

Supplementary Material

Comparative anti-cancer potentials of taxifolin and quercetin methylated derivatives against HCT-116 cell line: Effects of O-methylation on taxifolin and quercetin as preliminary natural leads

Hamdoon A. Mohammed^{1,2*}, Suliman A. Almahmoud¹, El-Sayed M. El-Ghaly², Firdos Alam Khan³, Abdul-Hamid Emwas⁴, Mariusz Jaremko⁵, Fatimah Almulhim⁵, Riaz A. Khan¹, and Ehab A. Ragab^{2*}

¹Department of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, Qassim University, Qassim 51452, Saudi Arabia

²Department of Pharmacognosy and Medicinal Plants, Faculty of Pharmacy, Al-Azhar University, Cairo 11884, Egypt

³Department of Stem Cell Research, Institute for Research and Medical Consultations (IRMC); Imam Abdulrahman Bin Faisal University, 31441 Dammam-Saudi Arabia

⁴CoreLabs, King Abdullah University of Science and Technology (KAUST), 23955-6900 Thuwal, Saudi Arabia.

⁵Smart-Health Initiative (SHI) and Red Sea Research Center (RSRC), Division of Biological and Environmental Sciences and Engineering (BESE), King Abdullah

University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

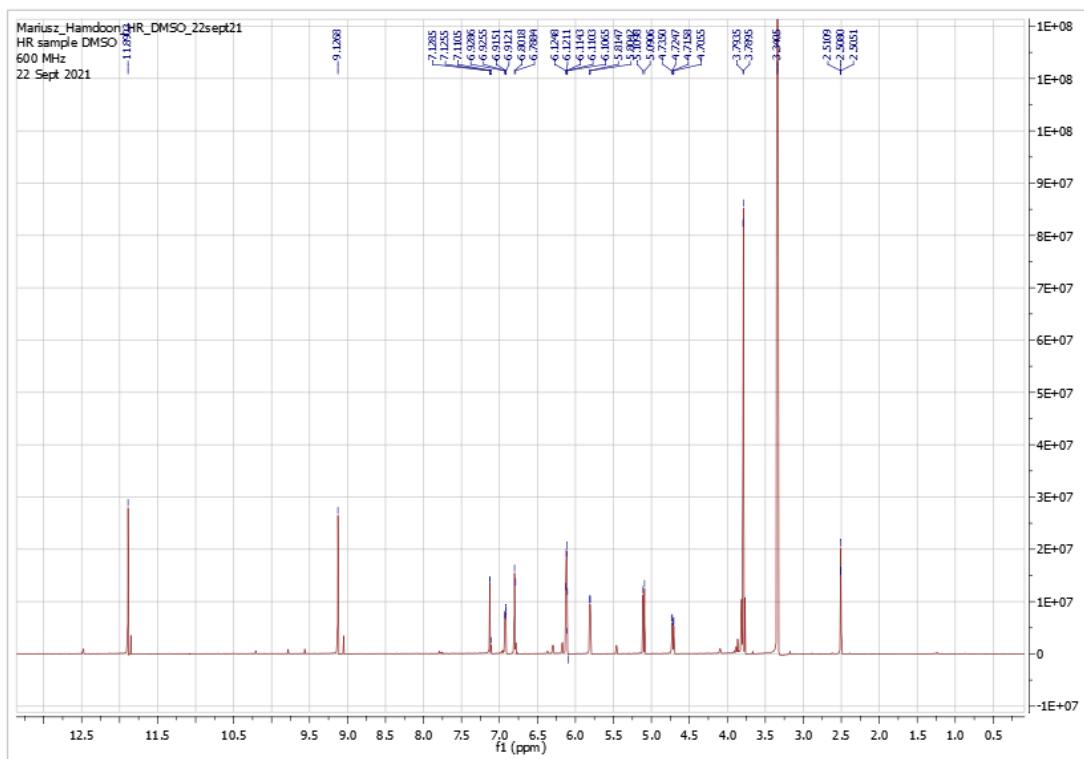


Figure S1: ^1H NMR spectrum of compound **1** (DMSO- d_6 , 600 MHz)

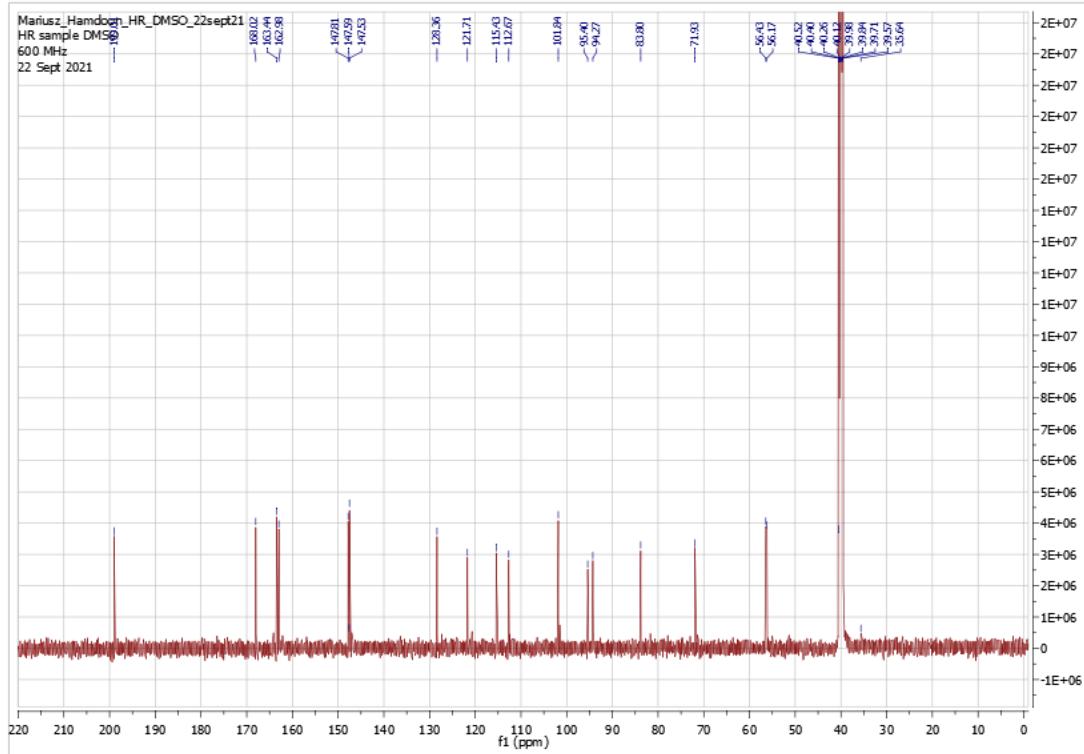


Figure S2: ^{13}C NMR spectrum of compound **1** (DMSO- d_6 , 150 MHz)

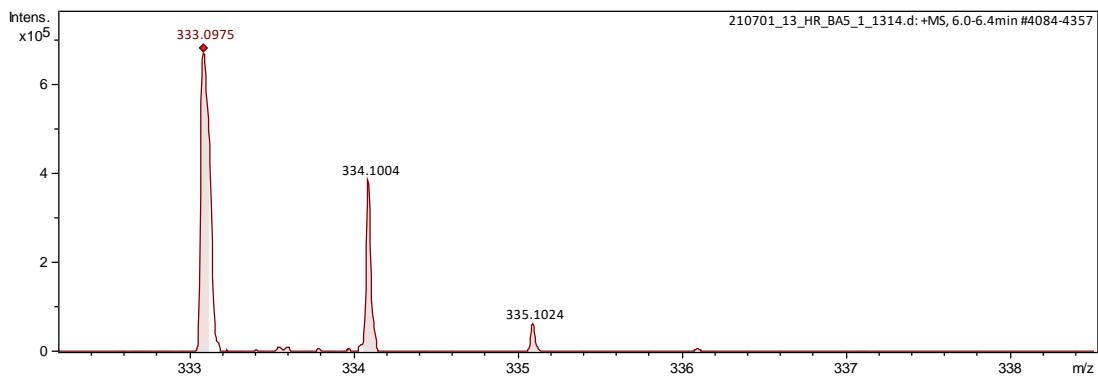


Figure S3: +ESIMS of compound **1**

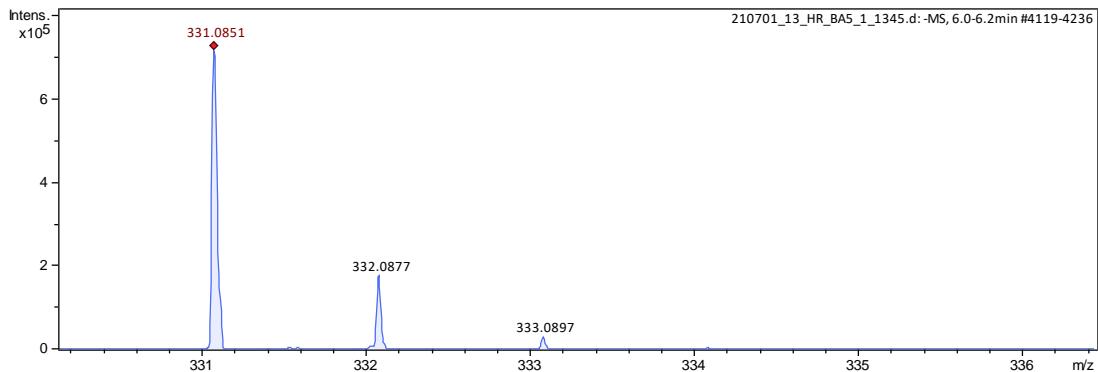


Figure S4: -ESIMS of compound **1**

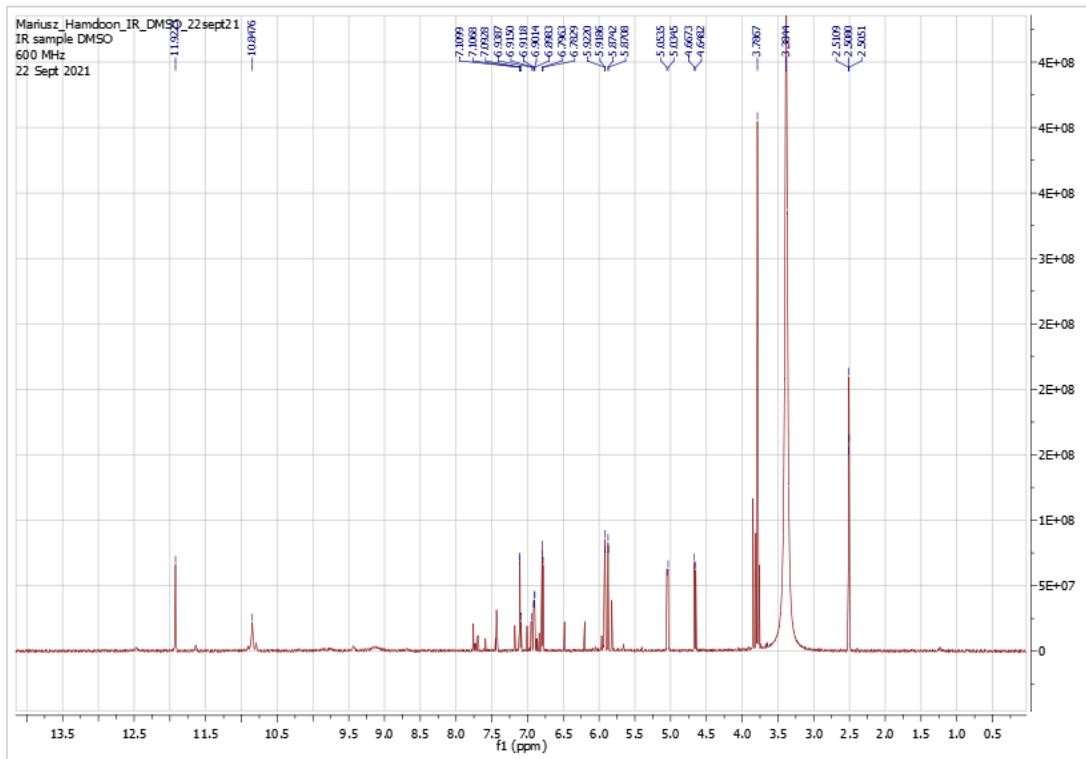


Figure S5: ^1H NMR spectrum of compound **2** (DMSO- d_6 , 600 MHz)

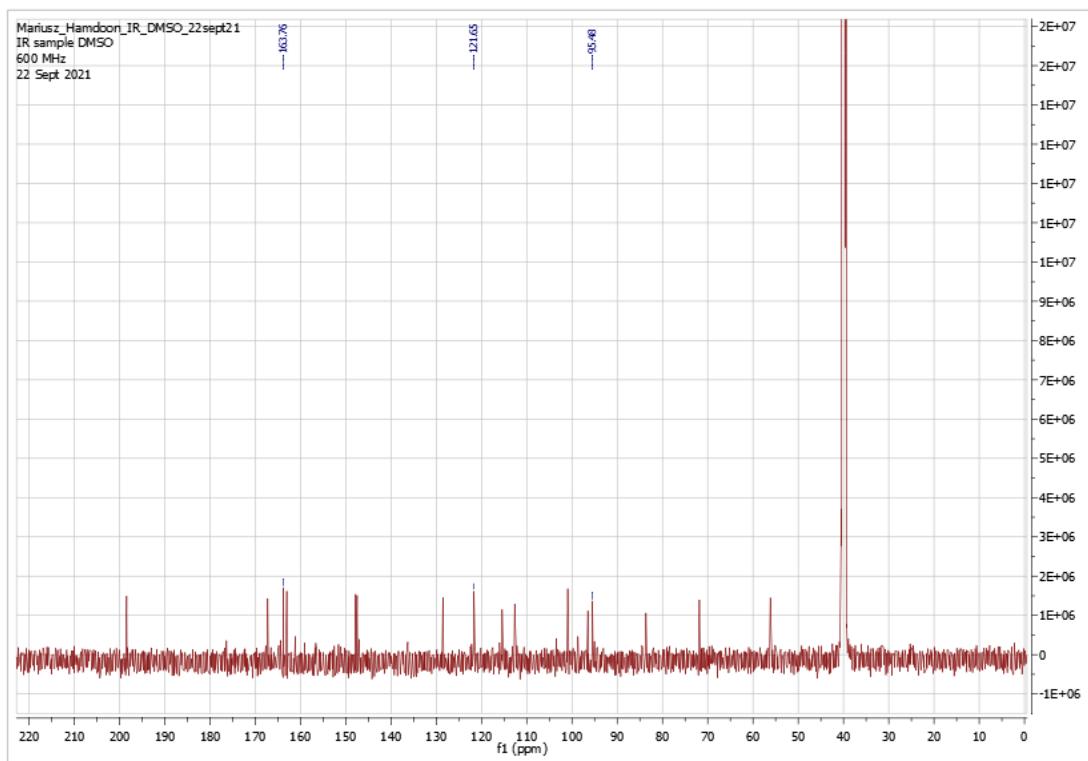


Figure S6: ^{13}C NMR spectrum of compound 2 (DMSO- d_6 , 150 MHz)

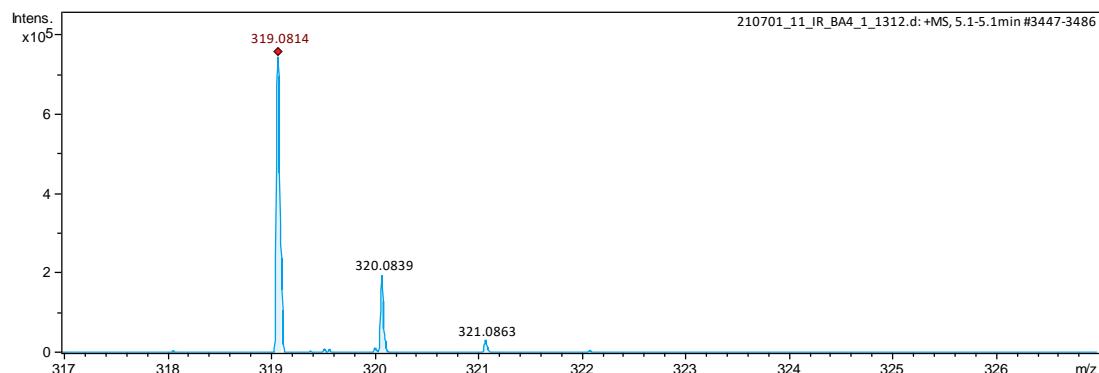


Figure S7: +ESIMS of compound 2

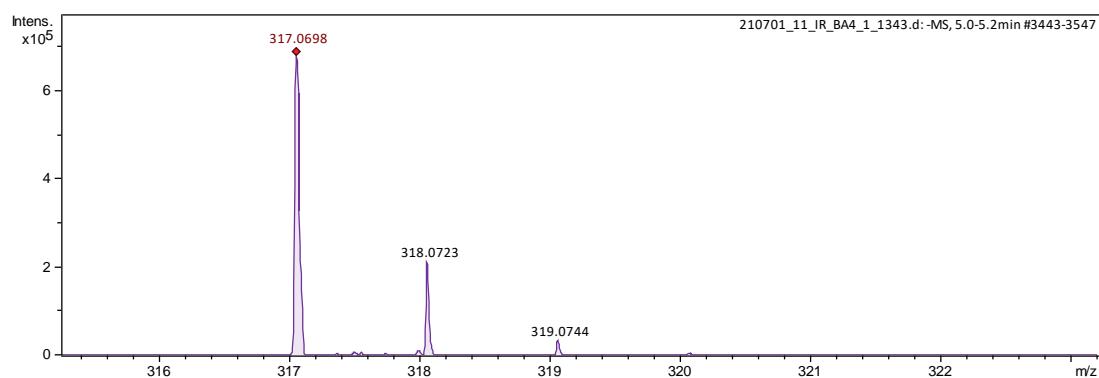


Figure S8: -ESIMS of compound 2

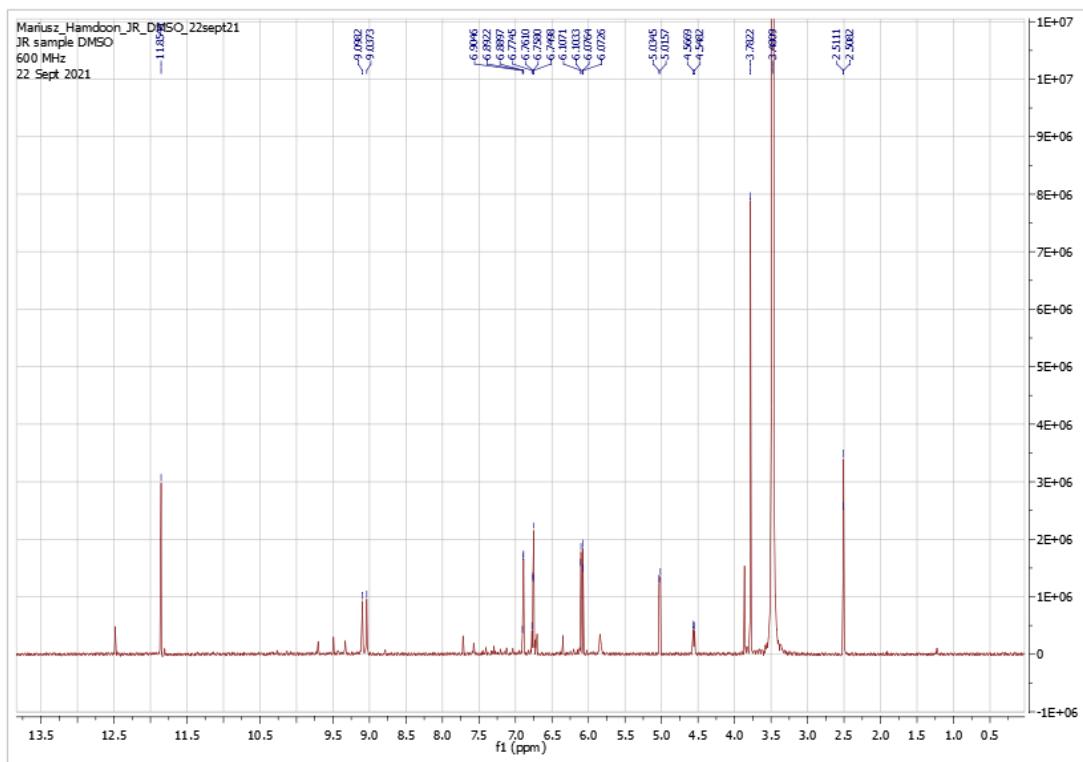


Figure S9: ^1H NMR spectrum of compound **3** (DMSO- d_6 , 600 MHz)

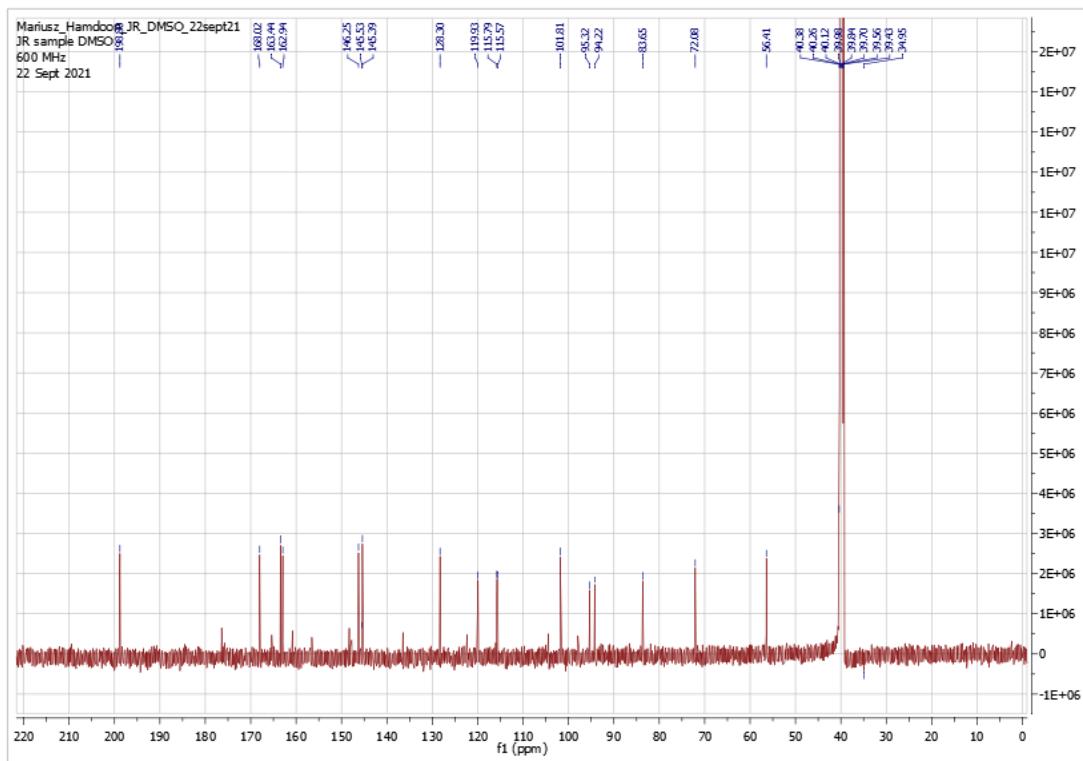


Figure S10: ^{13}C NMR spectrum of compound **3** (DMSO- d_6 , 150 MHz)

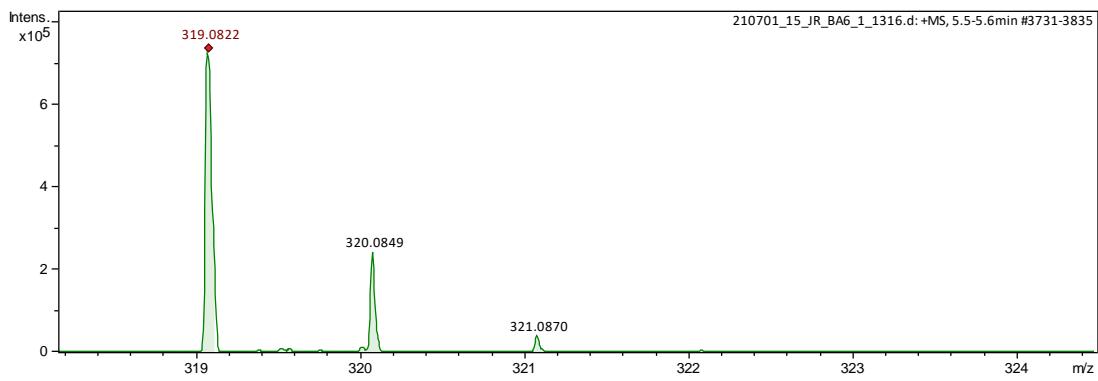


Figure S11: +ESIMS of compound 3

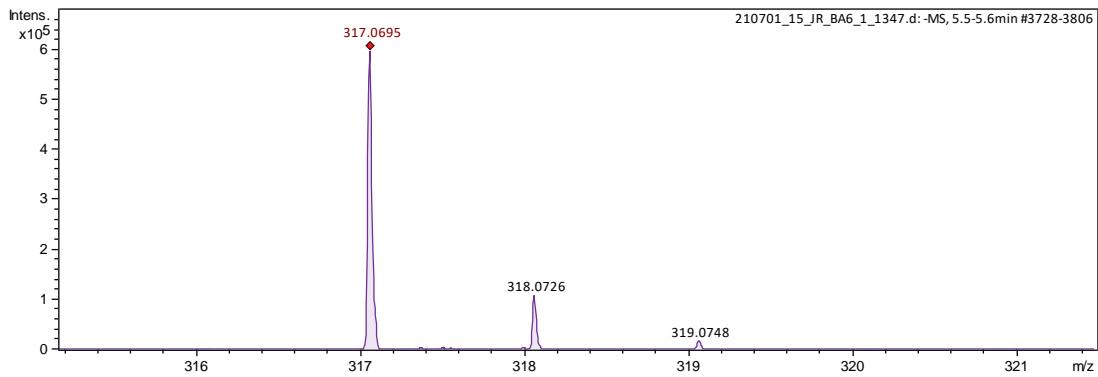


Figure S12: -ESIMS of compound 3

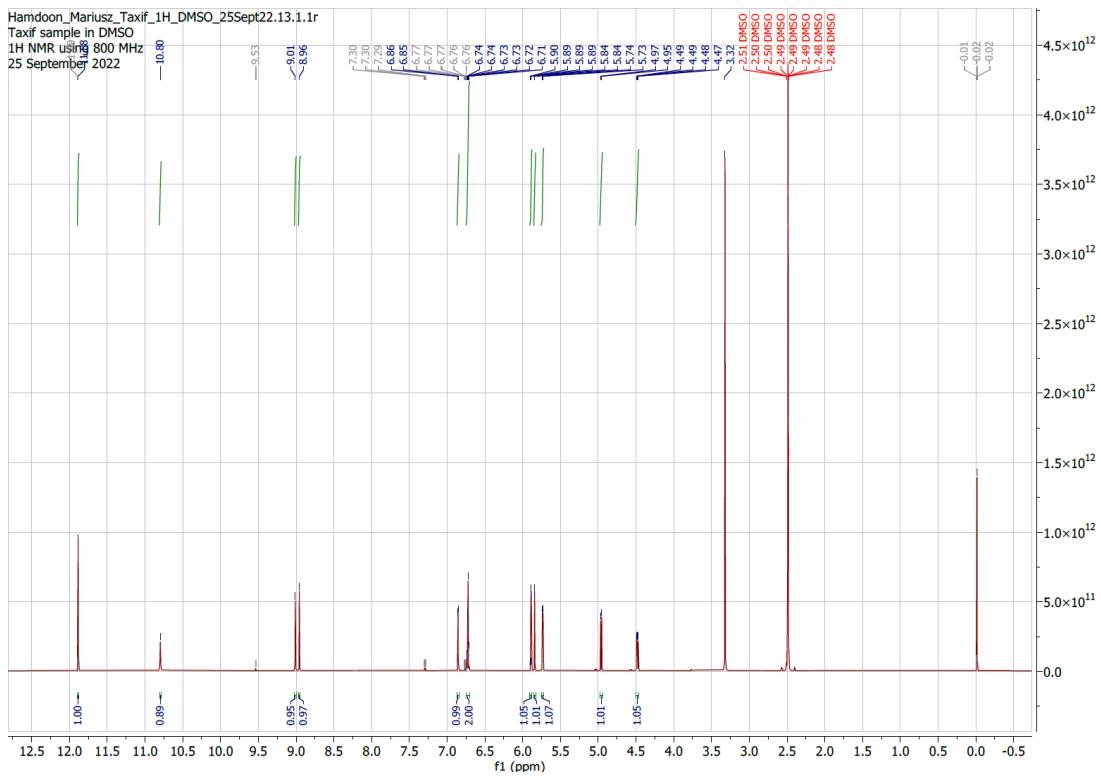


Figure S13: ^1H NMR spectrum of compound 4 (DMSO- d_6 , 800 MHz)

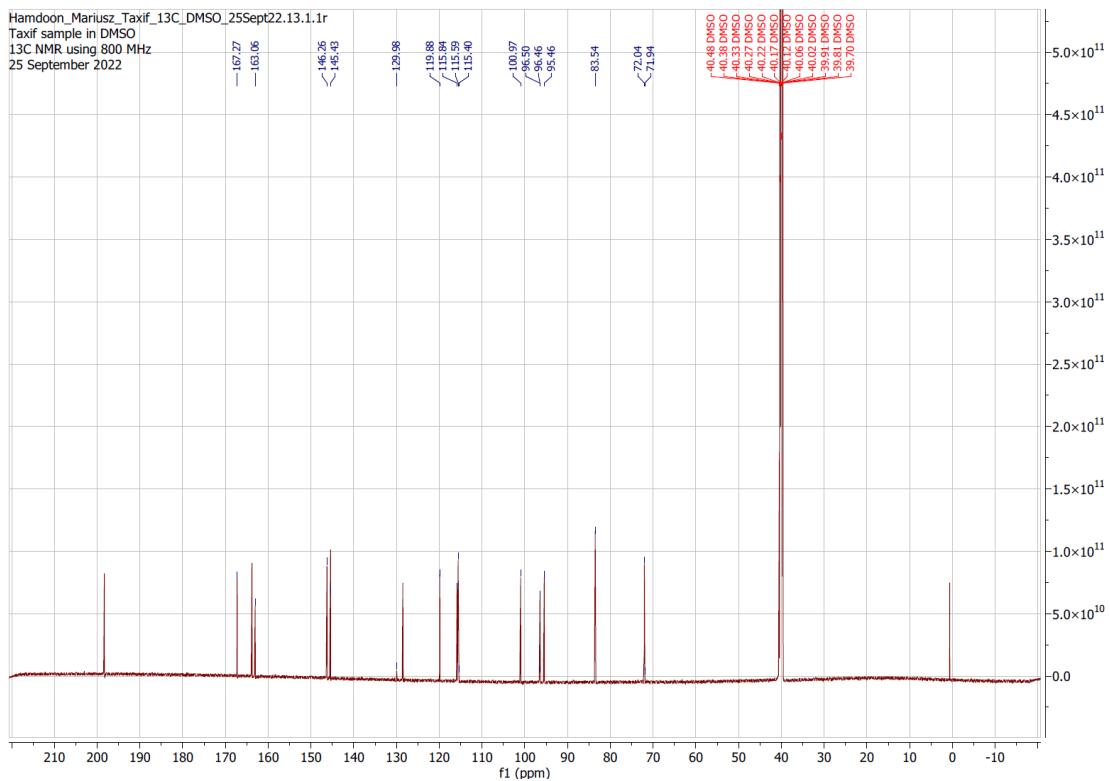


Figure S14: ¹³C NMR spectrum of compound 4 (DMSO-*d*₆, 200 MHz)

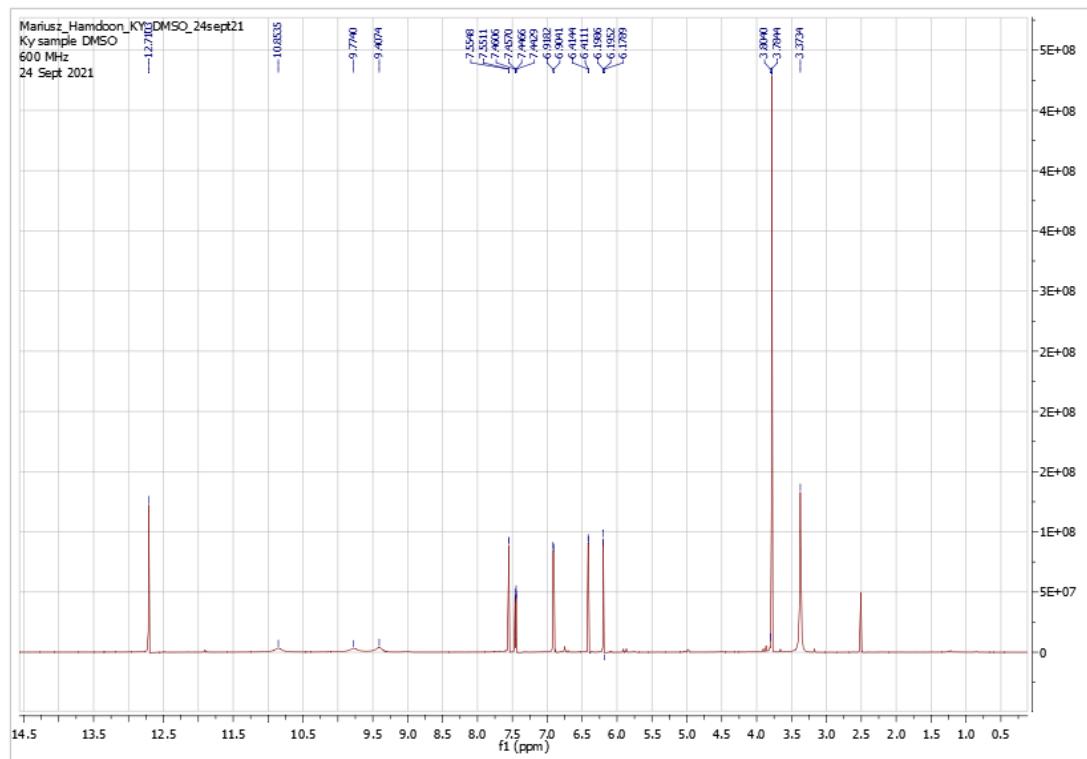


Figure S15: ¹H NMR spectrum of compound 5 (DMSO-*d*₆, 600 MHz)

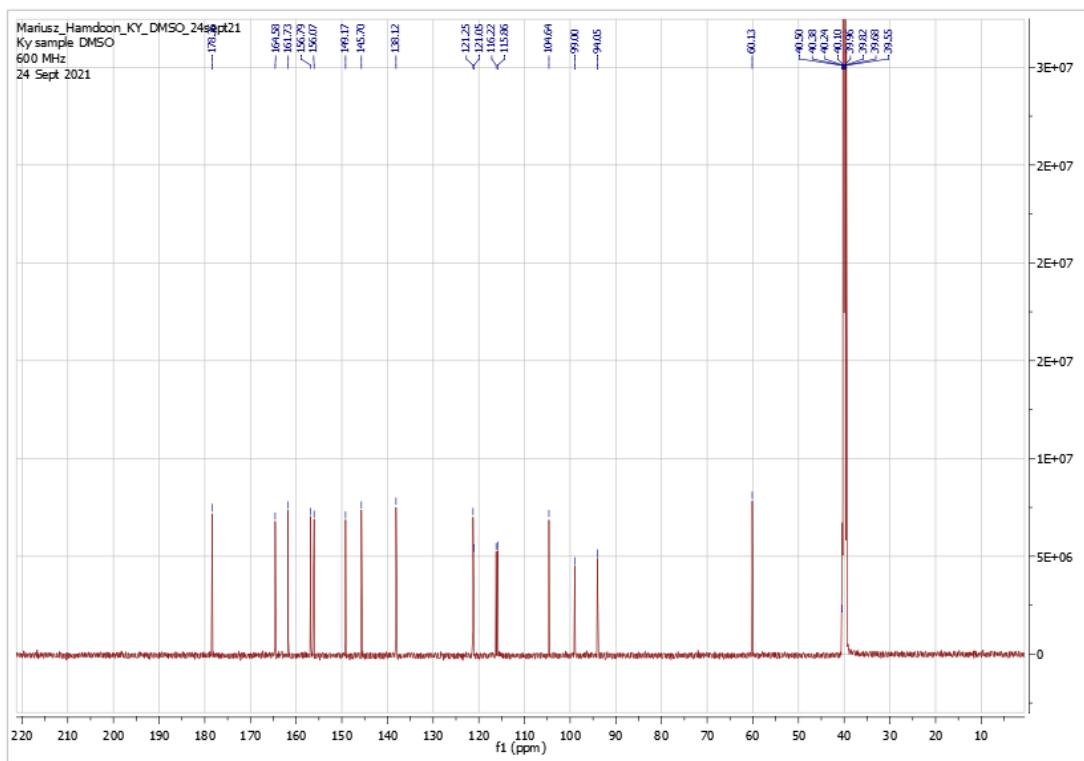


Figure S16: ^{13}C NMR spectrum of compound **5** (DMSO- d_6 , 150 MHz)

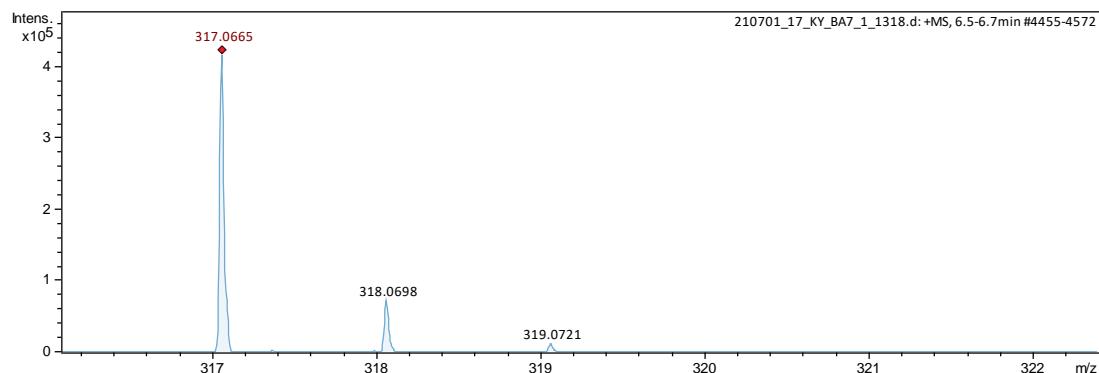


Figure S17: +ESIMS of compound **5**

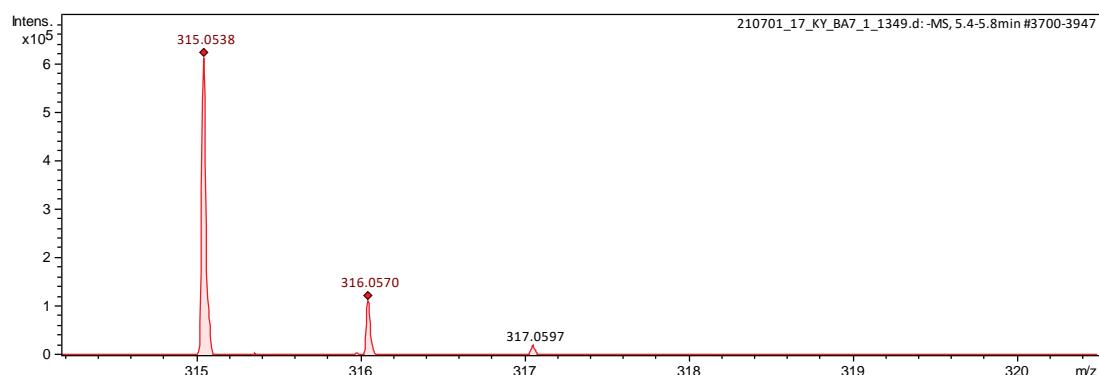


Figure S18: -ESIMS of compound **5**

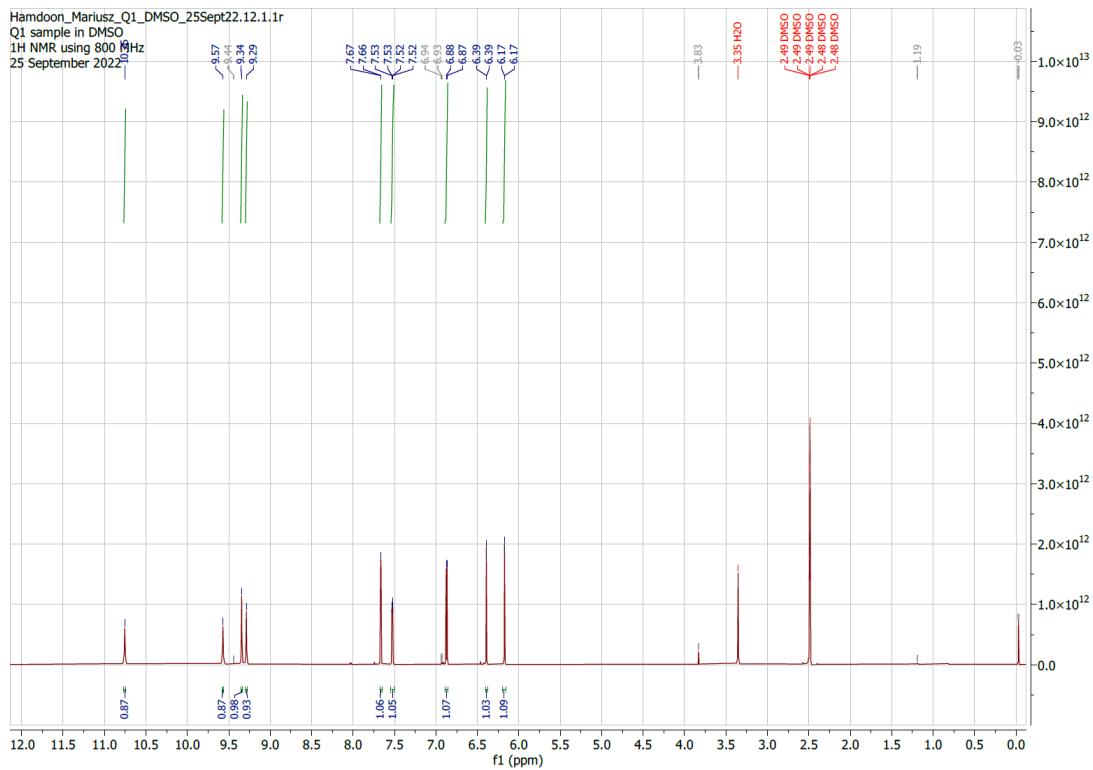


Figure S19: ${}^1\text{H}$ NMR spectrum of compound **6** (DMSO-*d*₆, 800 MHz)

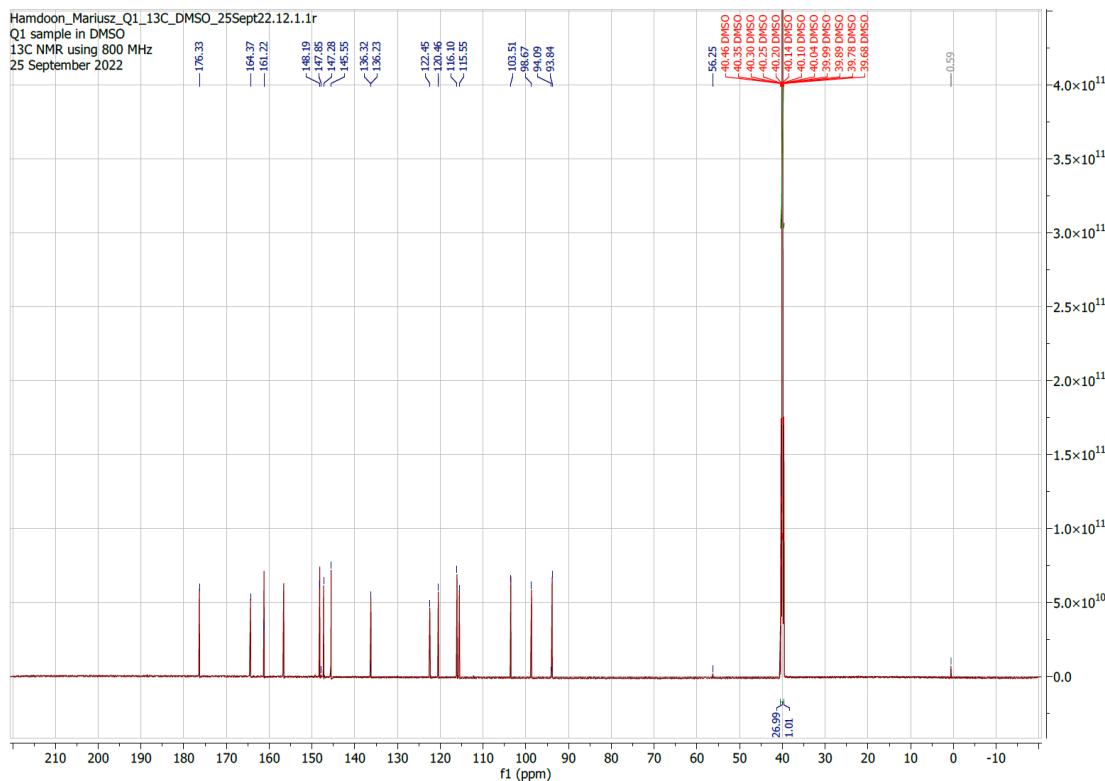


Figure S20: ${}^{13}\text{C}$ NMR spectrum of compound **6** (DMSO-*d*₆, 200 MHz)