

3(2H)-Furanone as a promising scaffold for the synthesis of novel fluorescent organic dyes: An experimental and theoretical investigation.

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Supporting Information

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Figure S1. The ^1H NMR spectrum (CDCl_3) of 5-phenyl -3(2H) -furanone

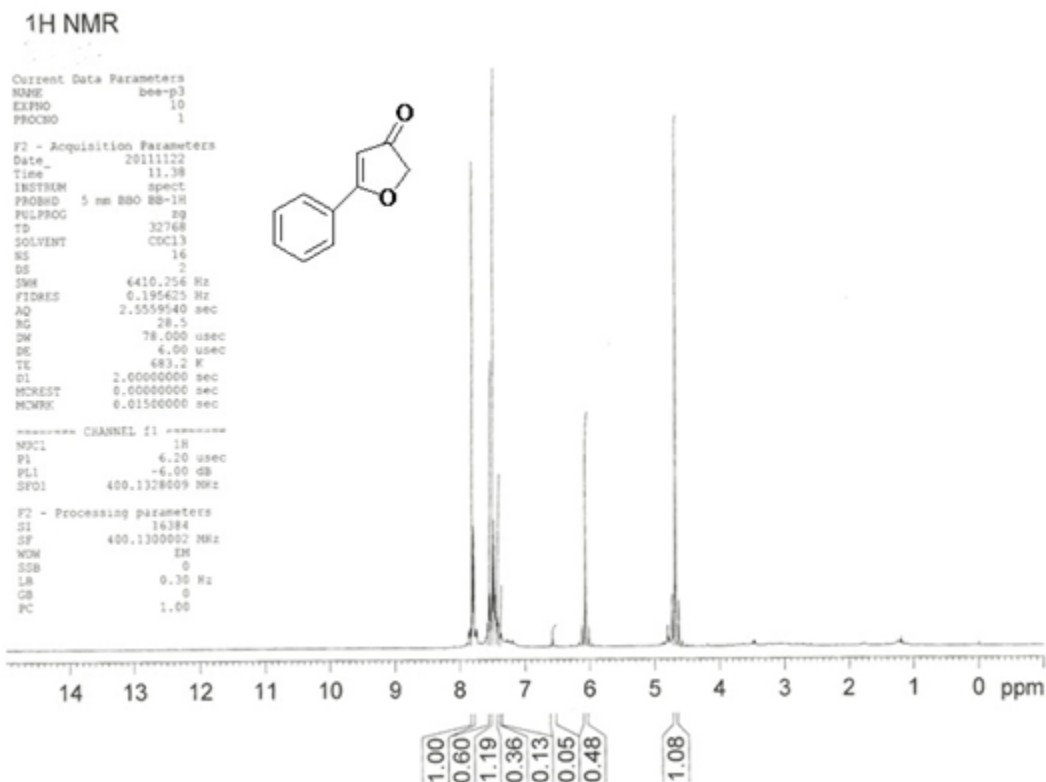


Figure S2. The ^{13}C NMR spectrum (CDCl_3) of 5-phenyl -3(2H) -furanone

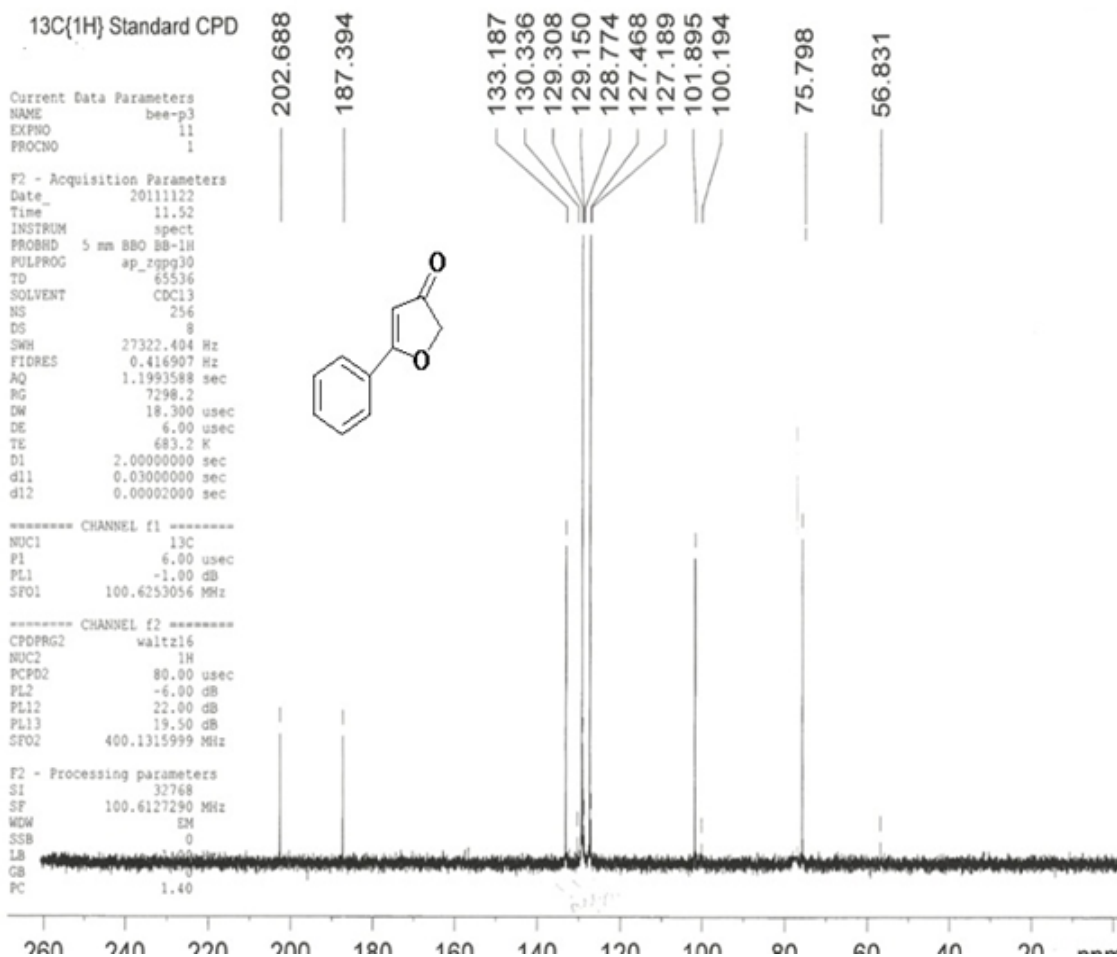


Figure S3. The ^1H NMR spectrum (CDCl_3) of FNPF

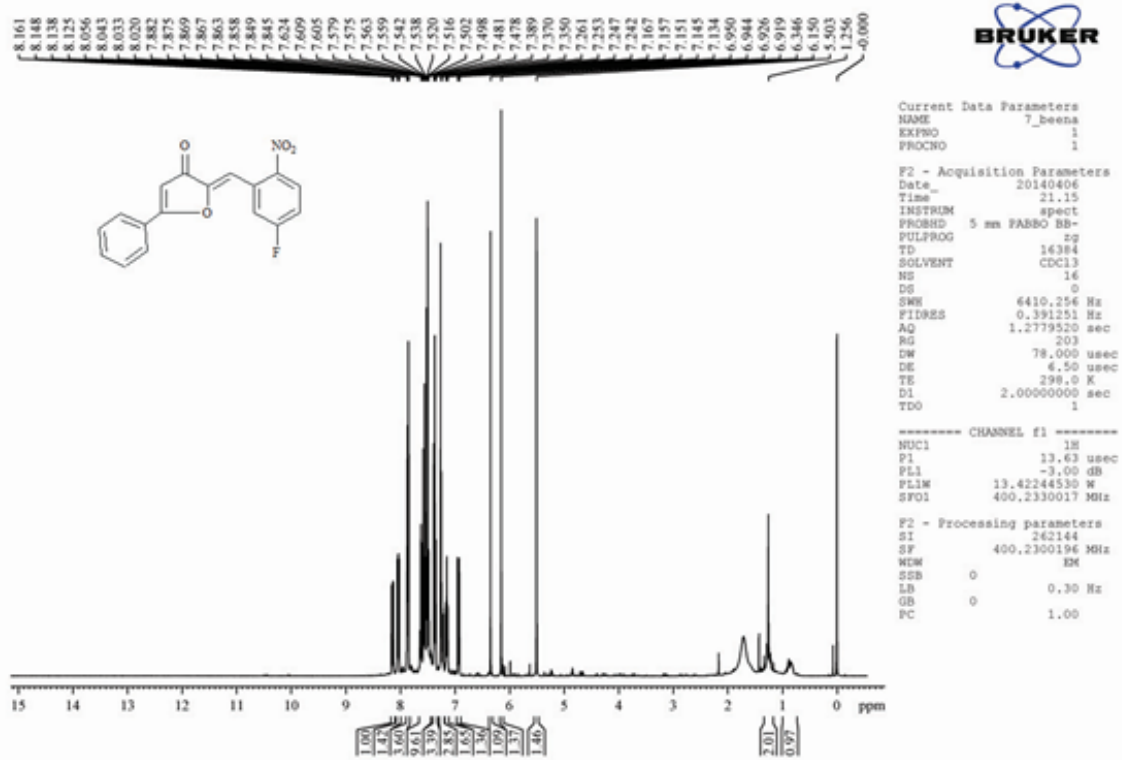


Figure S4. The ^{13}C NMR spectrum (CDCl_3) of FNPF

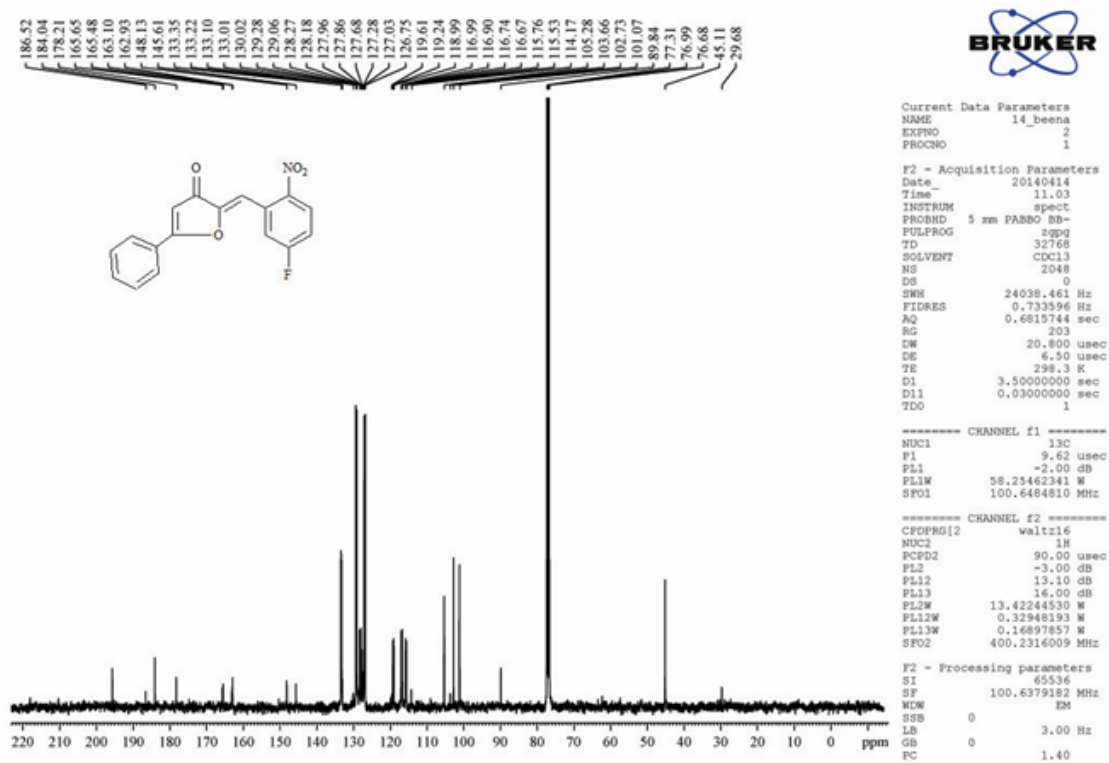


Figure S5. The DEPT (135) NMR spectrum (CDCl₃) of FNPF

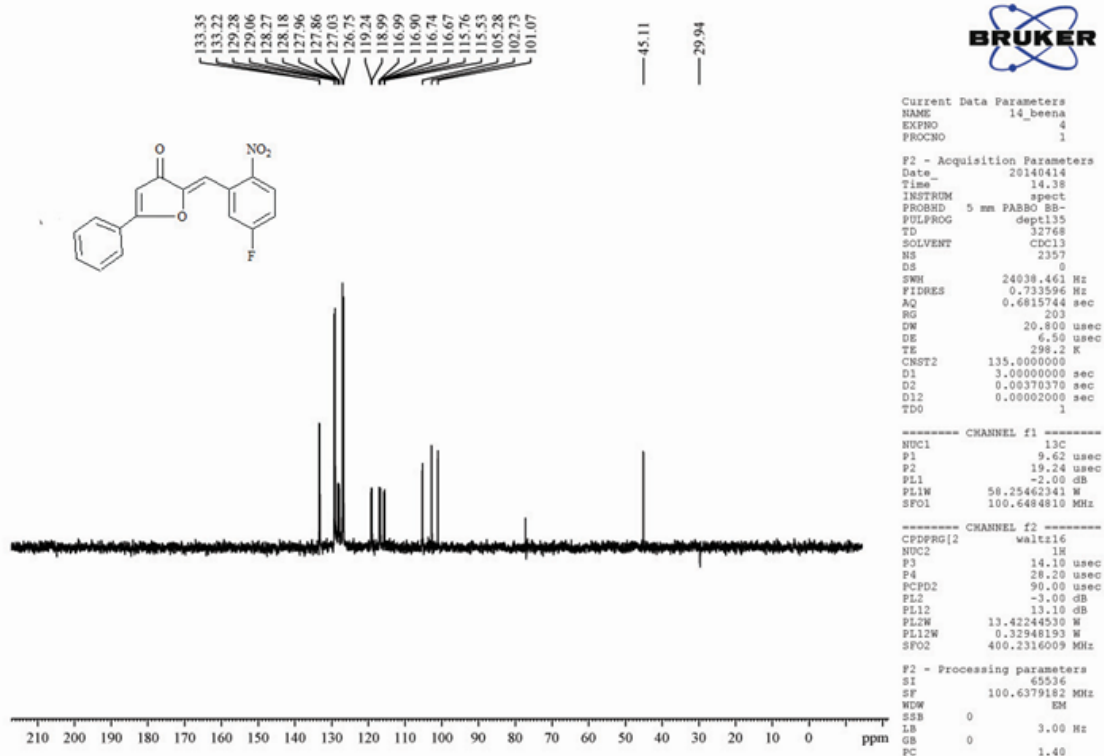


Figure S6. The DEPT (90) NMR spectrum (CDCl₃) of FNPF

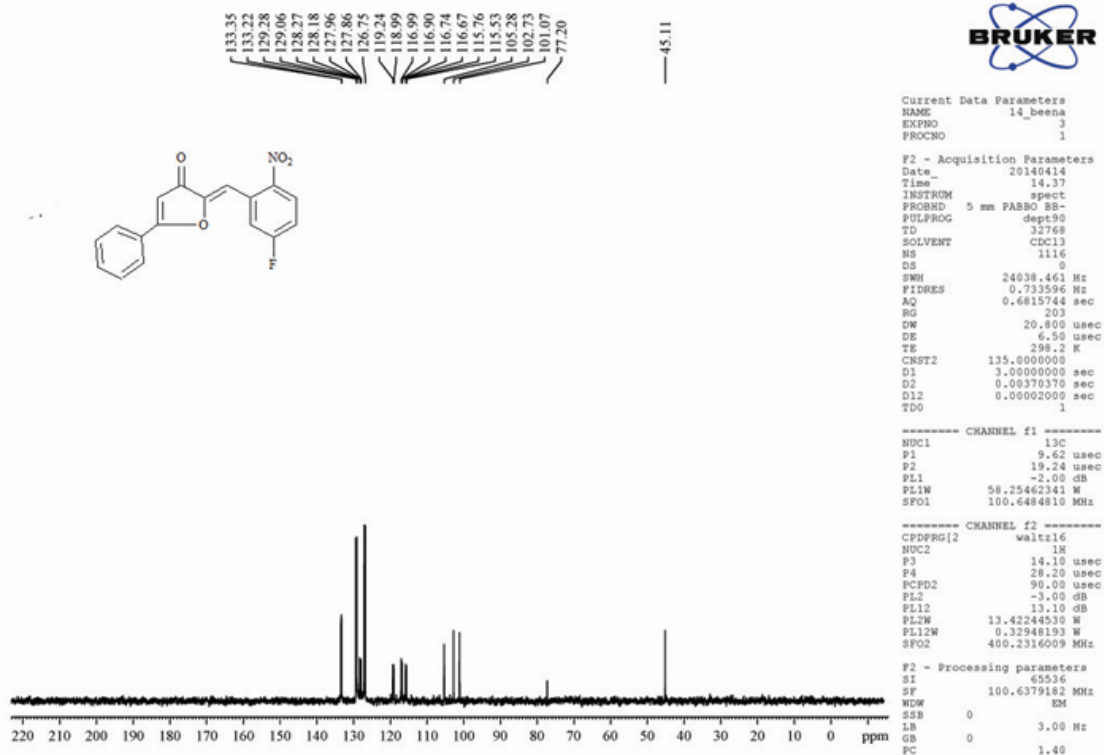
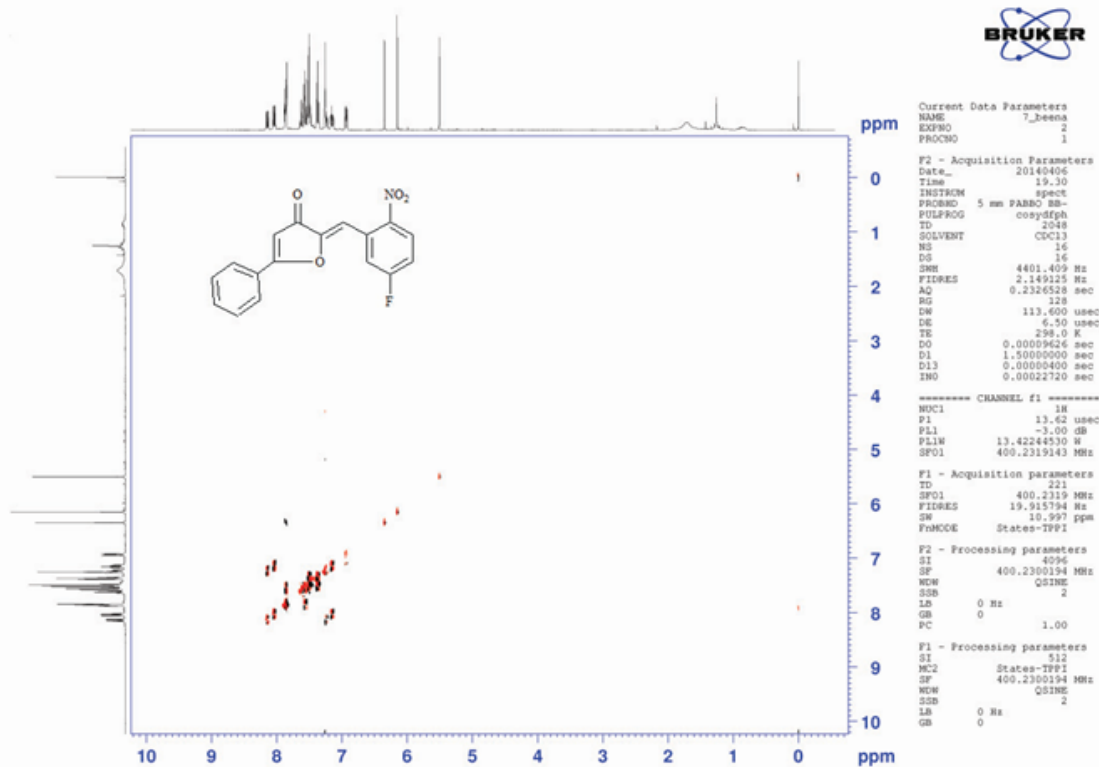


Figure S7. The ^1H , ^1H -COSY NMR spectrum (CDCl_3) of FNPF



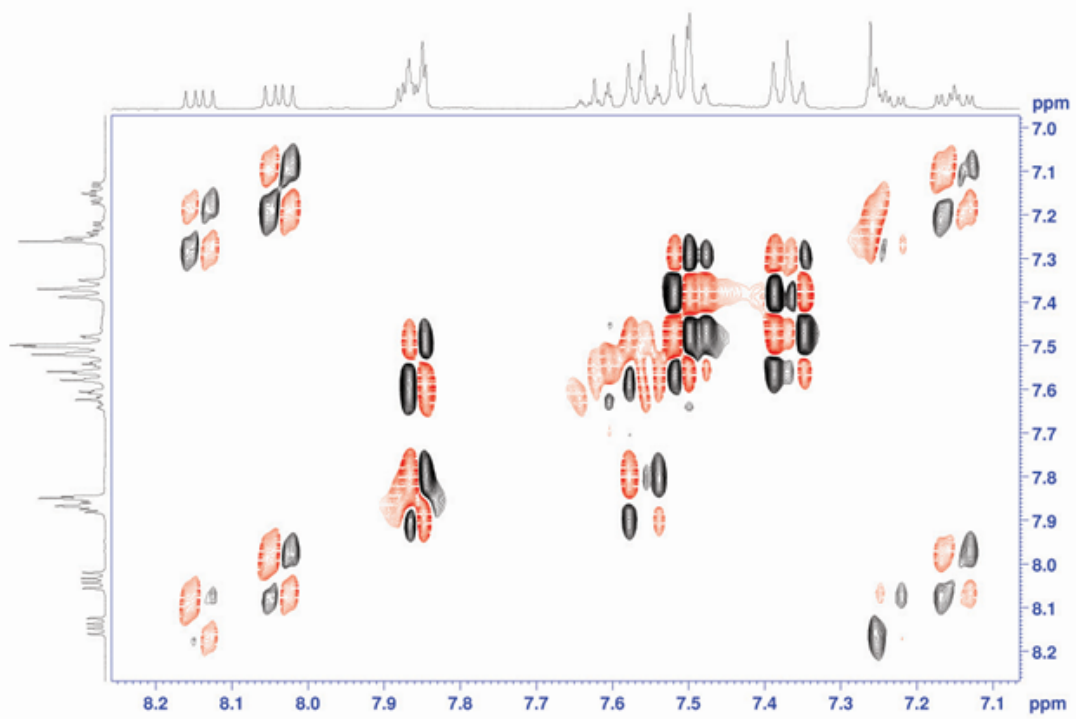


Figure S8. The LC-MS spectrum of FNPF

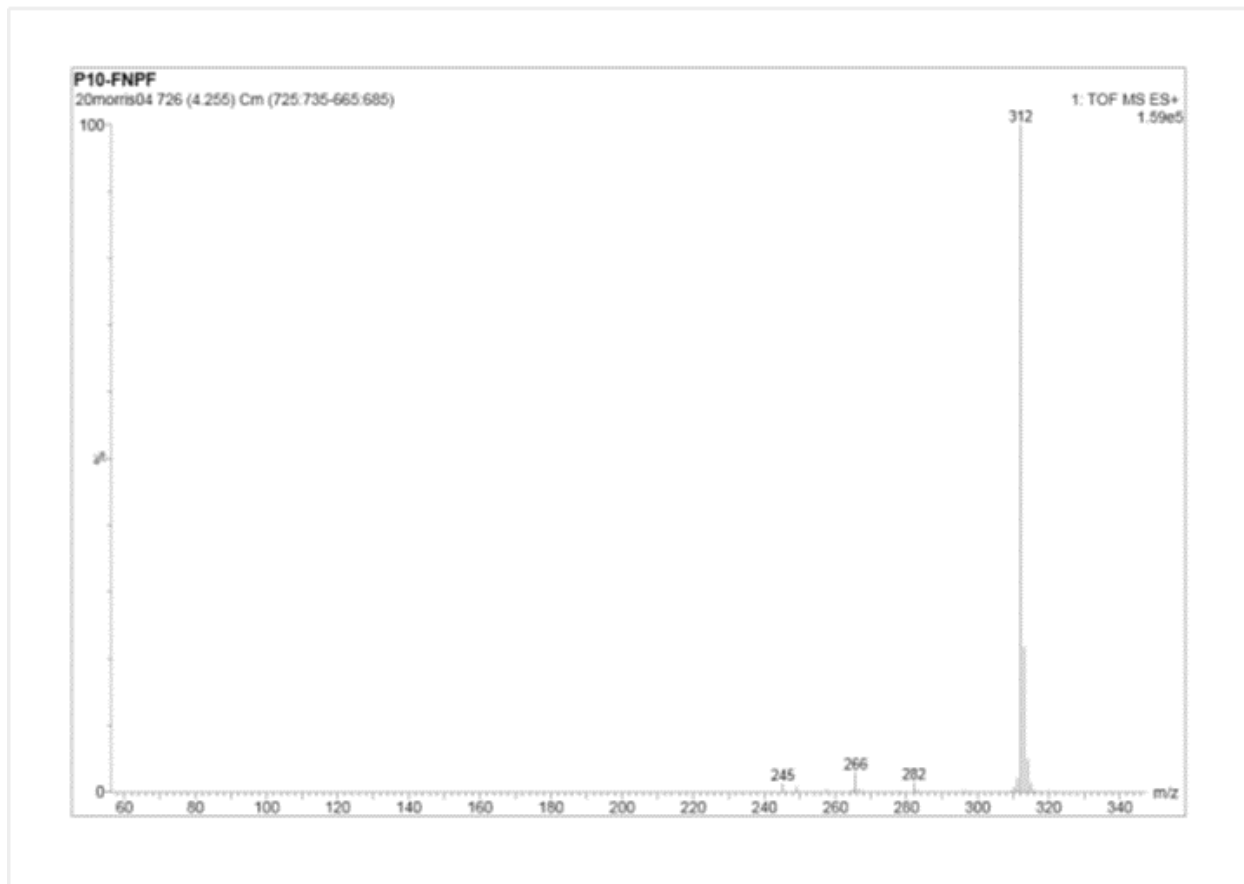


Figure S9. The ^1H NMR spectrum (CDCl_3) of CBPF

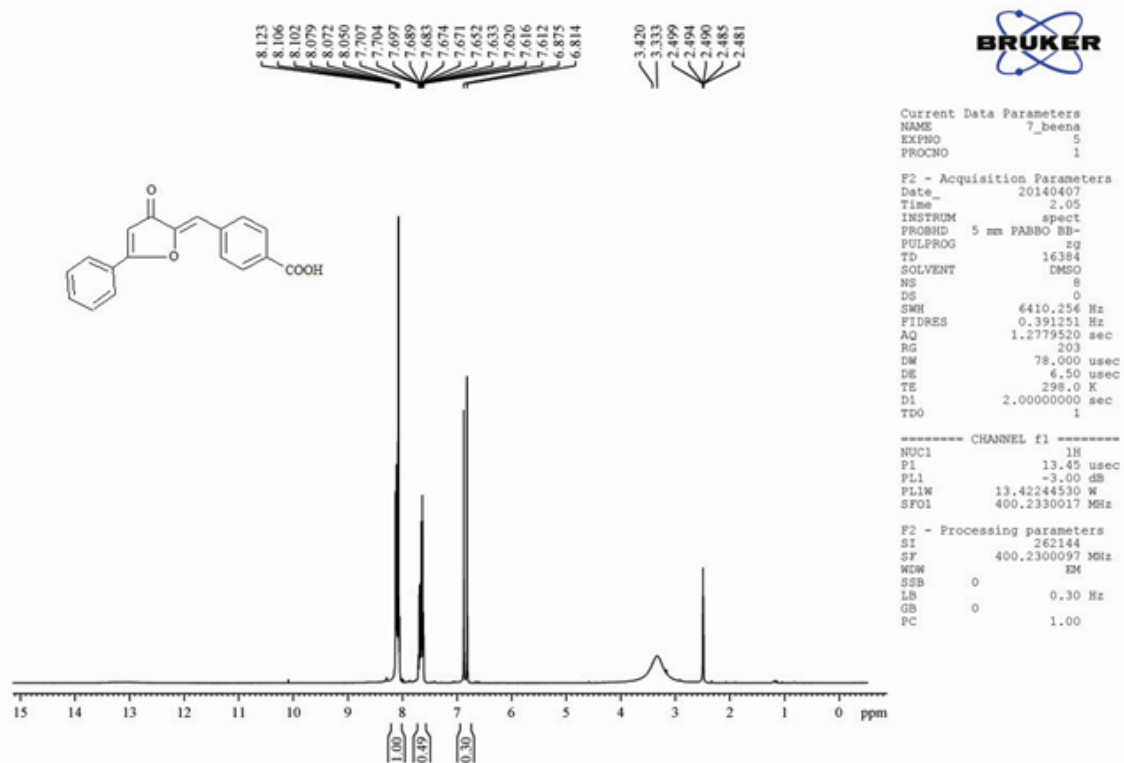


Figure S10. The ^{13}C NMR spectrum (CDCl_3) of CBPF

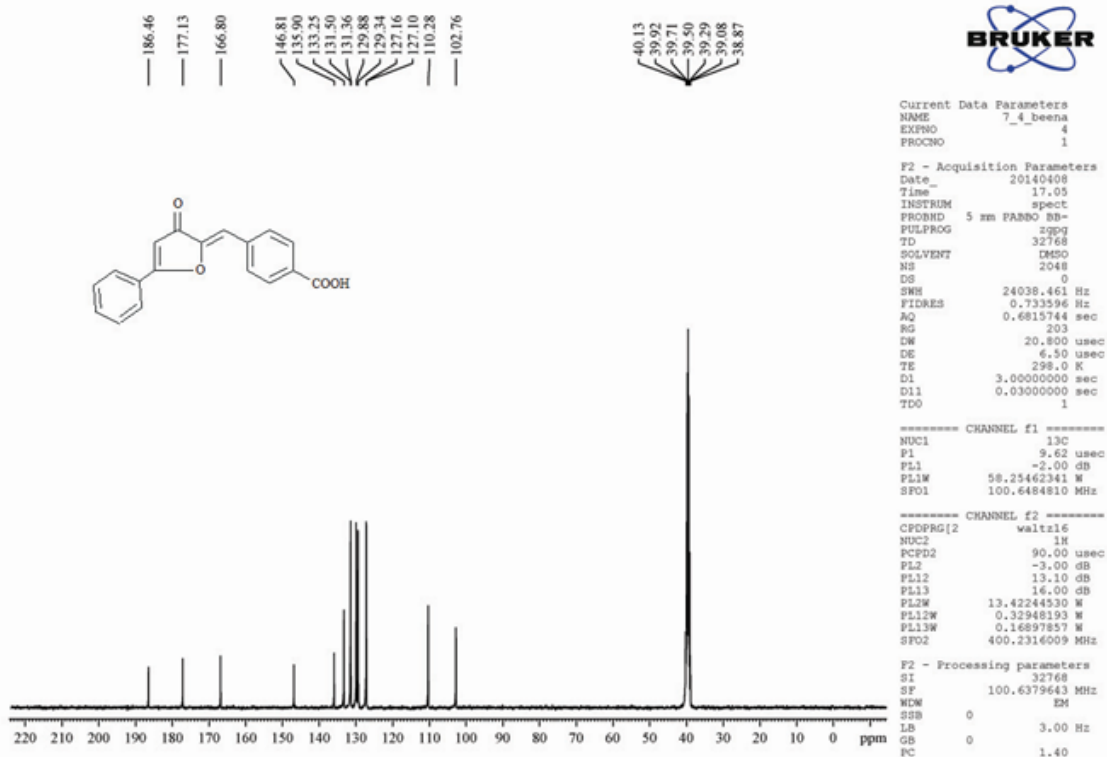


Figure S11. The DEPT (135) NMR spectrum (CDCl₃) of CBPF

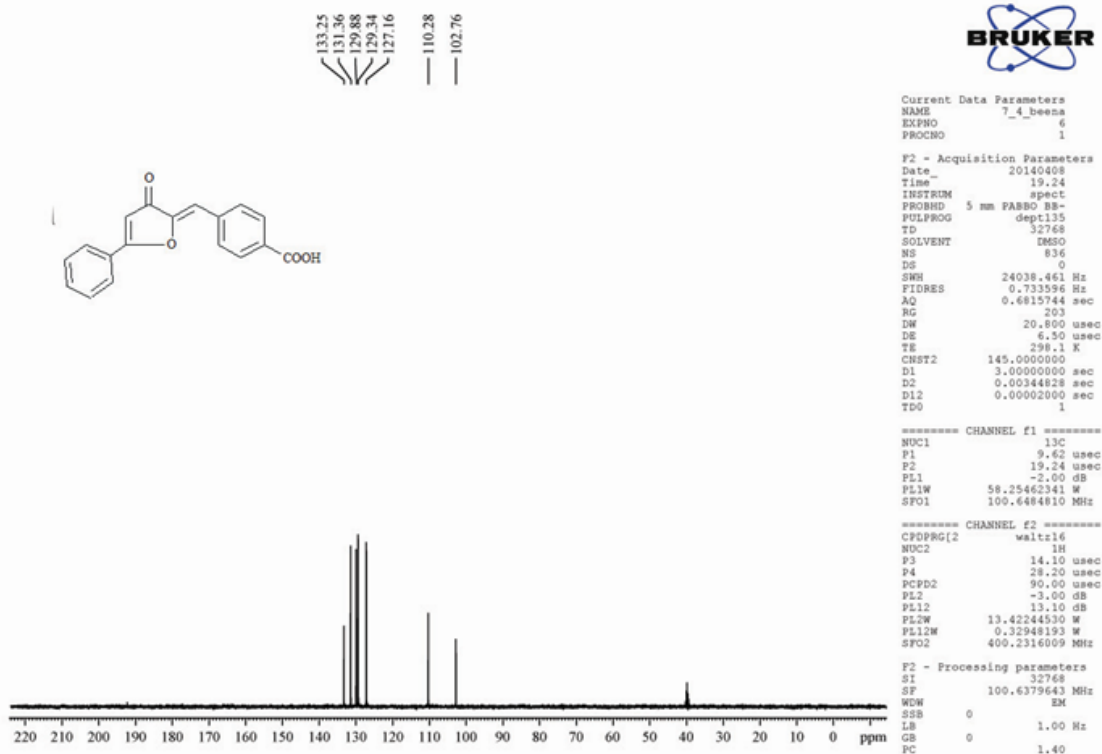


Figure S12. The DEPT (90) NMR spectrum (CDCl₃) of CBPF

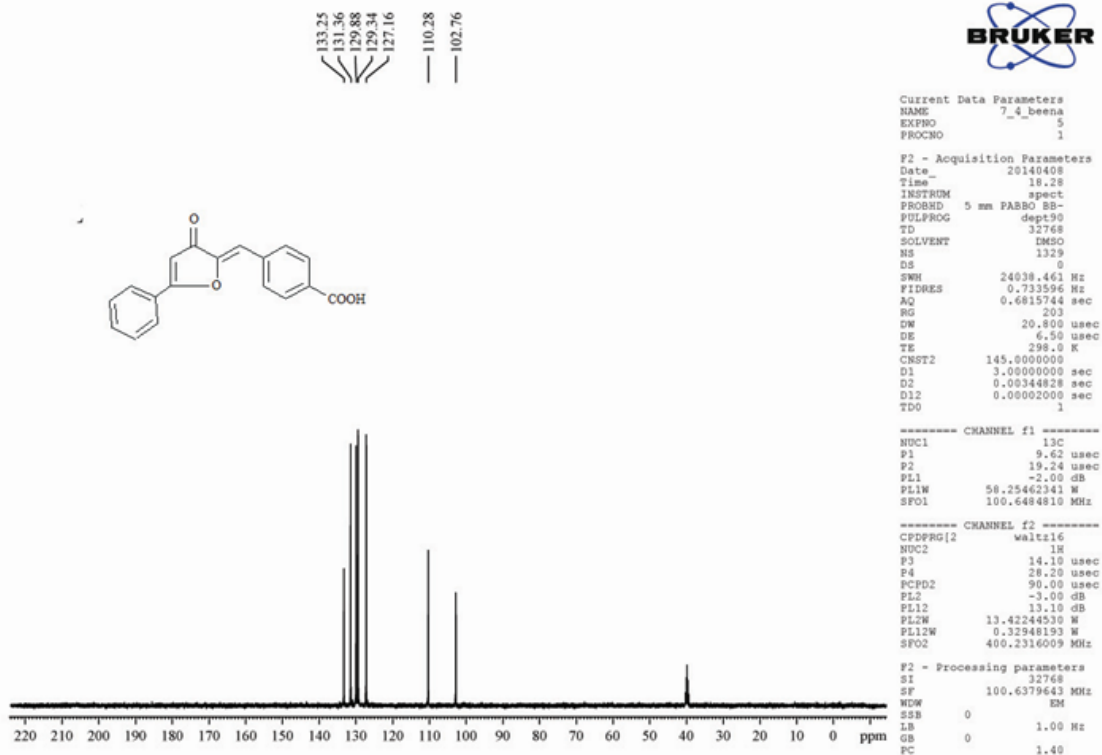
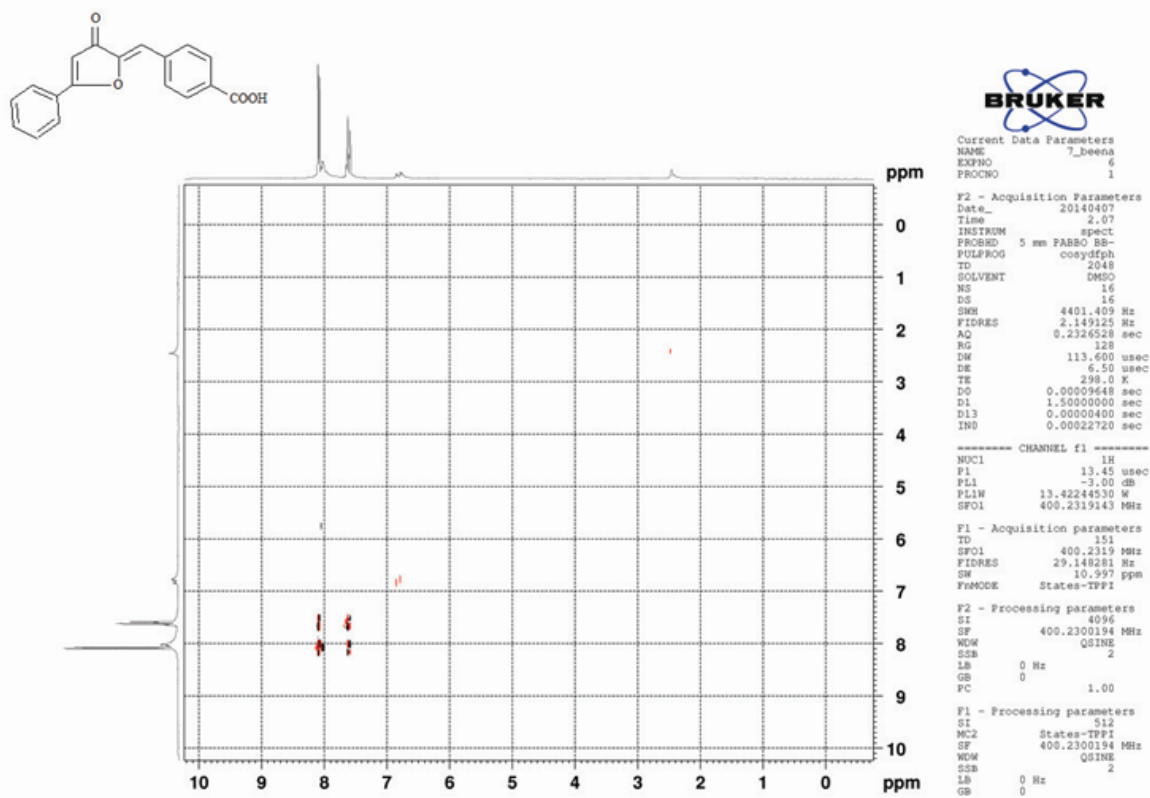


Figure S13. The ^1H , ^1H -COSY NMR spectrum (CDCl_3) of FNPF



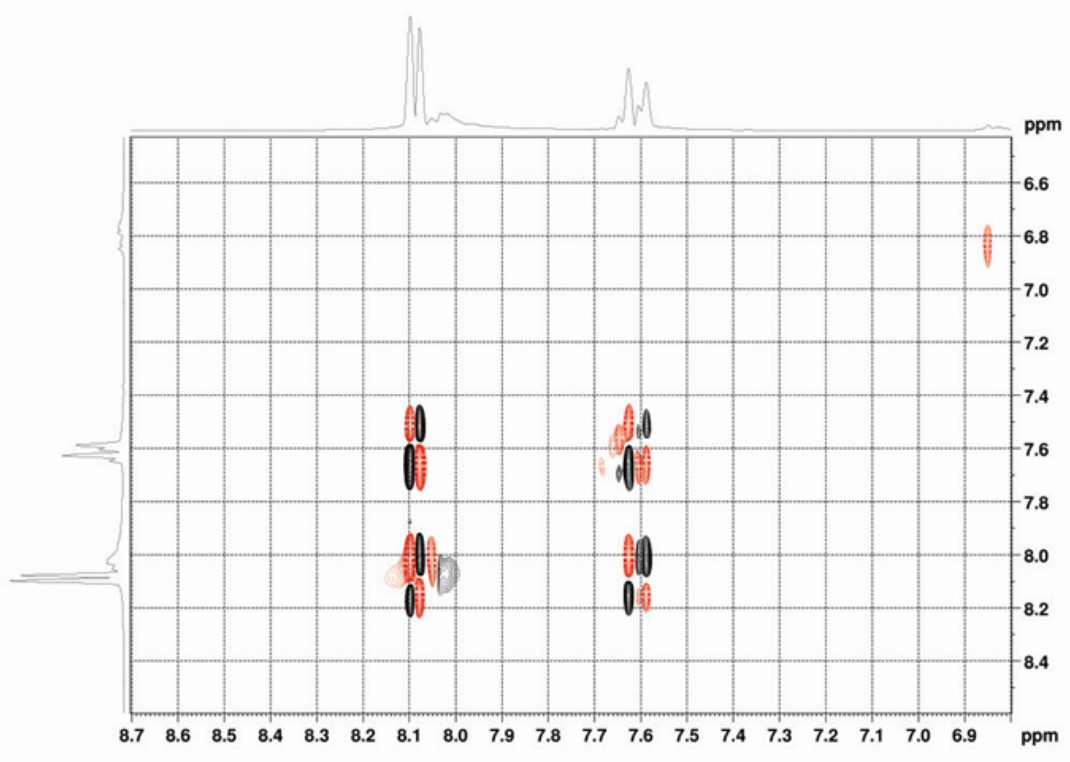


Figure S14. The LC-MS spectrum of CBPF

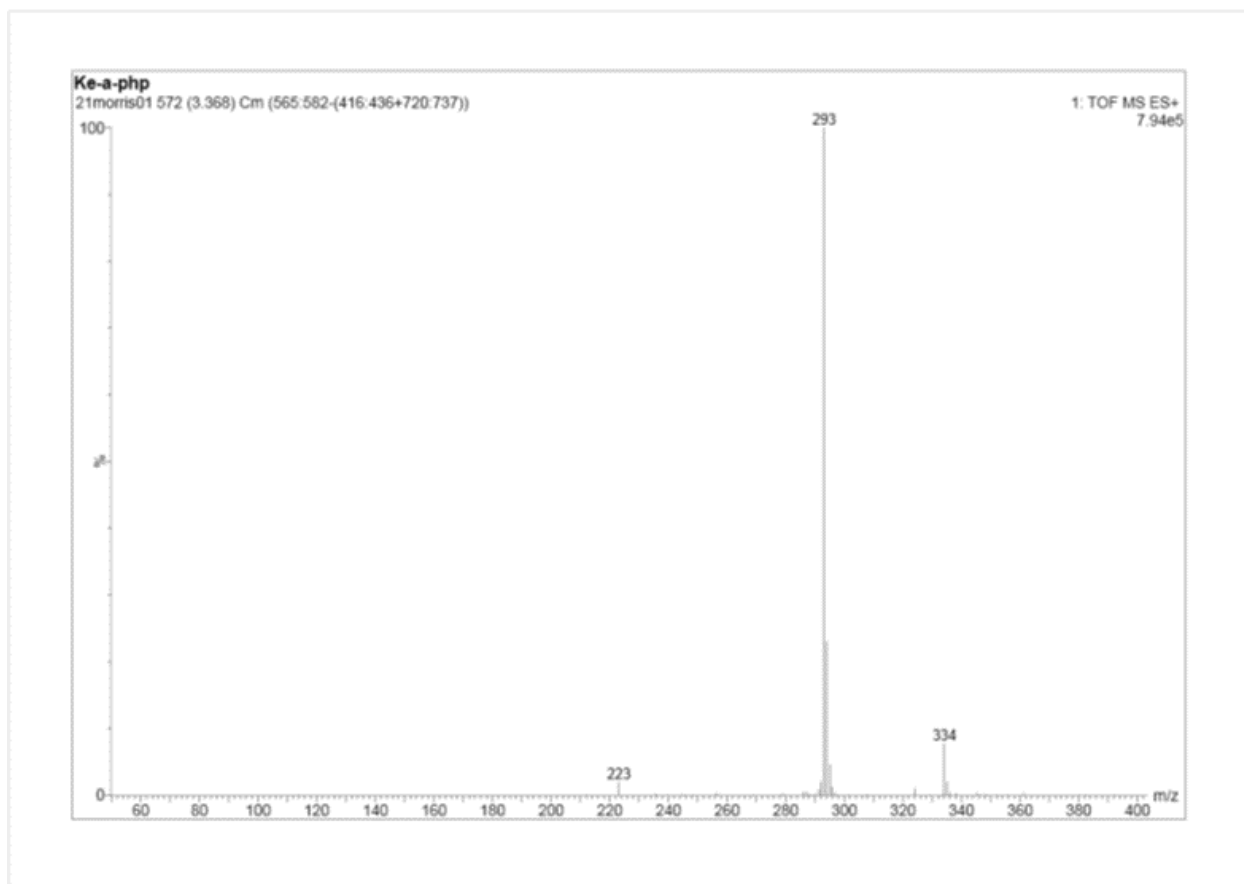
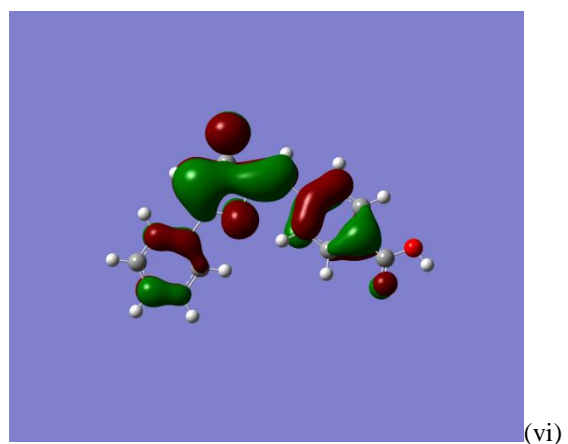
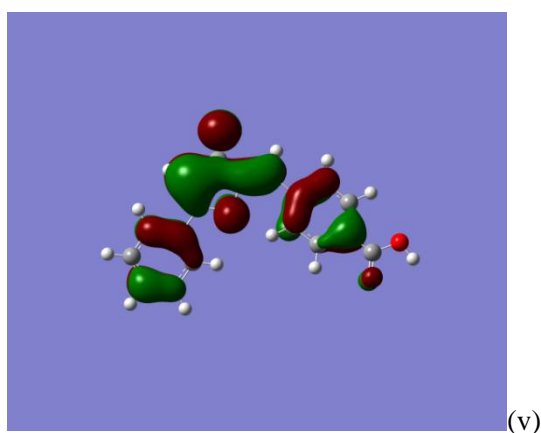
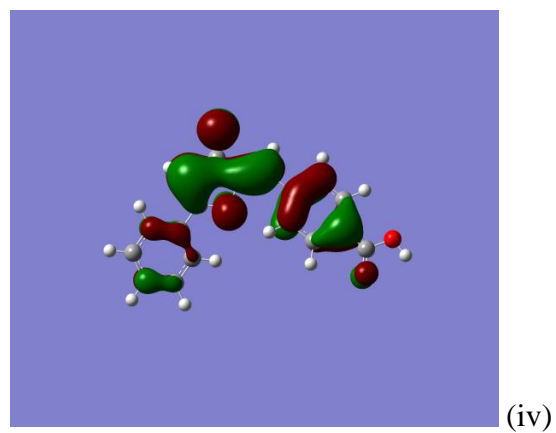
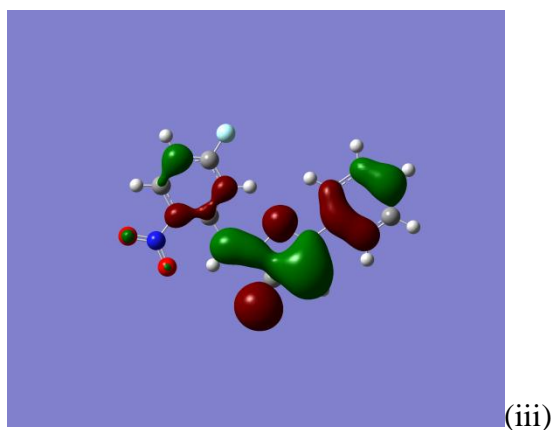
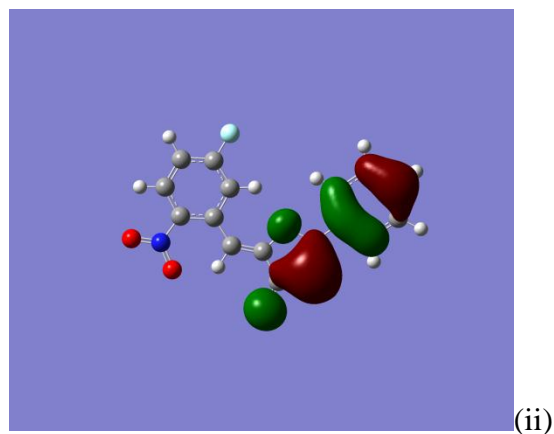
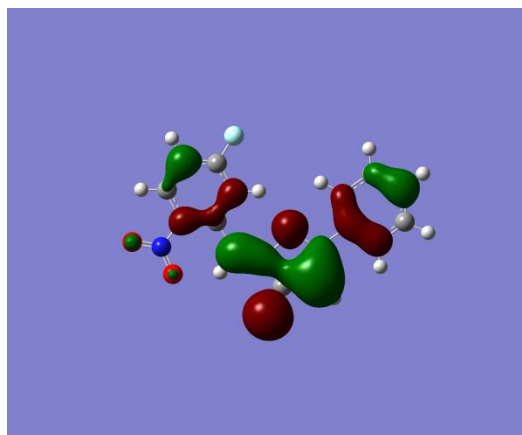
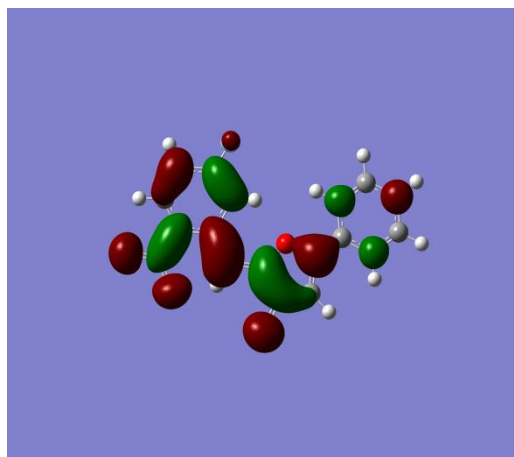
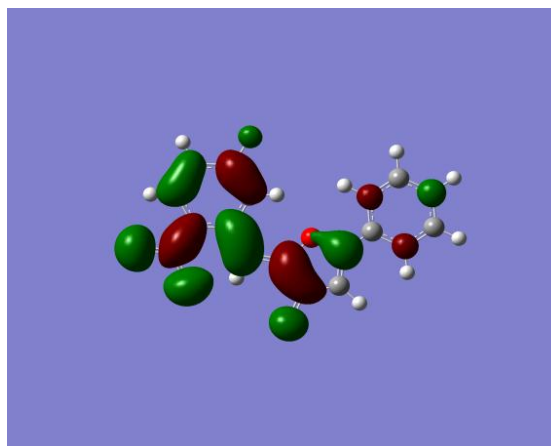


Figure S15. Frontier orbitals of FNPF and CBPF calculated by the TD-DFT/ B3LYP/6-31G+ method on excited state (i) FNPF_{HOMO} (G.P), (ii) FNPF_{HOMO} (wr), (iii) FNPF_{HOMO} (cyhx), (iv) CBPF_{HOMO}(G.P), (v) CBPF_{HOMO}(wr), (vi) CBPF(cyhx), (vii) FNPF_{LUMO} (G.P), (viii) FNPF_{LUMO} (wr), (ix) FNPF_{LUMO}(cyhx), (x) CBPF_{LUMO}(G.P), (xi) CBPF_{LUMO} (wr), (xii) CBPF_{LUMO}(cyhx).

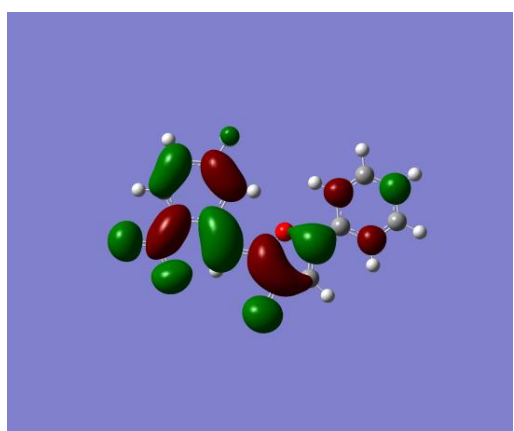




(vii)



(viii)



(ix)