

A sustainable improvement of ω -bromoalkylphosphonates synthesis to access novel KuQuinones

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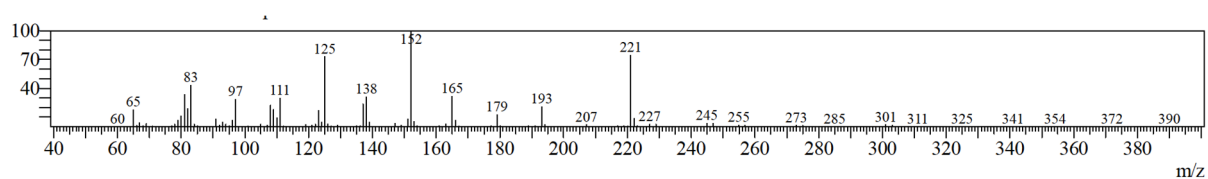
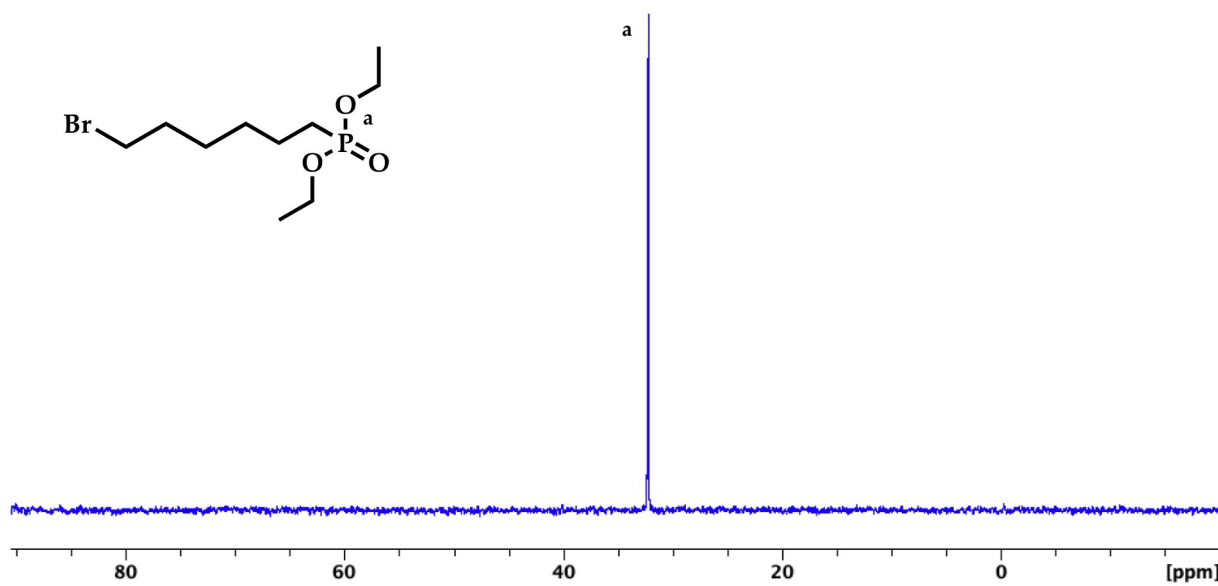
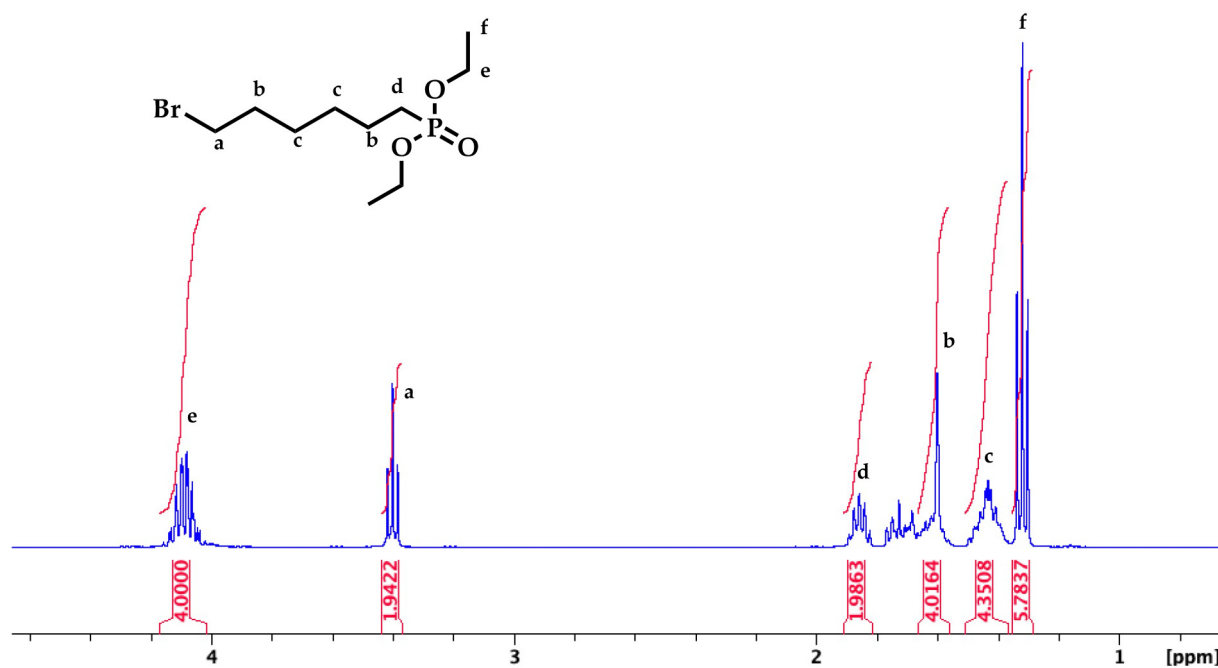
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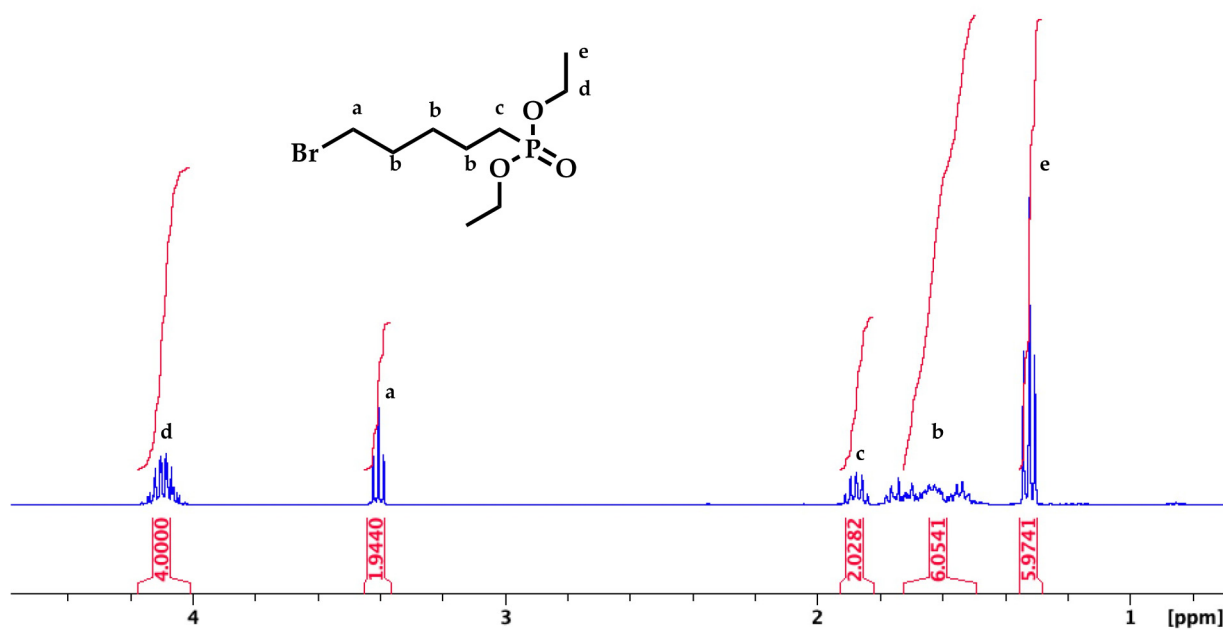


Figure S4. ¹H NMR spectrum of **2** in CDCl₃. ¹H NMR: δ 1.322 (t, J=7.06, 6H), δ 1.475-1.739 (m, 6H), δ 1.826-1.920 (m, 2H), δ 3.404 (t, J=6.72 Hz, 2H), δ 4.013-4.166 (m, 4H).

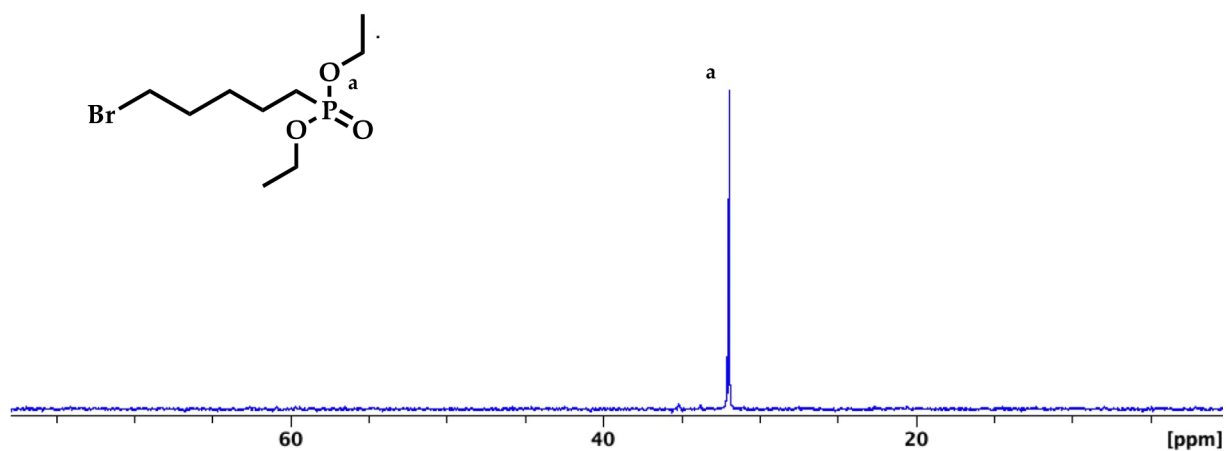


Figure S5. ³¹P NMR spectrum of **2** in CDCl₃. ³¹P NMR: δ 31.928 (s, 1P).

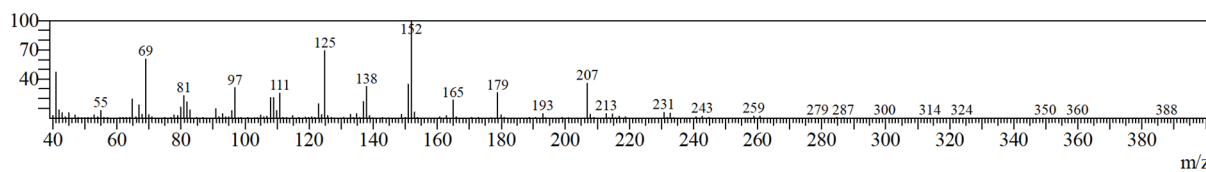


Figure S6. Mass spectrum of **2** (EI, 70 eV): $m/z = 207$ [M-Br]⁺; $m/z = 152$ [[•]CH₂P(=OH)(OCH₂CH₃)₂]⁺; $m/z = 125$ [152-C₂H₅]⁺.

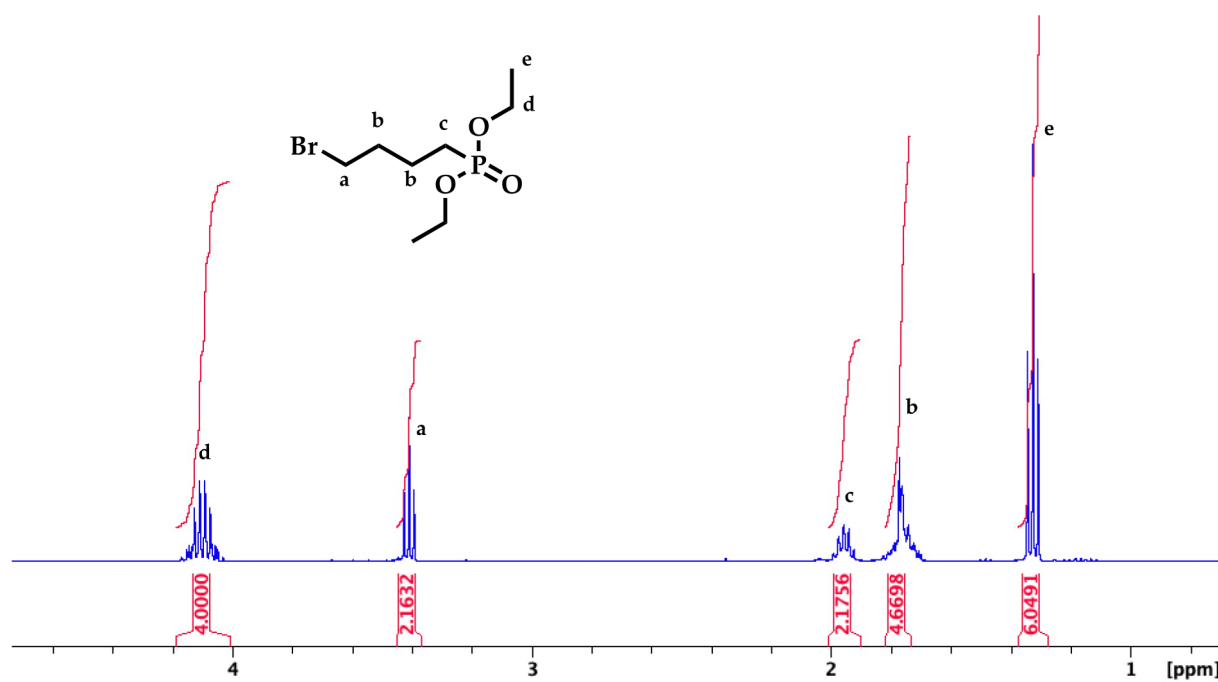


Figure S7. ¹H NMR spectrum of 3 in CDCl₃. ¹H NMR: δ 1.326 (t, J=7.05, 6H), δ 1.730-1.821 (m, 4H), δ 1.918-2.002 (m, 2H), δ 3.409 (t, J=6.56 Hz, 2H), δ 4.042-4.156 (m, 4H).

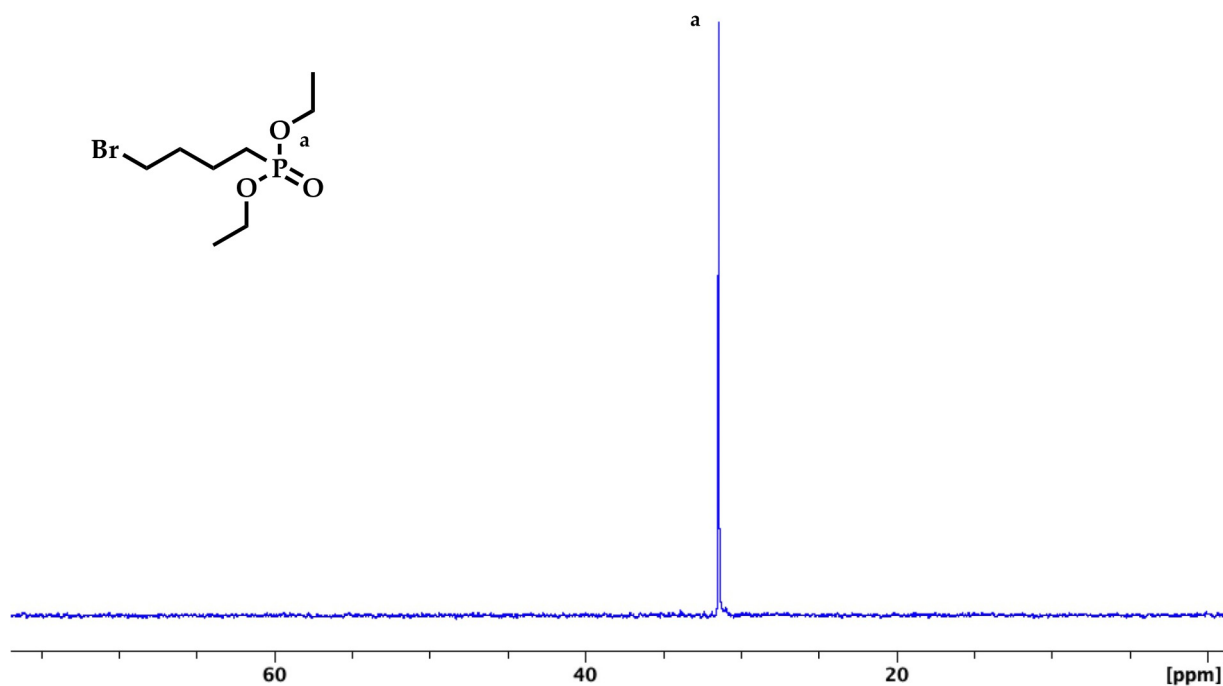


Figure S8. ³¹P NMR spectrum of 3 in CDCl₃. ³¹P NMR: δ 31.400 (s, 1P).

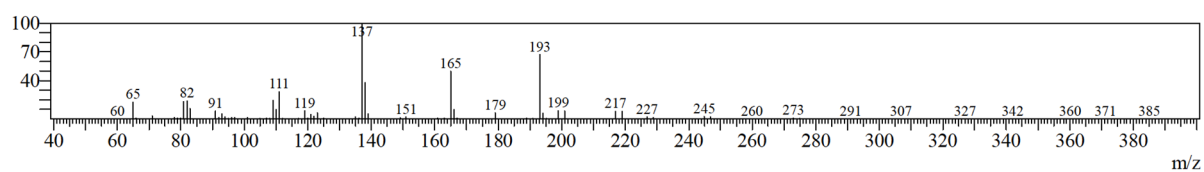
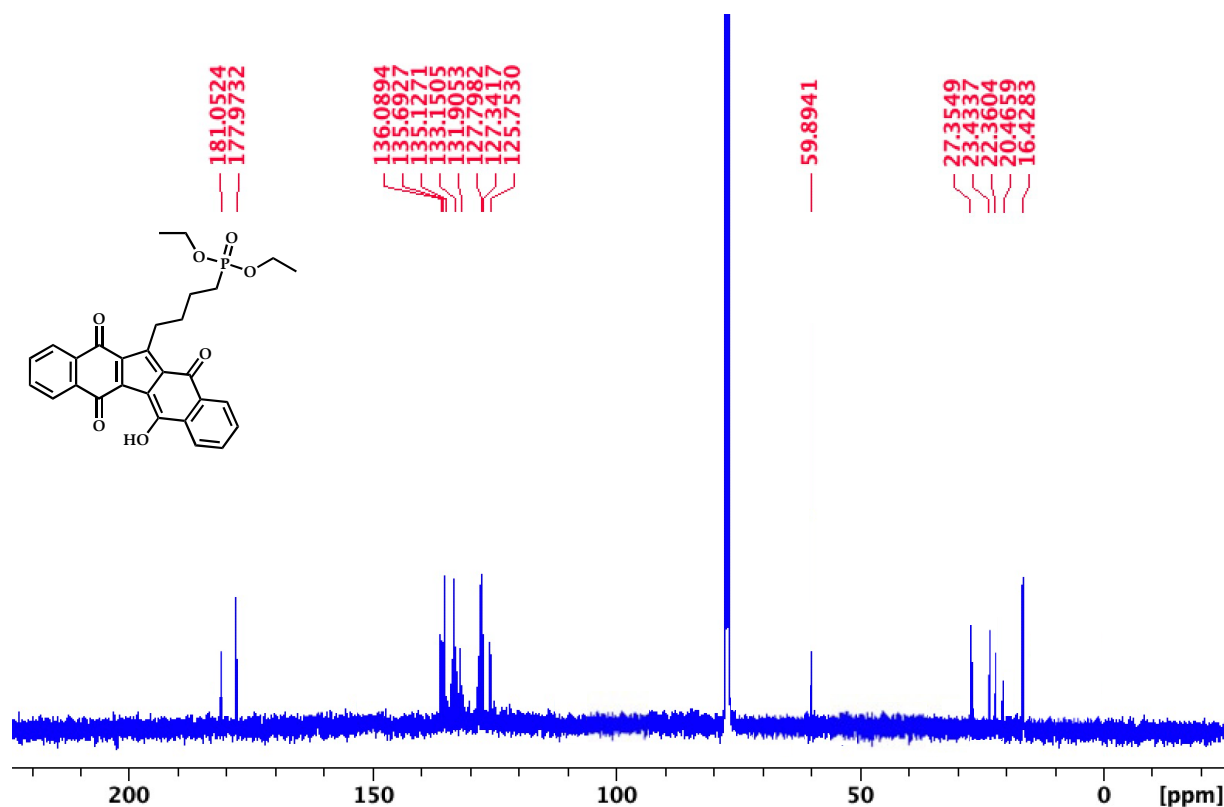
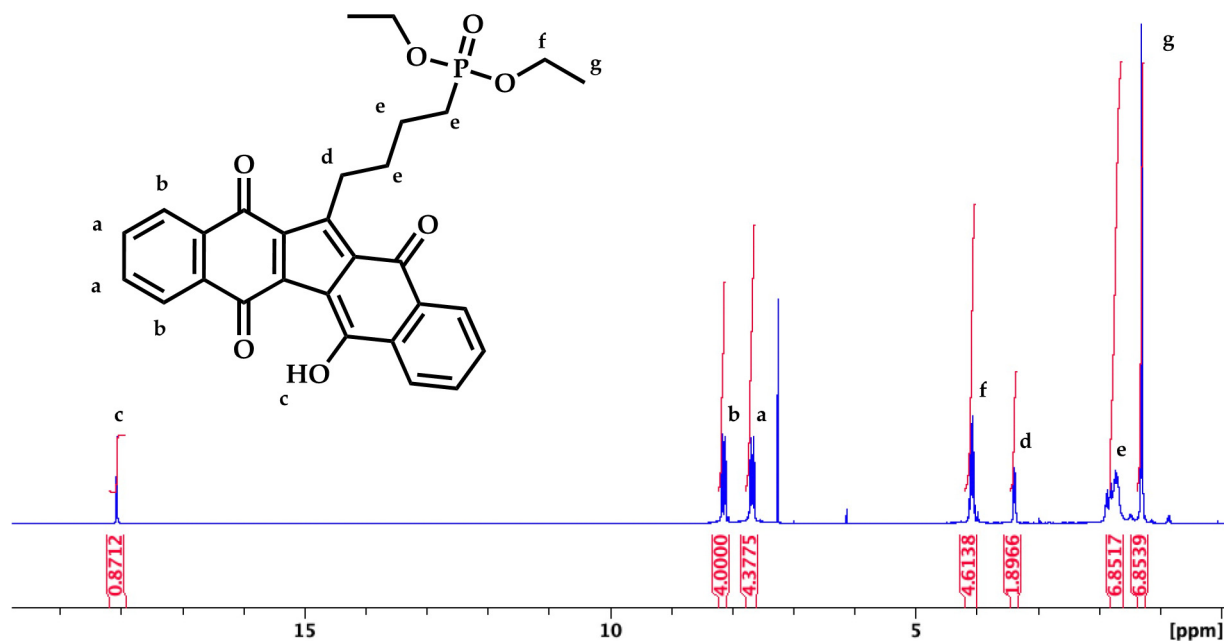


Figure S9. Mass spectrum of 3 MS (EI, 70 eV): $m/z = 193$ [M-Br]⁺; $m/z = 165$ [193-C₂H₄]⁺; $m/z = 137$ [165-C₂H₄]⁺.



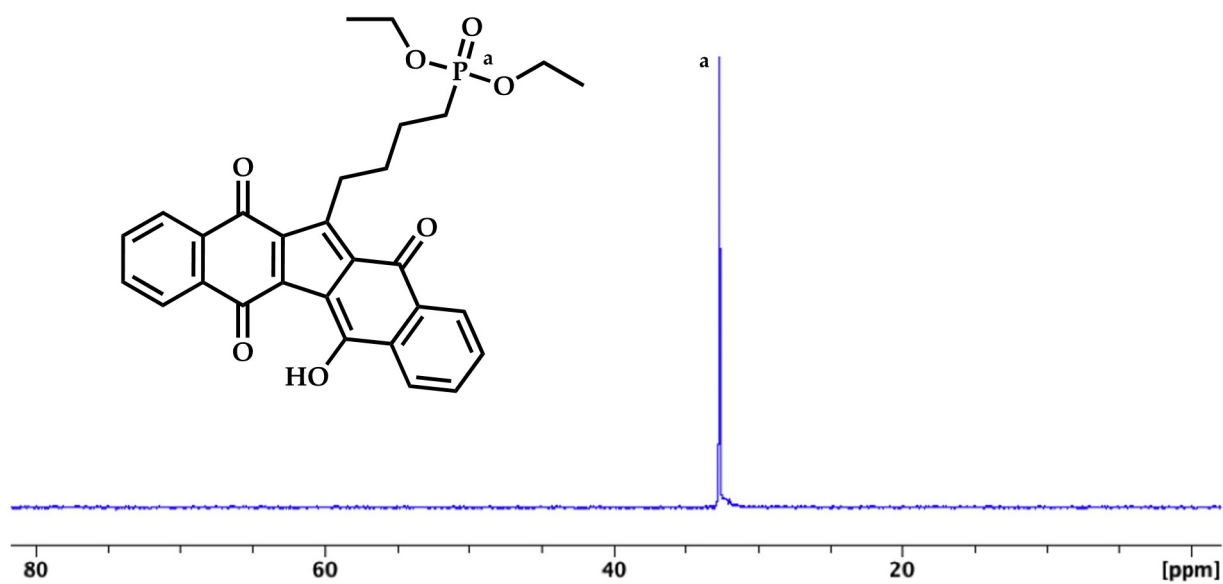


Figure S12. ³¹P NMR spectrum of **4** in CDCl₃. ³¹P NMR: δ 32.686 (s, 1P).

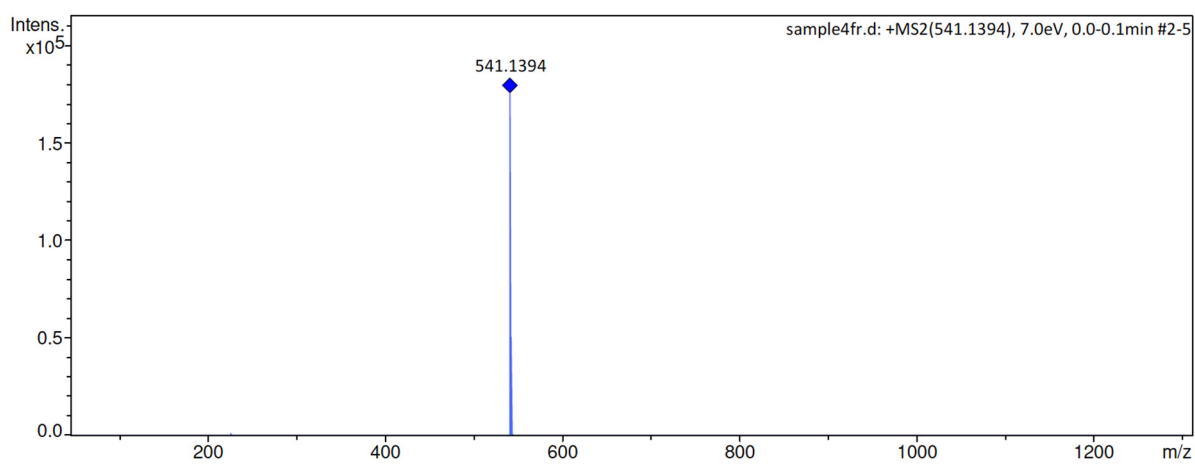


Figure S13. HRMS spectrum of **4**. *m/z*: [M + Na]⁺ calcd for C₂₉H₂₇NaO₇P 541.1387; found 541.1394.

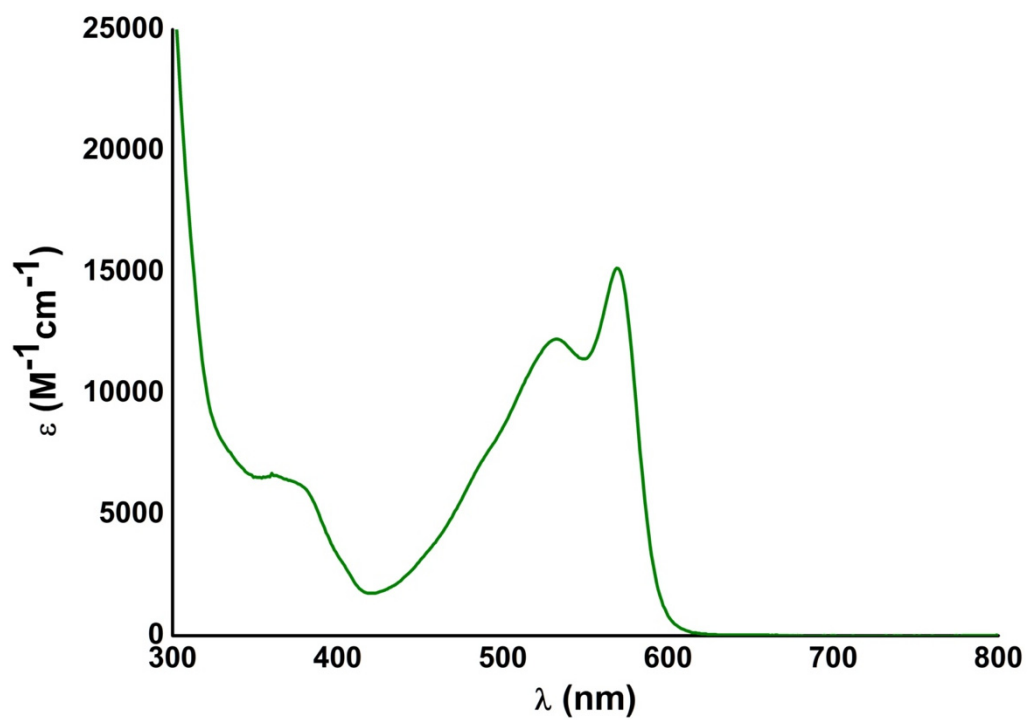


Figure S14. UV-vis spectrum of 4 in CHCl₃.

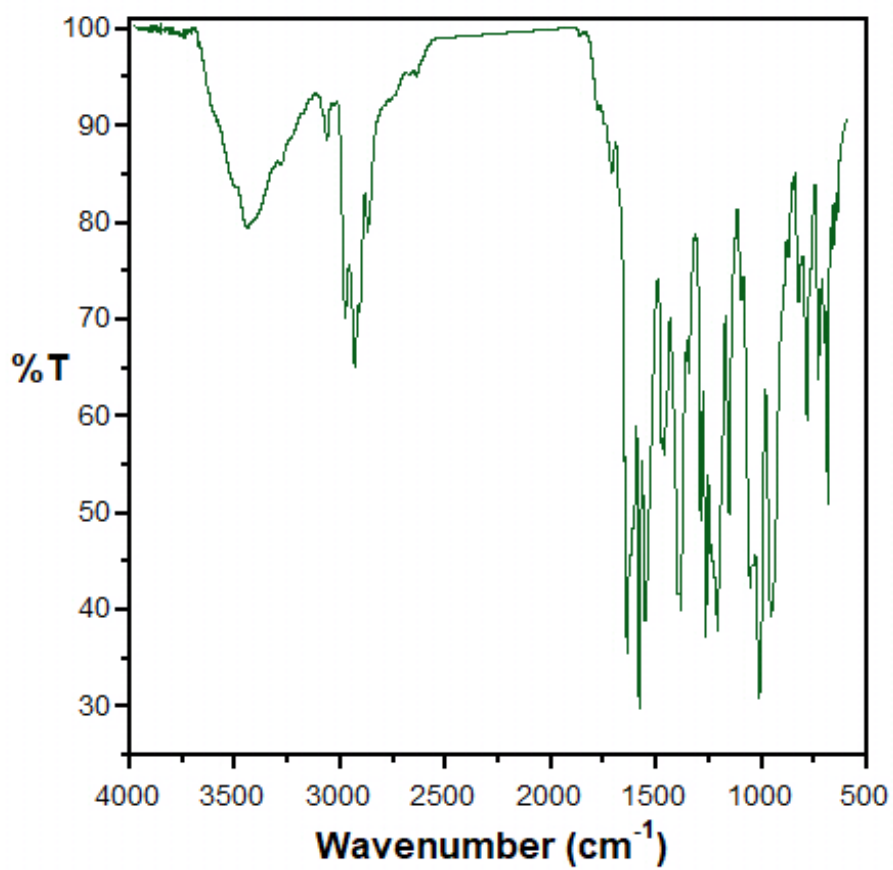


Figure S15. ATR-IR spectrum of 4.

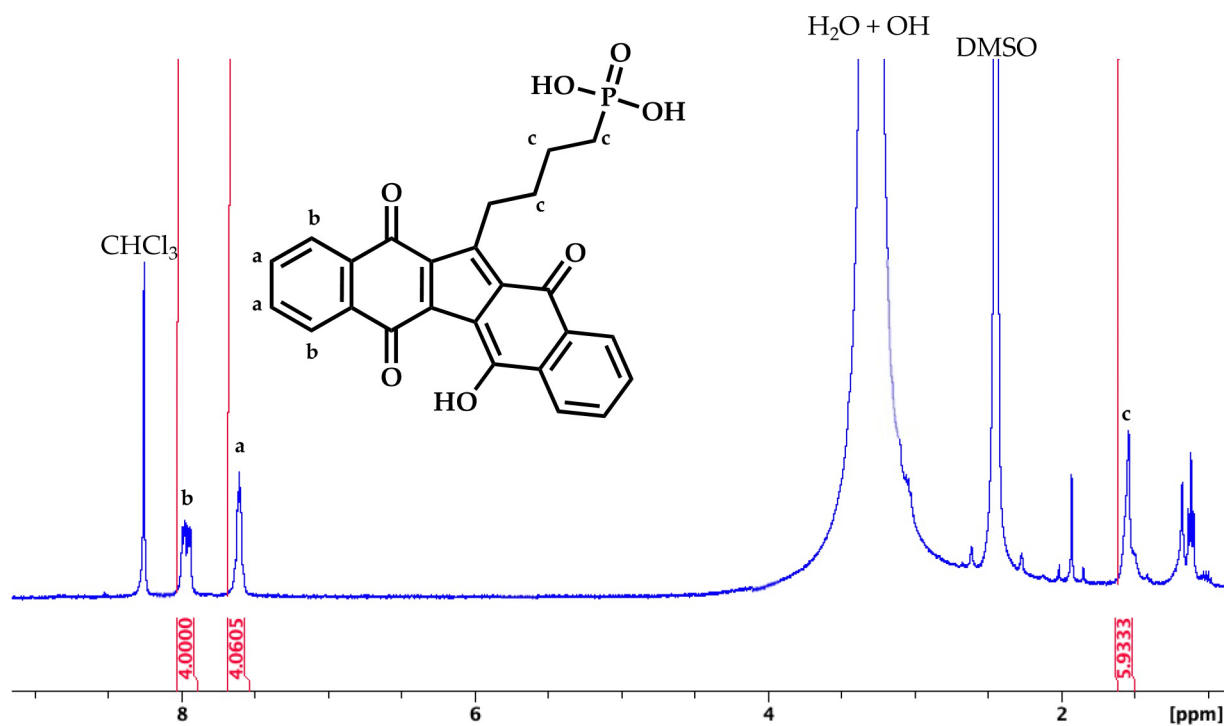


Figure S16. ^1H NMR spectrum of 7 in $\text{DMSO}-d_6$. ^1H NMR: δ 1.493-1.617 (m, 6H), δ 7.529-7.697 (m, 4H), δ 7.891-8.035 (m, 4H).

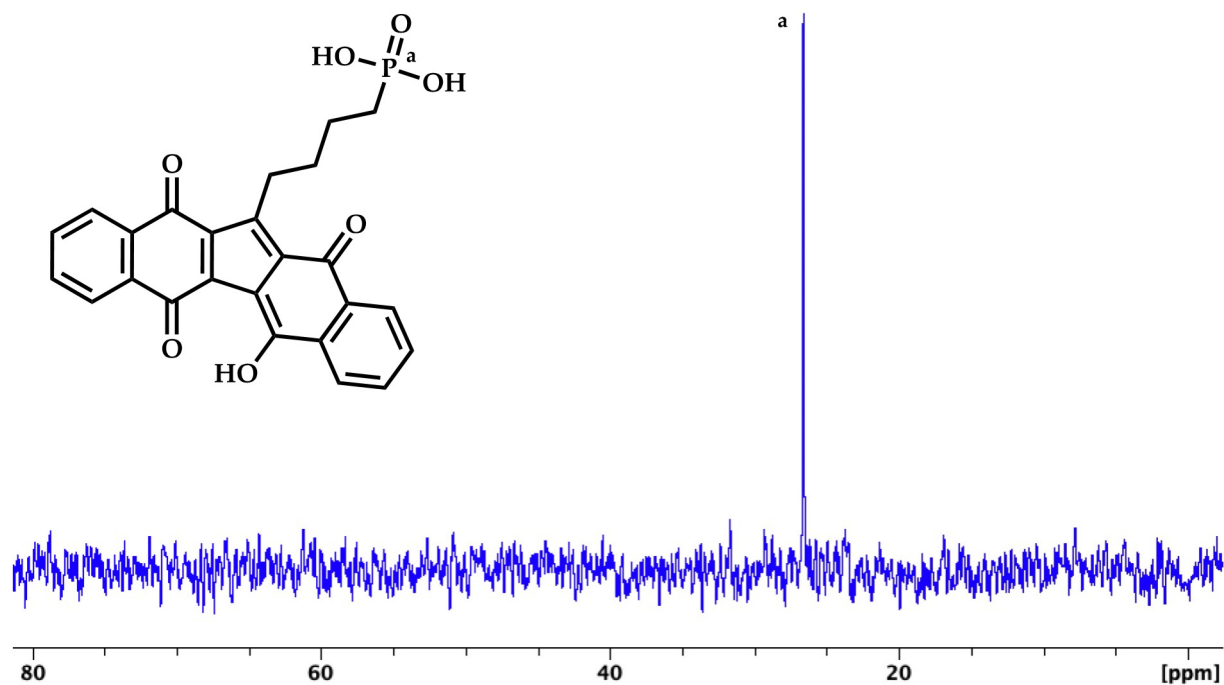


Figure S17. ^{31}P NMR spectrum of 7 in $\text{DMSO}-d_6$; δ 26.653 (s, 1P).

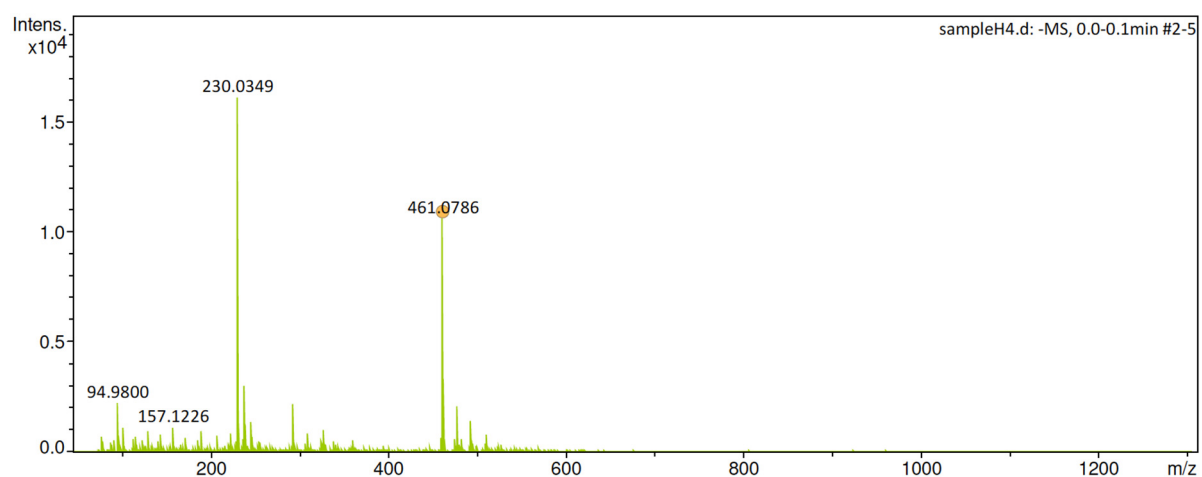


Figure S18. HRMS spectrum of 7. m/z : $[M - H]^-$ calcd for $C_{25}H_{18}O_7P$ 461.0796; found 461.0786.

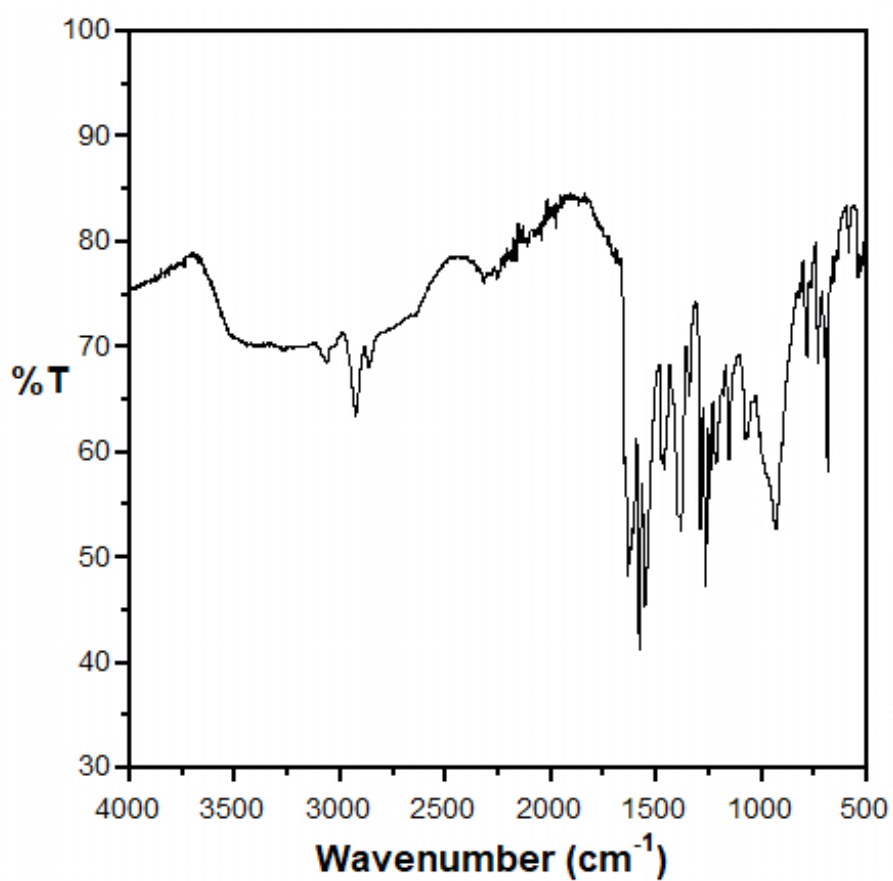


Figure S19. ATR-IR spectrum of 7.

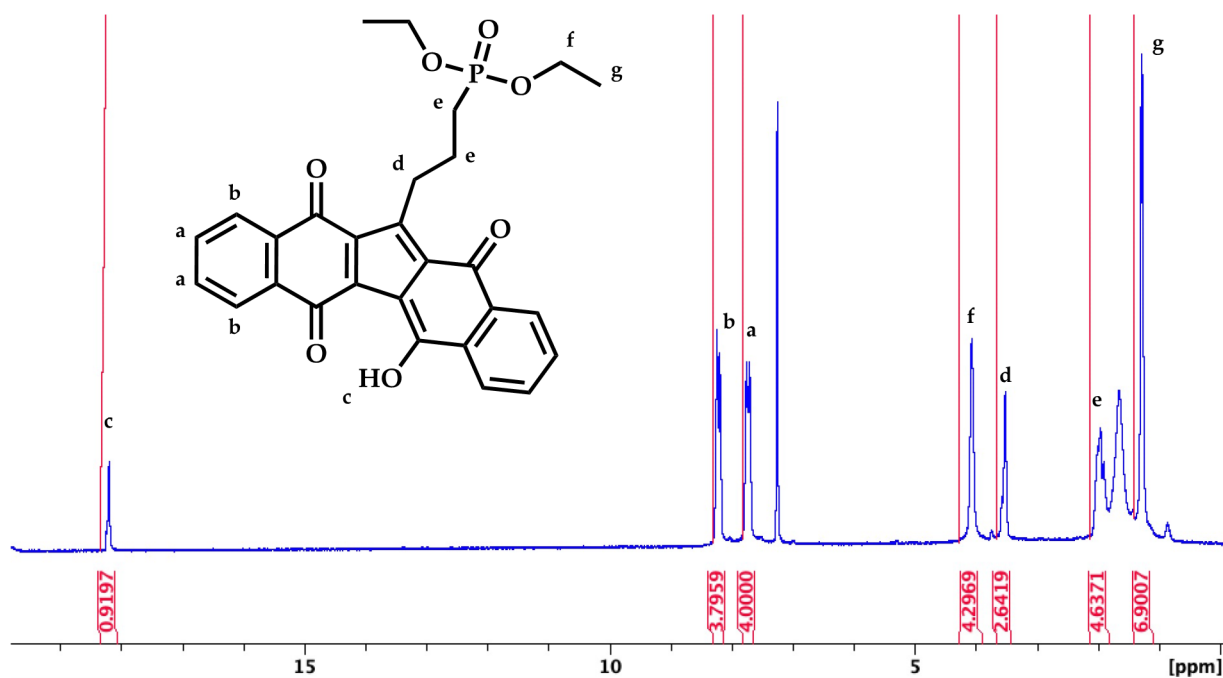


Figure S20. ^1H NMR spectrum of **5** in CDCl_3 . ^1H NMR: δ 1.281 (t, $J=7.08$ Hz, 6H), δ 1.862-2.053 (m, 4H), δ 3.486 (t, $J=7.09$, 2H), δ 3.991-4.152 (m, 4H), δ 7.628-7.780 (m, 4H), δ 8.120-8.238 (m, 4H), δ 18.150 (s, 1H).

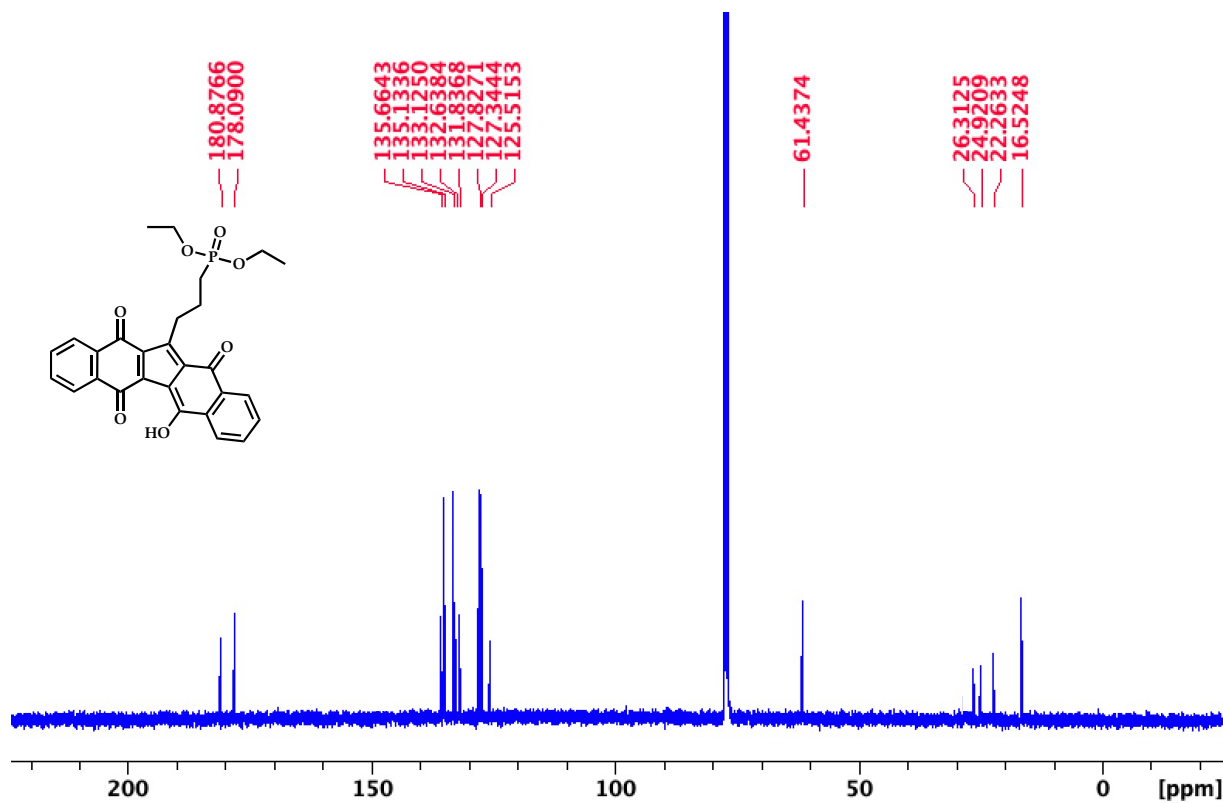


Figure S21. ^{13}C NMR spectrum of **5** in CDCl_3 . ^{13}C NMR: δ 180.876 and 178.090 (C=O); δ 135.664, 135.133, 133.125, 132.638, 131.836, 127.827, 127.344, 125.515 (aromatic carbons); δ 61.437, 26.312, 24.920, 22.263, 16.524 (aliphatic carbons).

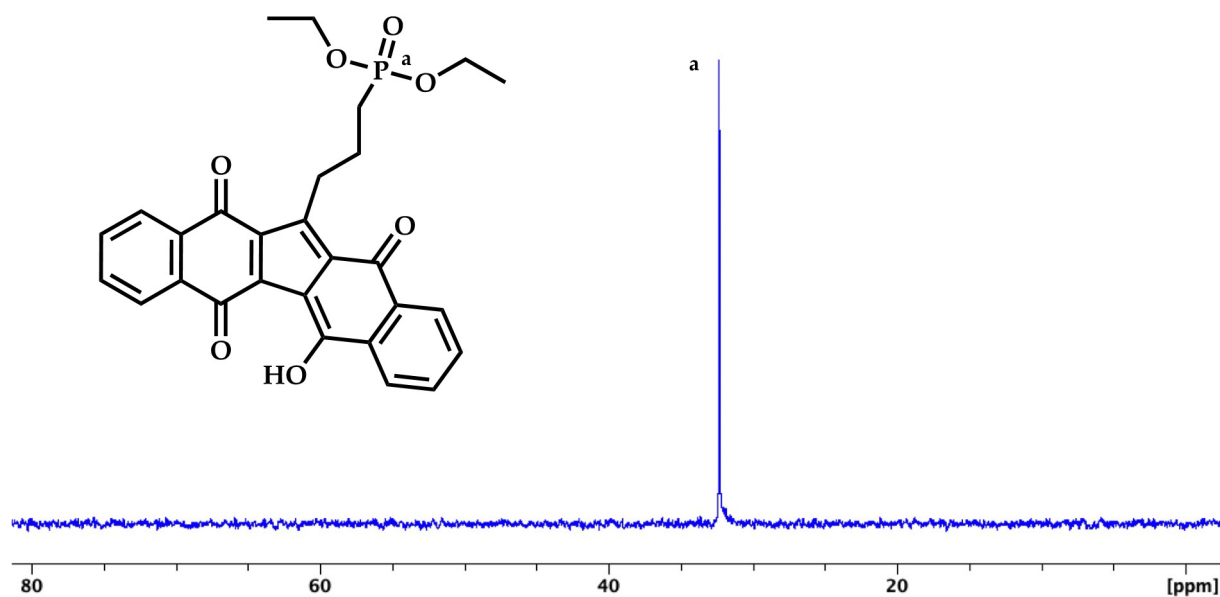


Figure S22. ³¹P NMR spectrum of 5 in CDCl₃. ³¹P NMR: δ 32.337 (s, 1P).

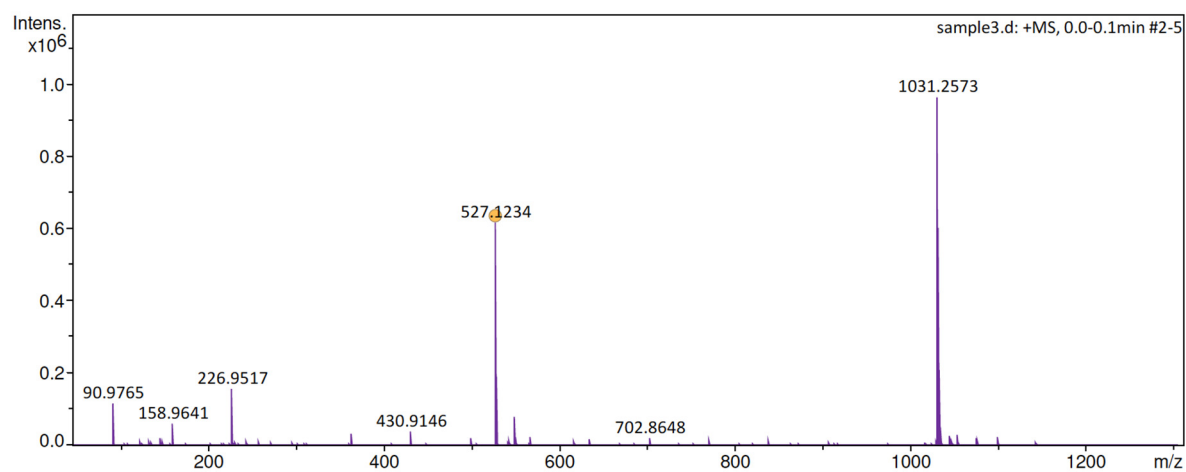


Figure S23. HRMS spectrum of 5. *m/z*: [M + Na]⁺ calcd for C₂₈H₂₅NaO₇P 527.1230; found 527.1234.

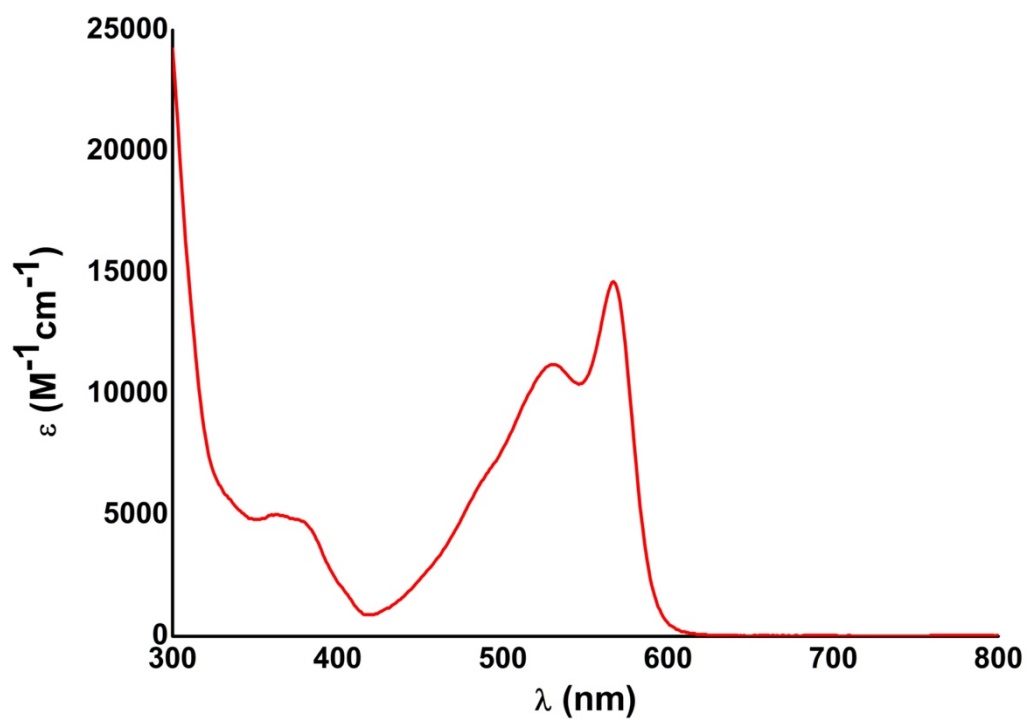


Figure S24. UV-vis spectrum of 5 in CHCl₃.

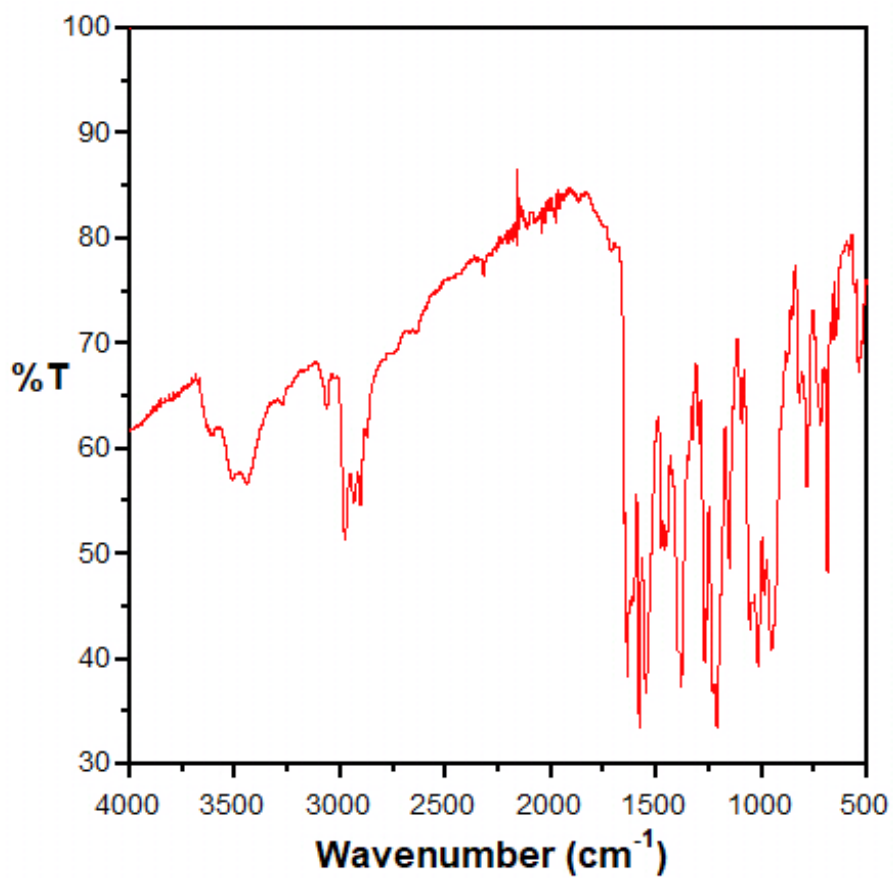


Figure S25. ATR-IR spectrum of 5.

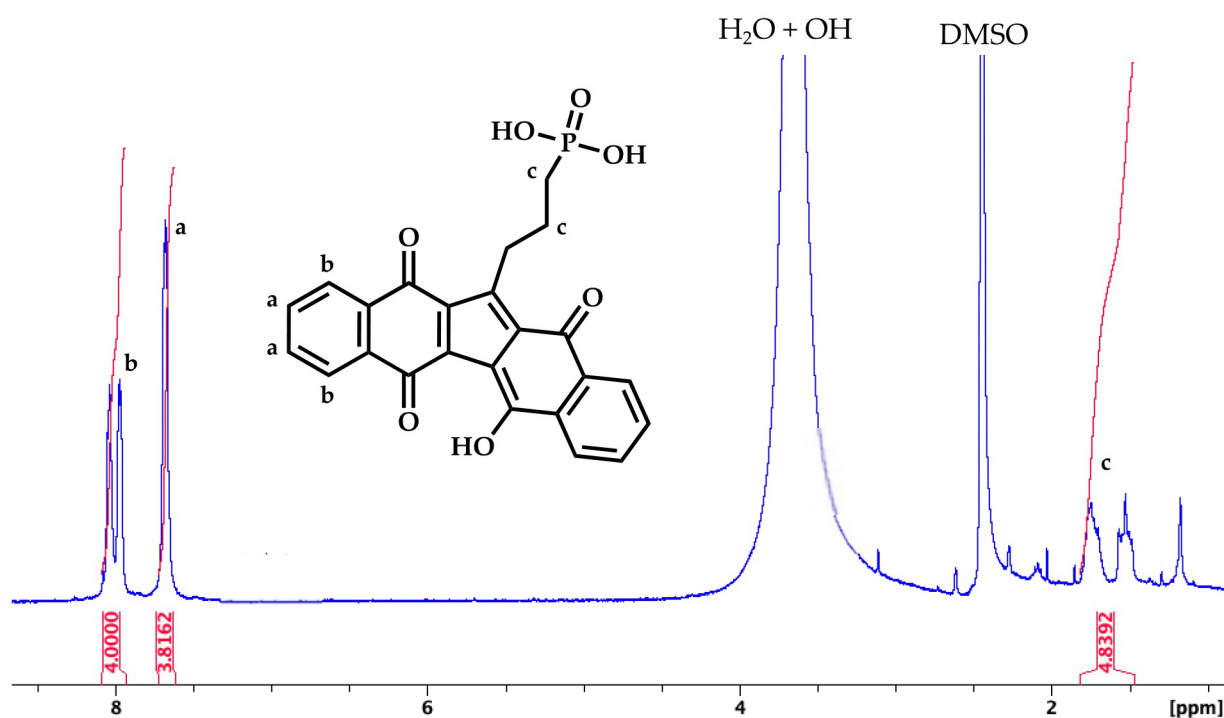


Figure S26. ^1H NMR spectrum of 8 in DMSO-d_6 . ^1H NMR: δ 1.493-1.801 (m, 4H), δ 7.609-7.725 (m, 4H), δ 7.924-8.084 (m, 4H).

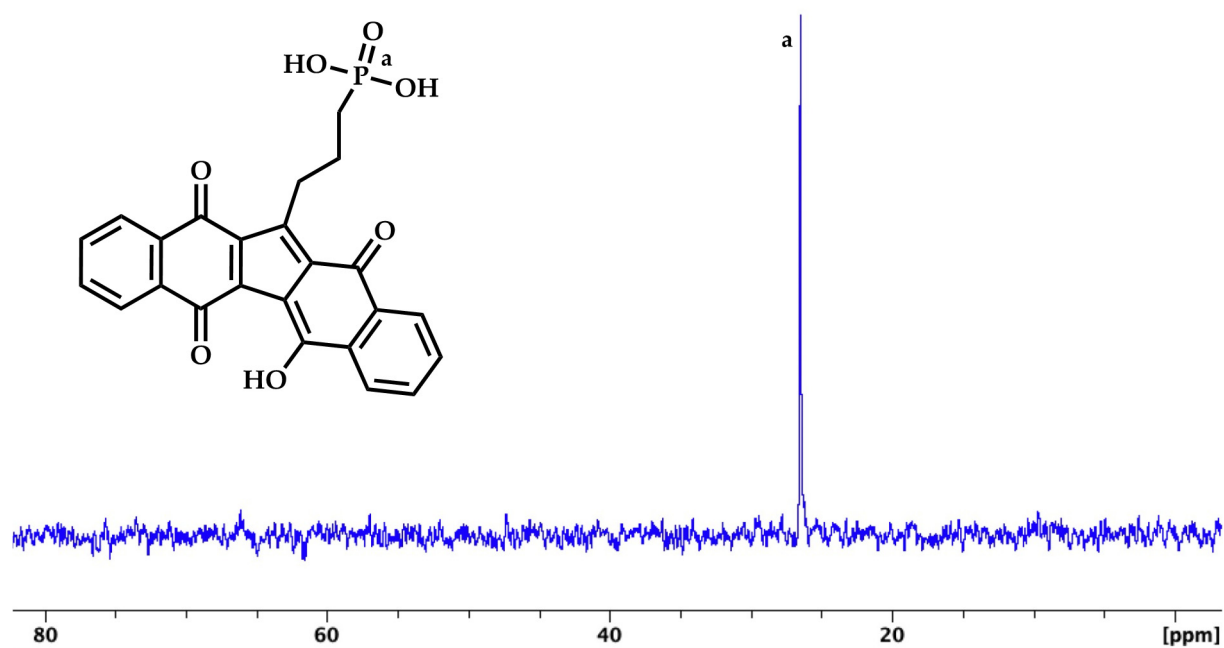


Figure S27. ^{31}P NMR spectrum of 8 in DMSO-d_6 : δ 26.534 (s, 1P).

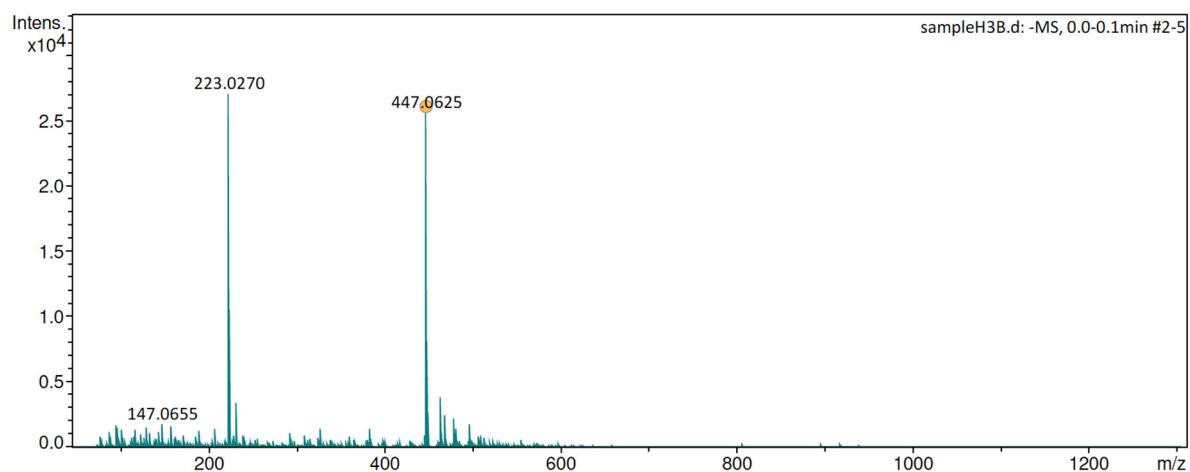


Figure S28. HRMS spectrum of 8. m/z : $[M - H]^-$ calcd for $C_{24}H_{16}O_7P$ 447.0639; found 447.0625.

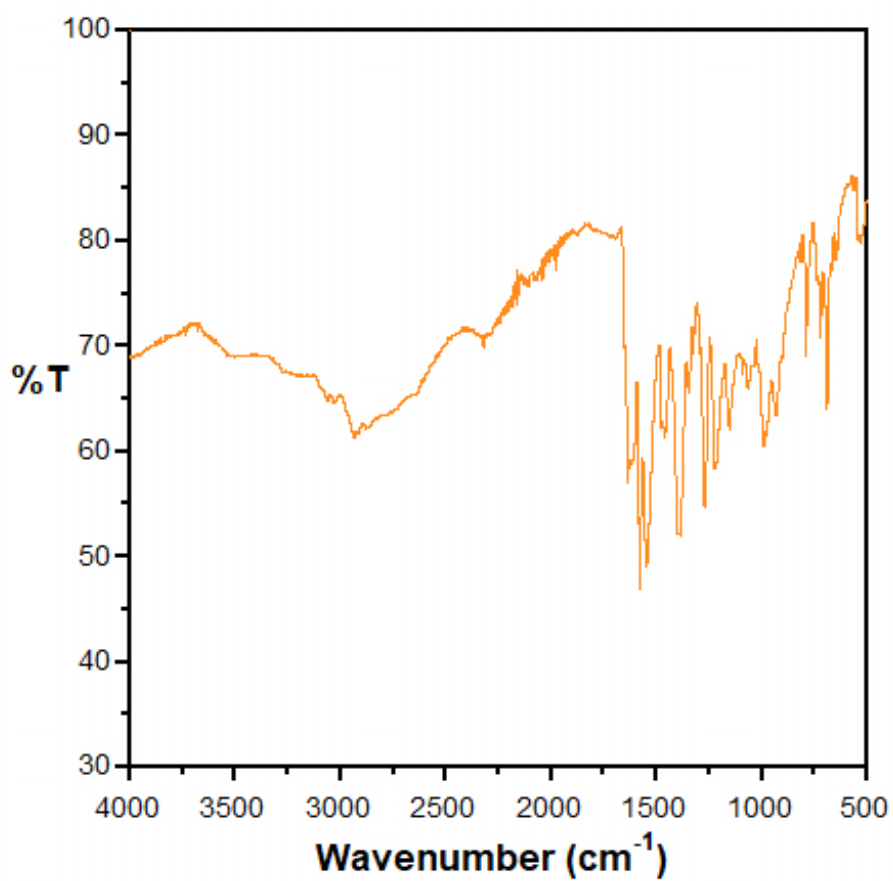


Figure S29. ATR-IR spectrum of 8.

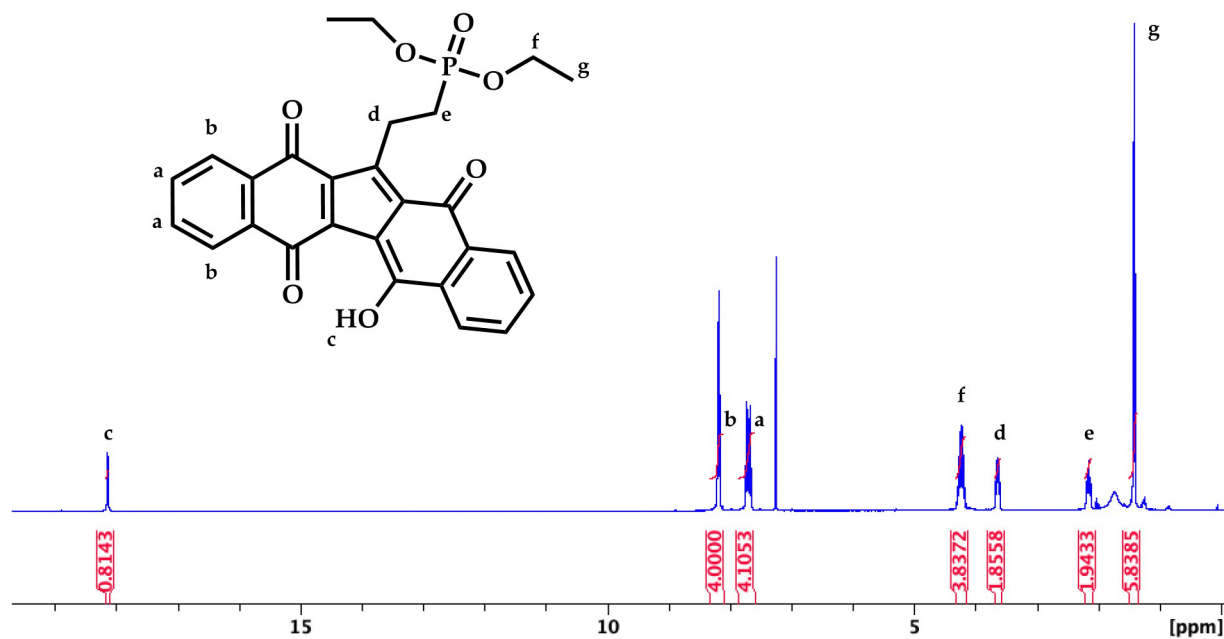


Figure S30. ^1H NMR spectrum of **6** in CDCl_3 . ^1H NMR: δ 1.423 (t, $J=7.00$ Hz, 6H), δ 2.102-2.224 (m, 2H), δ 3.602-3.702 (m, 2H), δ 4.157-4.320 (m, 4H), δ 7.645-7.764 (m, 4H), δ 8.163-8.228 (m, 4H), δ 18.147 (s, 1H).

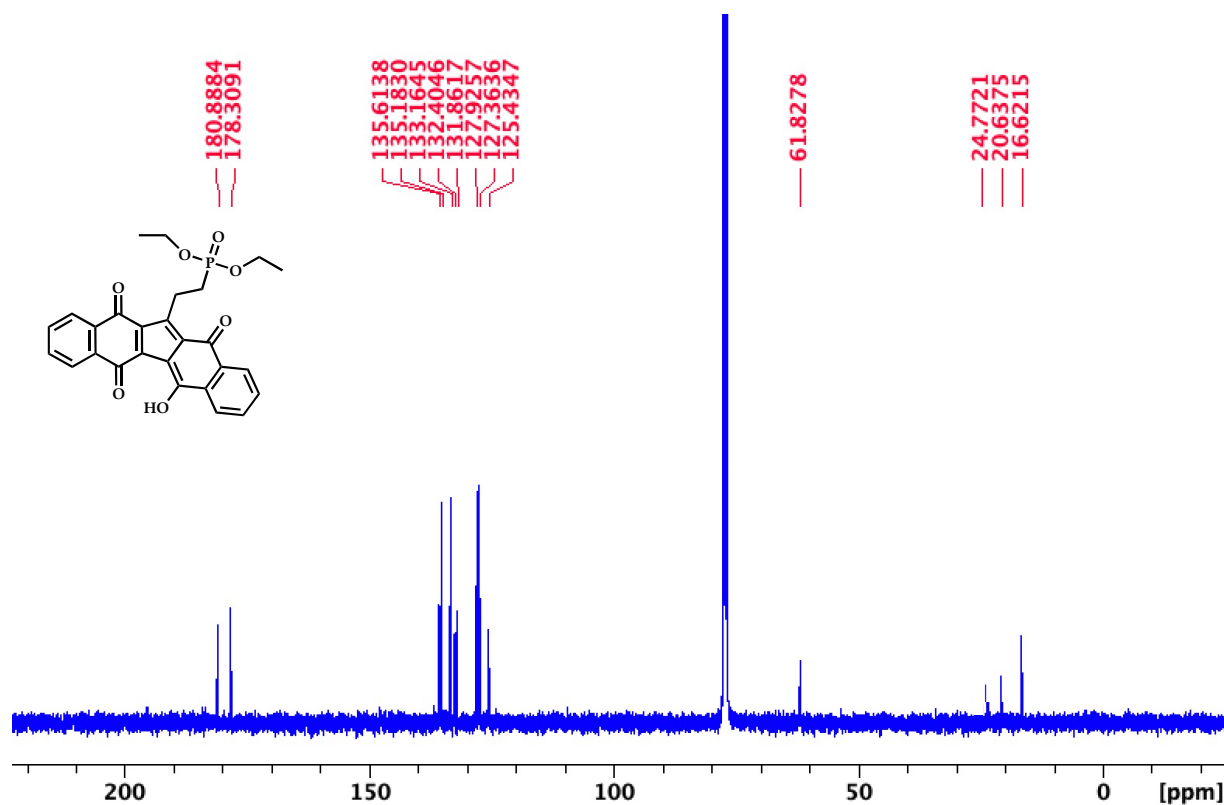


Figure S31. ^{13}C NMR spectrum of **6** in CDCl_3 . ^{13}C NMR: δ 180.888 and 178.309 (C=O); δ 135.613, 135.183, 133.164, 132.404, 131.861, 127.925, 127.363, 125.434 (aromatic carbons); δ 61.827, 24.772, 20.637, 16.621 (aliphatic carbons).

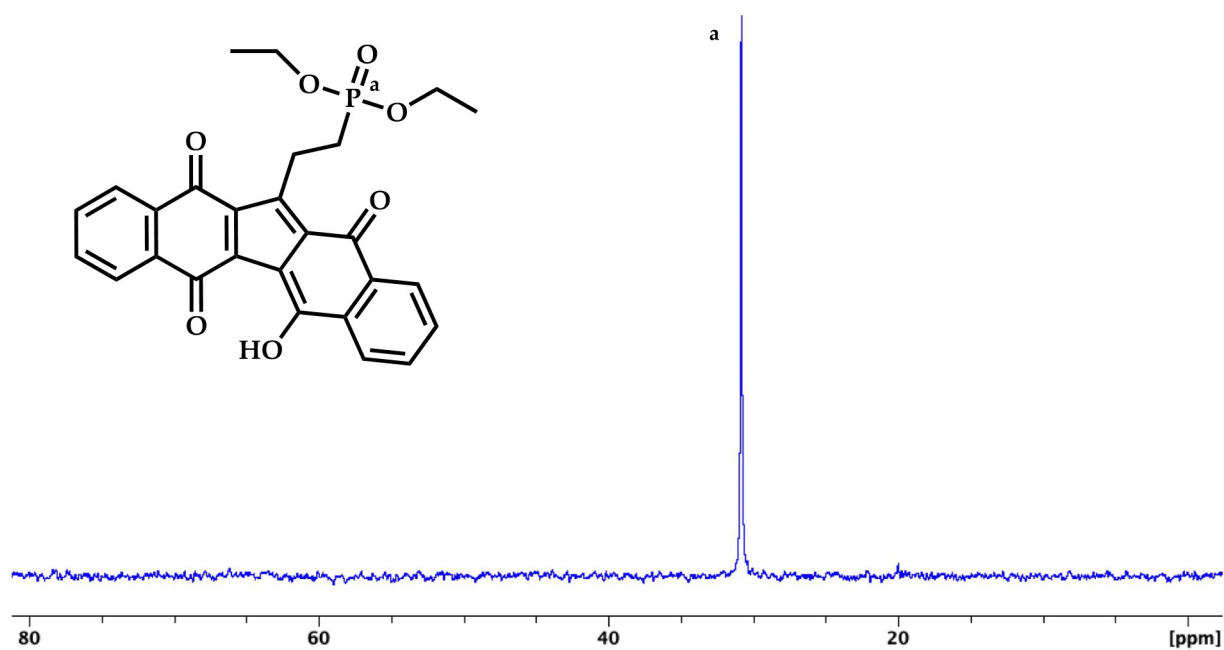


Figure S32. ³¹P NMR spectrum of **6** in CDCl₃. ³¹P NMR: δ 30.835 (s, 1P).

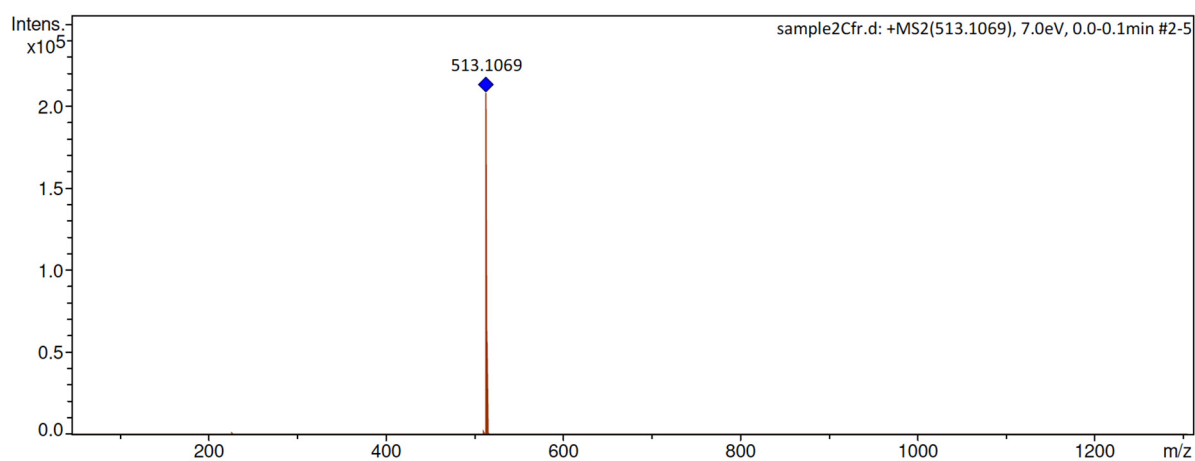


Figure S33. HRMS spectrum of **6**. *m/z*: [M + Na]⁺ calcd for C₂₇H₂₃NaO₇P 513.1074; found 513.1069.

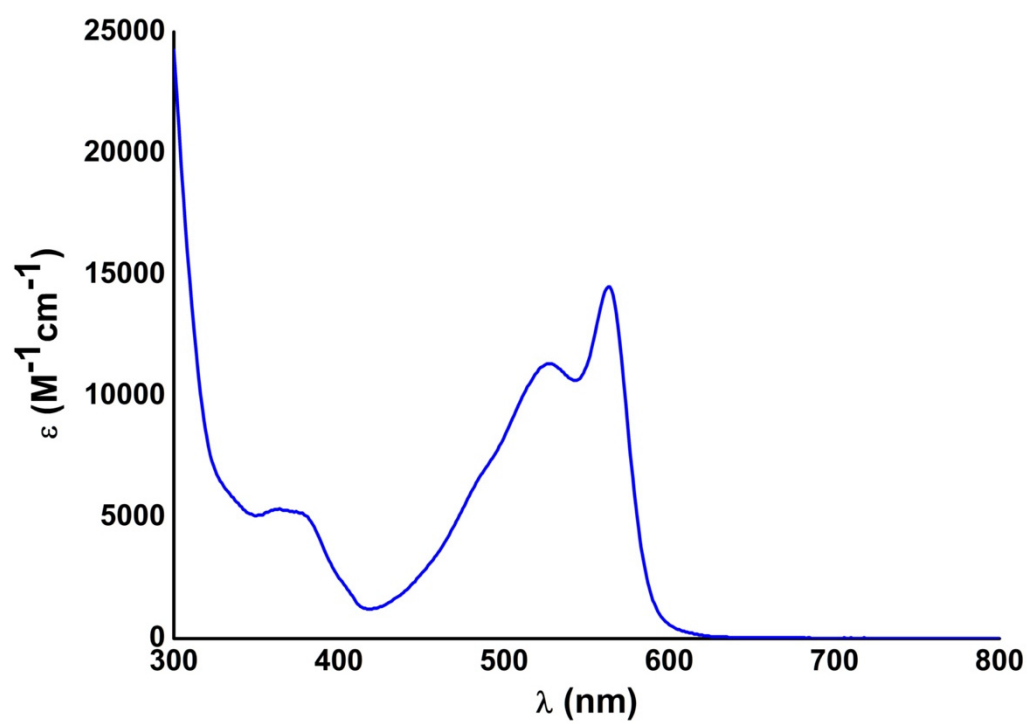


Figure S34. UV-vis spectra of 6 in CHCl₃.

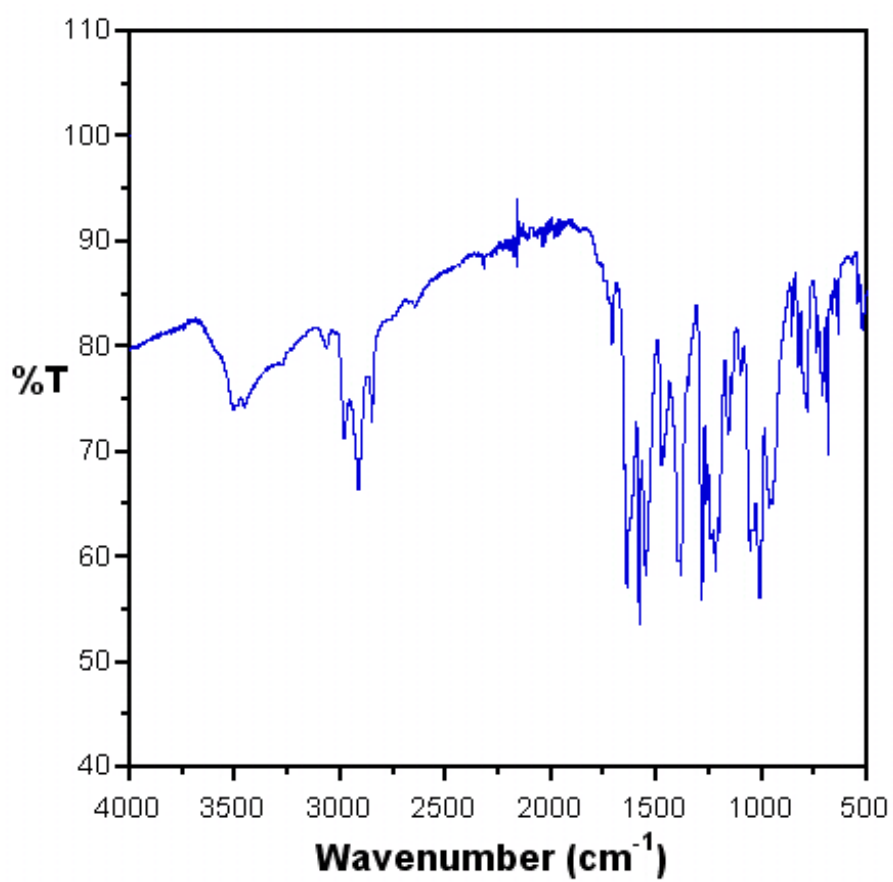


Figure S35. ATR-IR spectrum of 6.

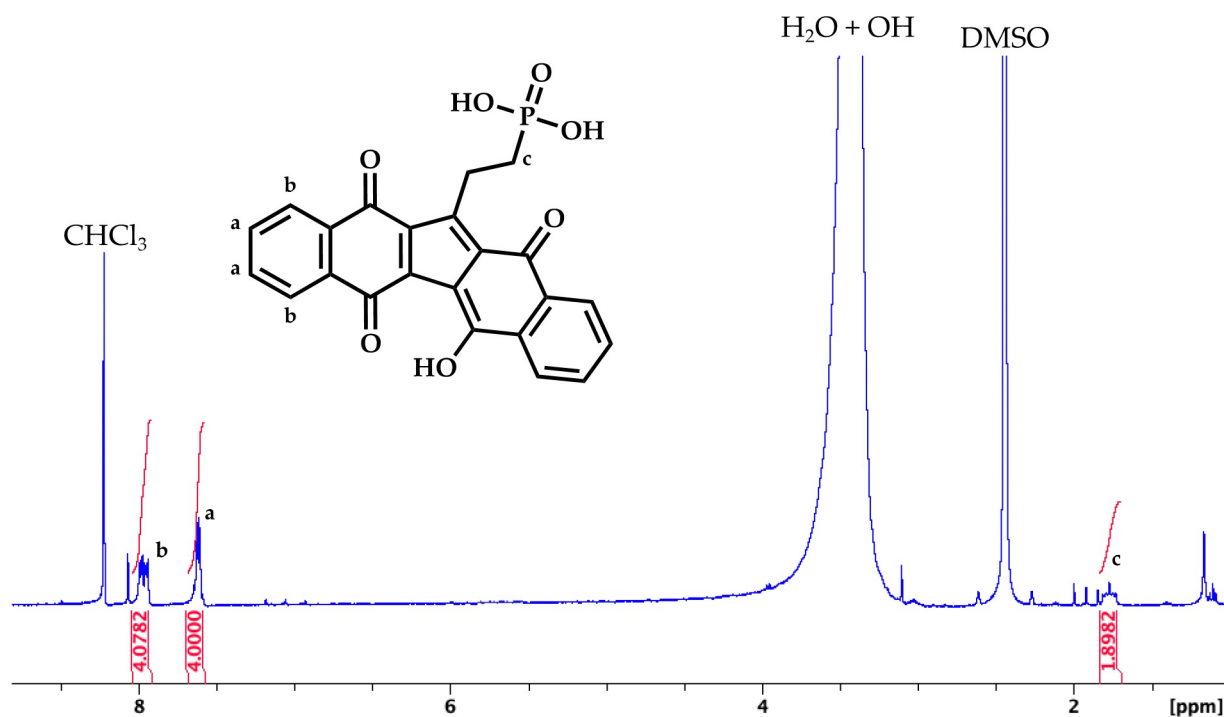


Figure S36. ¹H NMR spectrum of 9 in DMSO-d₆. ¹H NMR: δ 1.692-1.847 (m, 2H), δ 7.509-7.677 (m, 4H), δ 7.921-8.045 (m, 4H).

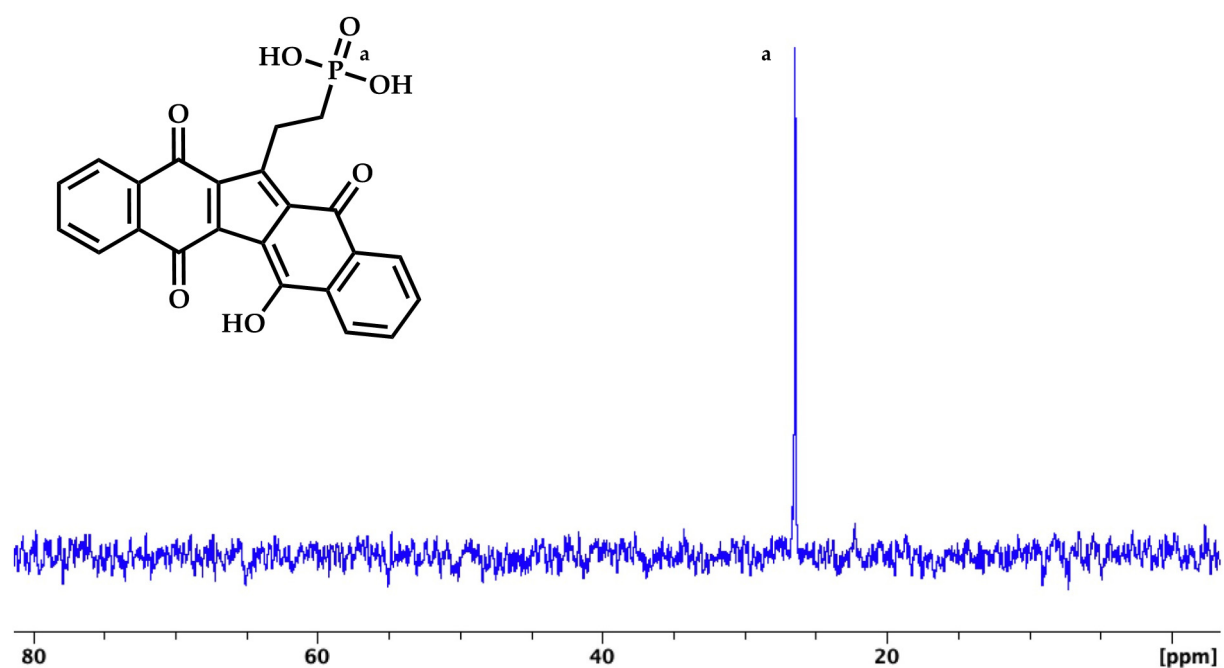


Figure S37. ³¹P NMR spectrum of 9 in DMSO-d₆: δ 26.483 (s, 1P).

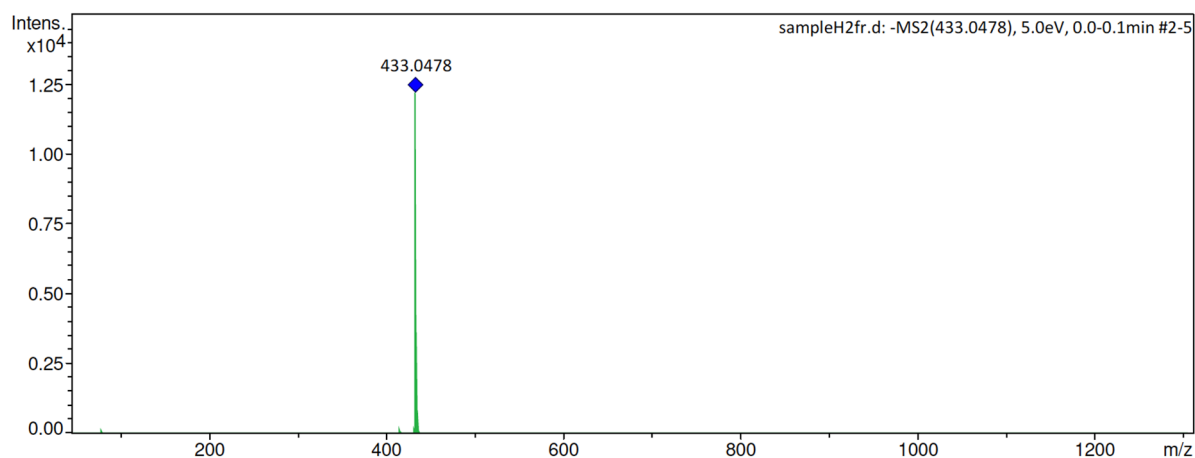


Figure S38. HRMS spectrum of **9**. m/z : $[M - H]^-$ calcd for $C_{23}H_{14}O_7P$ 433.0483; found 433.0478.

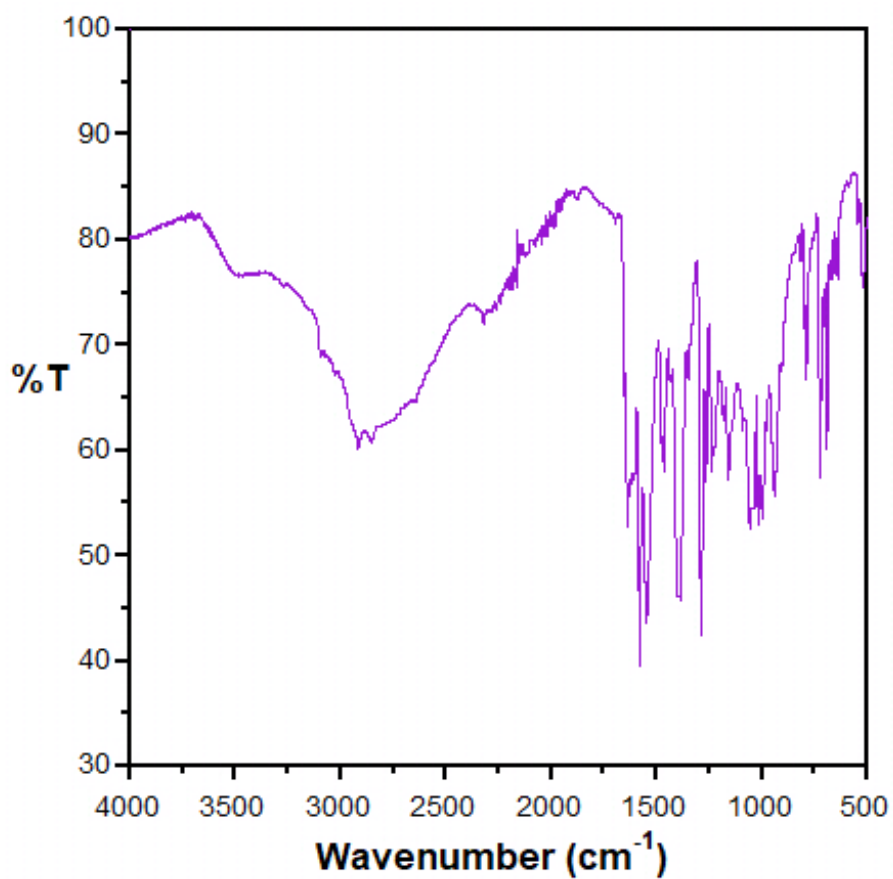


Figure S39. ATR-IR spectrum of **9**.