

Environmentally Friendly Synthesis of New Mono- and Bis-Pyrazole Derivatives; In Vitro Antimicrobial, Antifungal, and Antioxidant Activity; and In Silico Studies: DFT, ADMETox, and Molecular Docking

Oussama Merzouki ^{1,*}, Nadia Arrousse ², Elhachmia Ech-chihbi ³, Ashwag S. Alanazi ⁴, El Houssine Mabrouk ^{1,5}, Mohamed Hefnawy ⁶, Abdelfattah El Moussaoui ^{7,8}, Hanane Touijer ⁸, Azeddin El Barnossi ⁸ and Mustapha Taleb ¹

¹ Laboratory of Engineering Electrochemistry, Modeling, and Environment, Department of Chemistry, Faculty of Sciences Dhar Mahraz, Sidi Mohamed Ben Abdellah University, Fez 30000, Morocco

² School of Science and Engineering, Al Akhawayn University in Ifrane, Hassan II Avenue, Ifrane 53000, Morocco

³ Laboratory of Physics and Chemistry of Inorganic and Organic Materials, Higher Normal School, Mohammed V University, Rabat 30050, Morocco

⁴ Department of Pharmaceutical Sciences, College of Pharmacy, Princess Nourah Bint Abdulrahman University, Riyadh 11671, Saudi Arabia

⁵ Laboratory of Materials Engineering for the Environment and Natural Resources, Faculty of Sciences and Technics, University of Moulay Ismail, Meknes, B.P 509, Boutalamine, Errachidia 52000, Morocco

⁶ Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia

⁷ Plant Biotechnology Team, Faculty of Sciences, Abdelmalek Essaadi University, Tetouan 93002, Morocco

⁸ Laboratory of Biotechnology, Environment, Agrifood, and Health, Faculty of Sciences Dhar El Mahraz, Sidi Mohamed Ben Abdellah University, Fez 30050, Morocco

* Correspondence: oussama.merzouki@usmba.ac.ma



Figure S1. The ^1H -NMR spectrum of the compounds **O1**.

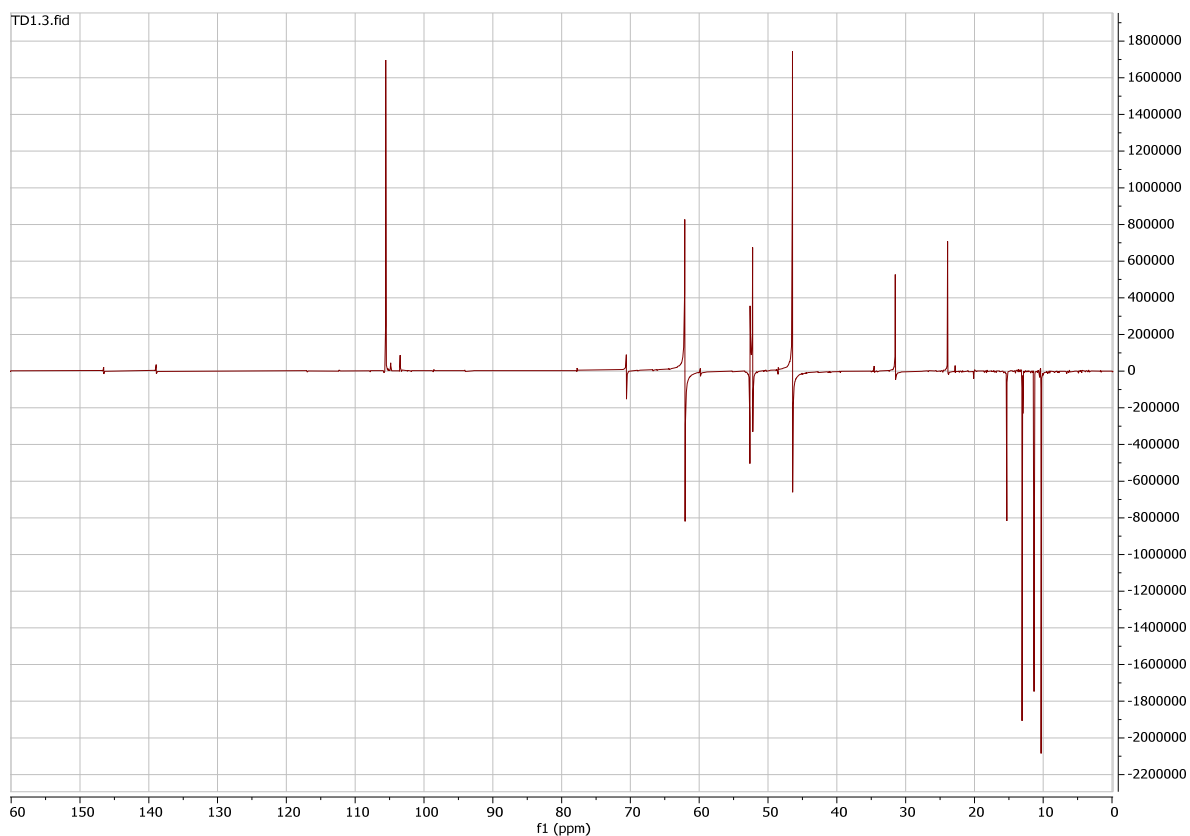


Figure S2. The ^{13}C -NMR spectrum of the compounds **O1**.

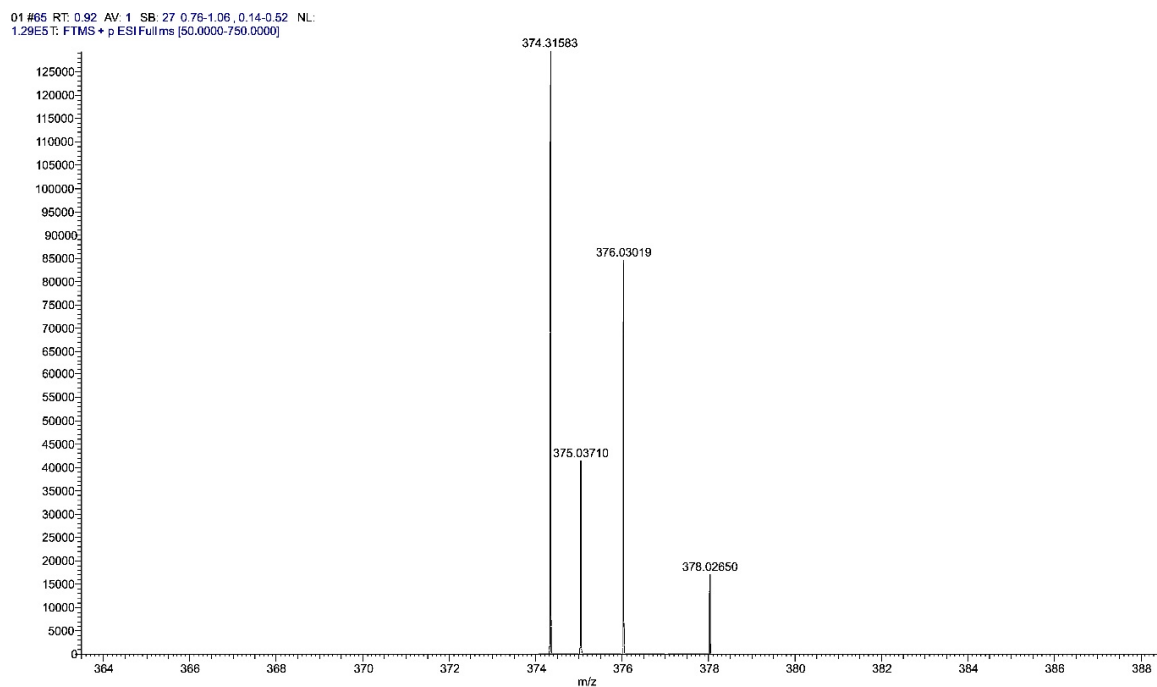


Figure S3. The Masse spectrum of the compounds **O1**.

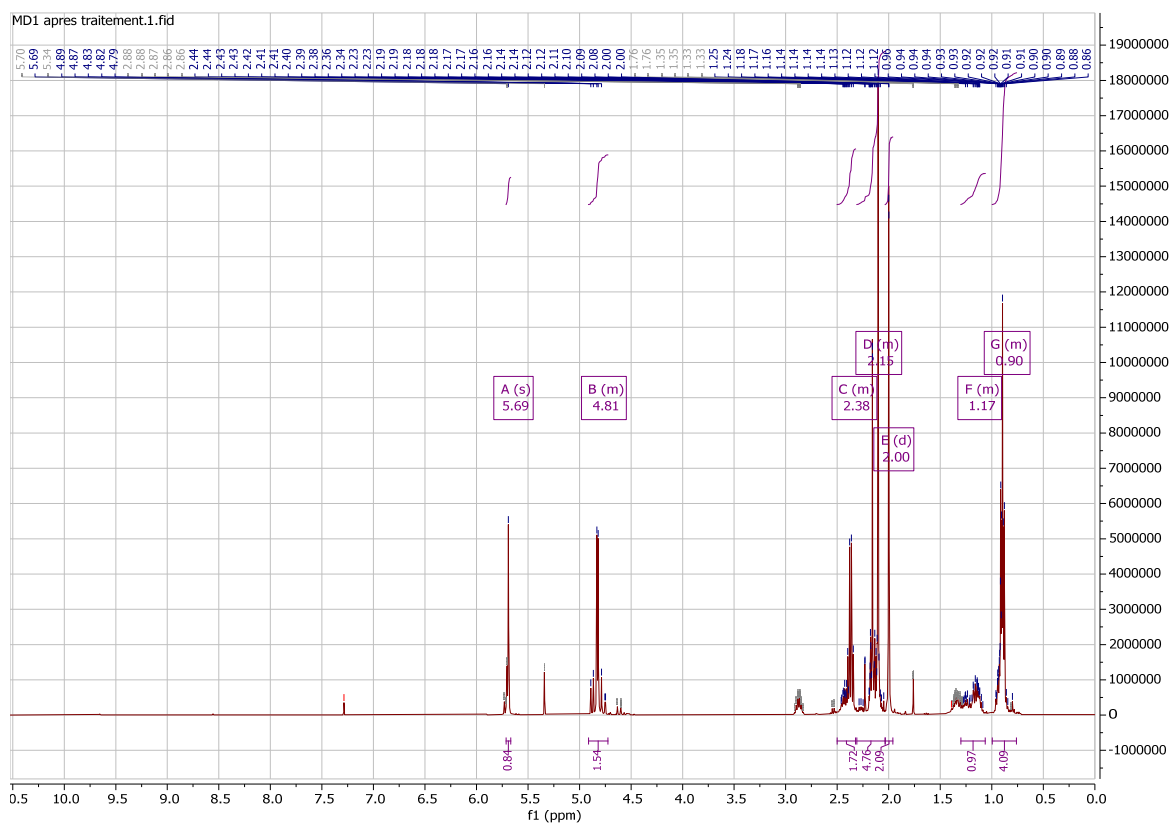


Figure S4. The ^1H -NMR spectrum of the compounds **O2**.

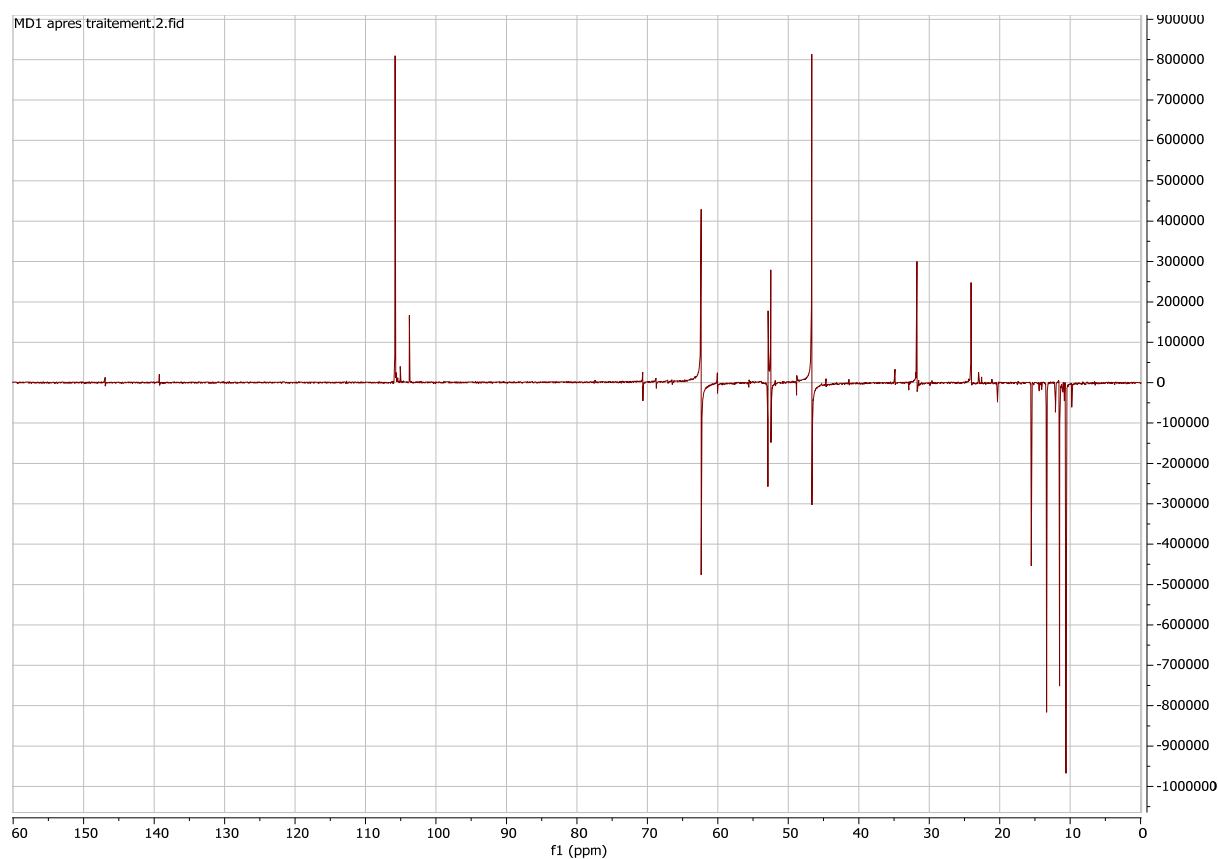


Figure S5. The ^{13}C -NMR spectrum of the compounds **O2**.

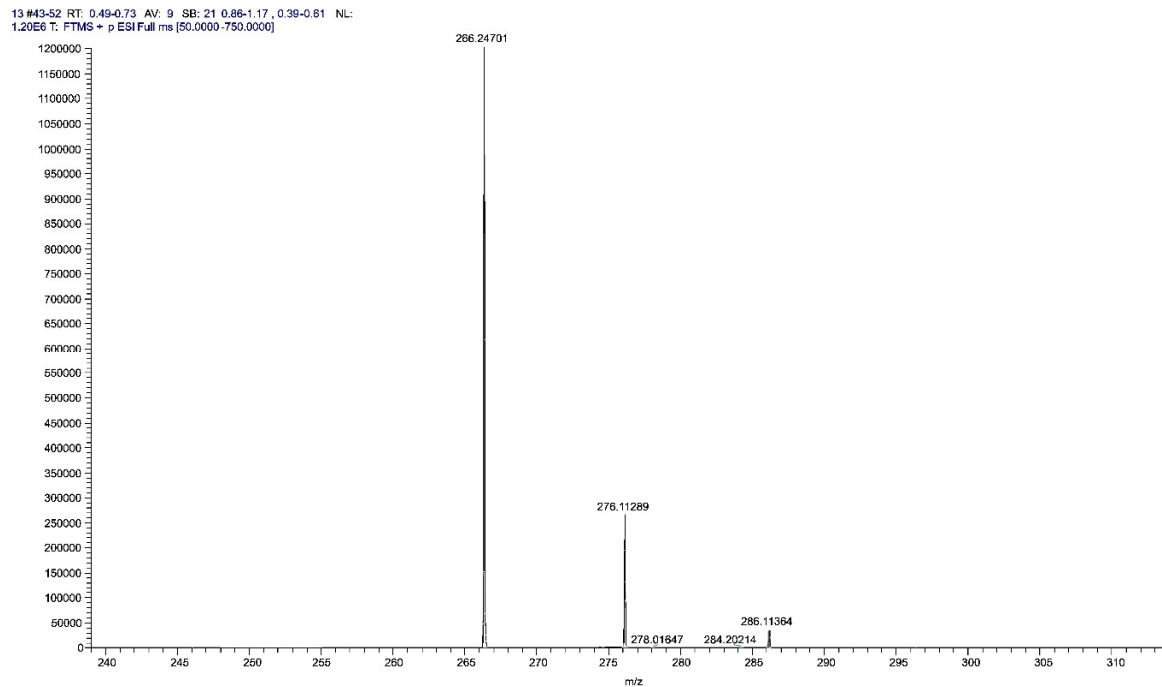


Figure S6. The masse spectrum of the compounds **O2**.

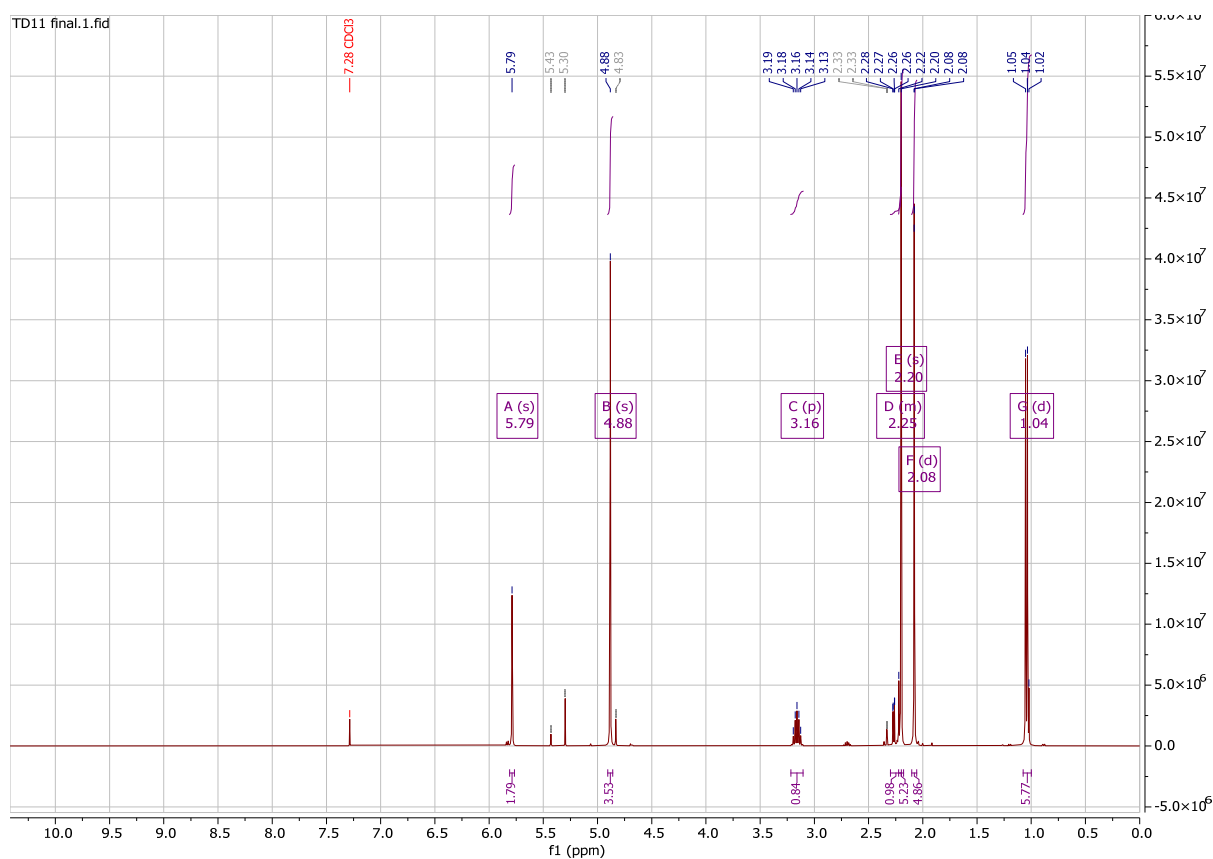
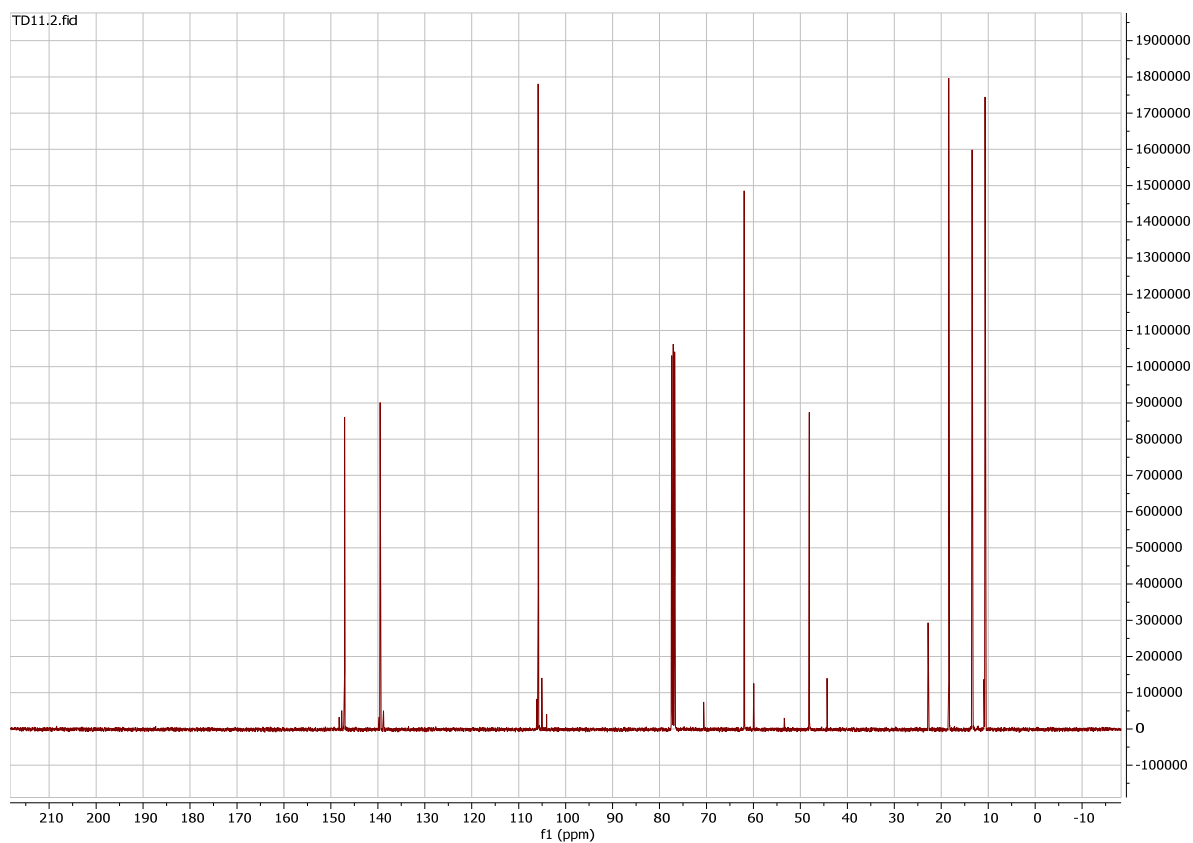


Figure S7. The ^1H -NMR spectrum of the compounds **O3**.



FigureS8. The ^{13}C -NMR spectrum of the compounds **O3**.

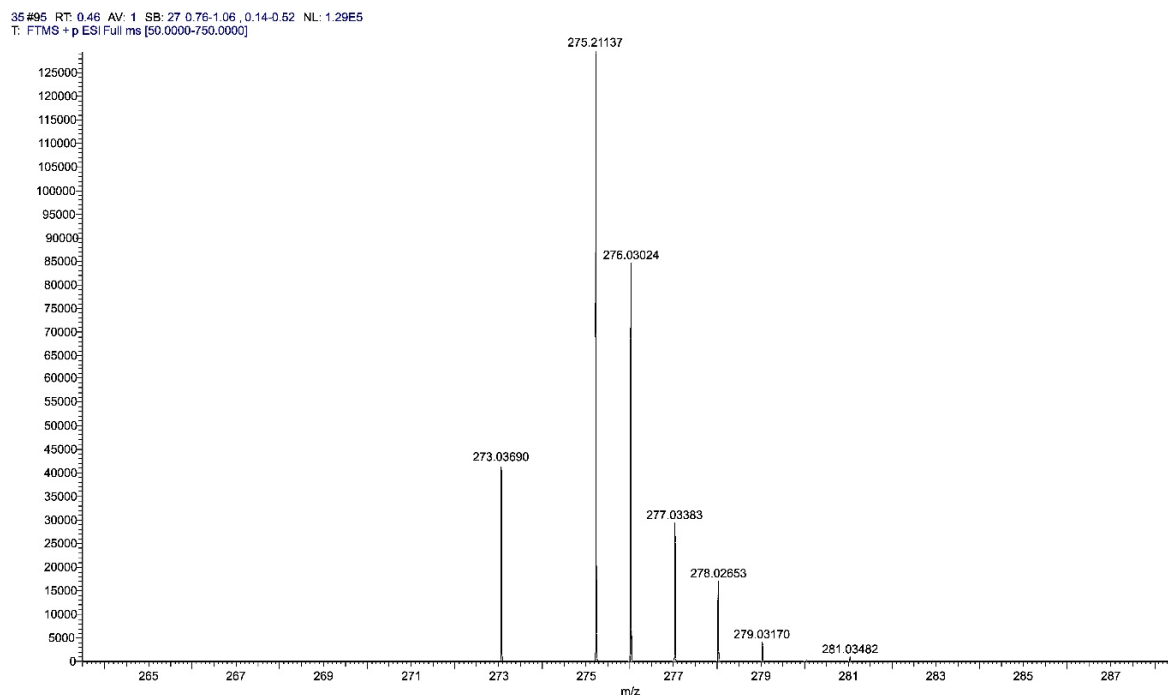


Figure S9. The masse spectrum of the compounds **O3**.

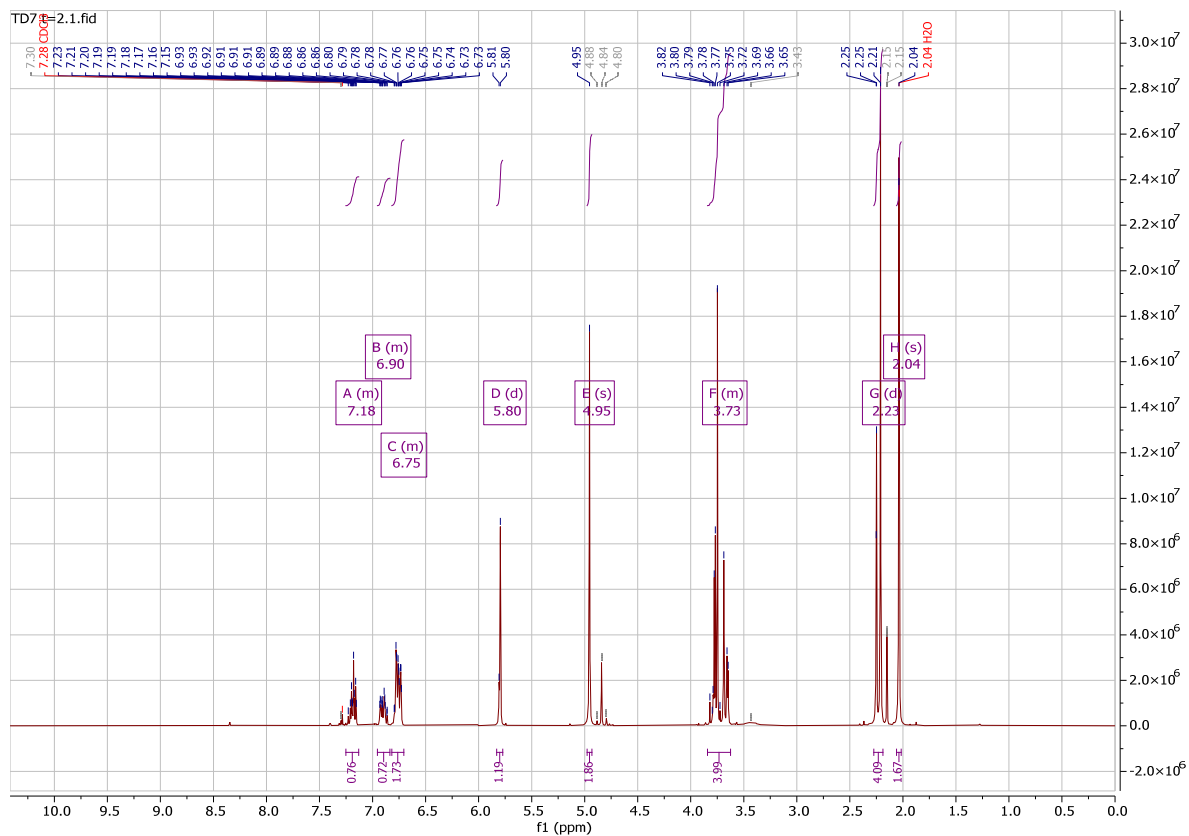


Figure S10. The ^1H -NMR spectrum of the compounds **O4**.

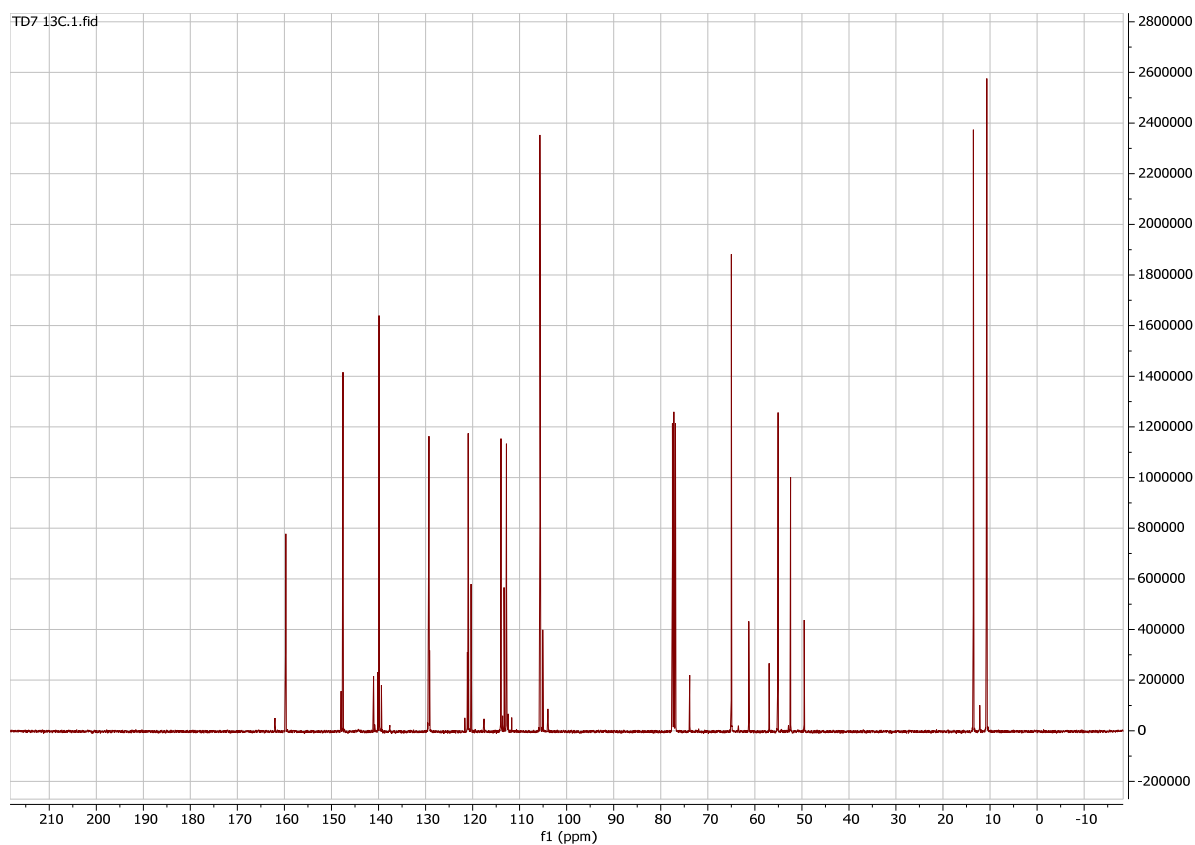


Figure S11. The ^{13}C -NMR spectrum of the compounds **O4**.

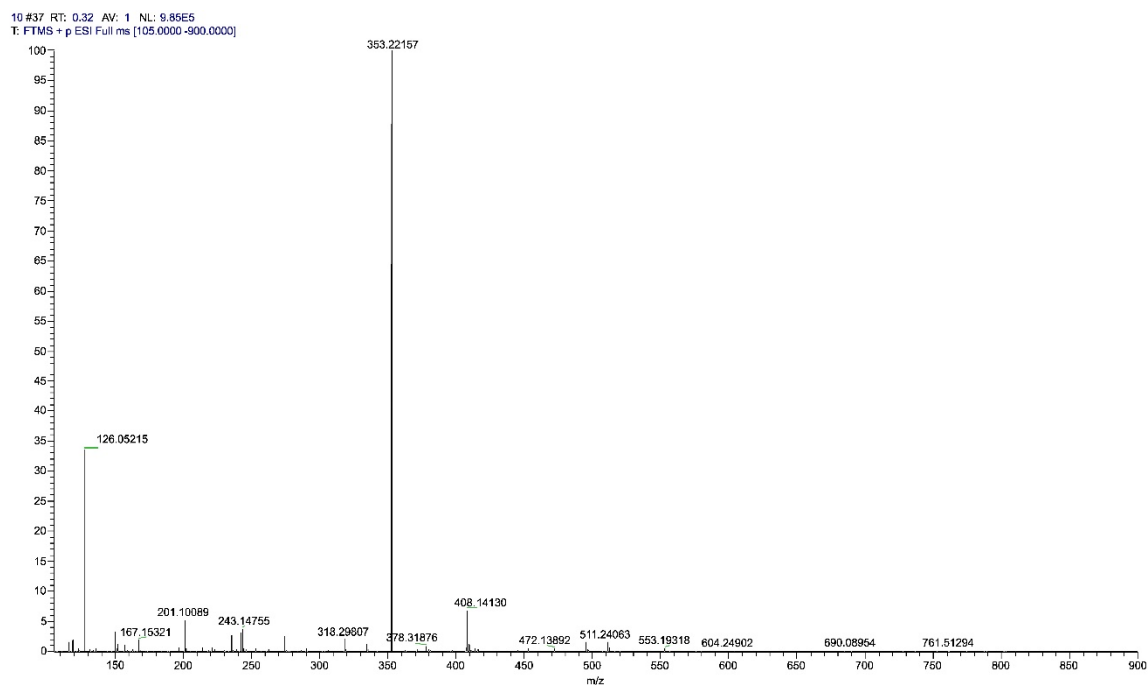


Figure S12. The masse spectrum of the compounds **O4**.



Figure S14. The ^{13}C -NMR spectrum of the compounds **O5**.

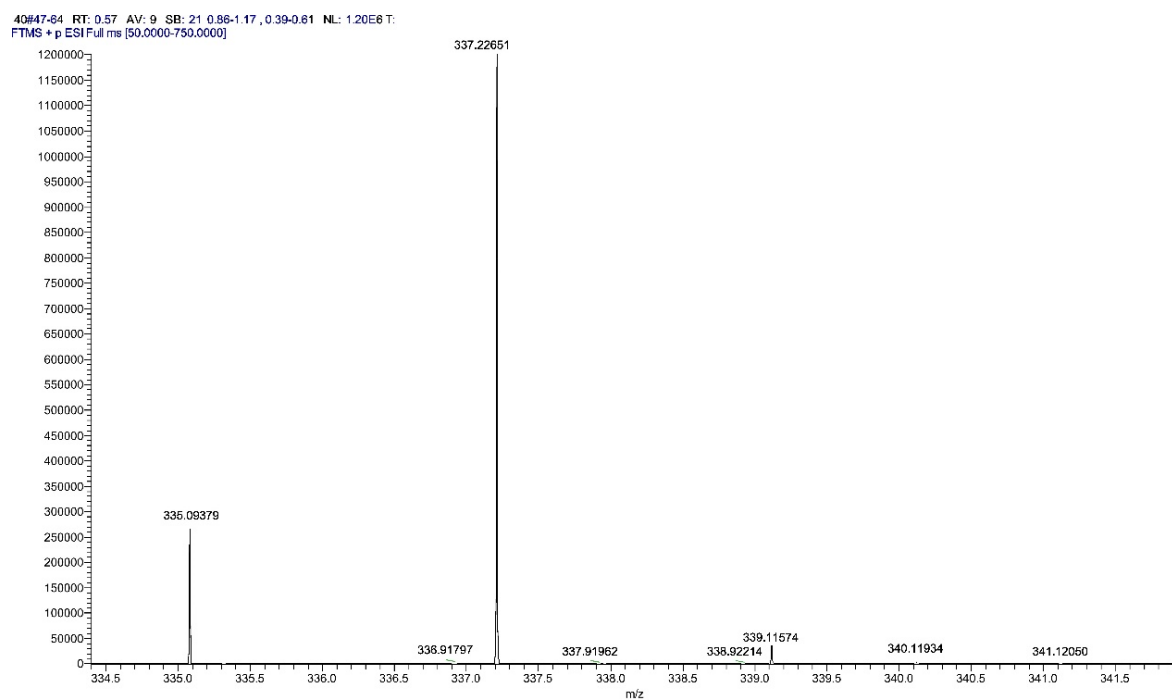


Figure S15. The ^1H -NMR spectrum of the compounds **O5**.