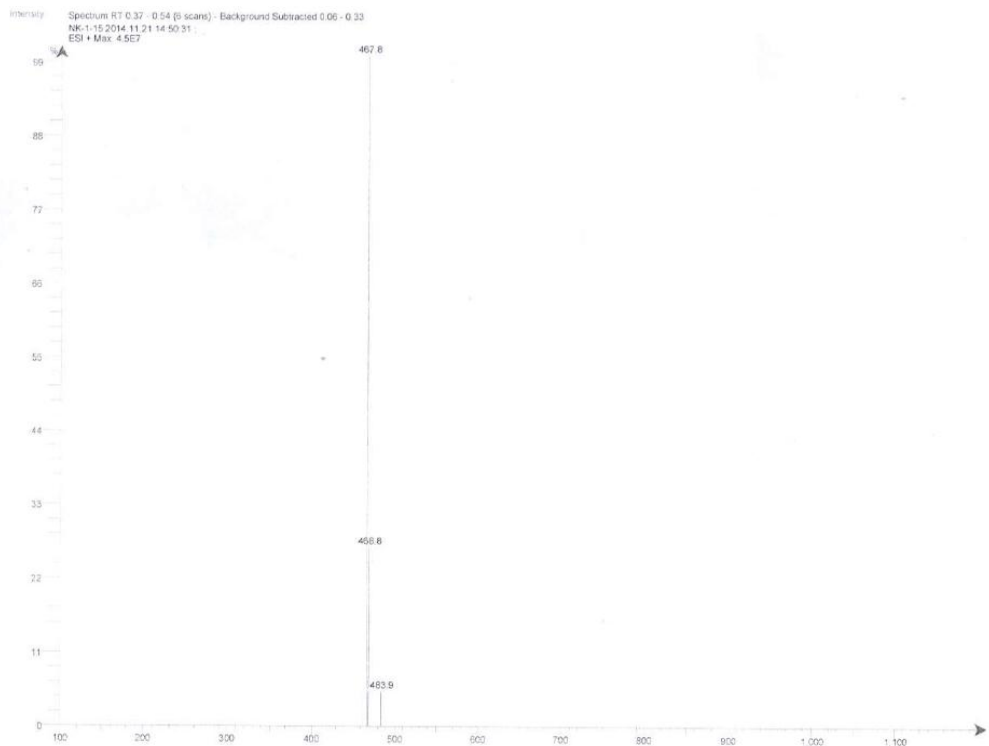


### 4-Amino-2-[4-(2,3-dichlorobenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (103)

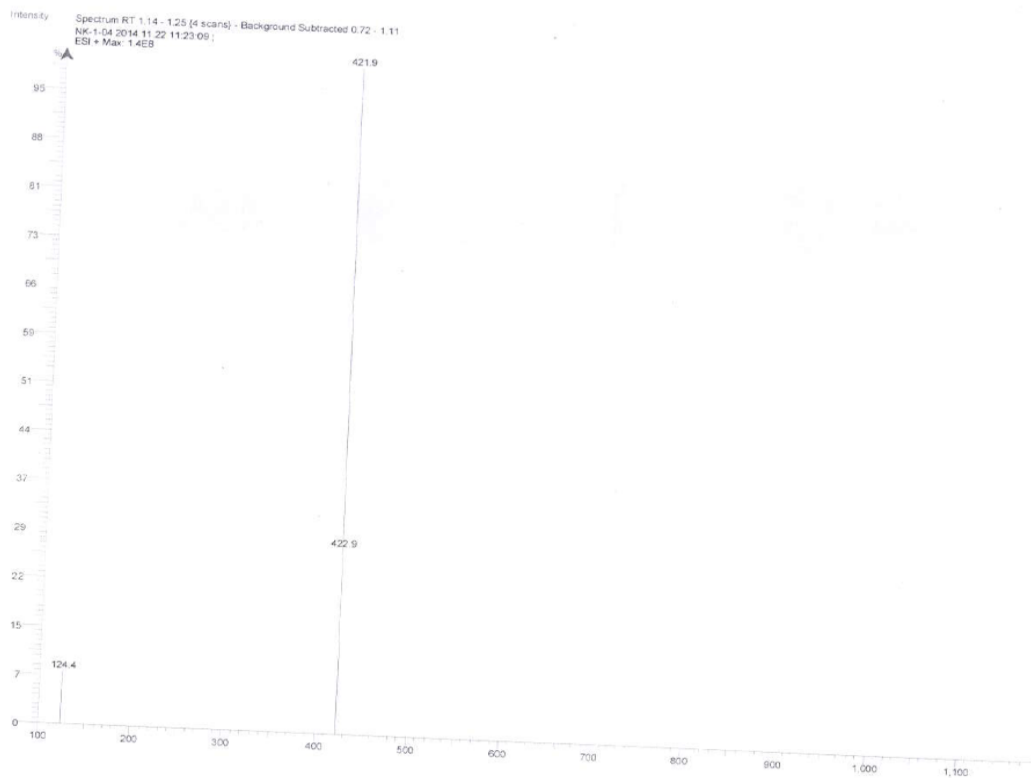




**4-Amino-2-[4-(2,3-dimethoxybenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (104)**



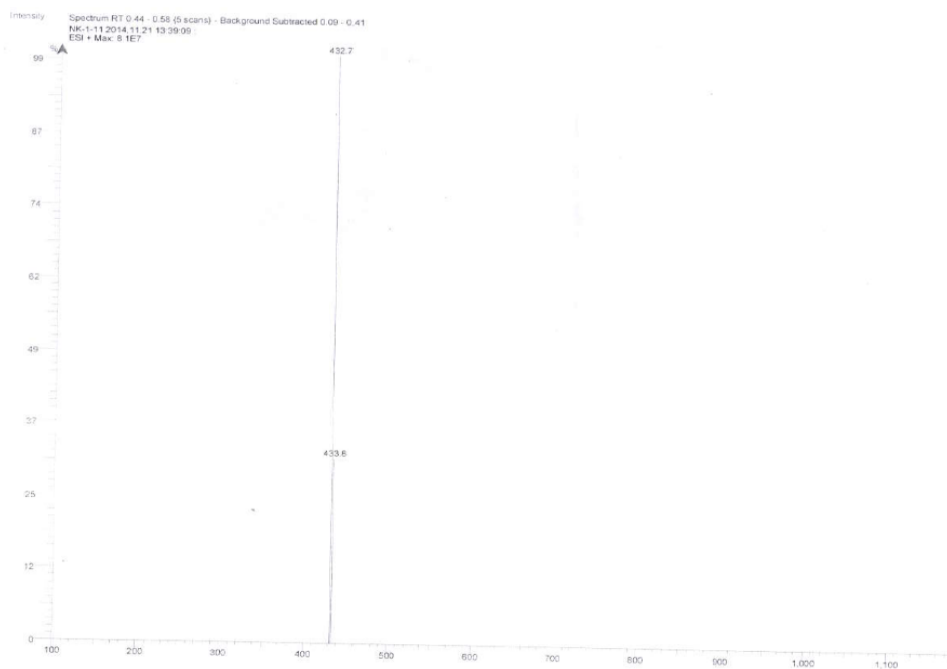
**4-Amino-2-[4-(3-methylbenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (105)**



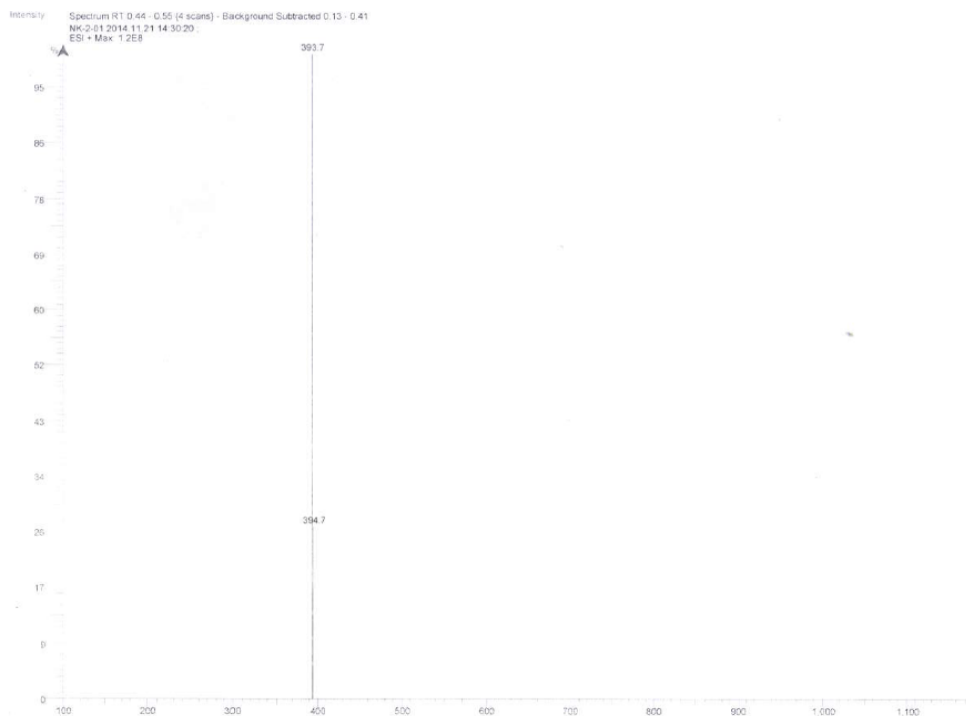
### 4-Amino-2-[4-(4-fluorobenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (106)



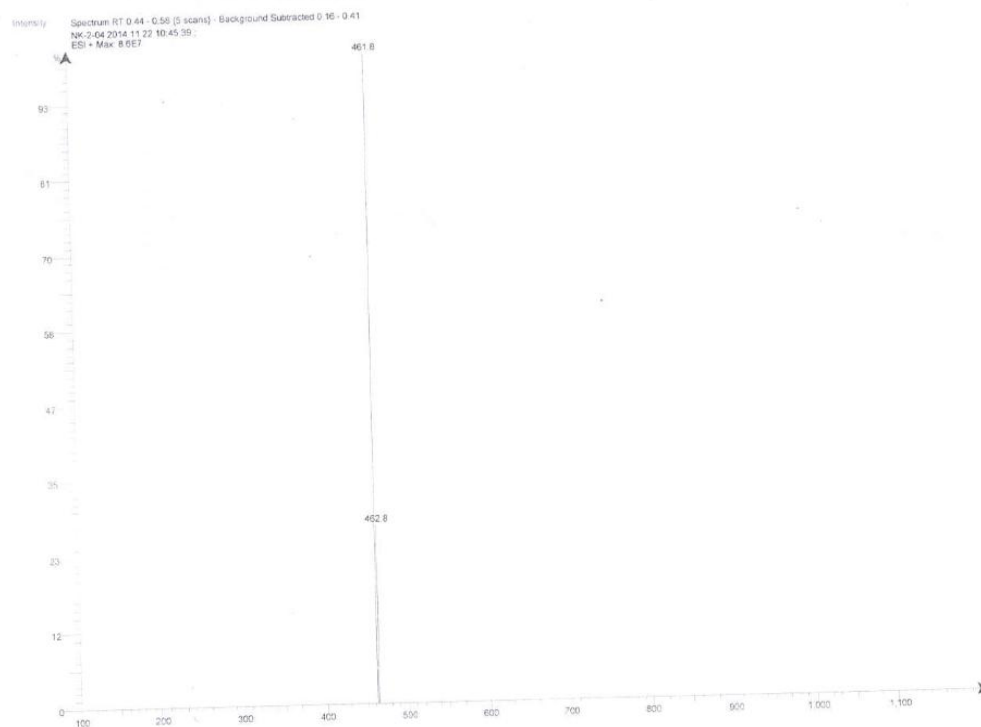
### 4-Amino-2-[4-(4-cyanobenzoyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (107)



### 4-Amino-2-[(4-benzylpiperazin-1-yl)methyl]-6,7-dimethoxyquinazoline (108)



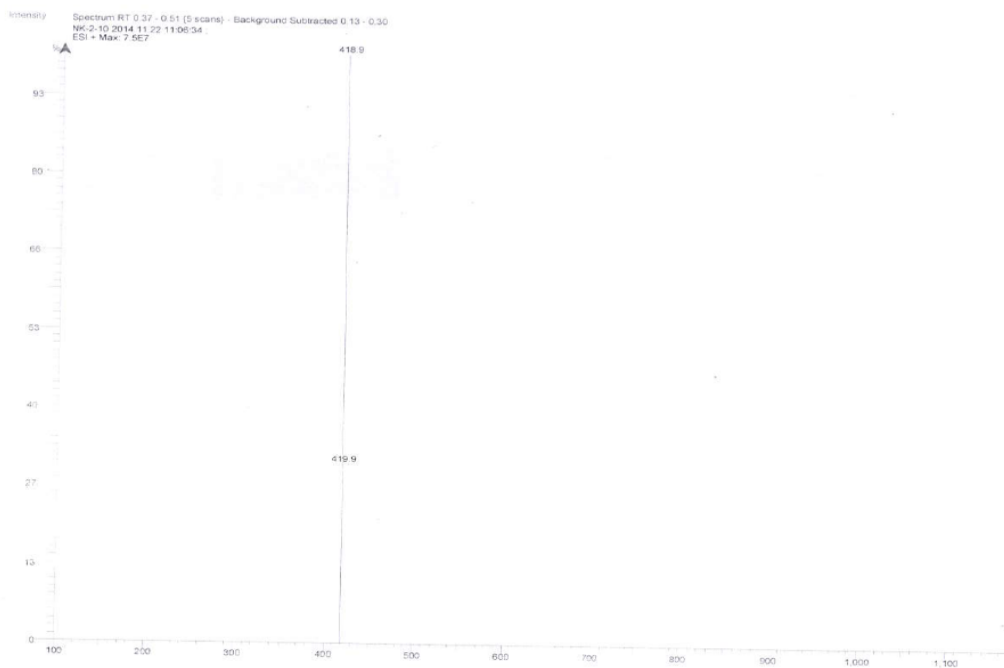
### 4-Amino-2-[4-(2-trifluoromethylbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (109)



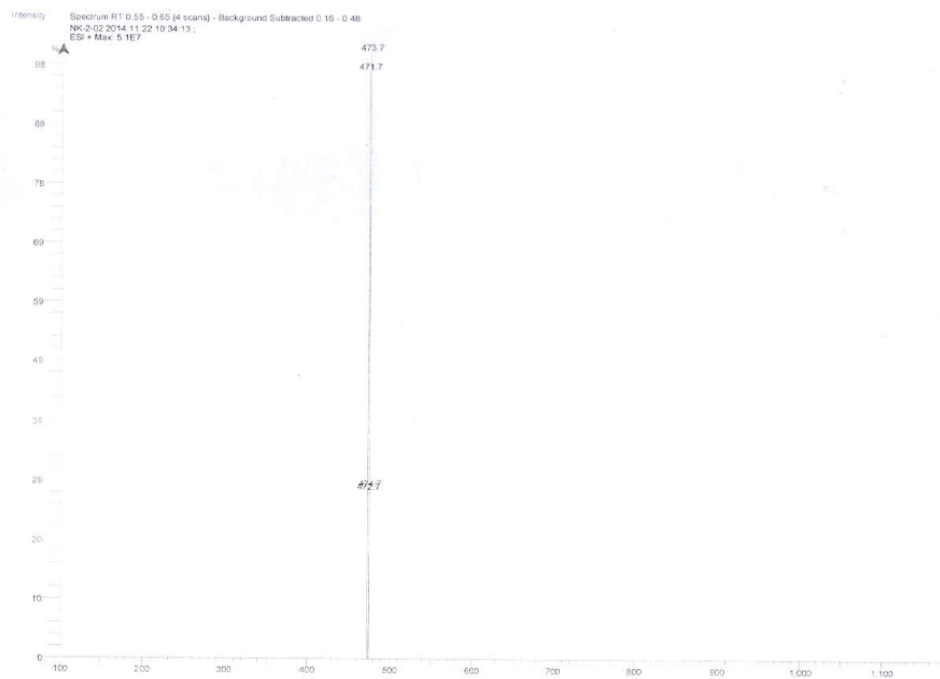
### 4-Amino-2-[4-(2-bromobenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (111)



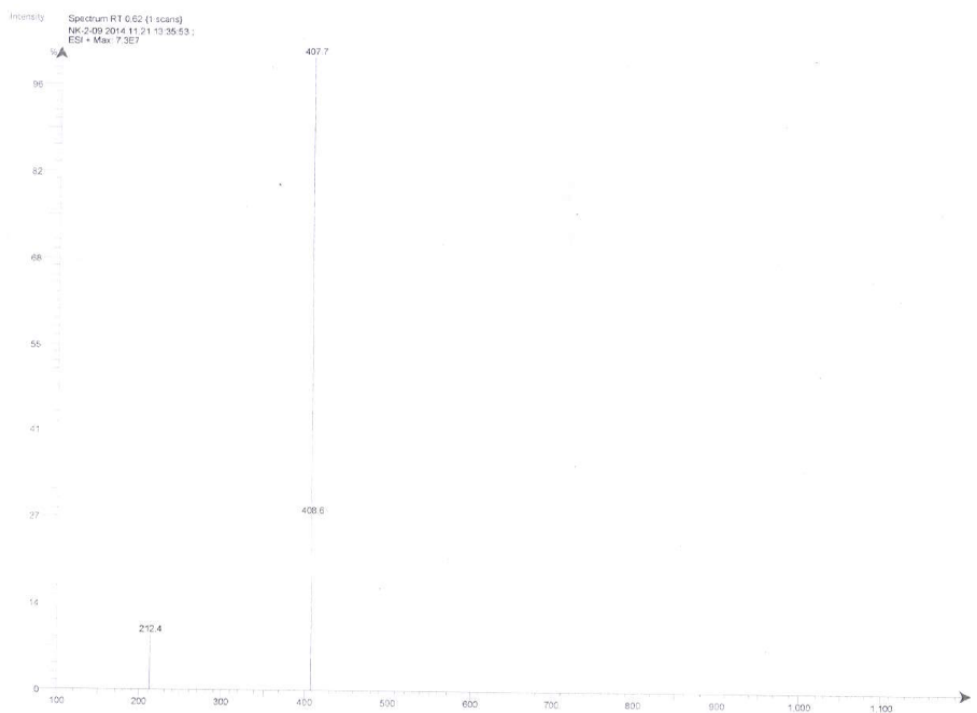
### 4-Amino-2-[4-(2-cyanobenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (112)



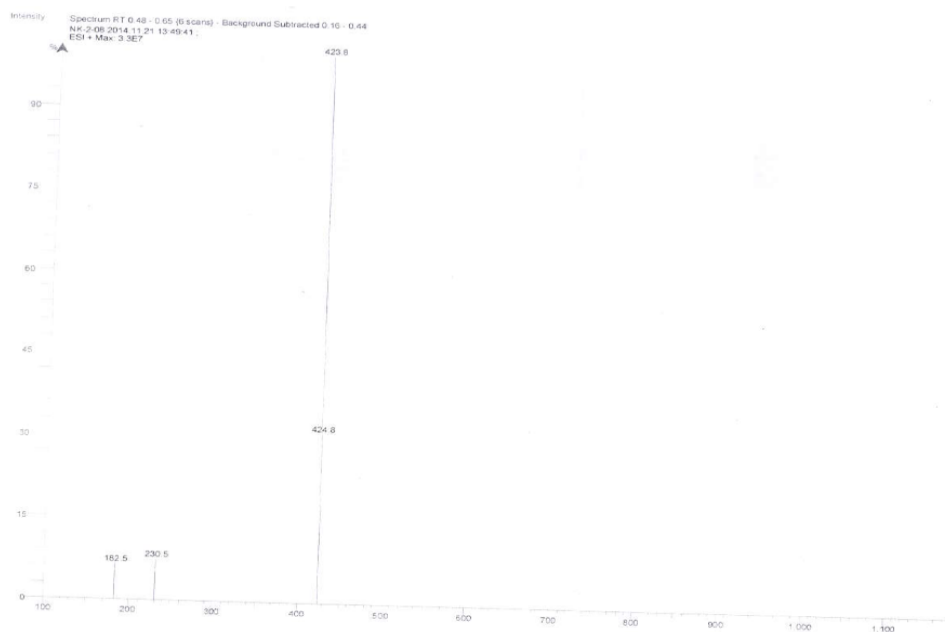
### 4-Amino-2-[4-(4-bromolbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (113)



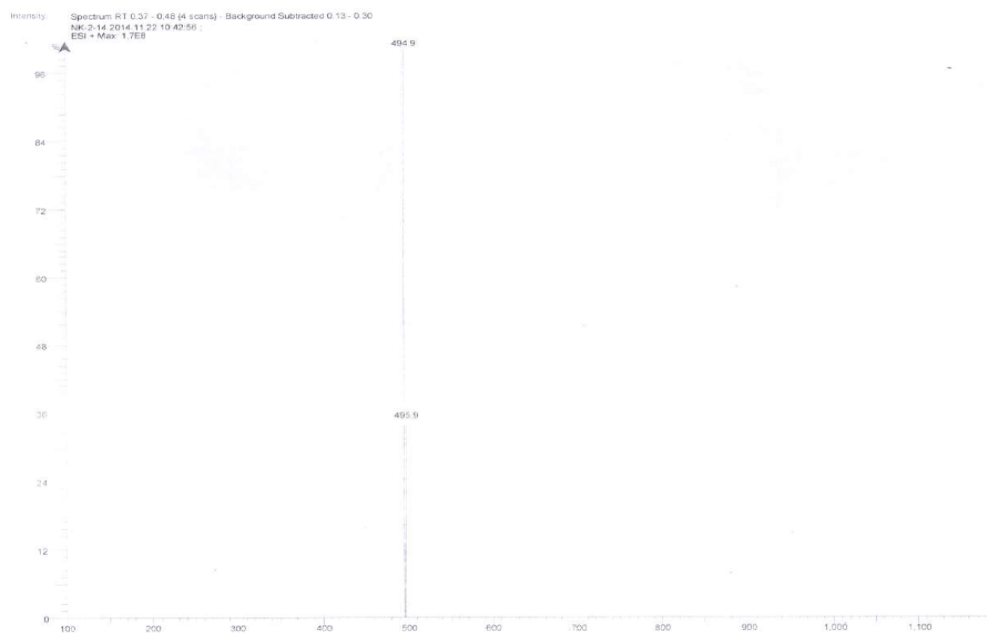
### 4-Amino-2-[4-(4-methylbenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (114)



### 4-Amino-2-[4-(4-methoxybenzyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (115)

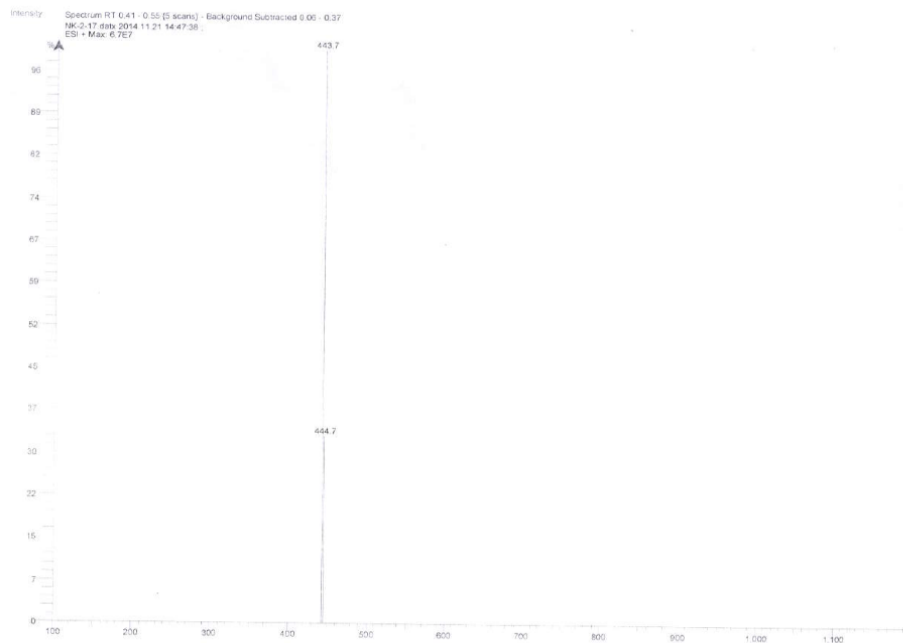


### 4-Amino-2-{4-[4-(2-cyanophenyl)benzyl]piperazin-1-ylmethyl}-6,7-dimethoxyquinazoline (117)





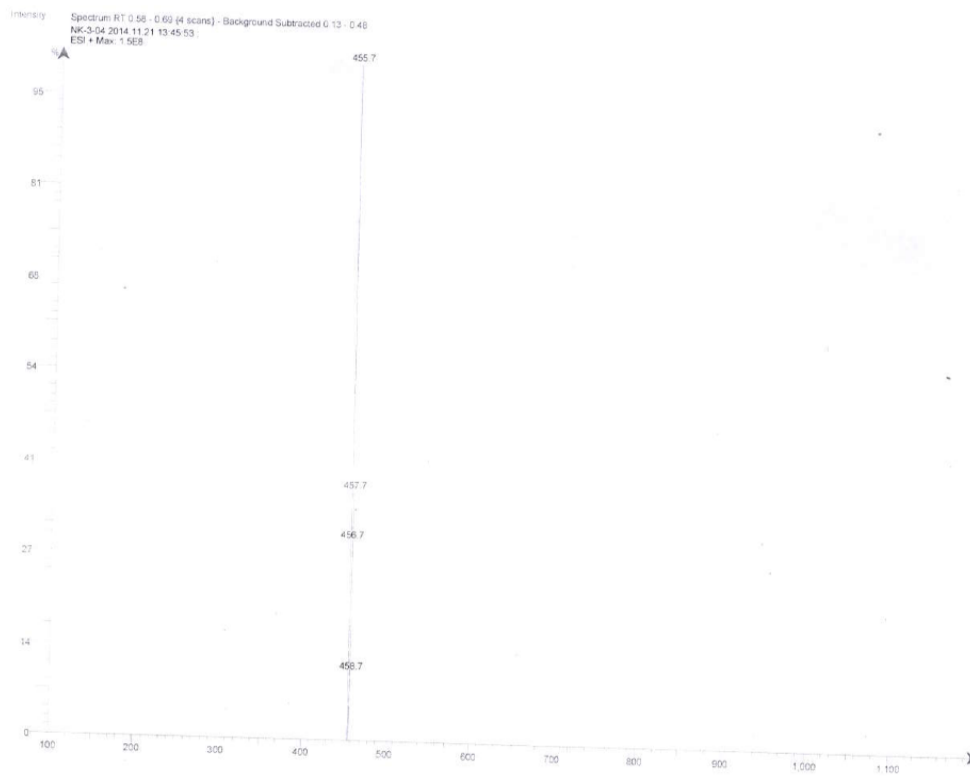
### 4-Amino-2-[4-(1-naphthylmethyl)piperazin-1-ylmethyl]-6,7-dimethoxyquinazoline (118)



### 1-[4-(4-Amino-6,7-dimethoxyquinazolin-2-yl)methylpiperazin-1-yl]-2-phenylethanone (121)



**1-[4-(4-Amino-6,7-dimethoxyquinazolin-2-yl)methylpiperazin-1-yl]-2-(3-chlorophenyl)ethanone (122)**



**1-[4-(4-Amino-6,7-dimethoxyquinazolin-2-yl)methylpiperazin-1-yl]-2-(4-methoxyphenyl)ethanone (123)**

