Supporting Information

For

Modulation of Chain-Breaking Antioxidant Activity of Phenolic Organochalcogens at Various pH and Co-antioxidants

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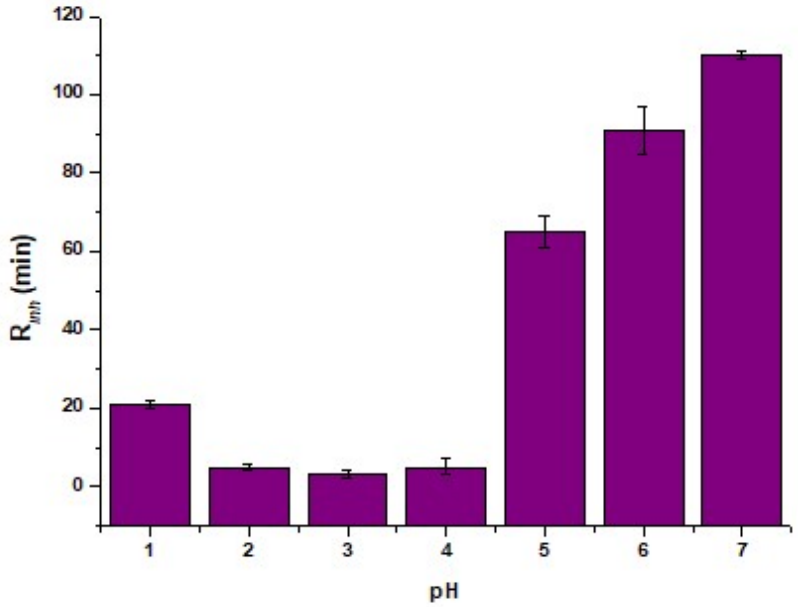


Figure S2. The T_{inh} profile of antioxidant **8** using NAC as co-antioxidant at pH 1-7 (HCl/NaOH regulated).

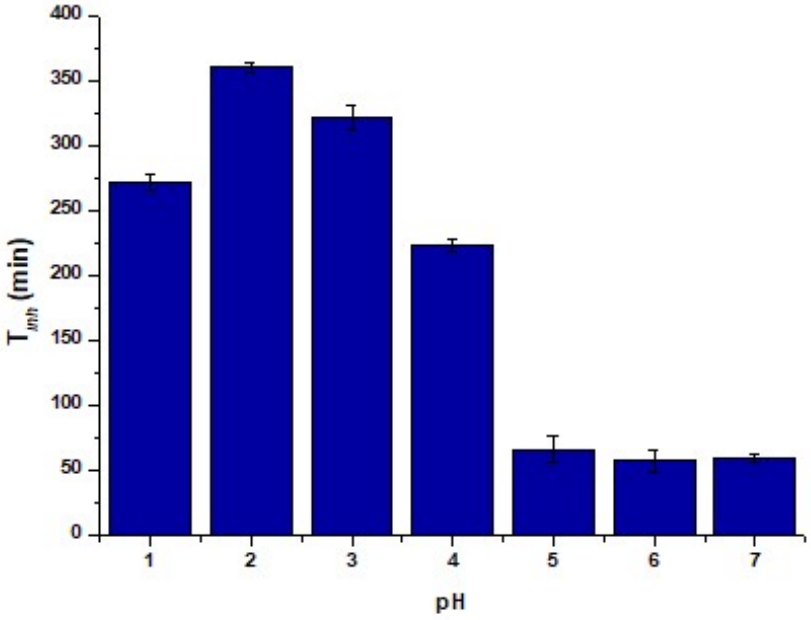


Figure S3. The R_{inh} profile of antioxidant **9** using NAC as co-antioxidant at pH 1-7 (HCl/NaOH regulated)

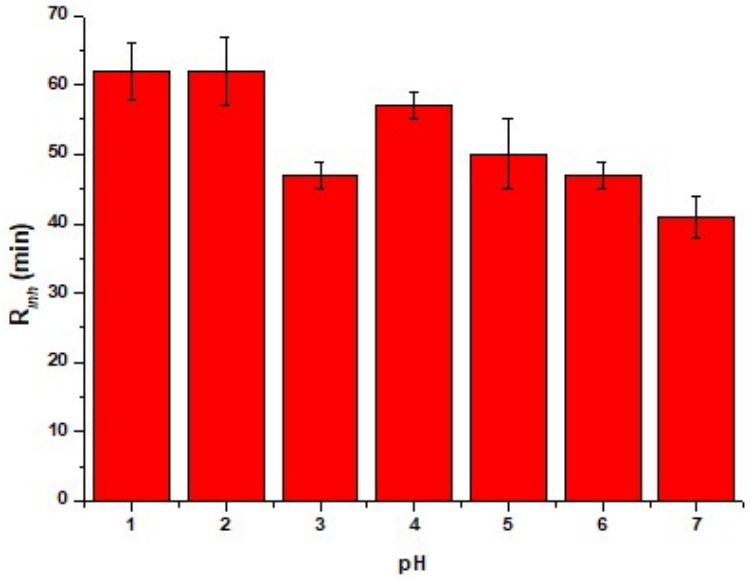


Figure S4. The T_{inh} profile of antioxidant **9** using NAC as co-antioxidant at pH 1-7 (HCl/NaOH regulated).

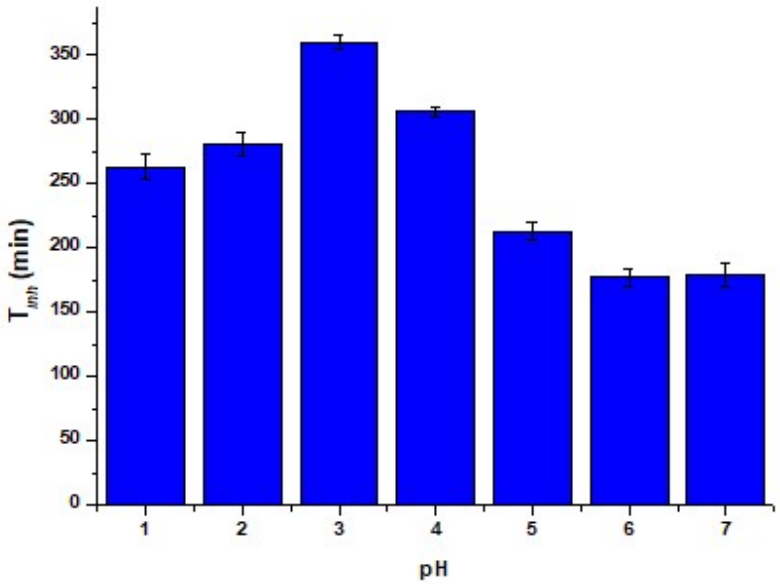


Figure S5. Control experiment without antioxidants (**8** and **9**) using NAC

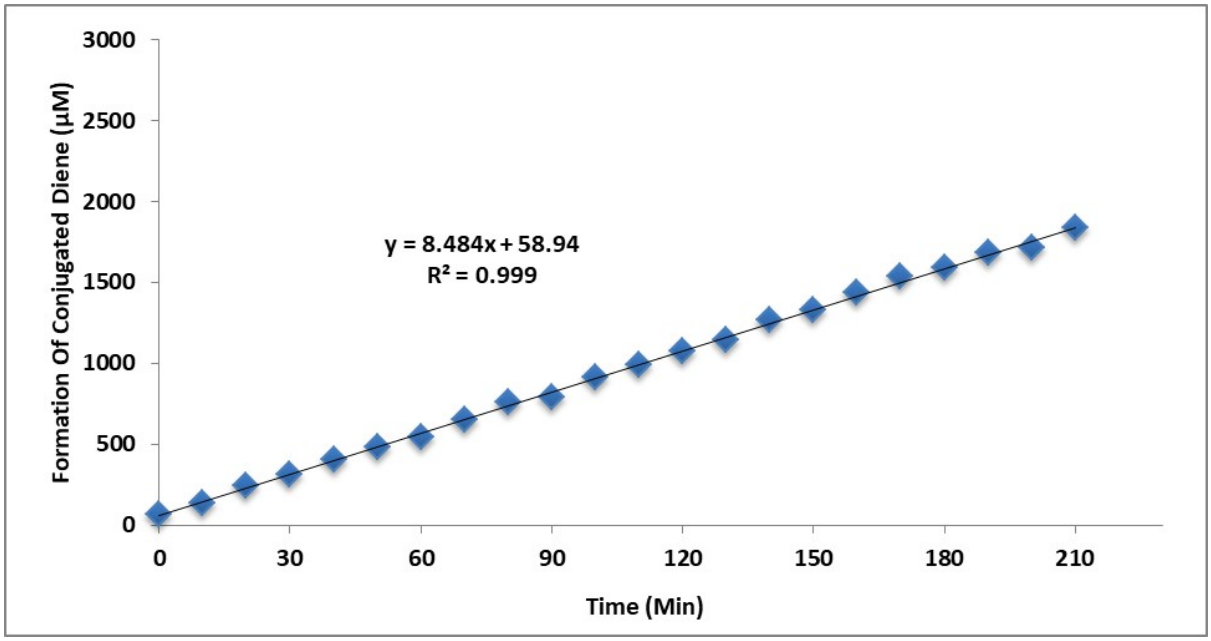


Figure S6. Control experiment without antioxidants (**8** and **9**) using GSH

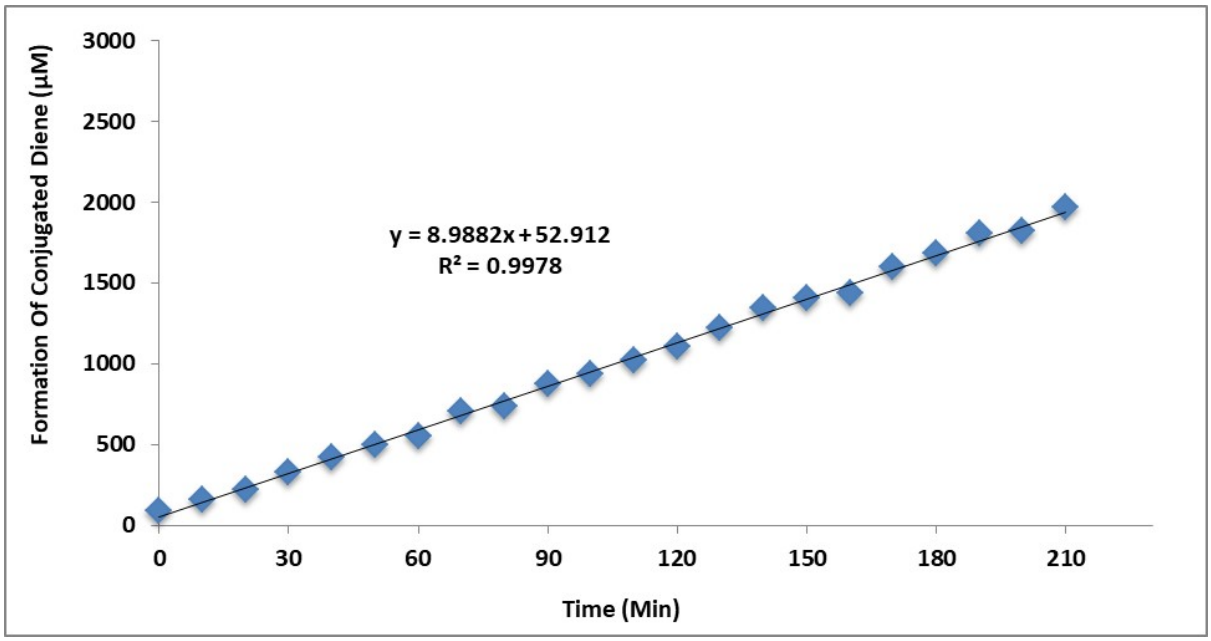


Figure S7. Control experiment without antioxidants (**8** and **9**) using DTT

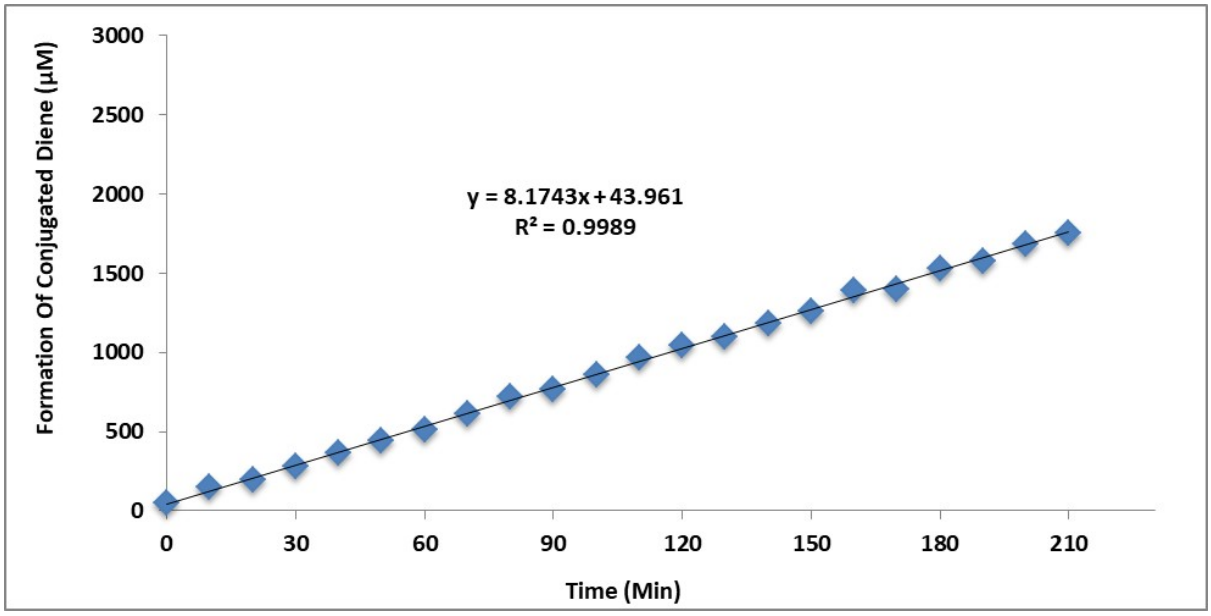


Figure S8. Control experiment without antioxidants (**8** and **9**) using AscOH

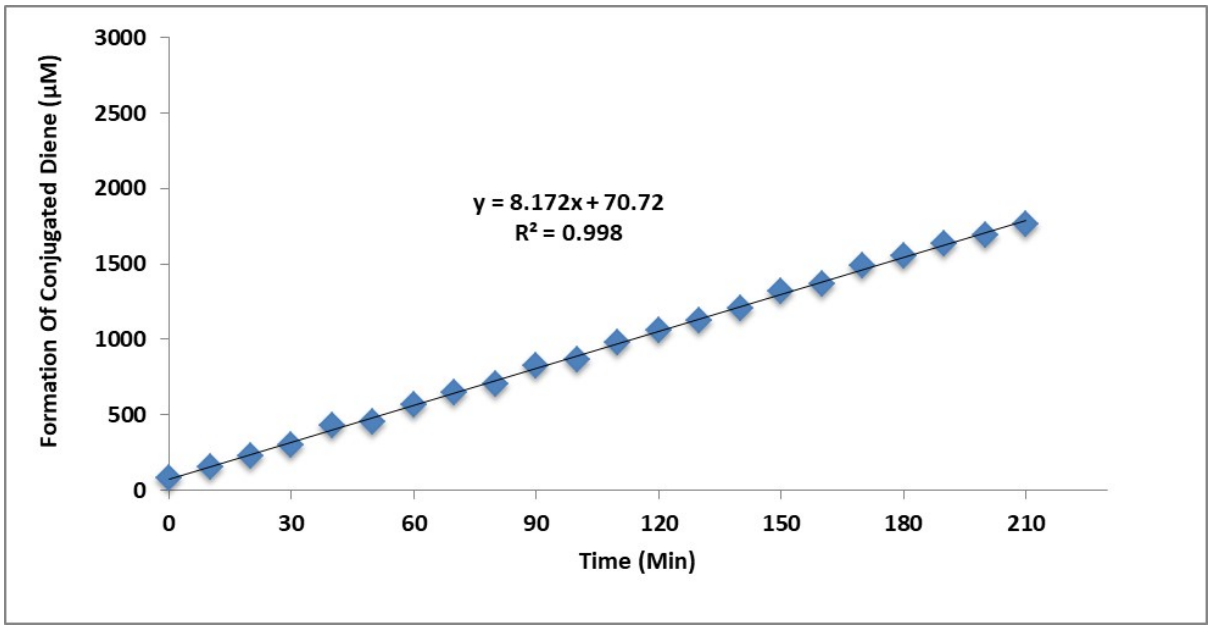


Figure S9. Control experiment without antioxidants (**8** and **9**) using sodium ascorbate

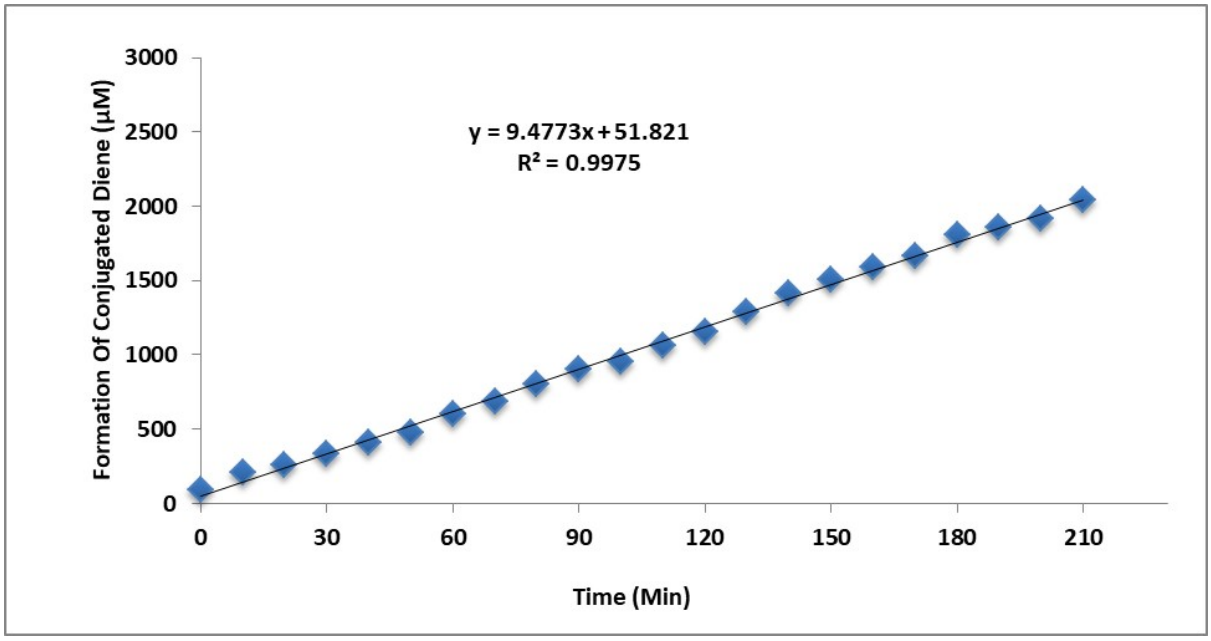


Figure S10. Control experiment without antioxidants (**8** and **9**) using $K_4[Fe(CN)_6].3H_2O$

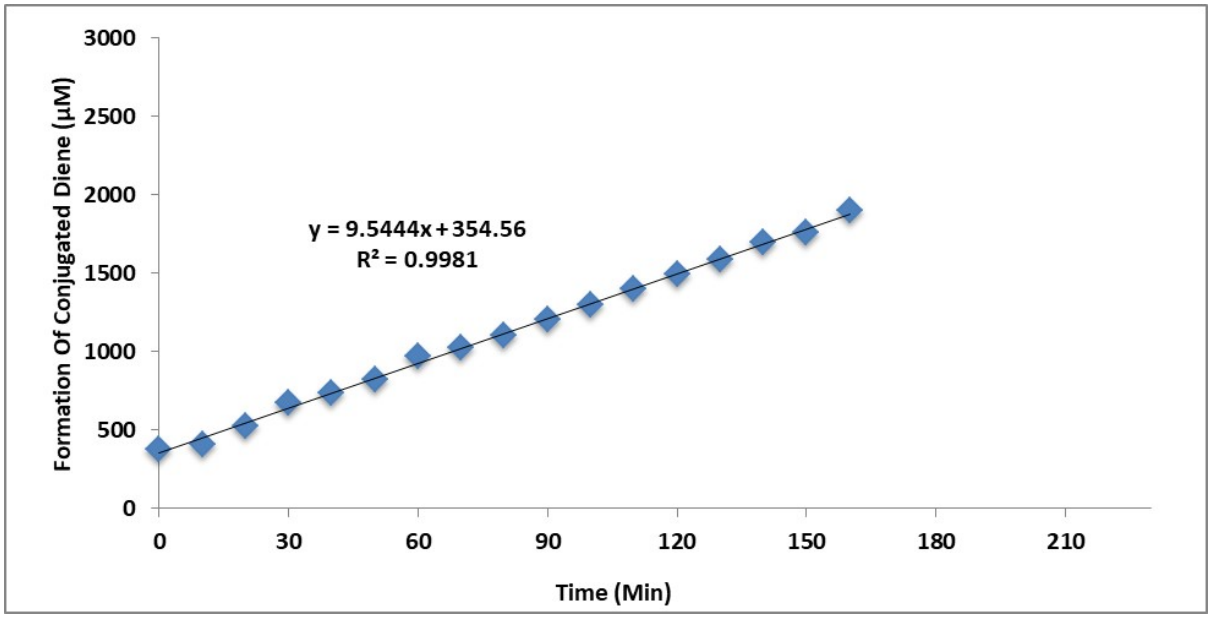


Figure S11. Control experiment without antioxidants (**8** and **9**) using $K_4[Fe(CN)_6].3H_2O$ + PTC

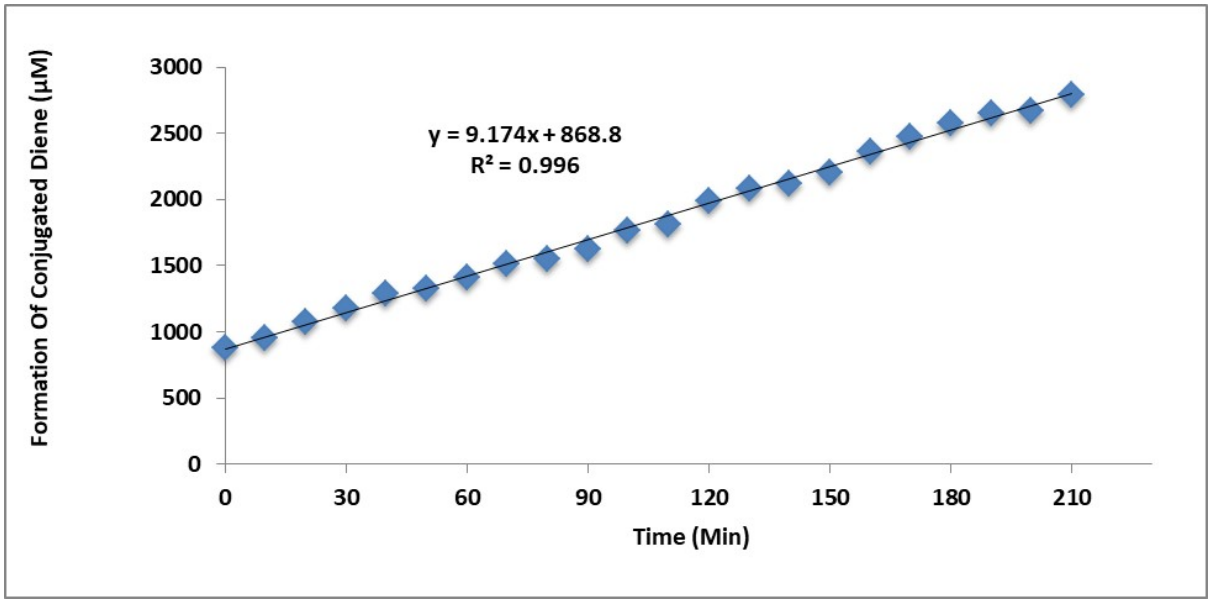


Figure S12. Control experiment without antioxidants (**8** and **9**) using $Na_2S_2O_5$

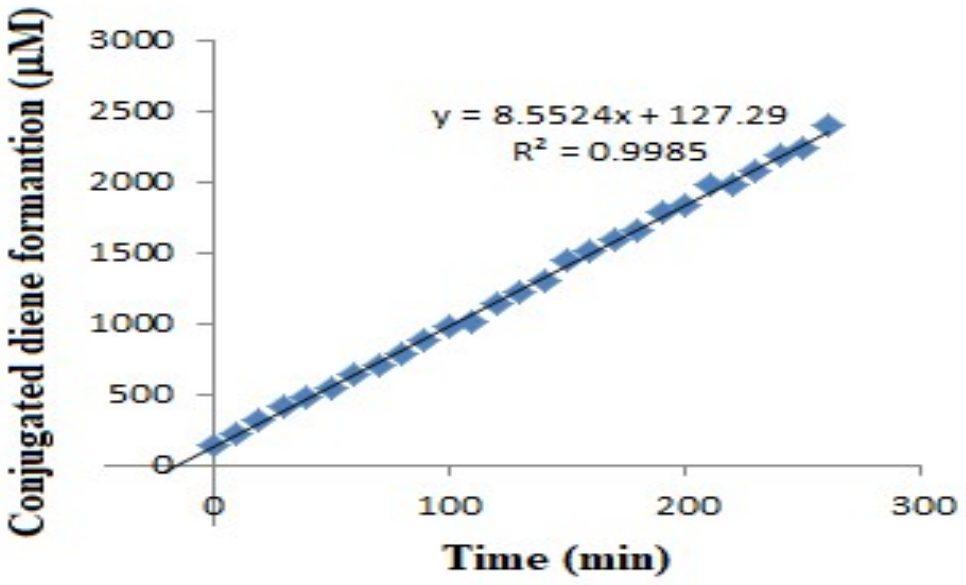


Figure S13. Control experiment without antioxidants (**8** and **9**) using $Na_2S_2O_5$ + PTC

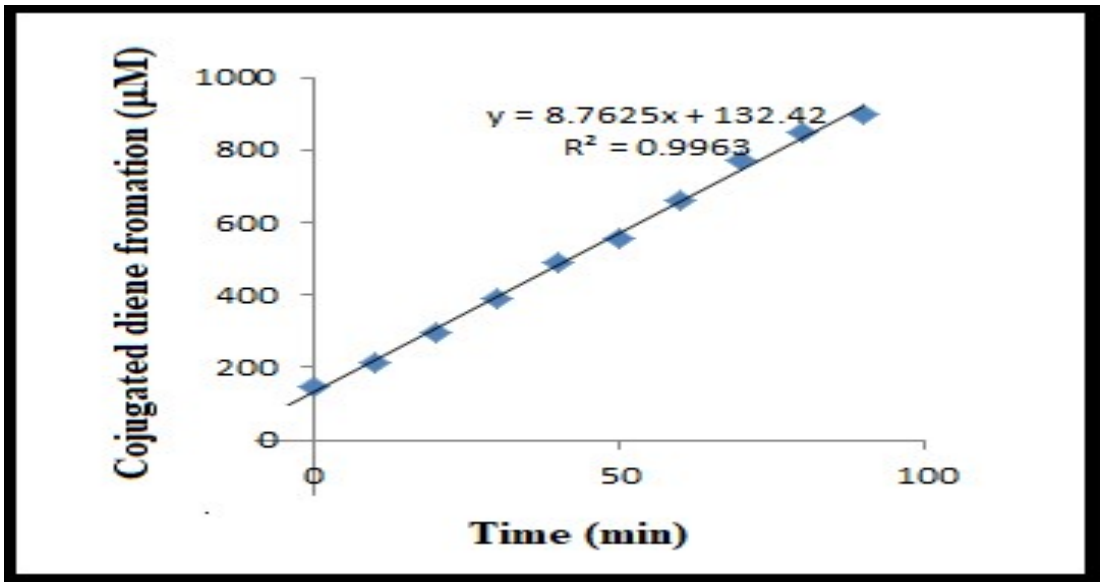


Figure S14. Control experiment without antioxidants (**8** and **9**) using TCEP

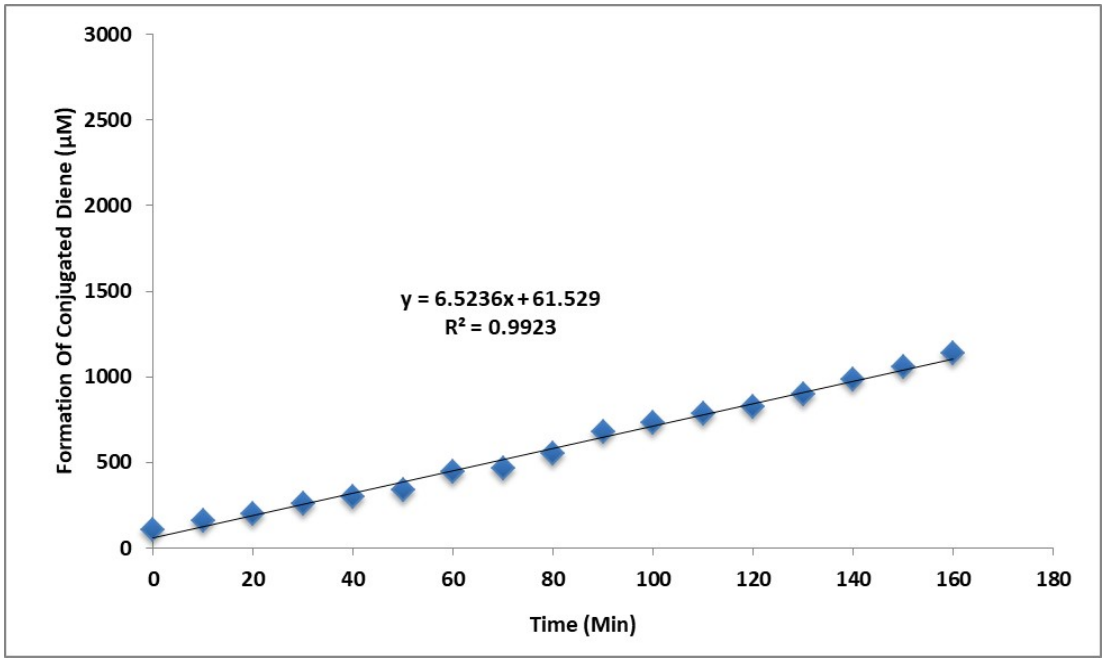
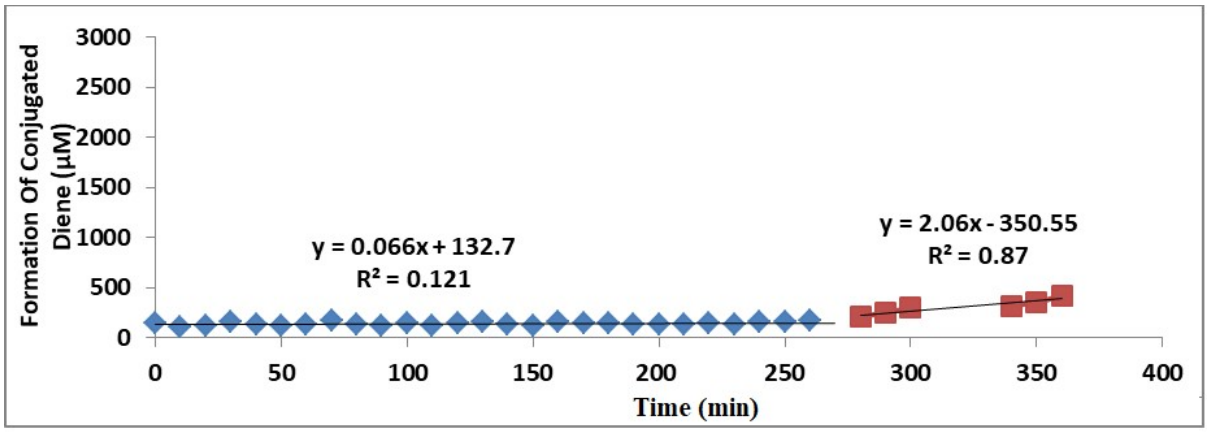
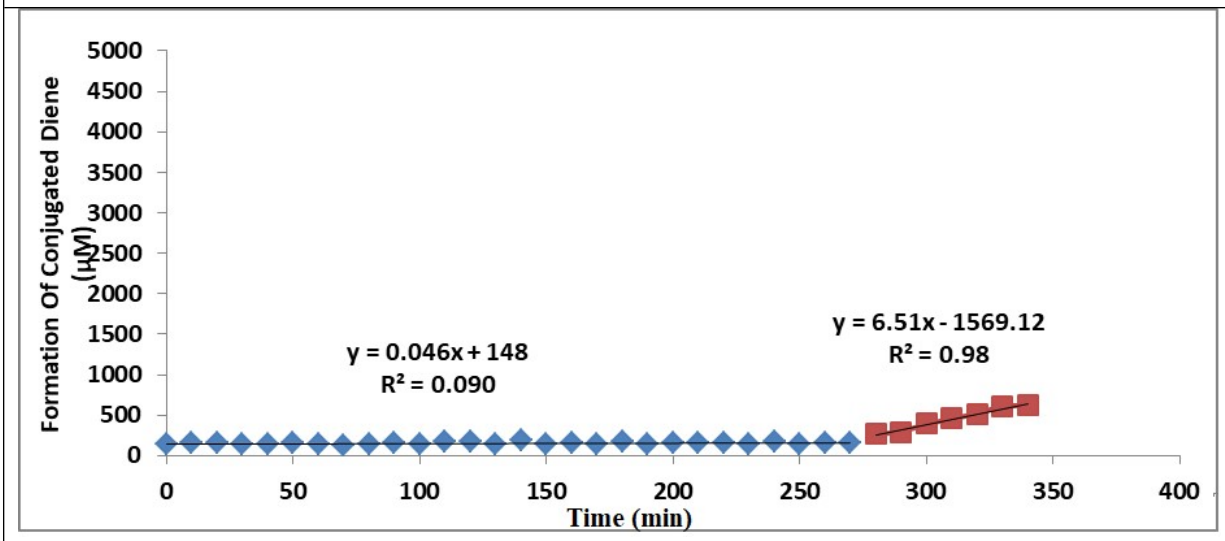


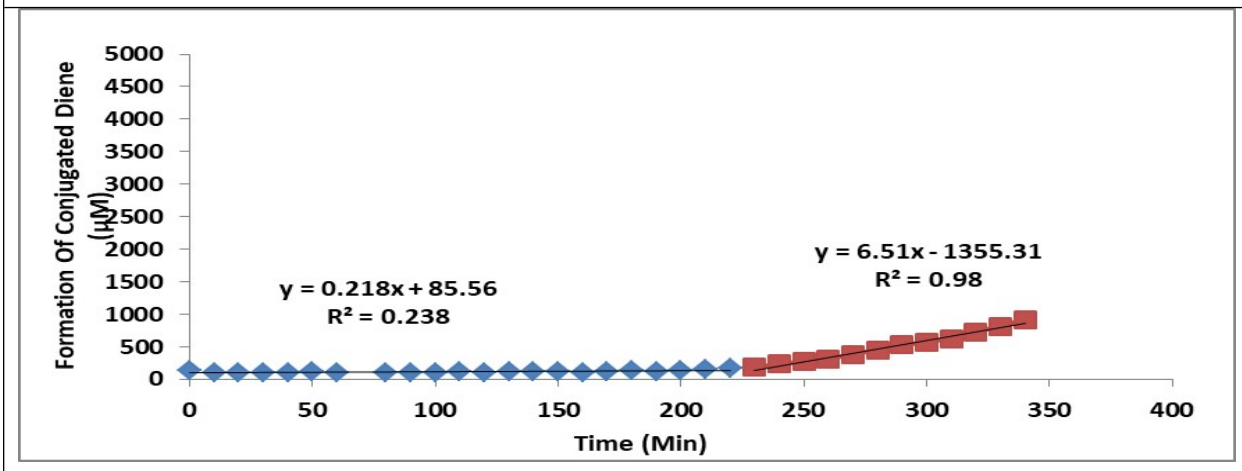
Figure S15. Experiment with antioxidant **8** using GSH



R_{inh} = 3.96 µM/min T_{inh} = 243 min

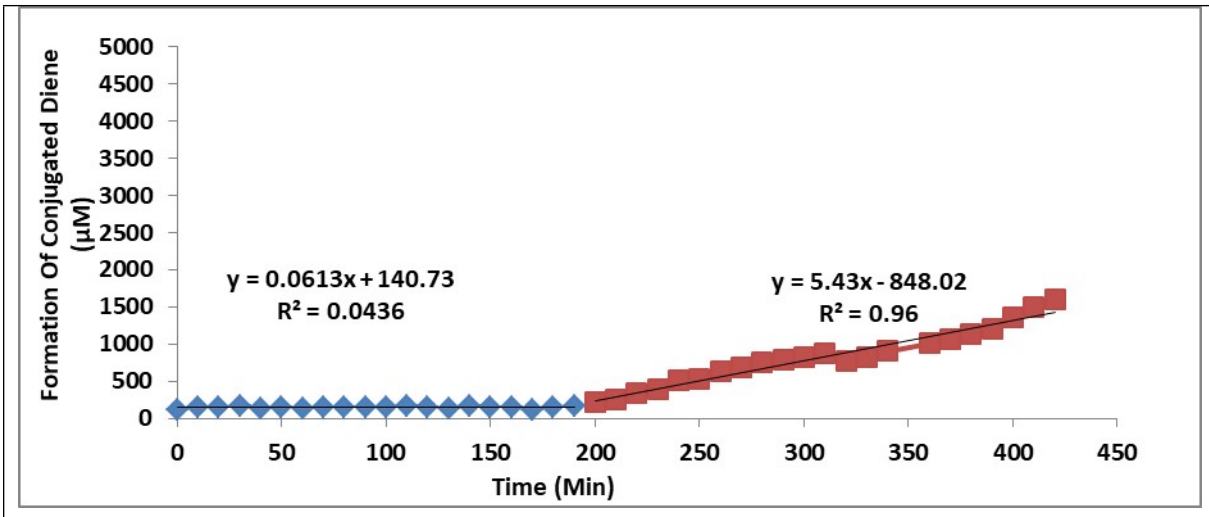


R_{inh} = 2.76 µM/min T_{inh} = 265 Min

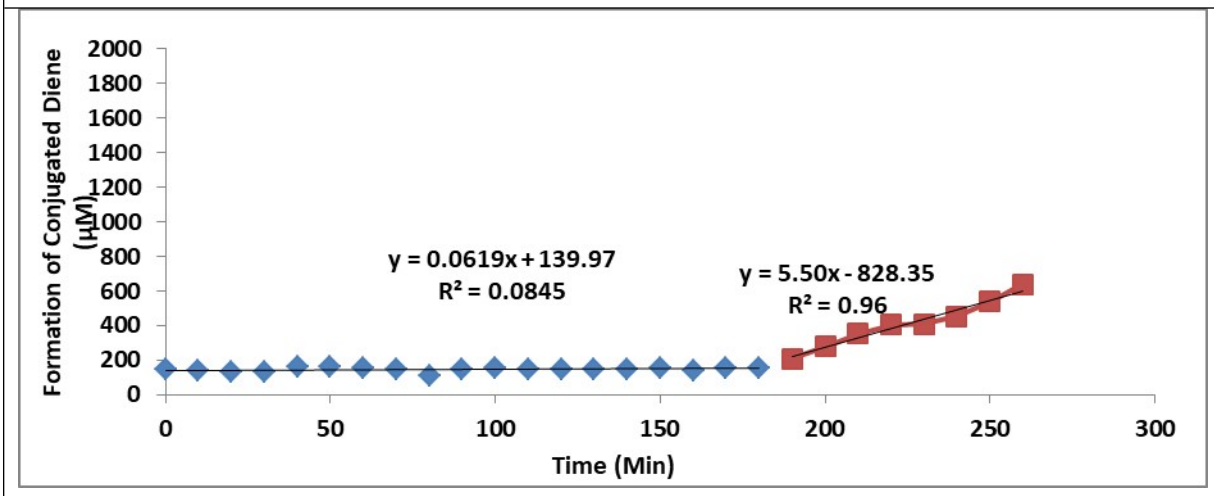


R_{inh} = 2.8 µM/min T_{inh} = 265 Min

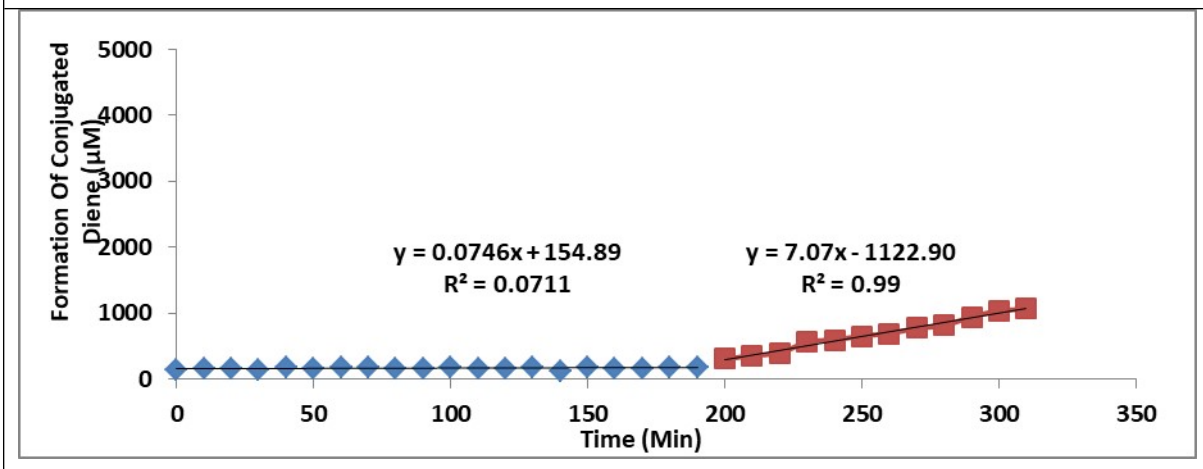
Figure S16. Experiment with antioxidant **8** using DTT



R_{inh} = 3.66 µM/min T_{inh} = 184 Min

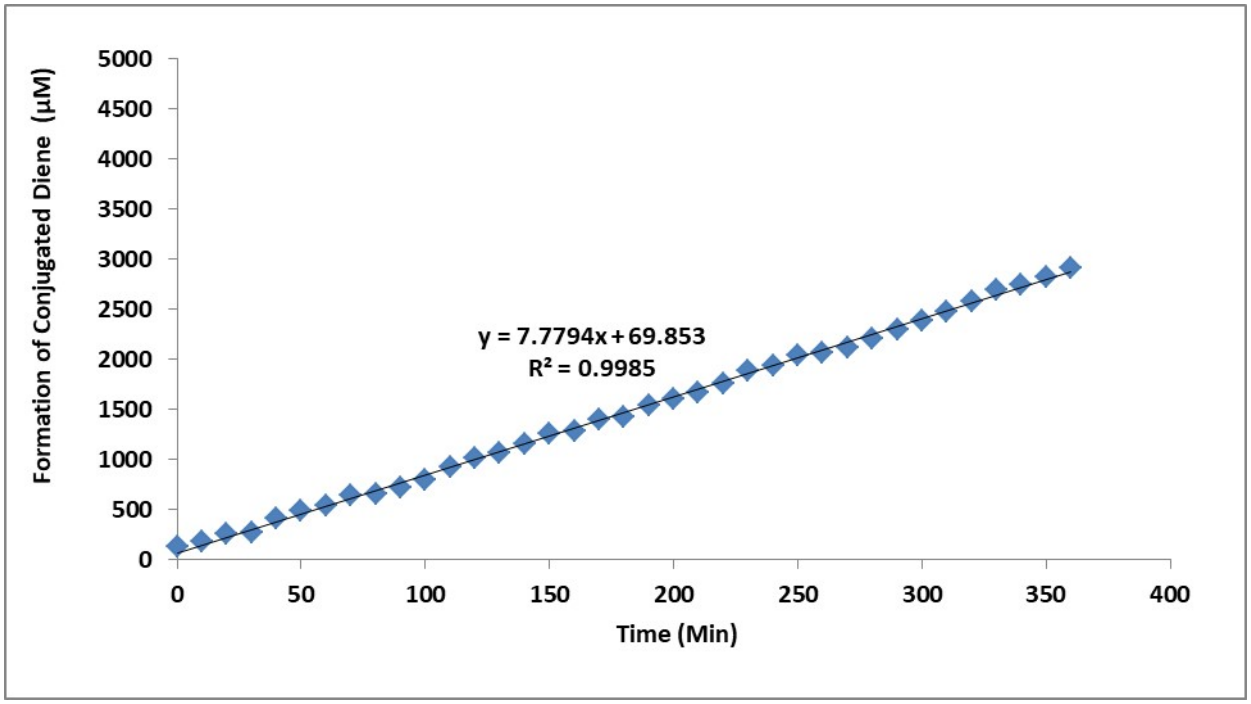


R_{inh} = 3.76 µM/min T_{inh} = 174 Min



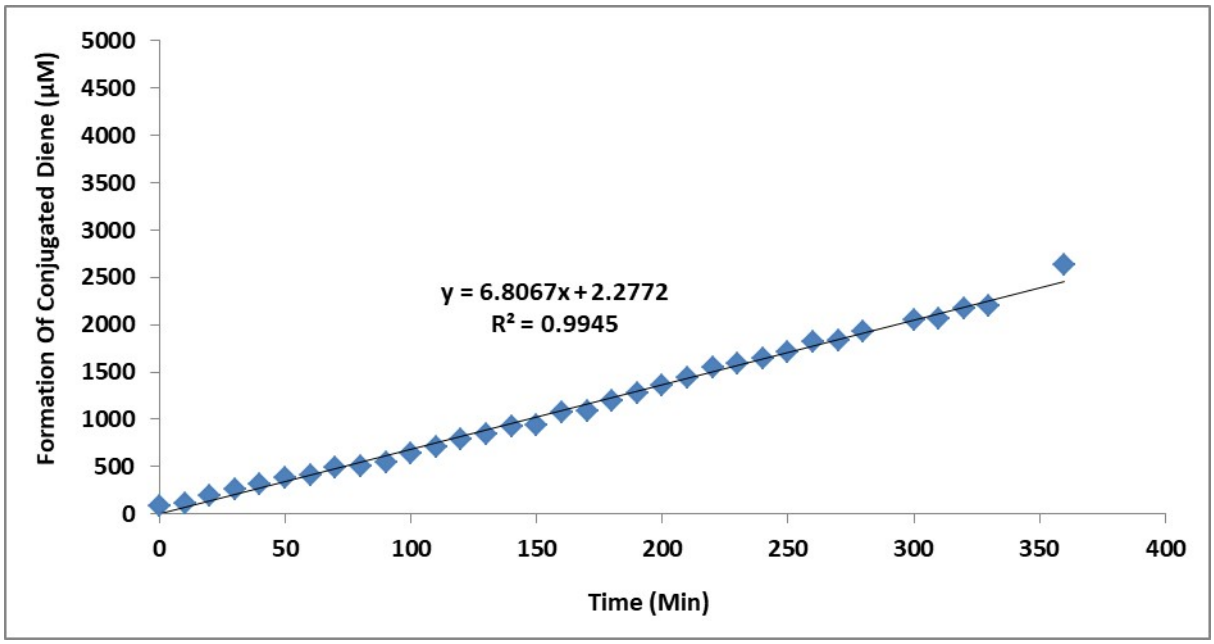
R_{inh} = 4.44 µM/min T_{inh} = 183 Min

Figure S17. Experiment with antioxidant **8** using AscOH



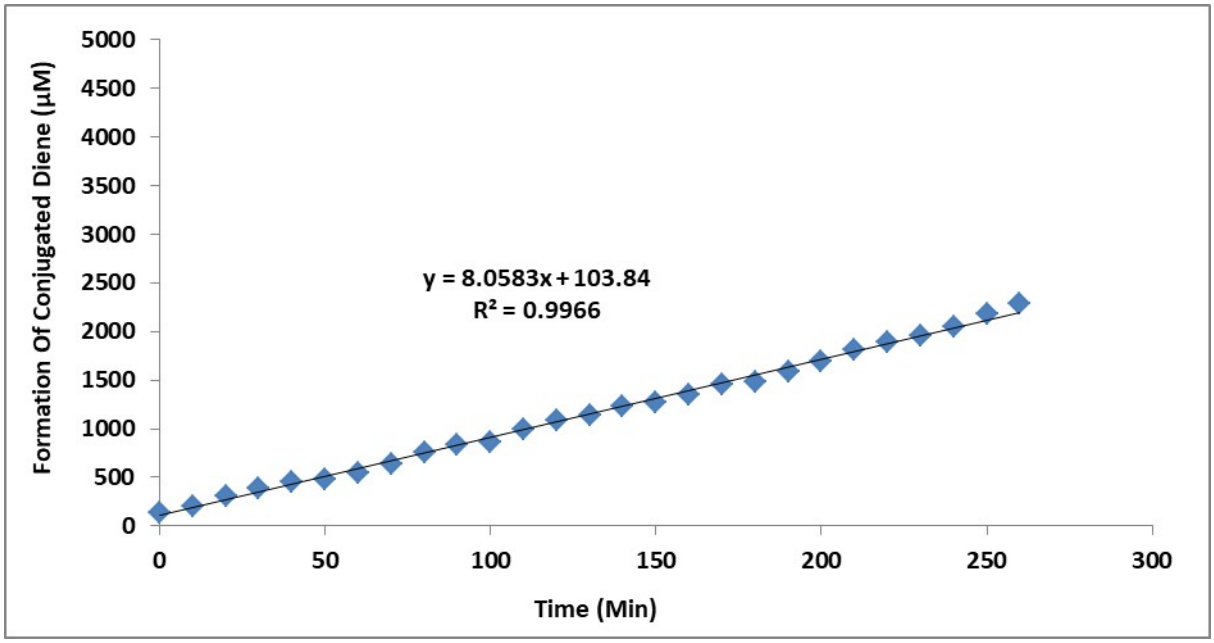
R_{inh} = 466.74 µM/min

Figure S18. Experiment with antioxidant **8** using sodium ascorbate



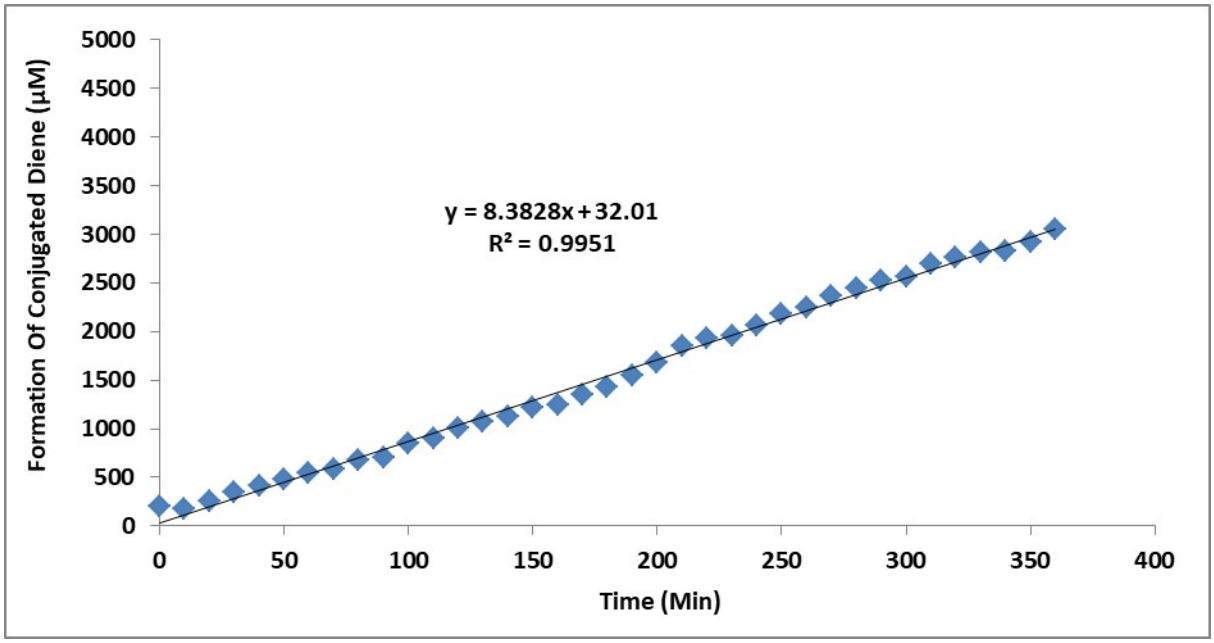
R_{inh} = 408 µM/min

Figure S19. Experiment with antioxidant **8** using $K_4[Fe(CN)_6].3H_2O$



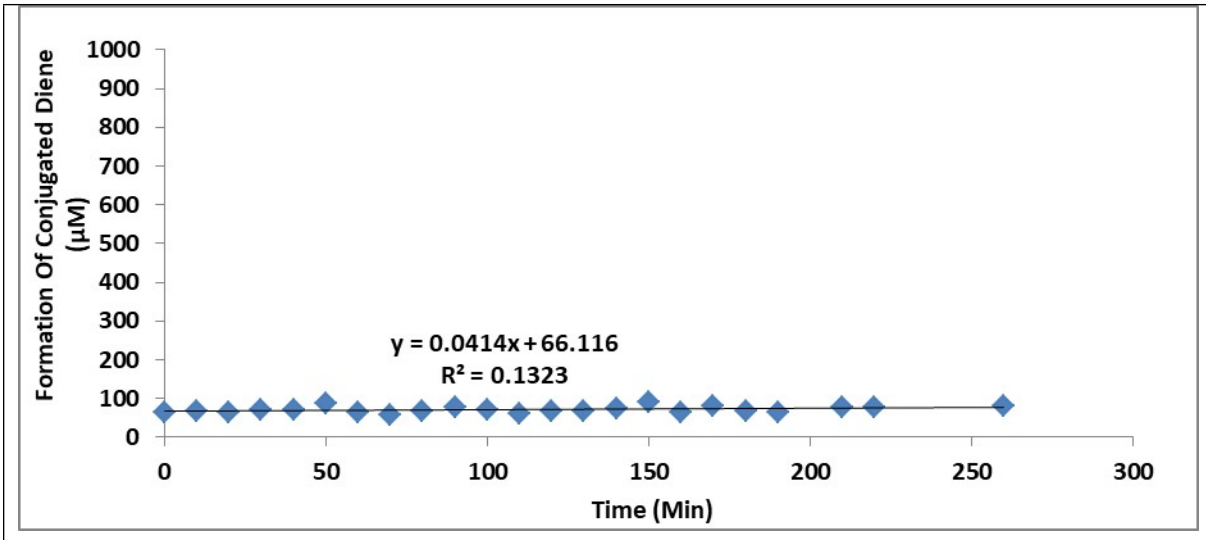
R_{inh} = 484 µM/min

Figure S20. Experiment with antioxidant **8** using $K_4[Fe(CN)_6].3H_2O$ + PTC

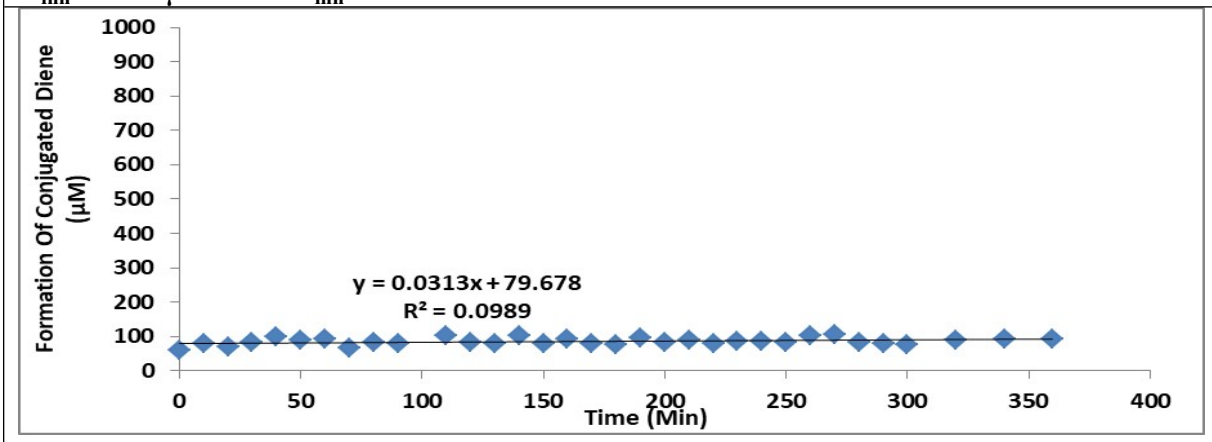


R_{inh} = 503 µM/min

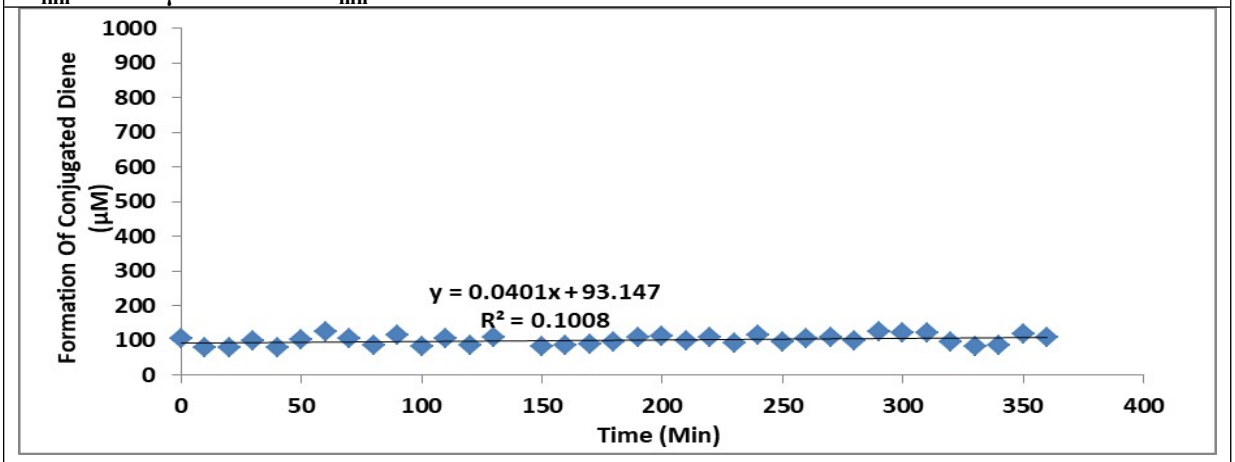
Figure S21. Experiment with antioxidant **8** using PCET



R_{inh} = 2.46 µM/min T_{inh} > 360 Min

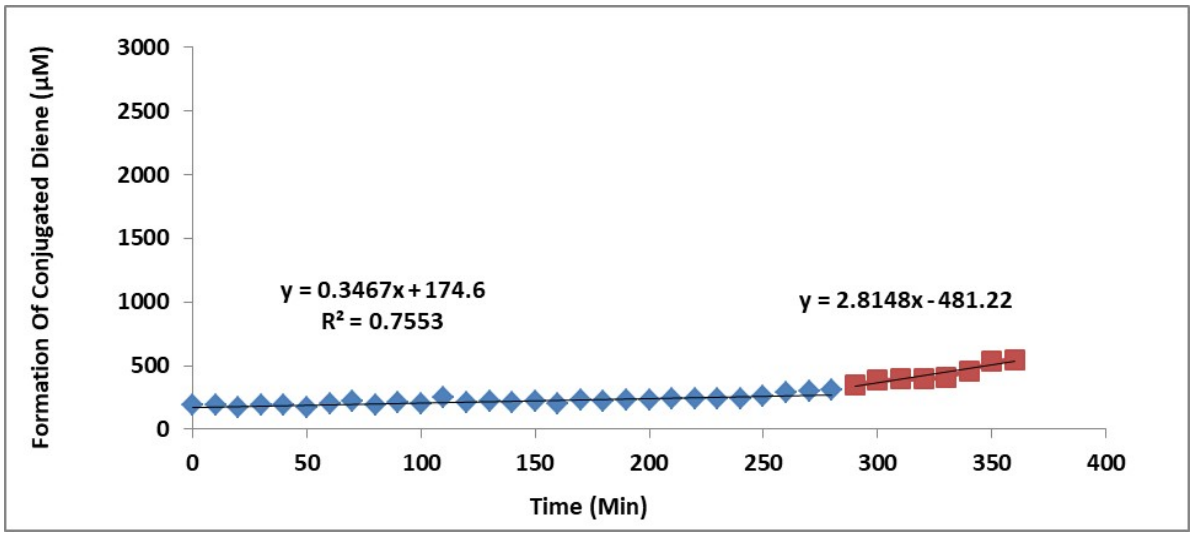


R_{inh} = 1.88 µM/min T_{inh} > 360 Min

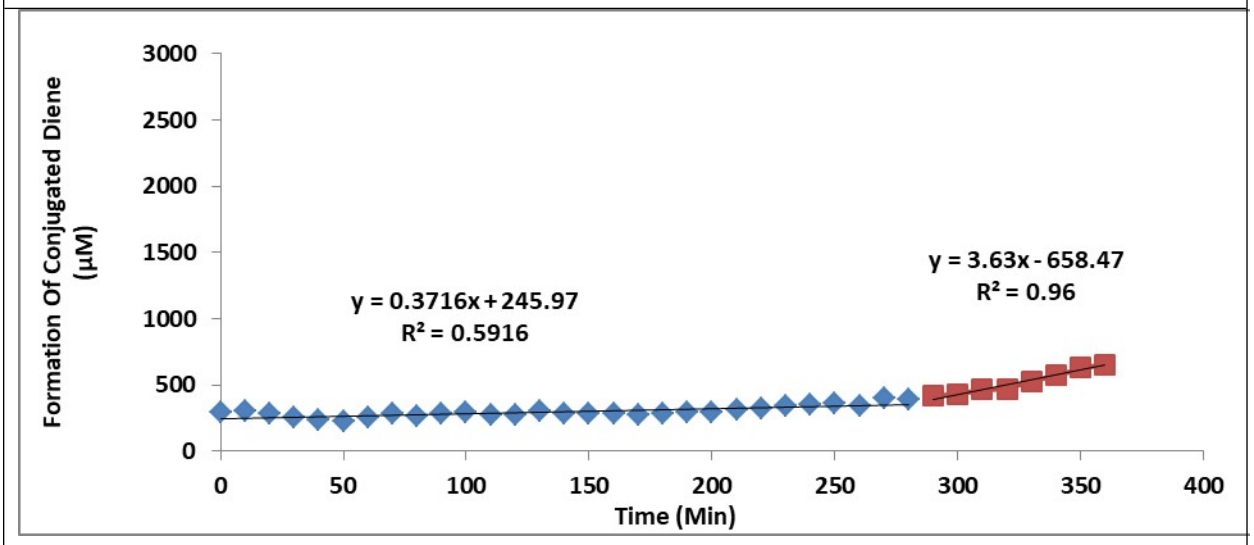


R_{inh} = 2.4 µM/min T_{inh} > 360 Min

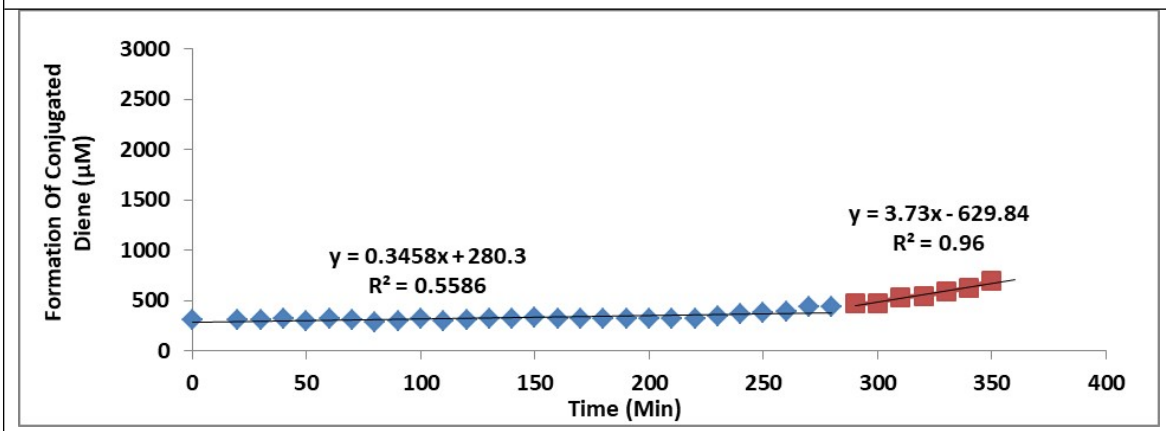
Figure S22. Experiment with antioxidant **8** using NAC pH = 1



R_{inh} = 20.8 µM/Min T_{inh} = 266 Min

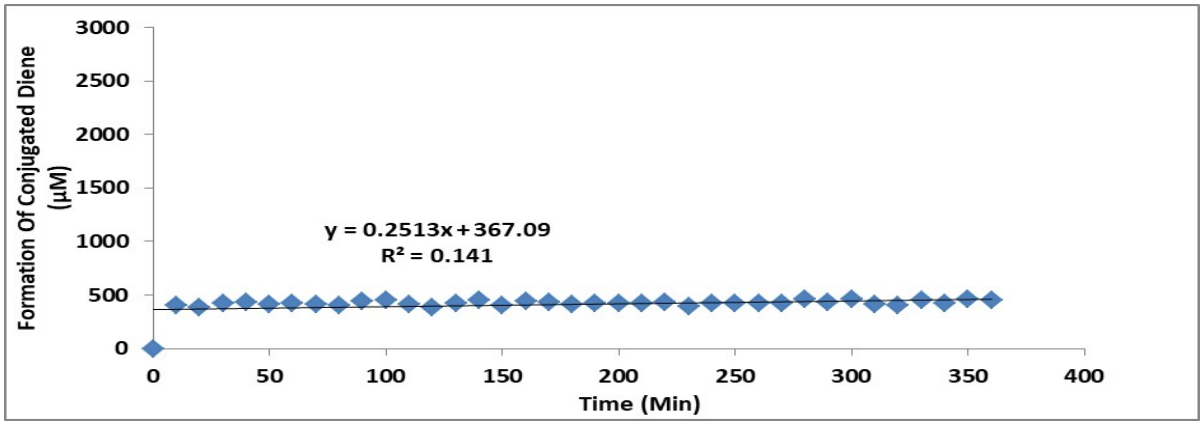


R_{inh} = 22.26 µM/Min T_{inh} = 278 Min

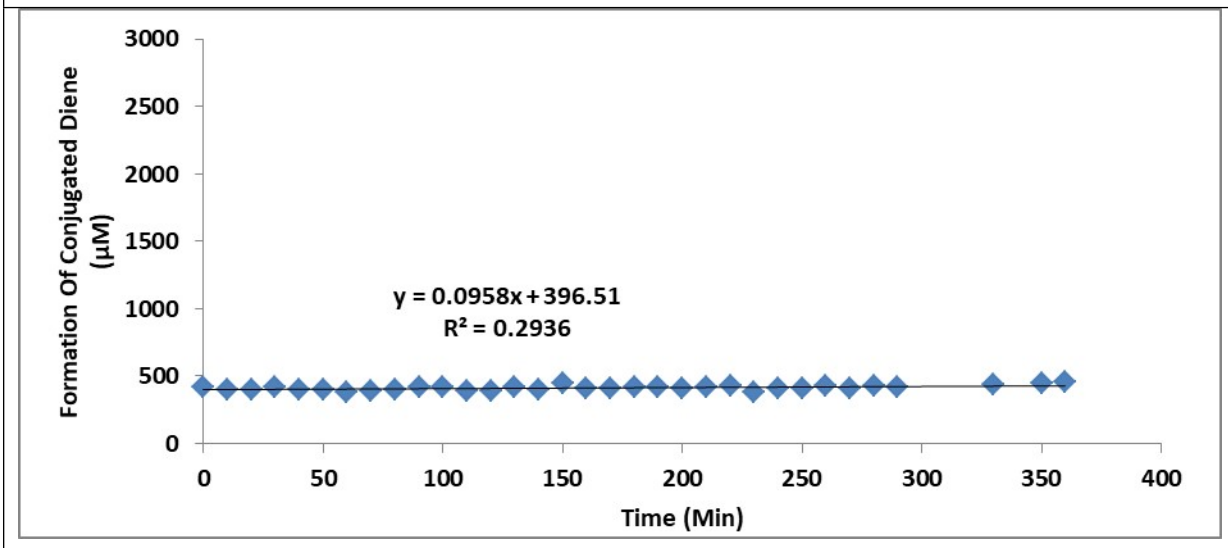


R_{inh} = 20.7 µM/Min T_{inh} = 269 Min

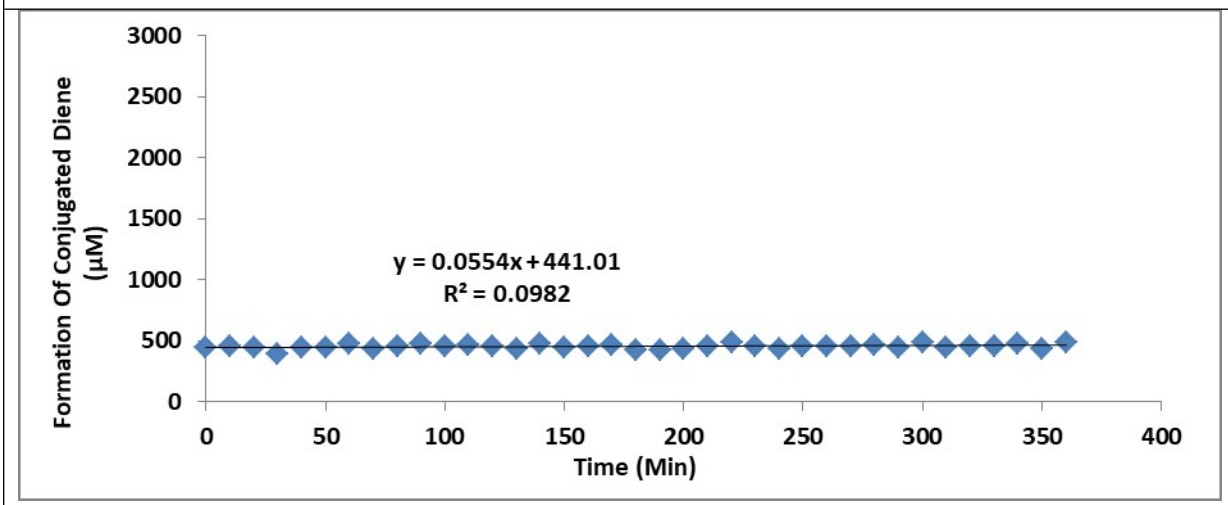
Figure S23. Experiment with antioxidant **8** using NAC pH = 2



R_{inh} = 5.06 µM/Min T_{inh} > 360 Min

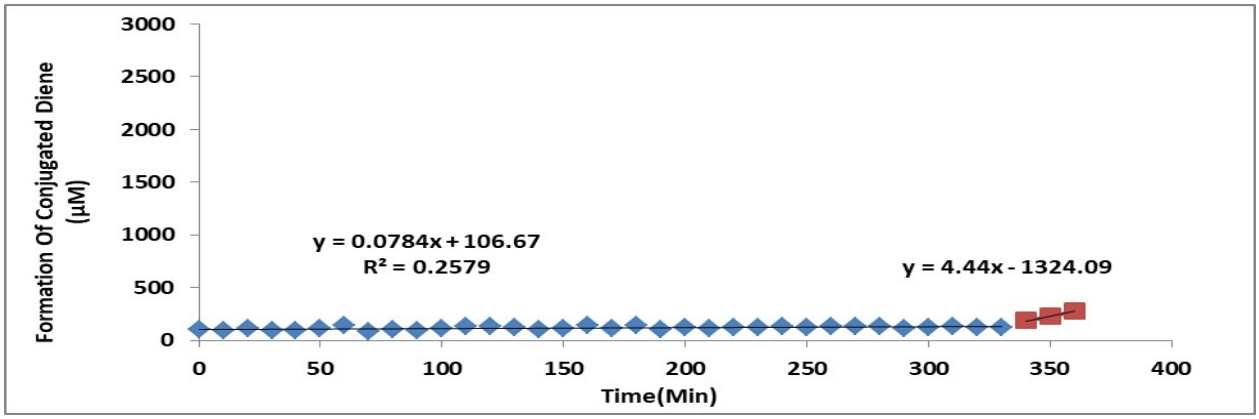


R_{inh} = 5.7 µM/Min T_{inh} > 360 Min

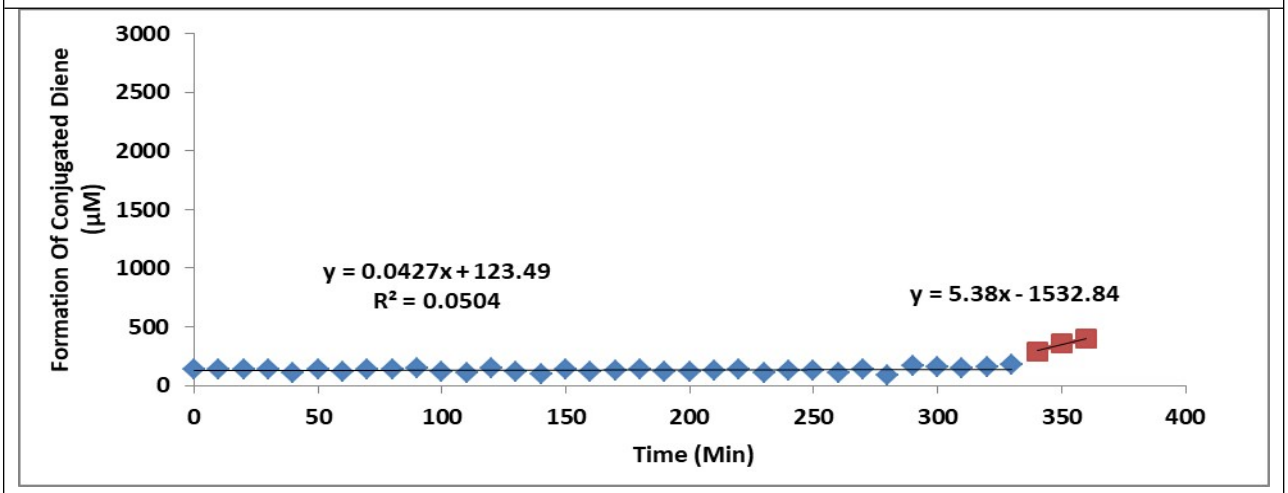


R_{inh} = 3.3 µM/Min T_{inh} > 360 Min

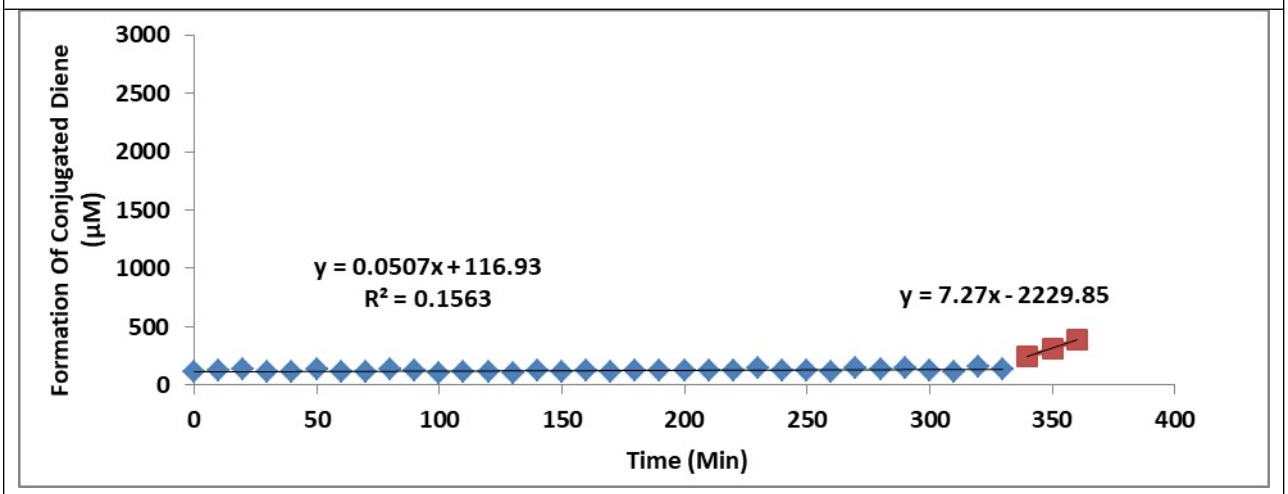
Figure S24. Experiment with antioxidant **8** using NAC pH = 3



R_{inh}=4.7 µM/Min T_{inh}=328 Min

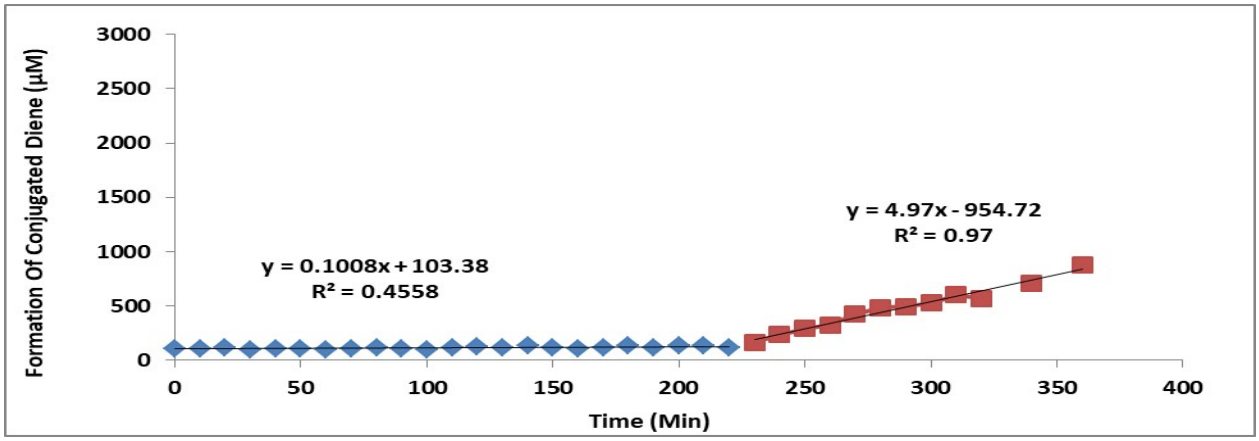


R_{inh}=2.52 µM/Min T_{inh}=311 Min

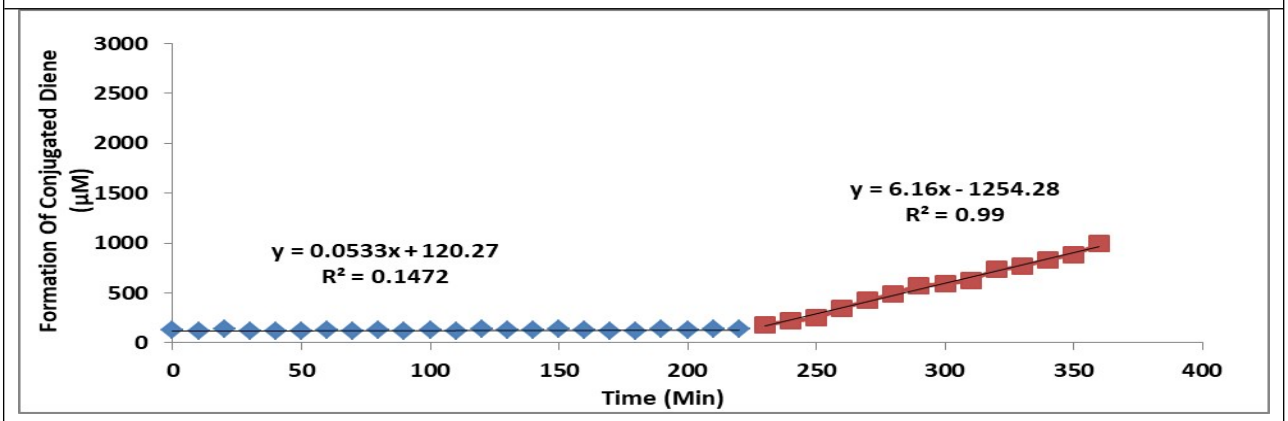


R_{inh} = 3.0 µM/Min T_{inh} = 325 Min

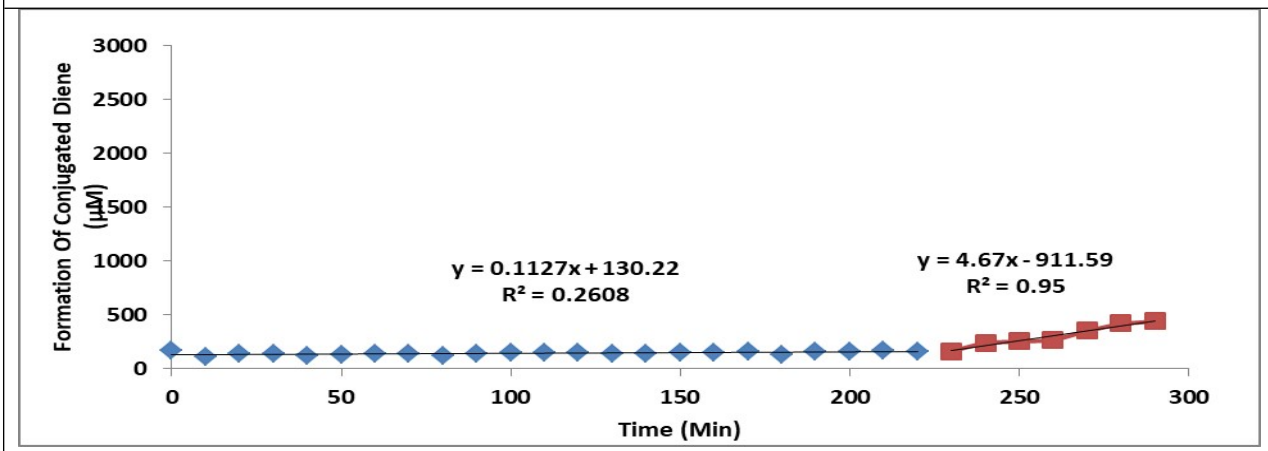
Figure S25. Experiment with antioxidant **8** using NAC pH = 4



R_{inh} = 6.05 µM/Min T_{inh} = 220 Min

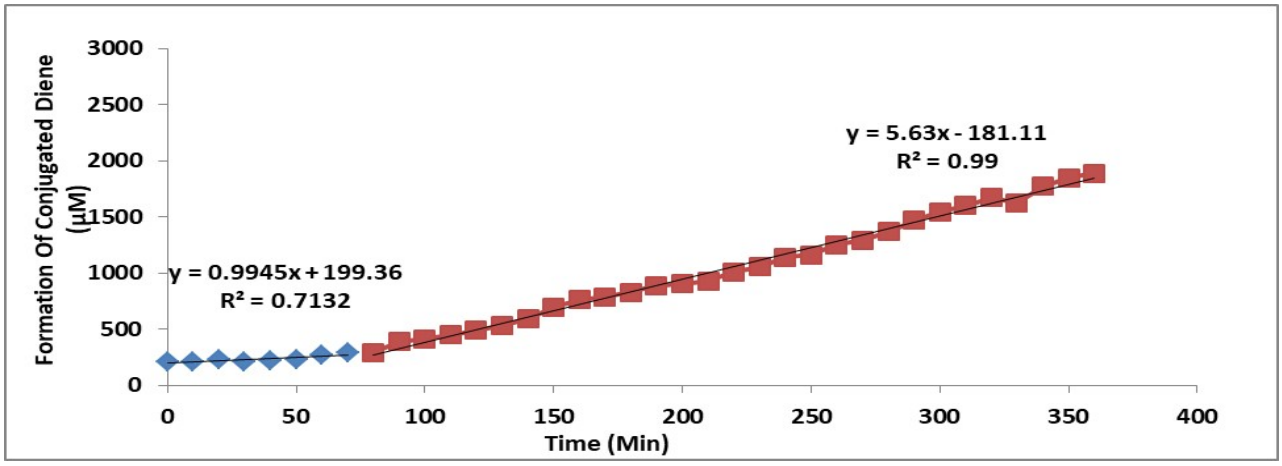


R_{inh} = 3.18µM/Min T_{inh} = 225 Min

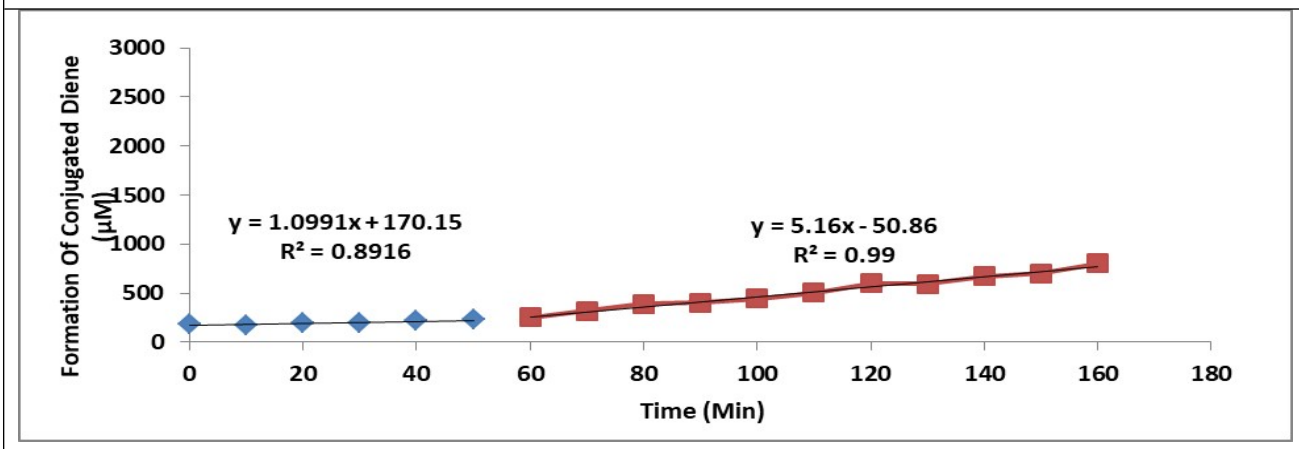


R_{inh} = 6.72µM/Min T_{inh} = 228 Min

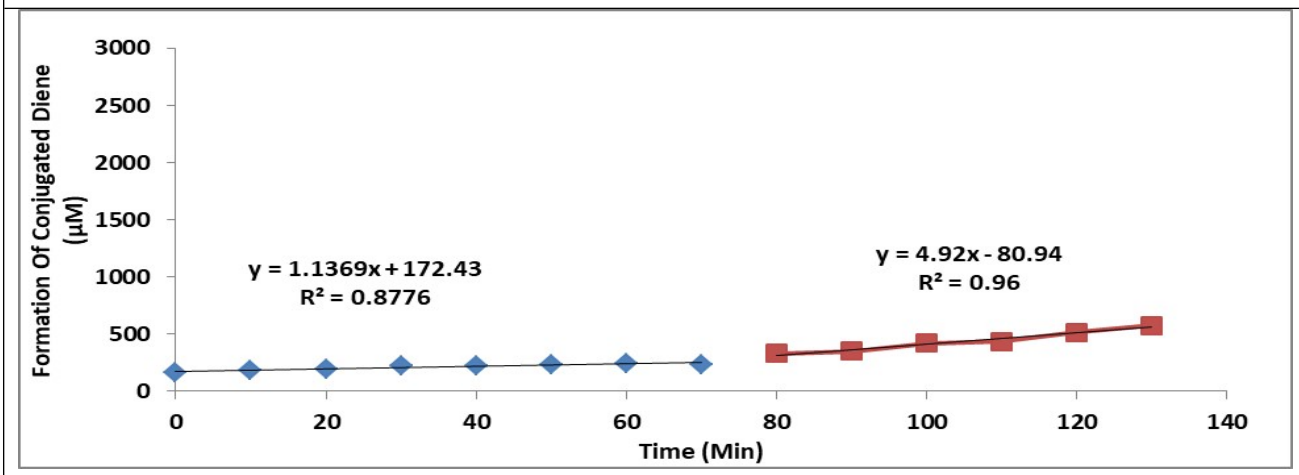
Figure S26. Experiment with antioxidant **8** using NAC pH = 5



R_{inh} = 59.64 µM/Min T_{inh} = 75 Min

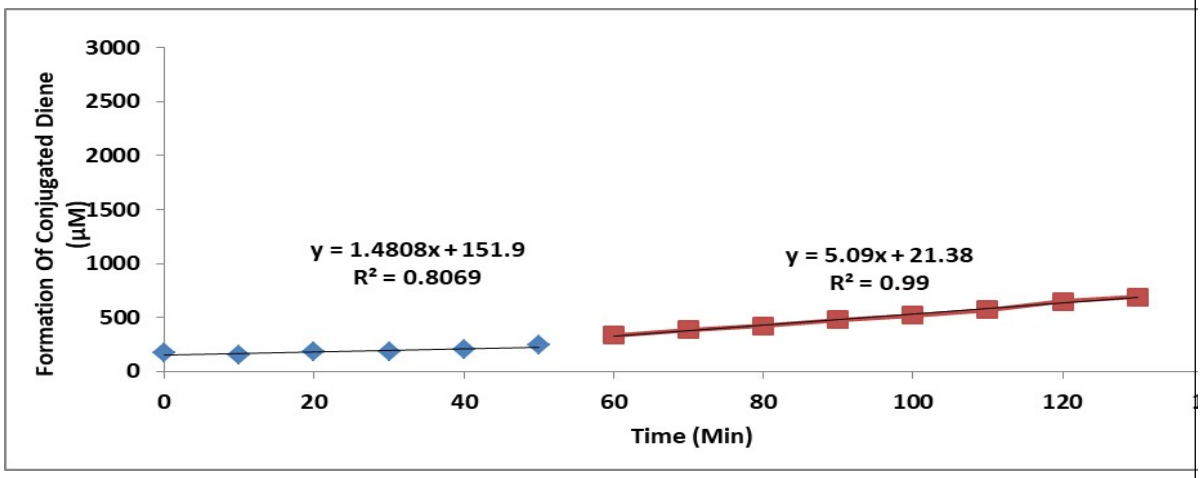


R_{inh} = 65.94 µM/Min T_{inh} = 55 Min

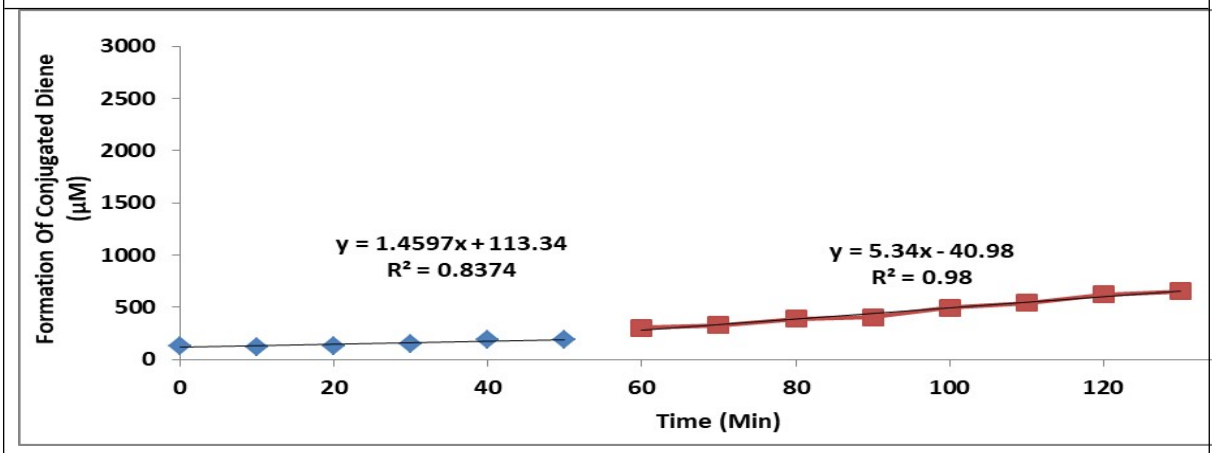


R_{inh} = 68.2 µM/Min T_{inh} = 67 Min

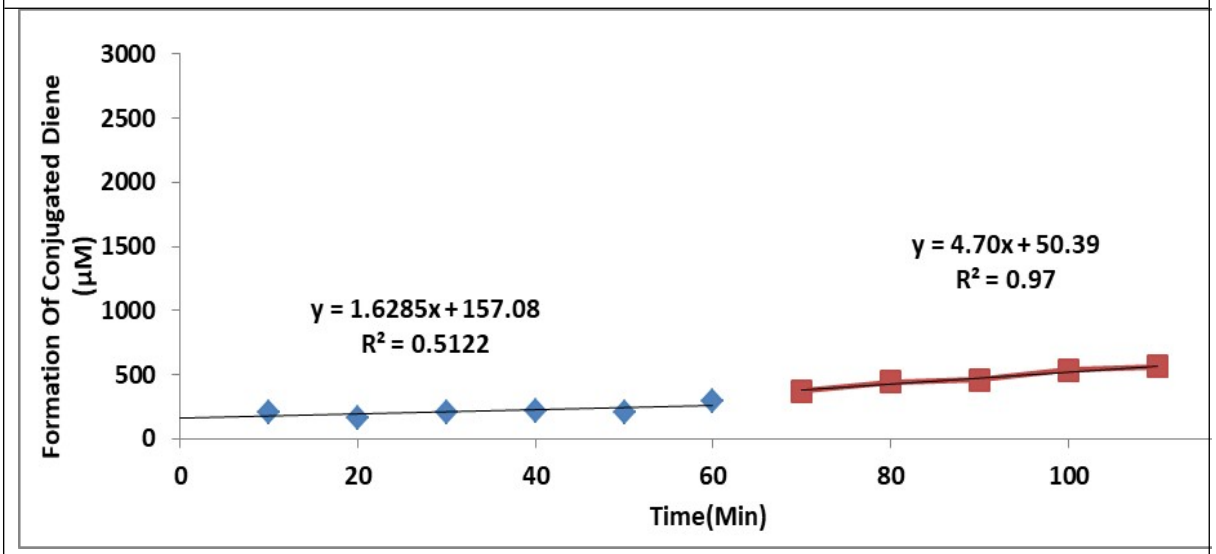
Figure S27. Experiment with antioxidant **8** using NAC pH = 6



R_{inh} = 88.8 µM/Min T_{inh} = 48 Min

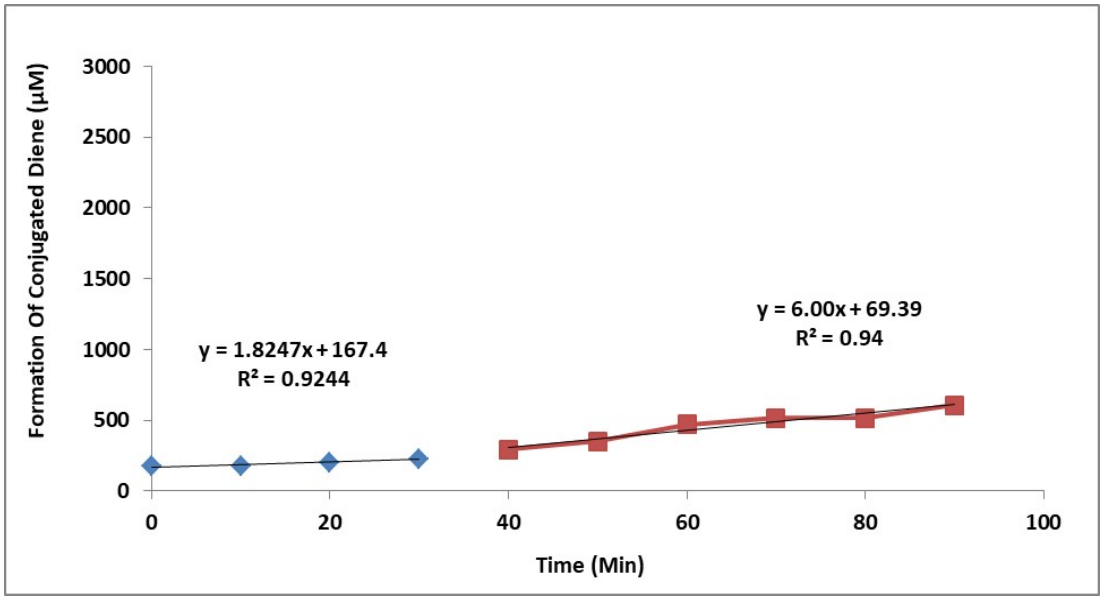


R_{inh} = 87.6 µM/Min T_{inh} = 55 Min

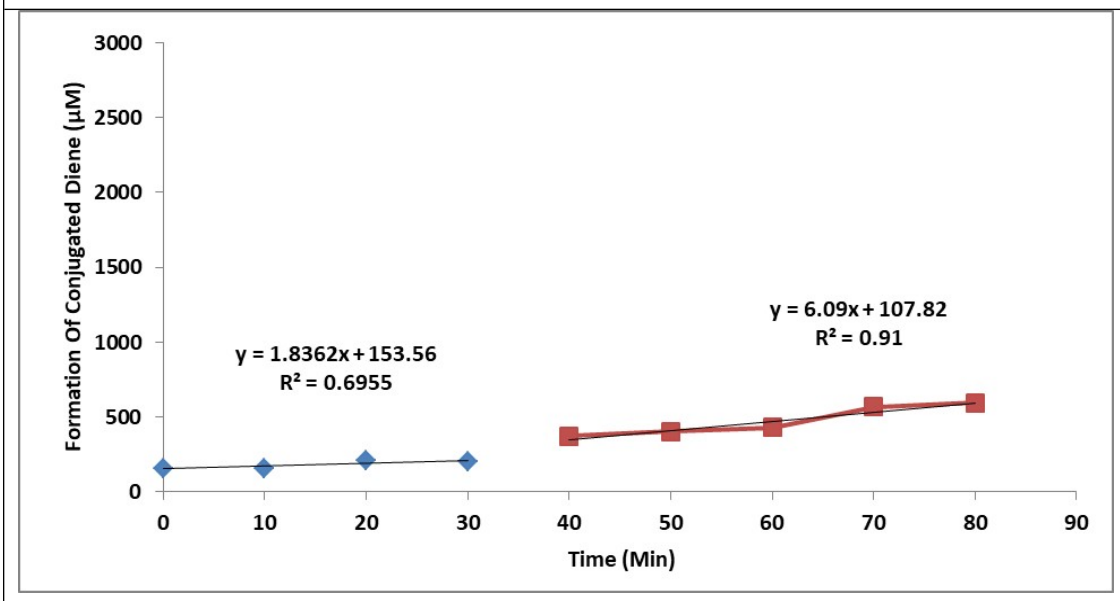


R_{inh} = 97.7 µM/Min T_{inh} = 60 Min

Figure S28. Experiment with antioxidant **8** using NAC pH = 7

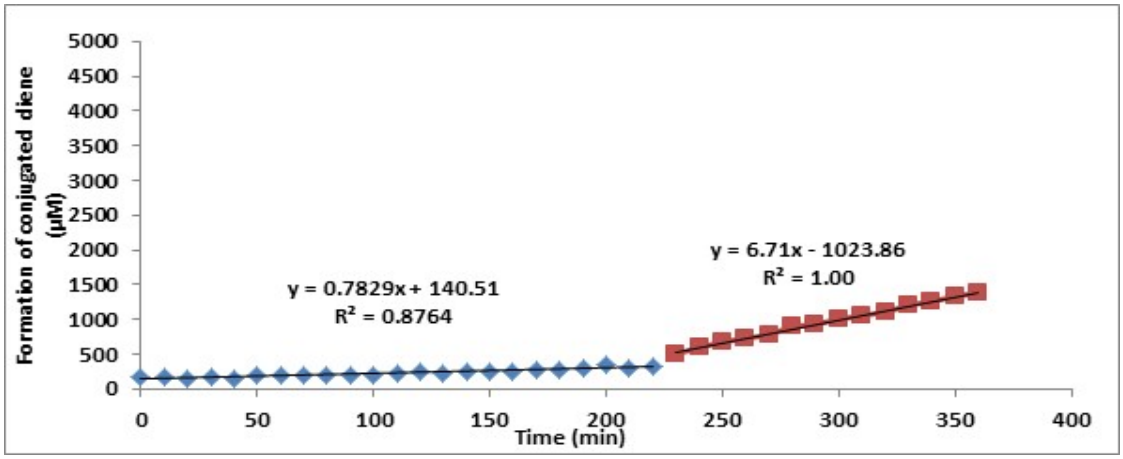


R_{inh} = 109.5 µM/Min T_{inh} = 57 Min

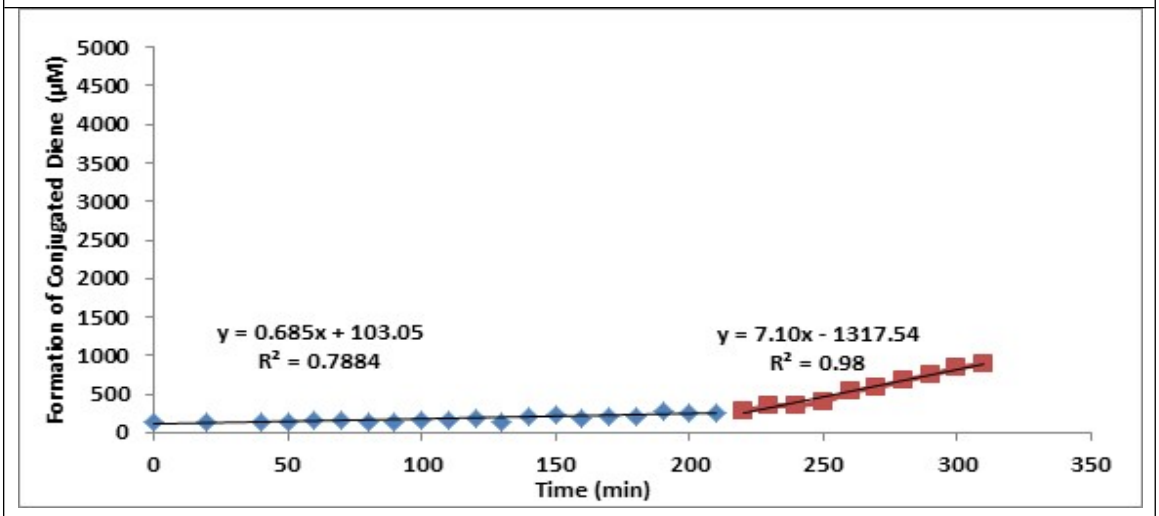


R_{inh} = 110.2 µM/Min T_{inh} = 61 Min

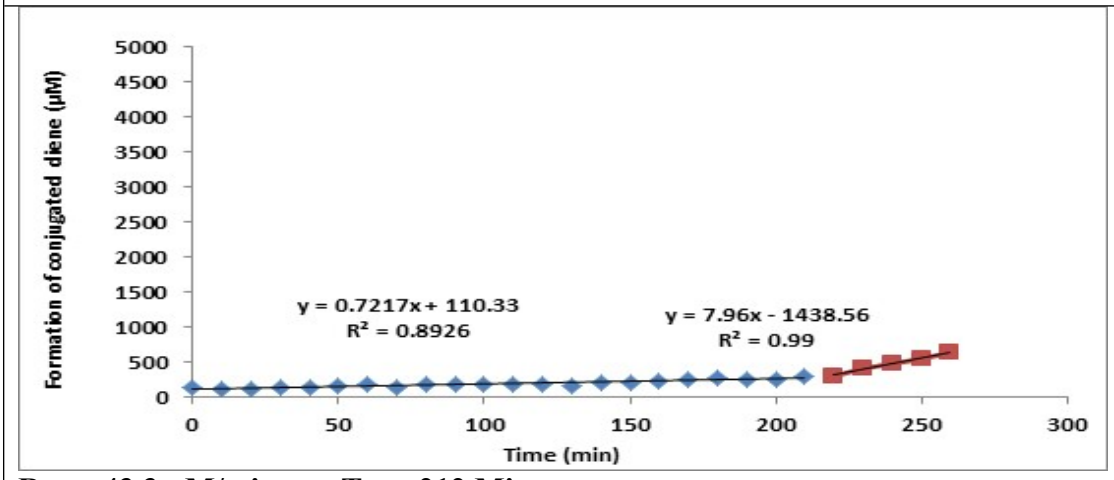
Figure S29. Experiment with antioxidant **9** using Ascorbic Acid



R_{inh}= 46.92 µM/min T_{inh}= 210 Min

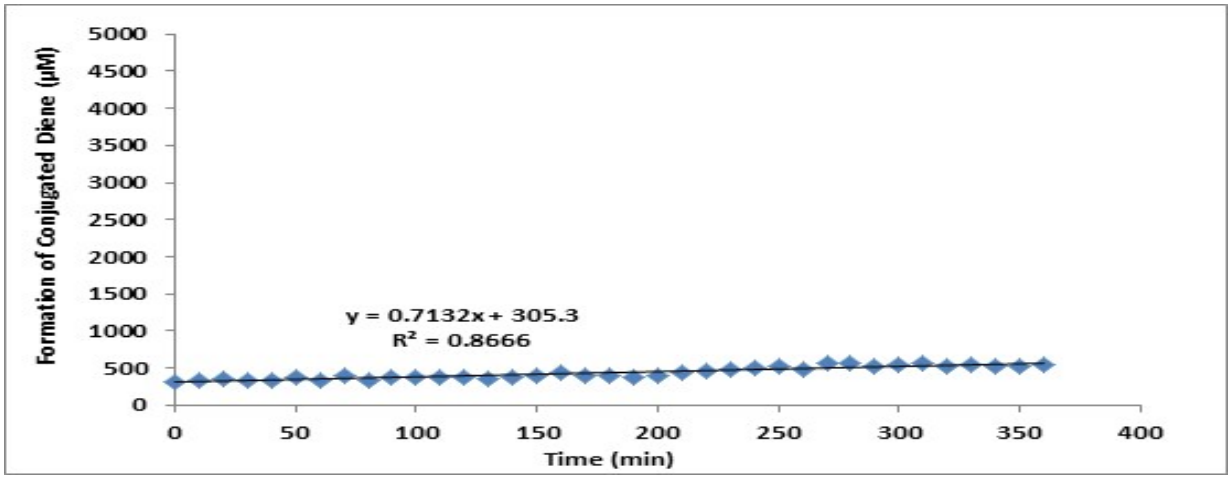


R_{inh} = 41.4 µM/min T_{inh} = 208 Min

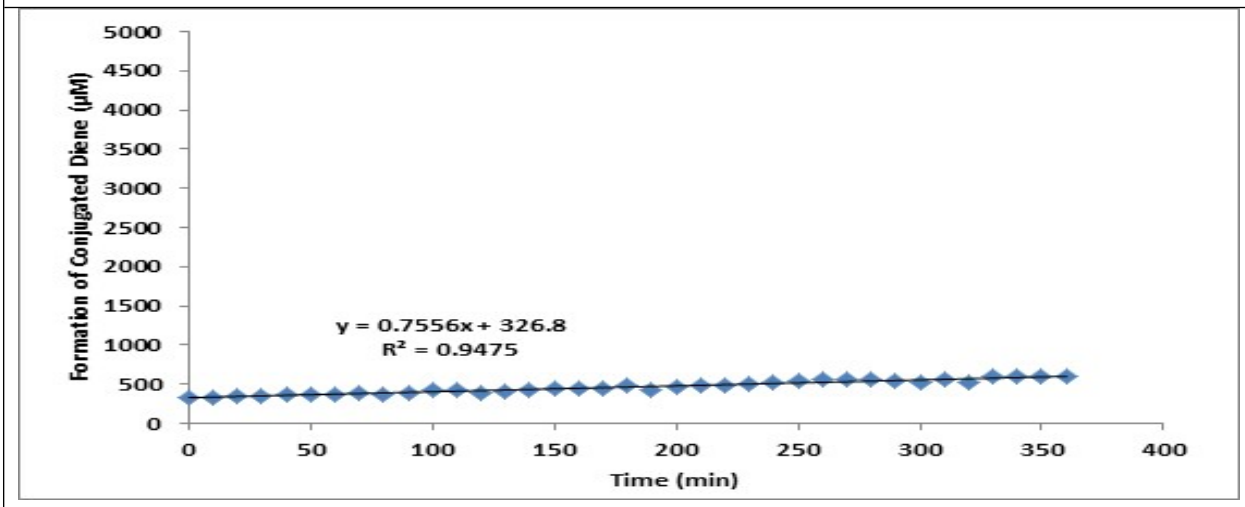


R_{inh} = 43.3 µM/min T_{inh}= 212 Min

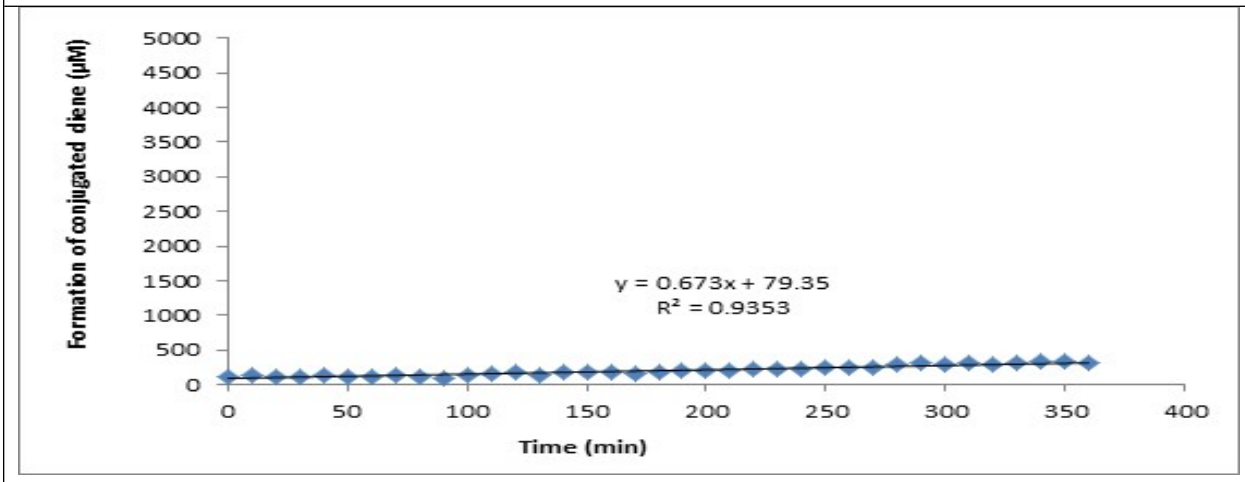
Figure S30. Experiment with antioxidant **9** using DTT



R_{inh} = 42.8 µm/min T_{inh} > 360 Min

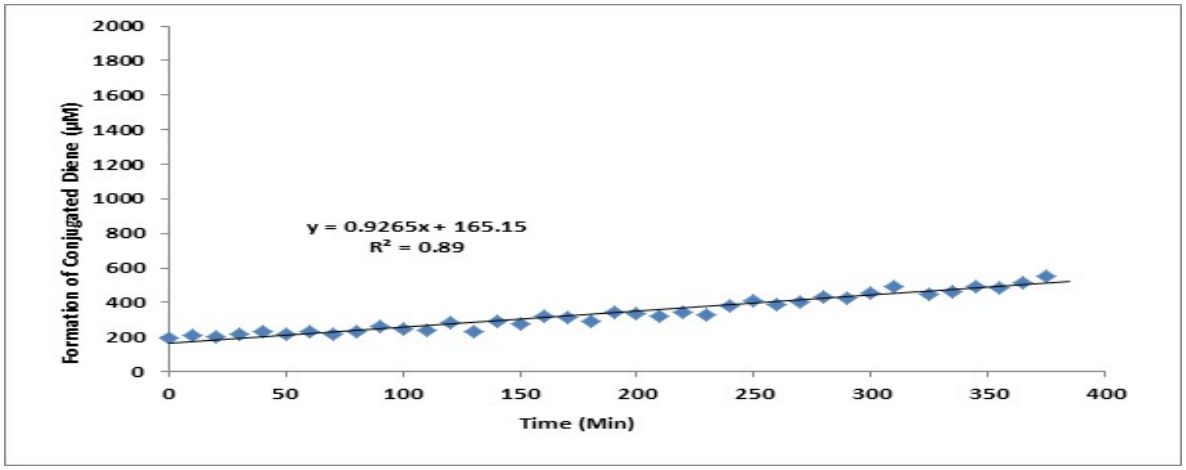


R_{inh} = 45.3 µM/min T_{inh} > 360 Min

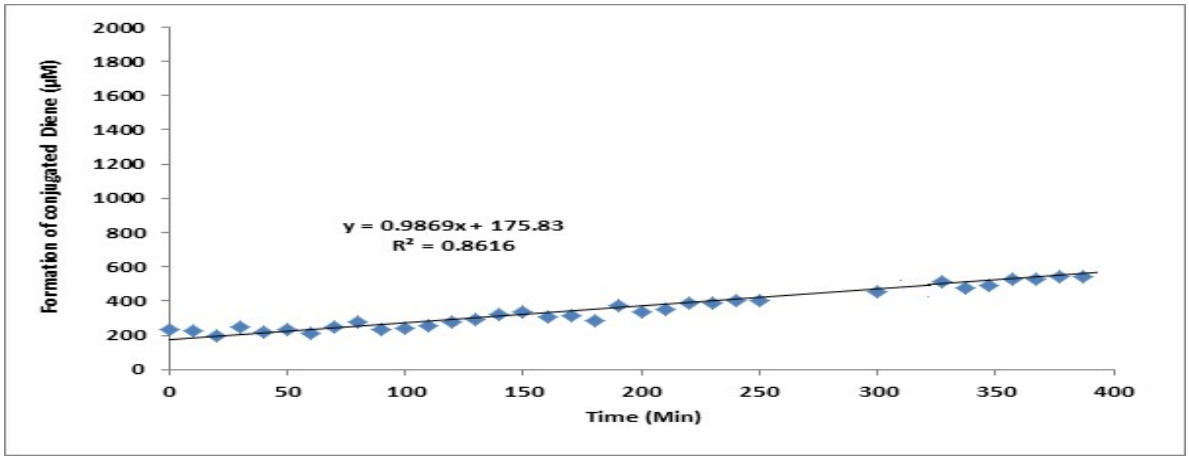


R_{inh} = 40.4 µm/min T_{inh} > 360 Min

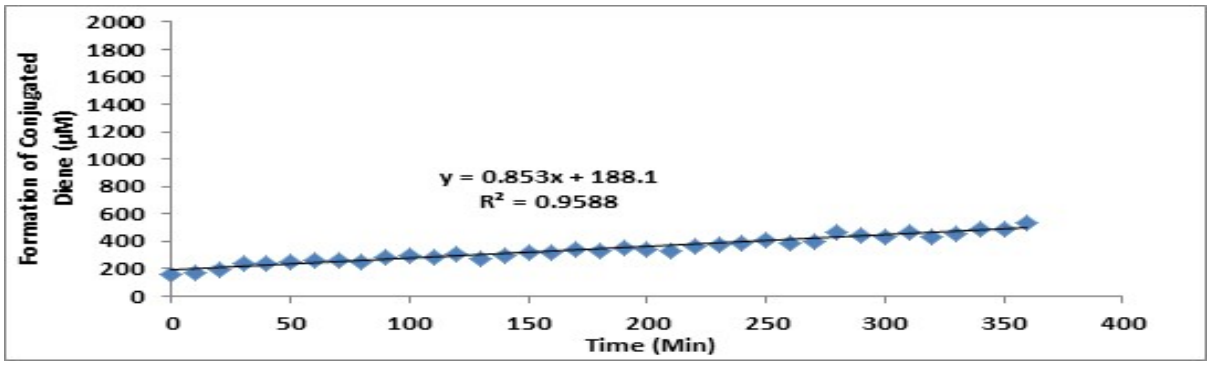
Figure S31. Experiment with antioxidant **9** using NAC



R_{inh} = 55.56 µM/min T_{inh} > 360 Min

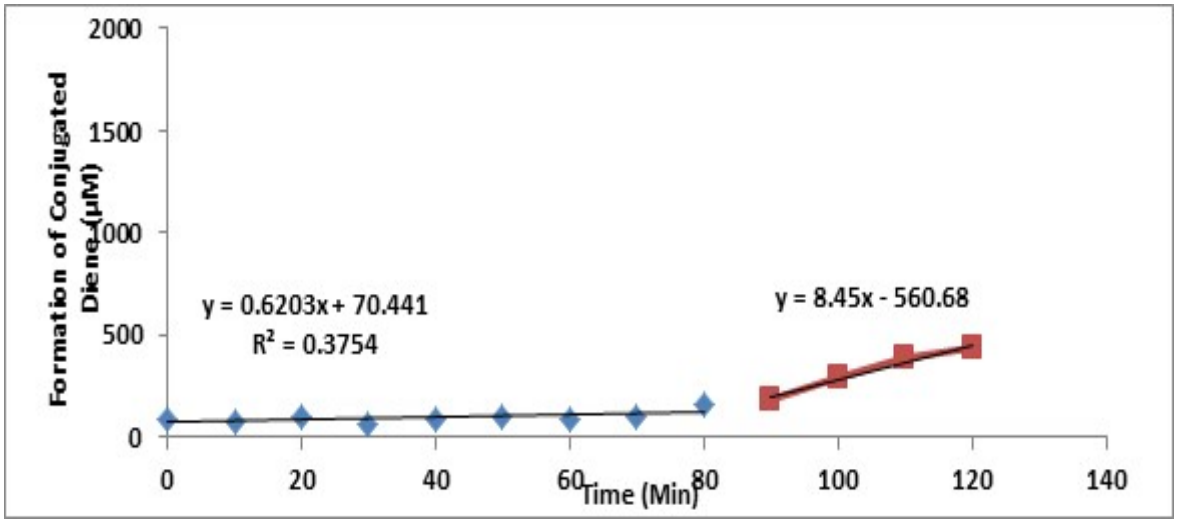


R_{inh} = 59.16 µM/min T_{inh} > 360 Min

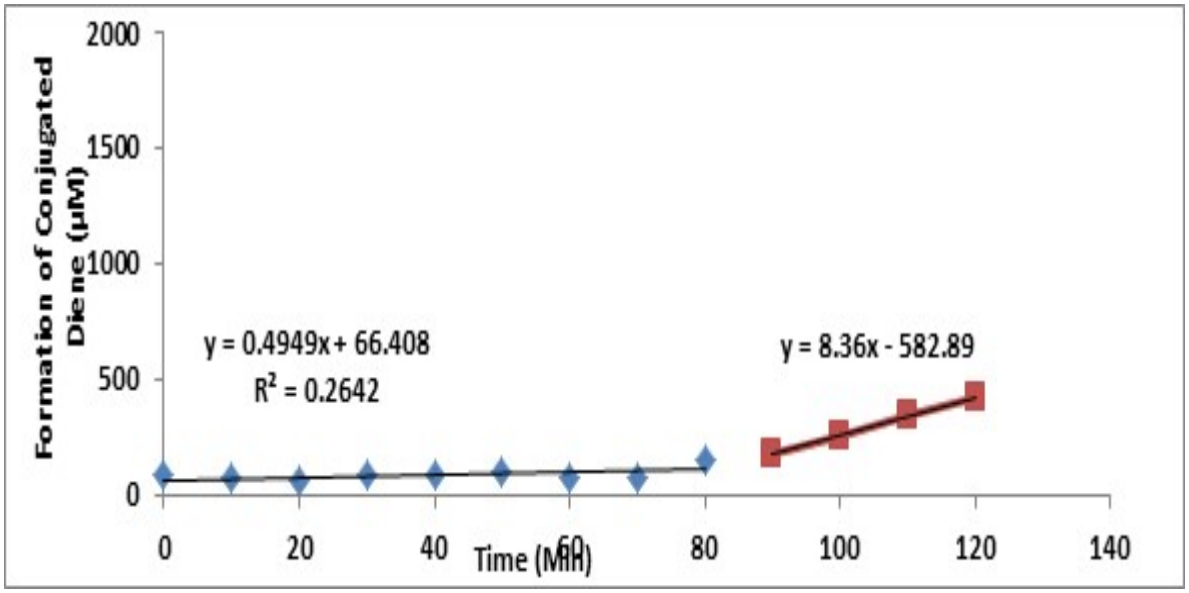


R_{inh} = 51.2 µM/min T_{inh} > 360 Min

Figure S32. Experiment with antioxidant **9** using $K_4Fe(CN_6).4H_2O$

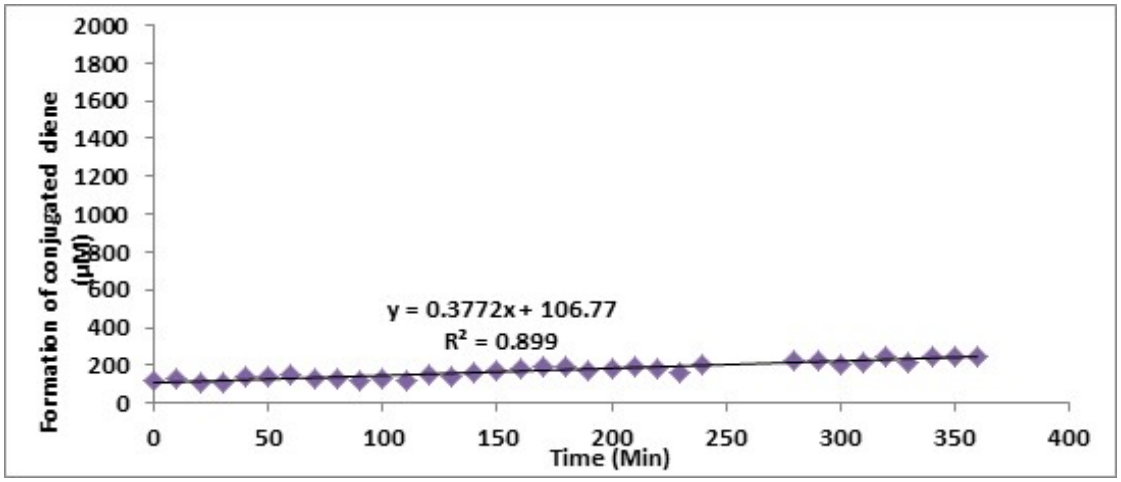


R_{inh} = 37.2 µM/min **T_{inh} = 80.602 Min**

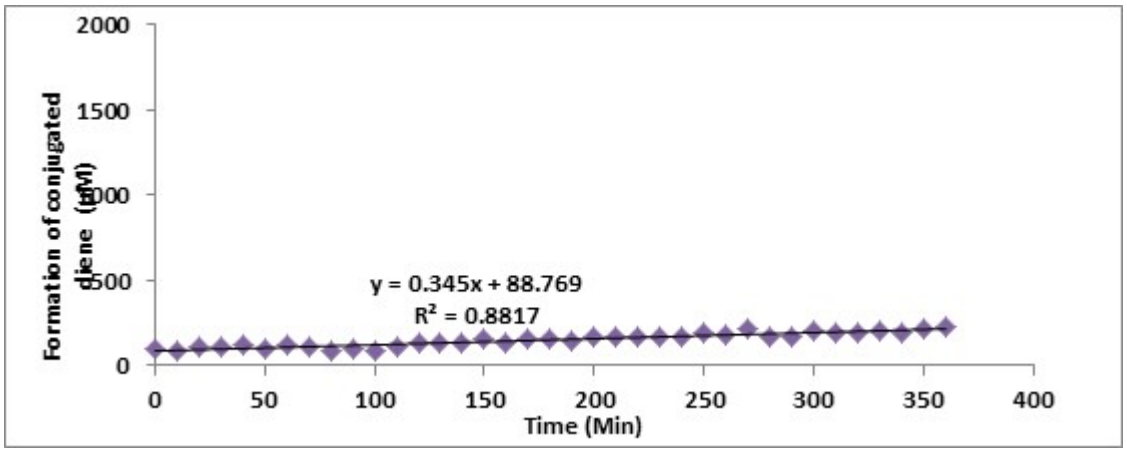


R_{inh} = 29.64 µM/min **T_{inh} = 82.54 Min**

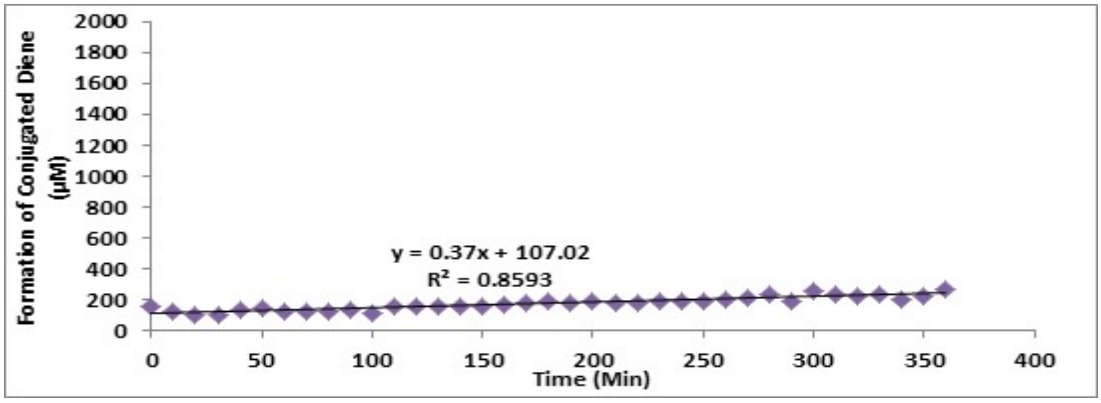
Figure S33. Experiment with antioxidant **9** using PTCP



R_{inh} = 22.62 µM/min T_{inh} > 360 Min

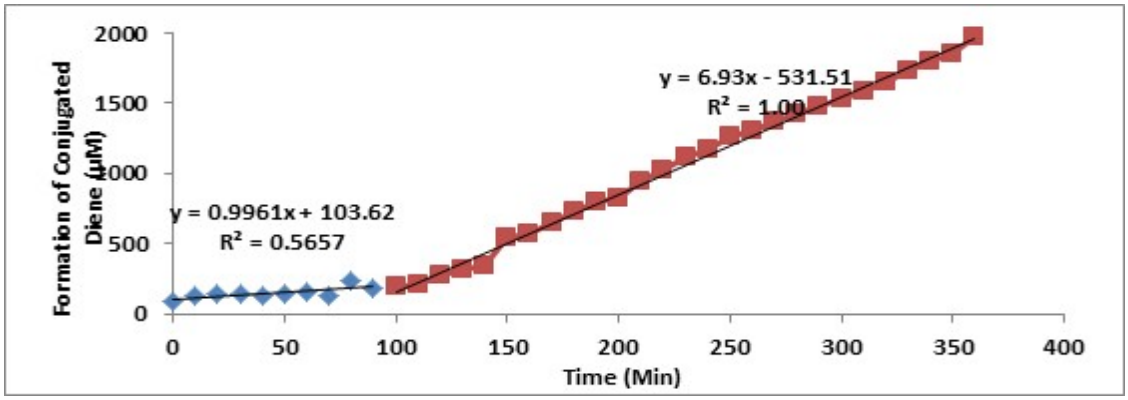


R_{inh} = 20.7 µM/min T_{inh} > 360 Min

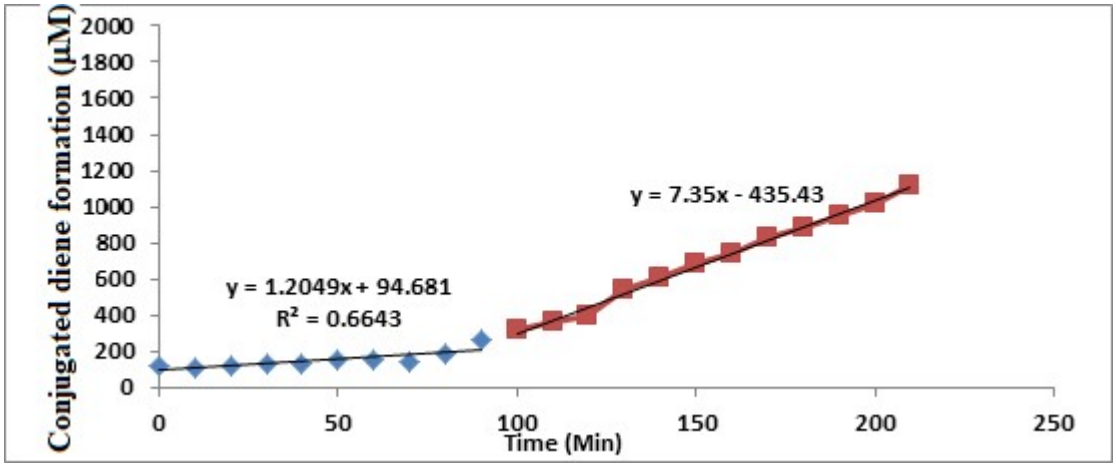


R_{inh} = 22.2 µM/min T_{inh} > 360 Min

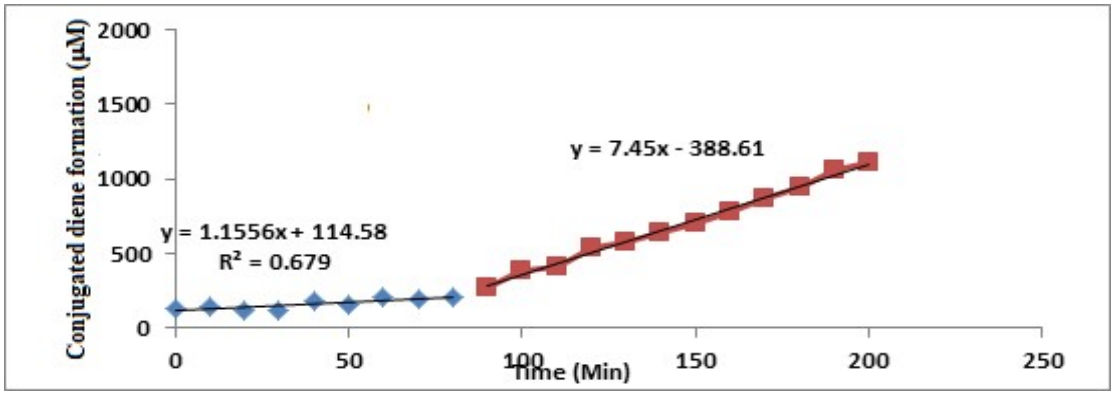
Figure S34. Experiment with antioxidant **9** using Sodium Ascorbate



R_{inh} = 59.76 µM/min **T_{inh} = 106.4 Min**

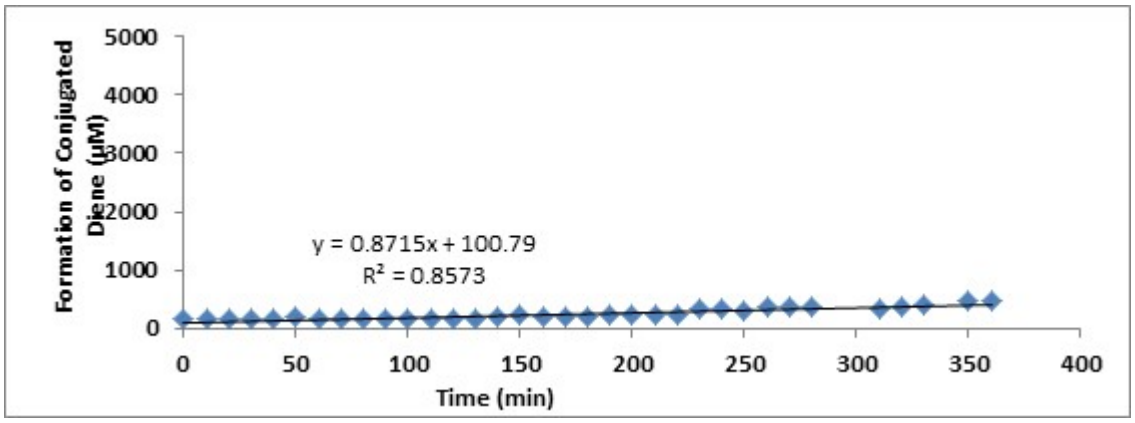


R_{inh} = 72.24 µM/min **T_{inh} = 86.2 Min**

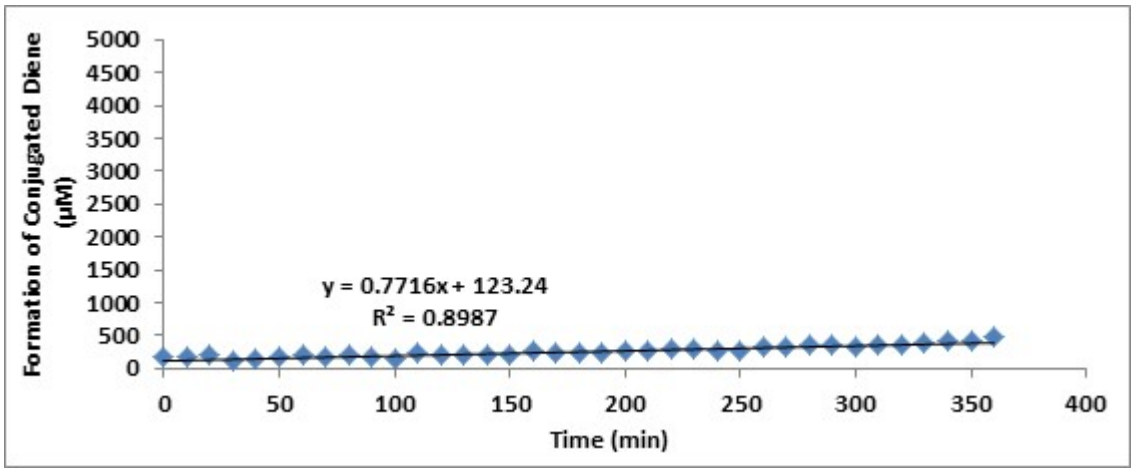


R_{inh} = 69.3µM/min **T_{inh} = 85.34 Min**

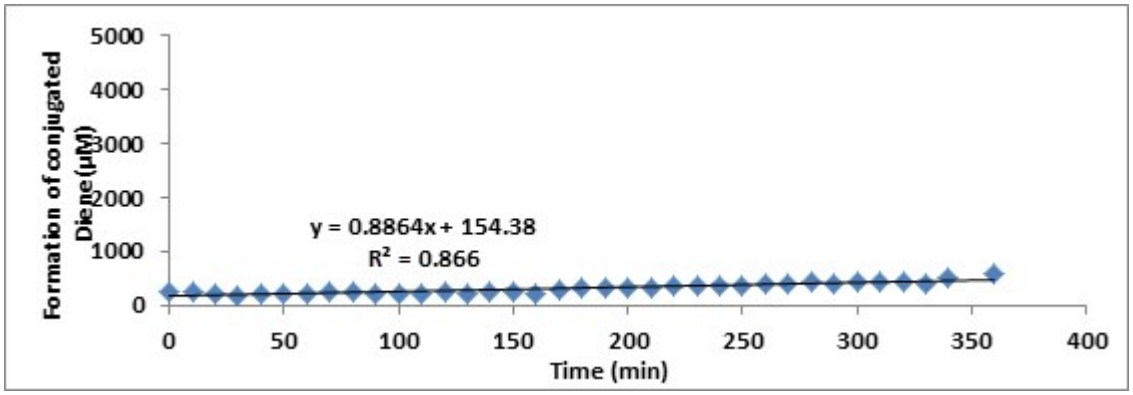
Figure S35. Experiment with antioxidant **9** using $K_4[Fe(CN)_6].3H_2O$ + PTC



R_{inh} = 52.26 µM/min T_{inh} > 360 Min

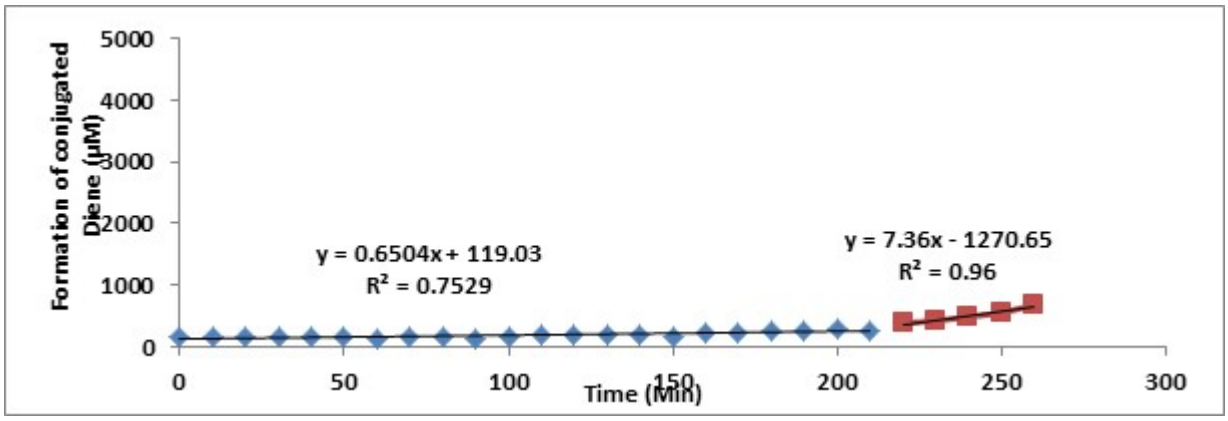


R_{inh} = 46.26 µM/min T_{inh} > 360 Min

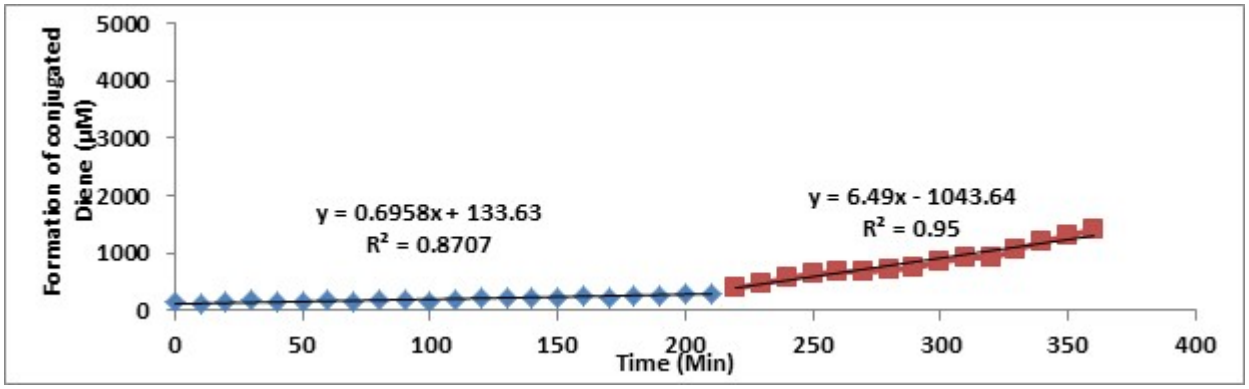


R_{inh} = 53.16 µM/min T_{inh} > 360 Min

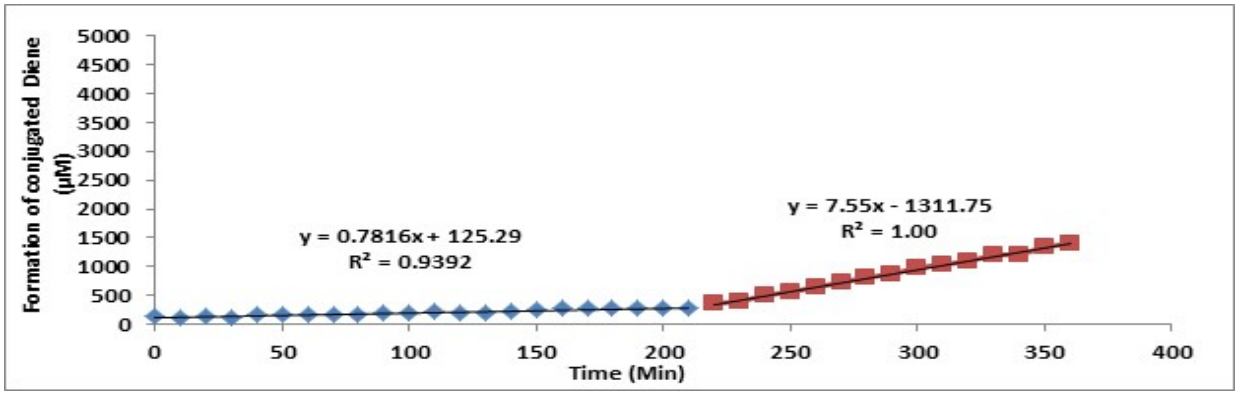
Figure S36. Experiment with antioxidant **9** using GSH



R_{inh} = 39 µM/min T_{inh} = 207.10 Min

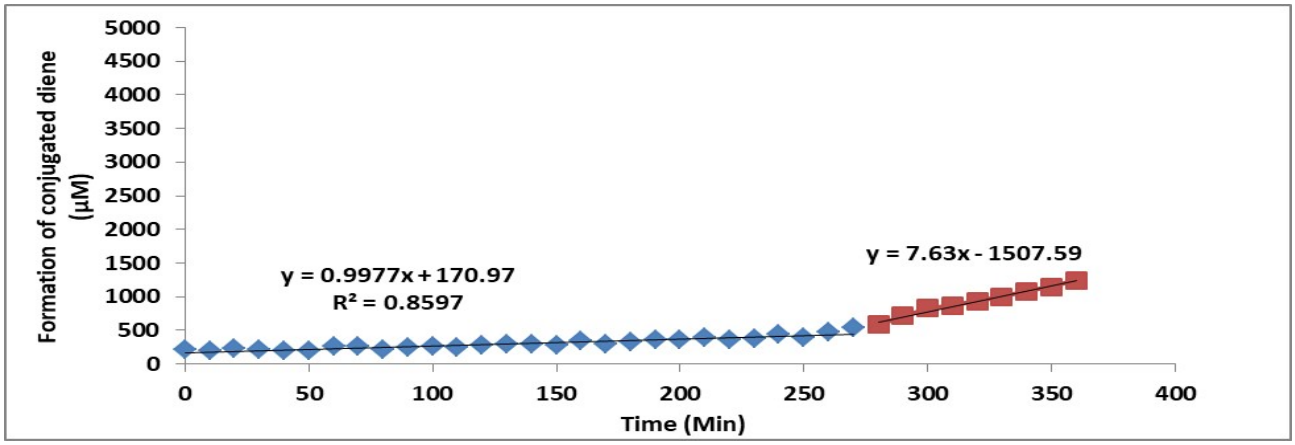


R_{inh} = 41.7 µM/min T_{inh} = 203.14 Min

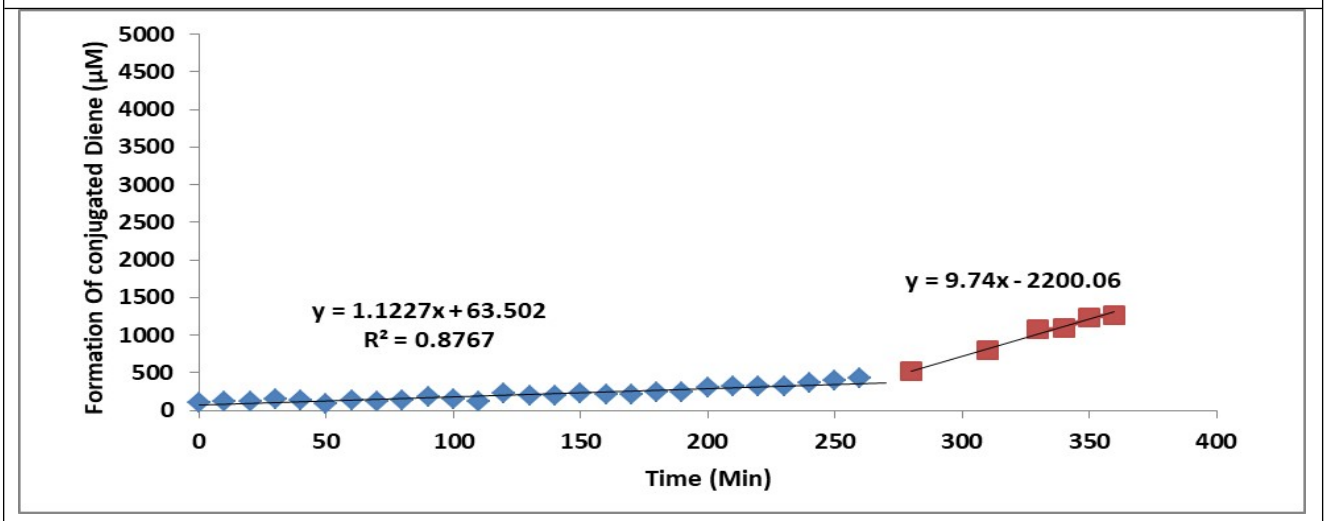


R_{inh} = 46.86 µM/min T_{inh} = 212.28 Min

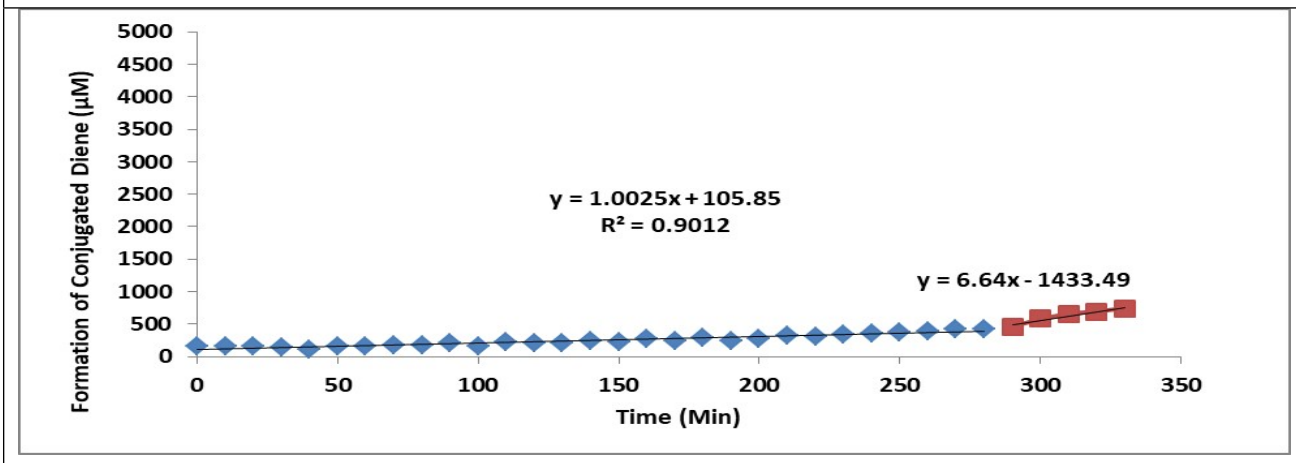
Figure S37. Experiment with antioxidant **9** using NAC pH 1



R_{inh} = 59.82 µM/Min **T_{inh} = 253 Min**

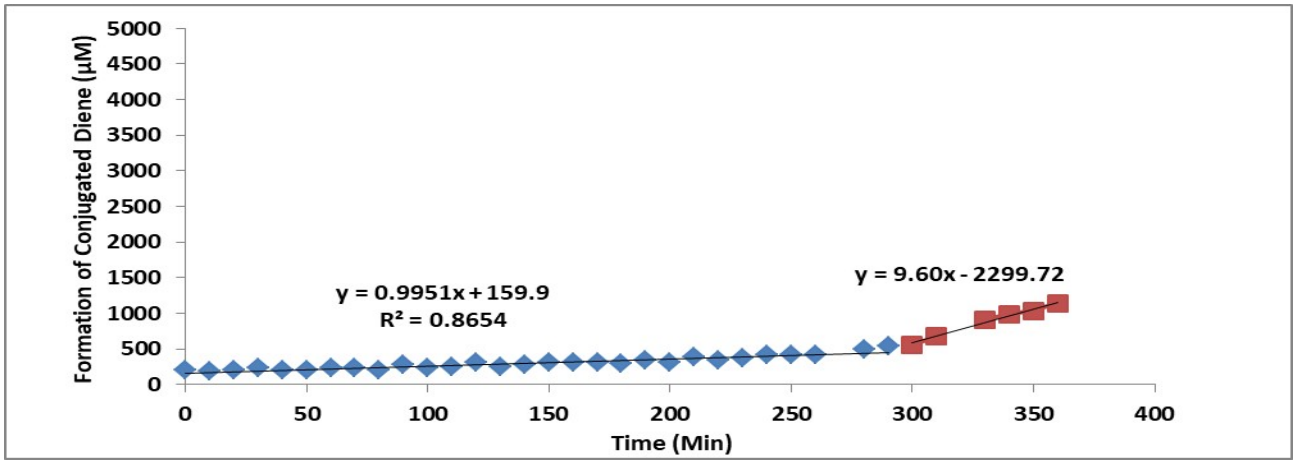


R_{inh} = 67.32 µM/Min **T_{inh} = 263 Min**

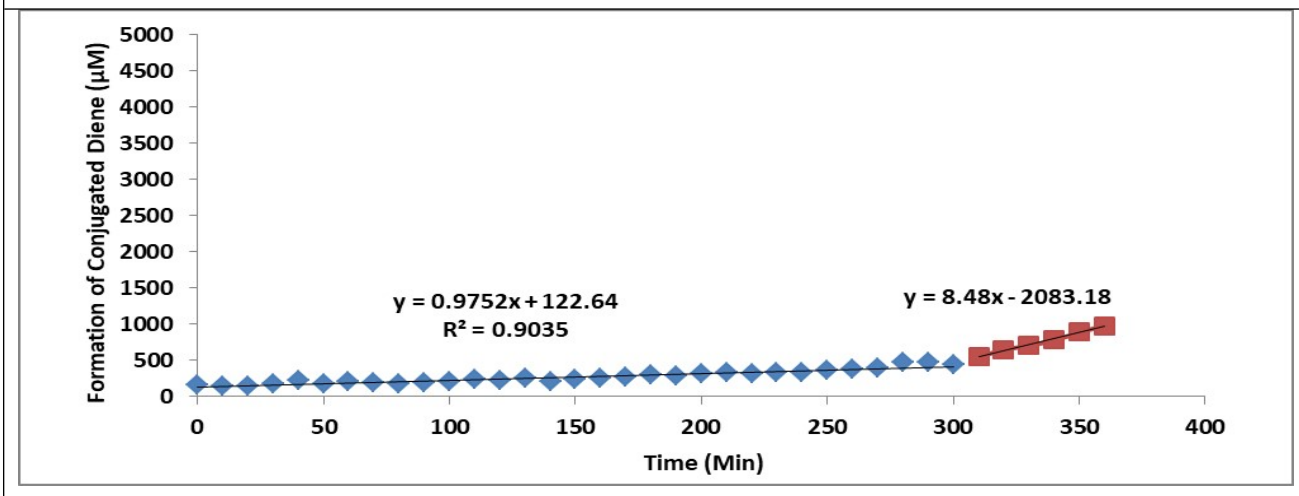


R_{inh} = 60.1 µM/Min **T_{inh} = 273 Min**

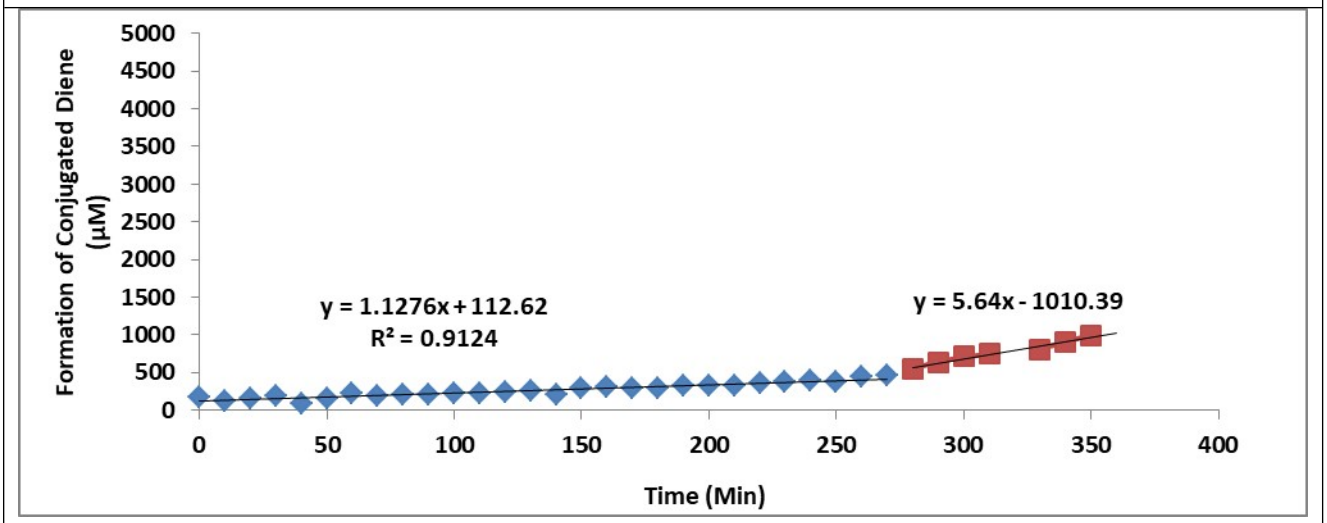
Figure S38. Experiment with antioxidant **9** using NAC pH 2



R_{inh} = 59.7 µM/Min **T_{inh} = 281 Min**

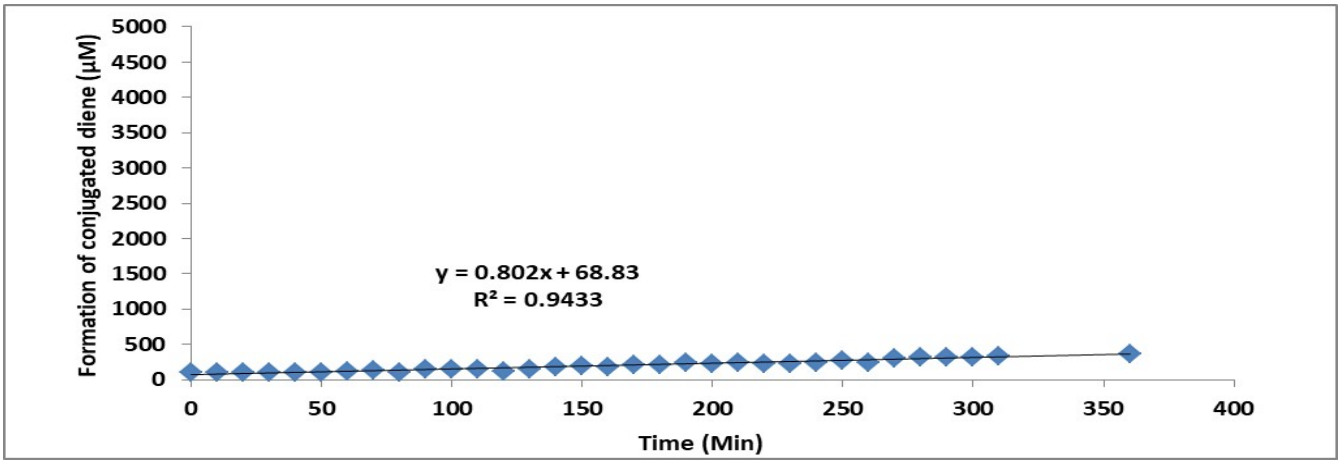


R_{inh} = 58.5 µM/Min **T_{inh} = 289 Min**

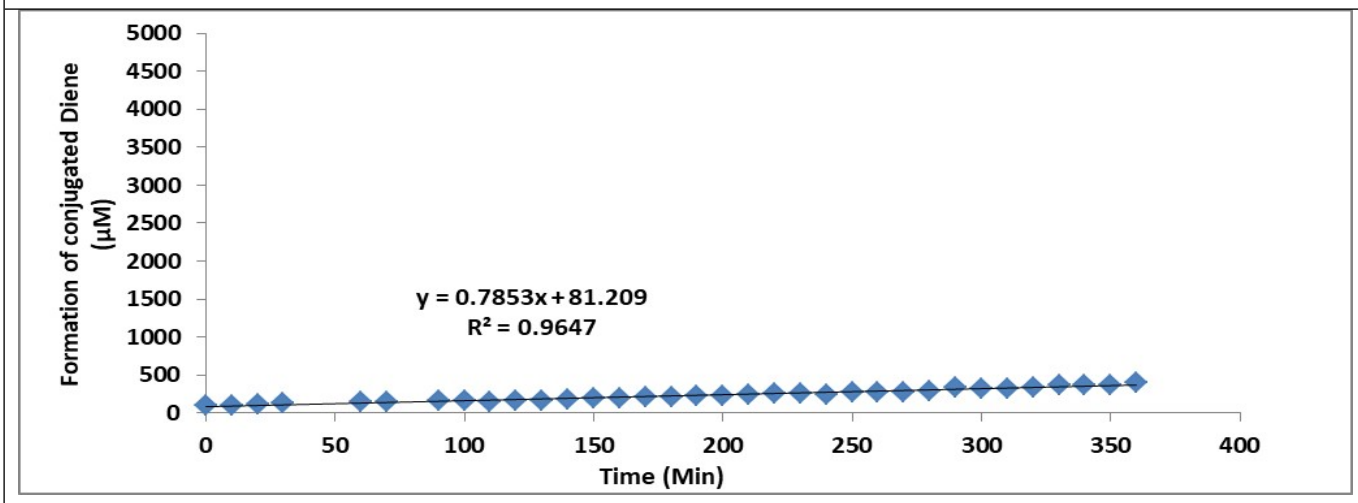


R_{inh} = 67.6 µM/Min **T_{inh} = 270 Min**

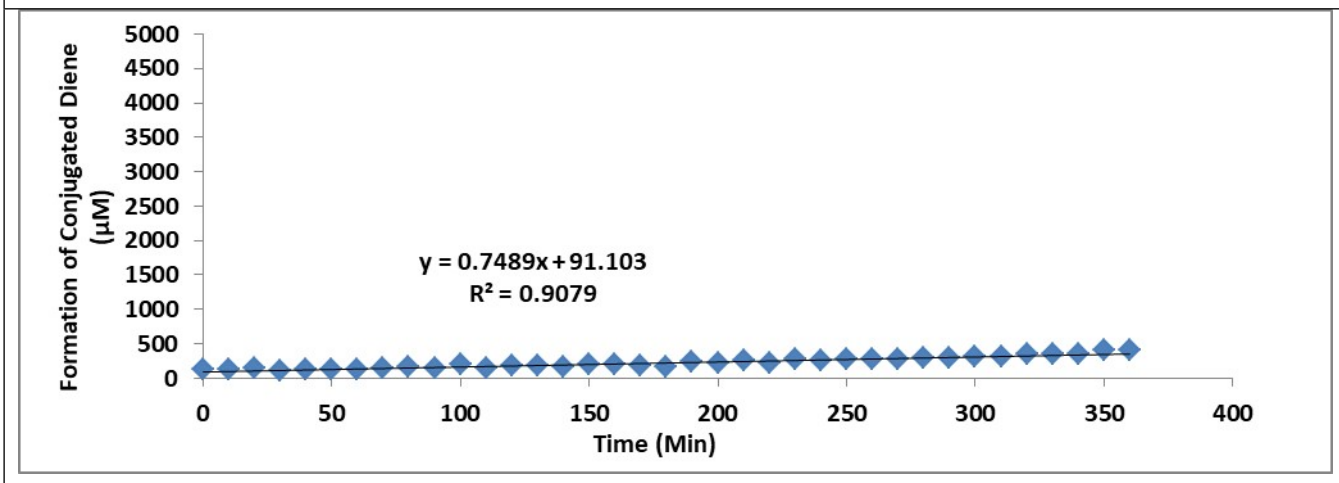
Figure S39. Experiment with antioxidant **9** using NAC pH 3



R_{inh} = 48.12µM/Min T_{inh} > 360 Min

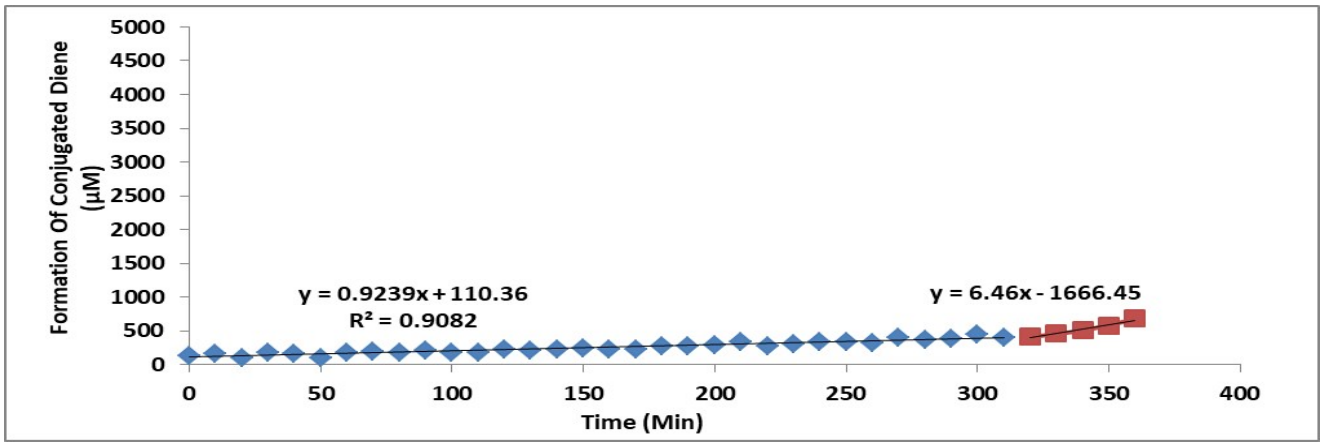


R_{inh} = 47.1 µM/Min T_{inh} > 360 Min

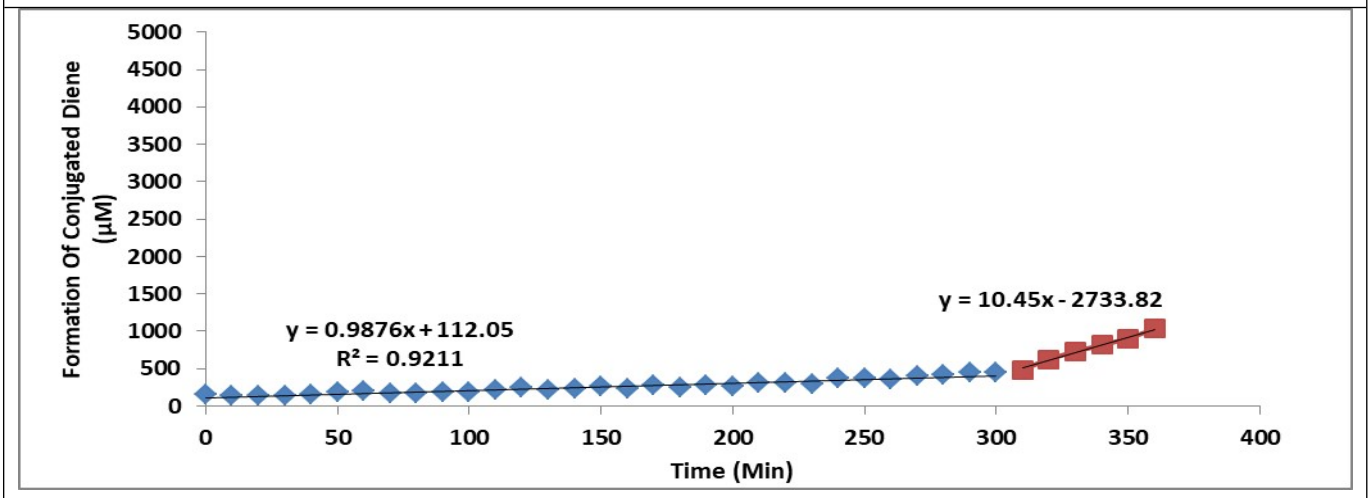


R_{inh} = 44.88 µM/Min T_{inh} > 360 Min

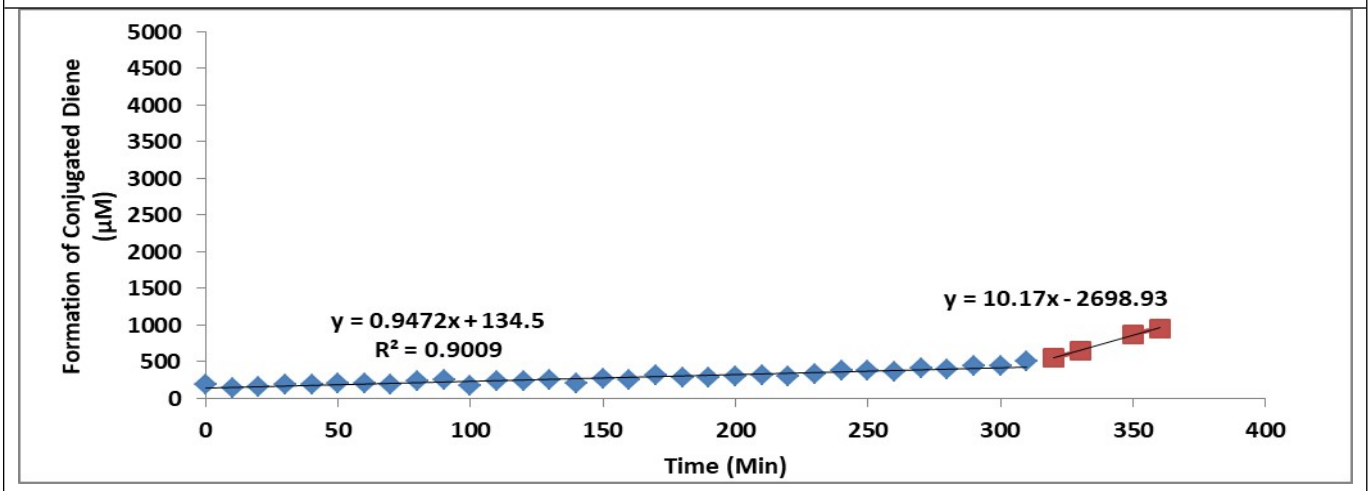
Figure S40. Experiment with antioxidant **9** using NAC pH 4



R_{inh} = 55.38 µM/Min **T_{inh} = 310 Min**

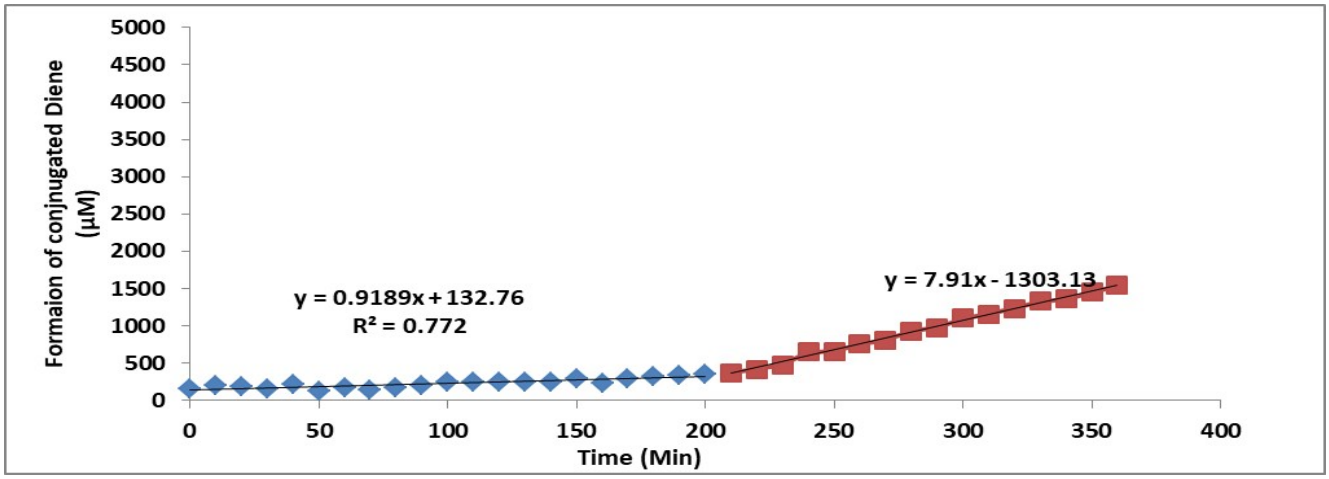


R_{inh} = 59.22 µM/Min **T_{inh} = 301 Min**

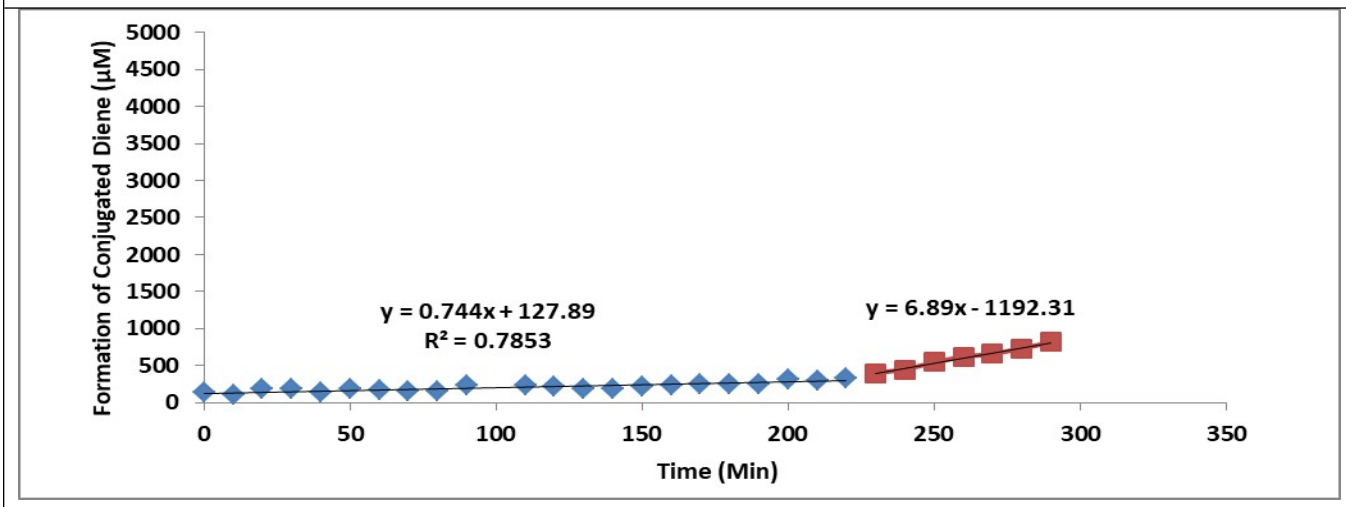


R_{inh} = 56.82 µM/Min **T_{inh} = 306 Min**

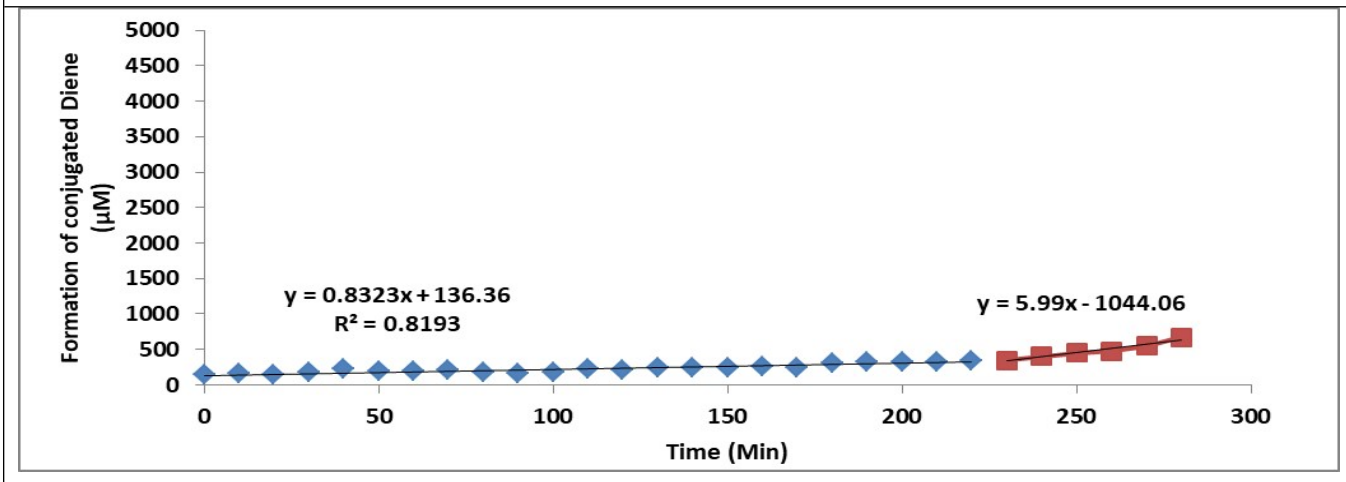
Figure S41. Experiment with antioxidant **9** using NAC pH 5



R_{inh} = 55.08 µM/Min T_{inh} = 205 Min

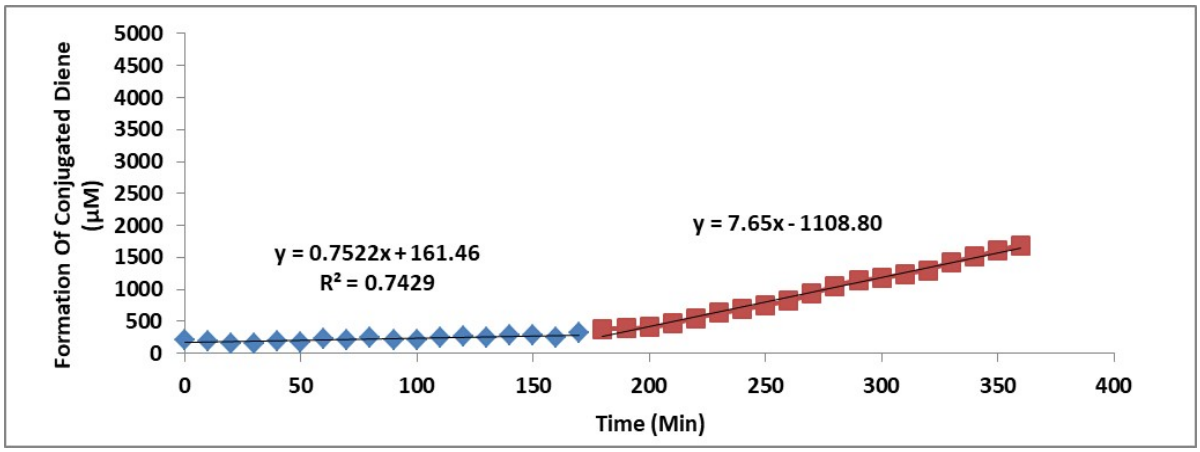


R_{inh} = 44.64 µM/Min T_{inh} = 214 Min

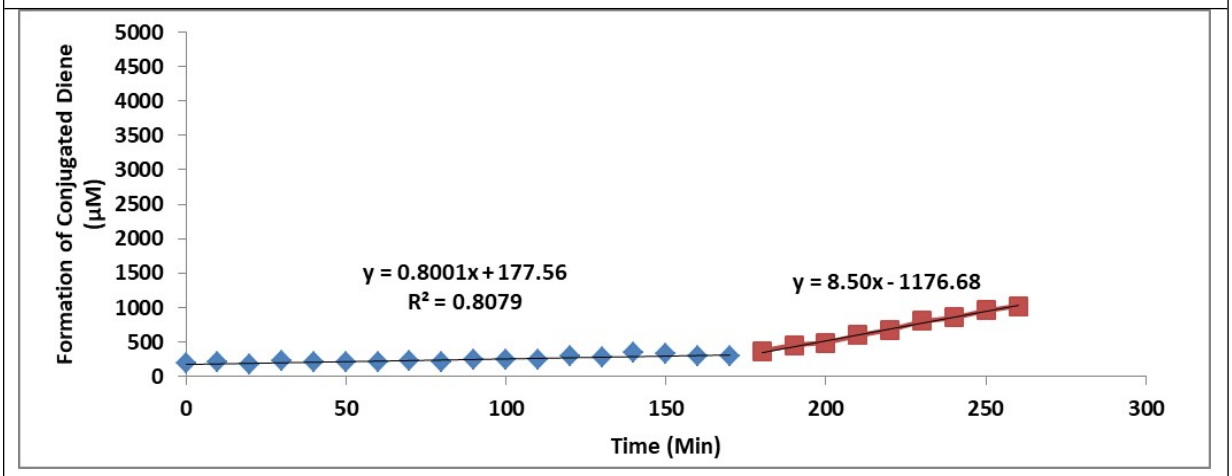


R_{inh} = 49.92 µM/Min T_{inh} = 220 Min

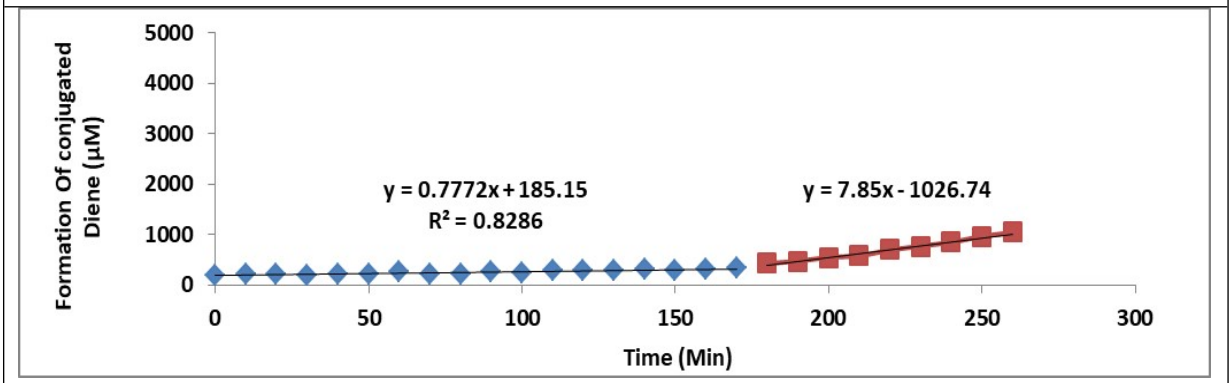
Figure S42. Experiment with antioxidant **9** using NAC pH 6



R_{inh} = 45.12 µM/Min T_{inh} = 184 Min

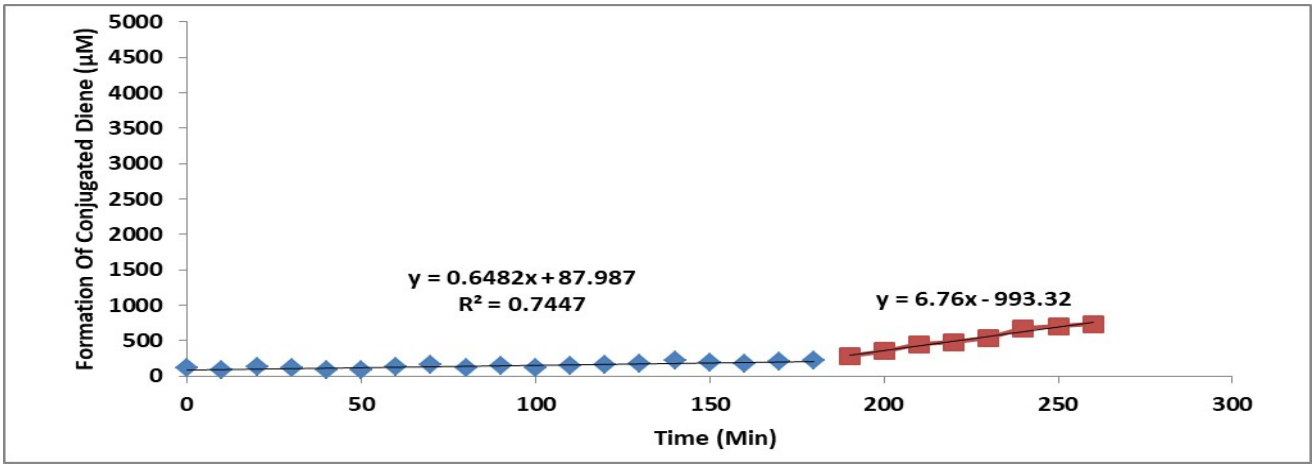


R_{inh} = 48 µM/Min T_{inh} = 176 Min

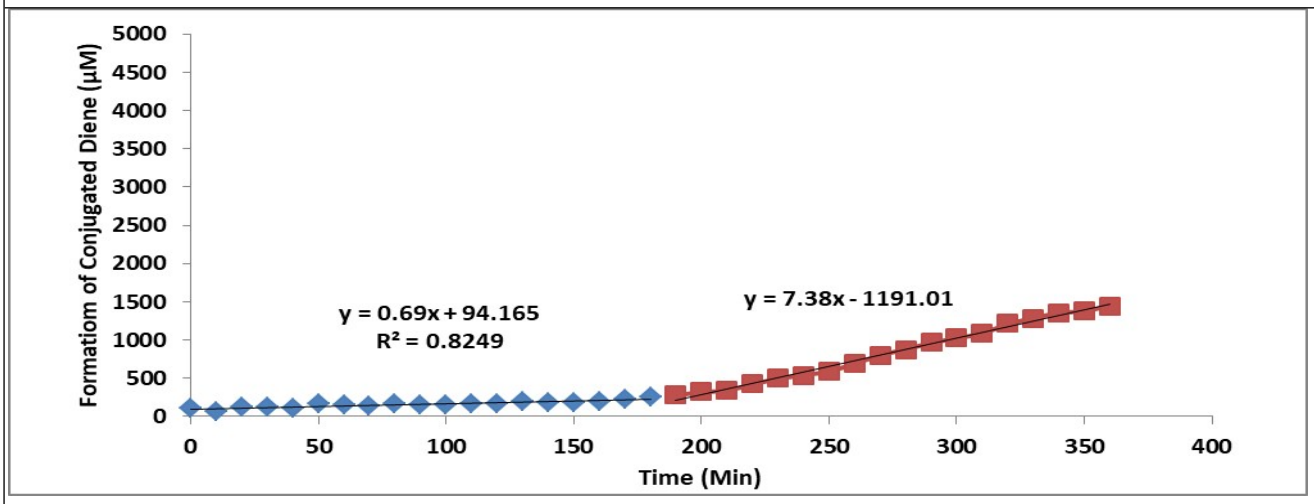


R_{inh} = 46.62 µM/Min T_{inh} = 171 Min

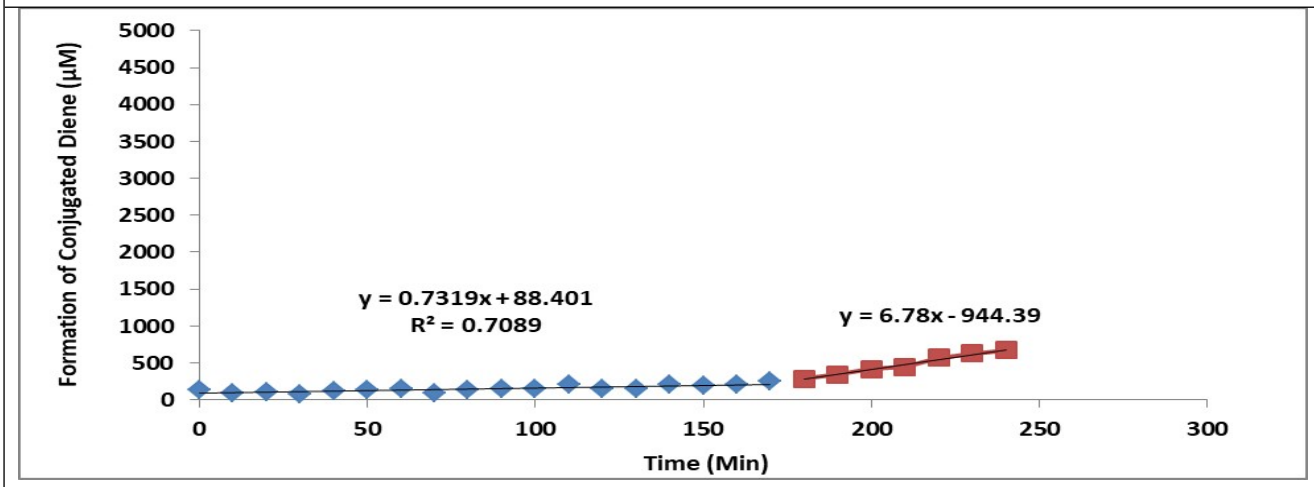
Figure S43. Experiment with antioxidant **9** using NAC pH 7



R_{inh} = 38.9 µM/Min **T_{inh} = 177 Min**



R_{inh} = 41.4 µM/Min **T_{inh} = 193 Min**



R_{inh} = 43.9 µM/Min **T_{inh} = 171 Min**

Scheme S1. Proposed mechanism for the quenching of LOO• by antioxidant **9** in the presence of aqueous co-antioxidants.