

Supporting Information for

One-pot CuI/DBU-catalyzed Carboxylative Cyclization Toward Oxazolidinones Using Recyclable Molecular Sieves as Efficient Promotor for Fixation of CO₂ in Water Medium

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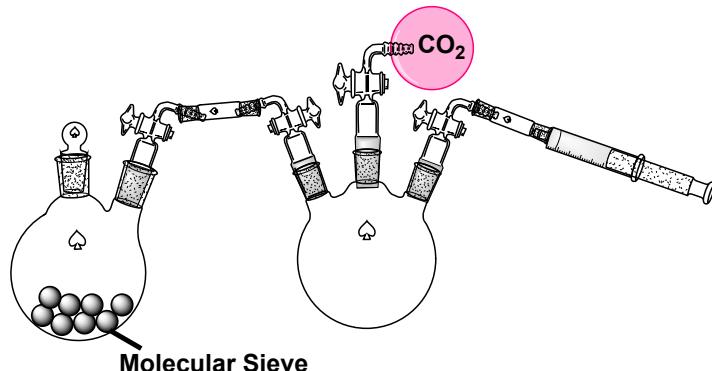
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1. The Measurement of CO₂ absorption by MS

(a) The set-up of measurement.



Entry	Sample	Conditions ^a	ΔV (mL) ^b
1	Only H ₂ O	193 mL H ₂ O for 5 h	0.5
2	MS/H ₂ O	30.0 g of MS + 193 mL H ₂ O for 5 h	4.5
3	MS/H ₂ O/DBU	30.0 g of MS + 193 mL H ₂ O + 15 mol% DBU for 5 h	5.8

^a H₂O was degassed by N₂ for 10 mins and concentration of conditions were same as standard condition; ^b the V(volume) of CO₂ absorbed was read from the change of 10 mL syringe. The syringe was filled with CO₂ and reached equilibrium in the beginning.

(b)

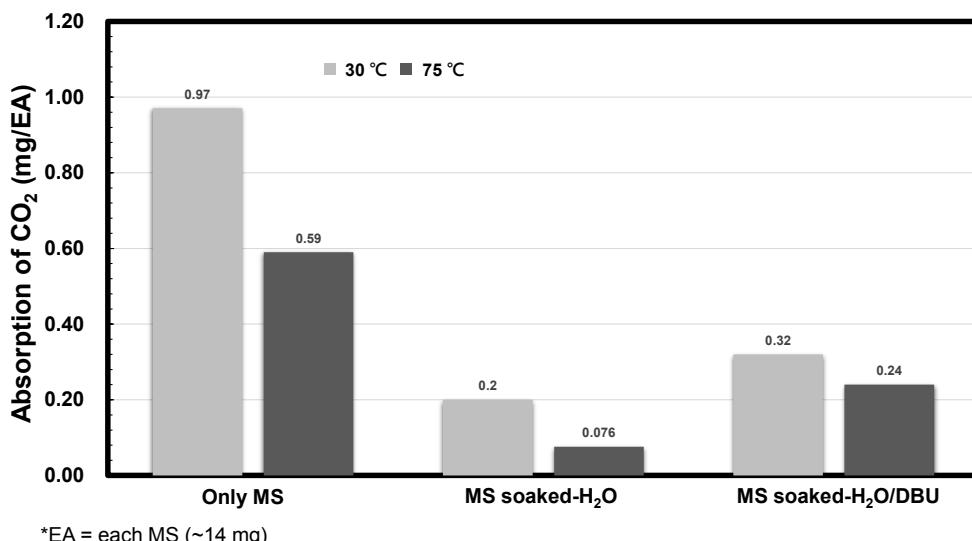


Figure S1. (a) The Measurement of CO₂ Absorption of H₂O, MS/H₂O, MS/H₂O/DBU under 1 Atm of CO₂; (b) The Weight Increase of MS Samples Measured by a Sorption Analyzer.

1. ^1H and ^{13}C NMR Spectra for Compound 5.

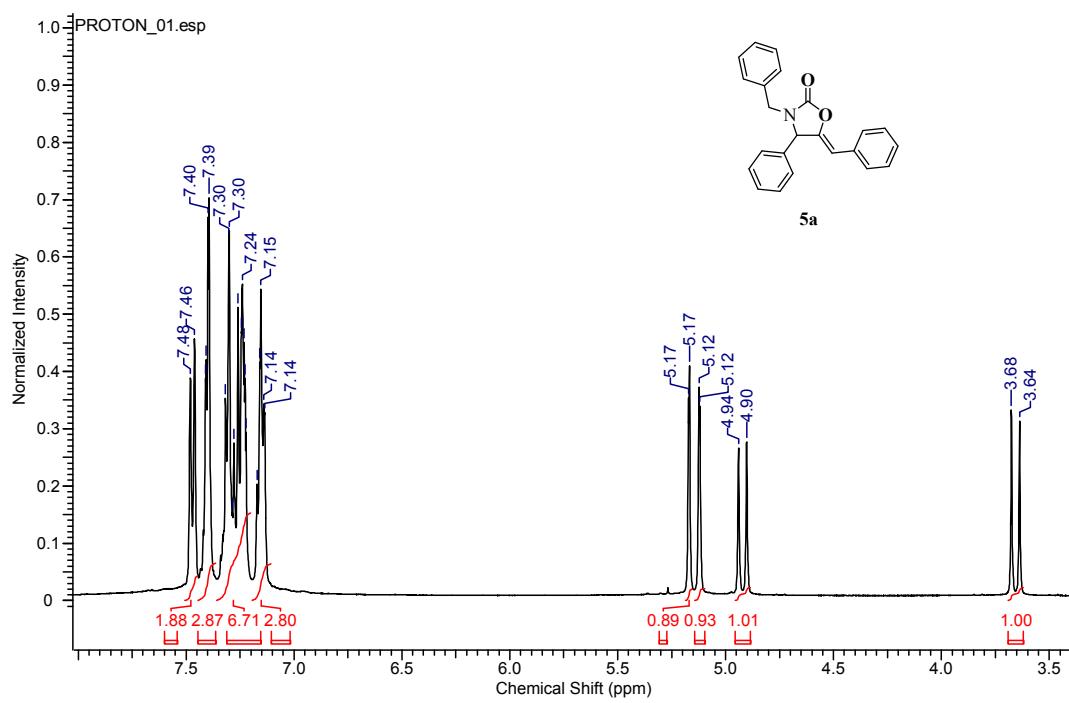


Figure S2. ^1H NMR (400 MHz, CDCl_3) of Compound 5a.

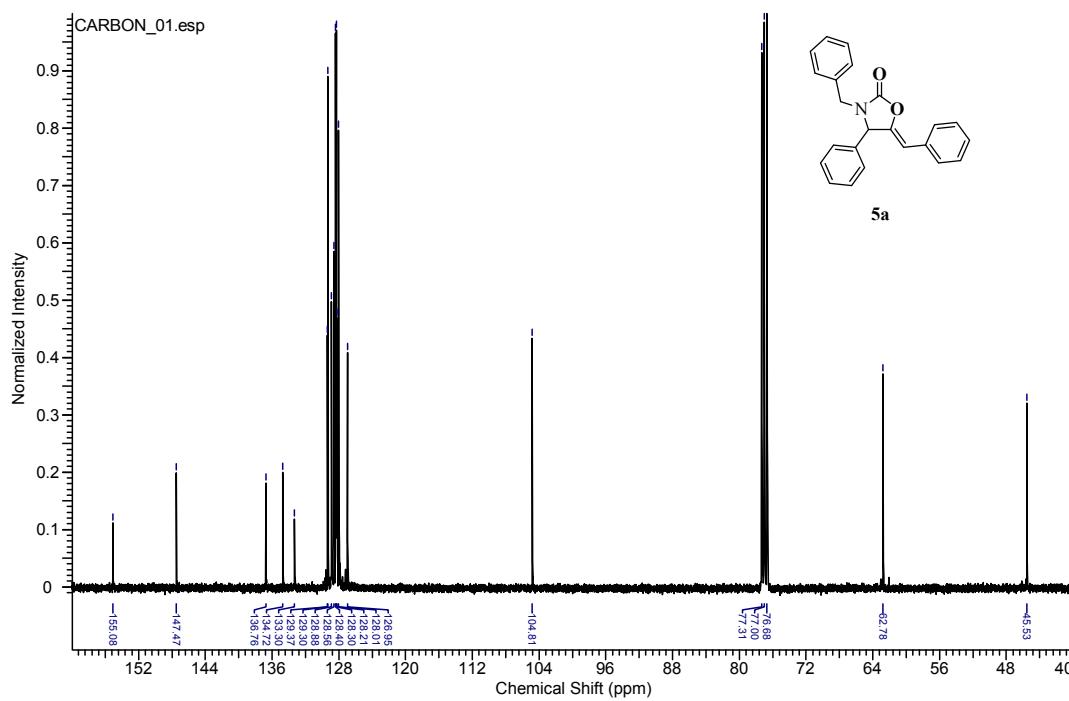


Figure S3. ^{13}C NMR (100 MHz, CDCl_3) of Compound 5a.

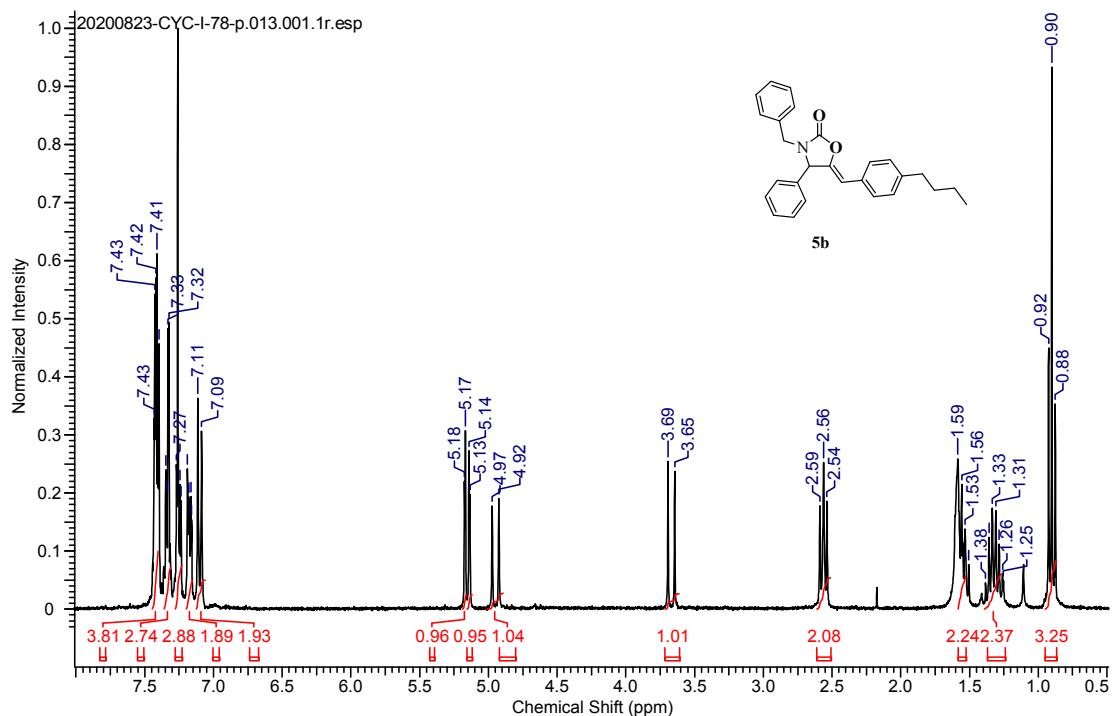


Figure S4. ^1H NMR (400 MHz, CDCl_3) of Compound 5b.

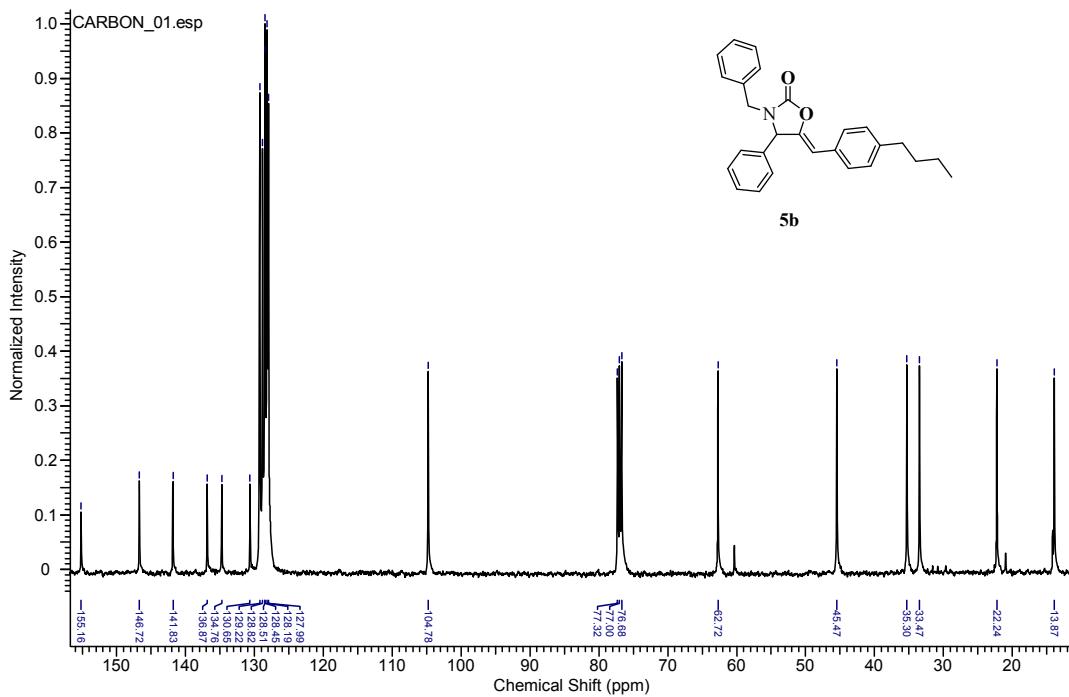


Figure S5. ^{13}C NMR (100 MHz, CDCl_3) of Compound 5b.

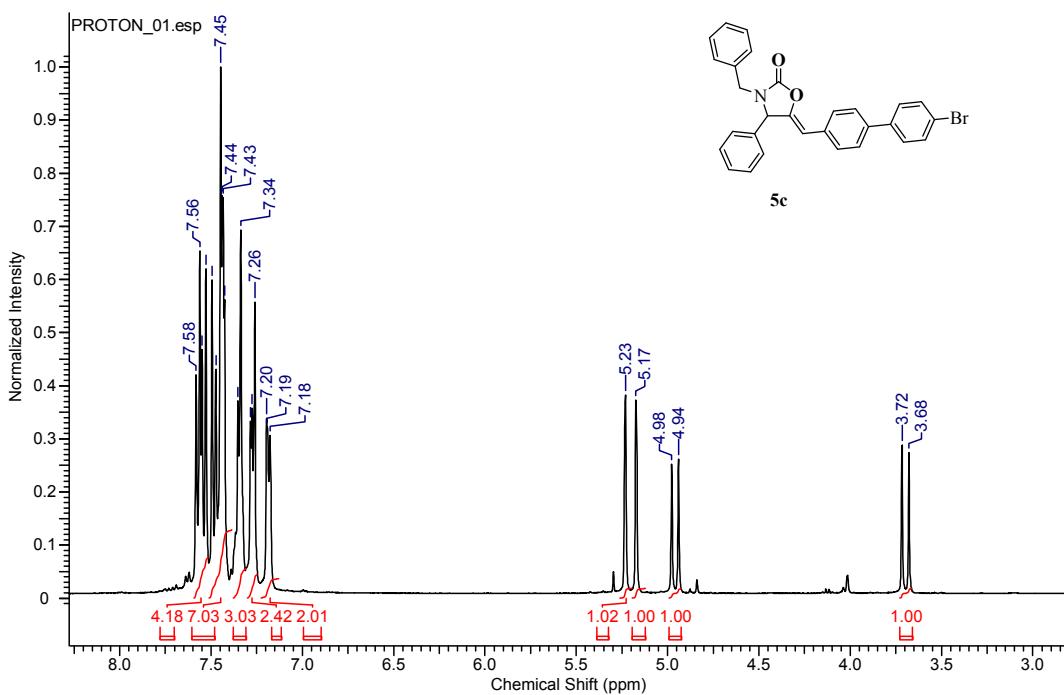


Figure S6. ^1H NMR (400 MHz, CDCl_3) of Compound 5c.

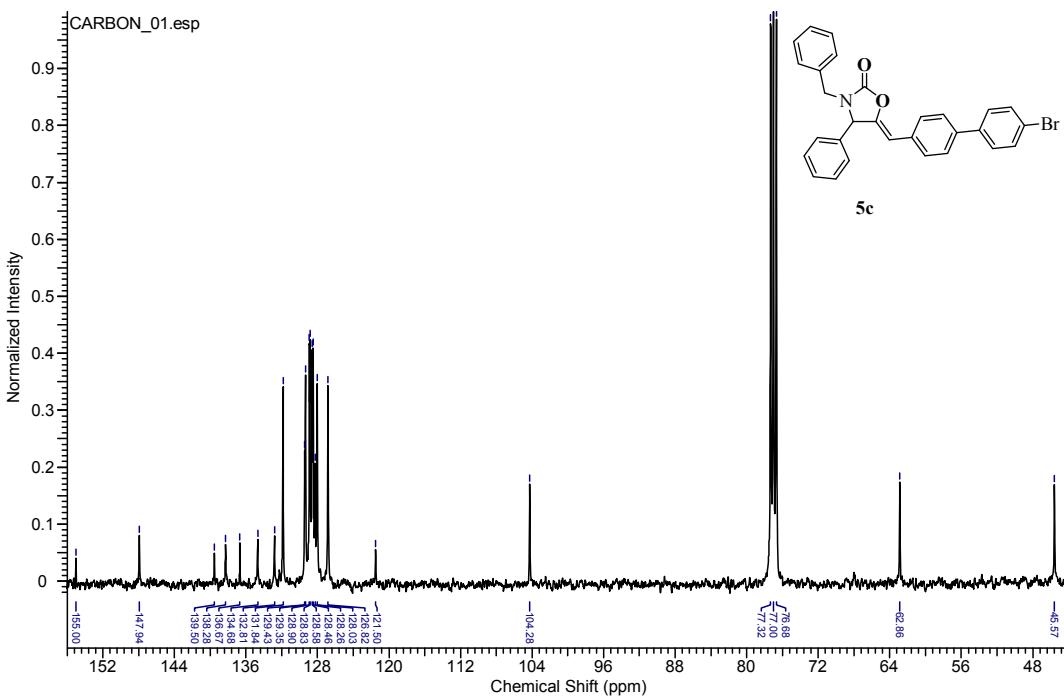


Figure S7. ^{13}C NMR (100 MHz, CDCl_3) of Compound 5c.

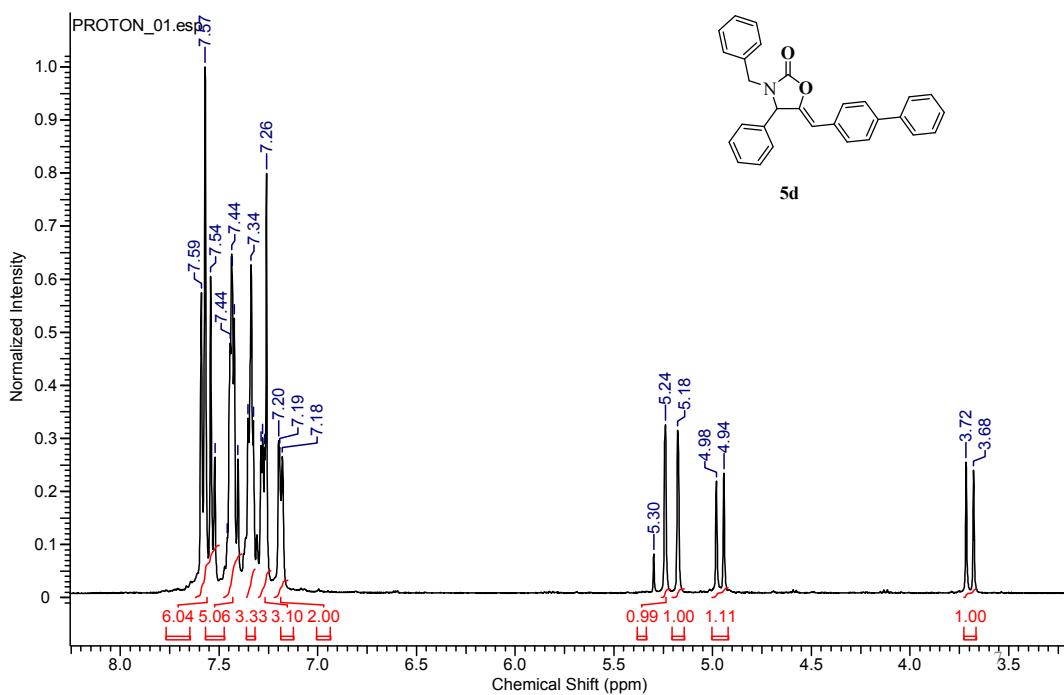


Figure S8. ^1H NMR (400 MHz, CDCl_3) of Compound 5d.

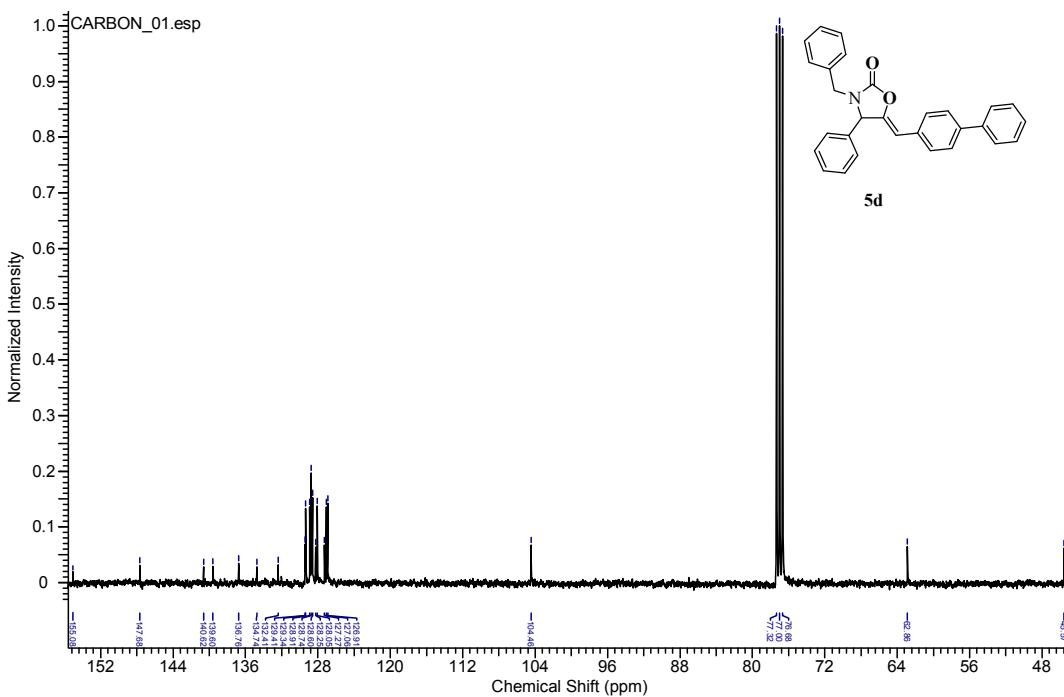


Figure S9. ^{13}C NMR (100 MHz, CDCl_3) of Compound 5d.

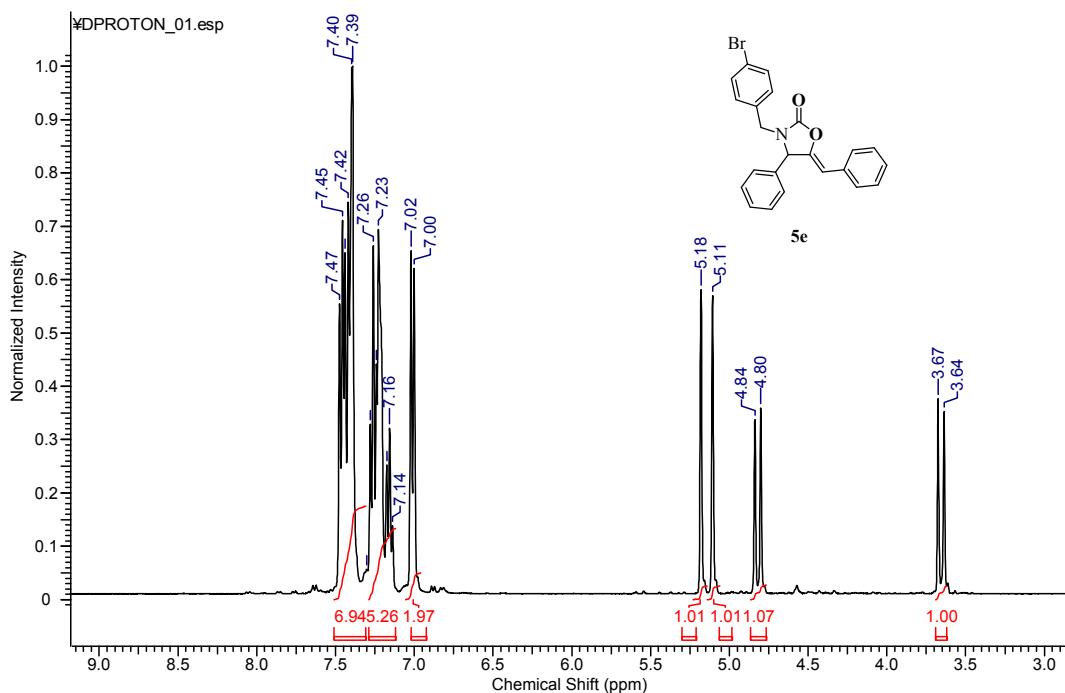


Figure S10. ^1H NMR (400 MHz, CDCl_3) of Compound 5e.

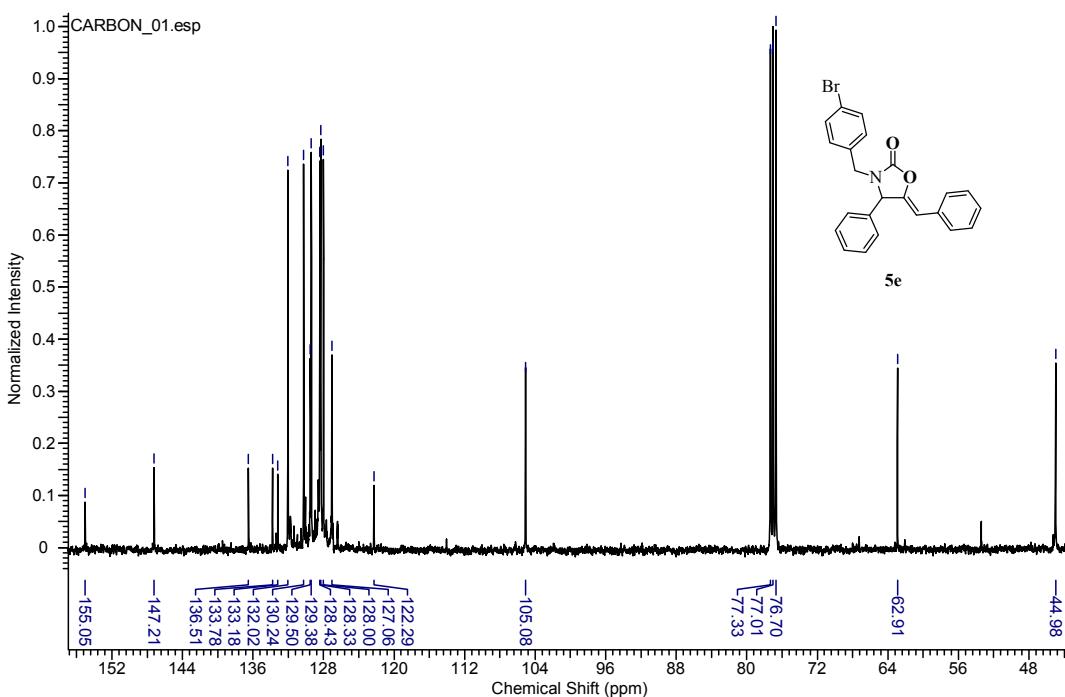


Figure S11. ^{13}C NMR (100 MHz, CDCl_3) of Compound 5e.

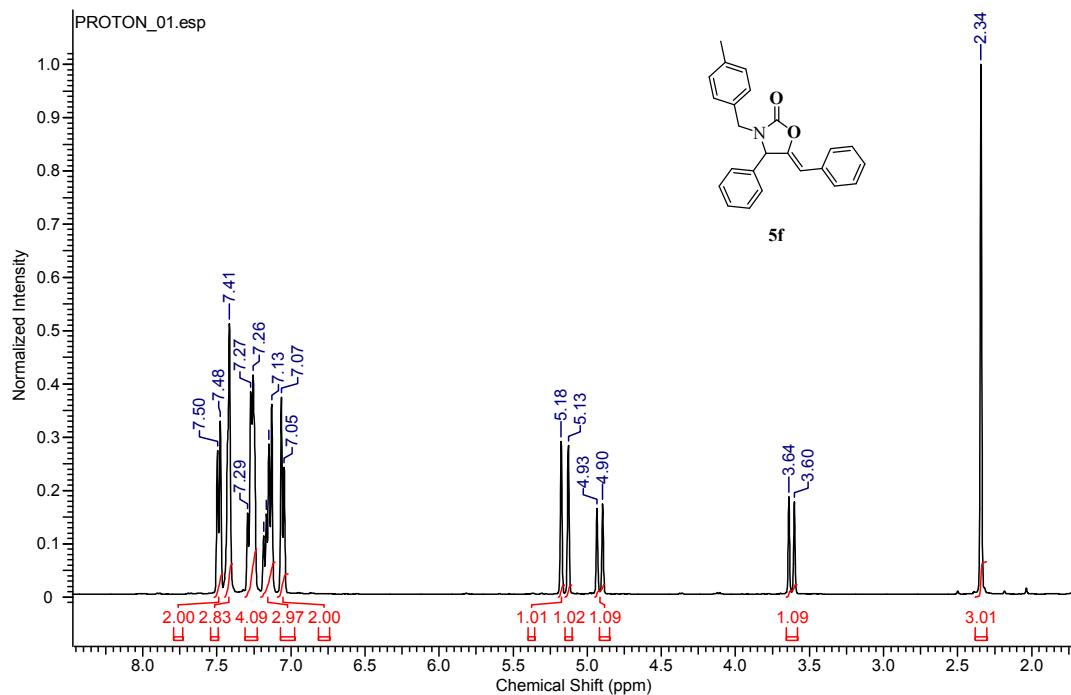


Figure S12. ^1H NMR (400 MHz, CDCl_3) of Compound 5f.

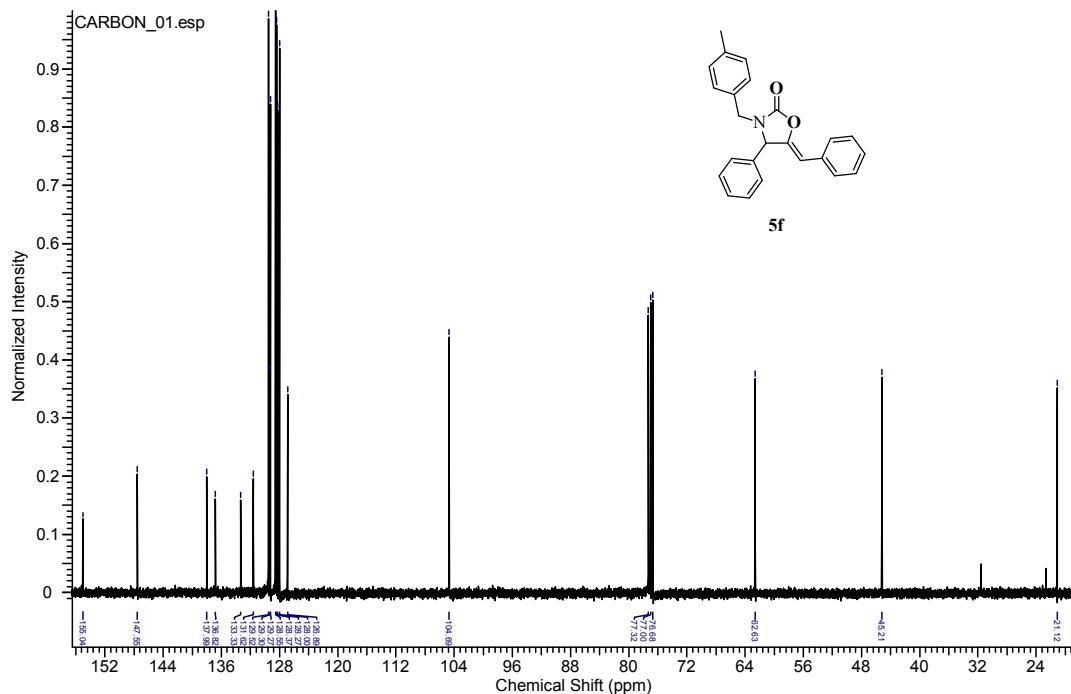


Figure S13. ^{13}C NMR (100 MHz, CDCl_3) of Compound 5f.

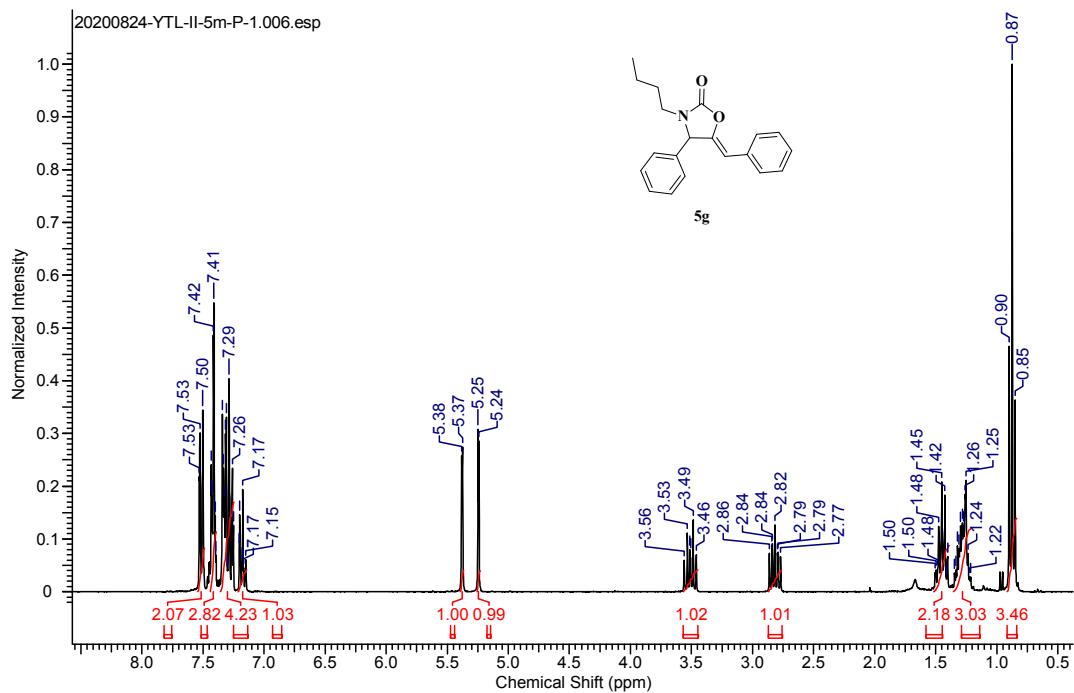


Figure S14. ^1H NMR (300 MHz, CDCl_3) of Compound **5g**.

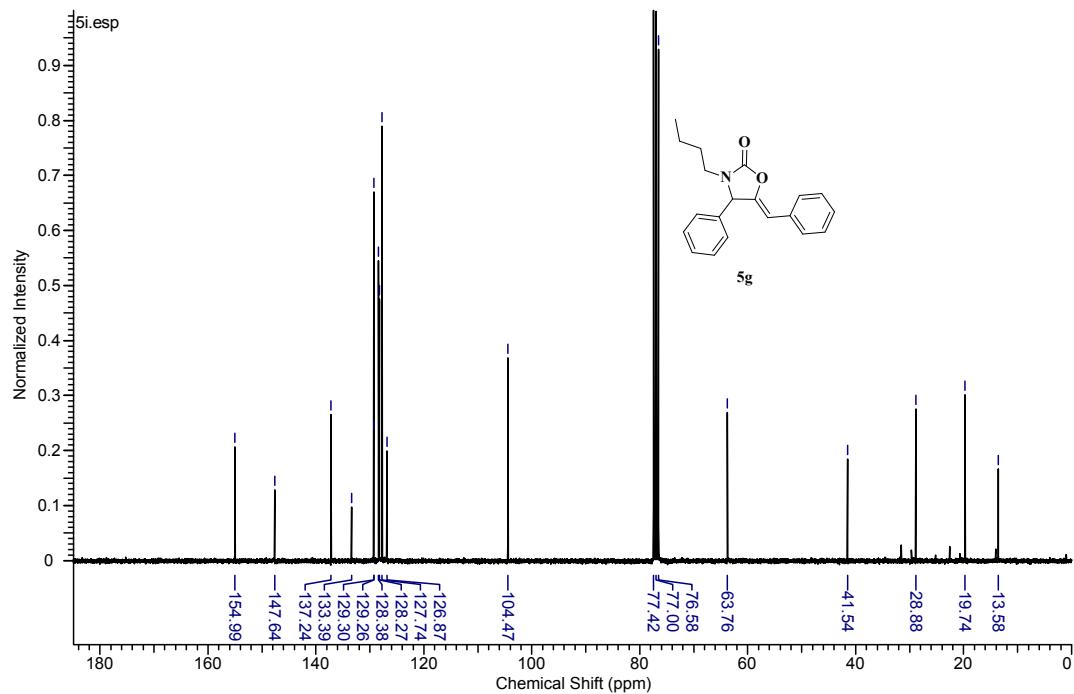


Figure S15. ^{13}C NMR (75 MHz, CDCl_3) of Compound **5g**.

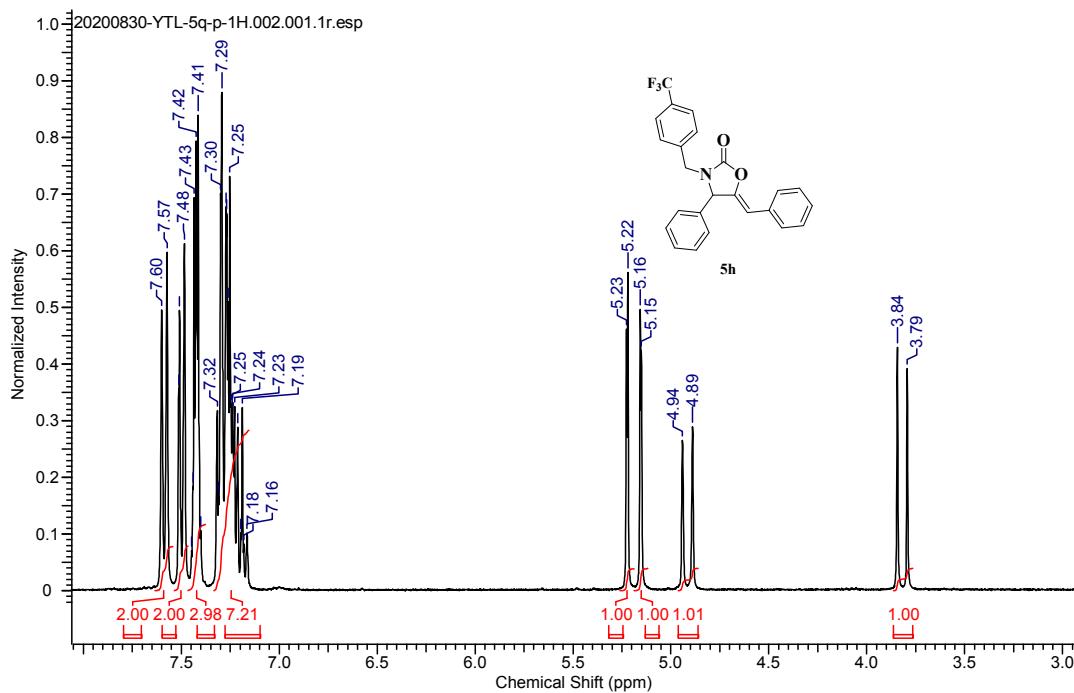


Figure S16. ^1H NMR (300 MHz, CDCl_3) of Compound 5h.

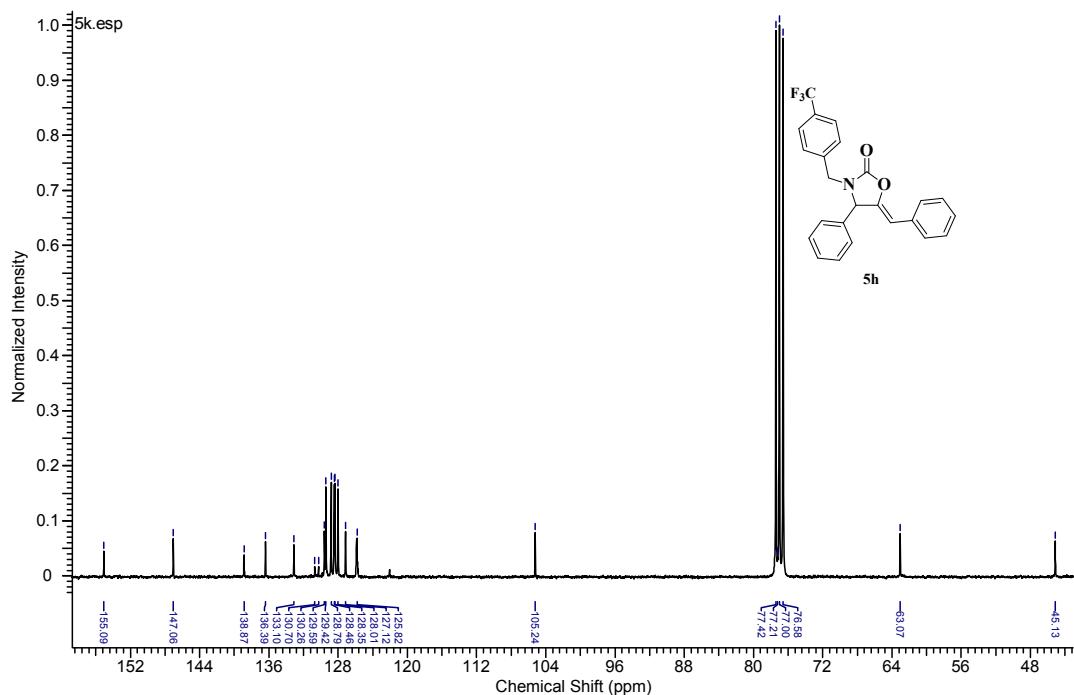


Figure S17. ^{13}C NMR (75 MHz, CDCl_3) of Compound 5h.

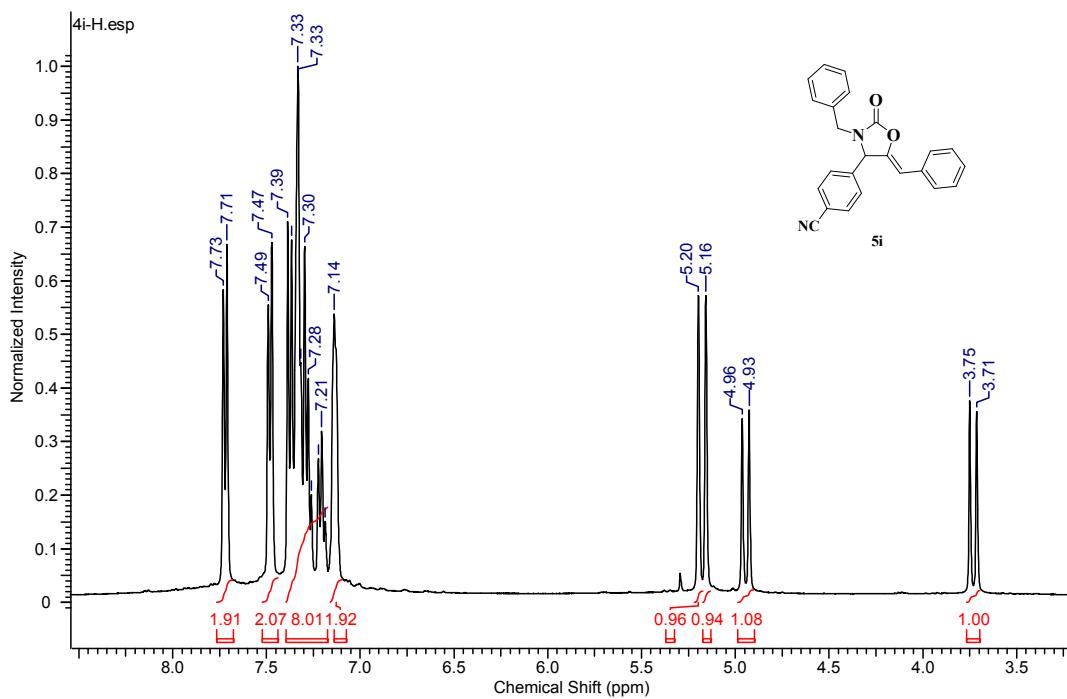


Figure S18. ^1H NMR (400 MHz, CDCl_3) of Compound 5i.

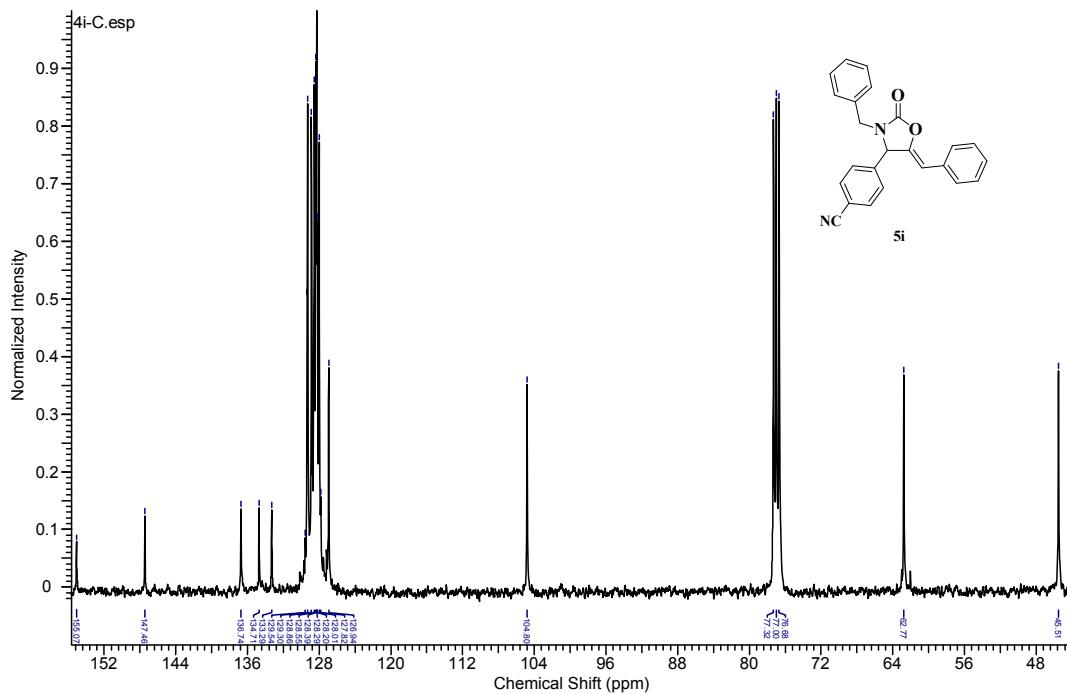


Figure S19. ^{13}C NMR (100 MHz, CDCl_3) of Compound 5i.

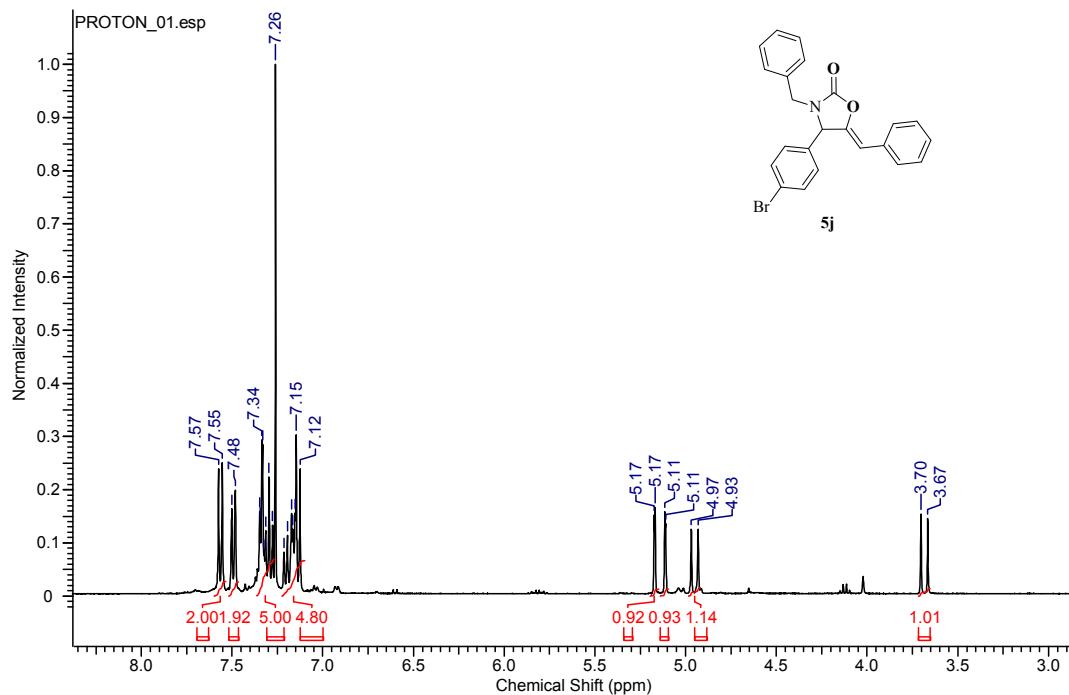


Figure S20. ^1H NMR (400 MHz, CDCl_3) of compound 5j.

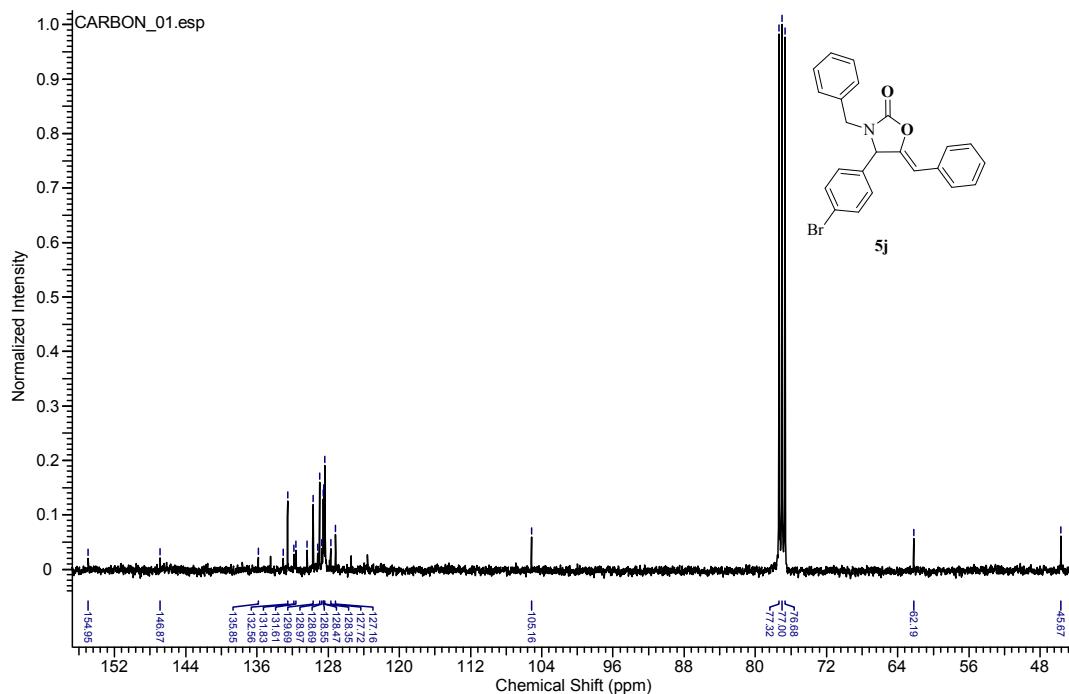


Figure S21. ^{13}C NMR (100 MHz, CDCl_3) of compound 5j.

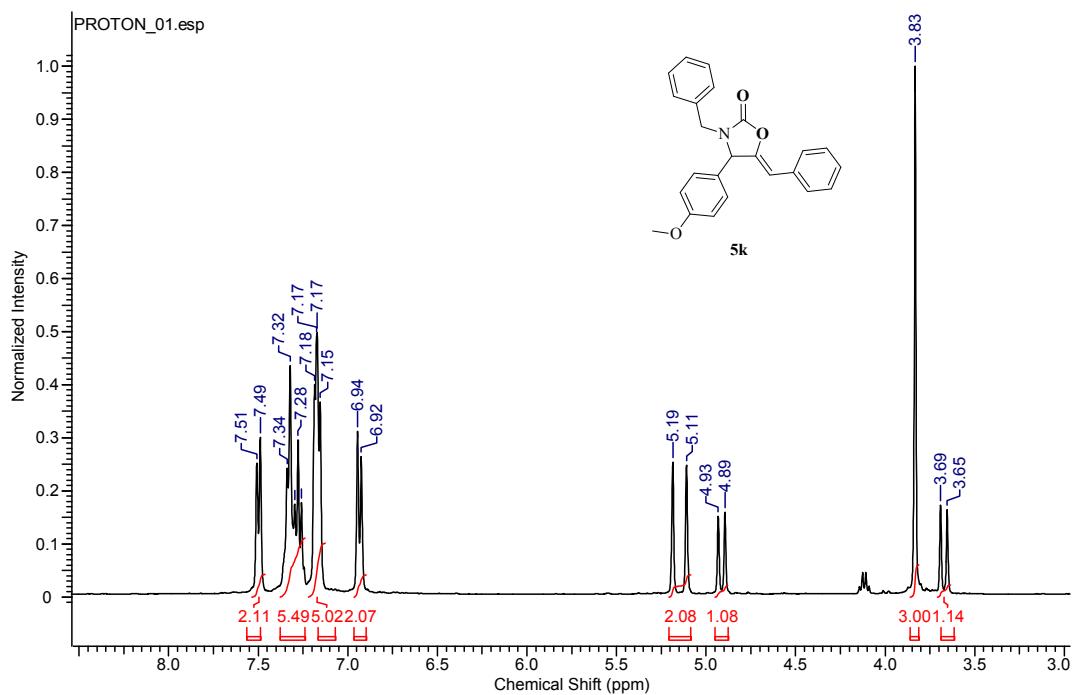


Figure S22. ^1H NMR (400 MHz, CDCl_3) of Compound 5k.

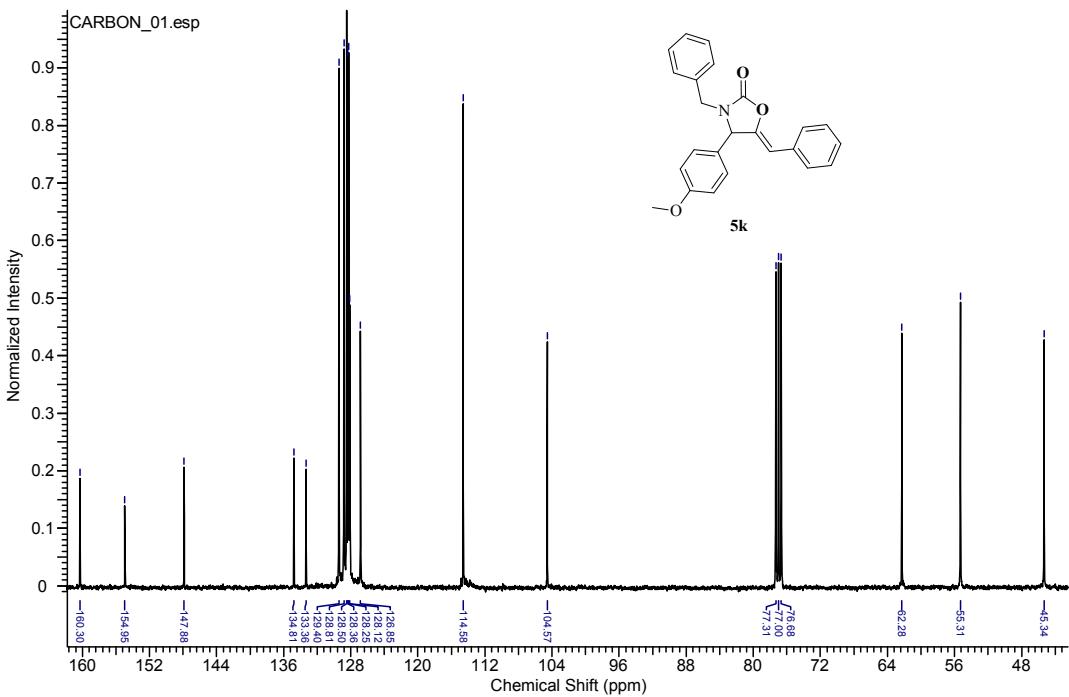


Figure S23. ^{13}C NMR (100 MHz, CDCl_3) of Compound 5k.

2. Mass Spectra for Compound 5.

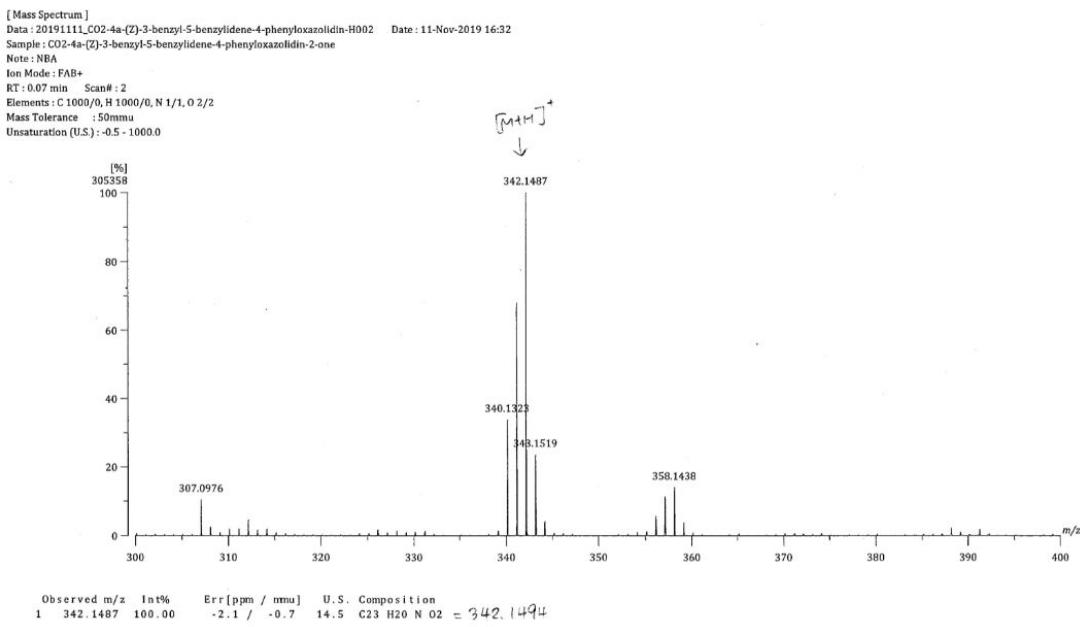


Figure S24. The Mass Spectrum of Compound 5a.

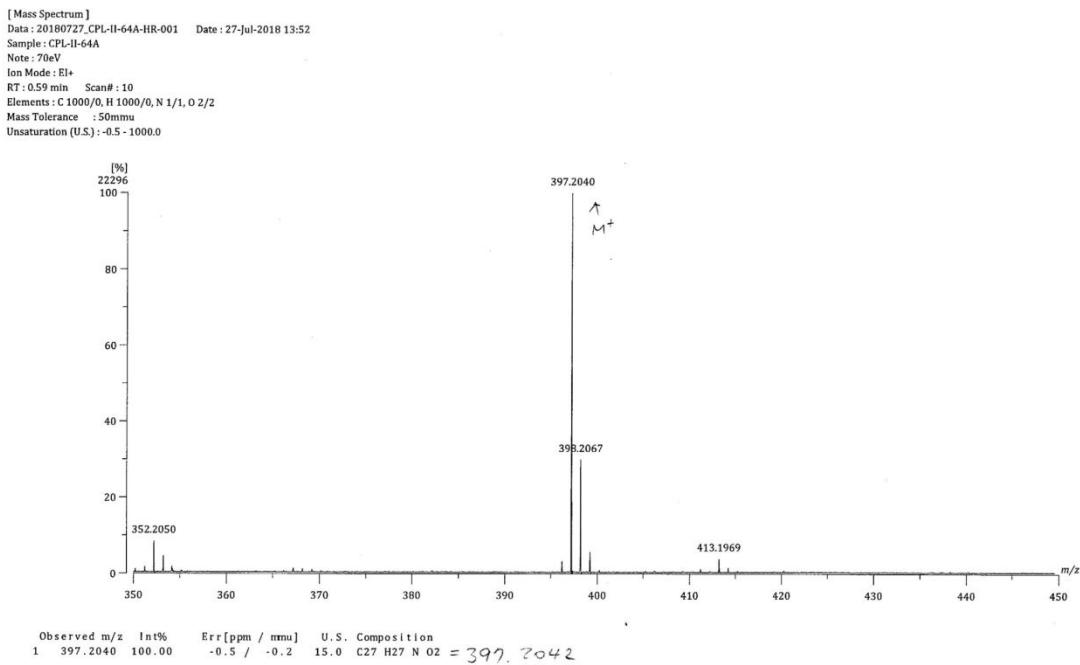


Figure S25. The Mass Spectrum of Compound 5b.

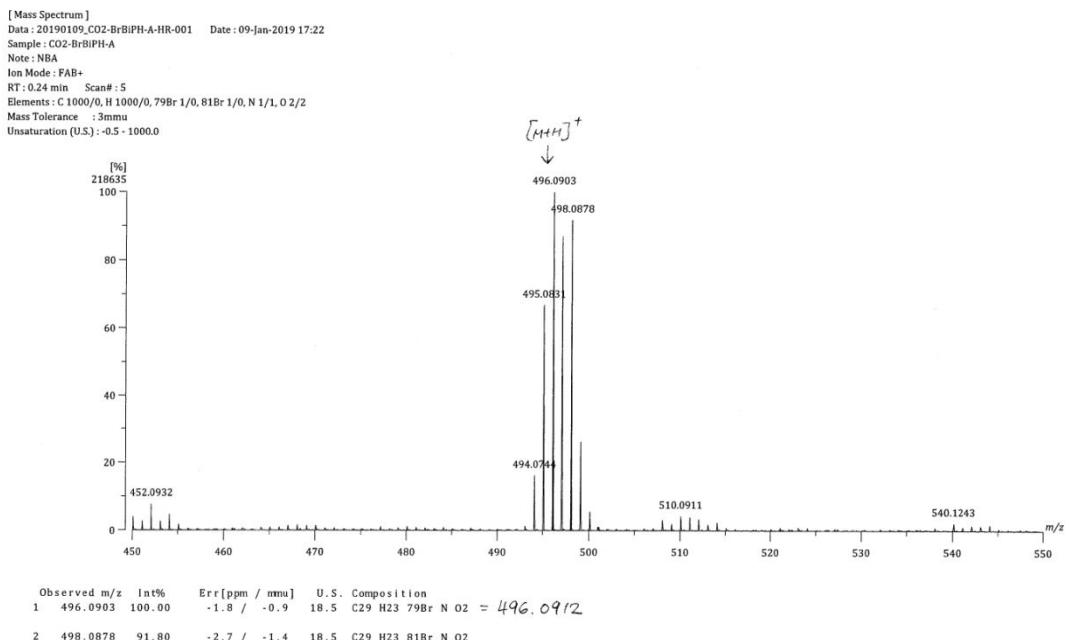


Figure S26. The Mass Spectrum of Compound 5c.

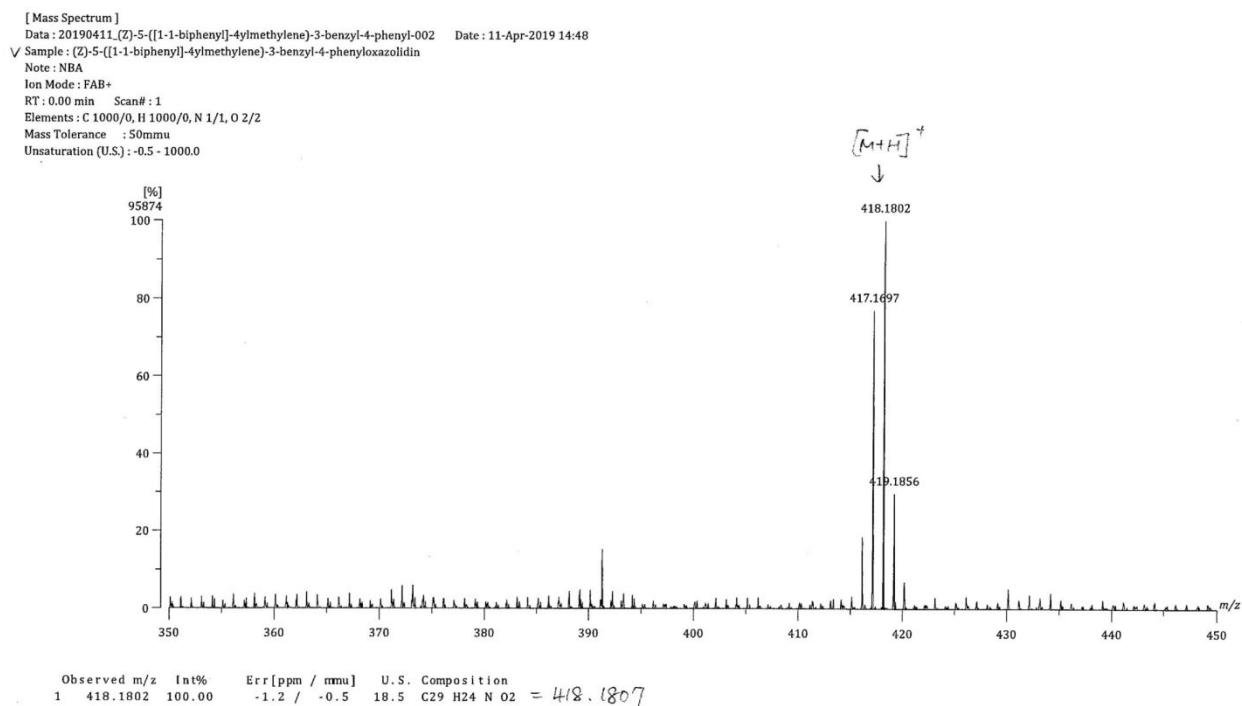


Figure S27. The Mass Spectrum of Compound 5d.

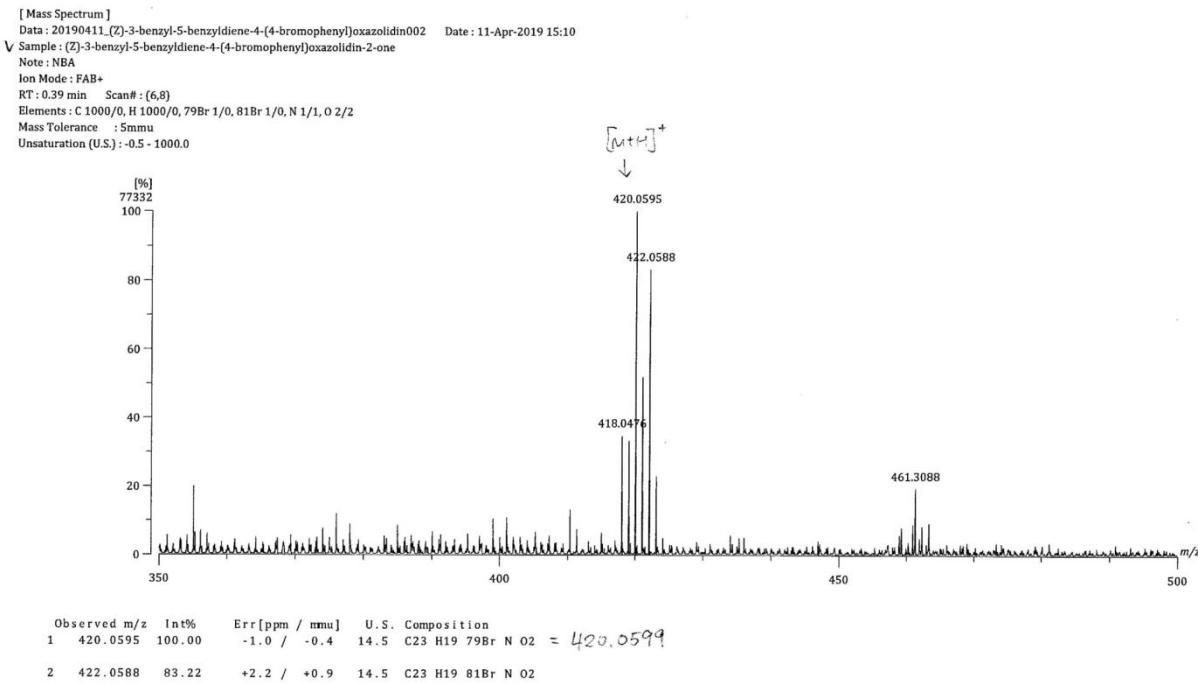


Figure S28. The Mass Spectrum of Compound 5e.

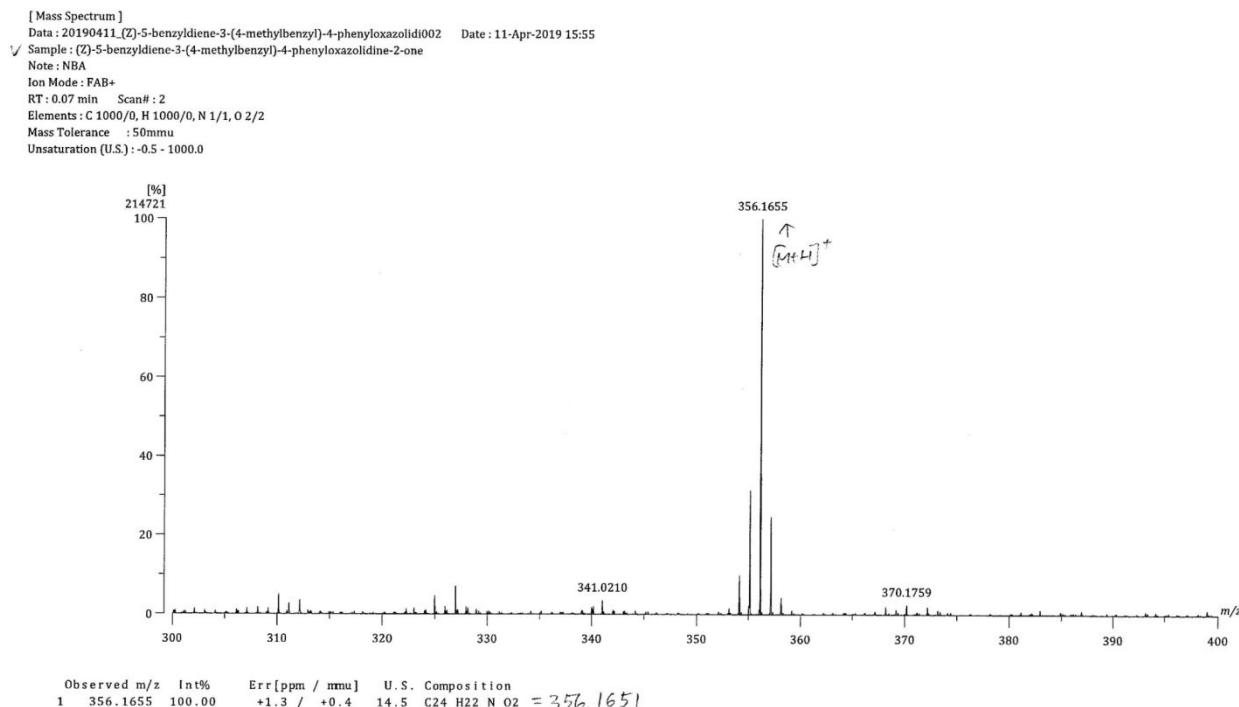
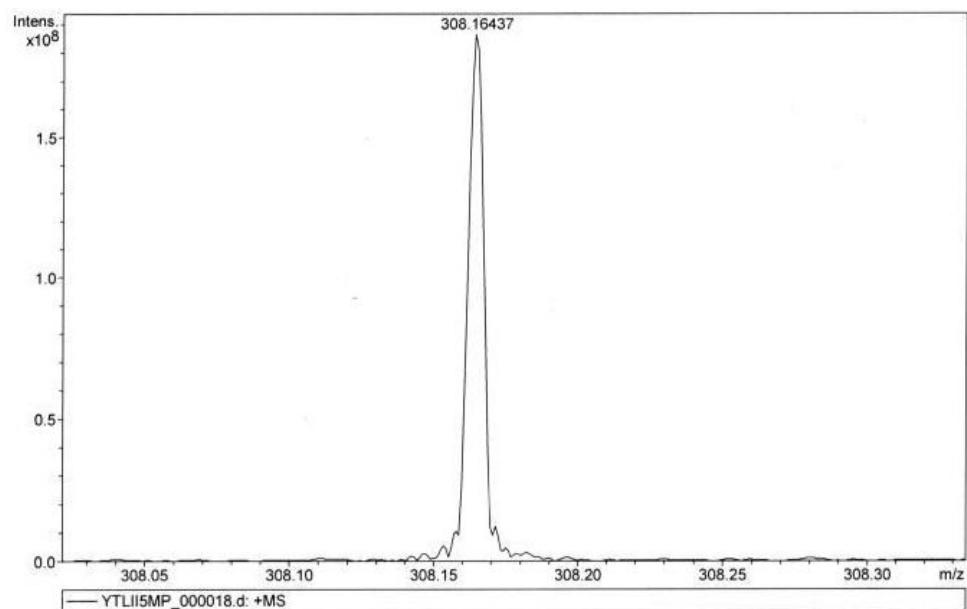
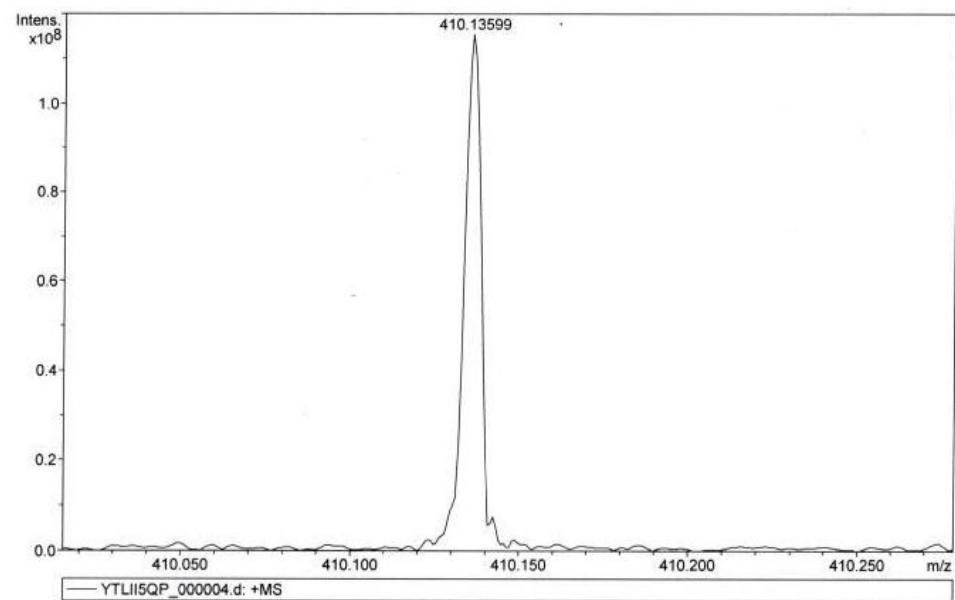


Figure S29. The Mass Spectrum of Compound 5f.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	N-Rule
308.16437	1	C ₂₀ H ₂₂ N ₂ O ₂	100.00	308.16451	0.14	0.44	6.8	10.5	even	ok

Figure S30. The Mass Spectrum of Compound 5g.



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e^- Conf	N-Rule
410.13599	1	C ₂₄ H ₁₉ F ₃ N ₂ O ₂	100.00	410.13624	0.25	0.60	4.5	14.5	even	ok

Figure S31. The Mass Spectrum of Compound 5h.

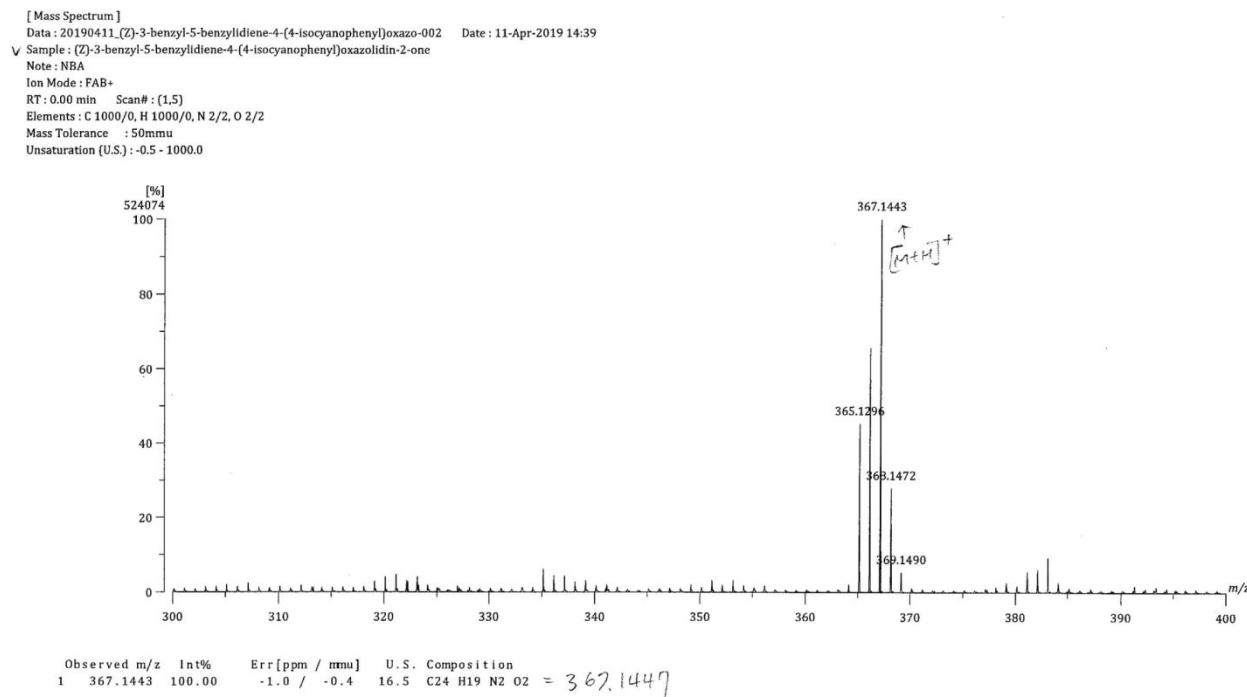


Figure S32. The Mass Spectrum of Compound 5i.

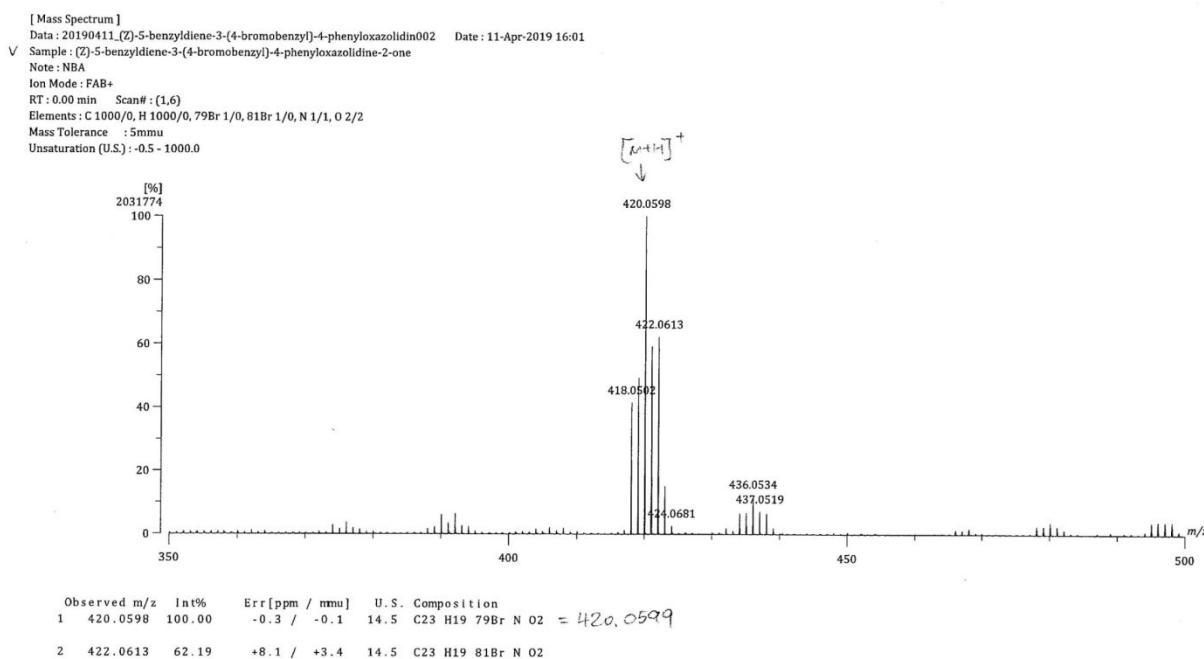


Figure S33. The Mass Spectrum of Compound 5j.

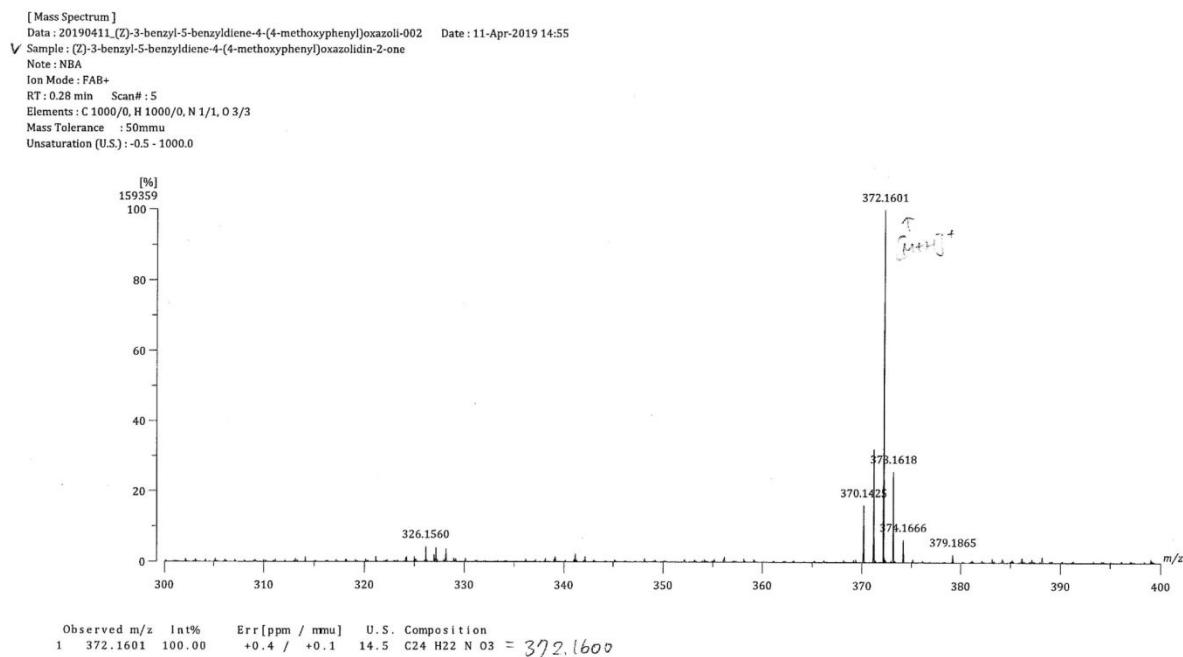


Figure S34. The Mass Spectrum of Compound 5k.

3. Single-crystal X-ray diffraction data of **5d** and **5k**

Crystals of **5d** and **5k** were grown by slow evaporation of petroleum ether/ethyl acetate and petroleum ether/ethyl acetate solutions at room temperature (30 °C) respectively. Both X-ray diffraction data were collected on a Bruker Kappa Apex Duo diffractometer at 120 K and 100 K, respectively.

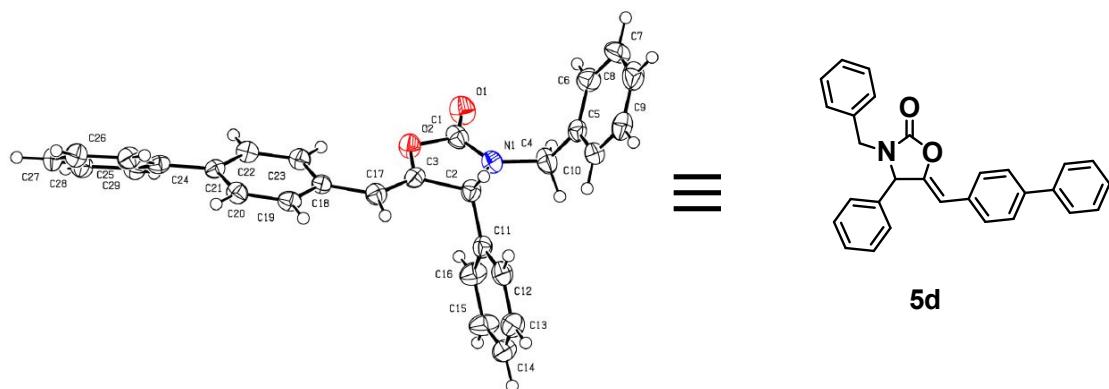


Figure S35. Crystal Structure of **5d** with Thermal Ellipsoids at 50% Probability.

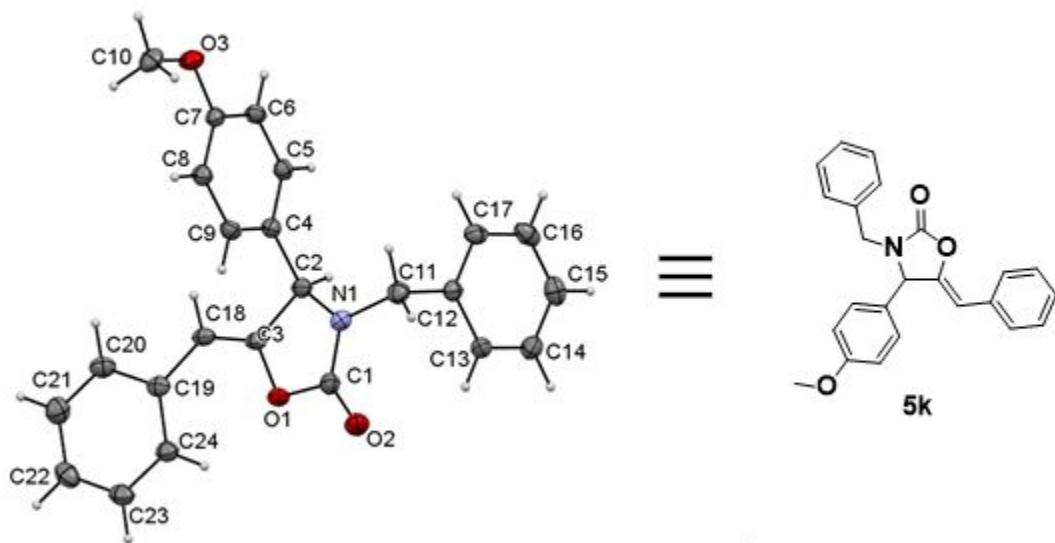


Figure S36. Crystal Structure of **5k** with Thermal Ellipsoids at 50% Probability.

Table S1. Crystal Data and Structure Refinement Parameters for the salts **5d and **5k**.**

	5d	5k
Empirical formula	C ₂₉ H ₂₃ NO ₂	C ₂₄ H ₂₁ NO ₃
Formula weight	417.48	371.42
Crystal system	Triclinic	Orthorhombic
T(K)	120.0 (2)	100.0 (2)
Space group	P-1	C222 ₁
a/Å	6.1618 (5)	13.4355 (4)
b/Å	8.7522 (6)	14.6914 (4)
c/Å	20.3805 (17)	19.5353 (6)
α(°)	88.042 (6)	90
β(°)	84.239 (7)	90
γ(°)	78.625 (6)	90
V/Å ³	1071.96 (15)	3856.0 (2)
Z	2	8
D _c /g cm ⁻³	1.283	1.280
μ/mm ⁻¹	0.081	0.676
θ/deg	3.014 to 27.498	4.459 to 72.386
Range <i>h</i>	-7 to 7	-16 to 16
Range <i>k</i>	-11 to 11	-18 to 18
Range <i>l</i>	-26 to 26	-23 to 24
Ref. collected	10408	44258
Ref. unique	5180	3825
Data/restraints/parameters	5180/0/290	3825/0/254
<i>R</i> _I ^a , <i>wR</i> ₂ ^b [I > 2σ(I)]	0.0564, 0.1379	0.0256, 0.0662
<i>R</i> _I ^a , <i>wR</i> ₂ ^b (all data)	0.1434, 0.1547	0.0262, 0.0667
GOF	1.009	1.093
CCDC number		

$$^a R_I = \Sigma(|F_o| - |F_c|)/\Sigma |F_o|; ^b wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$$