

SUPPLEMENTARY MATERIAL

Synthesis and molecular docking of new 1,3,4-oxadiazole incorporated 1,2,3-triazole moiety as a potential anticancer agent targeting thymidylate synthase.

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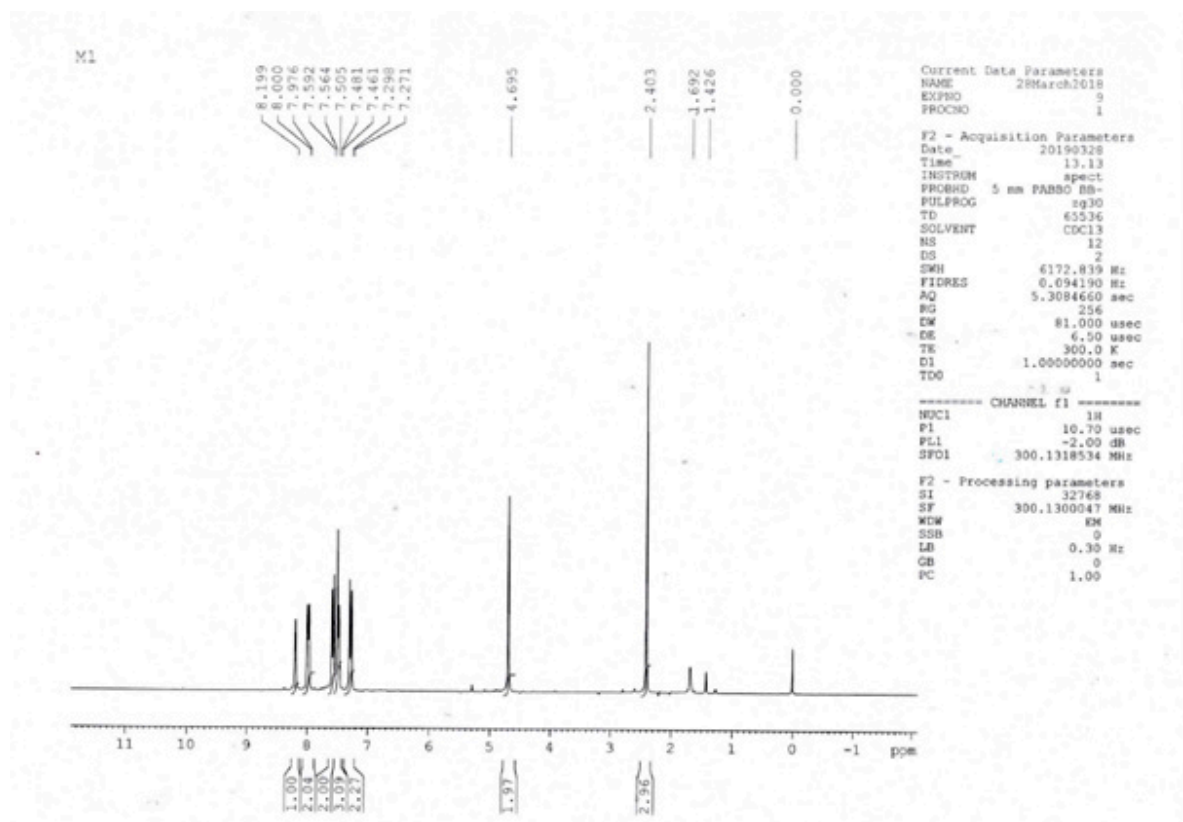


Figure S1: ^1H NMR of compound 6

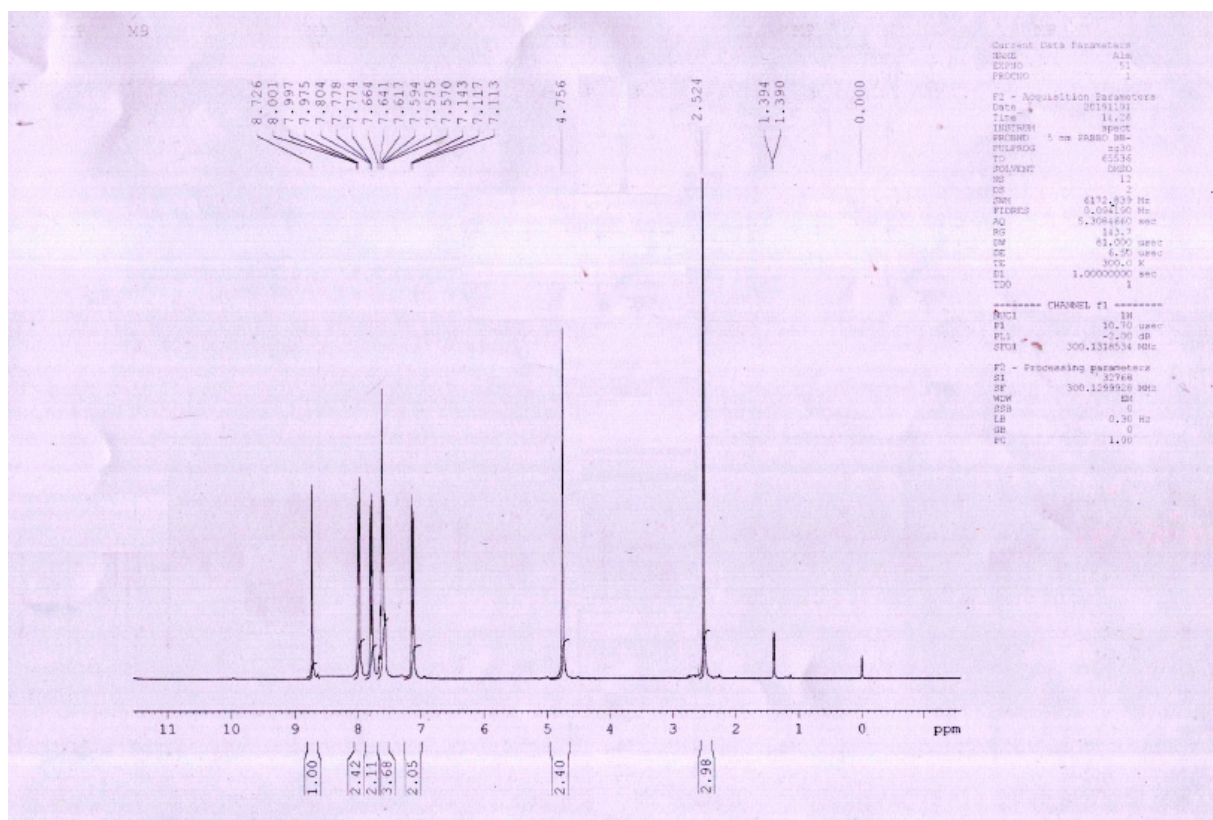


Figure S2: ¹H NMR of compound 7

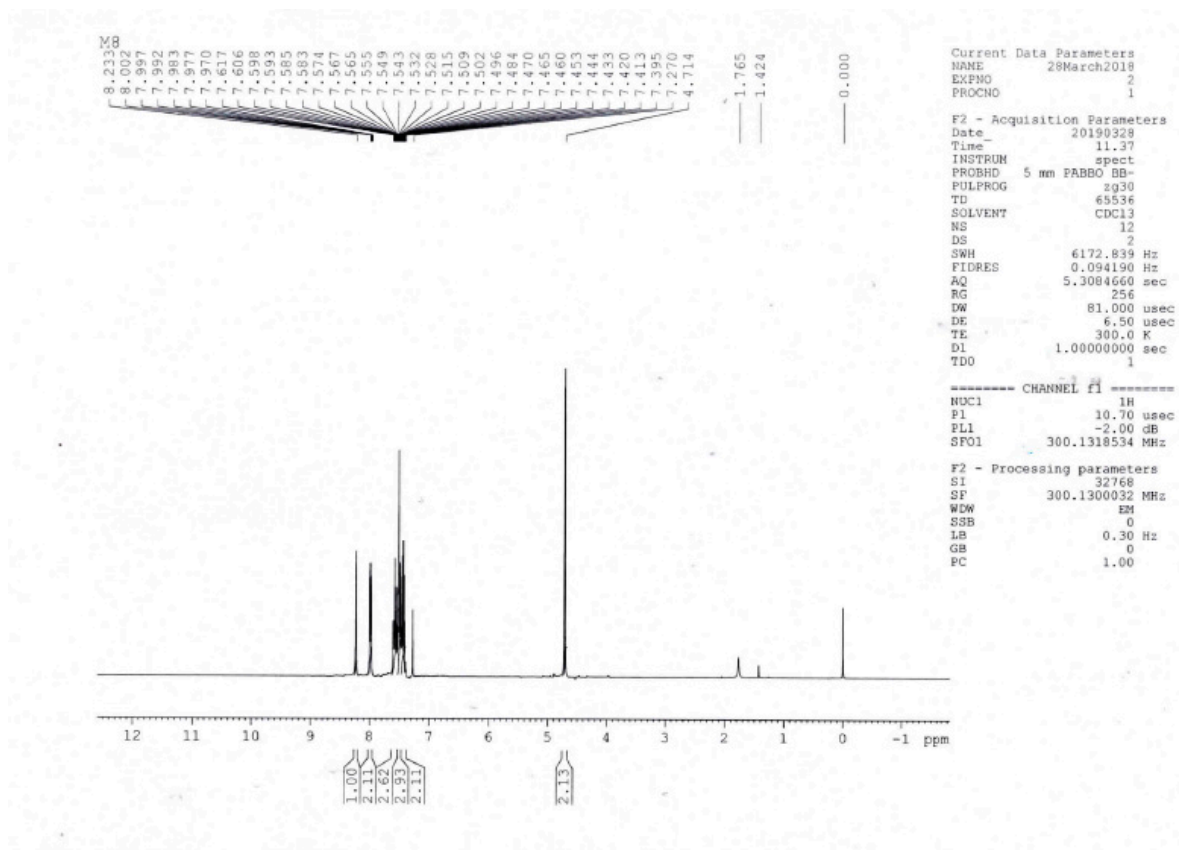


Figure S3: ^1H NMR of compound 8

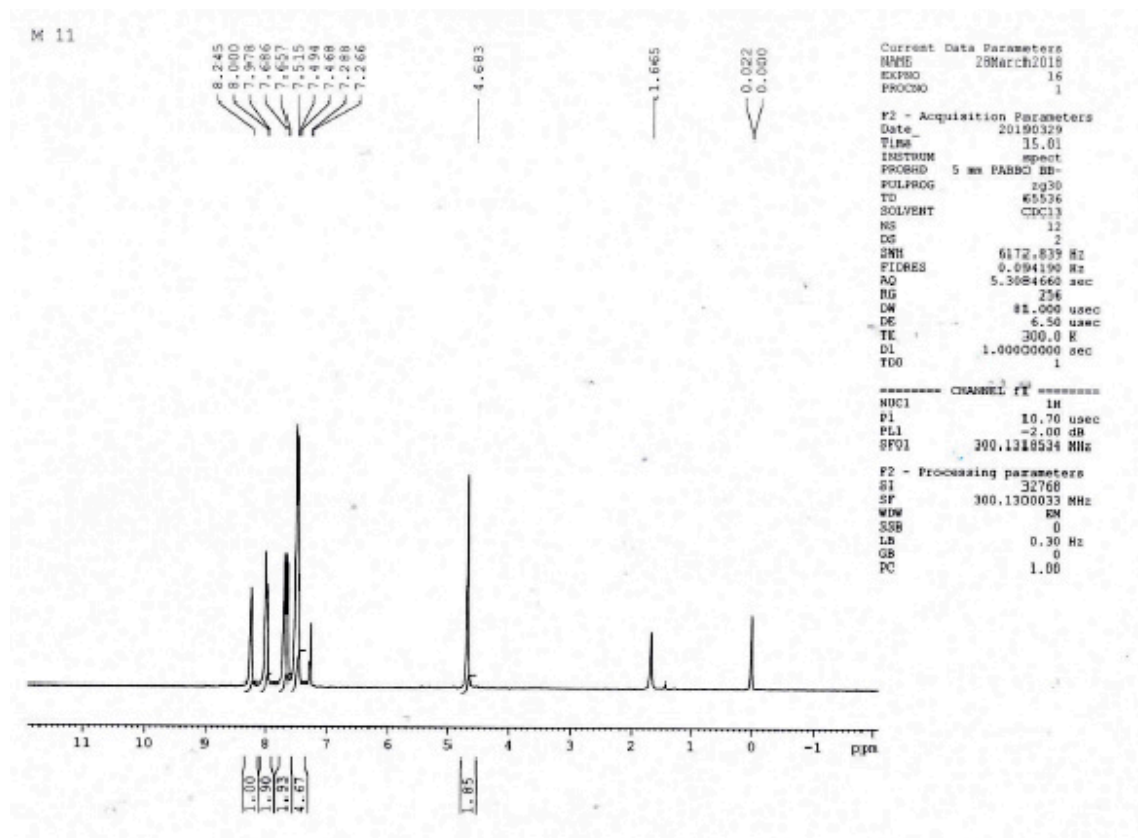


Figure S4: ^1H NMR of compound 9

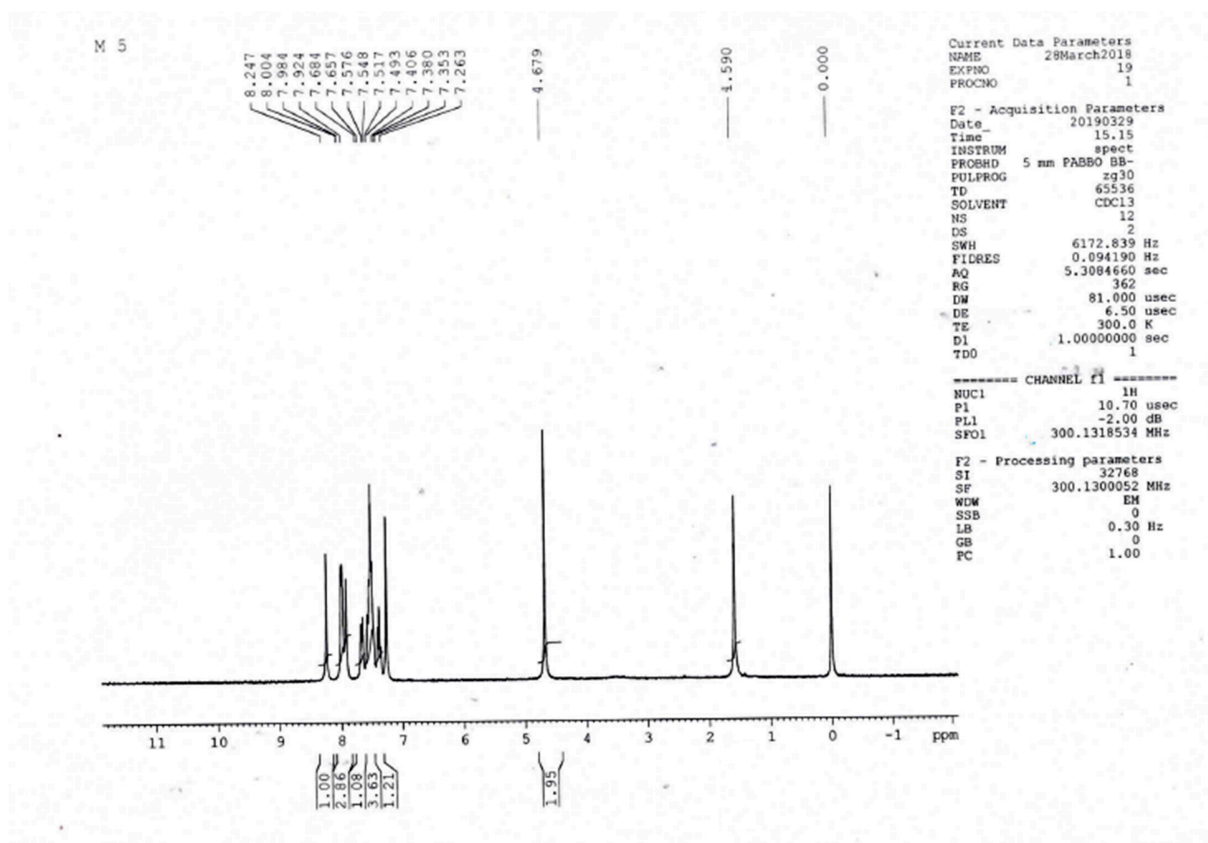


Figure S5: ¹H NMR of compound 10

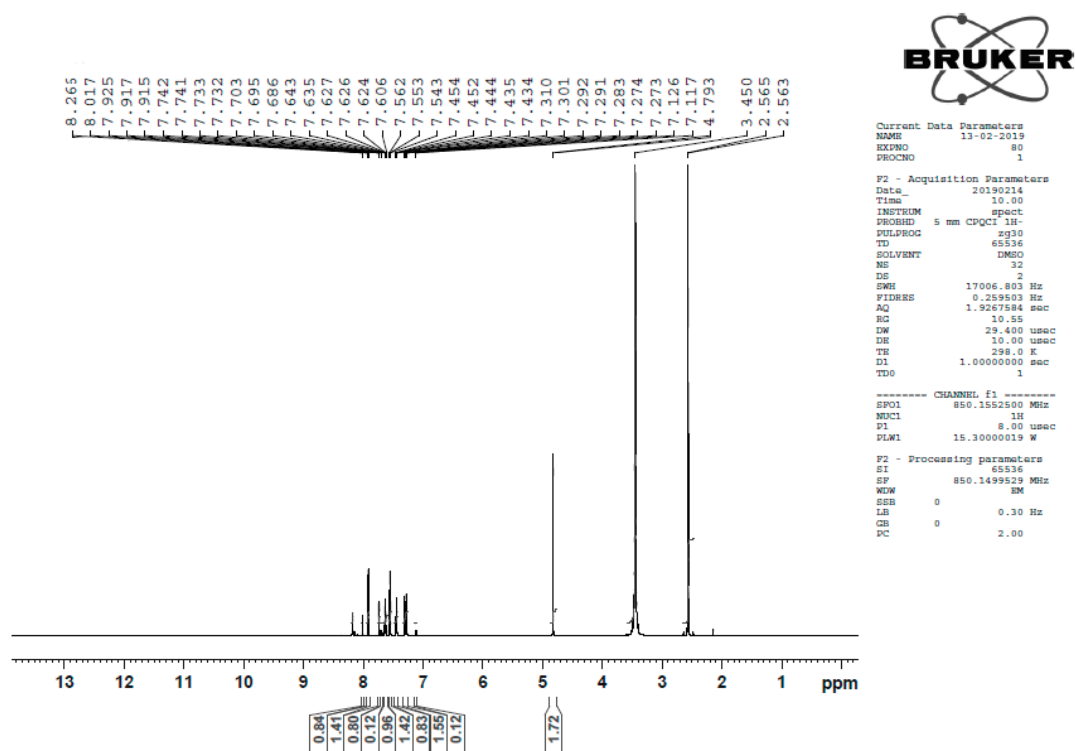


Figure S6: ¹H NMR of compound 11

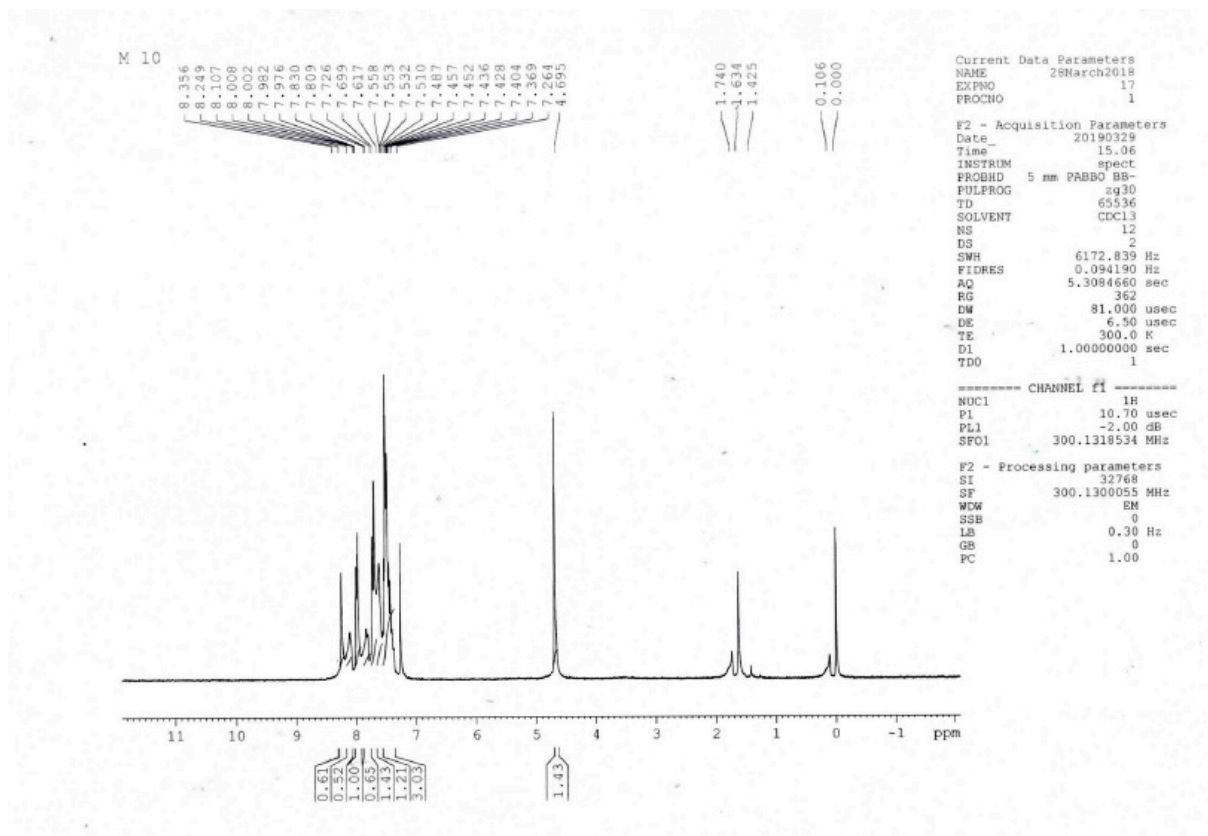


Figure S7: ^1H NMR of compound 12

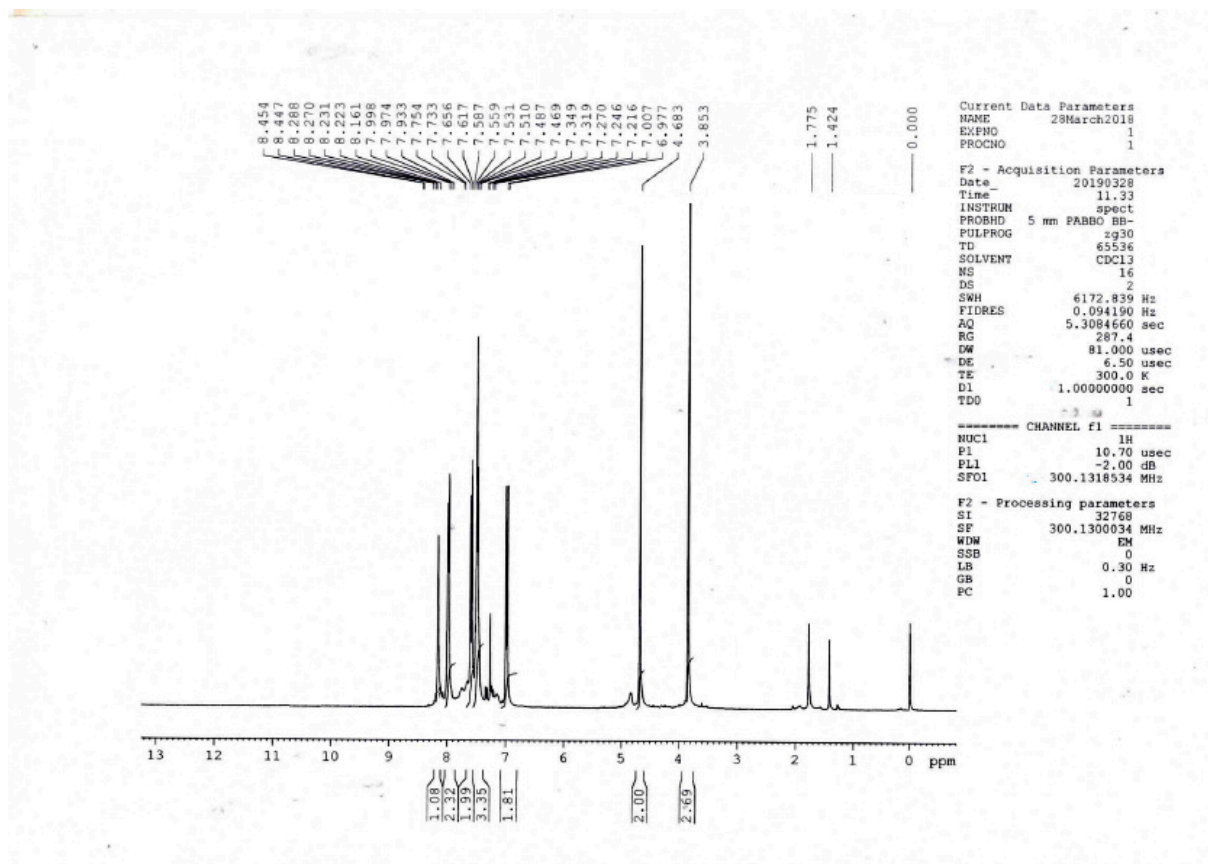


Figure S8: ^1H NMR of compound 13

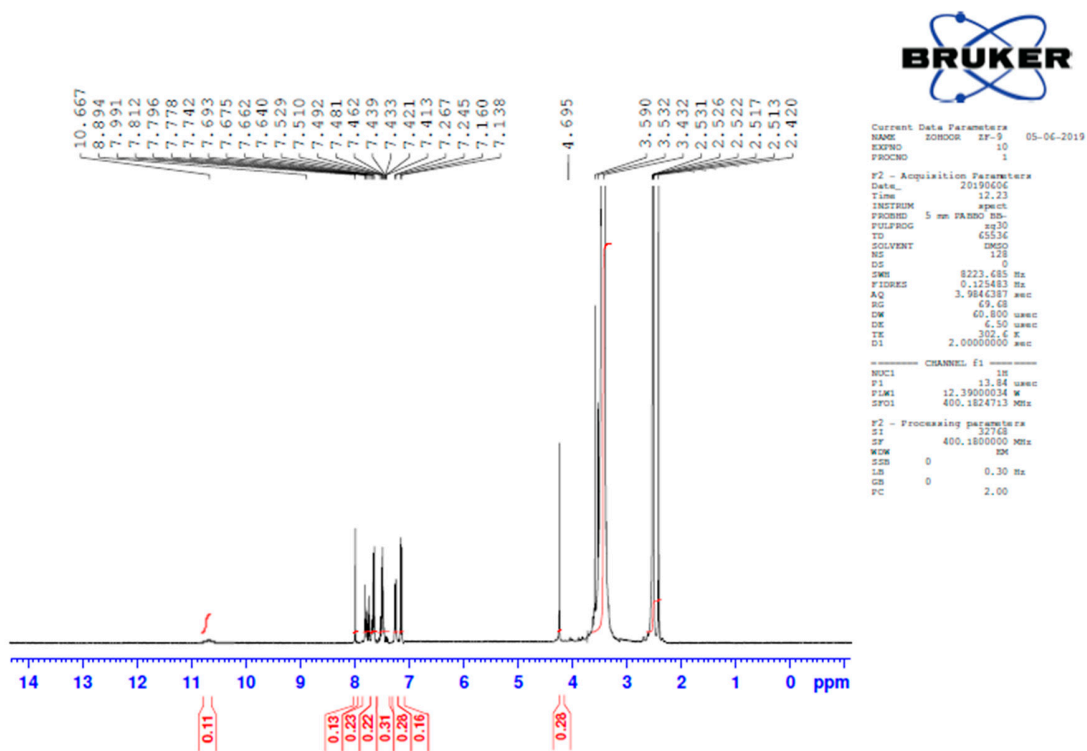


Figure S9: ¹H NMR of compound 14

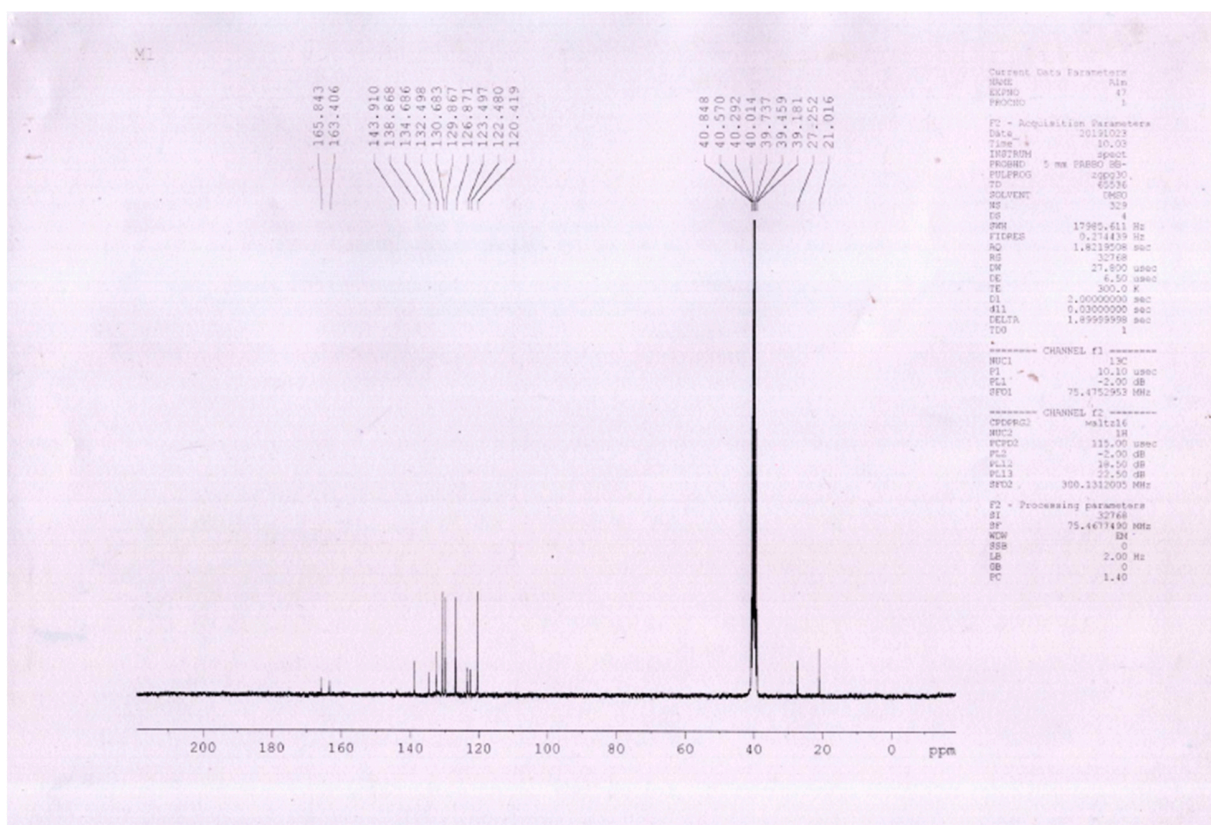


Figure S10: ^{13}C NMR of compound 6

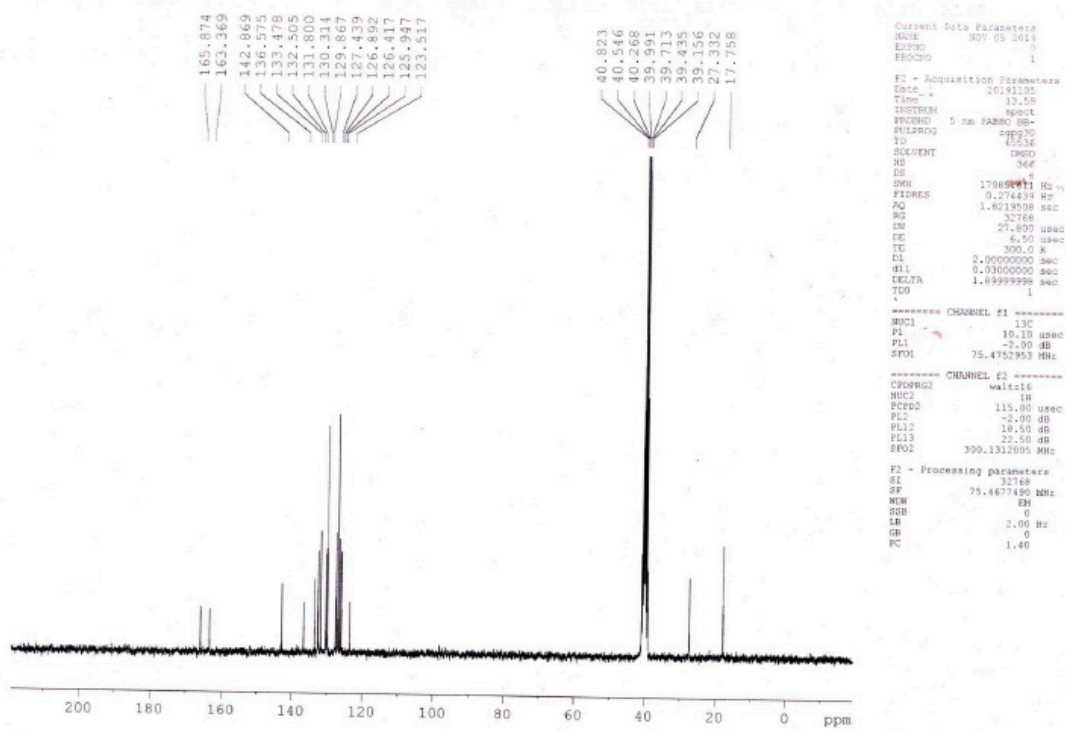


Figure S11: ¹³C NMR of compound 7

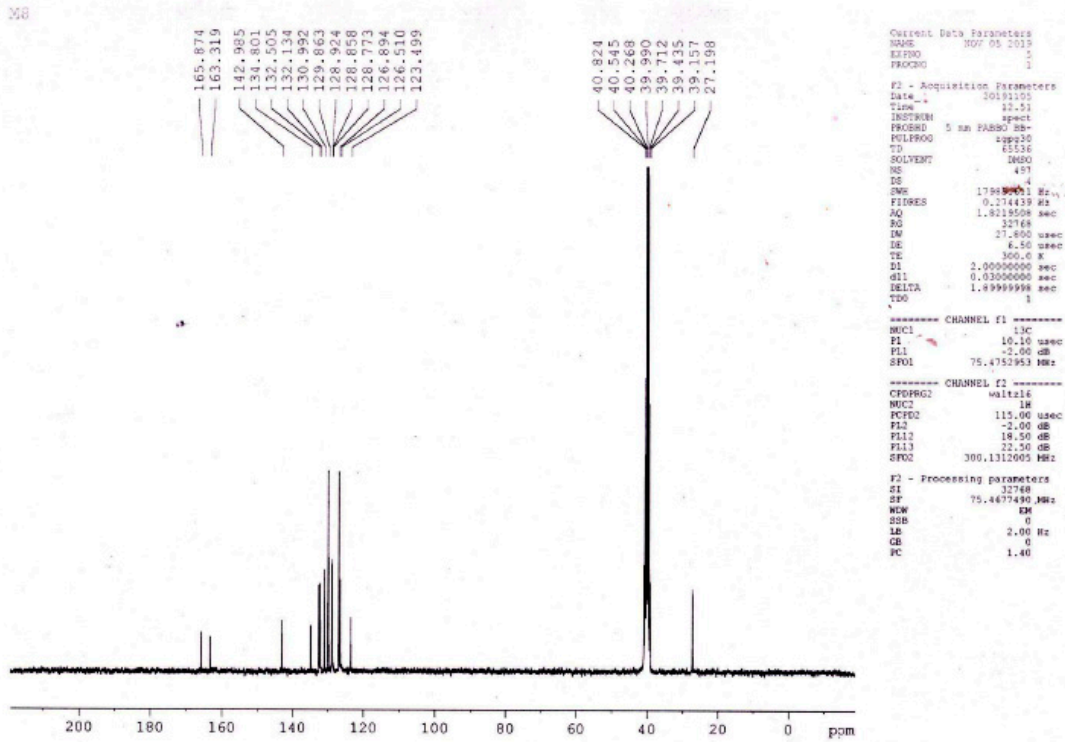


Figure S12: ¹³C NMR of compound 8

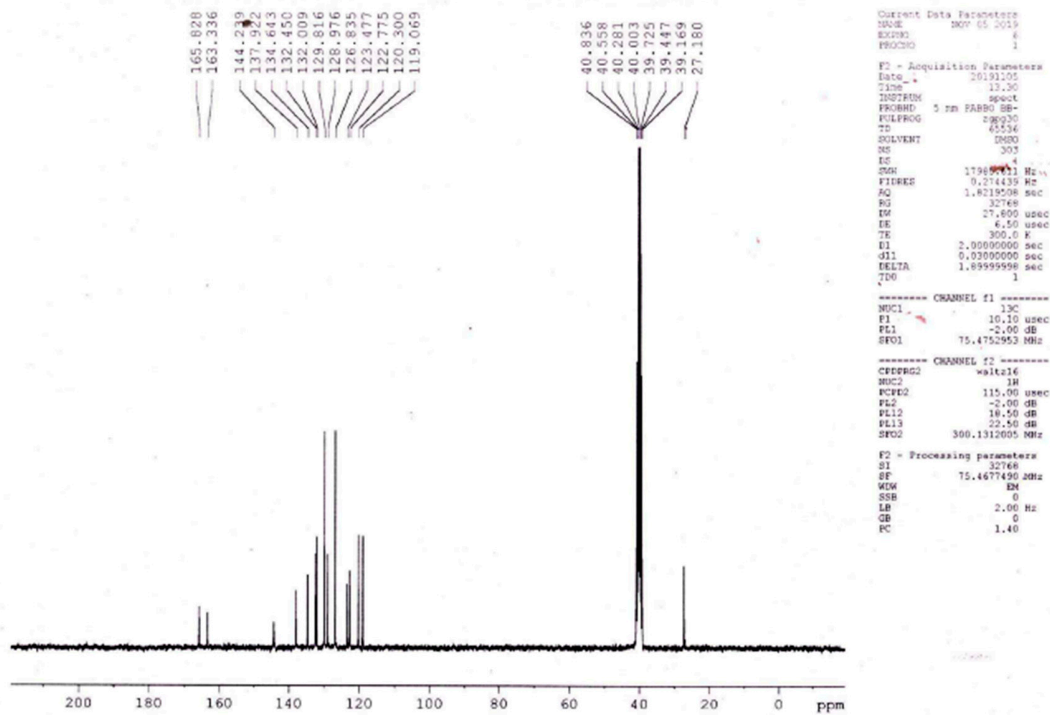


Figure S13: ^{13}C NMR of compound 9

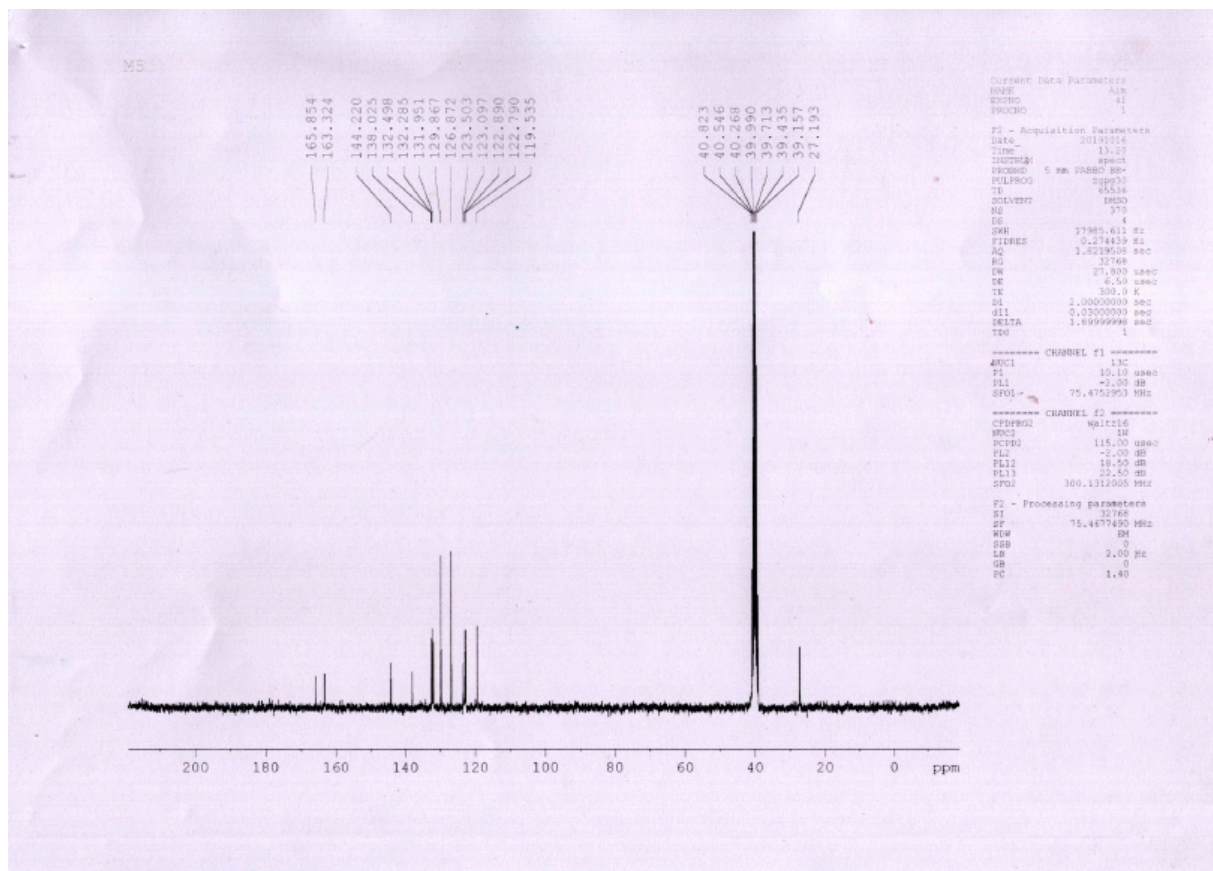


Figure S14: ^{13}C NMR of compound 10

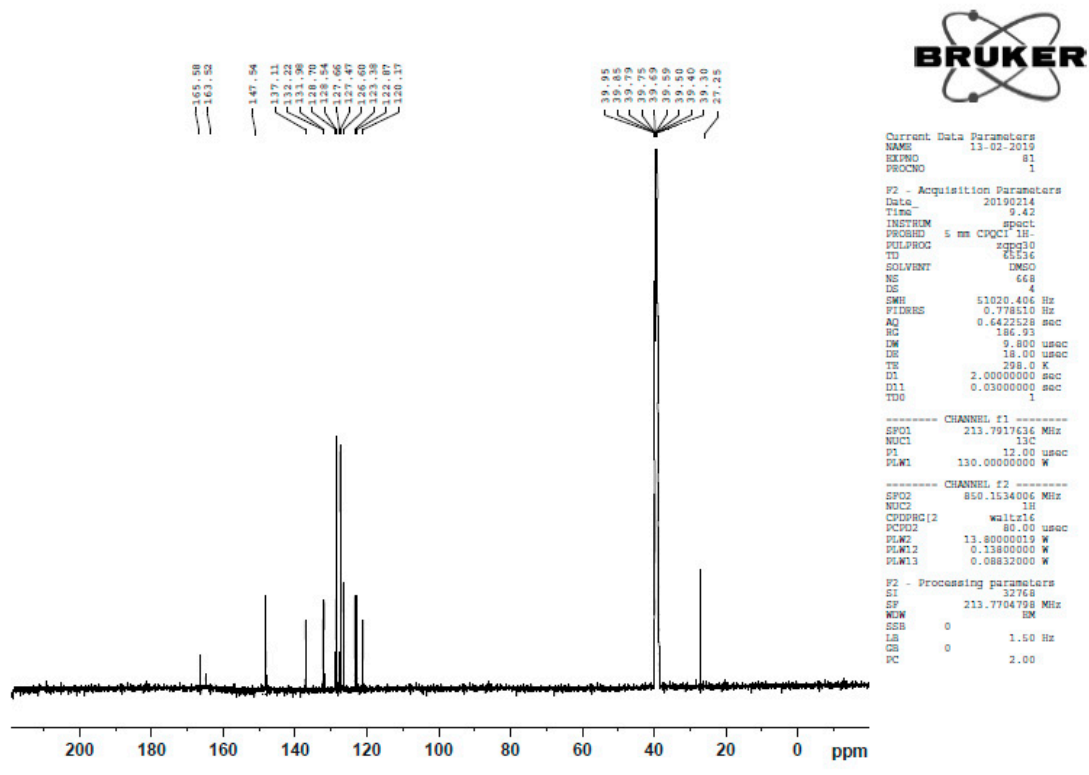


Figure S15: ¹³C NMR of compound 11

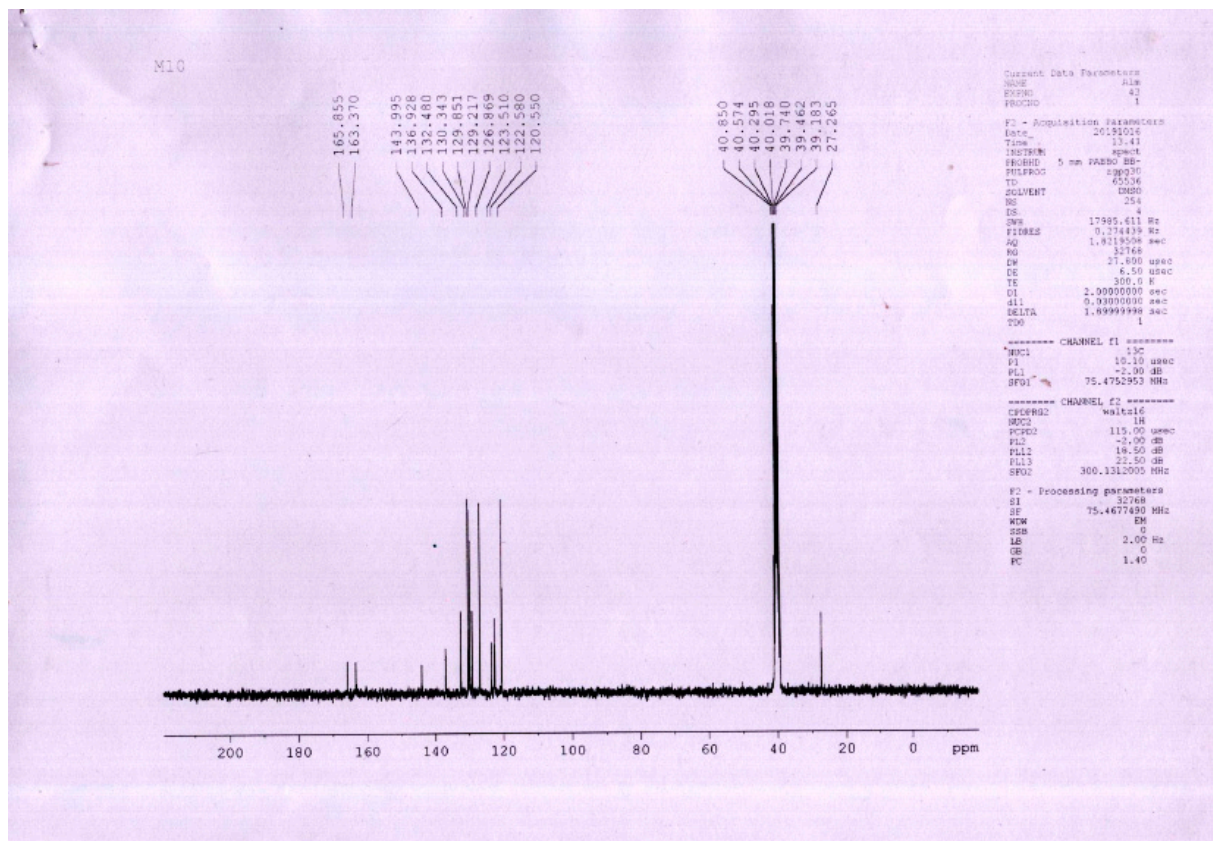


Figure S16: ^{13}C NMR of compound 12

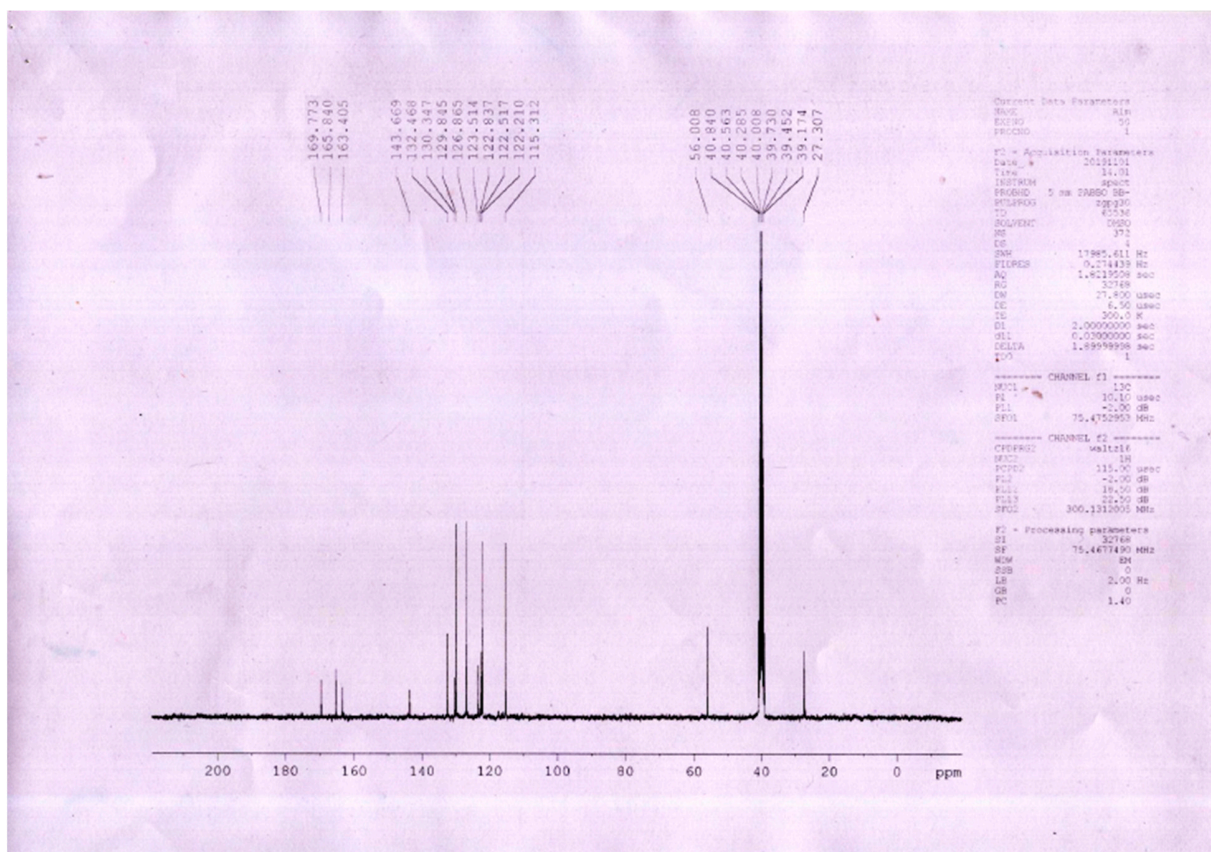


Figure S17: ¹³C NMR of compound 13

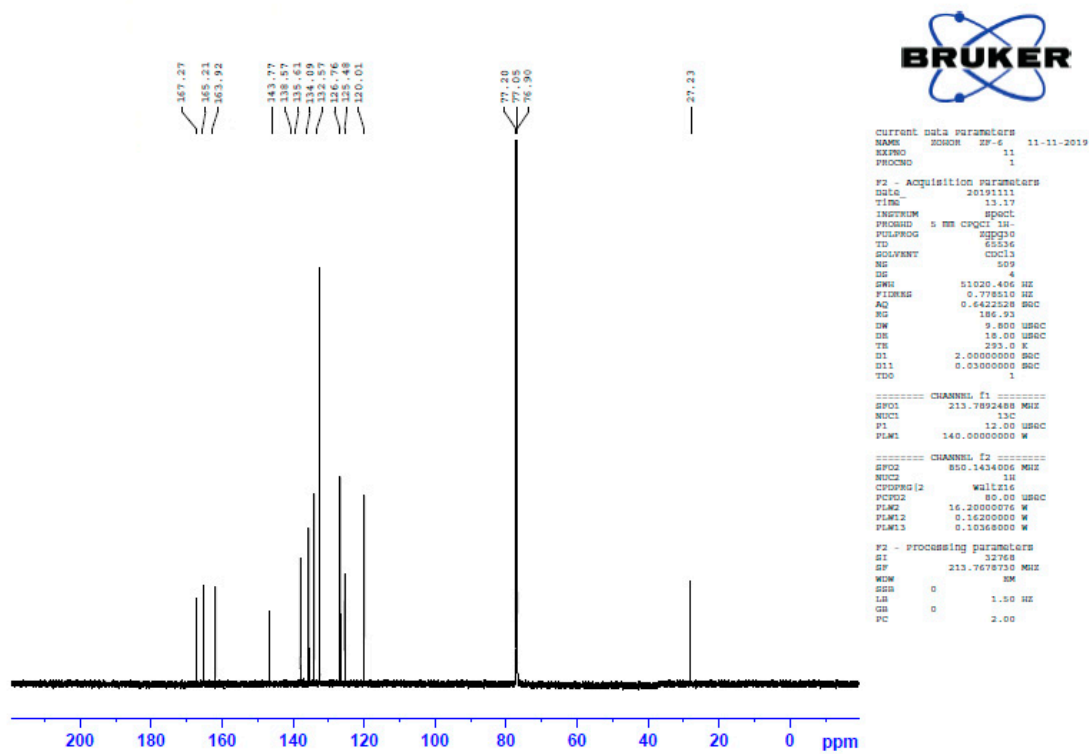


Figure S18: ¹³C NMR of compound 14

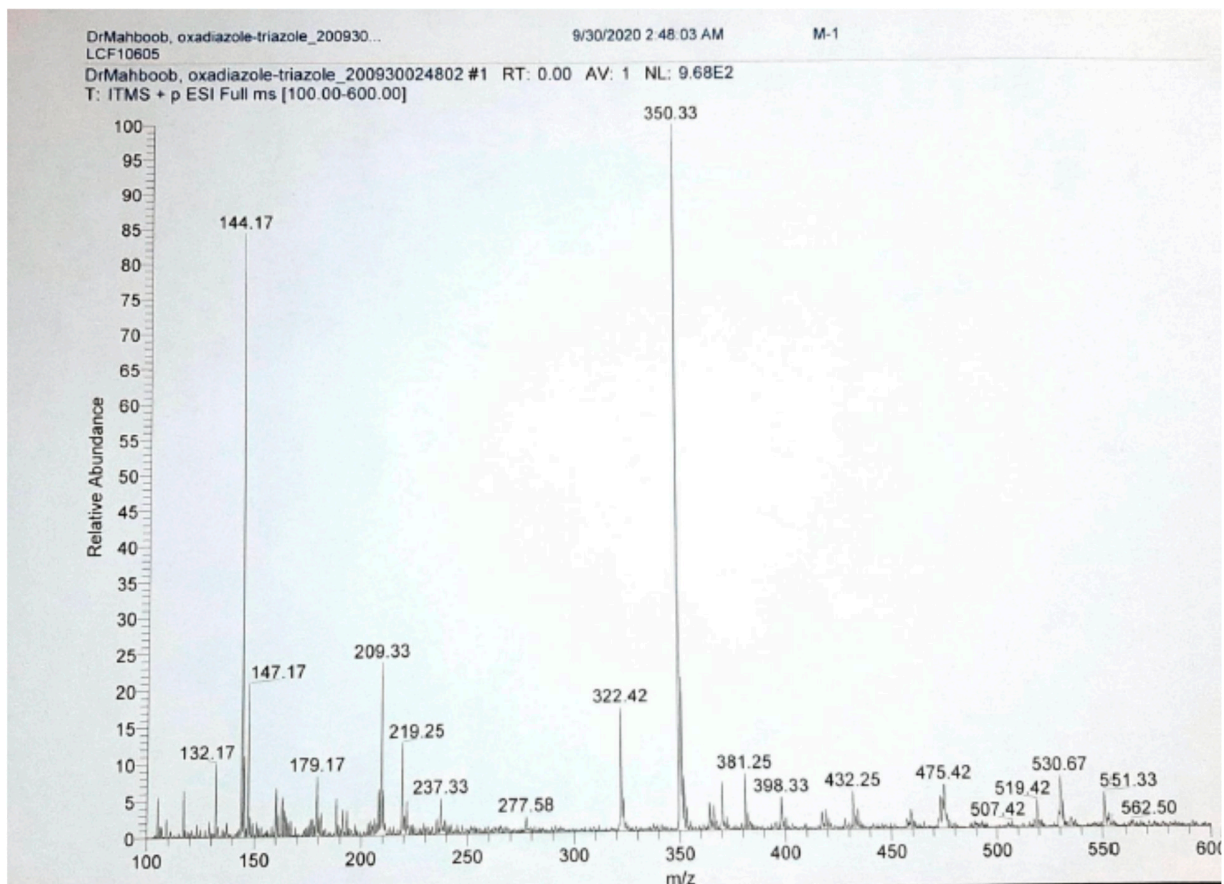


Figure S19: Mass of compound 6

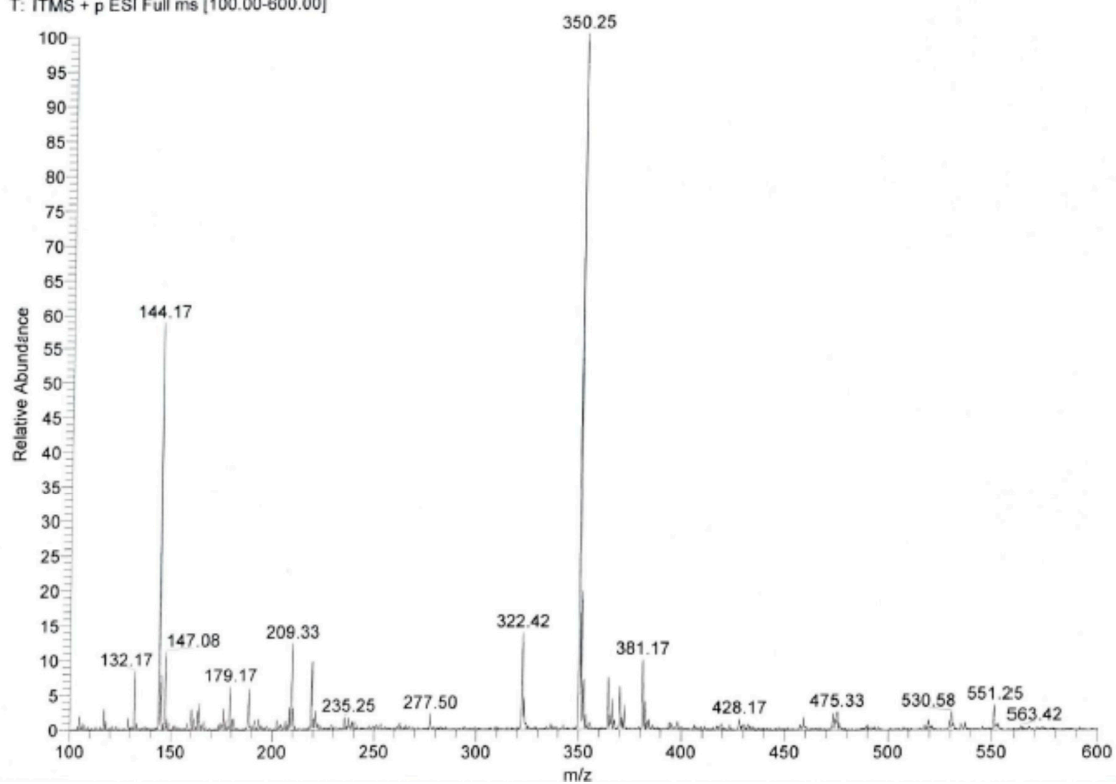


Figure S20: Mass of compound 7

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T: ITMS + p ESI Full ms [100.00-600.00]

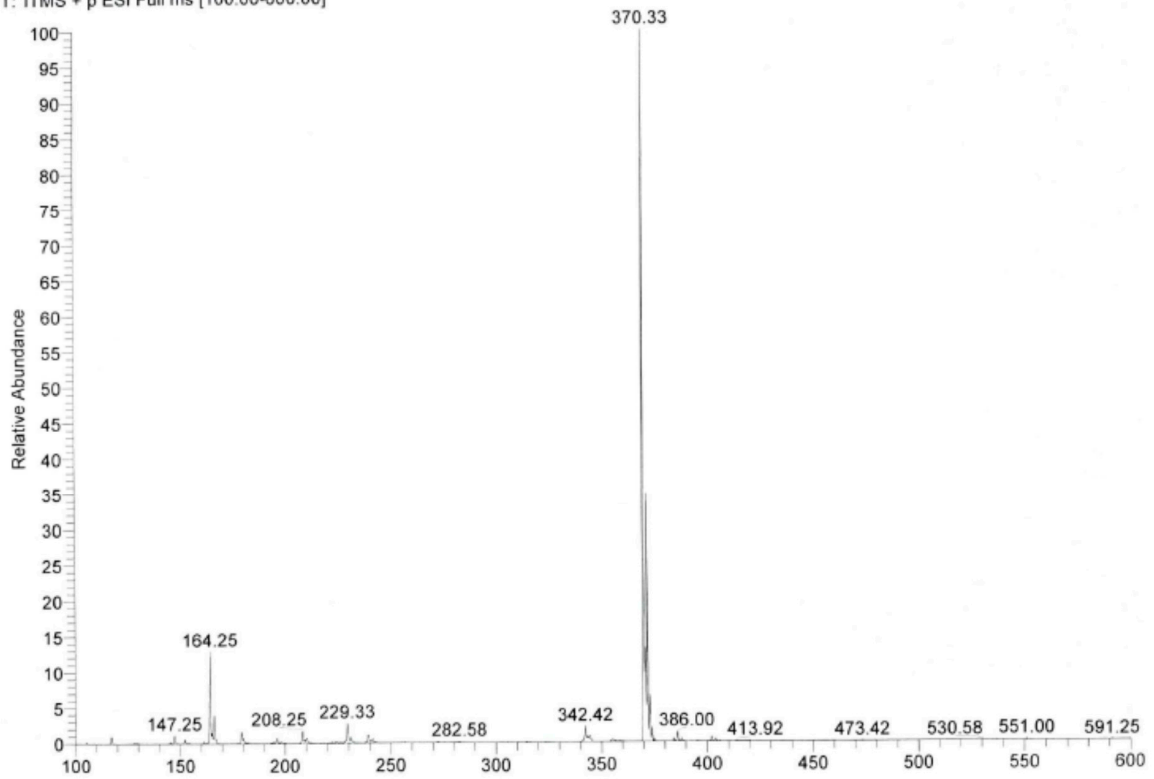


Figure S21: Mass of compound 8

DrMahboob, oxadiazole-triazole_200930...
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9/30/2020 2:31:47 AM

M-11

DrMahboob, oxadiazole-triazole_200930022940 #1 RT: 0.00 AV: 1 NL: 1.33E3
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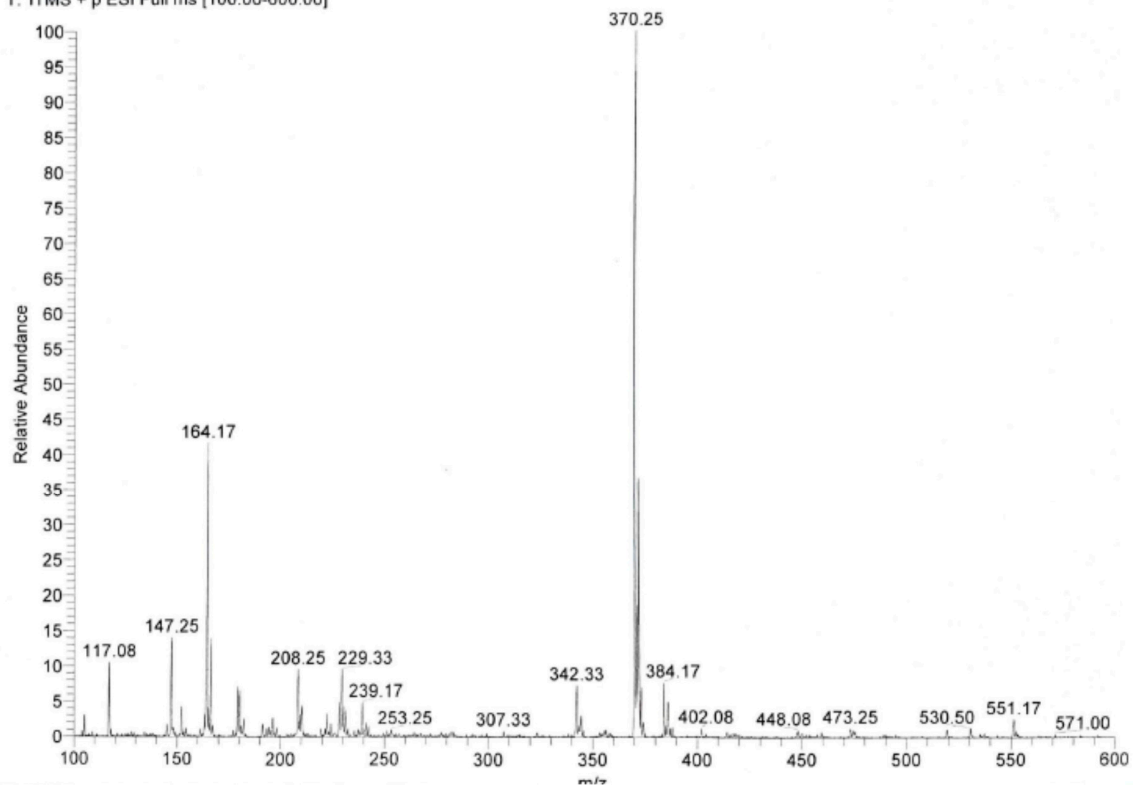


Figure S22: Mass of compound 9

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9/30/2020 3:32:33 AM

M-5

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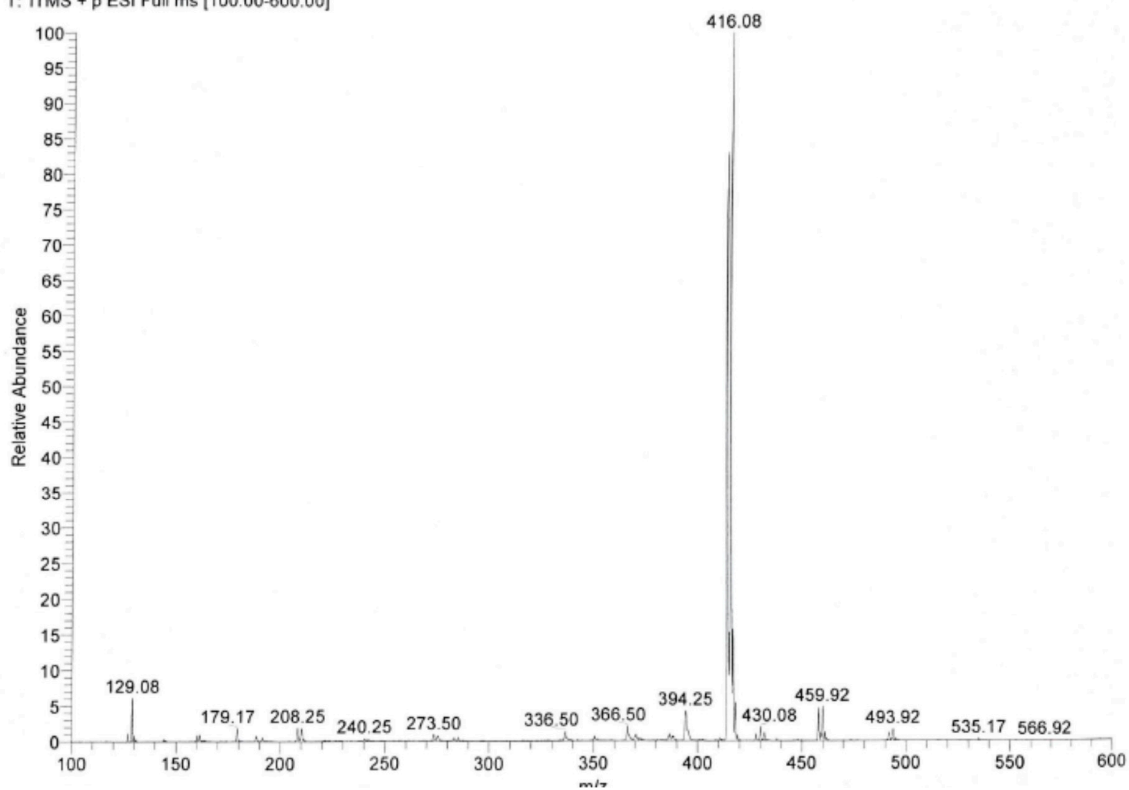


Figure S23: Mass of compound 10

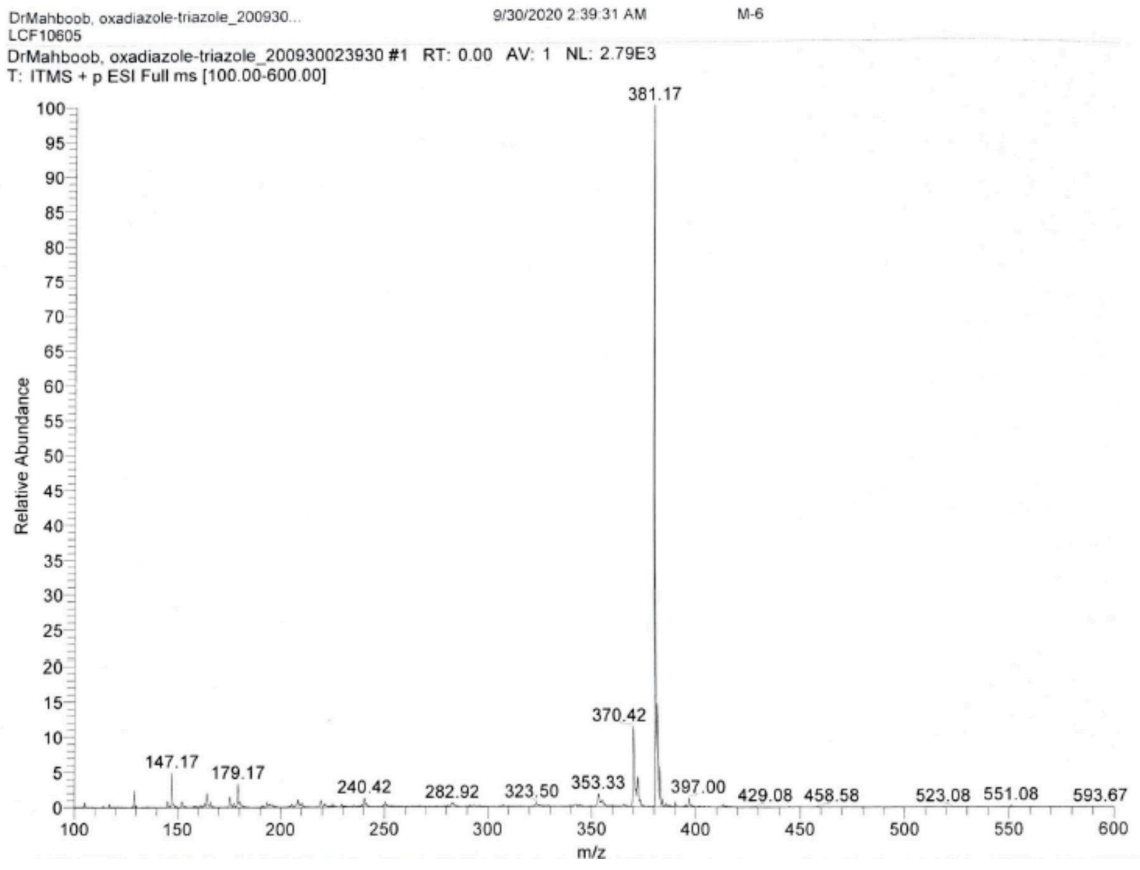


Figure S24: Mass of compound 11

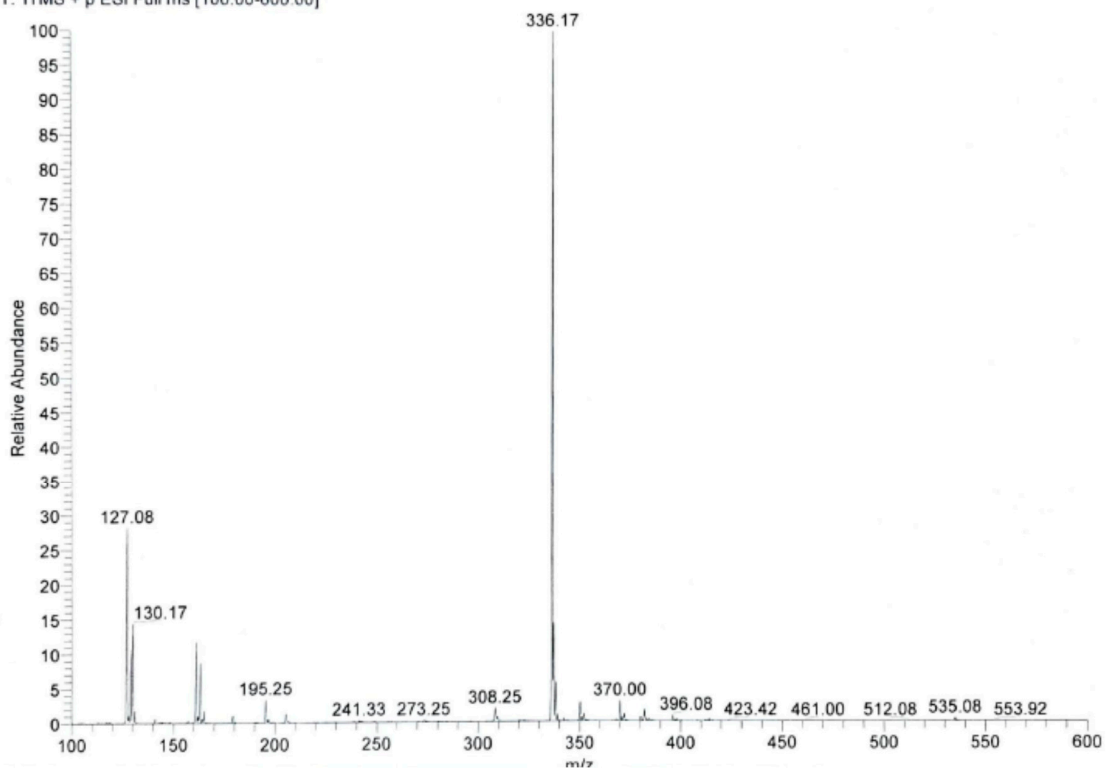


Figure S25: Mass of compound 12

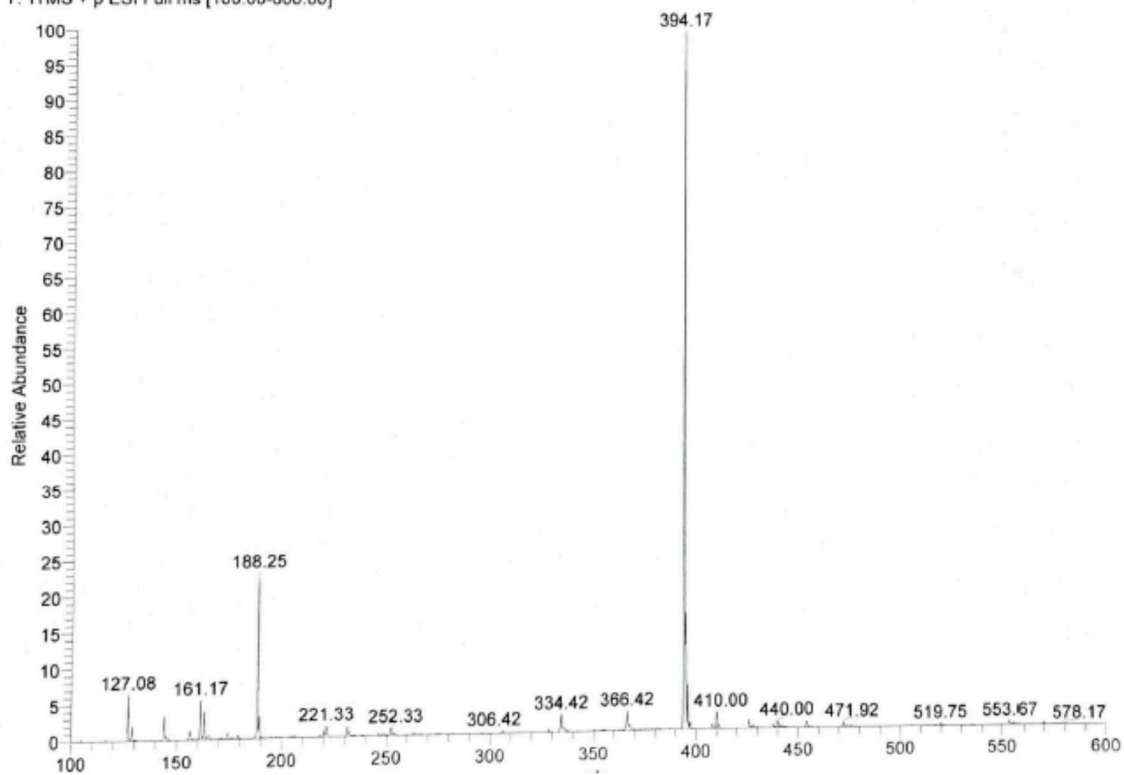


Figure S26: Mass of compound 13

C:\Thermo\ _200922051538
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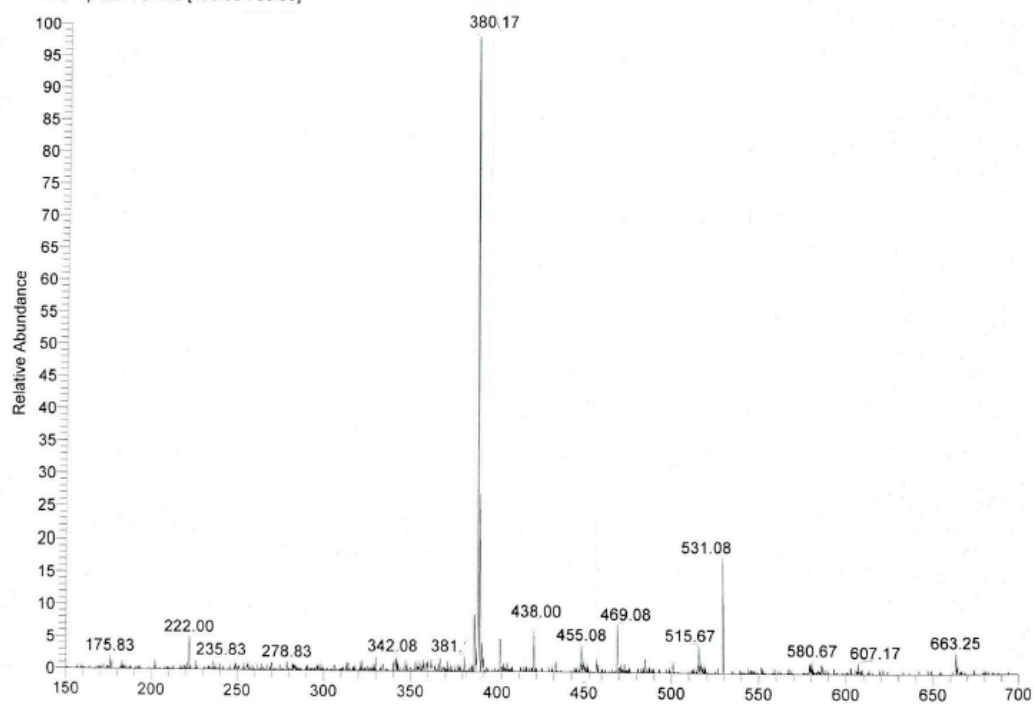


Figure S27: Mass of compound 14