

Supporting Information

9-arylacenaphtho[1,2-b]quinoxalines via Suzuki-Miyaura cross coupling reaction as cancer therapeutic and cellular imaging agent

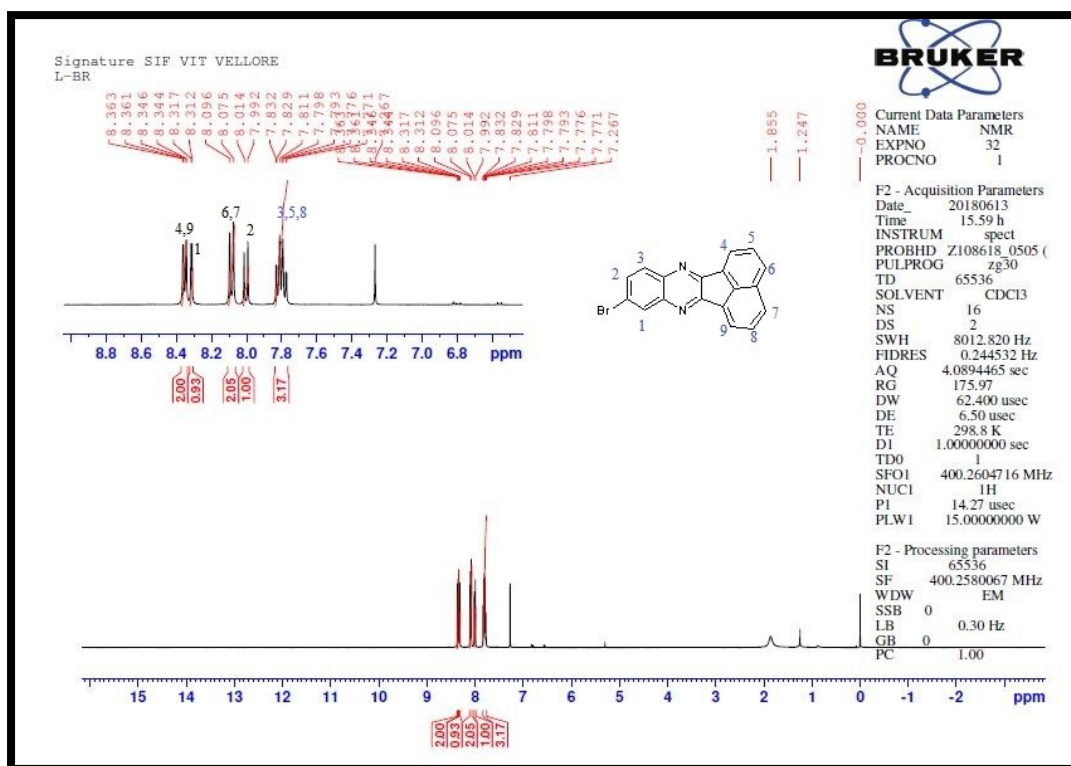
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Department of Chemistry, School of advanced sciences, Vellore Institute of Technology Vellore-632014, Tamilnadu, India, E-mail: priyankar.paira@vit.ac.in

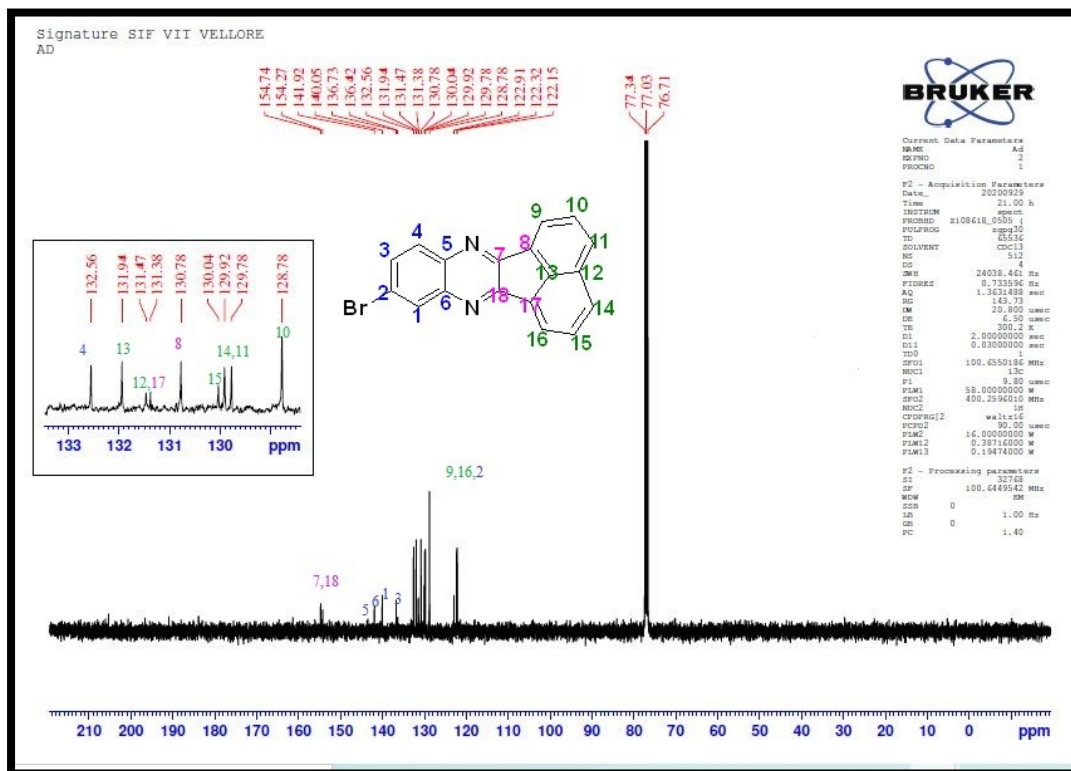
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NMR Spectra

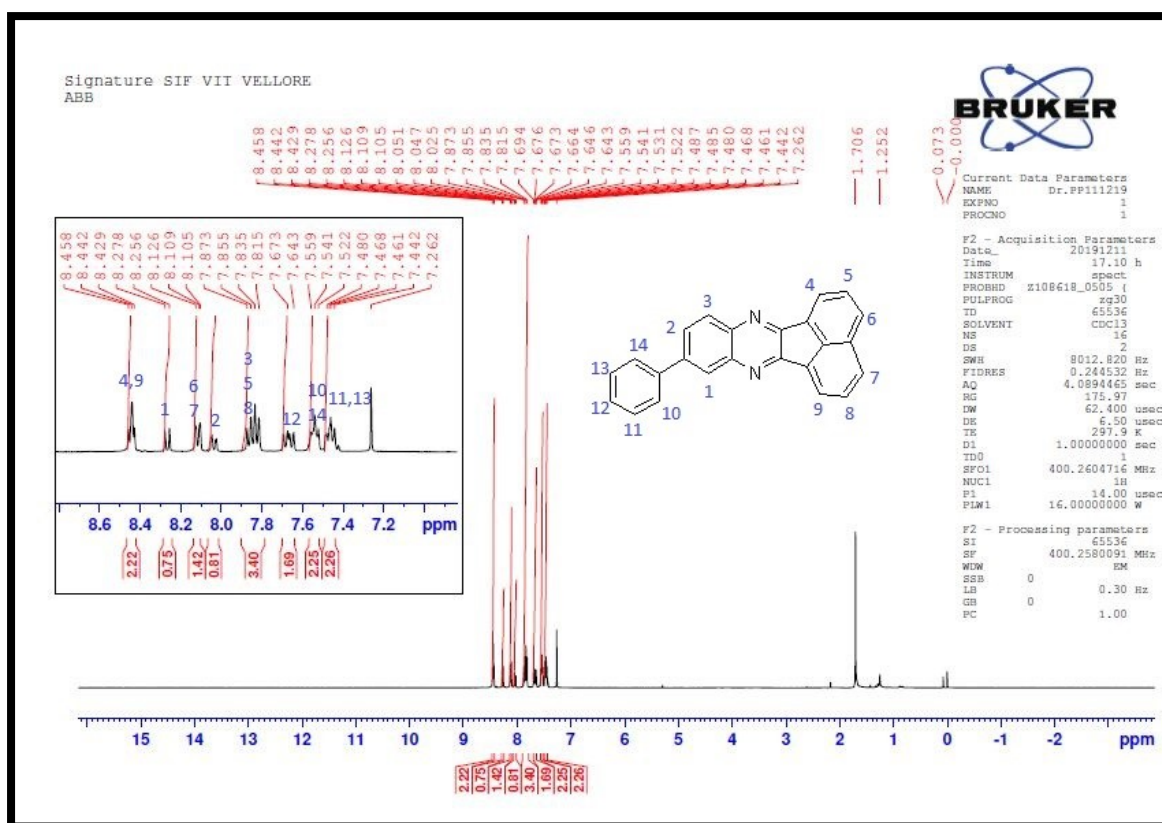
¹H NMR of compound 9-bromoacenaphtho[1,2-b]quinoxaline (3):



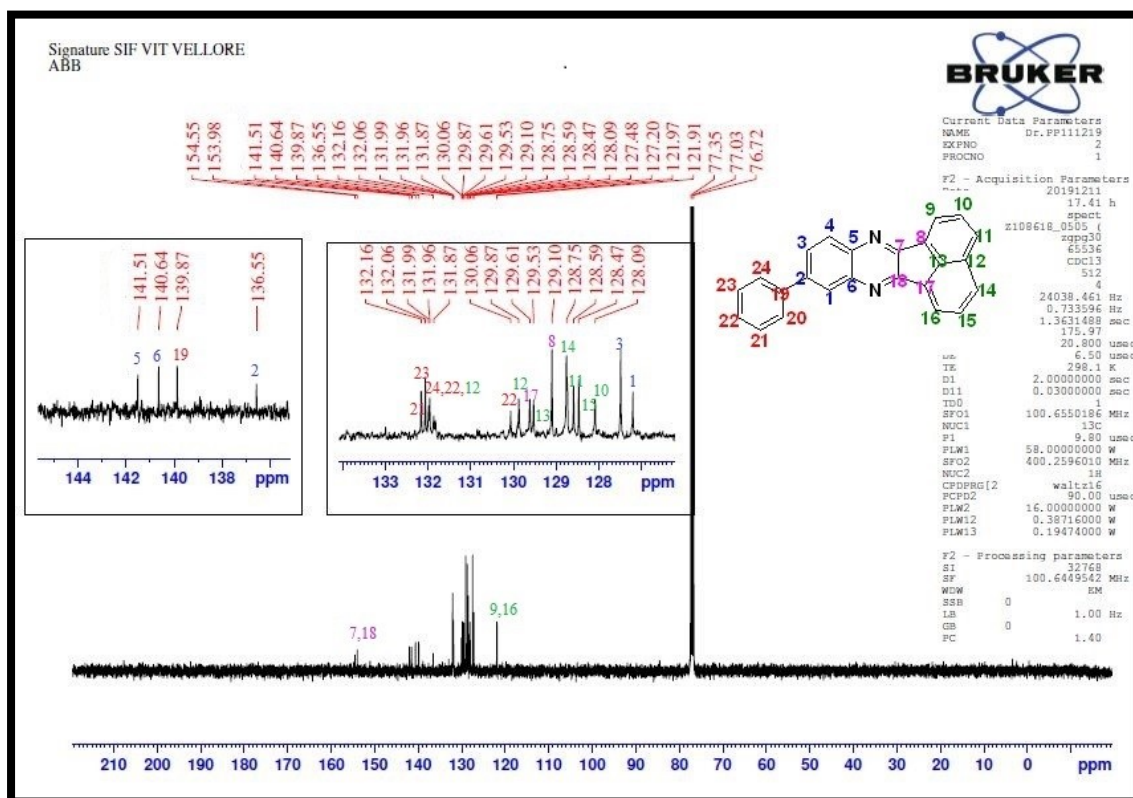
¹³C NMR of compound 9-bromoacenaphtho[1,2-b]quinoxaline (3):



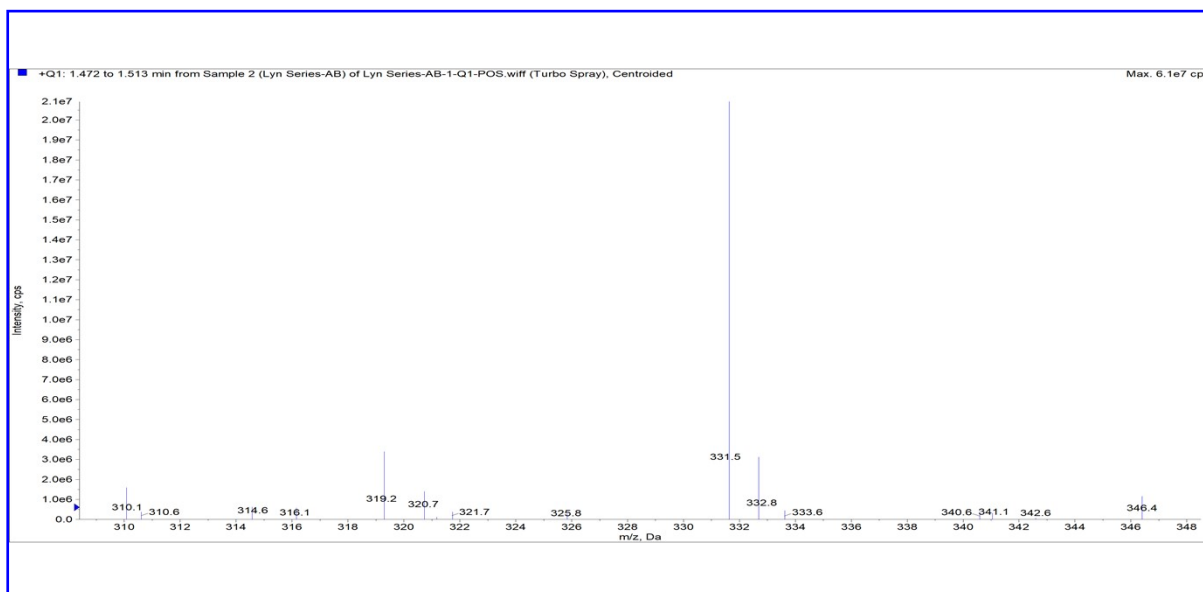
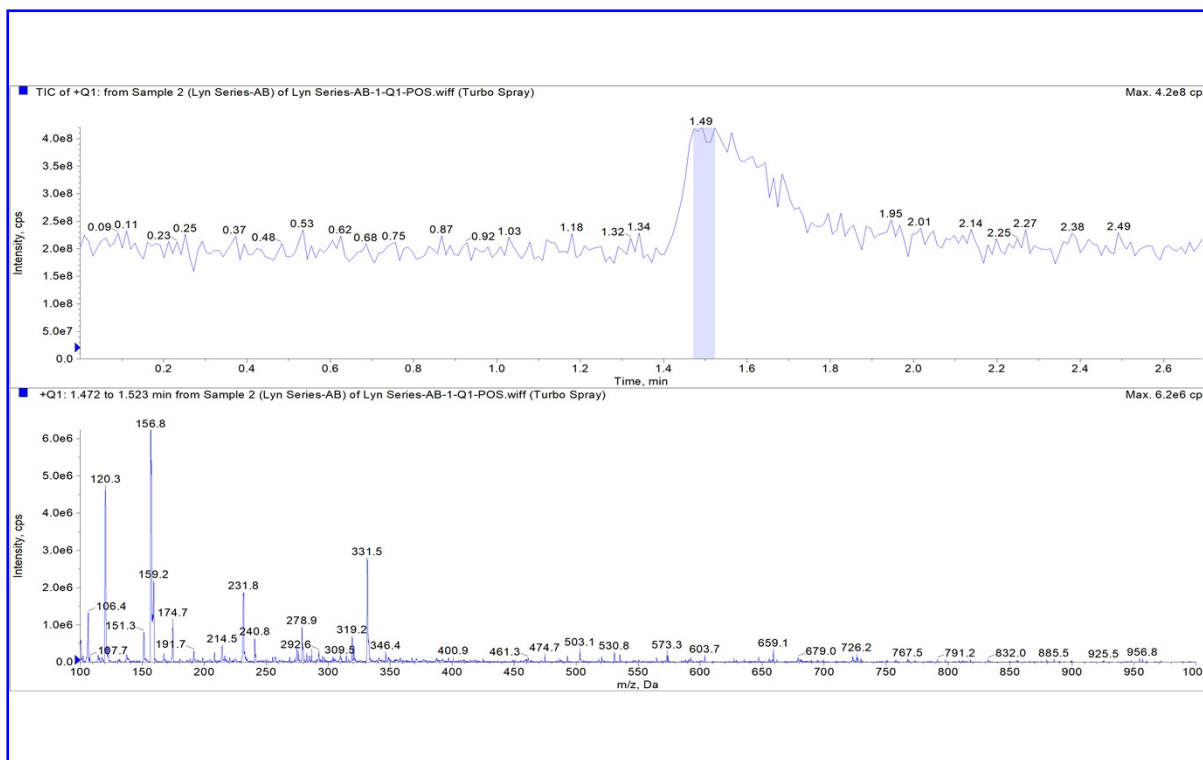
¹H NMR of compound 9-phenylacnaphtho[1,2-b]quinoxaline (5a)



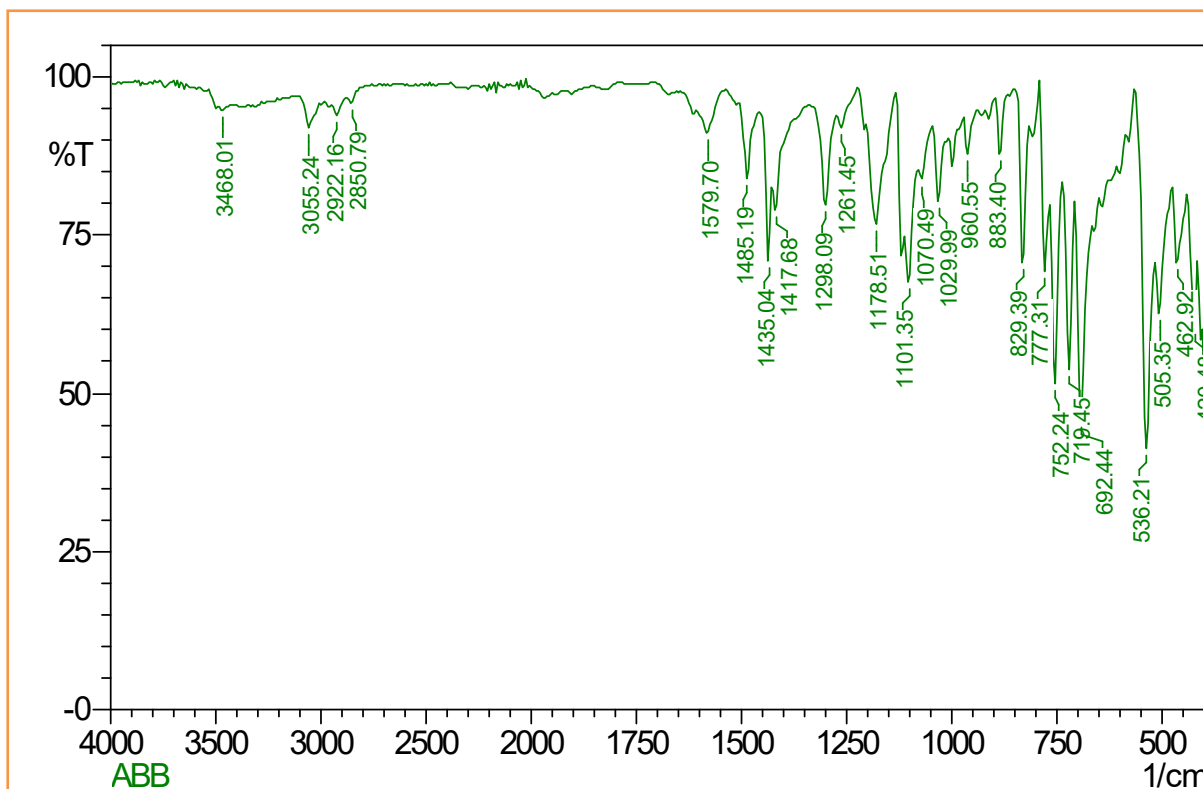
¹³C NMR of compound of 9-phenylacnaphtho[1,2-b]quinoxaline (5a):



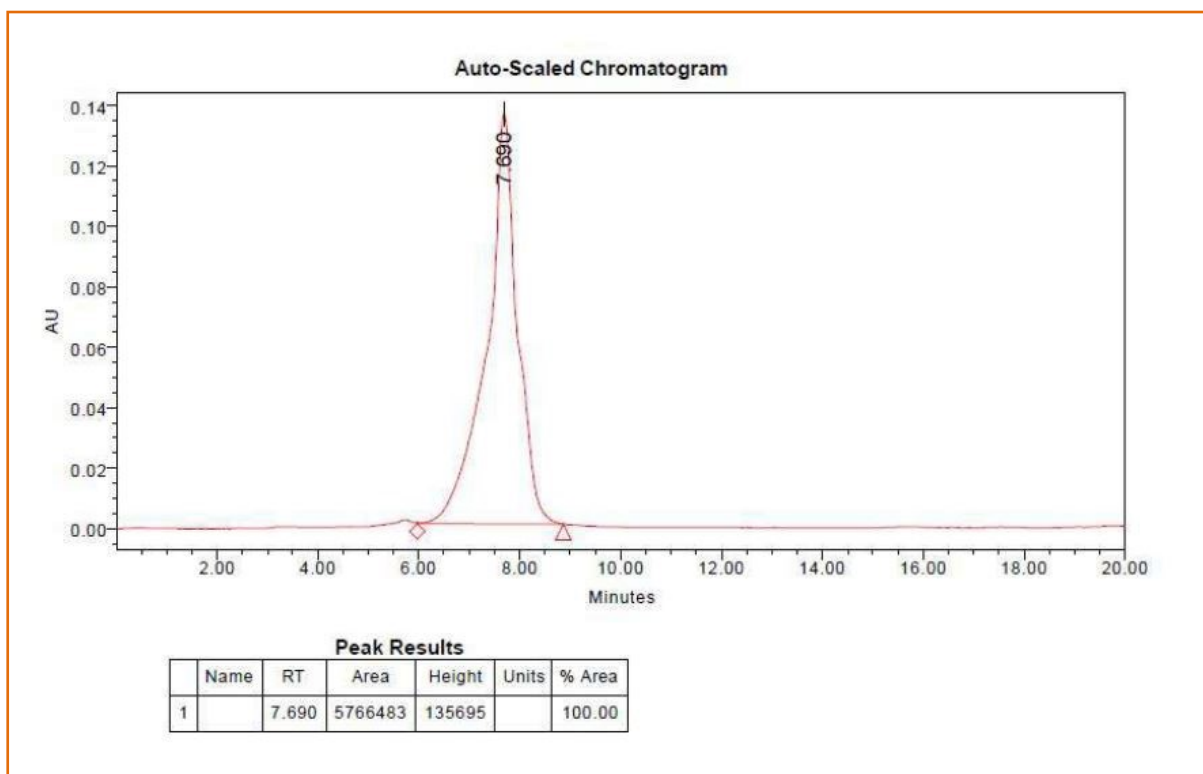
ESI-MS of compound 9-phenylacenaphtho[1,2-b]quinoxaline (5a)



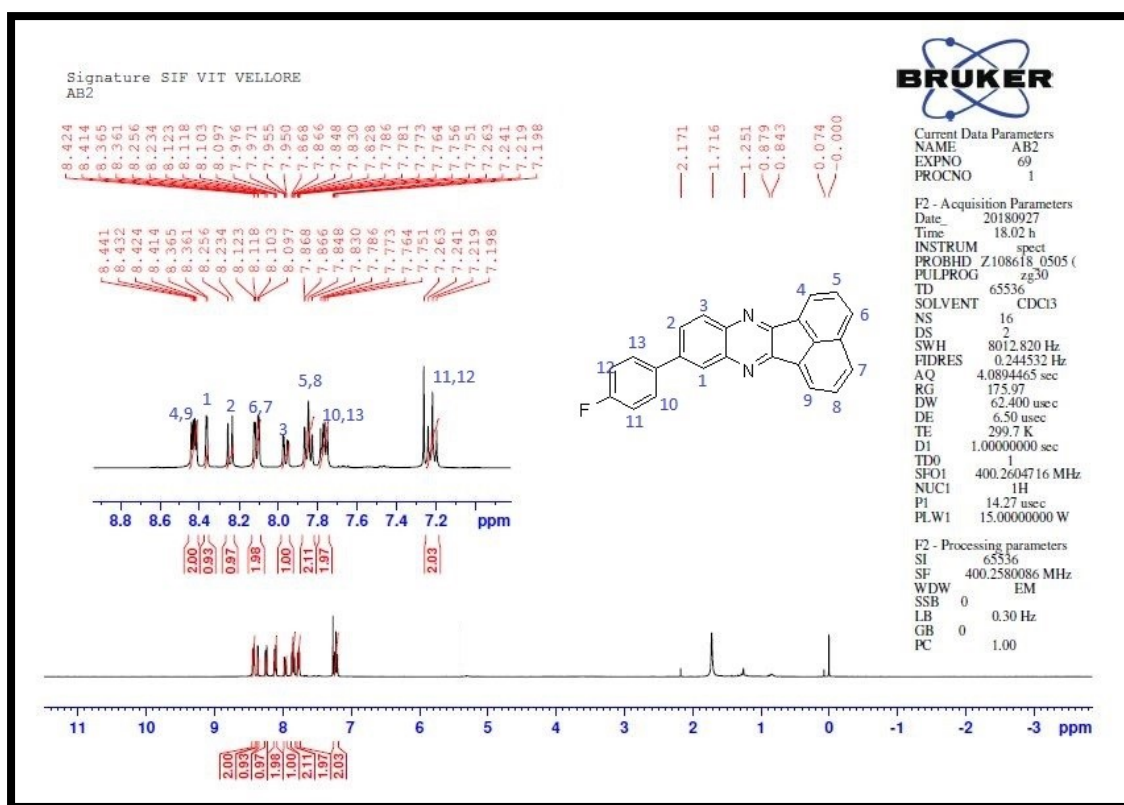
FT-IR of compound 9-phenylacnaphtho[1,2-b]quinoxaline (5a)



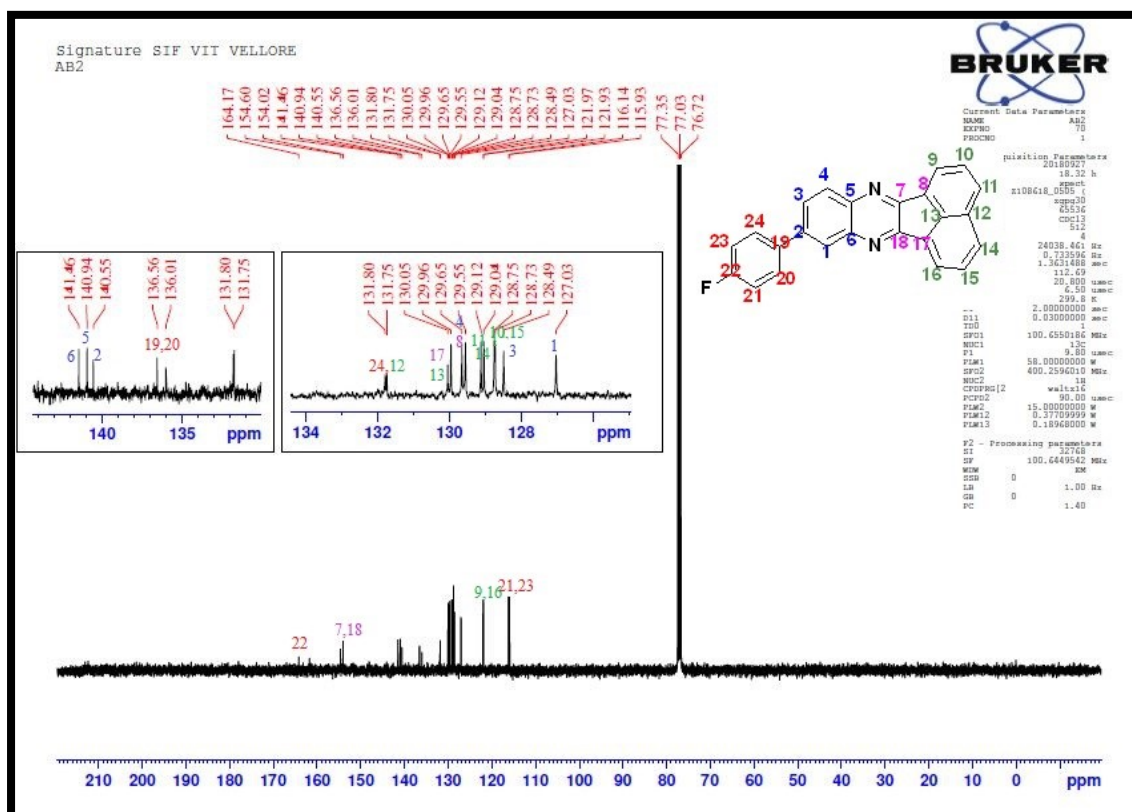
UPLC purity profile of compound 9-phenylacnaphtho[1,2-b]quinoxaline (5a)



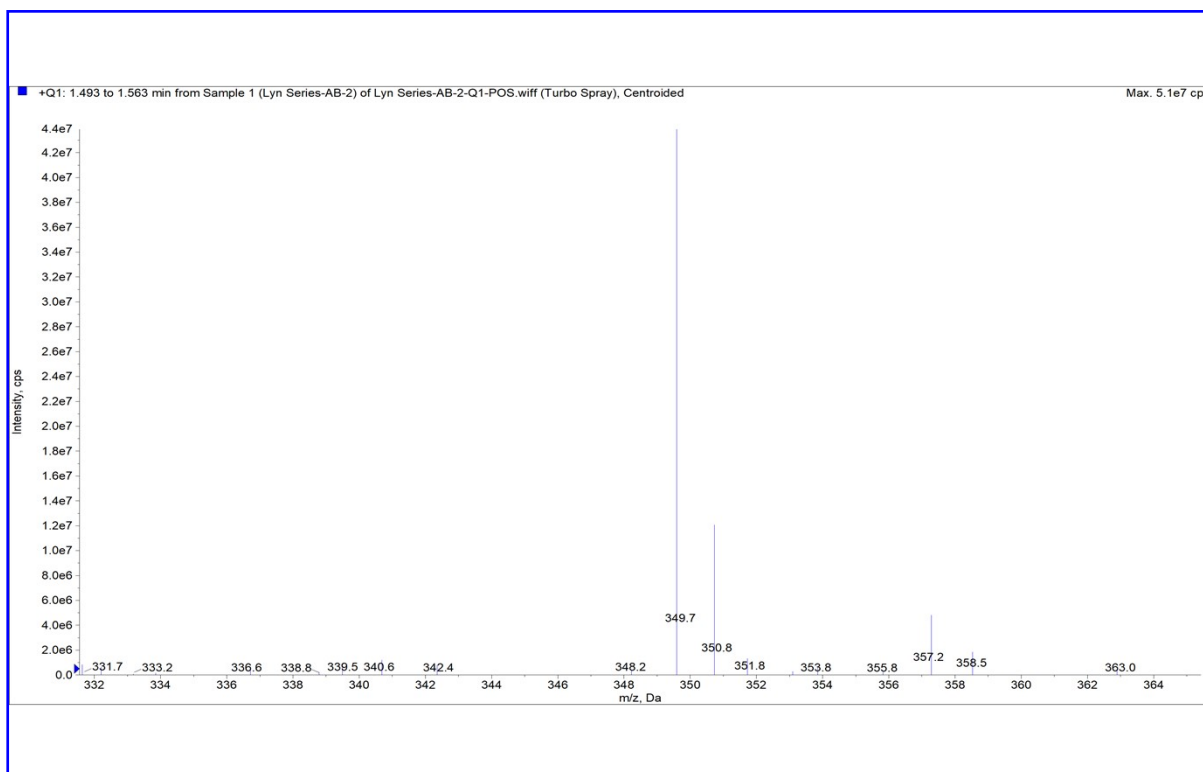
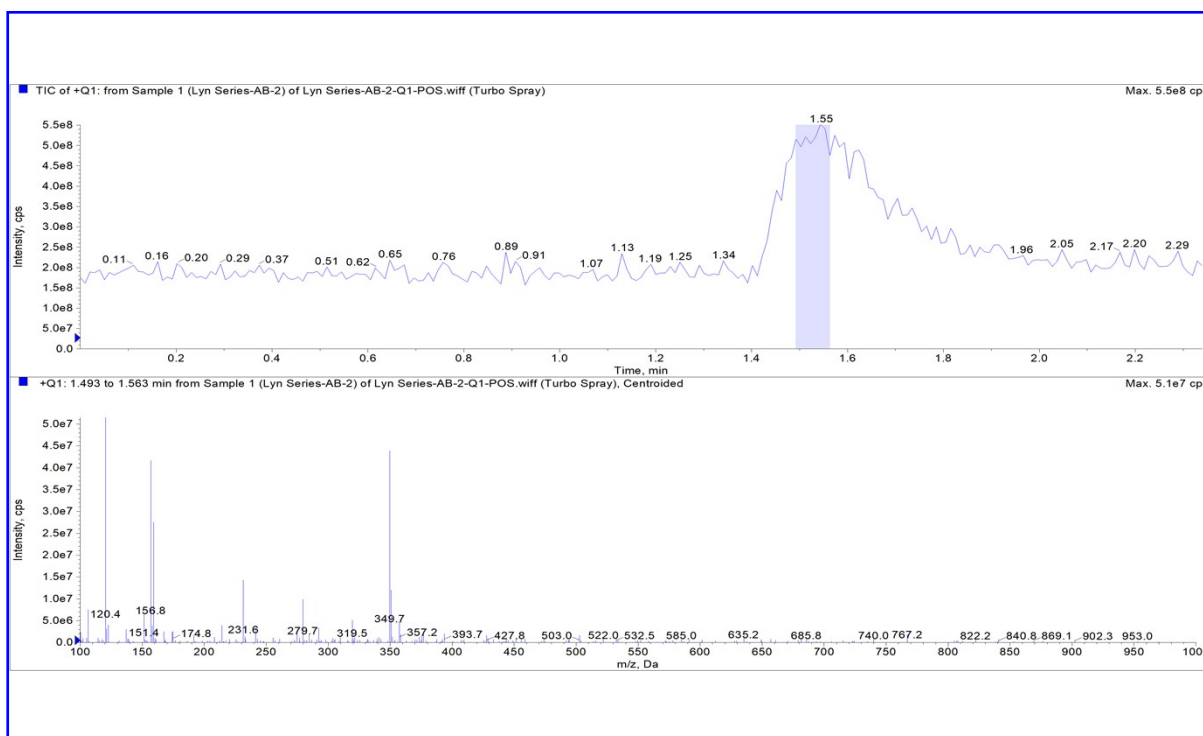
¹H NMR of compound 9-(4-fluorophenyl)acenaphtho[1,2-b]quinoxaline (5b)



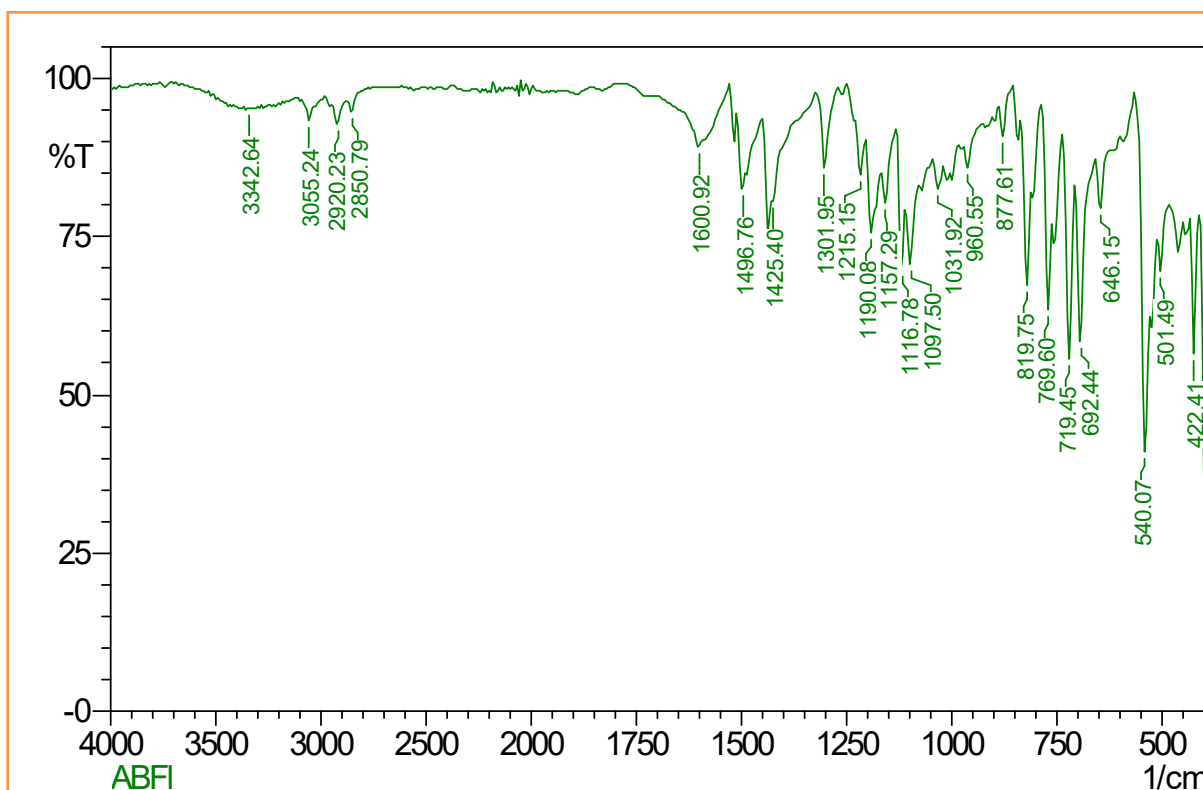
¹³C NMR spectrum of compound 9-(4-fluorophenyl)acenaphtho[1,2-b]quinoxaline (5b)



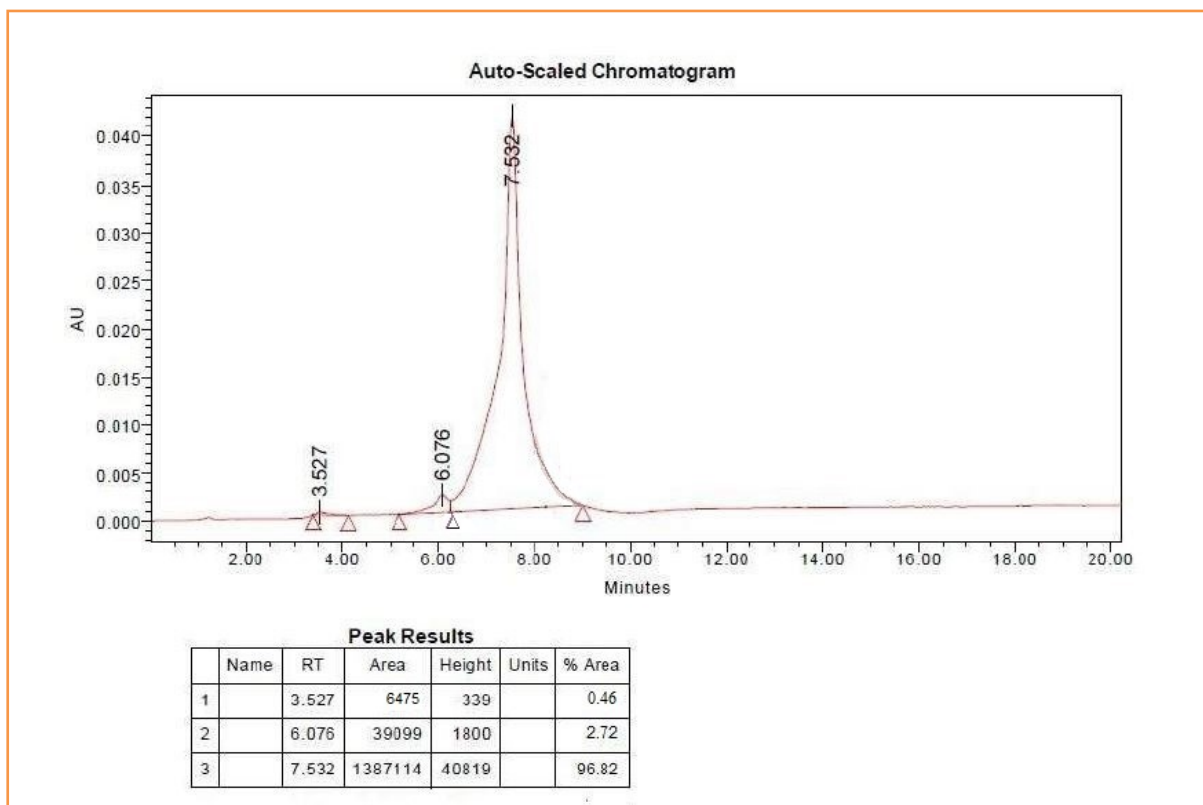
ESI-MS of compound 9-(4-fluorophenyl)acenaphtho[1,2-b]quinoxaline (5b)



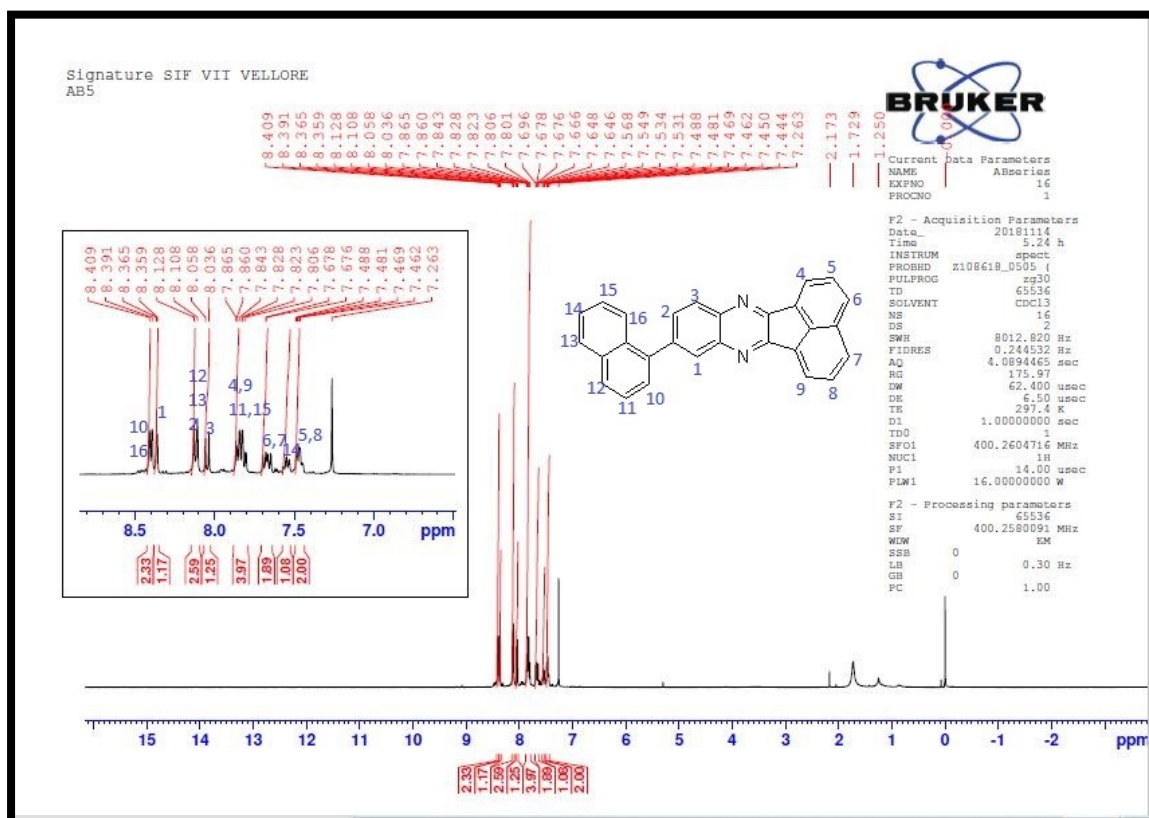
FTIR of compound 9-(4-fluorophenyl)acenaphtho[1,2-b]quinoxaline (5b)



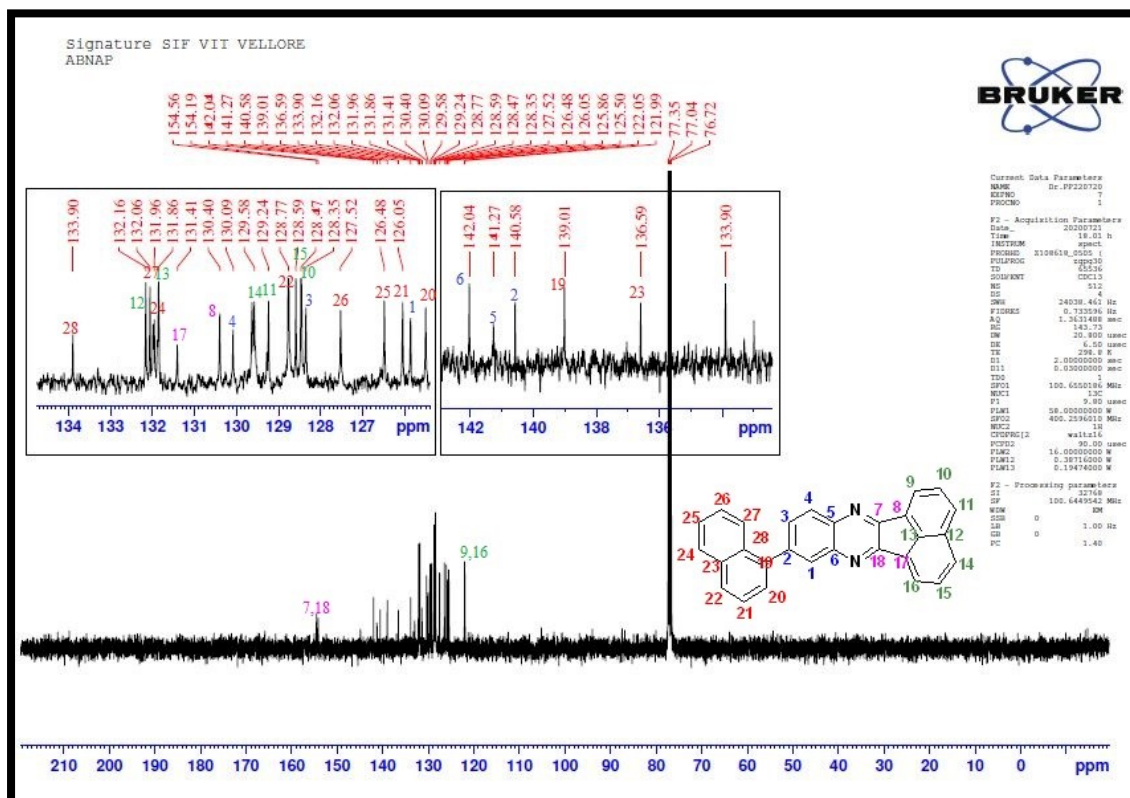
UPLC purity profile of compound 9-(4-fluorophenyl)acenaphtho[1,2-b]quinoxaline (5b)



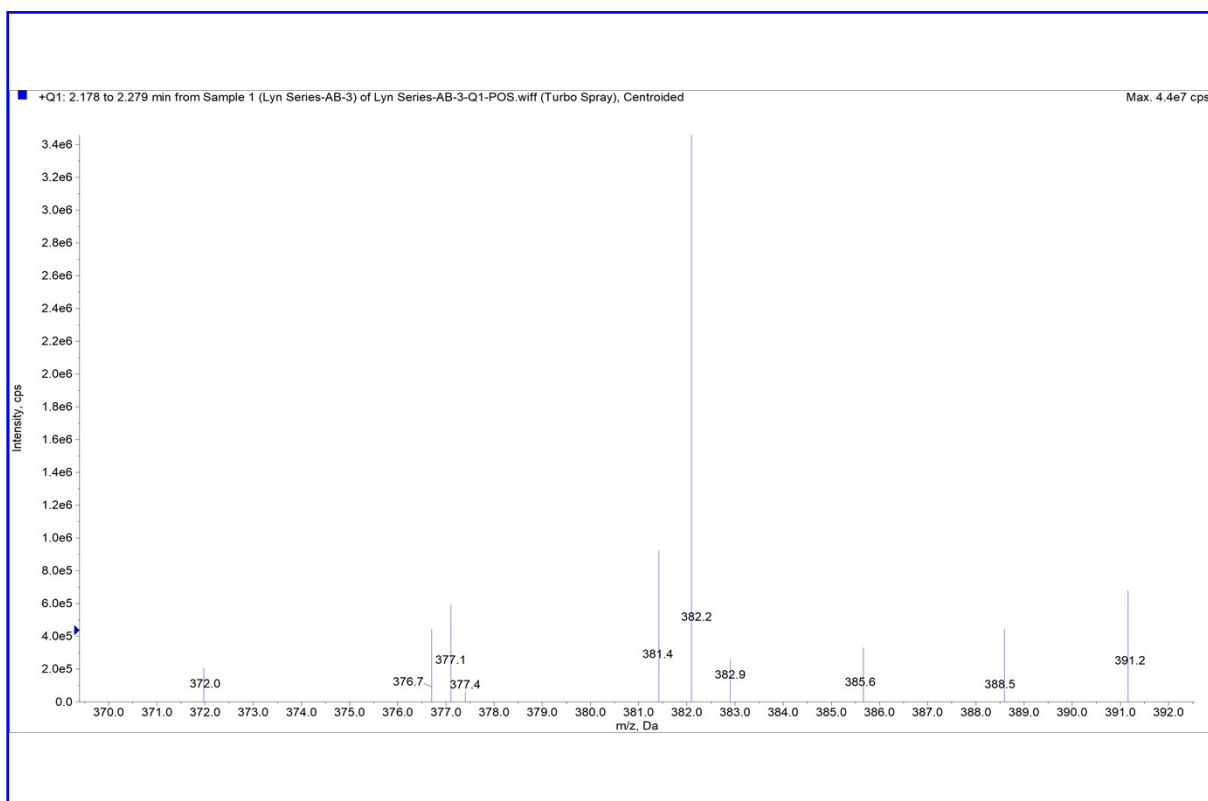
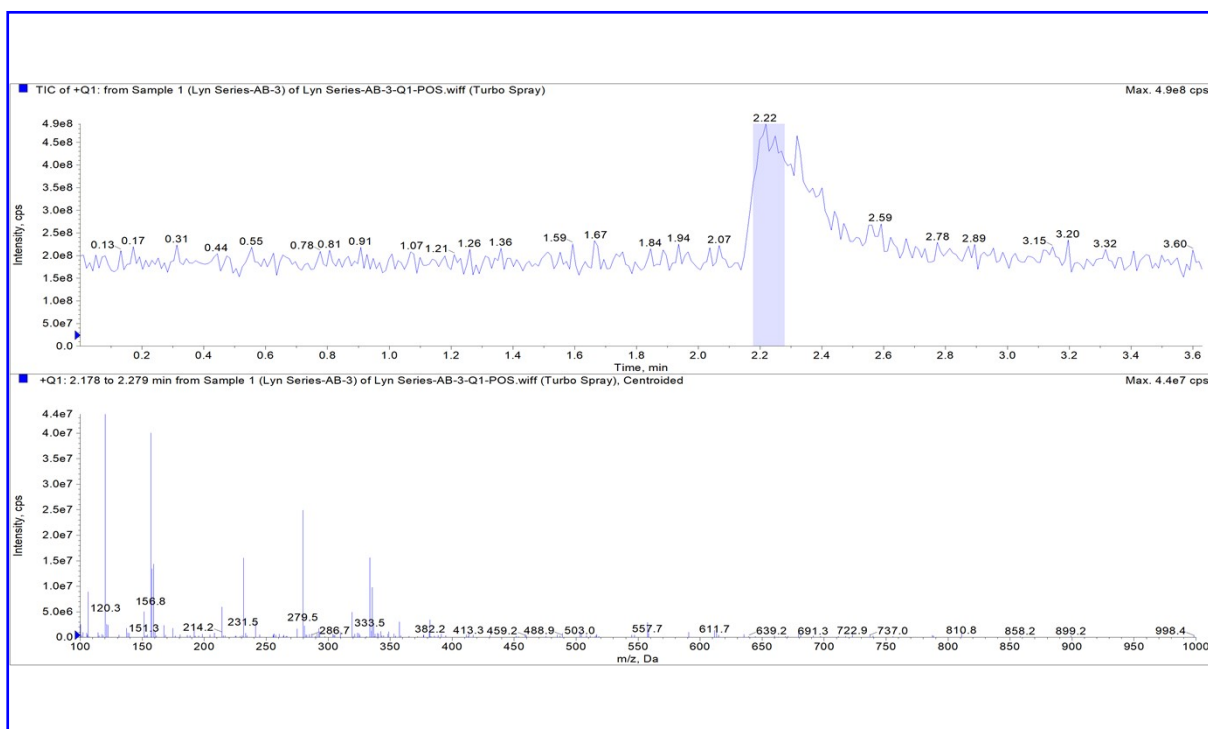
¹H NMR of compound 9-(naphthalen-1-yl)acenaphtho[1,2-b]quinoxaline (5c)



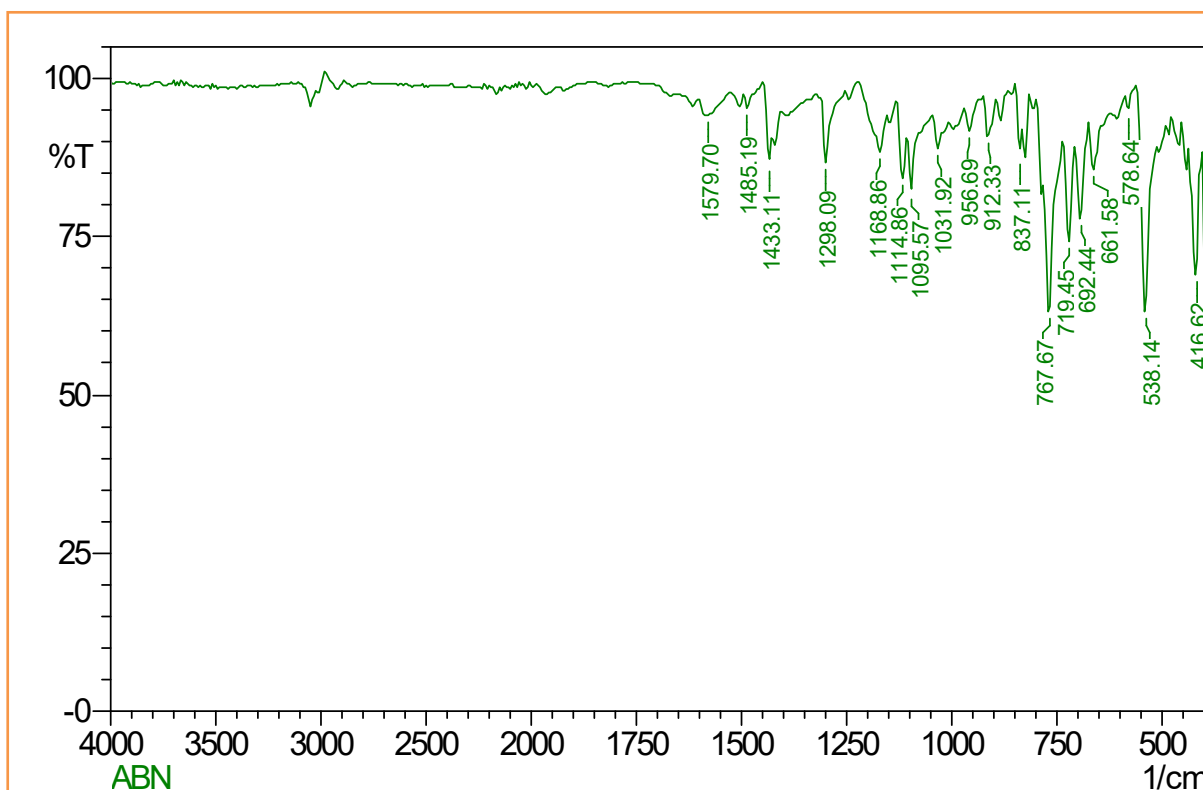
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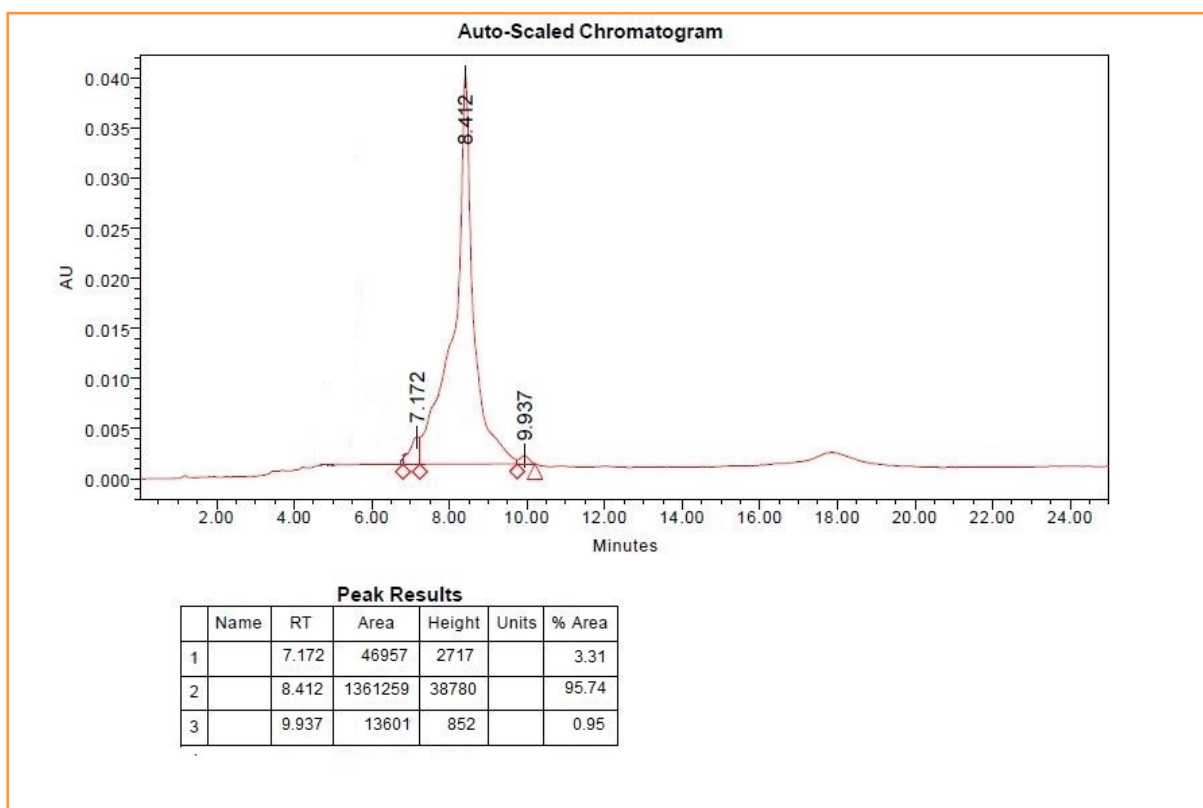
ESI-MS of compound 9-(naphthalen-1-yl)acenaphtho[1,2-b]quinoxaline (5c)



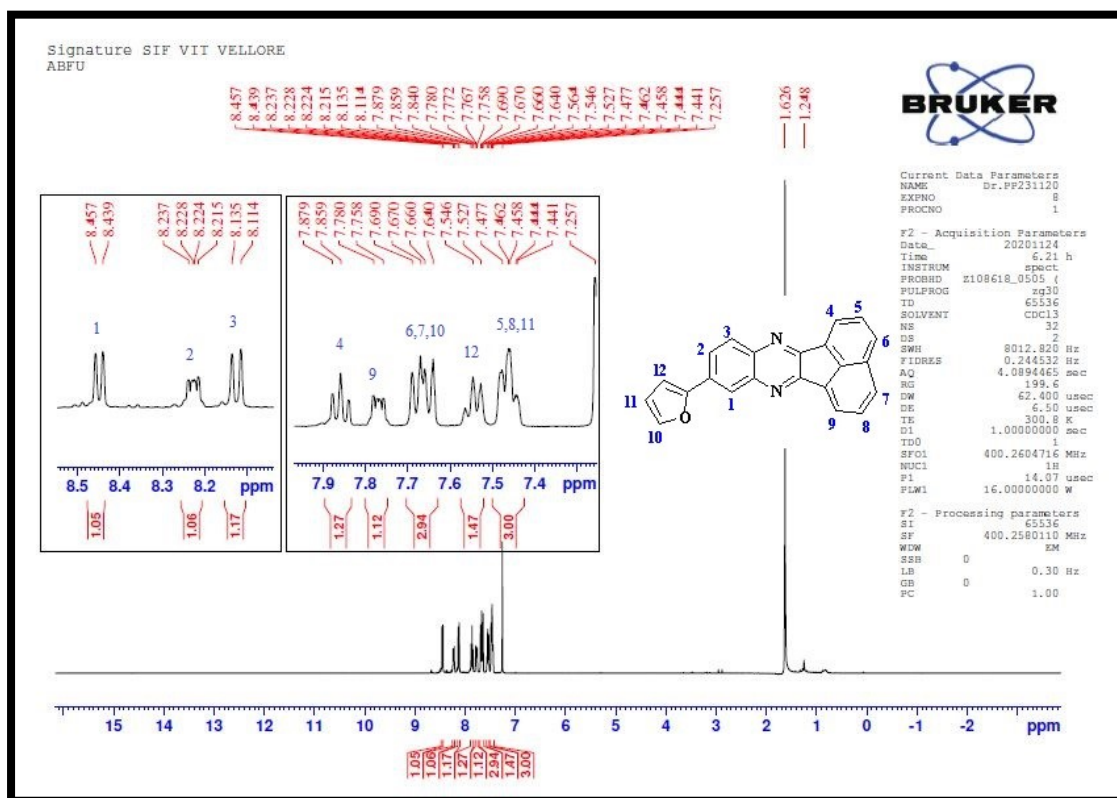
FTIR of compound 9-(naphthalen-1-yl)acenaphtho[1,2-b]quinoxaline (5c)



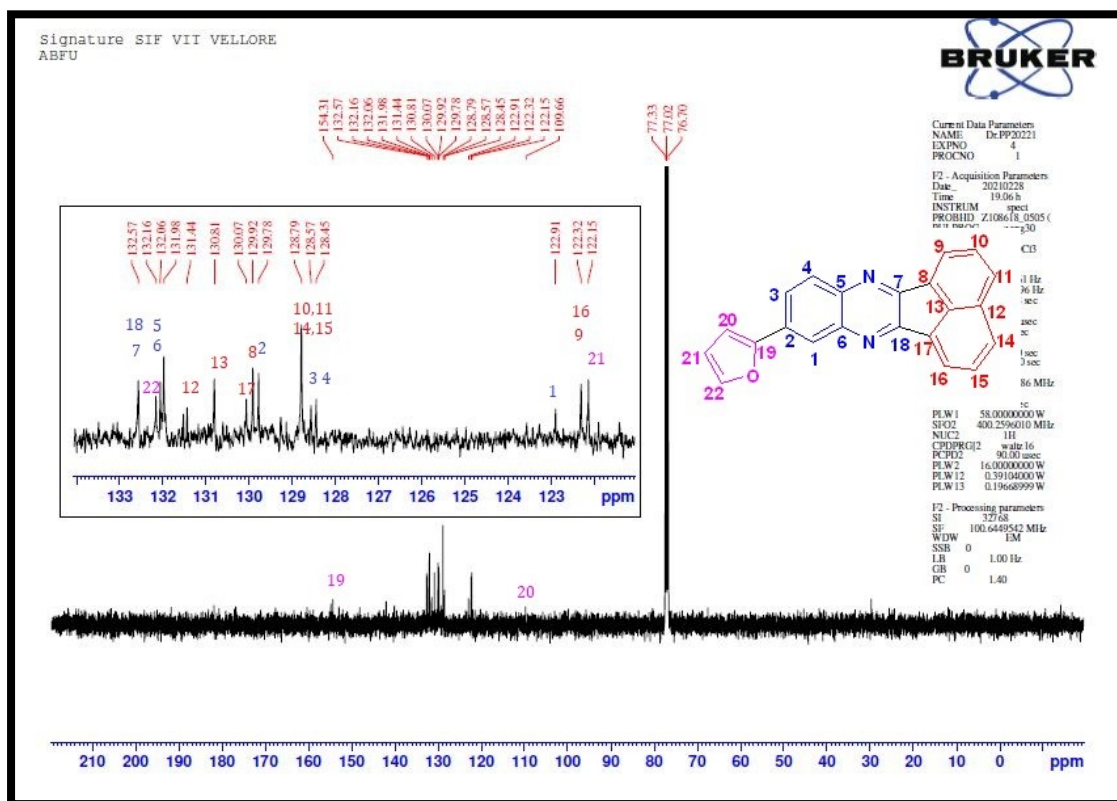
UPLC purity profile of compound 9-(naphthalen-1-yl)acenaphtho[1,2-b]quinoxaline (5c)



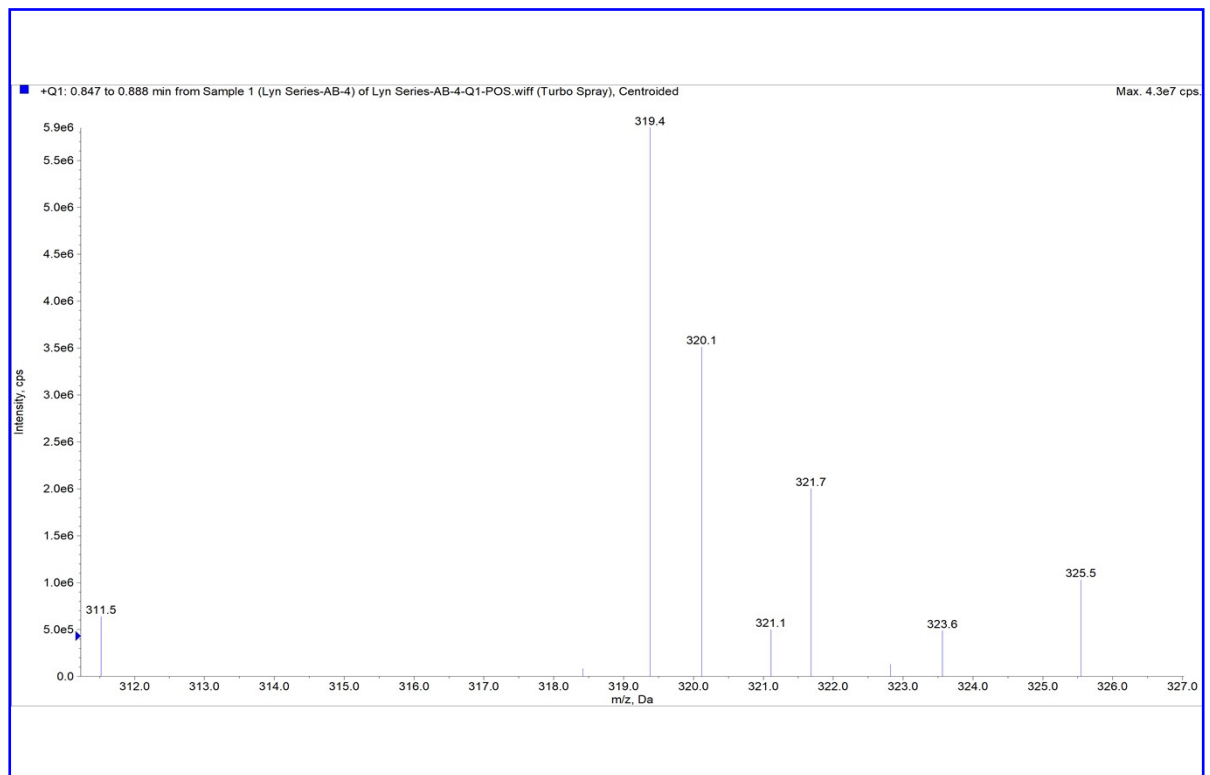
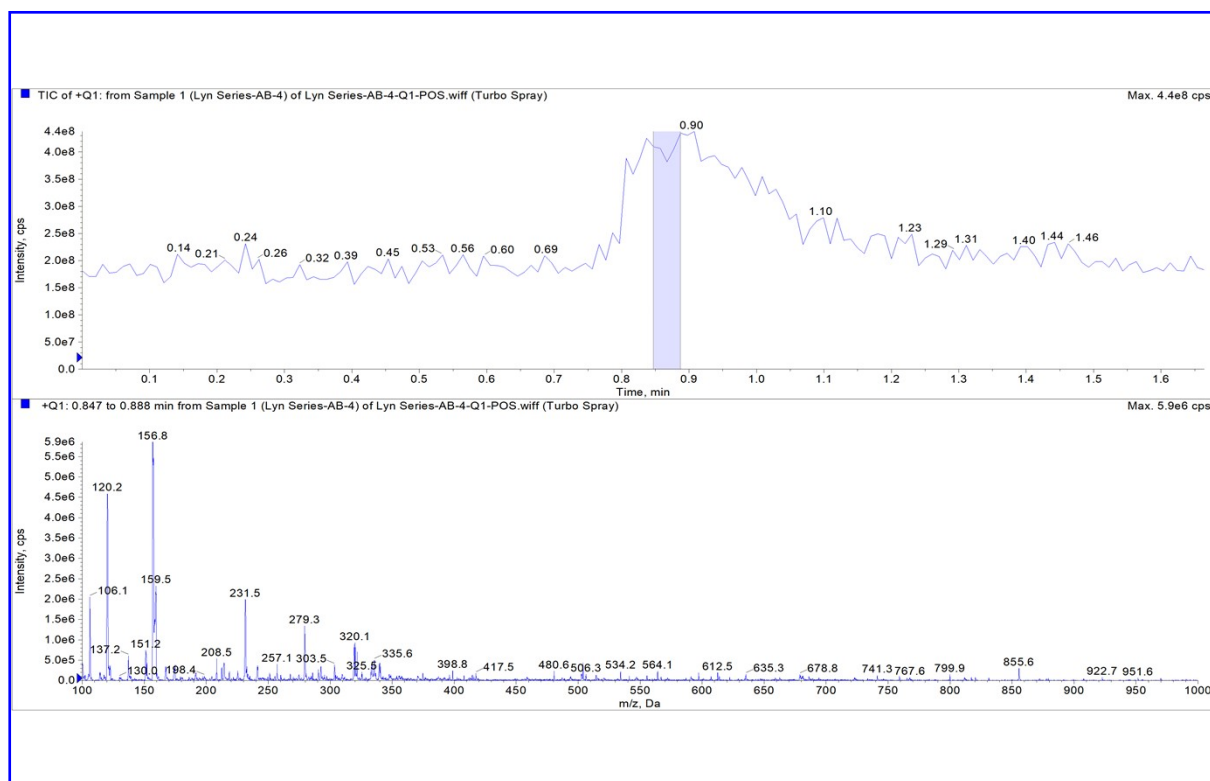
¹H NMR of compound 9-(furan-2-yl)acenaphtho[1,2-b]quinoxaline (5d)



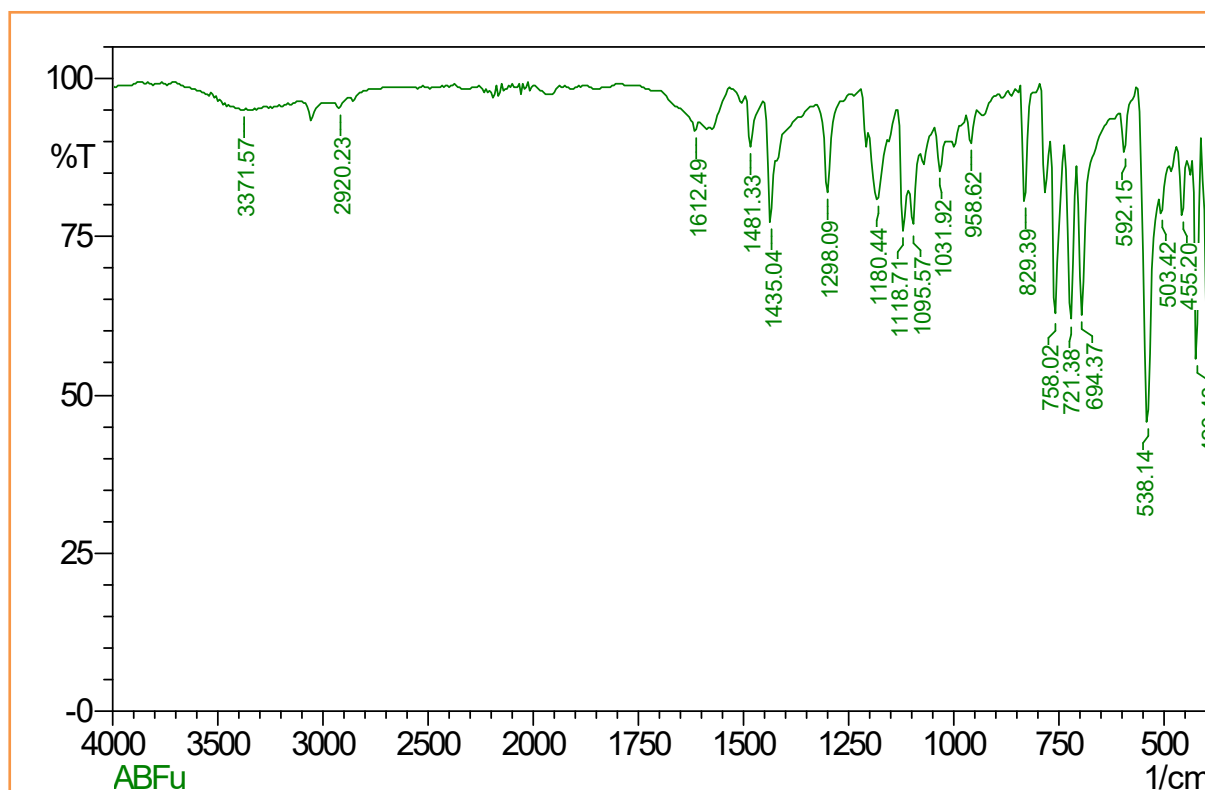
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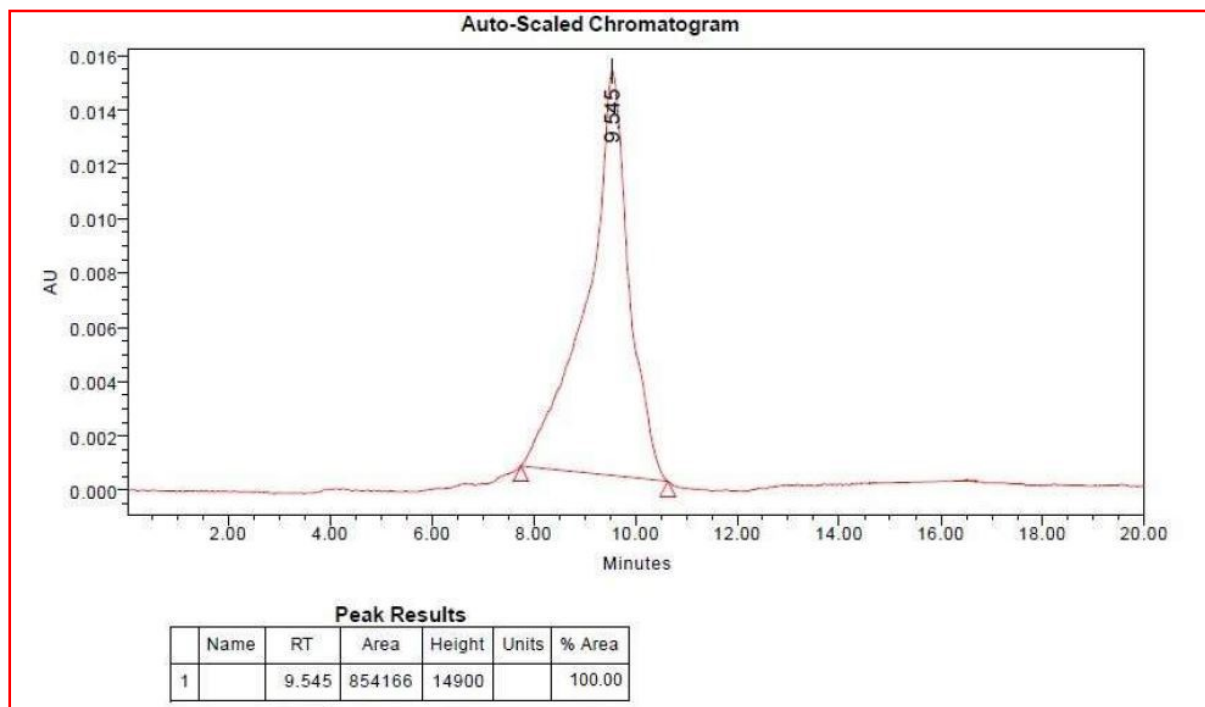
ESI-MS of compound 9-(furan-2-yl)acenaphtho[1,2-b]quinoxaline (5d)



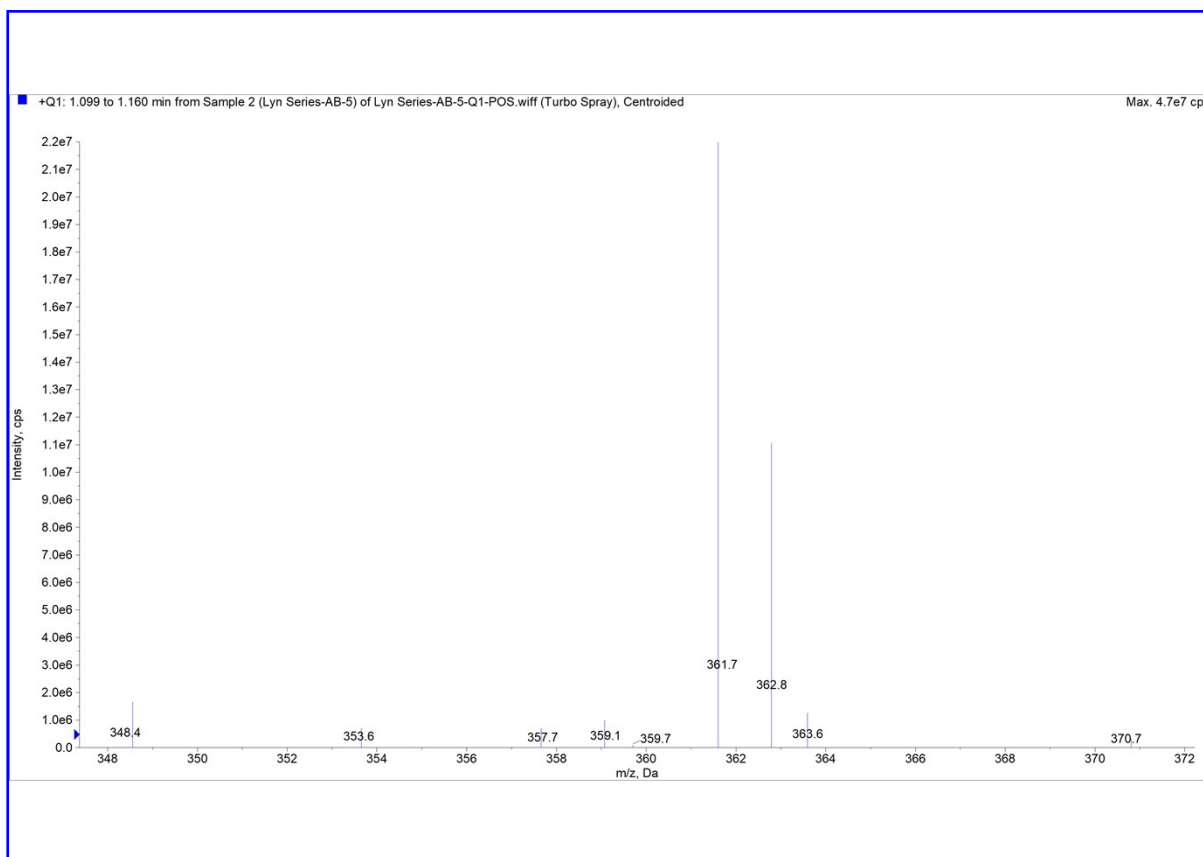
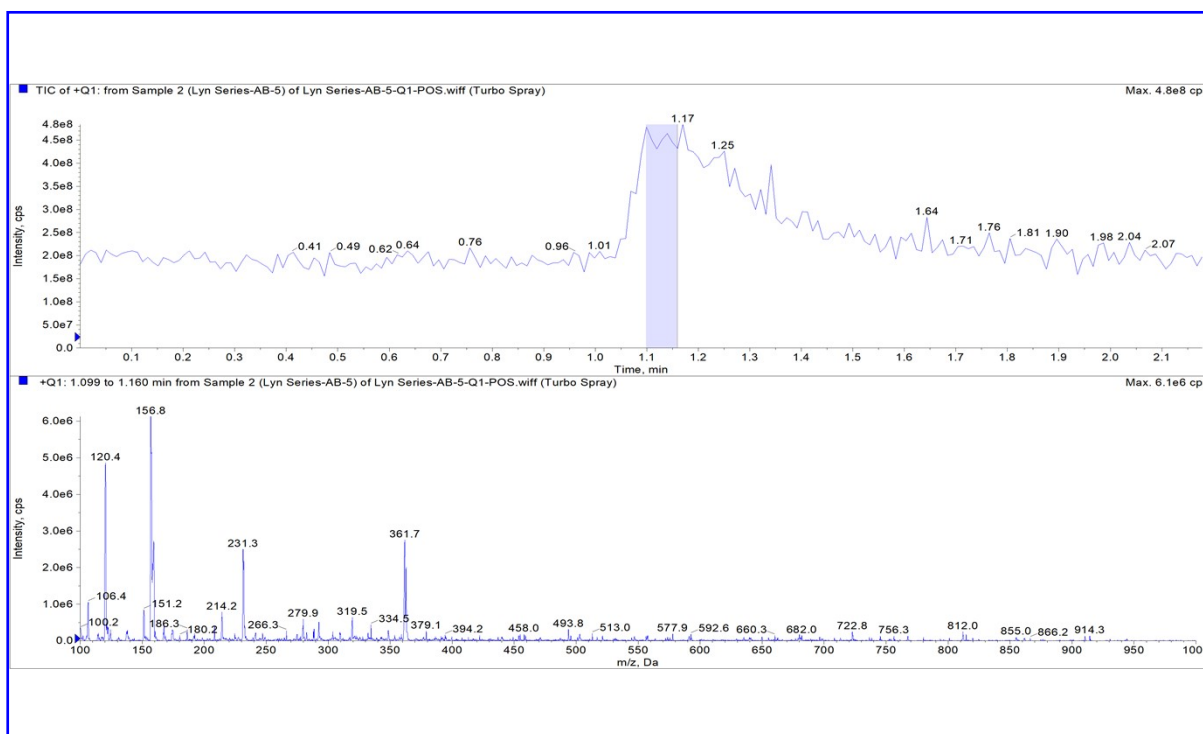
FTIR of compound 9-(furan-2-yl)acenaphtho[1,2-b]quinoxaline (5d)



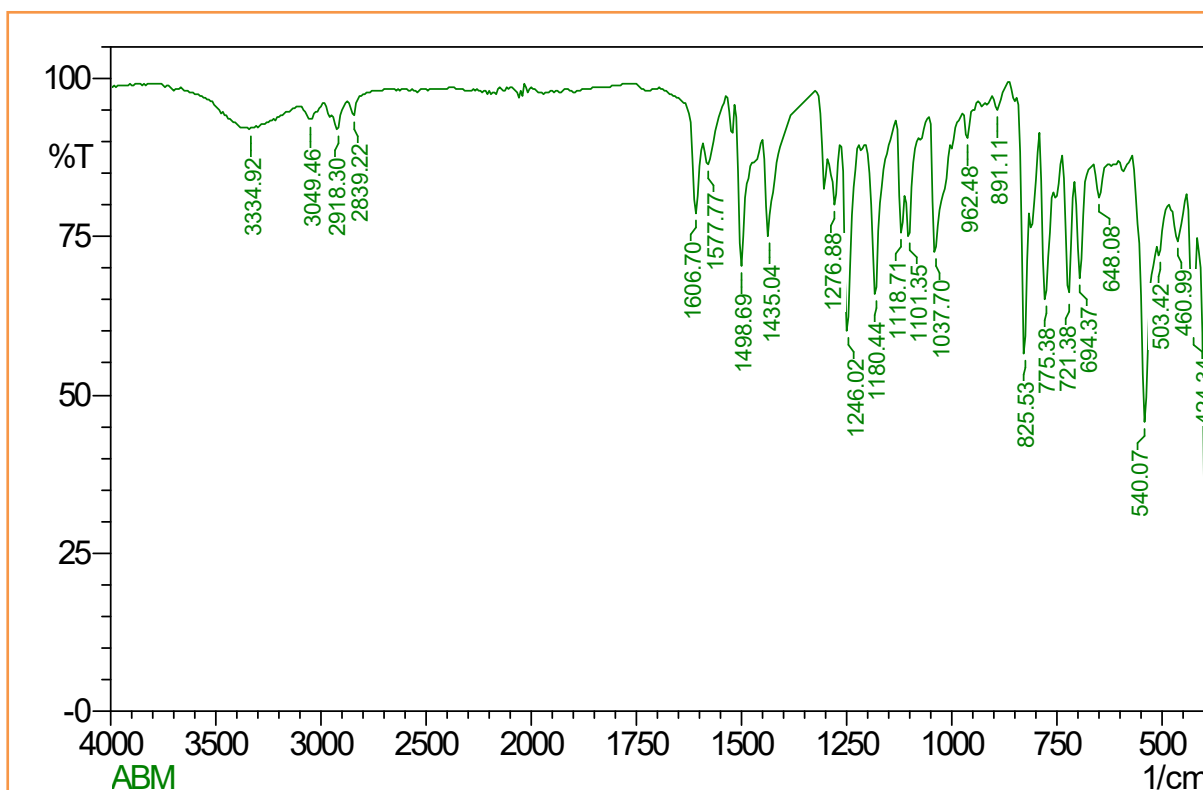
UPLC purity profile of compound 9-(furan-2-yl)acenaphtho[1,2-b]quinoxaline (5d)



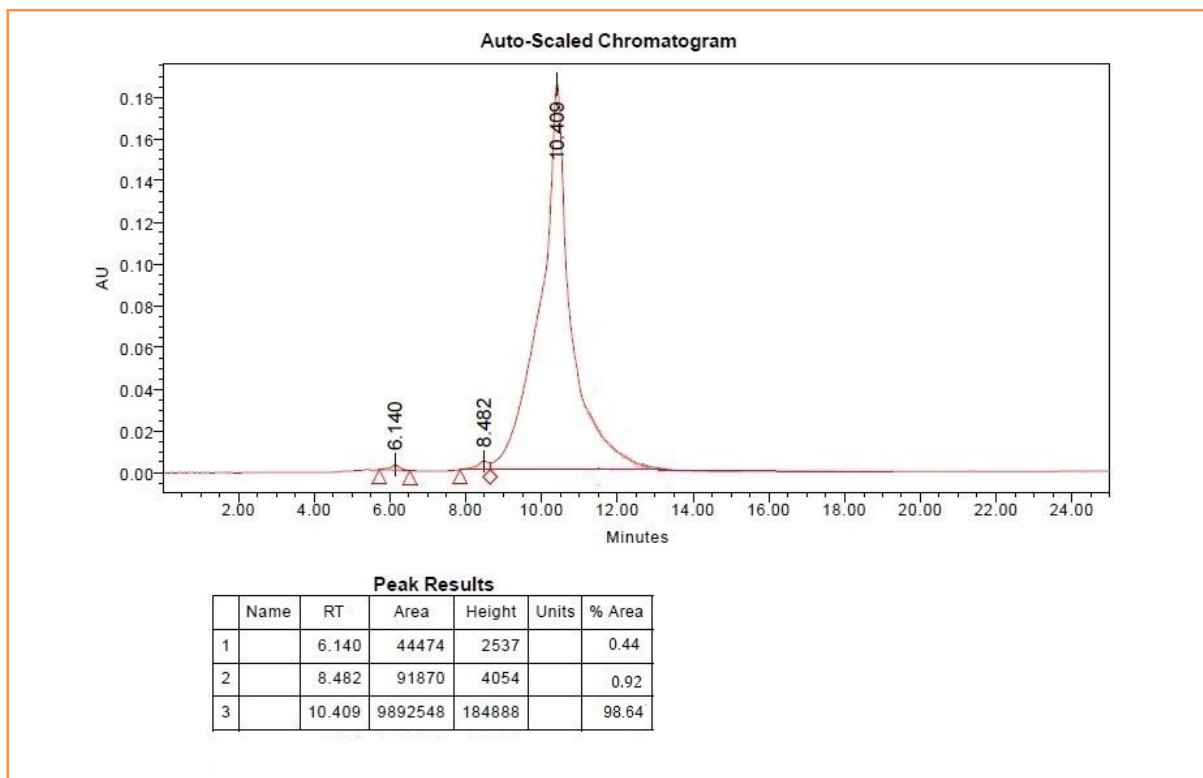
ESI-MS of compound 9-(4-methoxyphenyl)acenaphtho[1,2-b]quinoxaline (5e)



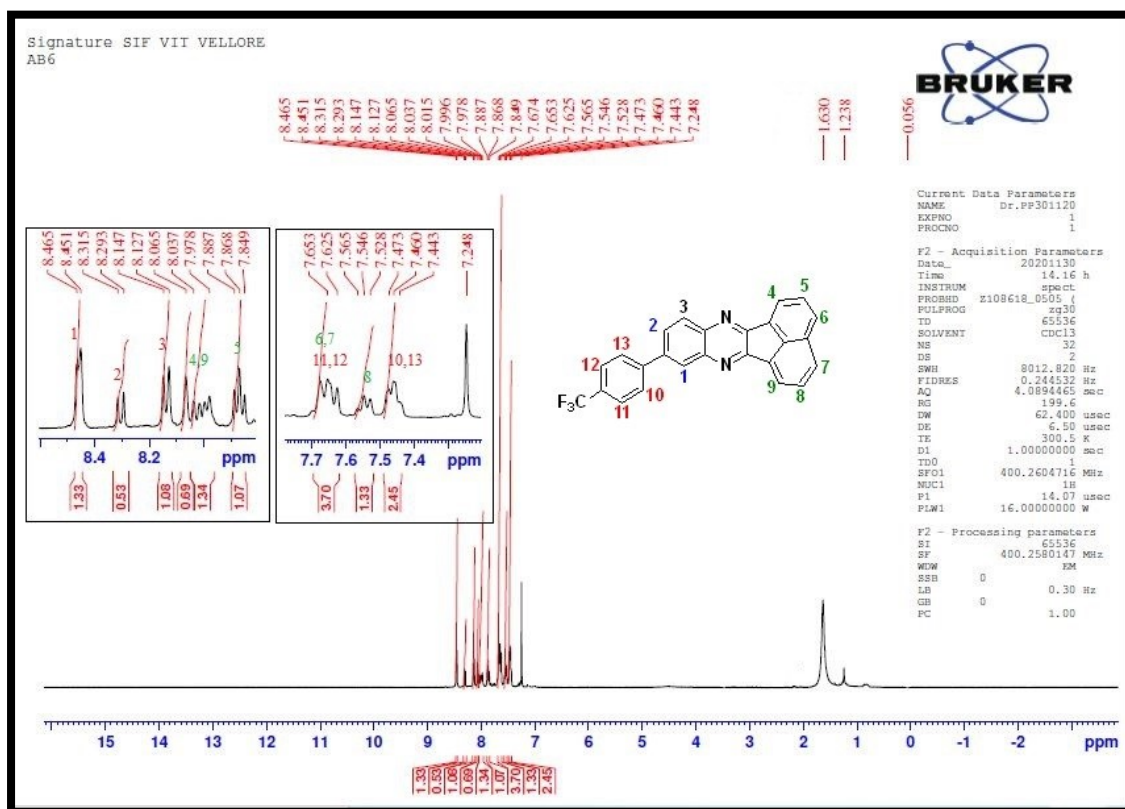
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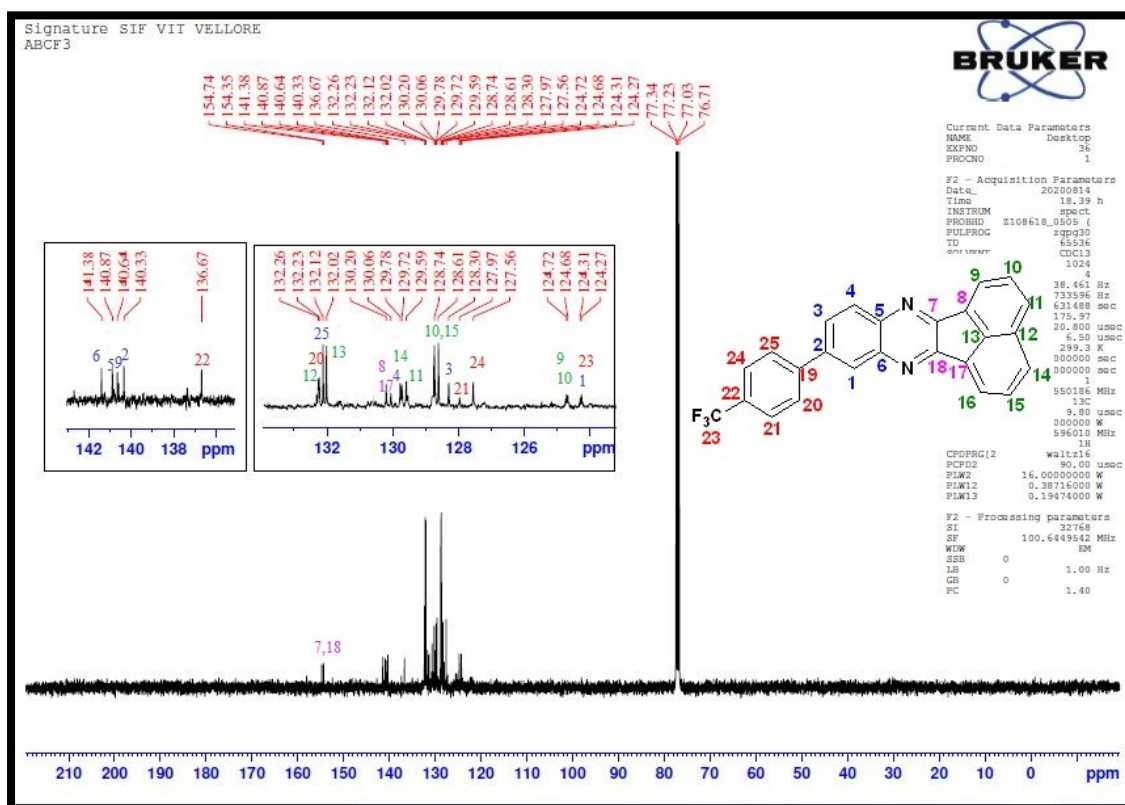
UPLC purity profile of compound 9-(4-methoxyphenyl)acenaphtho[1,2-b]quinoxaline (5e)



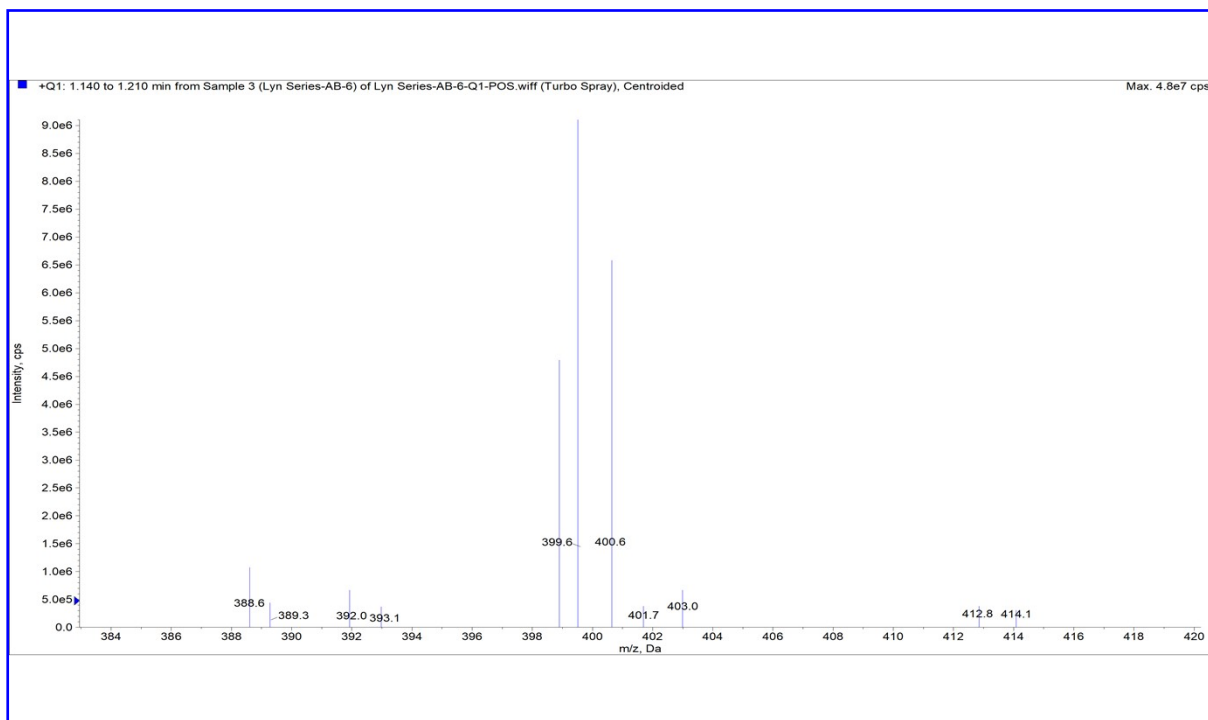
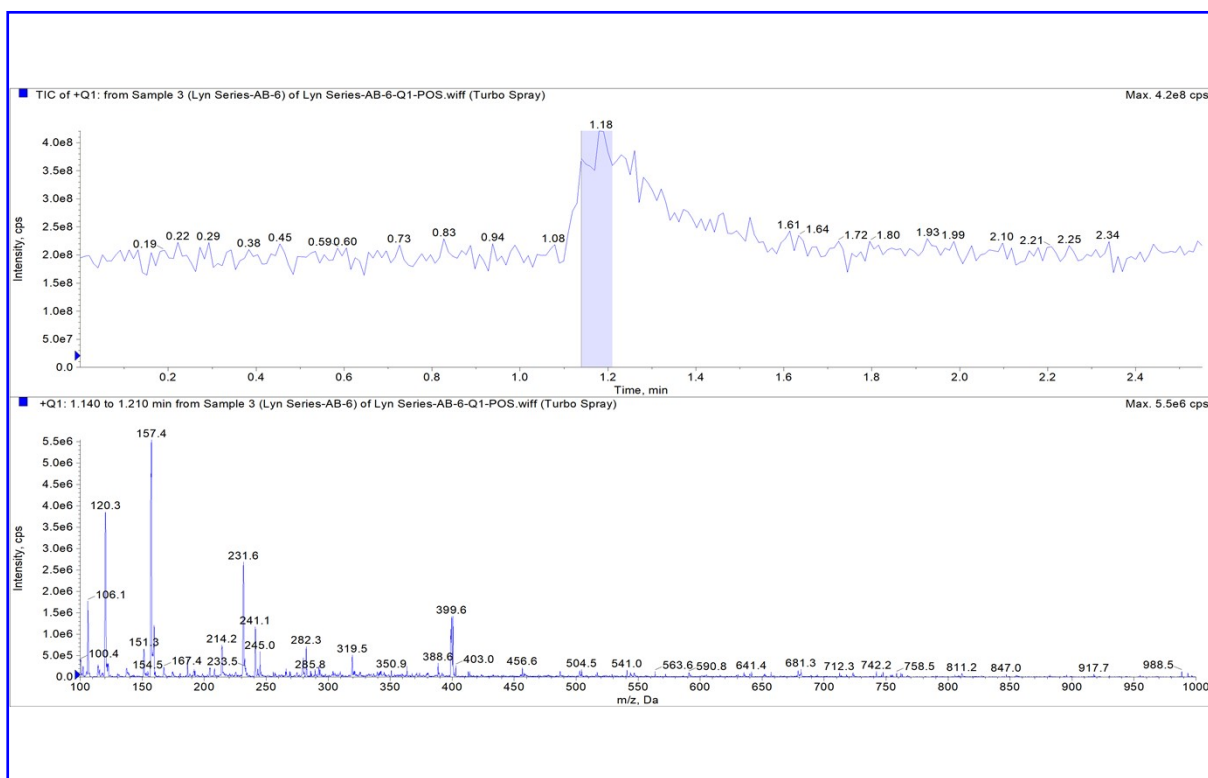
¹H NMR of compound 9-(4-(trifluoromethyl)phenyl)acenaphtho[1,2-b]quinoxaline (5f)



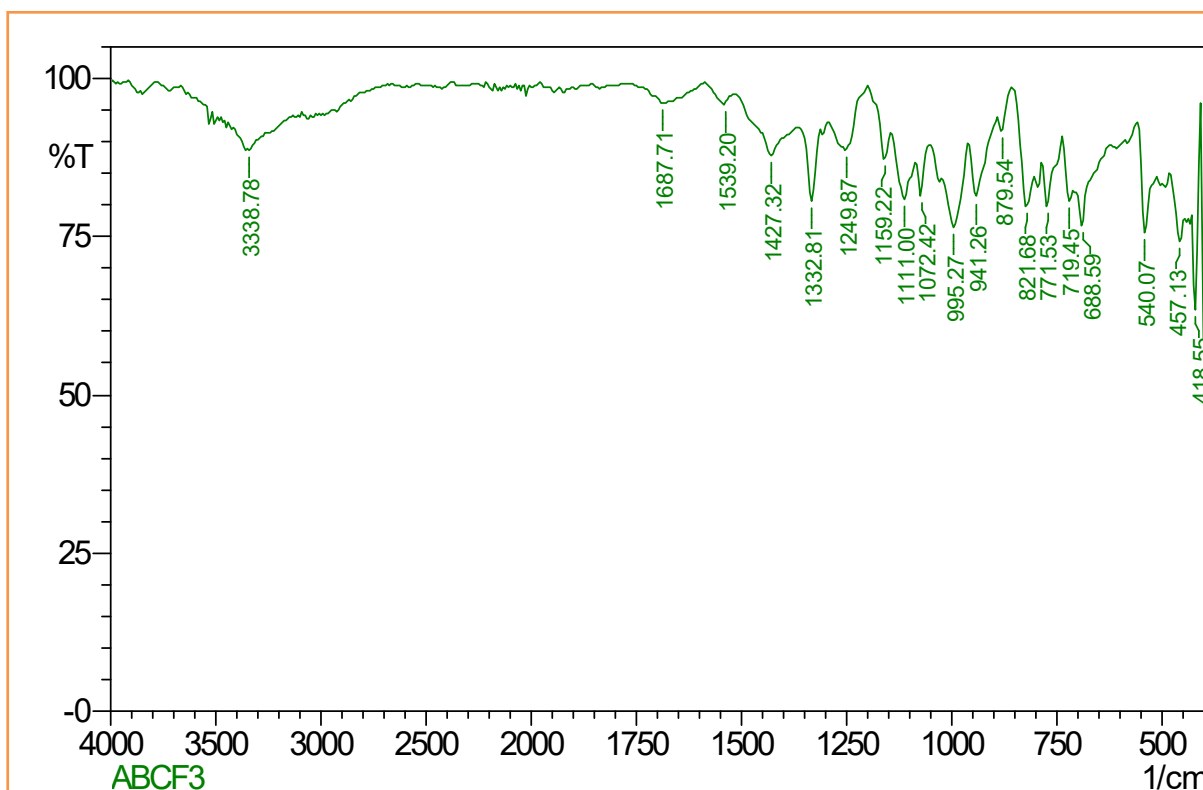
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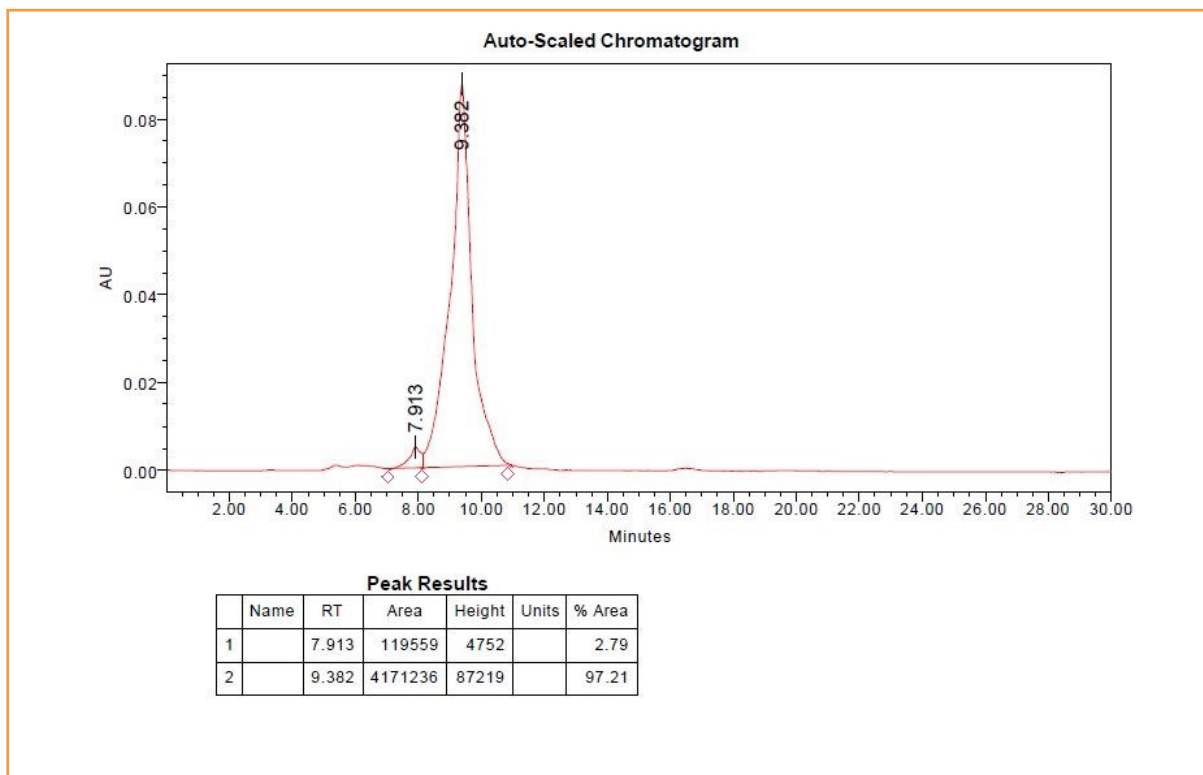
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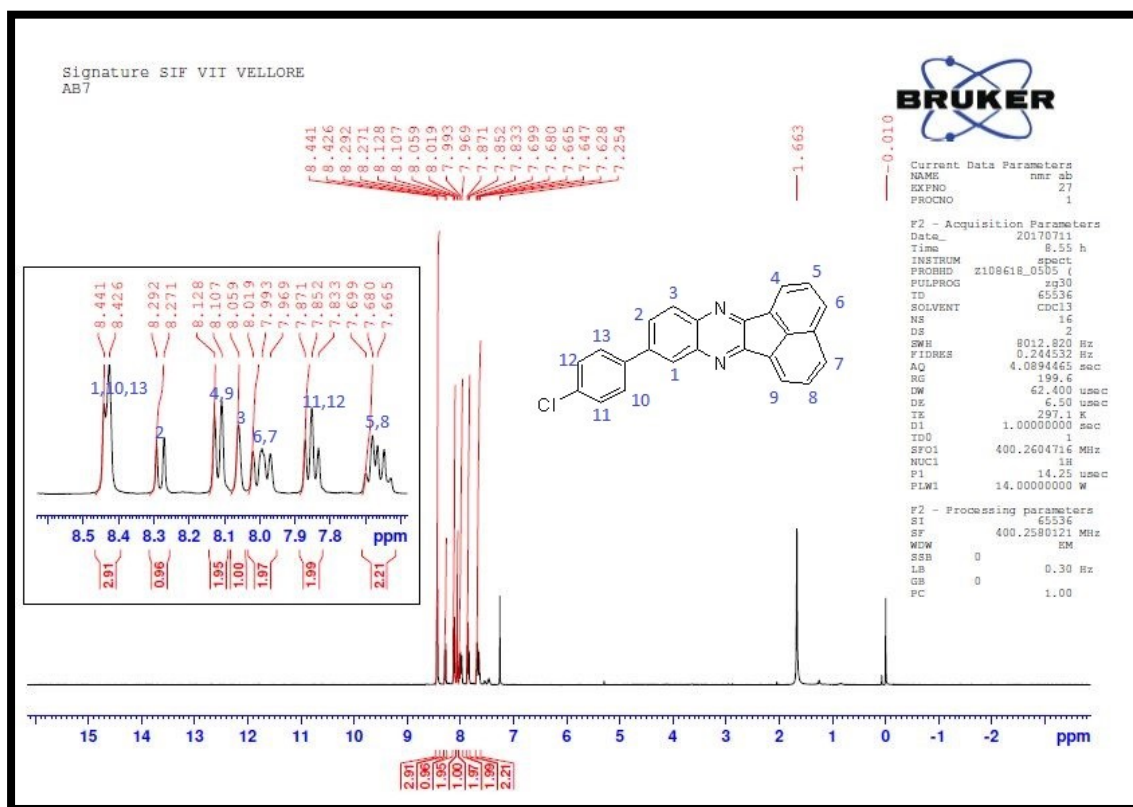
FTIR of compound 9-(4-(trifluoromethyl)phenyl)acenaphtho[1,2-b]quinoxaline (5f)



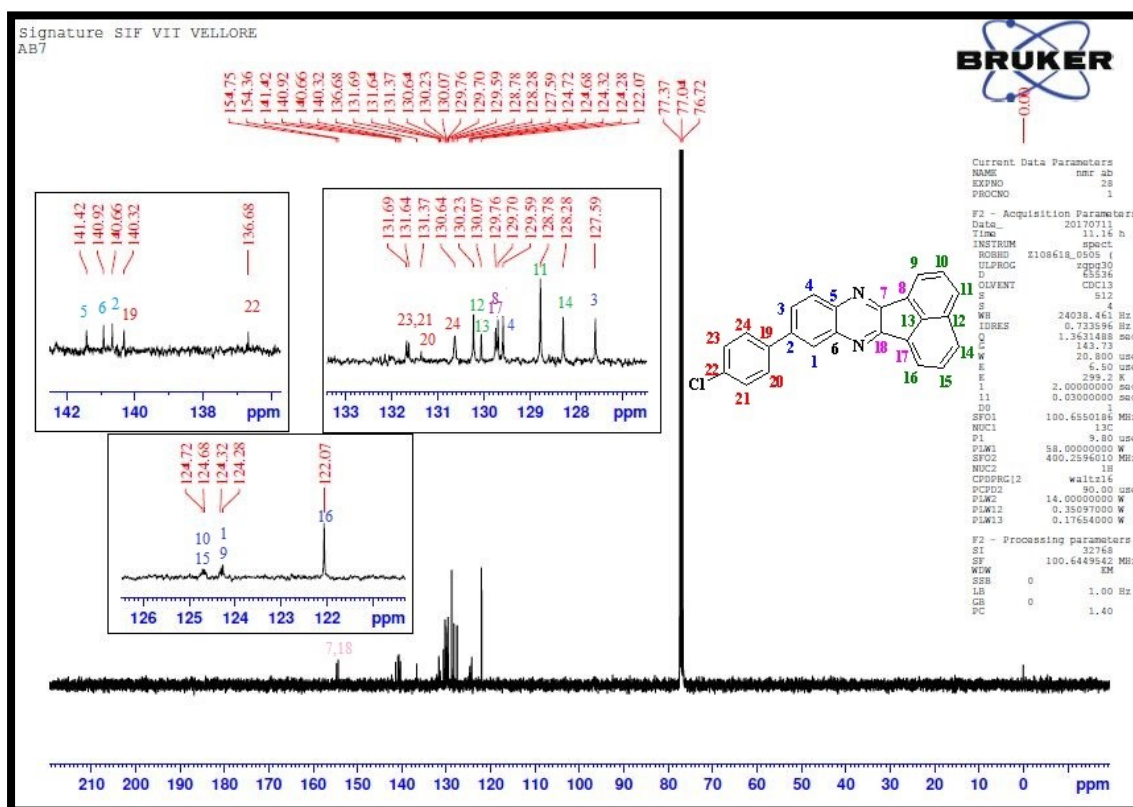
UPLC purity profile of compound 9-(4-(trifluoromethyl)phenyl)acenaphtho[1,2-b]quinoxaline (5f)



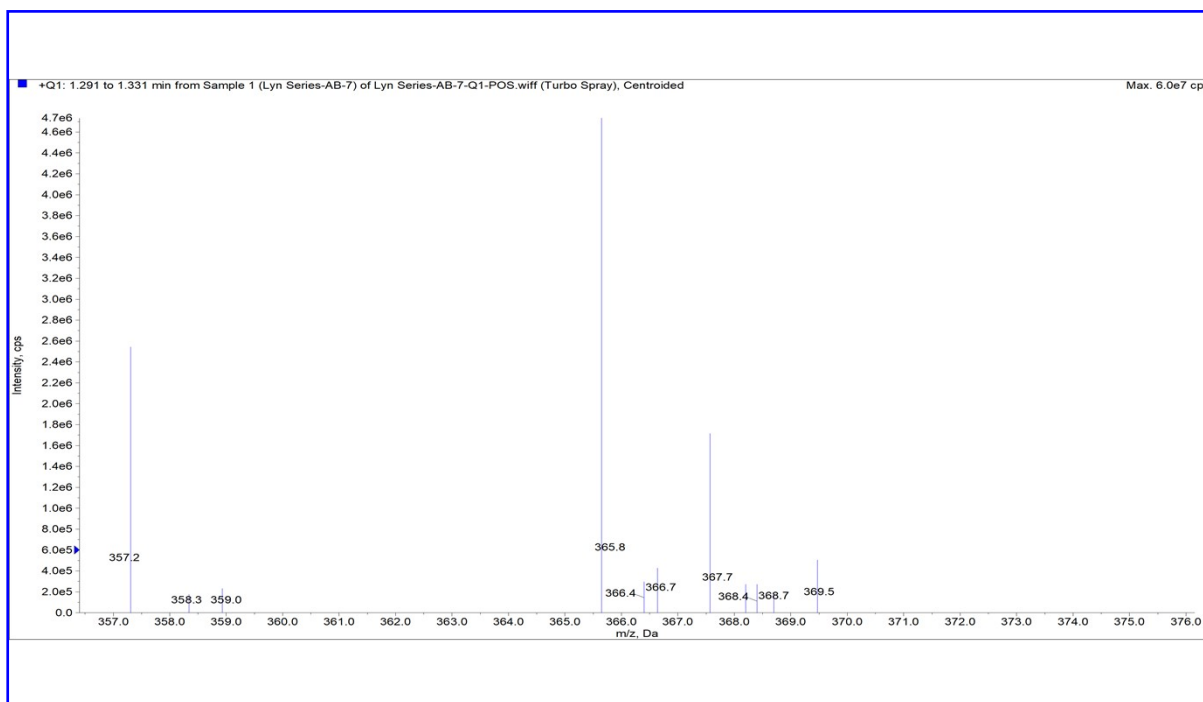
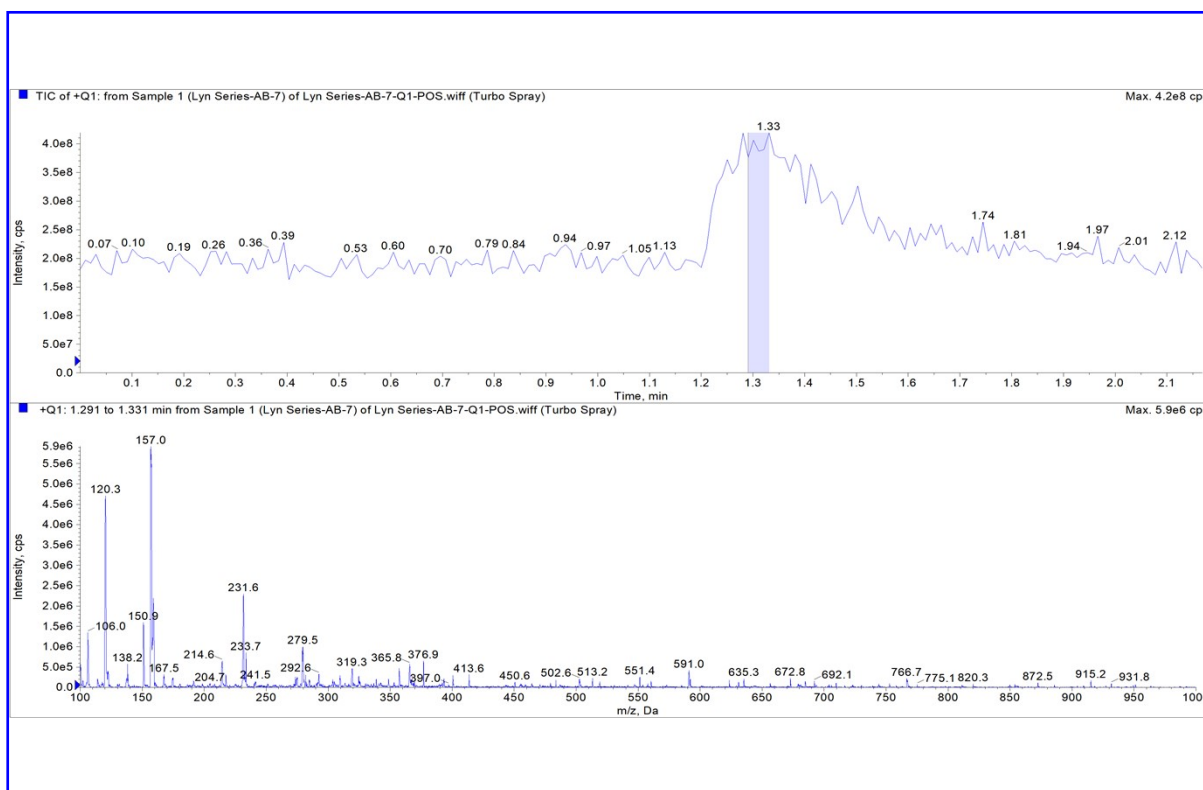
¹H NMR of compound 9-(4-chlorophenyl)acenaphtho[1,2-b]quinoxaline (5g)



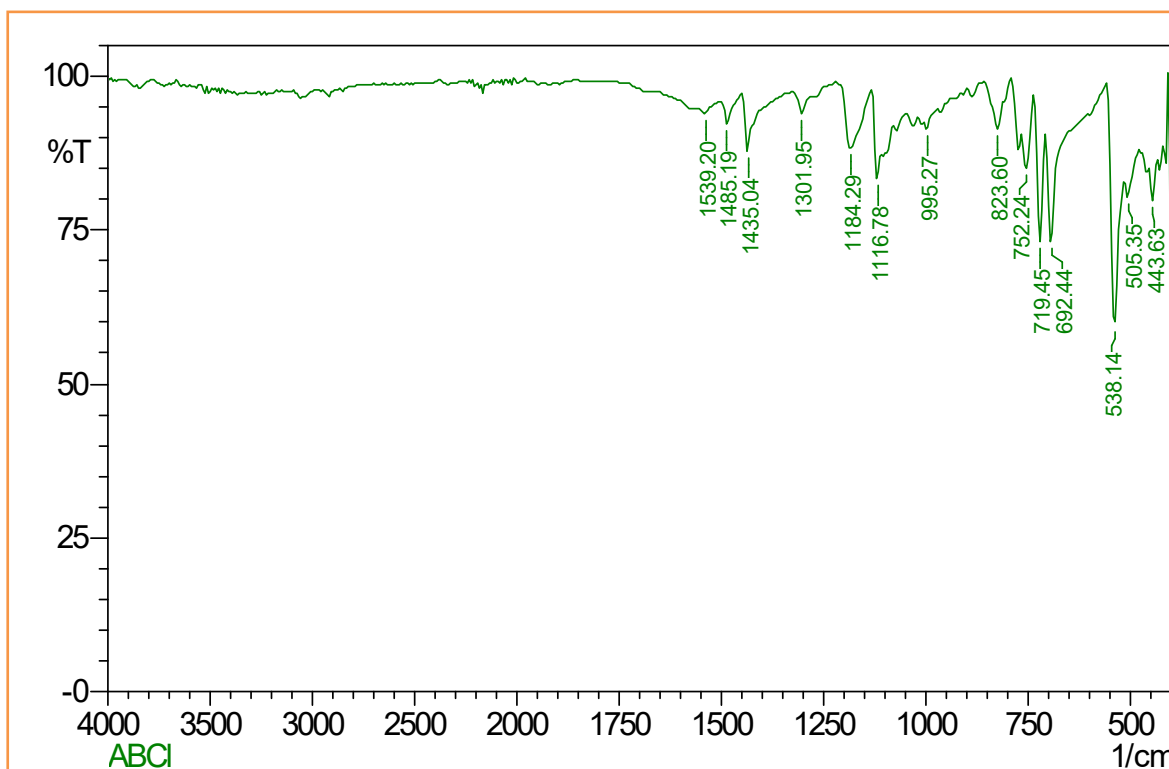
¹³C NMR spectrum of compound 9-(4-chlorophenyl)acenaphtho[1,2-b]quinoxaline (5g)



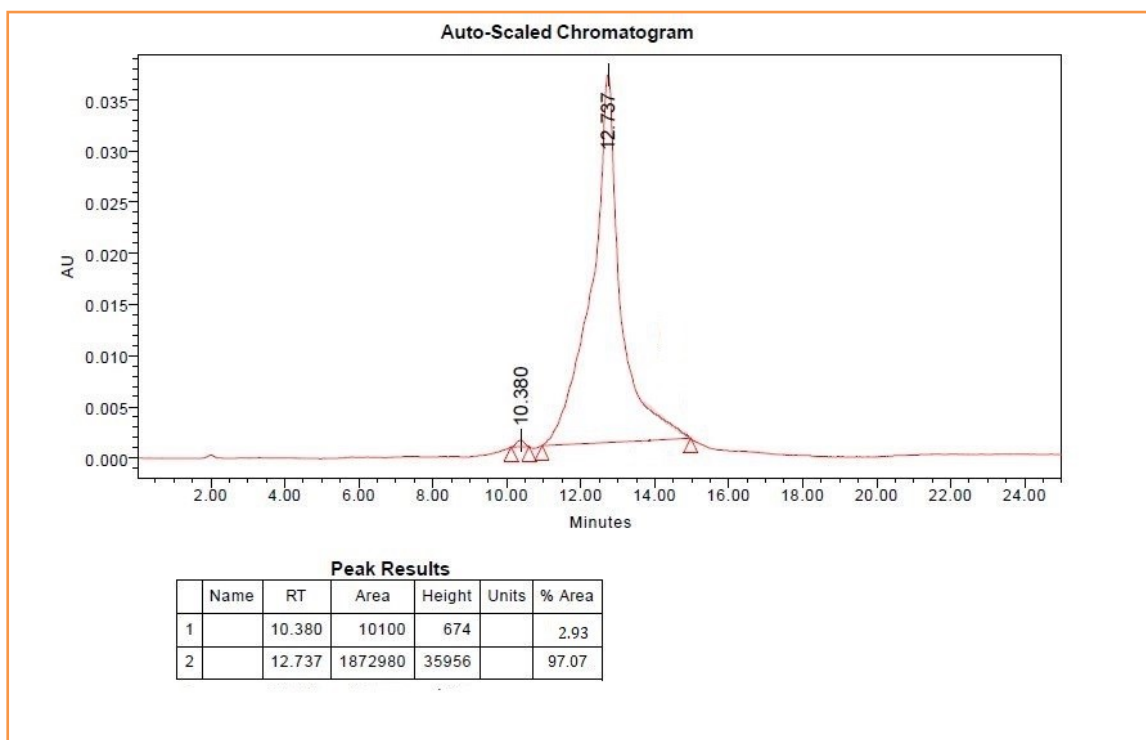
ESI-MS of compound 9-(4-chlorophenyl)acenaphtho[1,2-b]quinoxaline (5g)



FTIR of compound 9-(4-chlorophenyl)acenaphtho[1,2-b]quinoxaline (5g)



UPLC purity profile of compound 9-(4-chlorophenyl)acenaphtho[1,2-b]quinoxaline (5g)



Cell Viability Plot

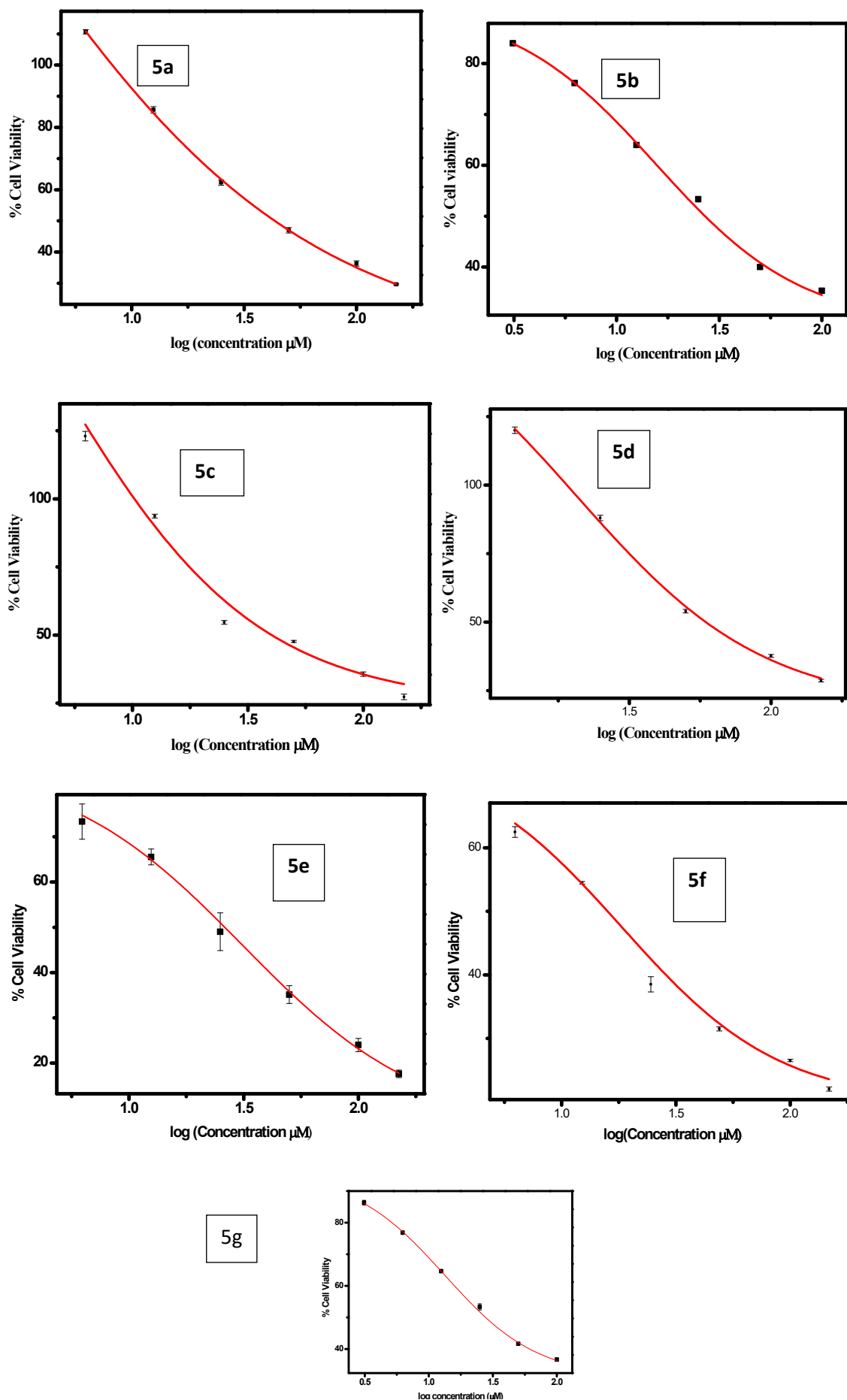


Fig S1: Cell viability vs log[5a-g] plot for HeLa cell line

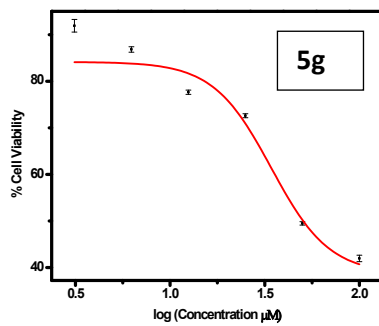
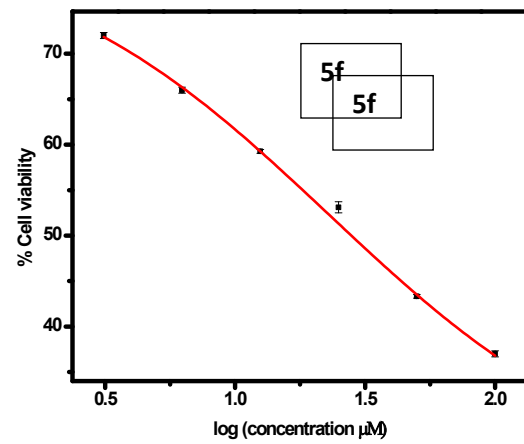
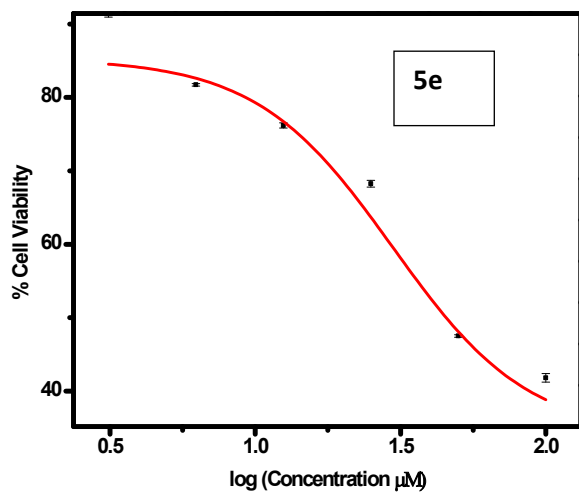
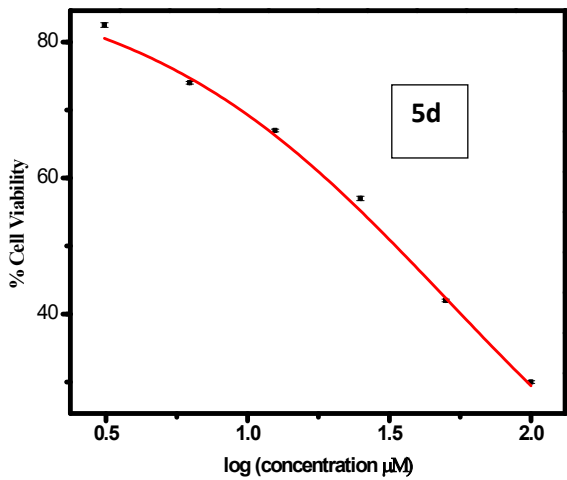
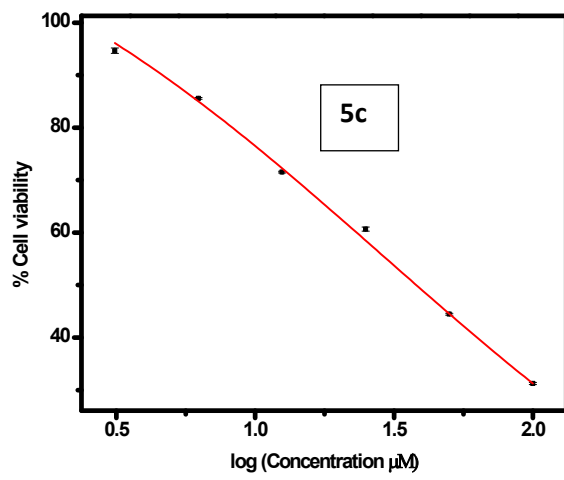
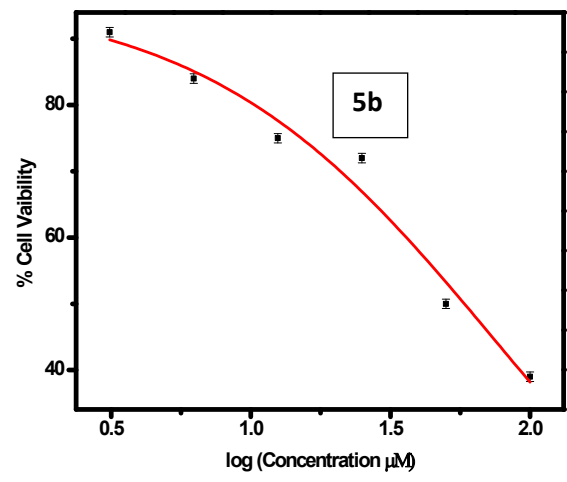
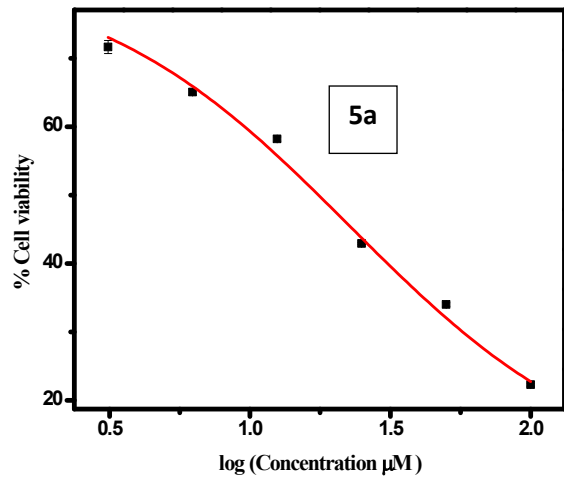


Fig S2: Cell viability vs log[5a-g] plot for U87MG cell line

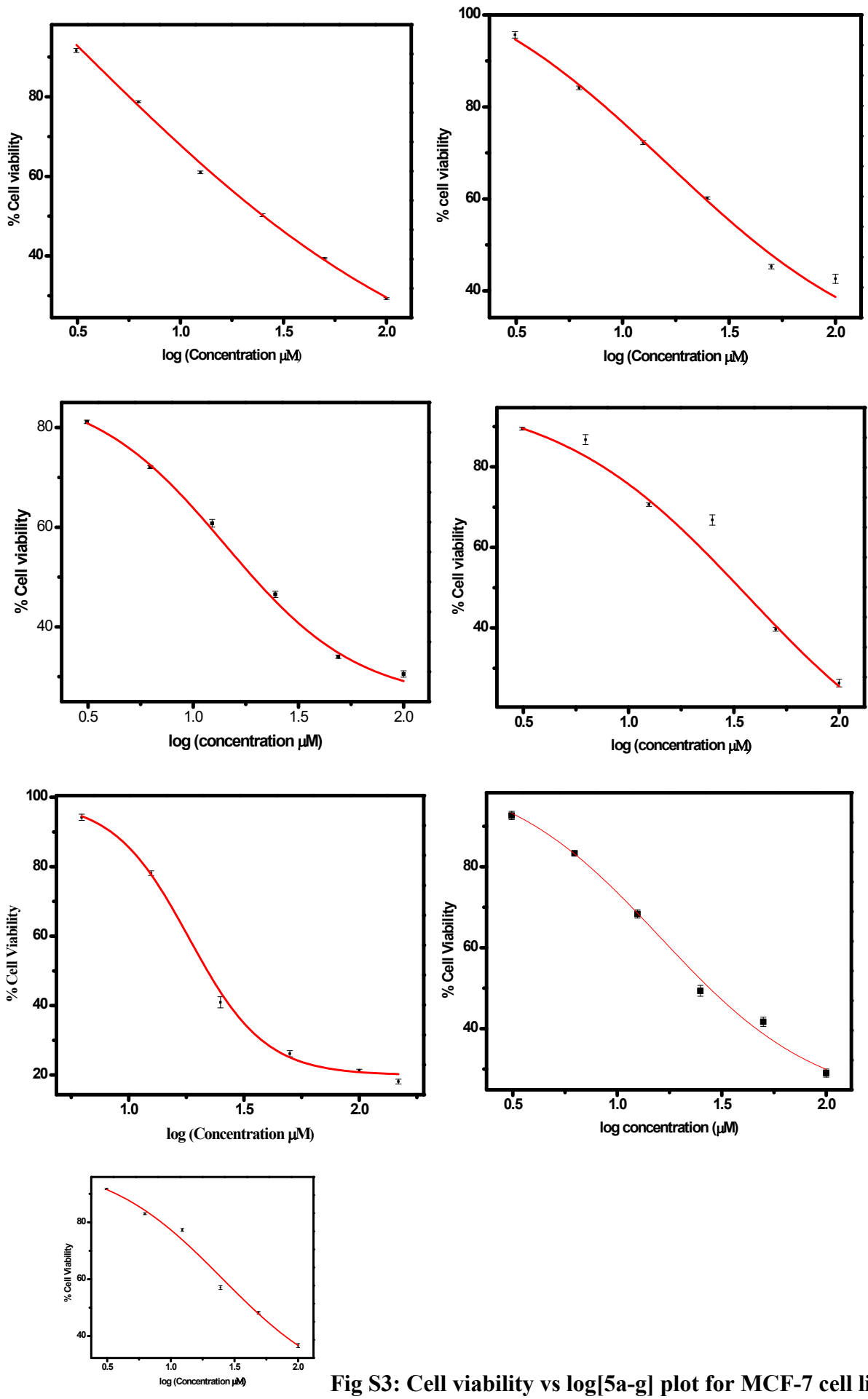


Fig S3: Cell viability vs log[5a-g] plot for MCF-7 cell line

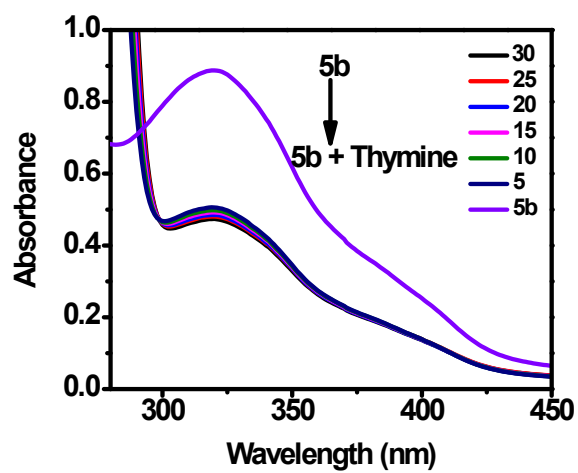
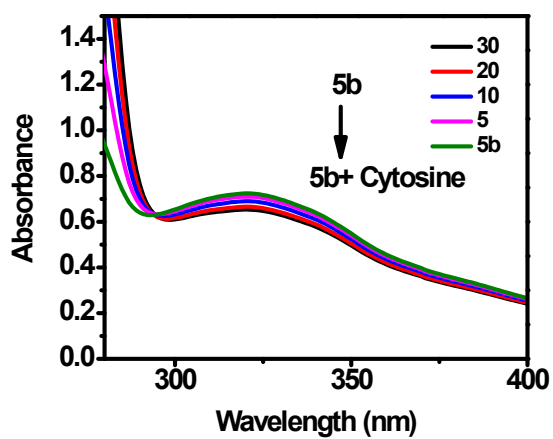
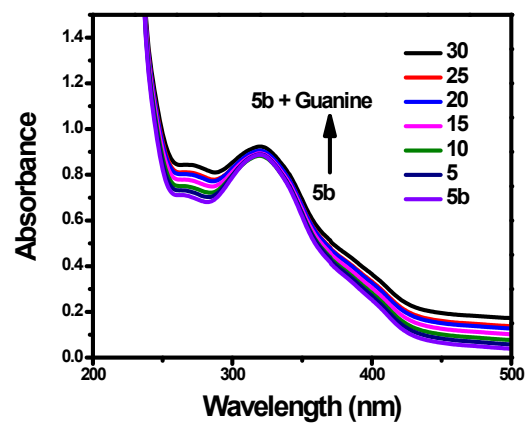
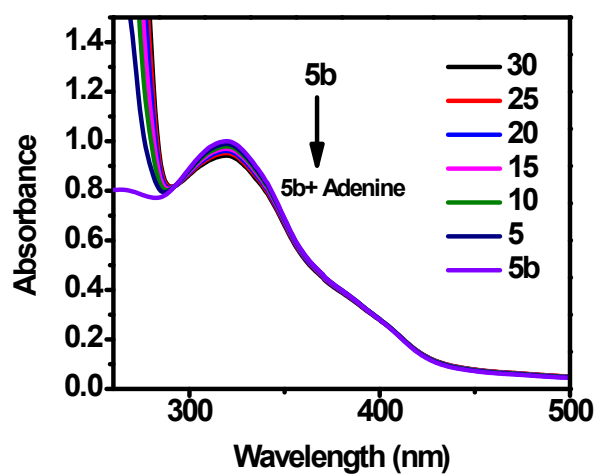


Fig. S4 ATGC titration with compound 5b