

Article

Supplementary Material: Antioxidant and Cytotoxic Activity of New Polyphenolic Derivatives of Quinazolin-4(3H)-one: Synthesis and In Vitro Activities Evaluation

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1. Figures

1.1. The IR spectra

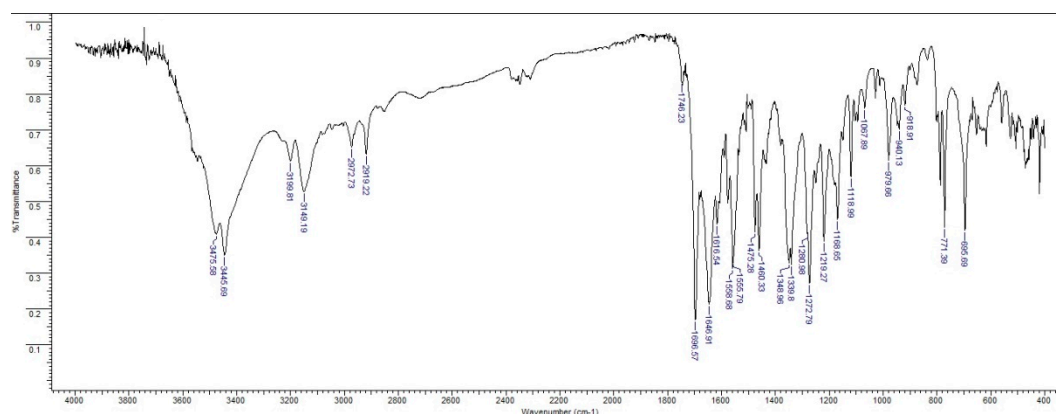


Figure S1. The IR spectrum for the compound 5a.

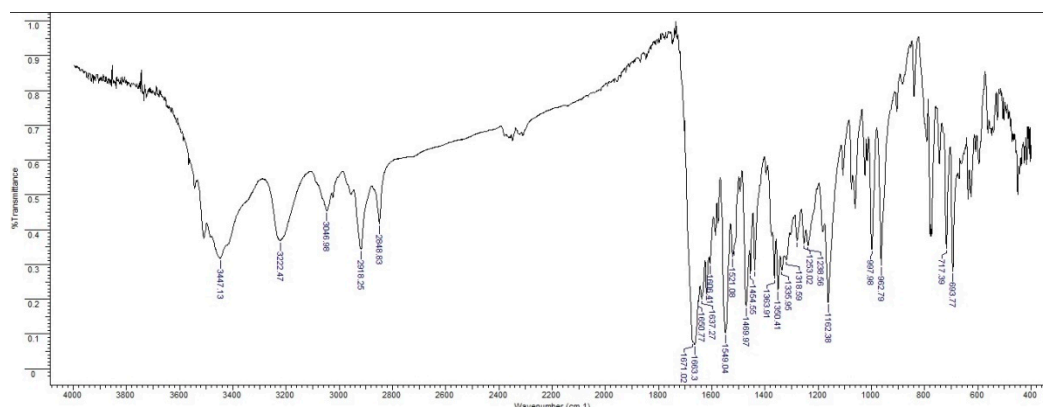


Figure S2. The IR spectrum for the compound 5b.

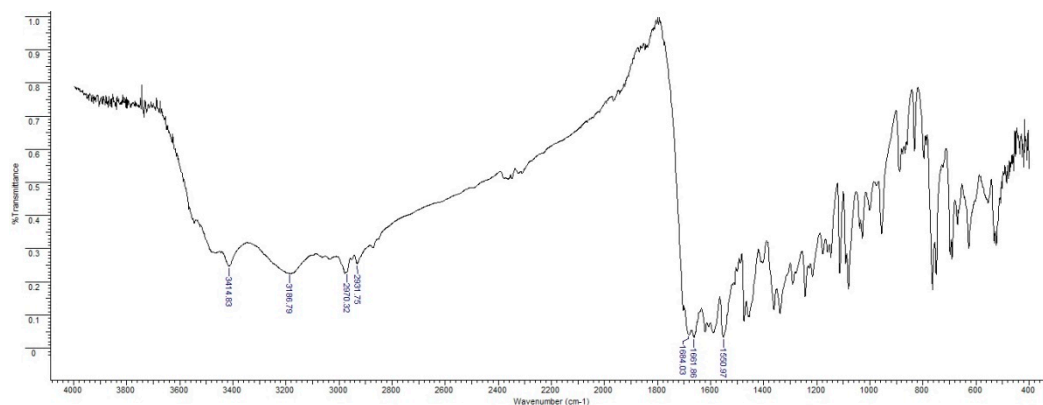


Figure S3. The IR spectrum for the compound **5c**.

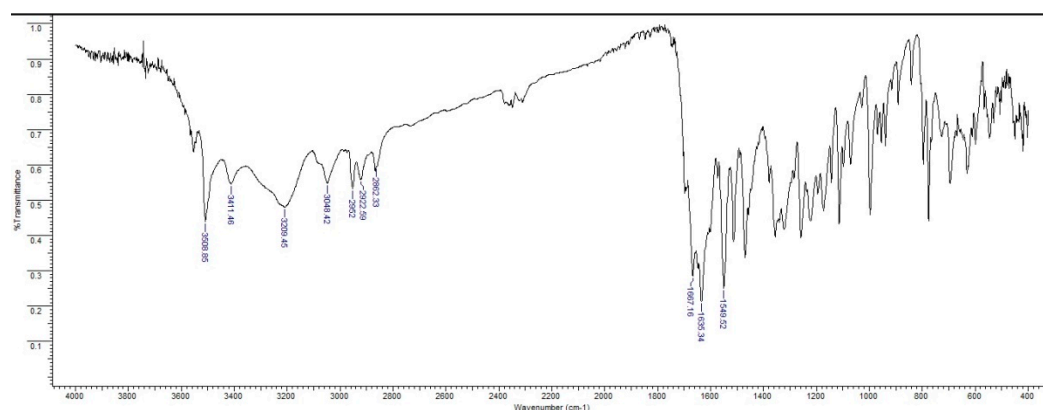


Figure S4. The IR spectrum for the compound **5d**.

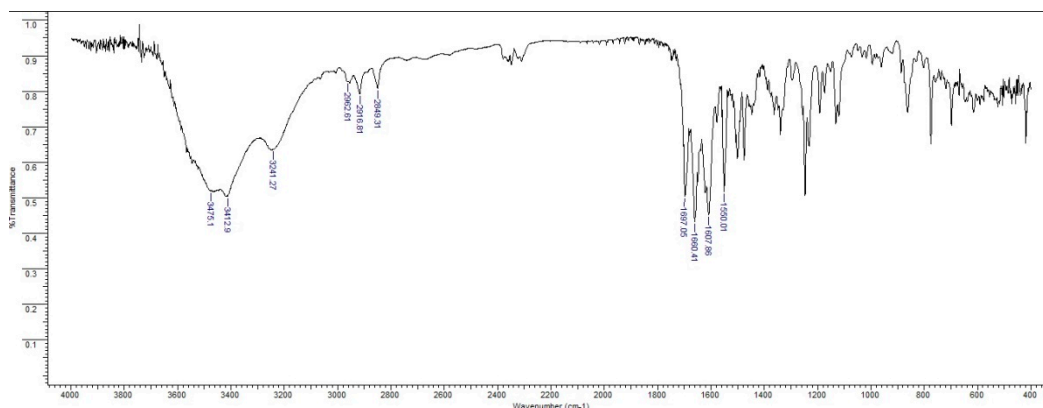


Figure S5. The IR spectrum for the compound **6a**.

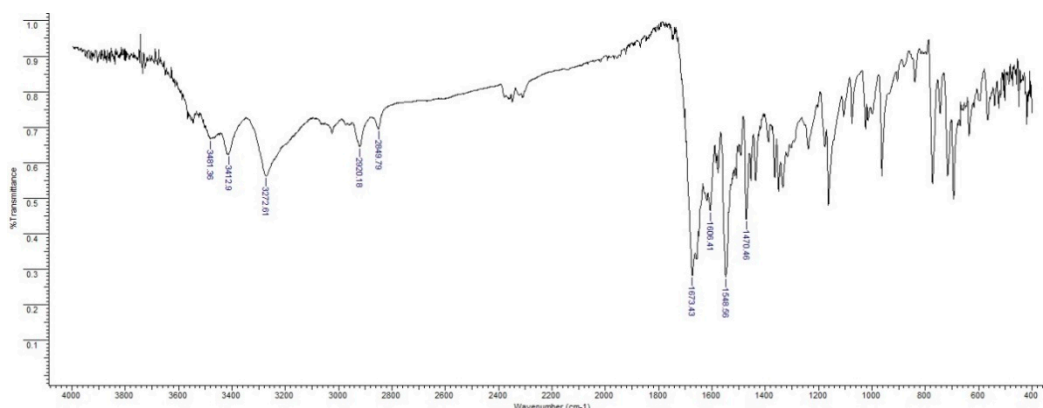


Figure S6. The IR spectrum for the compound **6b**.

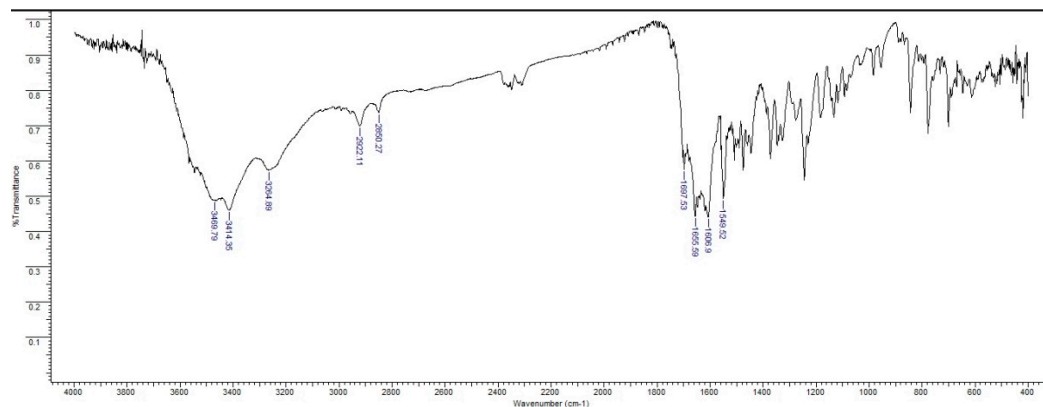


Figure S7. The IR spectrum for the compound 6c.

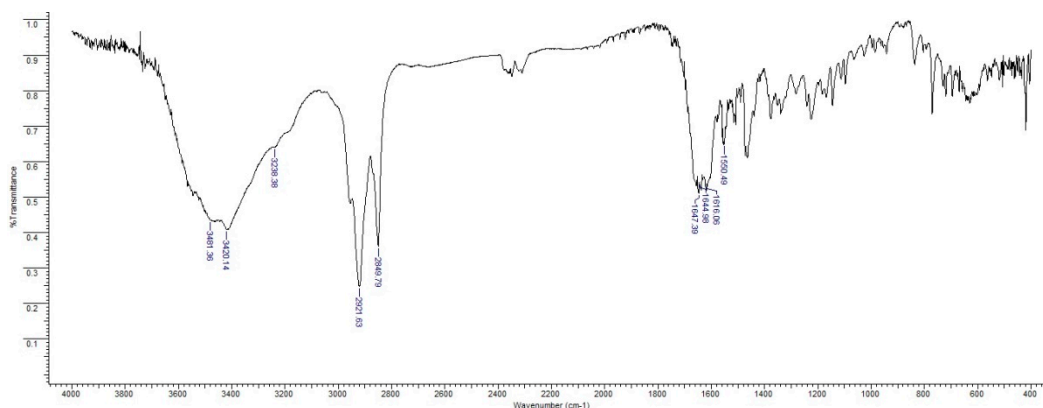


Figure S8. The IR spectrum for the compound 6d.

1.2. The MS spectra

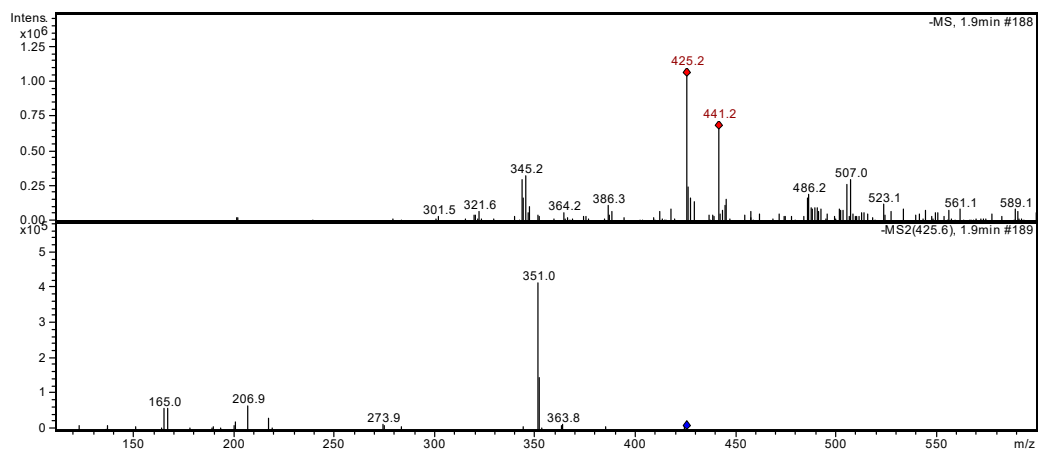


Figure S9. The MS spectrum for the compound 5a.

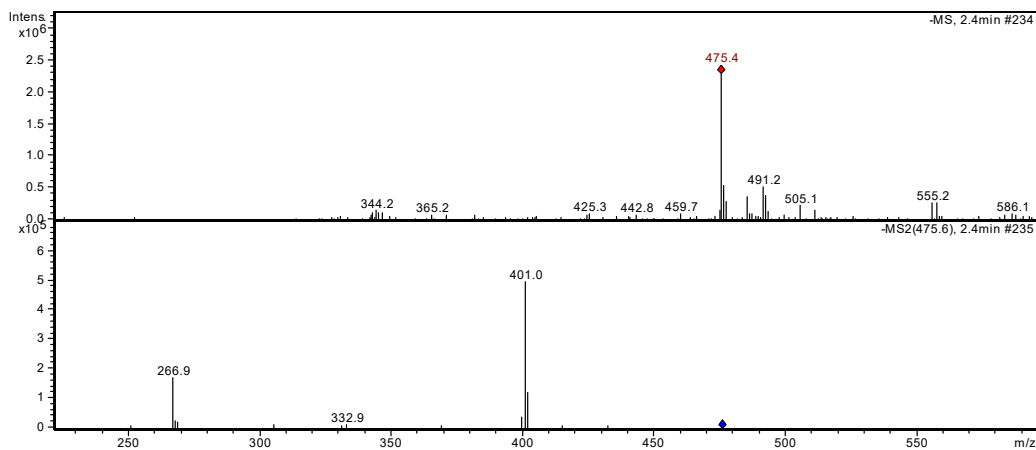


Figure S10. The MS spectrum for the compound 5b.

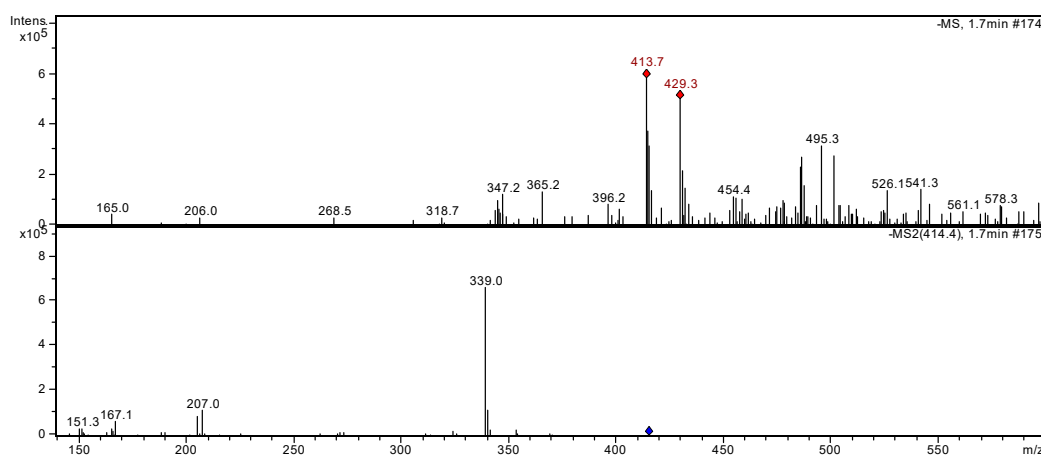


Figure S11. The MS spectrum for the compound 5c.

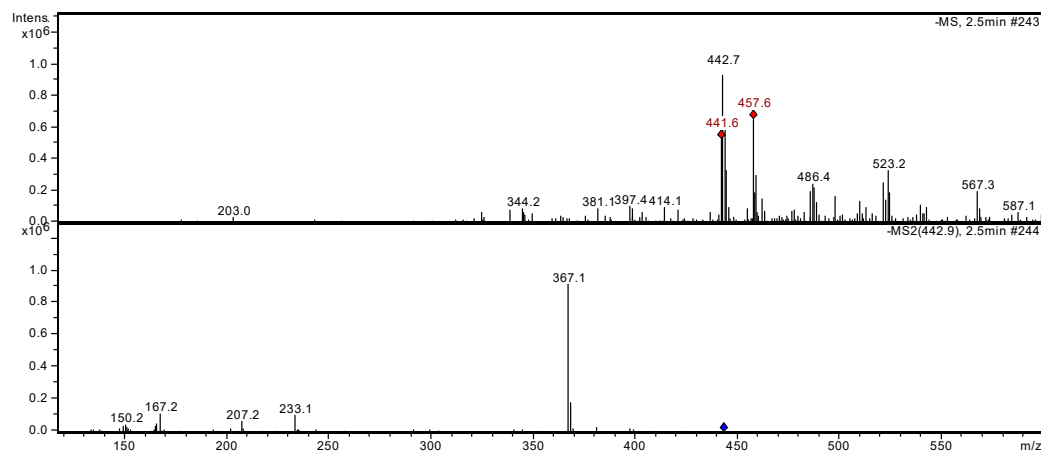


Figure S12. The MS spectrum for the compound 5d.

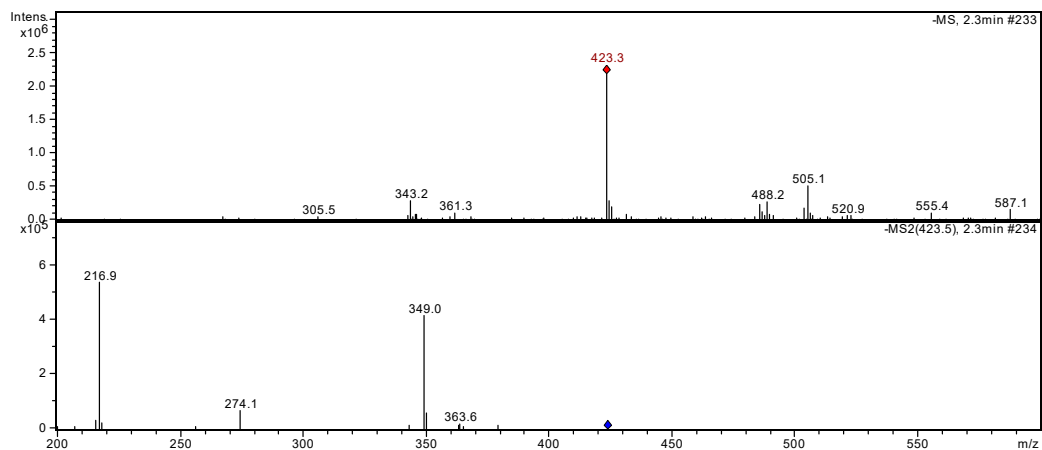


Figure S13. The MS spectrum for the compound 6a.

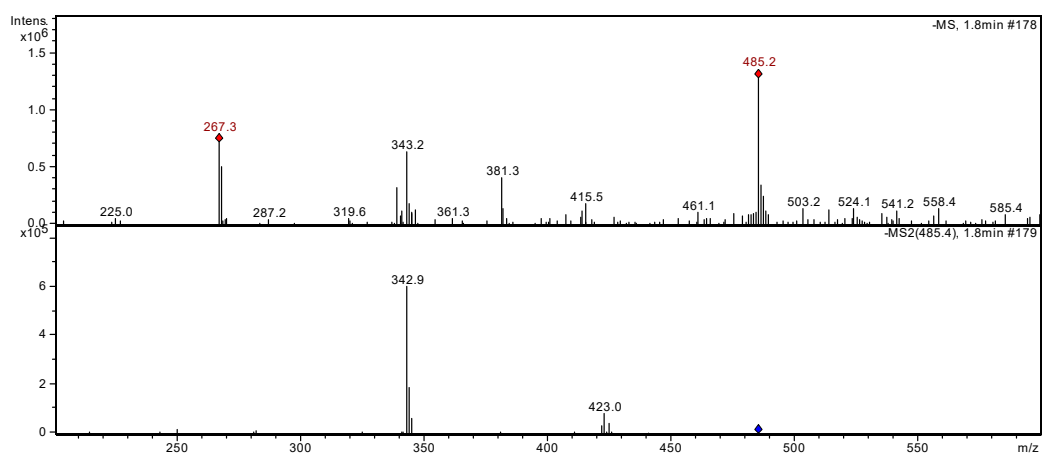


Figure S14. The MS spectrum for the compound 6b.

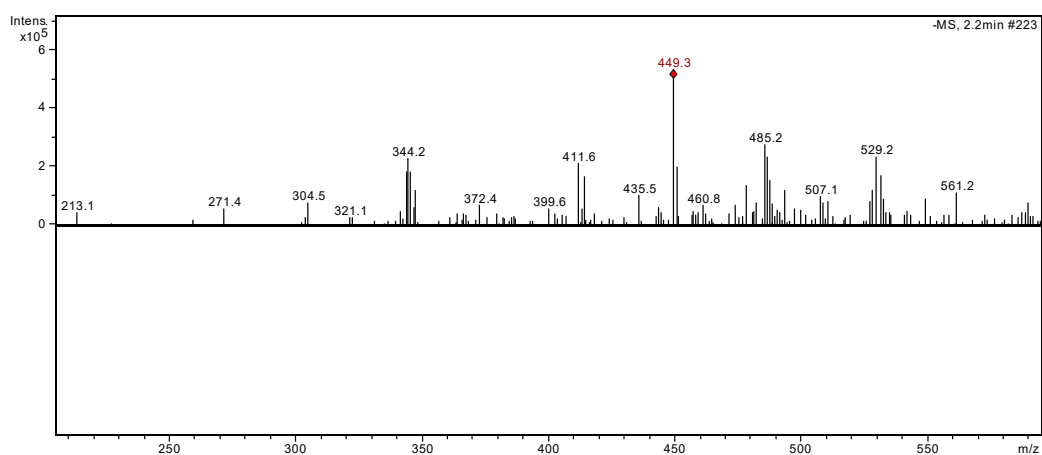


Figure S15. The MS spectrum for the compound 6c.

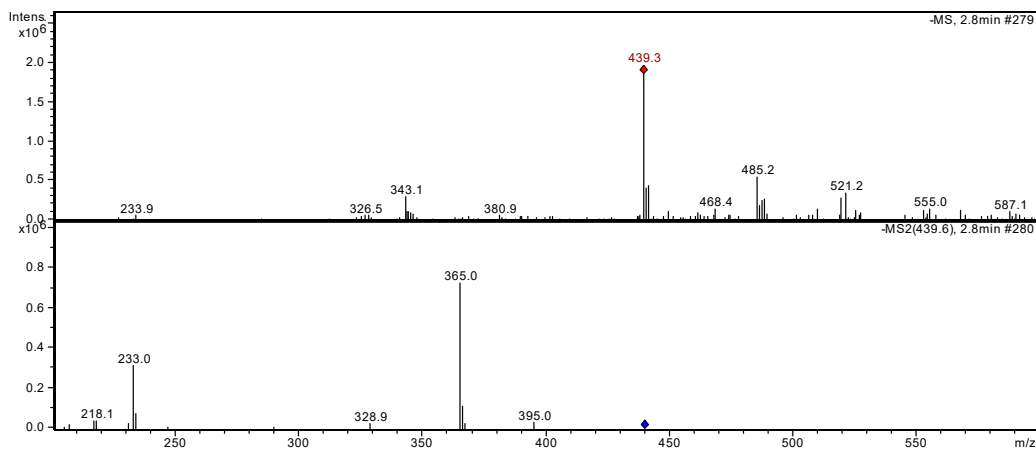


Figure S16. The MS spectrum for the compound 6d.

1.1. The ^1H -NMR spectrum

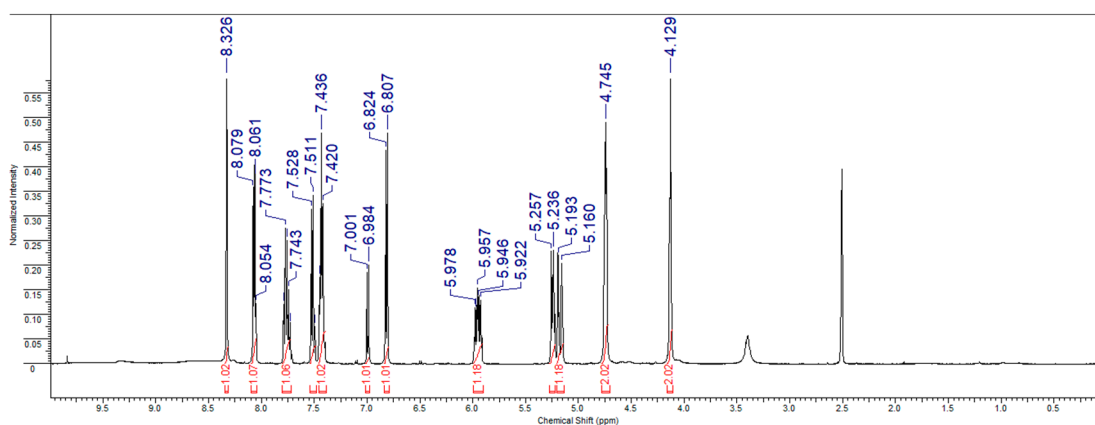


Figure S17. The ^1H -NMR spectrum for the compound 5a. The integral label for the triplet at 7.511 ppm is 1.04 and for the multiplet at 5.239 ppm is 1.04.

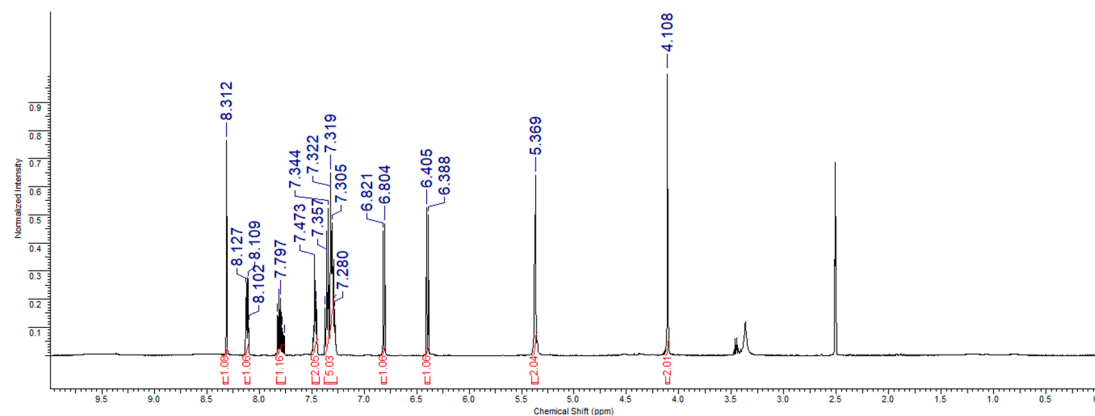


Figure S18. The ^1H -NMR spectrum for the compound 5b.

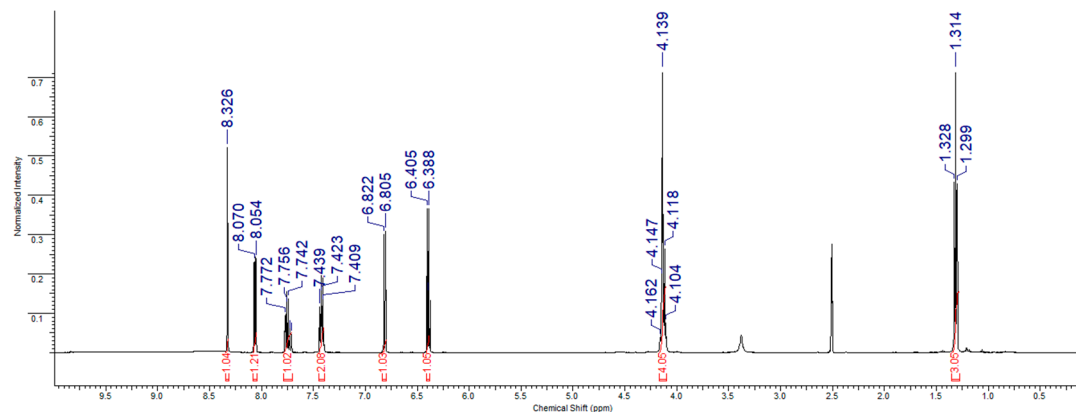


Figure S19. The ^1H -NMR spectrum for the compound **5c**.

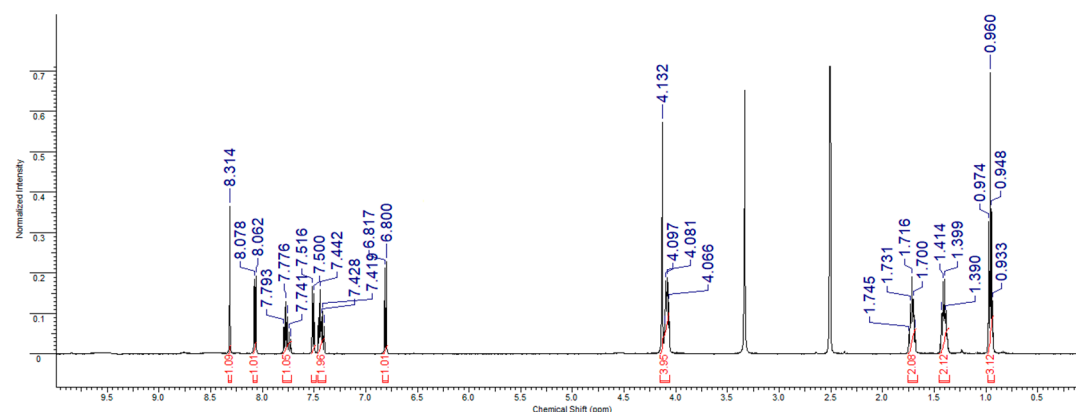


Figure S20. The ^1H -NMR spectrum for the compound **5d**. The integral label for the doublet at 7.508 ppm is 1.09.

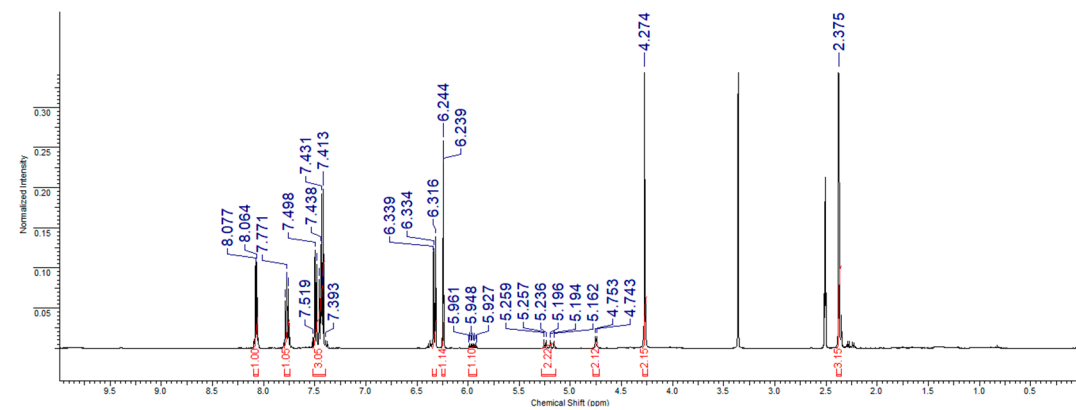
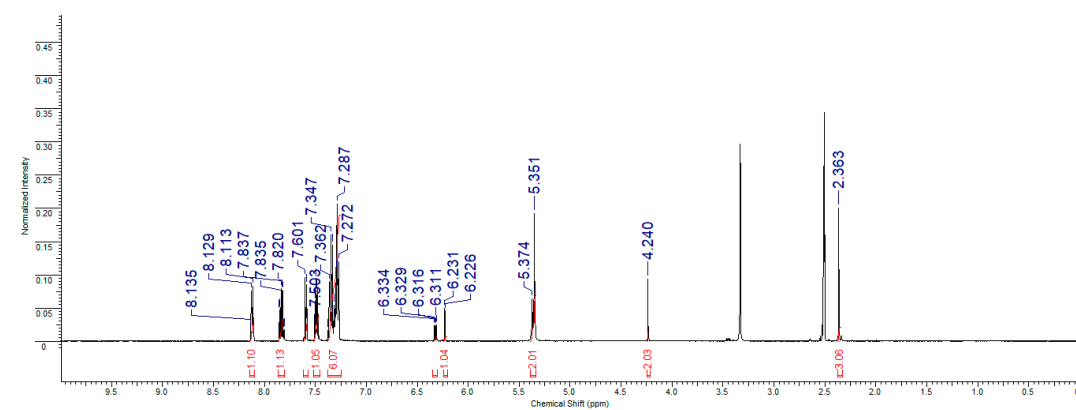


Figure S21. The ^1H -NMR spectrum for the compound **6a**. The integral label for the doublet of doublets at 6.327 ppm is 1.19.



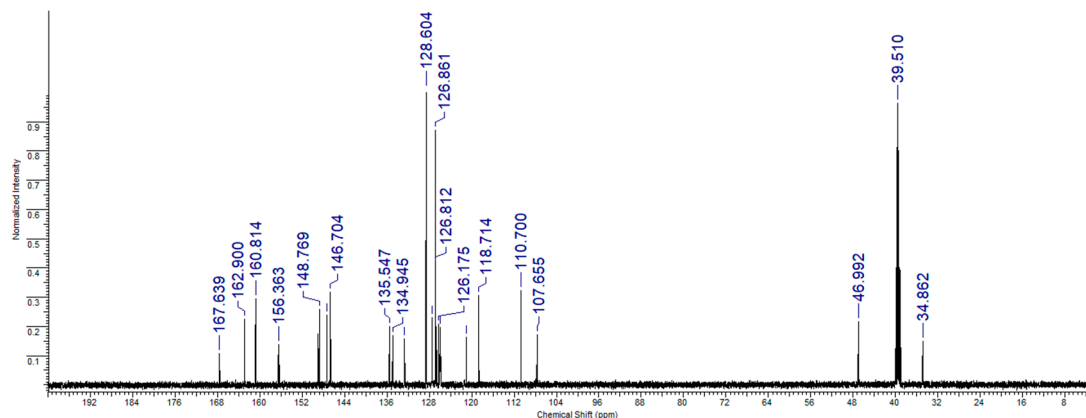


Figure S26. The ^{13}C -NMR spectrum for the compound **5b**.

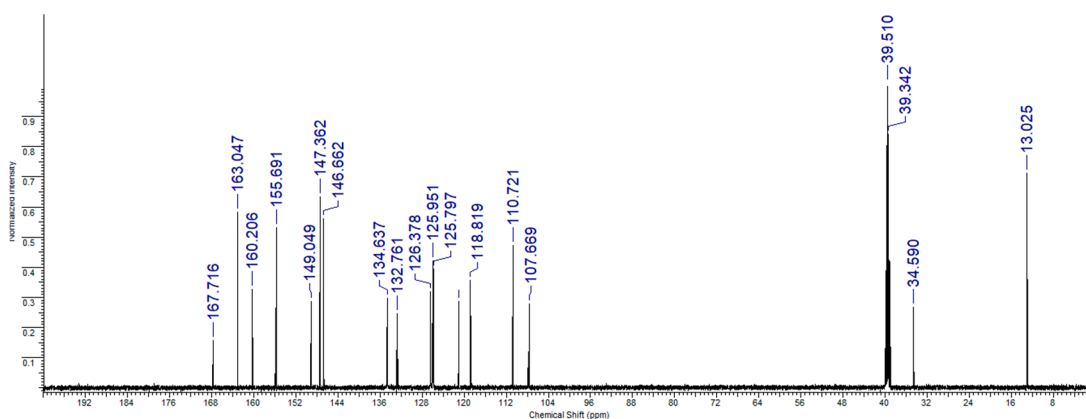


Figure S27. The ^{13}C -NMR spectrum for the compound **5c**.

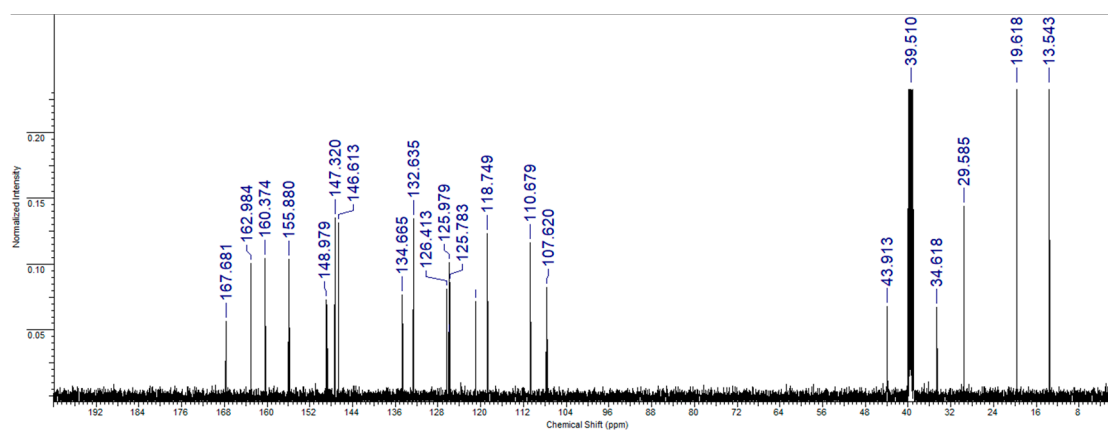


Figure S28. The ^{13}C -NMR spectrum for the compound **5d**.

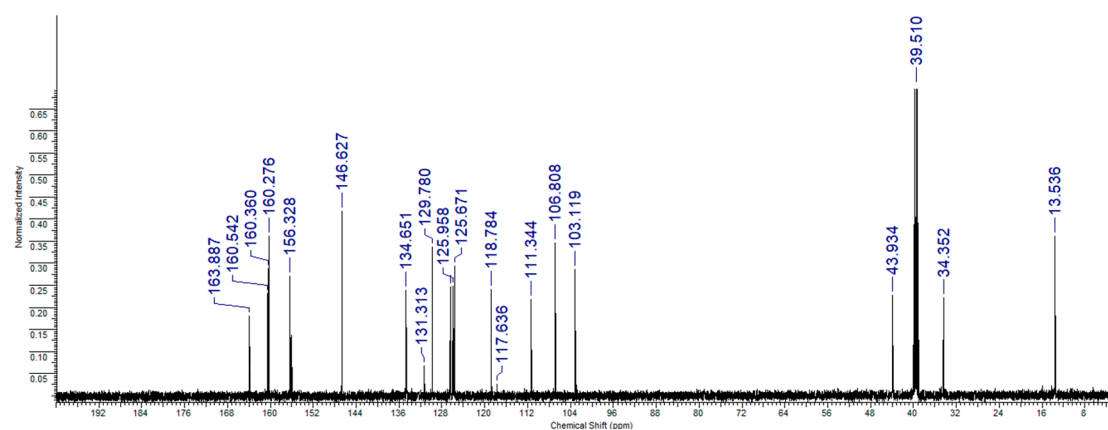


Figure S29. The ^{13}C -NMR spectrum for the compound **6a**.

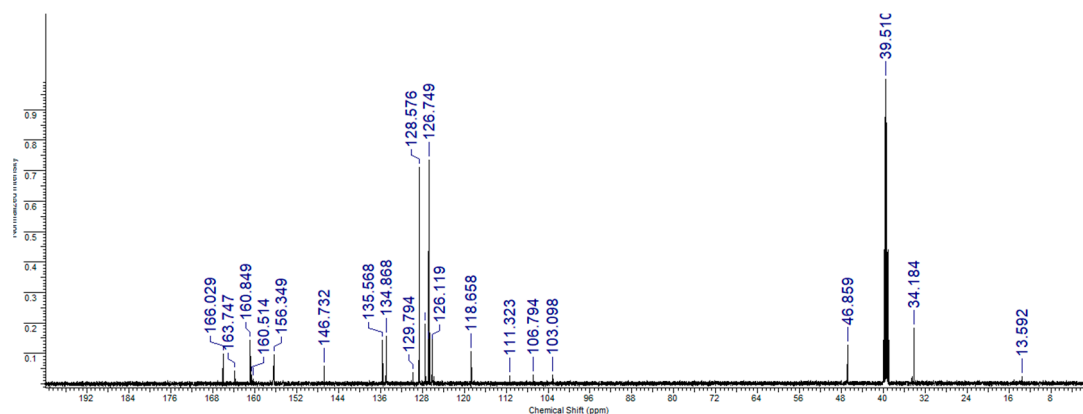


Figure S30. The ^{13}C -NMR spectrum for the compound **6b**.

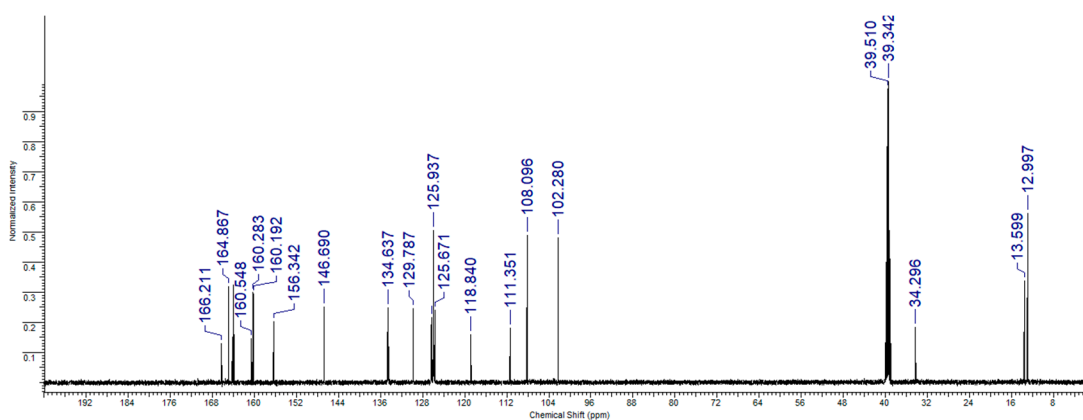


Figure S31. The ^{13}C -NMR spectrum for the compound **6c**.

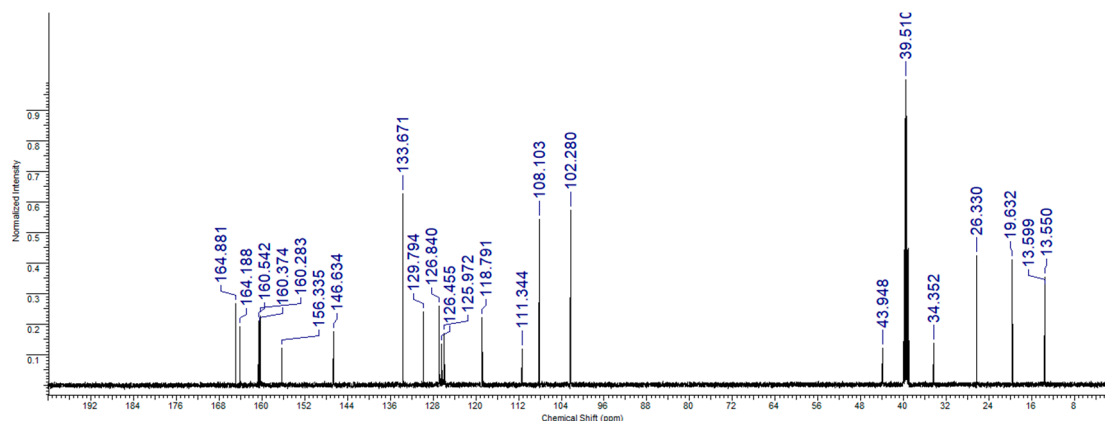


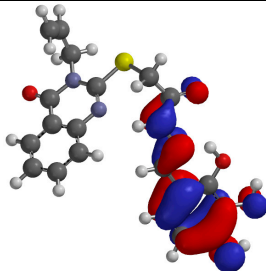
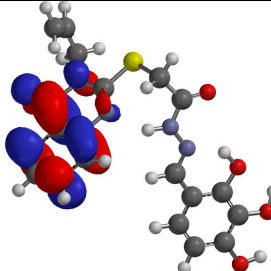
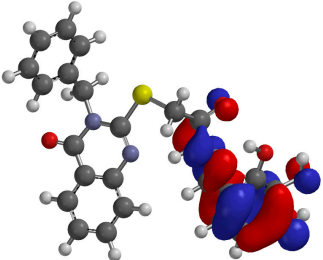
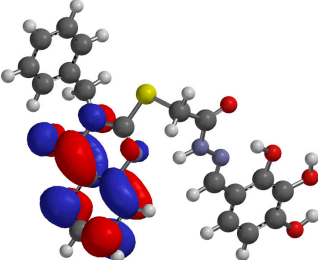
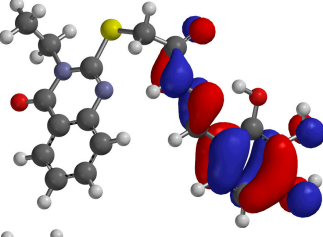
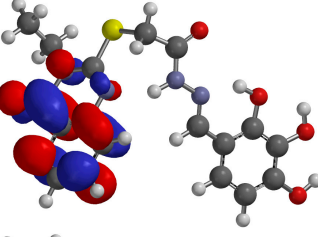
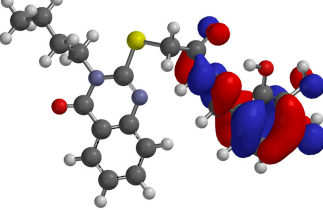
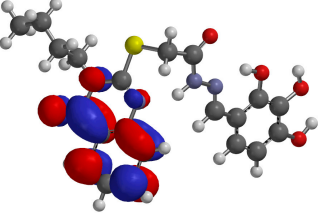
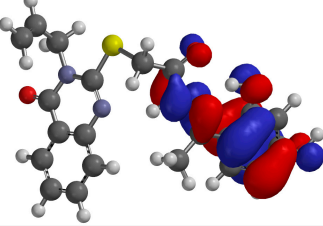
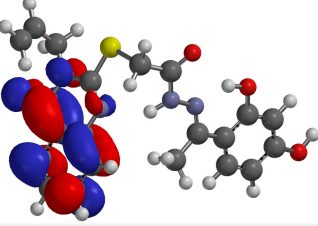
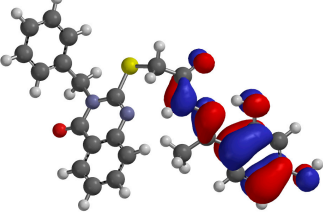
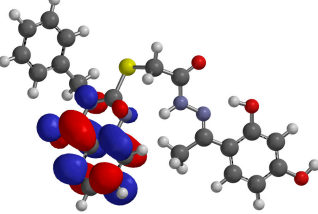
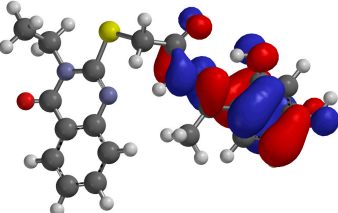
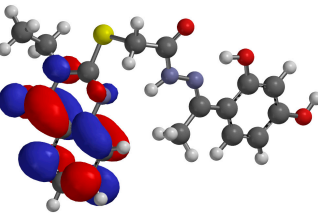
Figure S32. The ^{13}C -NMR spectrum for the compound **6d**.

2. Tables

2.1. The depiction of HOMO and LUMO and the depiction of the spin density maps of the phenol group radicalization for the compounds **5a-d** and **6a-d**

Table S1. The depiction of HOMO and LUMO for the compounds **5a-d** and **6a-d**

Compound	HOMO	LUMO
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Compound	HOMO	LUMO
5a		
5b		
5c		
5d		
6a		
6b		
6c		

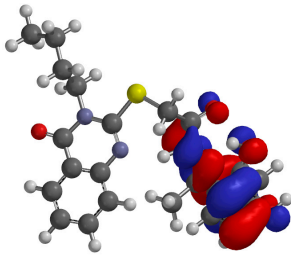
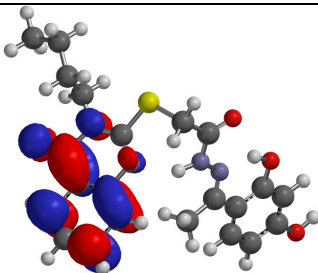
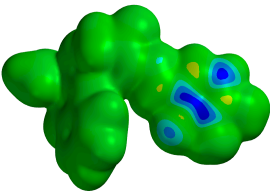
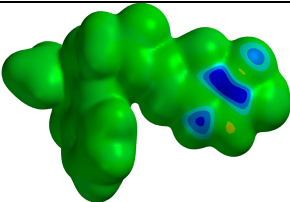
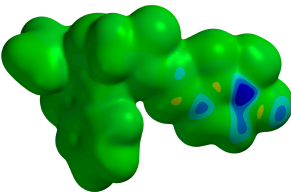
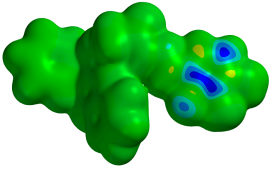
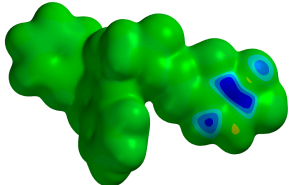
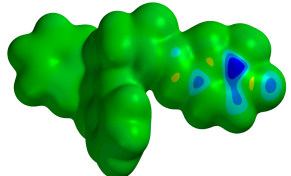
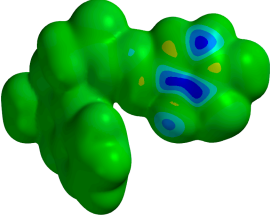
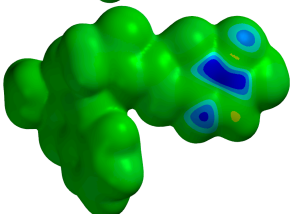
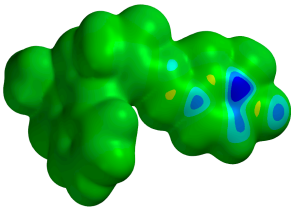
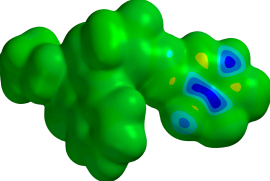
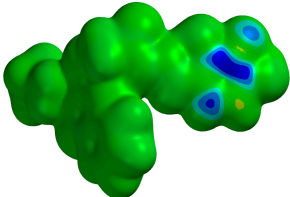
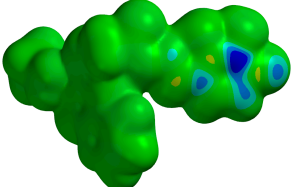
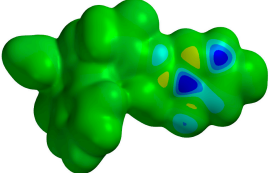
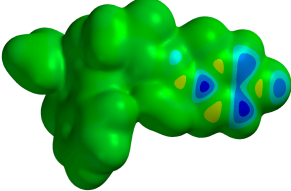
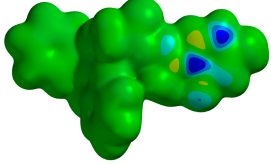
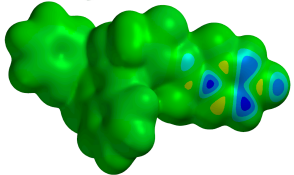
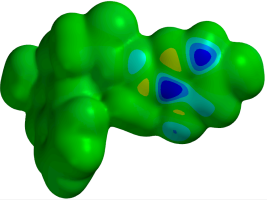
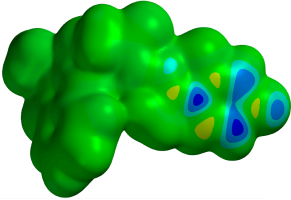
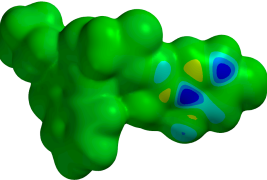
Compound	HOMO	LUMO
6d		

Table S2. The depiction of spin density maps for the phenol group radicalization for the compounds 5a-d and 6a-d

Compound	Spin density map depending on the phenolic radical		
	ortho (H1)	meta (H2)	para (H3)
5a			
5b			
5c			
5d			
6a		N/A	
6b		N/A	

Compound	Spin density map depending on the phenolic radical		
	ortho (H1)	meta (H2)	para (H3)
6c		N/A	
6d		N/A	