

SUPPORTING INFORMATION

FOR

Synthesis, characterization of steroidal heterocyclic compounds, DNA condensation and molecular docking studies and their *in vitro* anticancer and acetylcholinesterase inhibition activities

**Abad Ali^a, Mohd Asif^a, Hena Khanam^a, Ashraf Mashrai^a, Mohd. Asif Sherwani^b,
Mohammad Owais^b, Shamsuzzaman^{a*}**

^a*Steroid Research Laboratory, Department of Chemistry, Aligarh Muslim University, Aligarh 202 002, India*

^b*Interdisciplinary Biotechnology Unit, Aligarh Muslim University, Aligarh 202 002, India*

**Corresponding author, E-mail address: shamsuzzaman9@gmail.com; phone no +919411003465*

Figures of ^1H NMR and ^{13}C NMR Spectra

Please note that some peaks in ^{13}C NMR spectra are merged due to complex steroidal skeleton. That's why chemical shift values of only those peaks are given in experimental section, which are clear in the spectra.

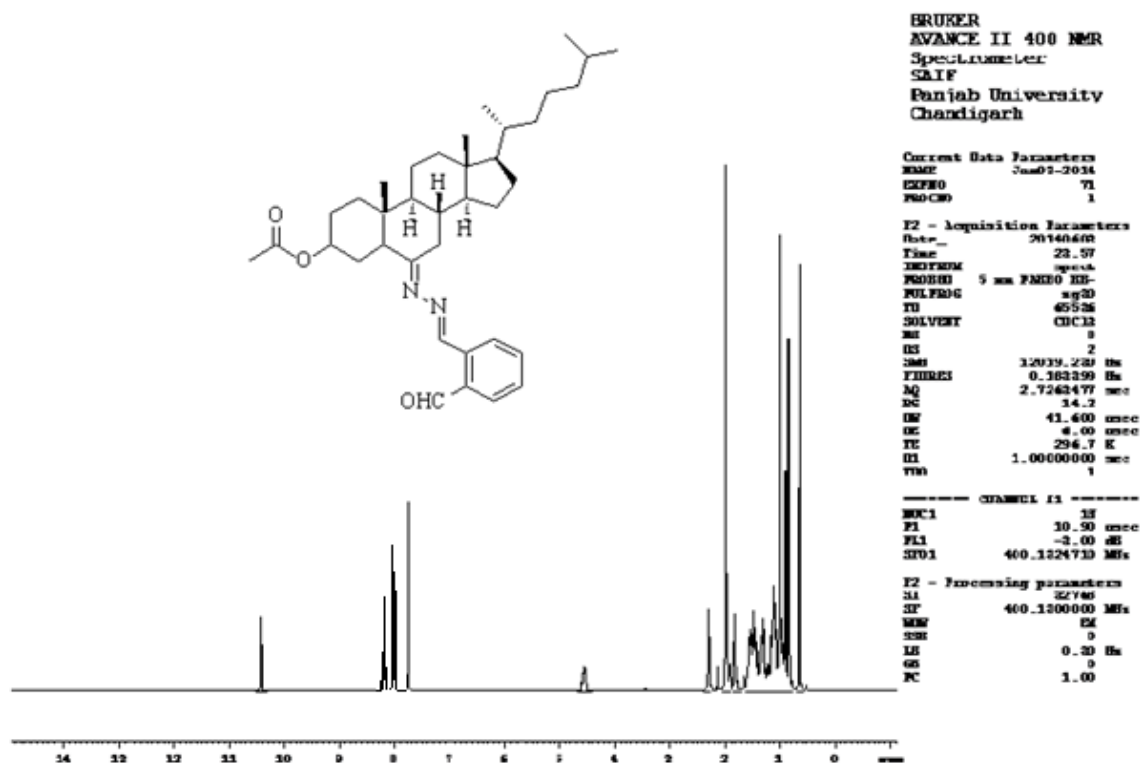


Fig S1. ^1H NMR of 3β -Acetoxy- 5α -cholestan-6-(iminohydrazono)-2-methylbenzaldehyde (**1e**)

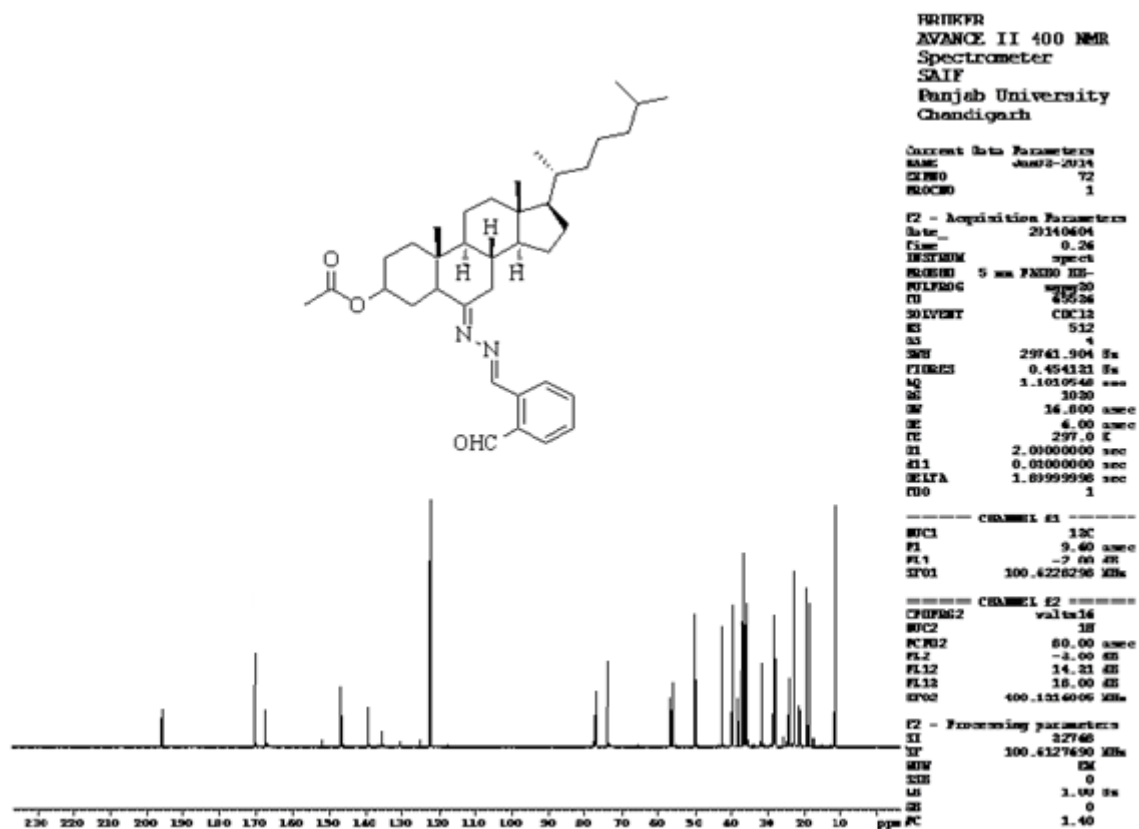


Fig S2. ^{13}C NMR of 3 β -Acetoxy-5 α -cholestan-6-(iminohydrazono)-2-methylbenzaldehyde (**1e**)

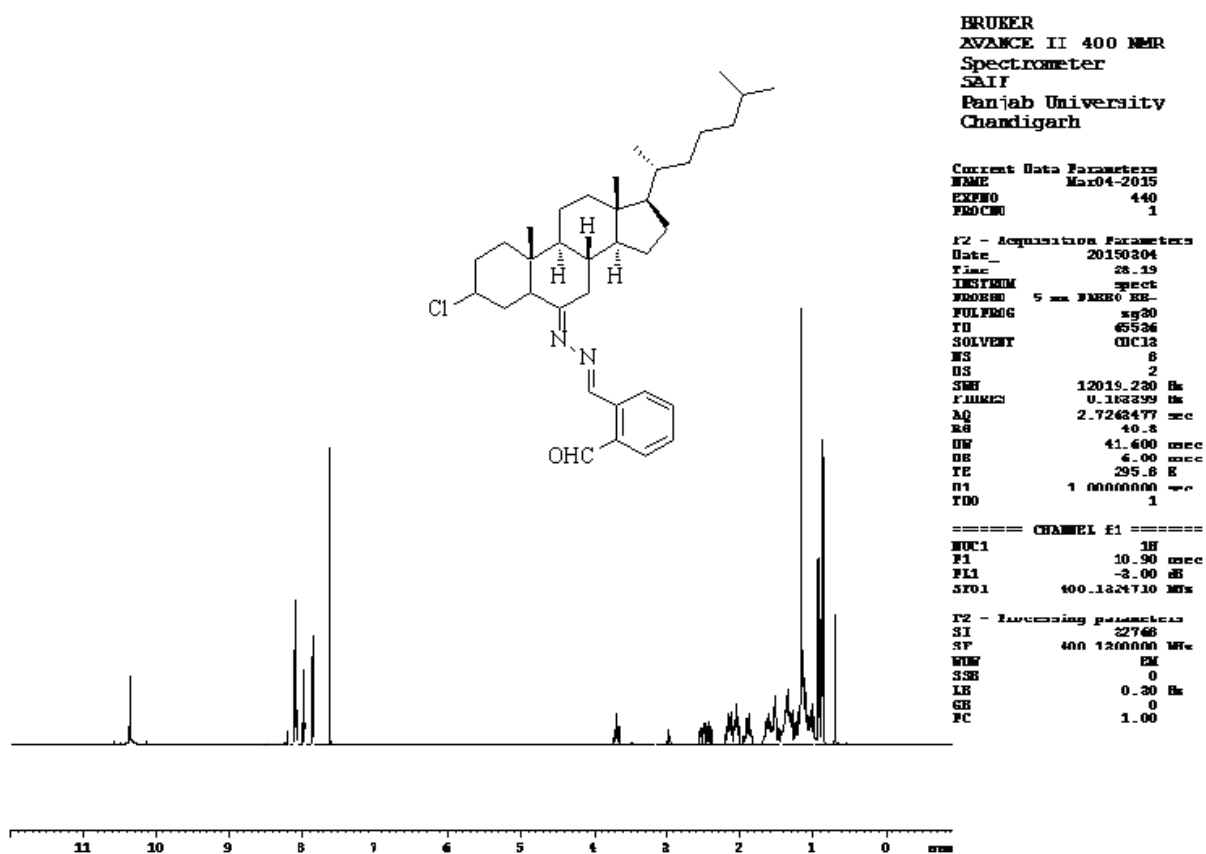


Fig S3. ^1H NMR of 3 β -Chloro-5 α -cholestan-6-(iminohydrazono)-2-methylbenzaldehyde (**2e**)

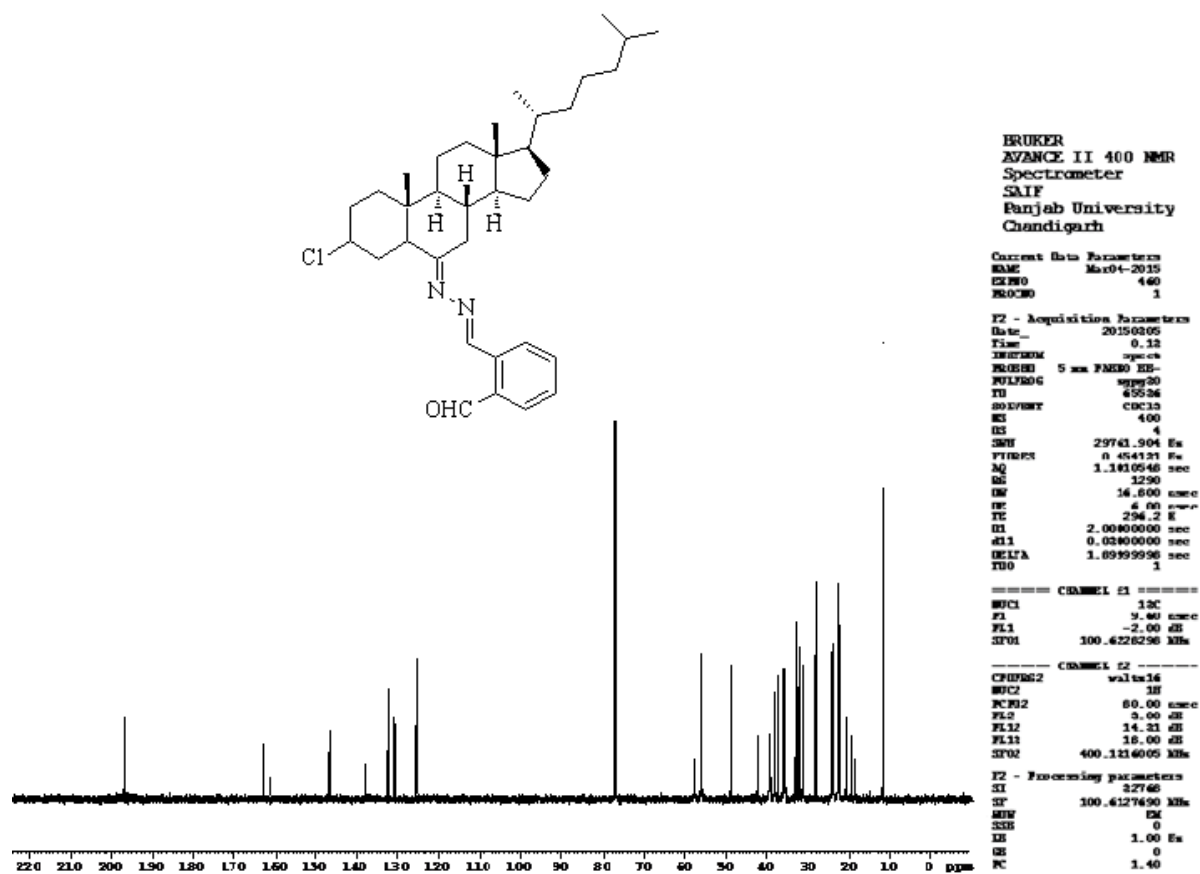


Fig S4. ^{13}C NMR of 3 β -Chloro-5 α -cholestan-6-(iminohydrazono)-2-methylbenzaldehyde (2e)

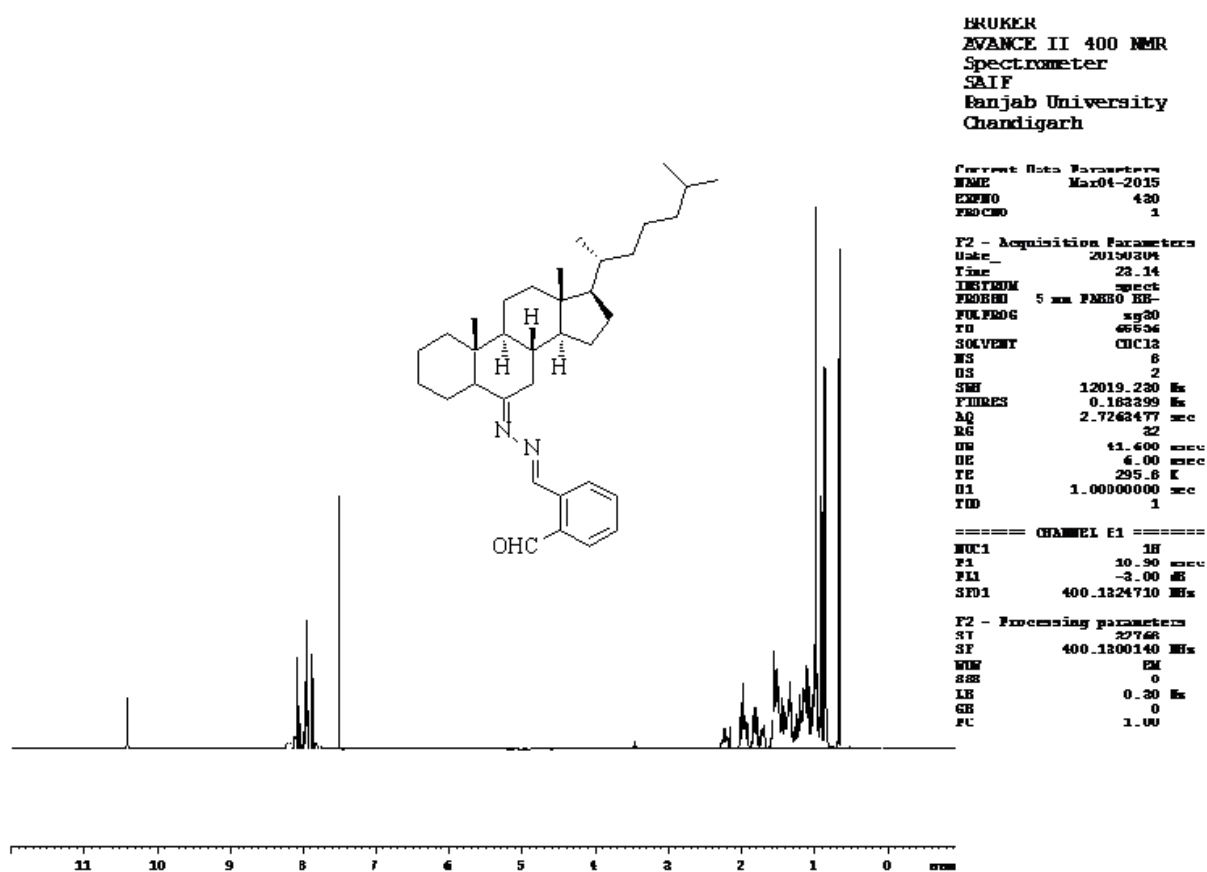


Fig S5. ^1H NMR of *5 α -cholestan-6-(iminohydrazono)-2-methylbenzaldehyde (3e)*

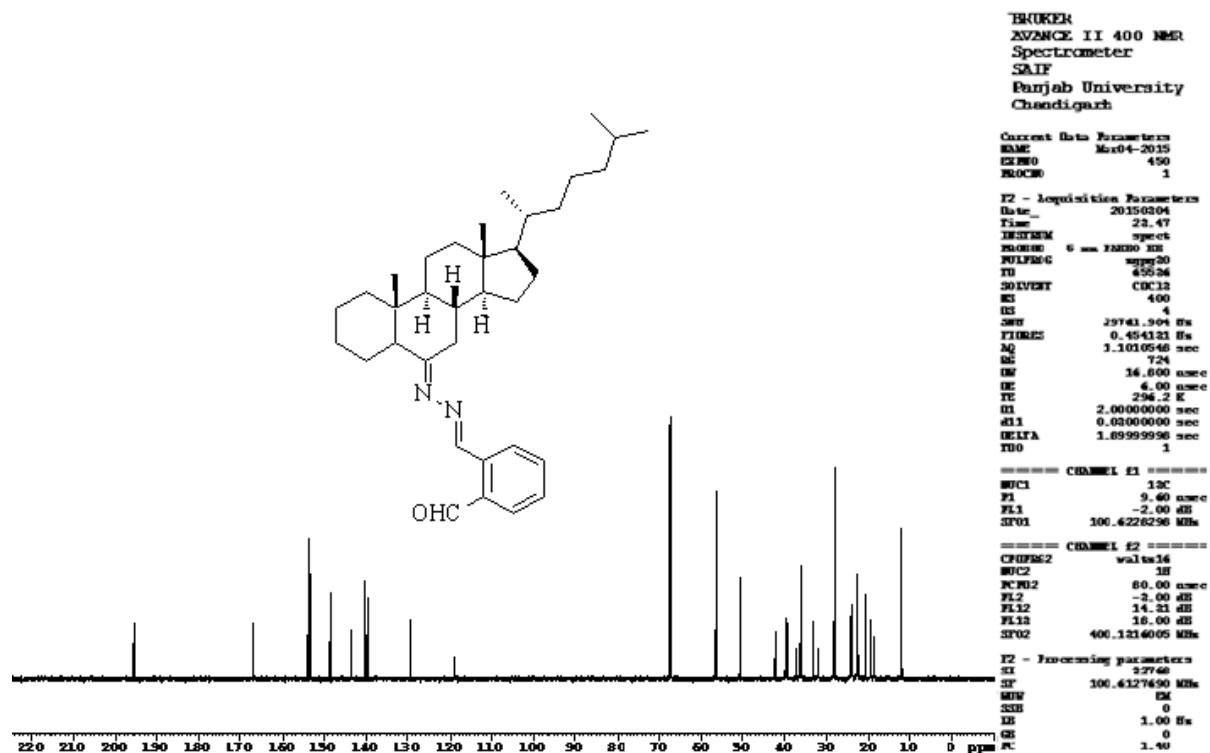


Fig S6. ^{13}C NMR of 5α -cholestan-6-(iminohydrazono)-2-methylbenzaldehyde (**3e**)

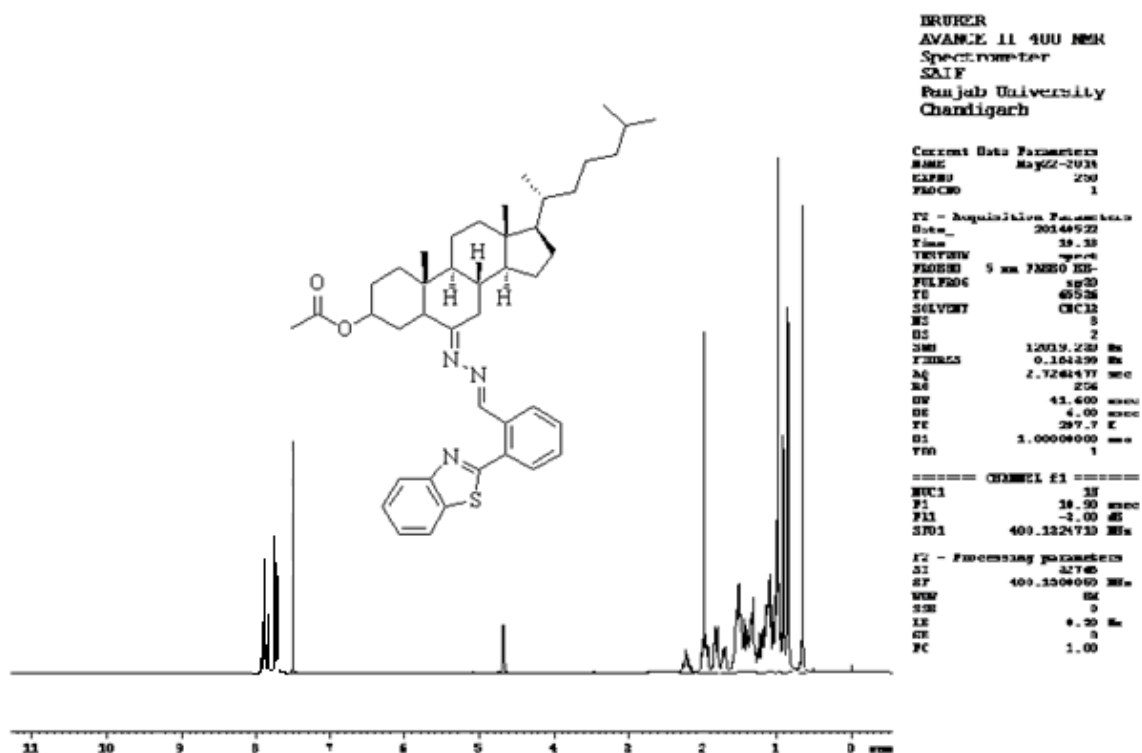


Fig S7. ^1H NMR of 3β -Acetoxy- 5α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo- $[d]$ -thiazole (**4**)

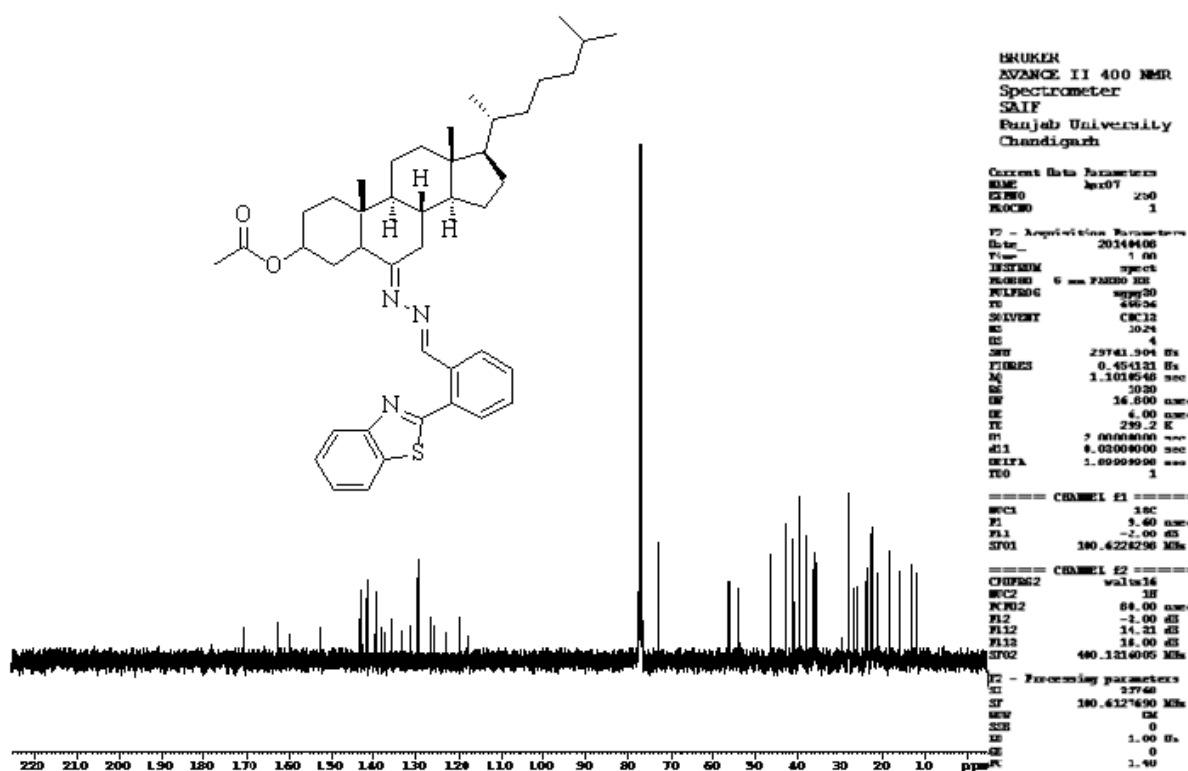


Fig S8. ^{13}C NMR of 3β -Acetoxy- 5α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo- $[d]$ -thiazole (**4**)

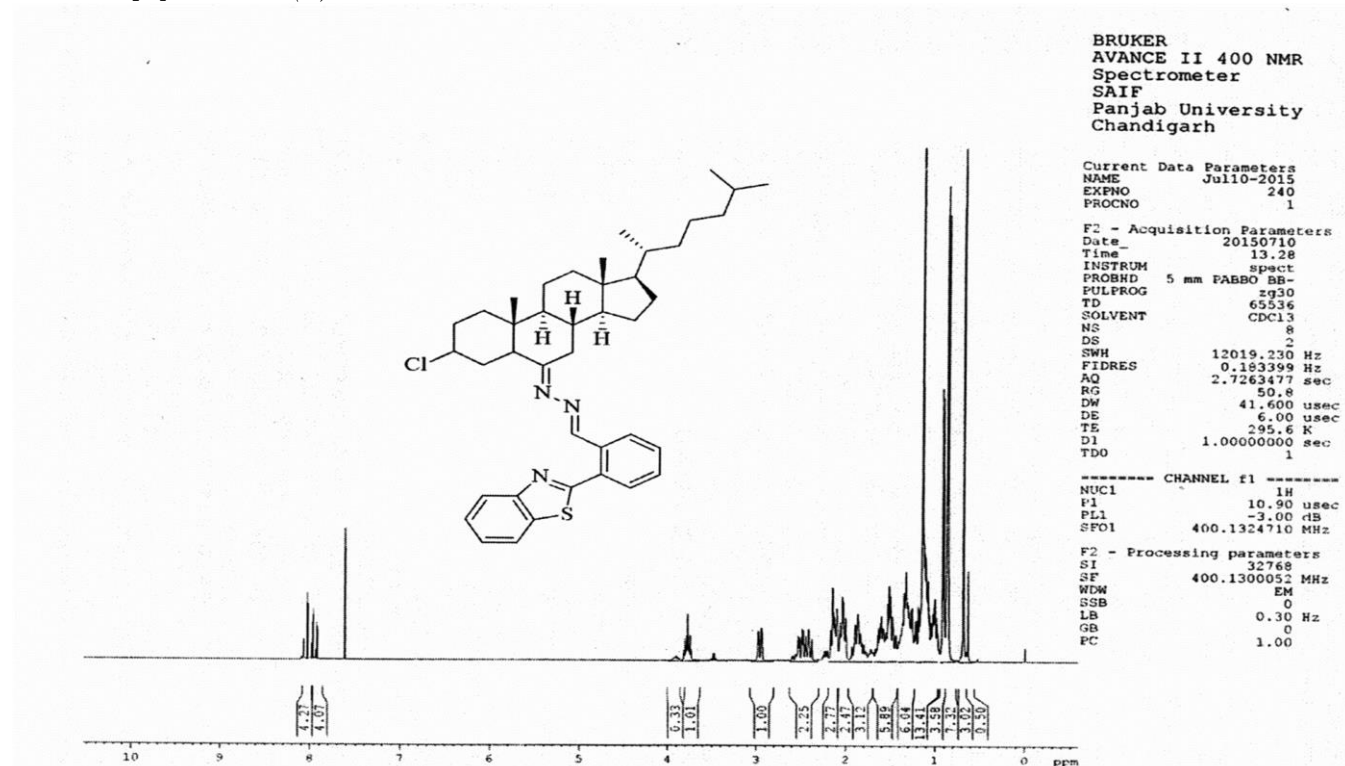


Fig S9. ^1H NMR of 3β -Chloro- 5α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo- $[d]$ -thiazole (**5**)

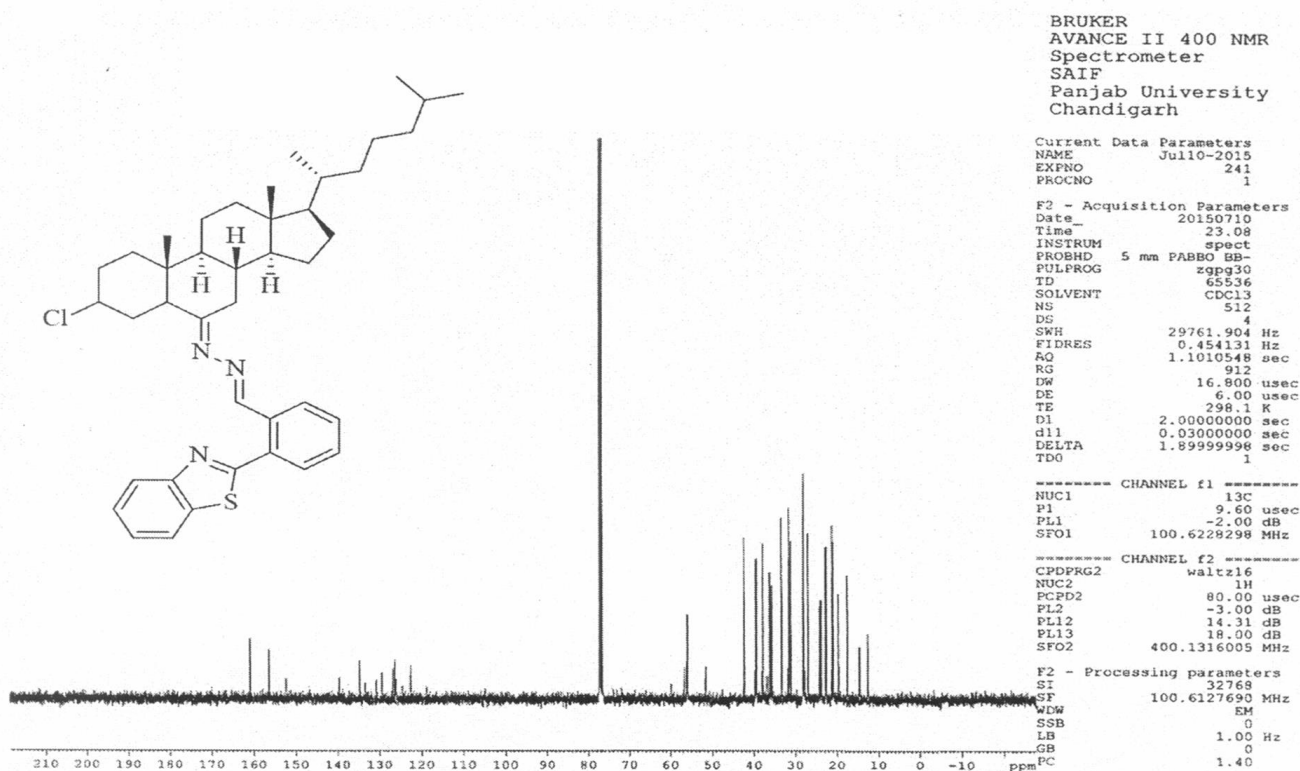


Fig S10. ¹³CNMR of 3 β -Chloro-5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-[d]-thiazole (5)

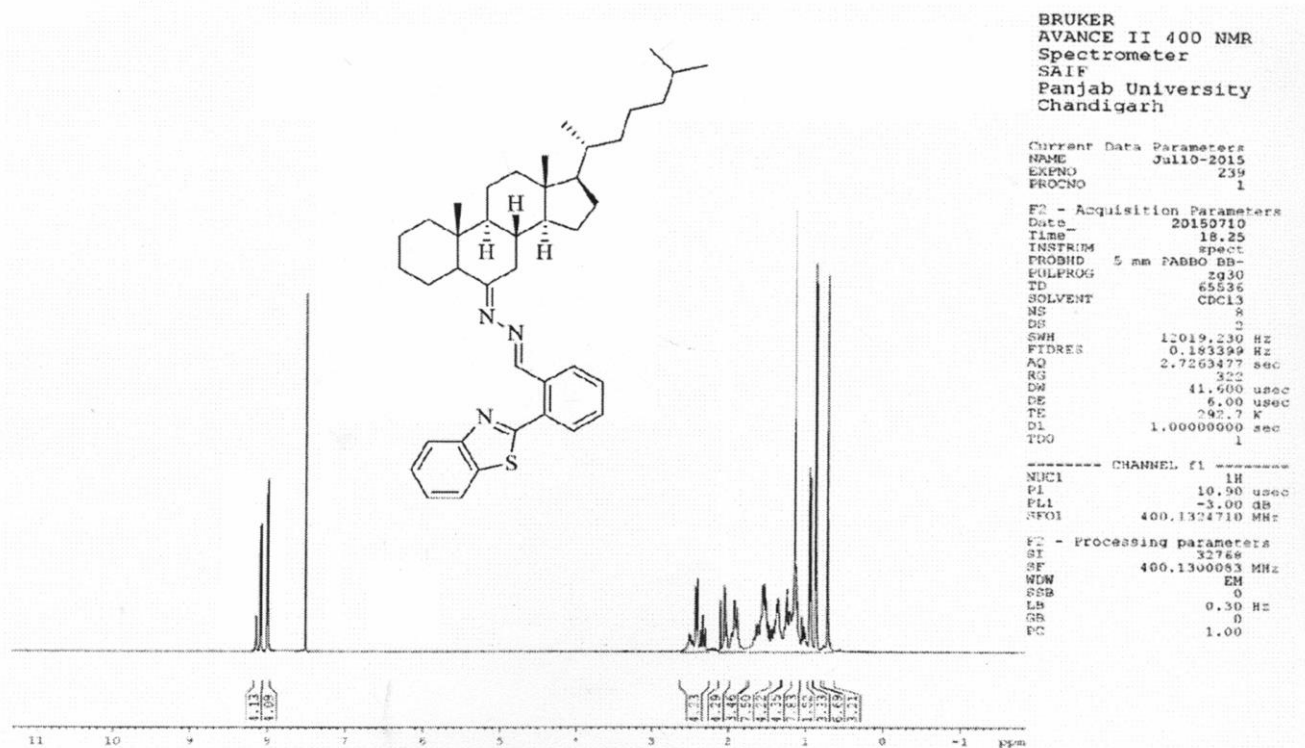


Fig S11. ¹HNMR of 5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-[d]-thiazole (6)

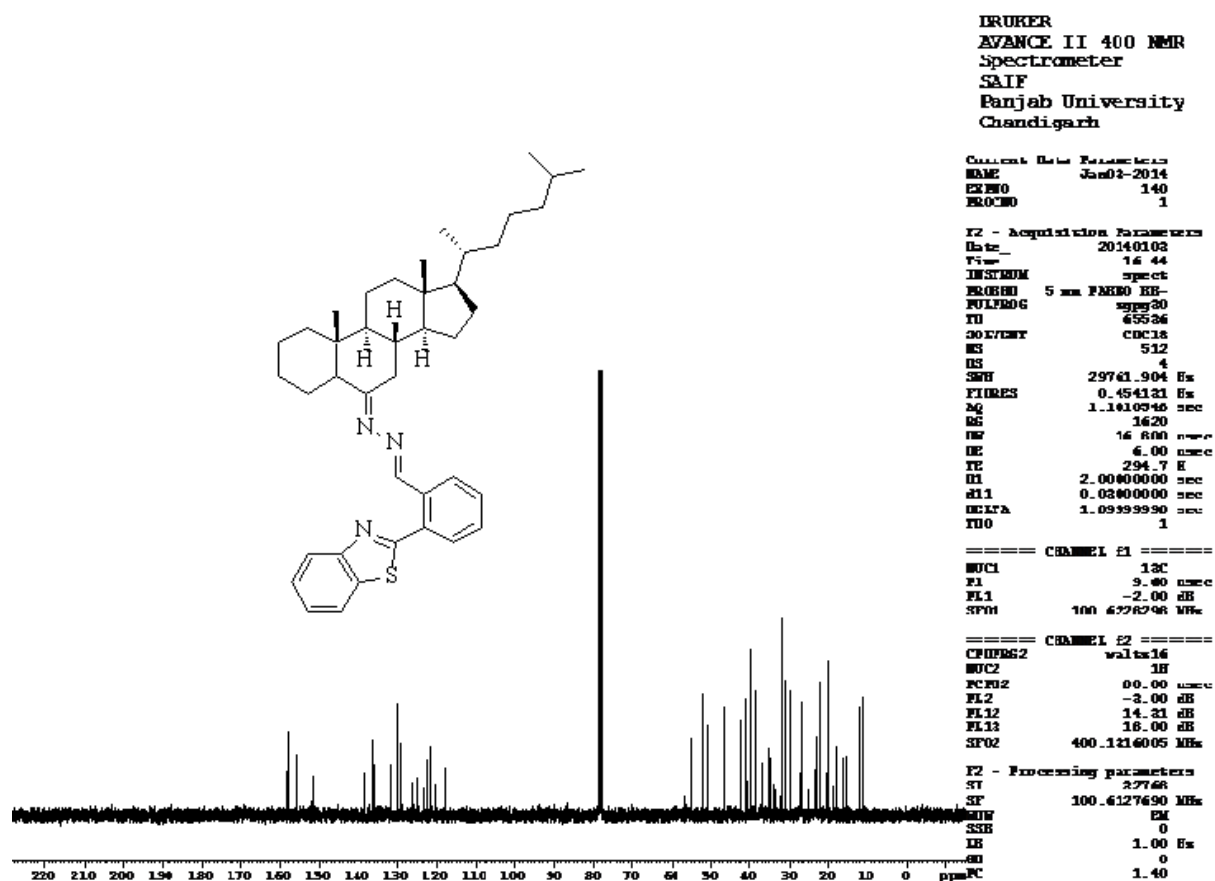


Fig S12. ^{13}C NMR of 5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-[d]-thiazole (6)

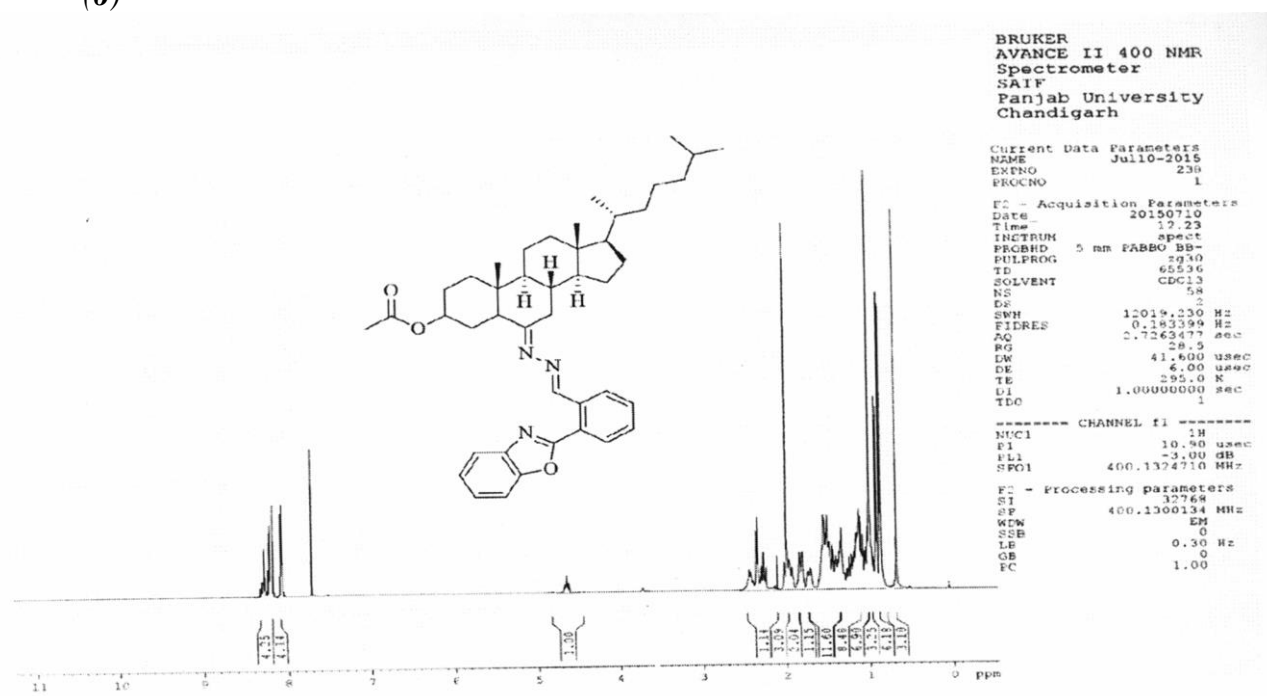


Fig S13. ^1H NMR of 3 β -Acetoxy-5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-[d]-oxazole (7)

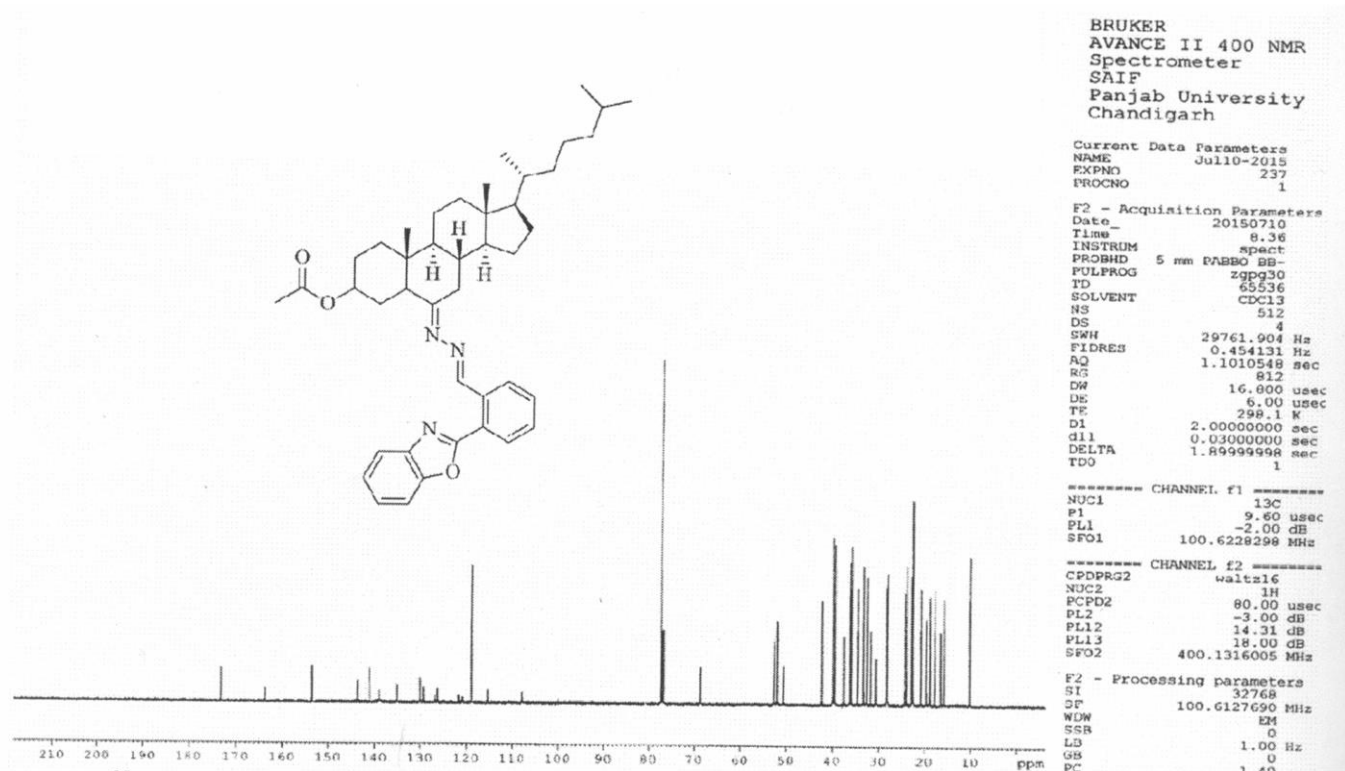


Fig S14. ^{13}C NMR of 3 β -Acetoxy-5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-*[d]*-oxazole (7)

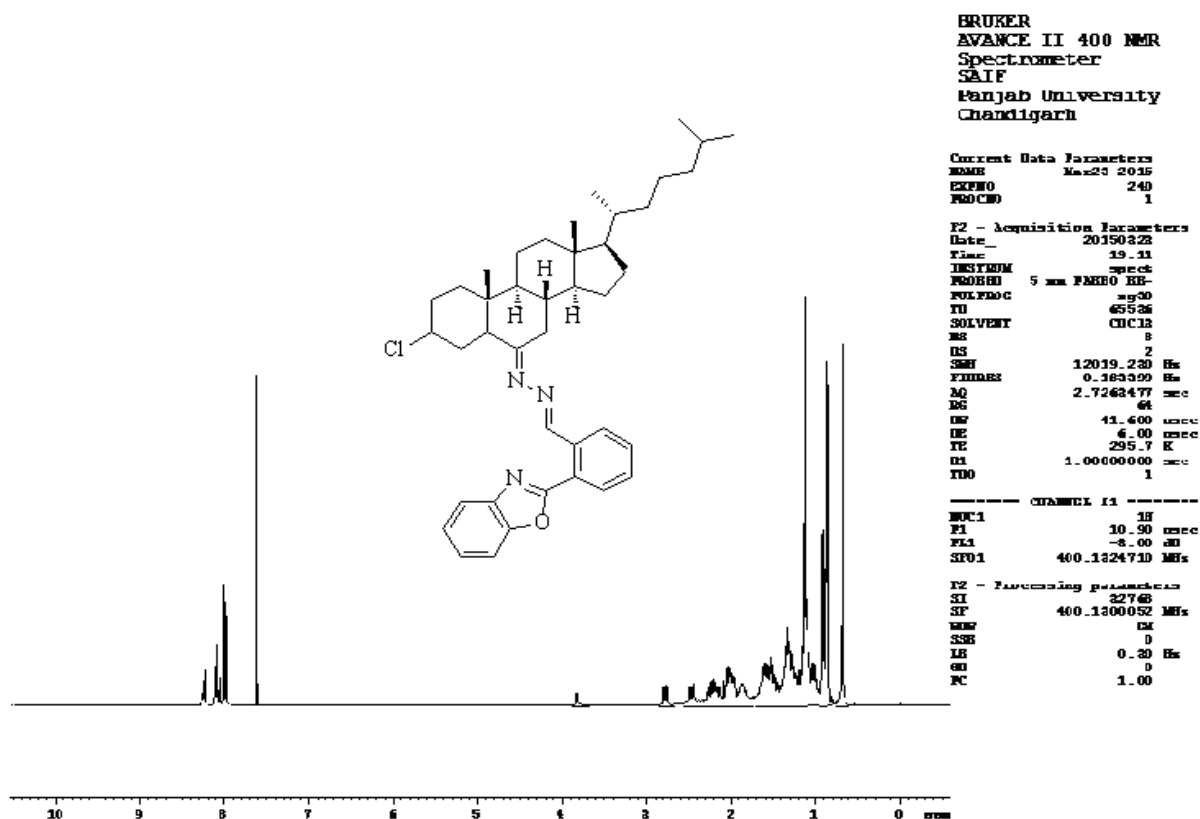


Fig S15. ^1H NMR of 3 β -Chloro-5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-*[d]*-oxazole (8)

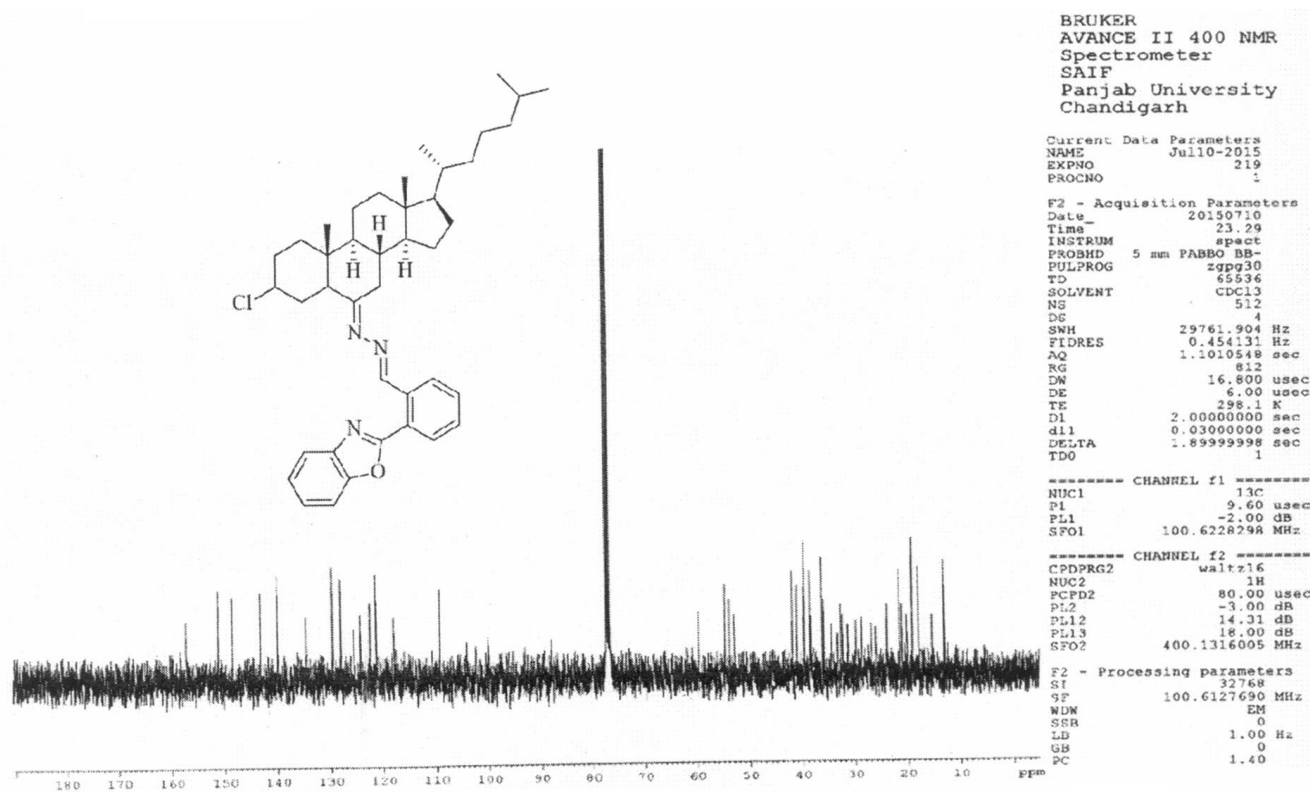


Fig S16. ^{13}C NMR of 3 β -Chloro-5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-[d]-oxazole (8)

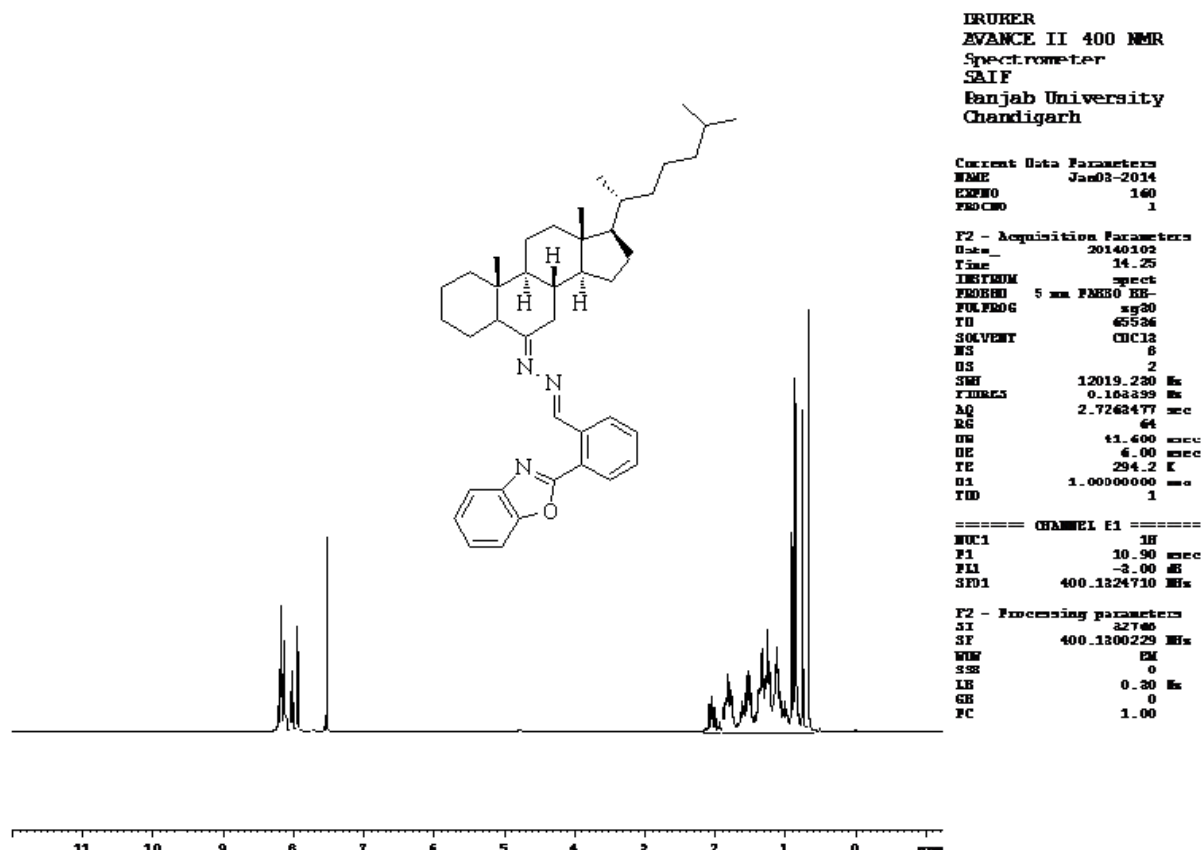


Fig S17. ^1H NMR of 5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-[d]-oxazole (9)

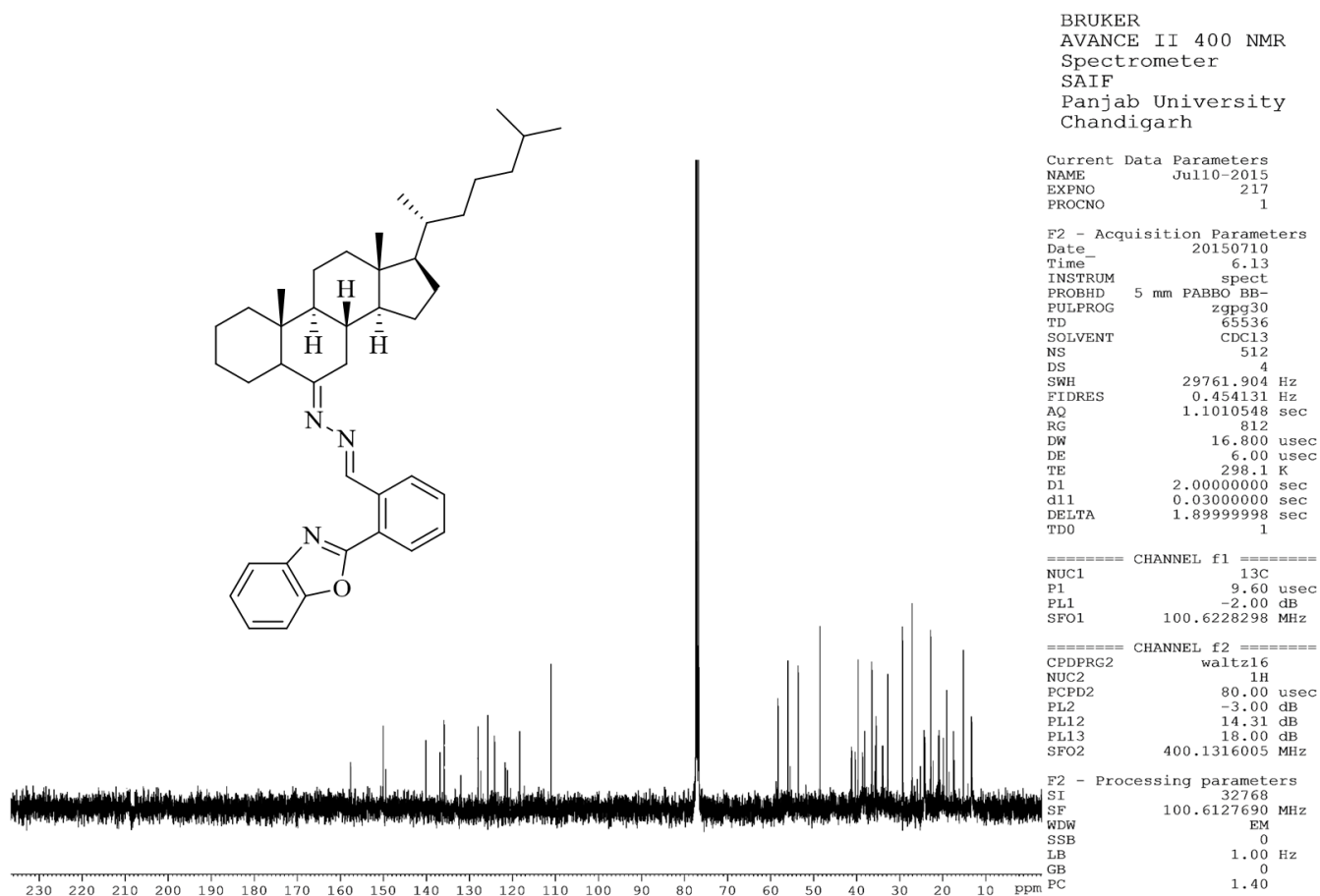


Fig S18. ^{13}C NMR of 5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-[d]-oxazole (9)

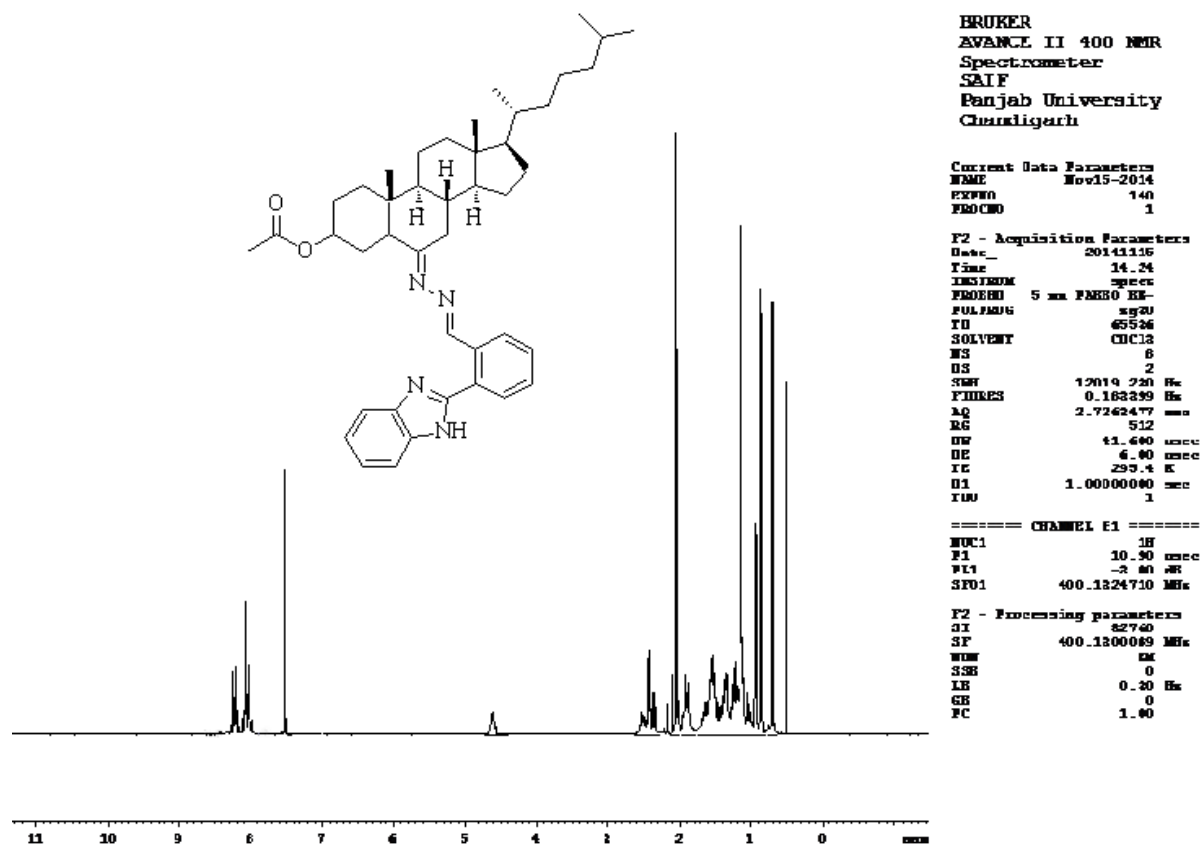


Fig S19. ^1H NMR of 3β -Acetoxy- 5α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo- $[d]$ -imidazole (**10**)

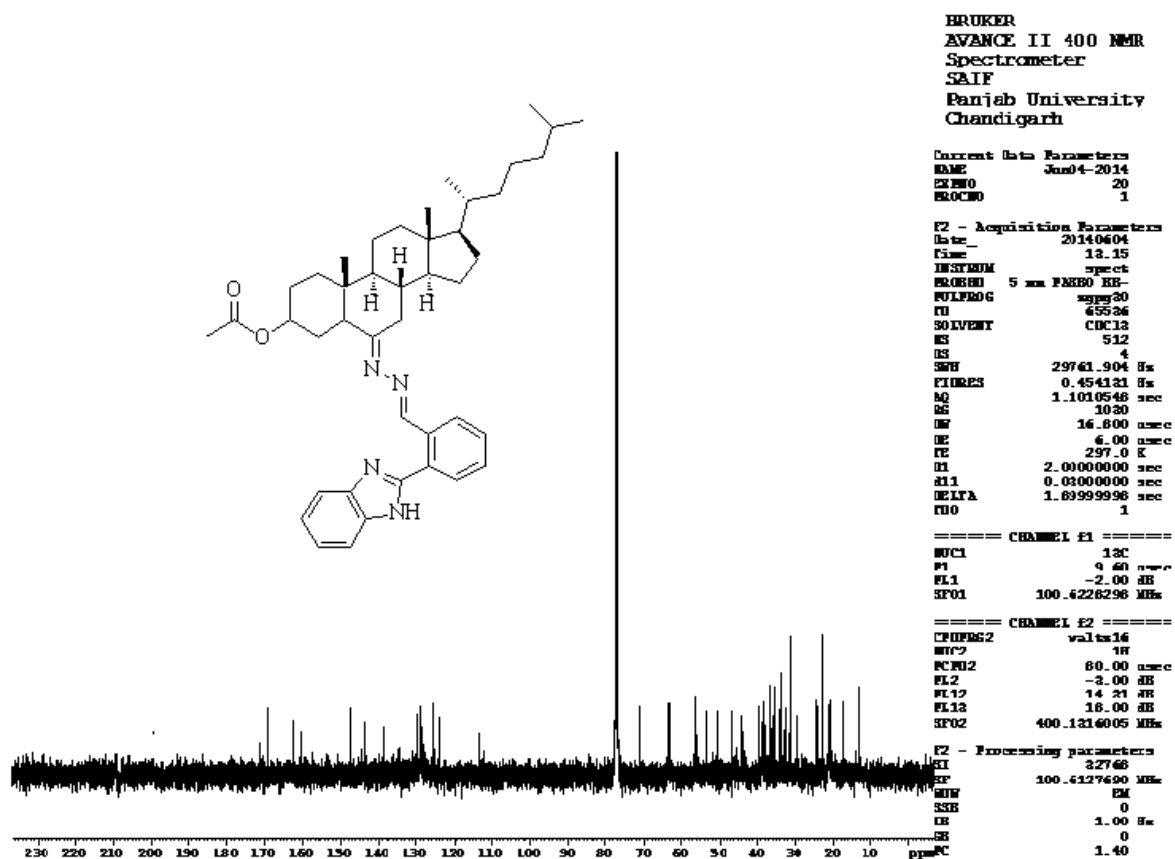


Fig S20. ^{13}C NMR of 3 β -Acetoxy-5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-*[d]*-imidazole (**10**)

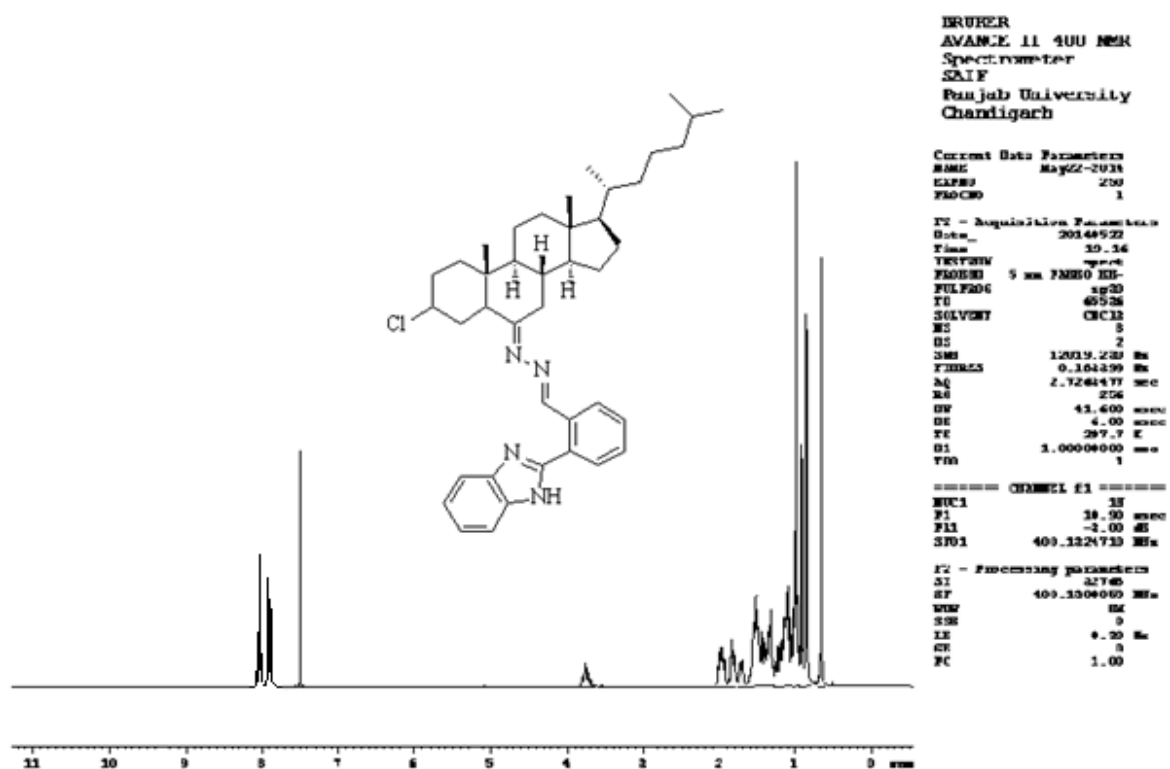


Fig S21. ^1H NMR of 3β -Chloro- 5α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo- $[d]$ -imidazole (**11**)

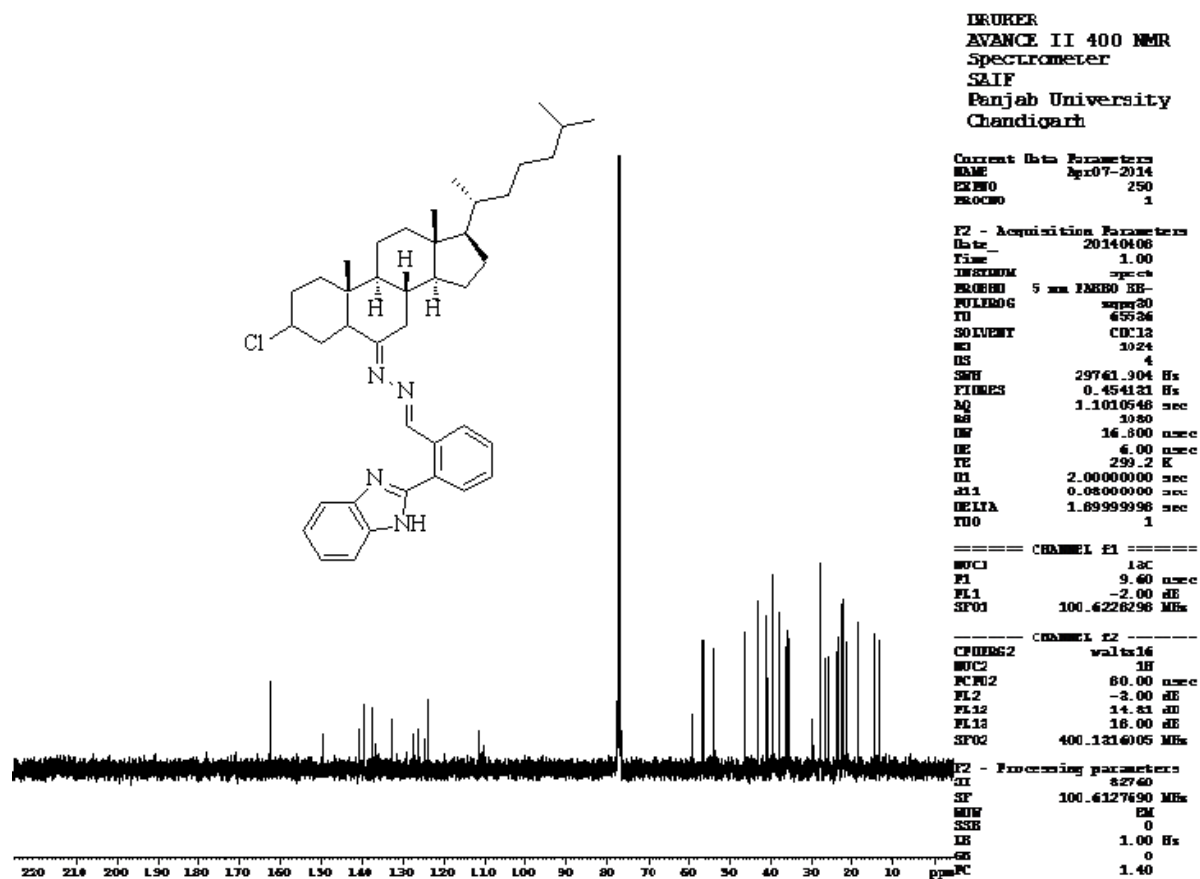


Fig S22. ^{13}C NMR of 3 β -Chloro-5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-*[d]*-imidazole (**11**)

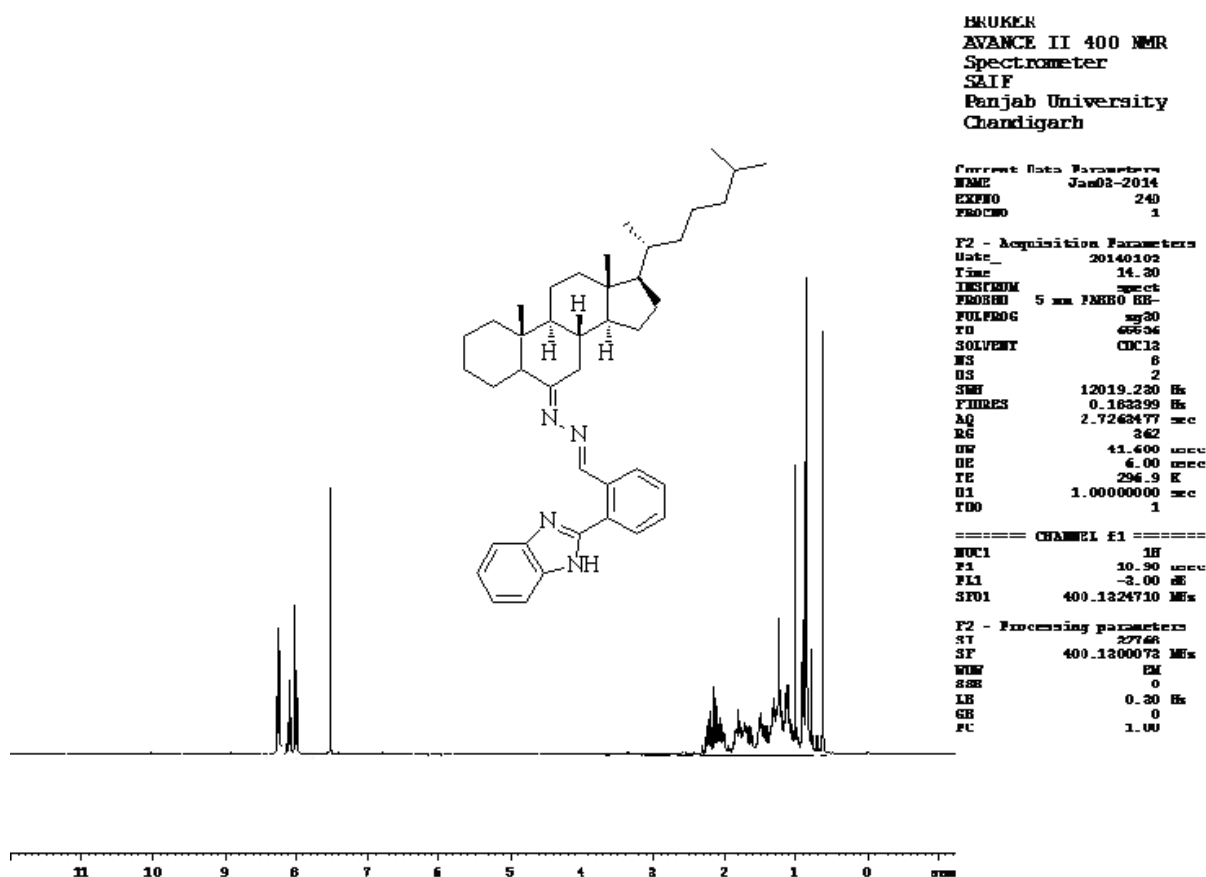


Fig S23. ^1H NMR of 5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-[d]-imidazole (**12**)

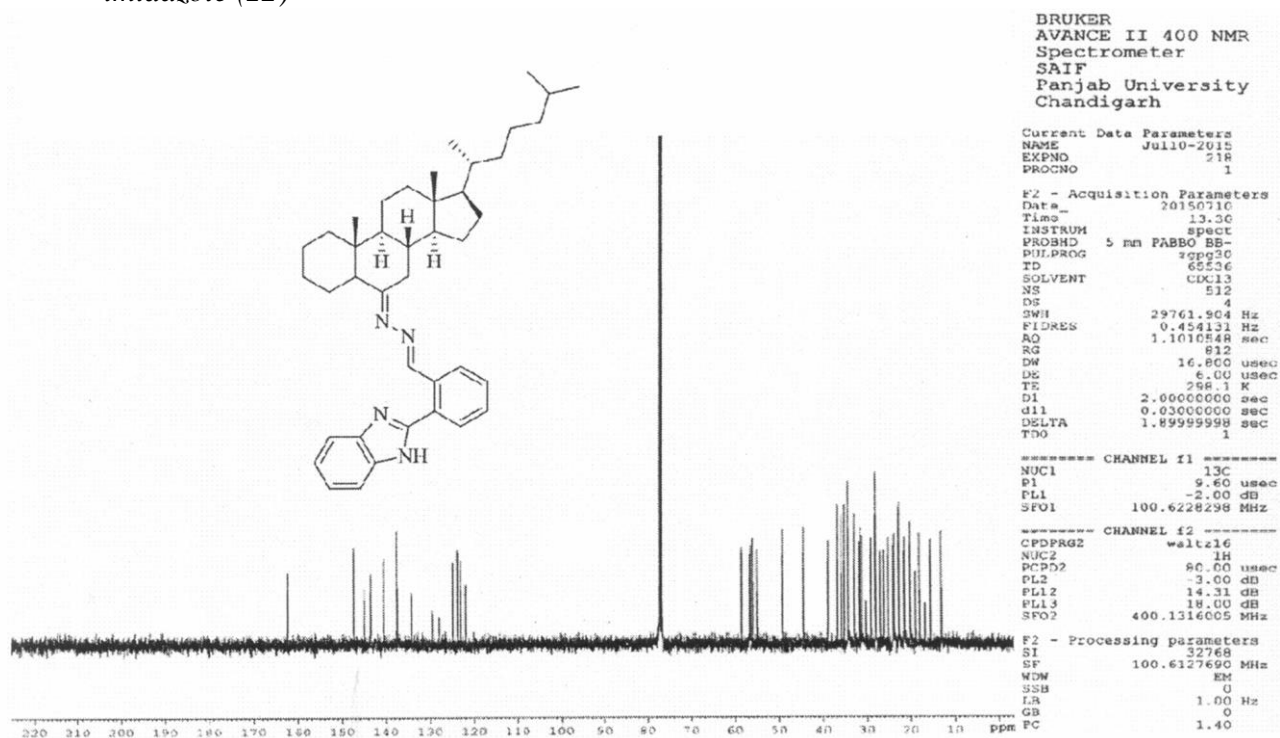
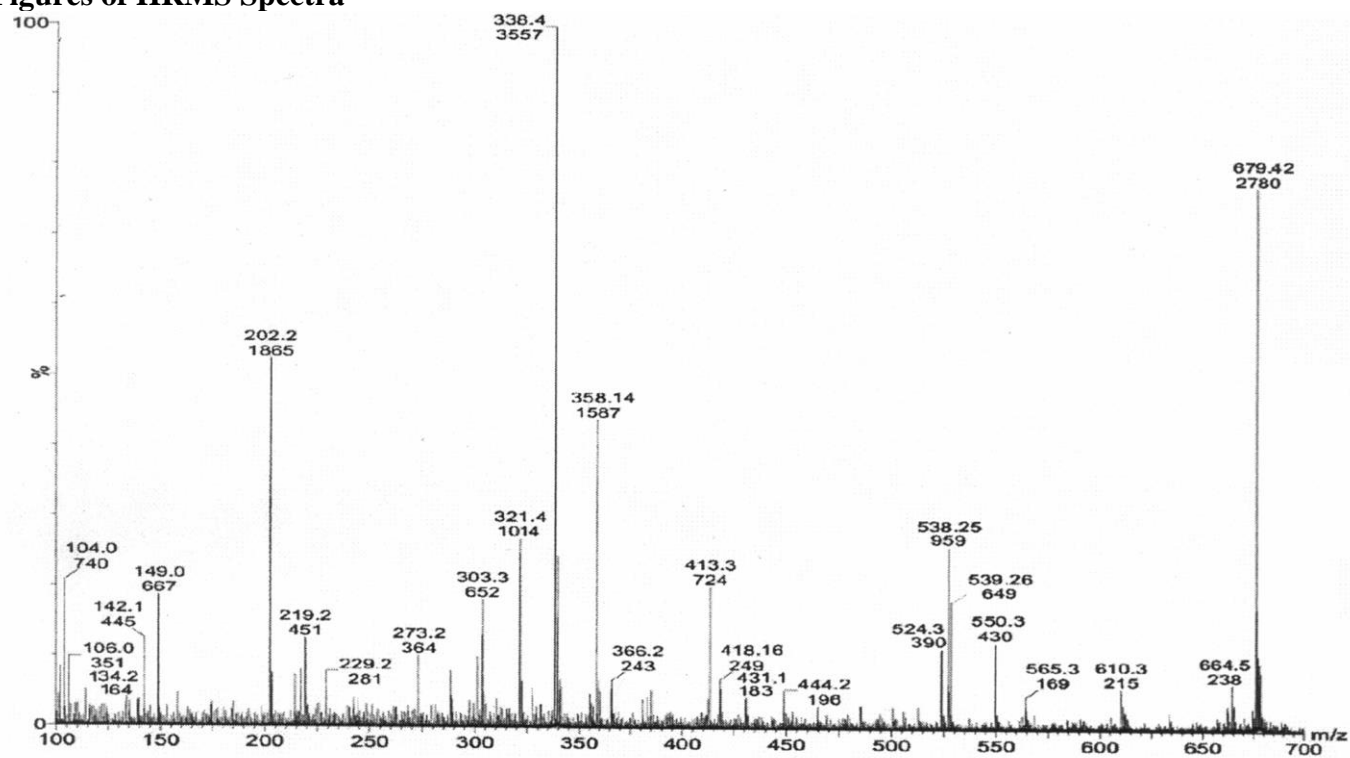
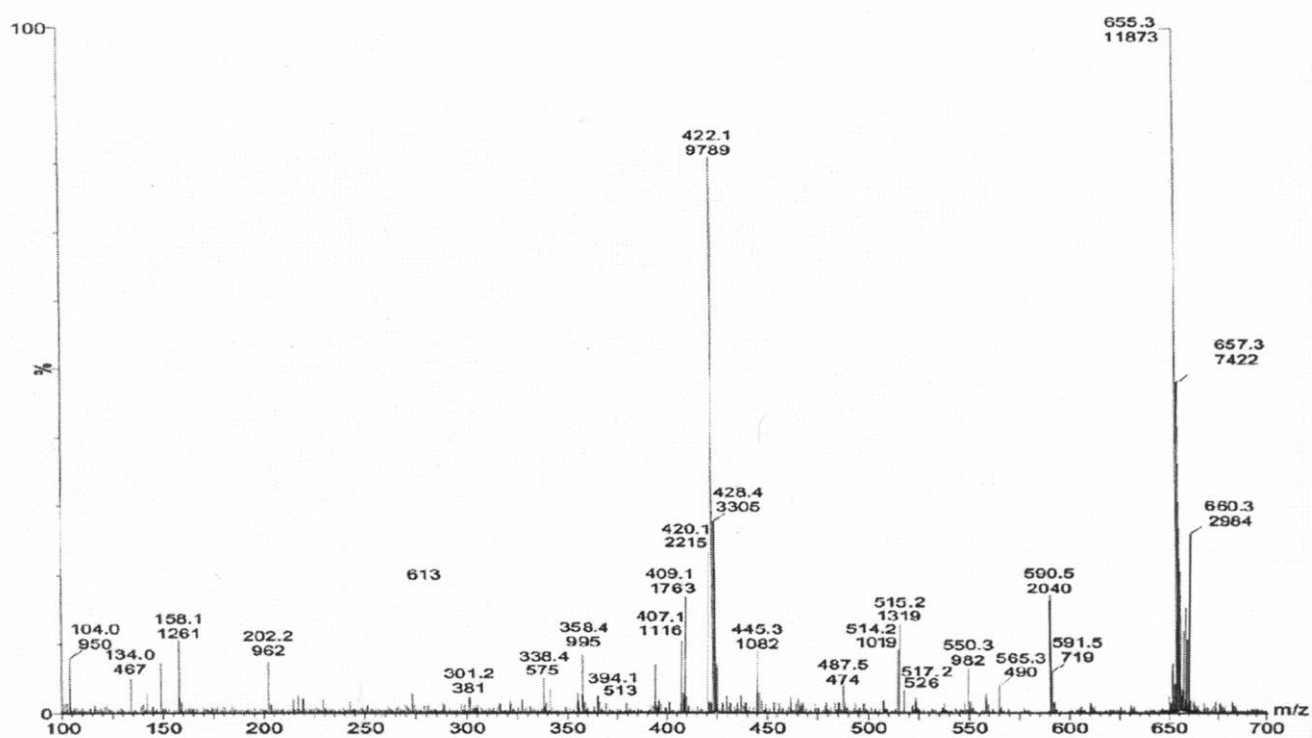


Fig S24. ^{13}C NMR of 5 α -cholestan-6-(iminohydrazonomethylphenyl-2-yl)-benzo-[d]-imidazole (**12**)

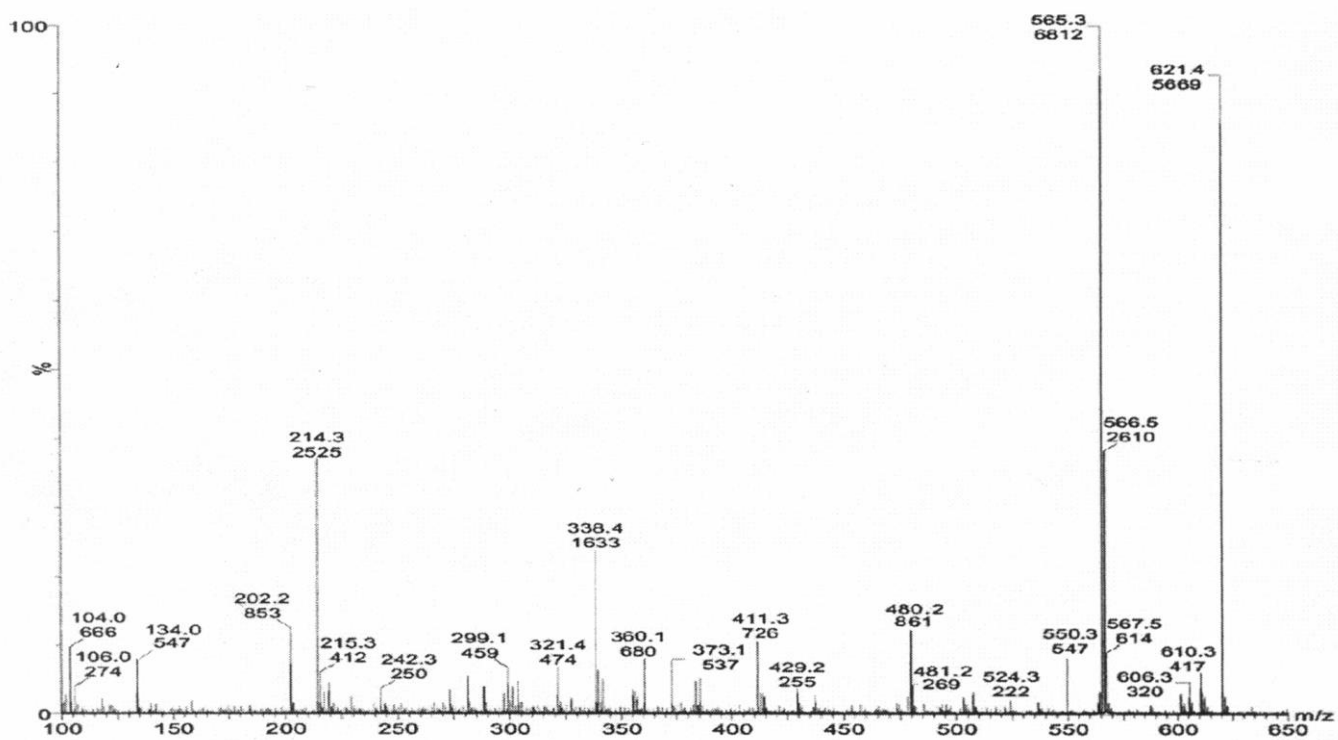
Figures of HRMS Spectra



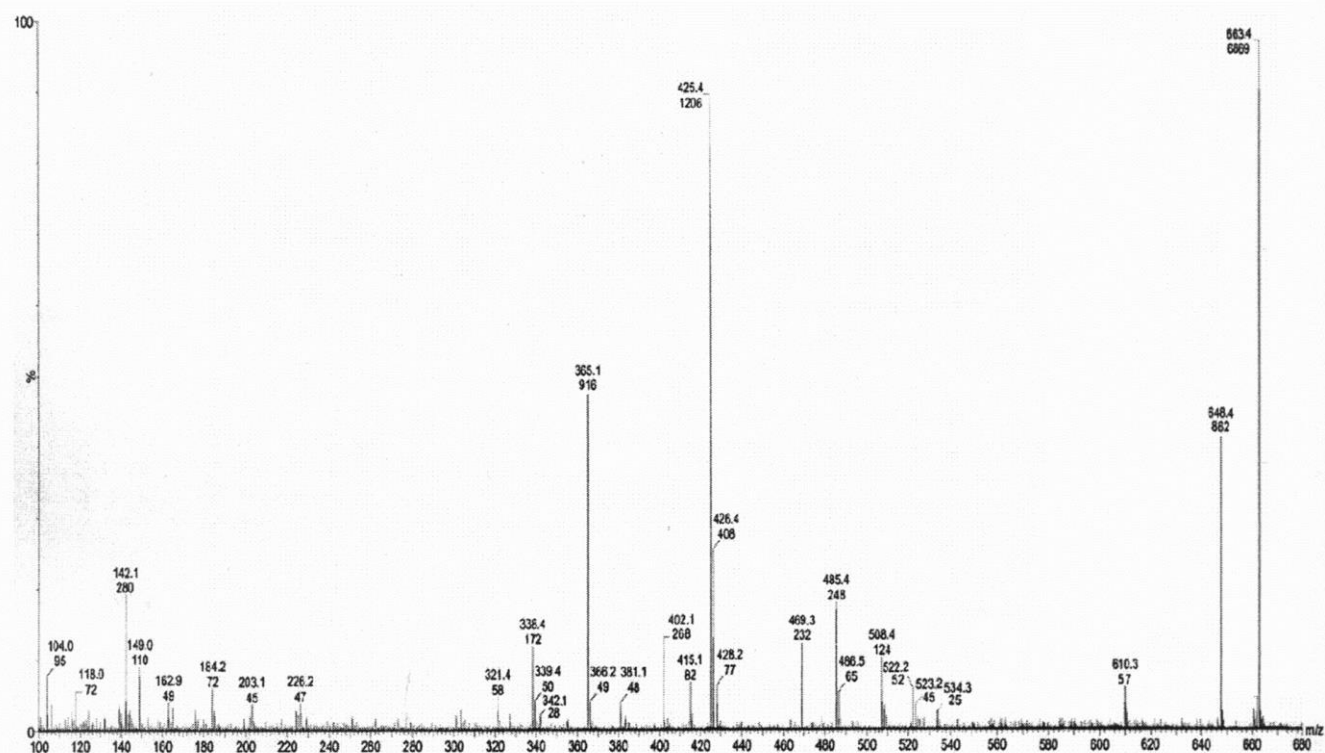
HRMS Spectra of compound 4



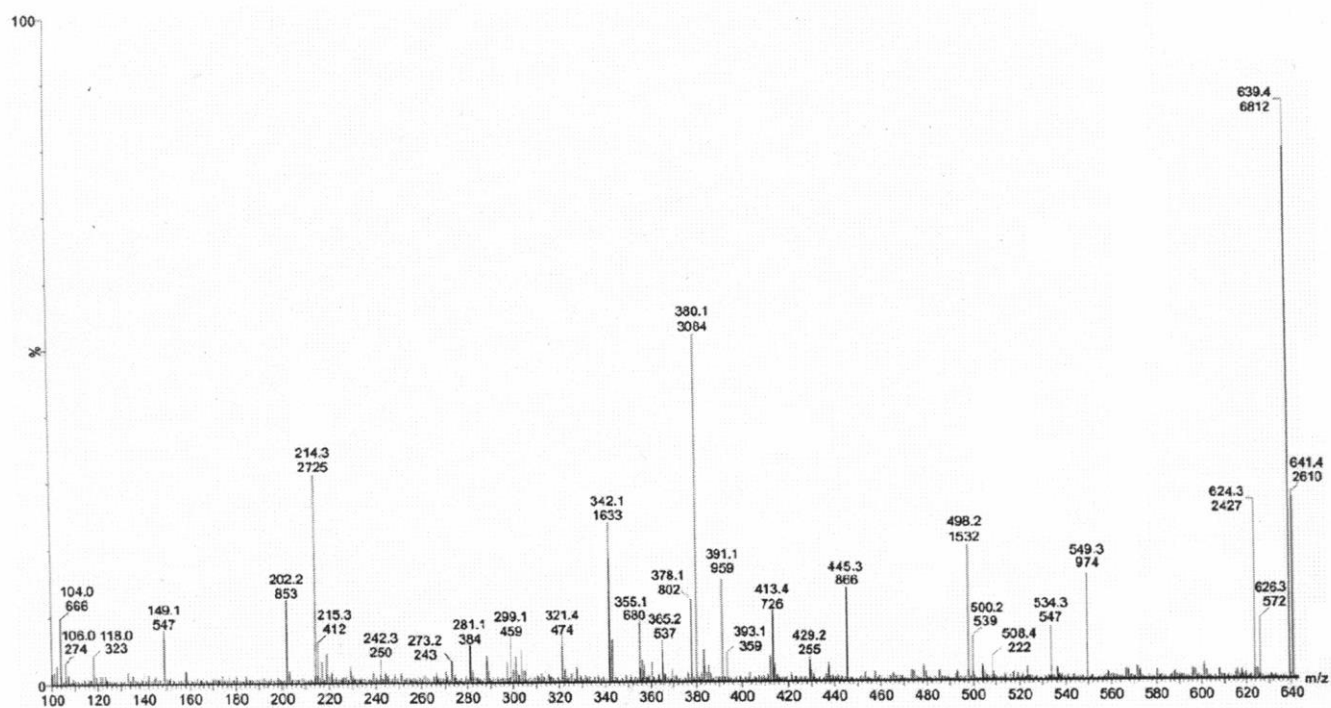
HRMS Spectra of compound 5



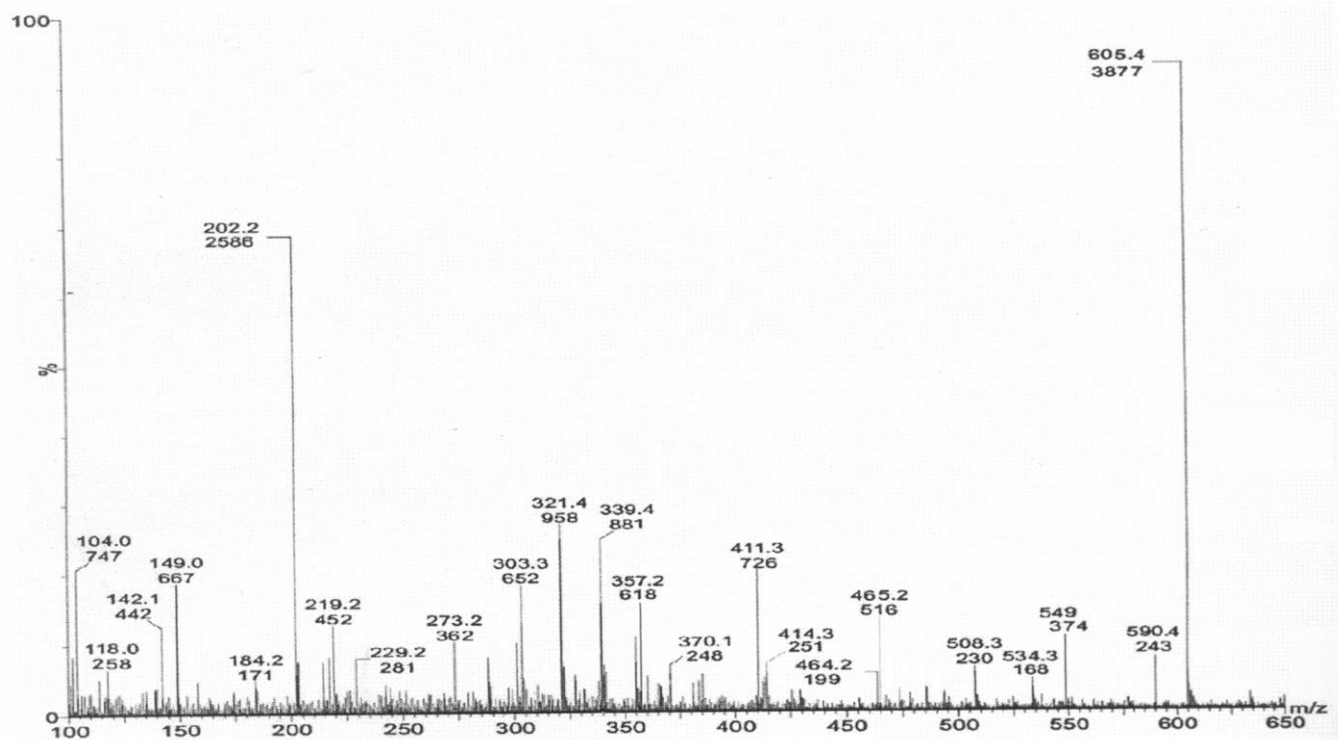
HRMS Spectra of compound 6



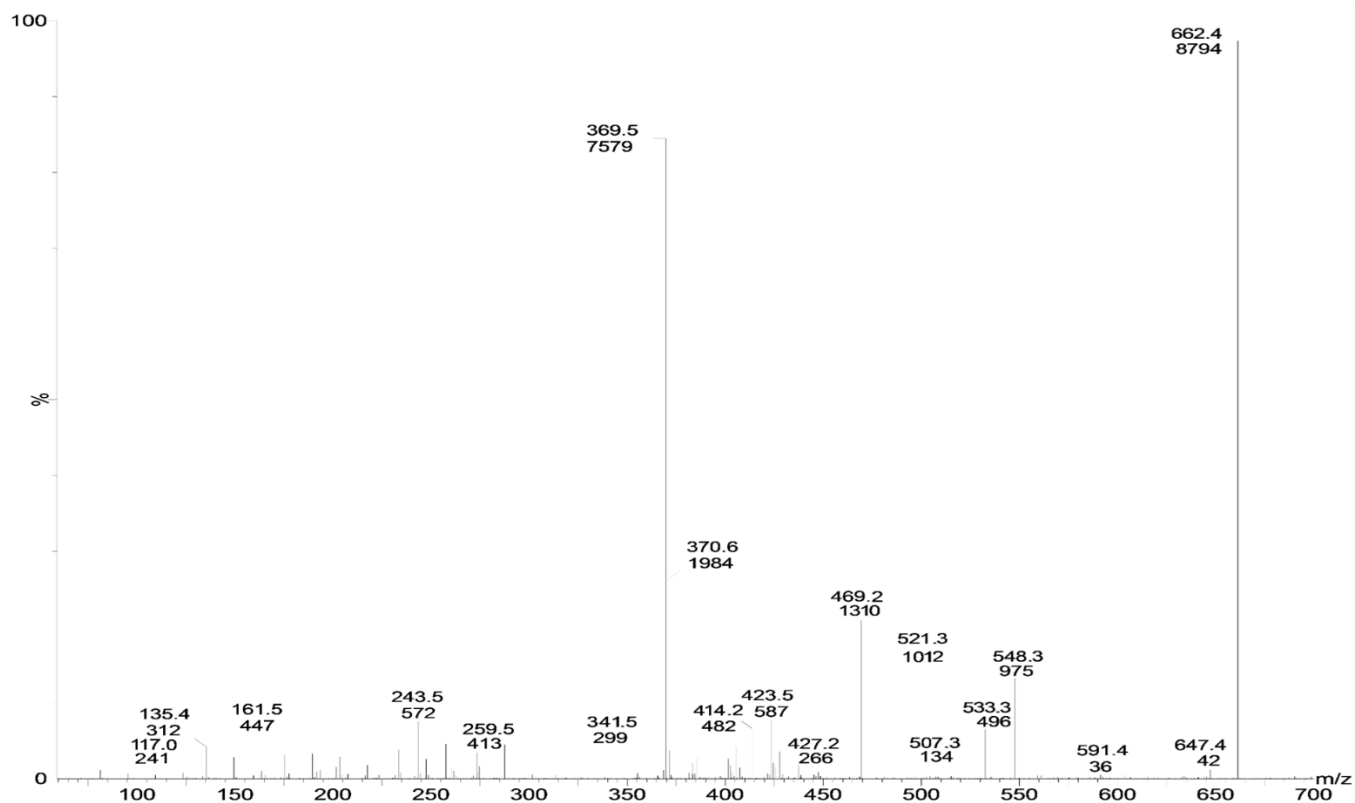
HRMS Spectra of compound 7



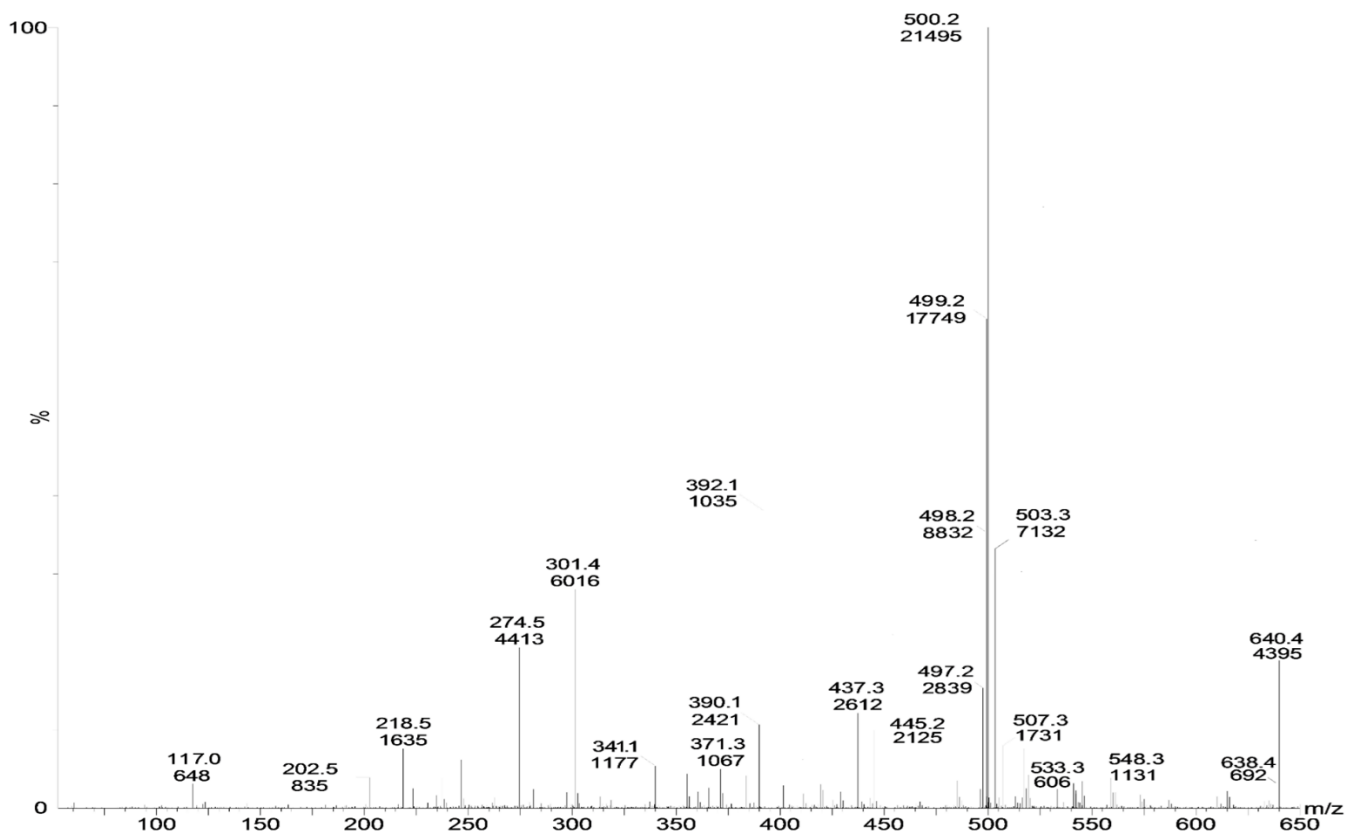
HRMS Spectra of compound 8



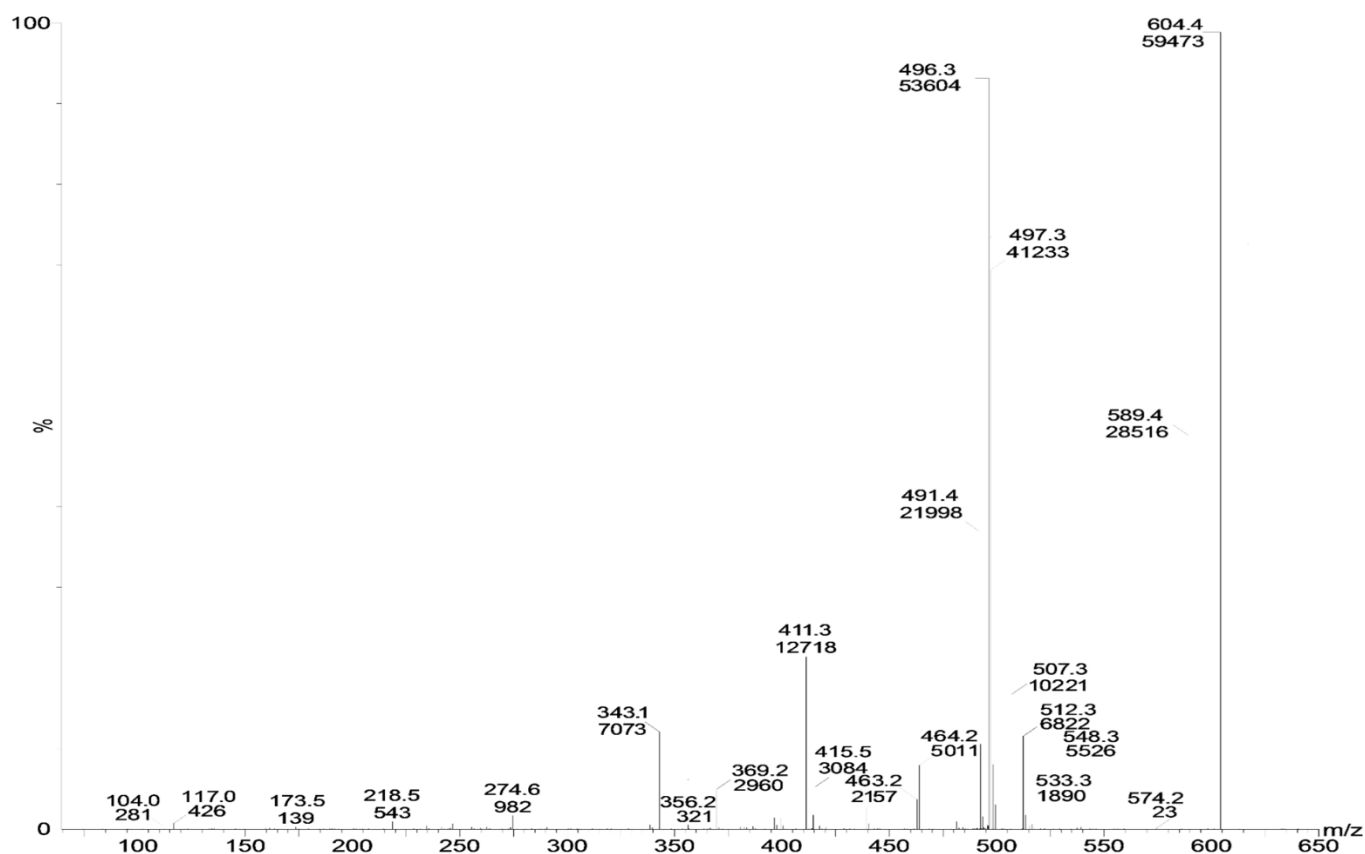
HRMS Spectra of compound 9



HRMS Spectra of compound 10



HRMS Spectra of compound 11



HRMS Spectra of compound **12**