

Supplementary file

2,5-Bis(2,2,2-trifluoroethoxy)phenyl-tethered 1,3,4-Oxadiazoles Derivatives: Synthesis, In Silico Studies, and Biological Assessment as Potential Candidates for Anti-Cancer and Anti-Diabetic Agent

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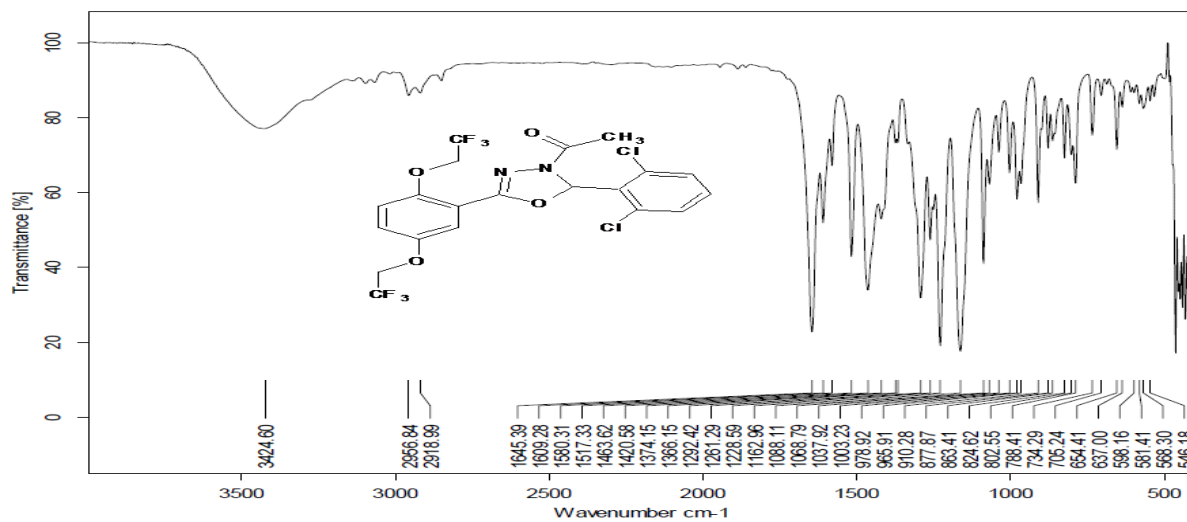
⁵ Central Research Laboratory, KS. Hegde Medical Academy, Nitte (Deemed to be University), Deralakatte, Mangalore 575018, India

⁶ Biophysical and Computational Chemistry Laboratory, Department of Chemistry, National Institute of Technology Karnataka, Surathkal, Mangalore 575025, India

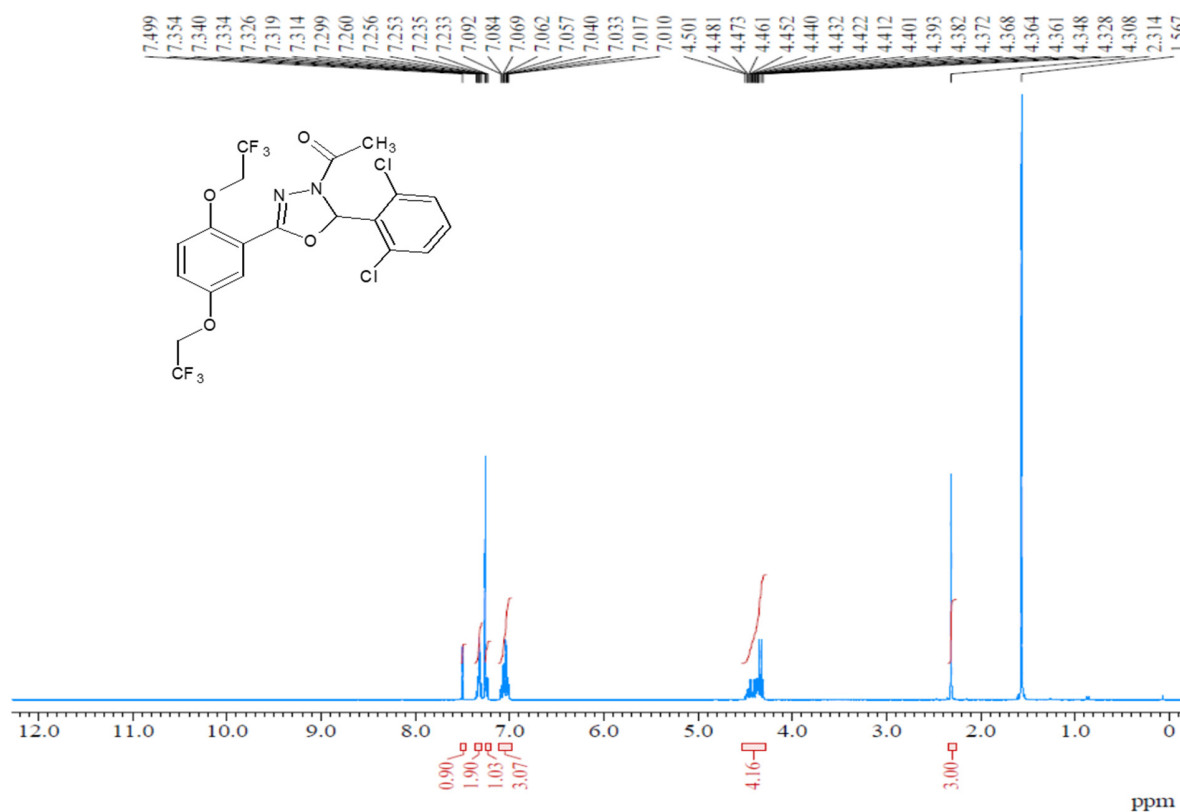
⁷ Department of Biochemistry, K.S. Hegde Medical Academy, Nitte (Deemed to be University), Deralakatte, Mangalore 575018, India

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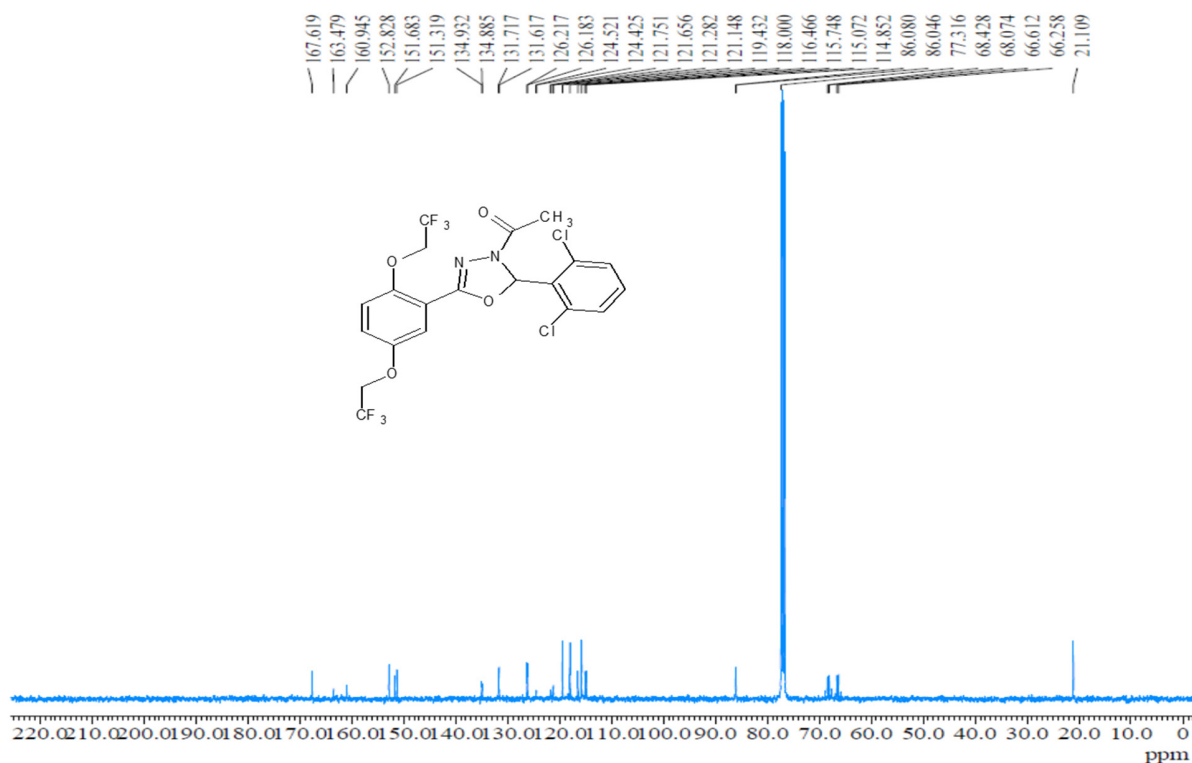
Supplementary file – Spectral data (IR, ^1H NMR, ^{13}C NMR, MASS Spectrum) of synthesized compounds



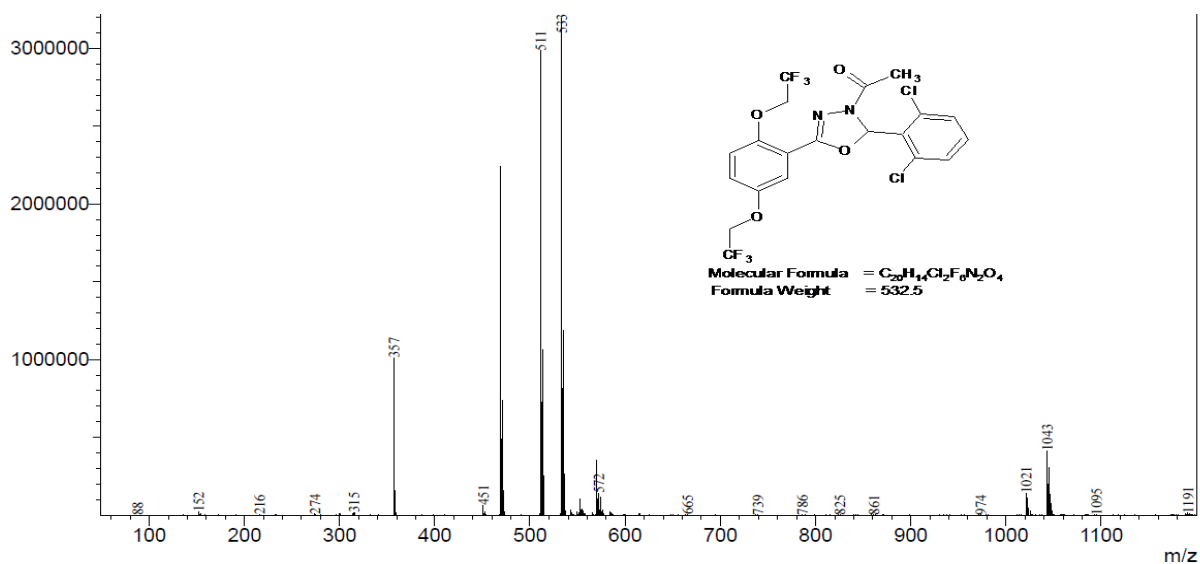
S.1: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,6-dichlorophenyl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5a)



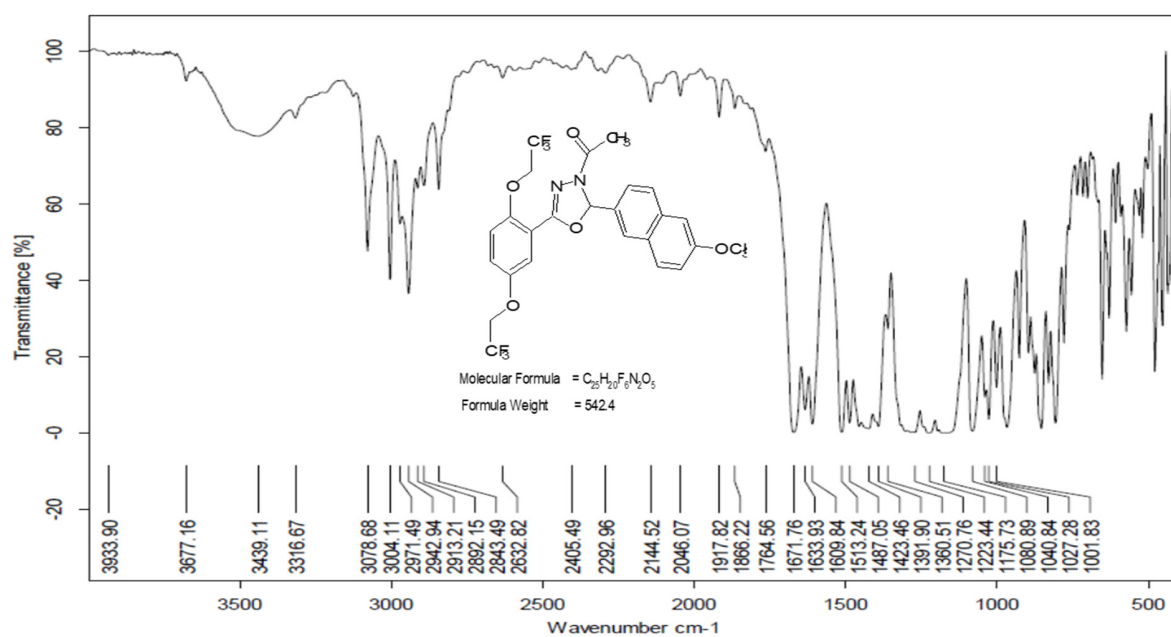
S.2: ^1H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,6-dichlorophenyl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5a)



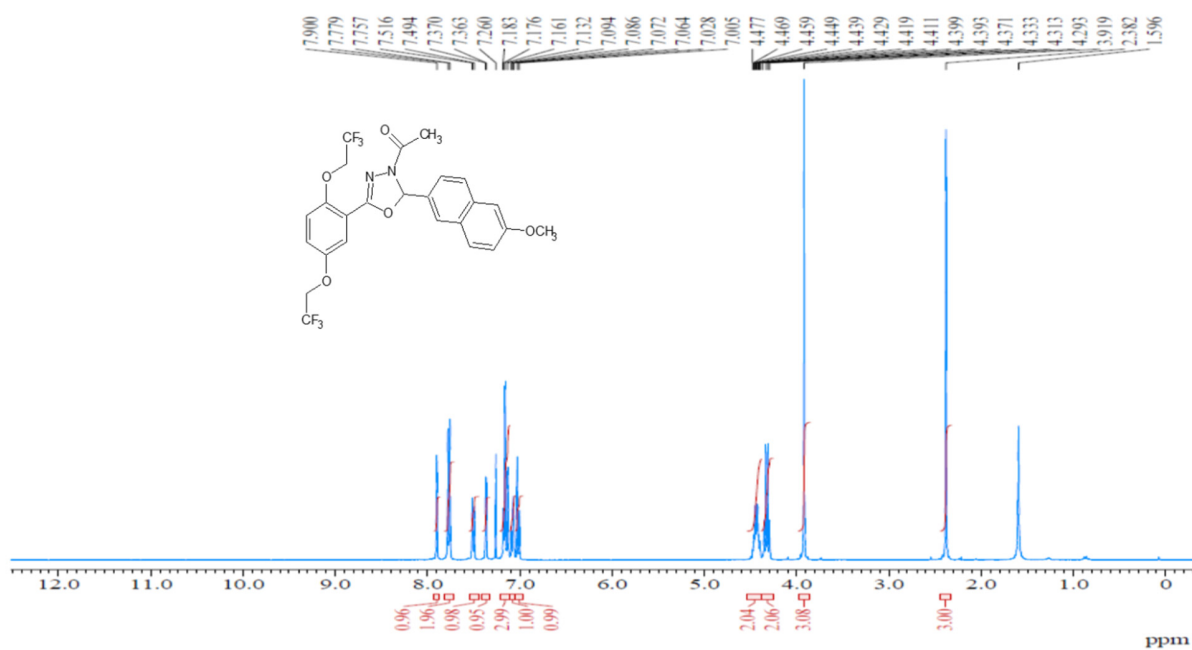
S.3: ¹³C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,6-dichlorophenyl)-1,3,4-oxadiazol-3(2H)-yl} ethanone(5a)



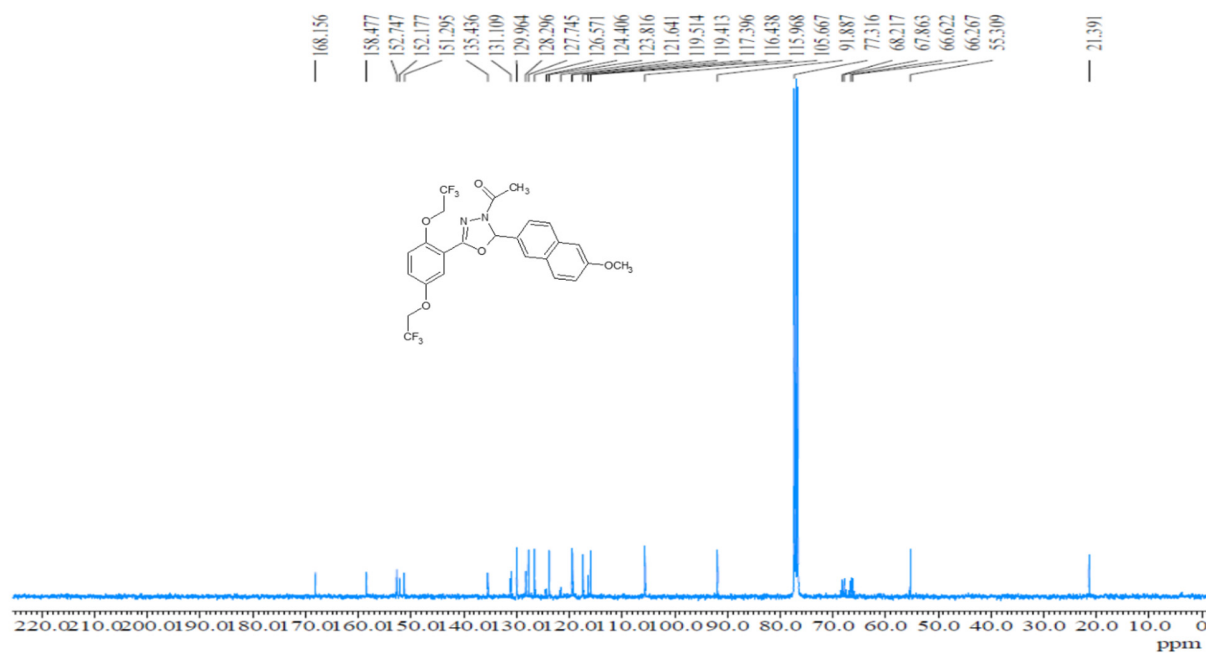
S.4: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,6-dichlorophenyl)-1,3,4-oxadiazol-3(2H)-yl} ethanone(5a)



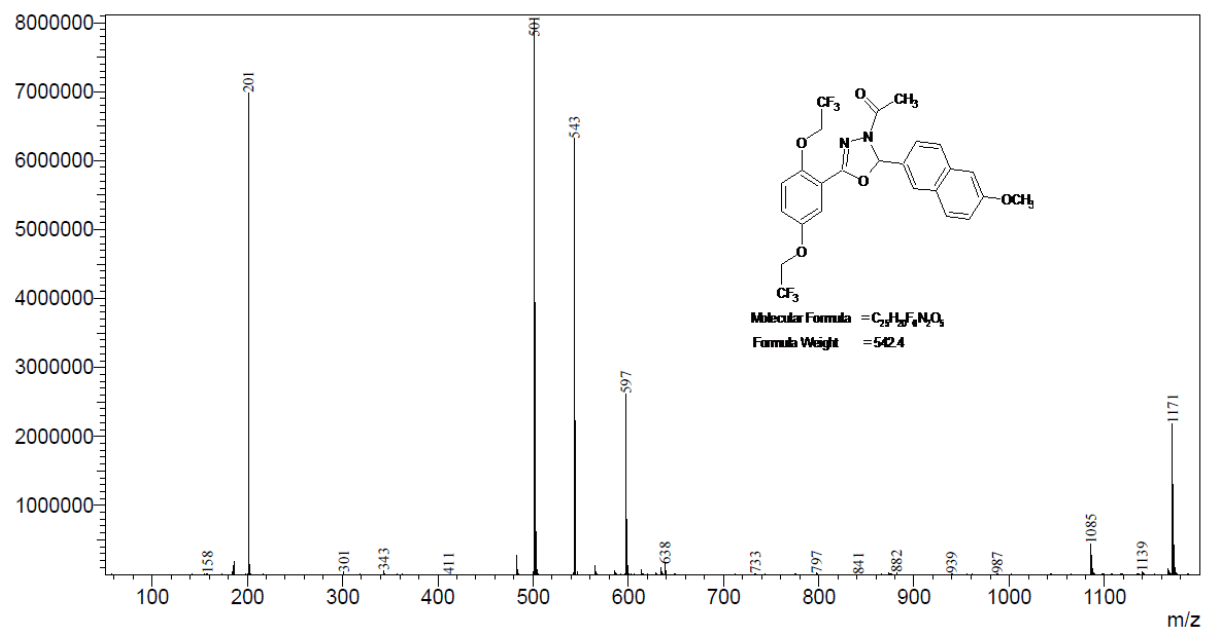
S.5: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(6-methoxy naphthalyl)-1,3,4-oxadiazol-3(2H)-yl} ethanone(5b)



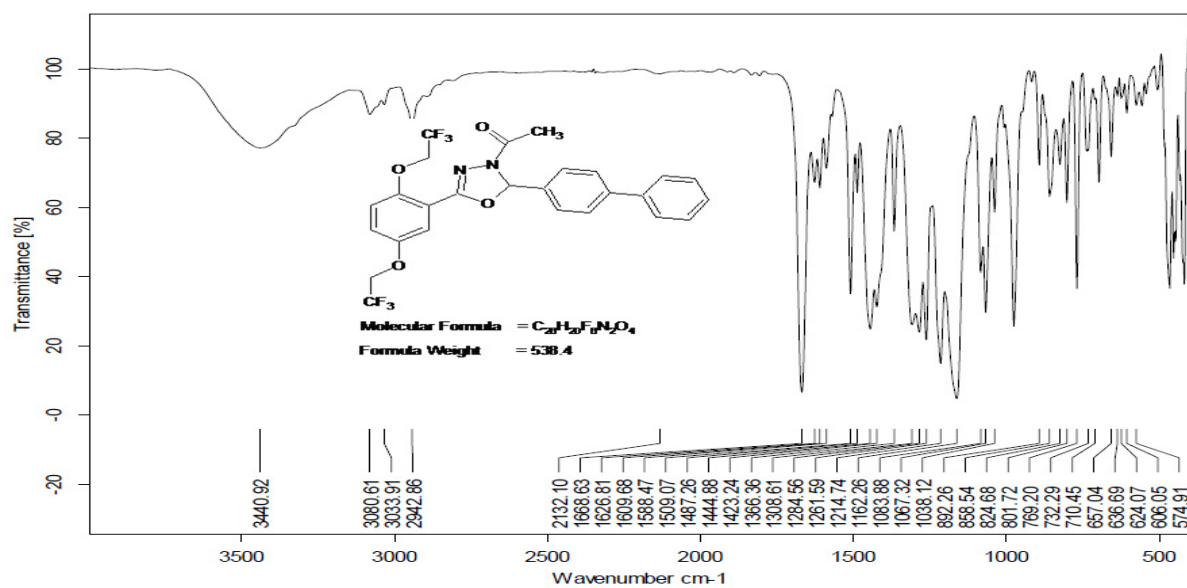
S.6: ¹H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(6-methoxy naphthalyl)-1,3,4-oxadiazol-3(2H)-yl} ethanone(5b)



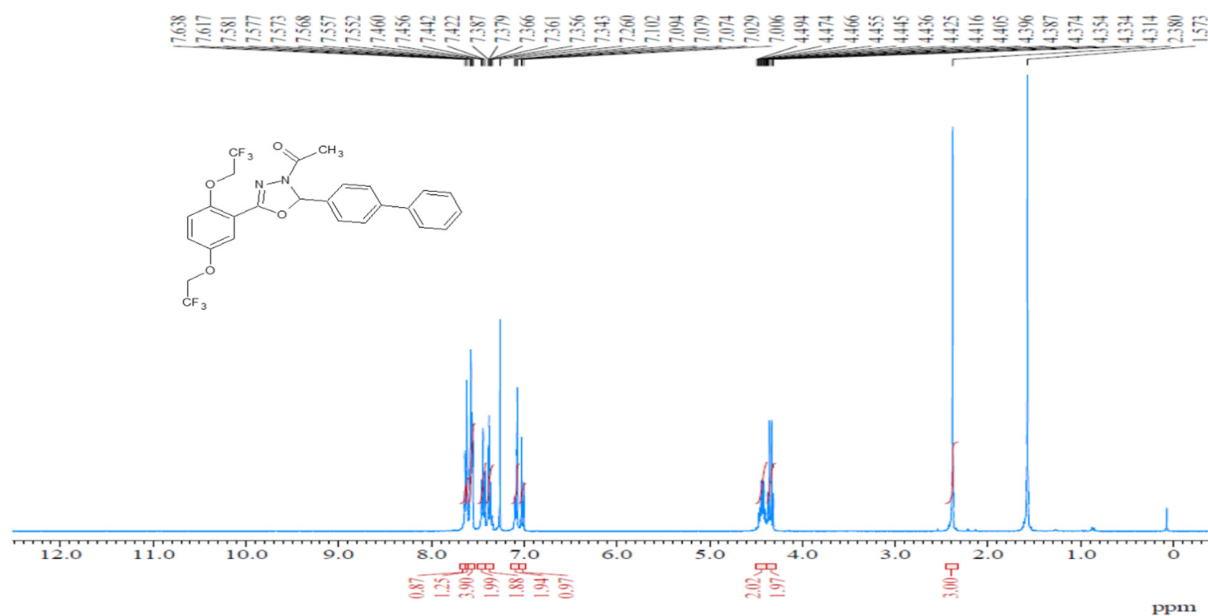
S.7: ^{13}C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(6-methoxy naphthyl)-1,3,4-oxadiazol-3(2*H*)-yl}ethanone(5b)



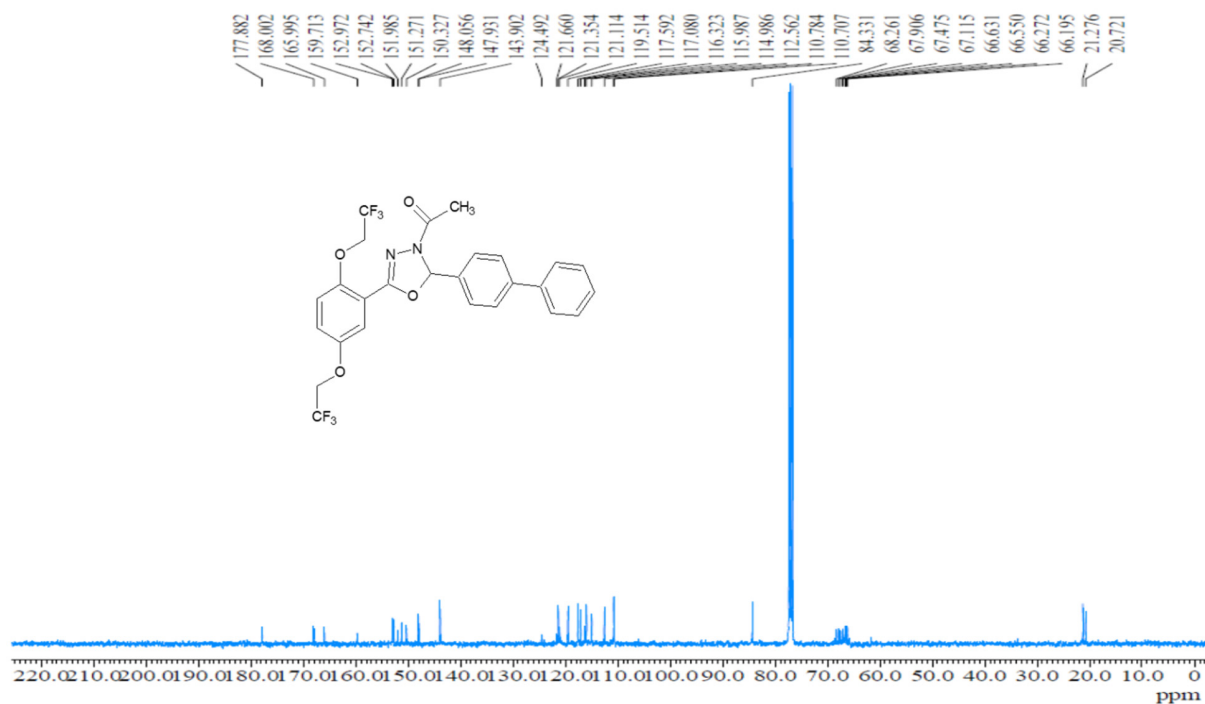
S.8: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(6-methoxy naphthyl)-1,3,4-oxadiazol-3(2*H*)-yl}ethanone(5b)



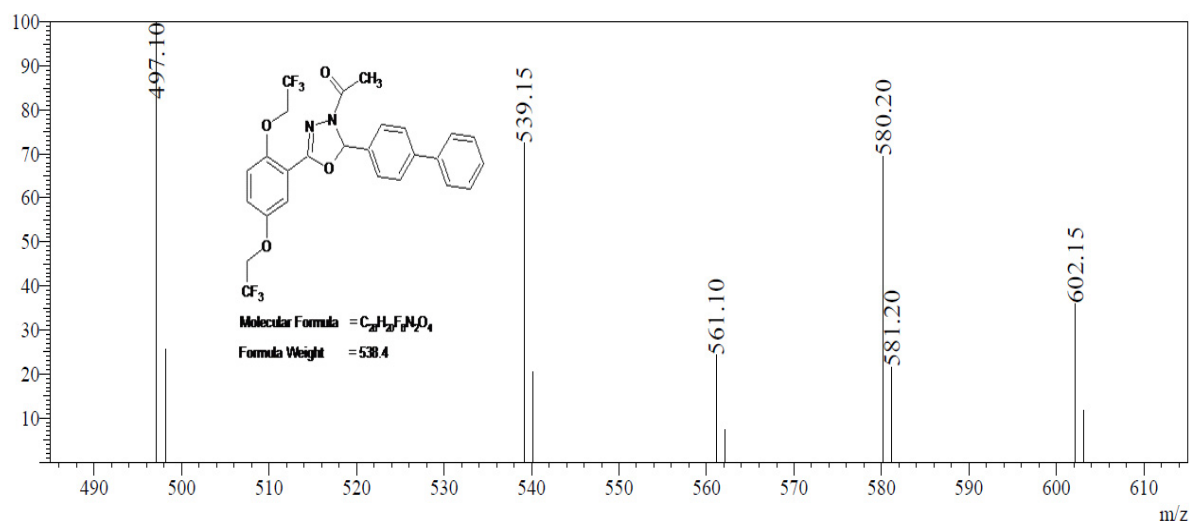
S.9: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-biphenyl)-1,3,4-oxadiazol-3(2*H*)-yl}ethanone(5c)



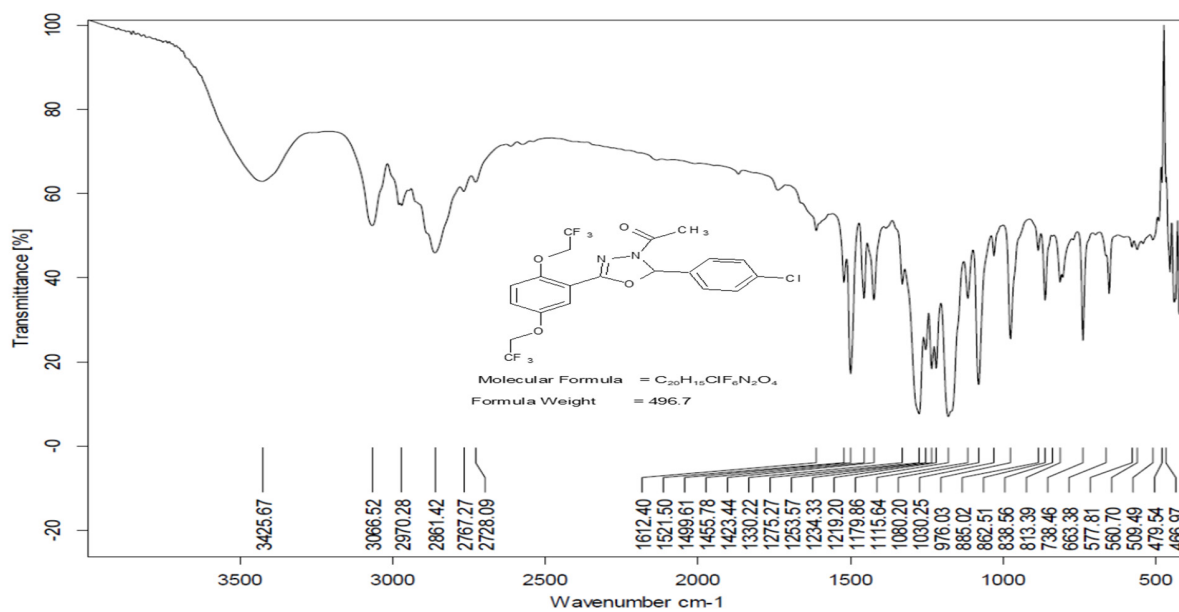
S.10: ¹H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-biphenyl)-1,3,4-oxadiazol-3(2*H*)-yl}ethanone(5c)



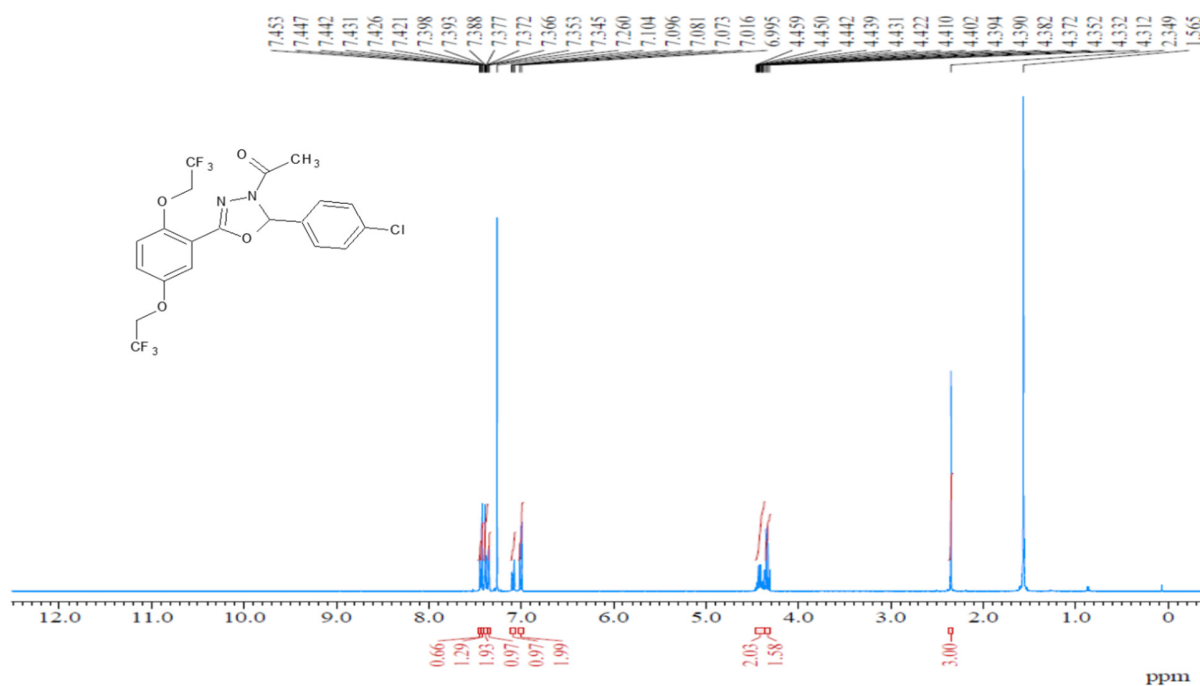
S.11: ^{13}C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-biphenyl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5c)



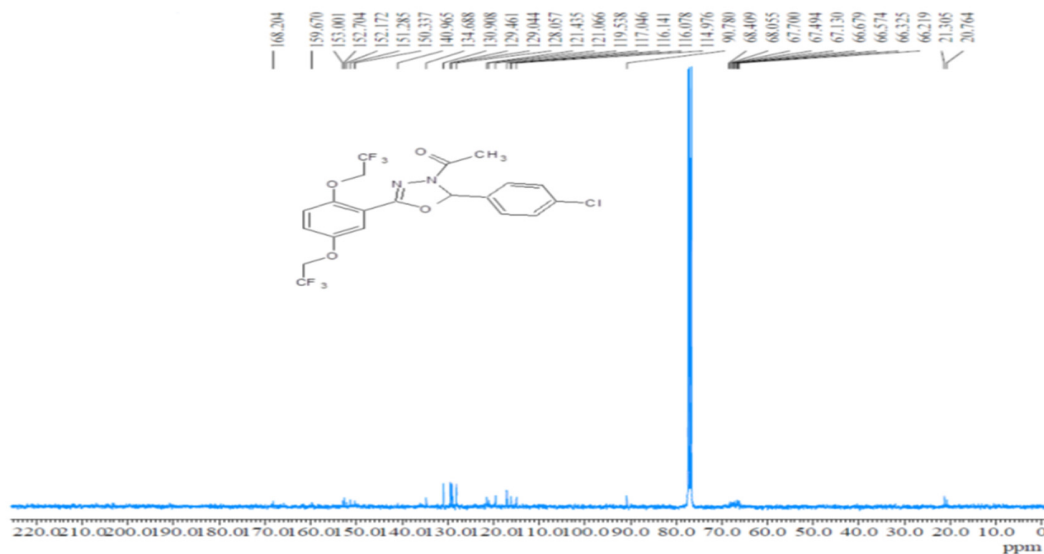
S.12: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-biphenyl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5c)



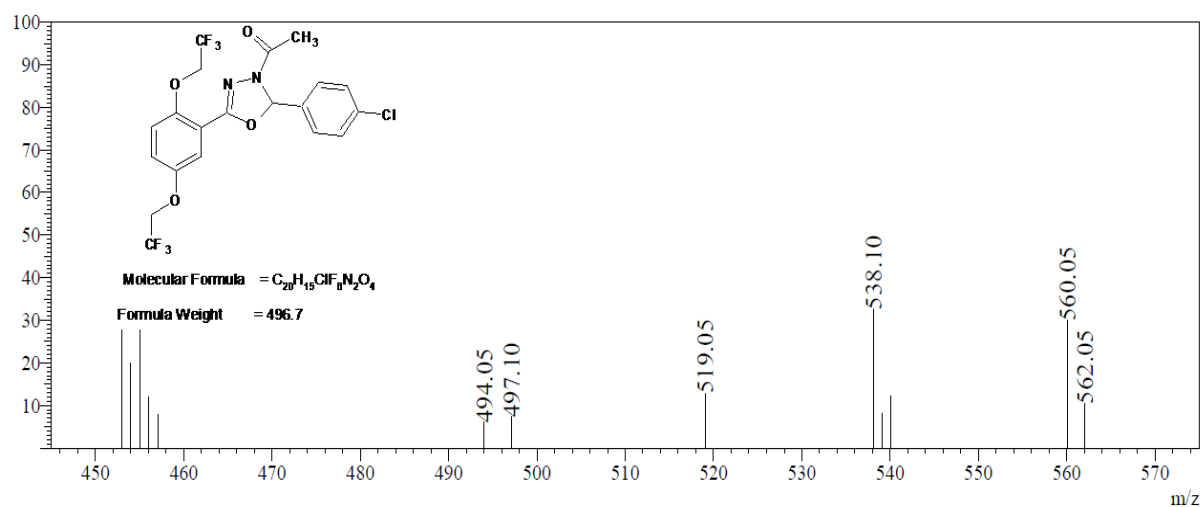
S.13: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-chloro phenyl)-1,3,4-oxadiazol-3(2*H*)-yl}ethanone(5d)



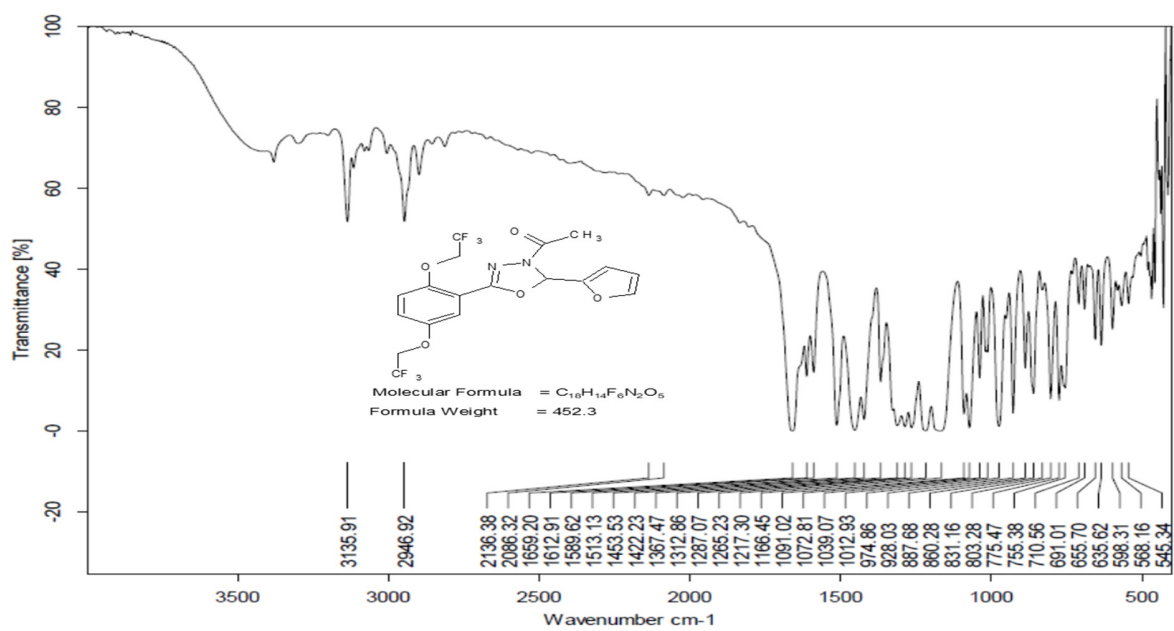
S.14: ¹H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-chloro phenyl)-1,3,4-oxadiazol-3(2*H*)-yl}ethanone(5d)



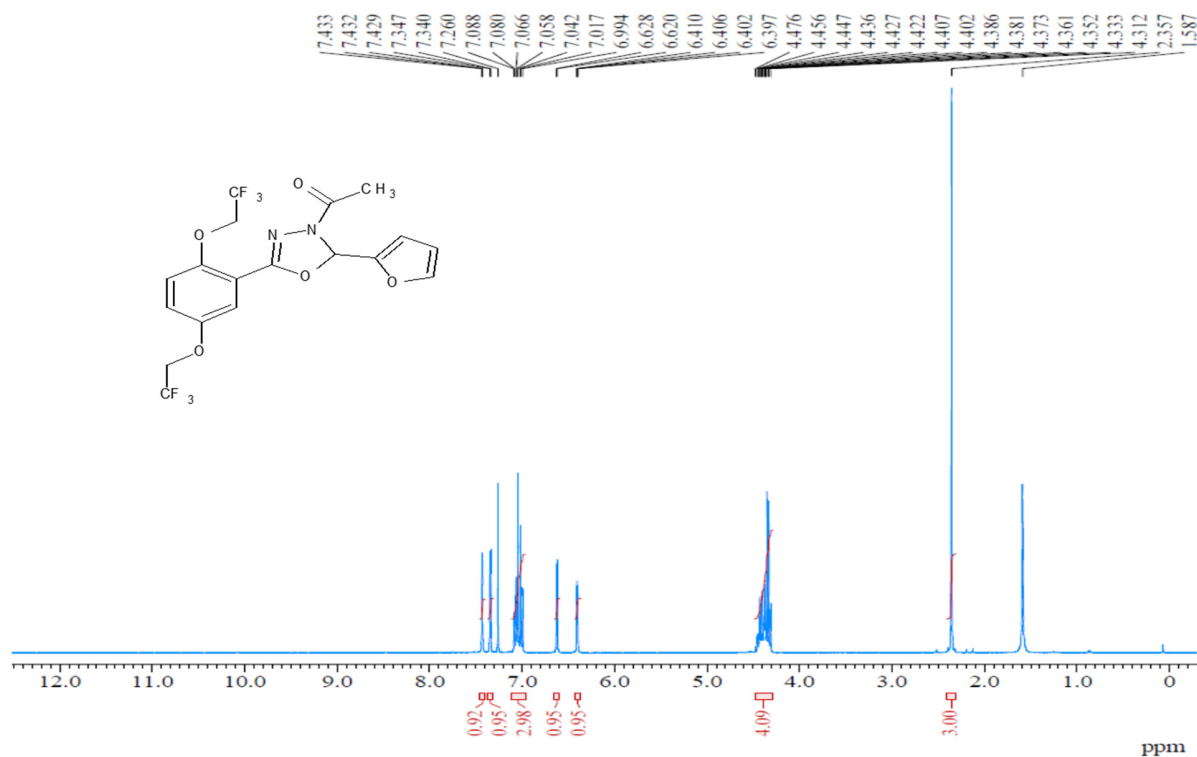
S.15: ¹³C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-chloro phenyl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5d)



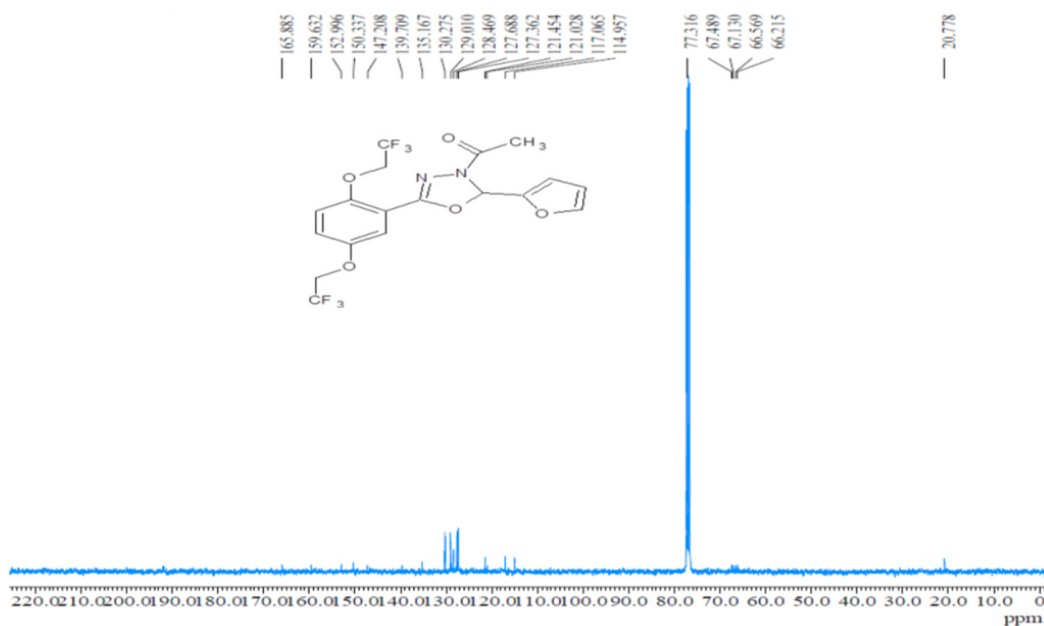
S.16: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-chloro phenyl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5d)



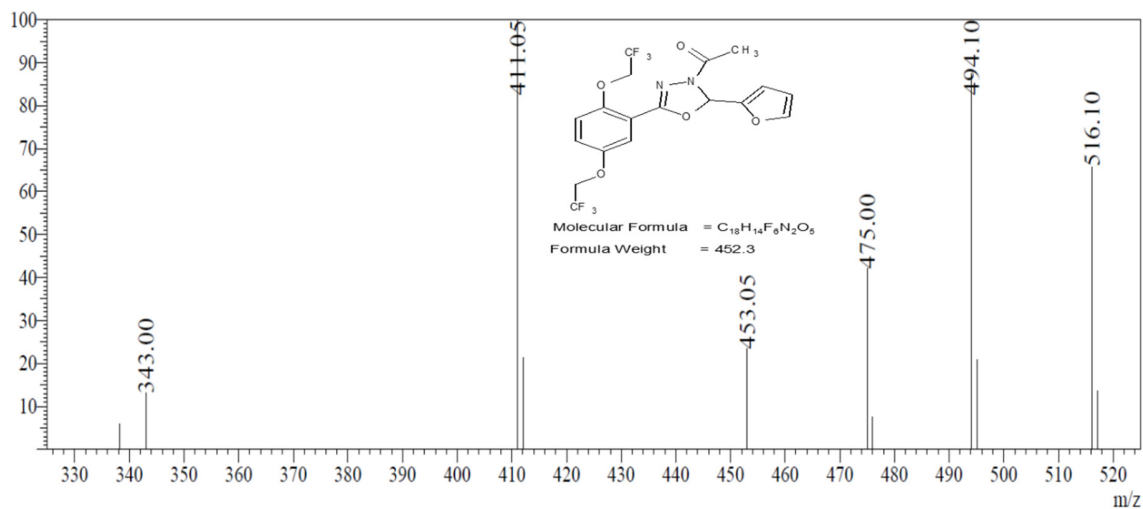
S.17: IR spectrum of of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(furfuryl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5e)



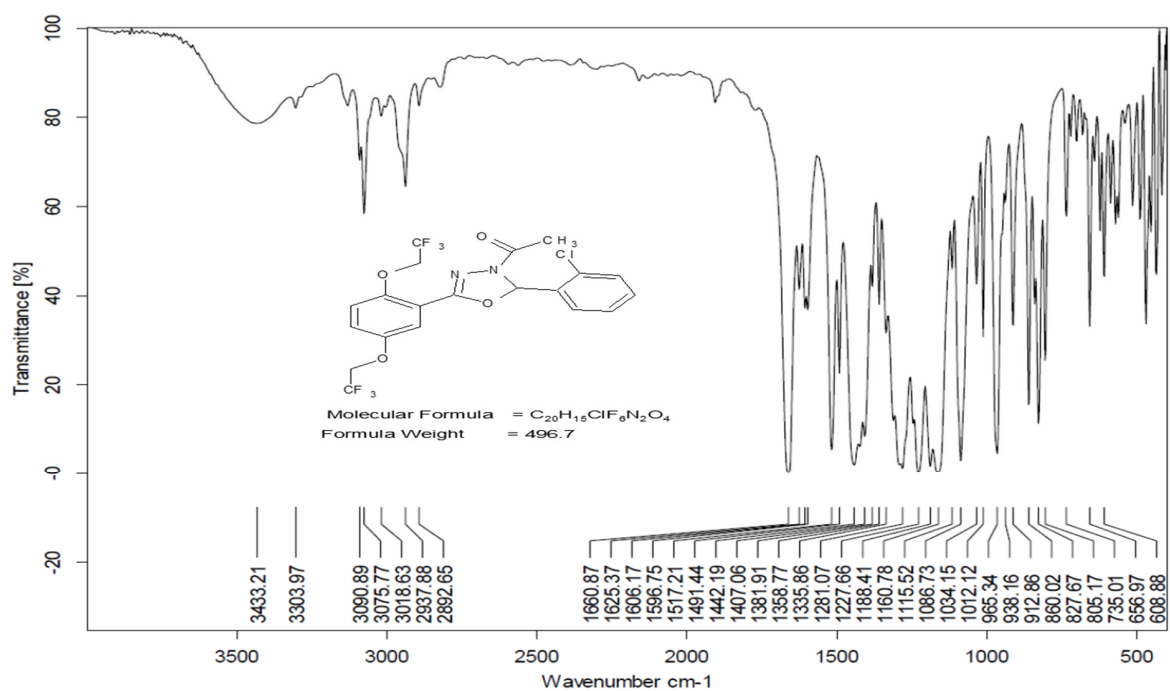
S.18: ¹H NMR spectrum of of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(furfuryl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5e)



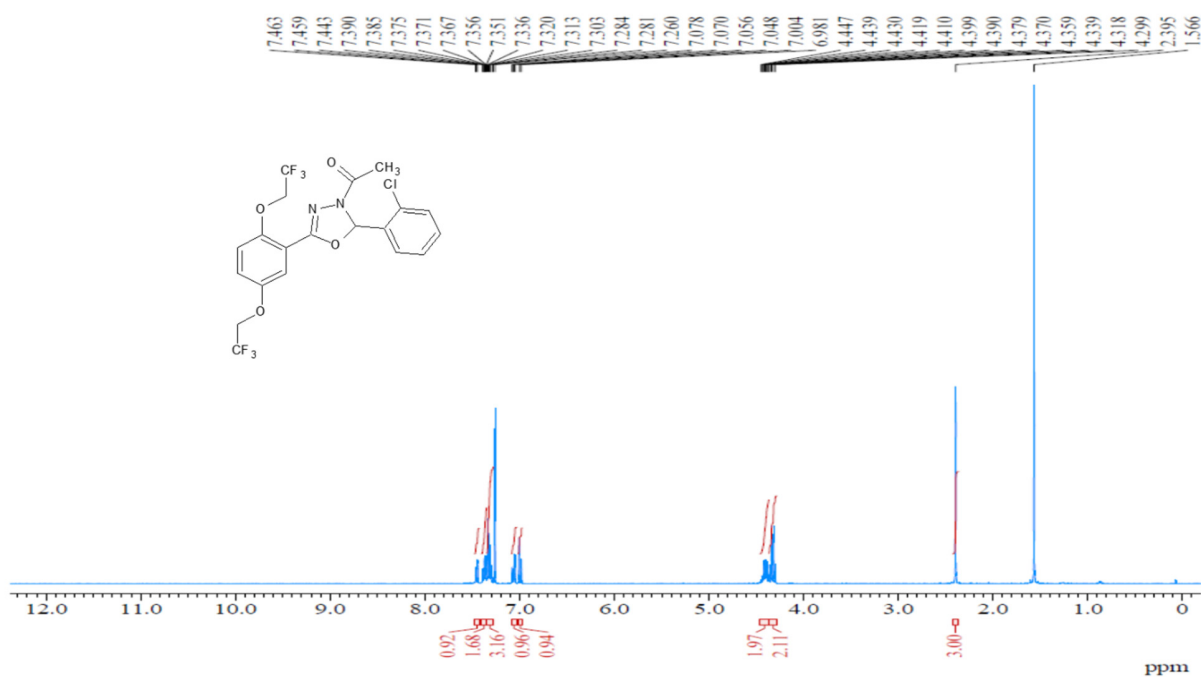
S.19: ^{13}C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(furfuryl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5e)



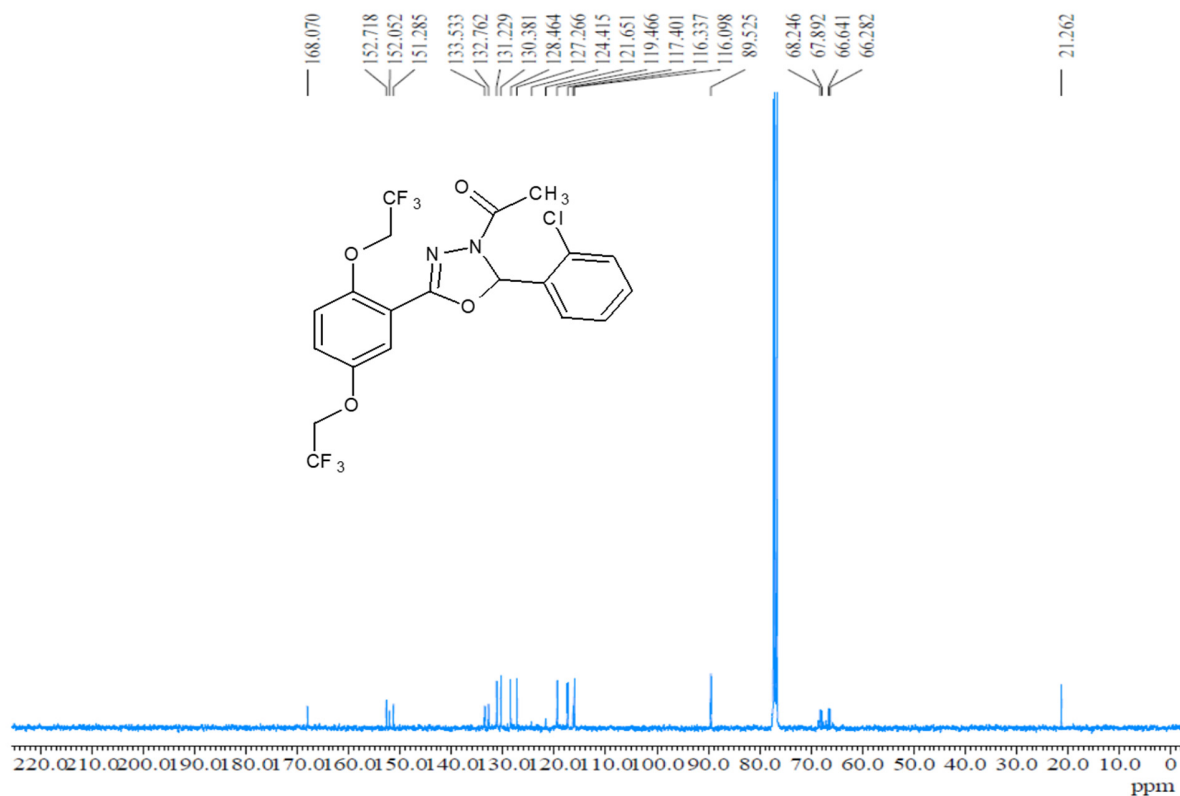
S.20: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(furfuryl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5e)



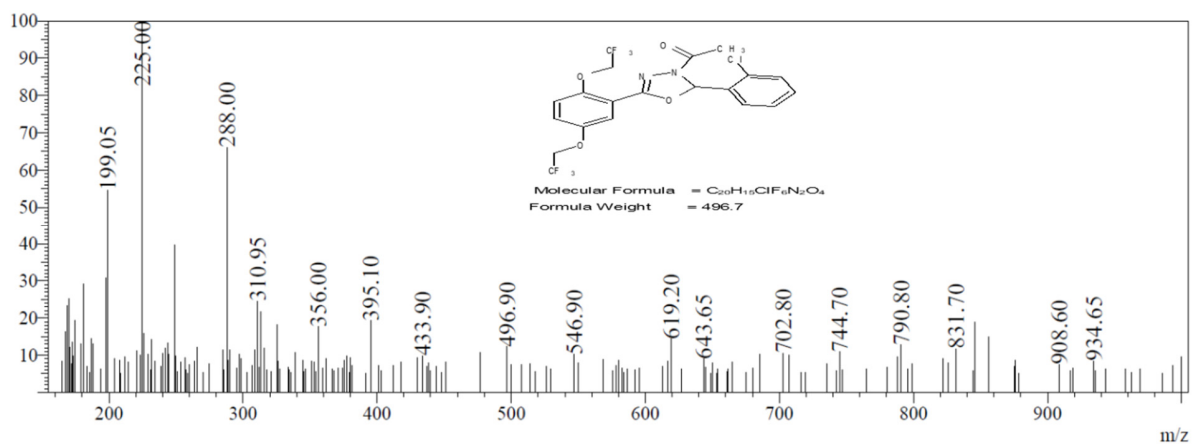
S.21: IR spectrum of of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2-chloro phenyl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5f)



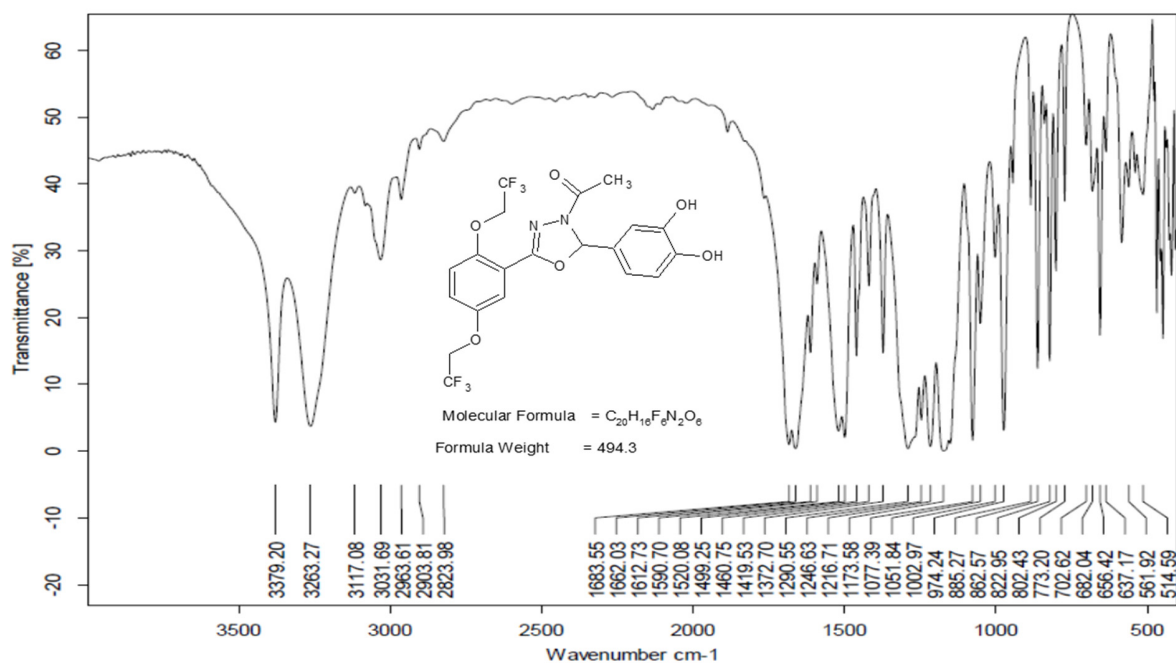
S.22: 1H NMR spectrum of of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2-chloro phenyl)-1,3,4-oxadiazol-3(2H)-yl}ethanone(5f)



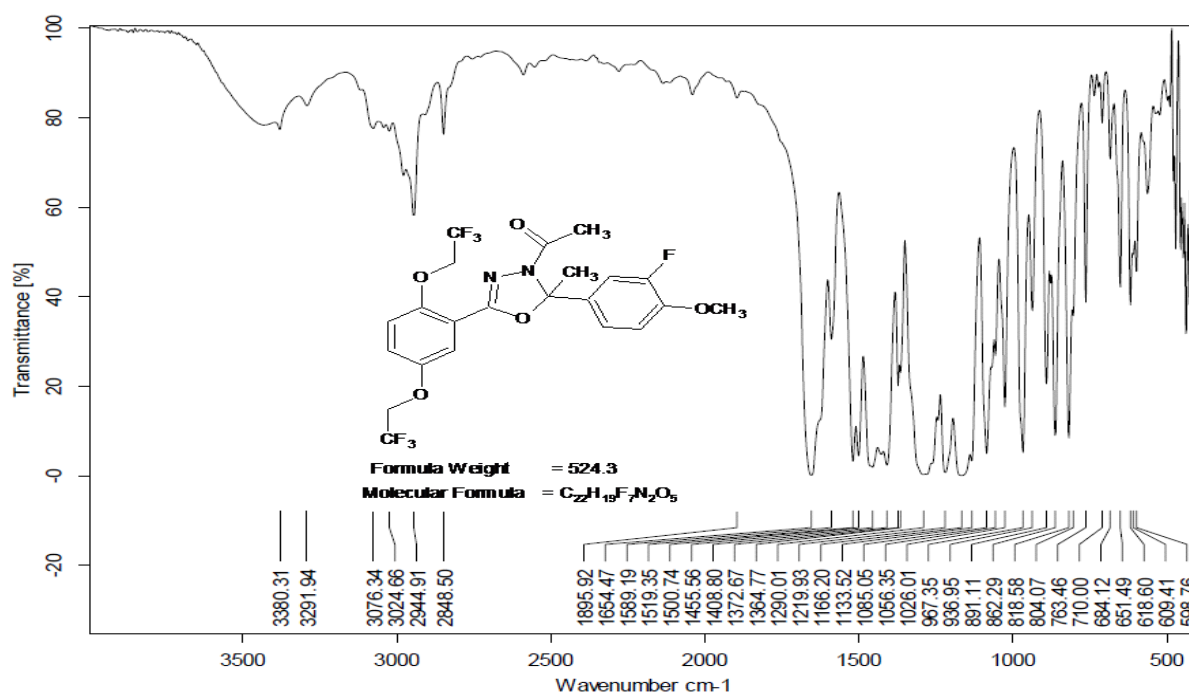
S.23: ¹³C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2-chloro phenyl)-1,3,4-oxadiazol-3(2H)-yl} ethanone(5f)



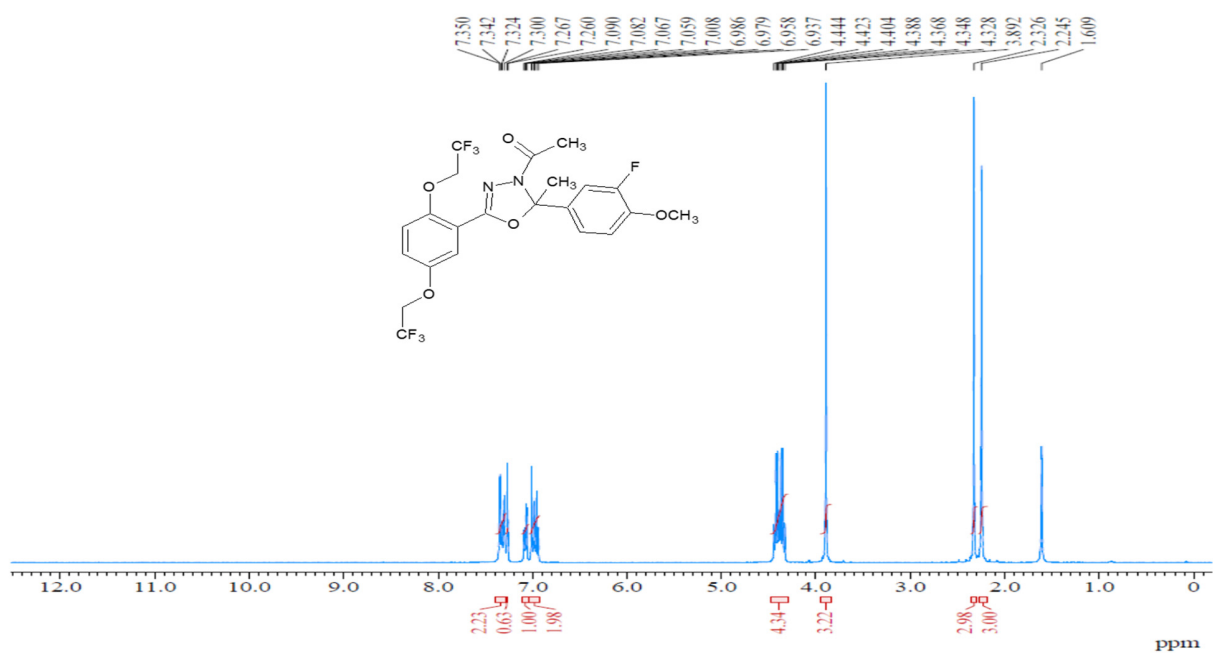
S.24: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2-chloro phenyl)-1,3,4-oxadiazol-3(2H)-yl} ethanone(5f)



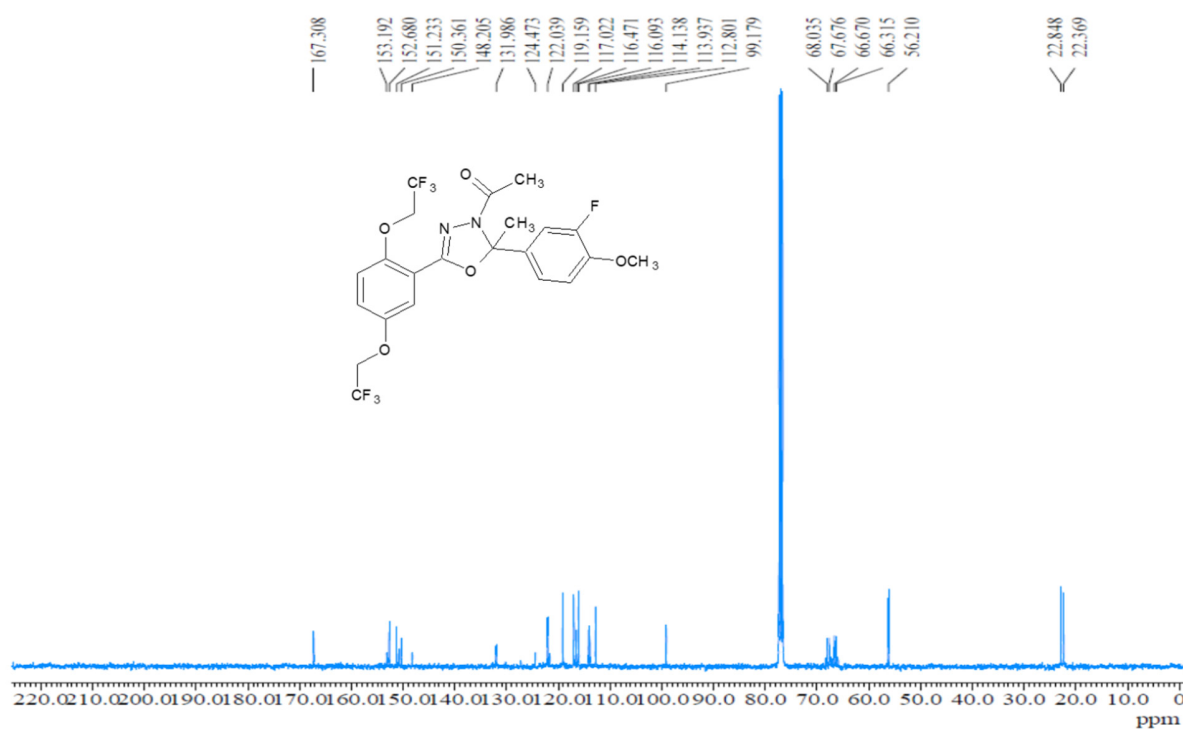
S.25: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(3,4-dihydroxy phenyl)-1,3,4-oxadiazol-3(2*H*)-yl}ethanone(5g)



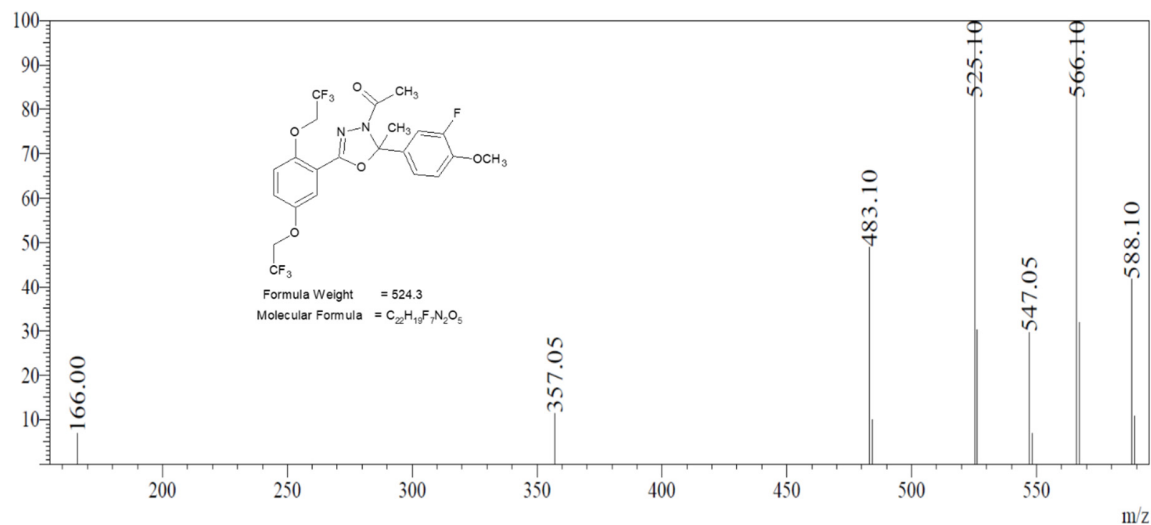
S.26: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(3-flouro-4-methoxy phenyl)-1,3,4-oxadiazol-3(2 *methyl*)-yl}ethanone(5i)



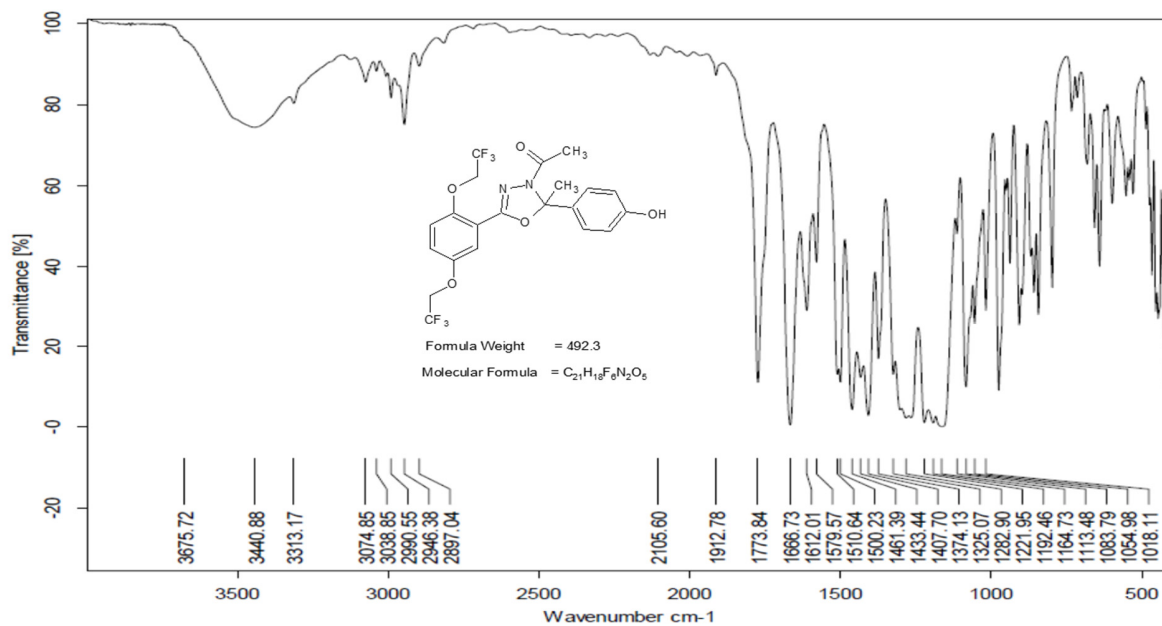
S.27: ¹H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(3-fluoro-4-methoxyphenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5i)



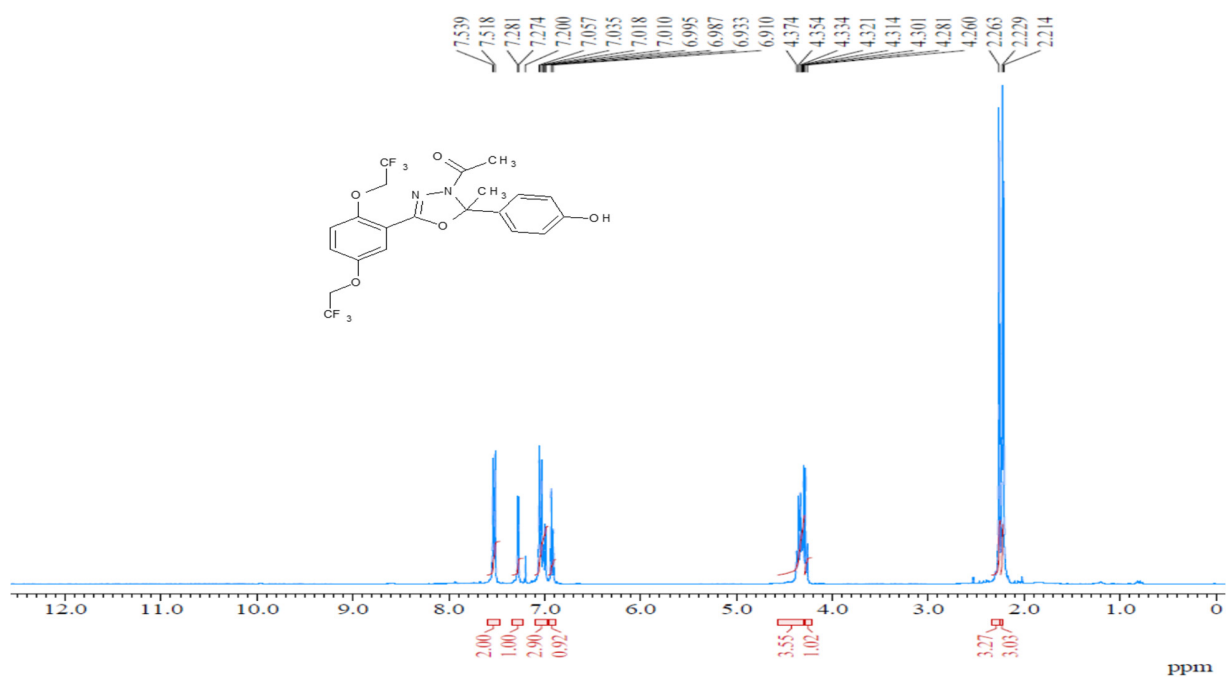
S.28: ¹³C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(3-fluoro-4-methoxyphenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5i)



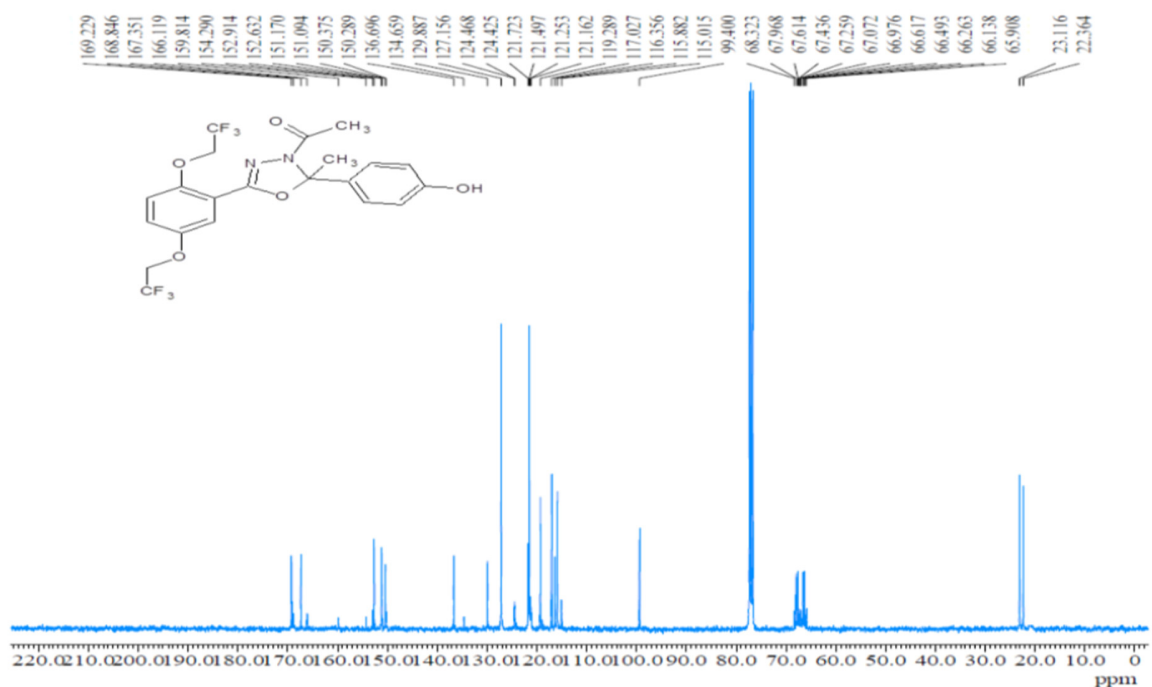
S.29: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(3-fluoro-4-methoxyphenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5i)



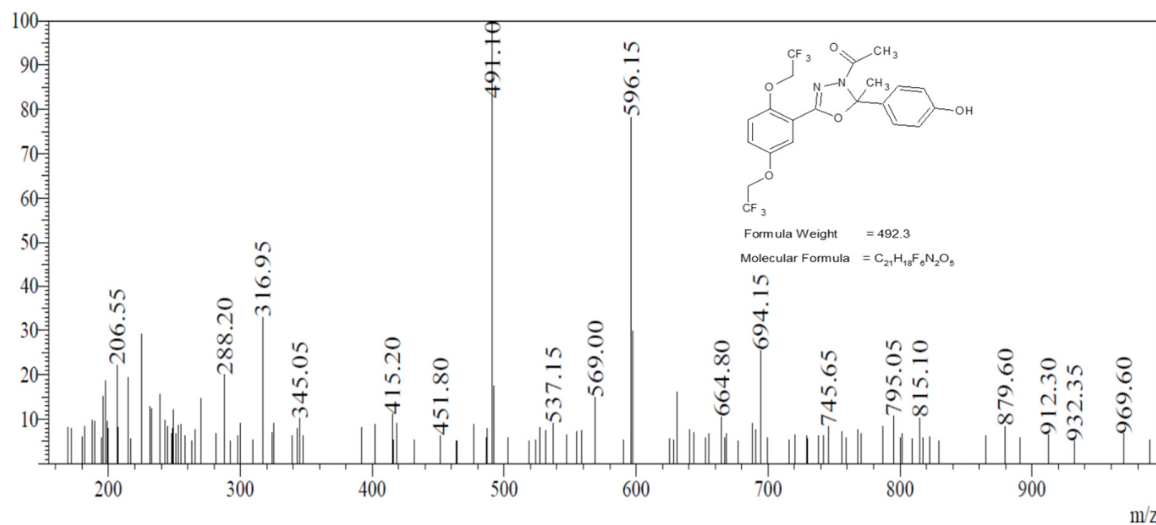
S.30: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-hydroxyphenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5j)



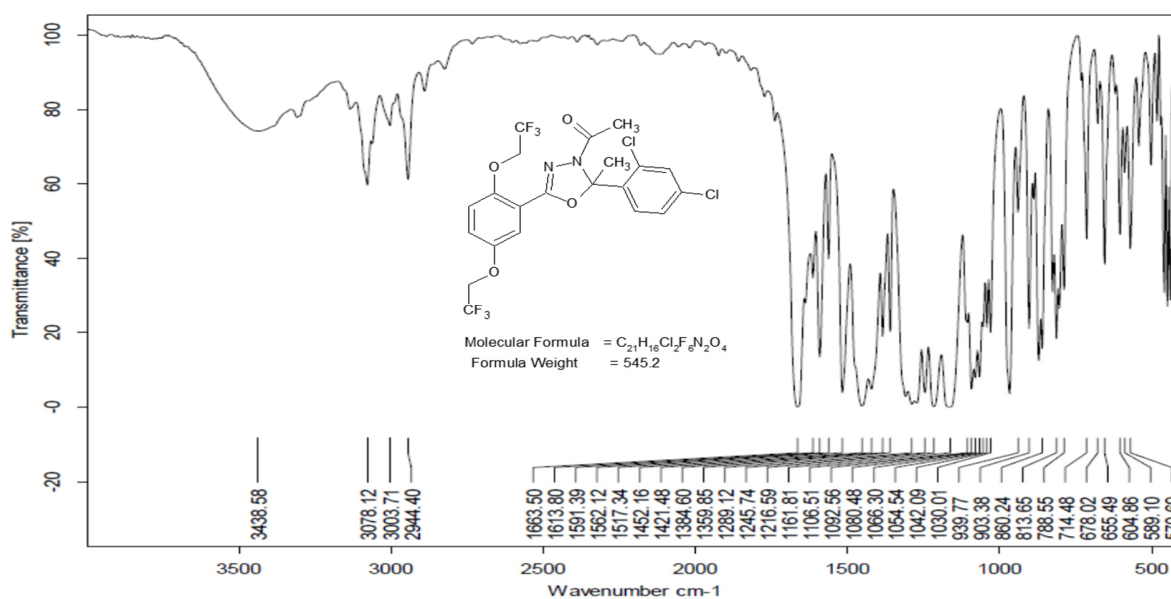
S.31: ¹H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-hydroxy phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5j)



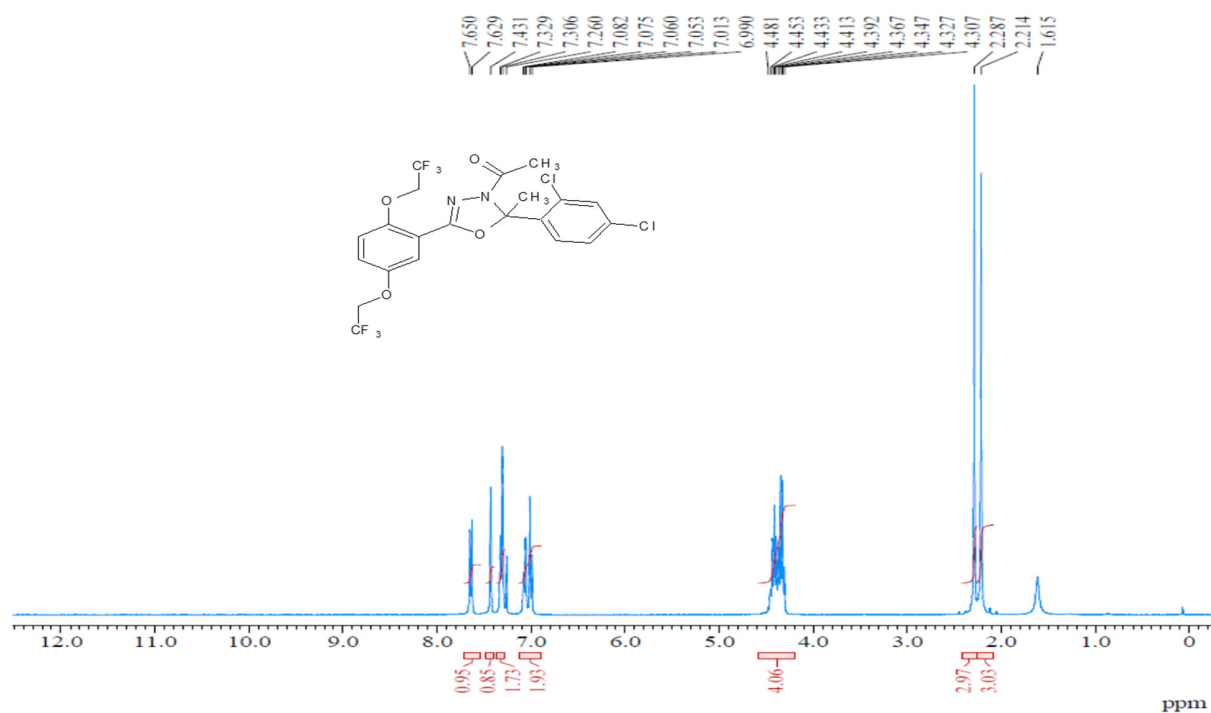
S.32: ¹³C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-hydroxy phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5j)



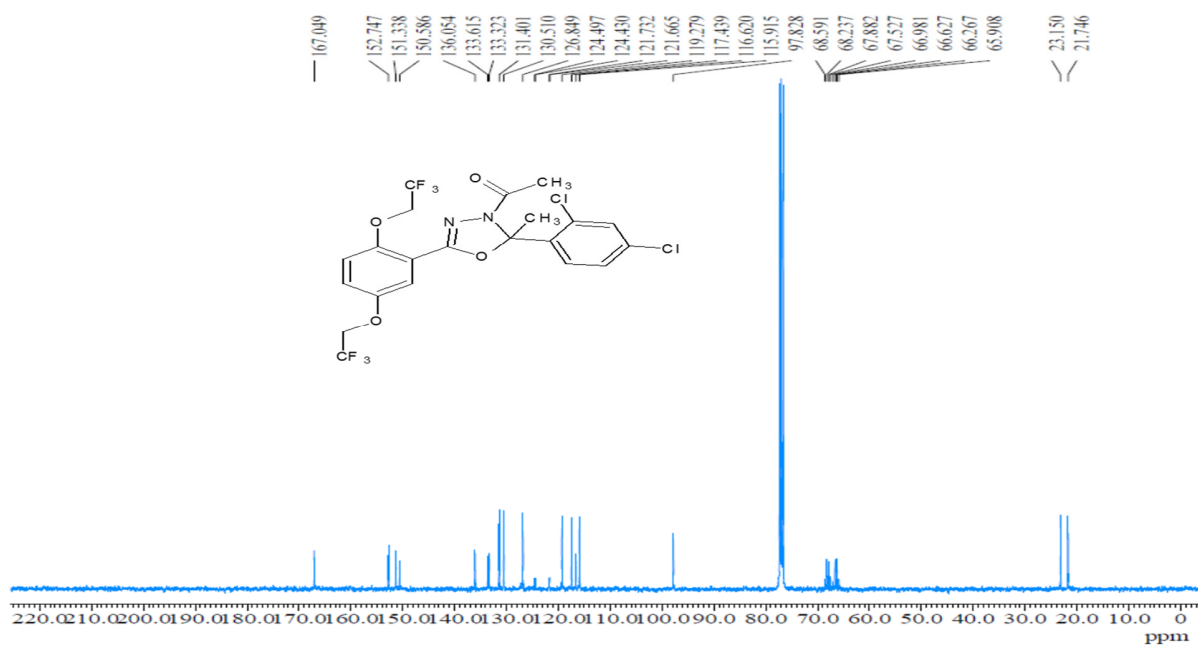
S.33: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-hydroxy phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5j)



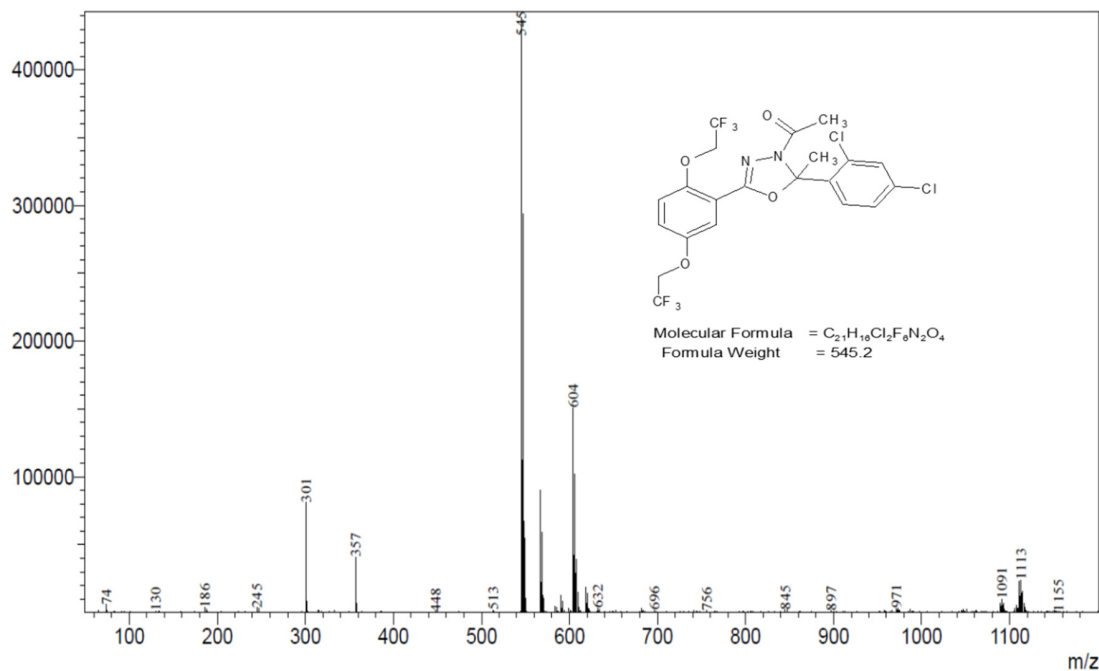
S.34: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,4-dichloro phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5k)



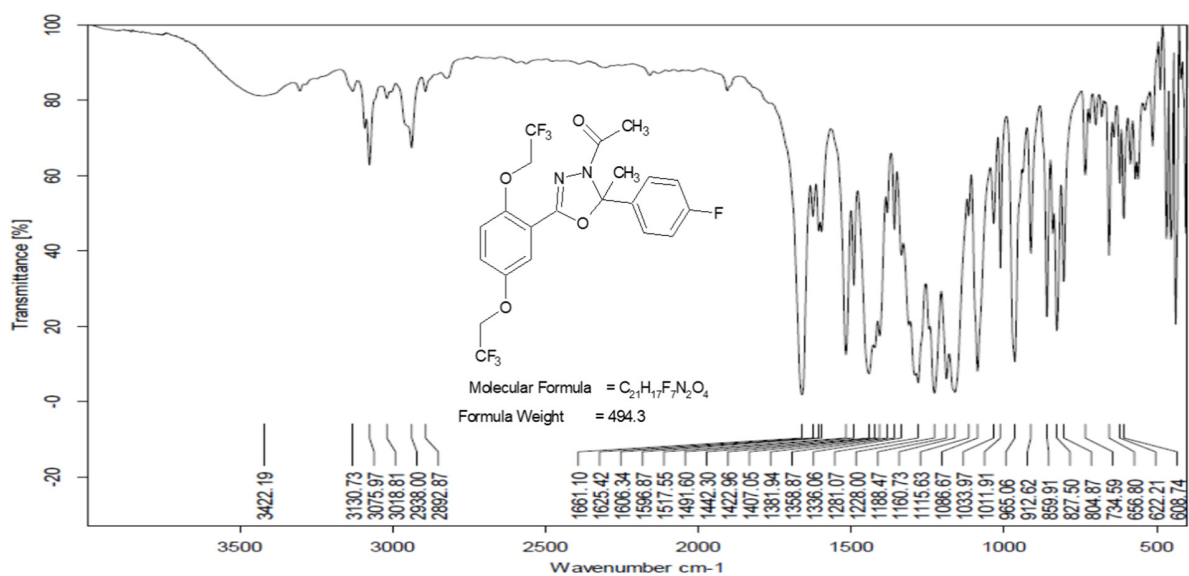
S.35: ¹H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,4-dichloro phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5k)



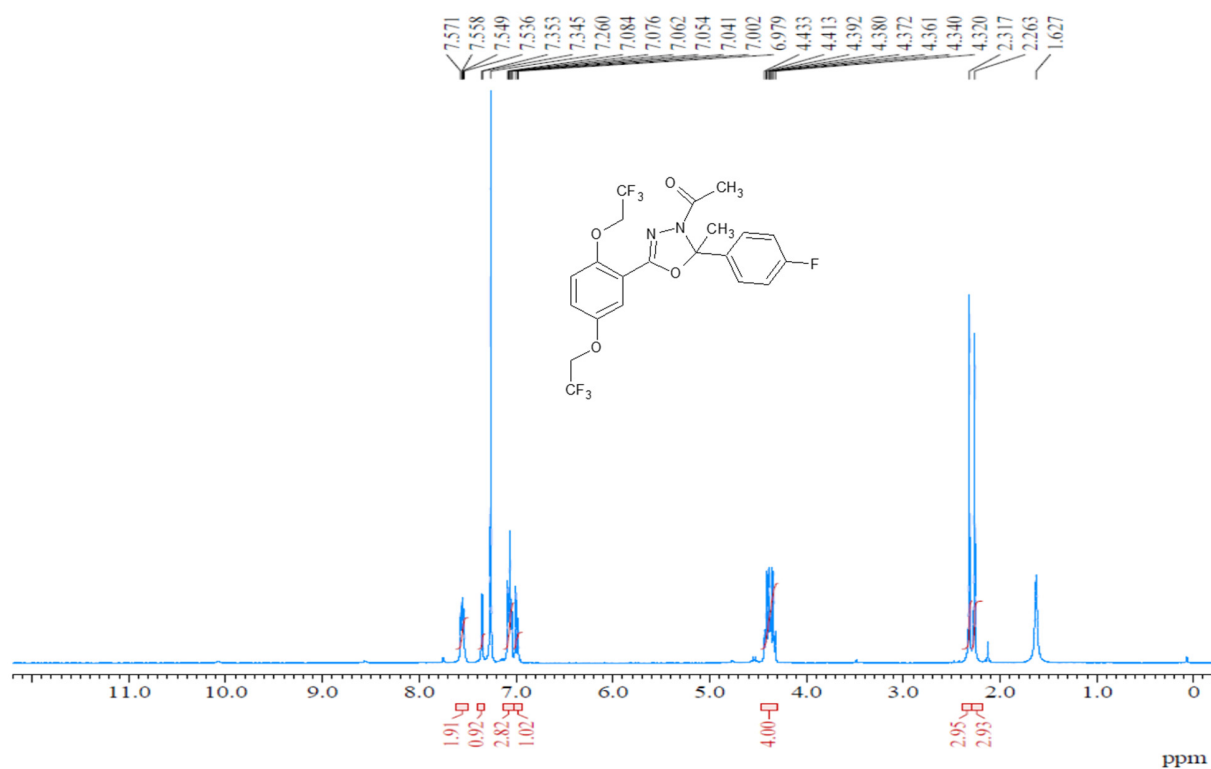
S.36: ¹³C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,4-dichloro phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5k)



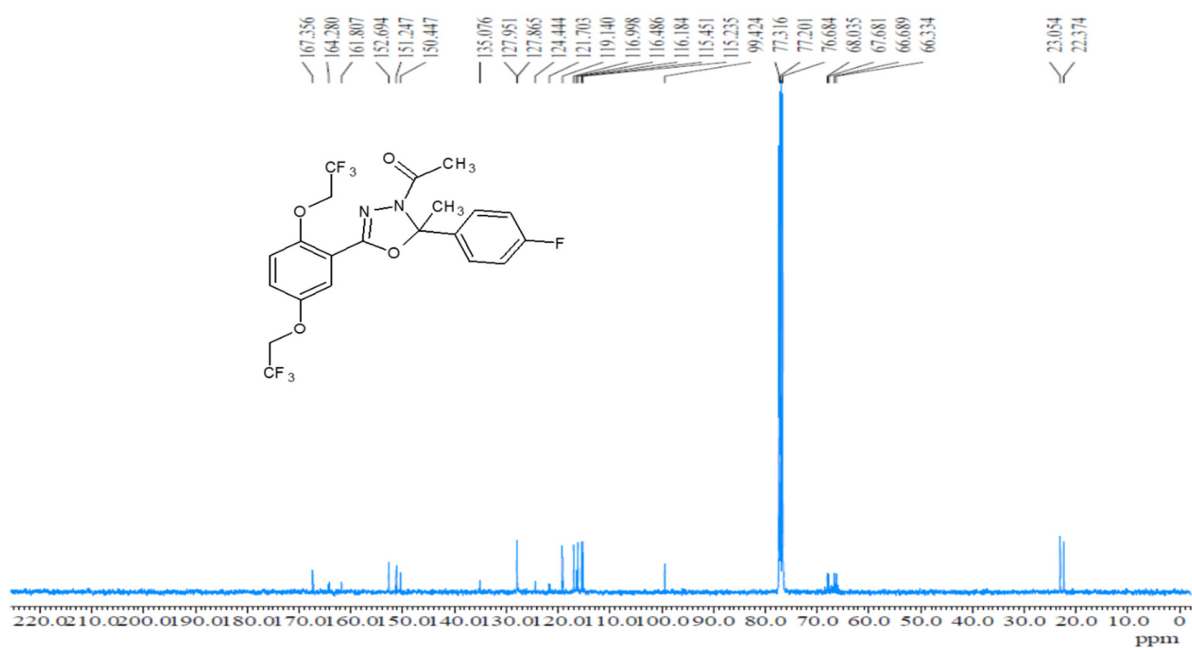
S.37: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,4-dichlorophenyl)-1,3,4-oxadiazol-3(2-methyl)-yl}ethanone(5k)



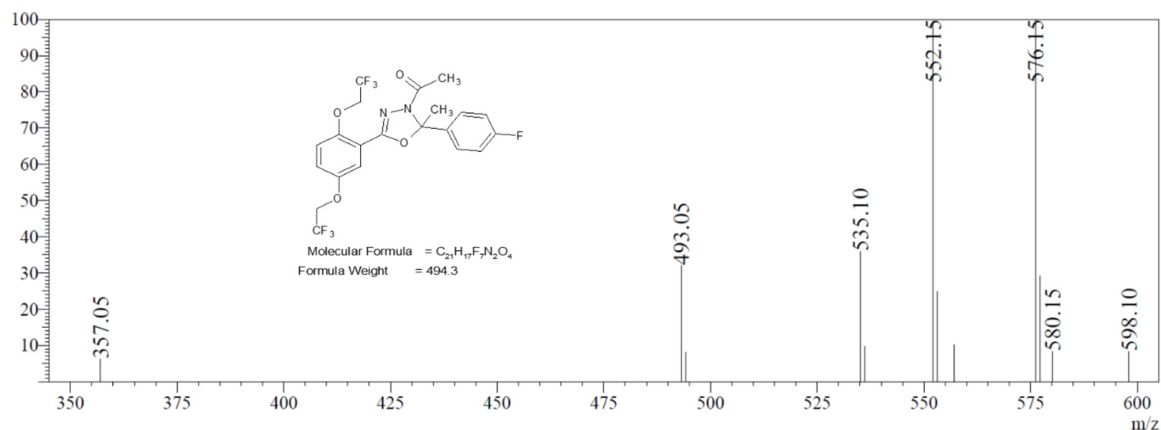
S.38: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-fluorophenyl)-1,3,4-oxadiazol-3(2-methyl)-yl}ethanone(5l)



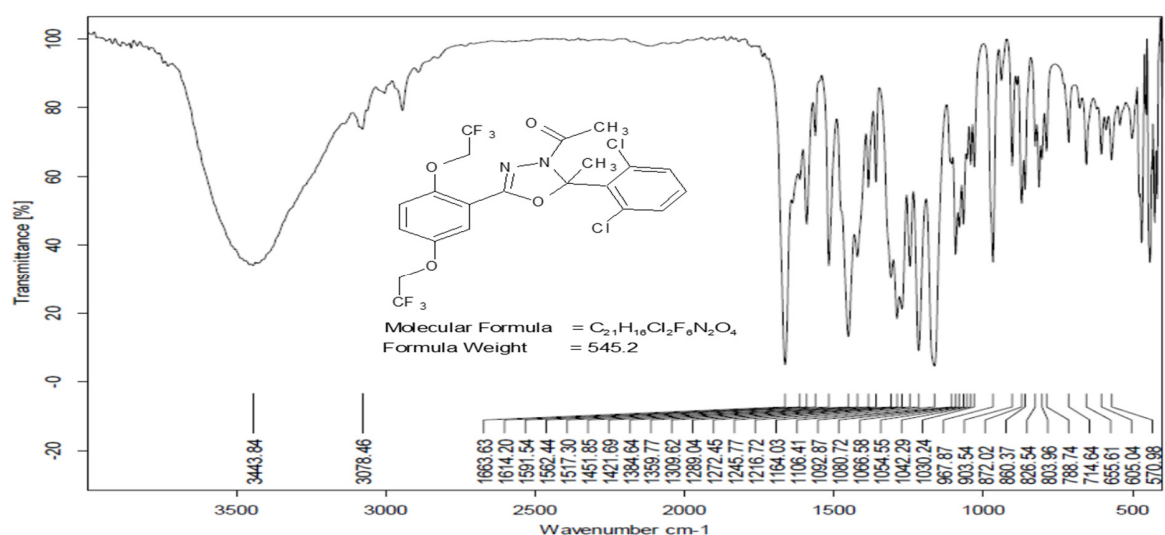
S.39: ¹H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-fluorophenyl)-1,3,4-oxadiazol-3(2-methyl)-yl}ethanone(51)



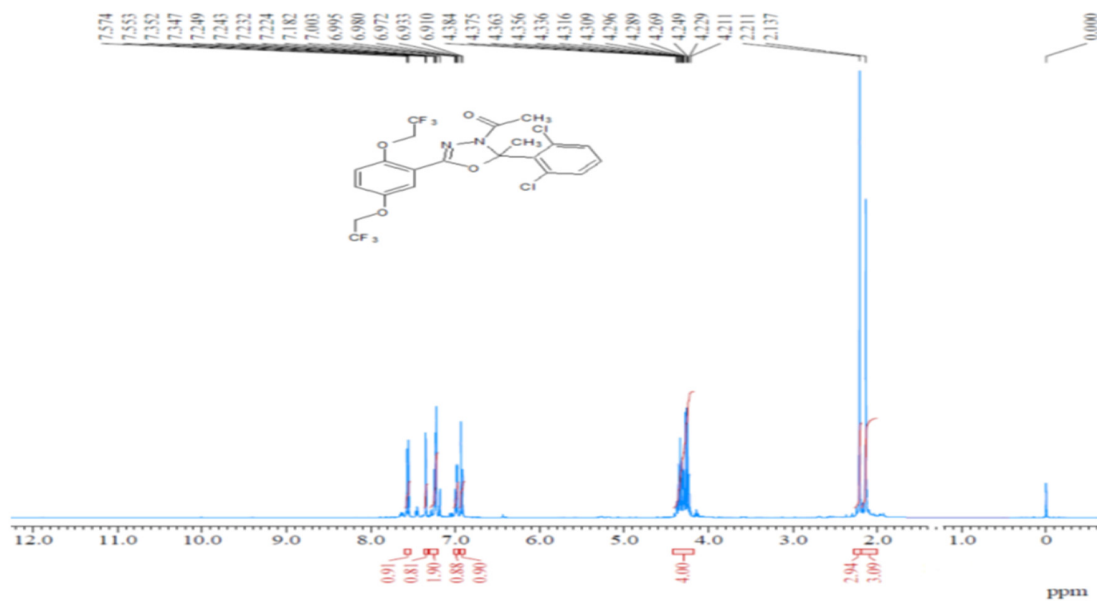
S.40: ¹³C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-fluorophenyl)-1,3,4-oxadiazol-3(2-methyl)-yl}ethanone(51)



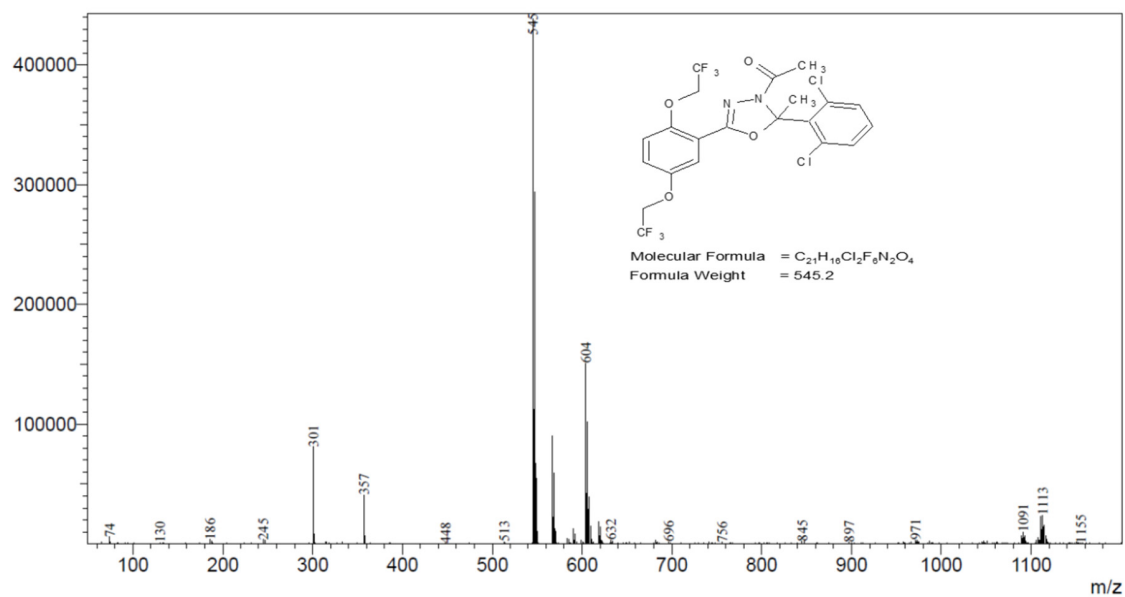
S.41: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-fluorophenyl)-1,3,4-oxadiazol-3(2-methyl)-yl}ethanone(51)



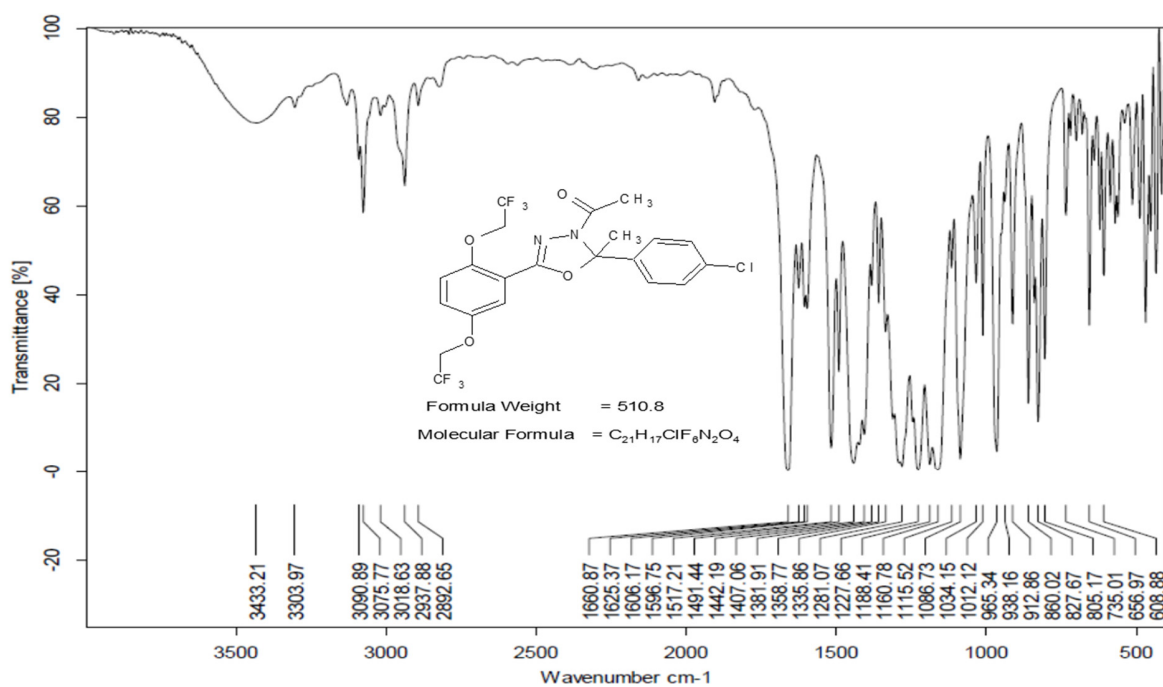
S.42: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,6-dichlorophenyl)-1,3,4-oxadiazol-3(2-methyl)-yl}ethanone(5m)



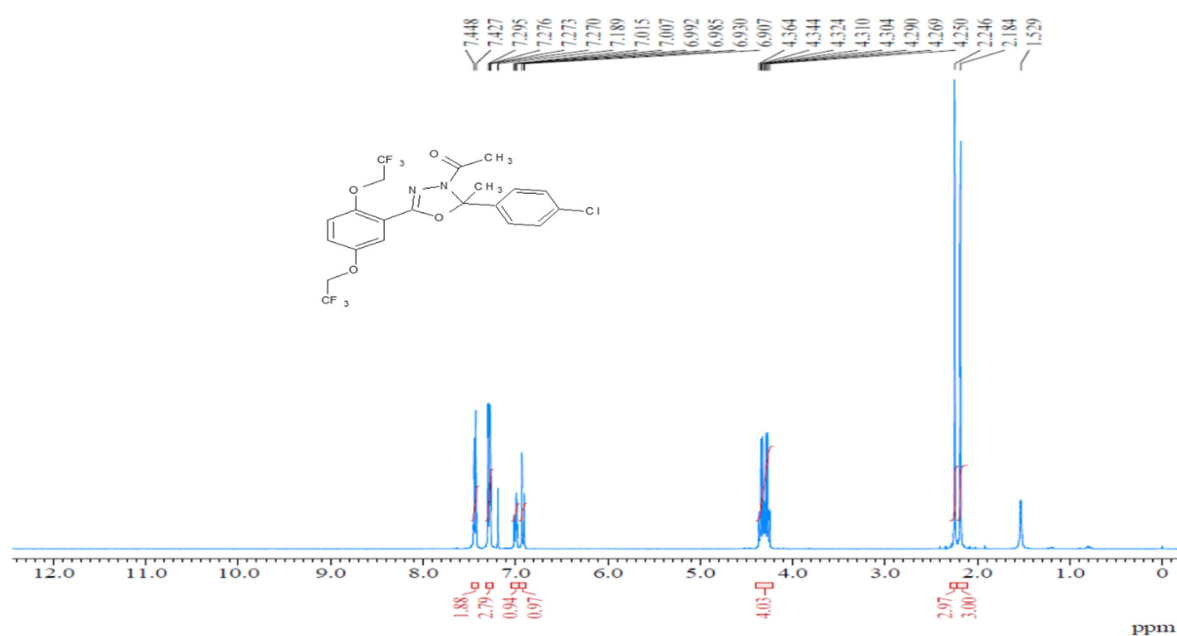
S.43: ^1H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,6-dichloro phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5m)



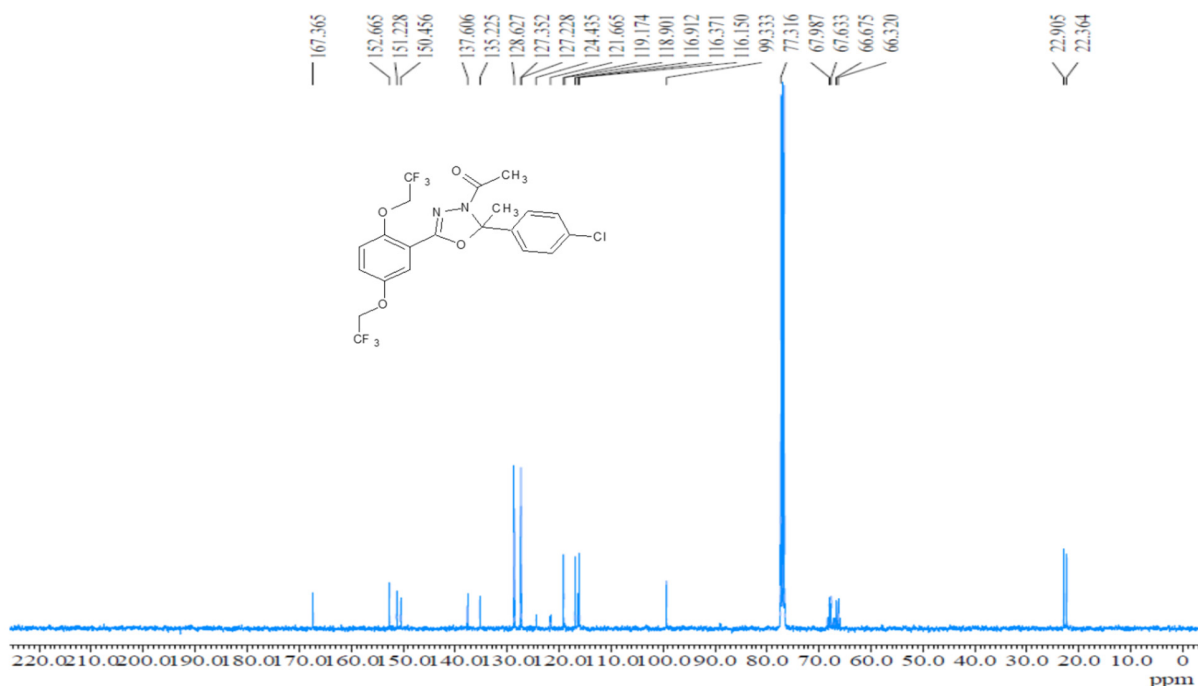
S.44: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(2,6-dichloro phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5m)



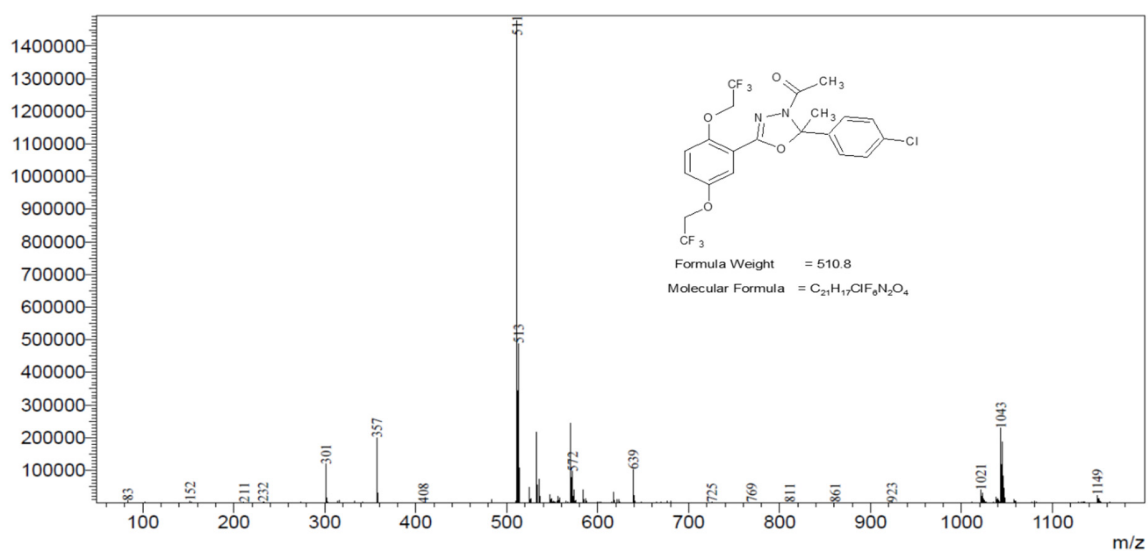
S.45: IR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-chloro phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5n)



S.46: ¹H NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-chloro phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5n)



S.47: ¹³C NMR spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-chloro phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5n)



S.48: Mass spectrum of 1-{5-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-2-(4-chloro phenyl)-1,3,4-oxadiazol-3(2-methyl)-yl} ethanone(5n)