

Synthesis, DFT Study, and In Vitro Evaluation of Antioxidant Properties and Cytotoxic and Cytoprotective Effects of New Hydrazones on SH-SY5Y Neuroblastoma Cell Lines

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Supplementary Materials

The IR, ^1H NMR and MS characterization spectra of the synthesized compounds.

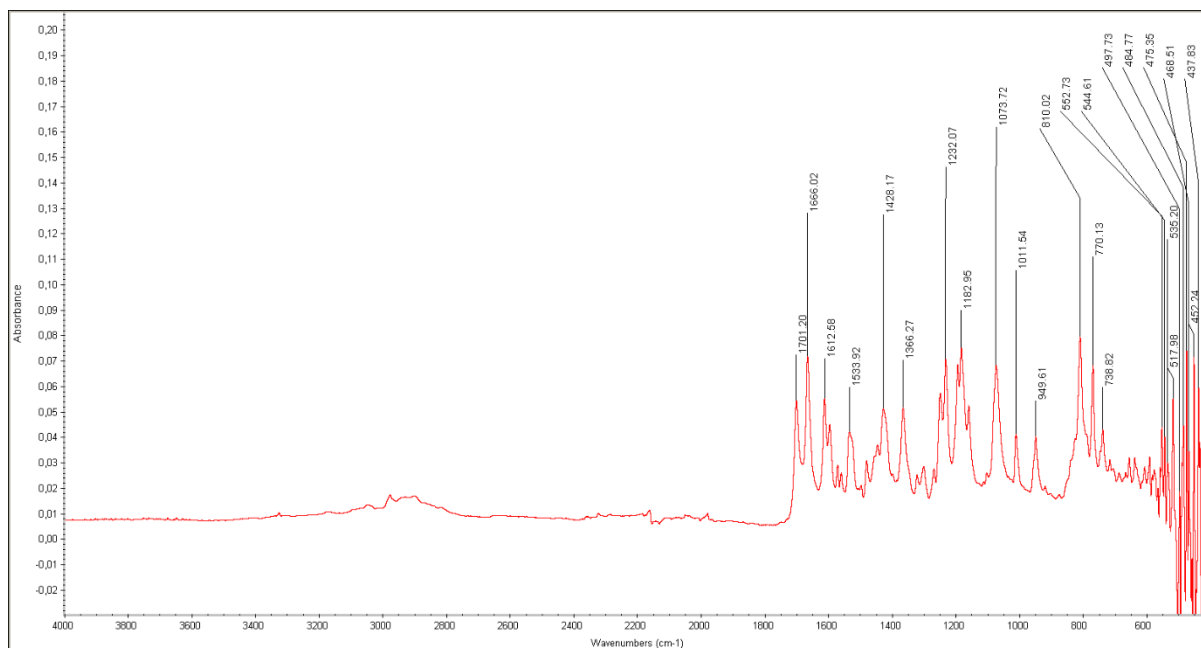


Figure S1. IR spectrum of ethyl 5-(4-bromophenyl)-1-(2-(2-(4-(dimethylamino)benzylidene)hydrazinyl)-2-oxoethyl)-2-methyl-1H-pyrrole-3-carboxylate (7a).

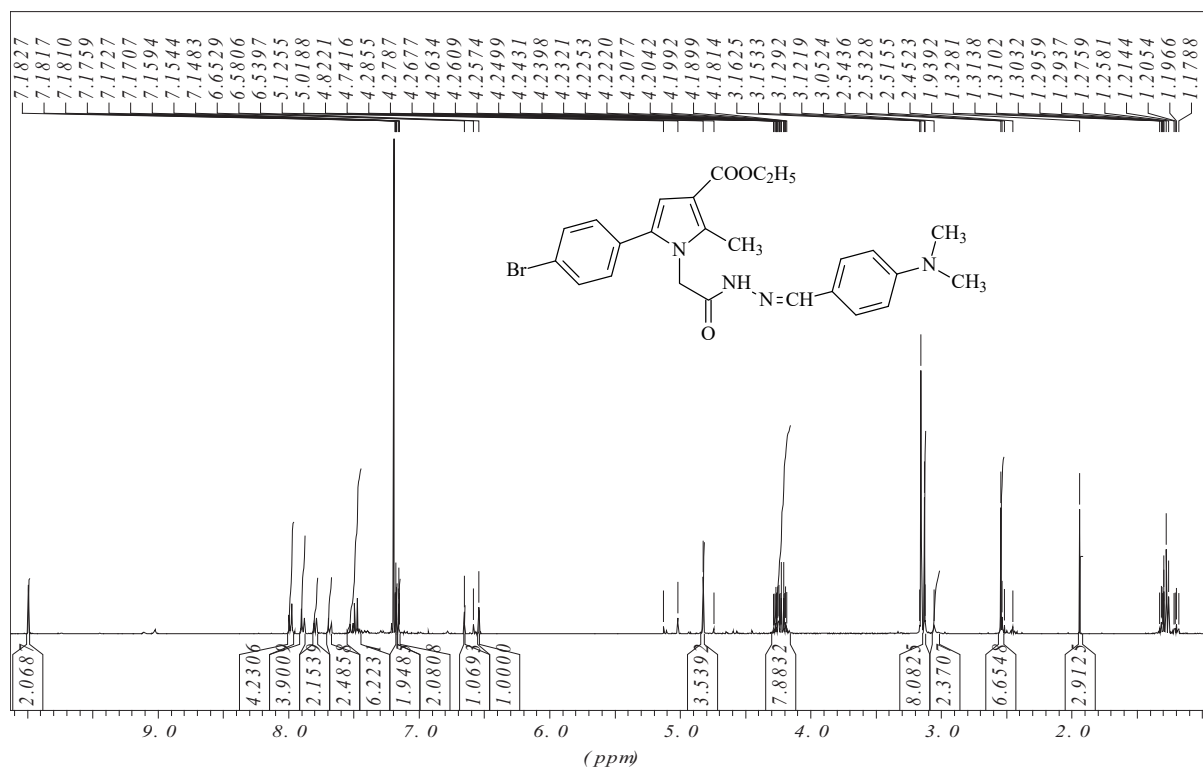


Figure S2. ^1H -NMR spectrum (CDCl_3 , 250 MHz) of compound 7a.

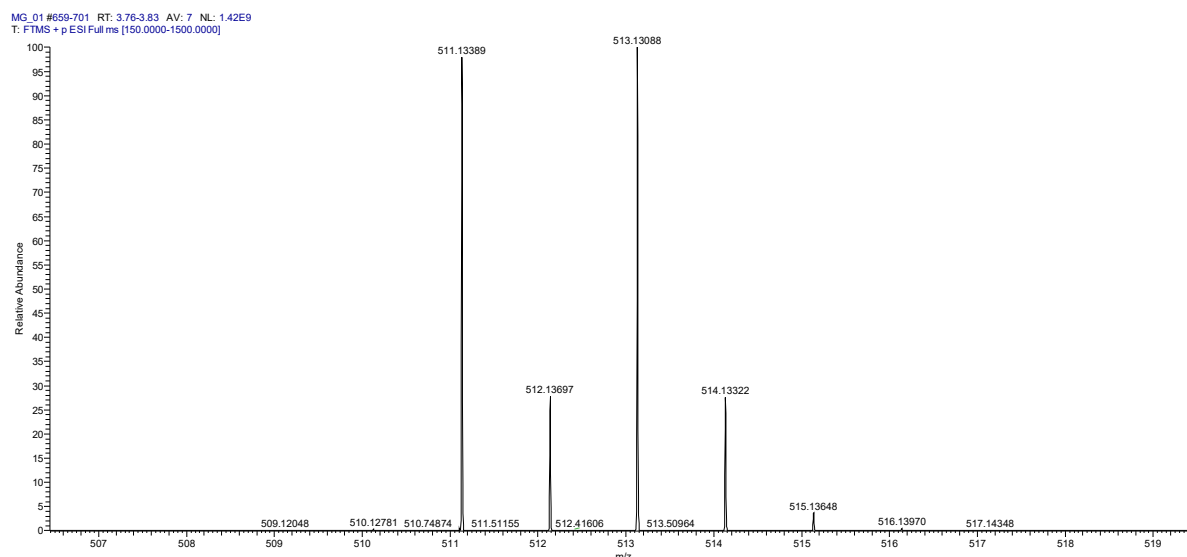


Figure S3. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-1-(2-(2-(4-(dimethylamino)benzylidene)hydrazinyl)-2-oxoethyl)-2-methyl-1H-pyrrole-3-carboxylate (7a).

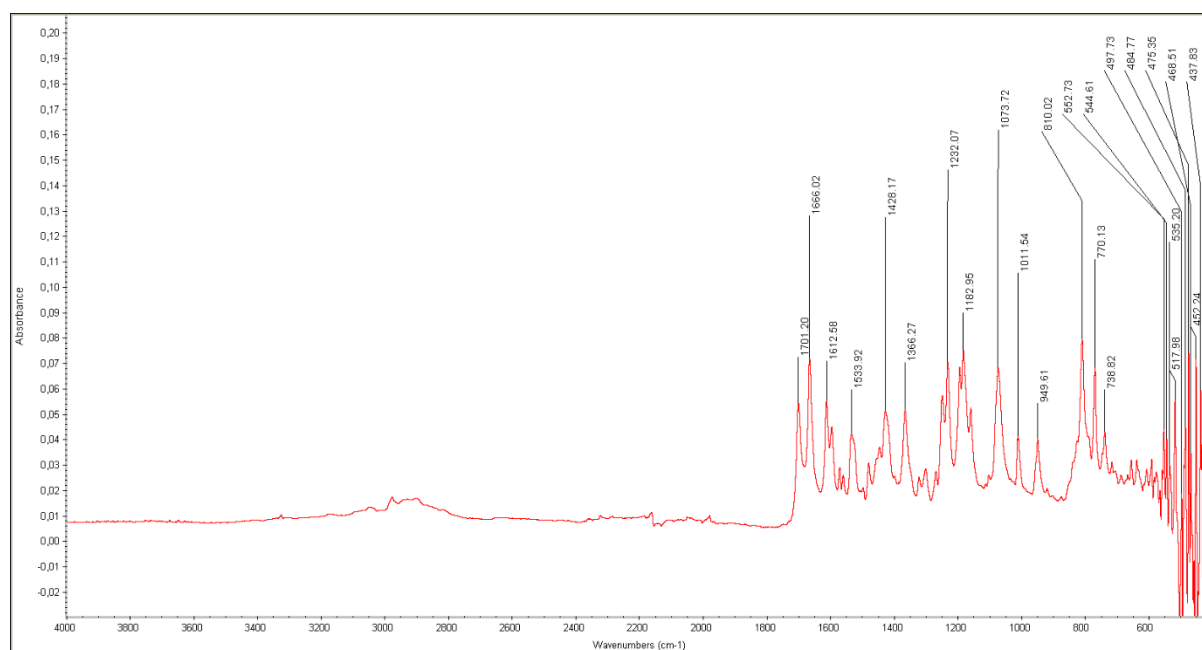


Figure S4. IR spectrum of ethyl 5-(4-bromophenyl)-1-(2-(2-(4-chlorobenzylidene)hydrazinyl)-2-oxoethyl)-2-methyl-1H-pyrrole-3-carboxylate (7b).

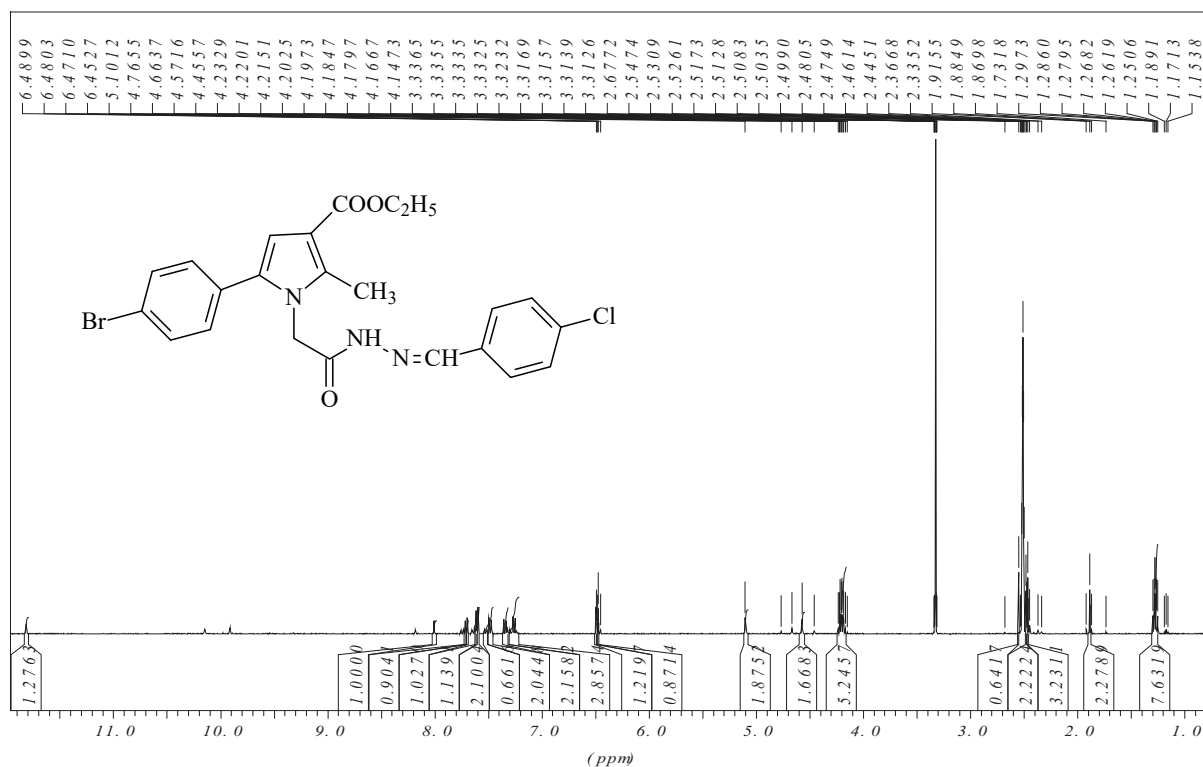


Figure S5. ^1H -NMR spectrum (CDCl_3 , 250 MHz) of compound 7b.

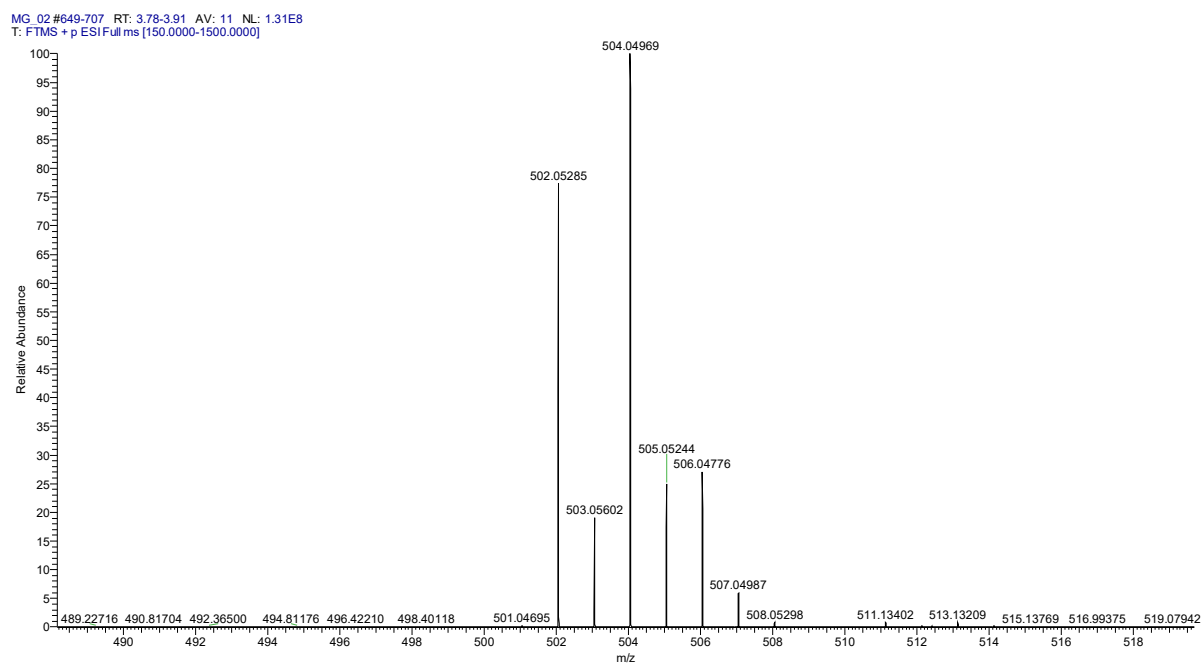


Figure S6. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-1-(2-(2-(4-chlorobenzylidene)hydrazinyl)-2-oxoethyl)-2-methyl-1H-pyrrole-3-carboxylate (7b).

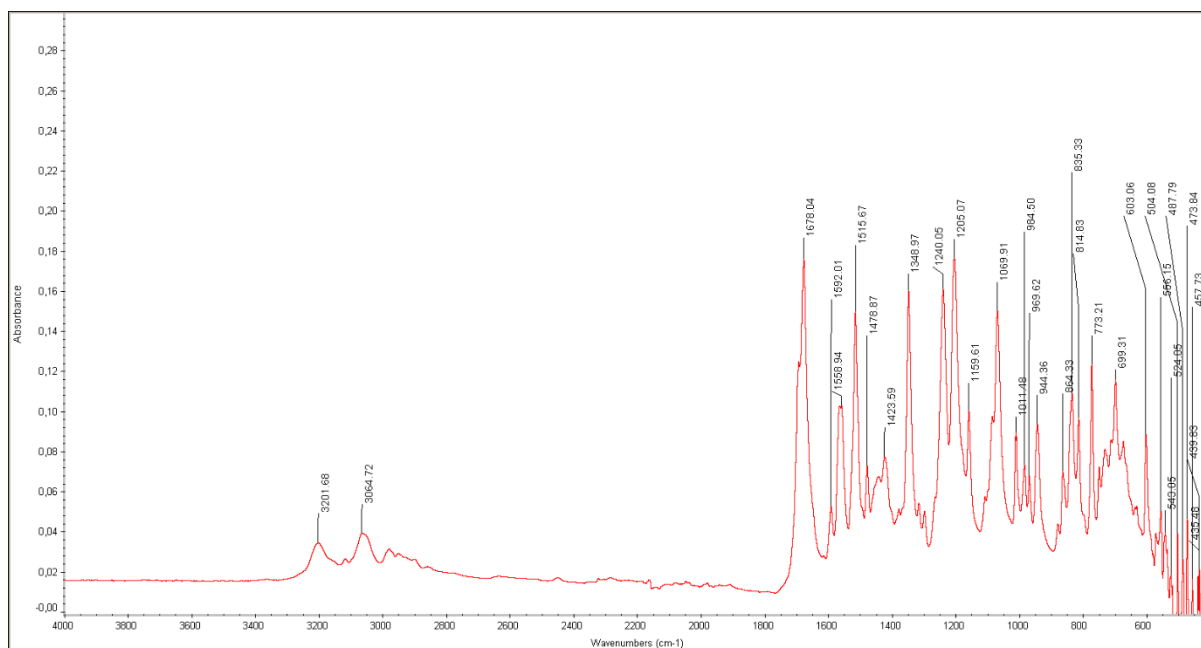


Figure S7. IR spectrum of ethyl 5-(4-bromophenyl)-2-methyl-1-(2-(2-(4-nitrobenzylidene)hydrazinyl)-2-oxo-ethyl)-1H-pyrrole-3-carboxylate (7c).

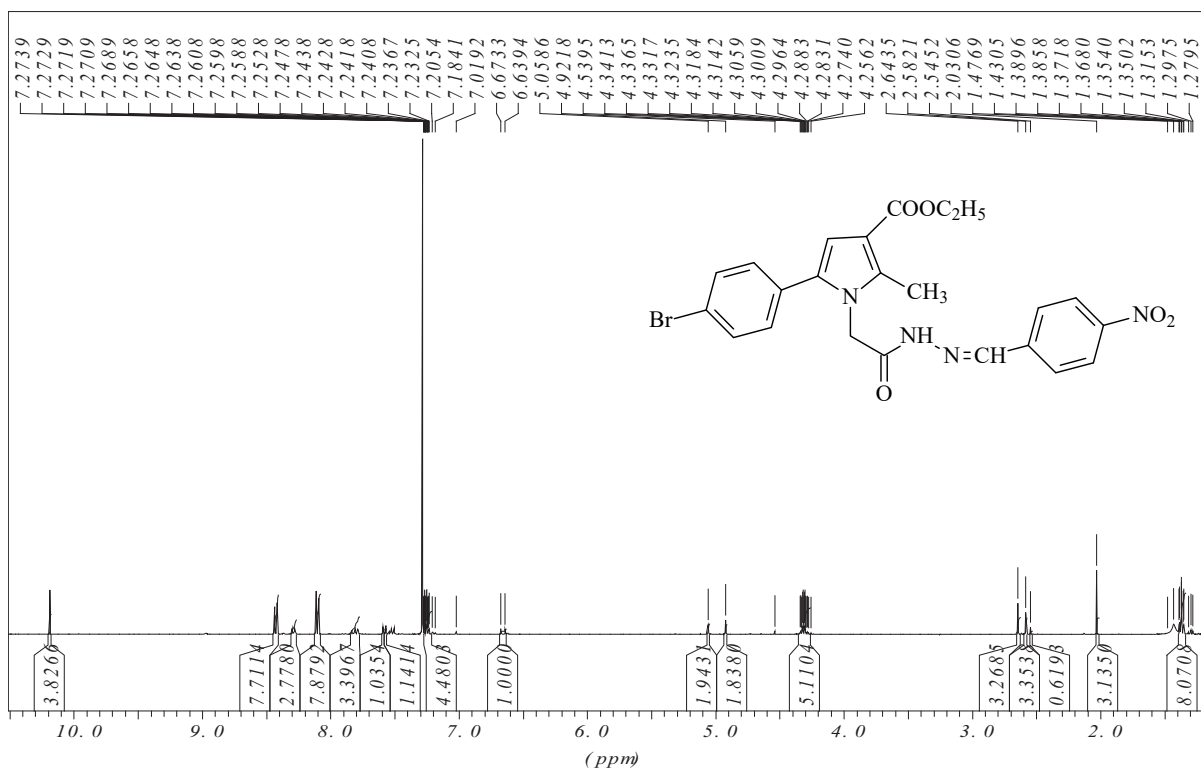


Figure S8. ¹H-NMR spectrum (CDCl₃, 250 MHz) of compound 7c.

MG_03 #559-614 RT: 3.60-3.71 AV: 10 NL: 1.57E8
T: FTMS + p ESIFull ms [150.0000-1500.0000]

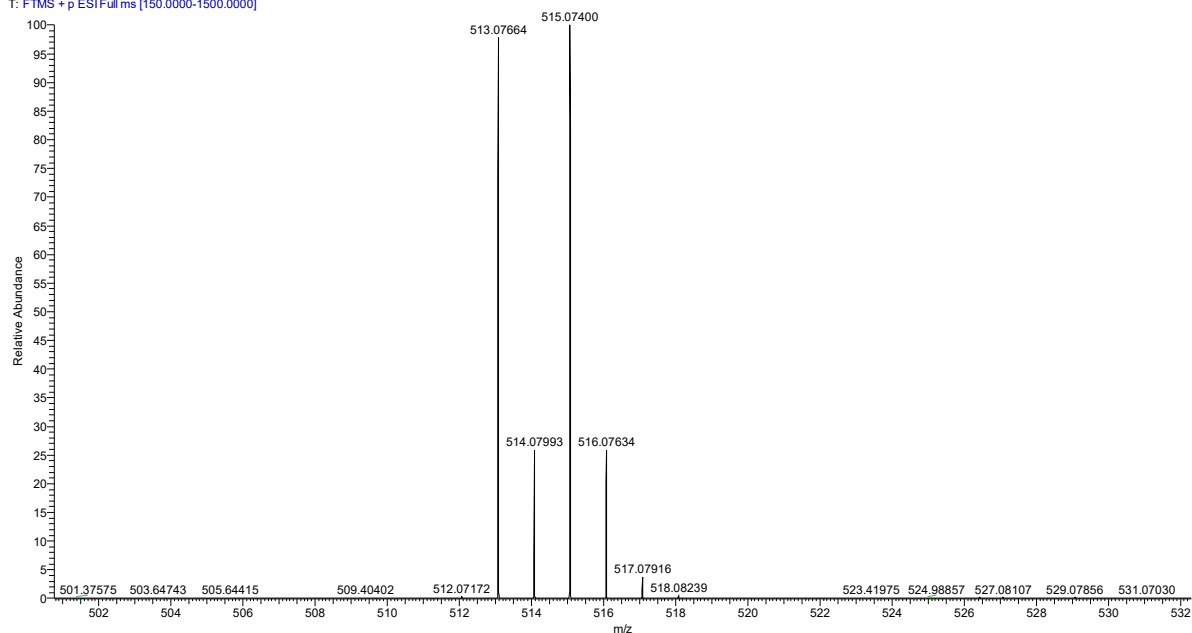


Figure S9. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-2-methyl-1-(2-(2-(4-nitrobenzylidene) hydrazinyl)-2-oxo-ethyl)-1H-pyrrole-3-carboxylate (7c).

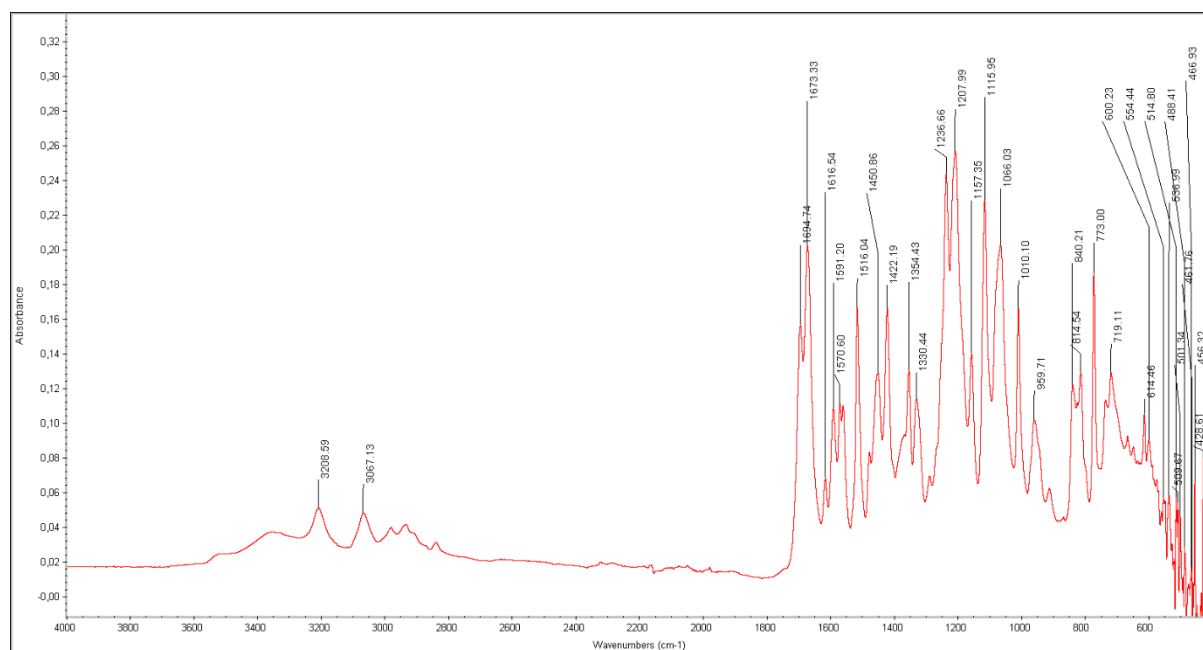


Figure S10. IR spectrum of ethyl 5-(4-bromophenyl)-1-(2-(2-(4-hydroxy-3,5-dimethoxybenzylidene)hydrazine-yl)-2-oxoethyl)-2-methyl-1H-pyrrole-3-carboxylate (7d).

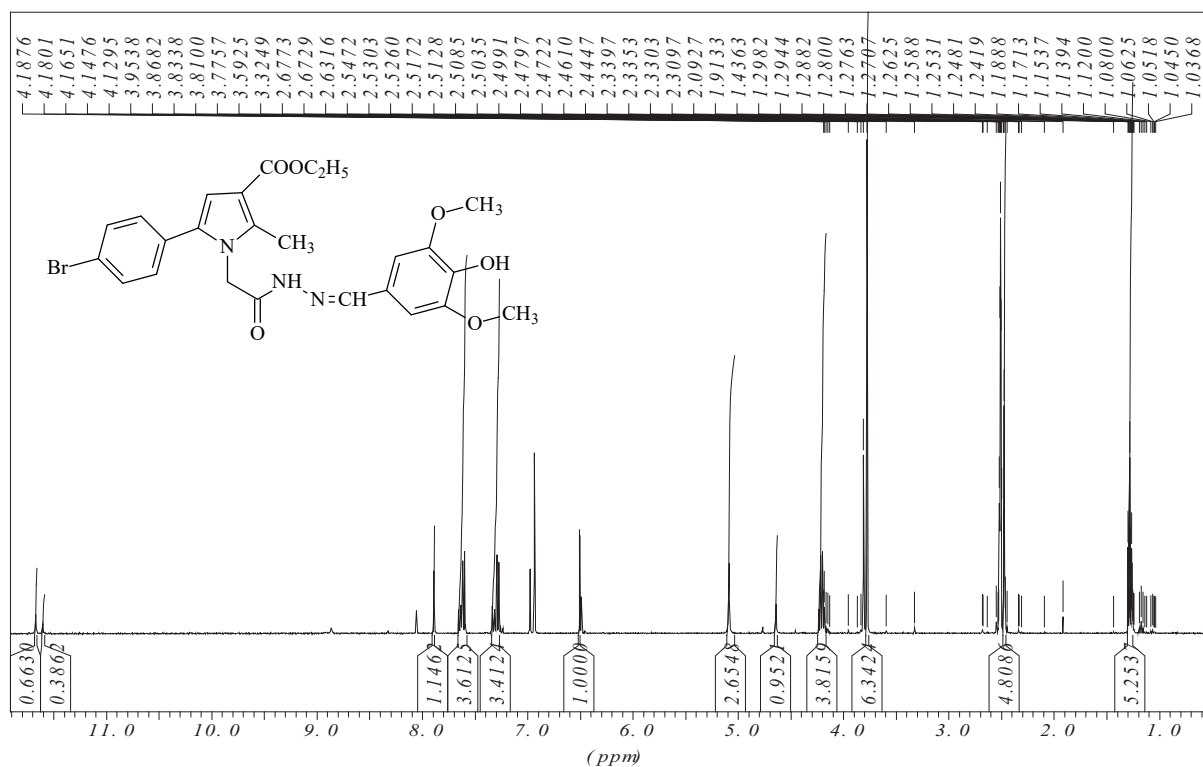


Figure S11. ^1H -NMR spectrum (CDCl_3 , 250 MHz) of compound 7d.

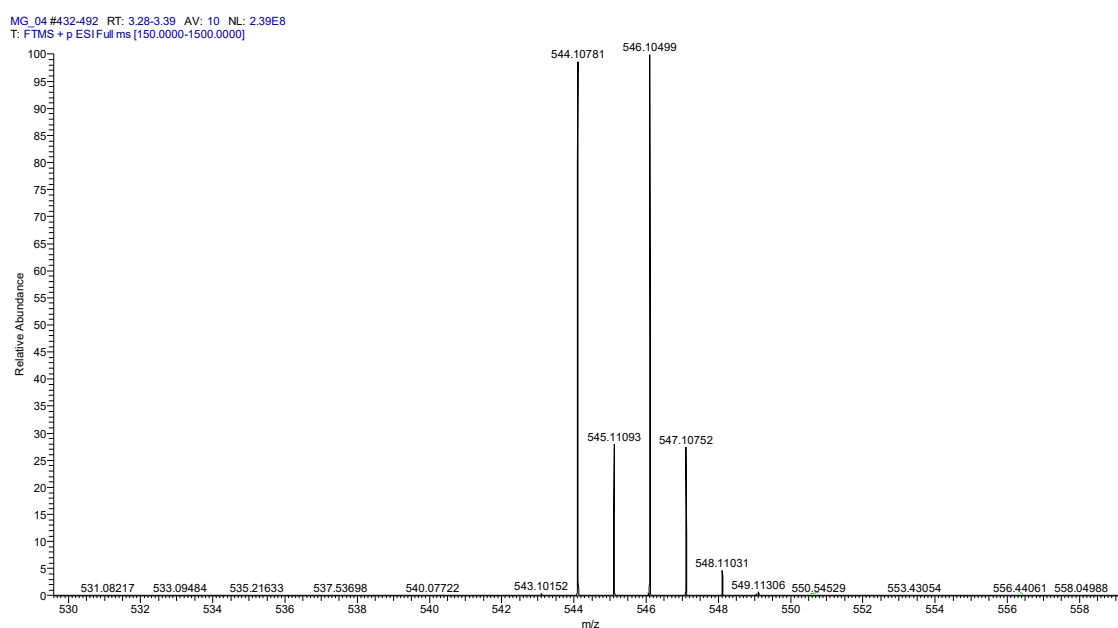
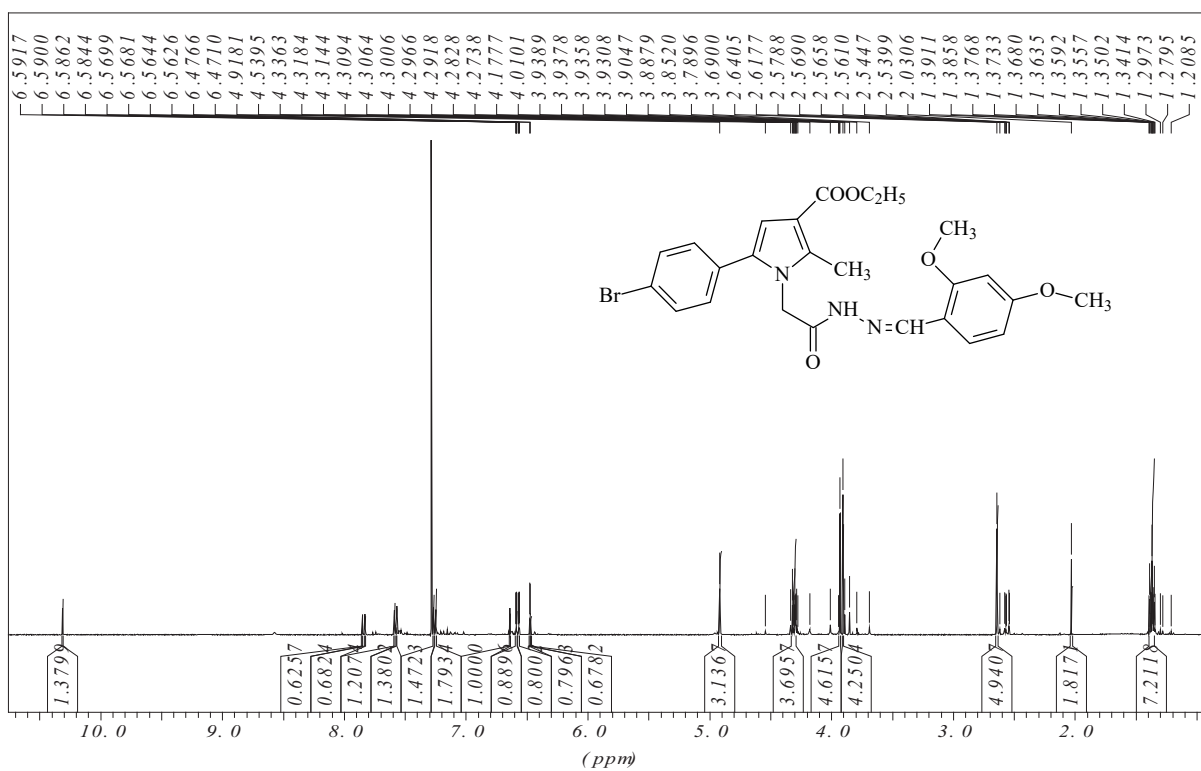
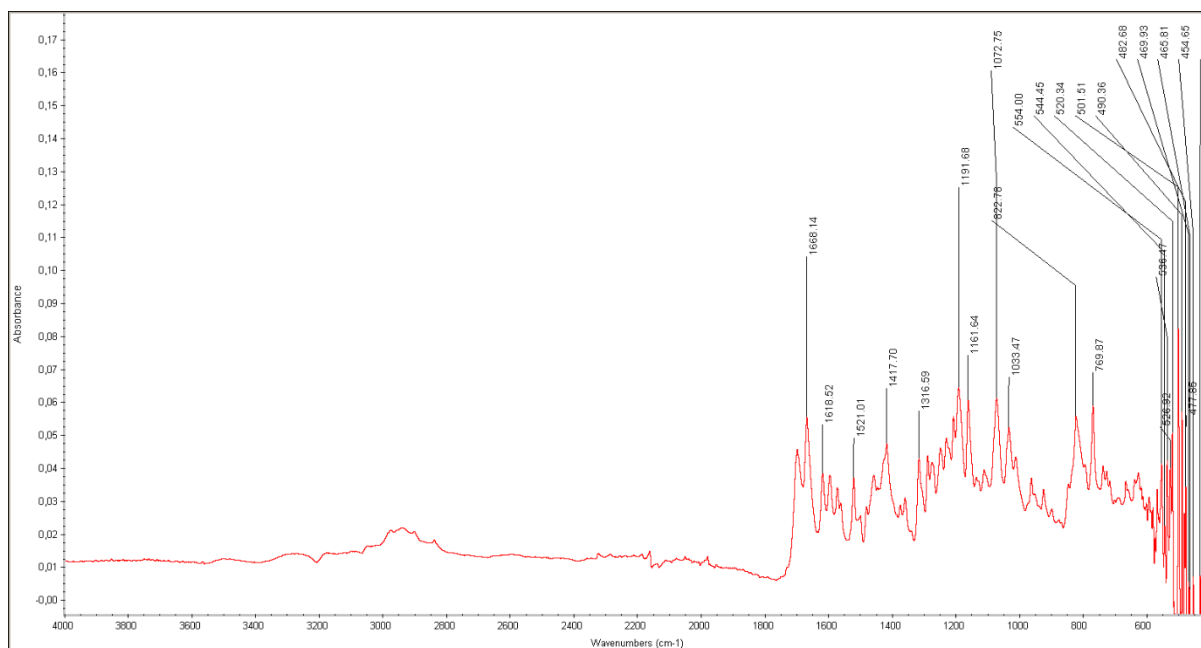


Figure S12. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-1-(2-(2-(4-hydroxy-3,5-dimethoxybenzylidene)hydrazine-yl)-2-oxoethyl)-2-methyl-1H-pyrrole-3-carboxylate (7d).



MG_05 #604-671 RT: 3.68-3.82 AV: 12 NL: 3.01E8
T: FTMS + p ESI Full ms [150.0000-1500.0000]

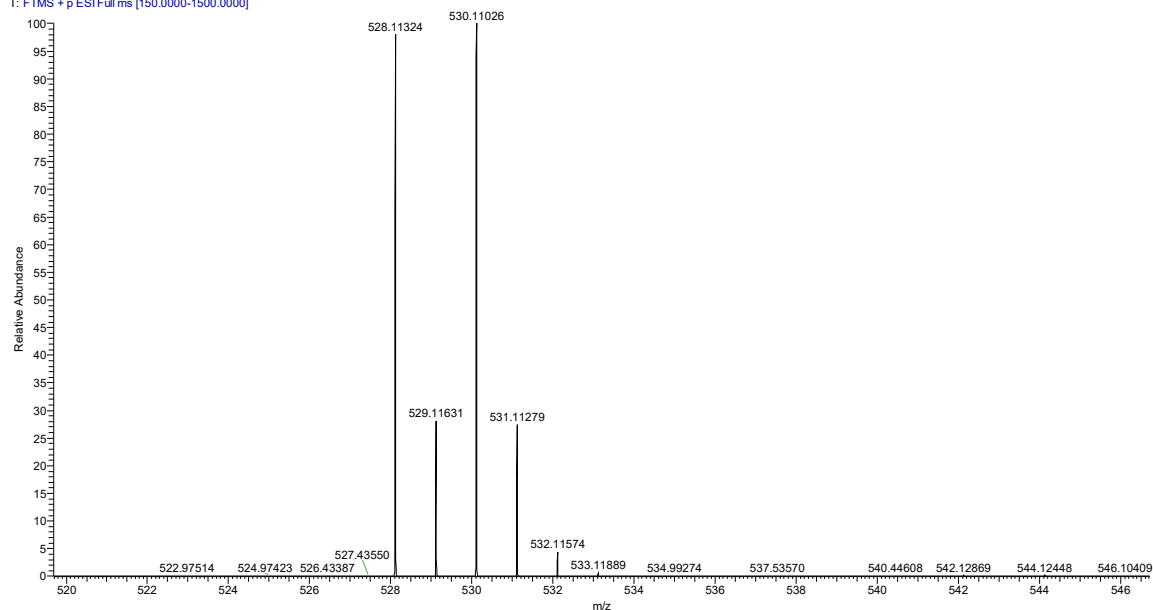


Figure S15. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-1-(2-(2-(2,4-dimethoxybenzylidene)hydrazinyl)-2-oxo-ethyl)-2-methyl-1H-pyrrole-3-carboxylate (7e).

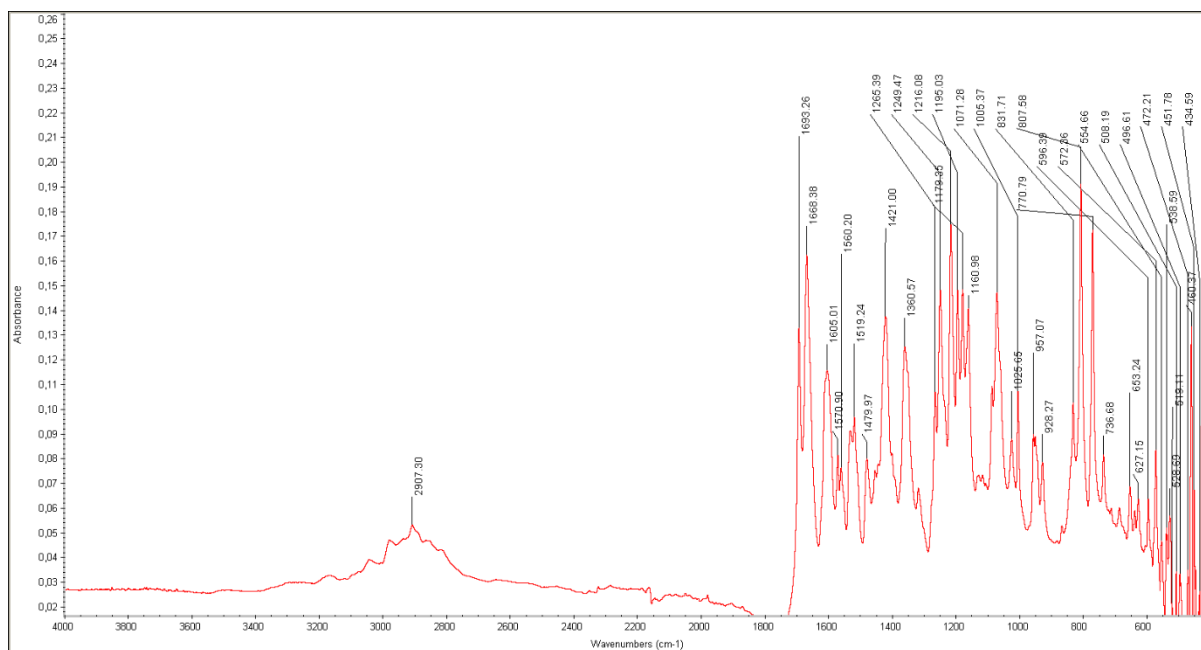


Figure S16. IR spectrum of ethyl 5-(4-bromophenyl)-1-(3-(2-(4-(dimethylamino)benzylidene)hydrazinyl)-3-oxopropyl)-2-methyl-1H-pyrrole-3-carboxylate (8a).

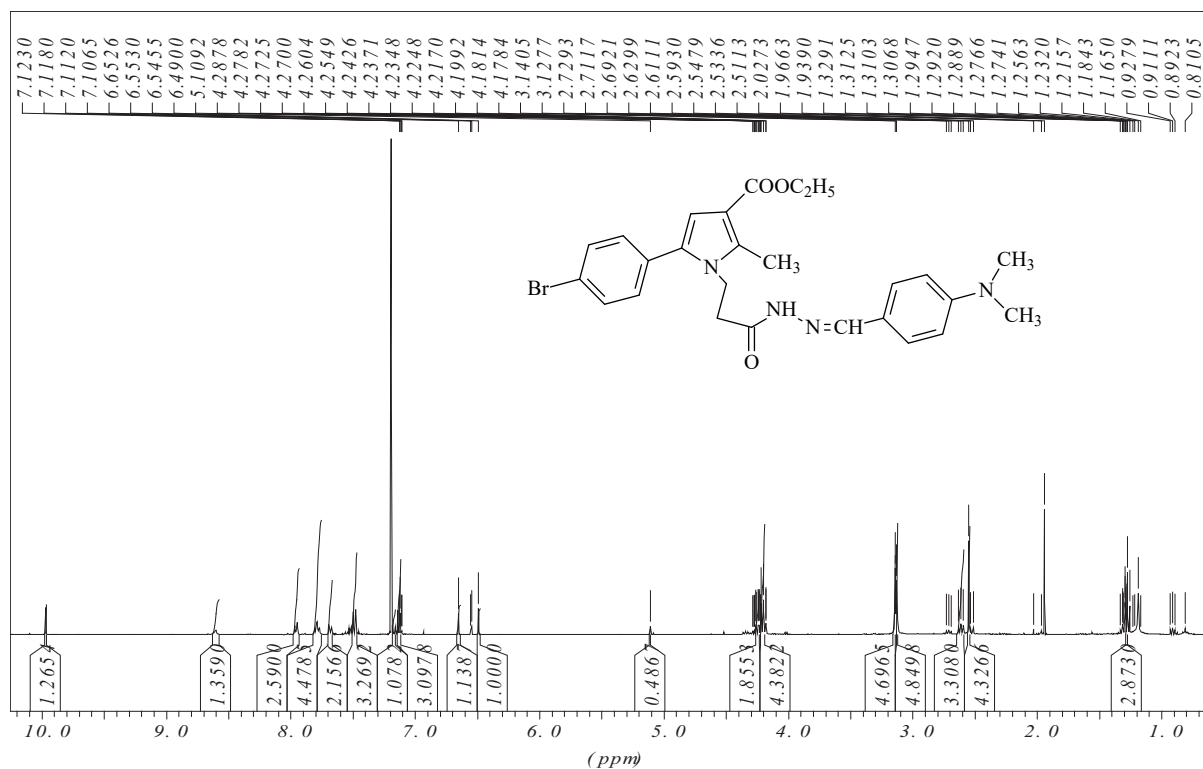


Figure S17. ¹H-NMR spectrum (CDCl₃, 250 MHz) of compound 8a.

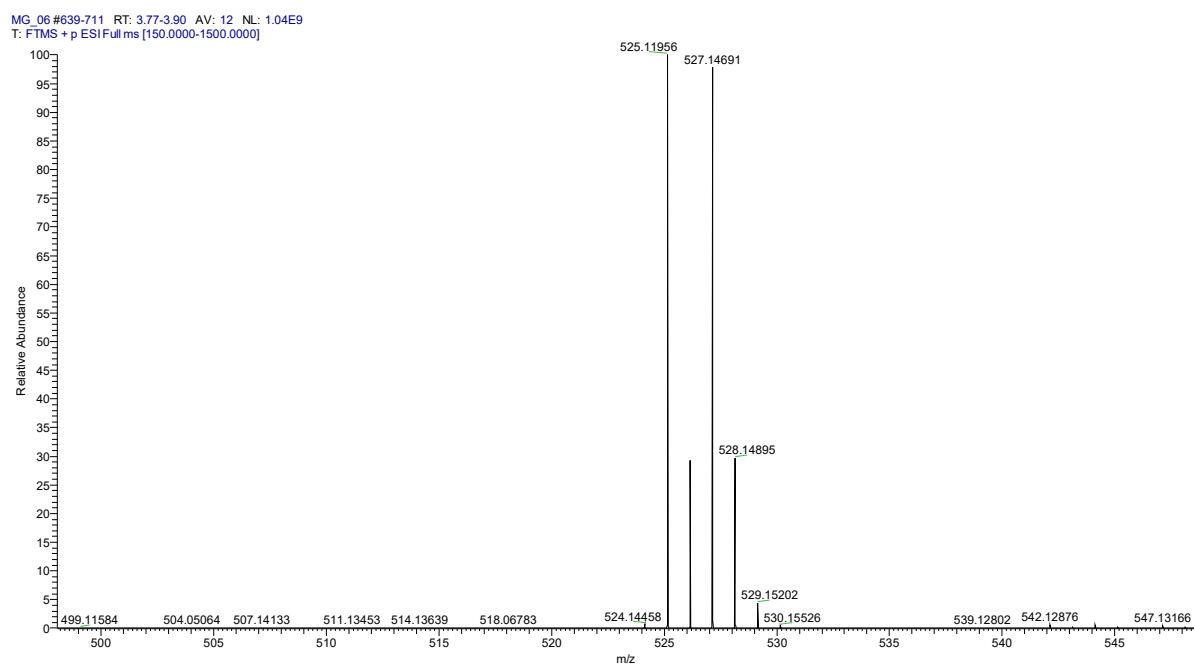


Figure S18. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-1-(3-(2-(4-(dimethylamino)benzylidene)hydrazinyl)-3-oxopropyl)-2-methyl-1H-pyrrole-3-carboxylate (8a).

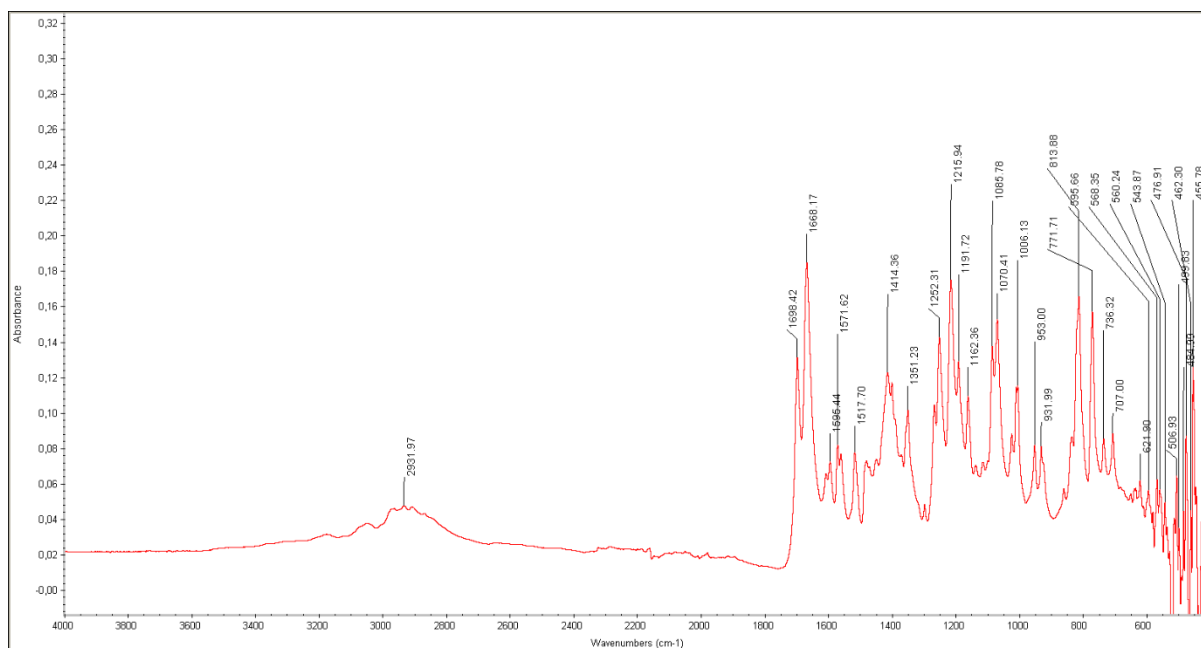


Figure S19. IR spectrum of ethyl 5-(4-bromophenyl)-1-(3-(2-(4-chlorobenzylidene)hydrazinyl)-3-oxopropyl)-2-methyl-1H-pyrrole-3-carboxylate (**8b**).

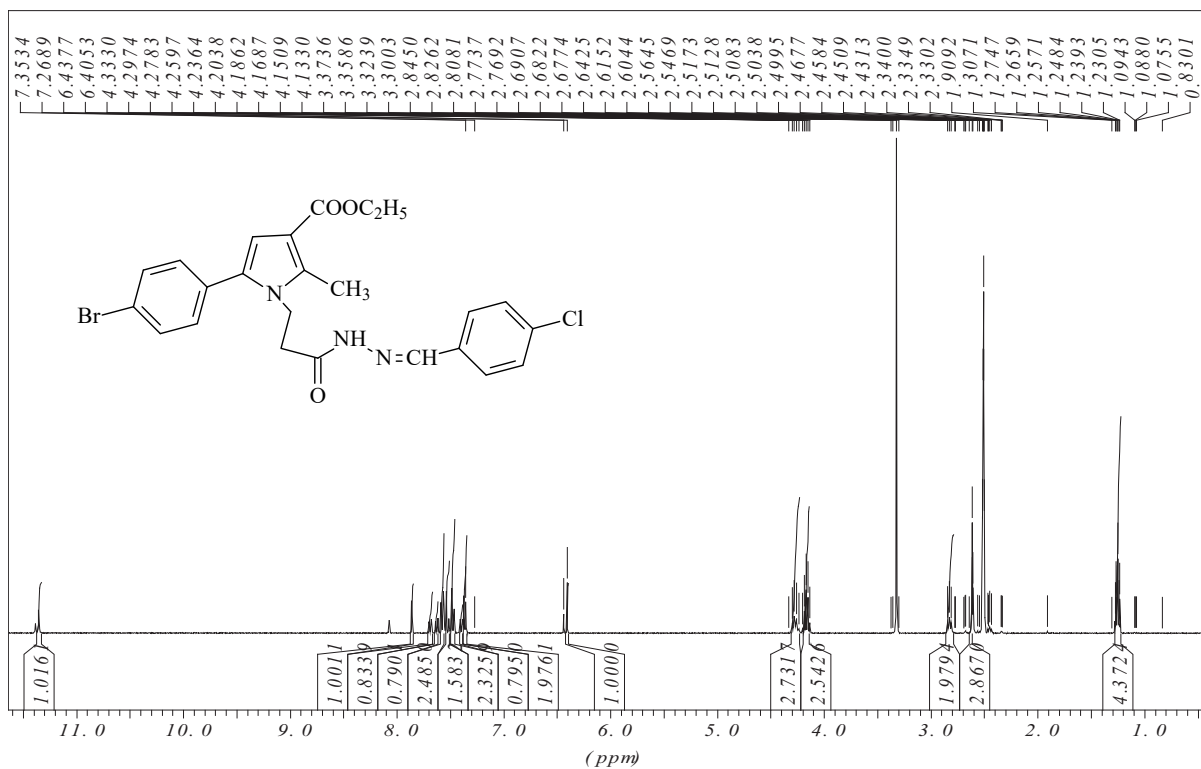


Figure S20. ^1H -NMR spectrum (CDCl_3 , 250 MHz) of compound **8b**.

MG_07 #641-691 RT: 3.82-3.92 AV: 9 NL: 3.49E8
T: FTMS + p ESIFull.ms [150.0000-1500.0000]

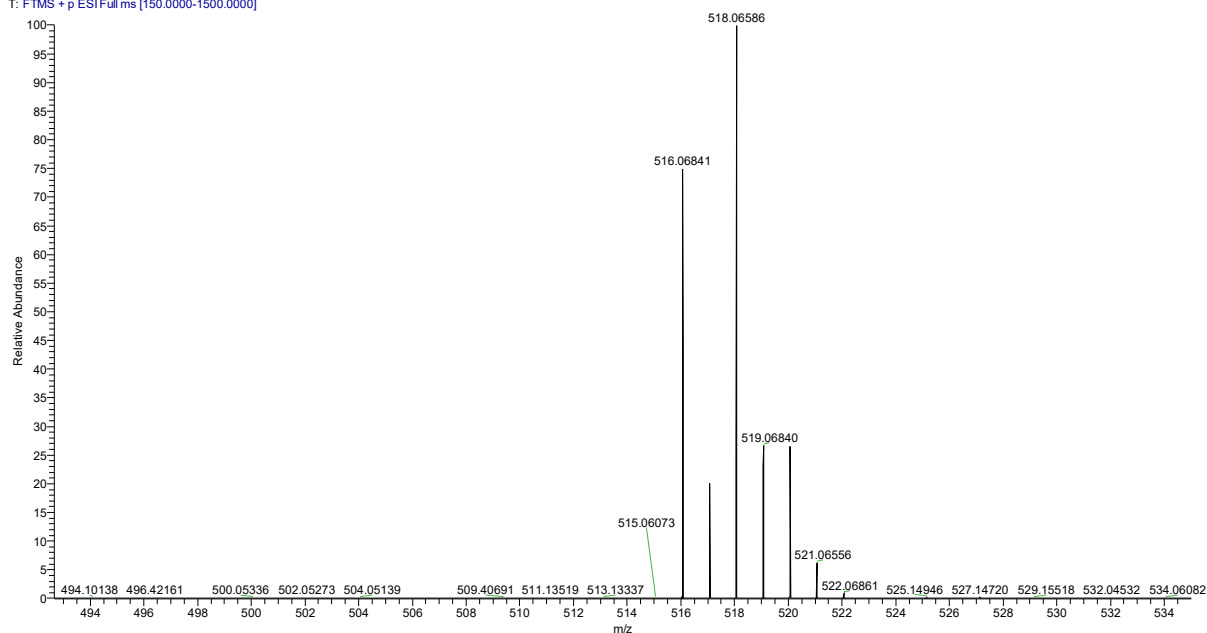


Figure S21. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-1-(3-(2-(4-chlorobenzylidene)hydrazinyl)-3-oxopropyl)-2-methyl-1H-pyrrole-3-carboxylate (8b).

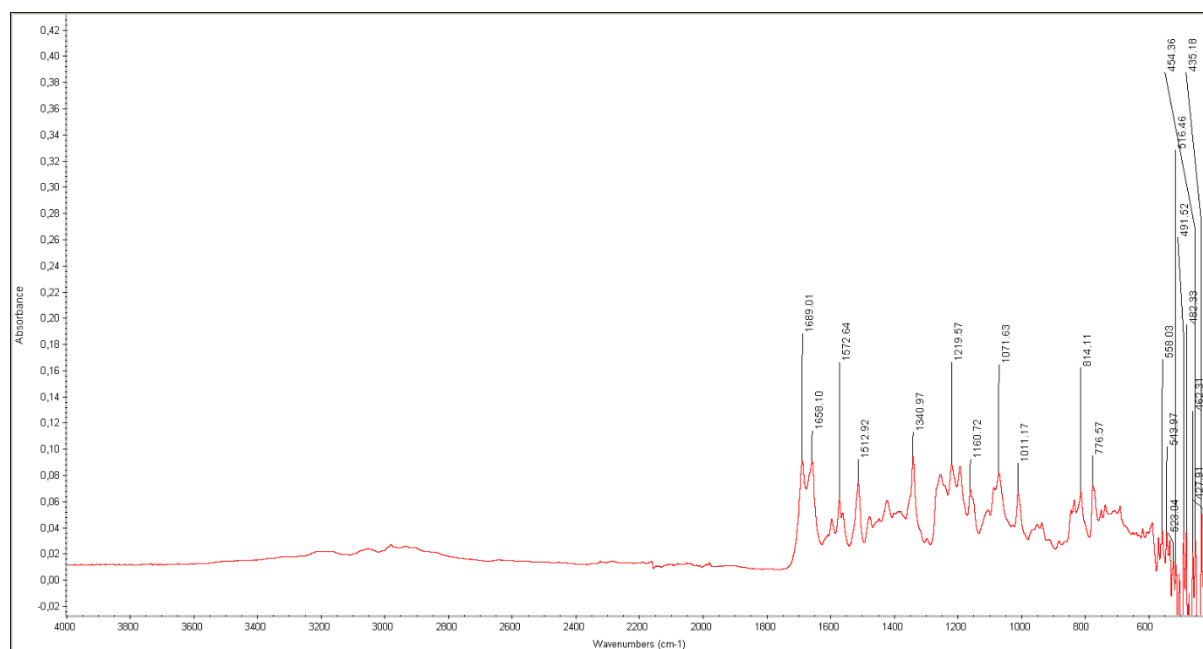


Figure S22. IR spectrum of ethyl 5-(4-bromophenyl)-2-methyl-1-(3-(2-(4-nitrobenzylidene)hydrazinyl)-3-oxo-propyl)-1H-pyrrole-3-carboxylate (8c).

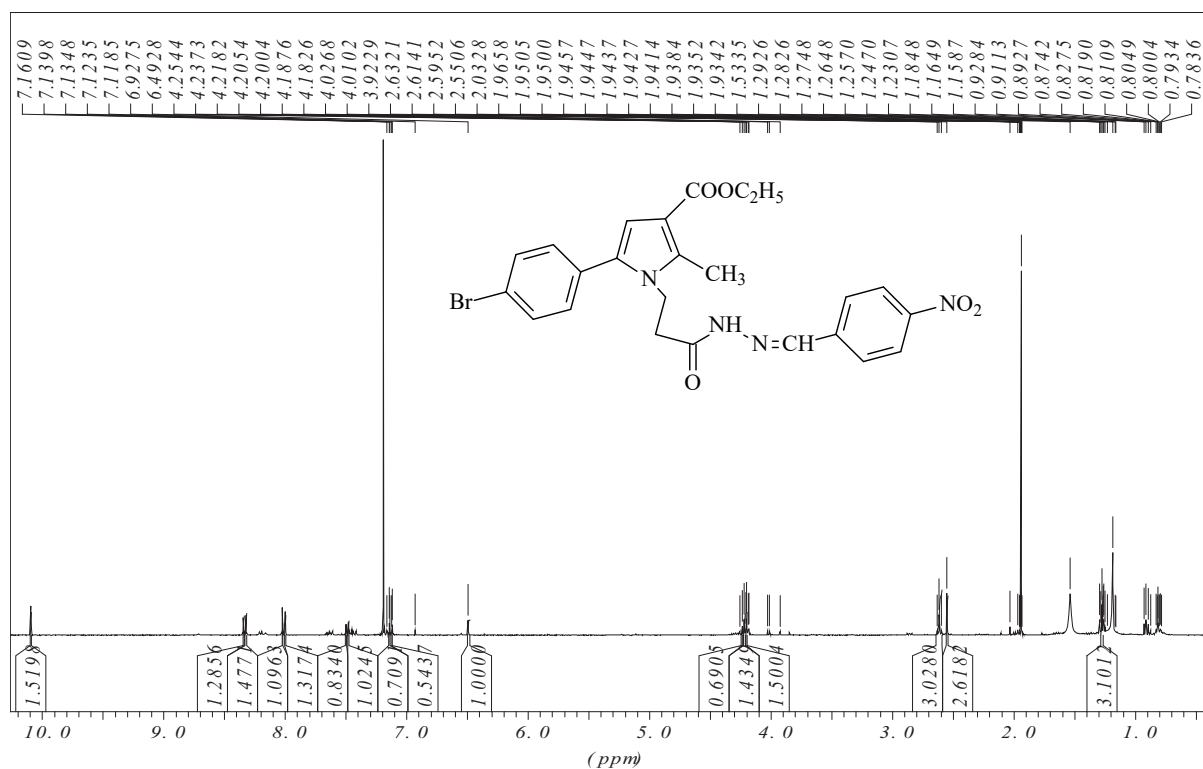


Figure S23. ¹H-NMR spectrum (CDCl₃, 250 MHz) of compound 8c.

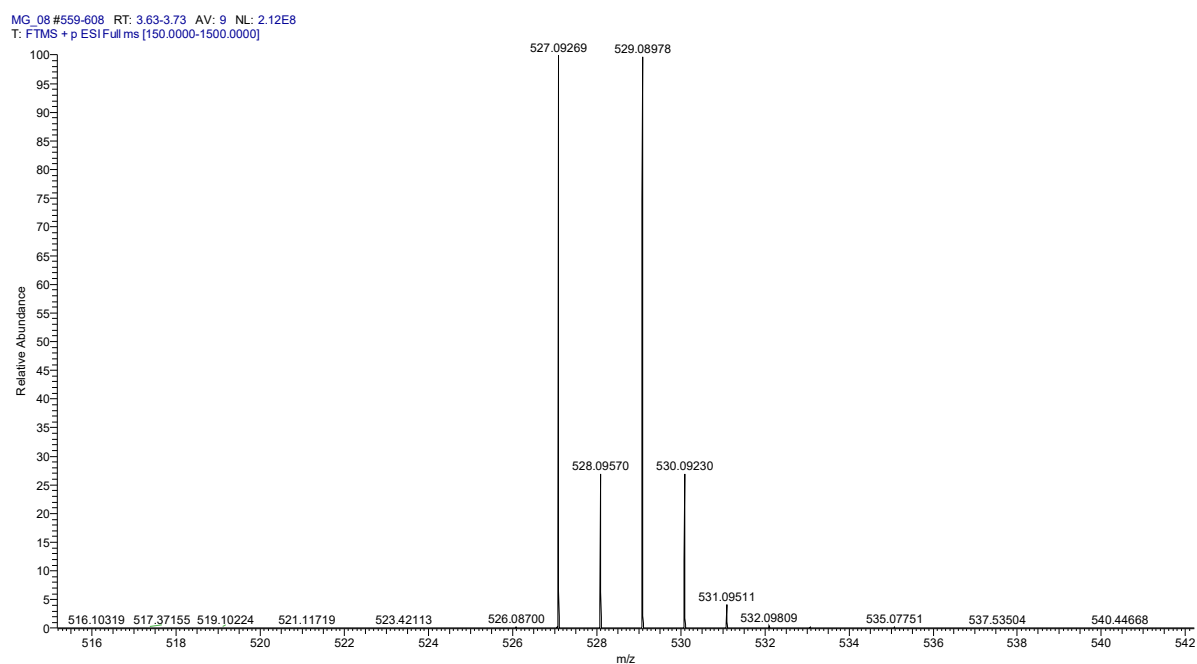
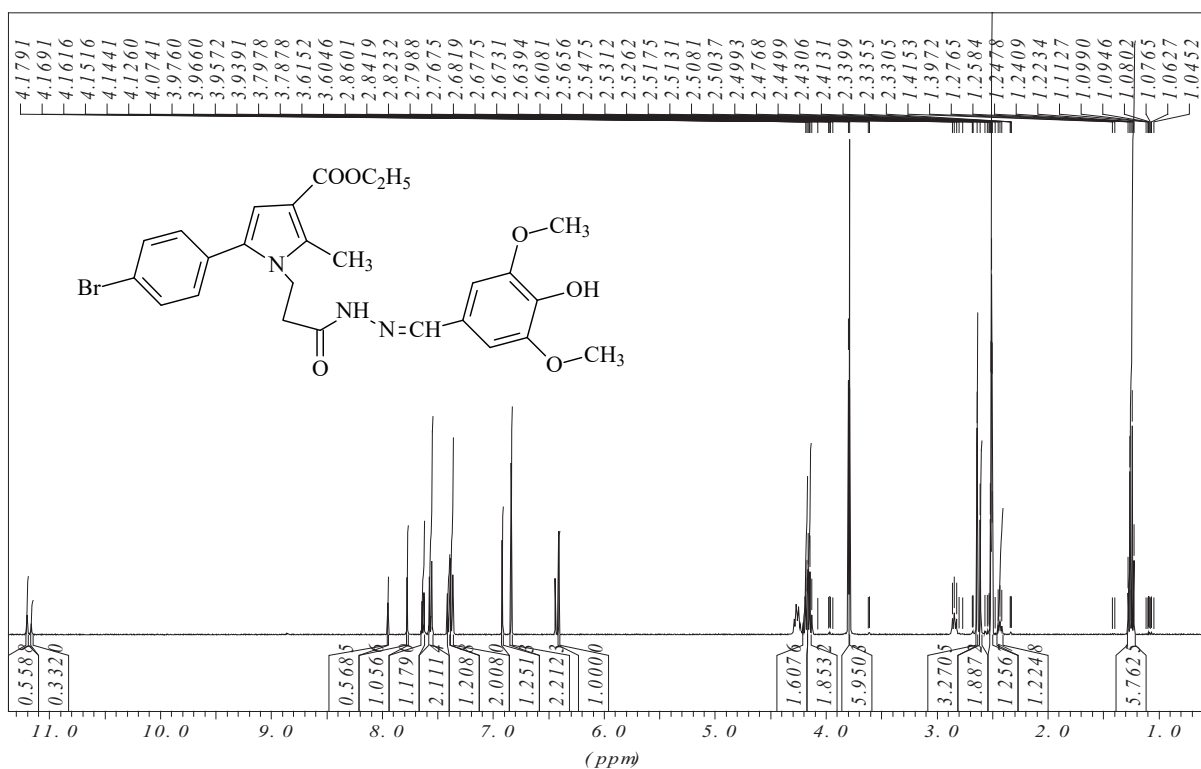
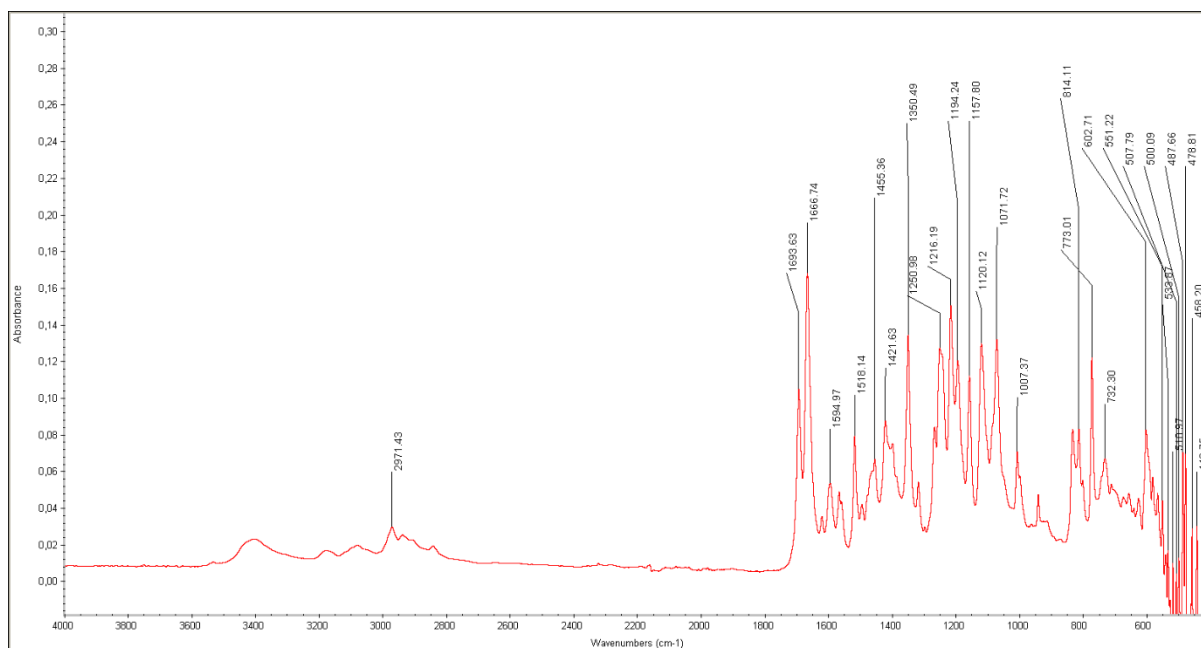


Figure S24. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-2-methyl-1-(3-(2-(4-nitrobenzylidene)hydrazinyl)-3-oxo-propyl)-1H-pyrrole-3-carboxylate (8c).



MG_09 #423-479 RT: 3.27-3.39 AV: 10 NL: 3.01E8
T: FTMS + p ESIFull.ms [150.0000-1500.0000]

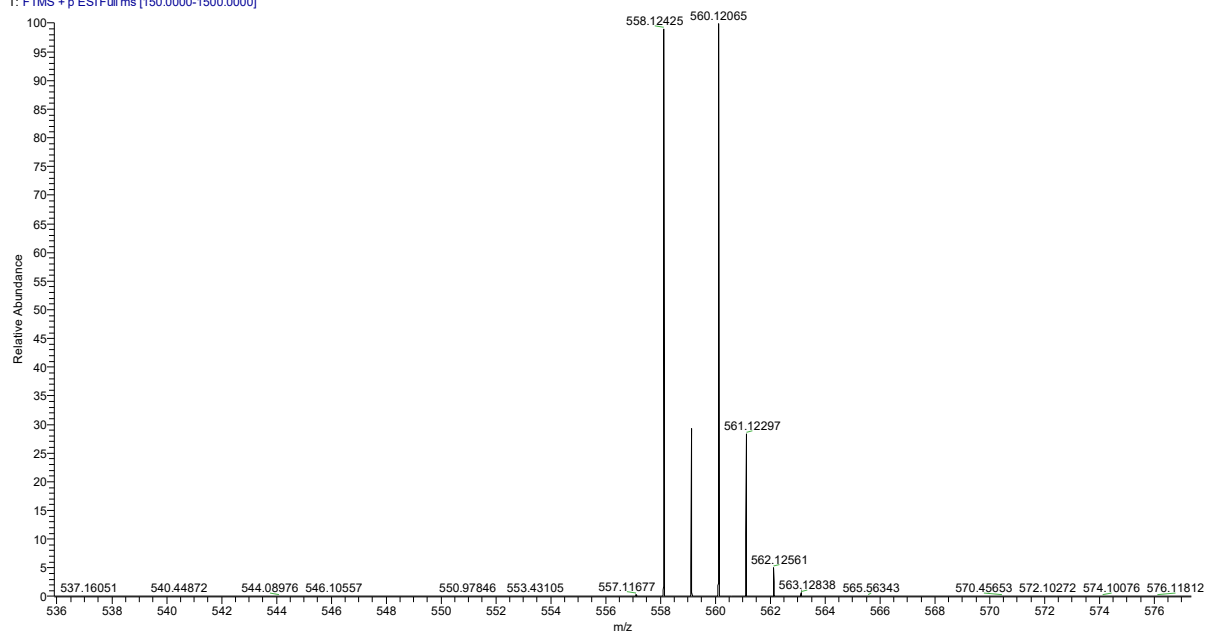


Figure S27. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-1-(3-(2-(4-hydroxy-3,5-dimethoxybenzylidene)hydrazine-yl)-3-oxopropyl)-2-methyl-1H-pyrrole-3-carboxylate (8d).

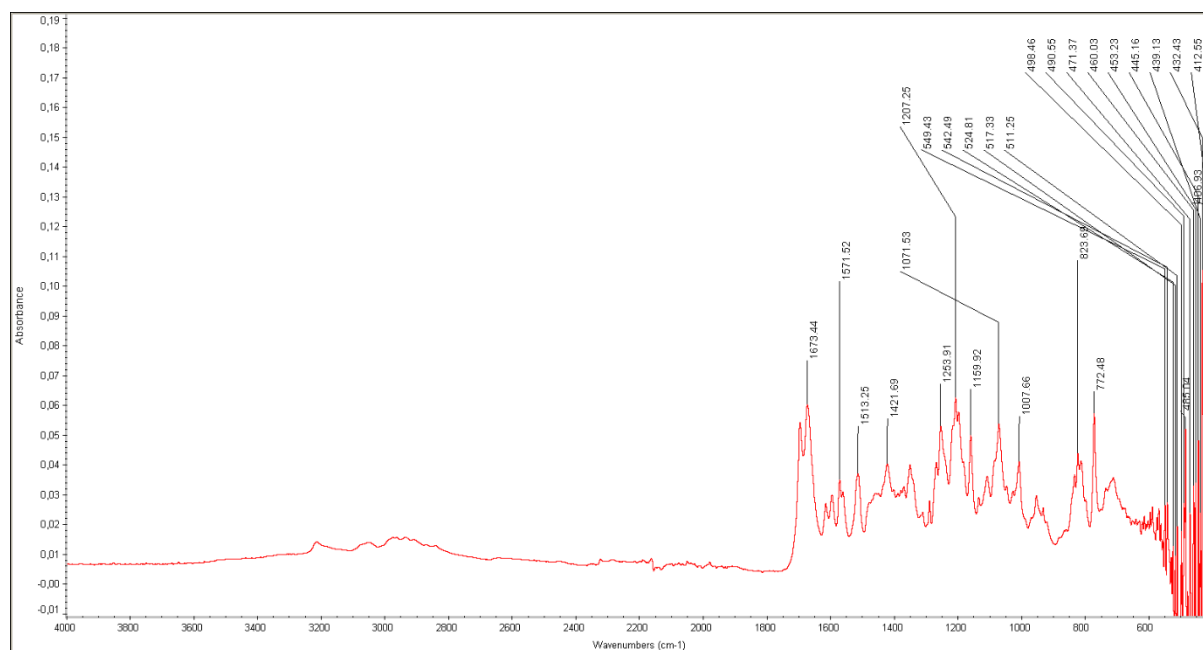


Figure S28. IR spectrum of ethyl 5-(4-bromophenyl)-1-(3-(2-(2,4-dimethoxybenzylidene)hydrazinyl)-3-oxo-propyl)-2-methyl-1H-pyrrole-3-carboxylate (8e).

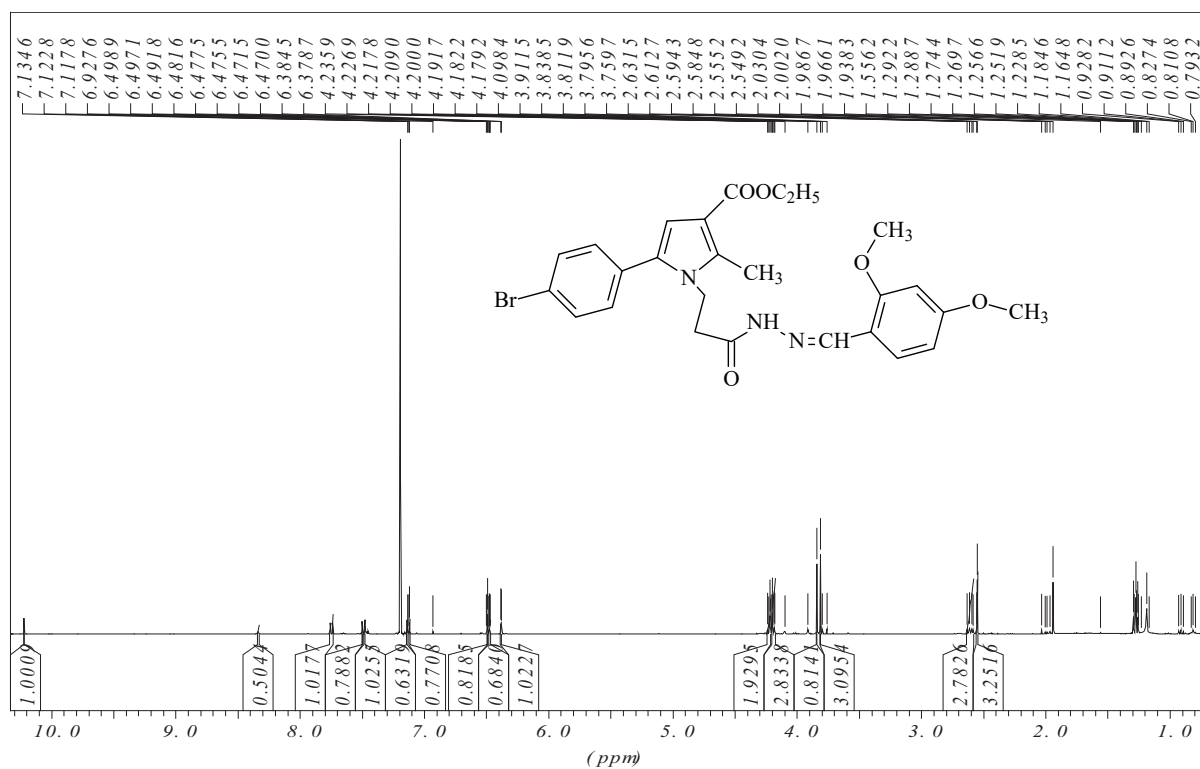


Figure S29. ¹H-NMR spectrum (CDCl₃, 600 MHz) of compound 8e.

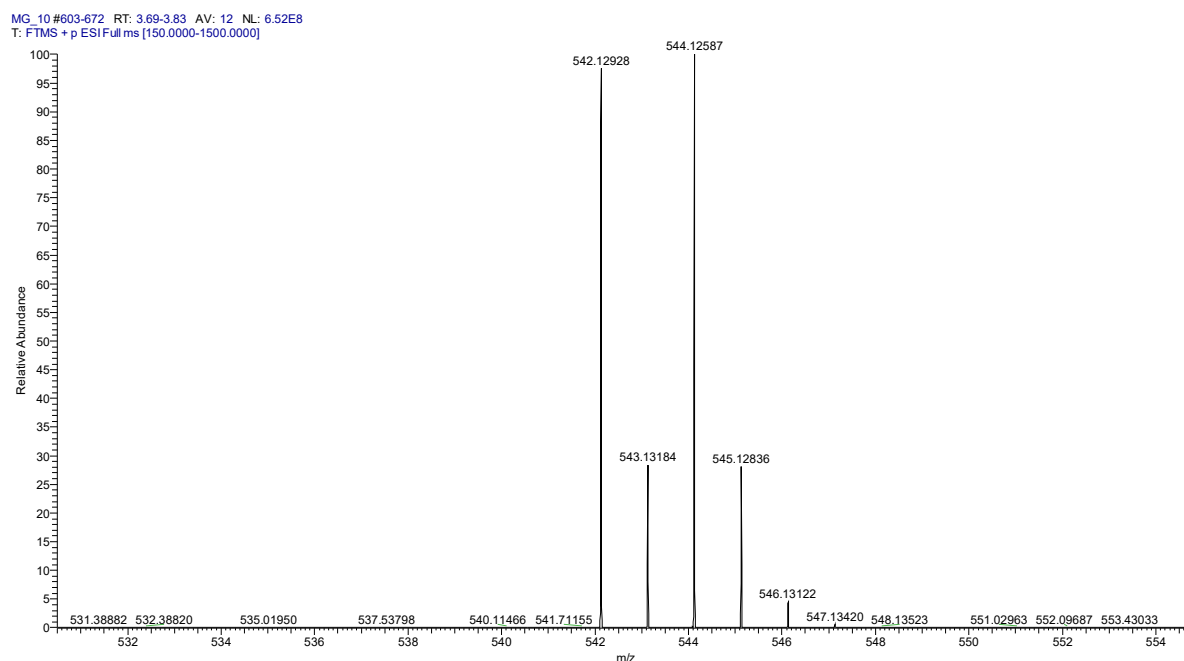


Figure S30. MS spectrum (ESI) of ethyl 5-(4-bromophenyl)-1-(3-(2-(2,4-dimethoxybenzylidene)hydrazinyl)-3-oxo-propyl)-2-methyl-1H-pyrrole-3-carboxylate (8e).