

Supplementary materials

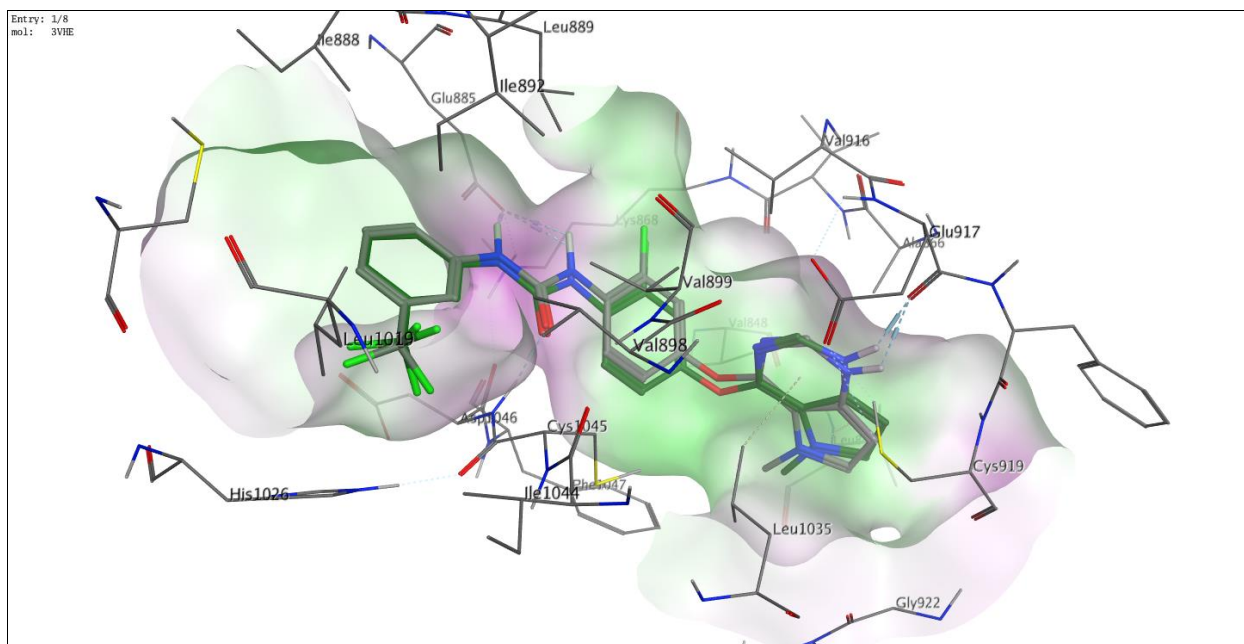


Figure S 1: Overlay of the redocked ligand (gray) and the co crystallized pose (green)

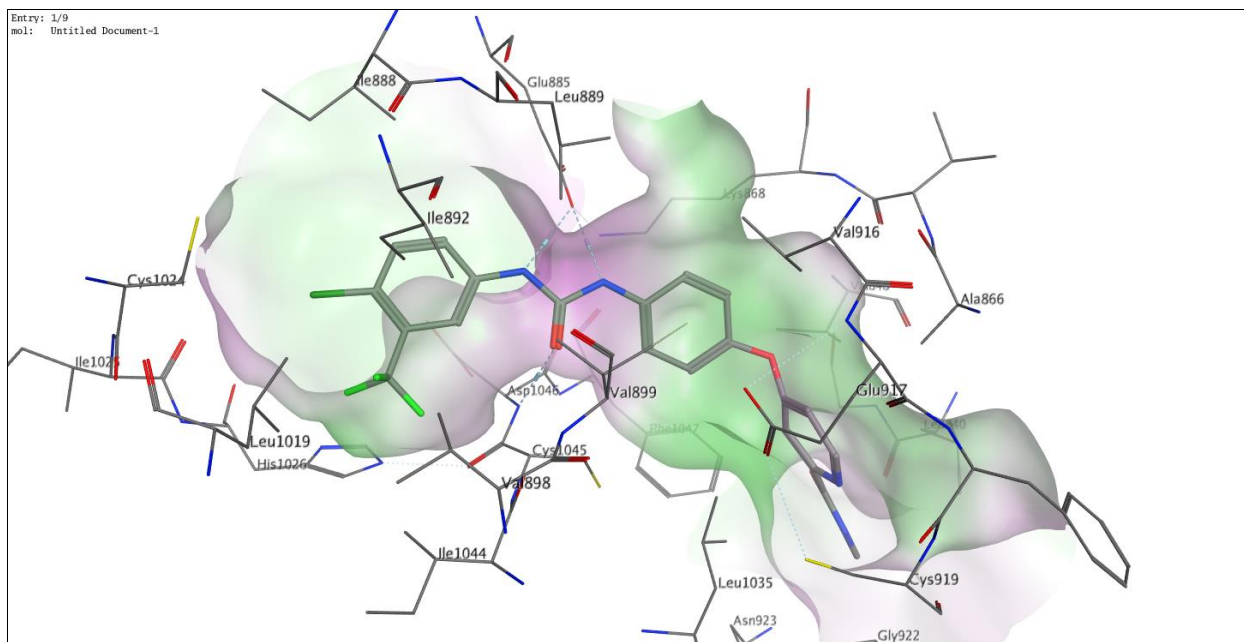


Figure S 2: Binding mode of sorafenib

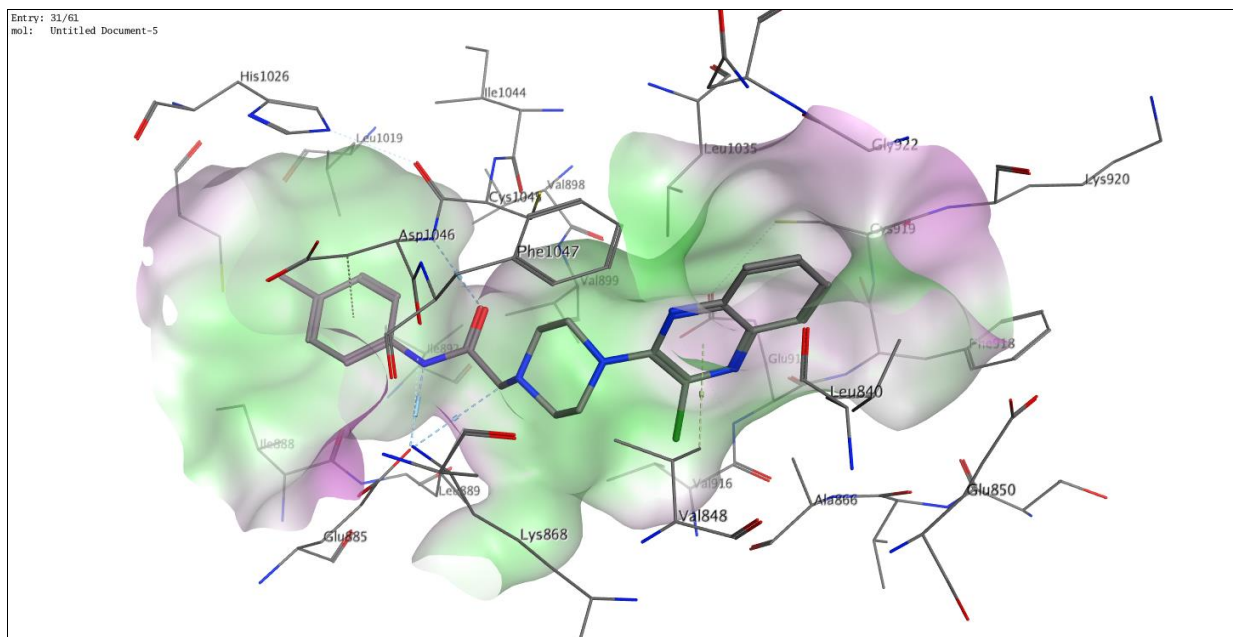


Figure S 3: 3D interaction of compound **10_e**

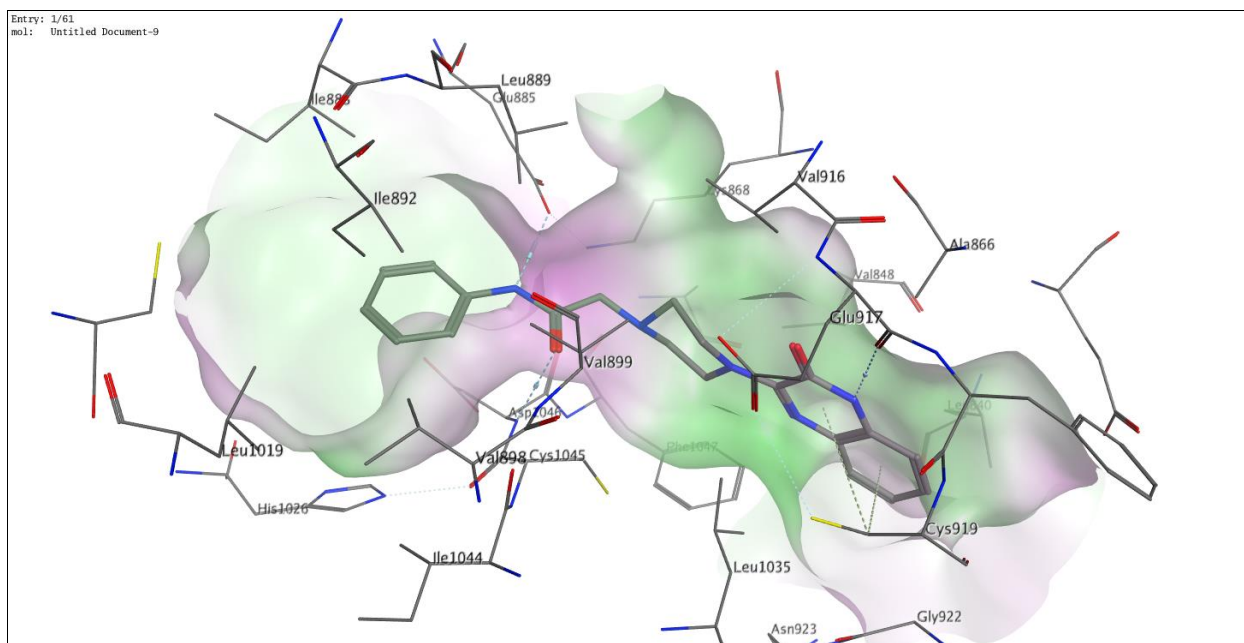


Figure S 4: Binding pattern of compound **13_a**

Abdallah ElSayed_H_401

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

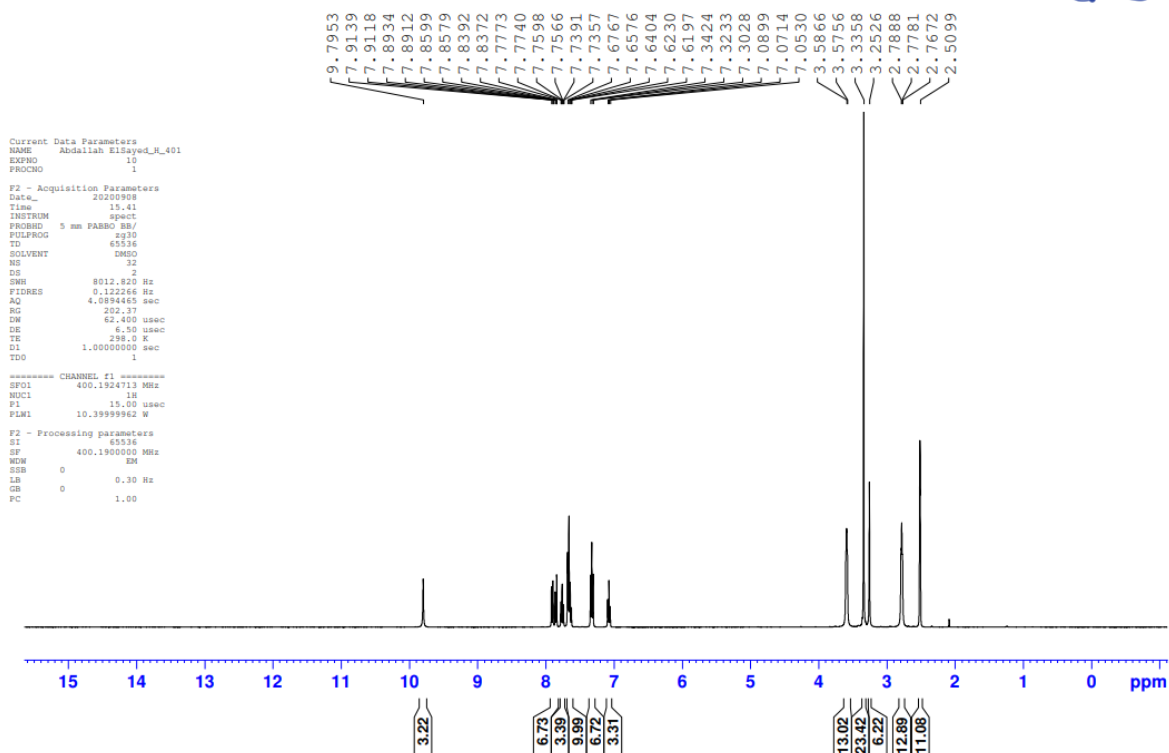


Figure S 5: ^1H NMR chart of compound **10_a**

Abdallah ElSayed_C_401

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

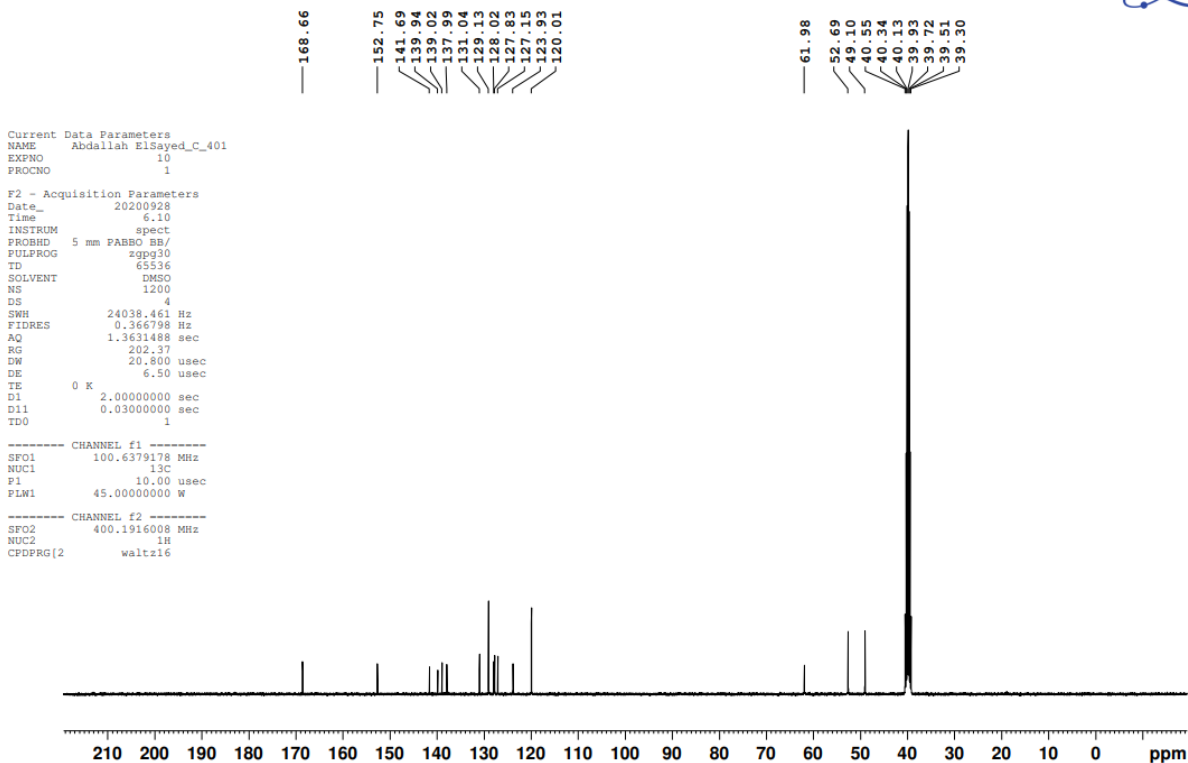


Figure S 6: ^{13}C NMR chart of compound **10a**

Abdallah ElSayed_H_402#

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

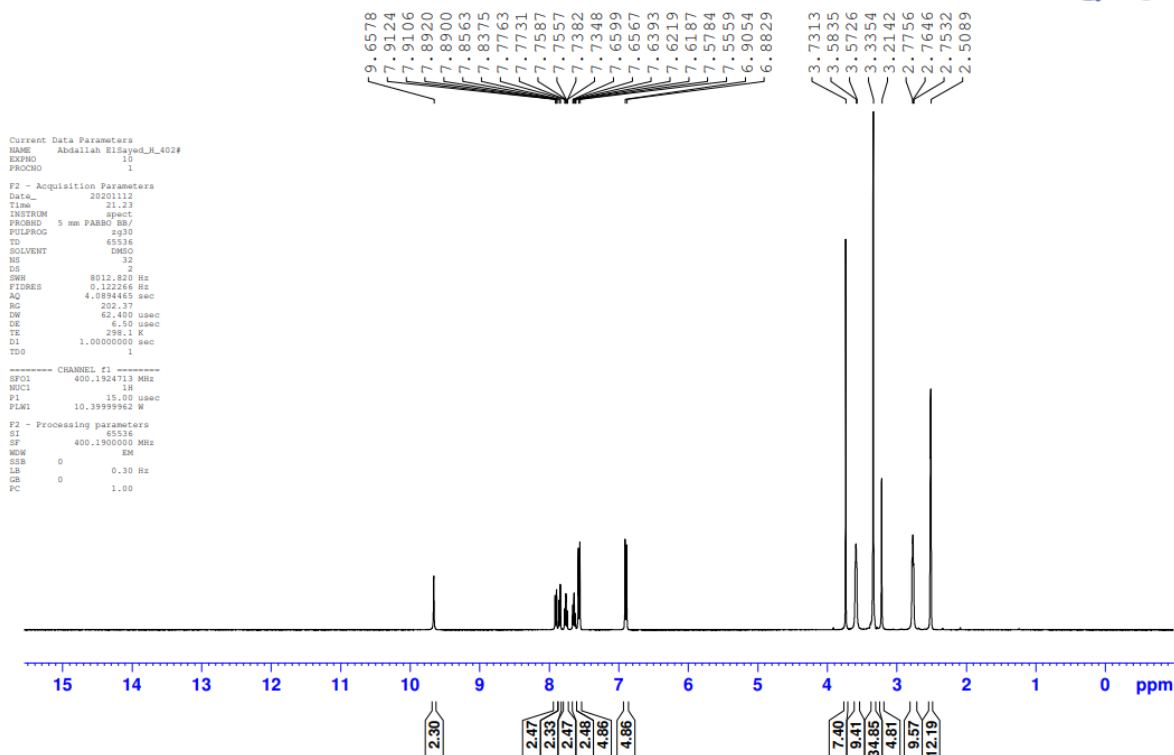


Figure S 7: ^1H NMR chart of compound **10b**

Abdallah ElSayed_C_402

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

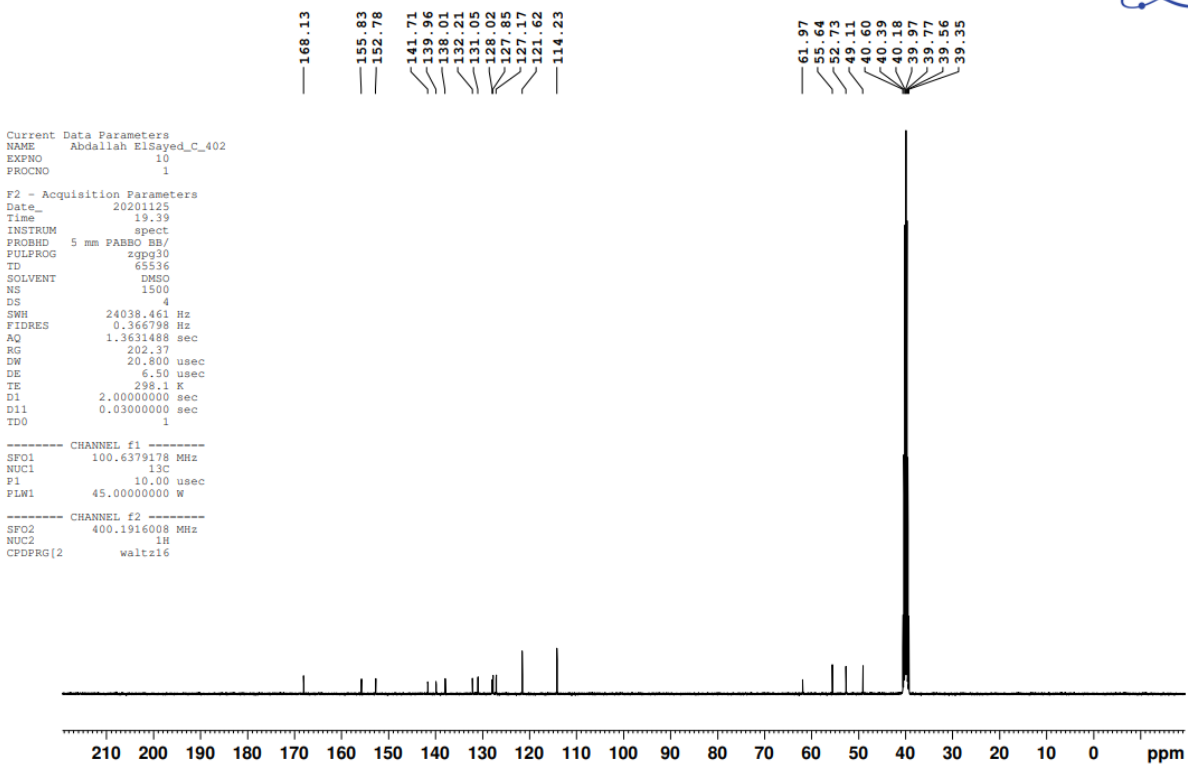
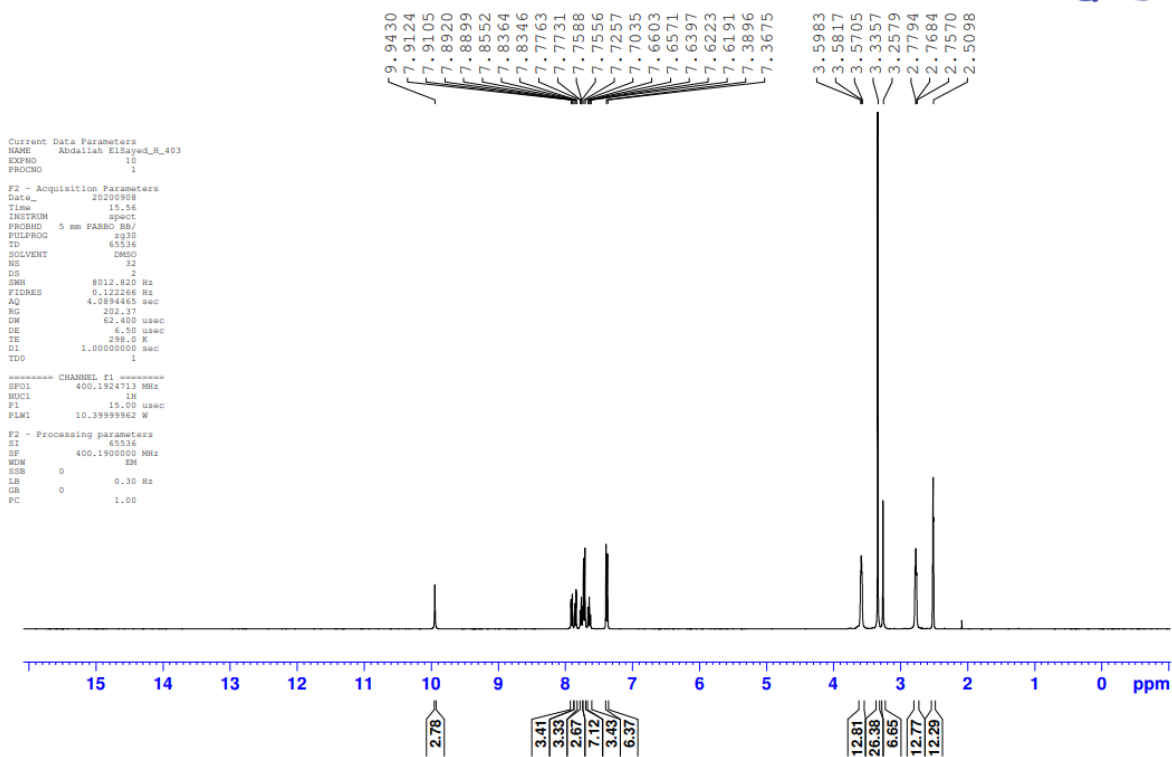
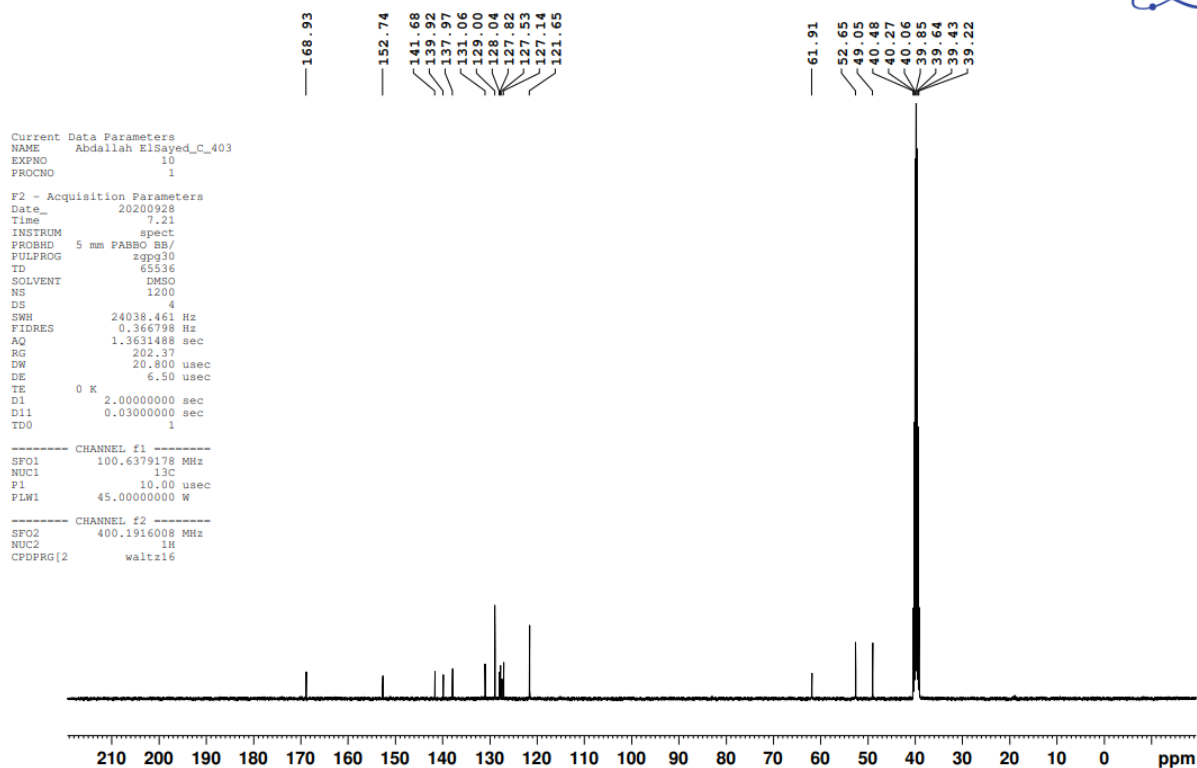


Figure S 8: ^{13}C NMR chart of compound **10_b**

Figure S 9: ^1H NMR chart of compound **10_c**

Figure S 10: ^{13}C NMR chart of compound **10c**

Abdallah ElSayed_H_404

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

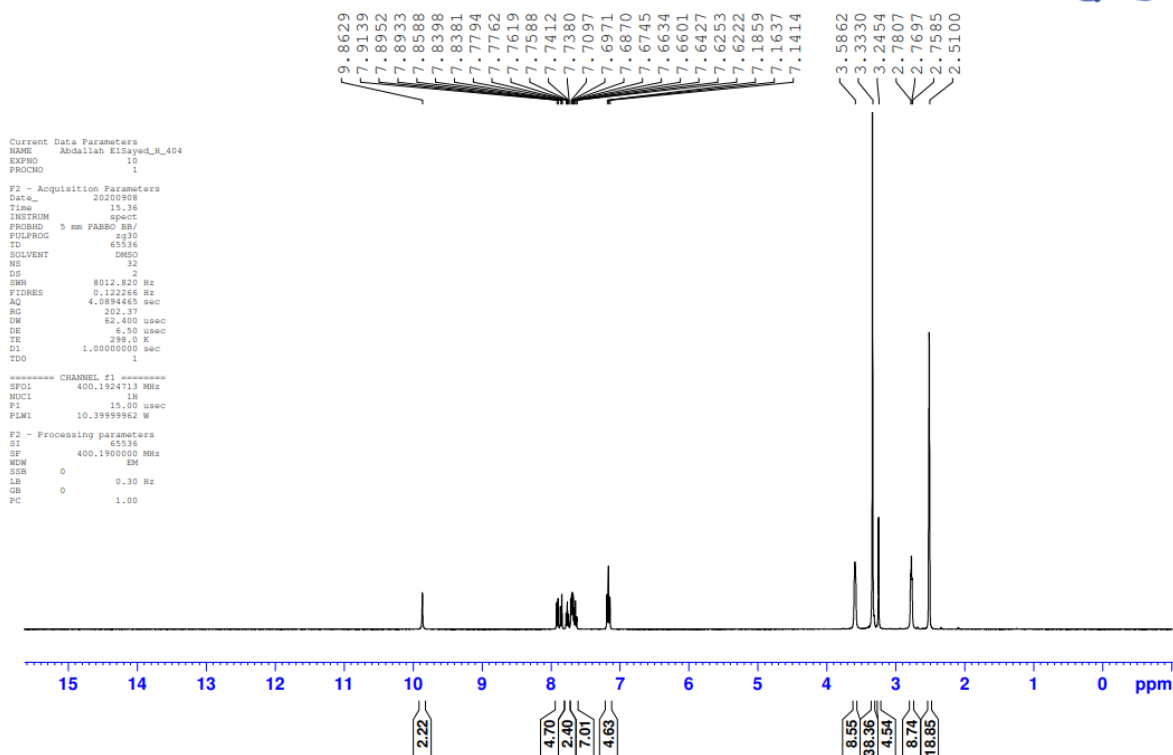


Figure S 11: ¹HNMR chart of compound **10_d**

Abdallah ElSayed_C_404

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

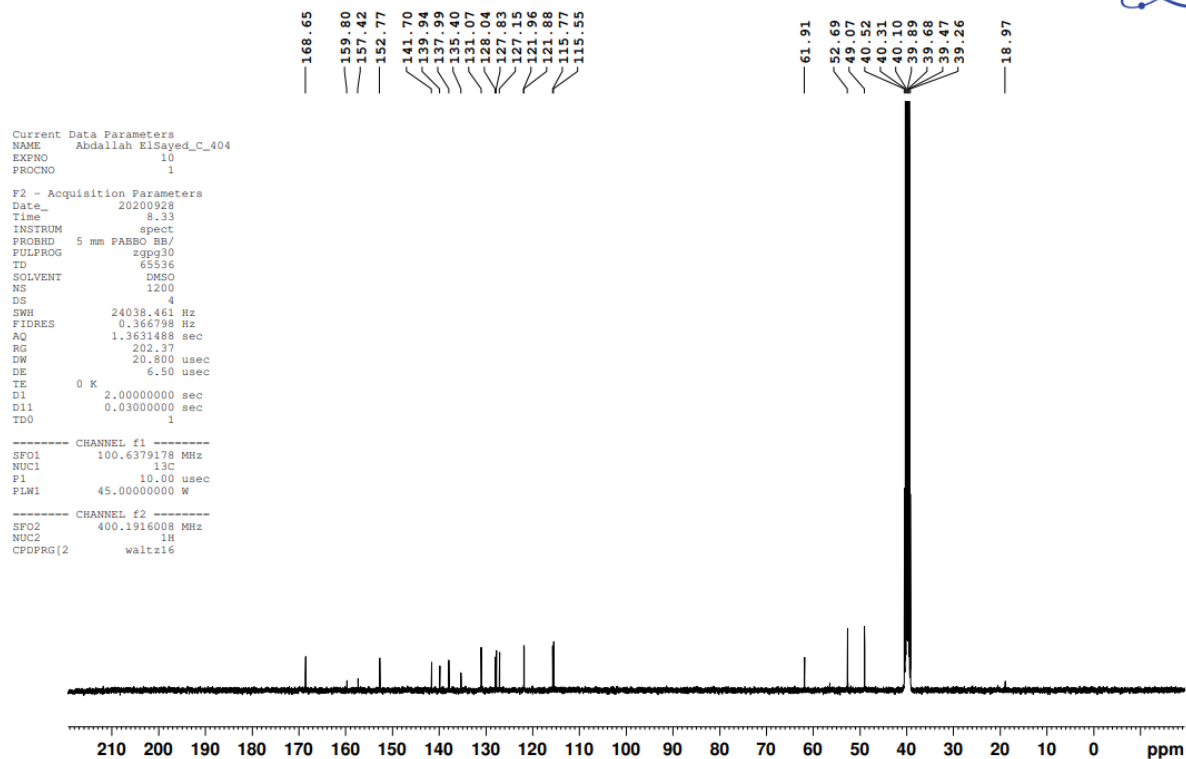
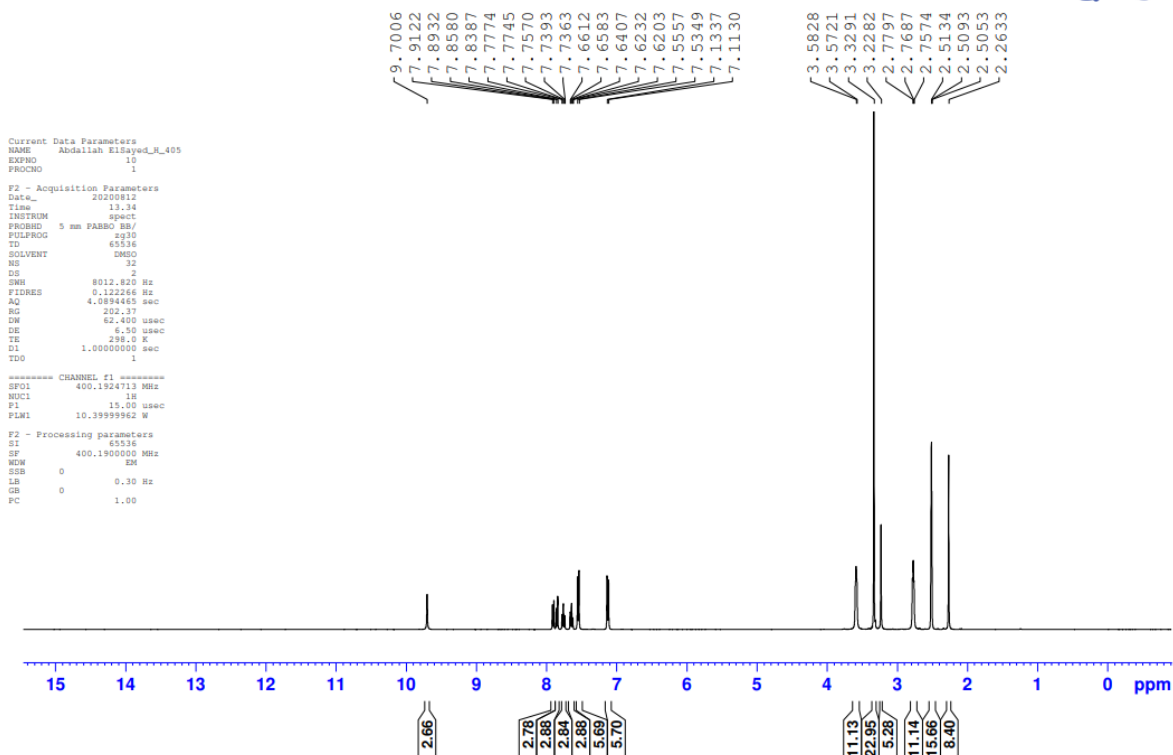
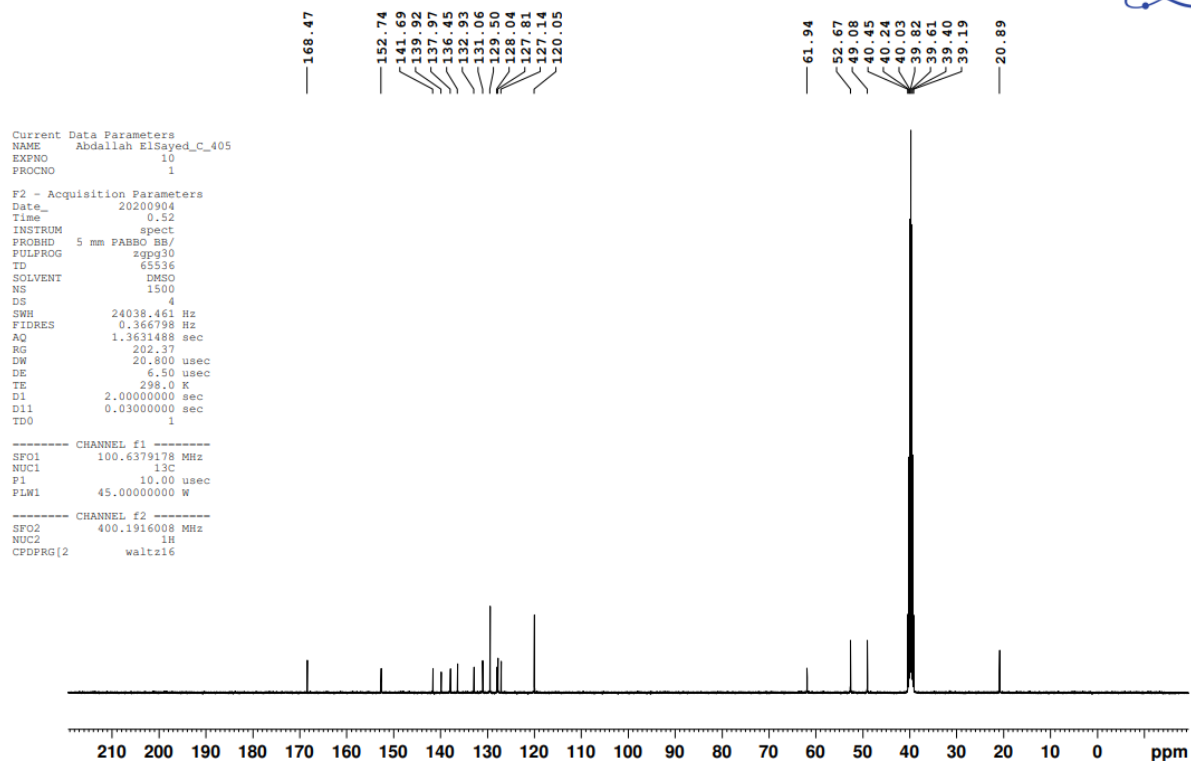


Figure S 12: ^{13}C NMR chart of compound 10_d

Figure S 13: ^1H NMR chart of compound **10e**

Figure S 14: ^{13}C NMR chart of compound **10e**

Abdallah ElSayed_H_406

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

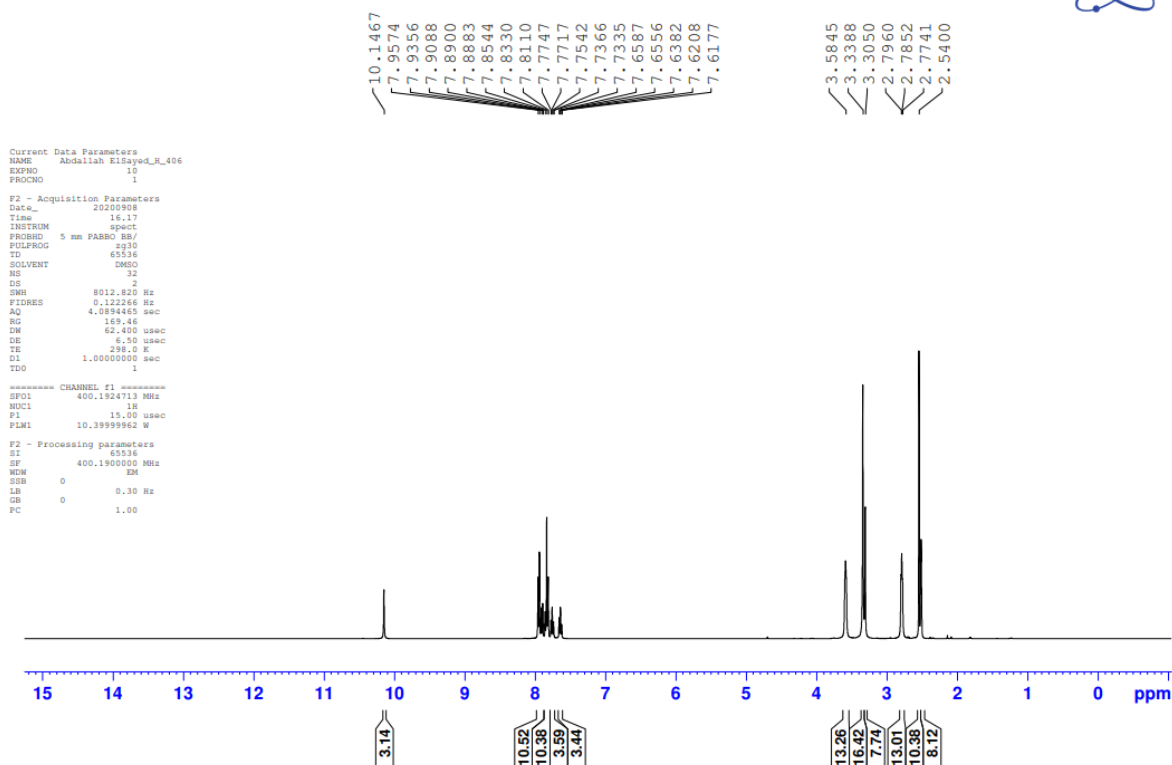


Figure S 15: ¹HNMR chart of compound 10j

Abdallah ElSayed_C_406

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

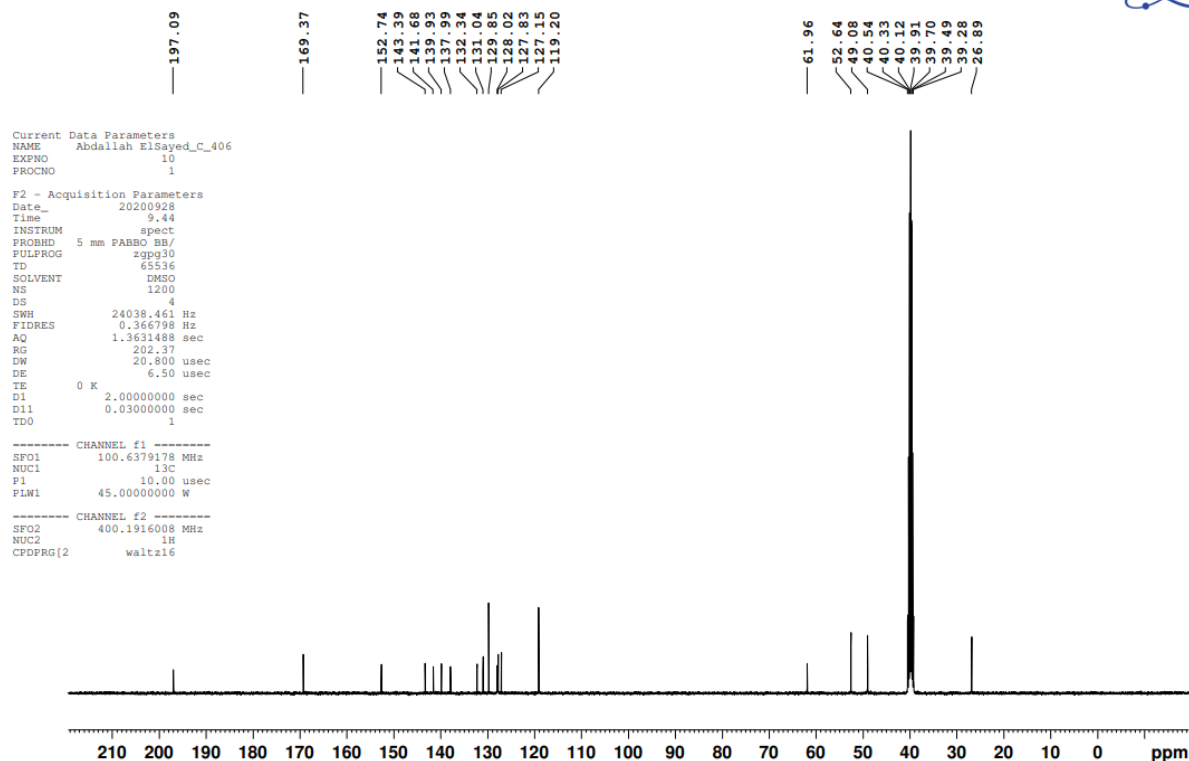
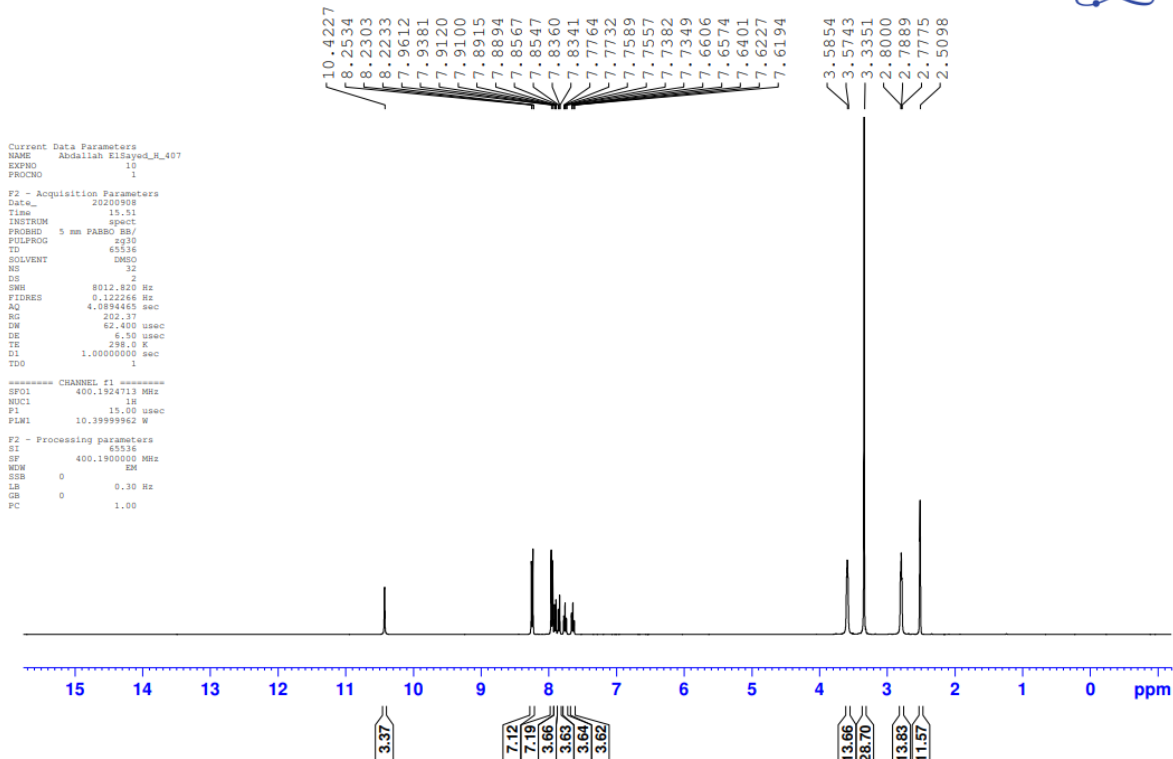


Figure S 16: ^{13}C NMR chart of compound 10_f

Figure S 17: ^1H NMR chart of compound 10_g

Abdallah ElSayed_H_407_D2O

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

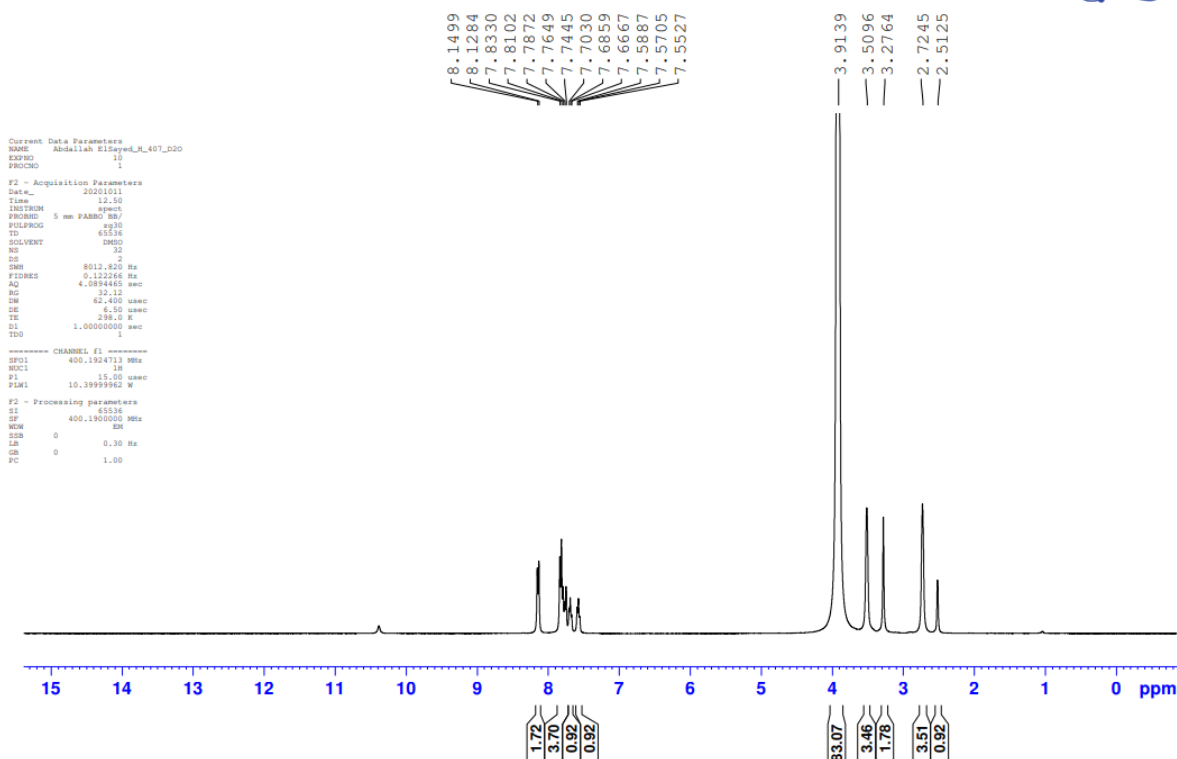
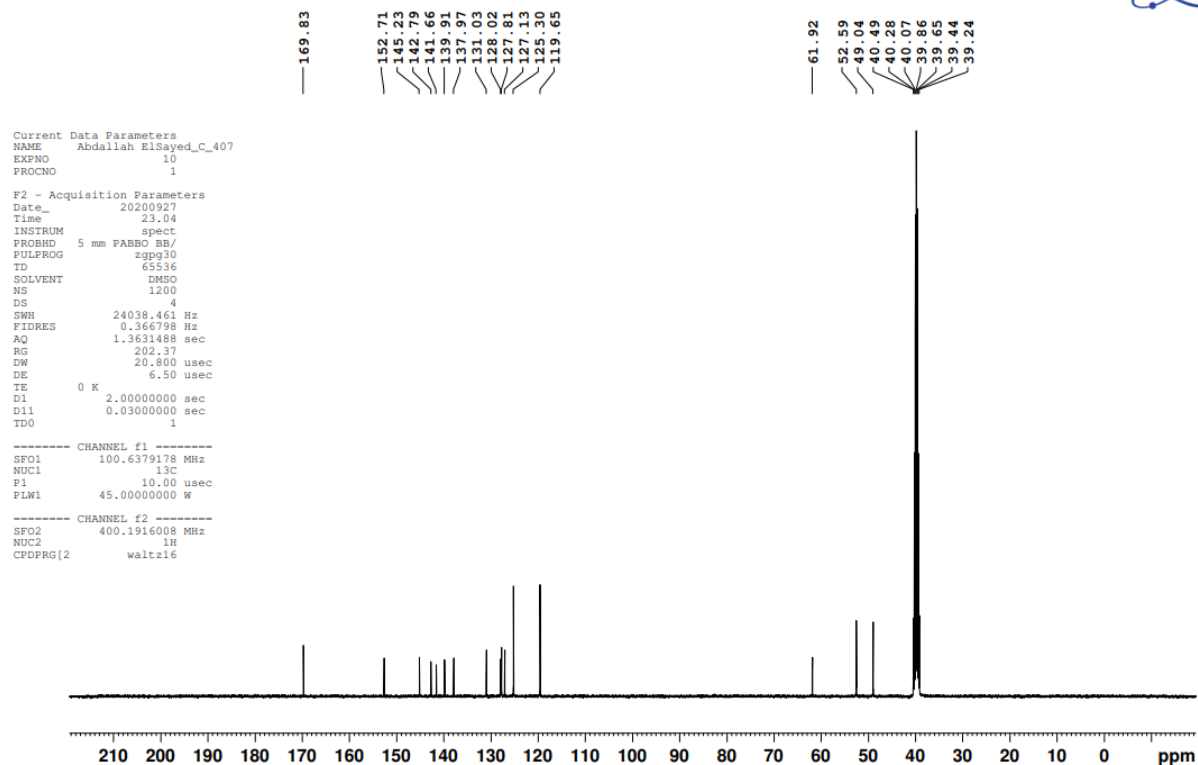


Figure S 18 : D₂O ¹H NMR chart of compound 10_g

Figure S 19: ^{13}C NMR chart of compound **10_g**

Abdallah ElSayed_H_409

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

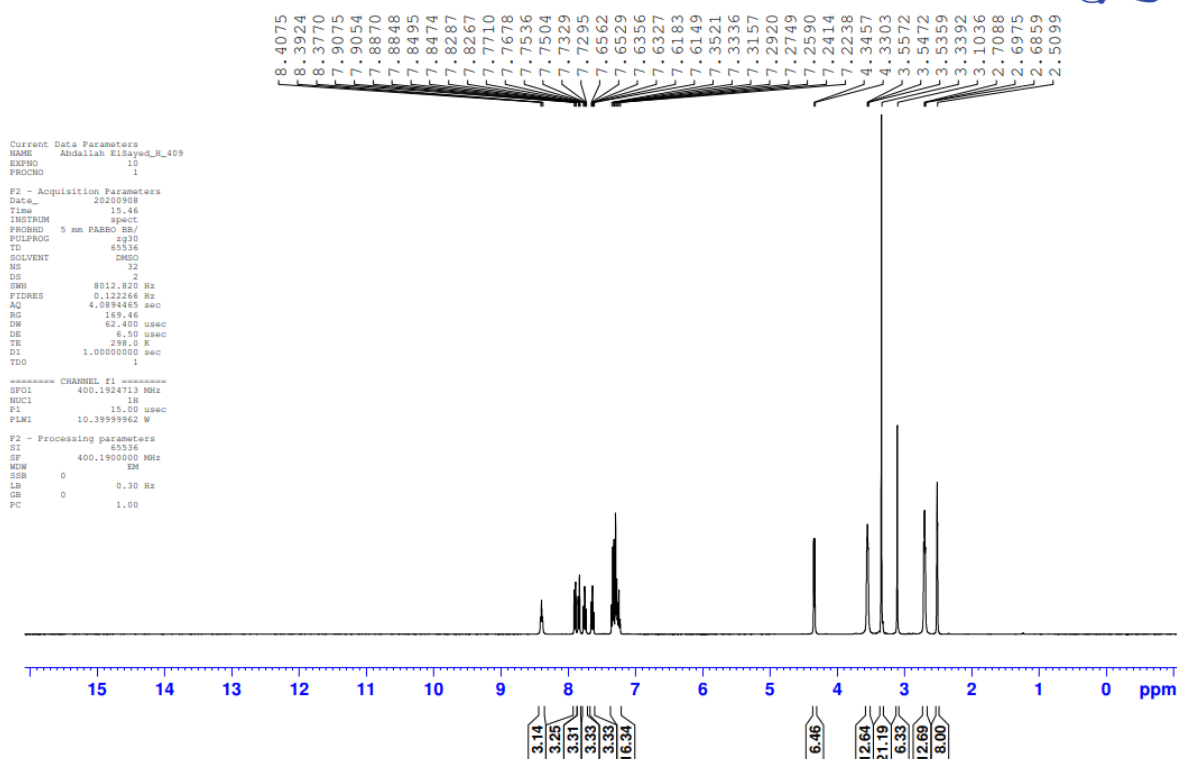
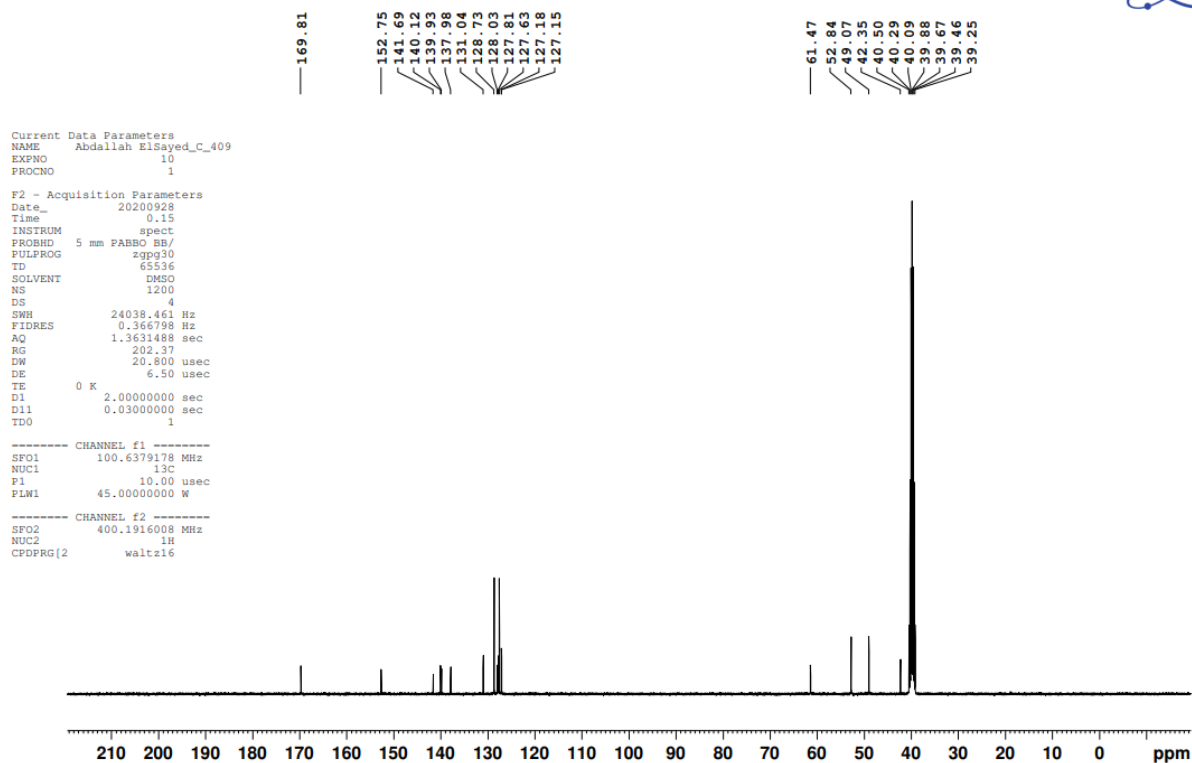
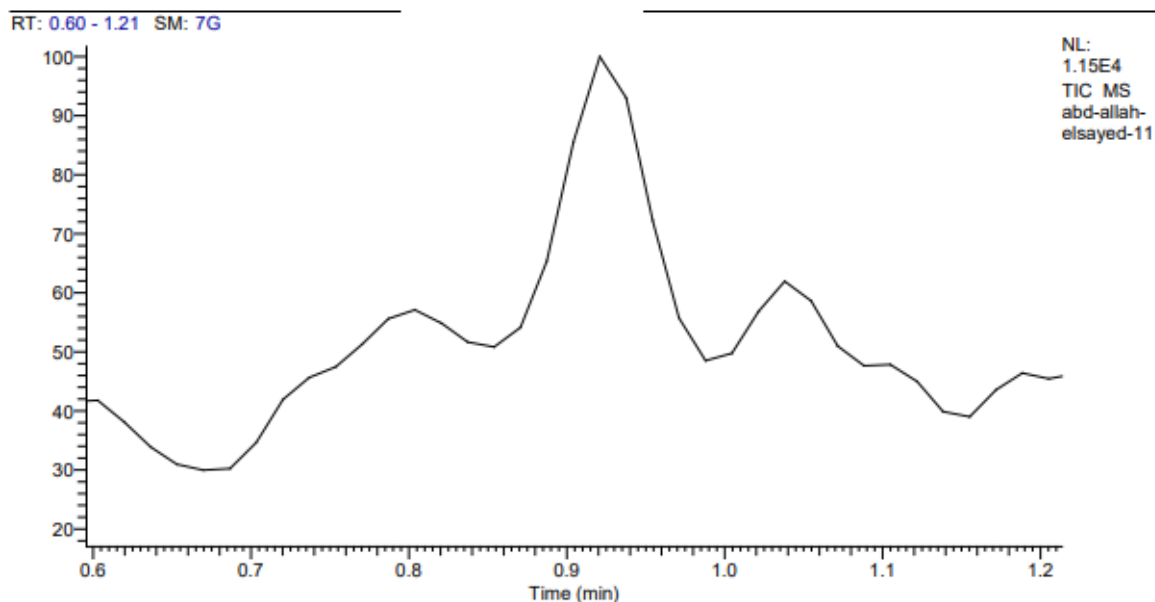


Figure S 20: ¹HNMR chart of compound 11

Figure S 21: ¹³CNMR chart of compound 11



abd-allah-elsayed-11 #54-59 RT: 0.92-1.00 AV: 6 NL: 1.03E2
T: + c EI Full ms [40.00-1000.00]

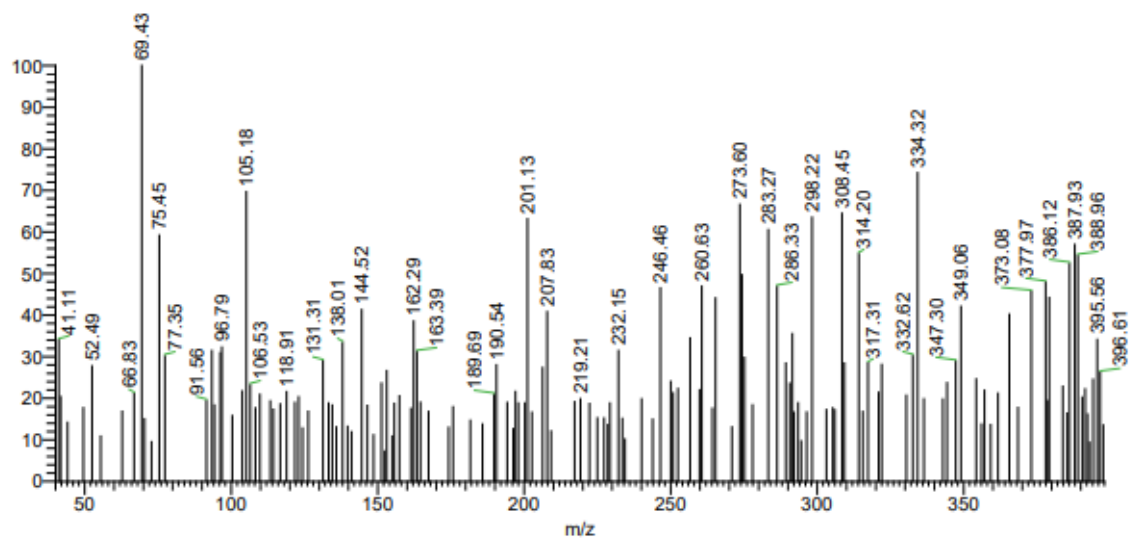


Figure S 22: Mass spec. of compound 11

Abdallah ElSayed_H_421

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

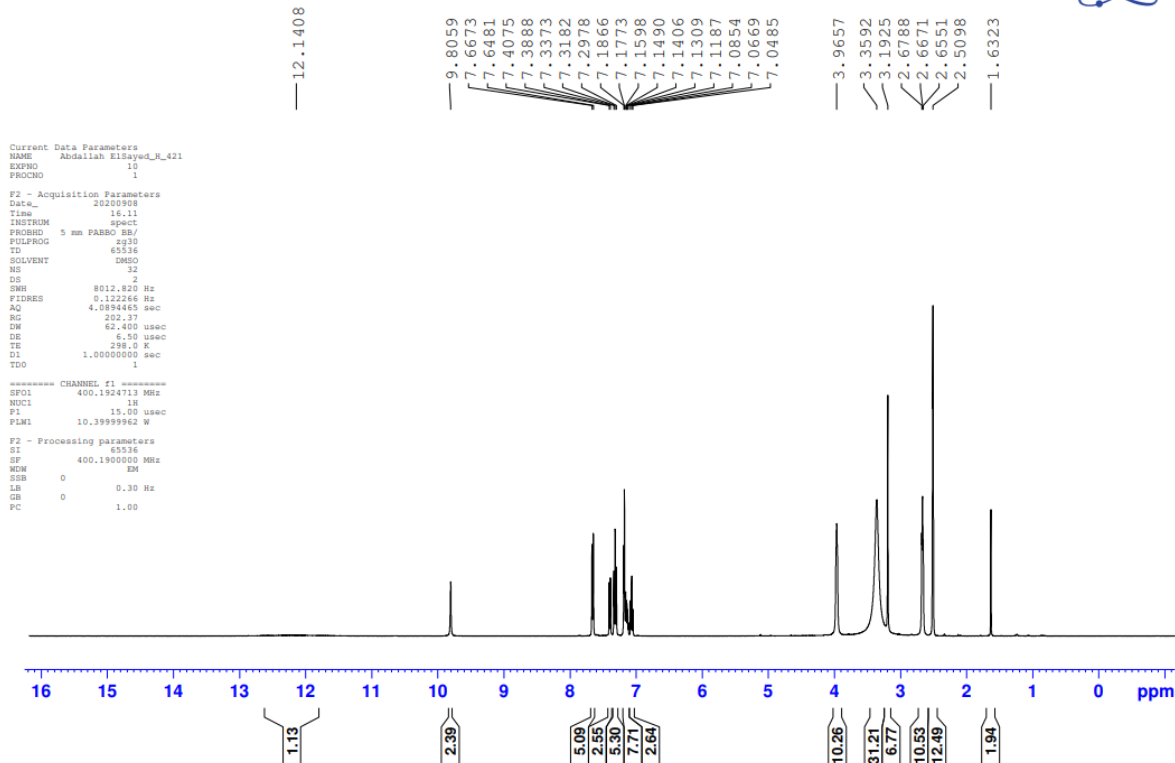


Figure S 23: ¹H NMR chart of compound **13_a**

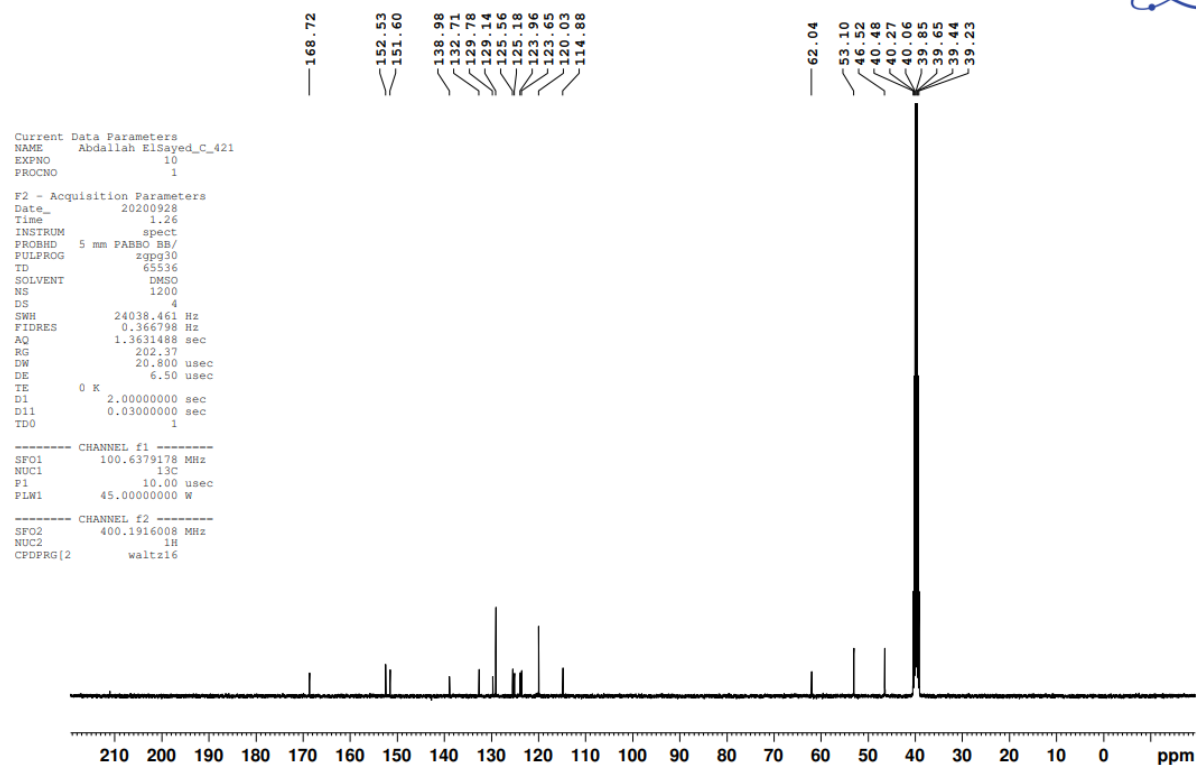


Figure S 24: ^{13}C NMR chart of compound **13_a**

Abdallah ElSayed_H_422

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

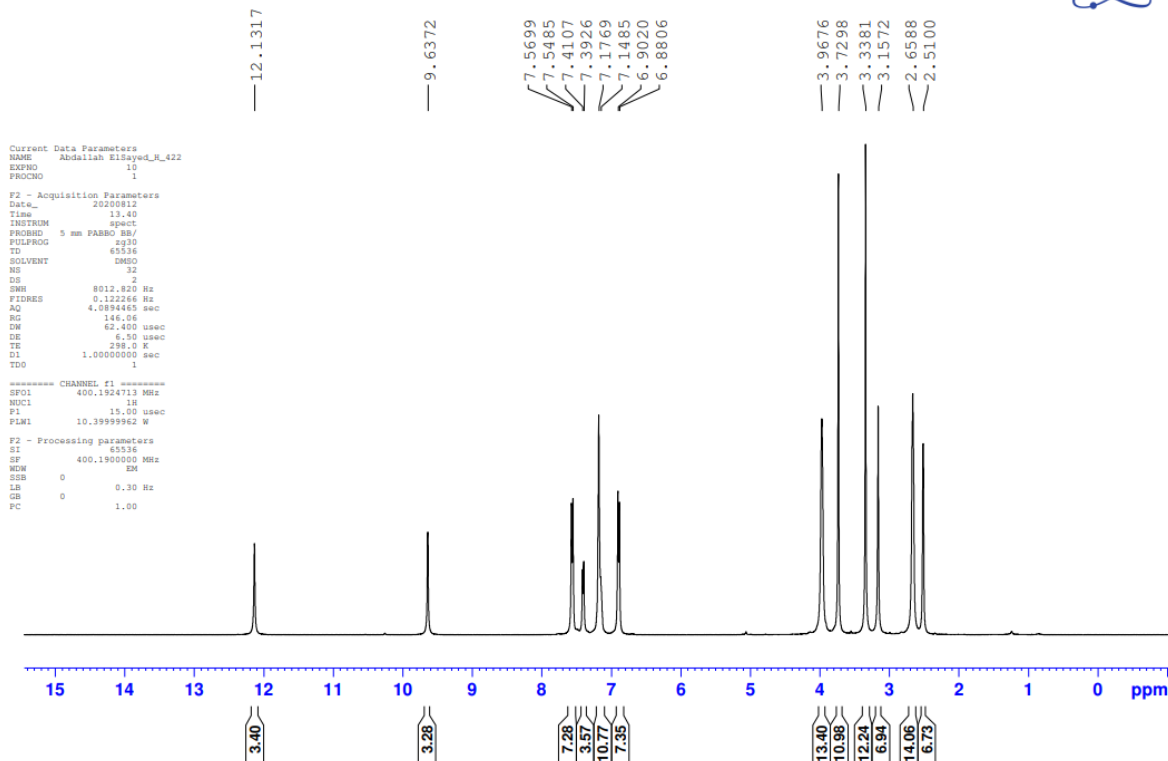
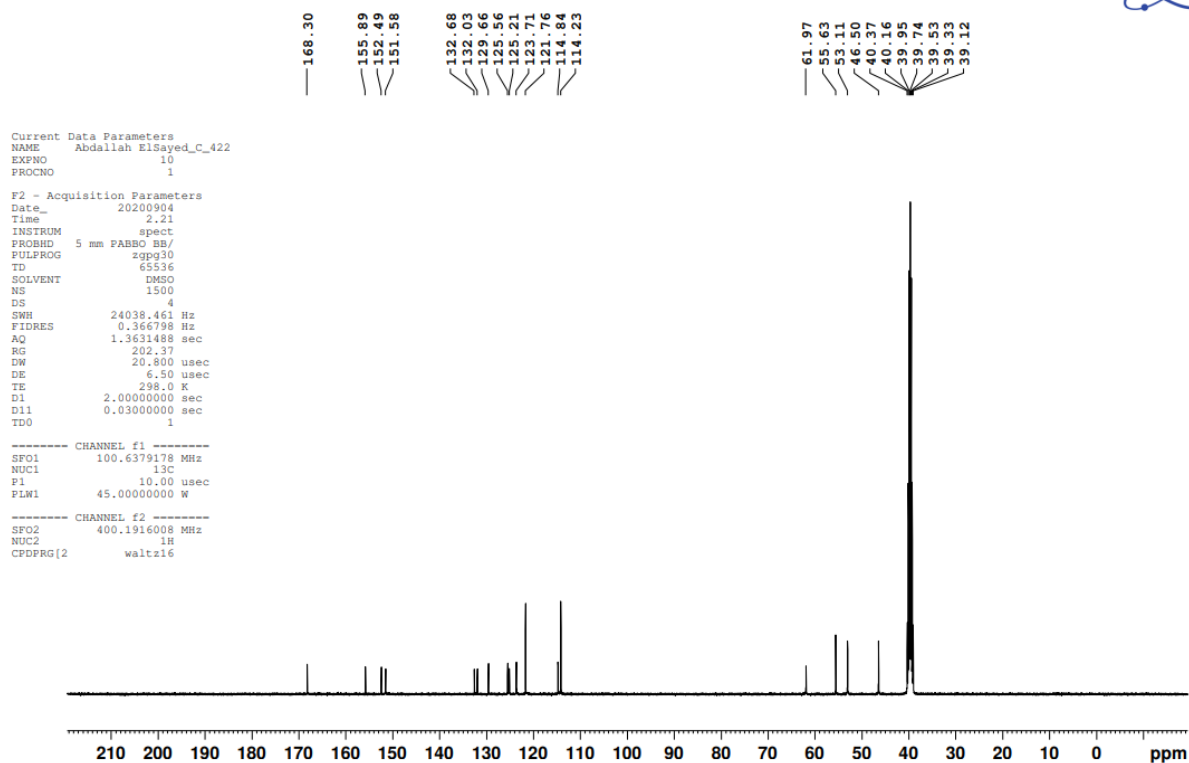


Figure S 25: ¹H NMR chart of compound **13_b**

Figure S 26: ^{13}C NMR chart of compound **13_b**

Abdallah ElSayed_H_423

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

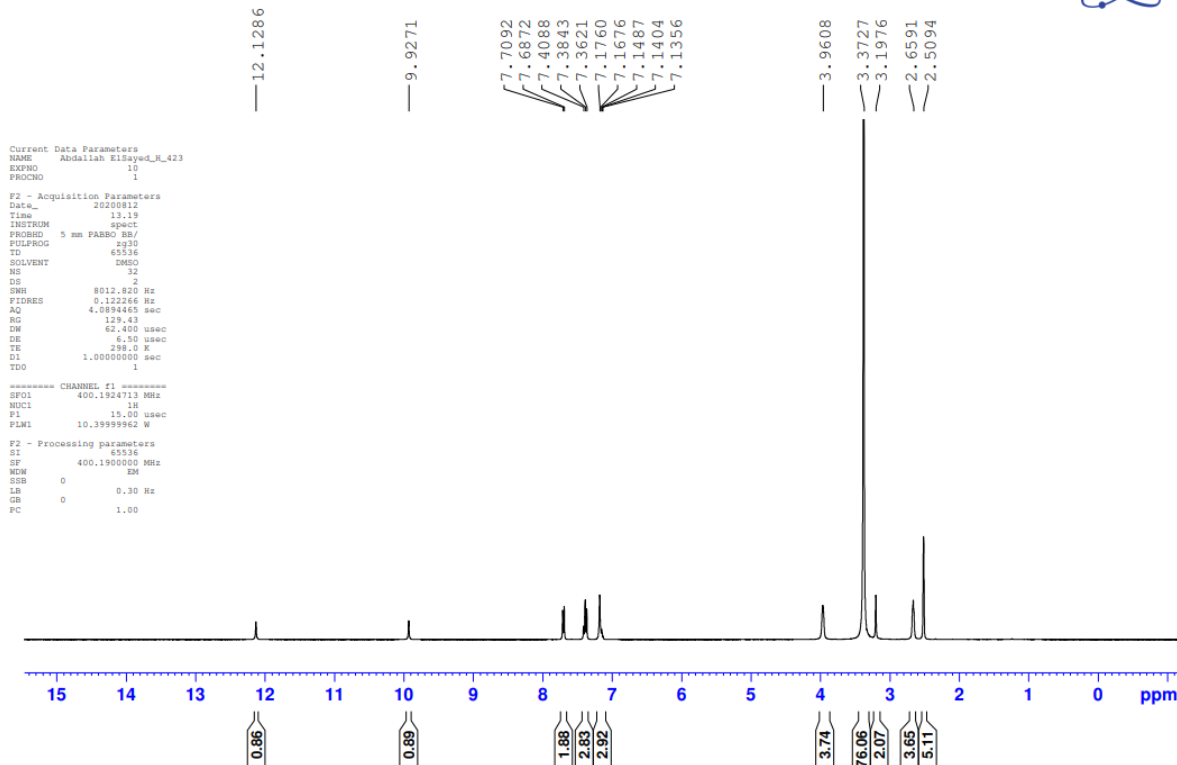


Figure S 27: ^1H NMR chart of compound **13c**.

Abdallah ElSayed_C_423

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

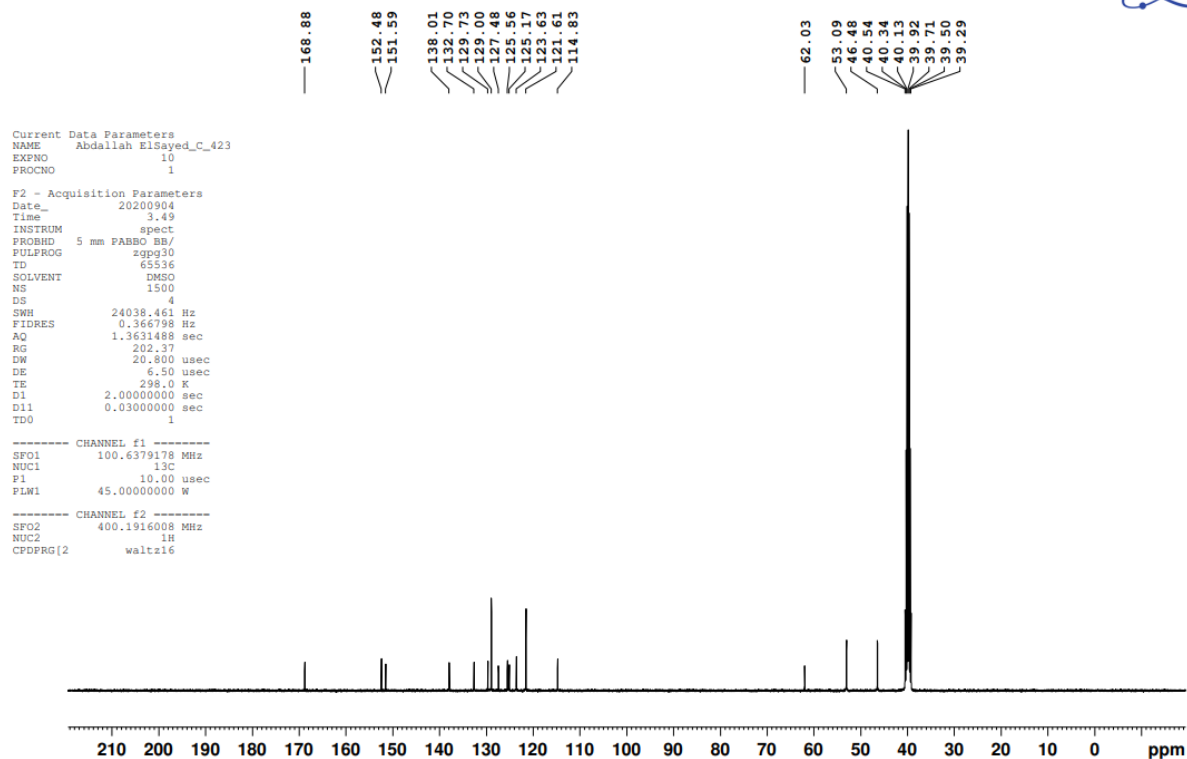


Figure S 28: ^{13}C NMR chart of compound **13c**

Abdallah ElSayed_H_424

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

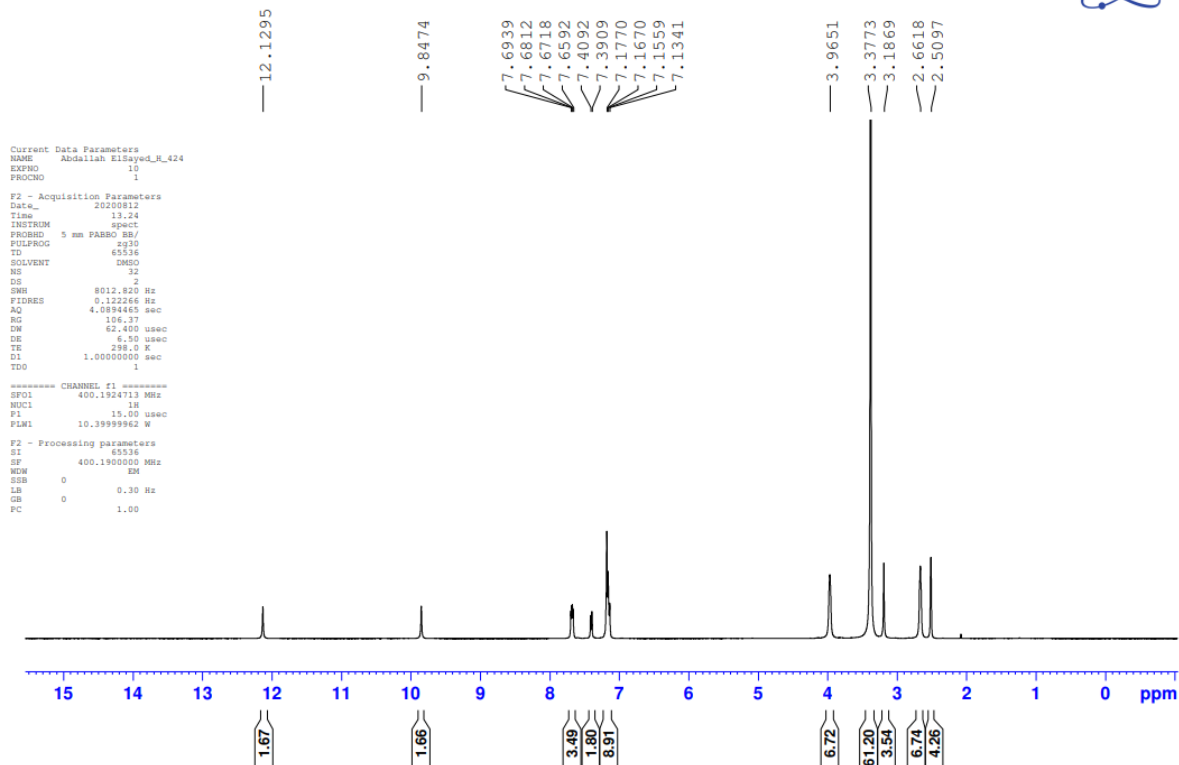
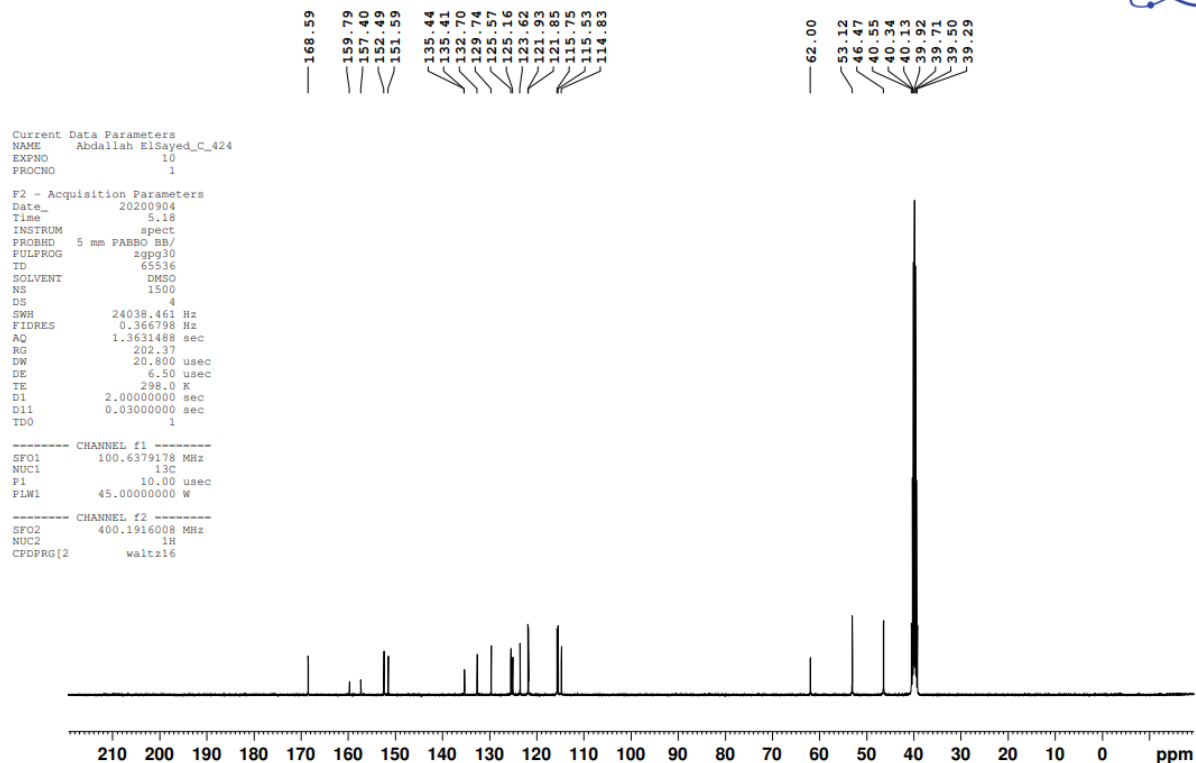


Figure S 29: ¹HNMR chart of compound **13d**

Figure S 30: ^{13}C NMR chart of compound **13_d**

Abdallah ElSayed_H_425

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

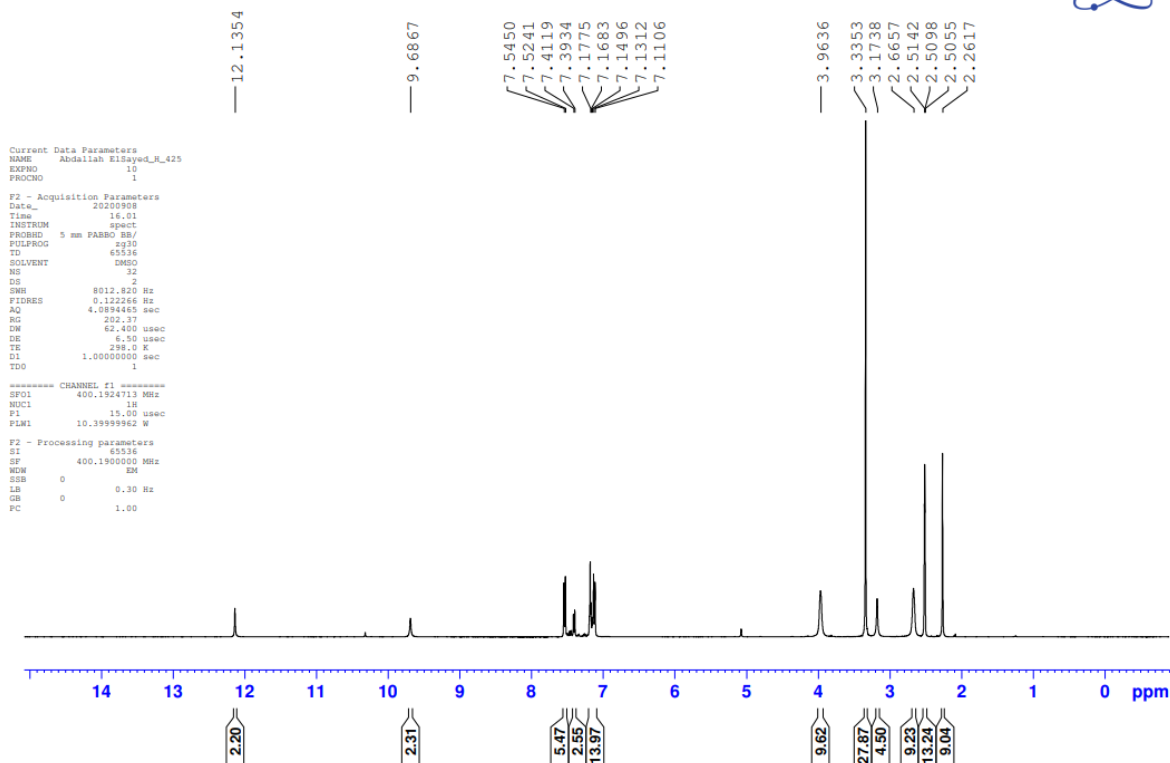
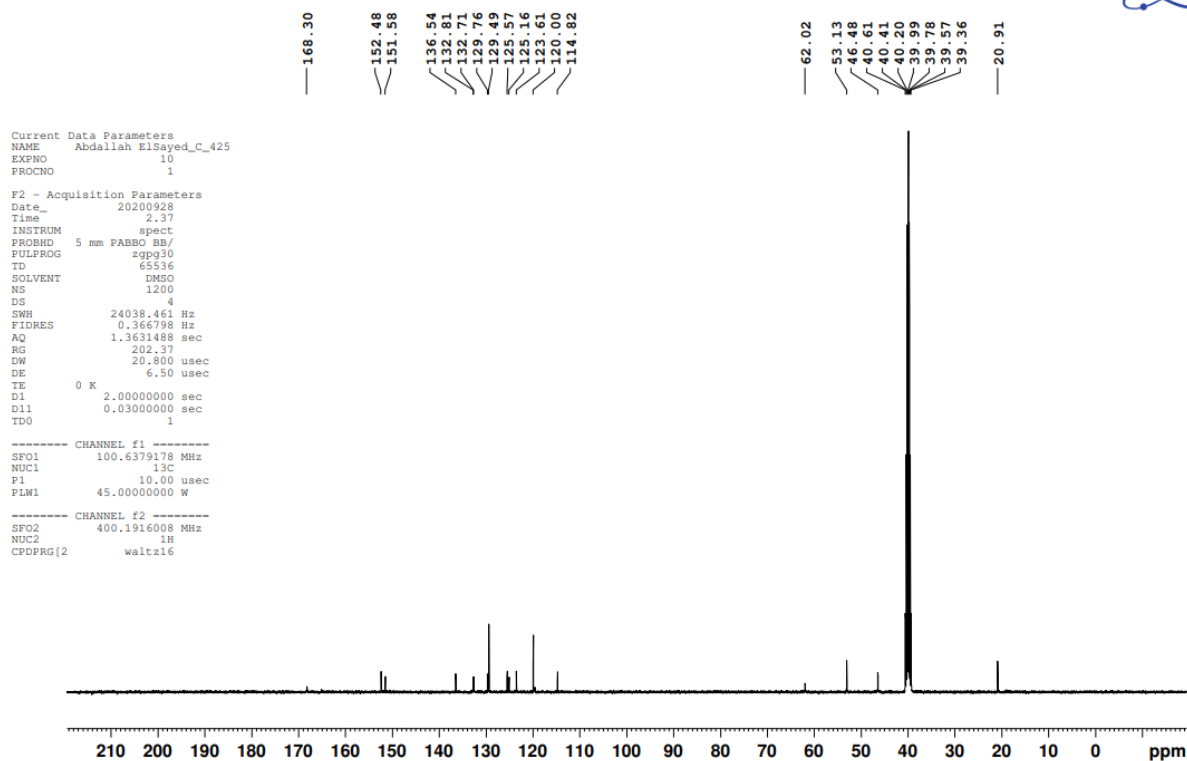


Figure S 31: ¹HNMR chart of compound **13_e**

Figure S 32: ^{13}C NMR chart of compound **13_e**

Abdallah ElSayed_H_426

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

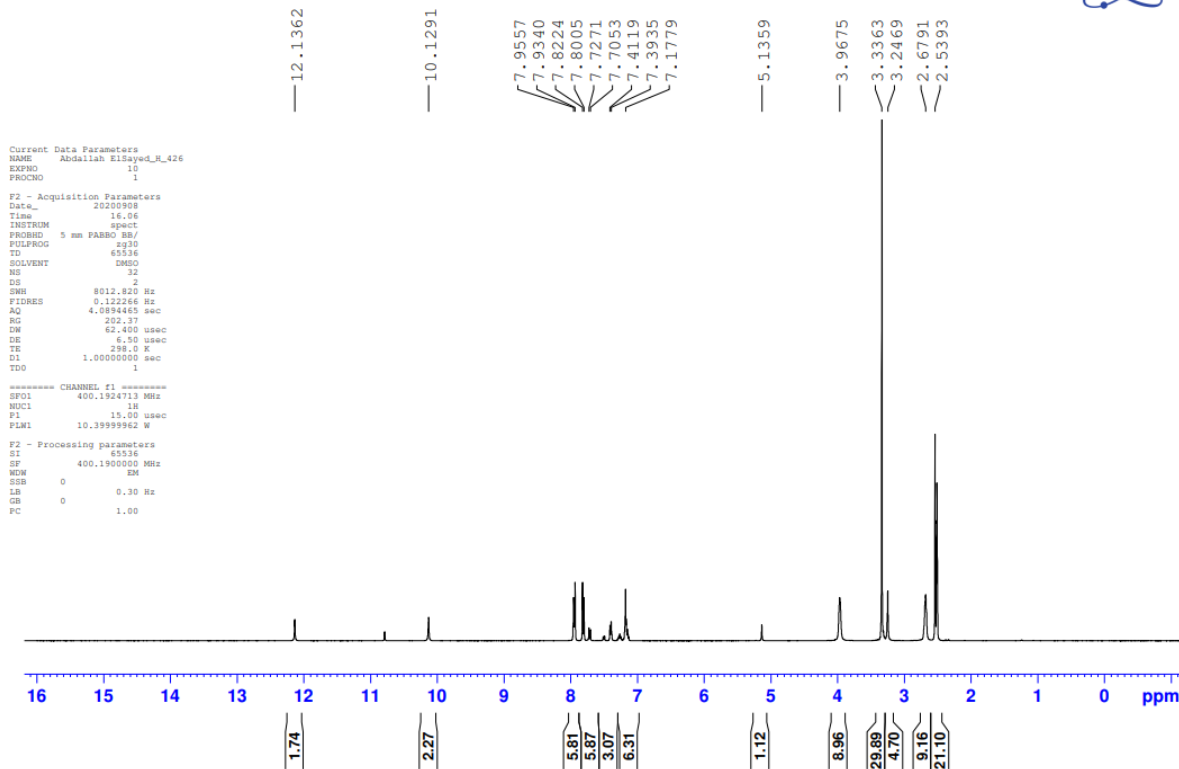


Figure S 33: ¹H NMR chart of compound **13f**

Abdallah ElSayed_C_426

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

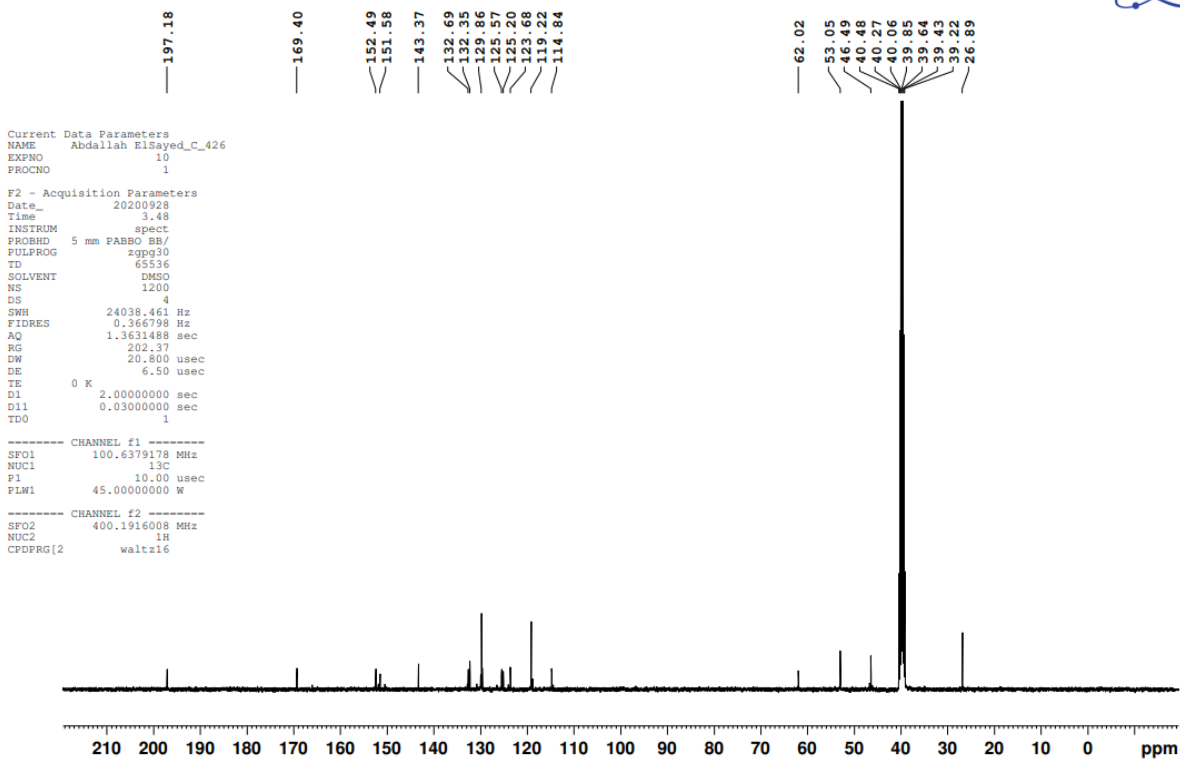
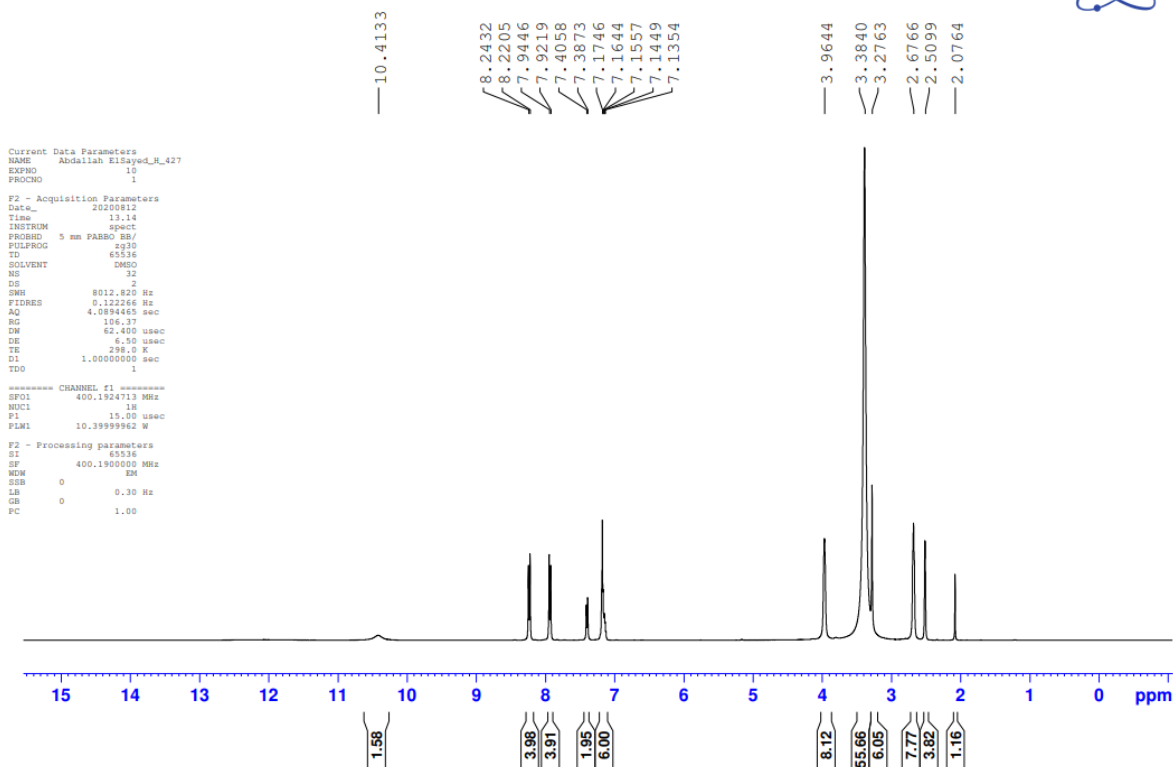


Figure S 34: ^{13}C NMR chart of compound 13_f

Figure S 35: ^1H NMR chart of compound **13_g**

Abdallah ElSayed_C_427

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

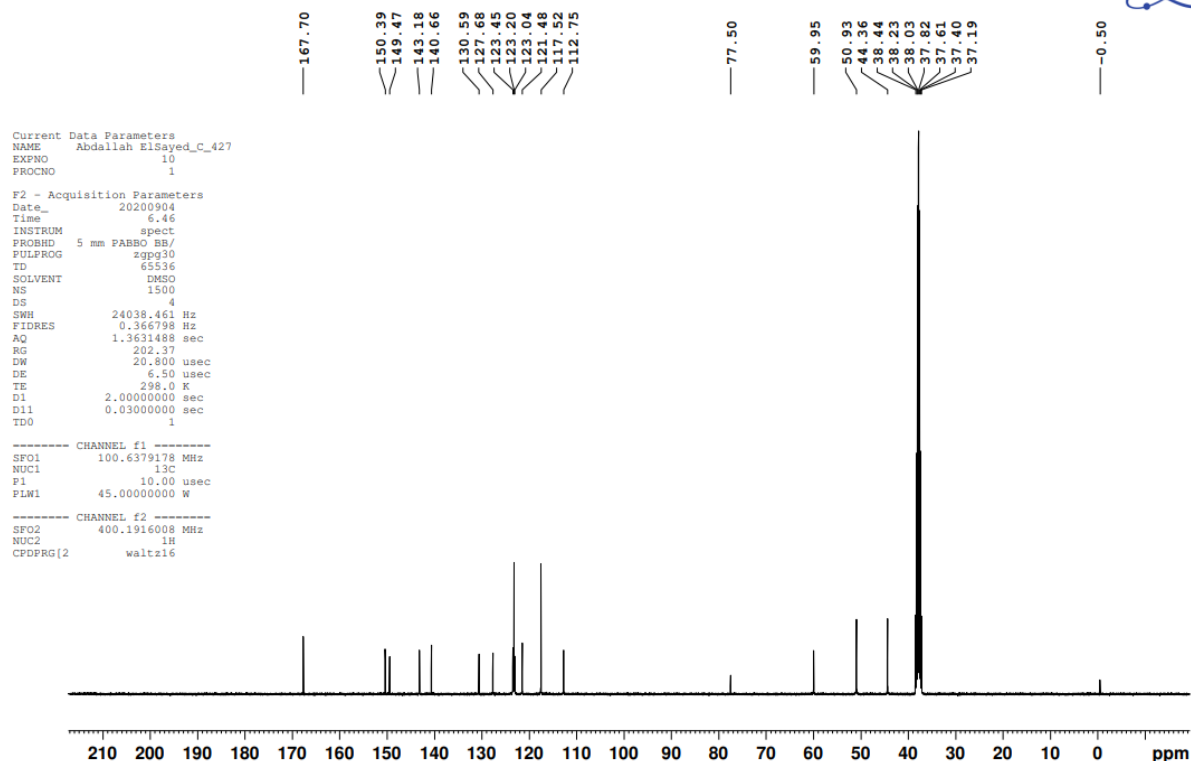


Figure S 36: ^{13}C NMR chart of compound **13_g**

Abdallah ElSayed_H_429

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

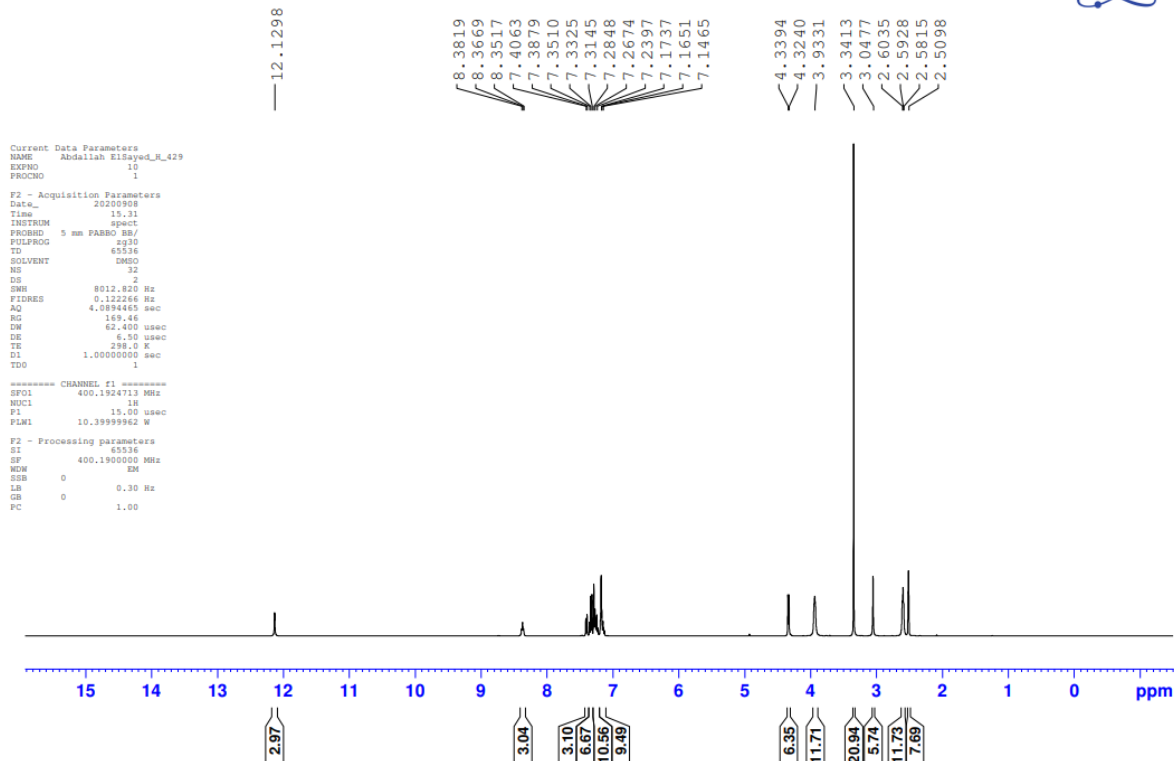
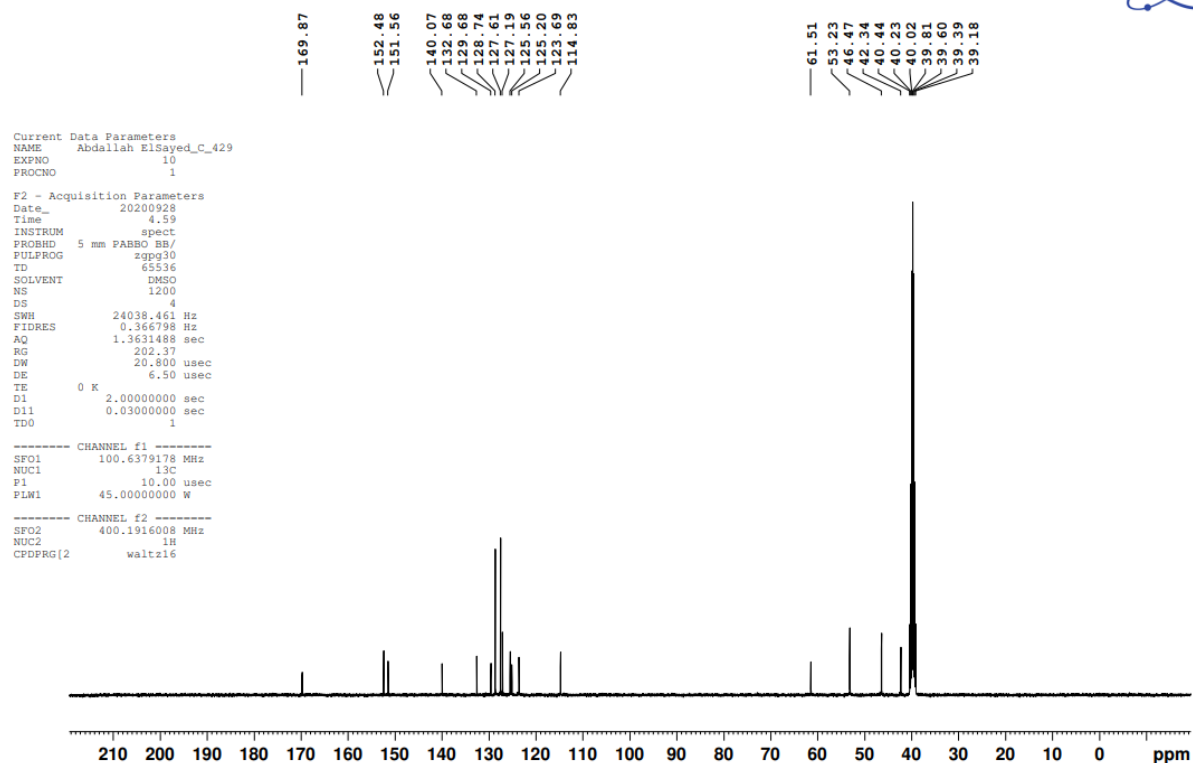


Figure S 37: ¹HNMR chart of compound 14

Figure S 38: ^{13}C NMR chart of compound 14