

Dark Blue Azo Dye Degradation by Electro-Fenton process and reaction mechanism prediction via theoretical Fukui Function Analysis

Nour El Houda Slama¹, Ghazza Masmoudi*¹, Maksym Fizer^{2,3}, Abdelkarim Mahdhi⁴, Ruslan Mariychuk⁵ and Hatem Dhaouadi¹

¹ Laboratory of Environmental Chemistry and Clean Processes, Faculty of Sciences of Monastir, University of Monastir, Tunisia.

² Department of Organic Chemistry, Educational Scientific Institute of Chemistry and Ecology, Uzhhorod National University, Fedinets, Str. 53/1, Uzhhorod, 88000, Ukraine.

³ Department of Chemistry, University of Nevada, Reno, 1664 N. Virginia Street, Reno, NV 89557-0216, USA

⁴ Laboratory of Analysis, Treatment and Valorization of Environmental Pollutants and Products, Faculty of Pharmacy, Monastir University, Monastir, Tunisia

⁵ Department of Ecology, Faculty of Humanities and Natural Sciences, University of Presov, 17th November str. 1, Presov, 08001, Slovakia.

*Corresponding author. Tel: +21650695670. Email. ghazza.massmoudi@fsm.u-monastir.tn
(Ghazza Masmoudi), 16-digit ORCID identifier 0000-0002-4236-2224

Supplementary information

Optimized structures and radical Fukui function plot of species considered in the degradation mechanism of DBA.

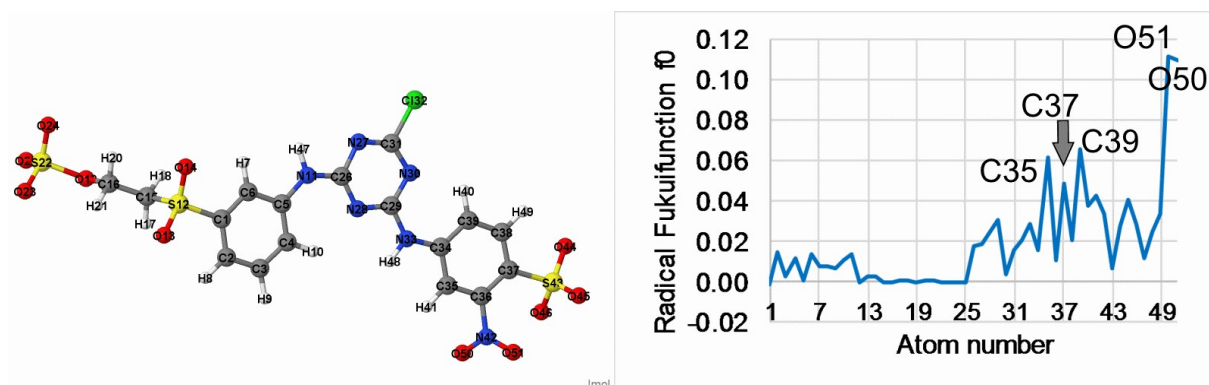


Figure S1. The optimized structure and radical Fukui function plot of A1.

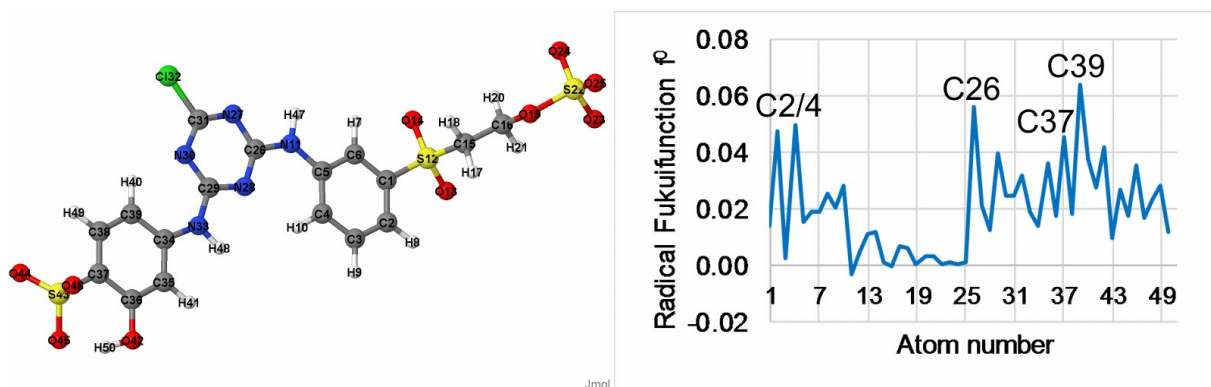


Figure S2. The optimized structure and radical Fukui function plot of A2.

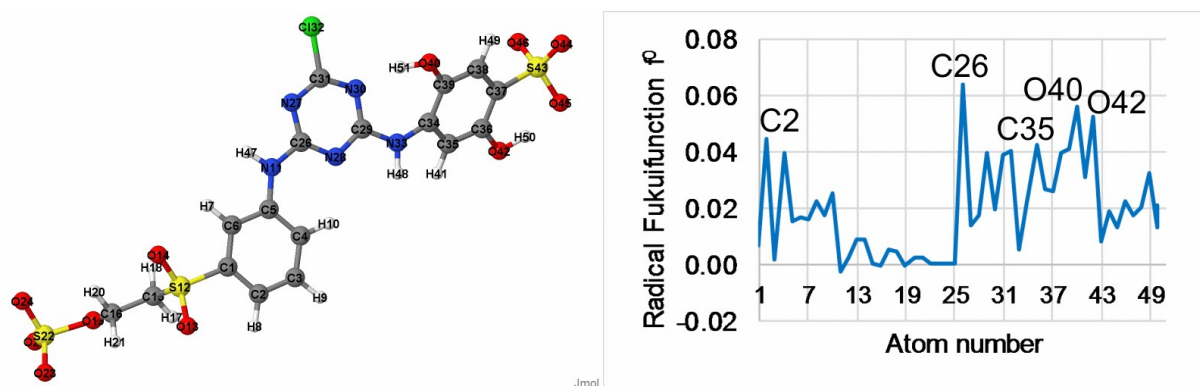


Figure S3. The optimized structure and radical Fukui function plot of A3.

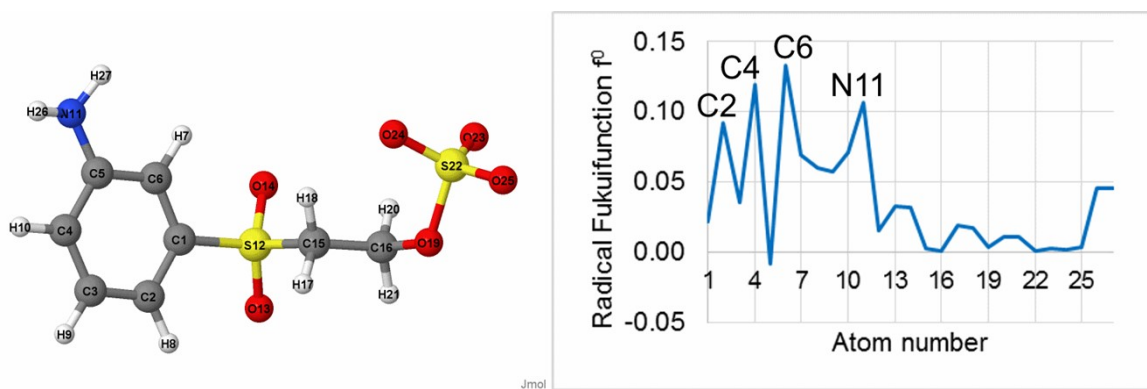
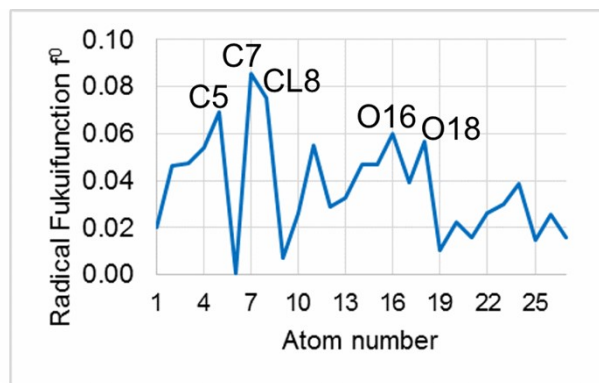
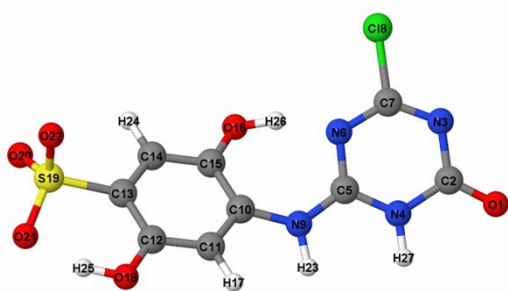
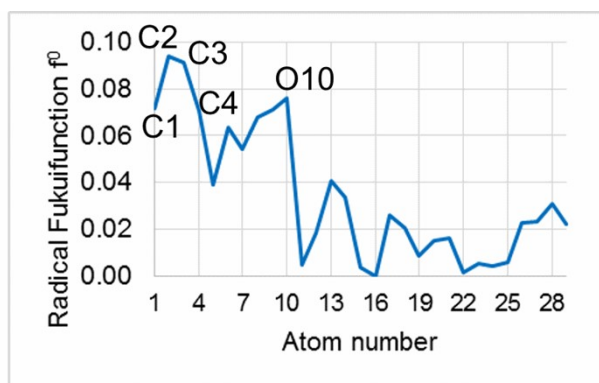
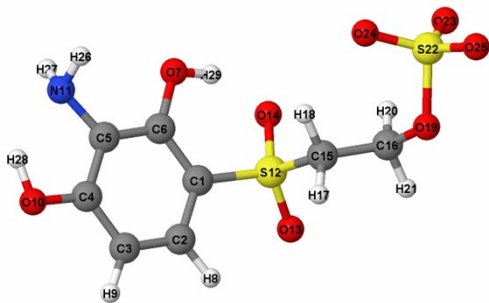


Figure S4. The optimized structure and radical Fukui function plot of A4a.



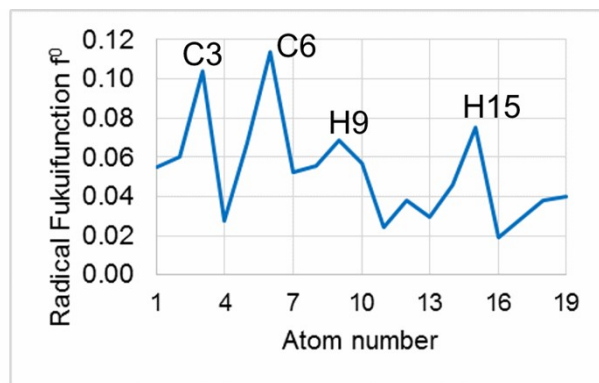
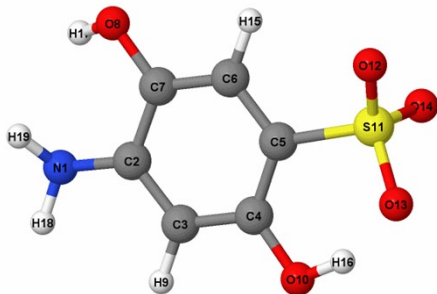
Jmol

Figure S5. The optimized structure and radical Fukui function plot of **A4b**.



Jmol

Figure S6. The optimized structure and radical Fukui function plot of **A5a**.



Jmol

Figure S7. The optimized structure and radical Fukui function plot of **A5b**.

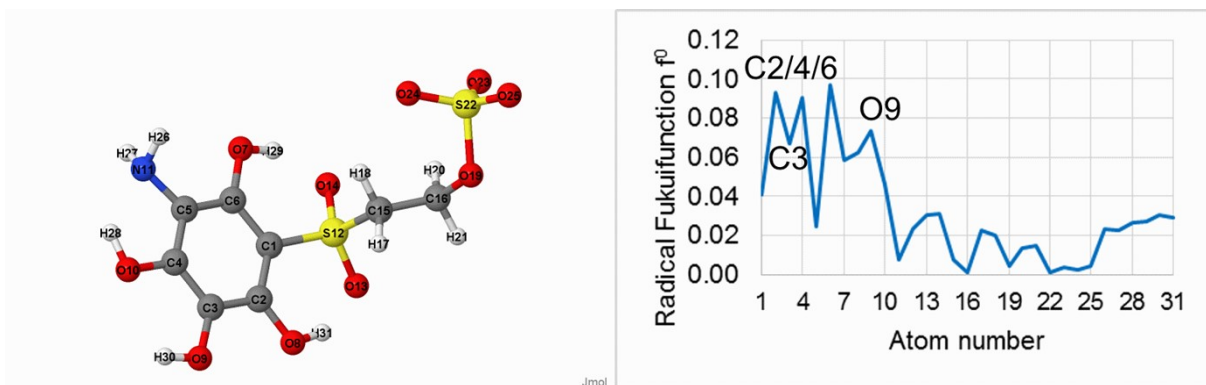


Figure S8. The optimized structure and radical Fukui function plot of **A6a**.

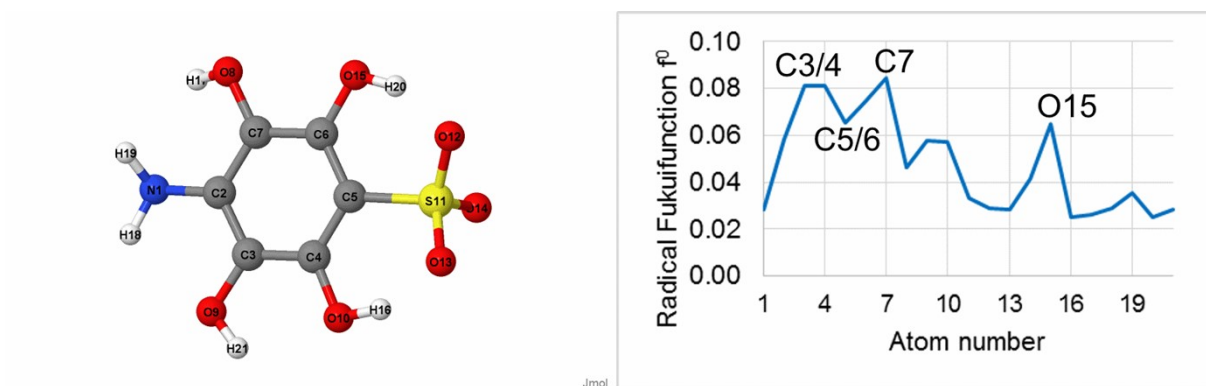


Figure S9. The optimized structure and radical Fukui function plot of **A6b**.

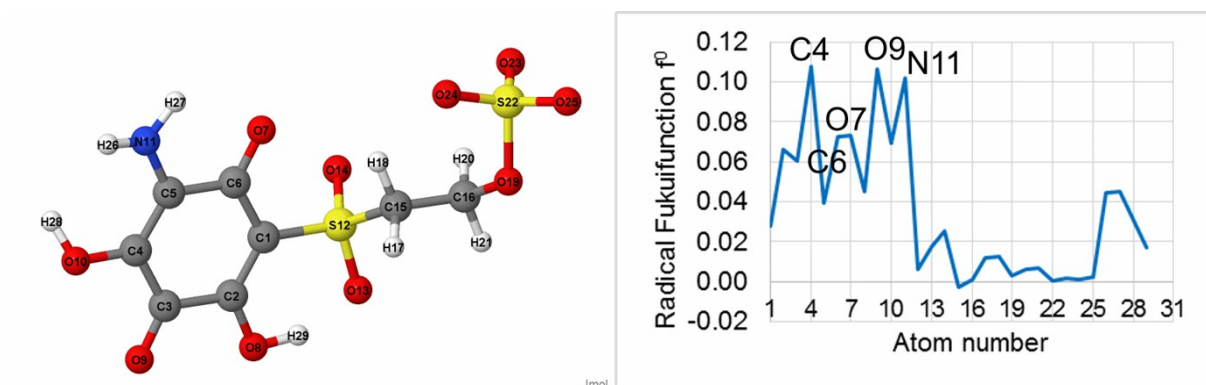
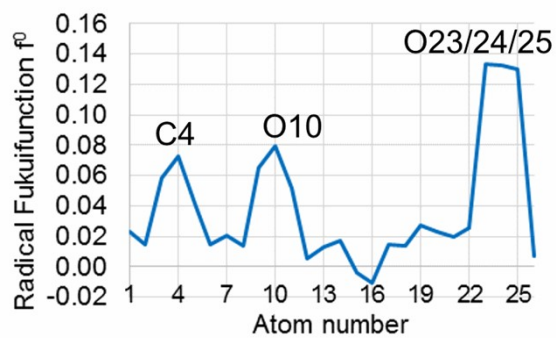
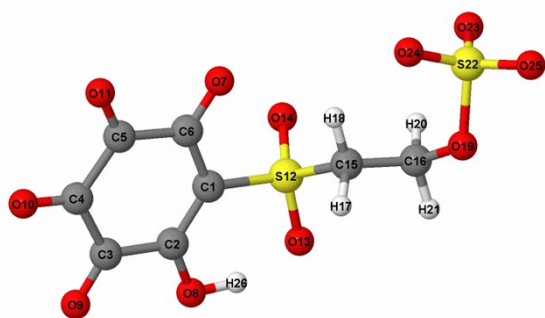
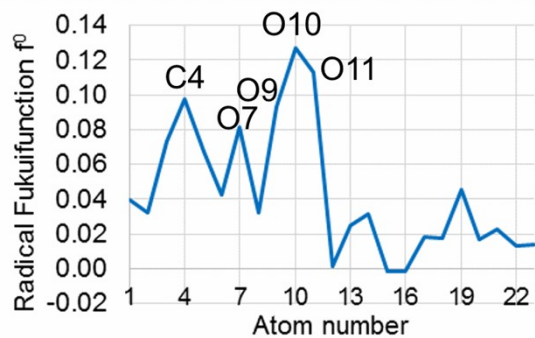
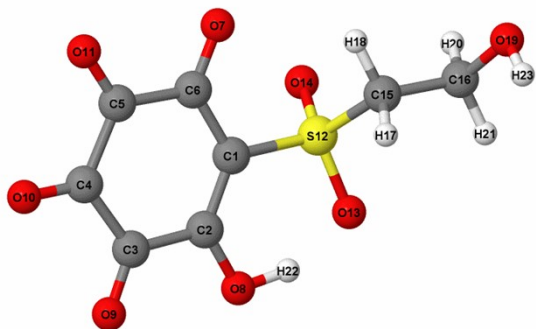


Figure S10. The optimized structure and radical Fukui function plot of **A7a**.



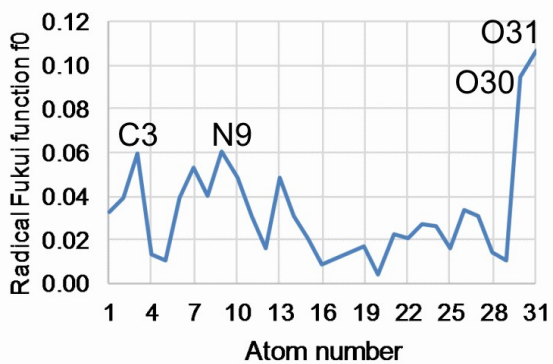
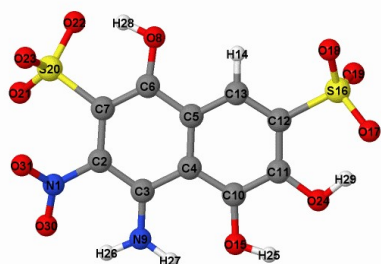
Jmol

Figure S11. The optimized structure and radical Fukui function plot of **A8a**.



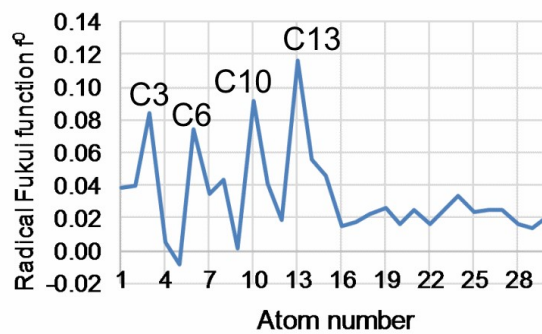
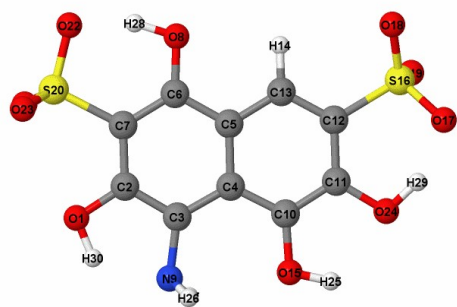
Jmol

Figure S12. The optimized structure and radical Fukui function plot of **A9a**.



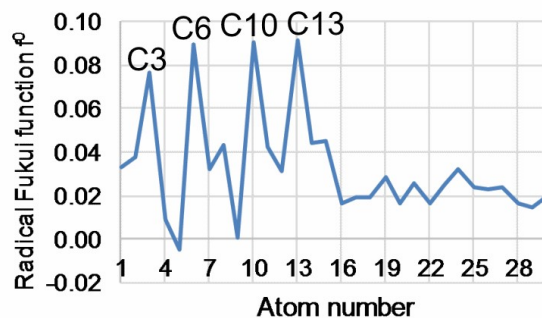
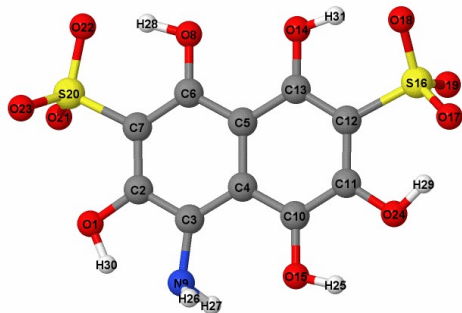
Jmol

Figure S13. The optimized structure and radical Fukui function plot of **B1**.



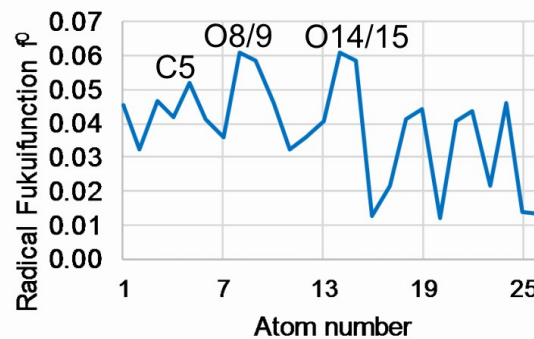
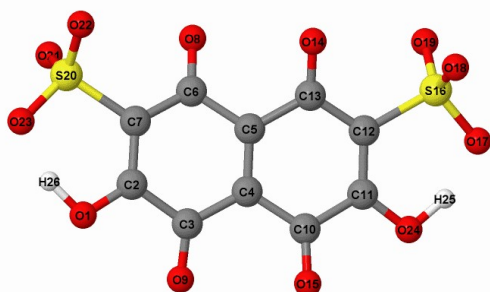
Jmol

Figure S14. The optimized structure and radical Fukui function plot of B2.



Jmol

Figure S15. The optimized structure and radical Fukui function plot of B3.



Jmol

Figure S16. The optimized structure and radical Fukui function plot of B4.

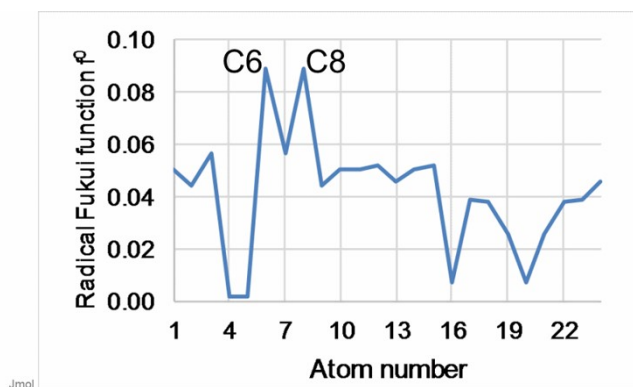


Figure S17. The optimized structure and radical Fukui function plot of C1.

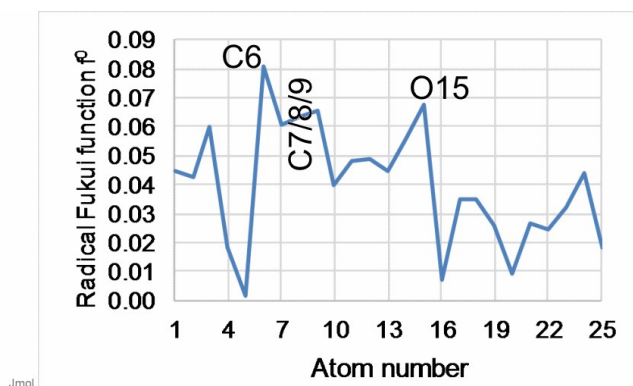
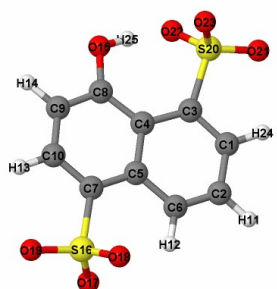


Figure S18. The optimized structure and radical Fukui function plot of C2.

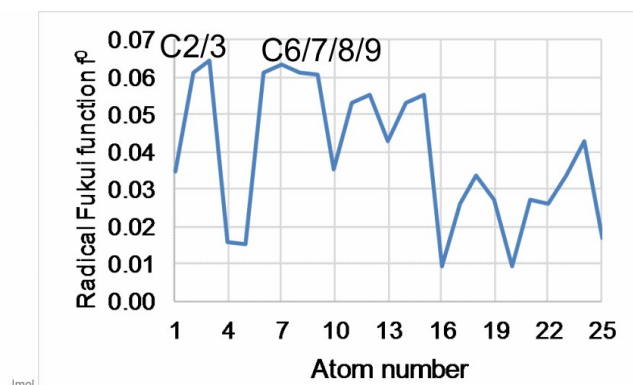
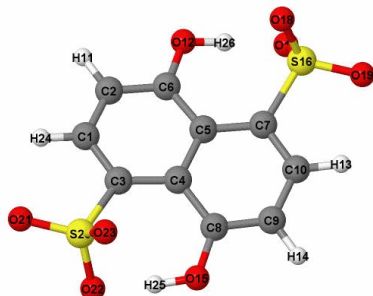


Figure S19. The optimized structure and radical Fukui function plot of C3.