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Supplementary Materials

Synthesis, Antioxidant Activity, In Silico Evaluation, and Cytotoxicity of Novel Polyphenolic–Methyliden–Hydrazono–Thiazole Derivatives

Alexandra Cătălina Cornea [1], Gabriel Marc [2,*], Ionel Fizeșan [3], Ioana Ionuț [1], Cristina Moldovan [1], Anca Stana [1], Brîndușa Tiperciuc [1], Ionuț-Valentin Creștin [3], Adrian Pîrnău [4], Laurian Vlase [5], Ilioara Oniga [6] and Ovidiu Oniga [1]

1. Figures

1.1. The IR spectra of the compounds E1-E8

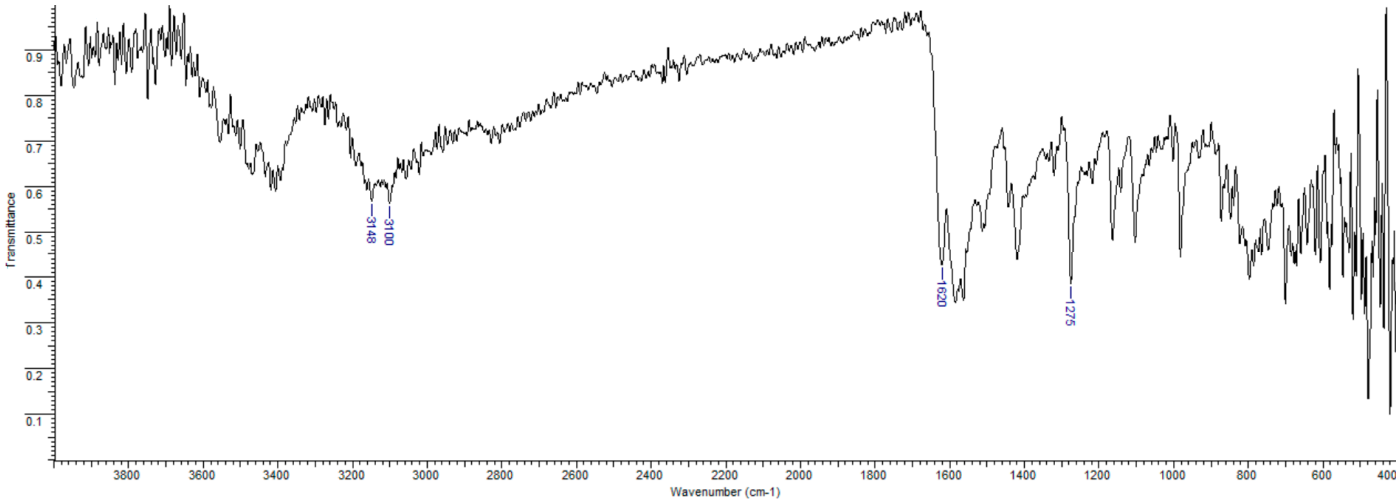


Figure S1. The IR spectrum of the compound **E1**

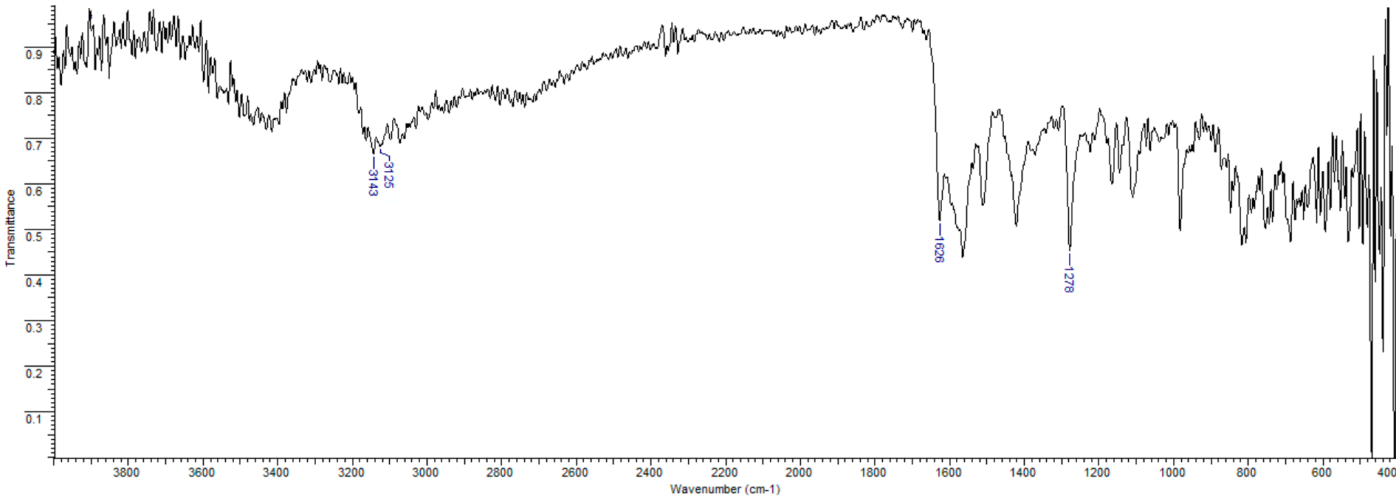


Figure S2. The IR spectrum of the compound **E2**

 https://doi.org/10.3390/molecules31203620

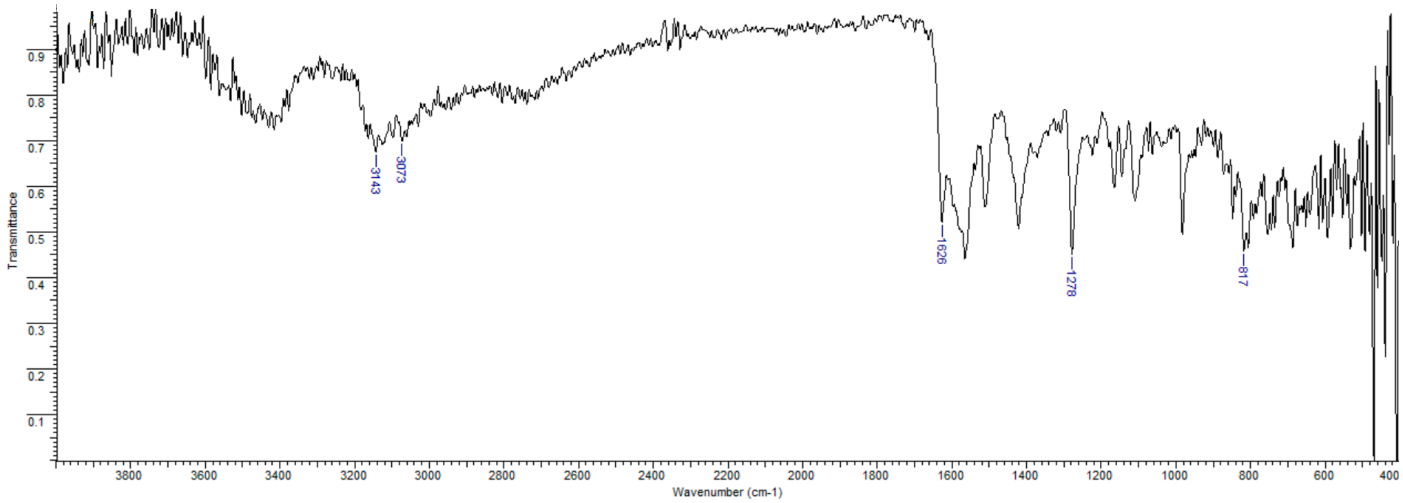


Figure S3. The IR spectrum of the compound **E3**

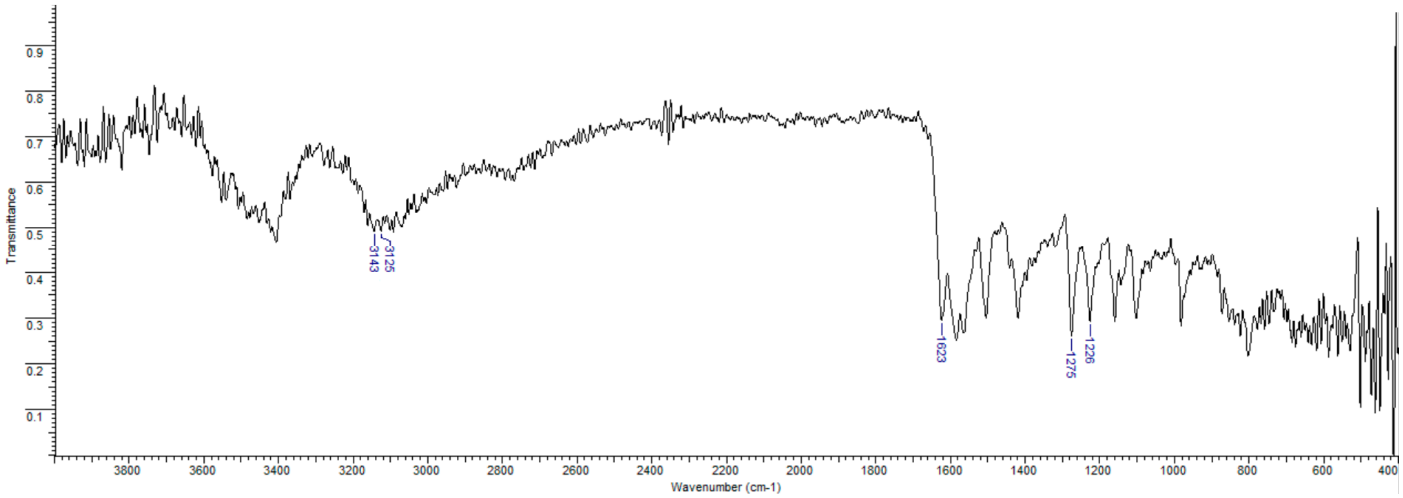


Figure S4. The IR spectrum of the compound **E4**

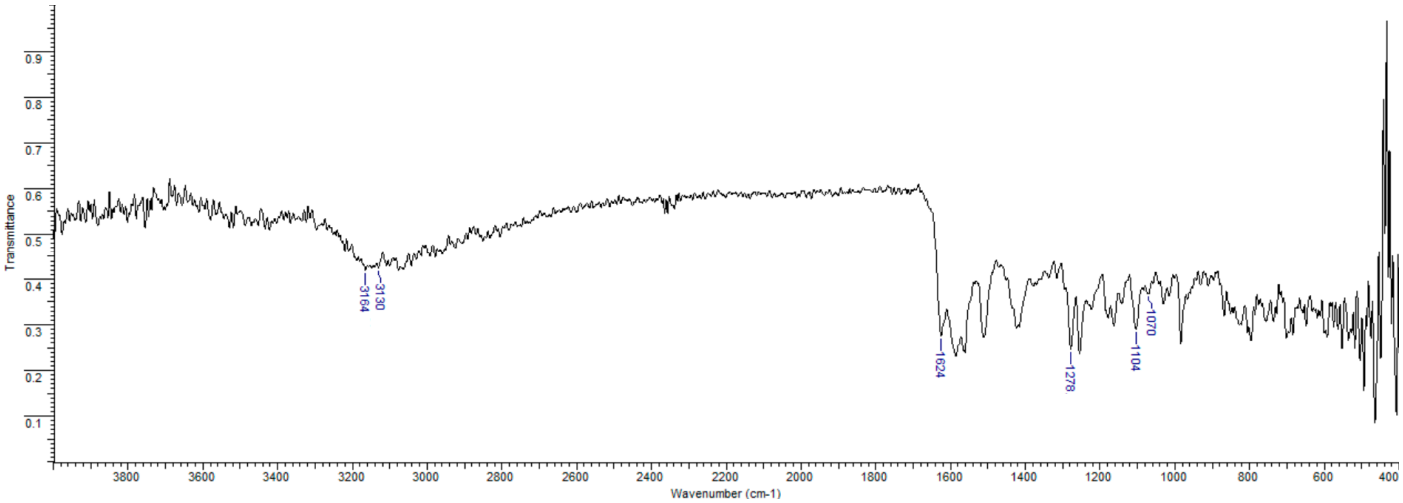


Figure S5. The IR spectrum of the compound **E5**

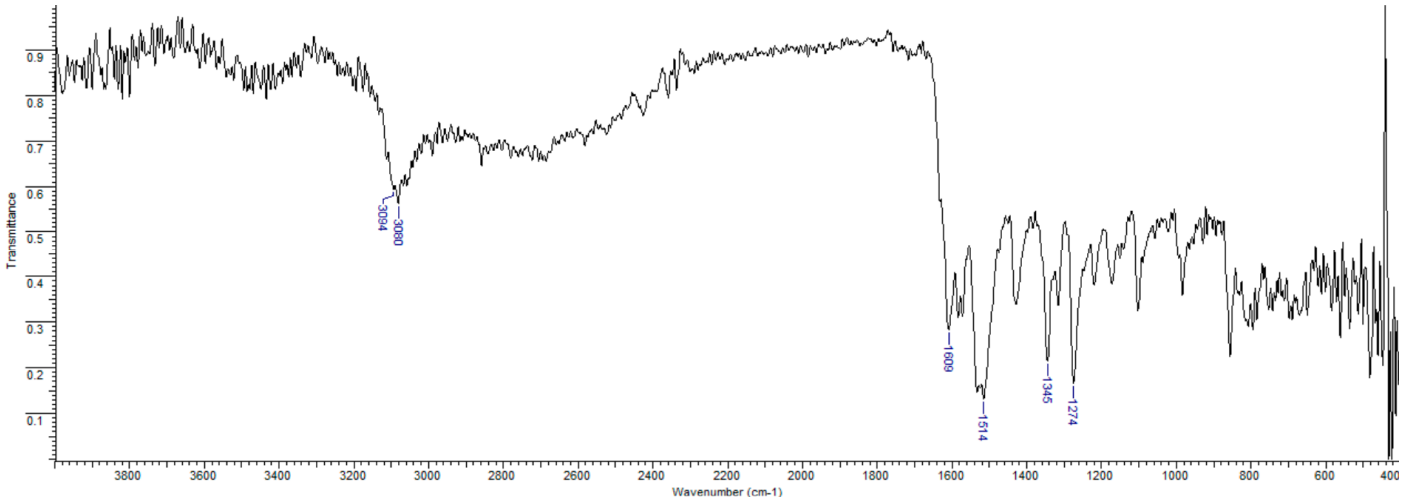


Figure S6. The IR spectrum of the compound **E6**

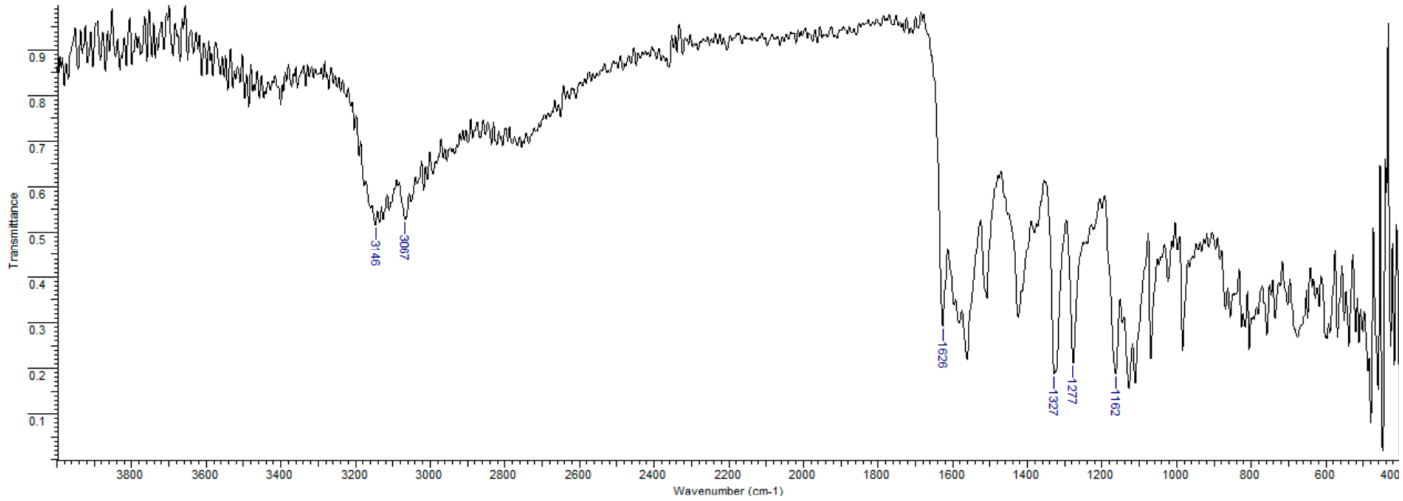


Figure S7. The IR spectrum of the compound **E7**

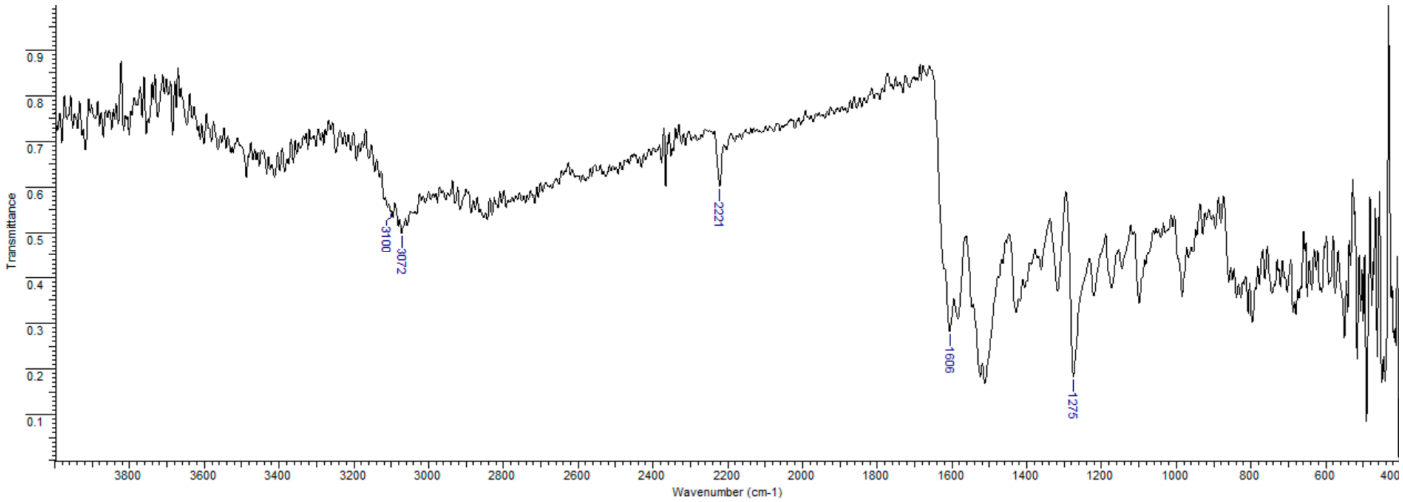


Figure S8. The IR spectrum of the compound **E8**

1.2 The ¹H-NMR spectra of the compounds E1-E8

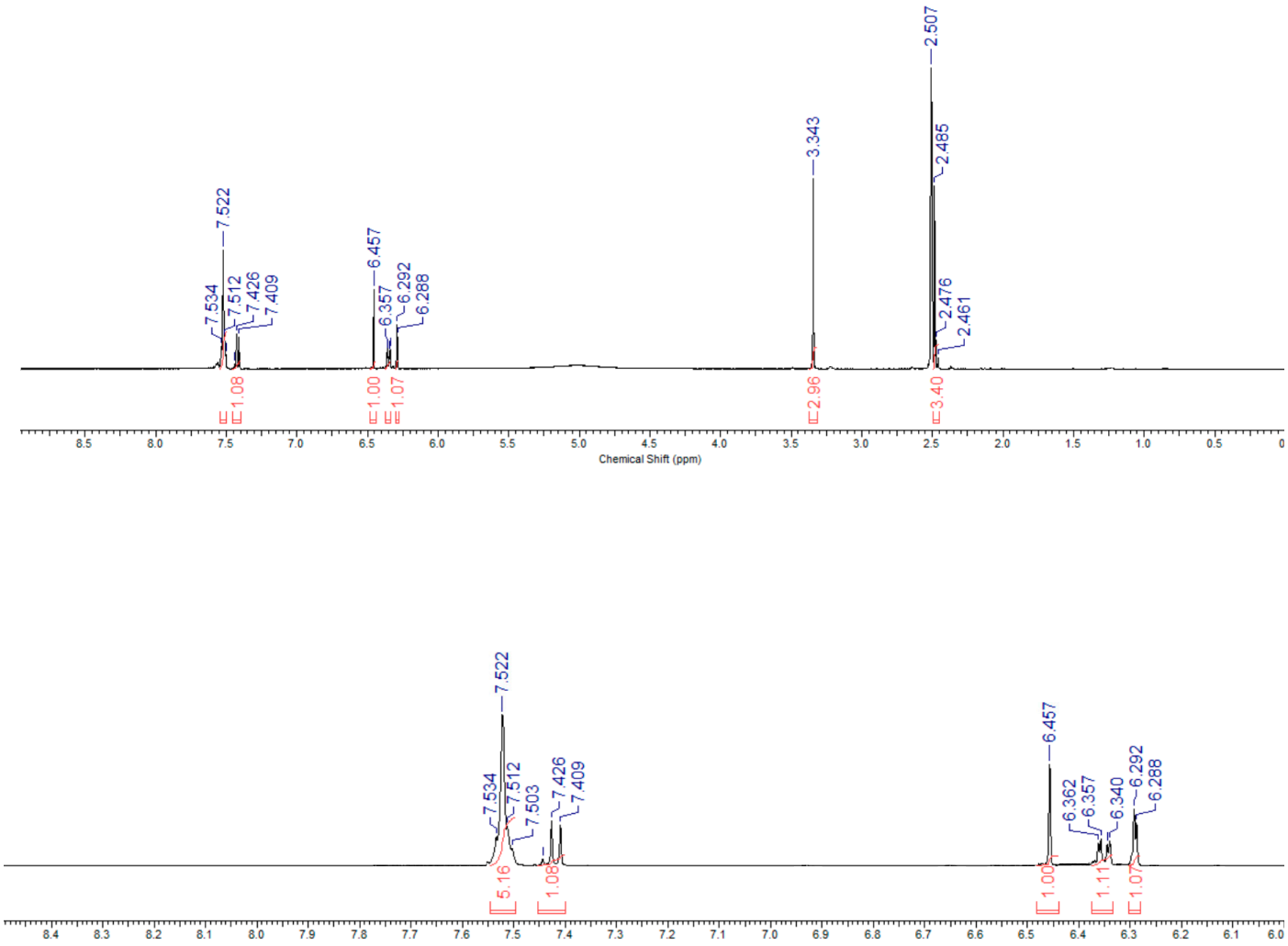
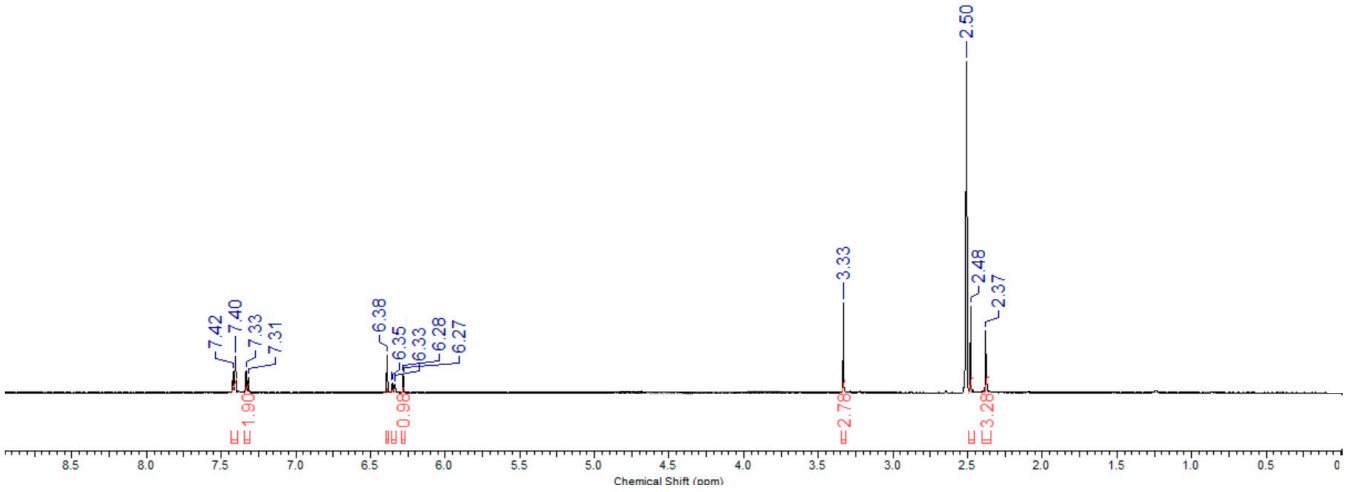


Figure S9. The ¹H-NMR spectrum of the compound **E1** (above) and zoom into aromatic area (below)



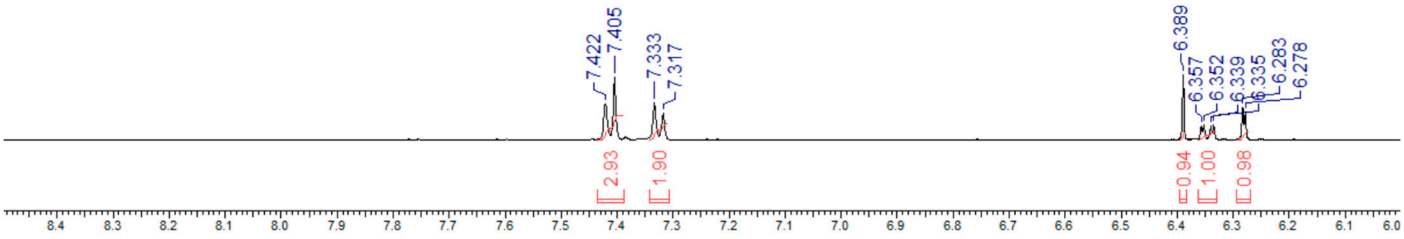


Figure S10. The ^{1}H-NMR spectrum of the compound **E2** (above) and zoom into aromatic area (below)

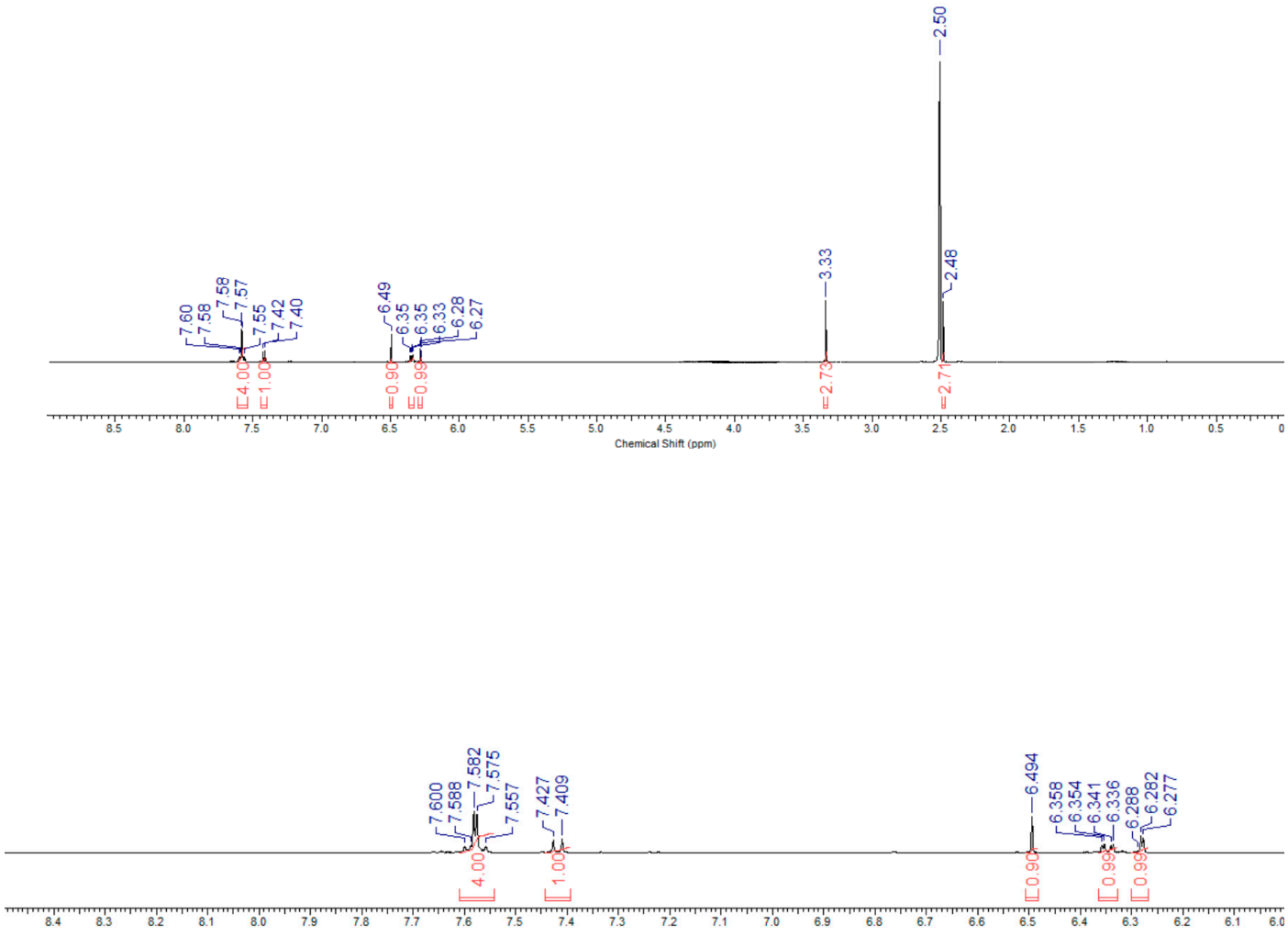


Figure S11. The ^{1}H-NMR spectrum of the compound **E3** (above) and zoom into aromatic area (below)

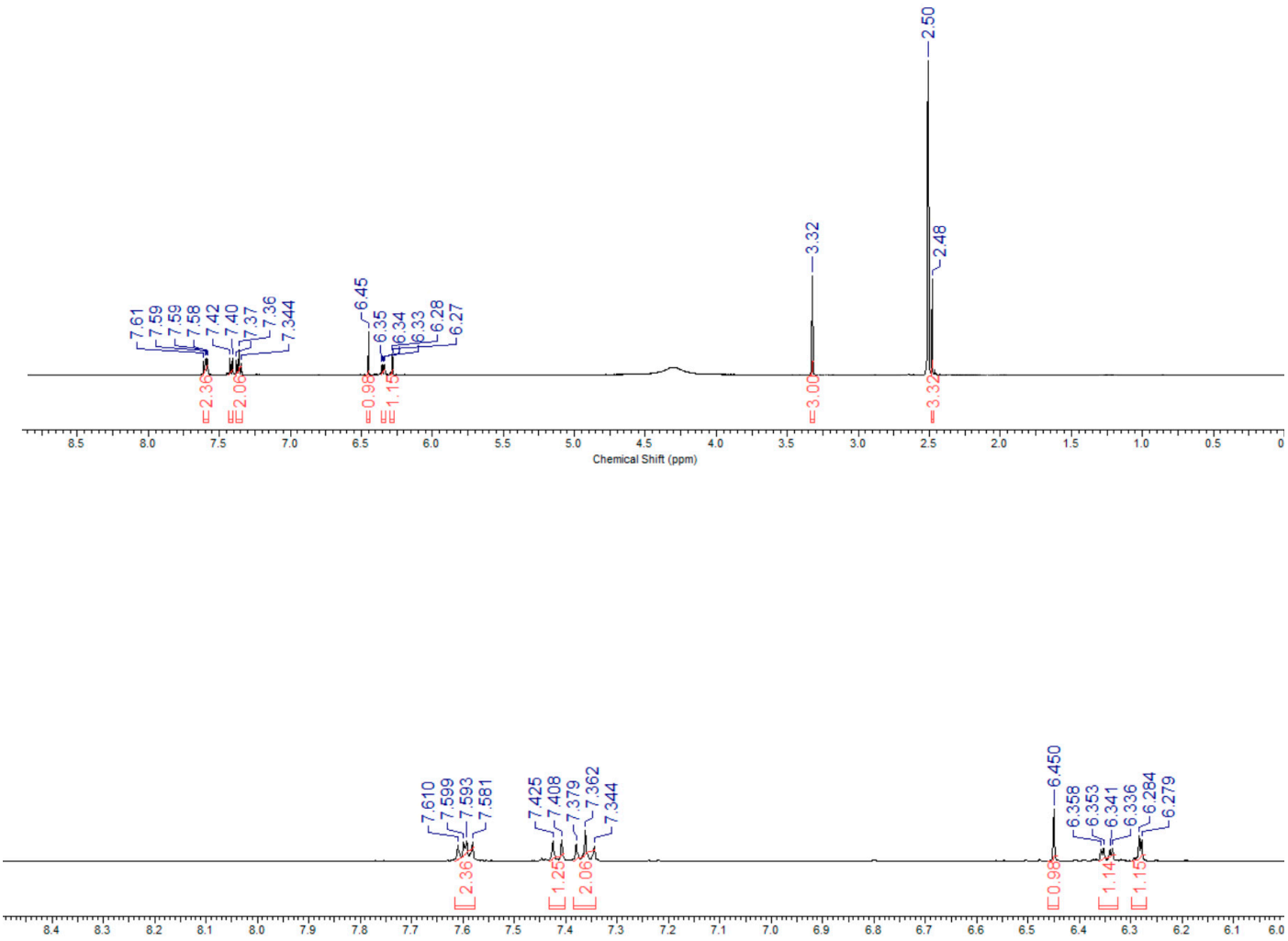
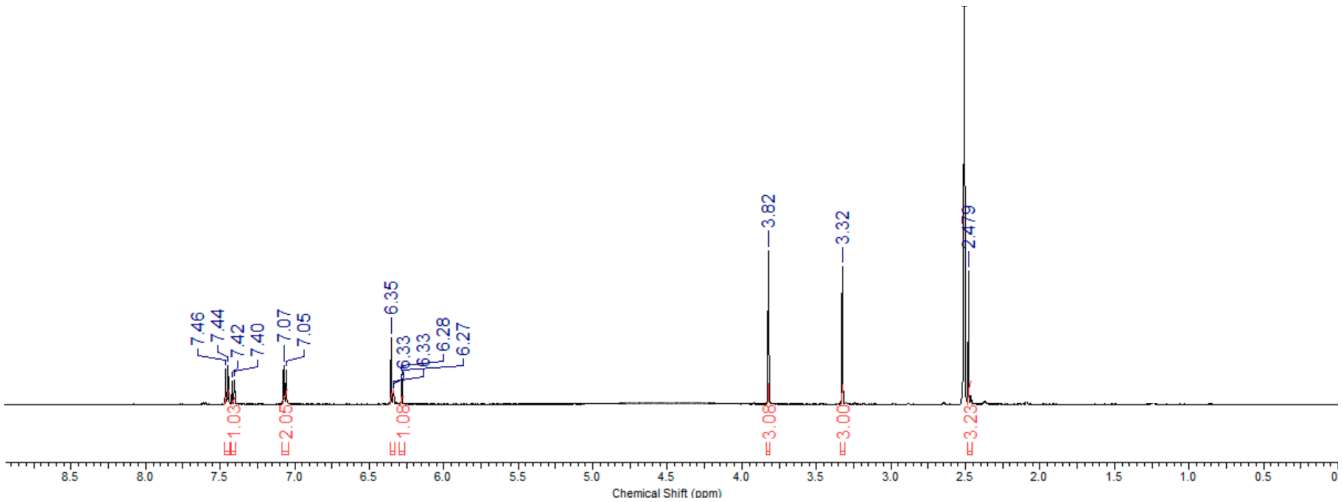


Figure S12. The ^{1}H-NMR spectrum of the compound **E4** (above) and zoom into aromatic area (below)



https://doi.org/10.3390/molecules31203620

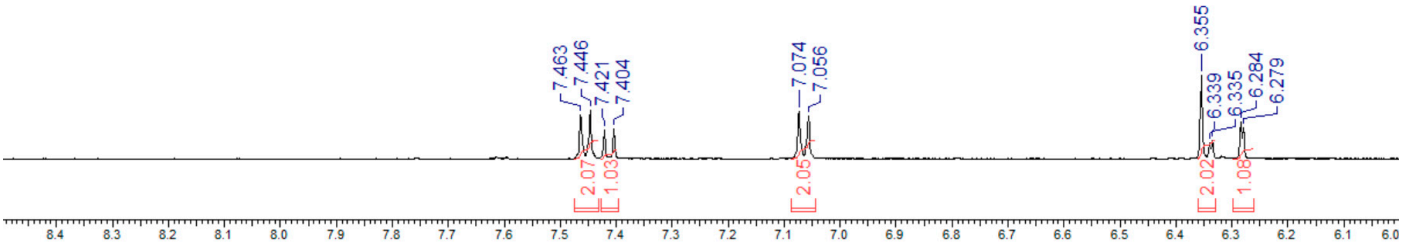


Figure S13. The ^{1}H-NMR spectrum of the compound **E5** (above) and zoom into aromatic area (below)

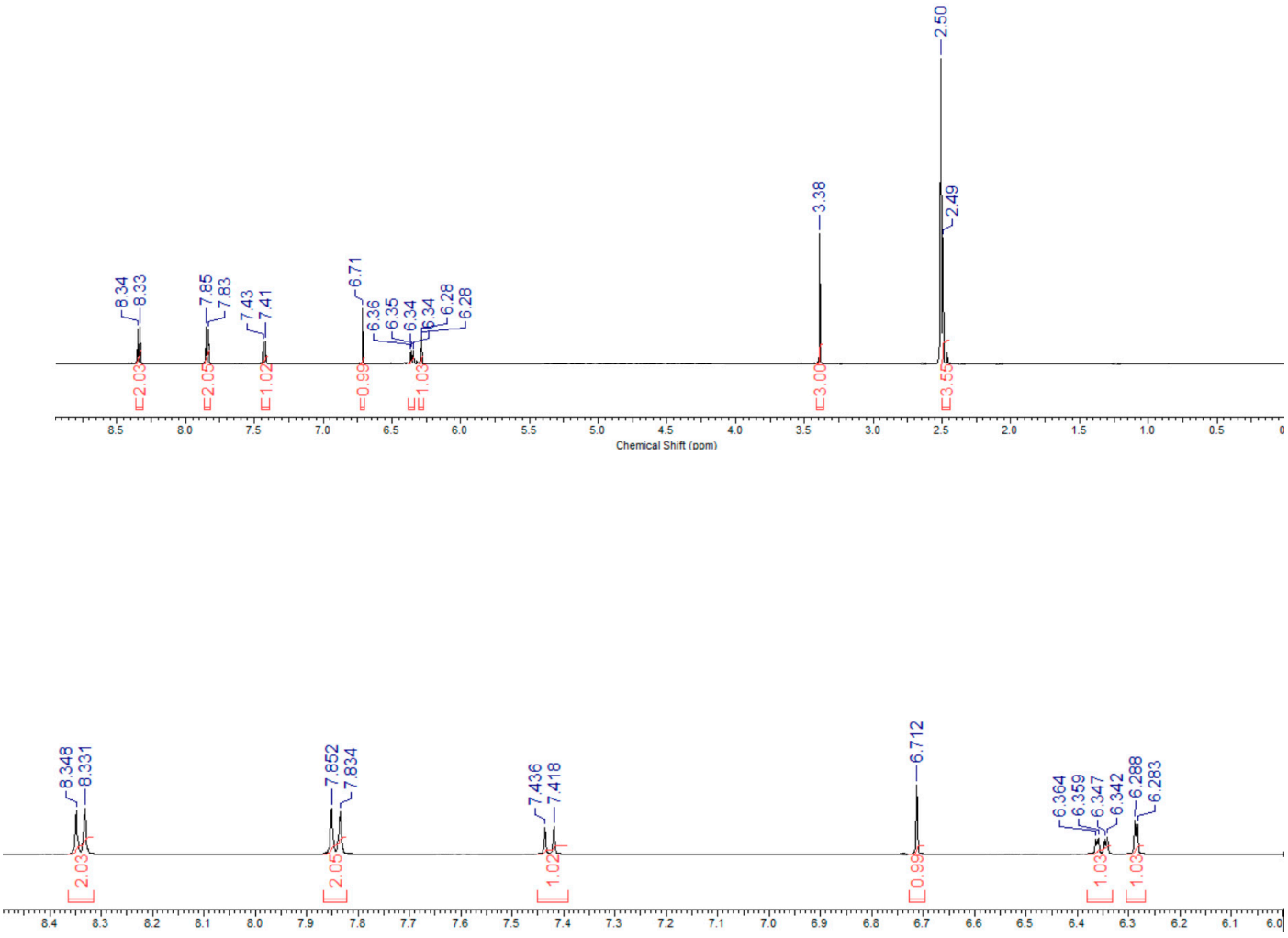


Figure S14. The ^{1}H-NMR spectrum of the compound **E6** (above) and zoom into aromatic area (below)

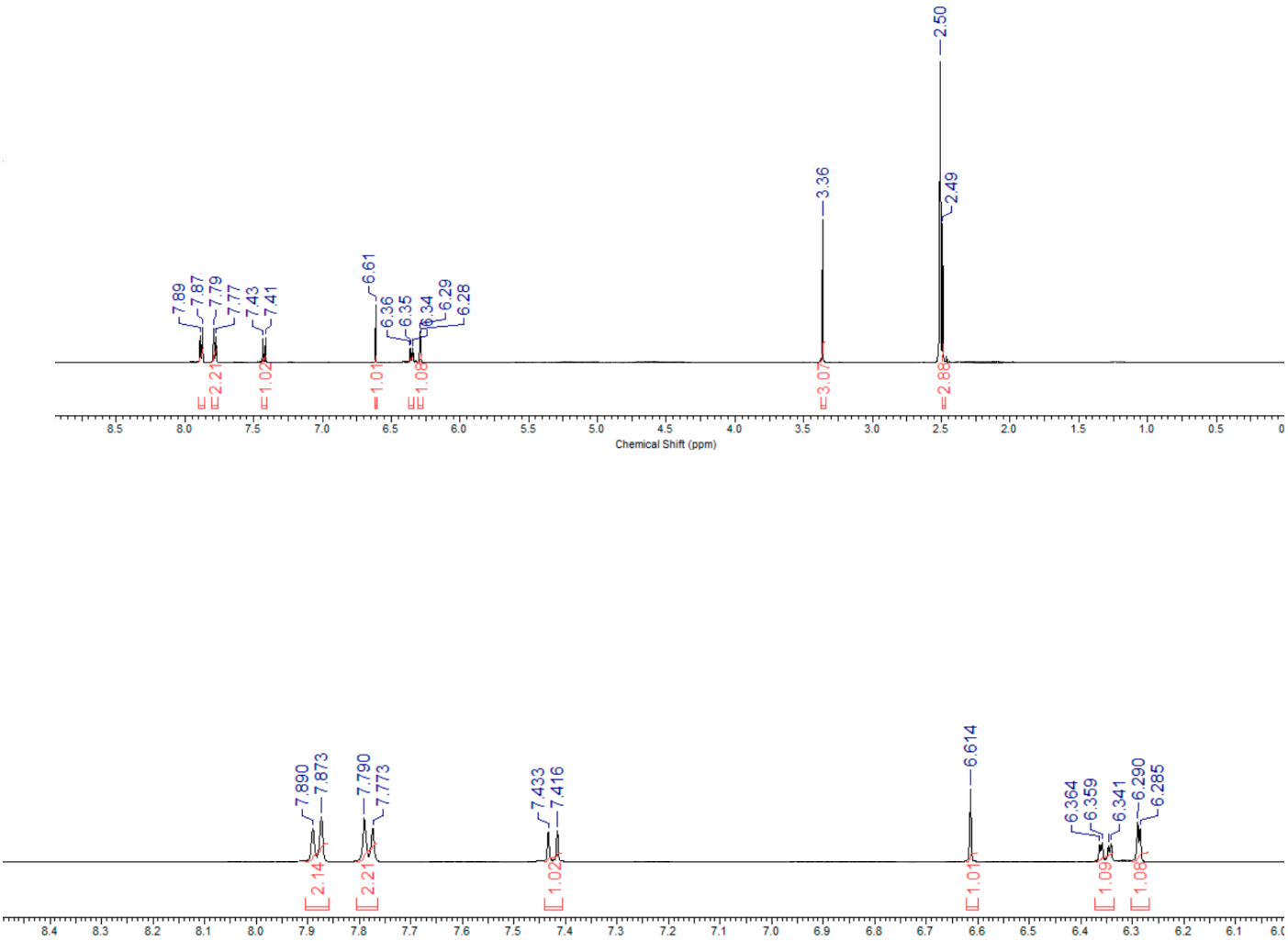
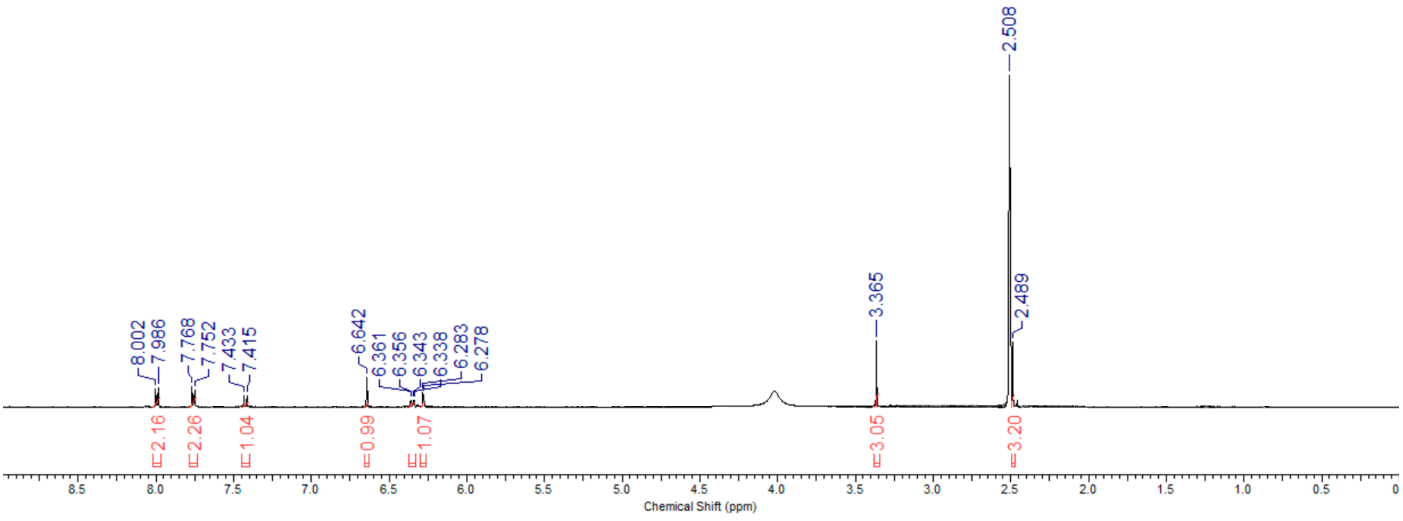


Figure S15. The ^{1}H-NMR spectrum of the compound **E7** (above) and zoom into aromatic area (below)



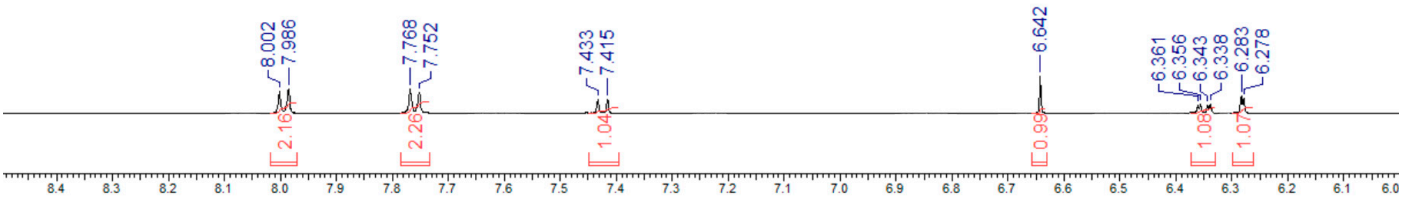


Figure S16. The ^{1}H-NMR spectrum if the compound **E8** (above) and zoom into aromatic area (below)

*1.3 The ^{13}C-NMR spectra of the compounds **E1-E8***

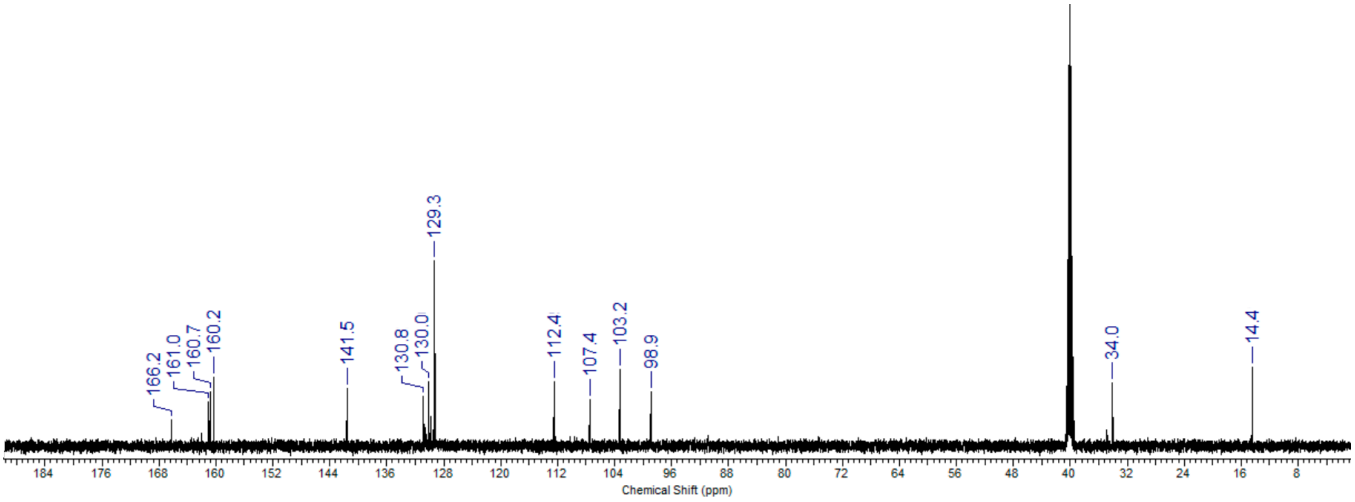


Figure S17. The ^{13}C-NMR spectrum of the compound **E1**

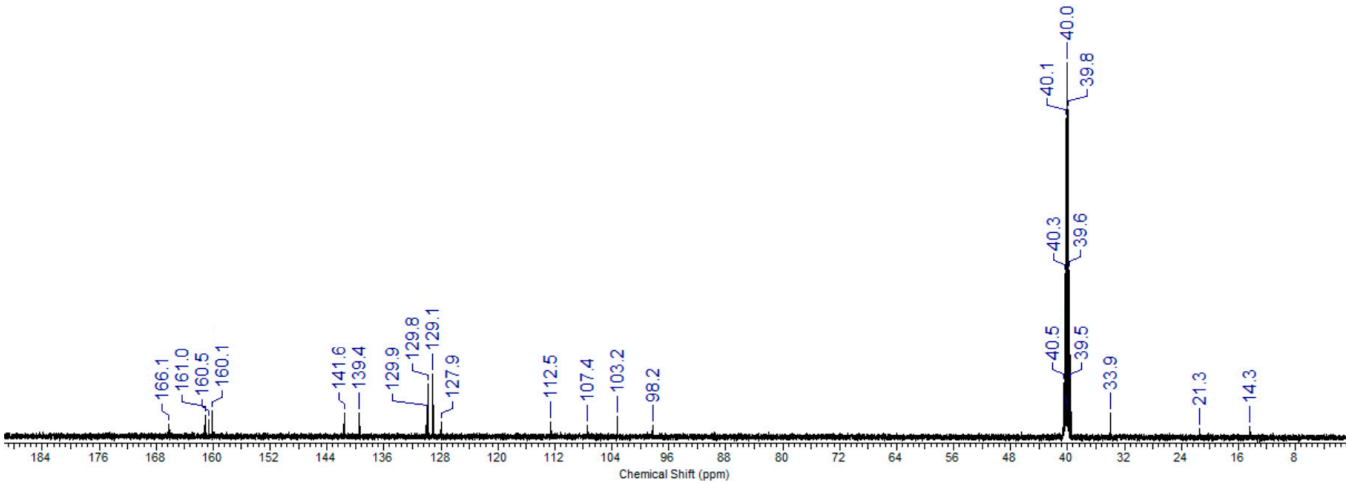


Figure S18. The ^{13}C-NMR spectrum of the compound **E2**

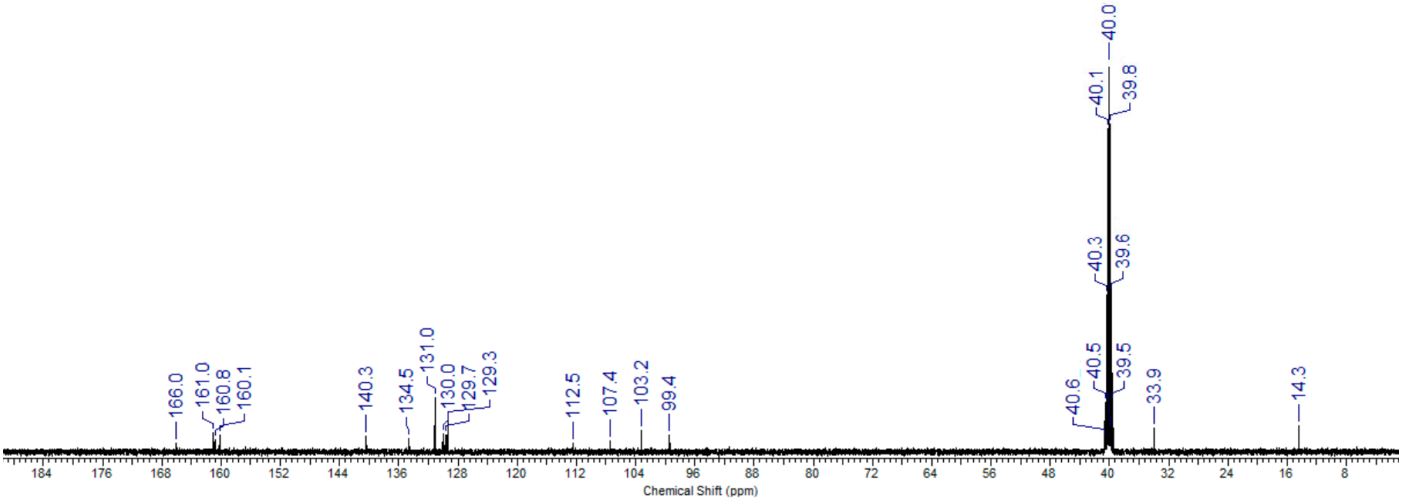


Figure S19. The ^{13}C-NMR spectrum of the compound **E3**

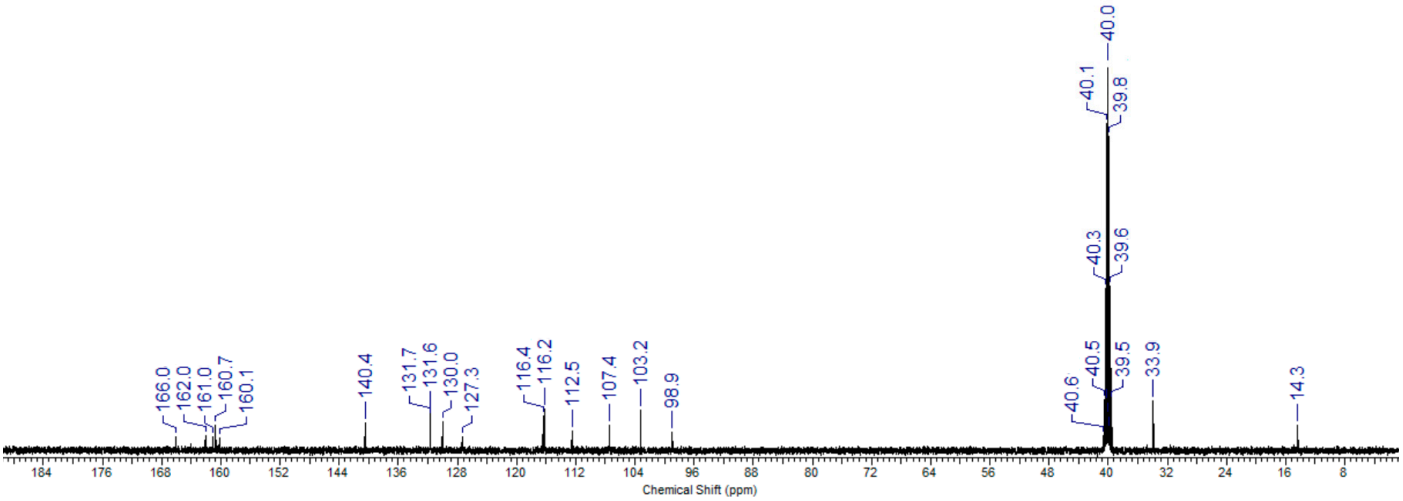


Figure S20. The ^{13}C-NMR spectrum of the compound **E4**

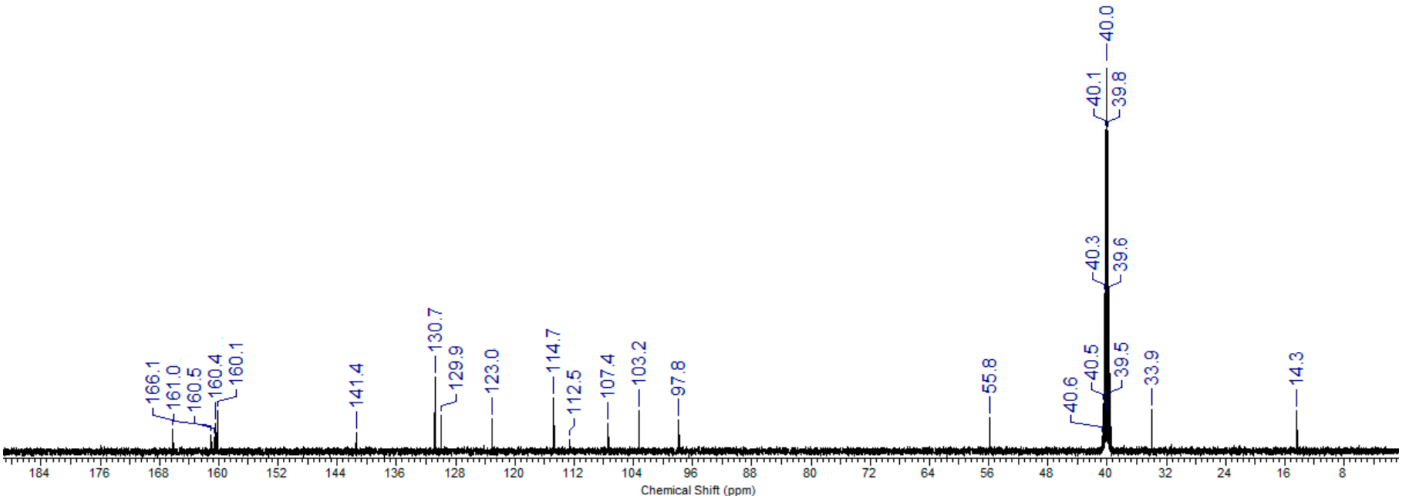


Figure S21. The ^{13}C-NMR spectrum of the compound **E5**

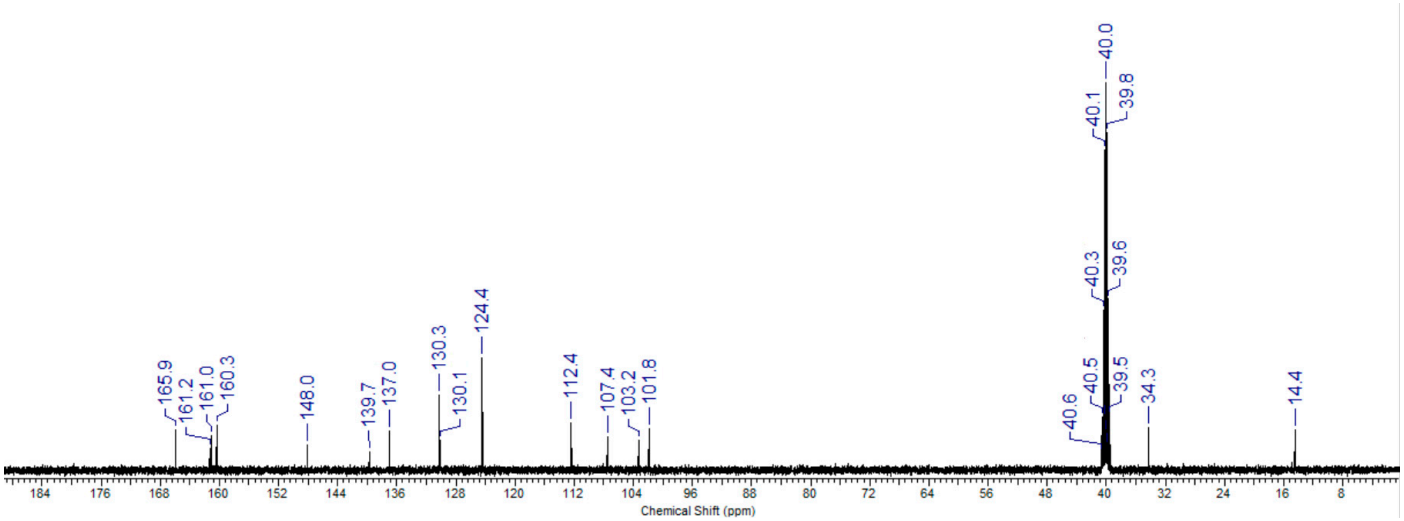


Figure S22. The ^{13}C-NMR spectrum of the compound **E6**

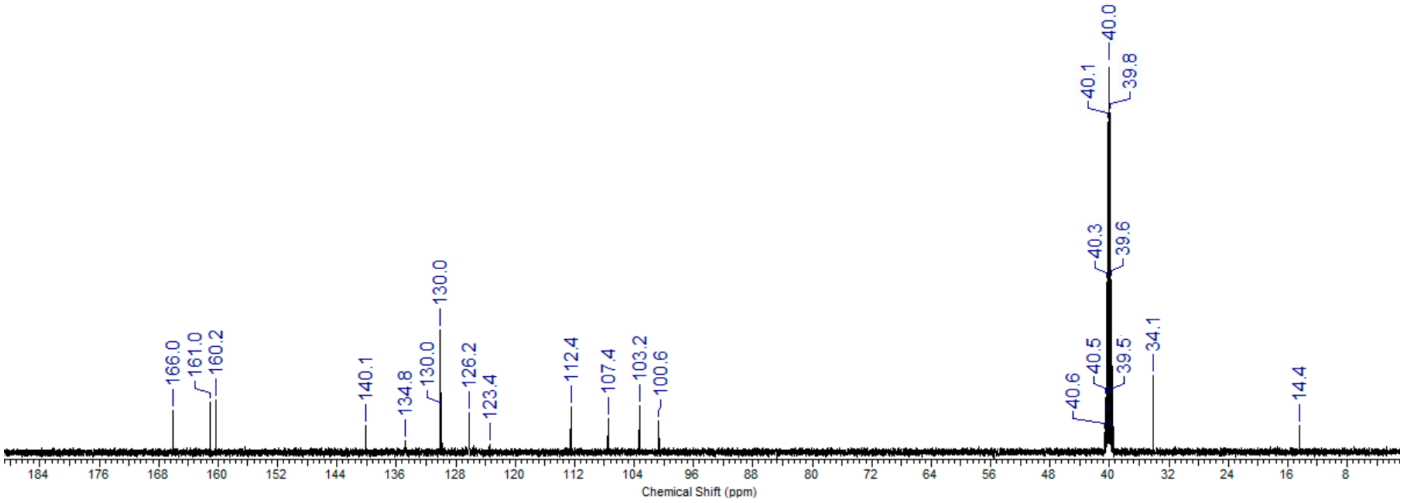


Figure S23. The ^{13}C-NMR spectrum of the compound **E7**

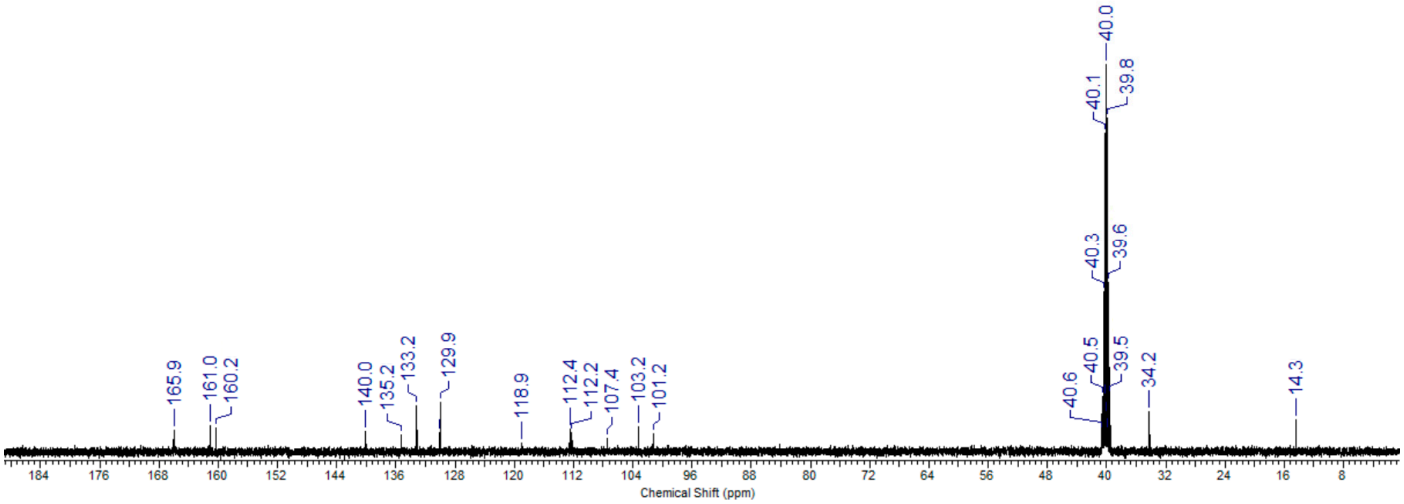


Figure S24. The ^{13}C-NMR spectrum of the compound **E8**

*1.4 The HRMS of the compounds **E1-E8***

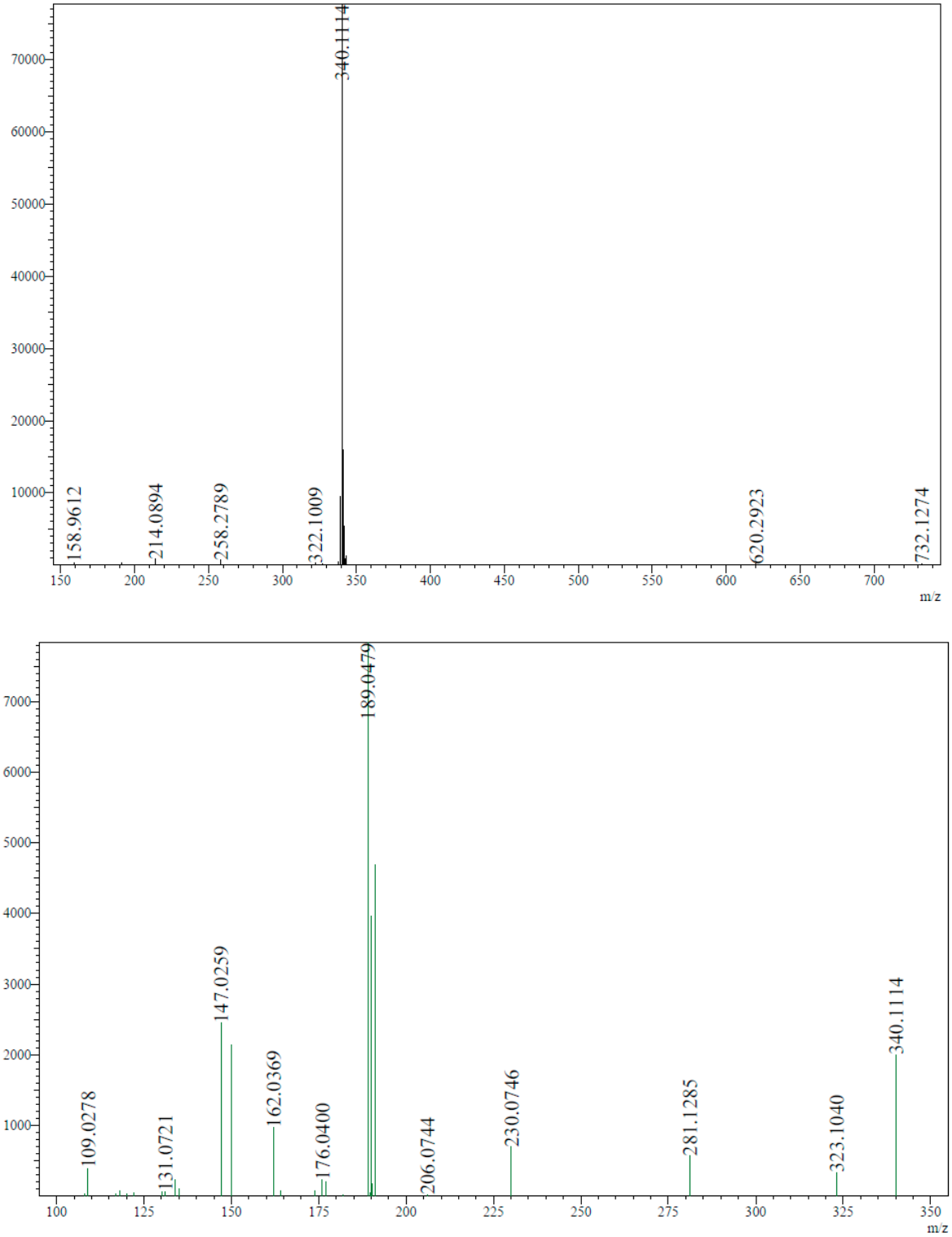


Figure S25. The HRMS spectrum of the compound **E1** (above) and MS/MS fragmentation spectrum of the corresponding molecular ion (below)

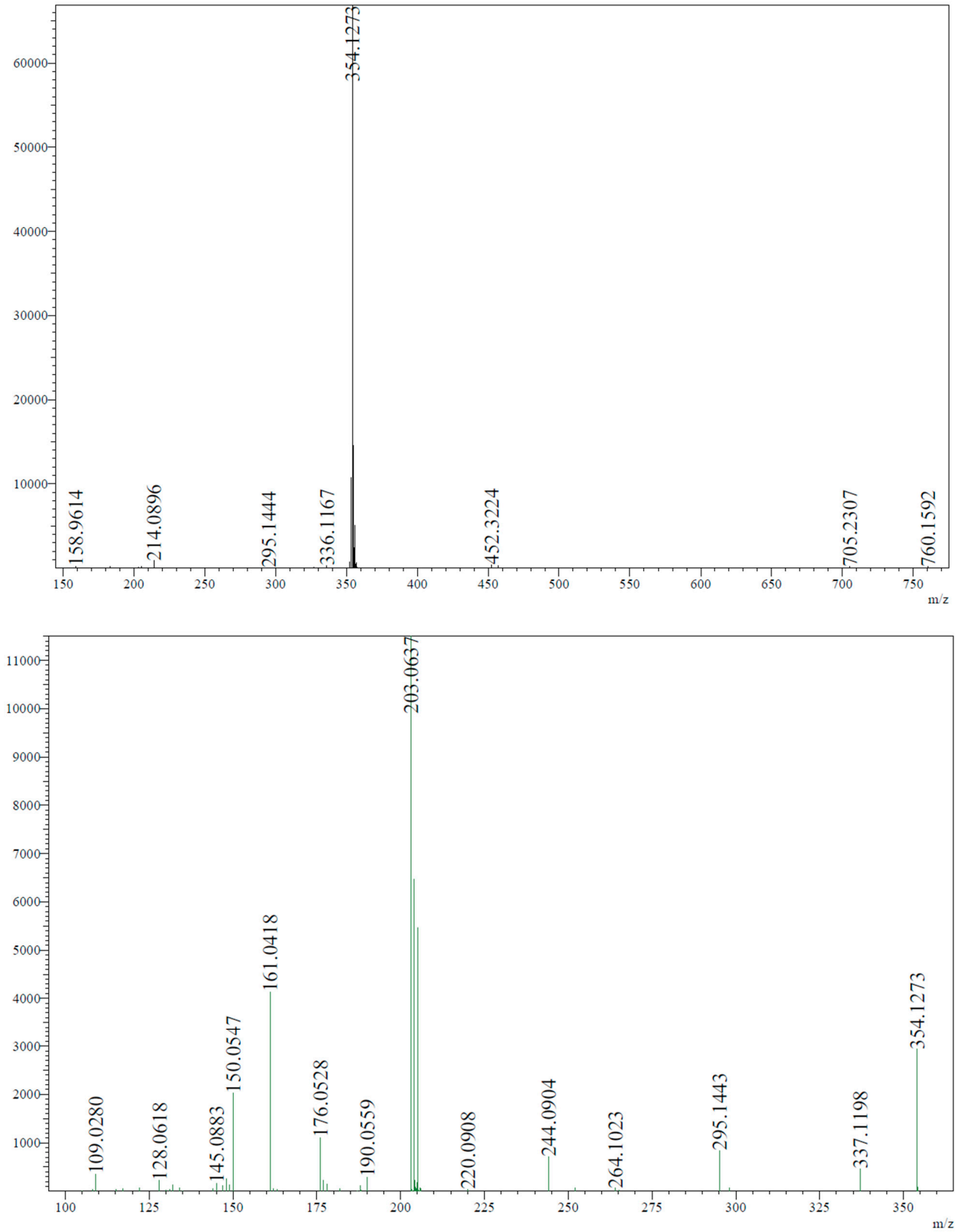


Figure S26. The HRMS spectrum of the compound **E2** (above) and MS/MS fragmentation spectrum of the corresponding molecular ion (below)

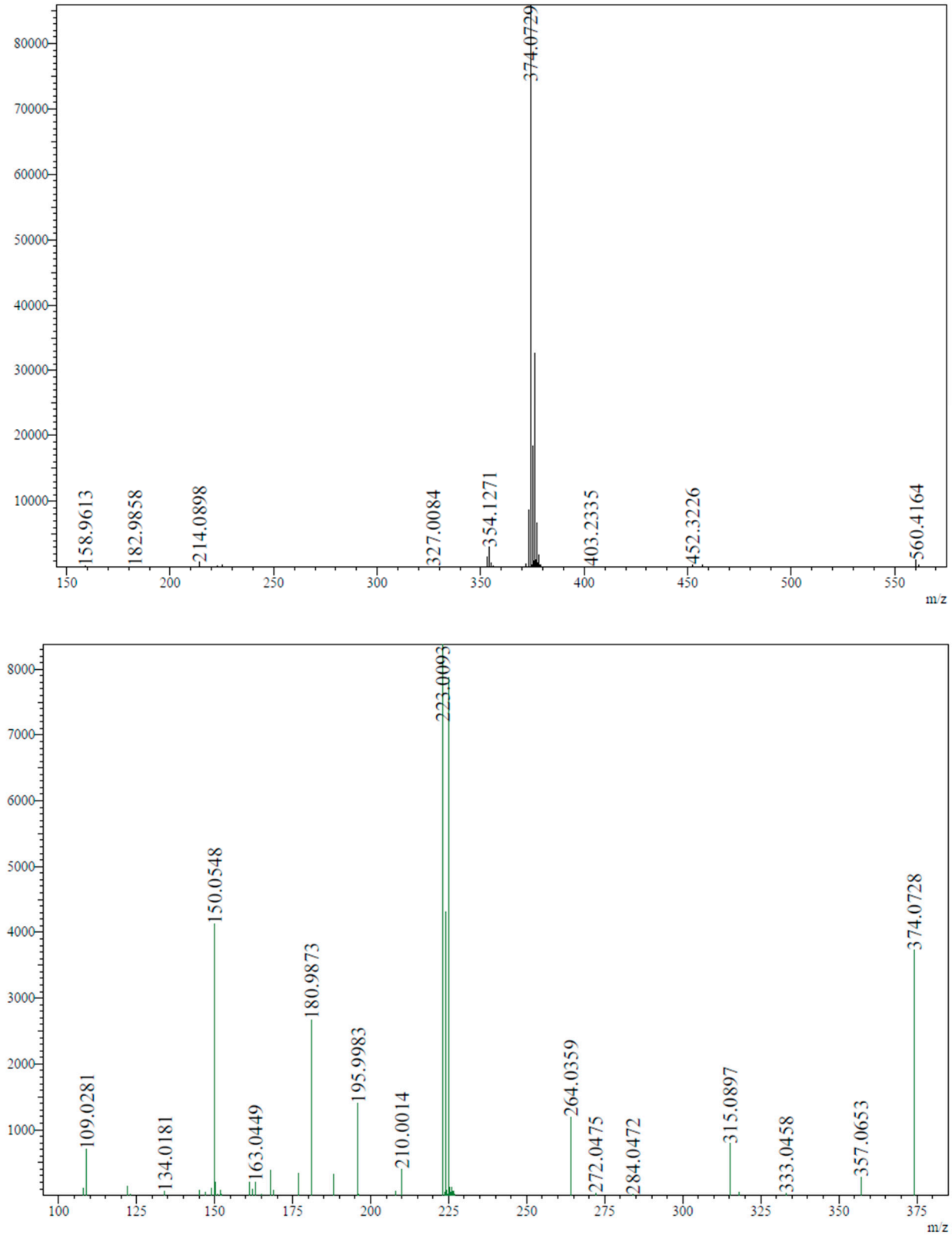


Figure S27. The HRMS spectrum of the compound **E3** (above) and MS/MS fragmentation spectrum of the corresponding molecular ion (below)

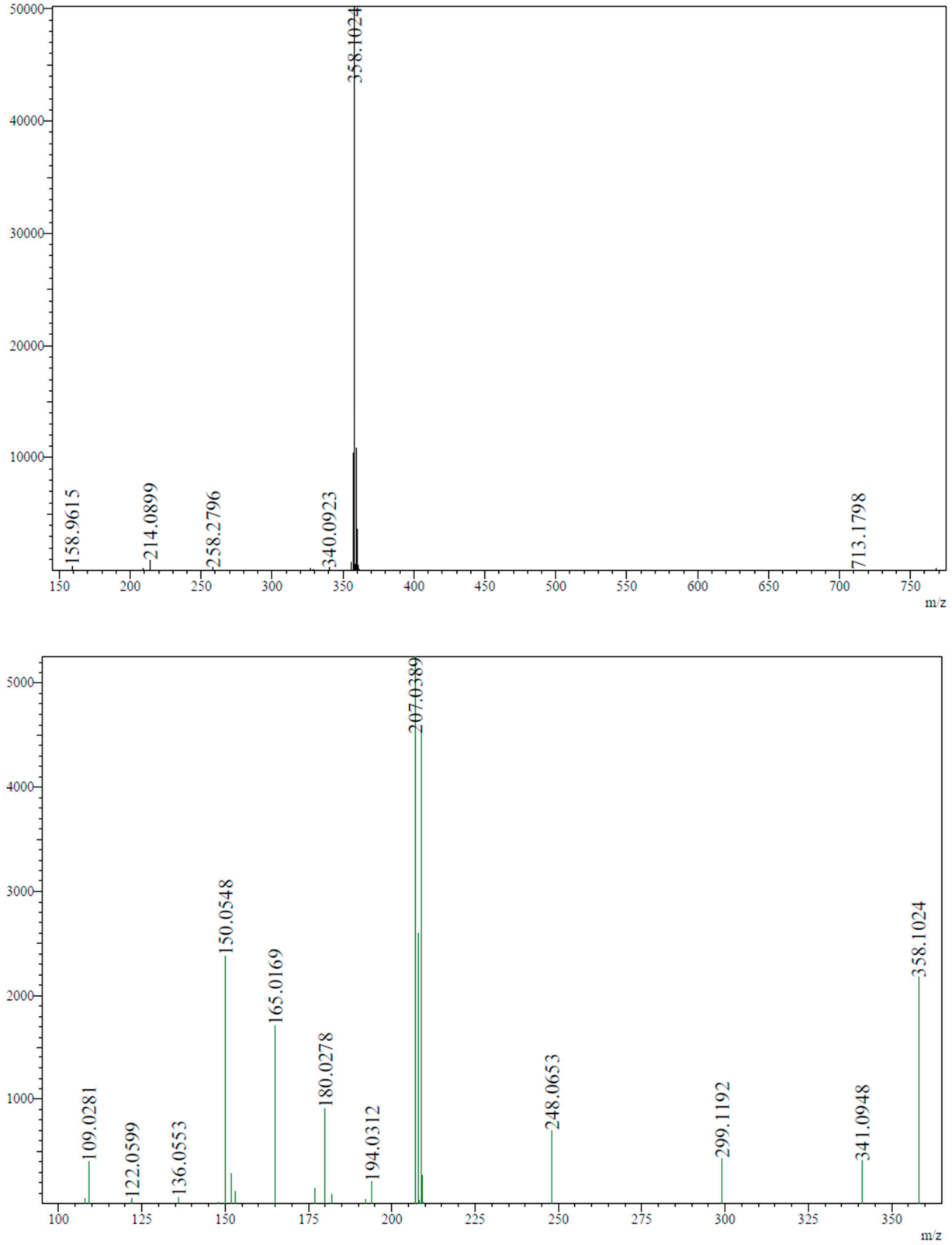


Figure S28. The HRMS spectrum of the compound **E4** (above) and MS/MS fragmentation spectrum of the corresponding molecular ion (below)

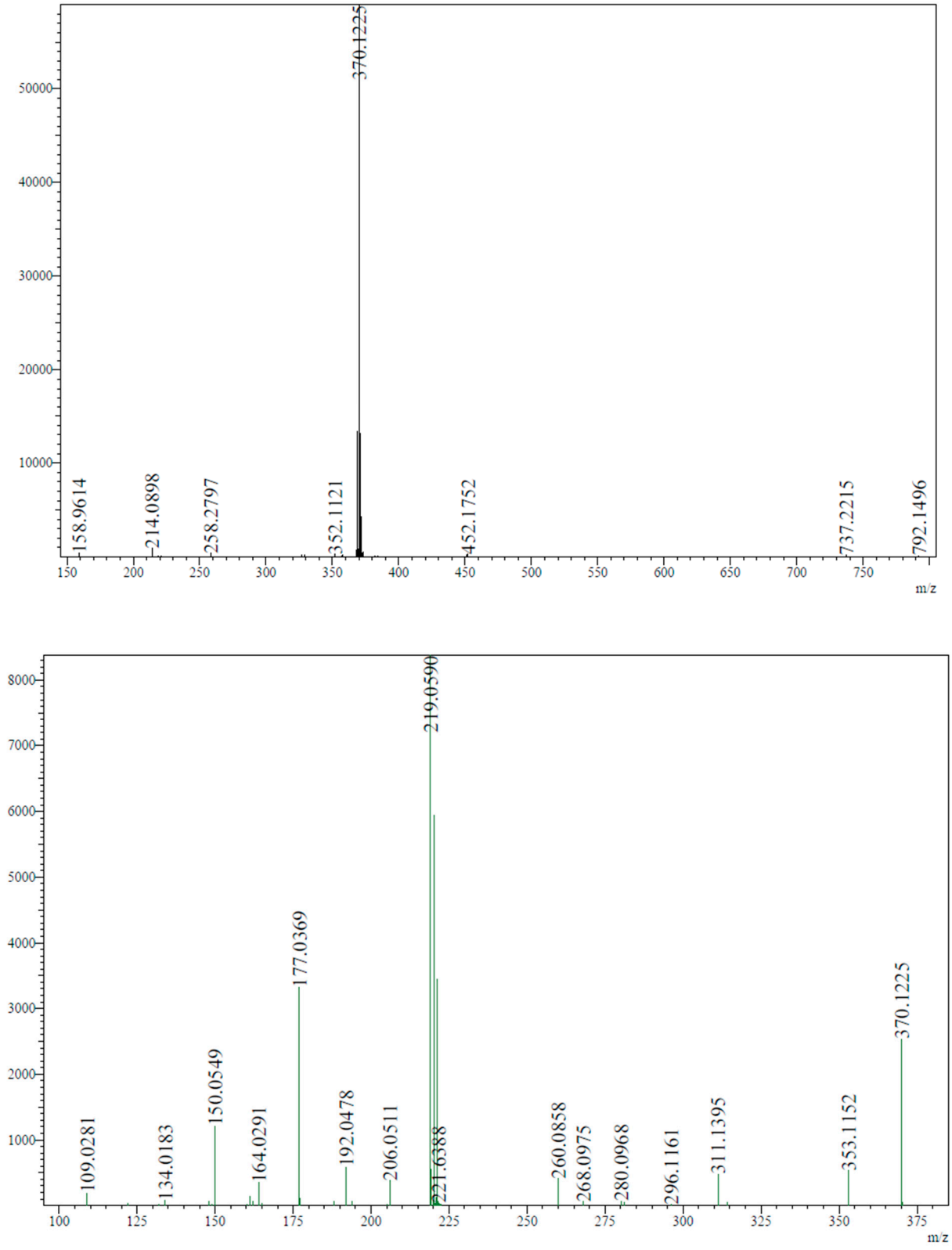


Figure S29. The HRMS spectrum of the compound **E5** (above) and MS/MS fragmentation spectrum of the corresponding molecular ion (below)

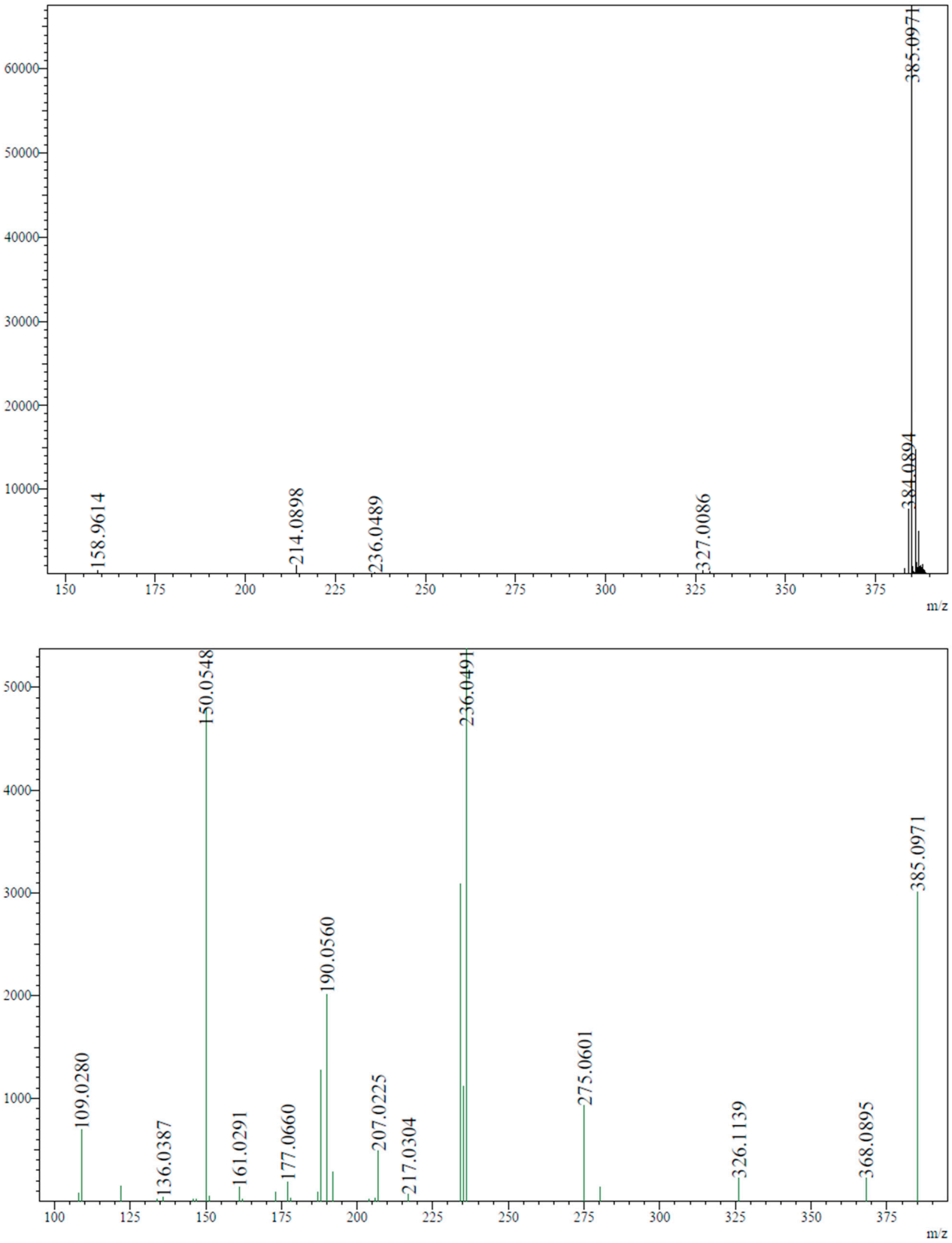


Figure S30. The HRMS spectrum of the compound **E6** (above) and MS/MS fragmentation spectrum of the corresponding molecular ion (below)

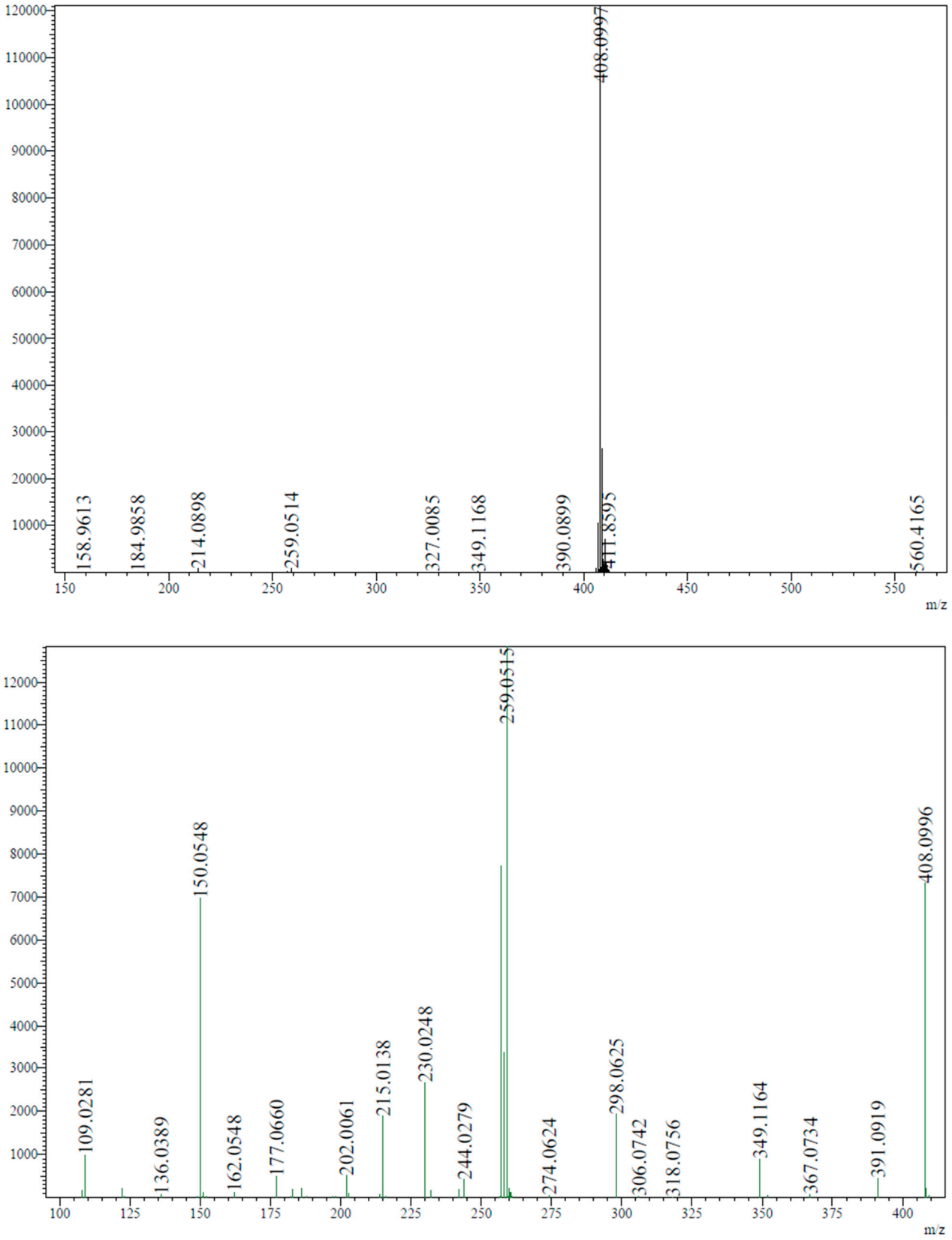


Figure S31. The HRMS spectrum of the compound **E7** (above) and MS/MS fragmentation spectrum of the corresponding molecular ion (below)

https://doi.org/10.3390/molecules31203620

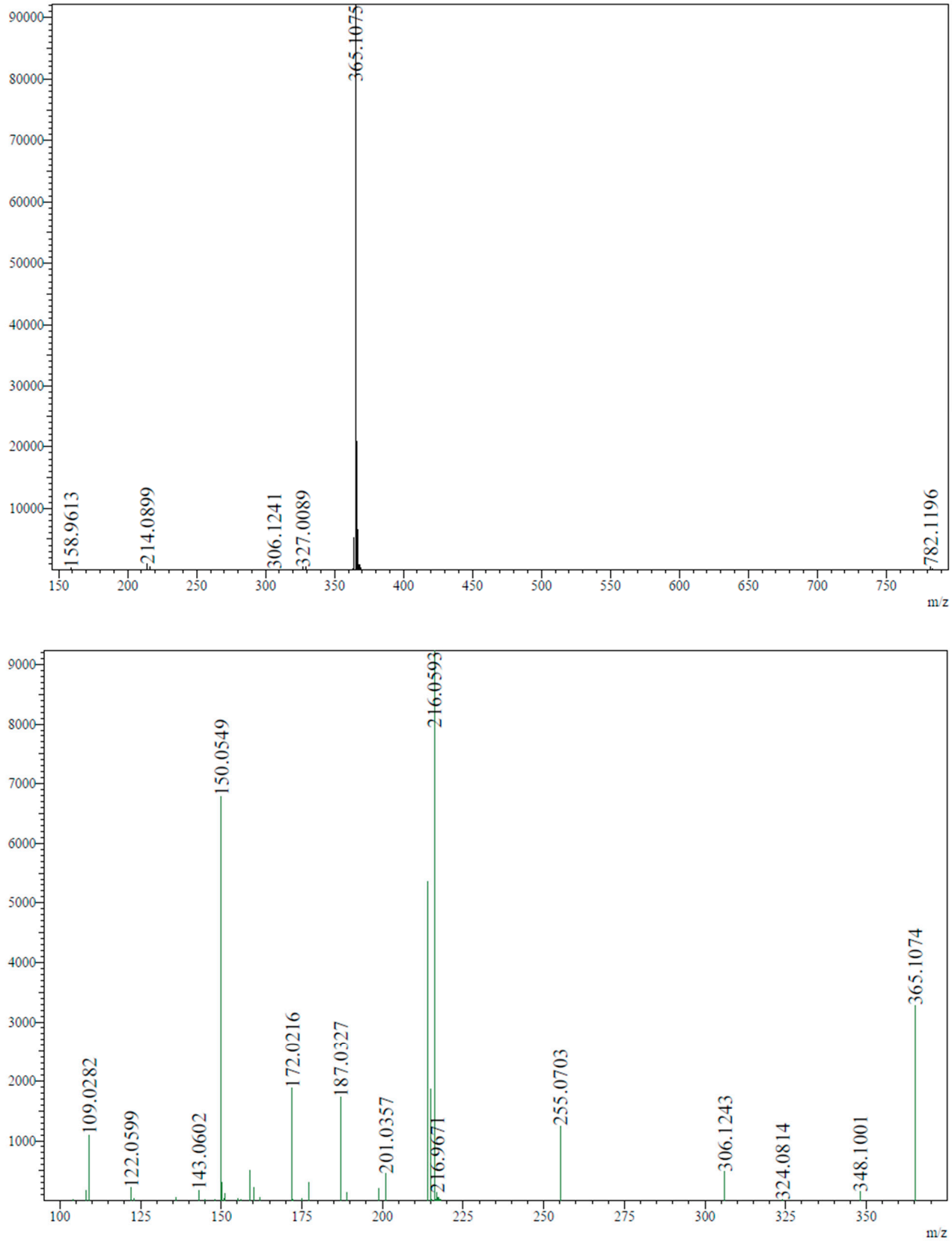


Figure S32. The HRMS spectrum of the compound **E8** (above) and MS/MS fragmentation spectrum of the corresponding molecular ion (below)

*1.5 The RP-HPLC chromatograms at 254 nm of the compounds **E1-E8***

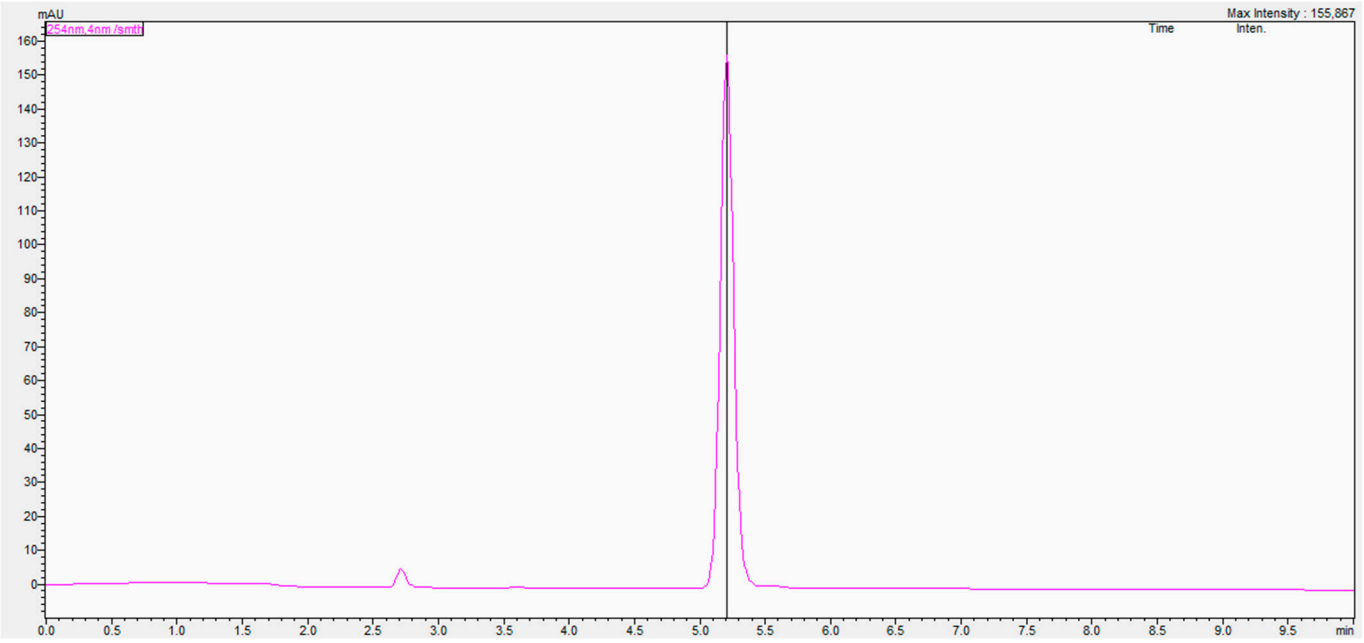


Figure S33. The RP-HPLC chromatogram of the compound **E1** recorded at 254 nm

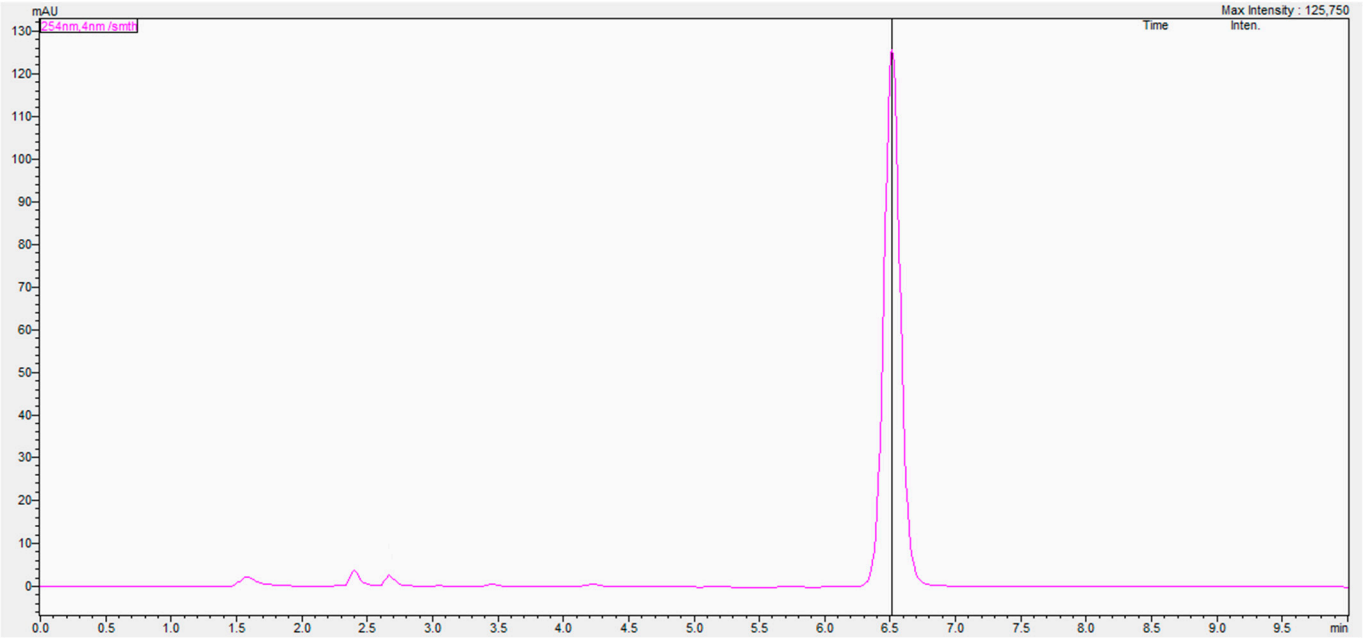


Figure S34. The RP-HPLC chromatogram of the compound **E2** recorded at 254 nm

https://doi.org/10.3390/molecules31203620

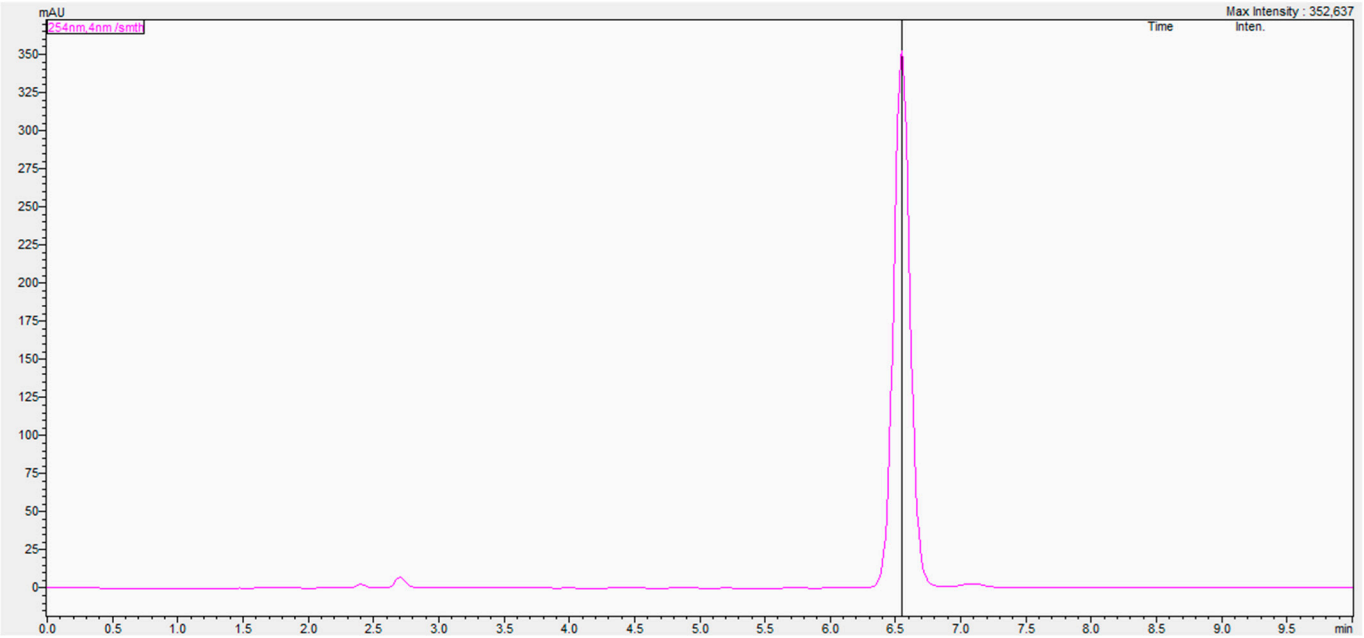


Figure S35. The RP-HPLC chromatogram of the compound **E3** recorded at 254 nm

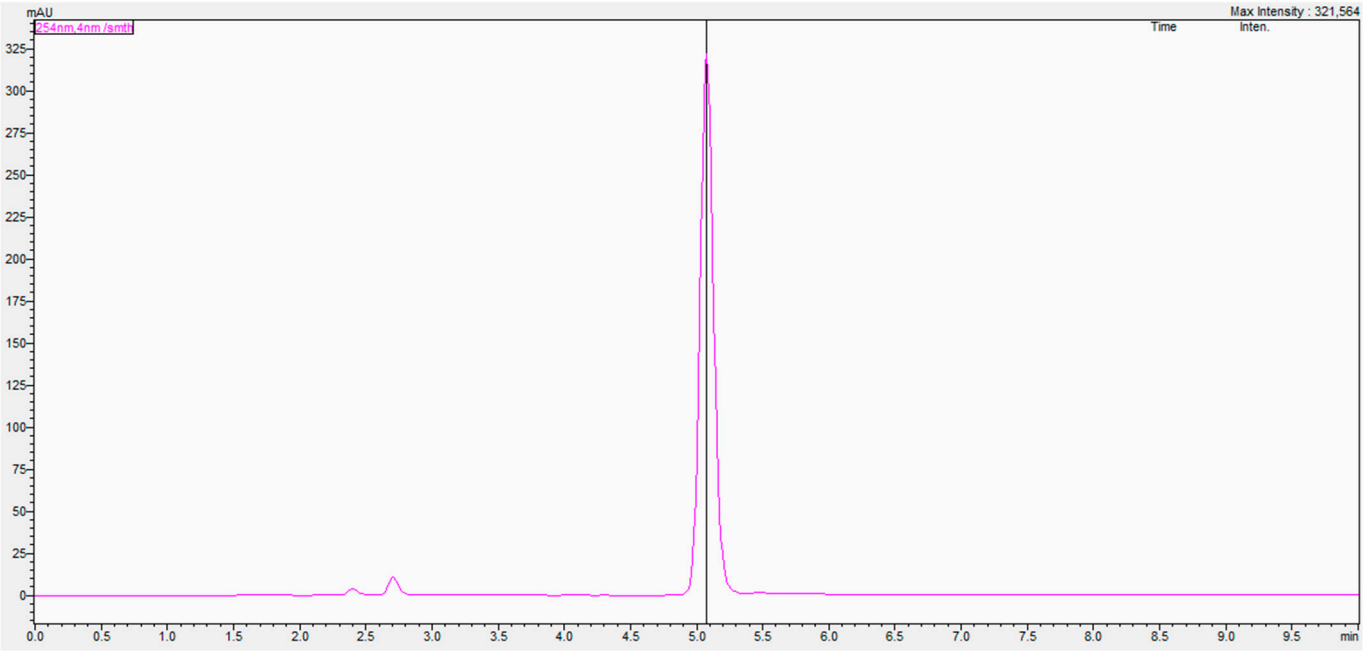


Figure S36. The RP-HPLC chromatogram of the compound **E4** recorded at 254 nm

https://doi.org/10.3390/molecules31203620

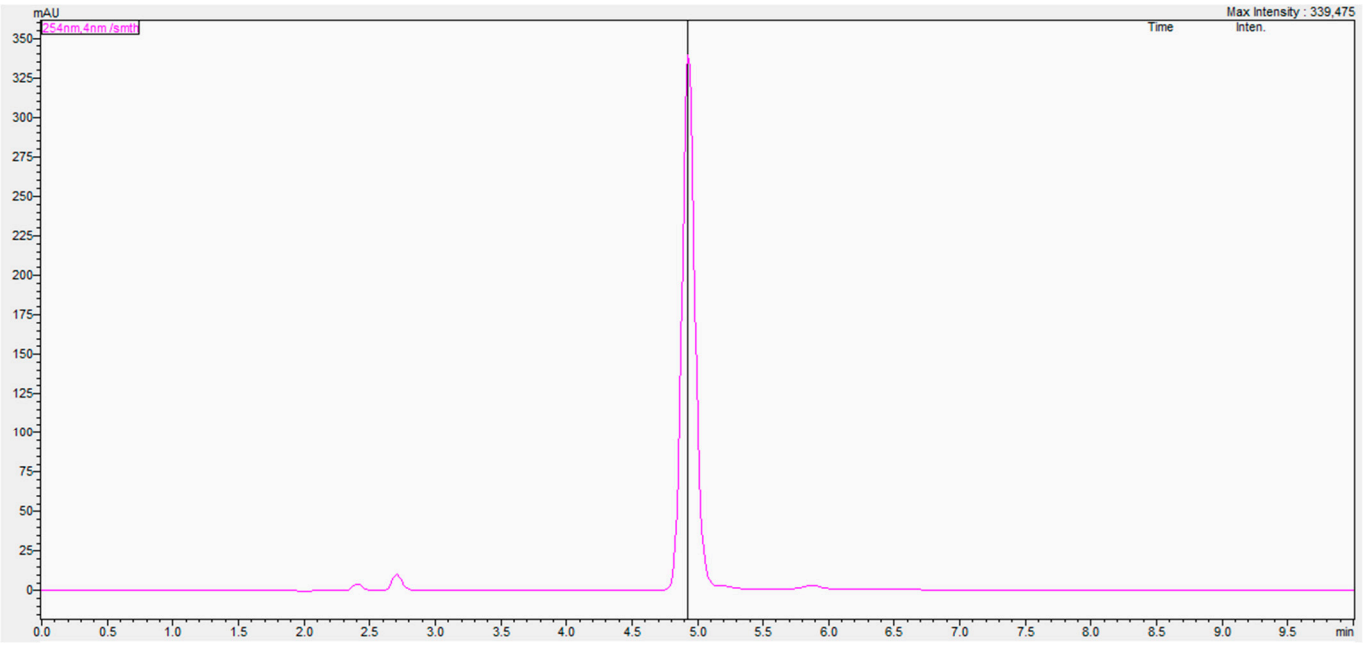


Figure S37. The RP-HPLC chromatogram of the compound **E5** recorded at 254 nm

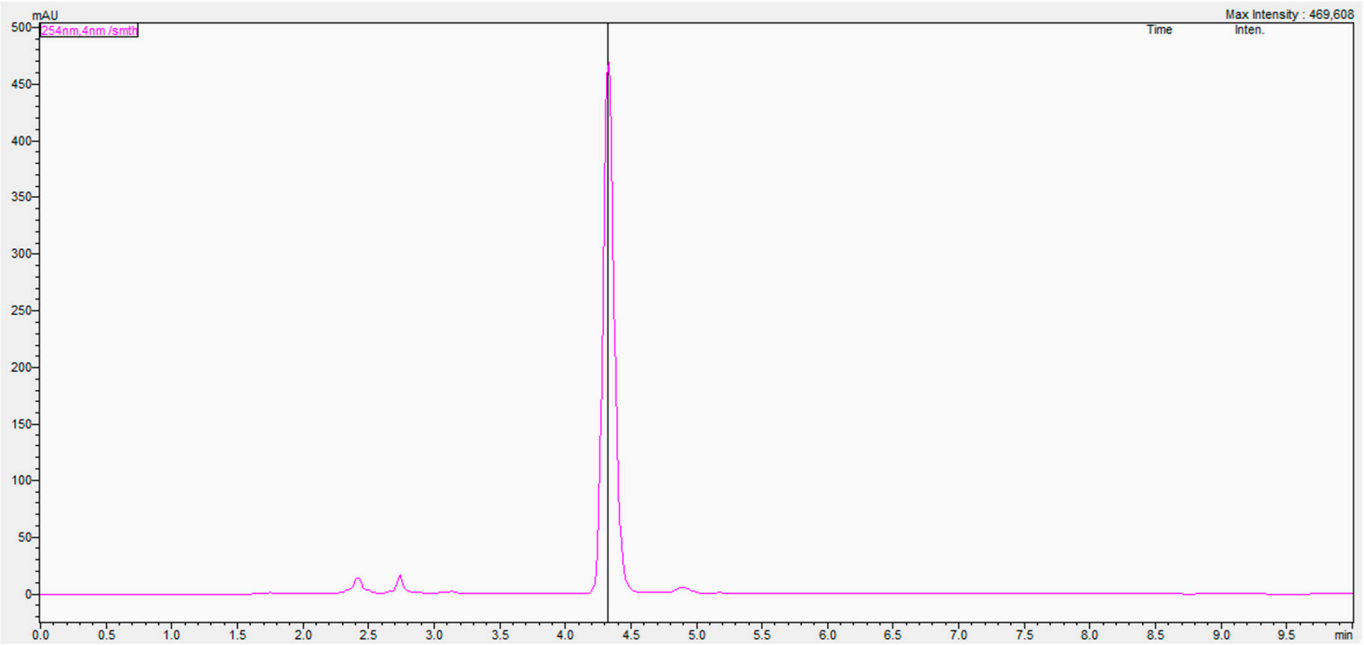


Figure S38. The RP-HPLC chromatogram of the compound **E6** recorded at 254 nm

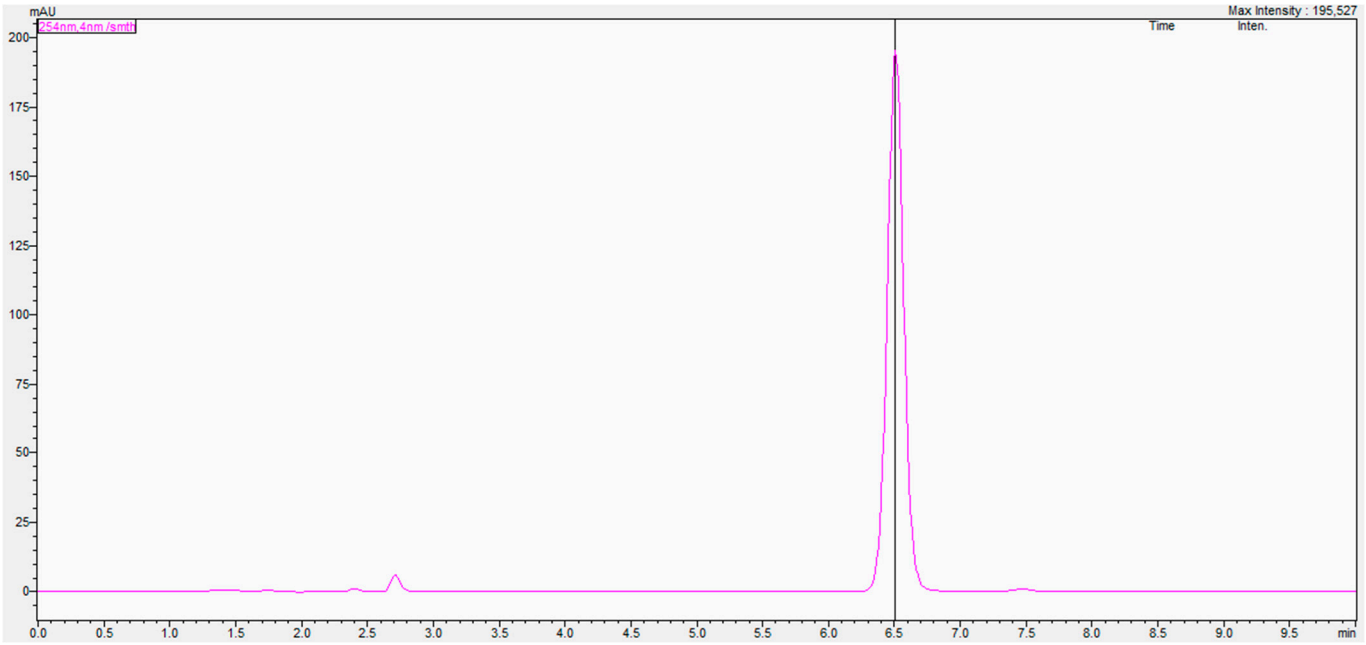


Figure S39. The RP-HPLC chromatogram of the compound **E7** recorded at 254 nm

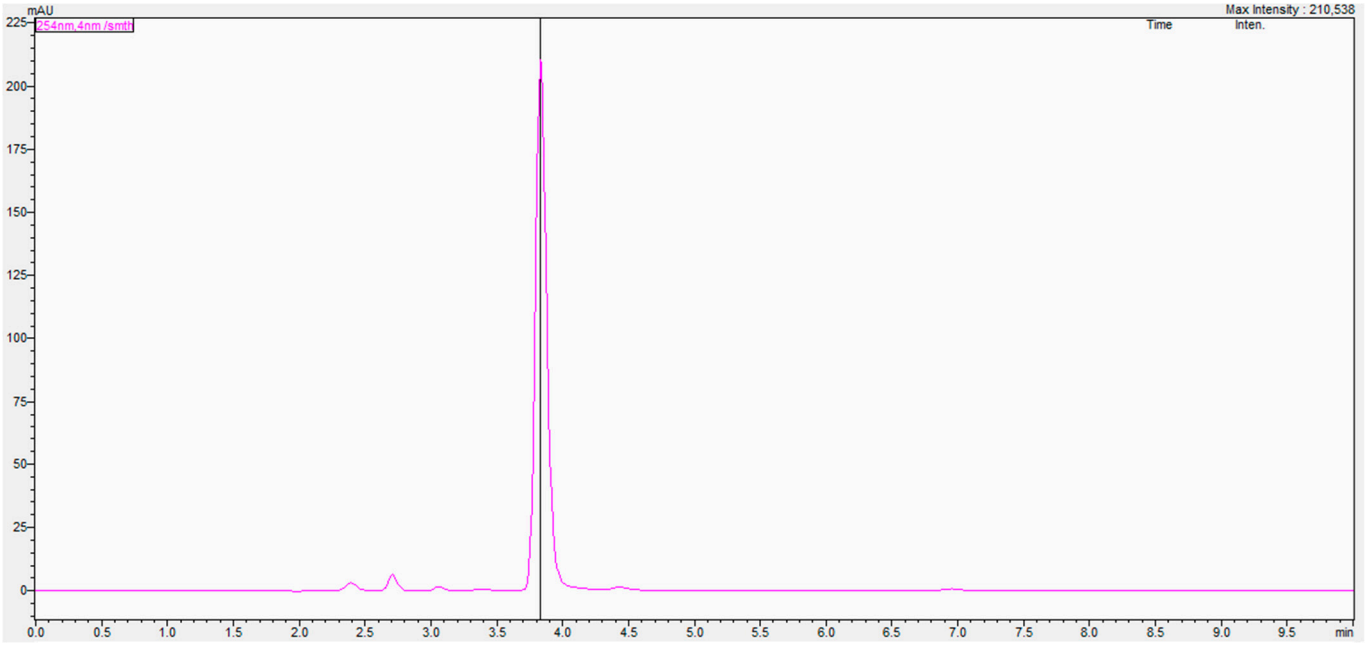


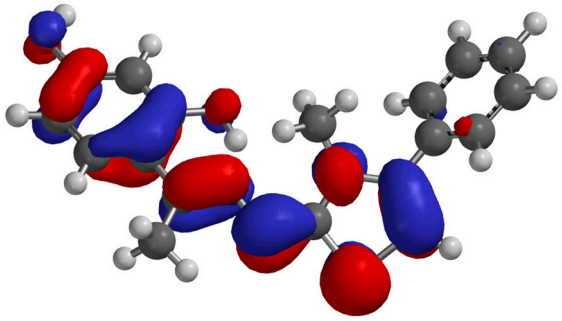
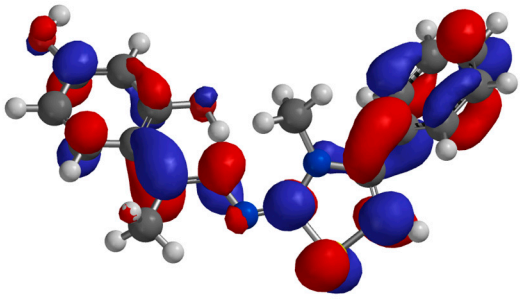
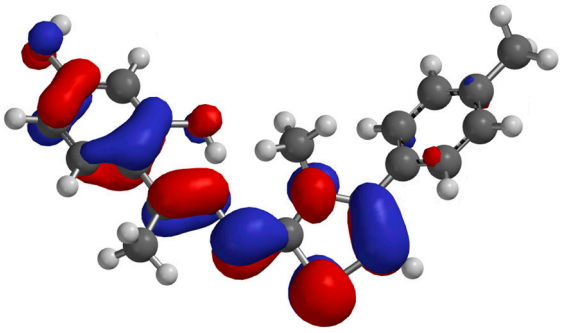
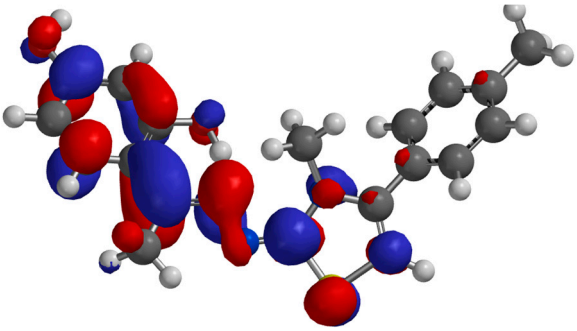
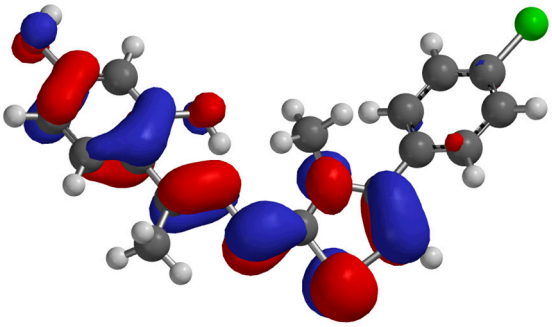
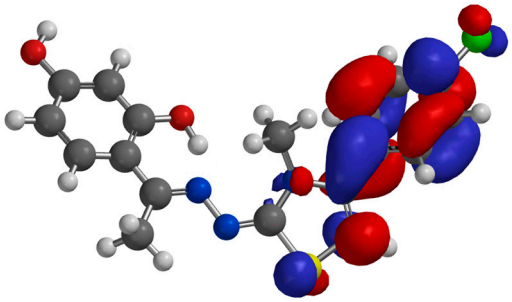
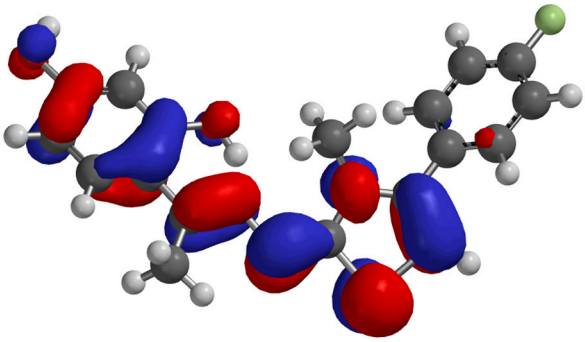
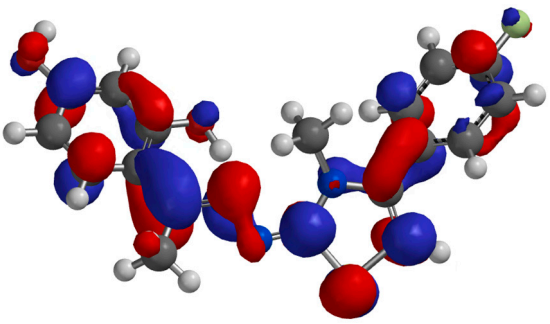
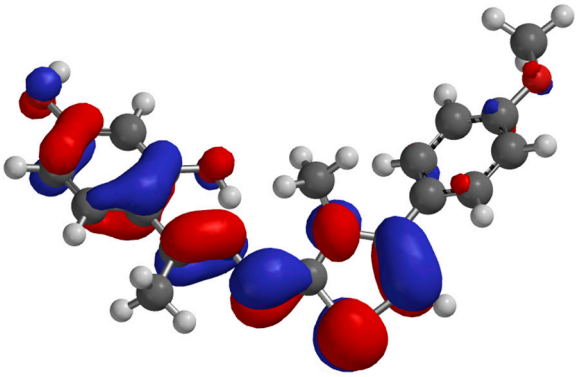
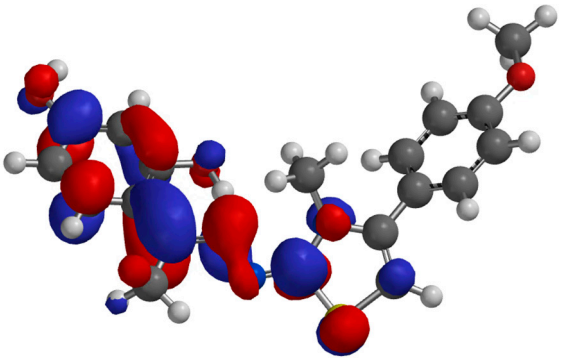
Figure S40. The RP-HPLC chromatogram of the compound **E8** recorded at 254 nm

2. Tables

*2.1. The depiction of HOMO and LUMO and the depiction of the spin density maps of compounds **E1-8***

Table S1. The depiction of HOMO and LUMO of the compounds **E1-8**

Compound	HOMO	LUMO

E1		
E2		
E3		
E4		
E5		

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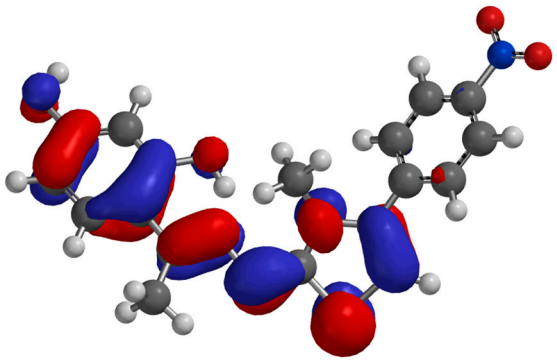
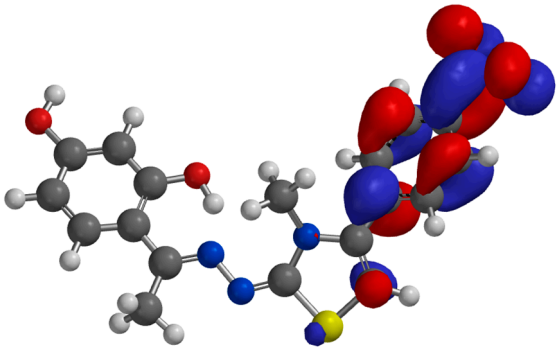
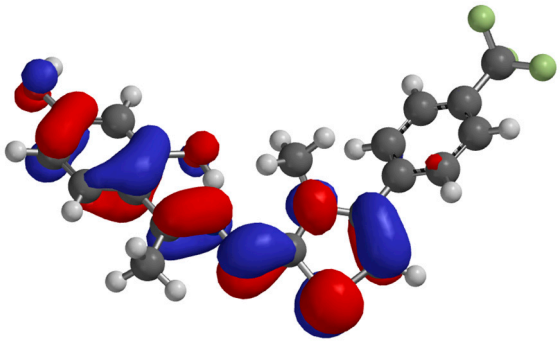
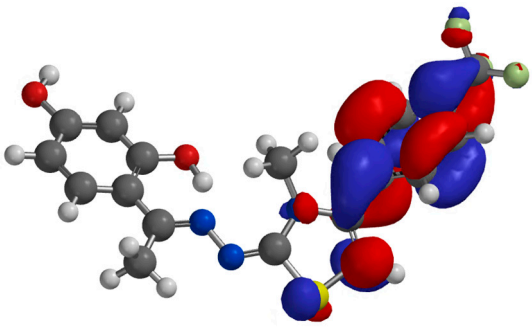
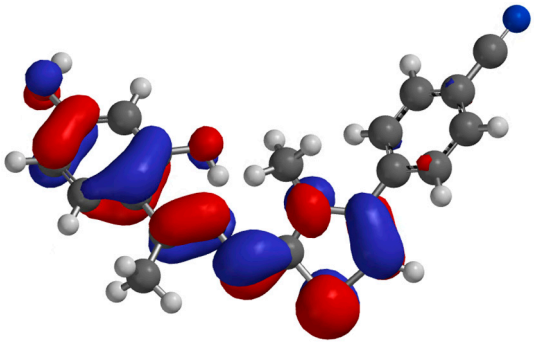
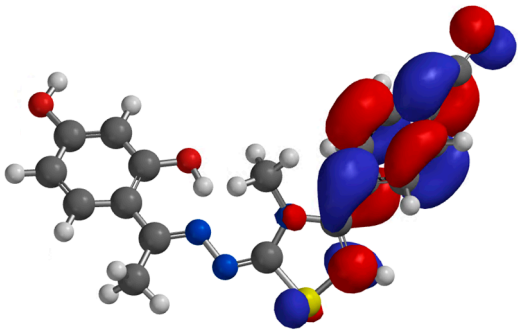
E6		
E7		
E8		

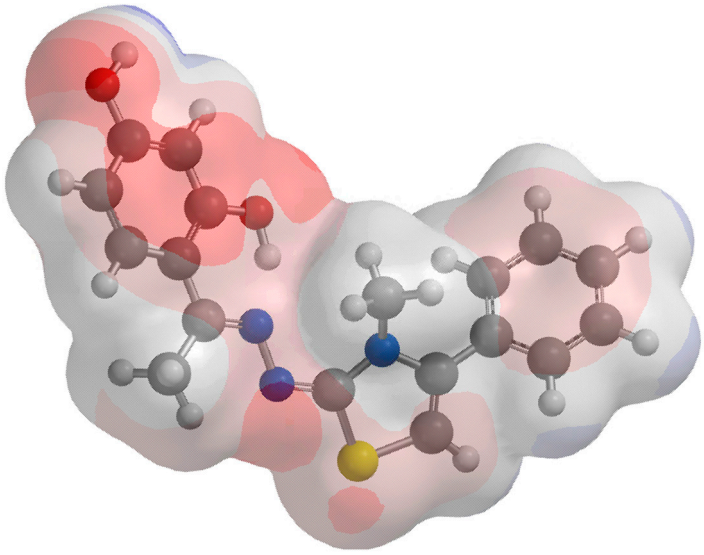
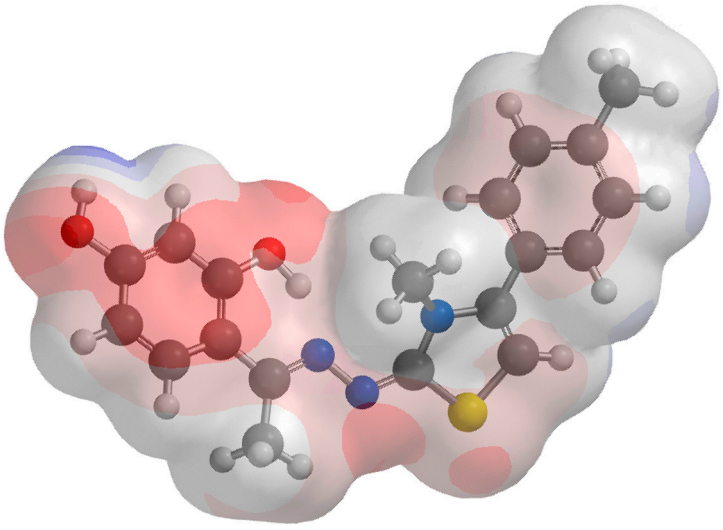
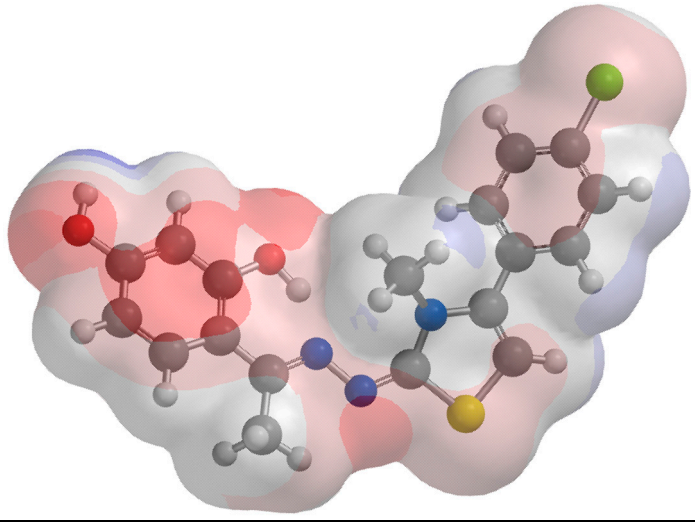
Table S2: The electrostatic potential maps of the compounds **E1-8**

Legend

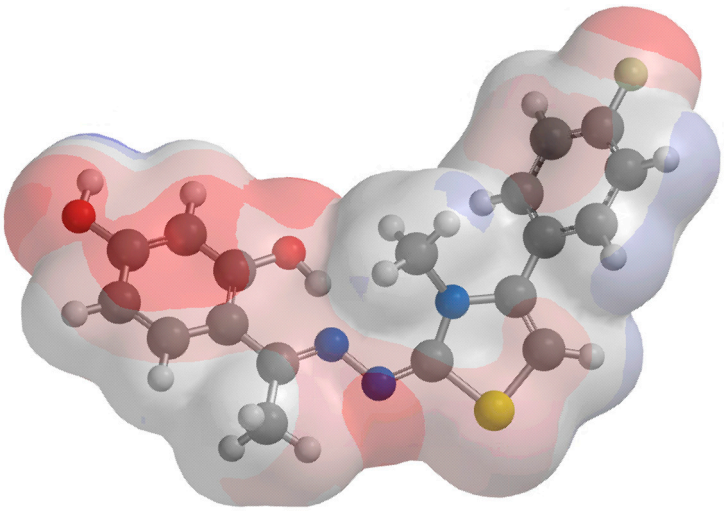
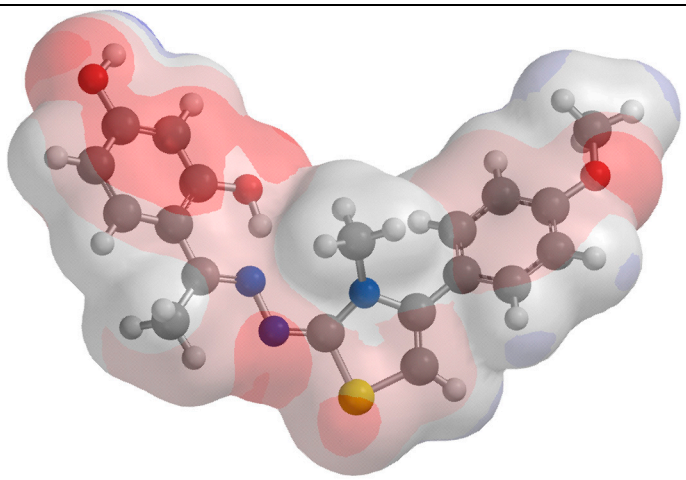
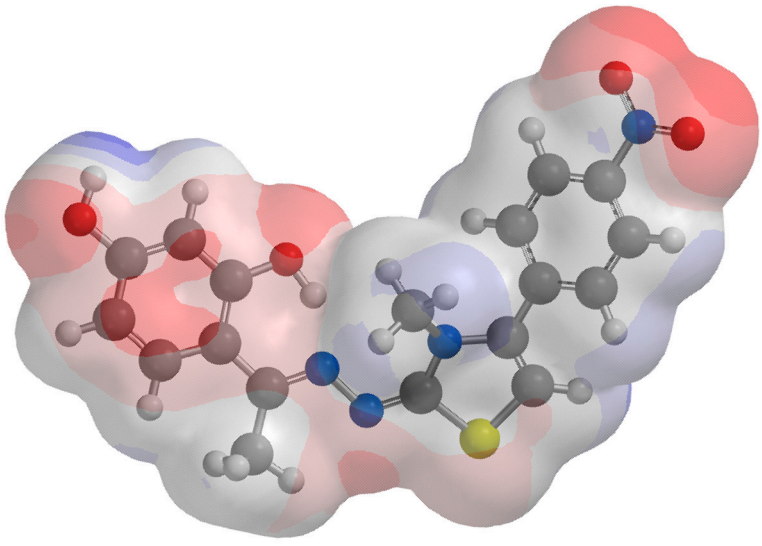


Compound	EPM

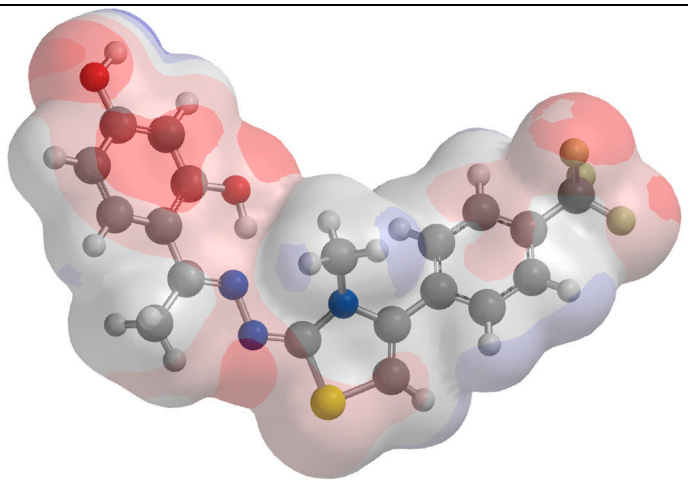
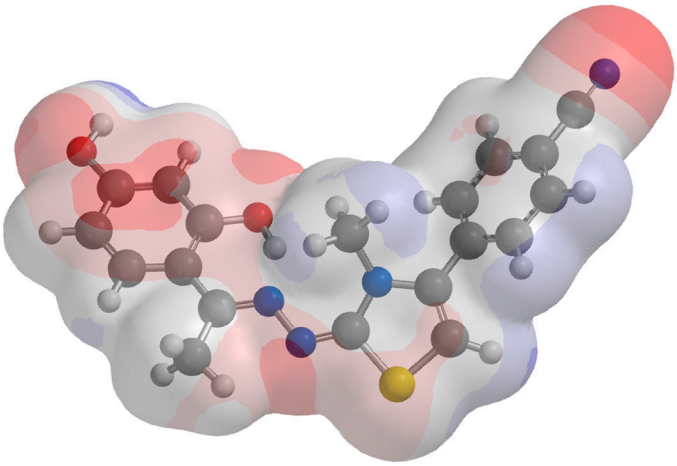
https://doi.org/10.3390/molecules31203620

E1	
E2	
E3	

https://doi.org/10.3390/molecules31203620

E4	
E5	
E6	

https://doi.org/10.3390/molecules31203620

E7	
E8	

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