

Supplementary Information

Synthesis of 4,4'-(arylmethylene)bis(3-methyl-1-phenyl-1H-pyrazol-5-ols) and evaluation of their antioxidant and anticancer activities

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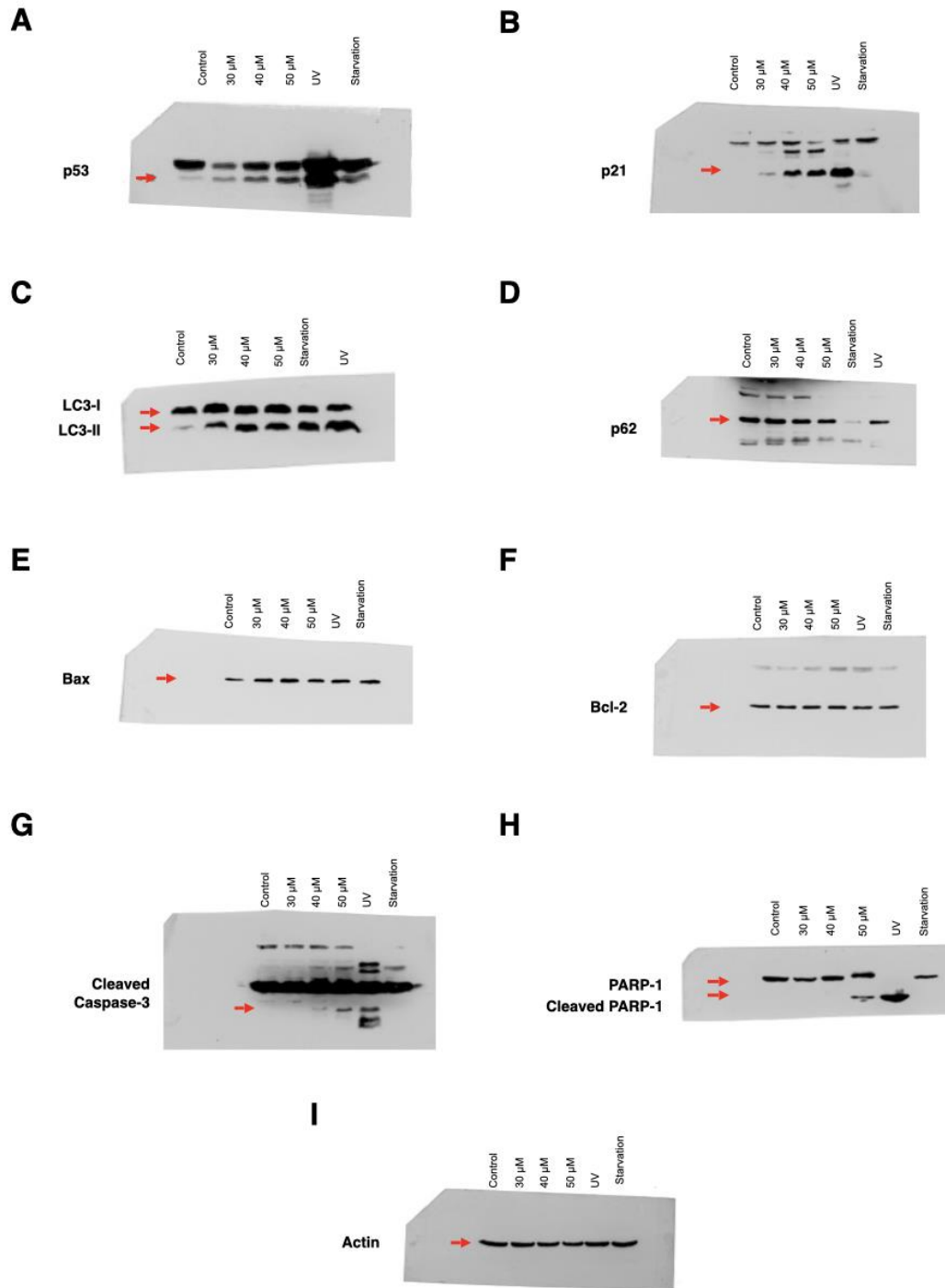


Fig. S1. Original western blots CL-X Posure™ films for Western blots. Each protein was detected in independent films at different times of exposure to the membrane. **A)** p53; **B)** p21; **C)** LC3-I and -II; **D)** p62; **E)** BAX; **F)** Bcl-2; **G)** Cleaved caspase-3; **H)** Active and cleaved PARP-1; **I)** Actin. Notice, for autophagy detection starvation control was first, in contrast to apoptosis control, which UV control was first.

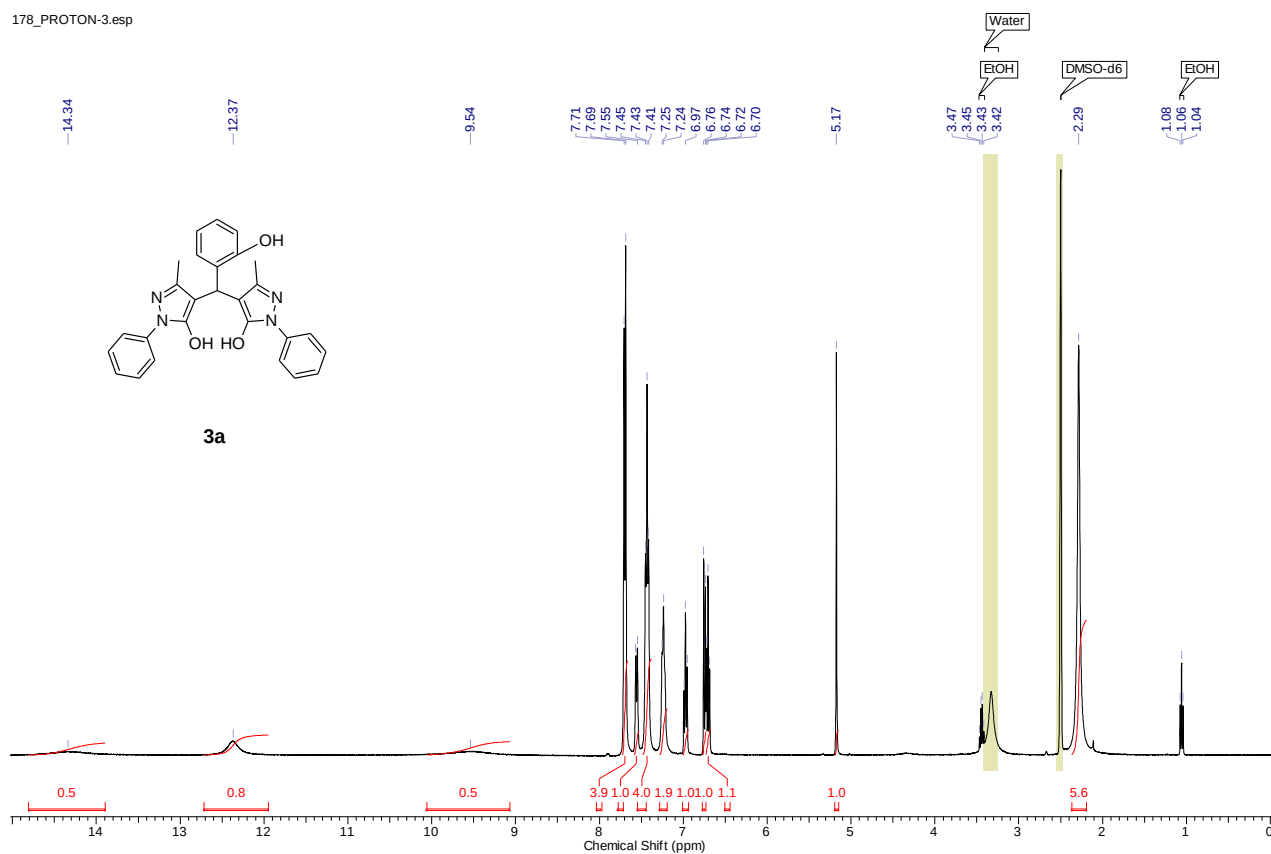


Fig. S2. ¹H NMR spectrum of compound **3a**.

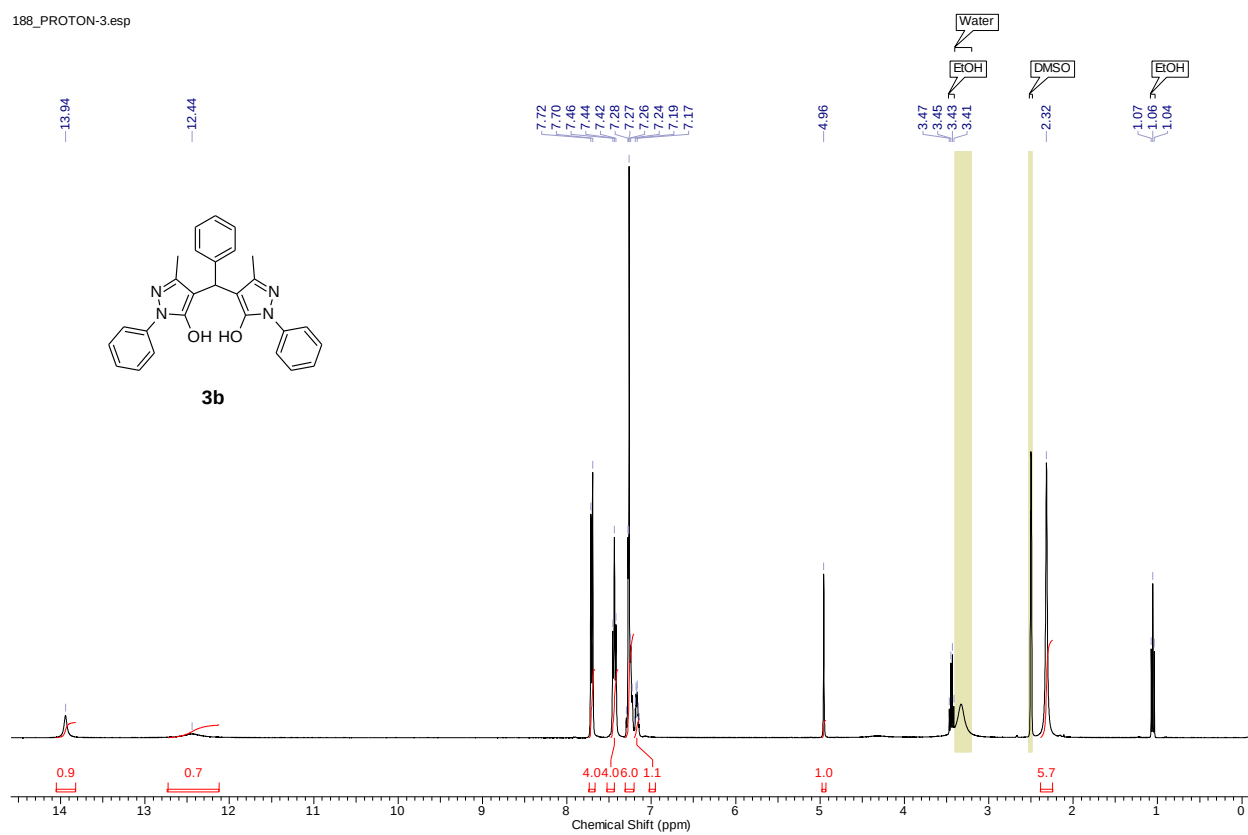


Fig. S3. ¹H NMR spectrum of compound **3b**.

182_PROTON-3.esp

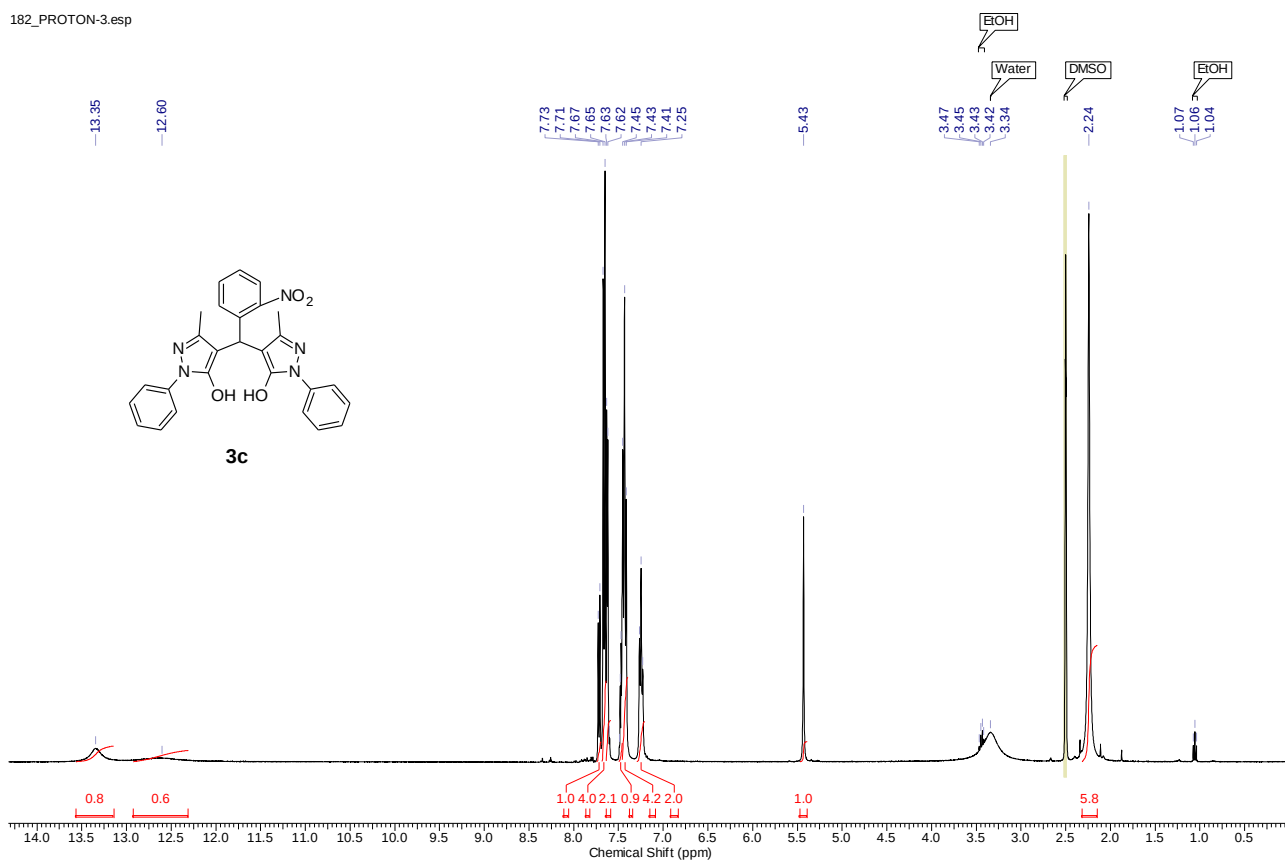


Fig. S4. ^1H NMR spectrum of compound **3c**.

187_PROTON-3.esp

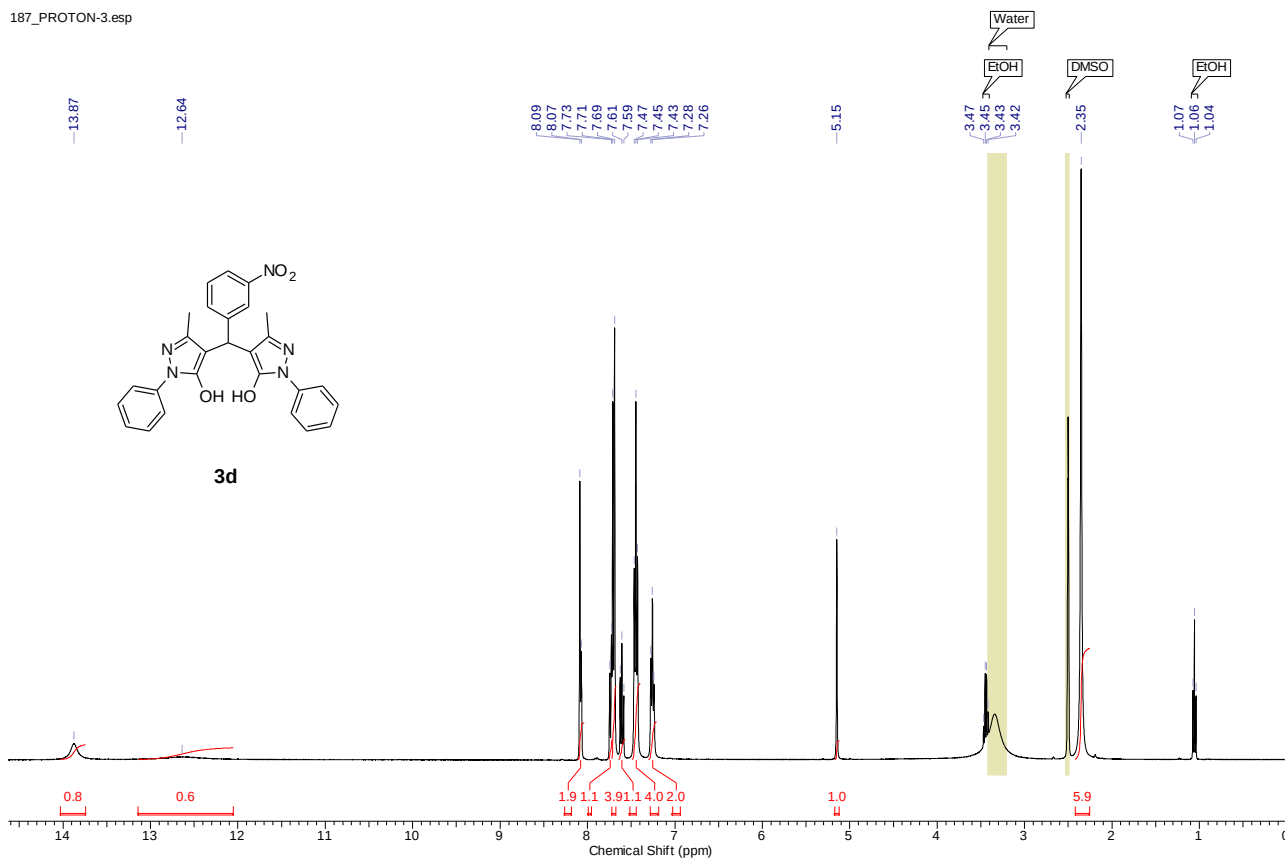


Fig. S5. ^1H NMR spectrum of compound **3d**.

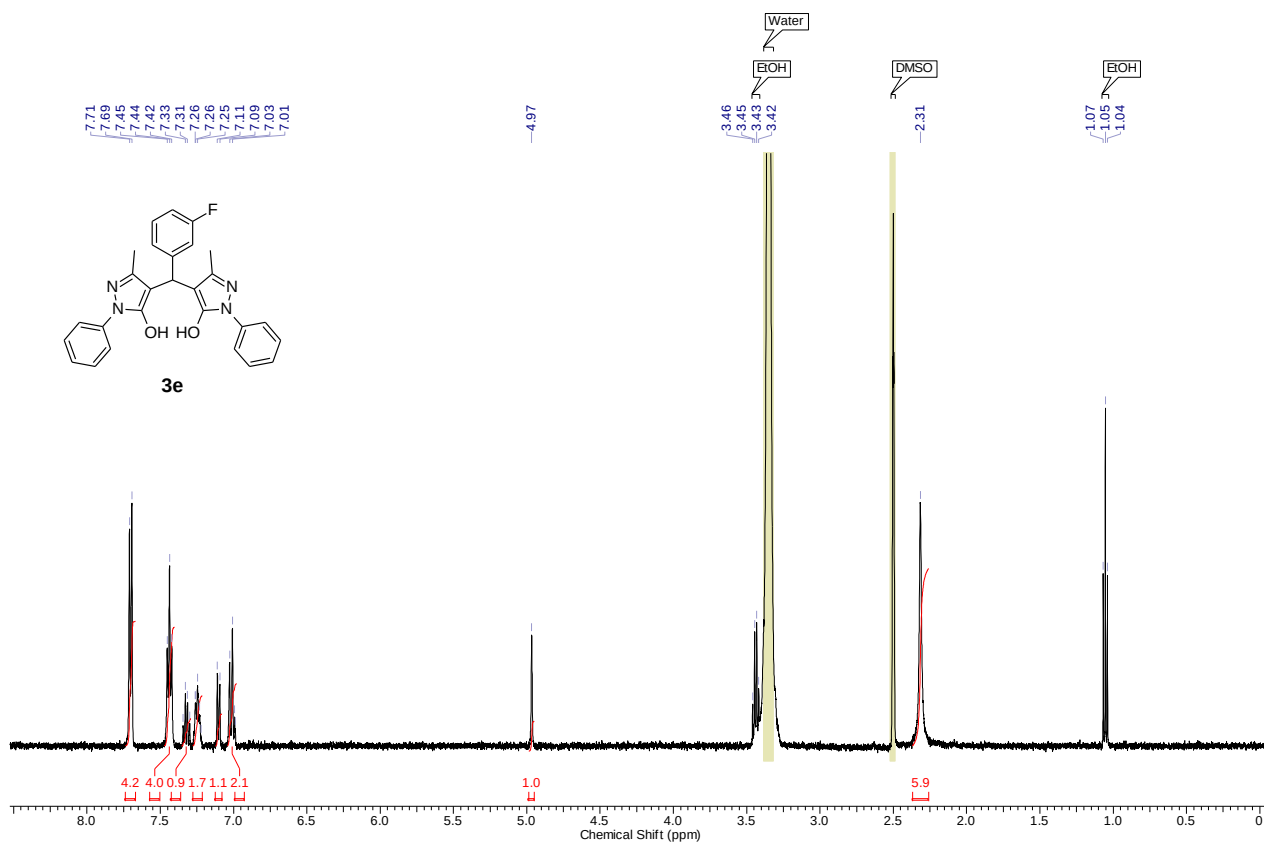


Fig. S6. ¹H NMR spectrum of compound **3e**.

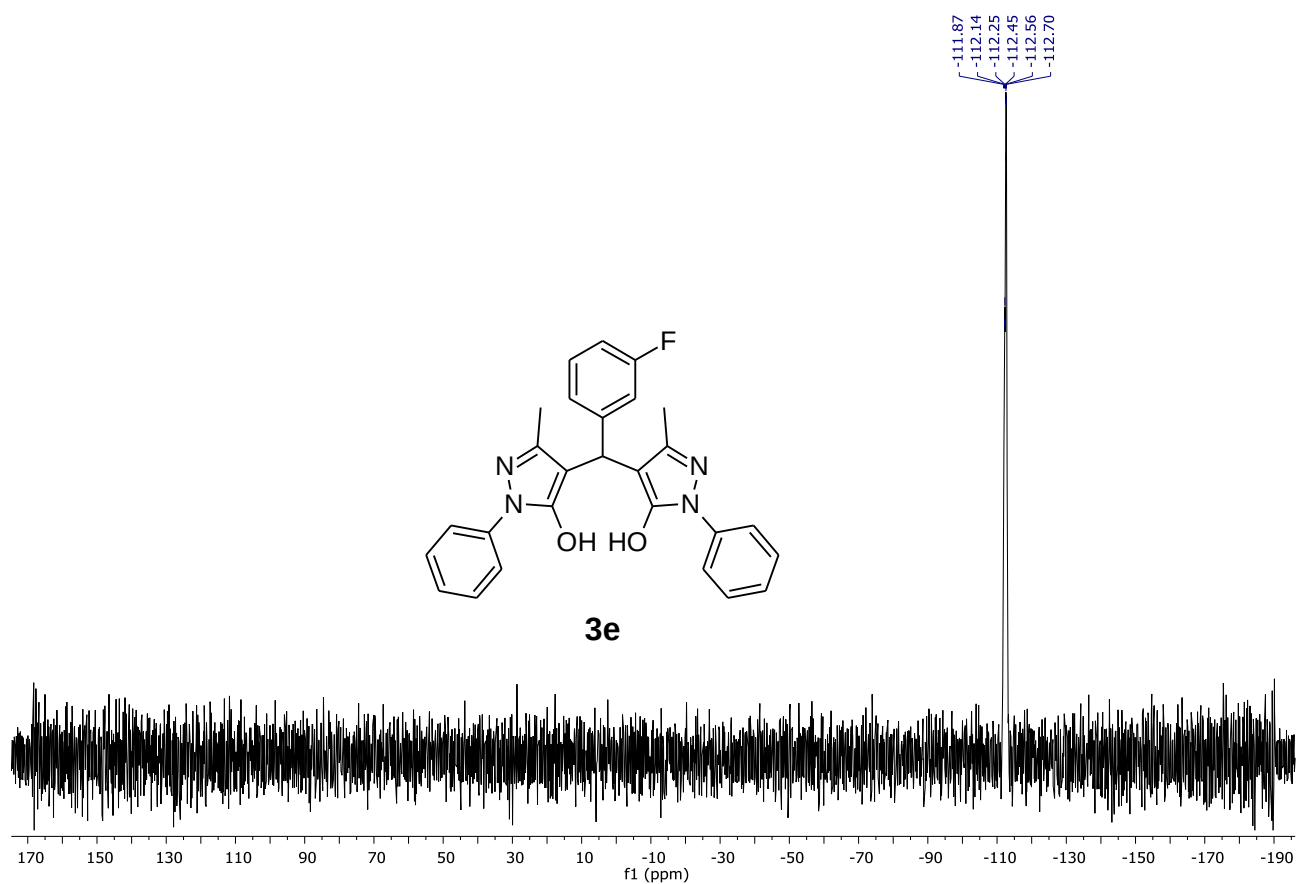


Fig. S7. ¹⁹F NMR spectrum of compound **2e**.

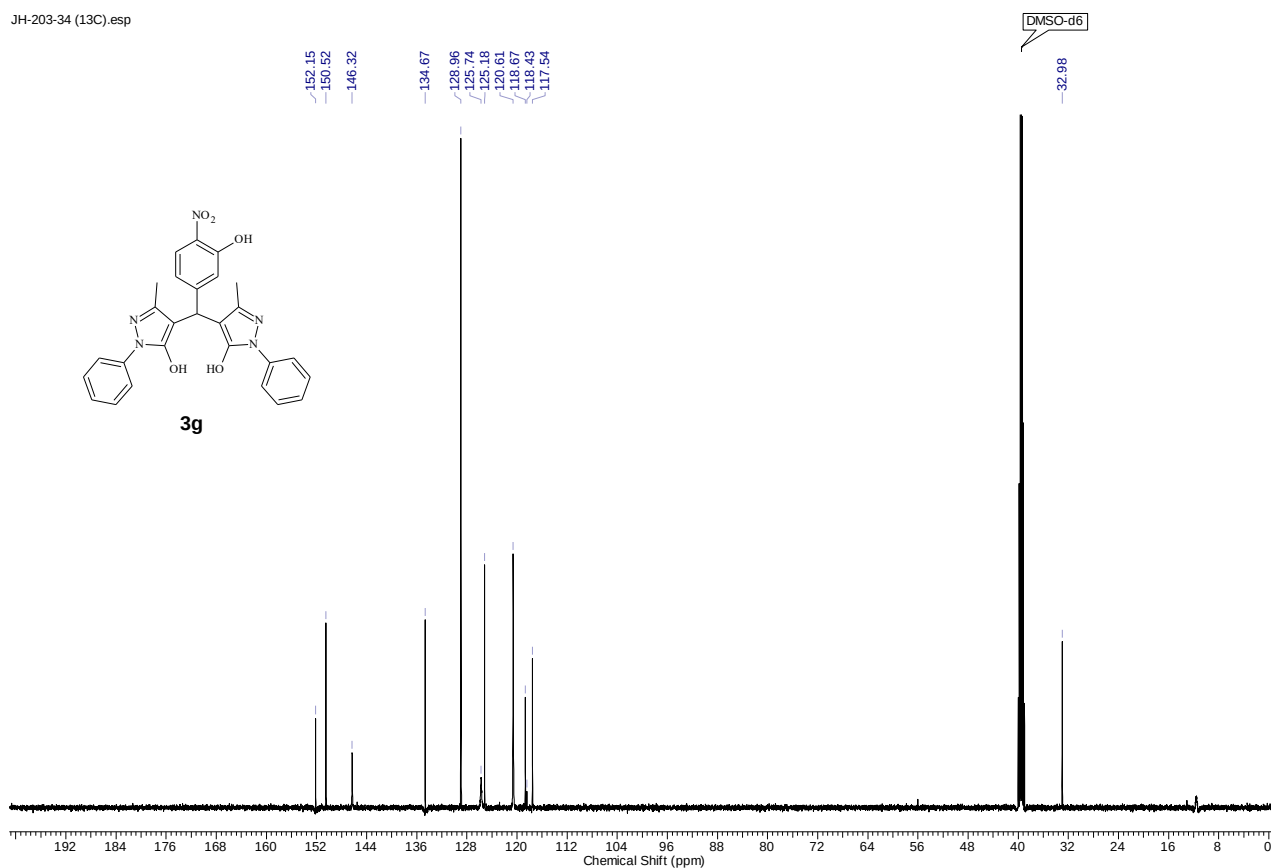


Fig. S10. ^{13}C NMR spectrum of compound **3g**.

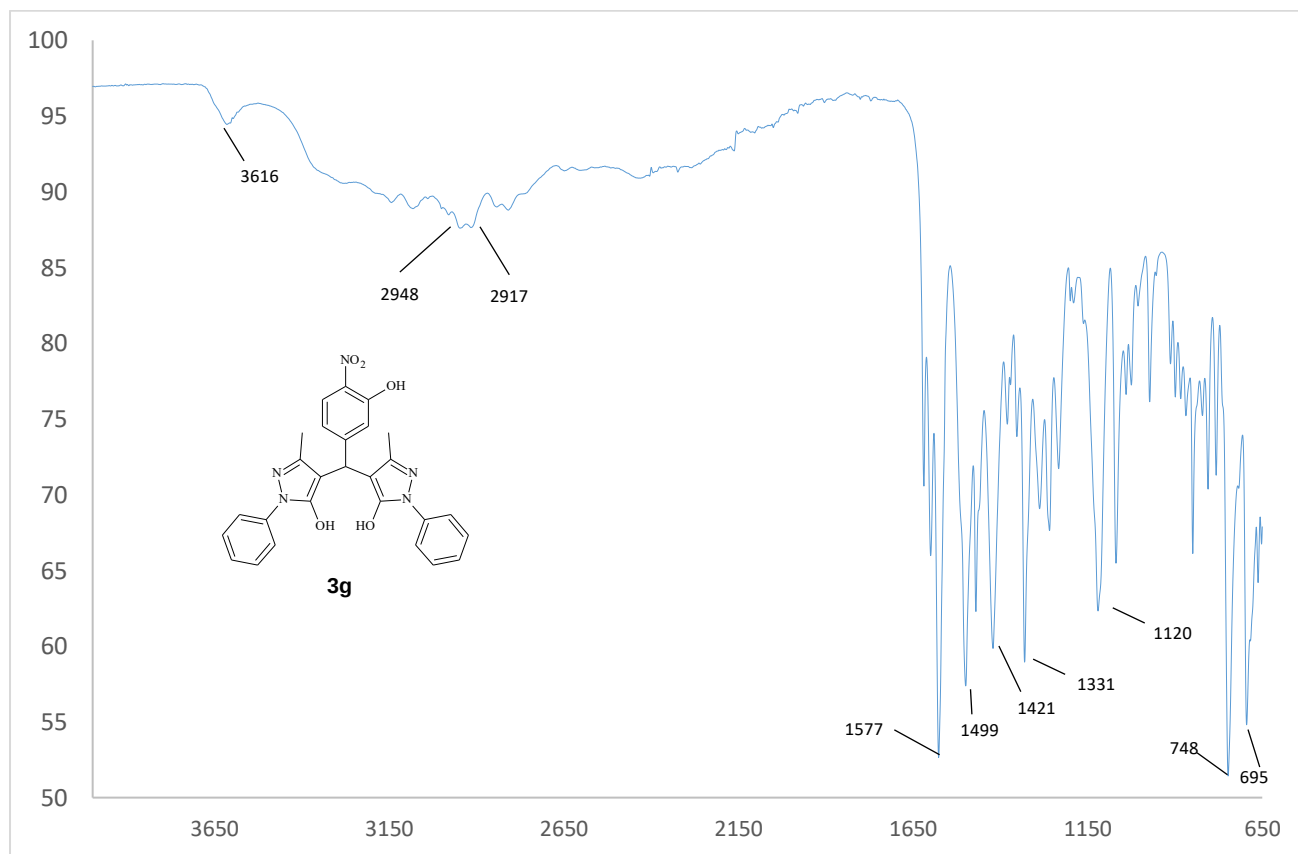


Fig. S11. FTIR spectrum of compound **3g**.

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	200 m/z	Scan End	600 m/z
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SPS Target Mass	400 m/z	Averages	5 Spectra	n/a	n/a

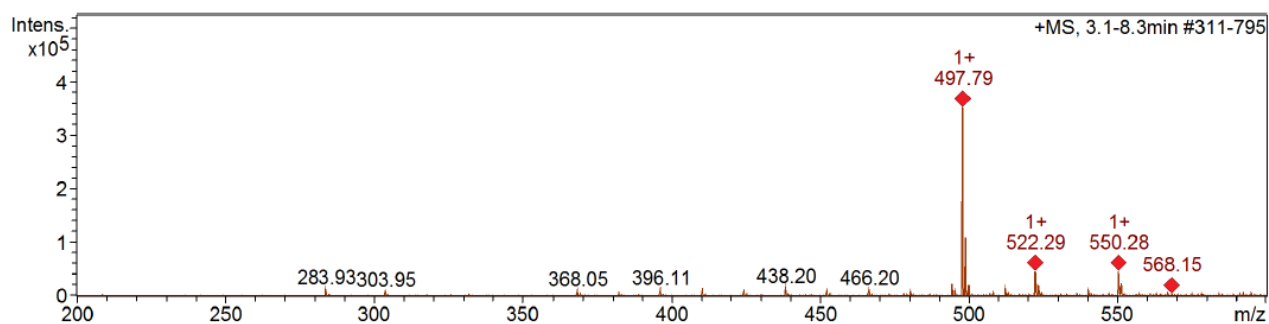


Fig. S12. ESI-MS spectrum of compound **3g**.

2h (3-OH-4-OMe).esp

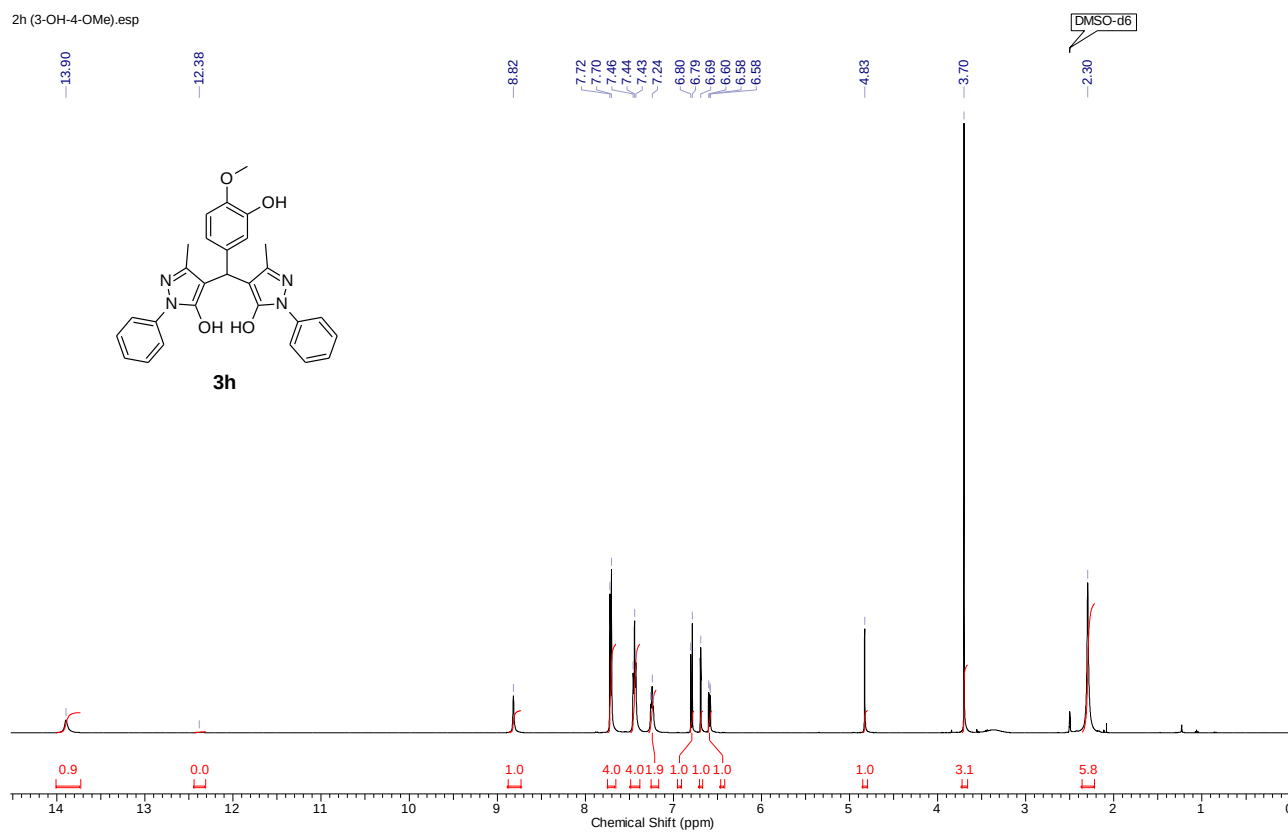


Fig. S13. ^1H NMR spectrum of compound **3h**.

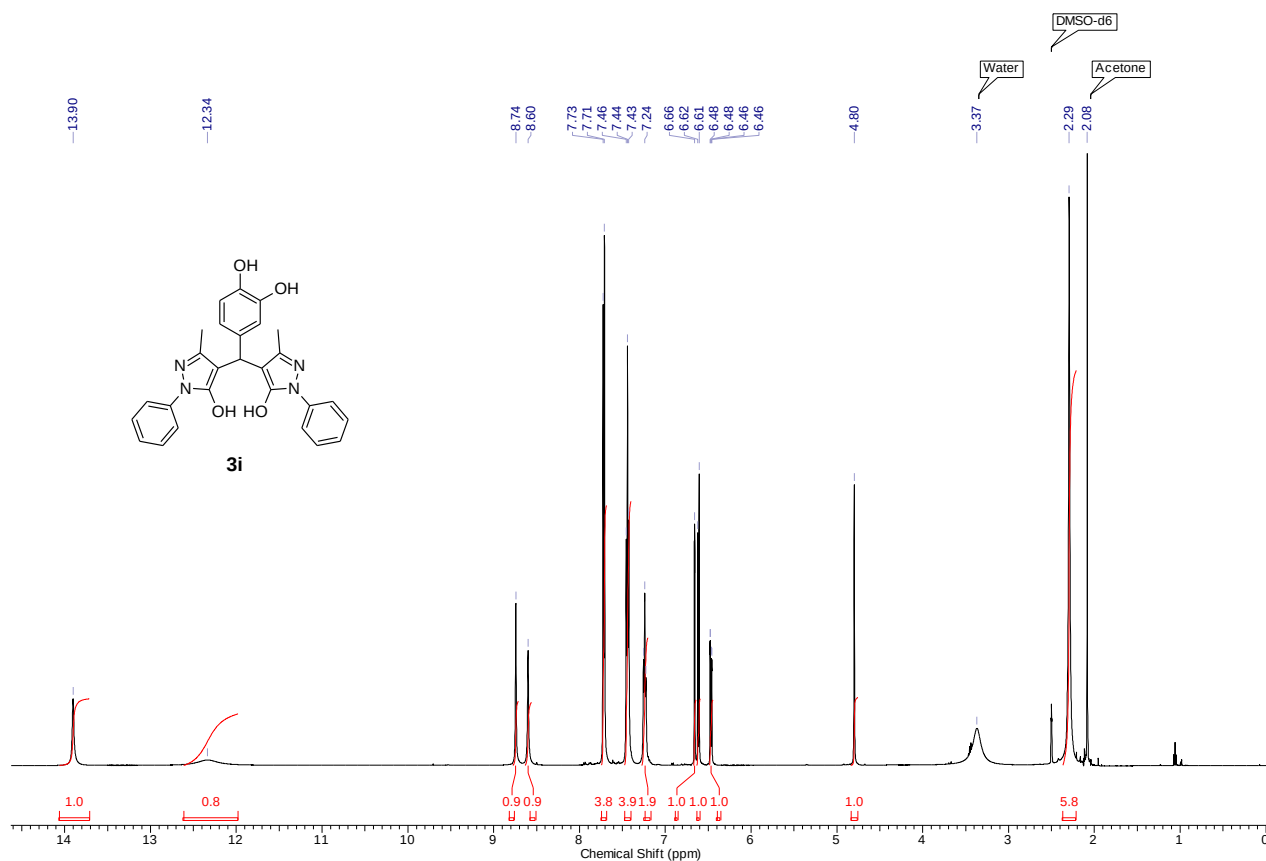


Fig. S14. ¹H NMR spectrum of compound **3i**.

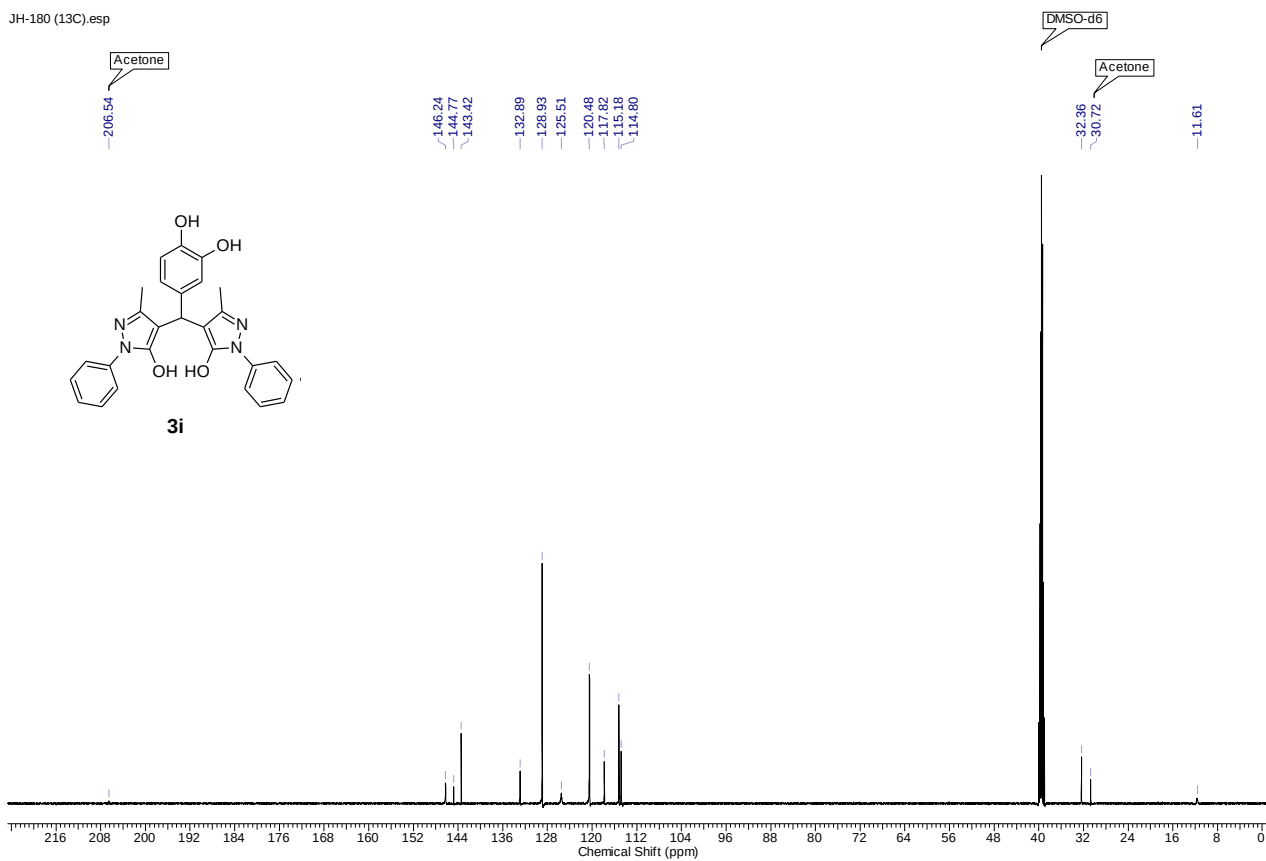


Fig. S15. ¹³C NMR spectrum of compound **3i**.

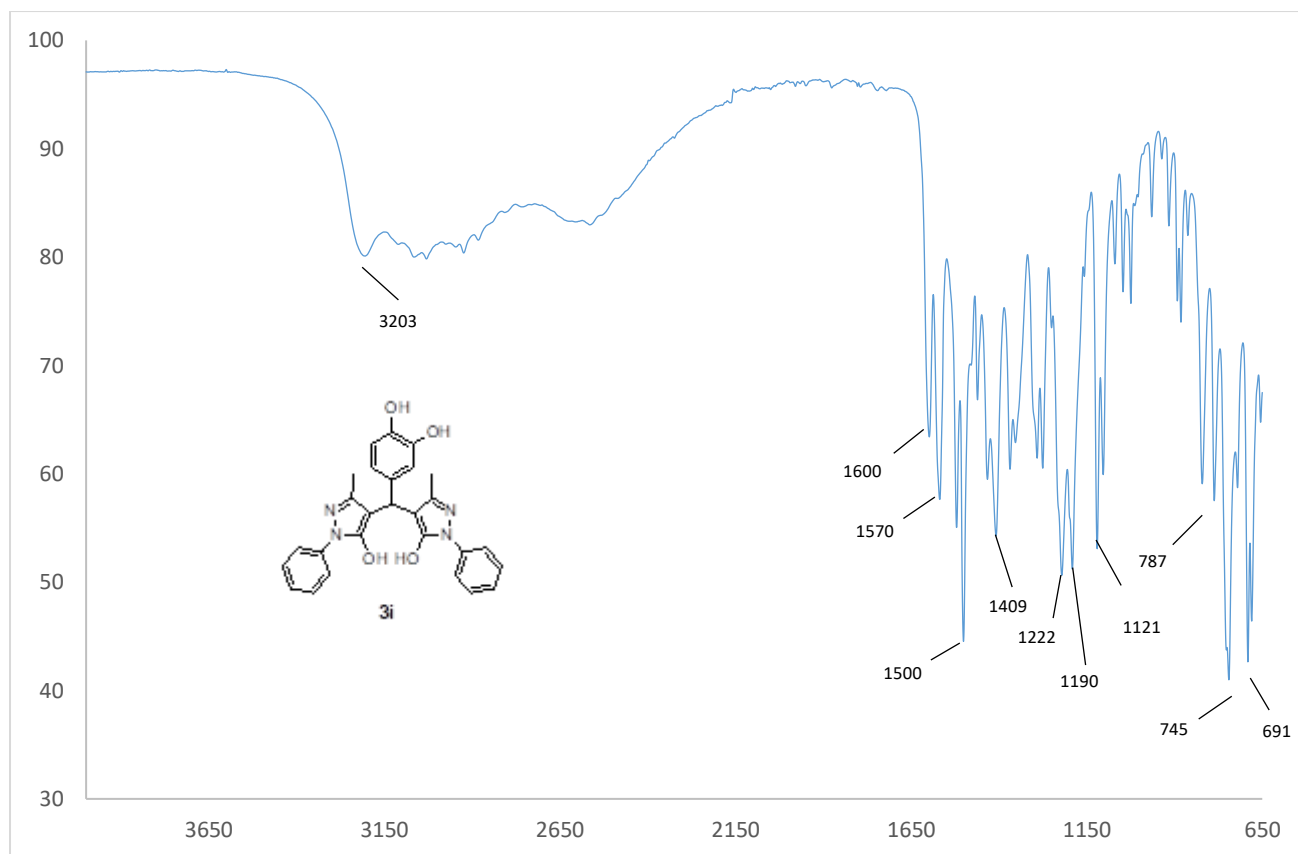


Fig. S16. FTIR spectrum of compound **3i**.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 mDa / DBE: min = -2.0, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

100 formula(e) evaluated with 3 results within limits (up to 19 closest results for each mass)

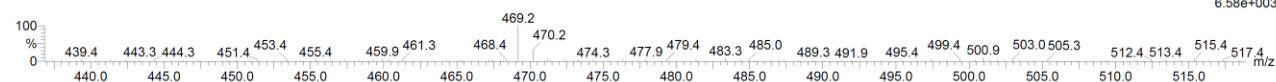
Elements Used:

C: 0-100 H: 0-200 N: 4-4 O: 0-30

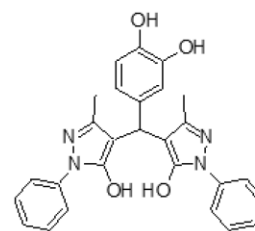
24-Jun-2016

jhm-24Jun16-180 212 (3.921) Cn (Cen,7, 50.00, Ar); Sm (SG, 3x5.00); Sb (12.5.00)

TOF MS ES+
6.58e+003



Minimum:					-2.0	
Maximum:		10.0	10.0		1000.0	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
469.1877	469.1876	0.1	0.2	17.5	8.3	C27 H25 N4 O4
	469.1935	-5.8	-12.4	8.5	70.8	C20 H29 N4 O9
	469.1782	9.5	20.2	4.5	172.4	C16 H29 N4 O12



Molecular Formula = C₂₇H₂₅N₄O₄
[M+H]⁺ = 469.187032 Da

Fig. S17. HRMS spectrum of compound **3i**.

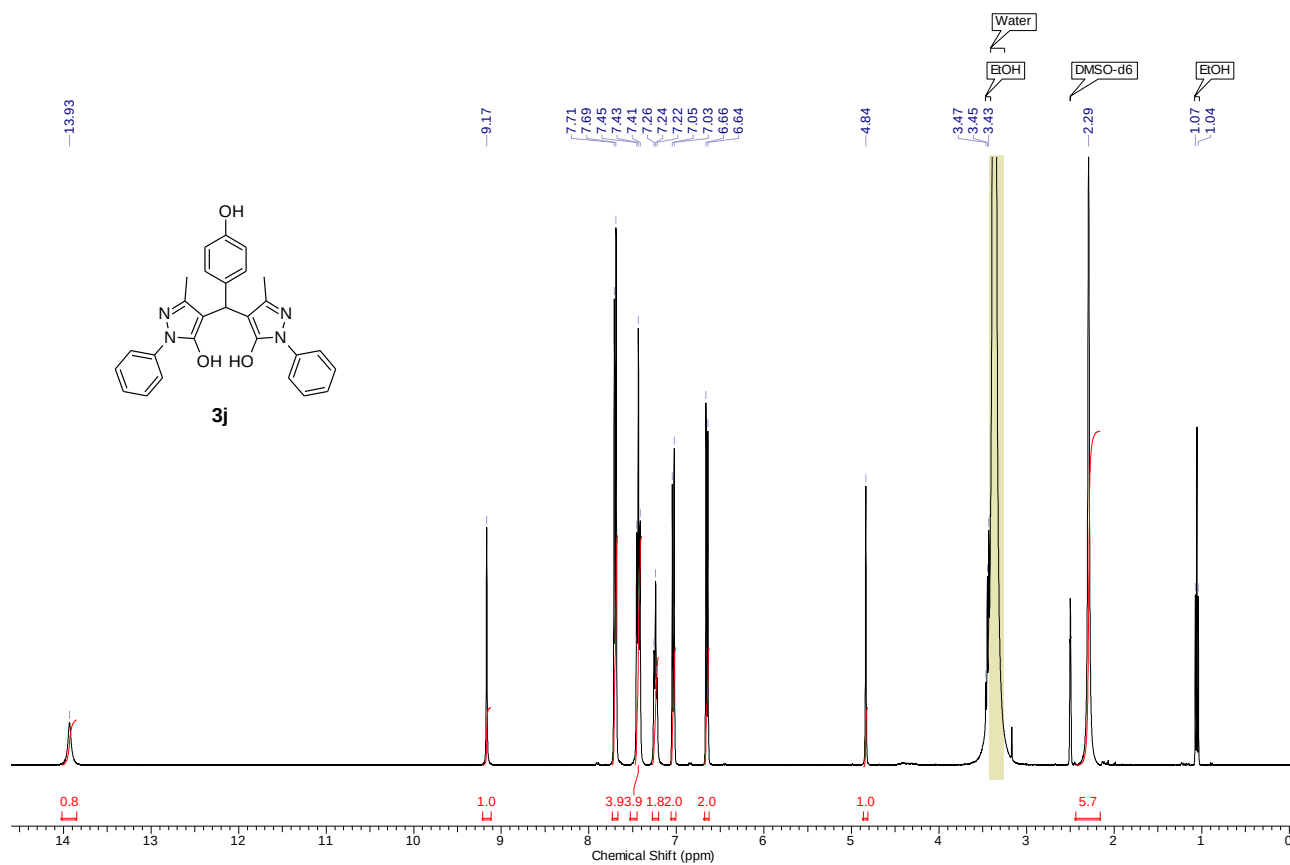


Fig. S18. ¹H NMR spectrum of compound **3j**.

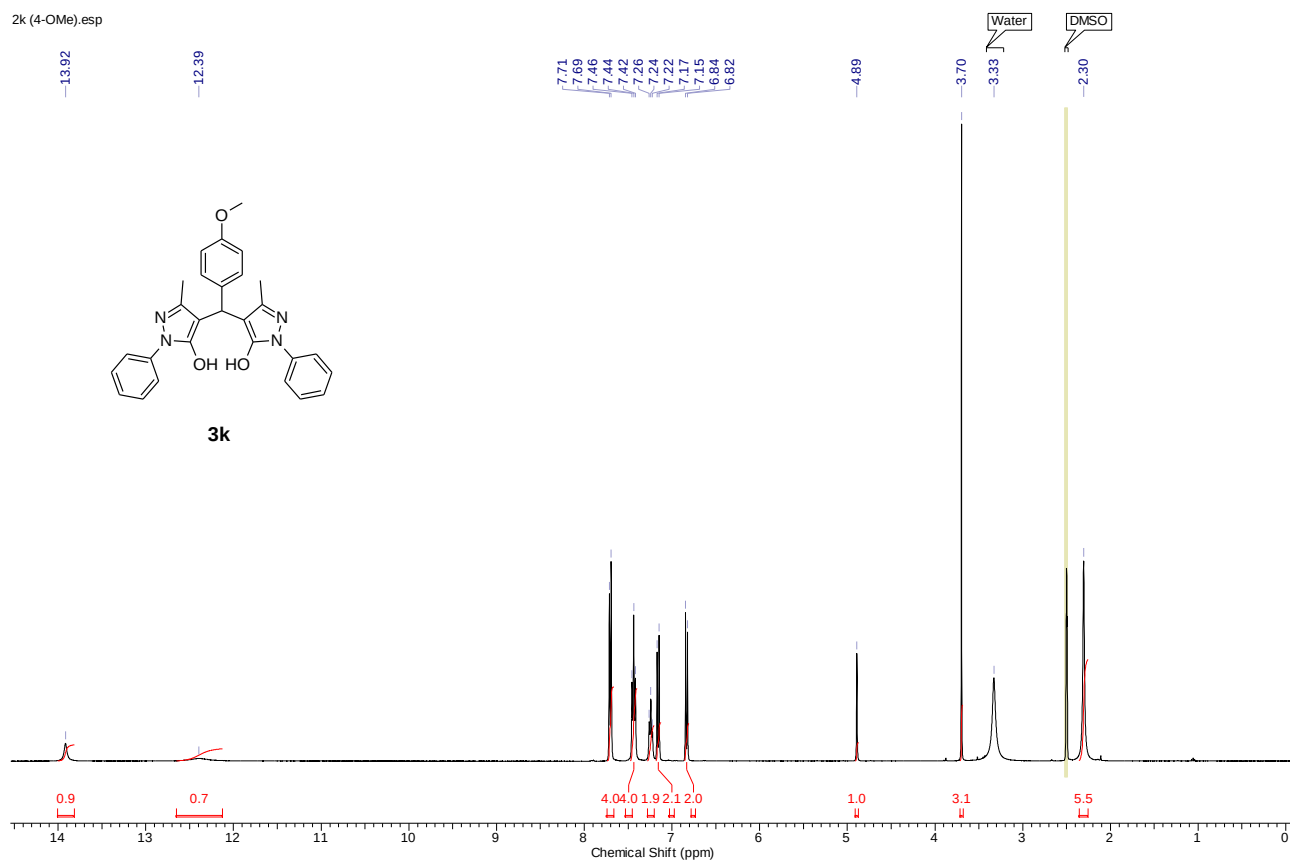


Fig. S19. ¹H NMR spectrum of compound **3k**.

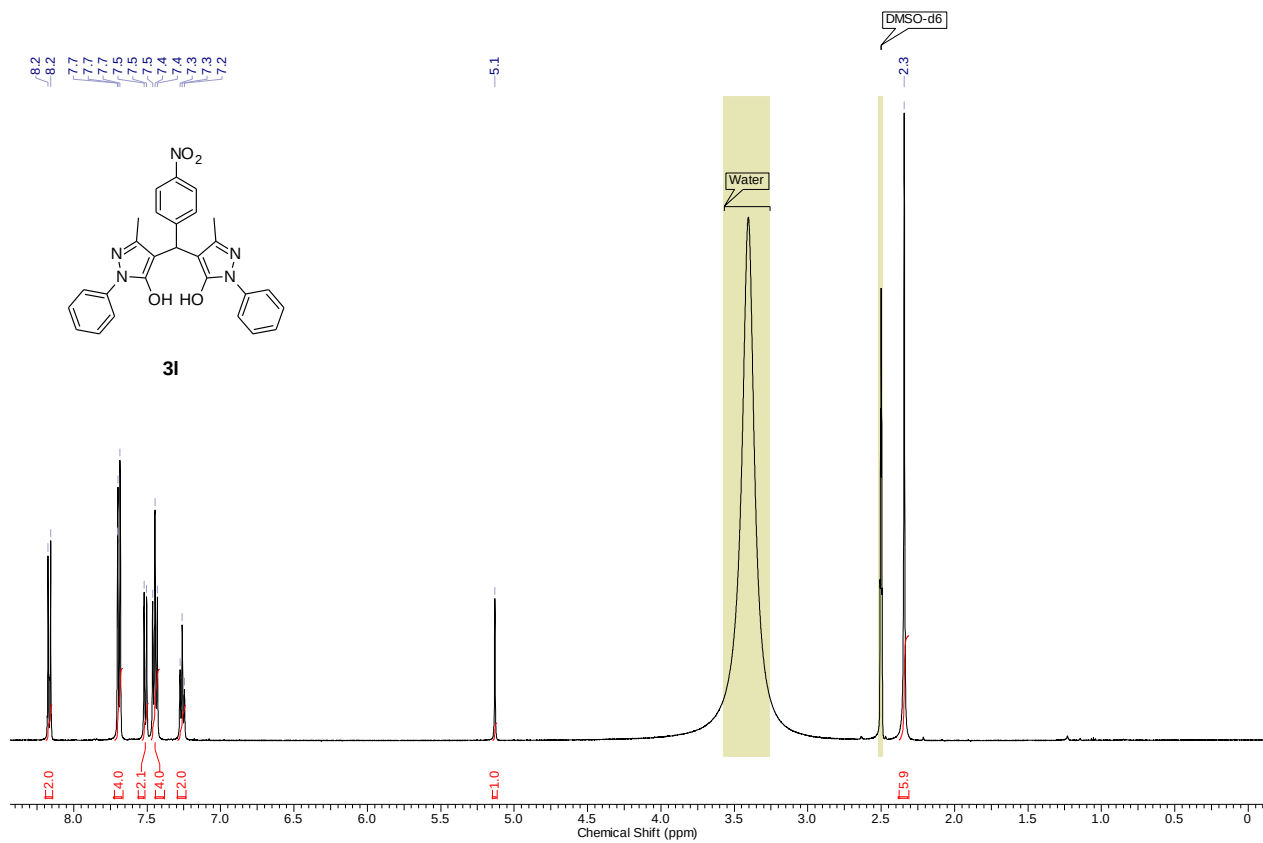


Fig. S20. ¹H NMR spectrum of compound **3l**.

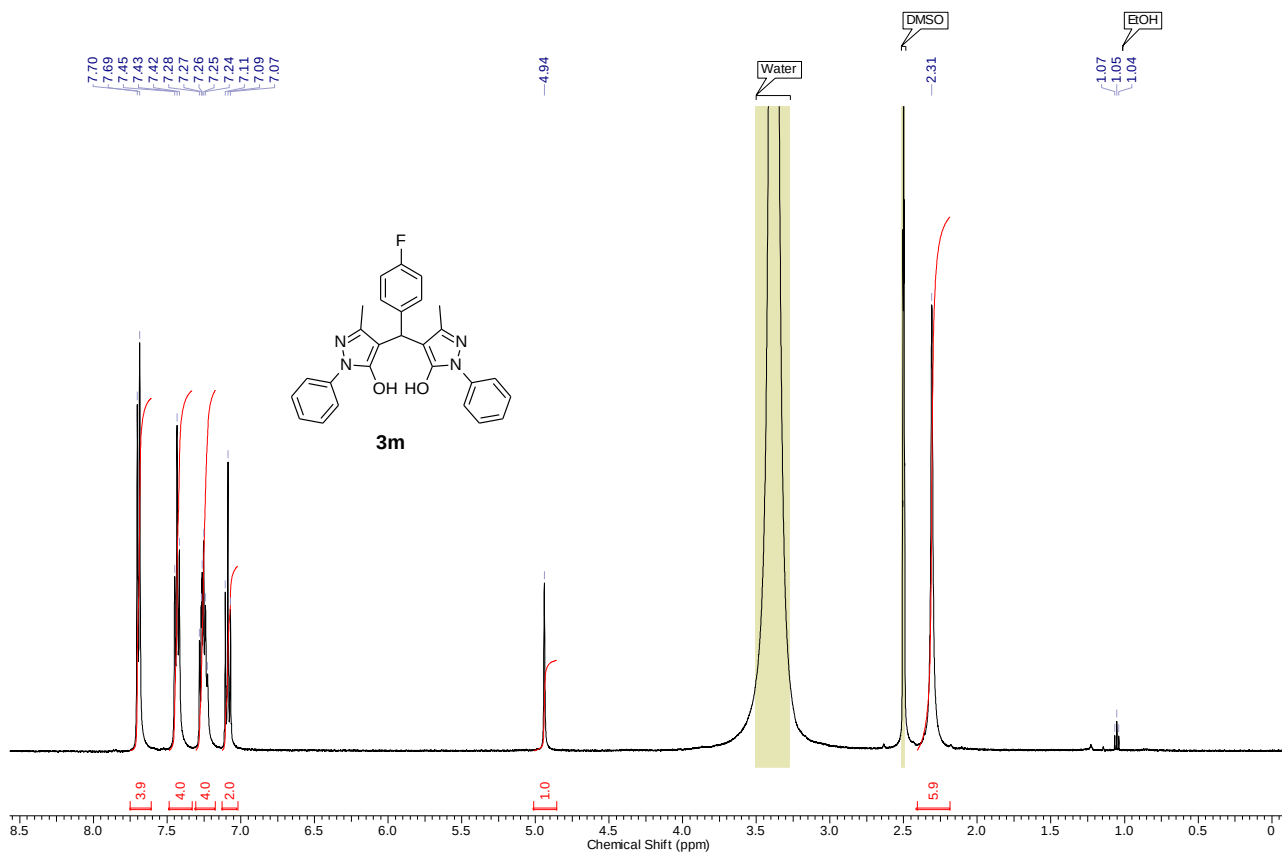


Fig. S21. ¹H NMR spectrum of compound **3m**.

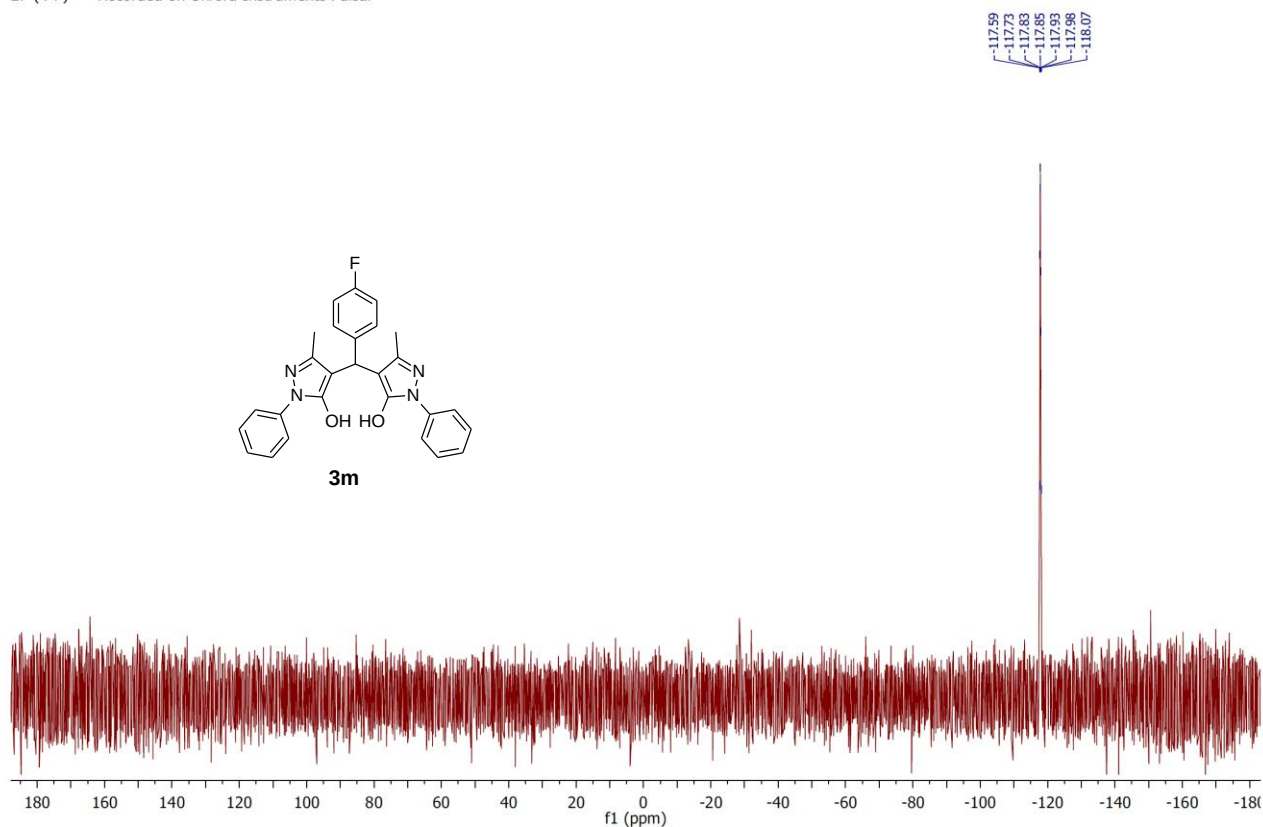


Fig. S22. ^{19}F NMR spectrum of compound **3m**.

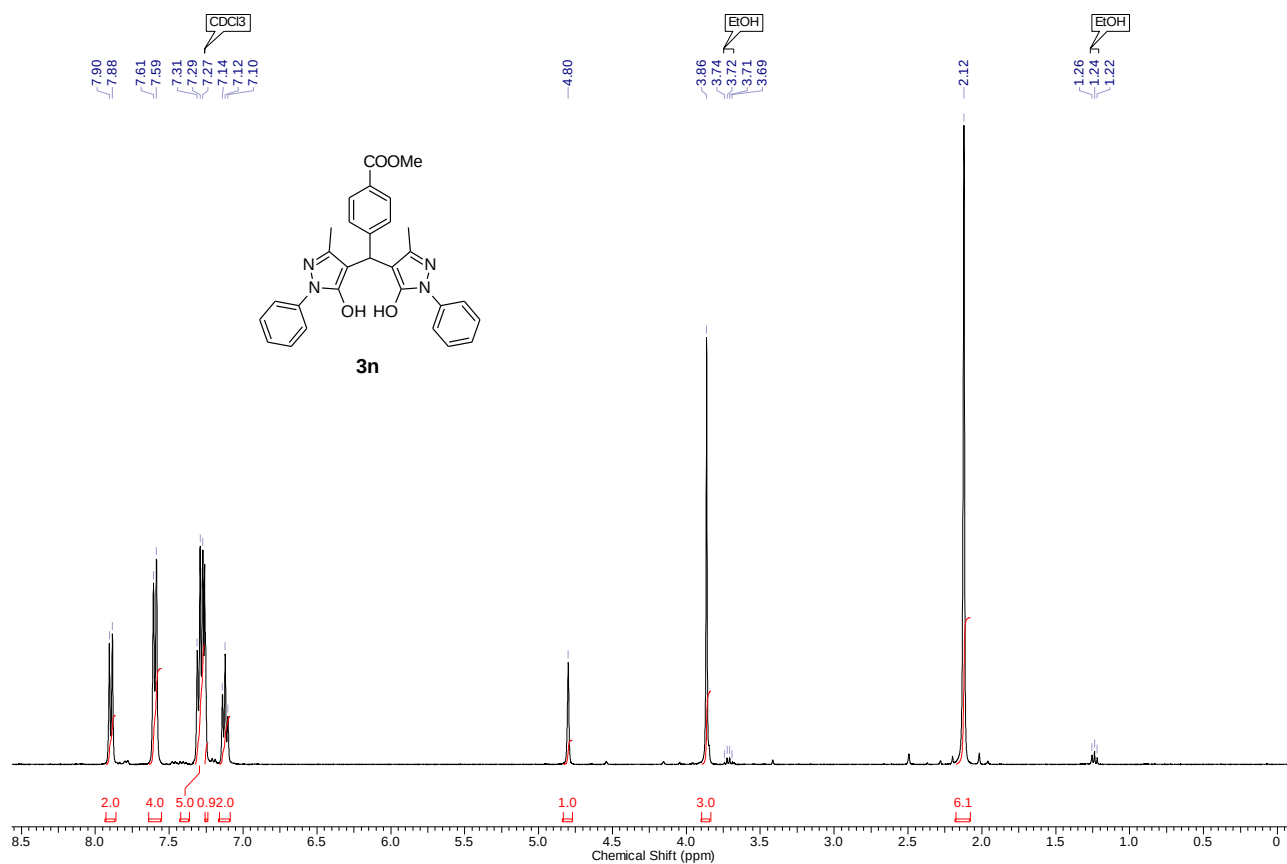


Fig. S23. ^1H NMR spectrum of compound **3n**.

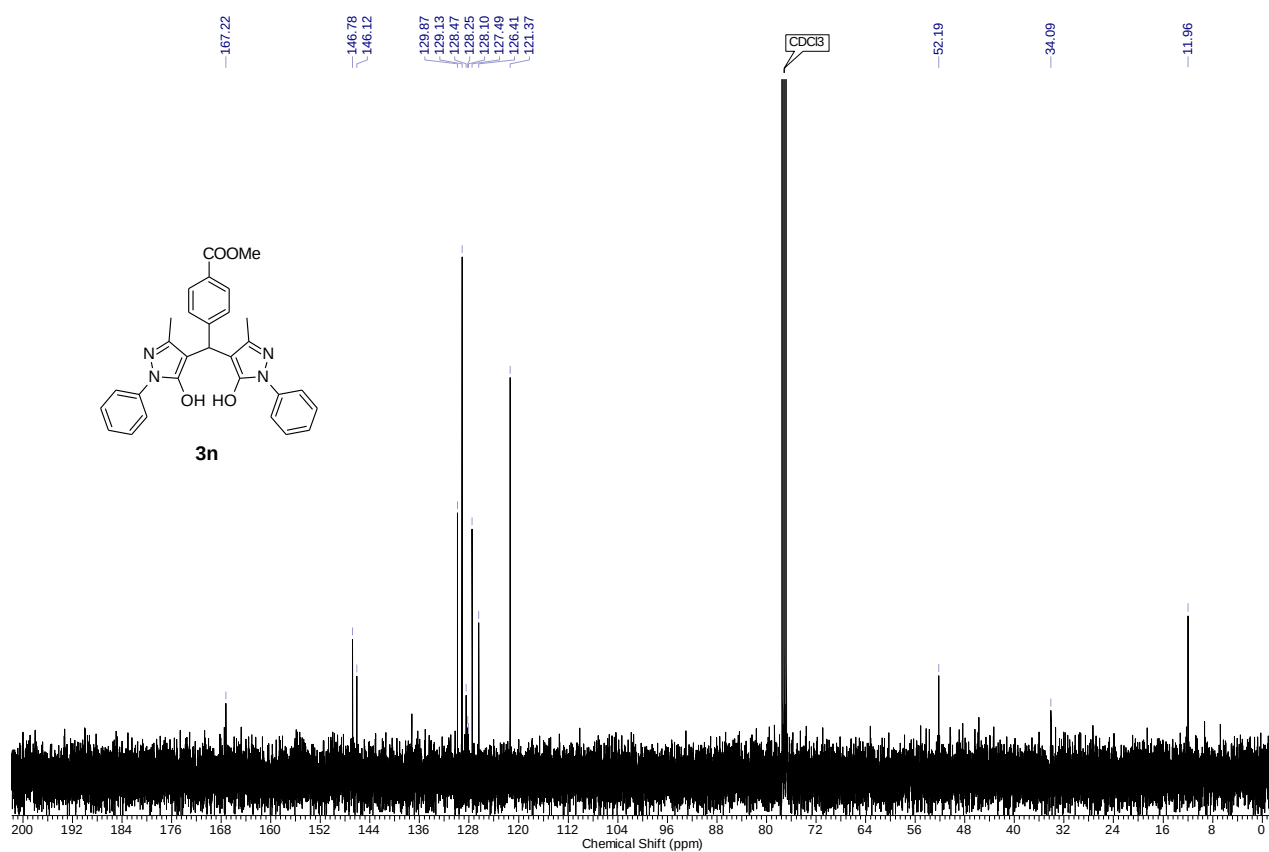


Fig. S24. ^{13}C NMR spectrum of compound **3n**.

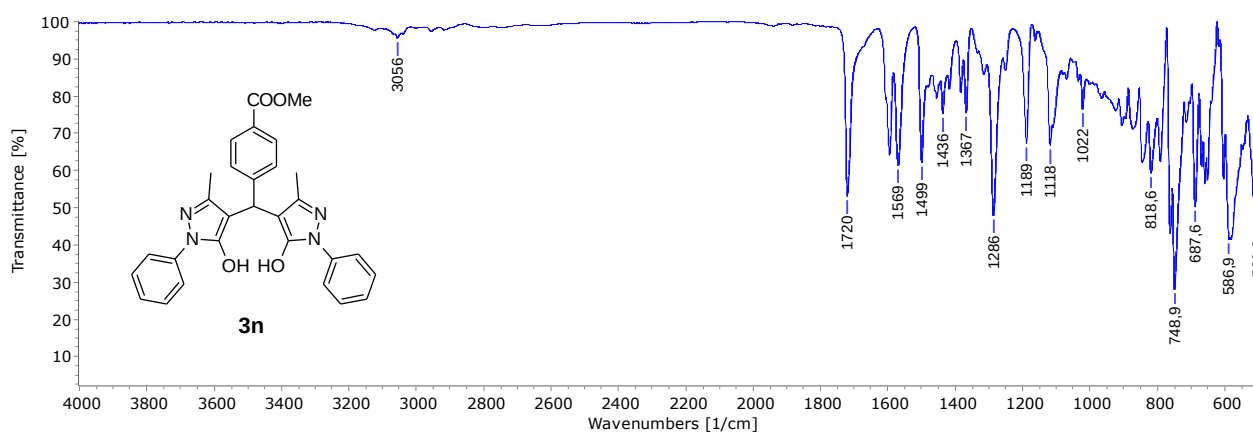


Fig. S25. FTIR spectrum of compound **3n**.

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	200 m/z	Scan End	600 m/z
Accumulation Time	100000 μ s	RF Level	63 %	Trap Drive	54.1
SPS Target Mass	400 m/z	Averages	5 Spectra	n/a	n/a

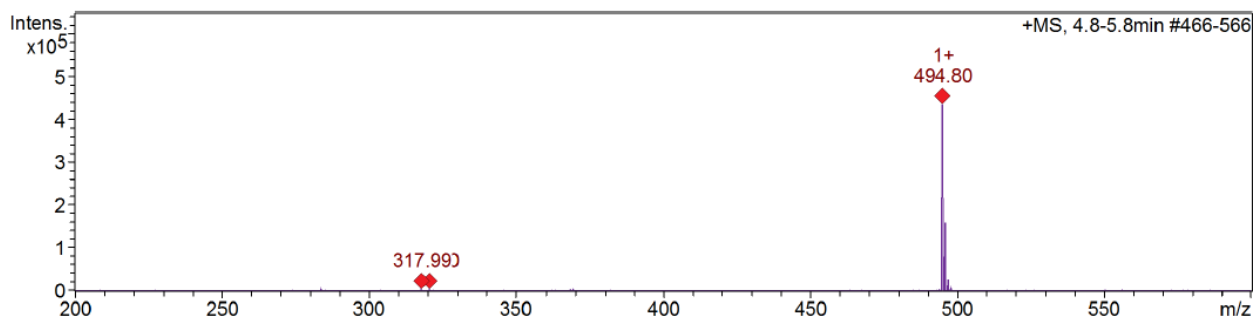


Fig. S26. ESI-MS spectrum of compound **3n**.

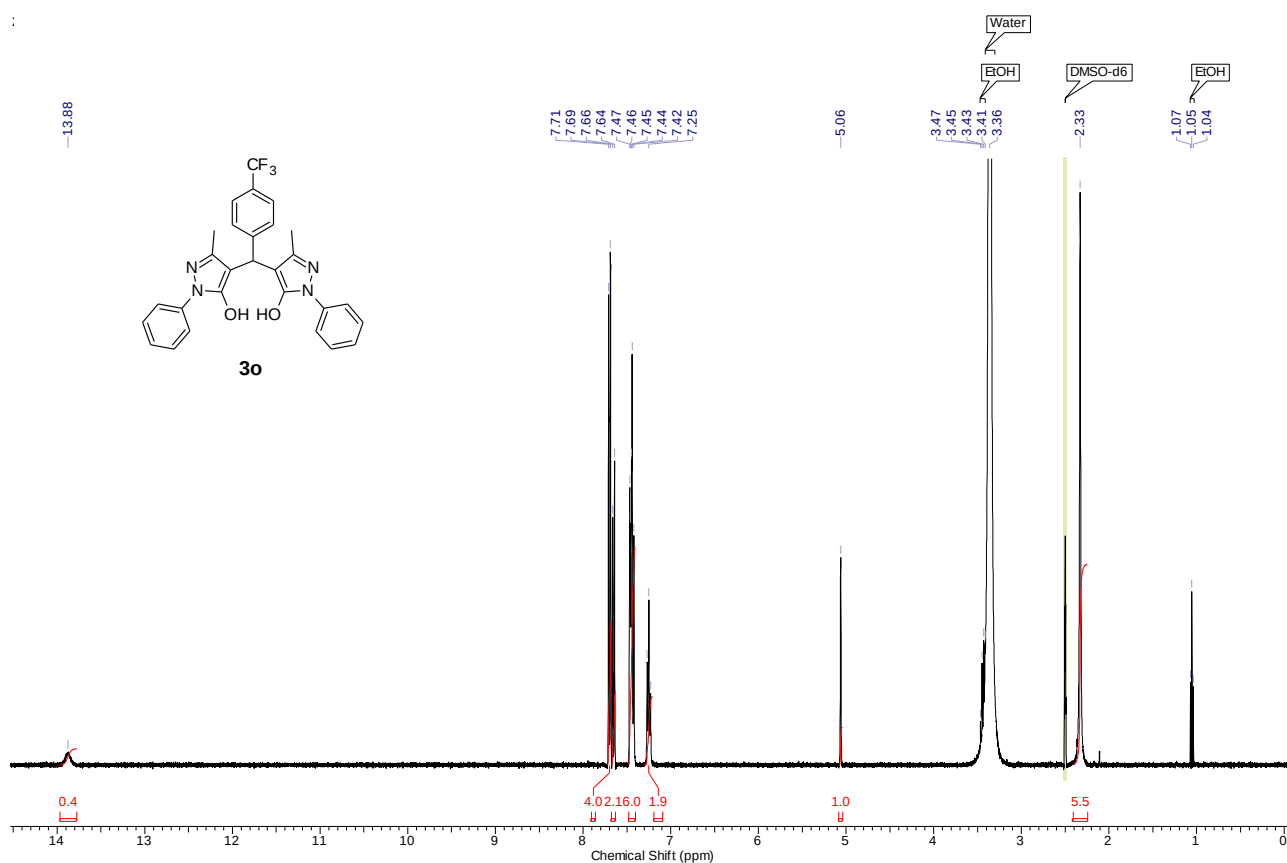


Fig. S27. ¹H NMR spectrum of compound **3o**.

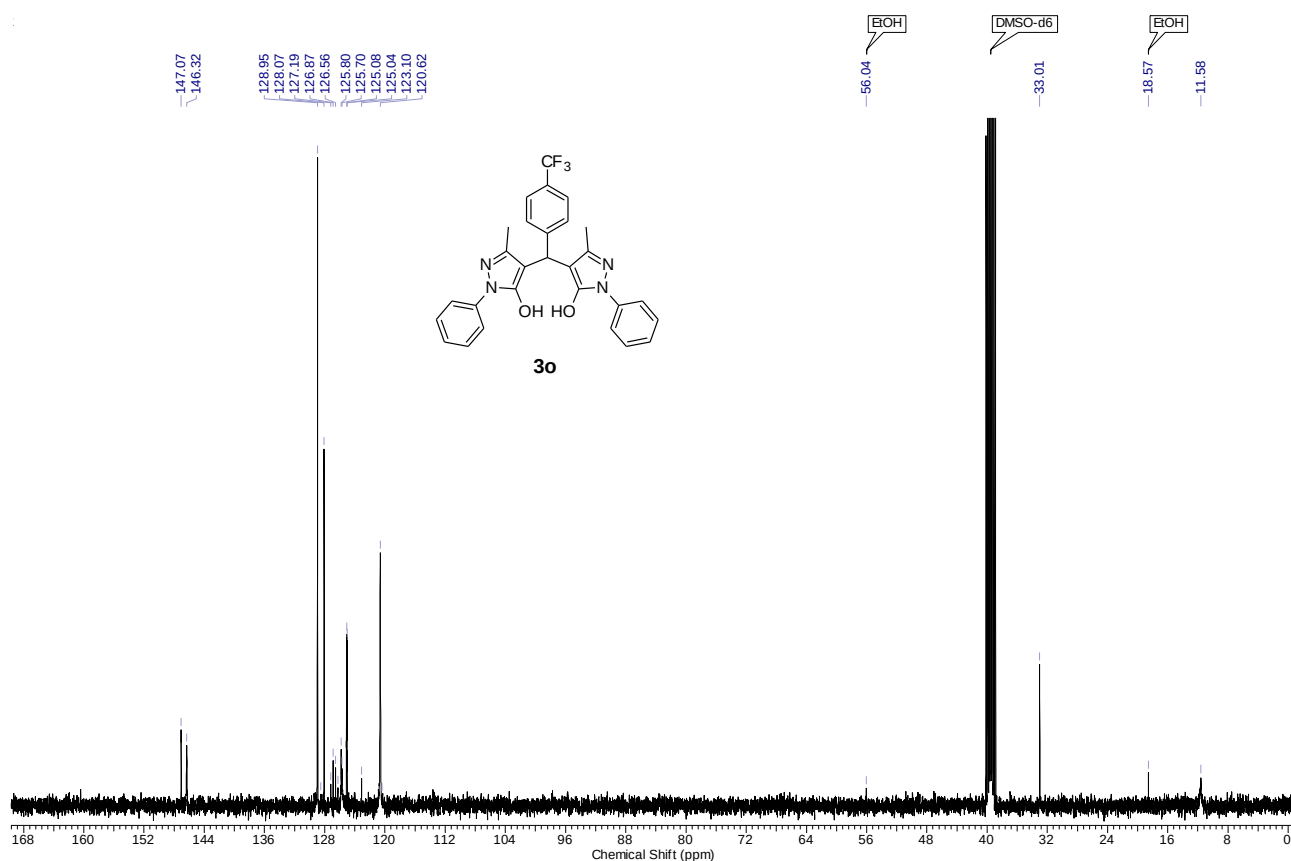


Fig. S28. ^{13}C NMR spectrum of compound **3o**.

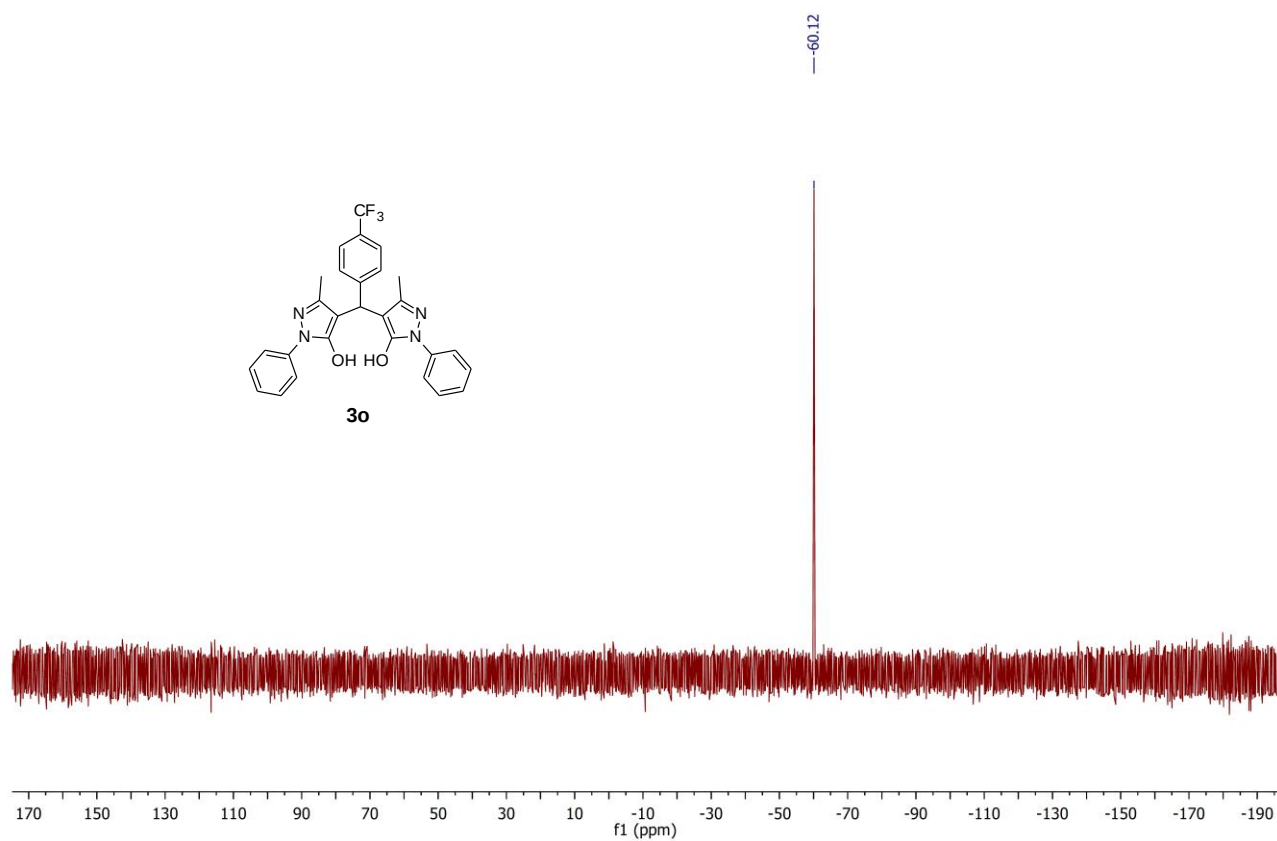


Fig. S29. ^{19}F NMR spectrum of compound **3o**.

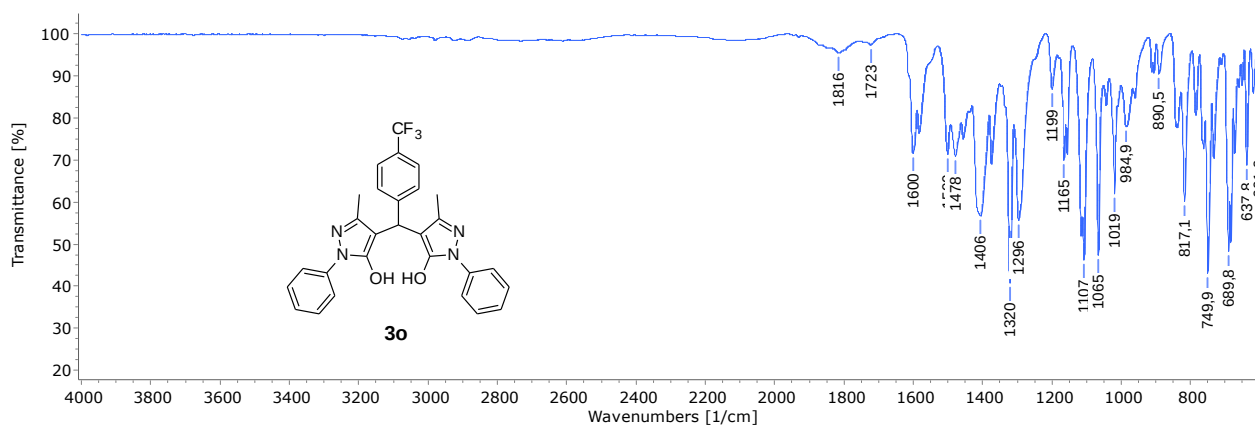


Fig. S30. FTIR spectrum of compound **3o**.

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	200 m/z	Scan End	600 m/z
Accumulation Time	517 μ s	RF Level	63 %	Trap Drive	54.1
SPS Target Mass	400 m/z	Averages	5 Spectra	n/a	n/a

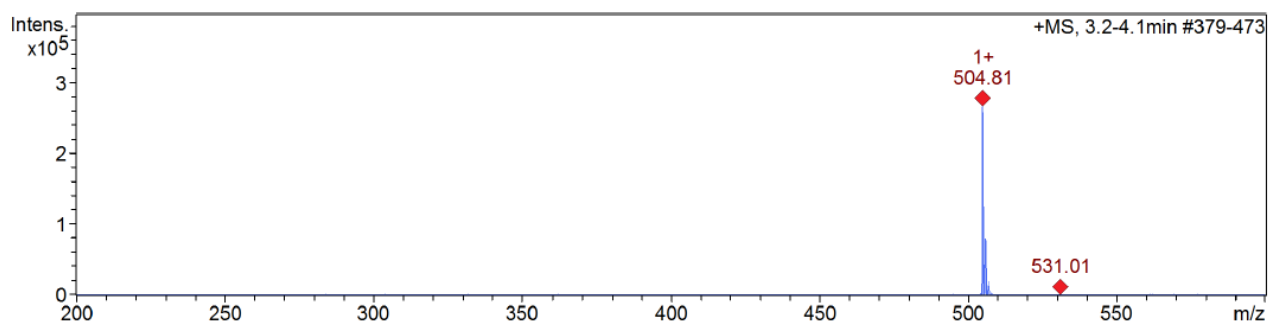


Fig. S31. ESI-MS spectrum of compound **3o**.

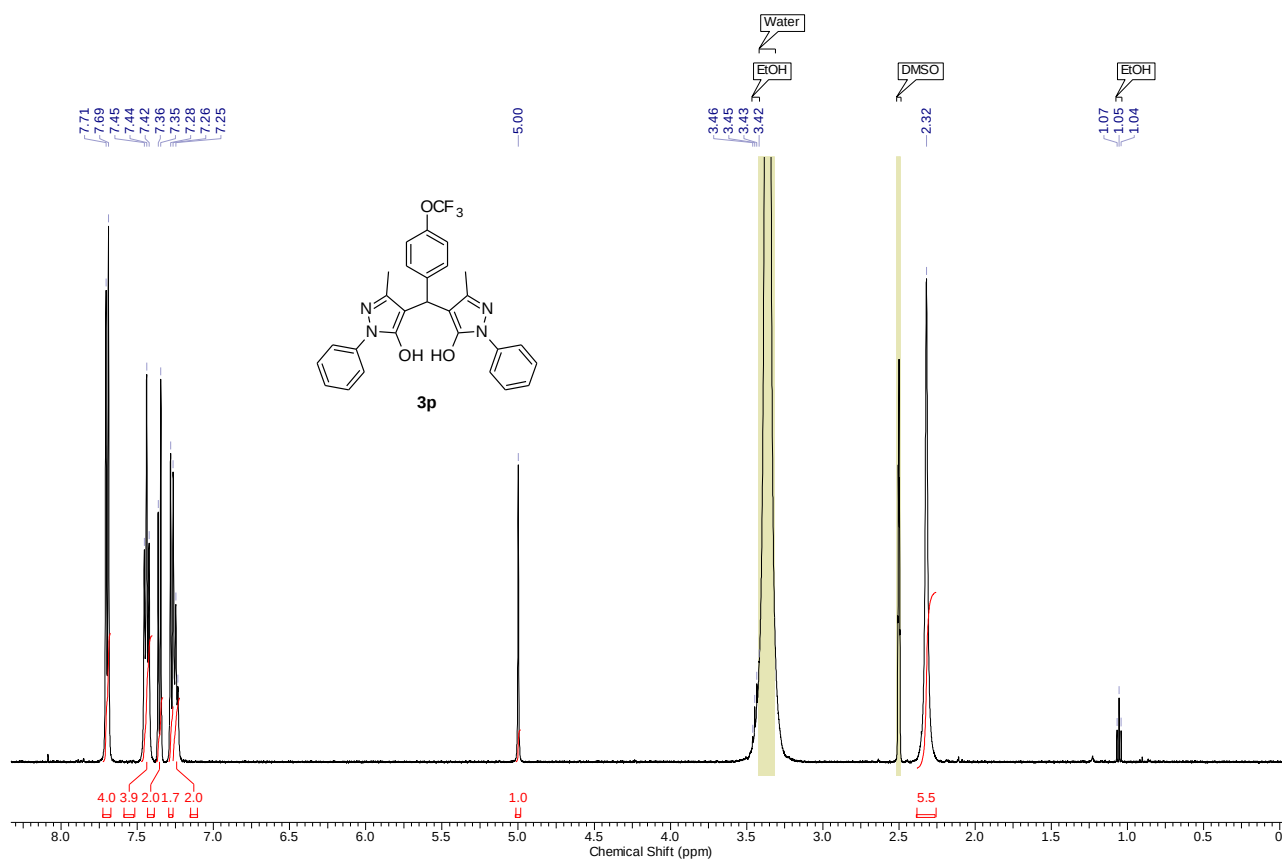


Fig. S32. ^1H NMR spectrum of compound **3p**.

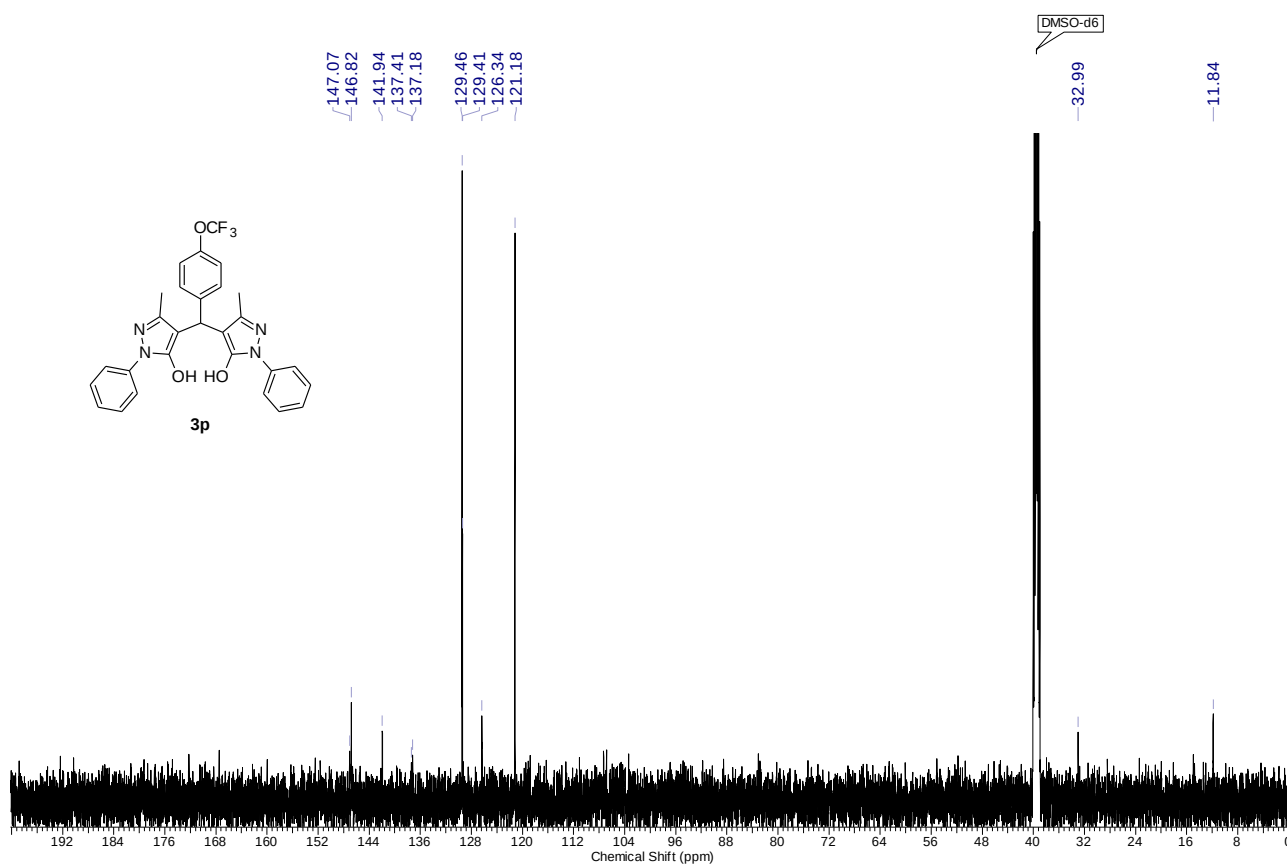


Fig. S33. ^{13}C NMR spectrum of compound **3p**.

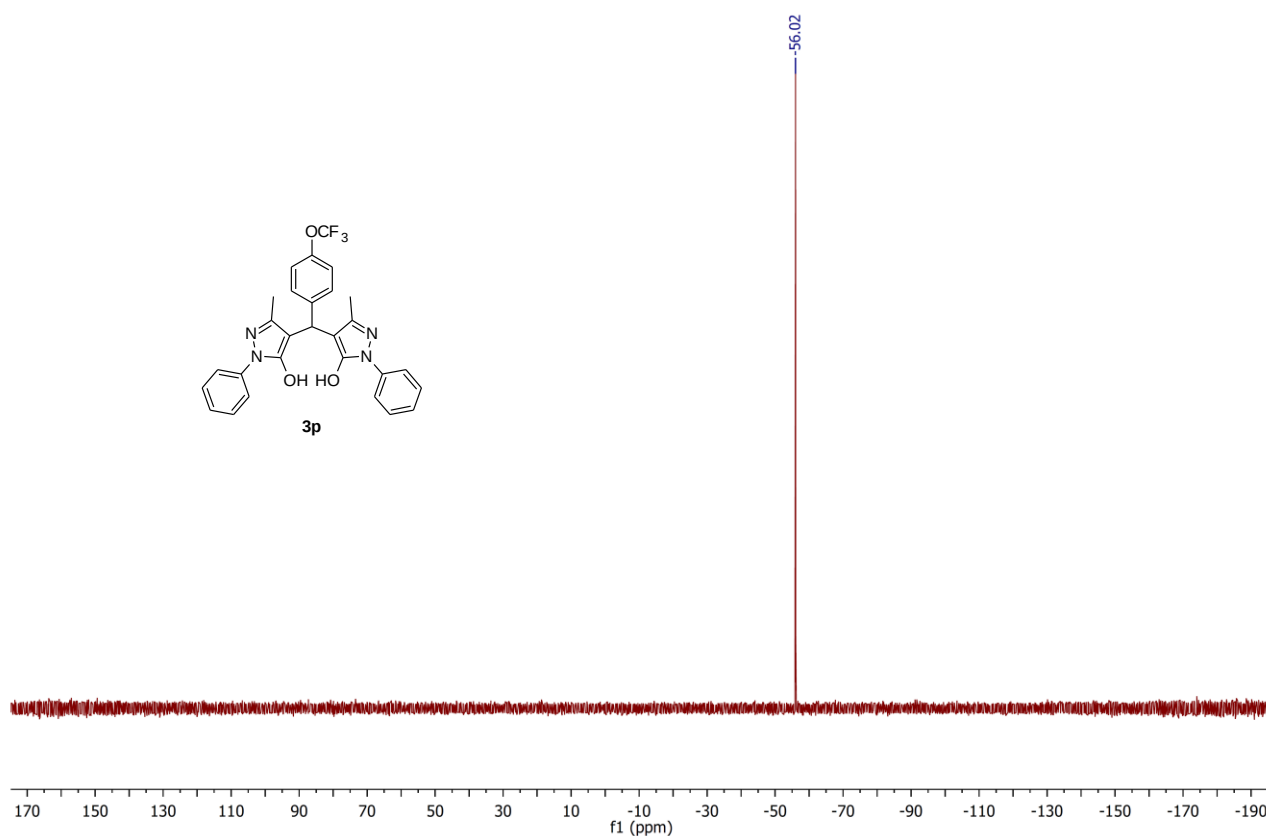


Fig. S34. ^{19}F NMR spectrum of compound **3p**.

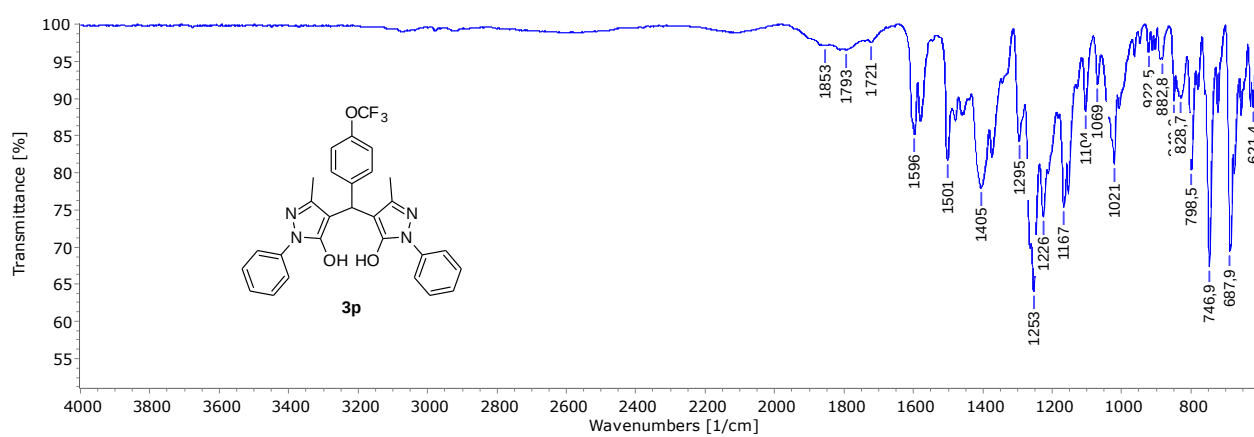


Fig. S35. FTIR spectrum of compound **3p**.



Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	UltraScan	Scan Begin	200 m/z	Scan End	600 m/z
Accumulation Time	1209 μ s	RF Level	63 %	Trap Drive	54.1
SPS Target Mass	400 m/z	Averages	5 Spectra	n/a	n/a

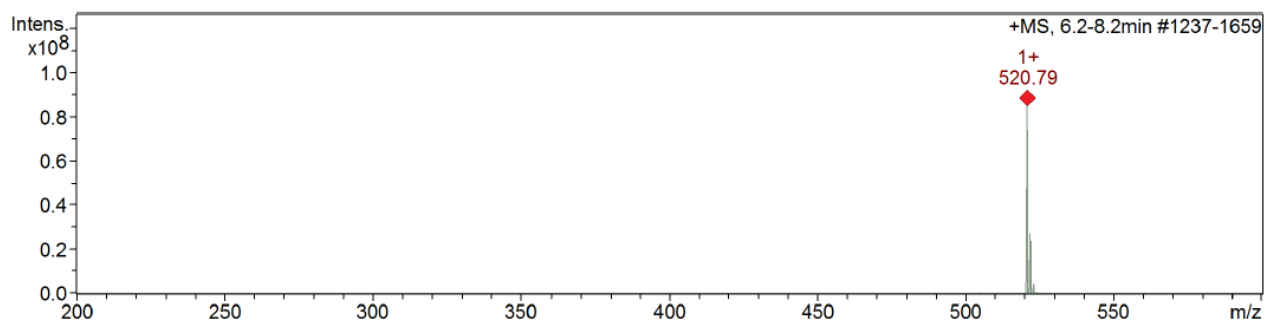


Fig. S36. ESI-MS spectrum of compound **3p**.

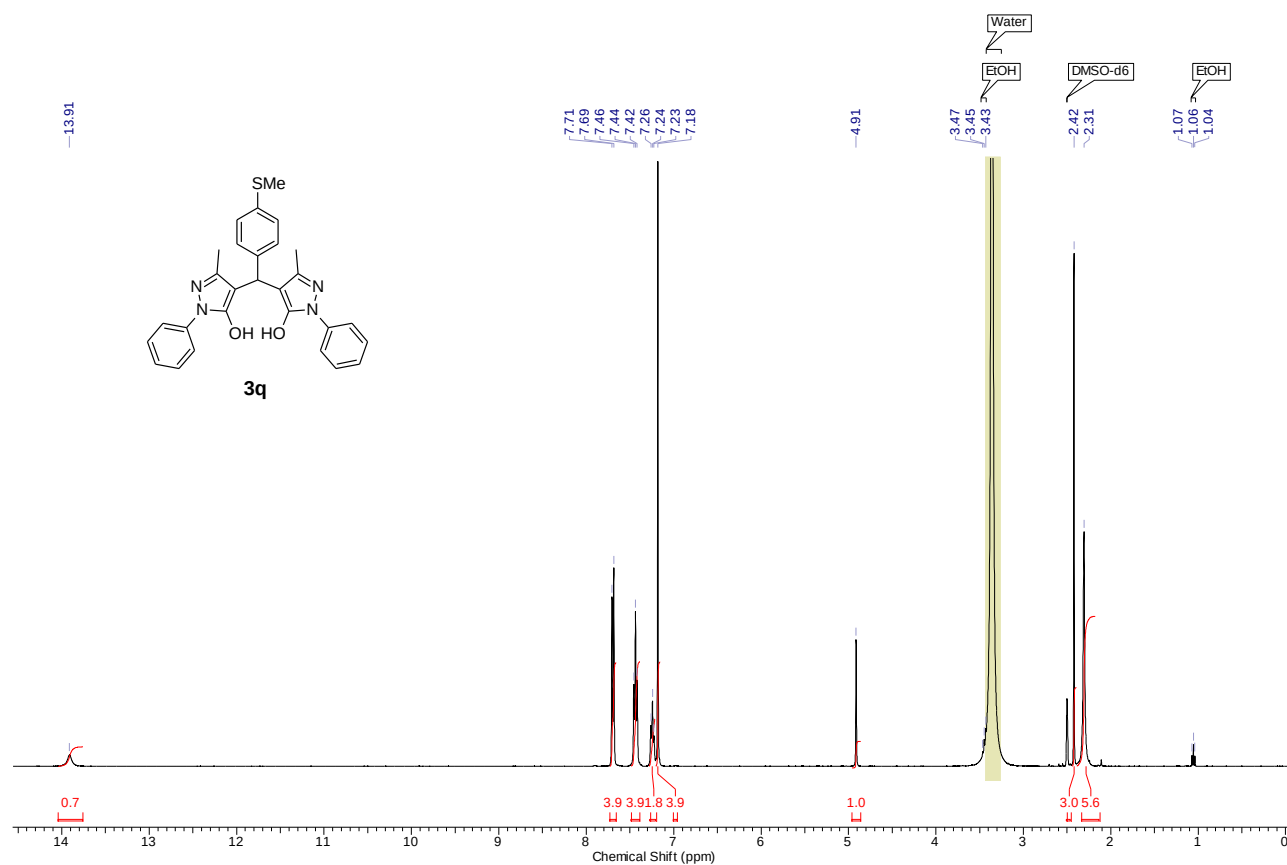


Fig. S37. ¹H NMR spectrum of compound **3q**.