

Supplementary Material

Novel 4-Anilinoquinazoline Derivatives as Potent Anticancer Agents: Design, Synthesis, Cytotoxic Activity, and Docking Study

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^ADepartment of Medicinal Chemistry, School of Pharmacy, Guilan University of Medical Sciences, Rasht 41491-73774, Iran.

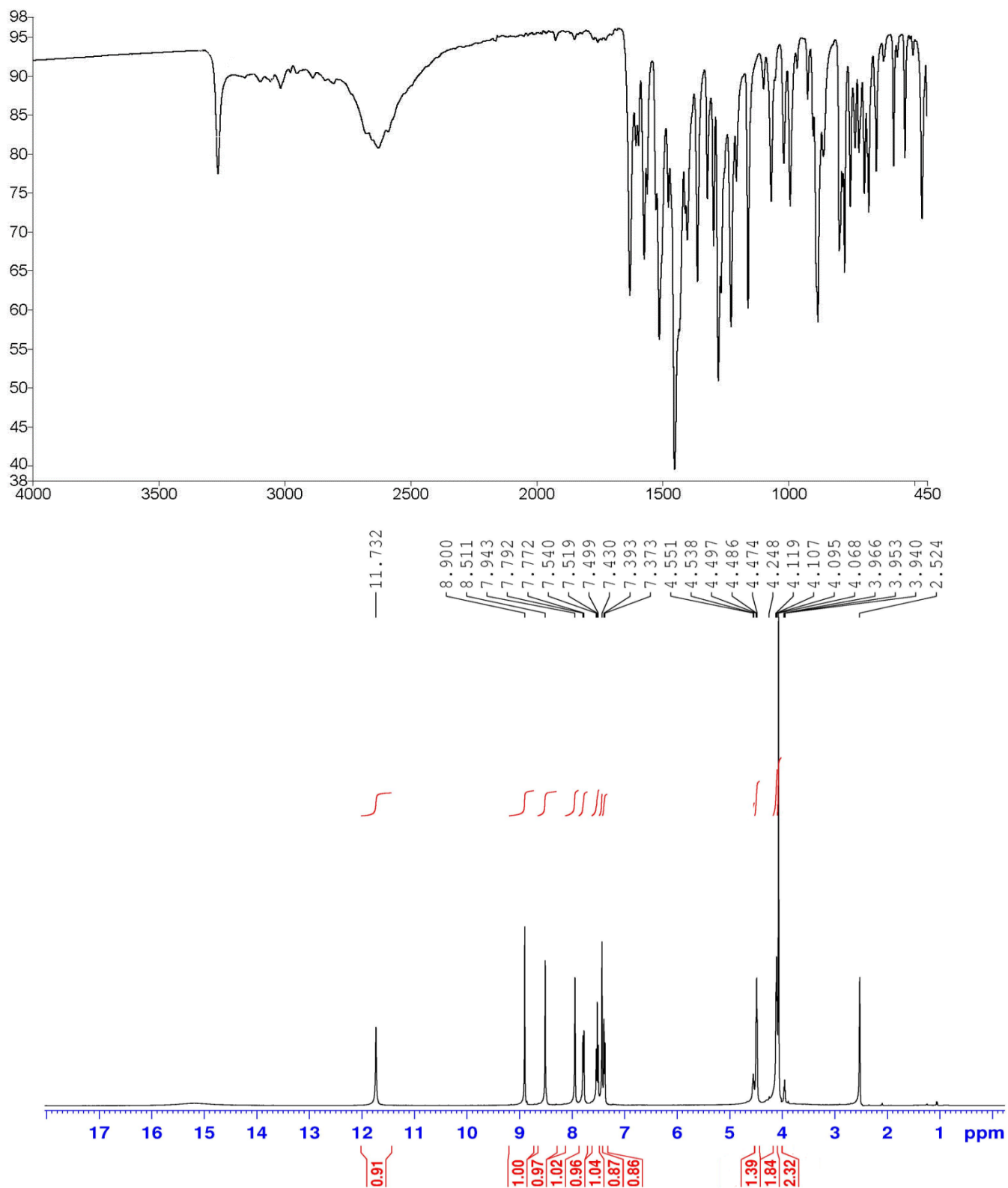
^BDepartment of Pharmaceutical Biotechnology, School of Pharmacy, Guilan University of Medical Sciences, Rasht 41491-73774, Iran.

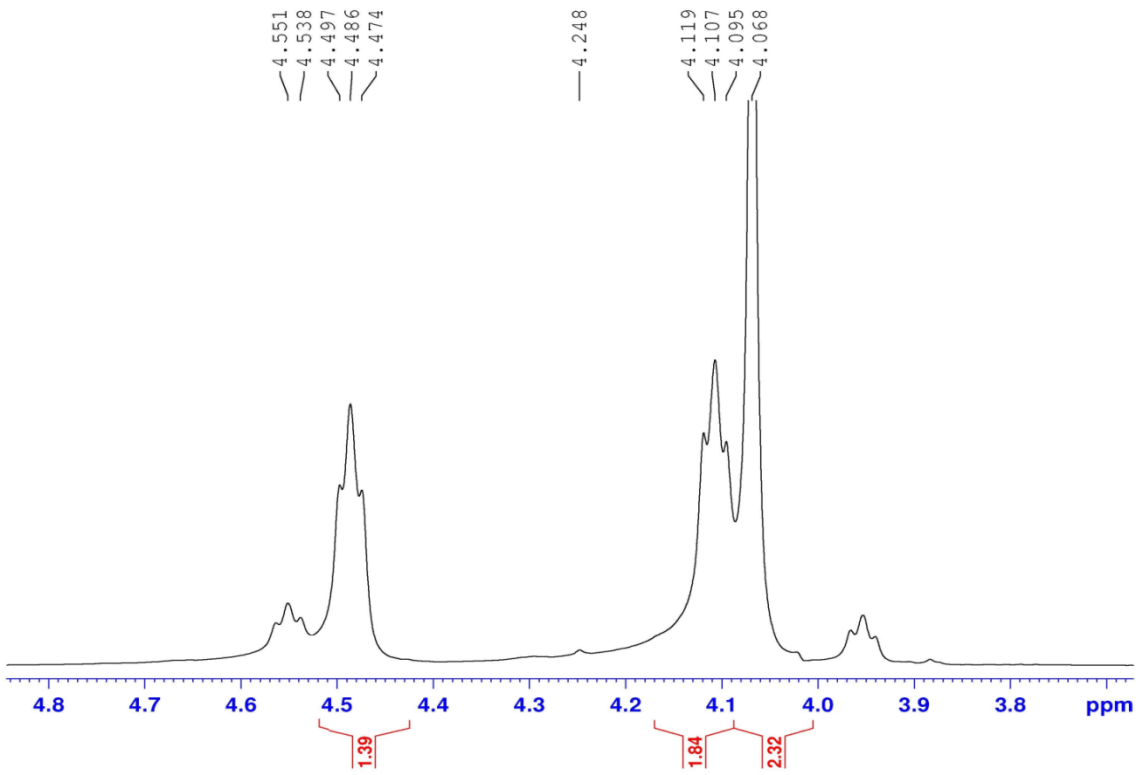
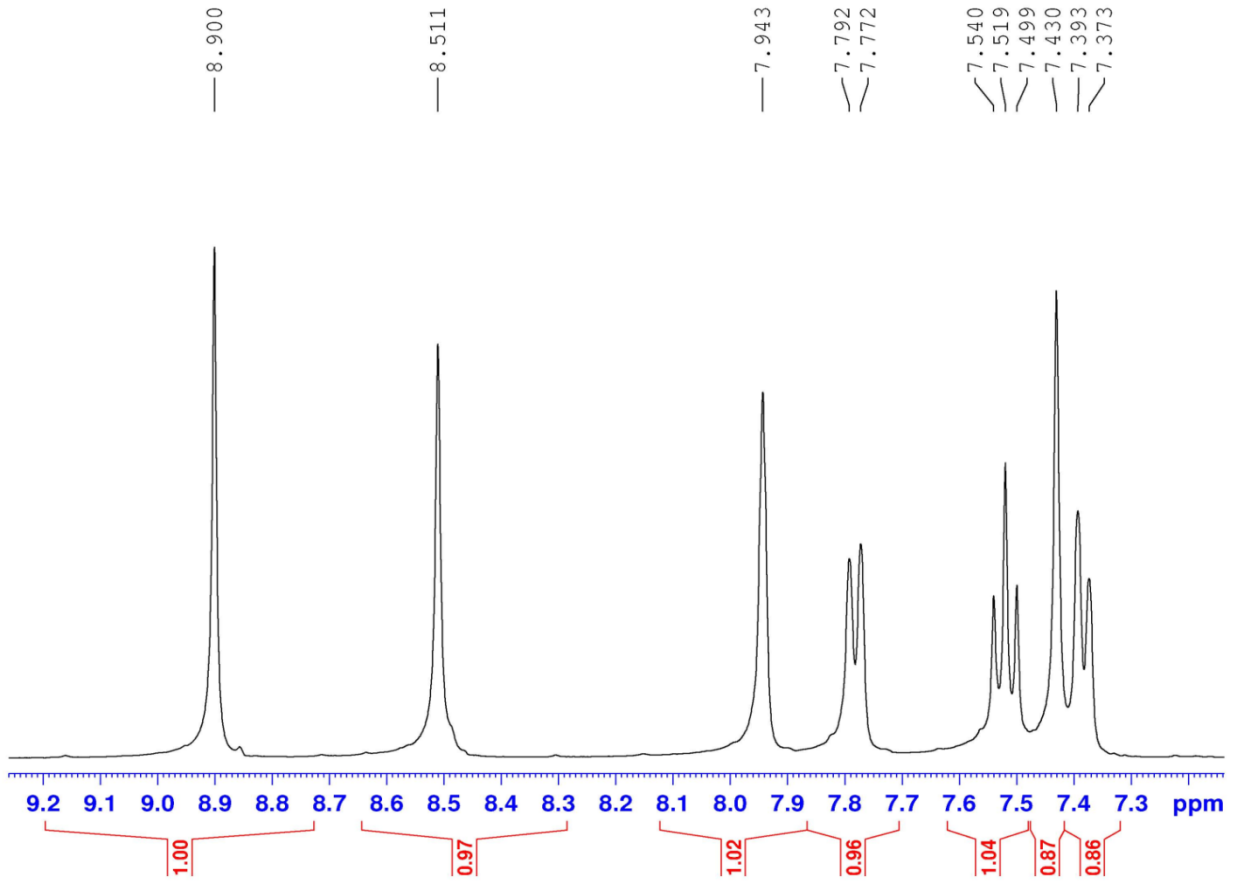
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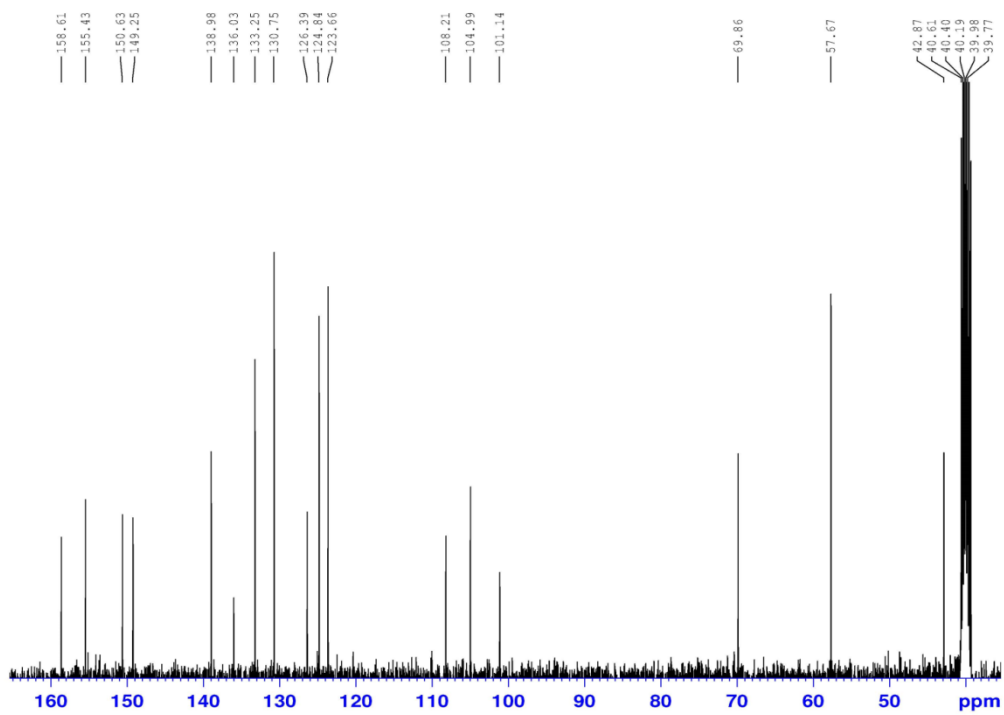
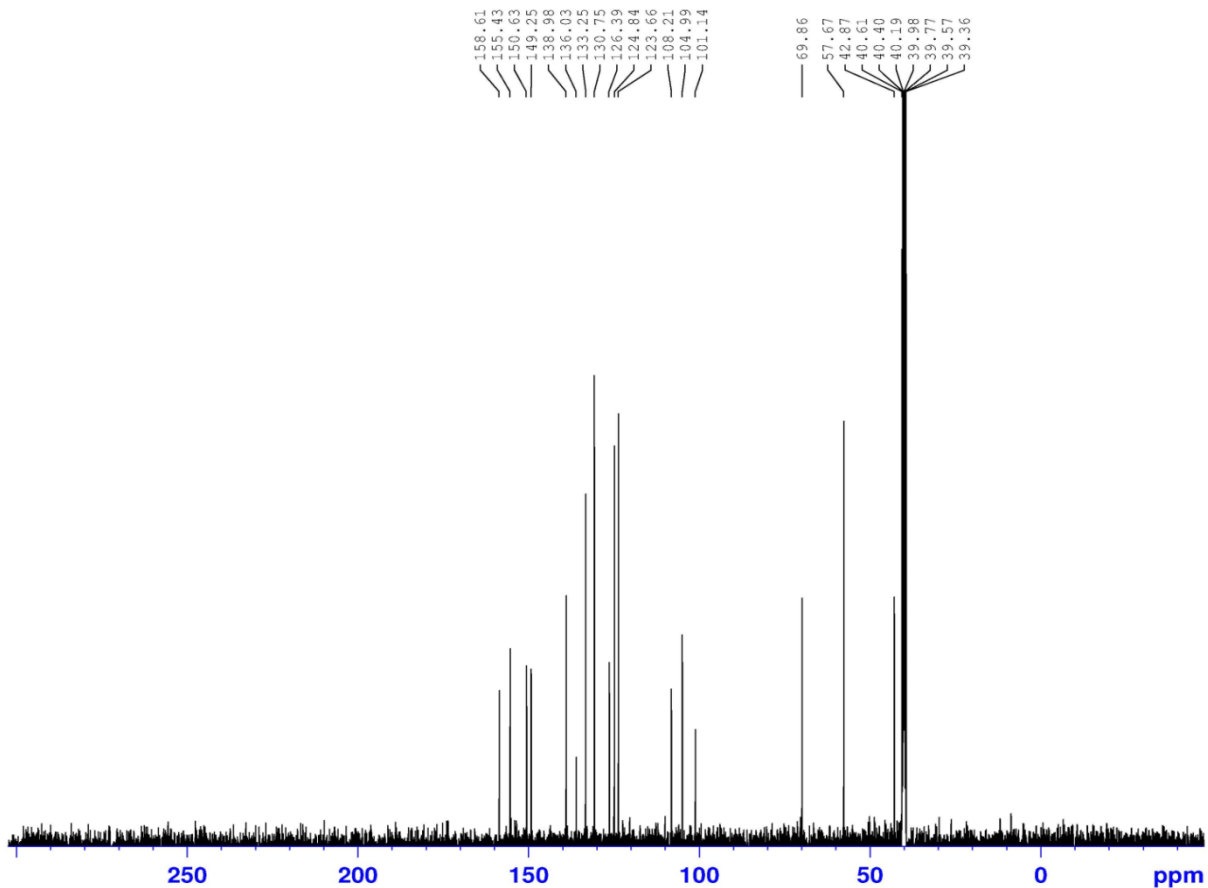
^DCorresponding author. Email: ghasemi_saeed@yahoo.com

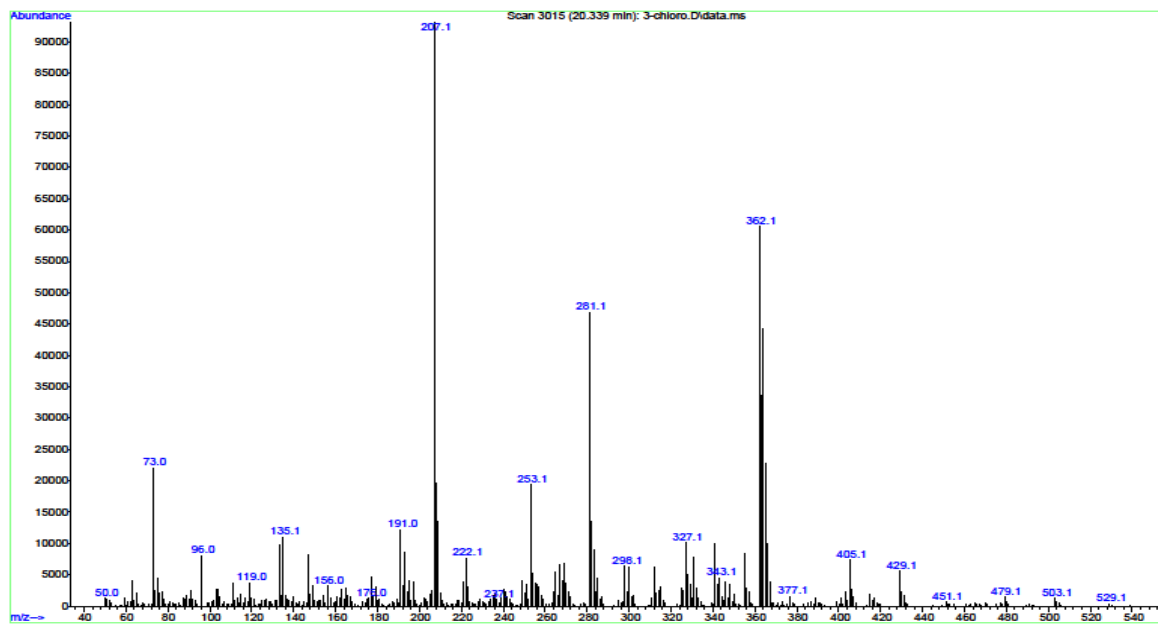
IR, ¹HNMR, ¹³CNMR, and Mass spectra of compounds 7a-7d and 8a-8l

7-(2-Chloroethoxy)-N-(3-chlorophenyl)-6-methoxyquinazolin-4-amine (7a)

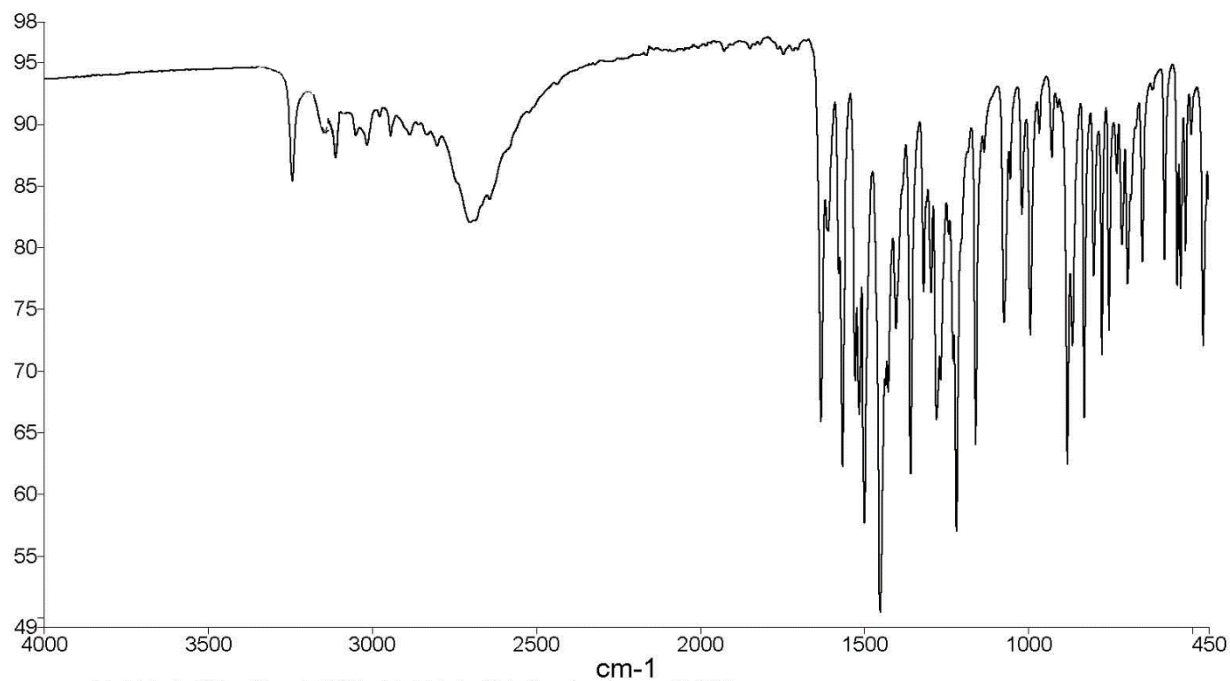


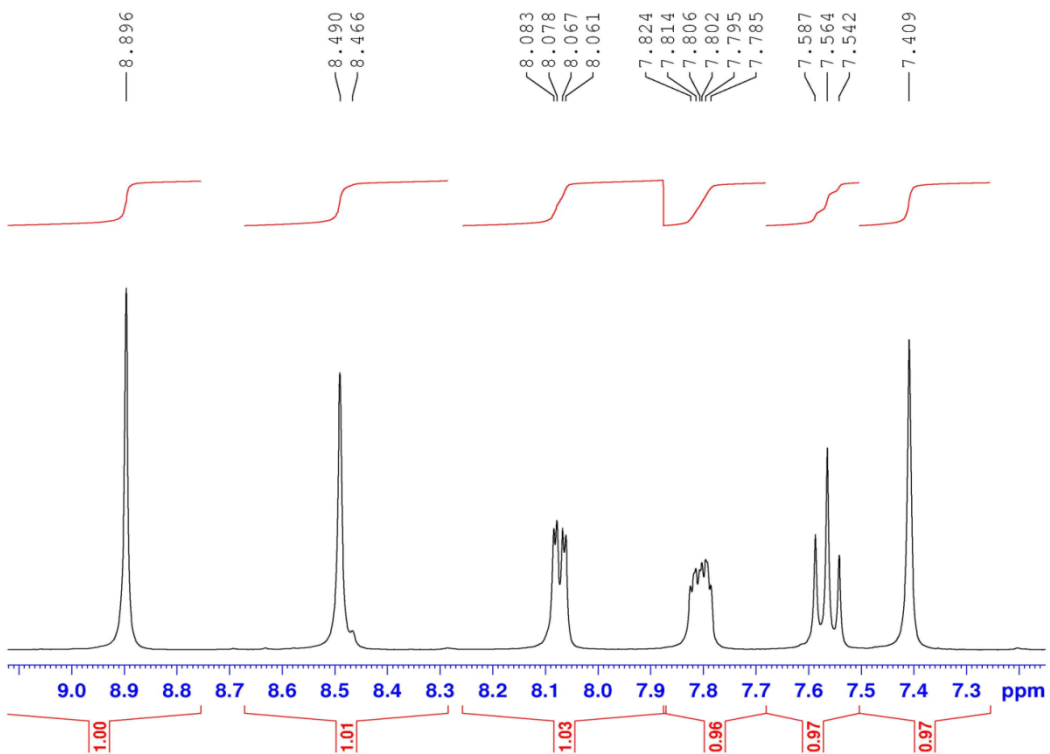
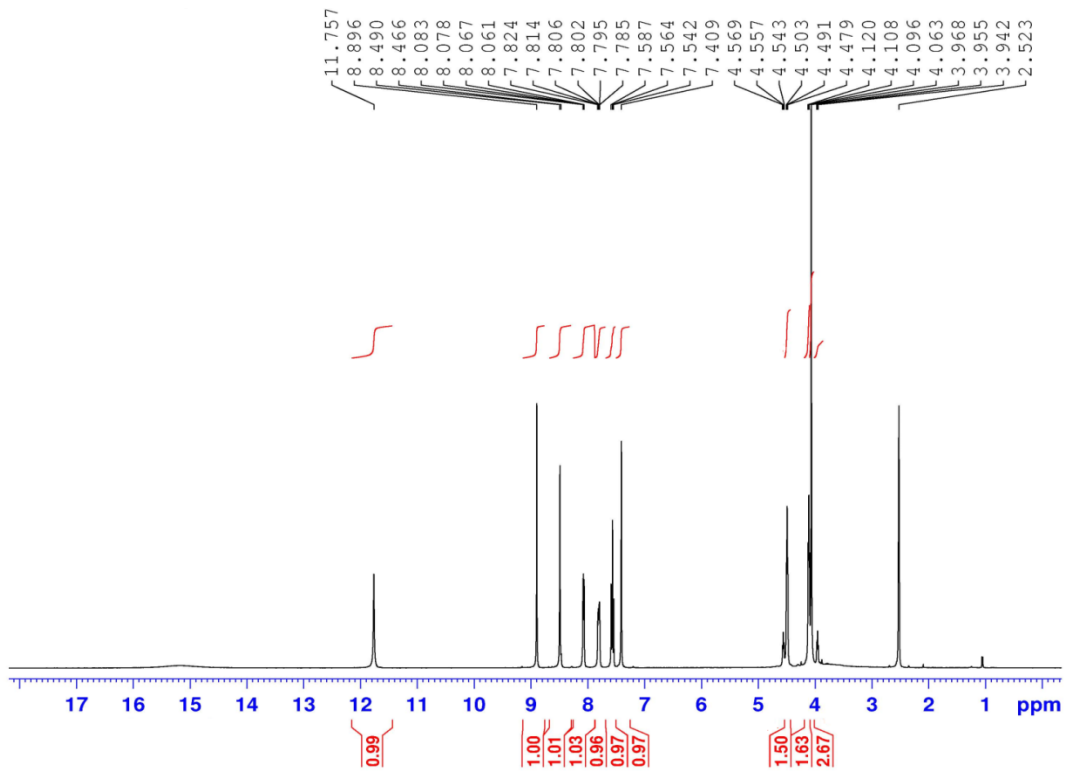






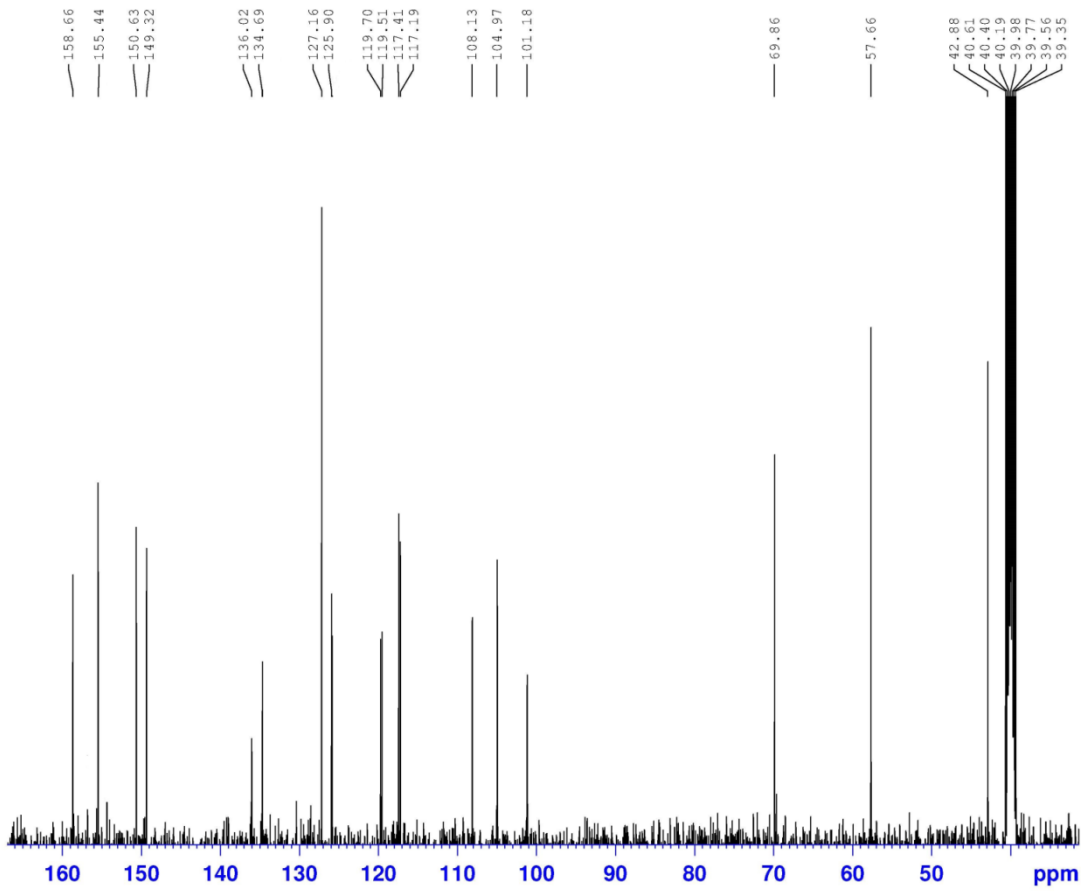
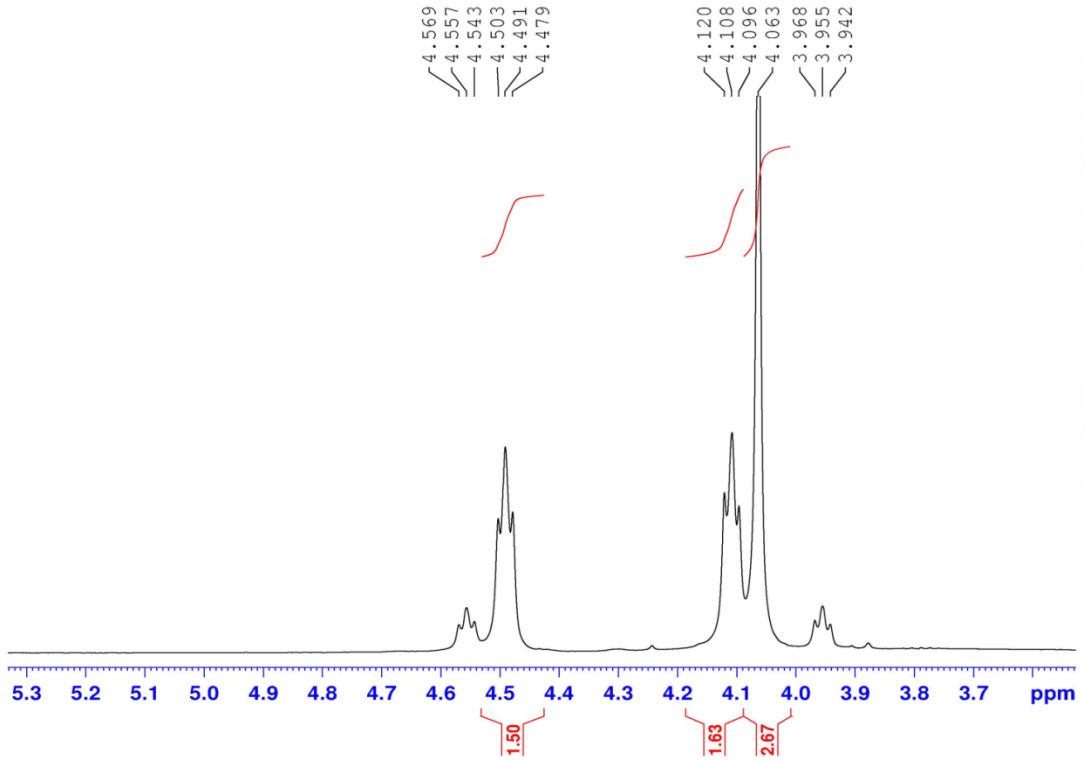
7-(2-Chloroethoxy)-N-(3-chloro-4-fluorophenyl)-6-methoxyquinazolin-4-amine (7b)

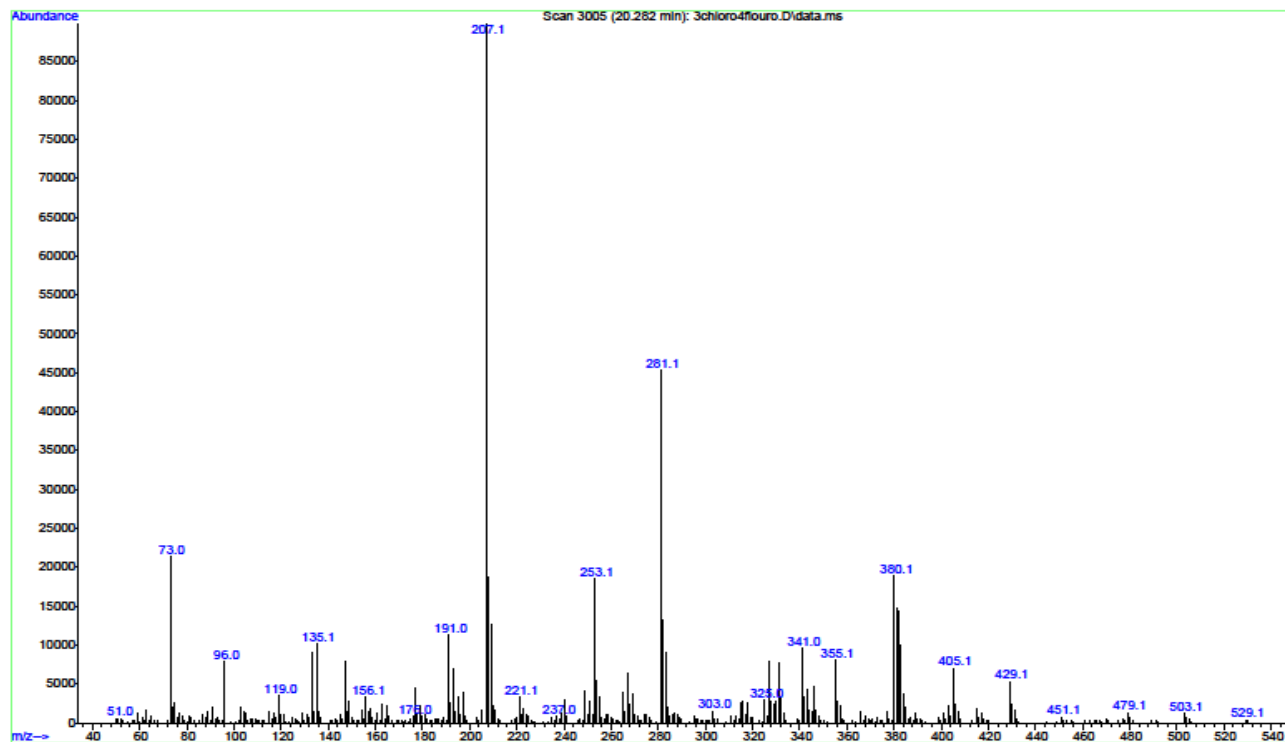




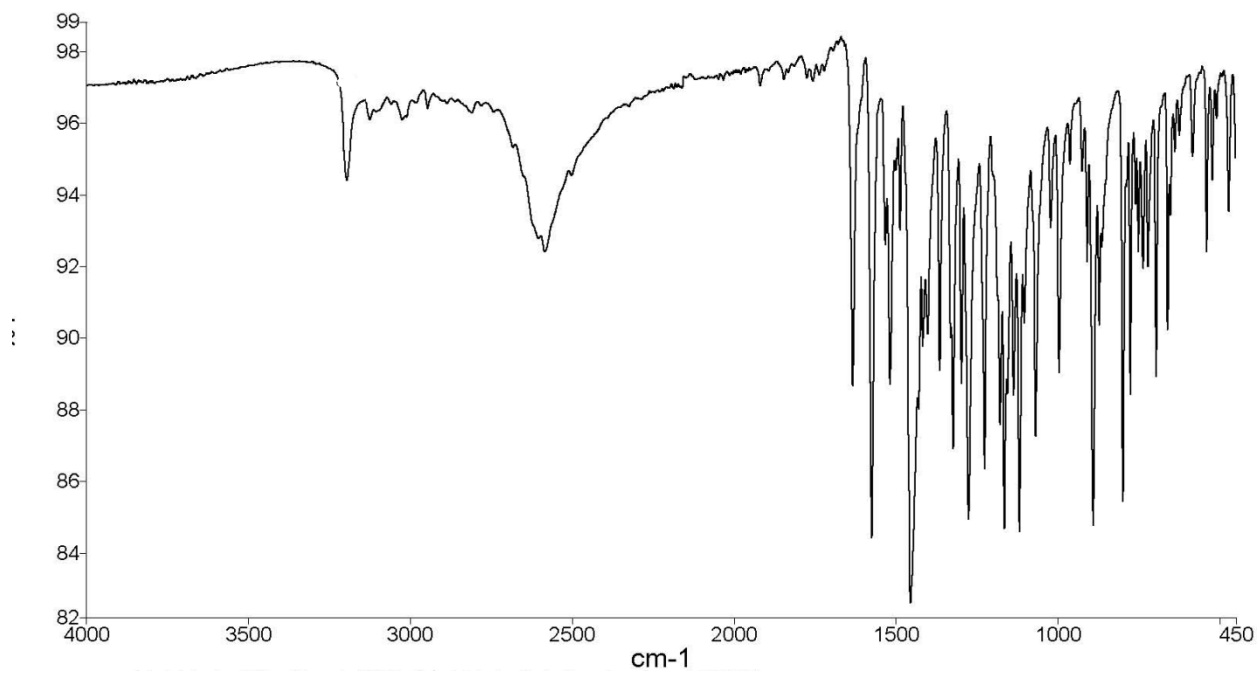
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8.490
8.466
8.083
8.078
8.067
8.061
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7.795
7.785
7.587
7.564
7.542
7.409
4.569
4.557
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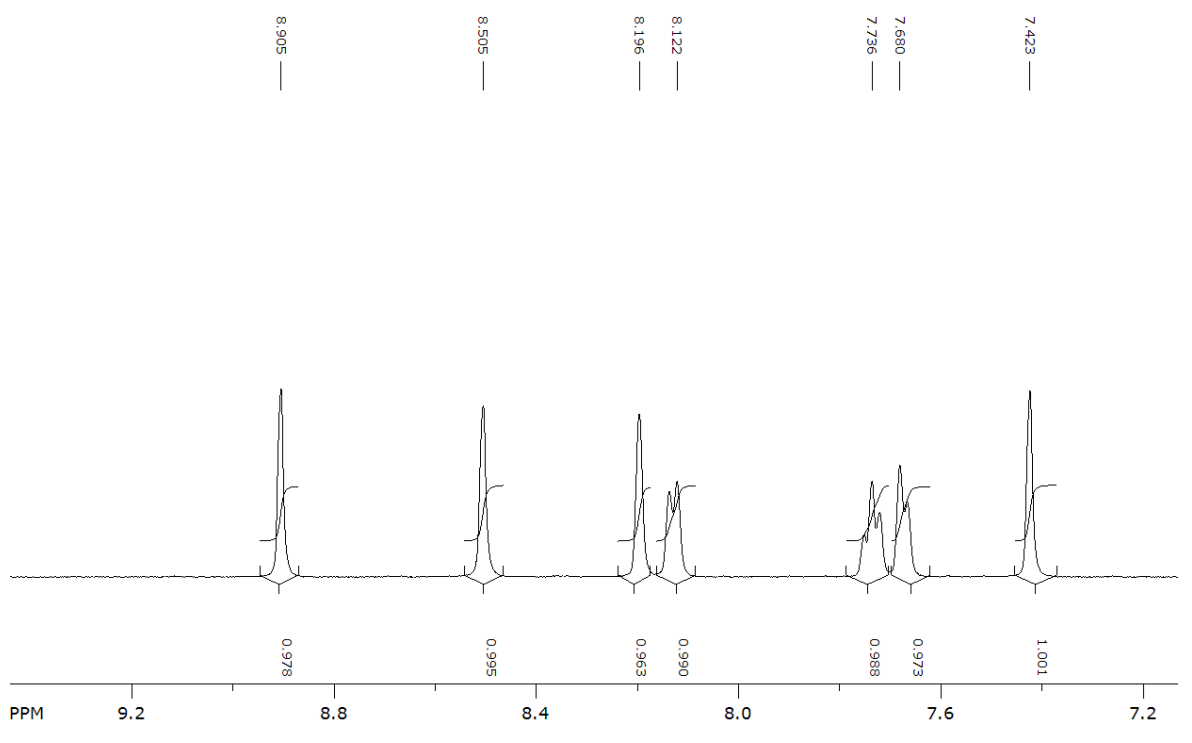
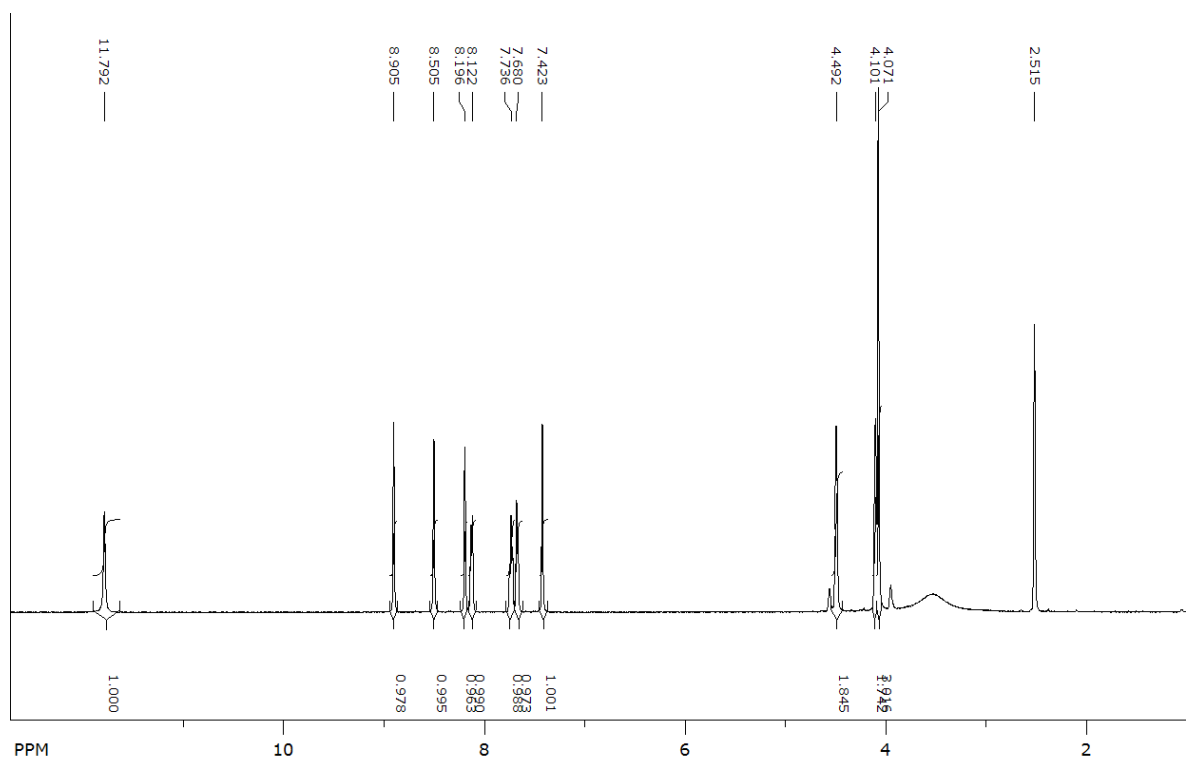
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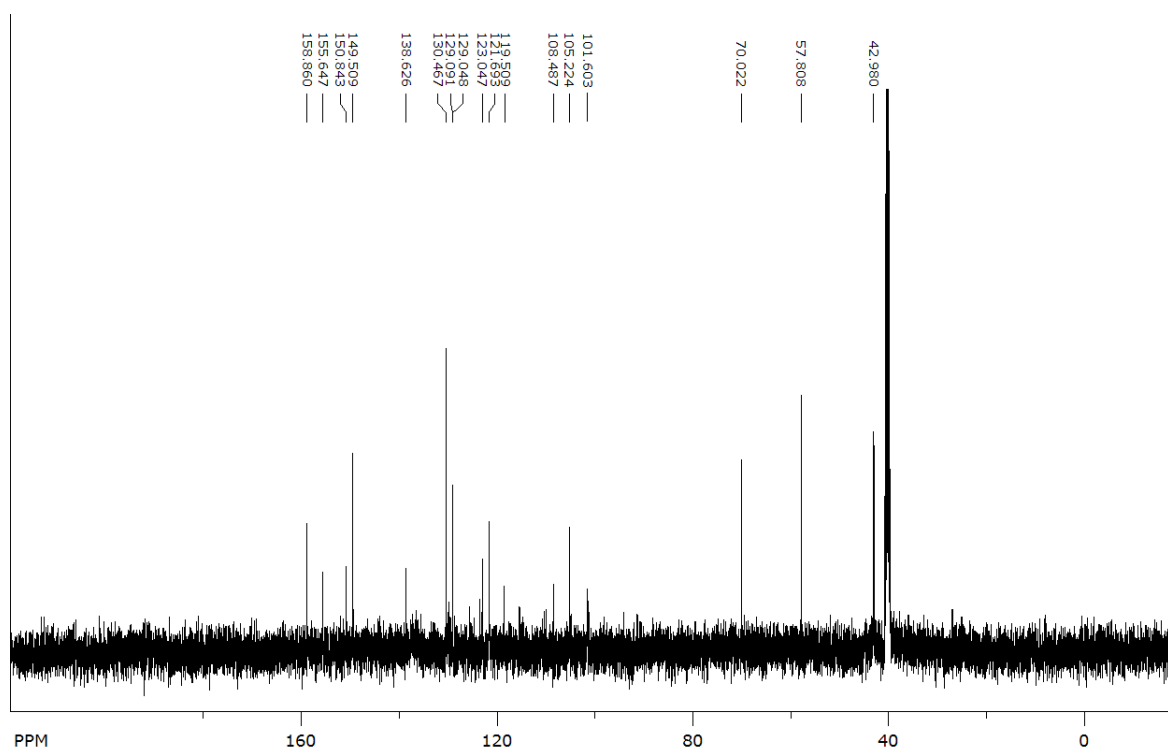
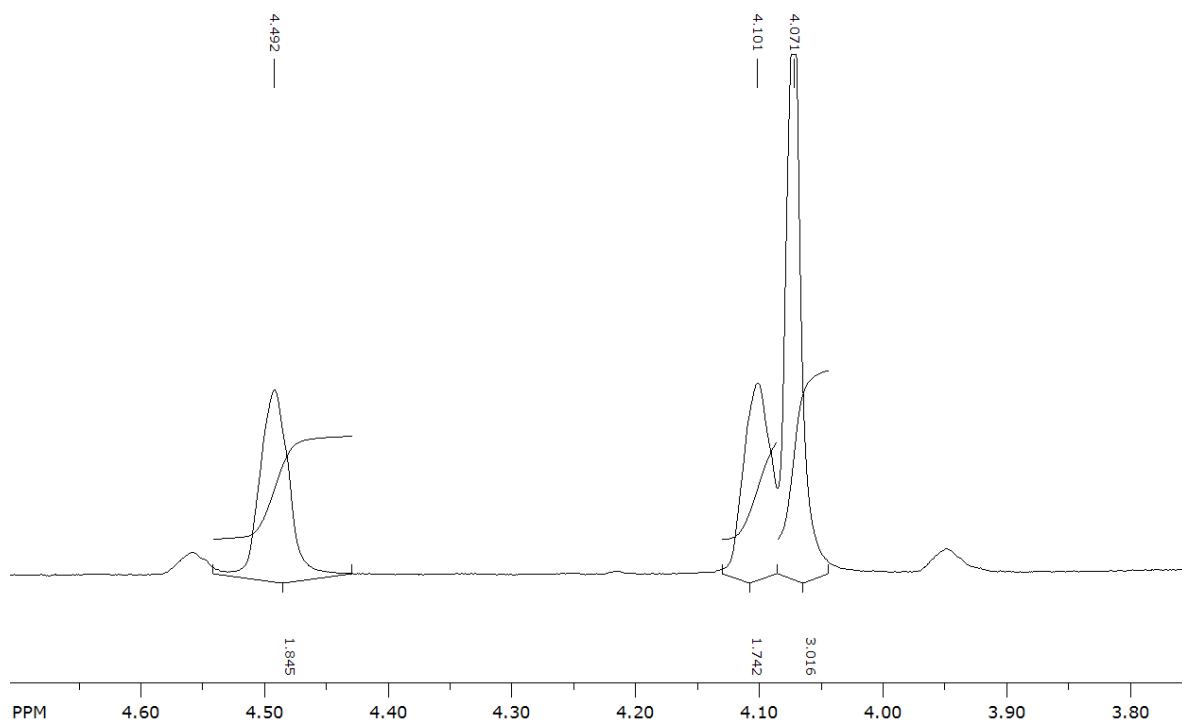


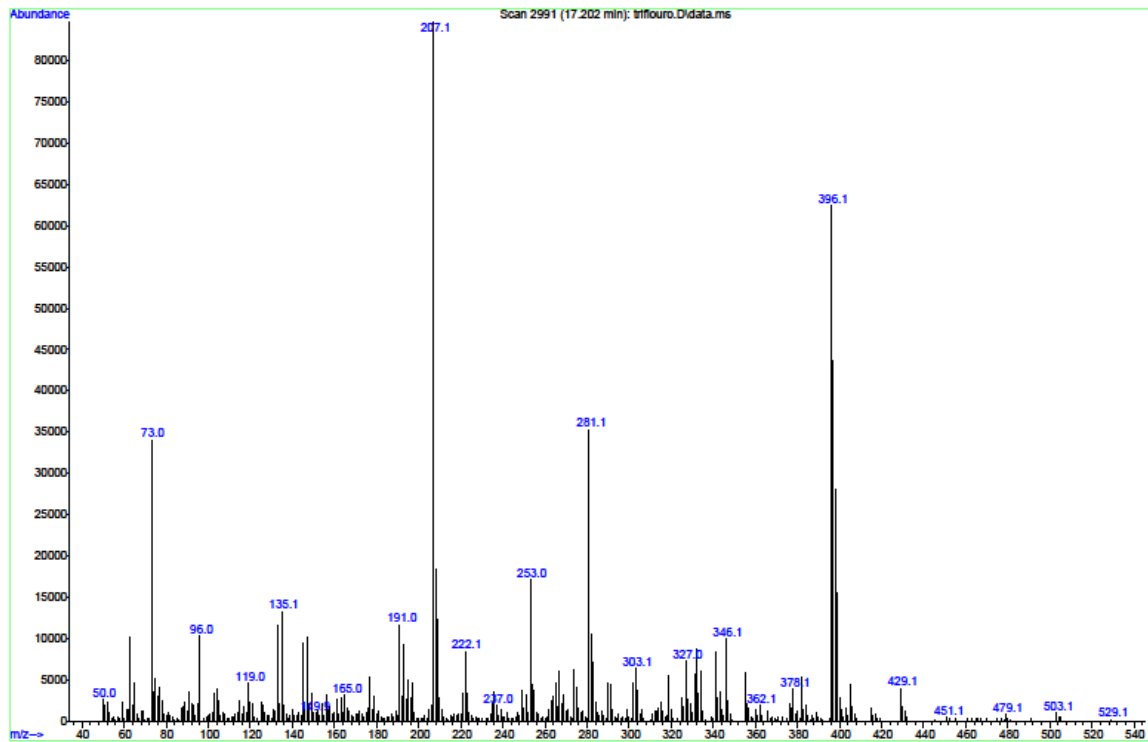


7-(2-Chloroethoxy)-N-(3-(trifluoromethyl)phenyl)-6-methoxyquinazolin-4-amine (7c)



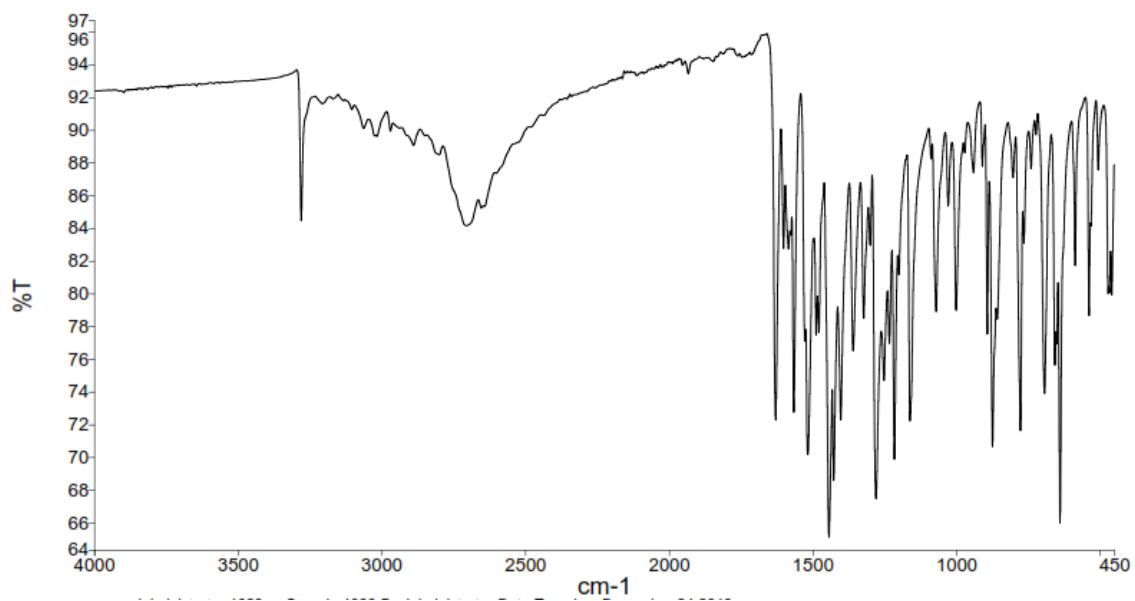


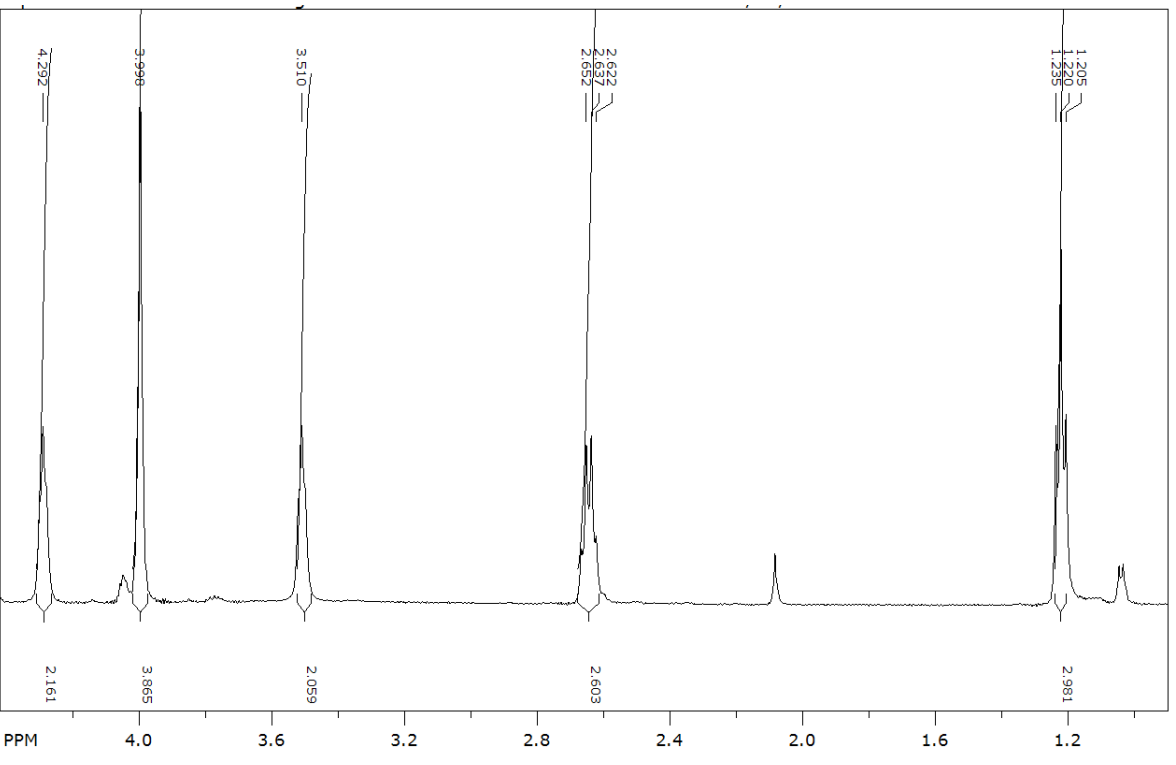
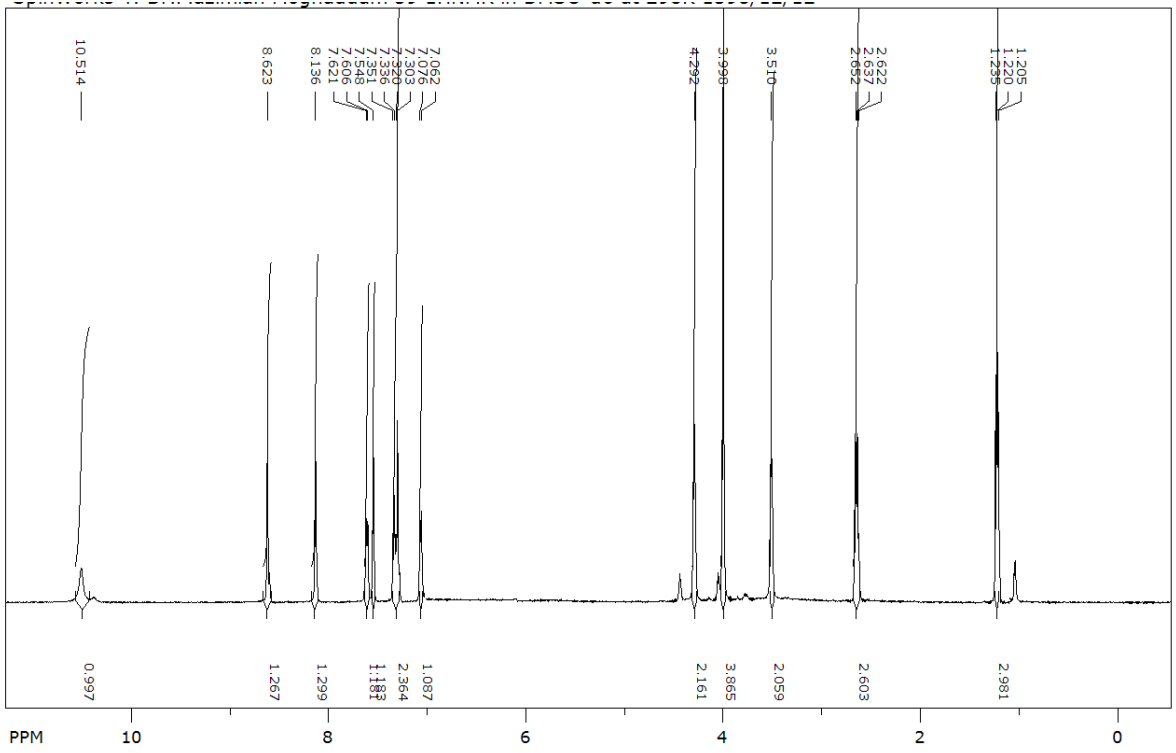


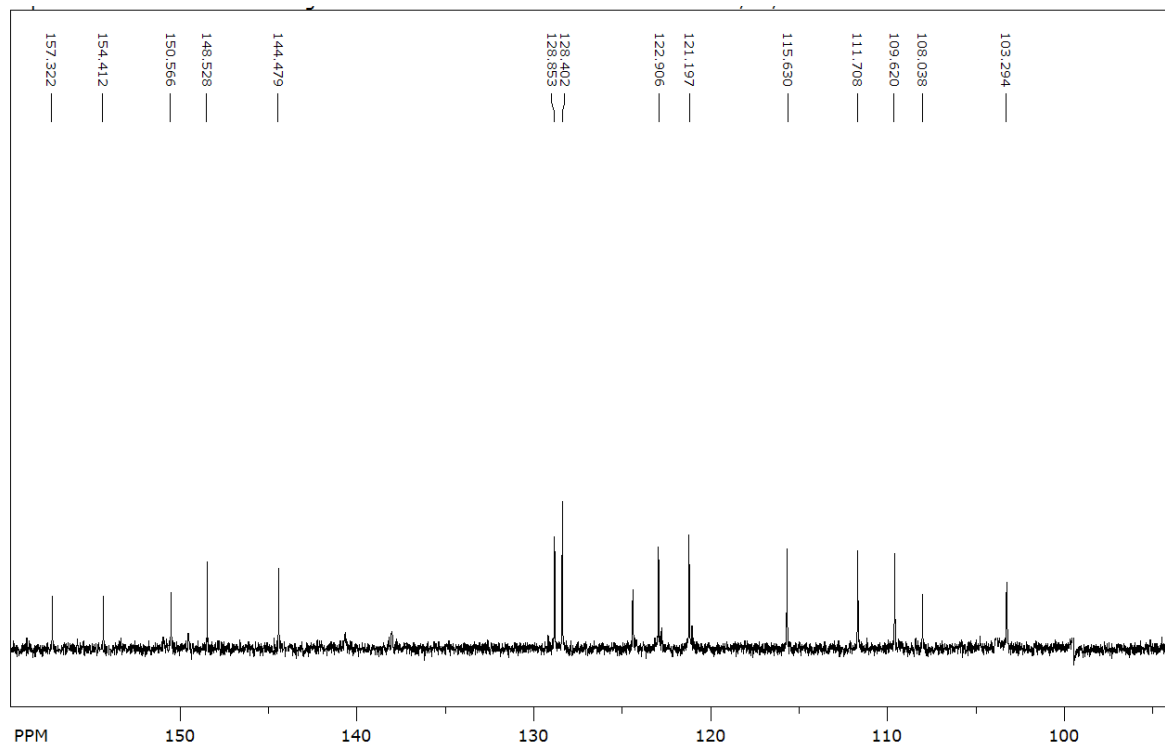
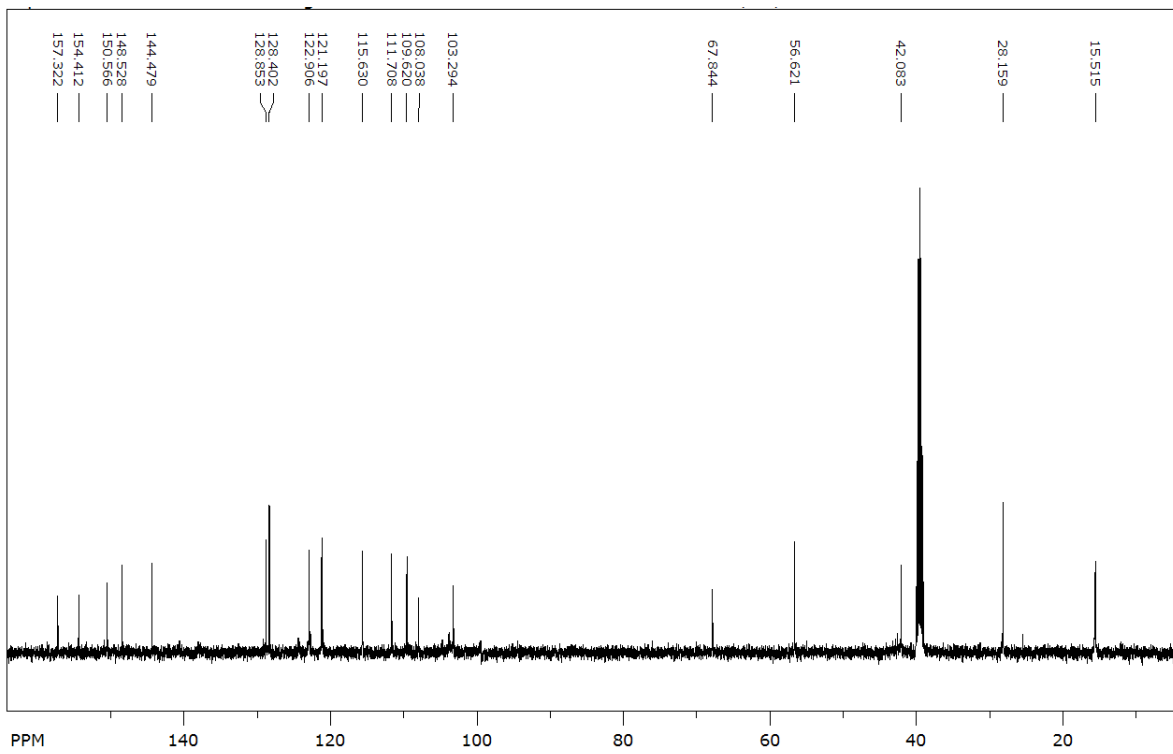


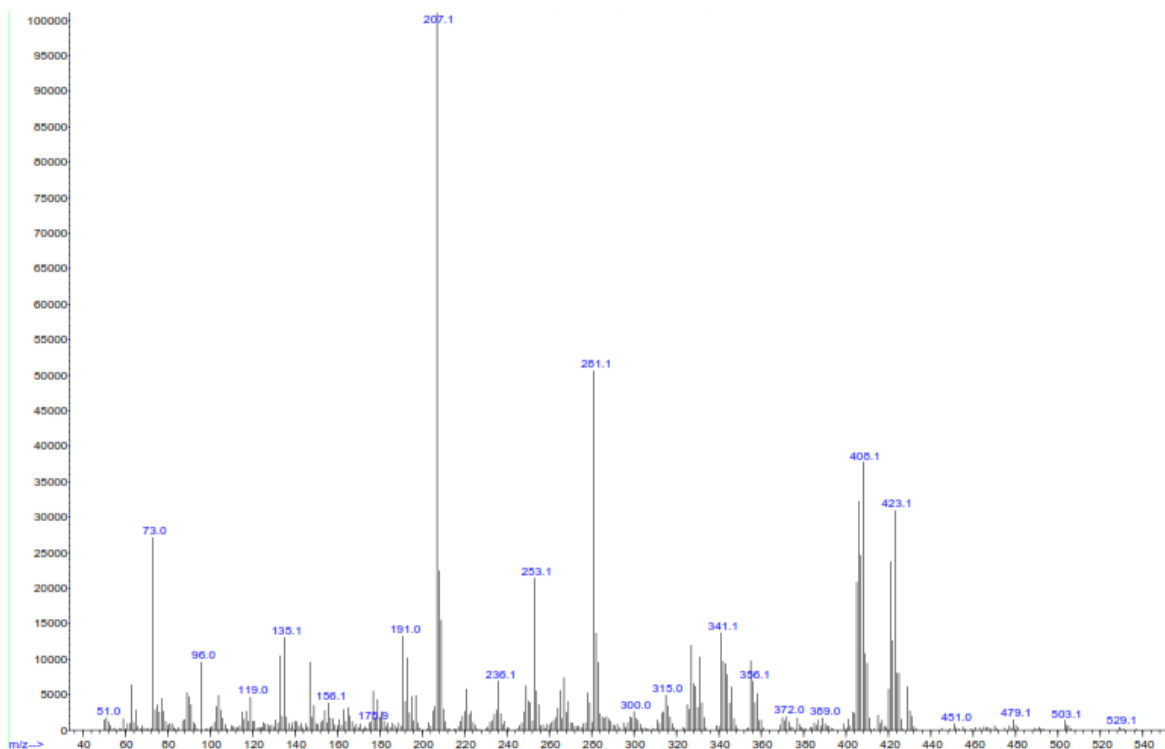
7-

(2-Chloroethoxy)-*N*-(3-ethylphenyl)-6-methoxyquinazolin-4-amine (7d)

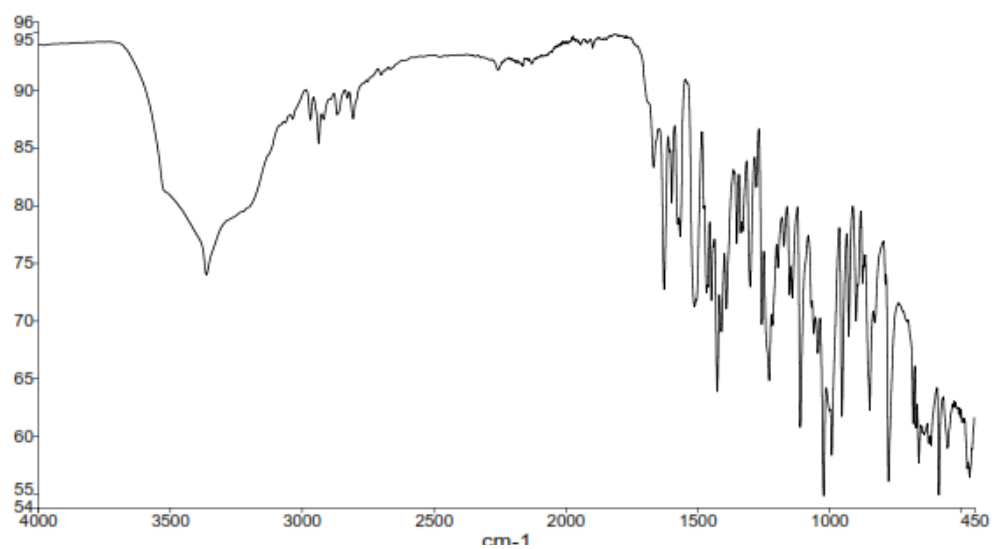


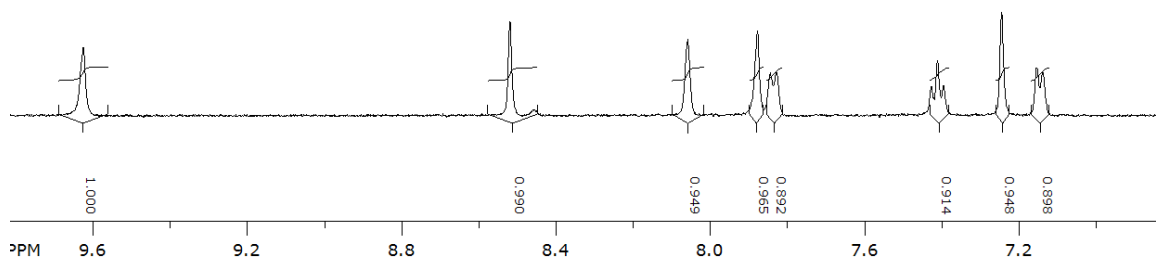
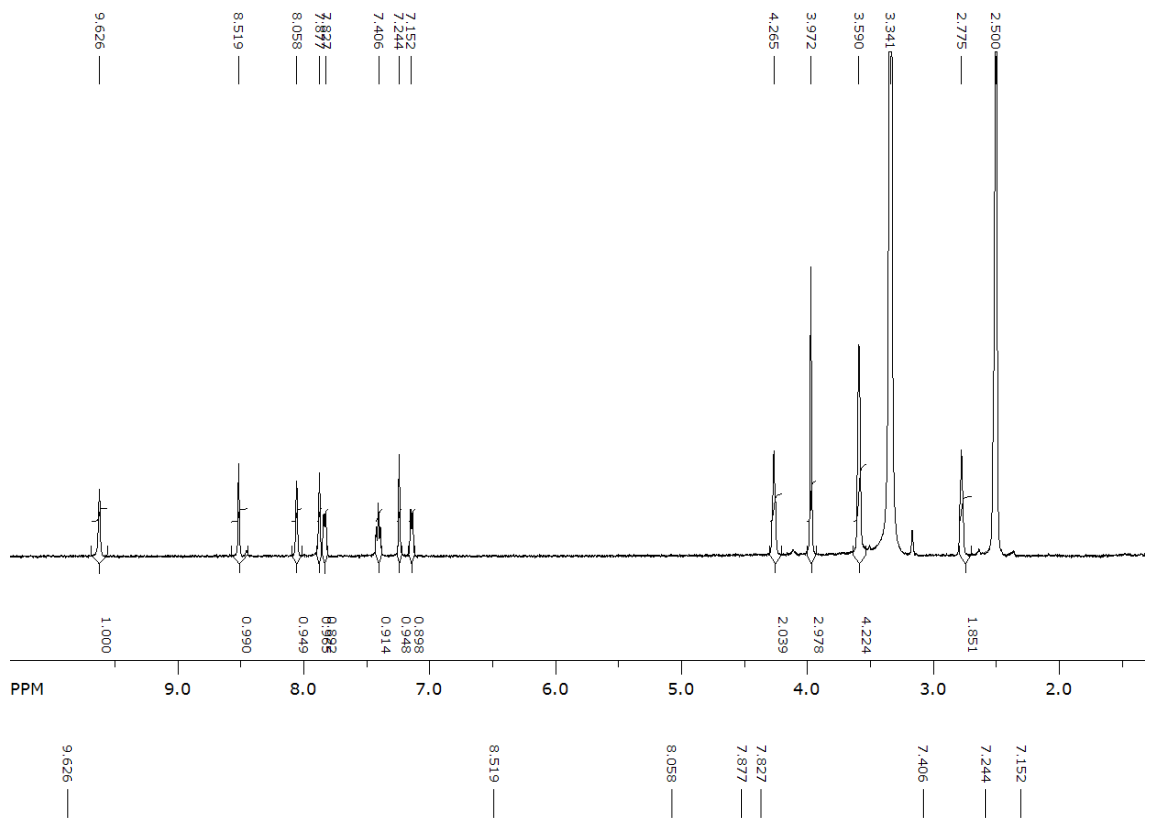


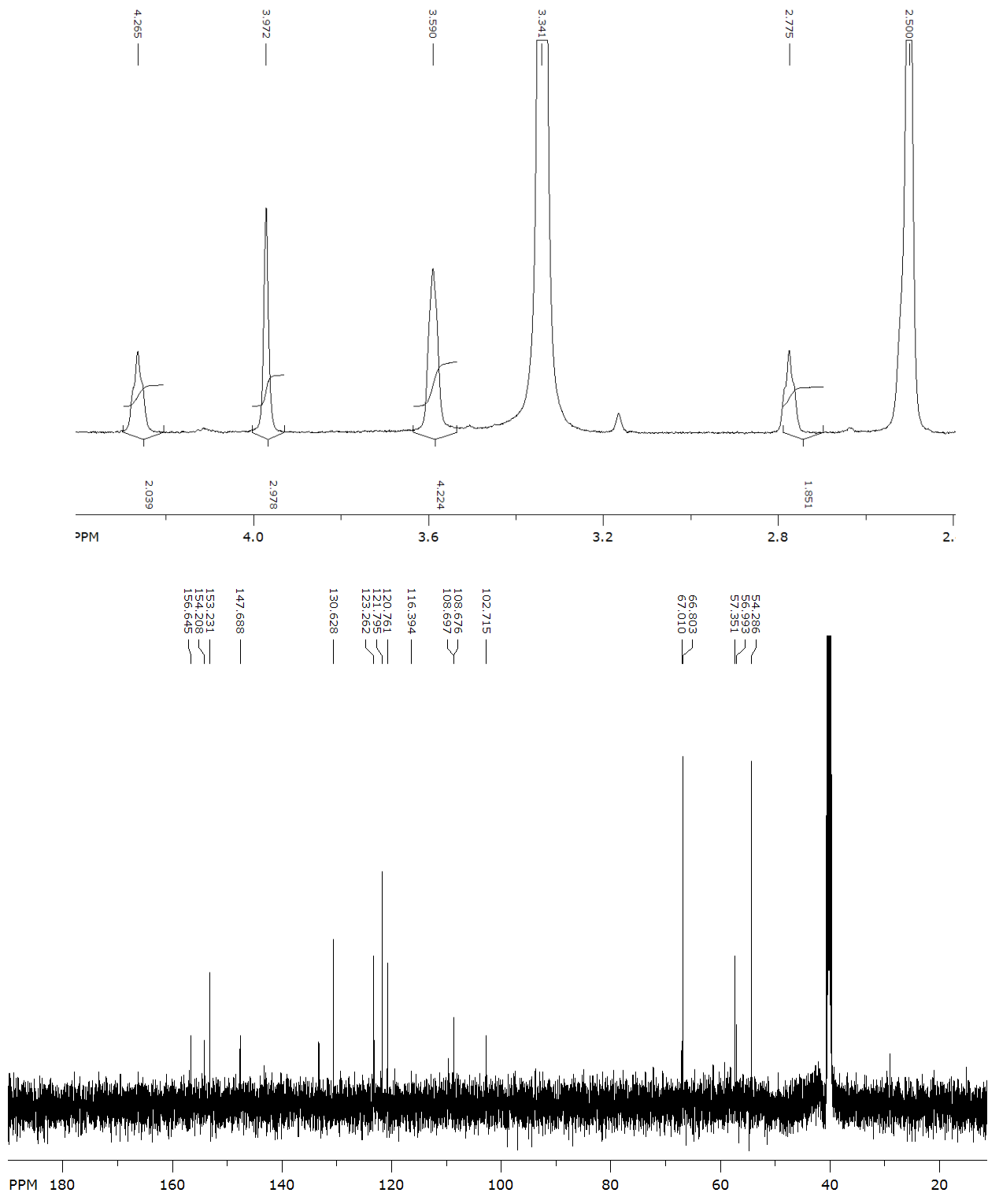


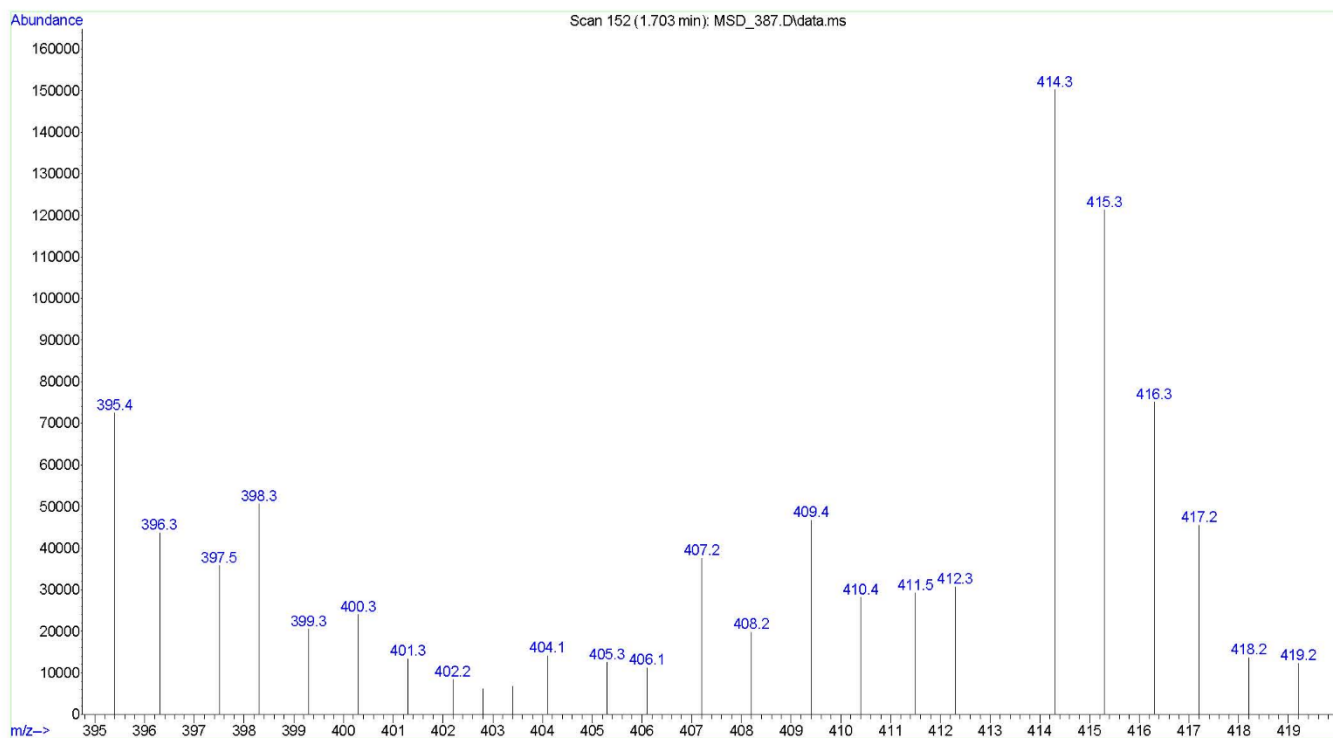


7-(2-morpholinoethoxy)-N-(3-chlorophenyl)-6-methoxyquinazolin-4-amine (8a)

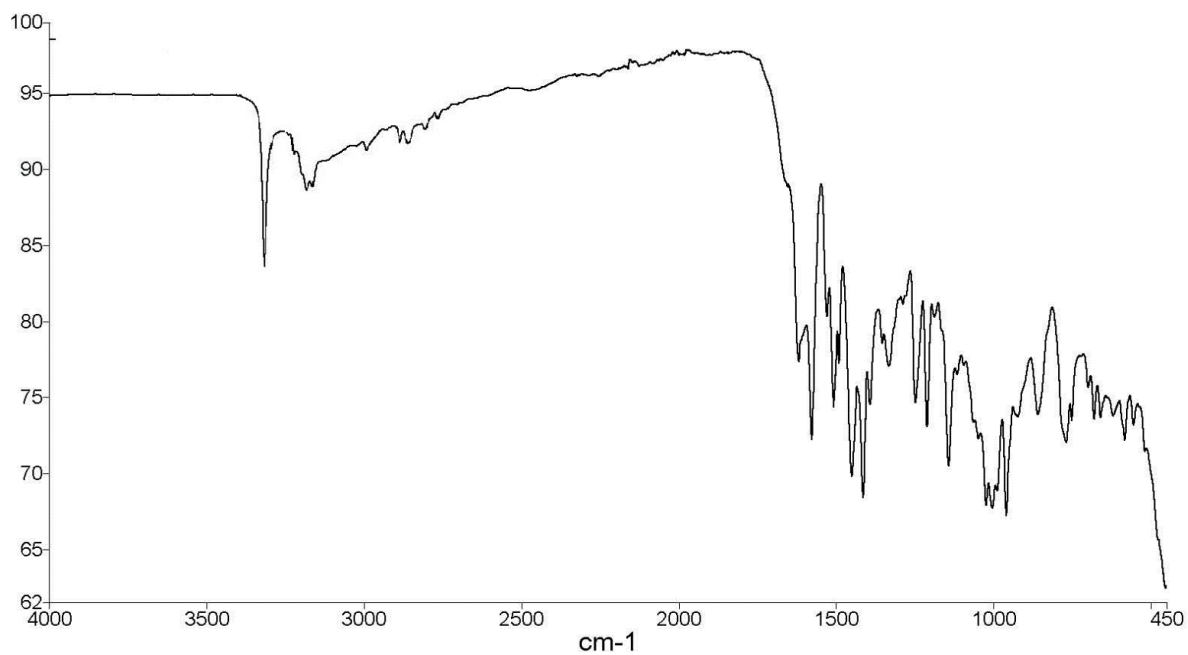


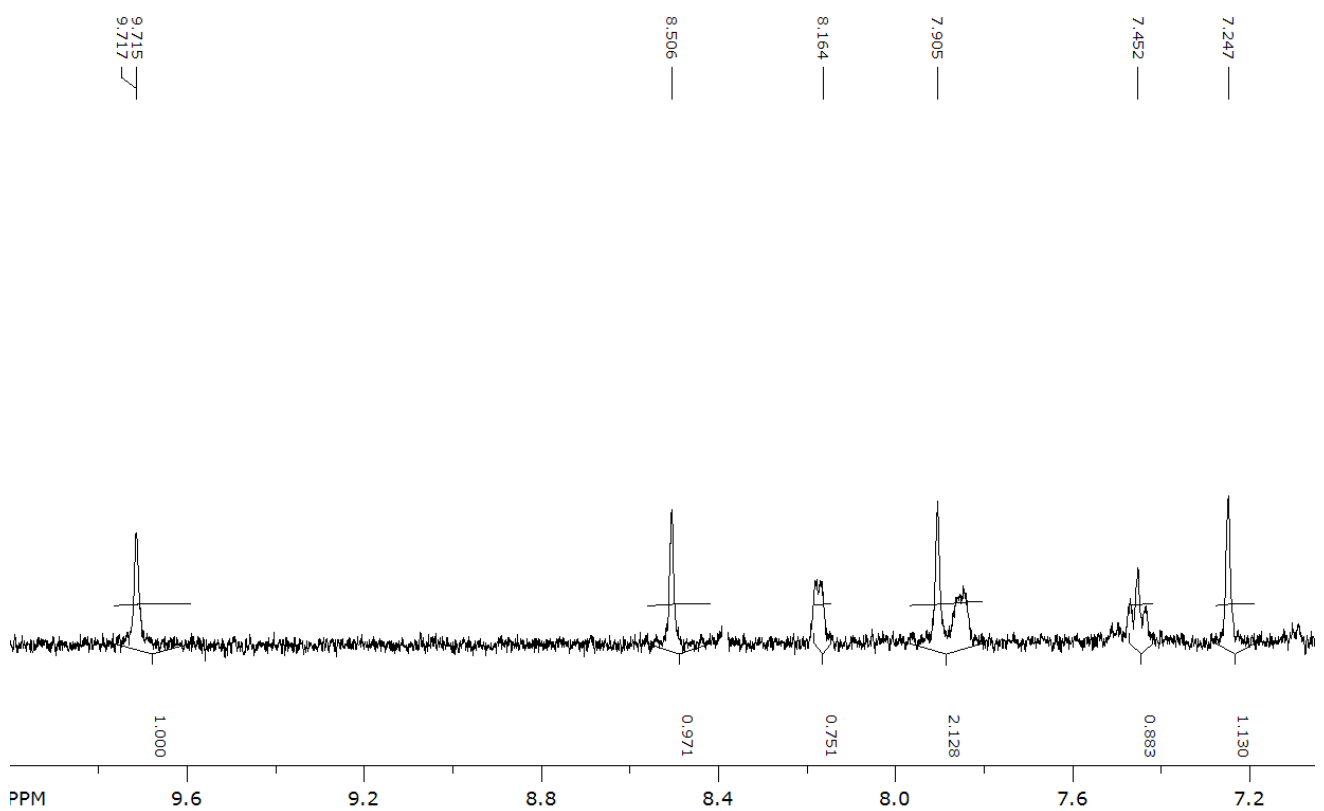
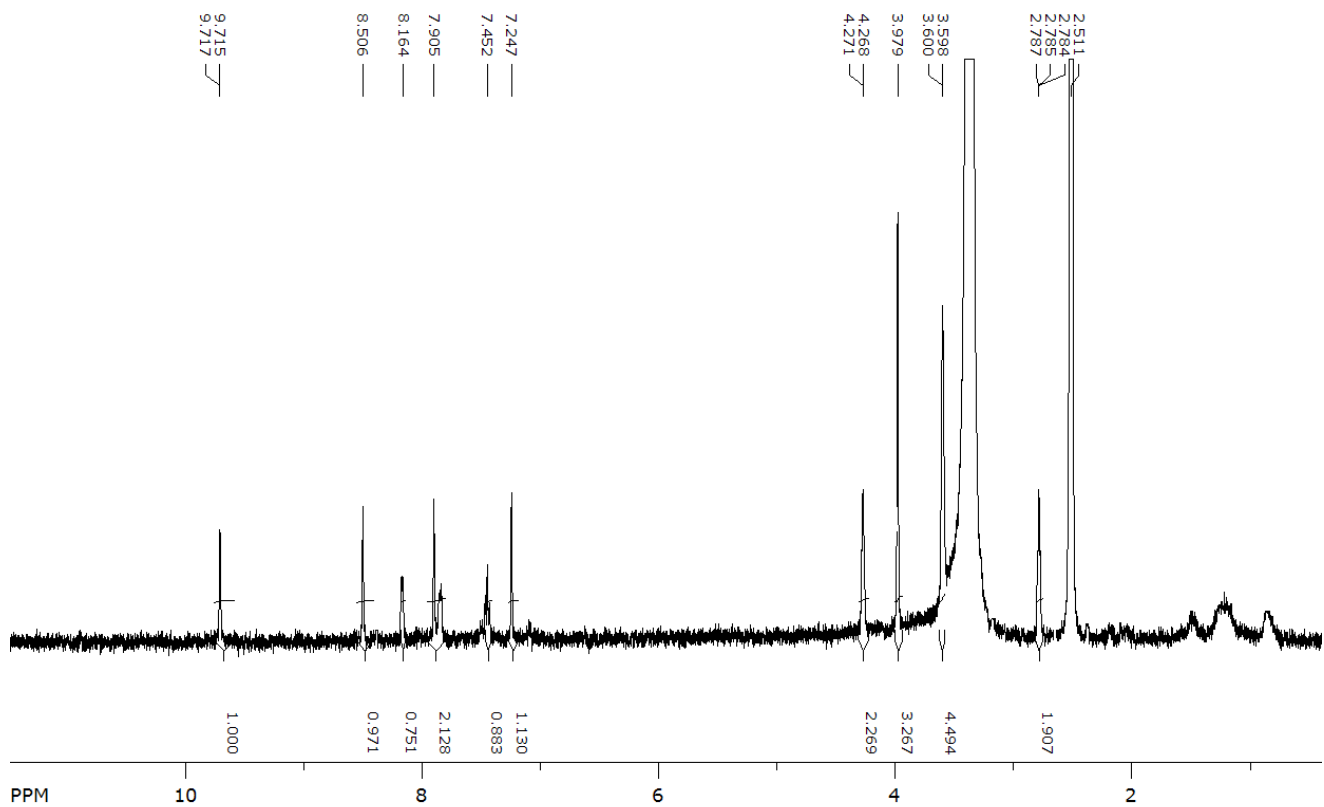


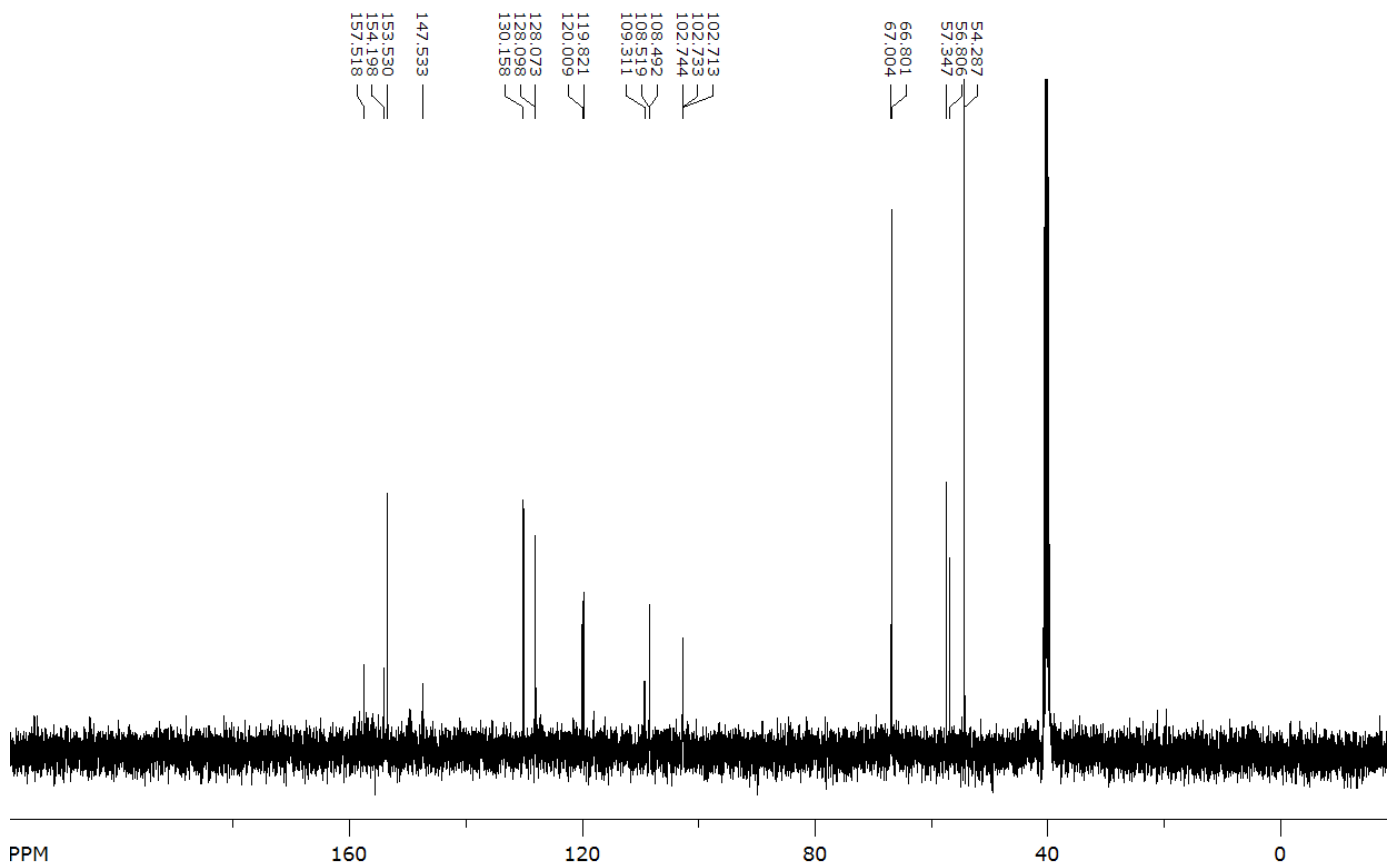
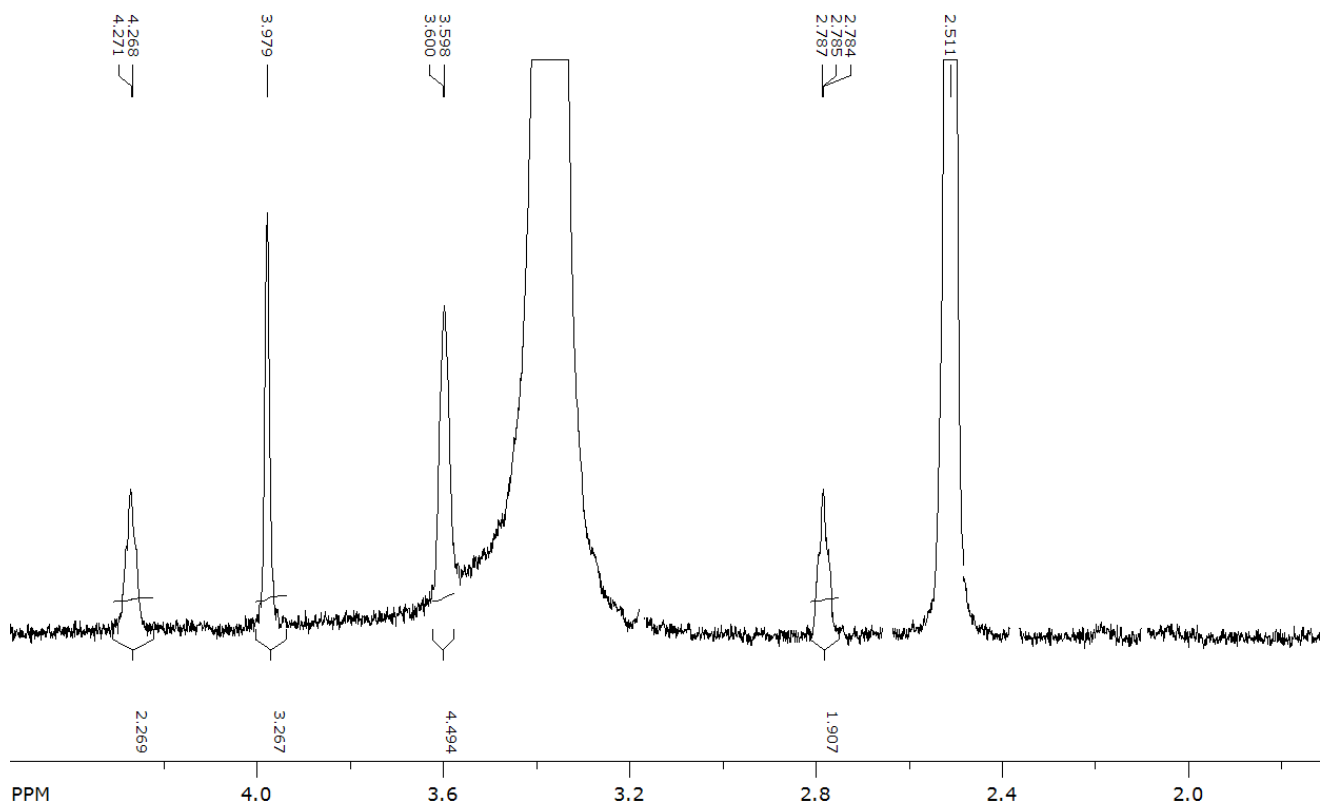


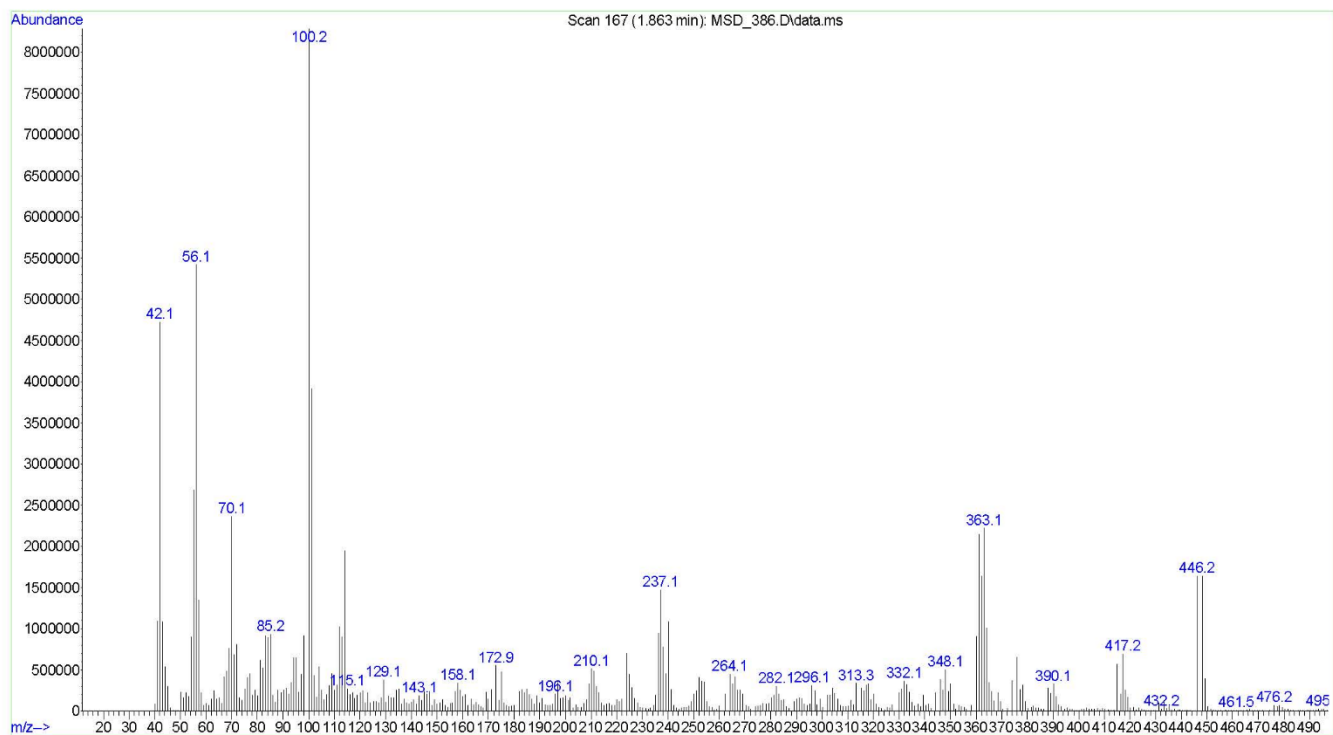


7-(2-morpholinoethoxy)-N-(3-chloro-4-fluorophenyl)-6-methoxyquinazolin-4-amine (8b)

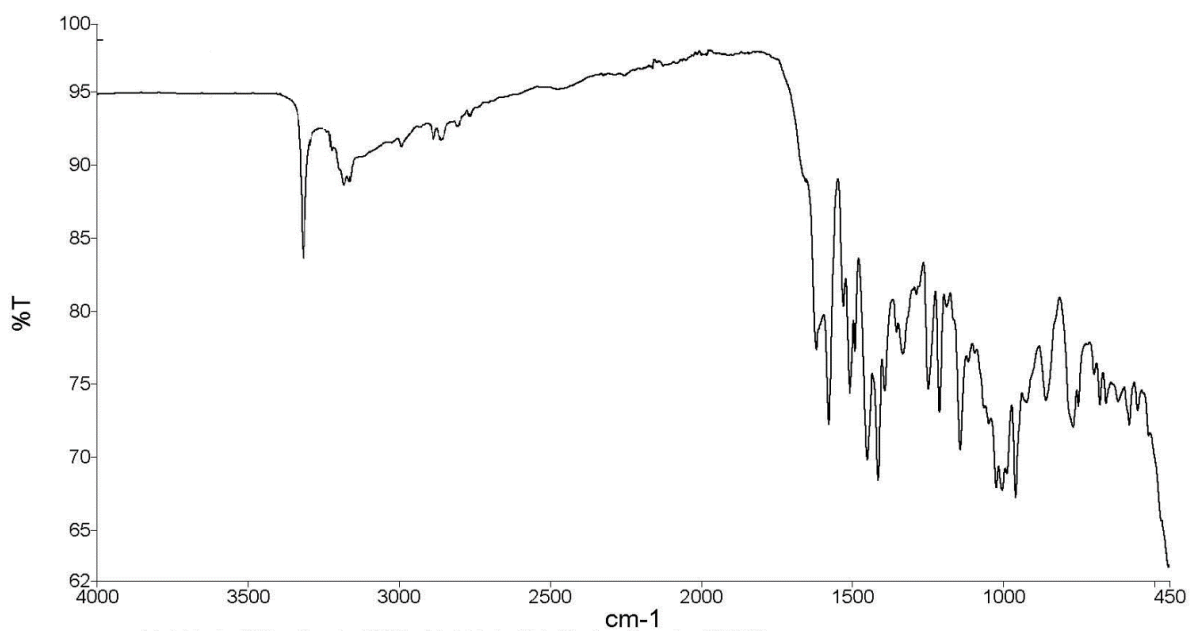


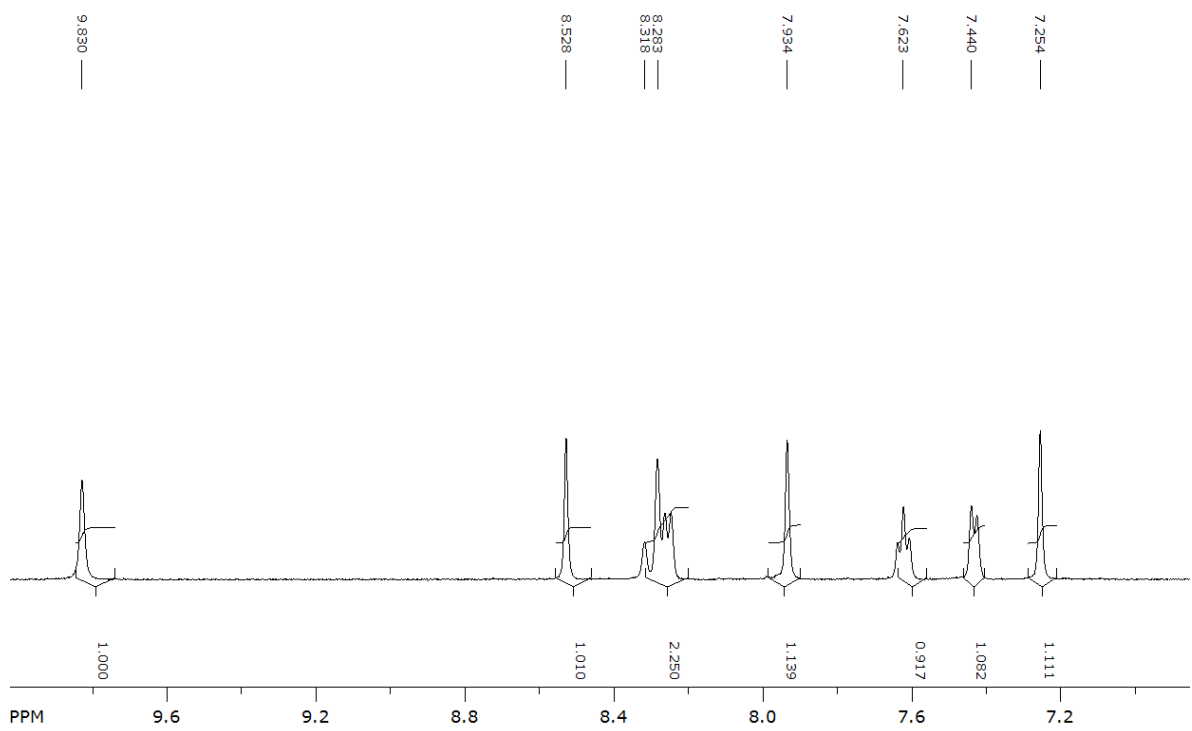


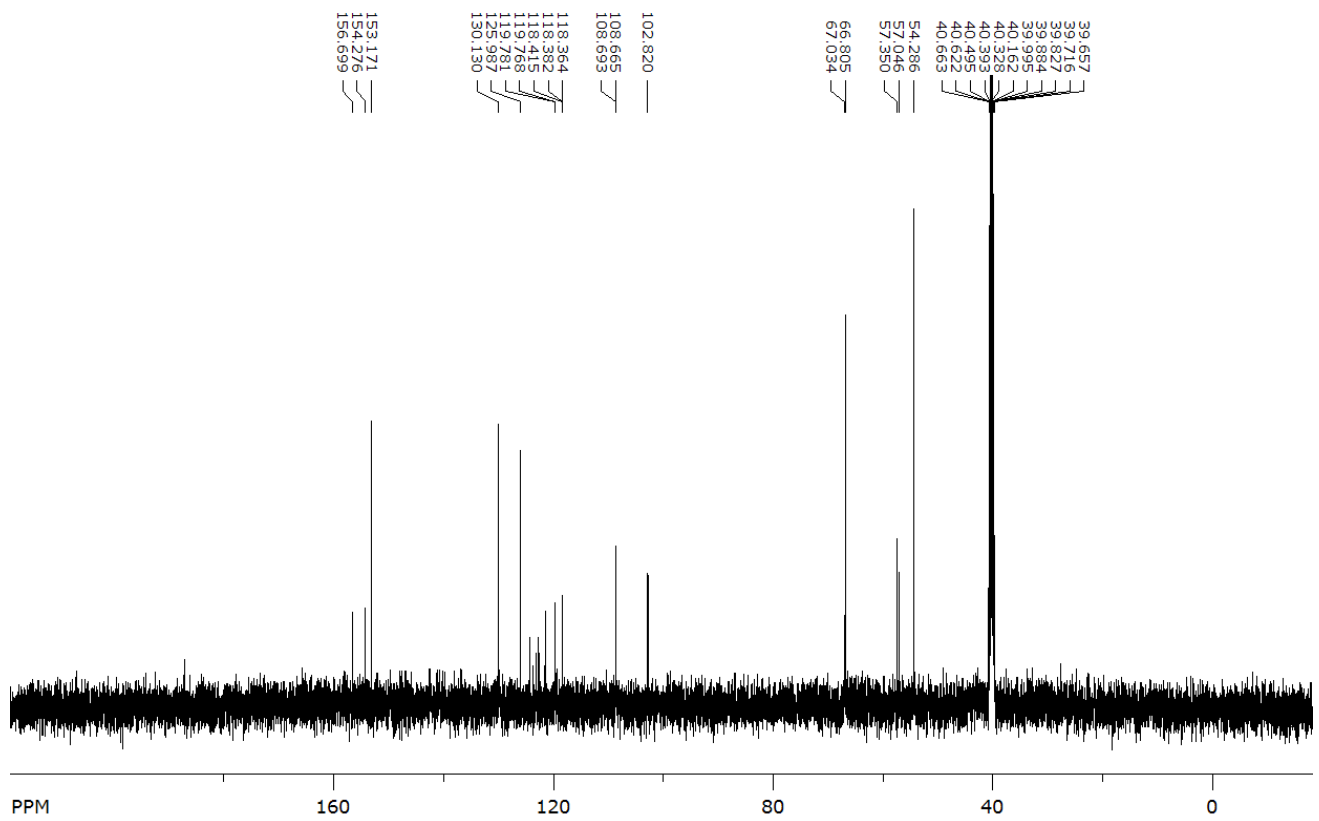
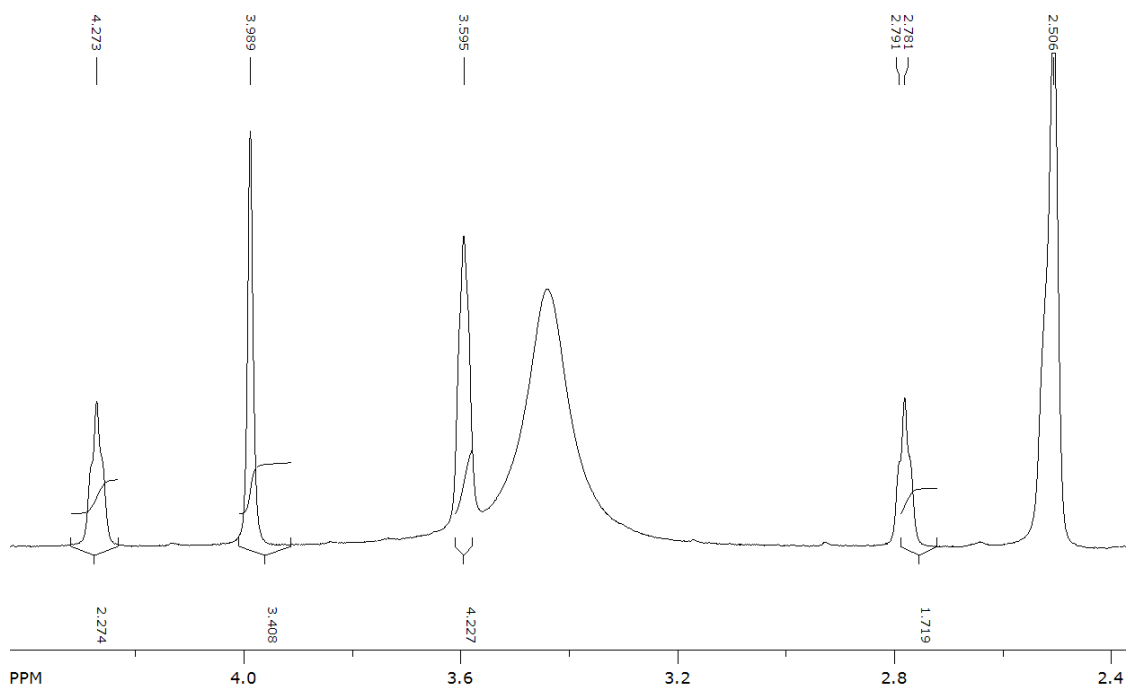


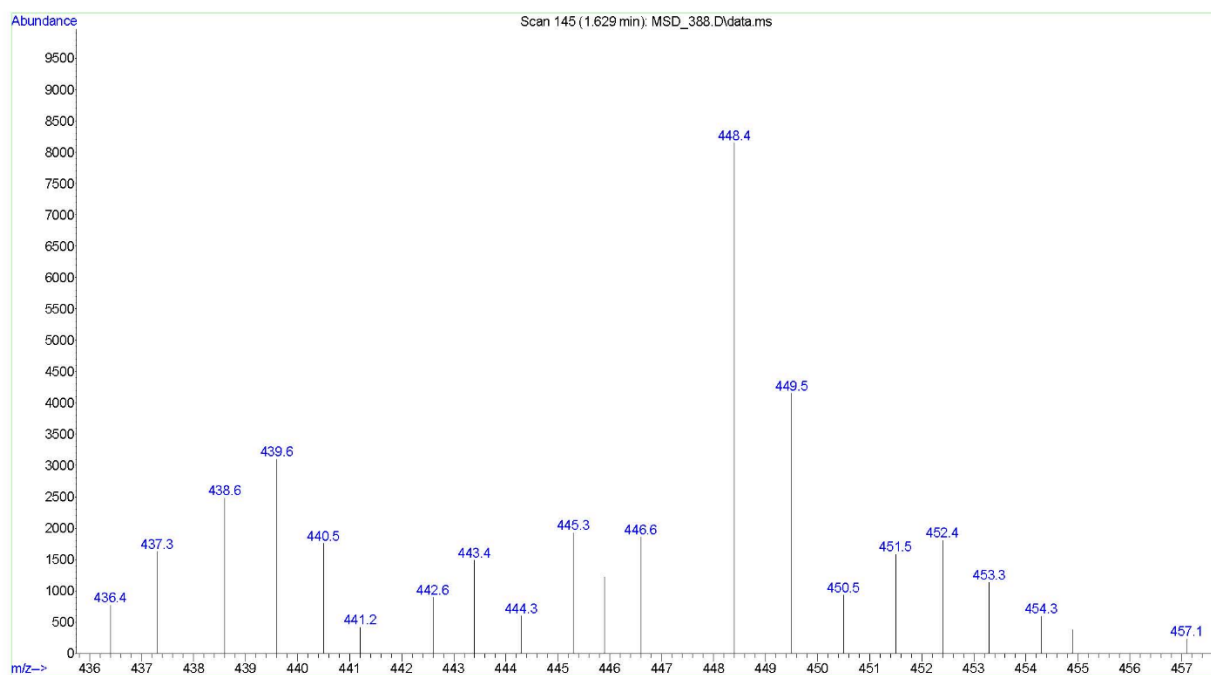
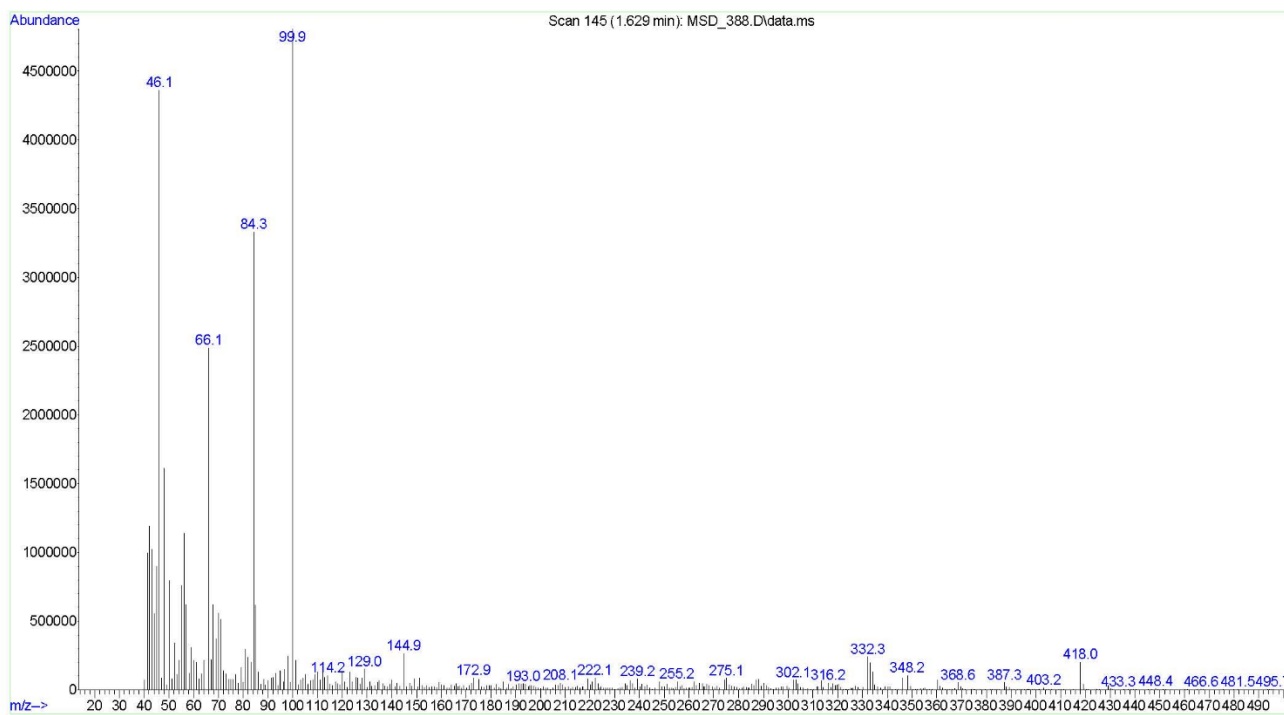


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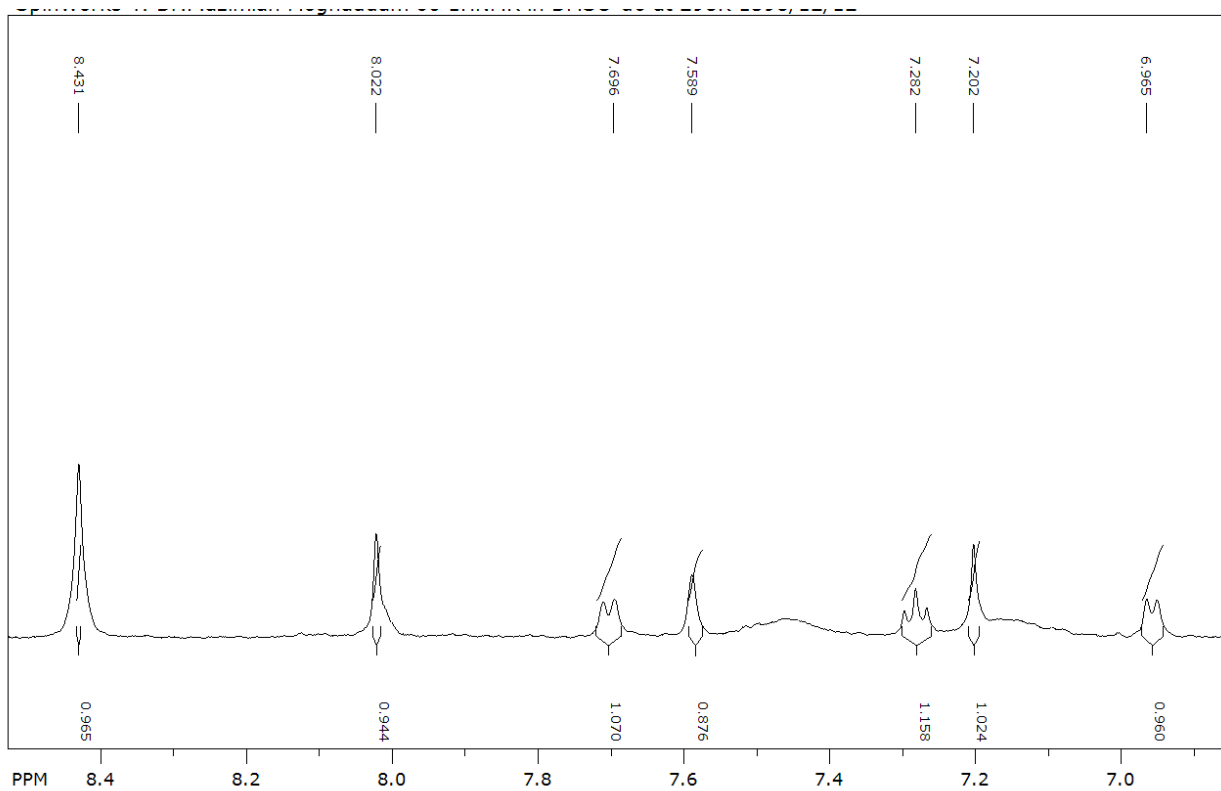
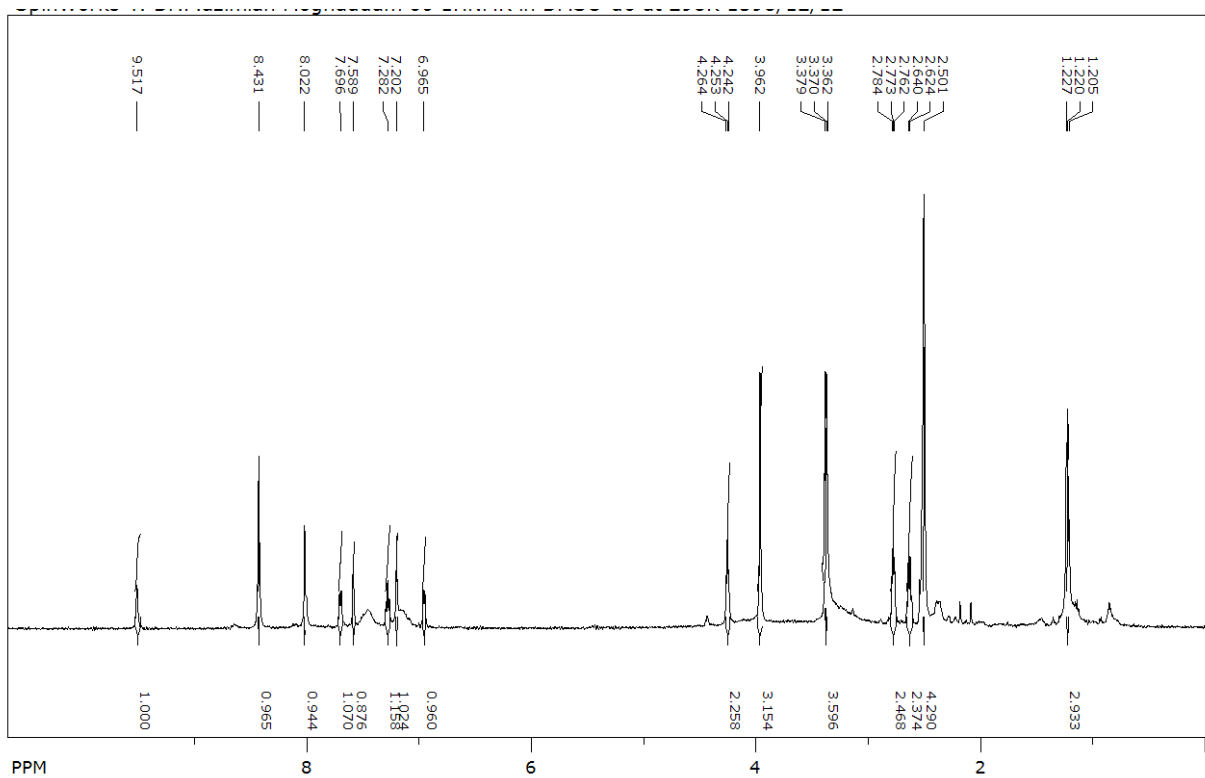


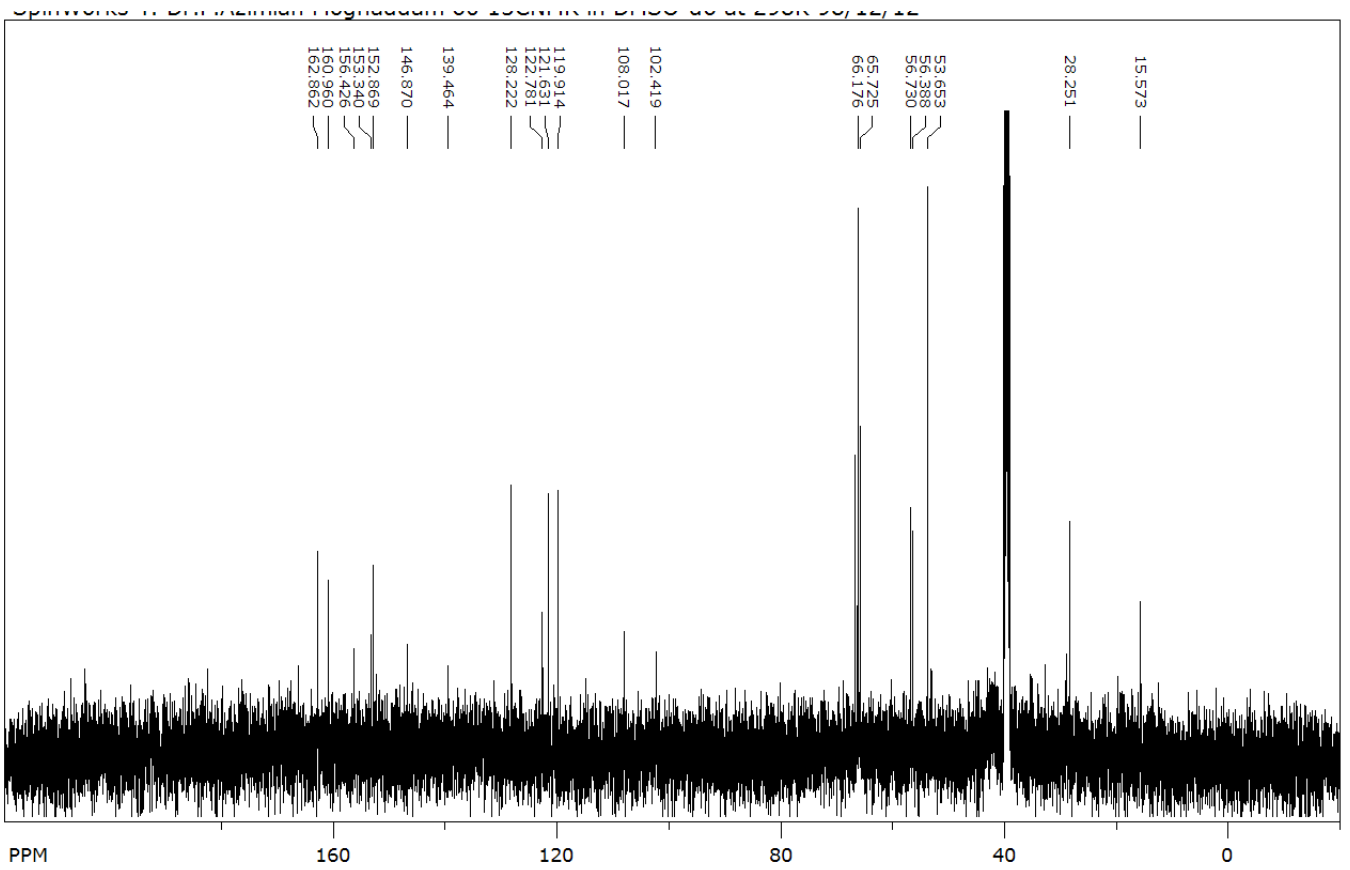
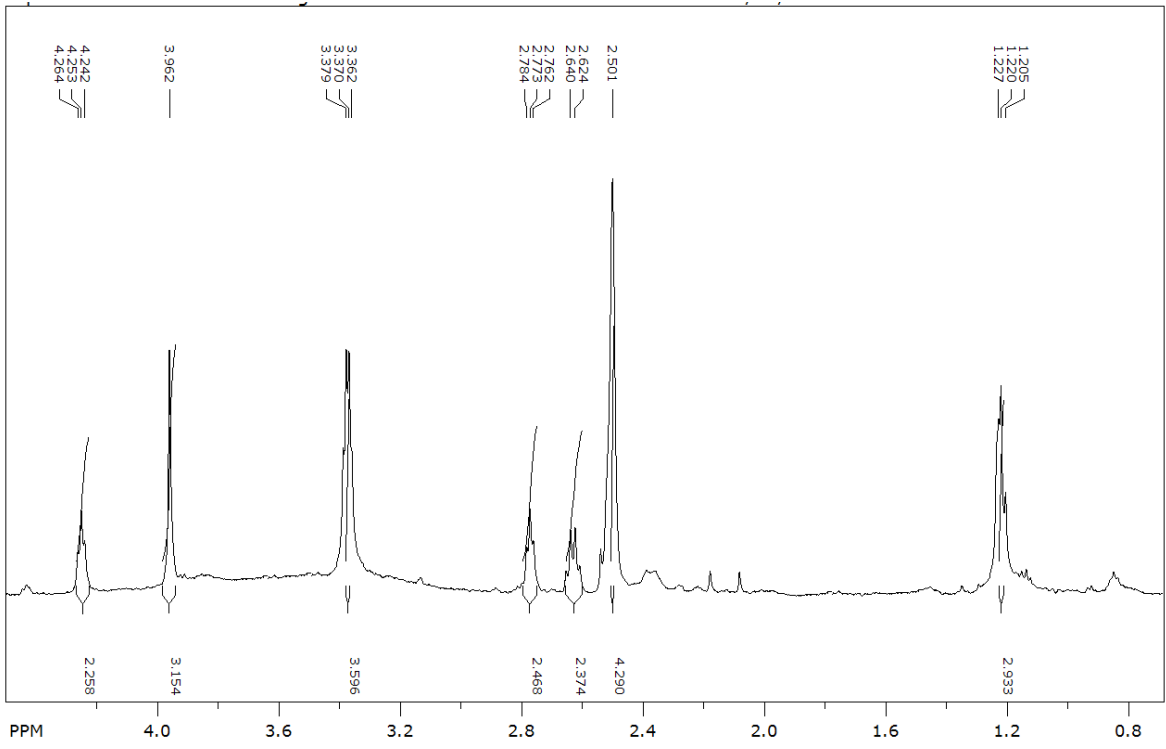


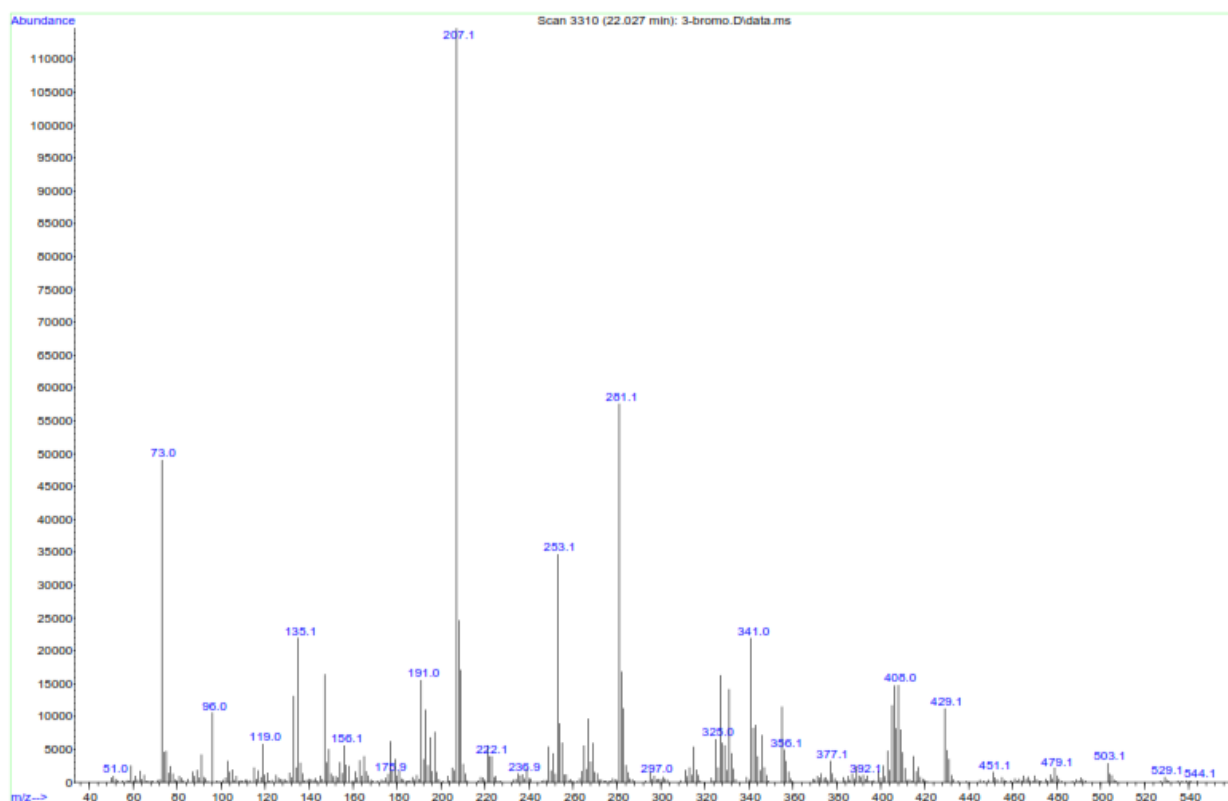


7-(2-morpholinoethoxy)-N-(3-ethylphenyl)-6-methoxyquinazolin-4-amine (8d)

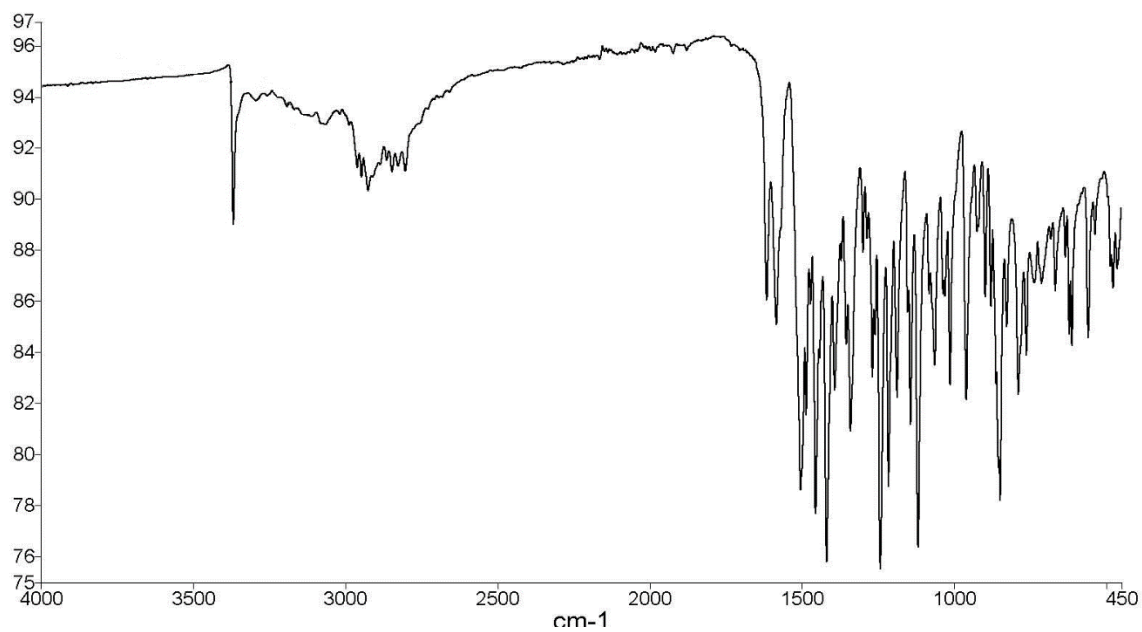


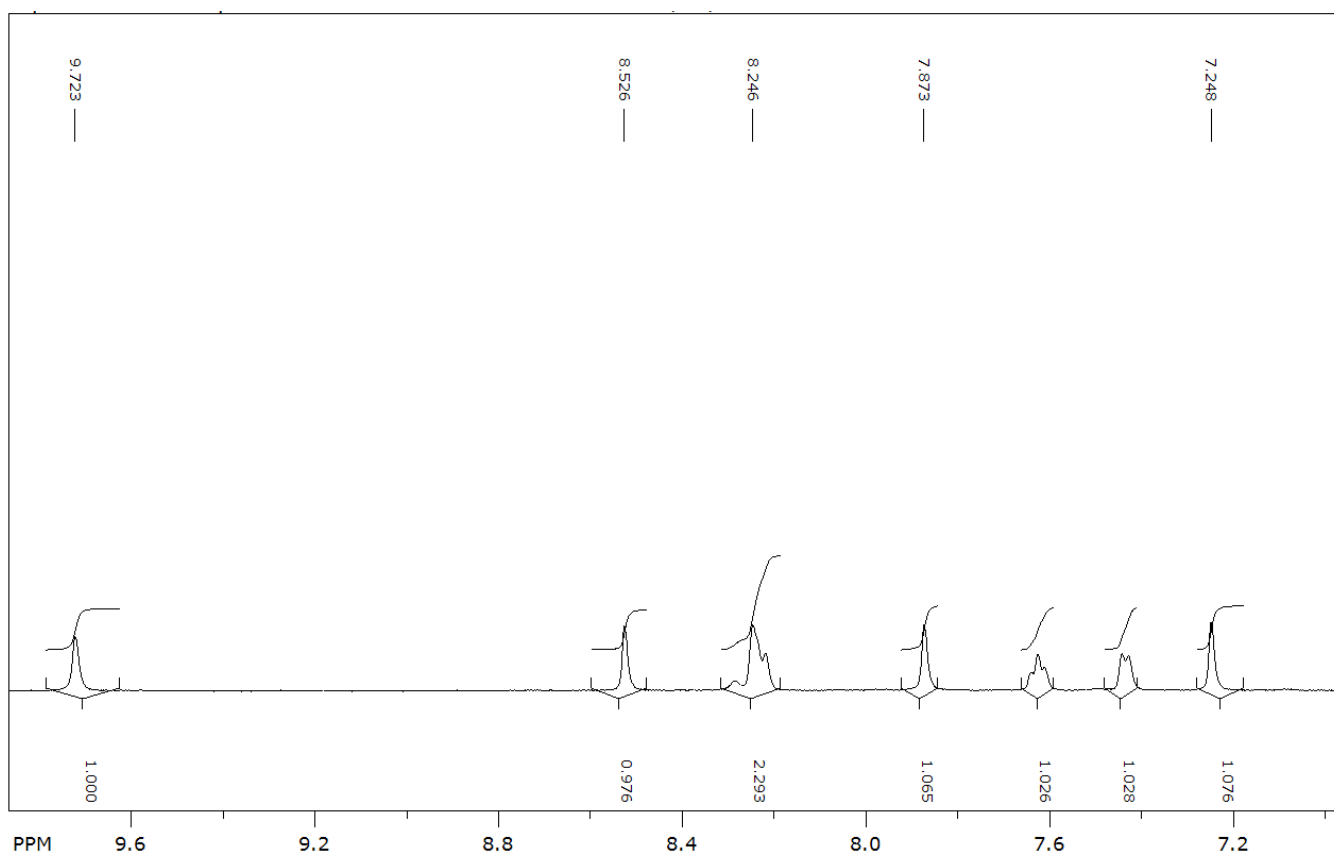
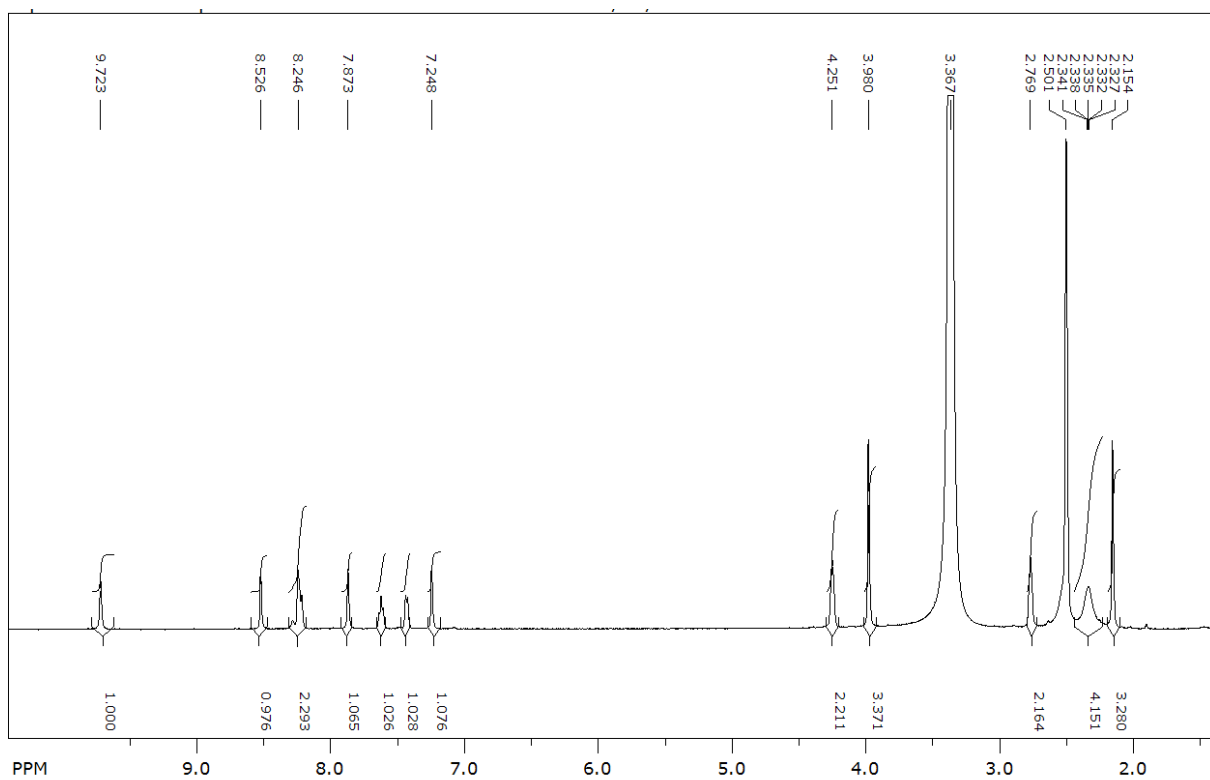


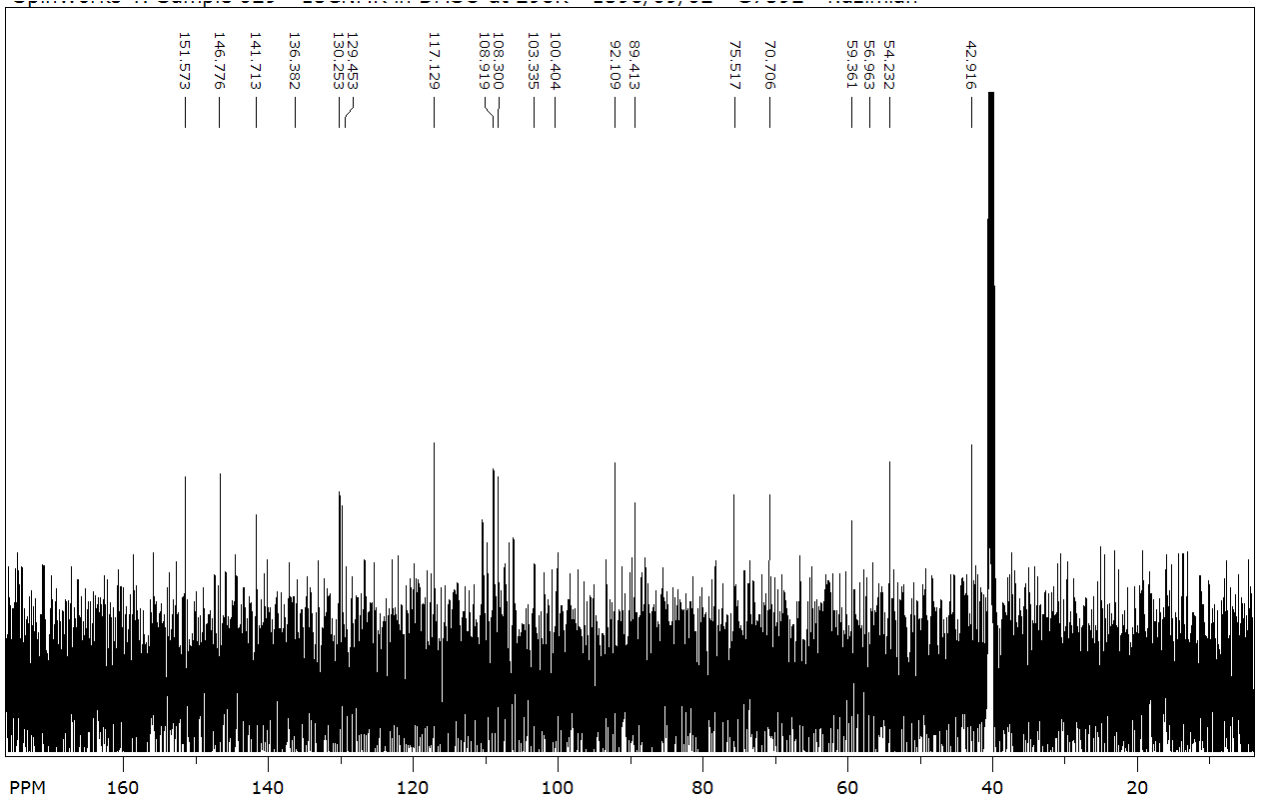
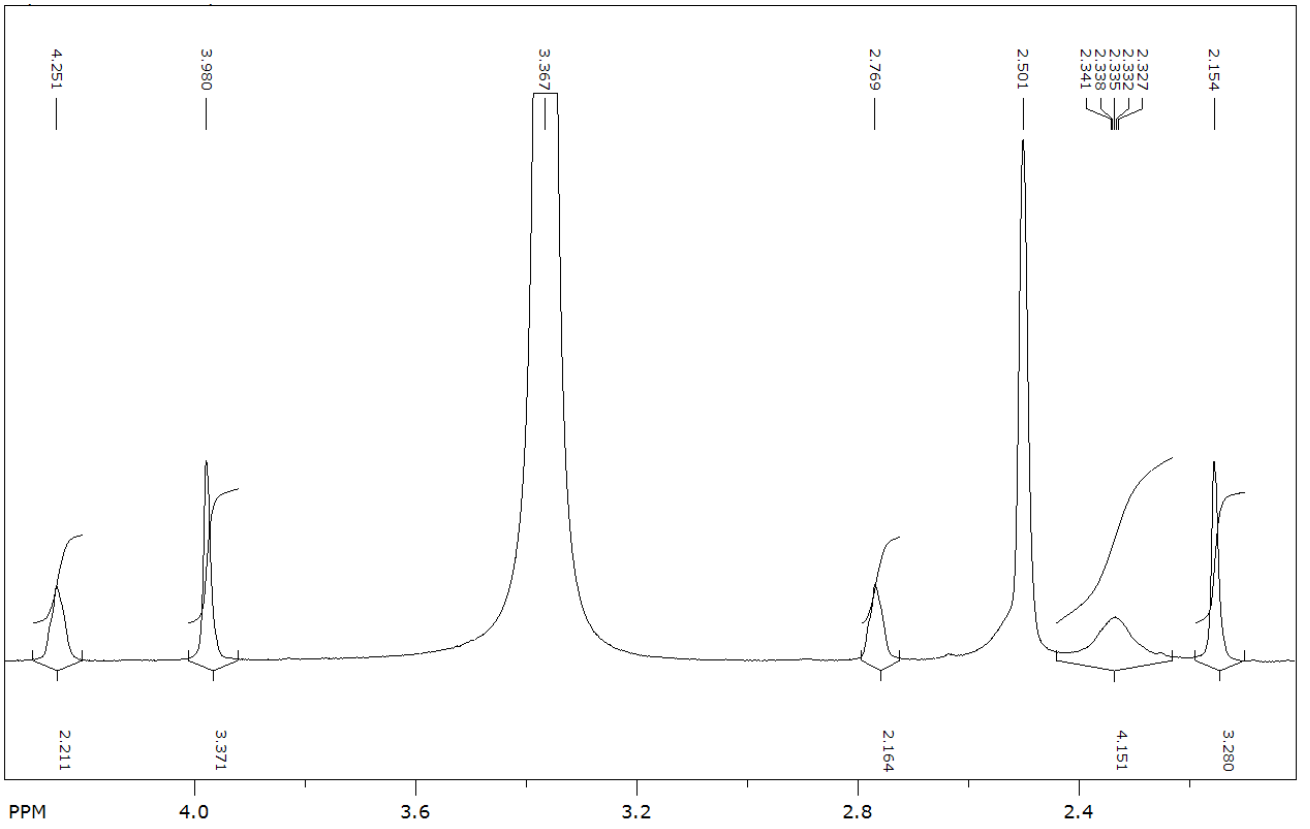


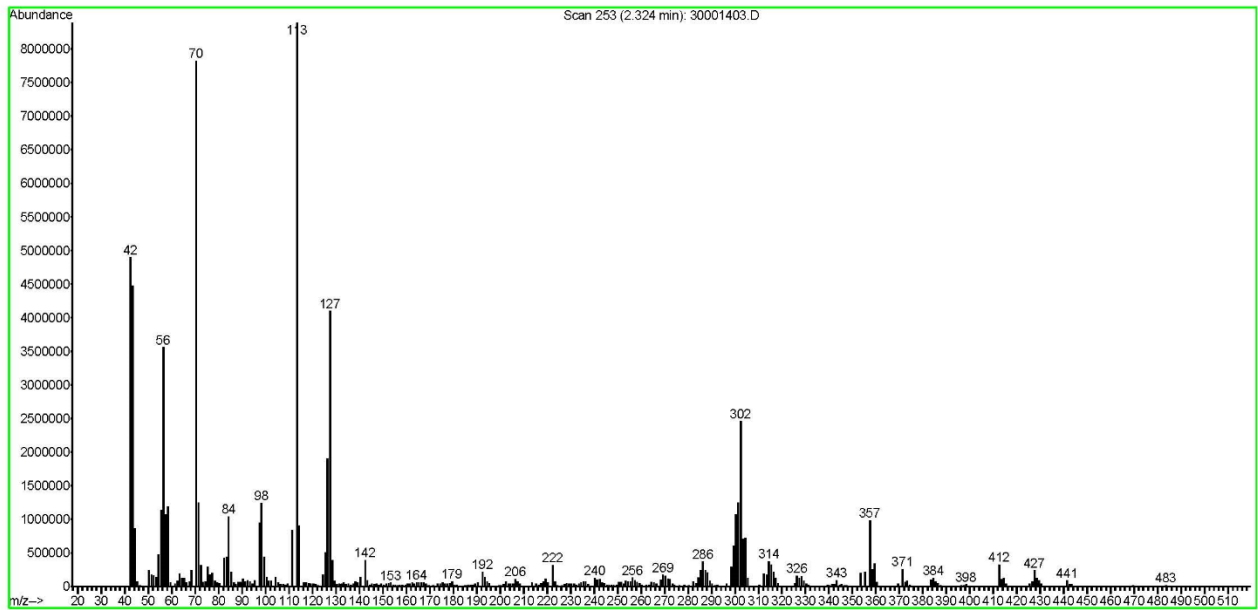


7-(2-(4-methylpiperazin-1-yl)ethoxy)-N-(3-chlorophenyl)-6-methoxyquinazolin-4-amine (8e)

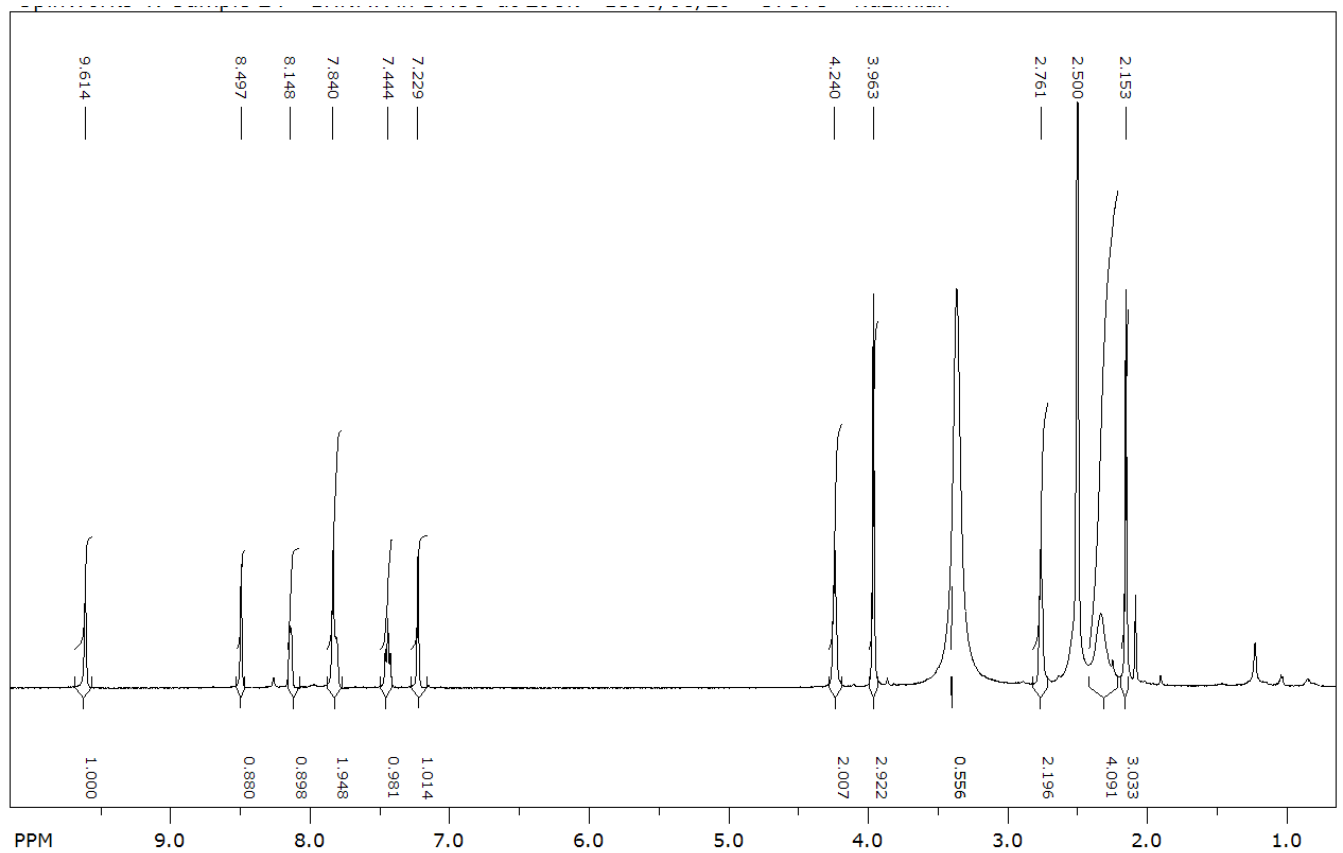


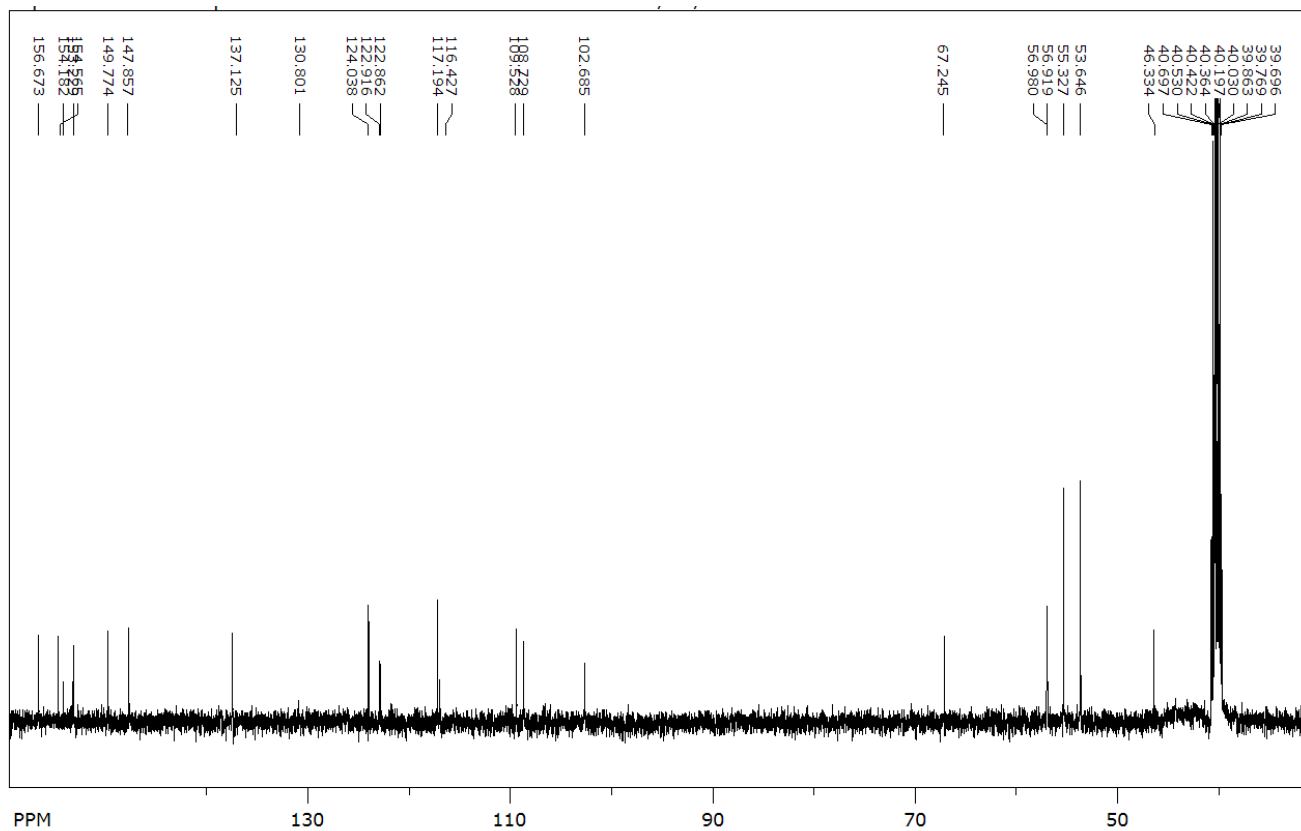
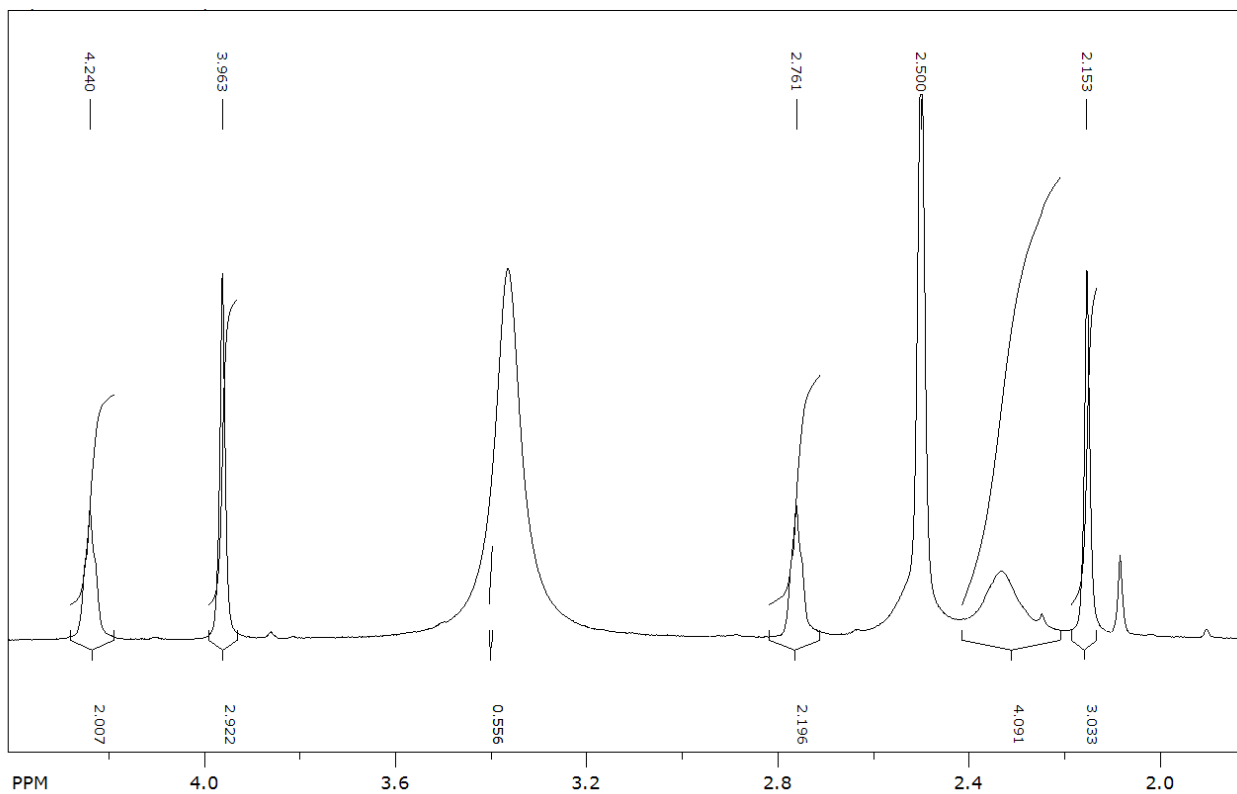


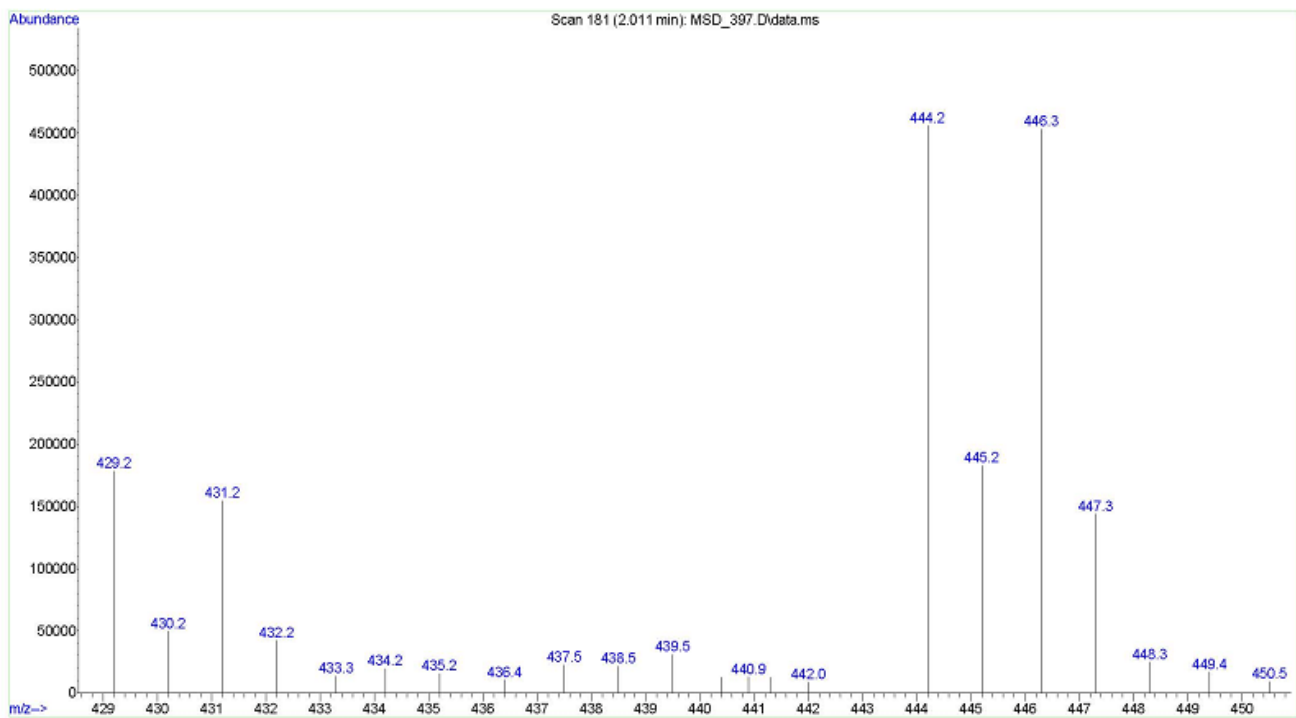




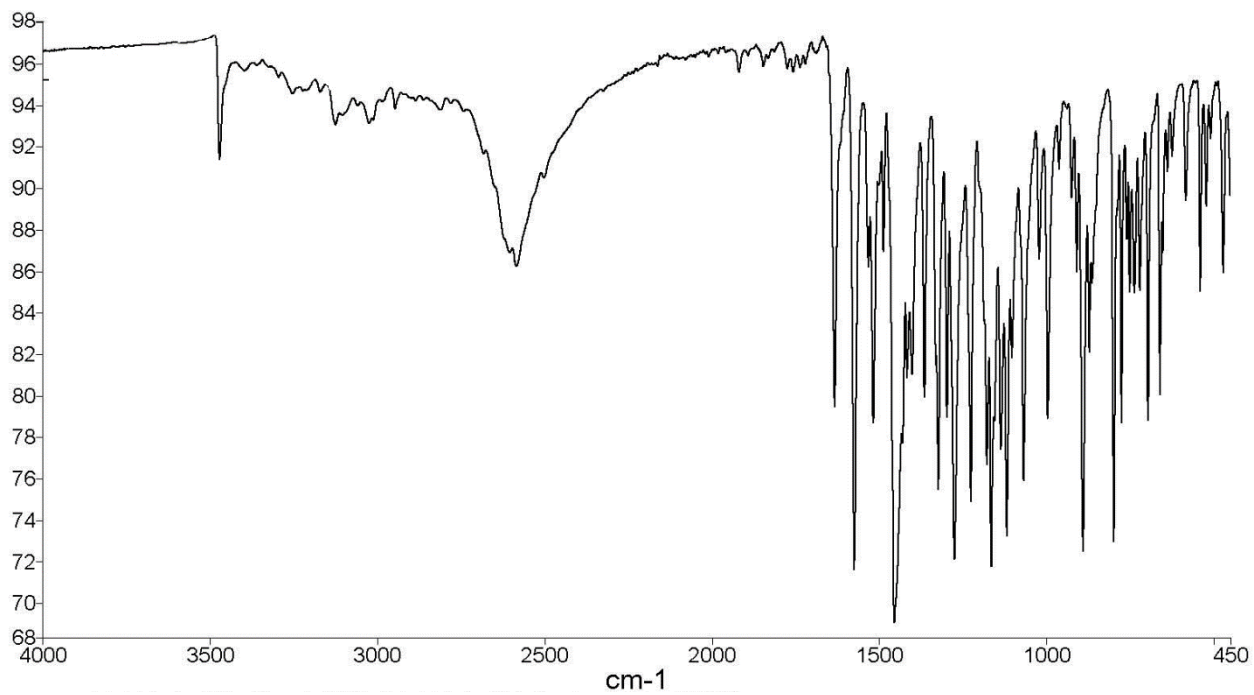
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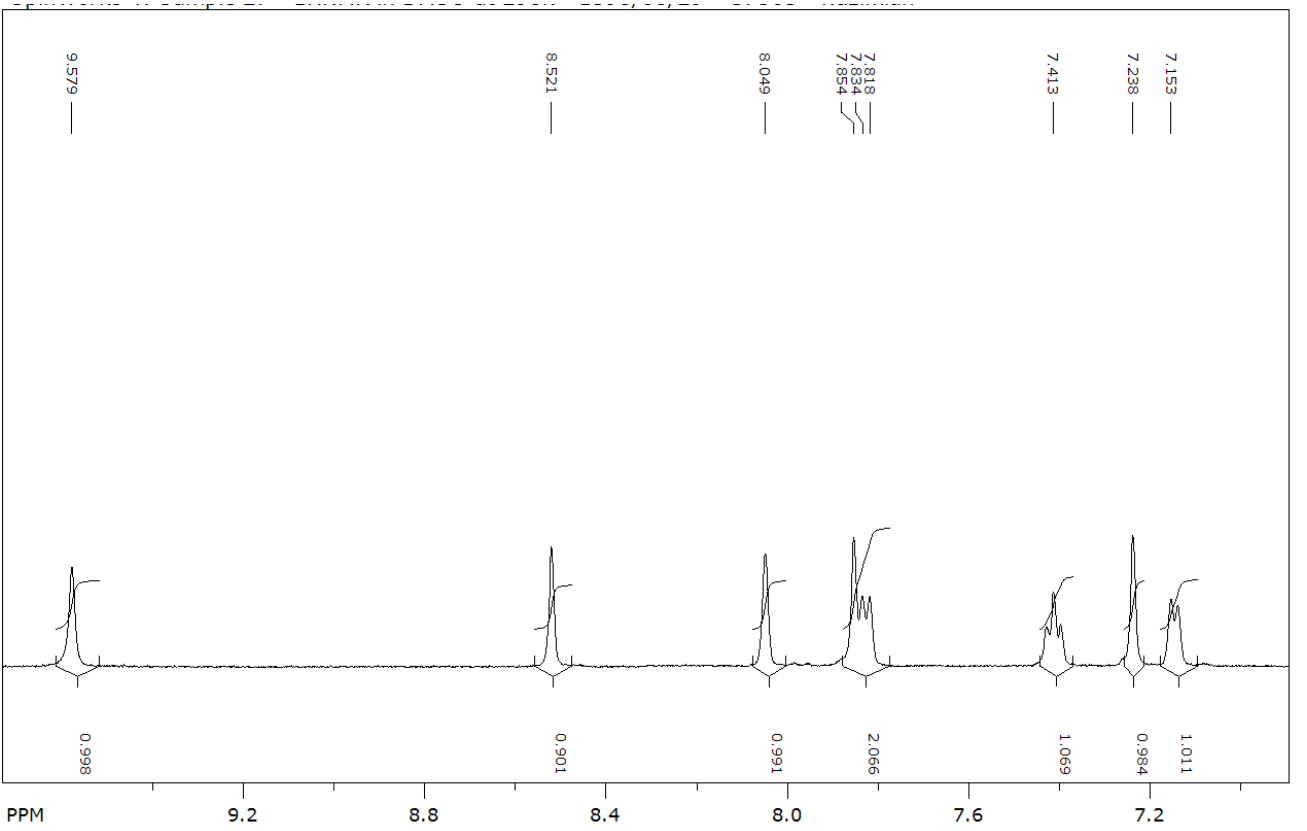
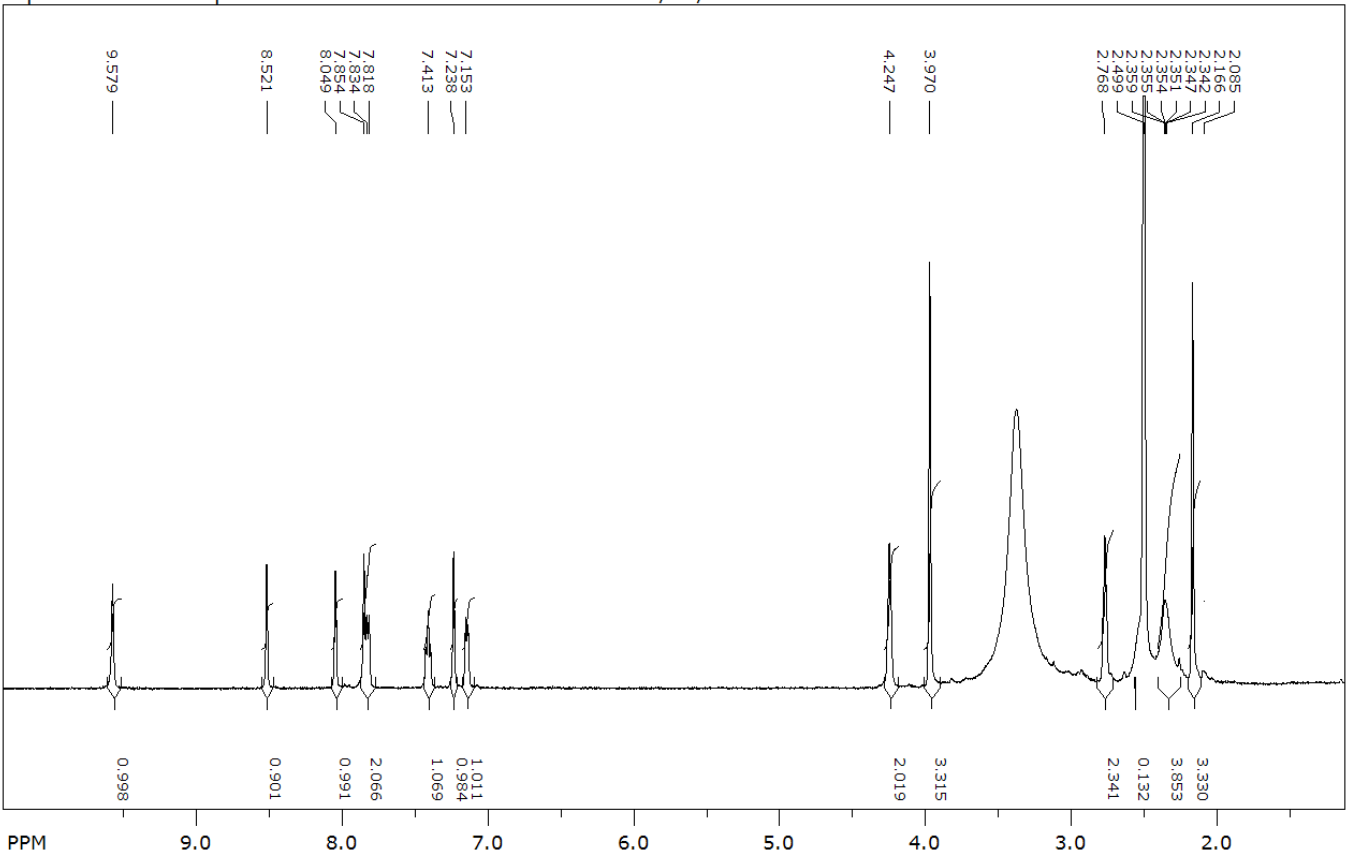


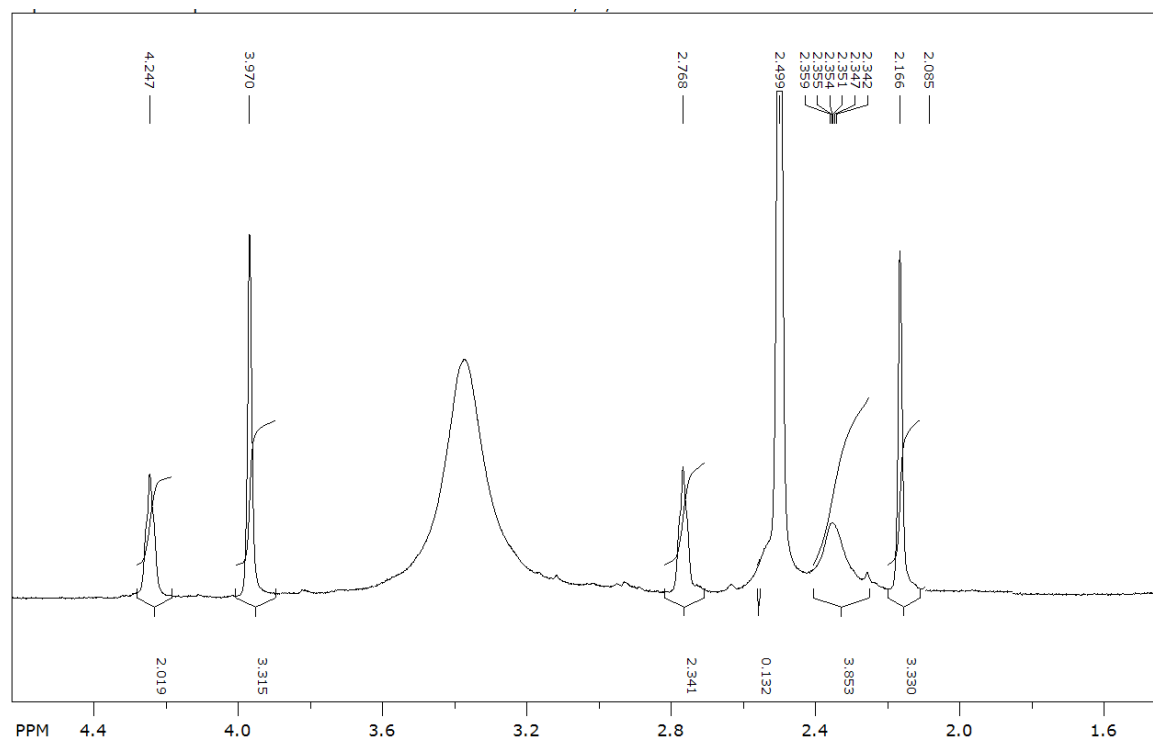


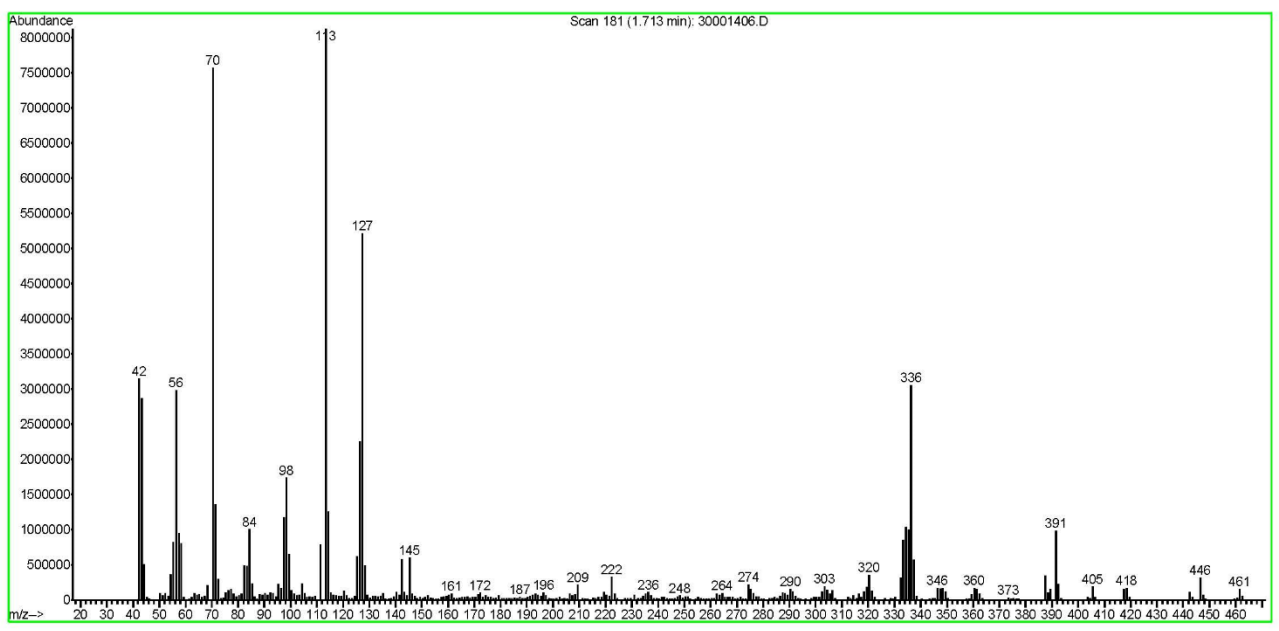
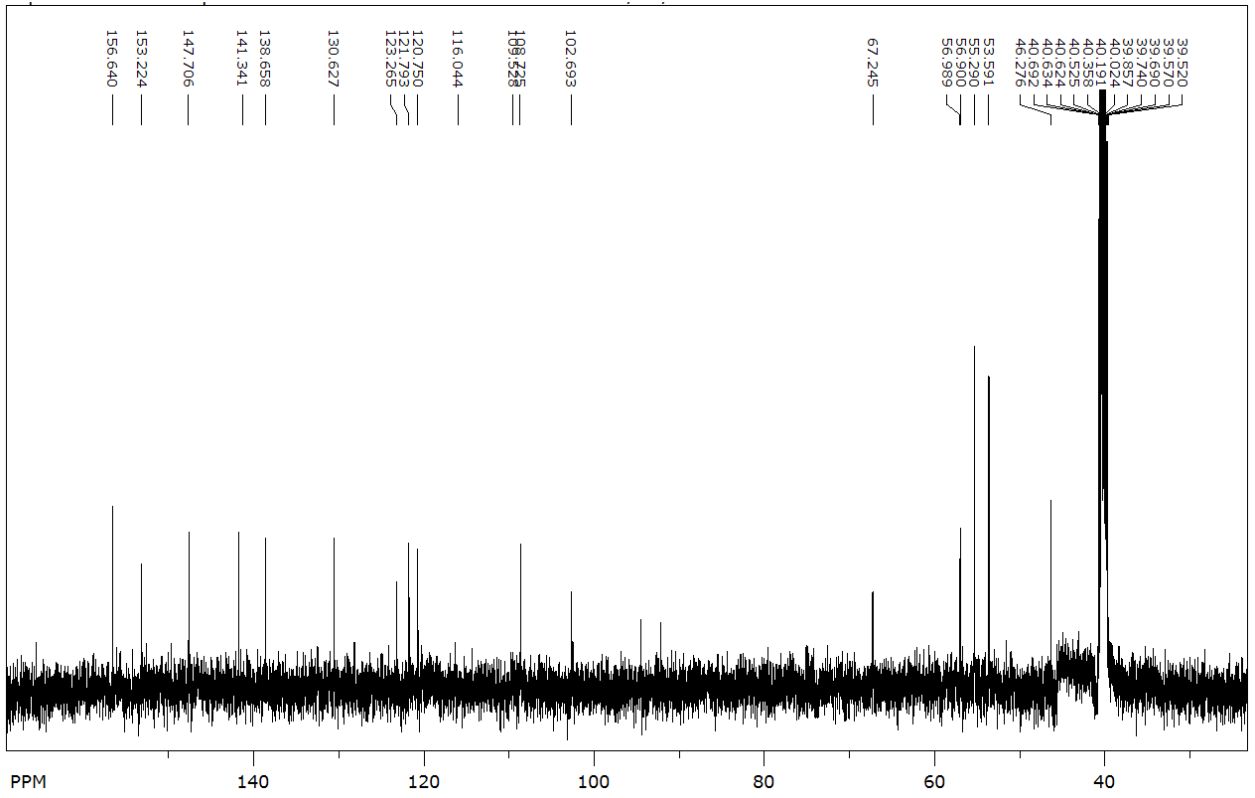


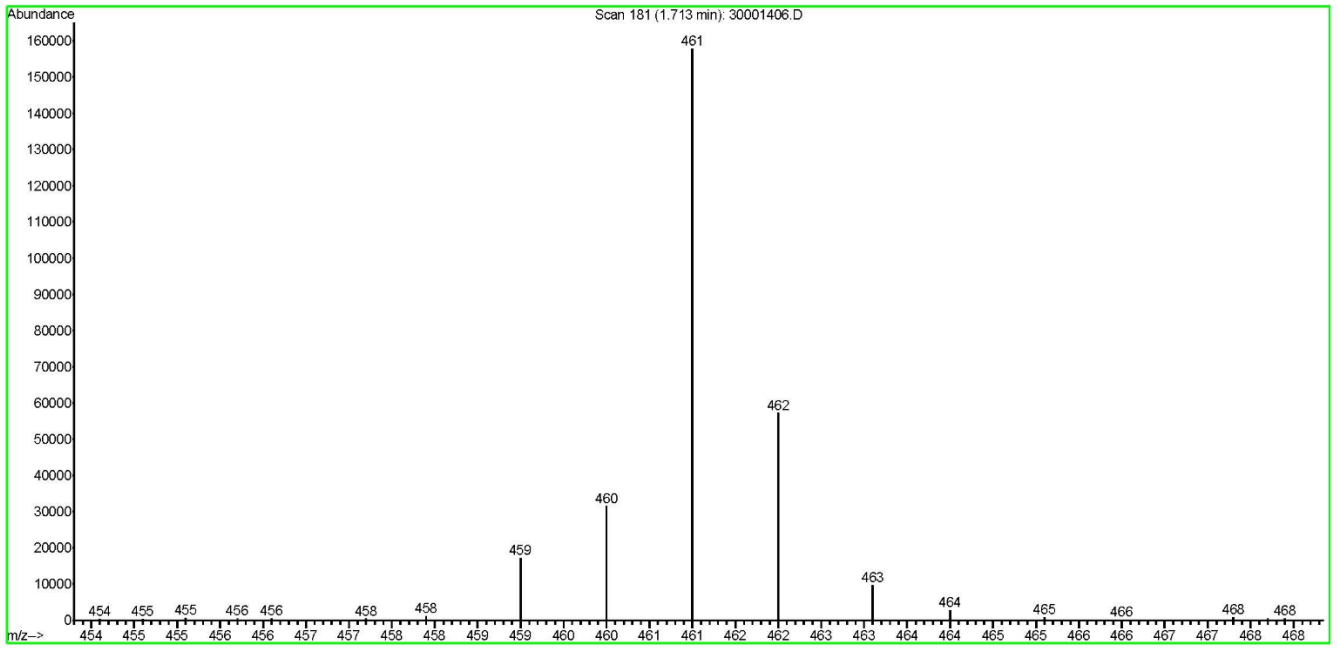
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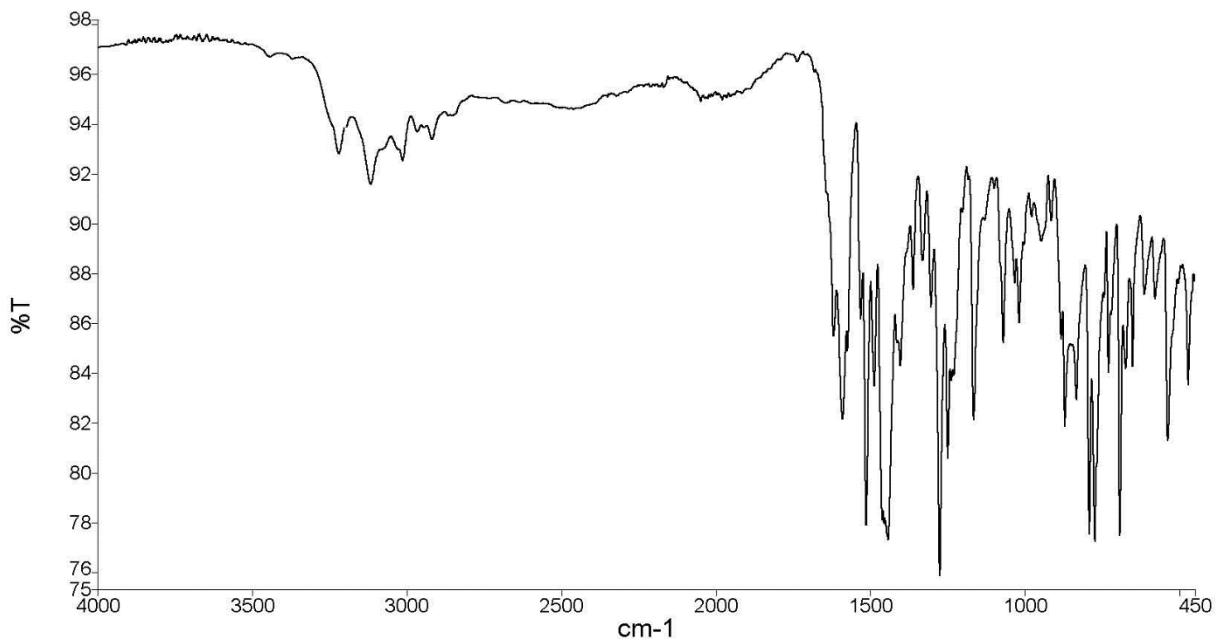


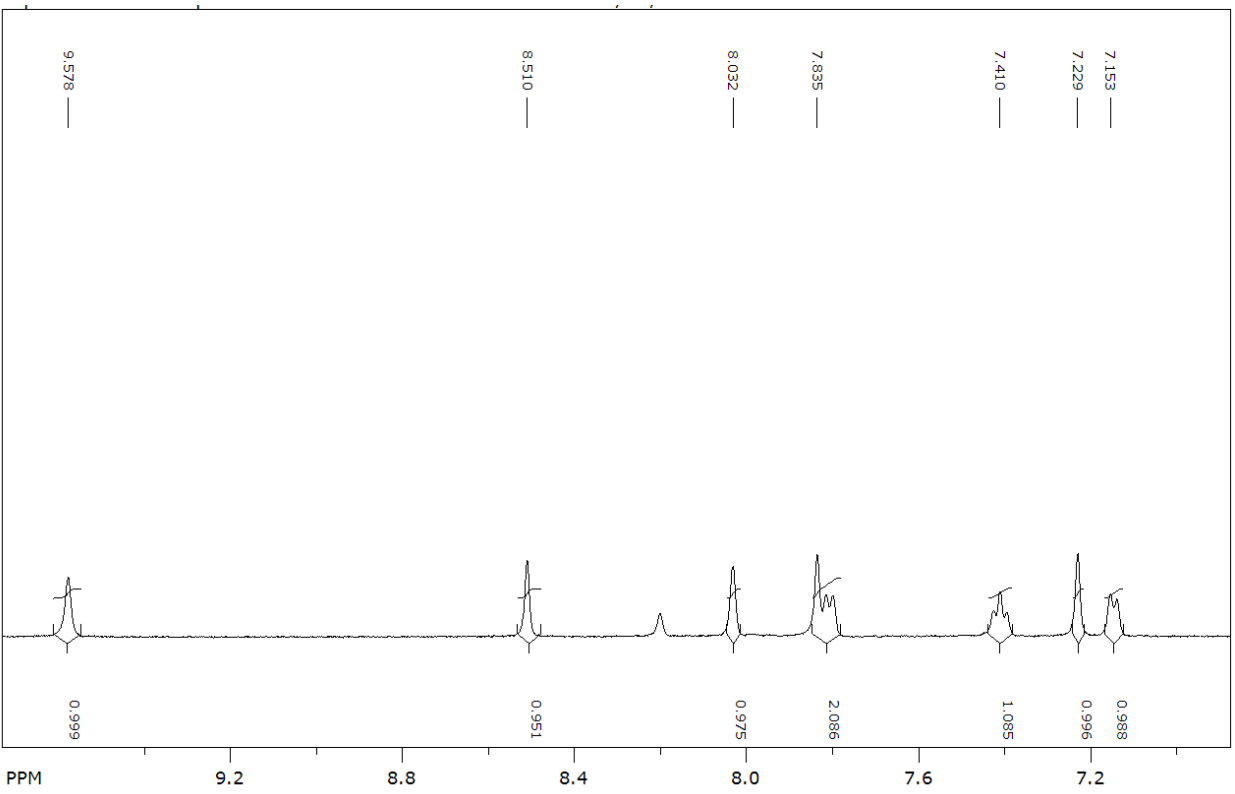
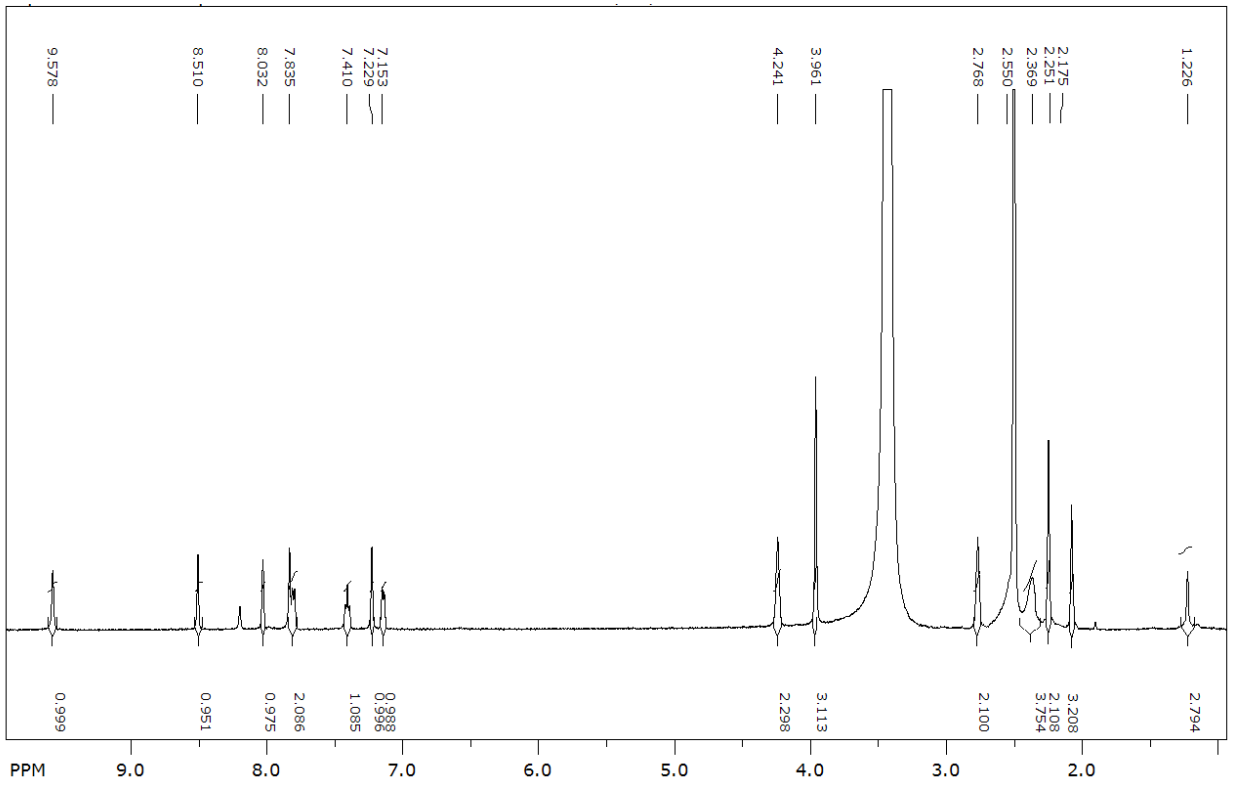


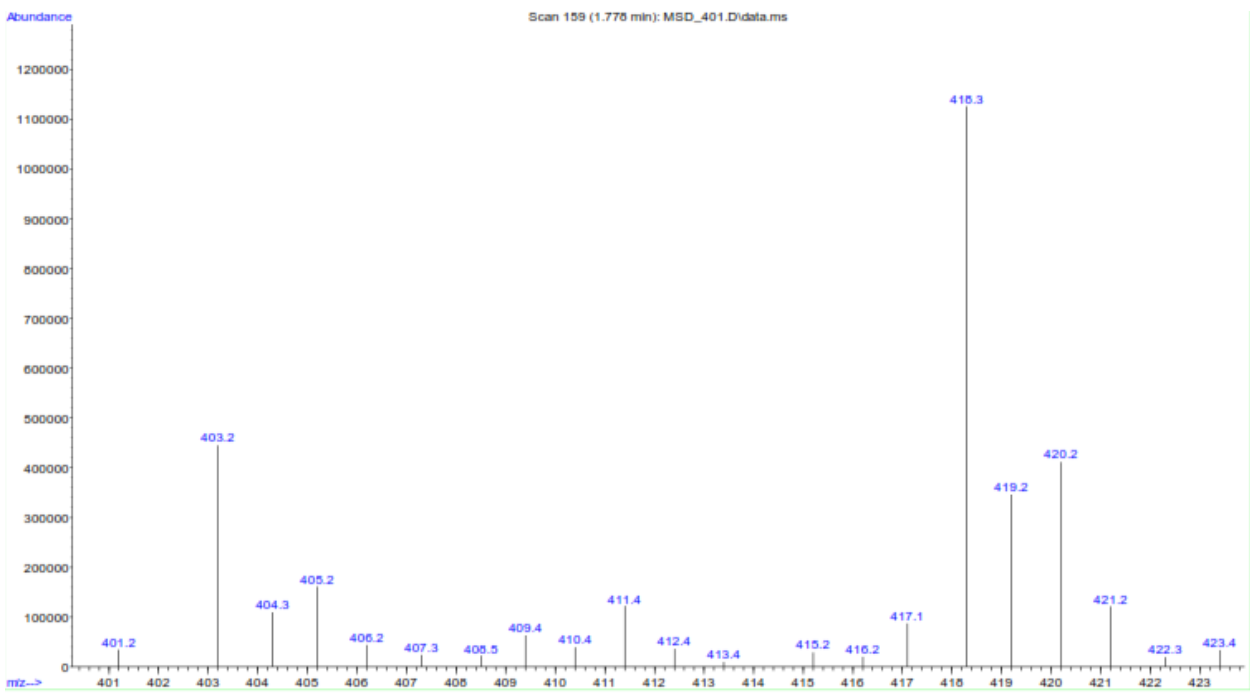
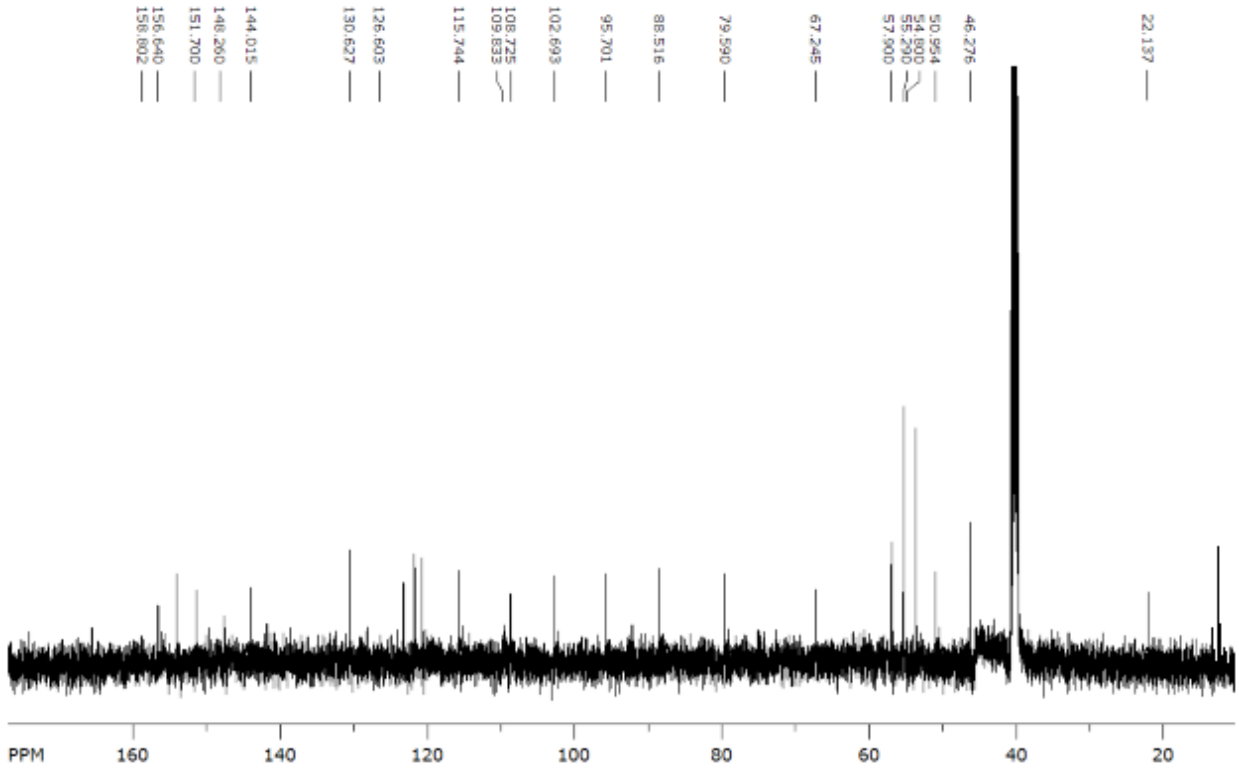




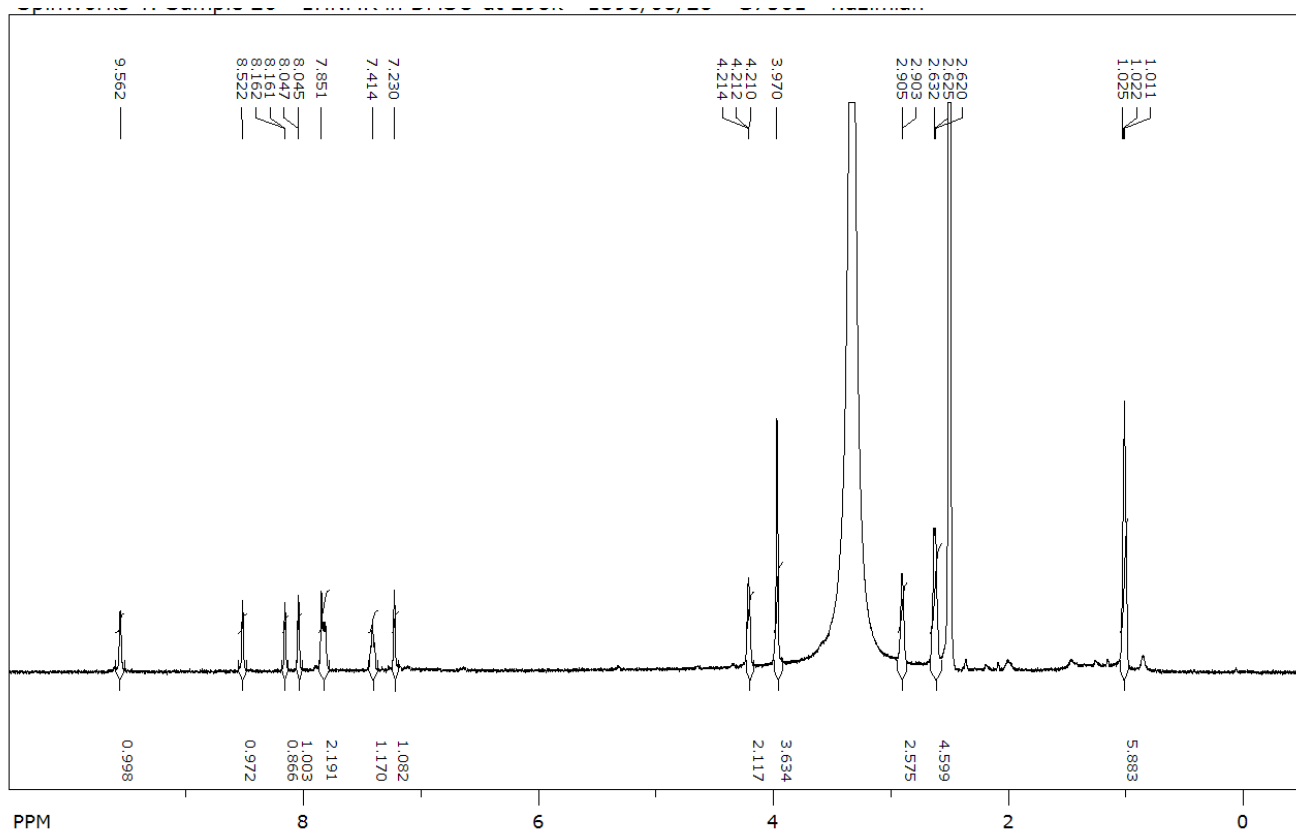
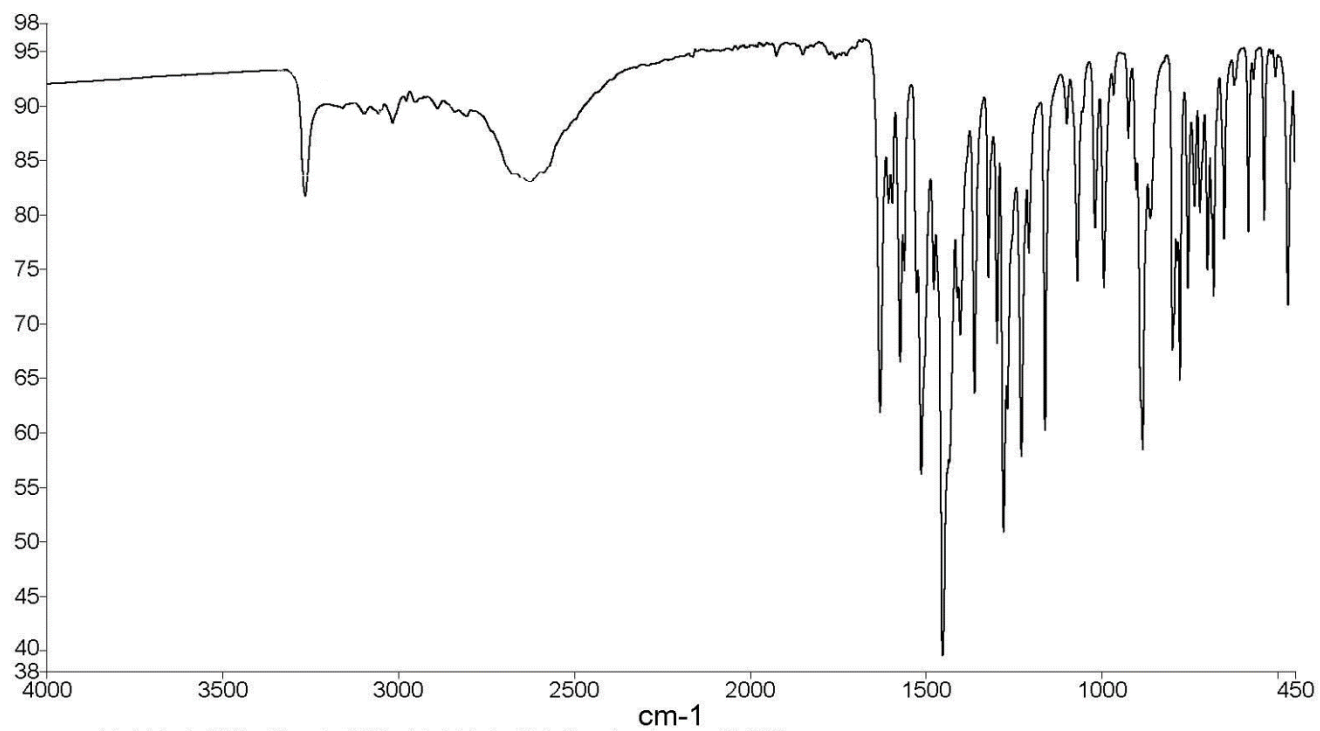
7-(2-(4-methylpiperazin-1-yl)ethoxy)-N-(3-ethylphenyl)-6-methoxyquinazolin-4-amine (8h)

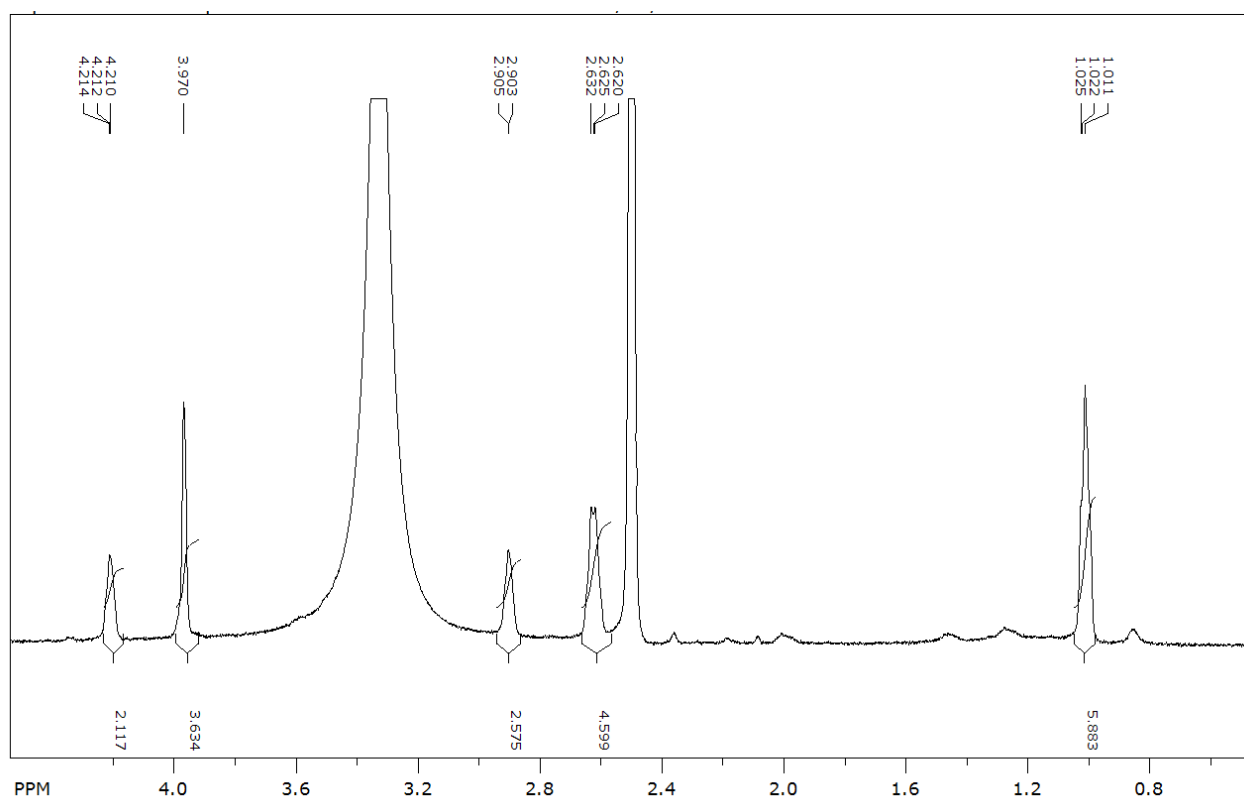
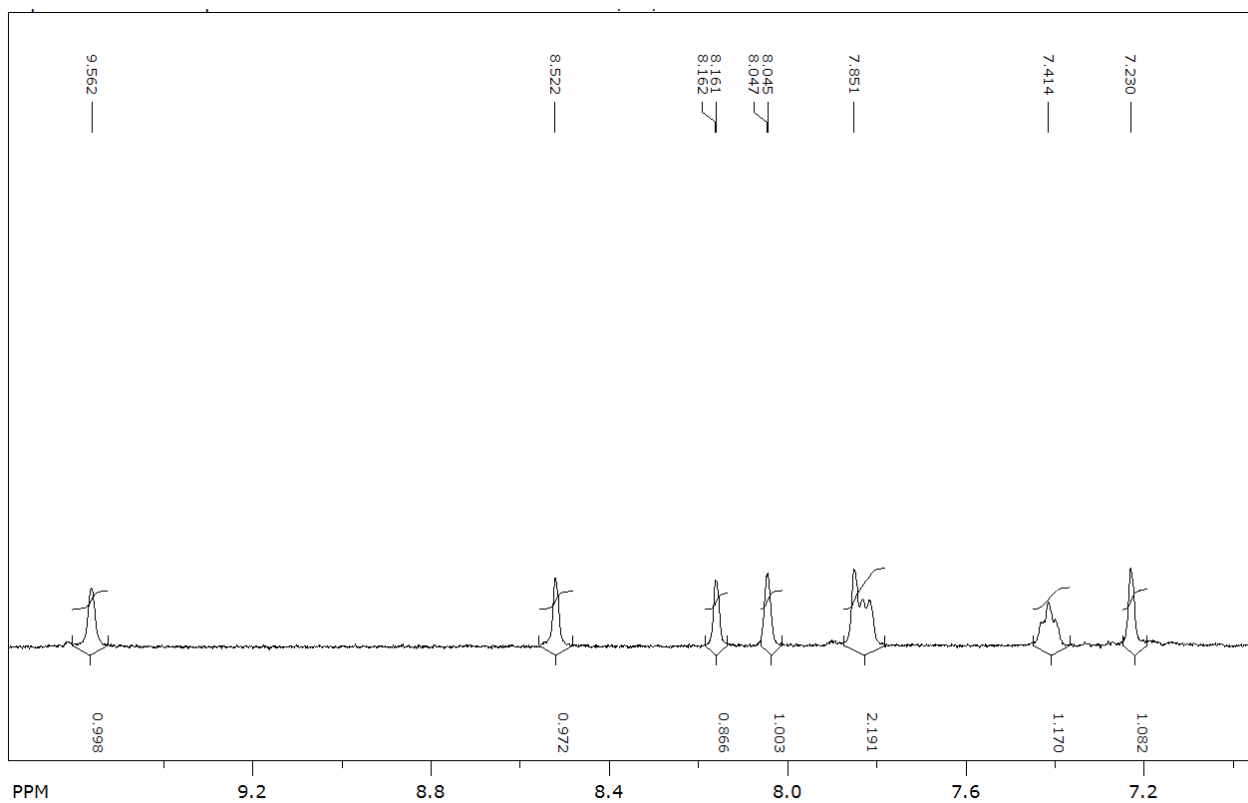


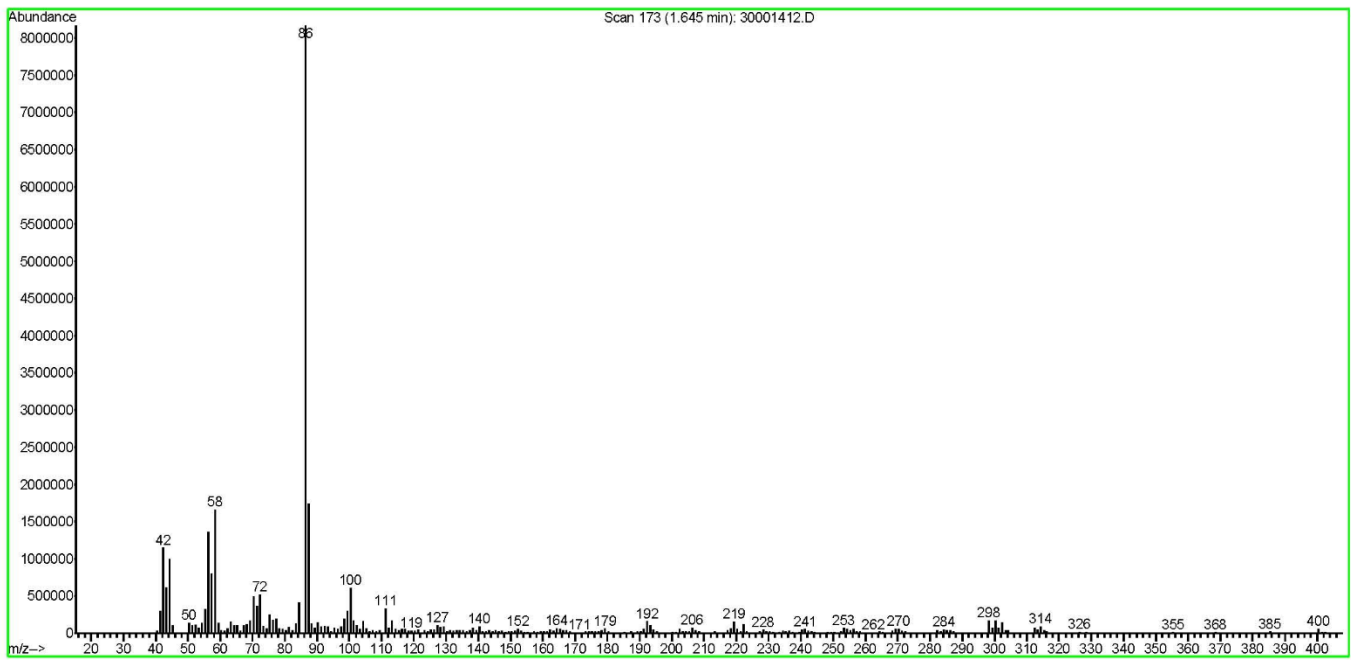
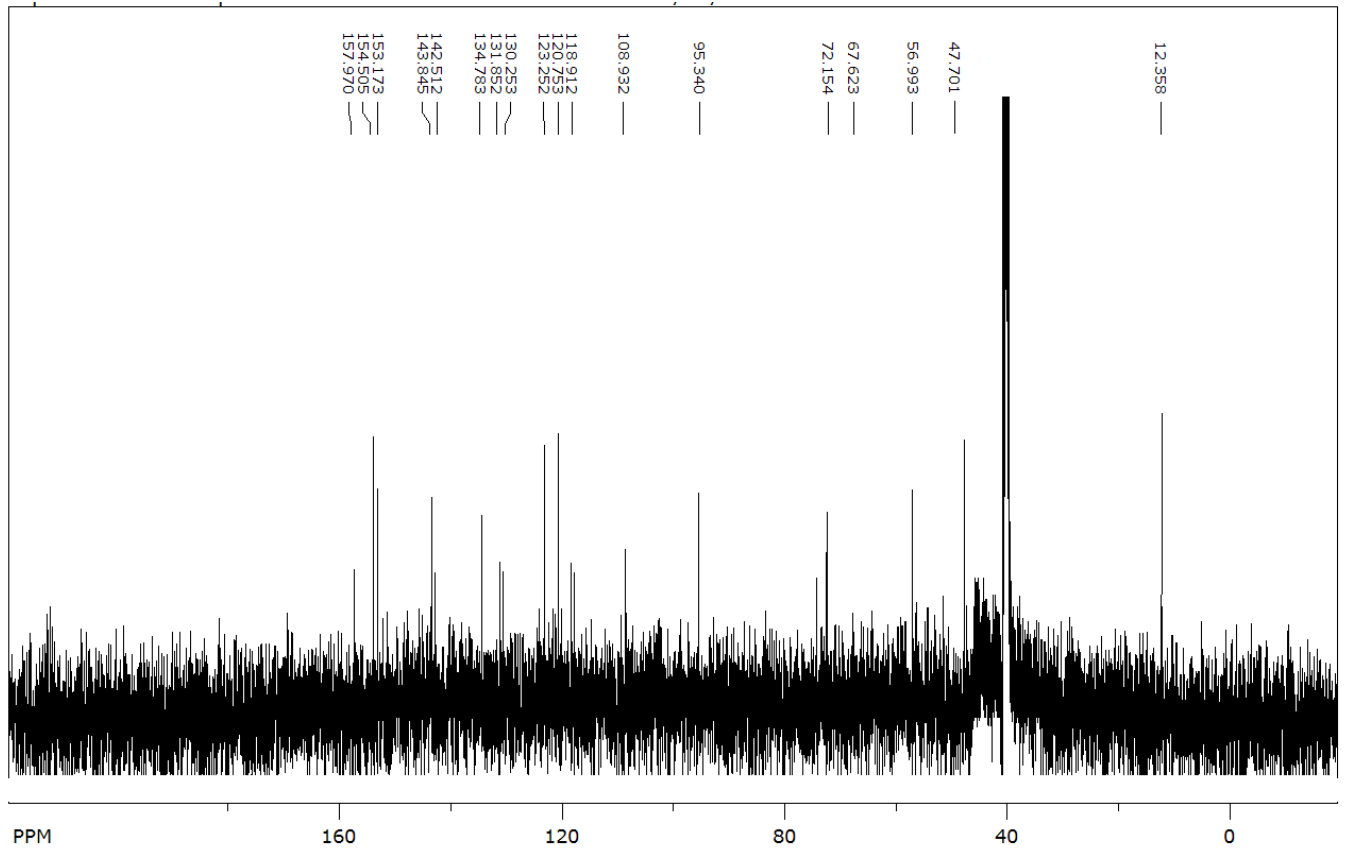


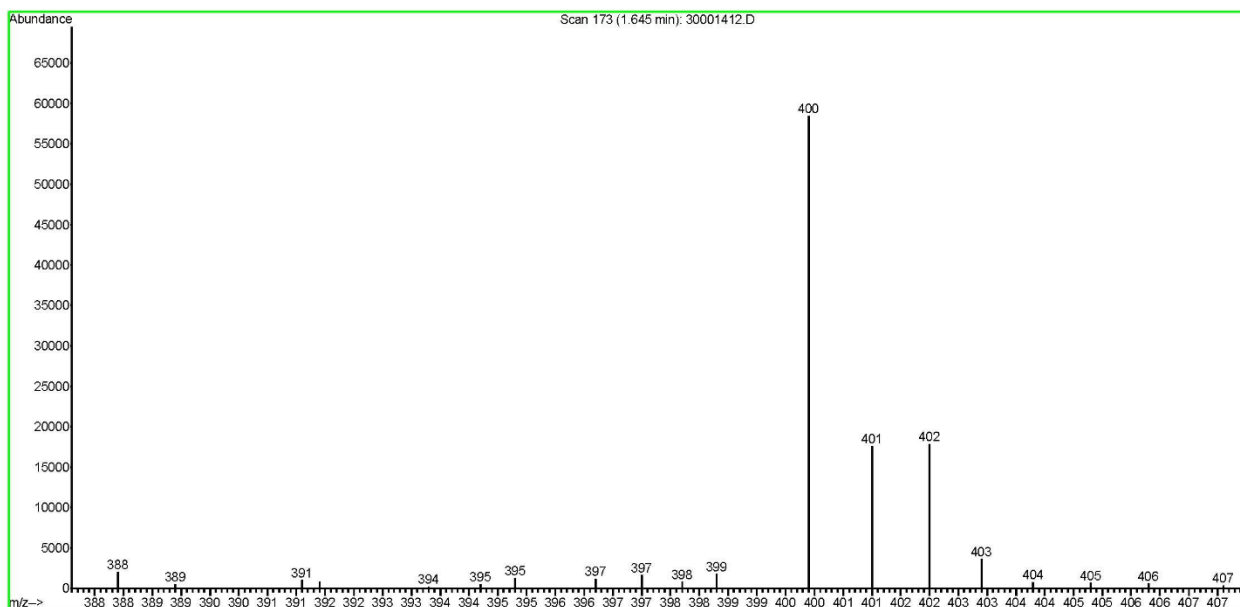


7-(2-(diethylamino)ethoxy)-N-(3-chlorophenyl)-6-methoxyquinazolin-4-amine (8i)

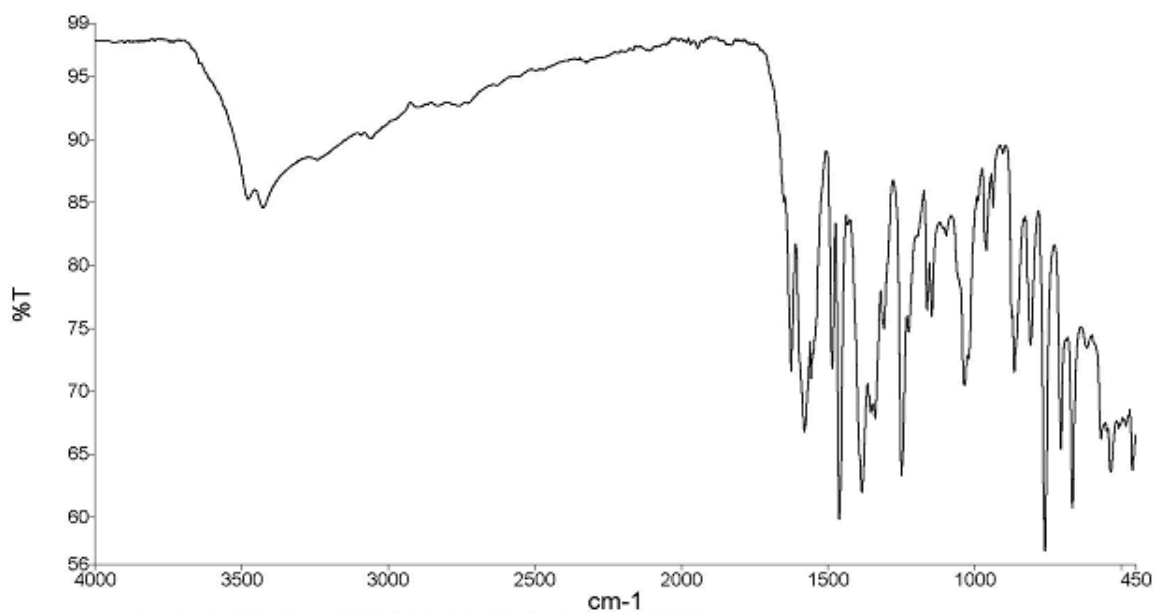


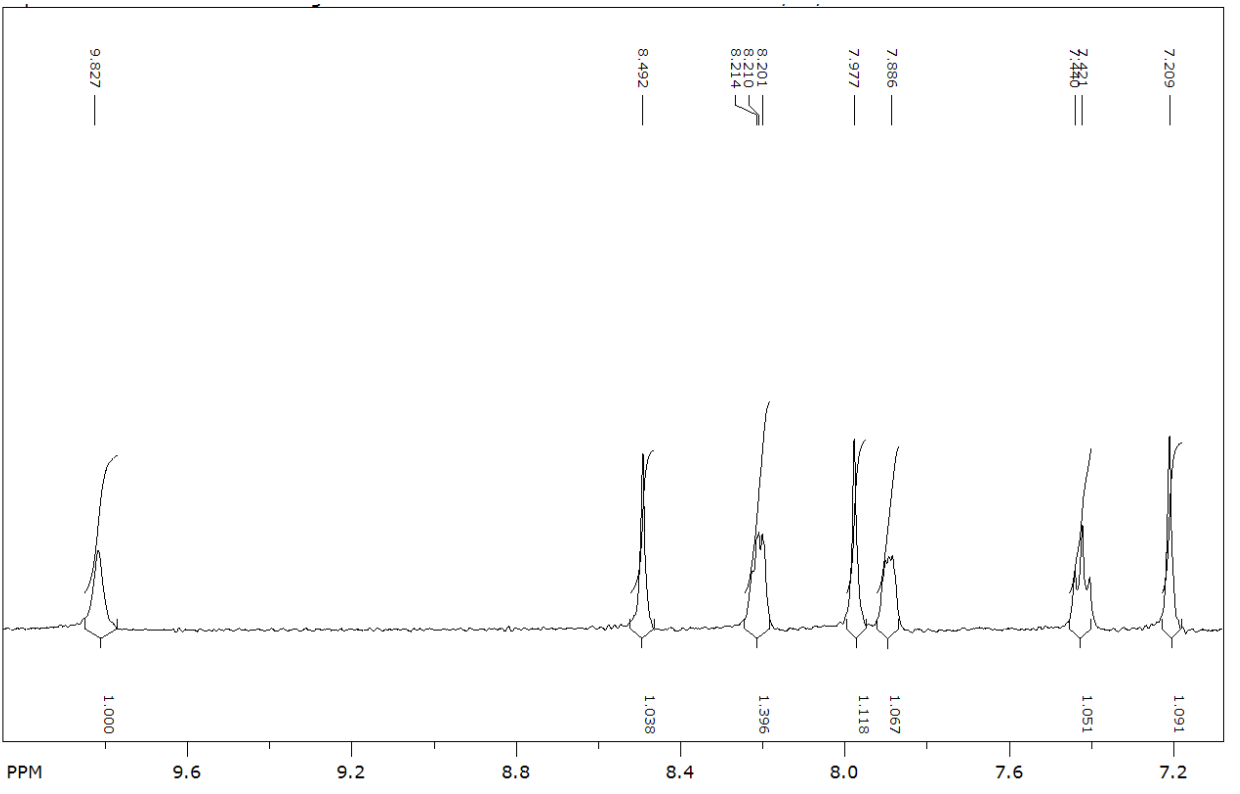
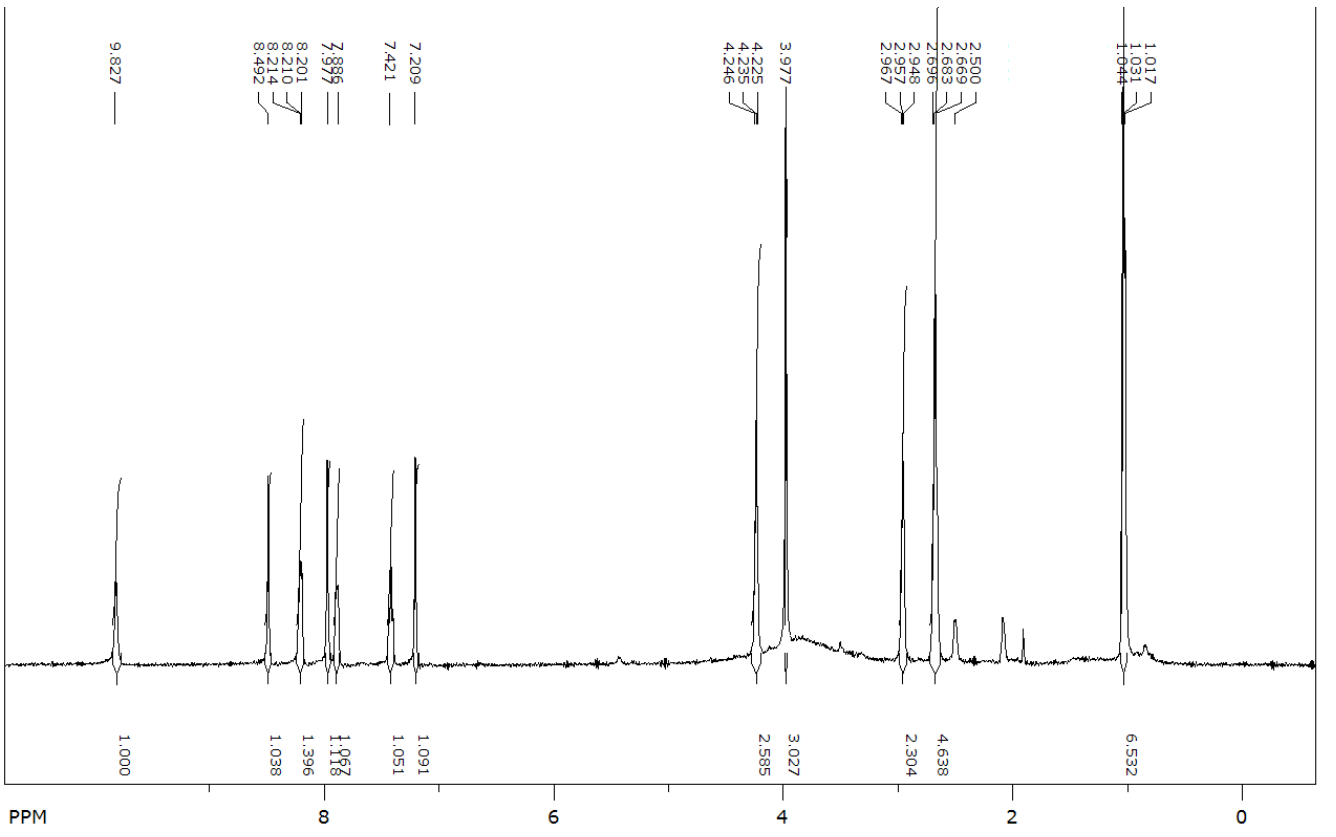


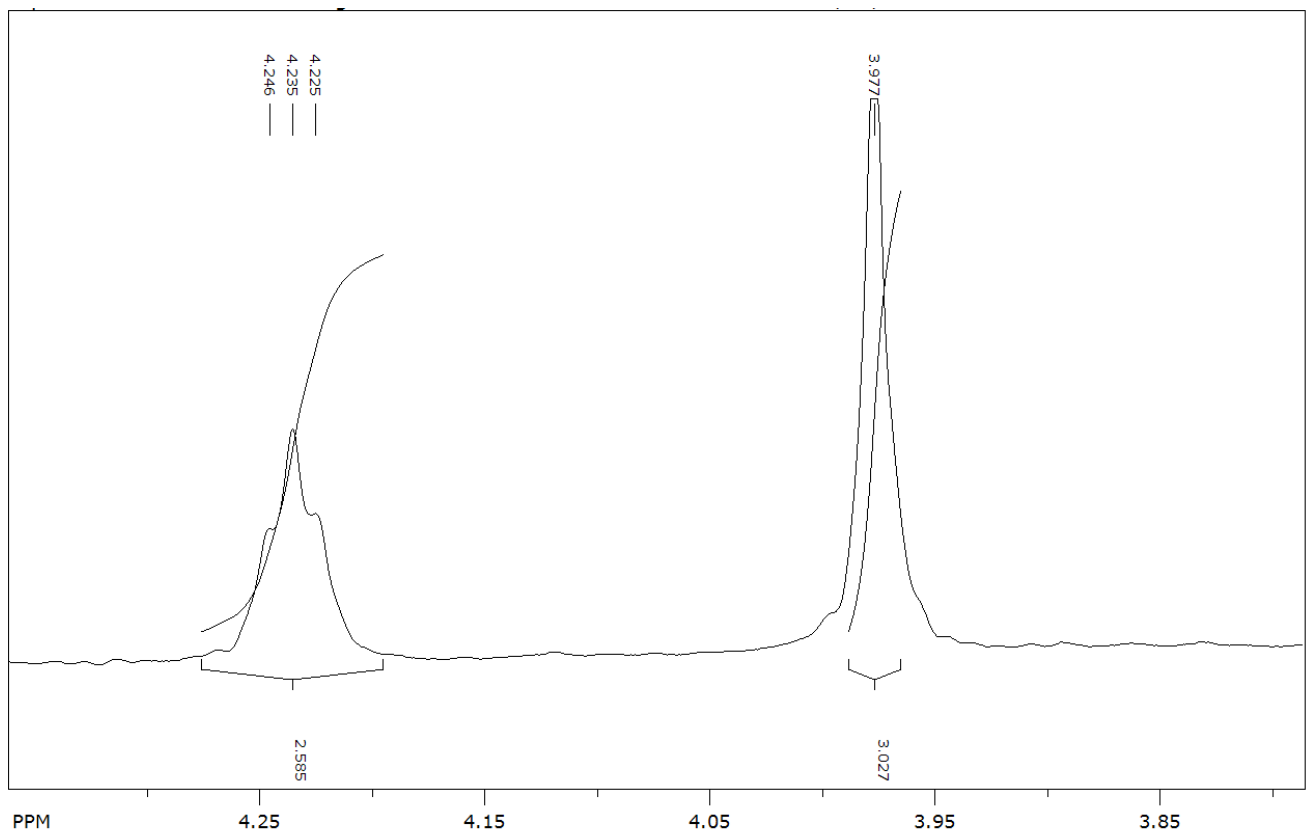
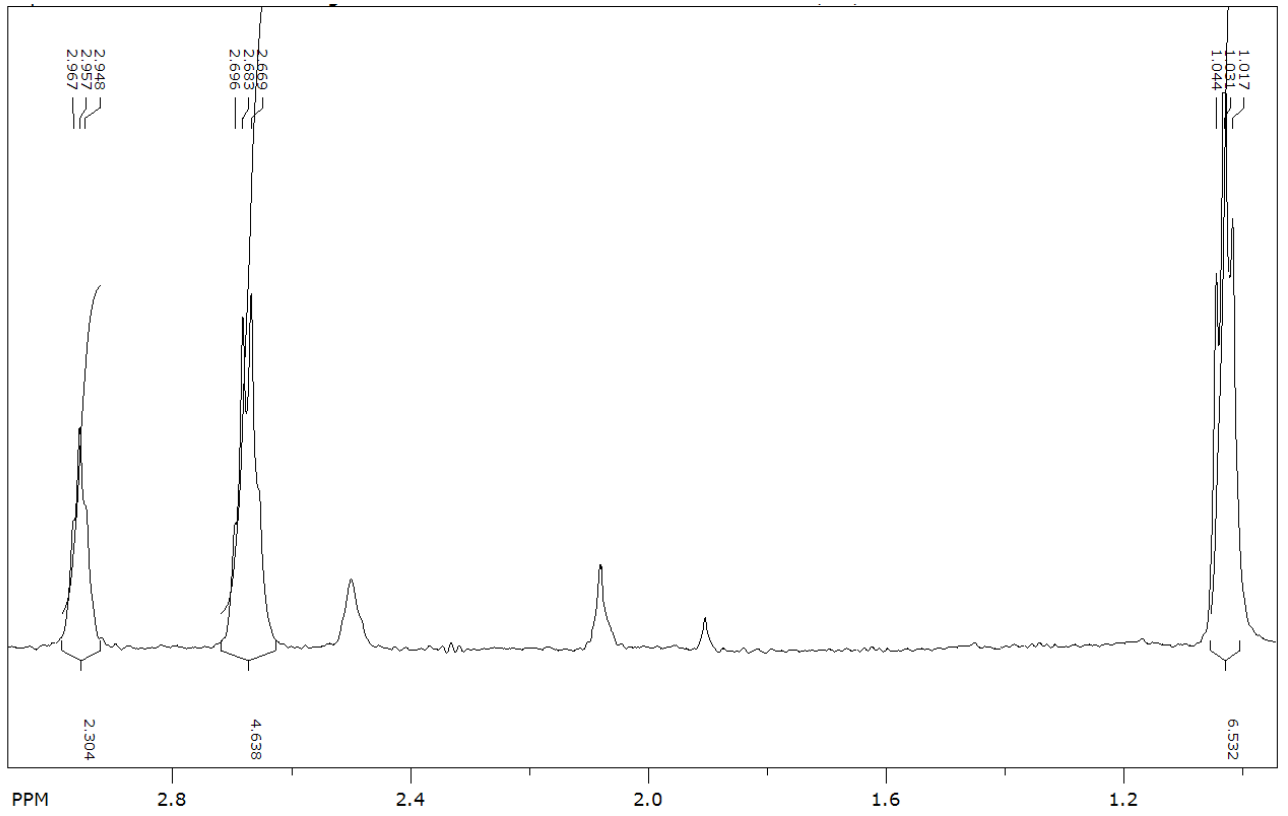


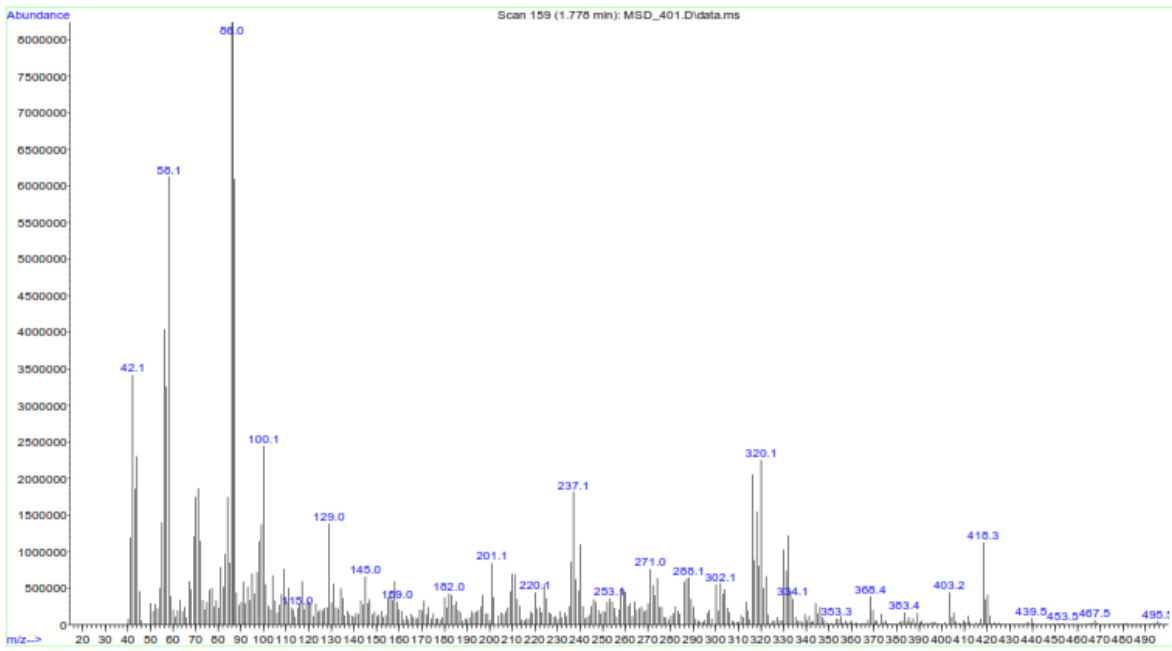
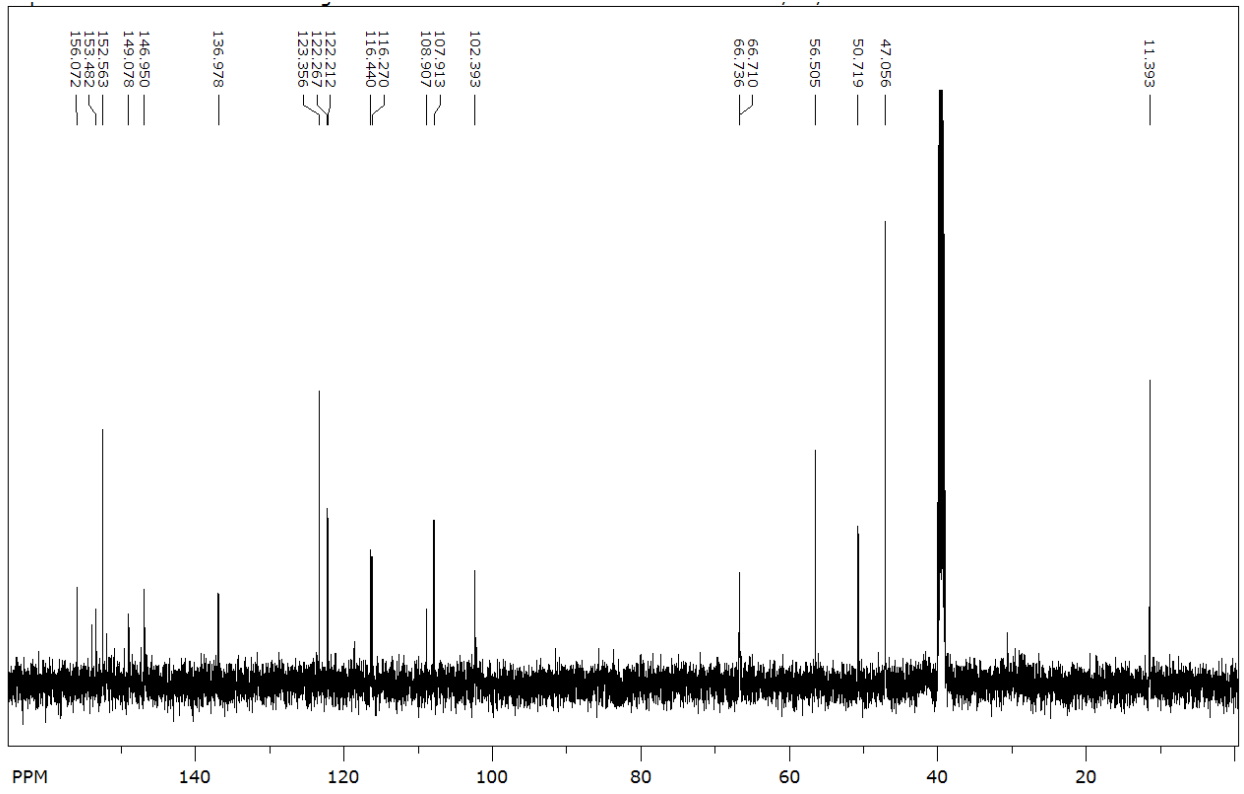


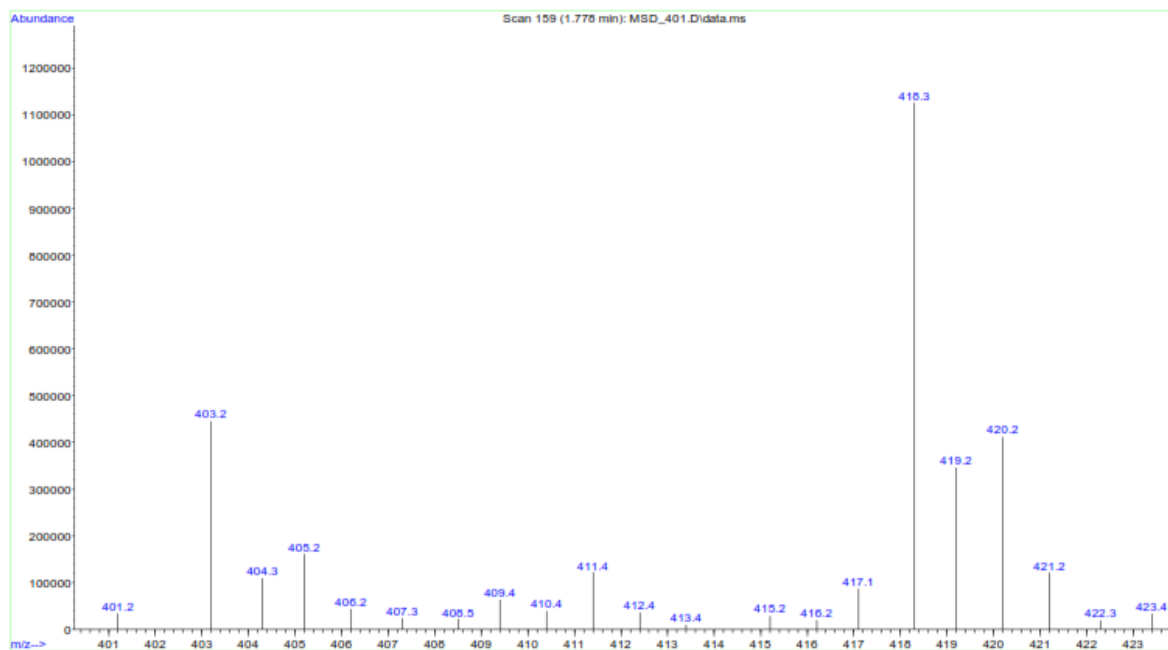
7-(2-(diethylamino)ethoxy)-N-(3-chloro-4-fluorophenyl)-6-methoxyquinazolin-4-amine (8j)



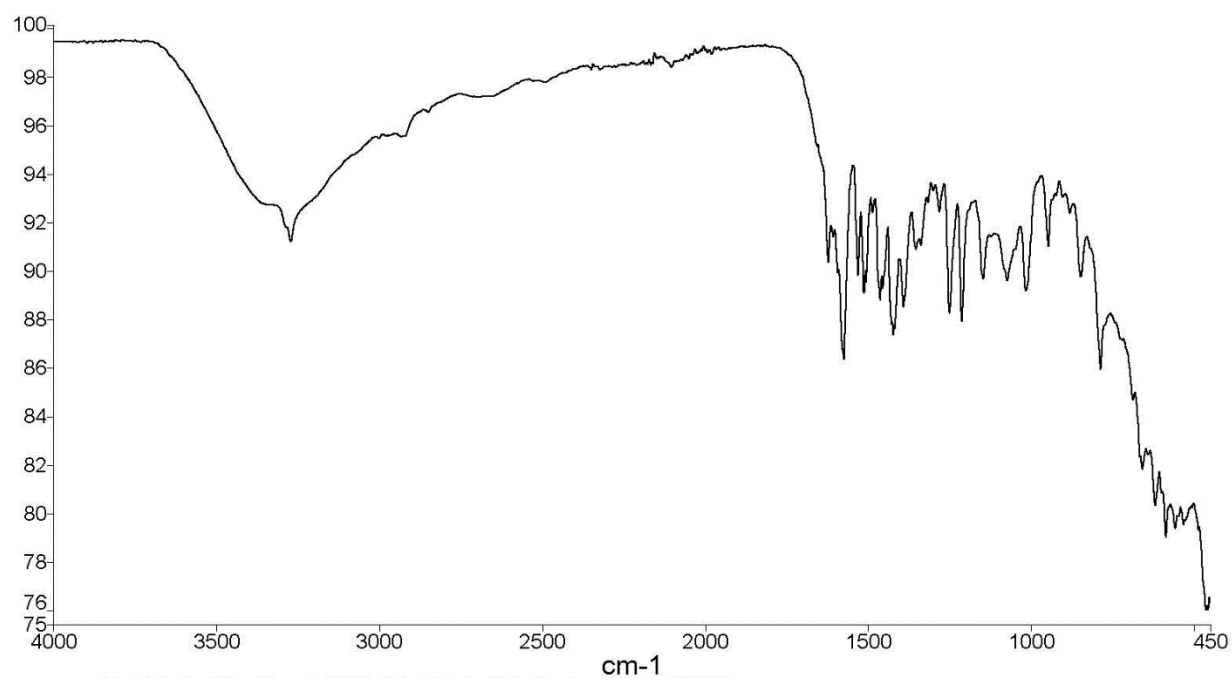


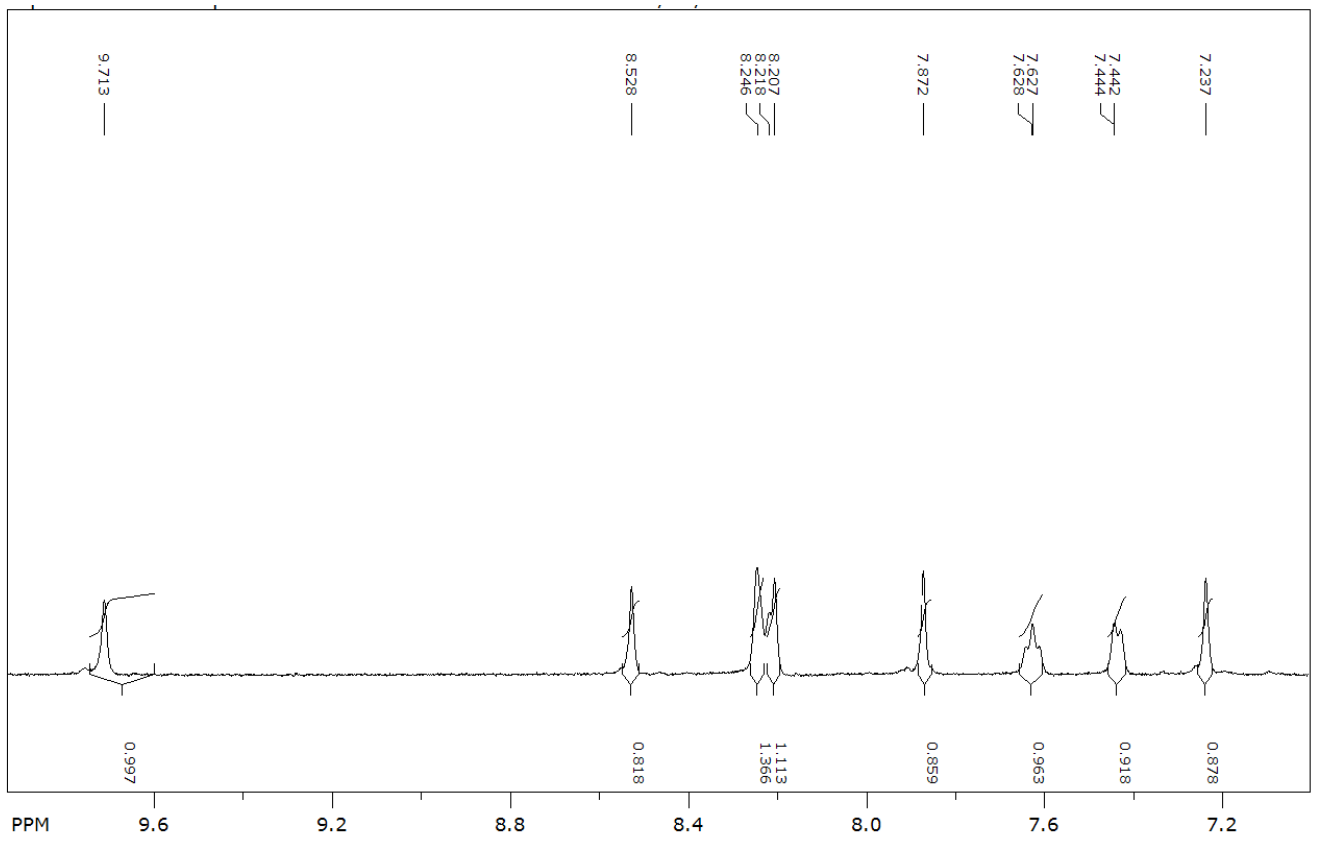
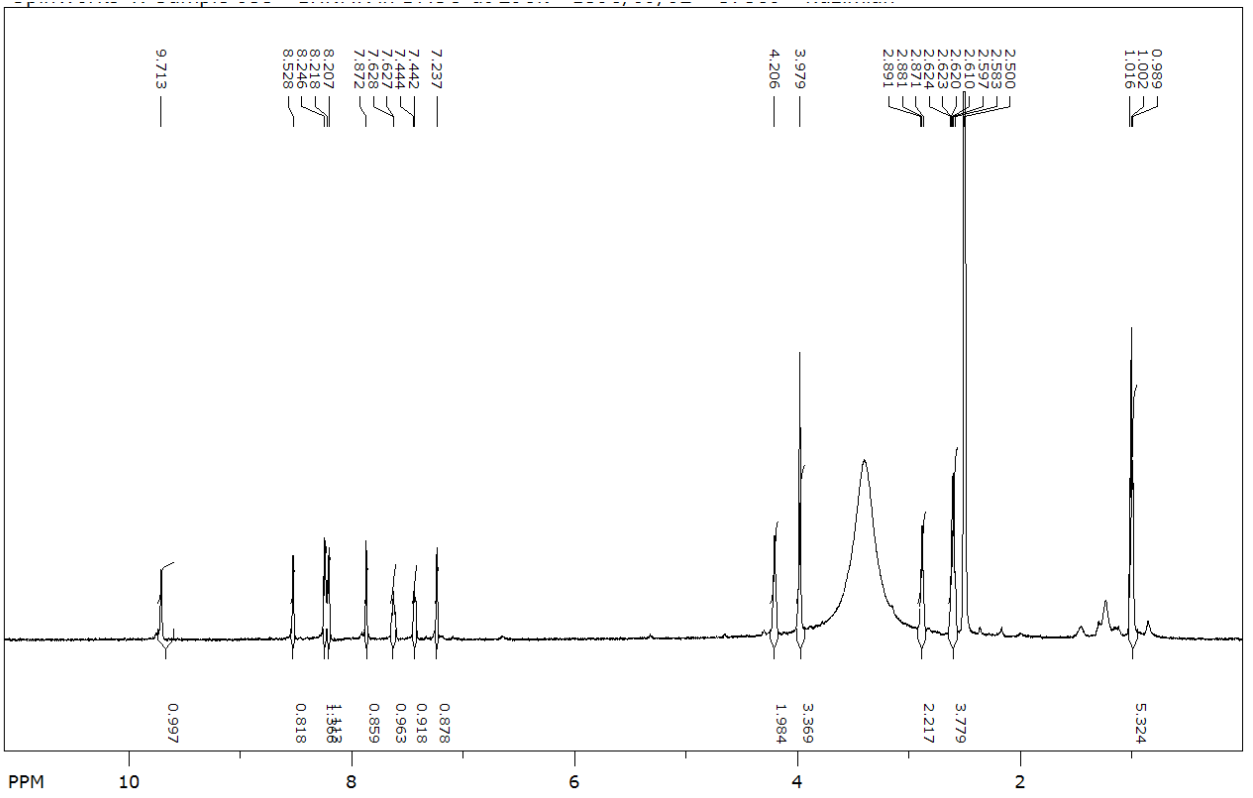


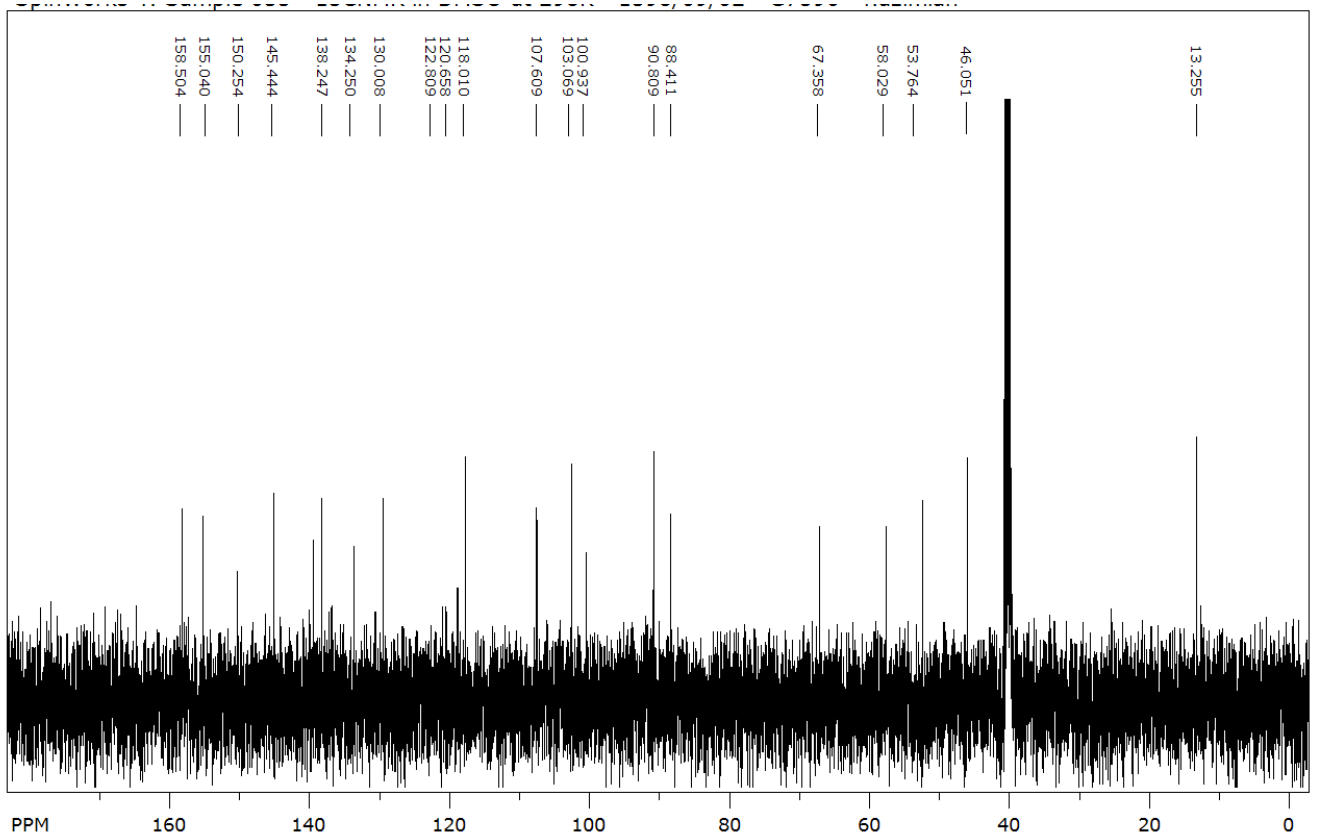
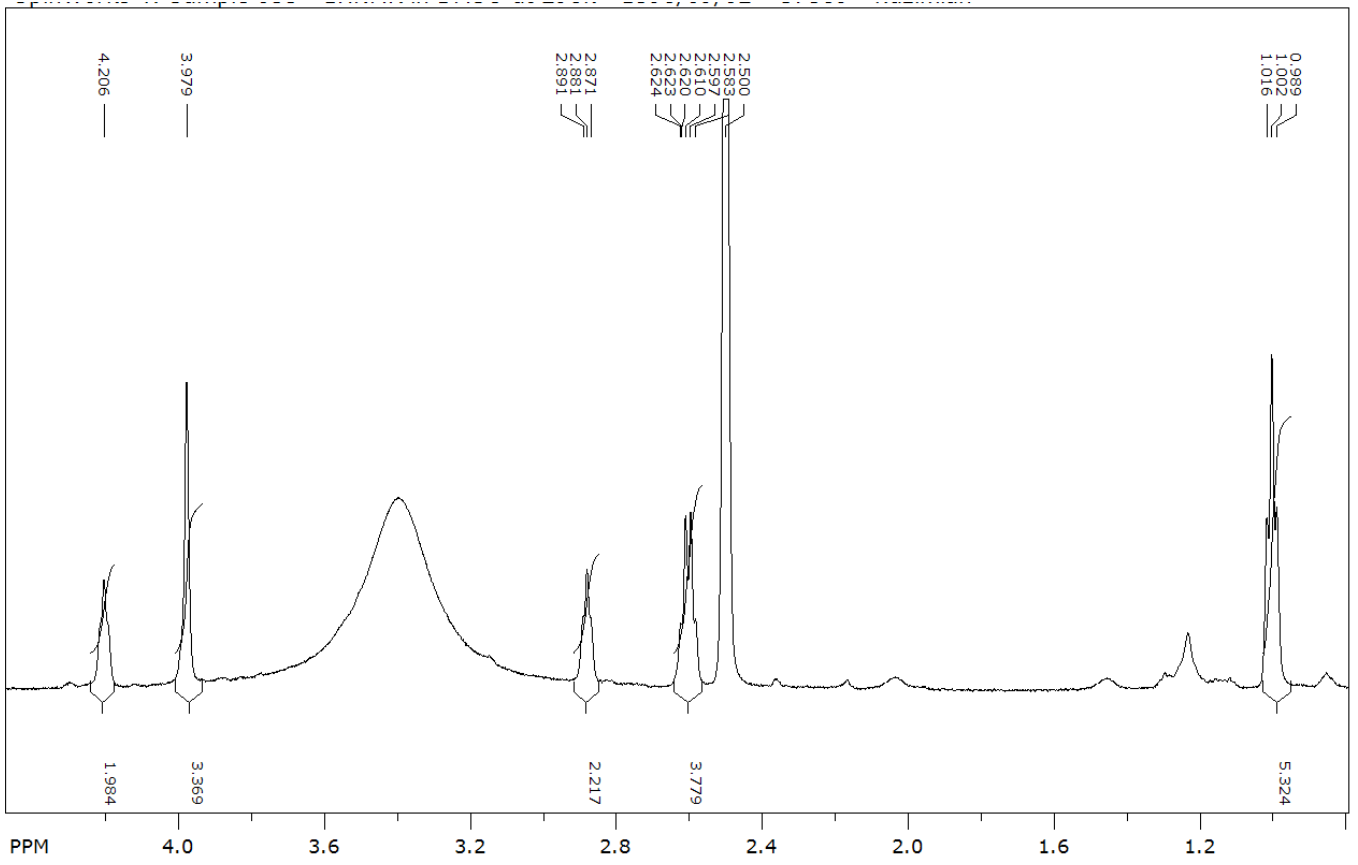


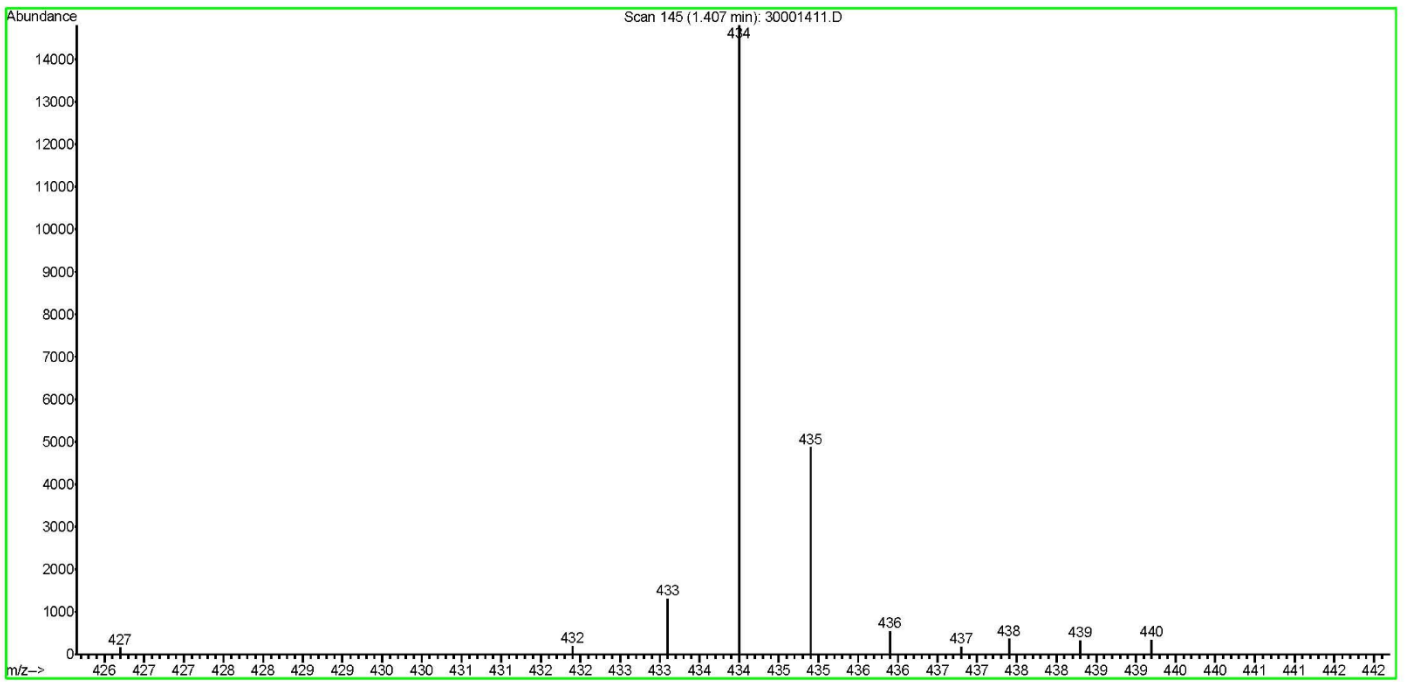
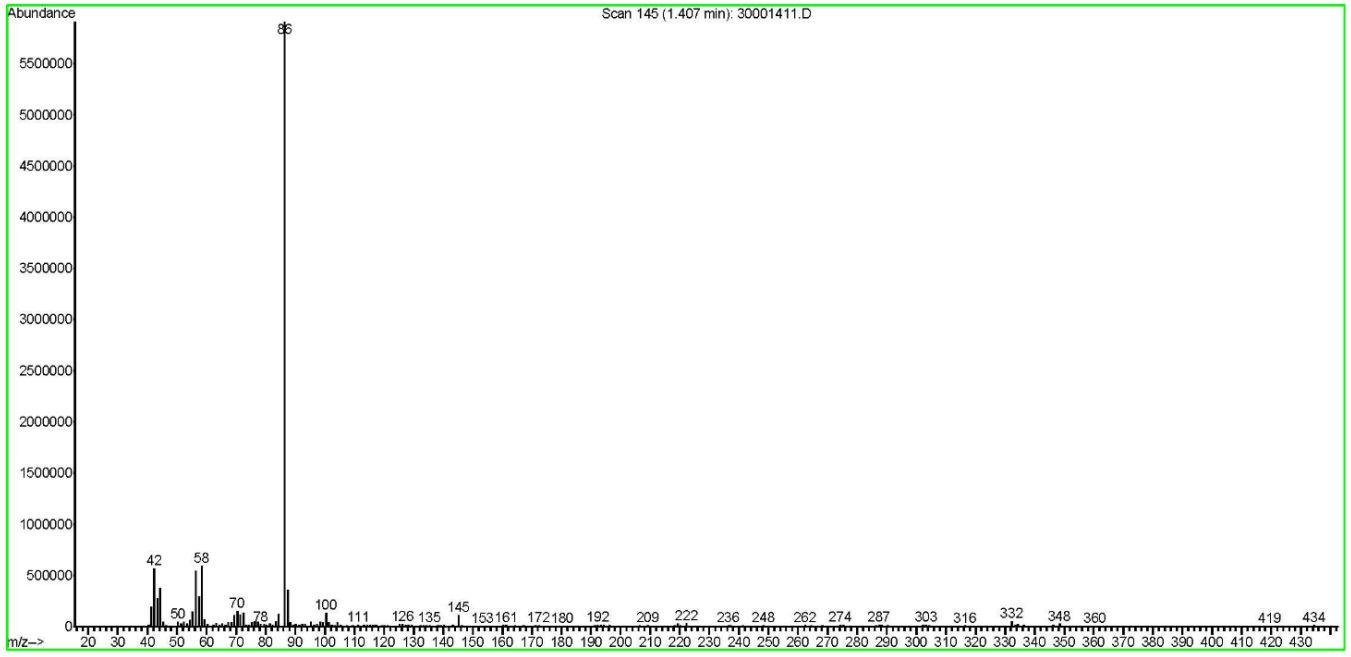


7-(2-(diethylamino)ethoxy)-N-(3-(trifluoromethyl)phenyl)-6-methoxyquinazolin-4-amine (8k)

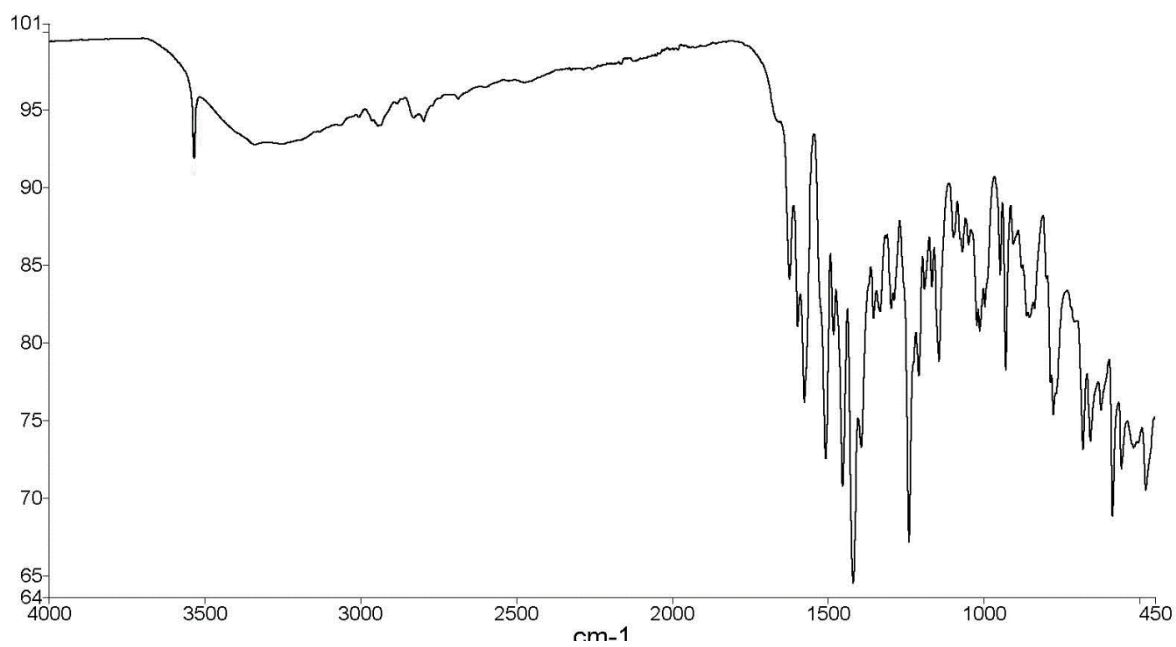


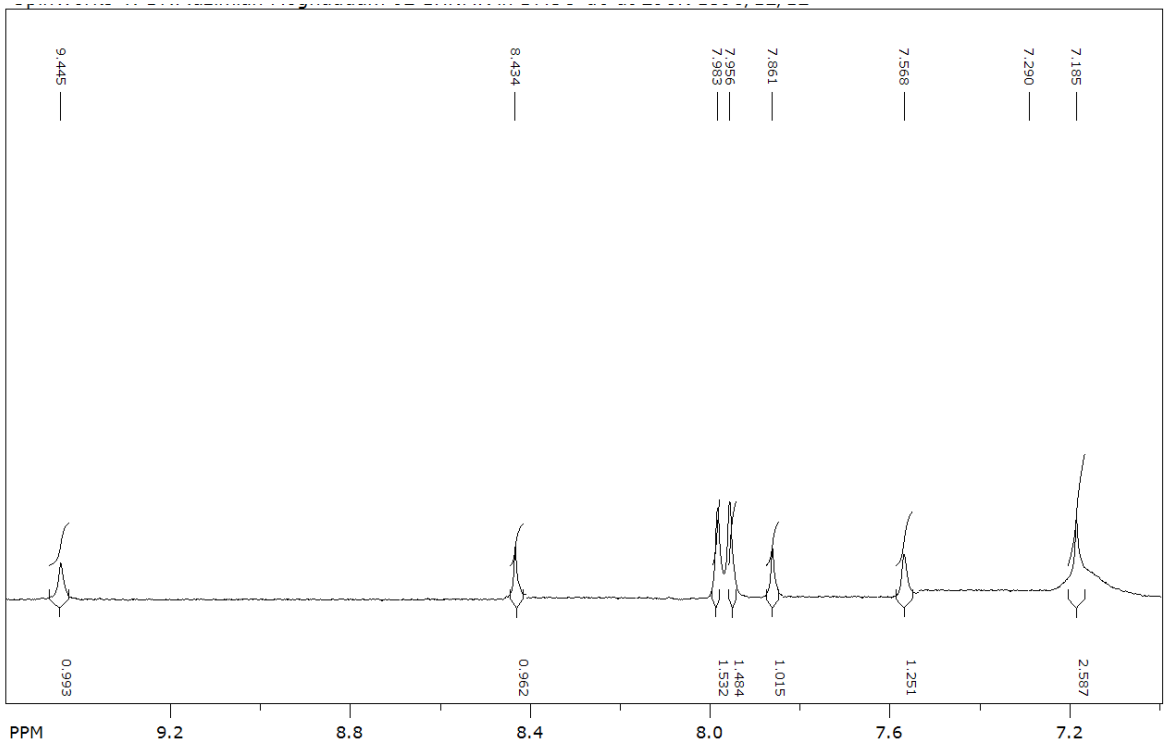
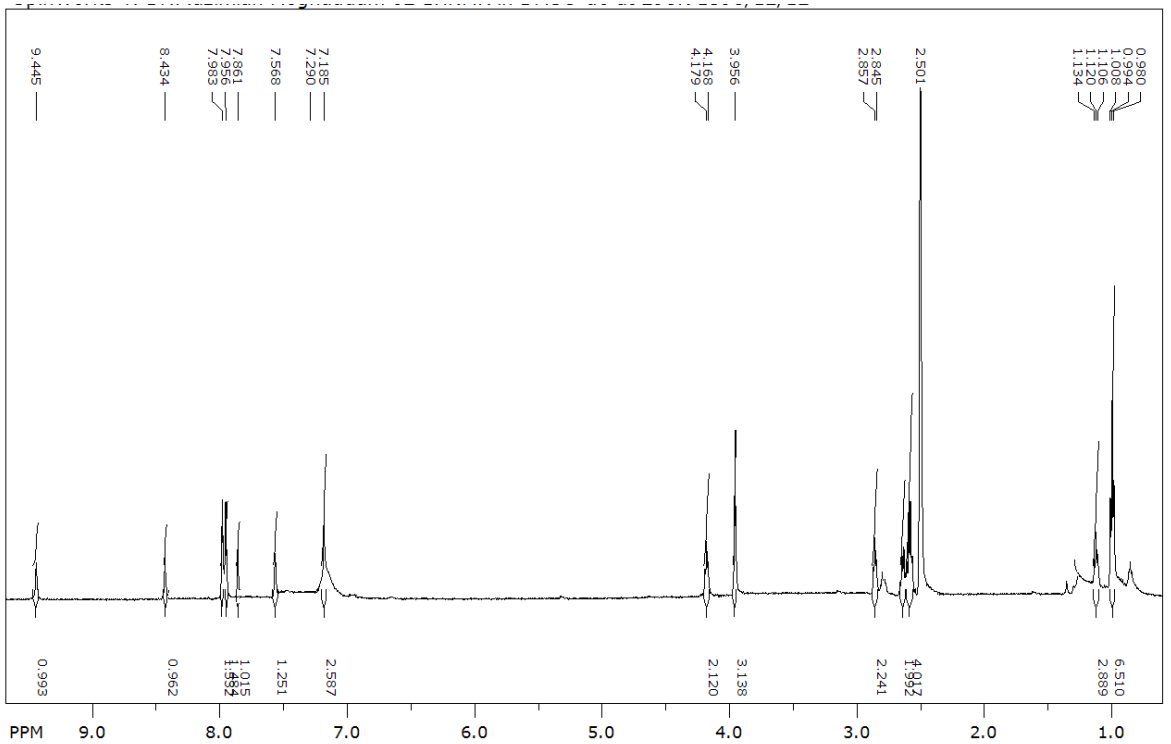


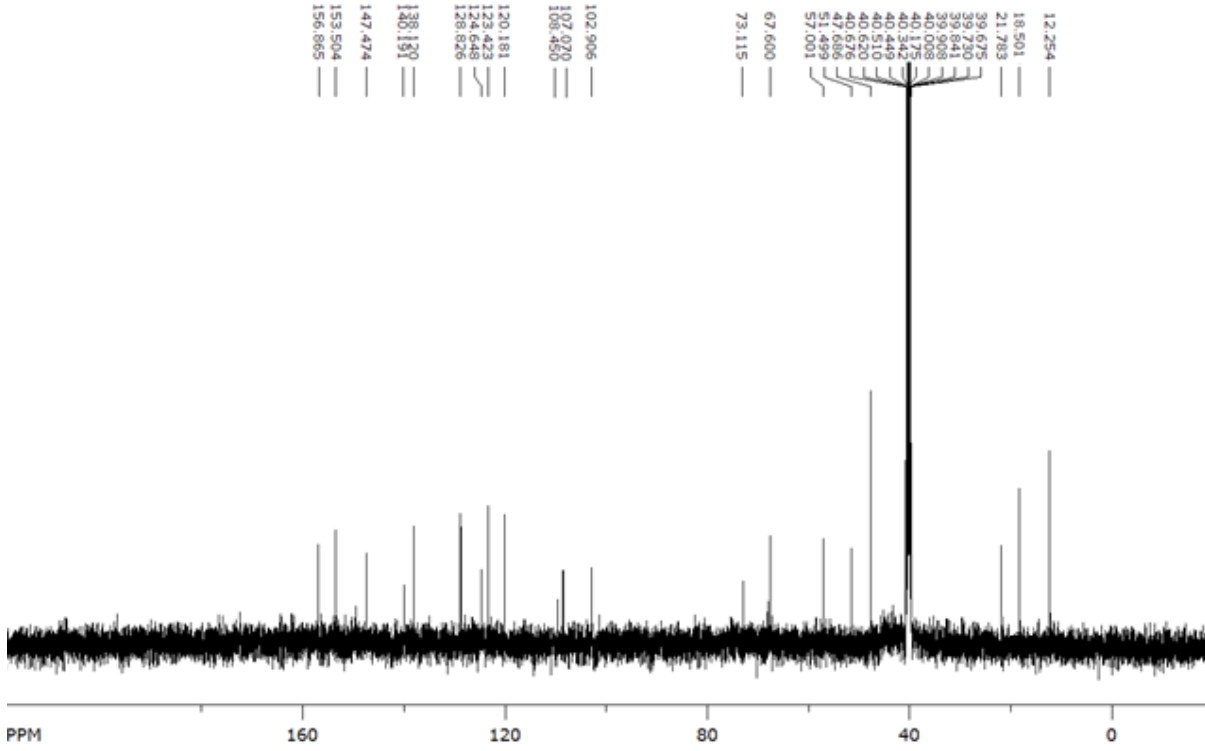
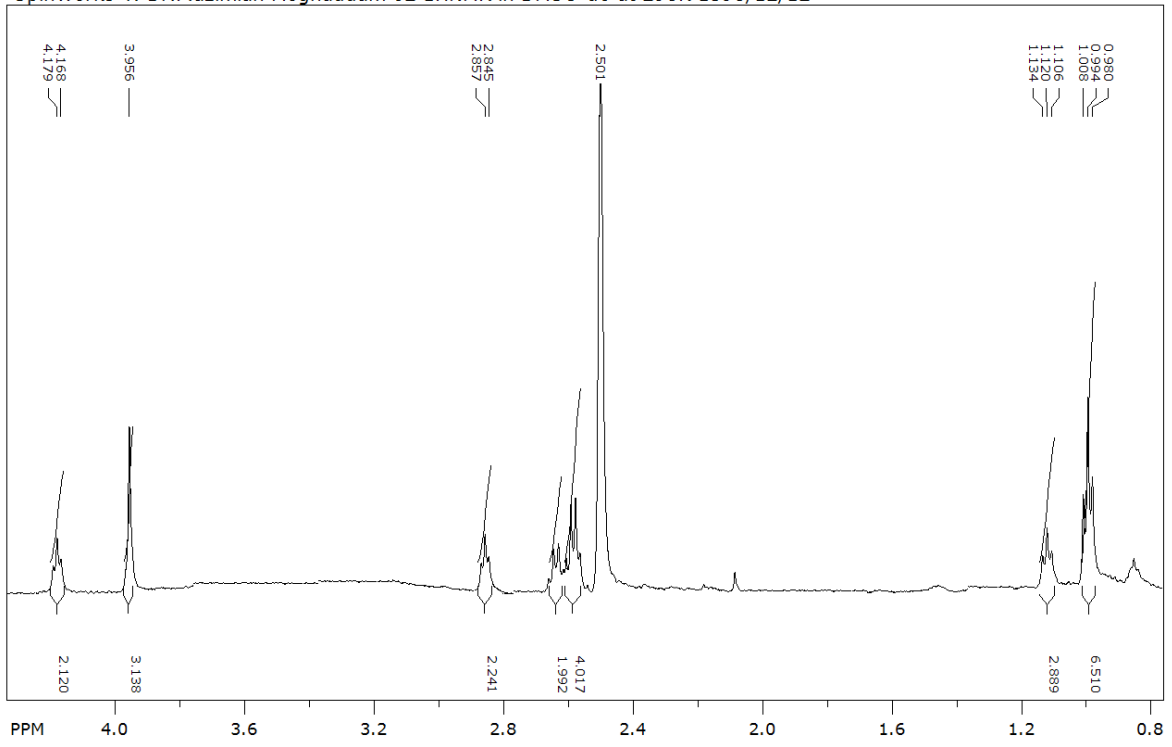


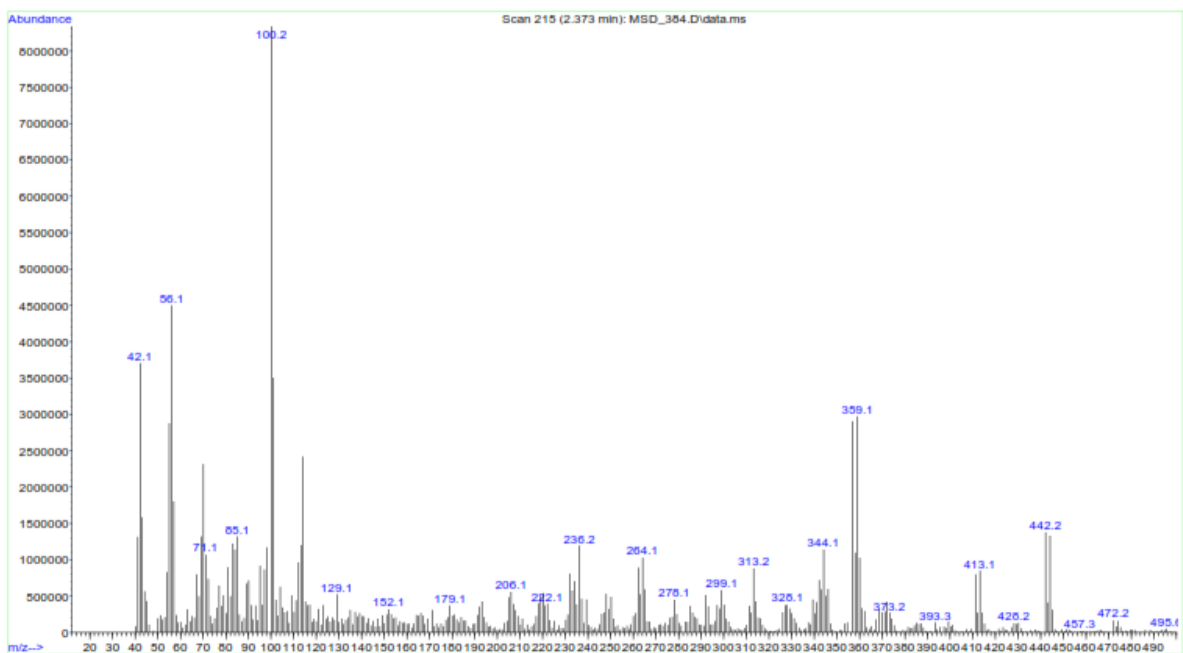


7-(2-(diethylamino)ethoxy)-N-(3-ethylphenyl)-6-methoxyquinazolin-4-amine (8I)

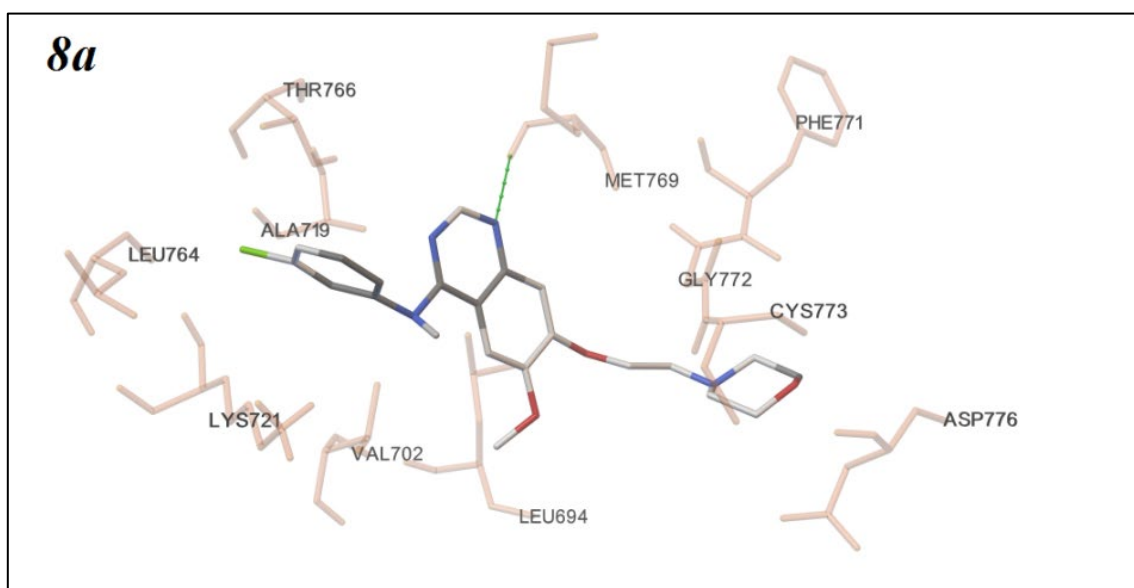




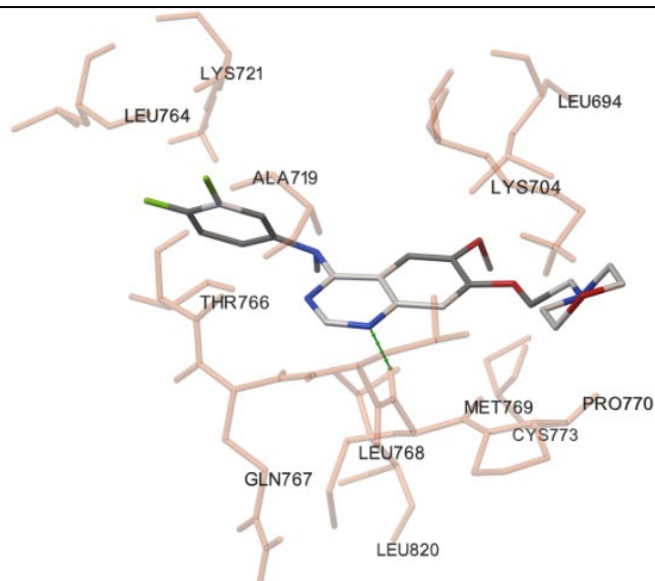




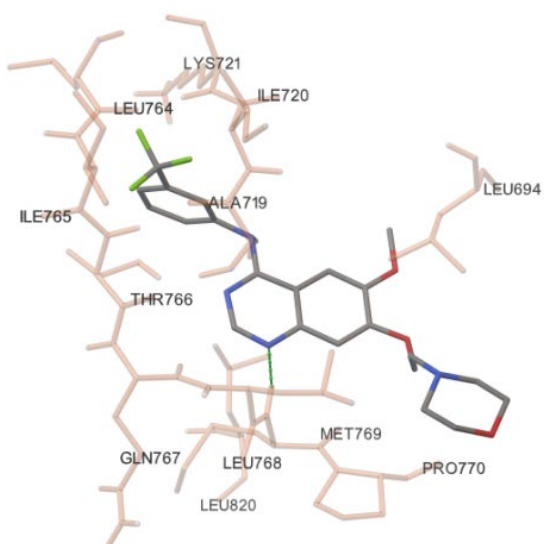
Docking interactions of compound 8a-8k with EGFR



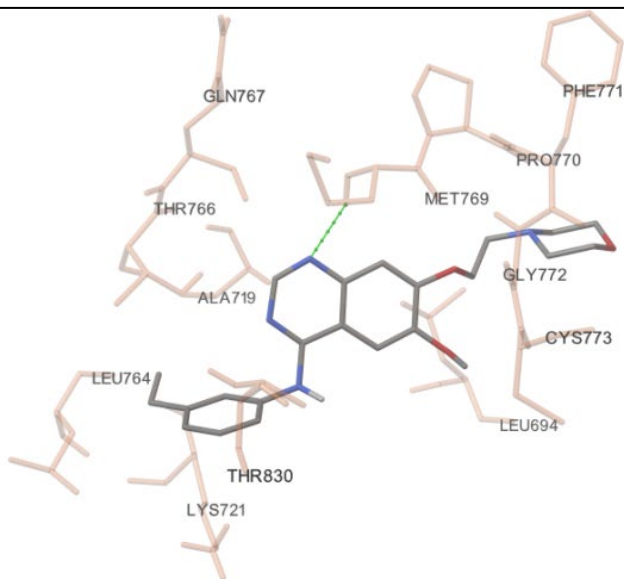
8b



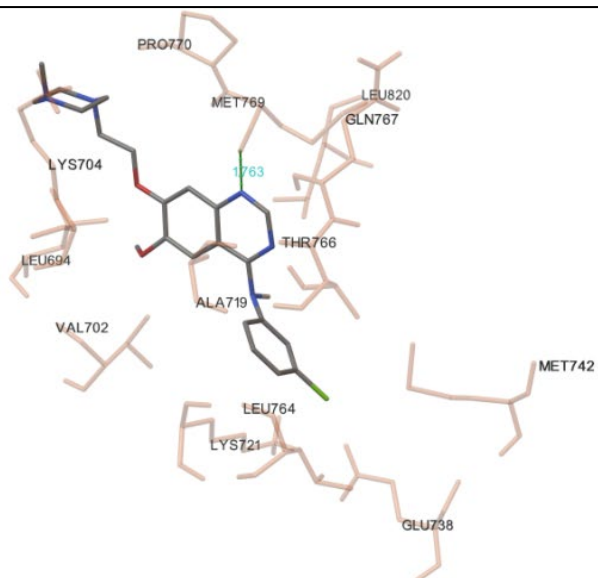
8c



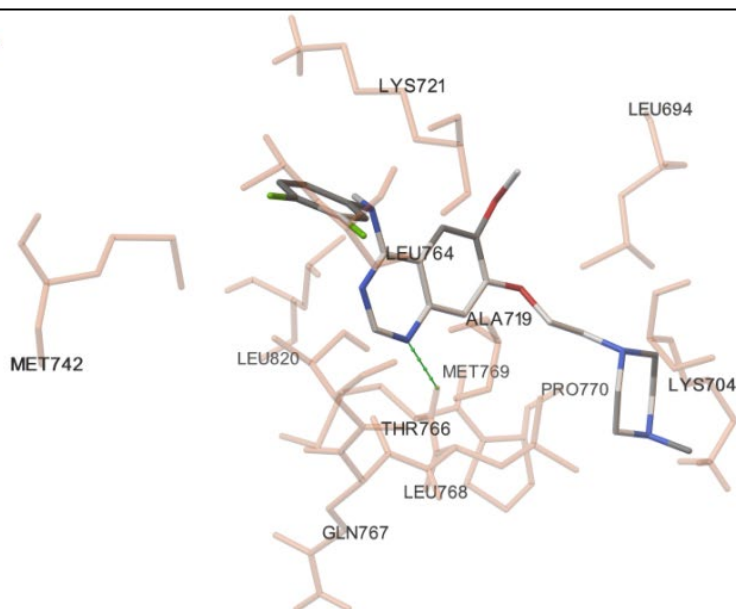
8d



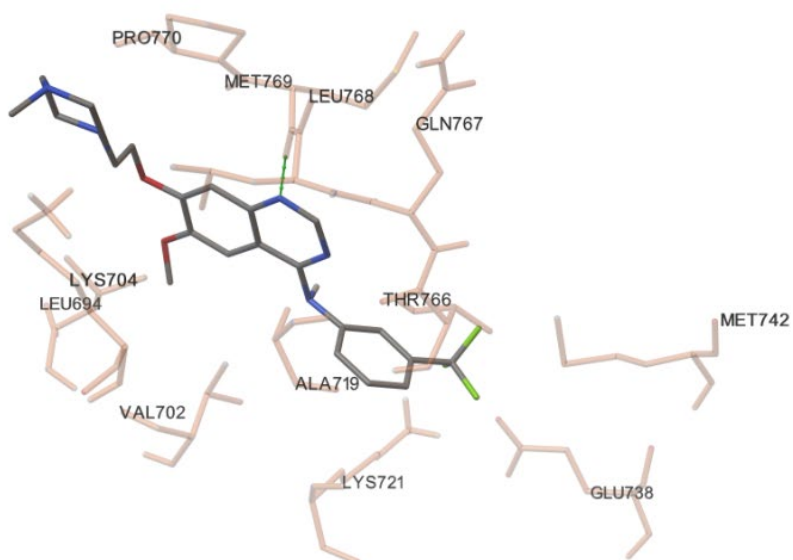
8e



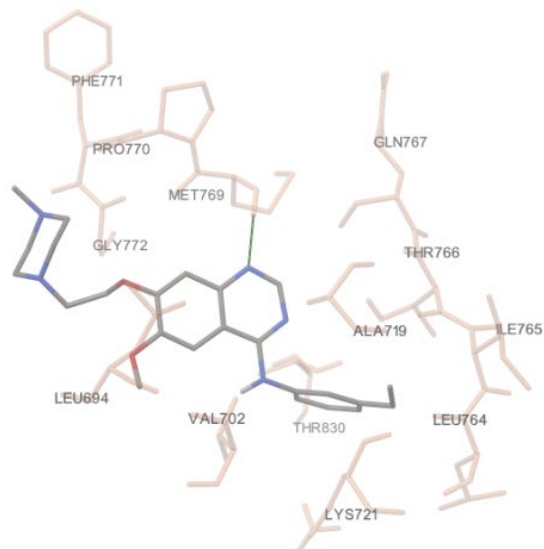
8f



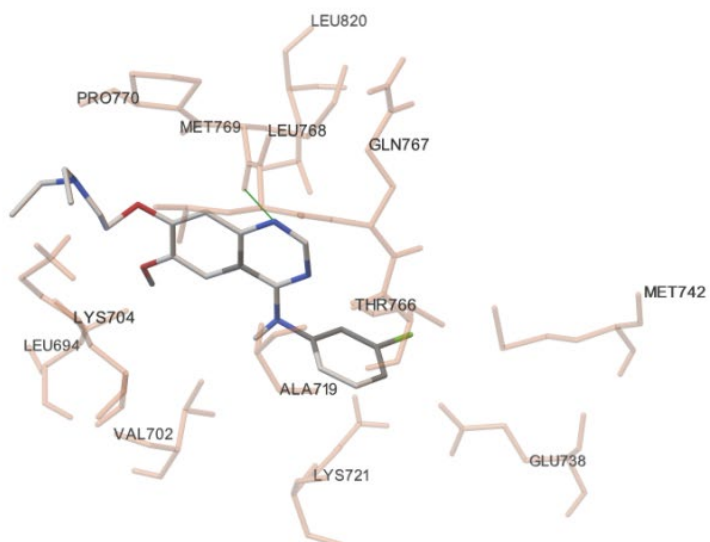
8g

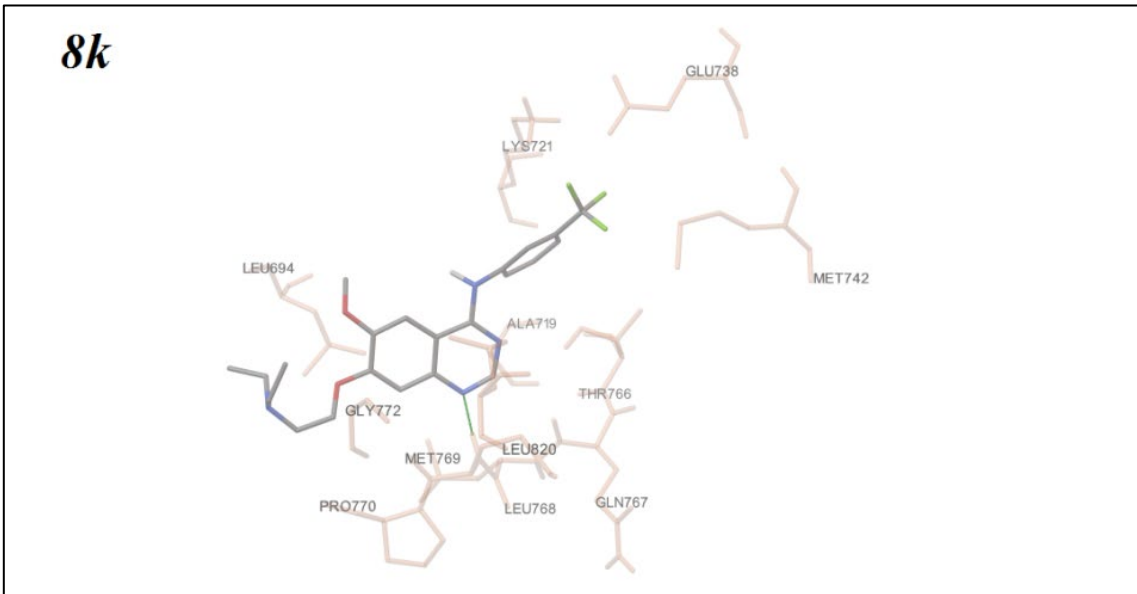
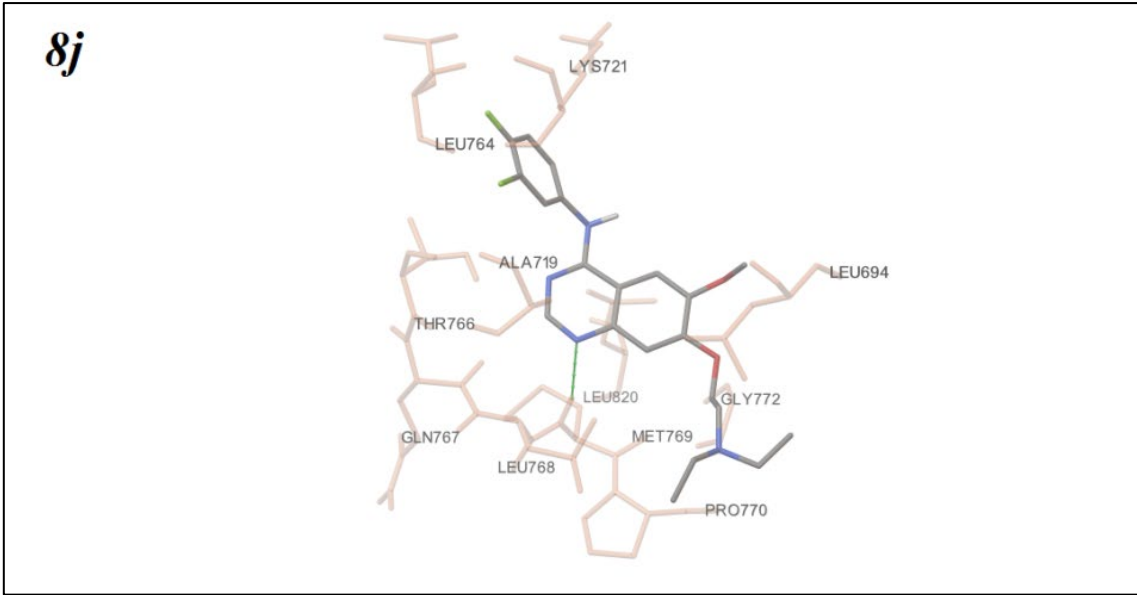


8h



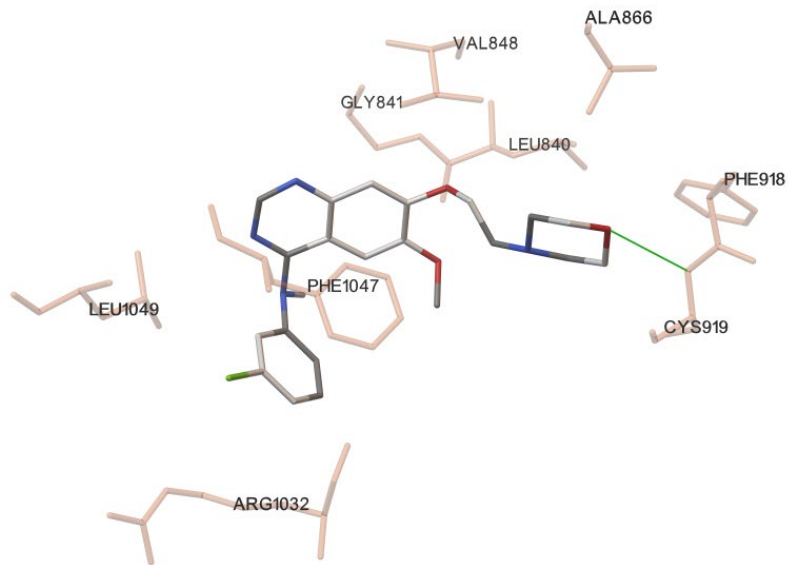
8i



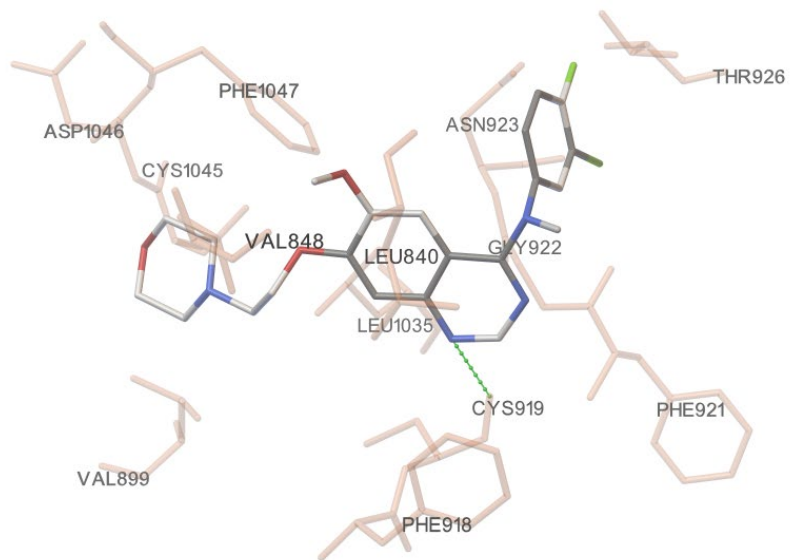


Docking interactions of compound 8a-8k with VEGFR

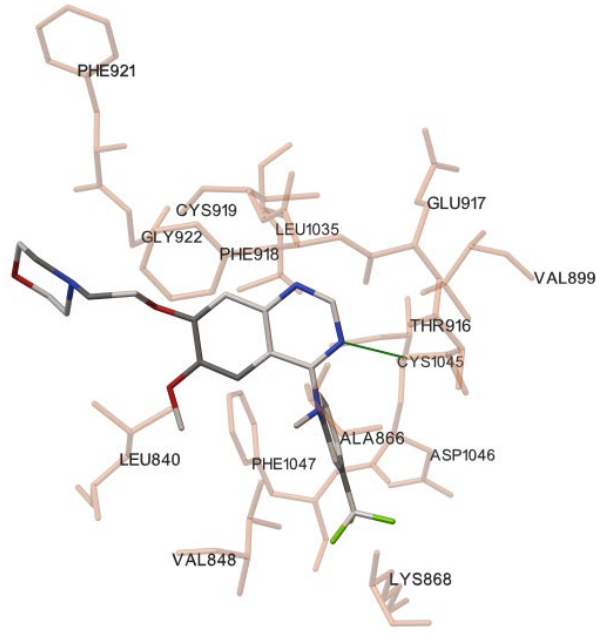
8a



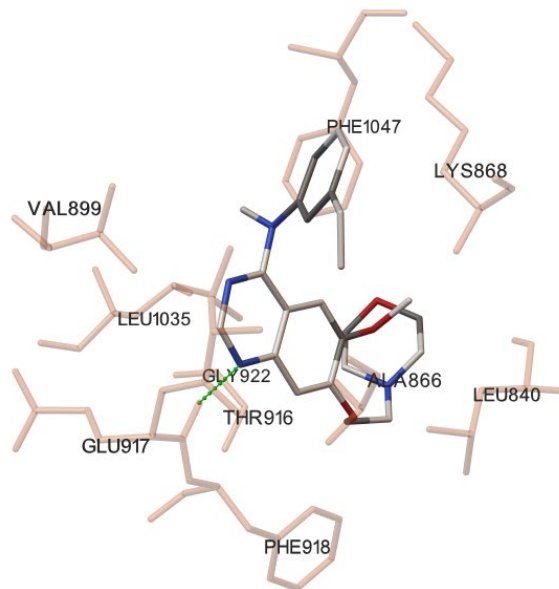
8b



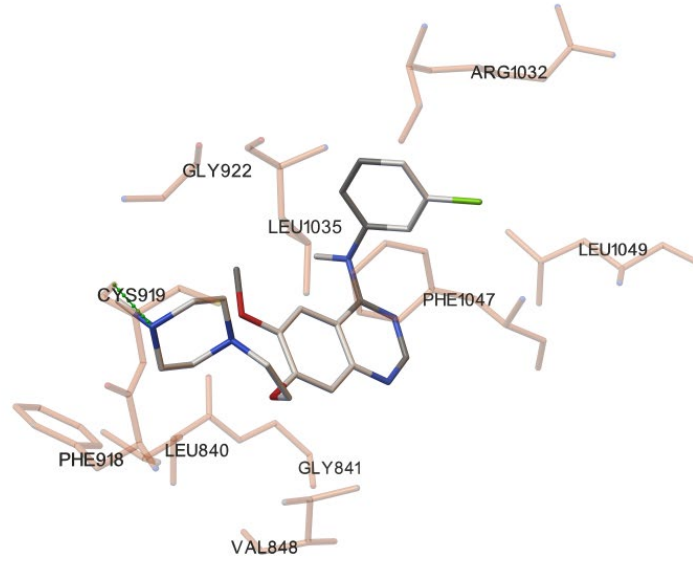
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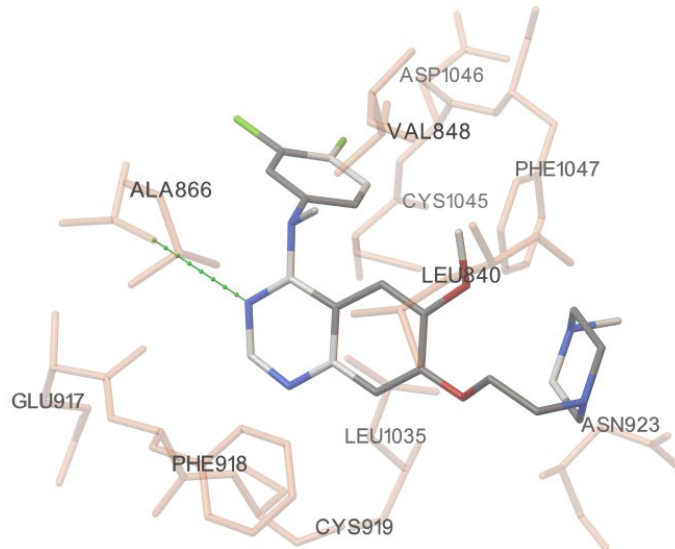
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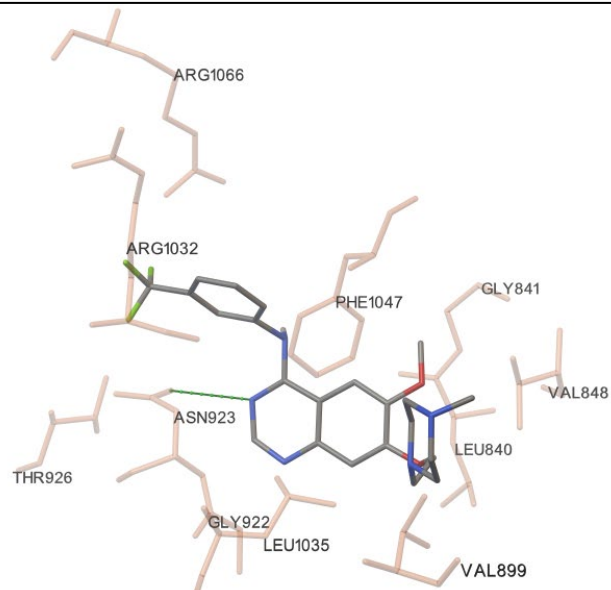
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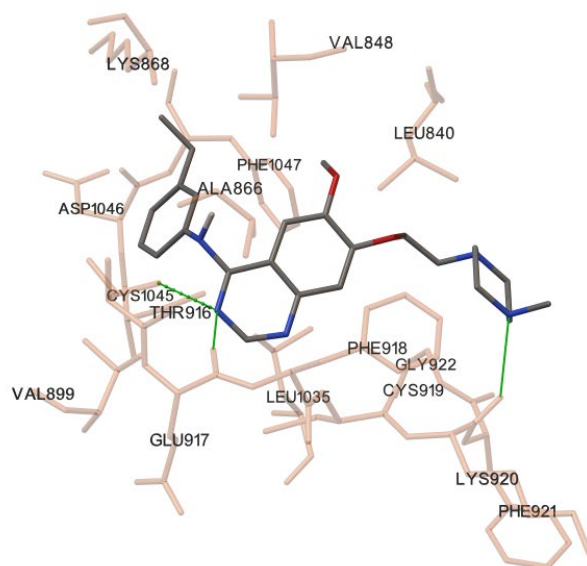
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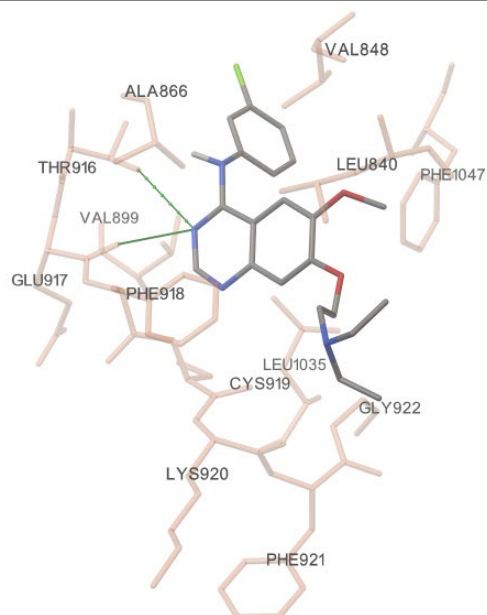
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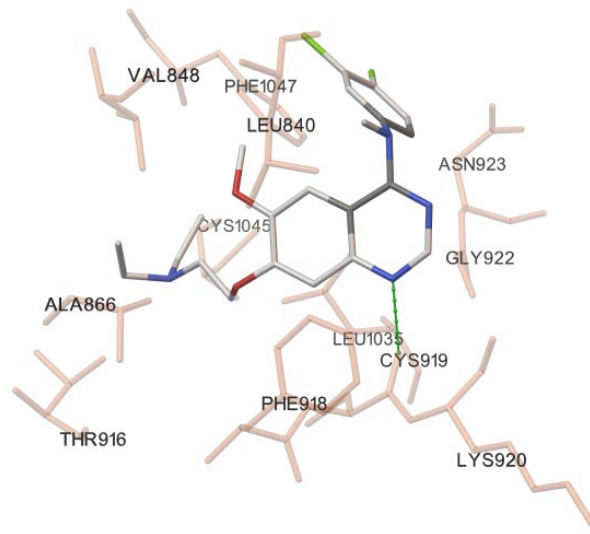
8h



8i



8j



8k

