

Supplementary Information

Synthesis of 1,2,4-oxadiazoles utilizing ethyl 2-cyano-2-(2-nitrophenylsulfonyloxyimino) acetate (*ortho*-nosylOXY) as a catalyst and dehydrating reagent under microwave irradiation

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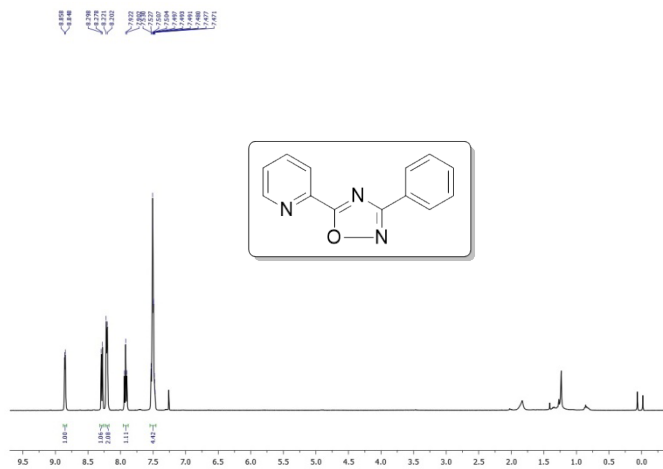


Fig. S1 — ¹H NMR spectrum of compound 3a

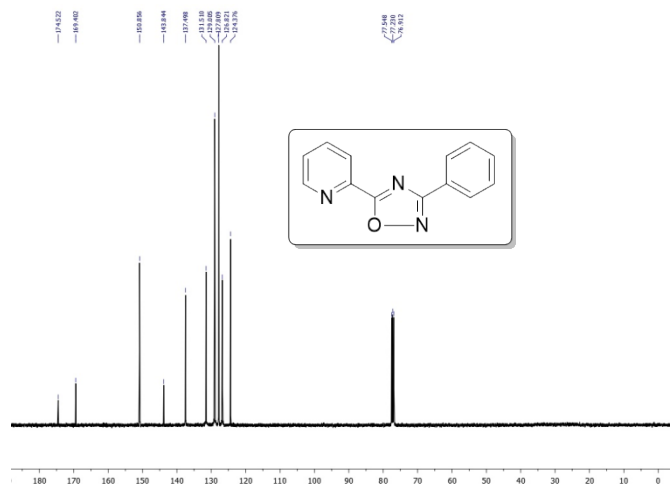


Fig. S2 — ¹³C NMR spectrum of compound 3a

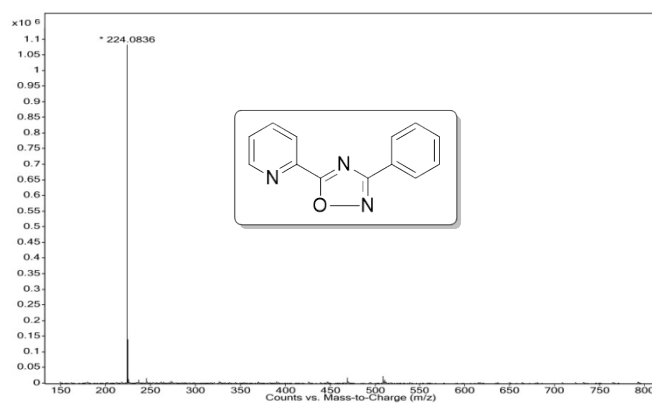


Fig. S3 — Mass spectrum of compound 3a

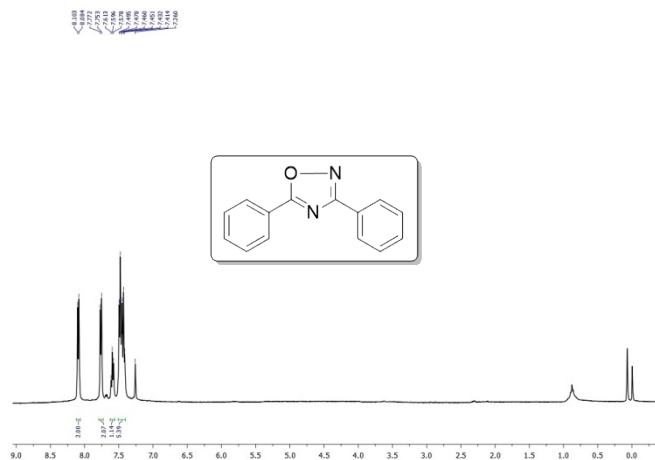


Fig. S4 — $^1\text{H NMR}$ spectrum of compound 3b

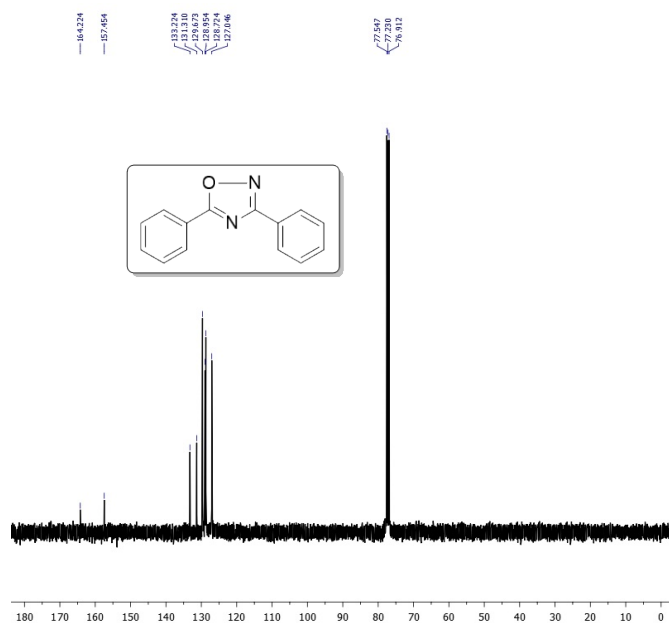


Fig. S5 — $^{13}\text{C NMR}$ spectrum of compound 3b

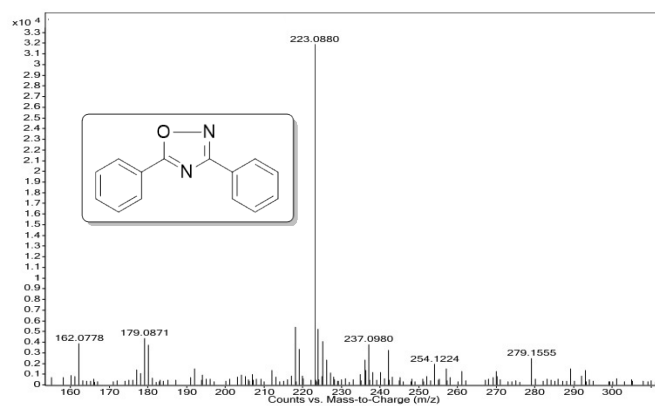


Fig. S6 — Mass spectrum of compound 3b

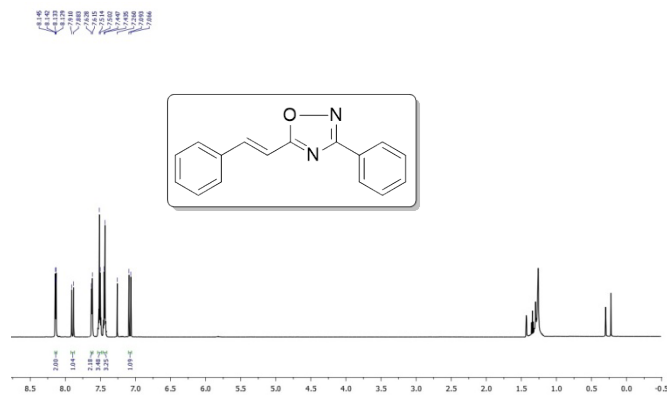


Fig. S7 — ¹H NMR spectrum of compound 3c

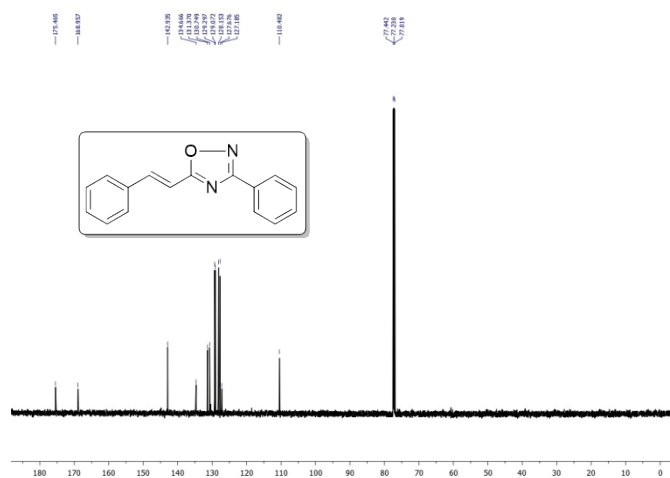


Fig. S8 — ¹³C NMR spectrum of compound 3c

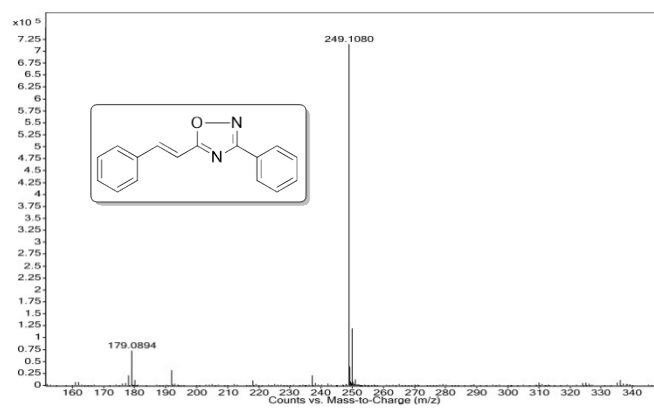


Fig. S9 — Mass spectrum of compound 3c

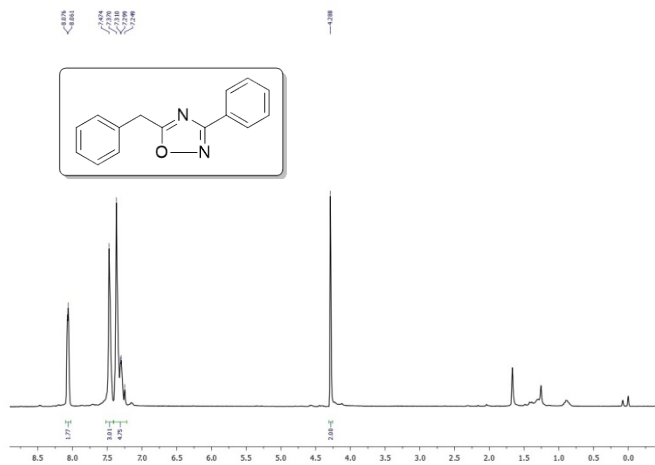
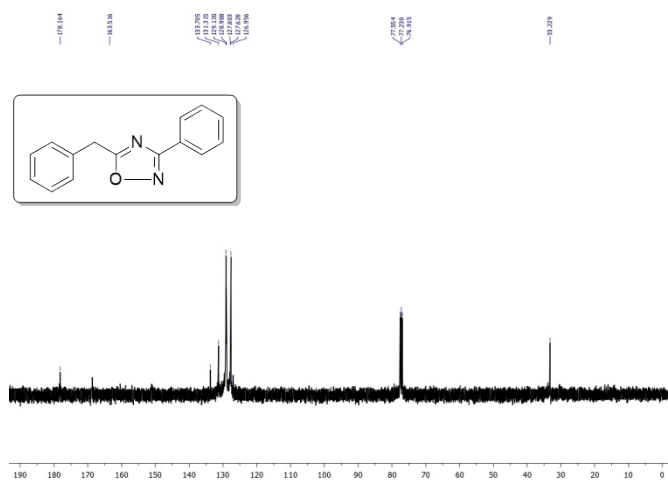


Fig. S10 — ^1H NMR spectrum of compound 3d



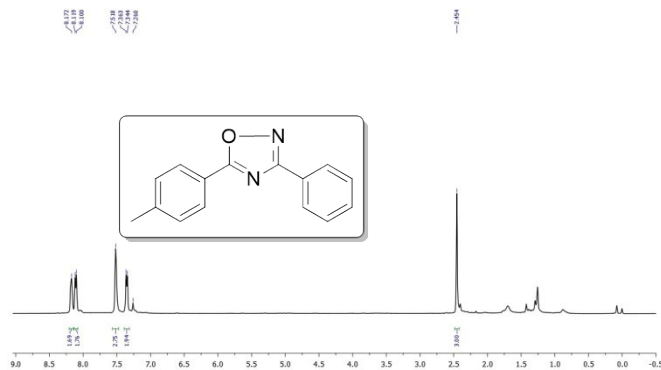


Fig. S13 — ^1H NMR spectrum of compound 3e

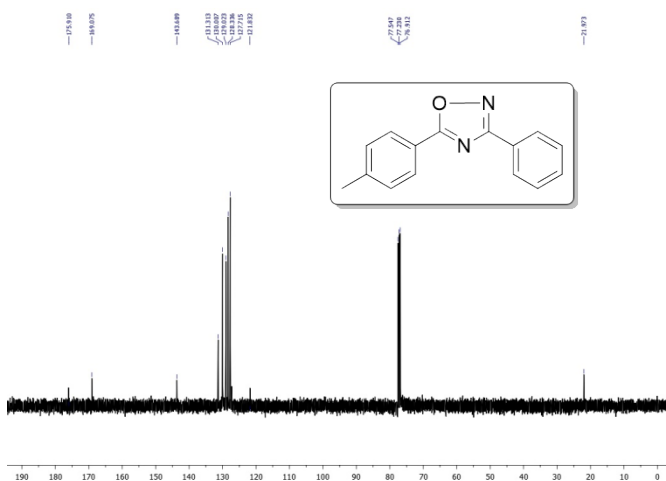


Fig. S14 — ^{13}C NMR spectrum of compound 3e

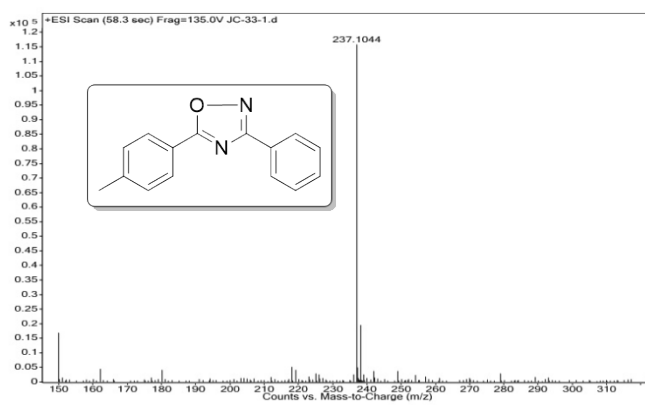


Fig. S15 — Mass spectra of compound 3e

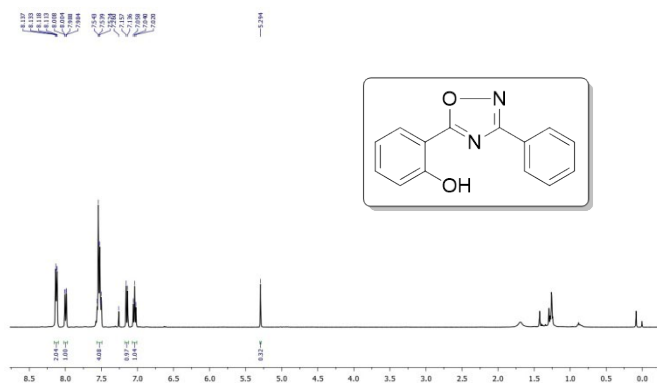


Fig. S16 — ¹H NMR spectrum of compound 3f

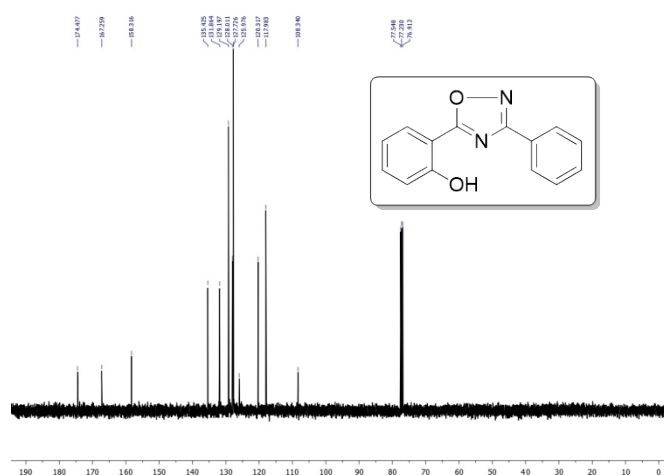


Fig. S17 — ¹³C NMR spectrum of compound 3f

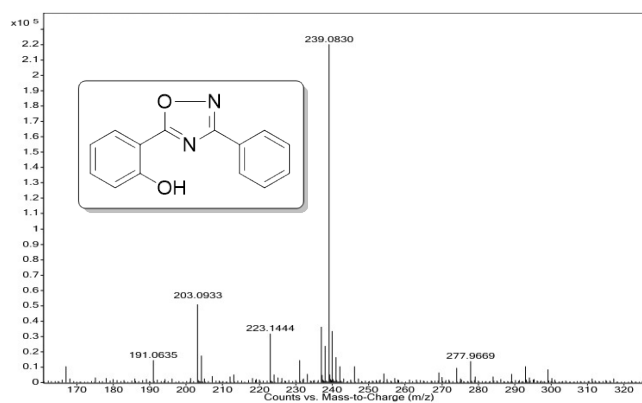


Fig. S18 — Mass spectrum of compound 3f

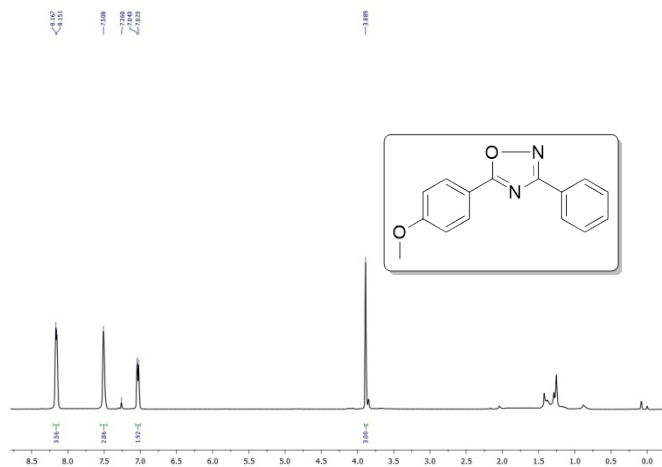


Fig. S19 — ^1H NMR spectrum of compound 3g

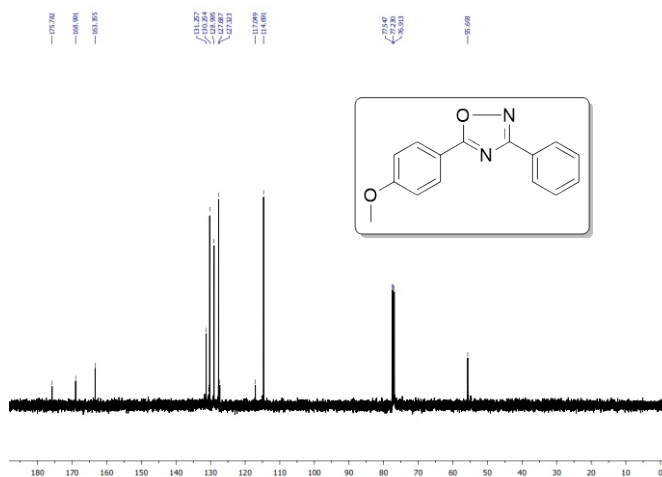


Fig. S20 — ^{13}C NMR spectrum of compound 3g

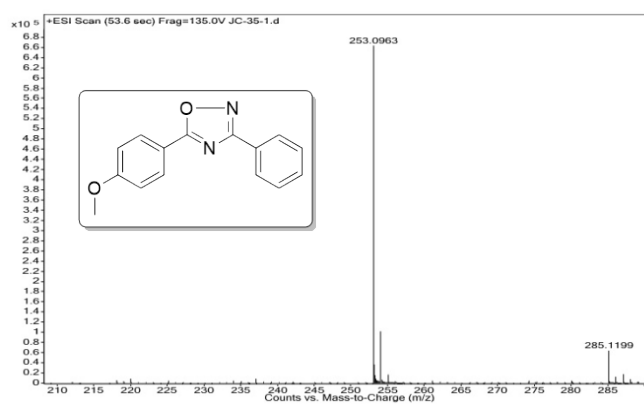


Fig. S21 — Mass spectrum of compound 3g

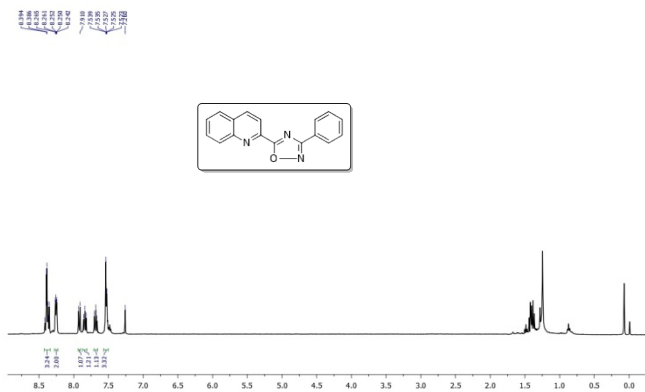


Fig. S25 — ¹H NMR spectrum of compound 3i

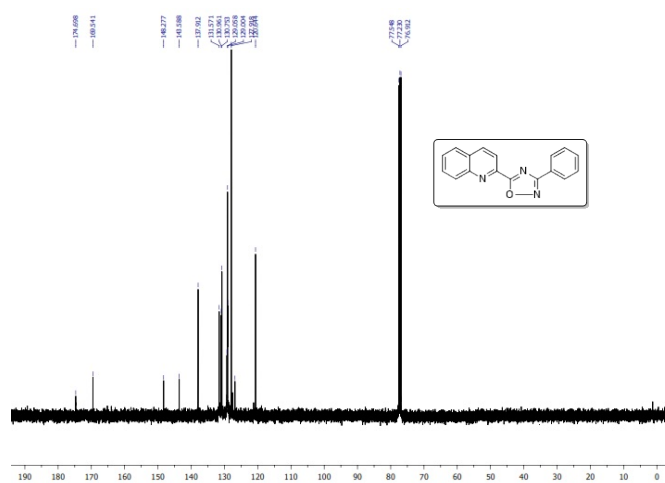


Fig. S26 — ¹³C NMR spectrum of compound 3i

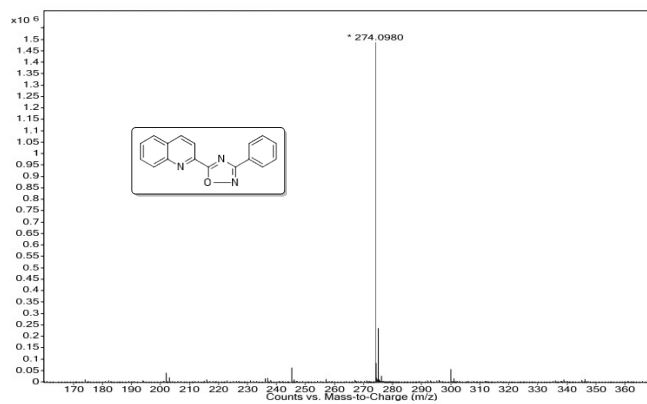


Fig. S27 — Mass spectrum of compound 3i

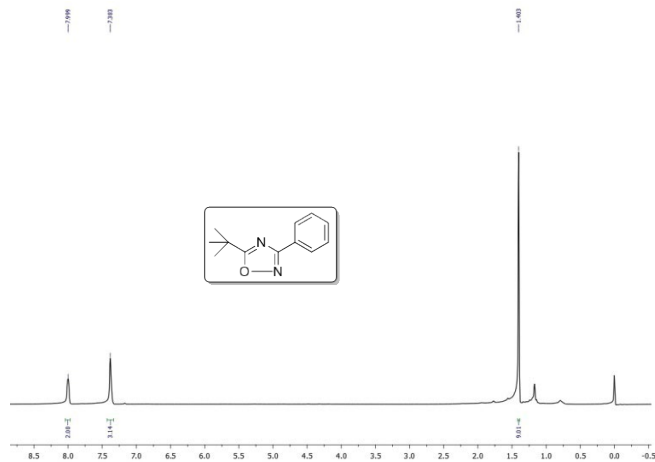


Fig. S28 — ^1H NMR spectrum of compound 3j

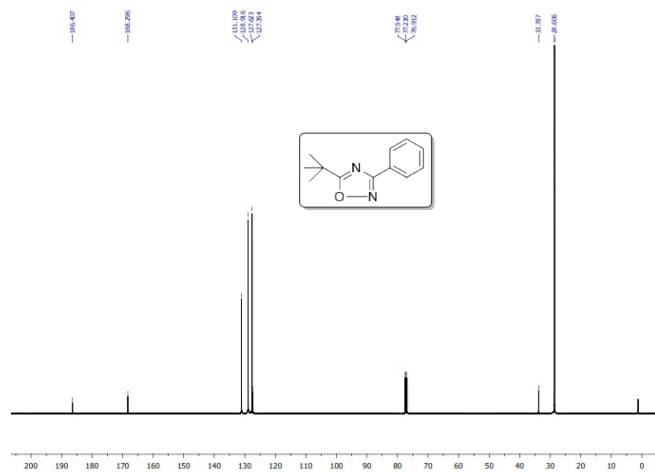


Fig. S29 — ^{13}C NMR spectrum of compound 3j

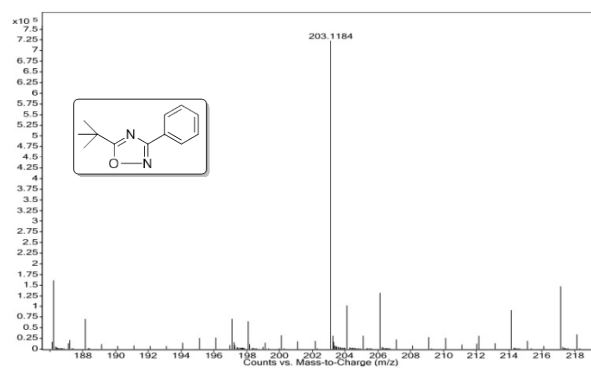


Fig. S30 — Mass spectrum of compound 3j

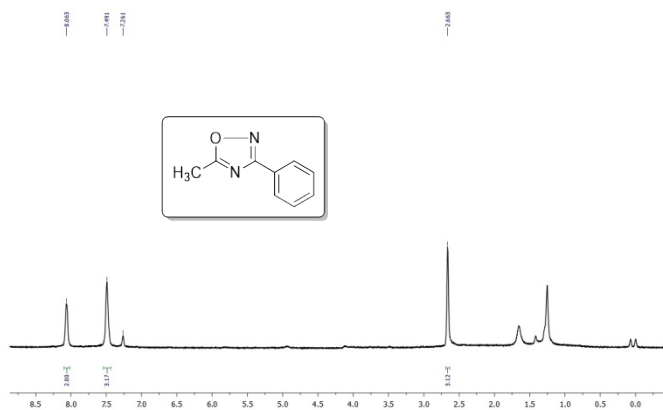


Fig. S31 — ^1H NMR spectrum of compound 3k

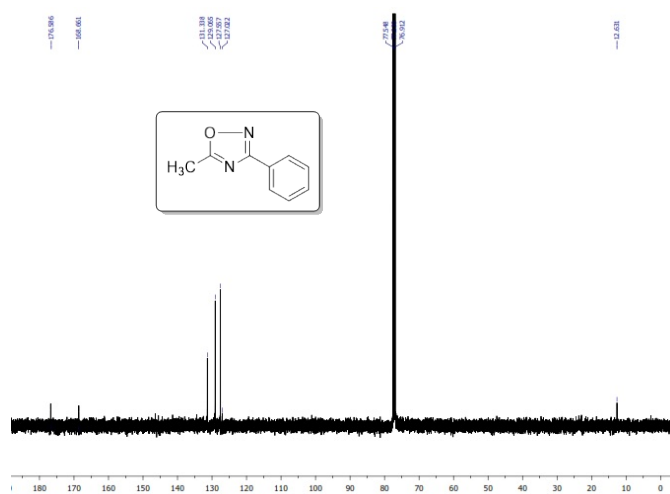


Fig. S32 — ^{13}C NMR spectrum of compound 3k

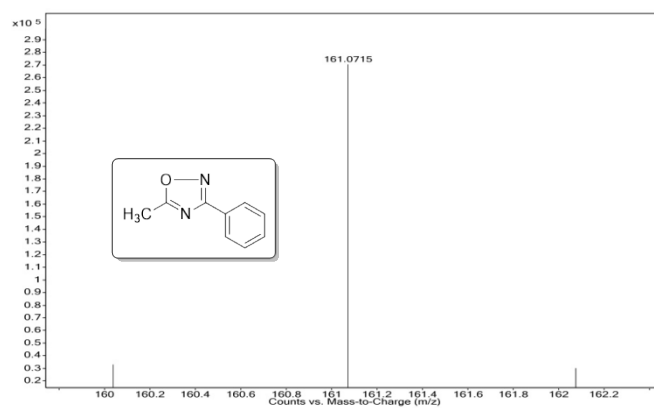


Fig. S33 — Mass spectrum of compound 3k

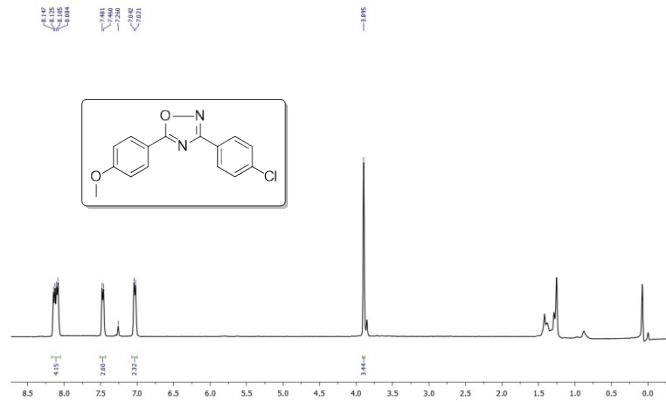


Fig. S34 — ^1H NMR spectrum of compound 4a

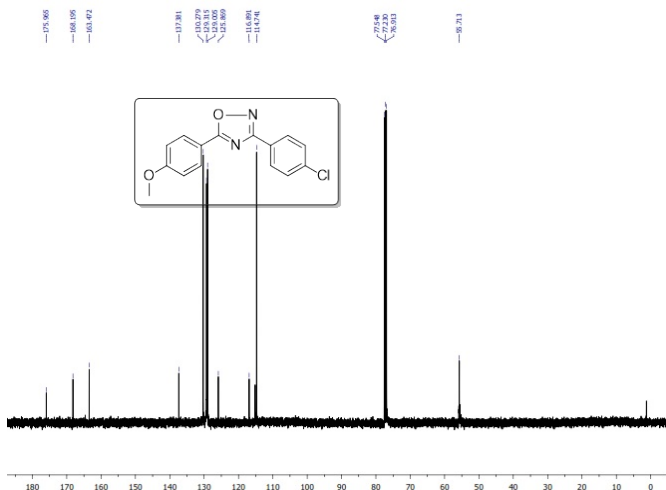


Fig. S35 — ^{13}C NMR spectrum of compound 4a

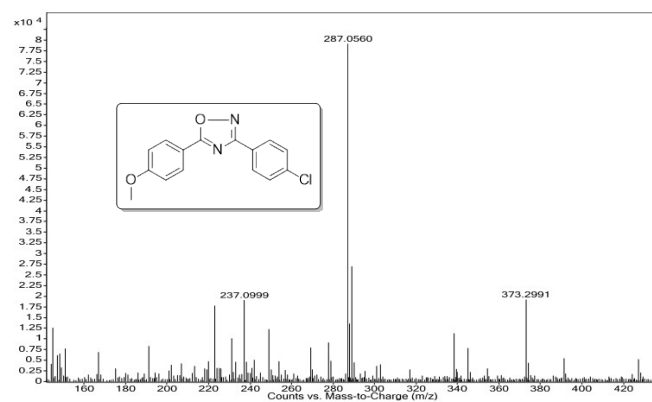


Fig. S36 — Mass spectrum of compound 4a

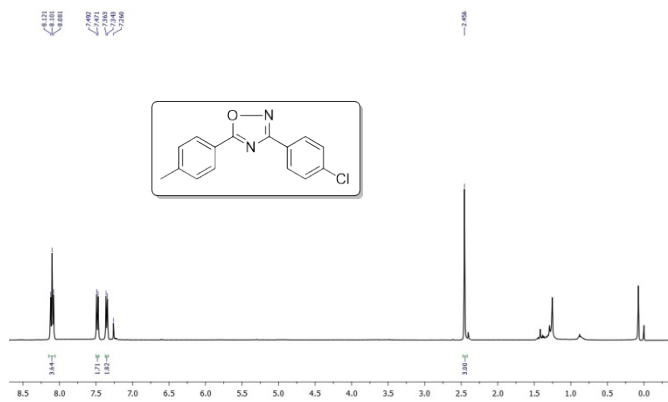


Fig. S37 — ^1H NMR spectrum of compound 4b

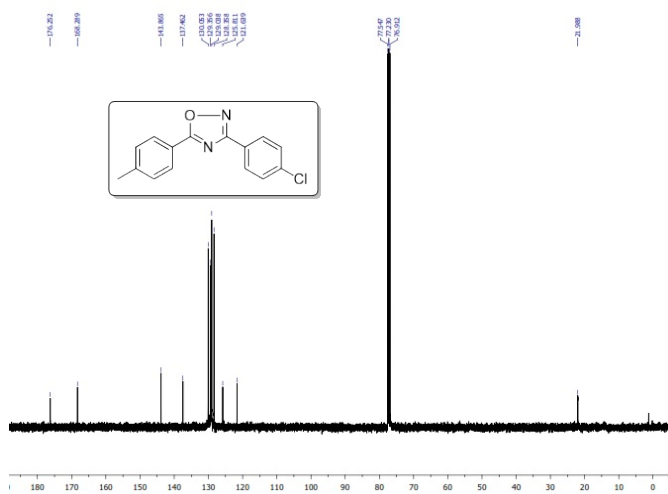


Fig. S38 — ^{13}C NMR spectrum of compound 4b

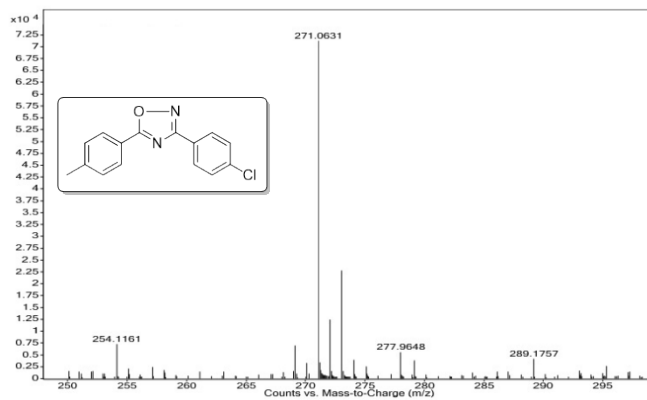


Fig. S39 — Mass spectrum of compound 4b

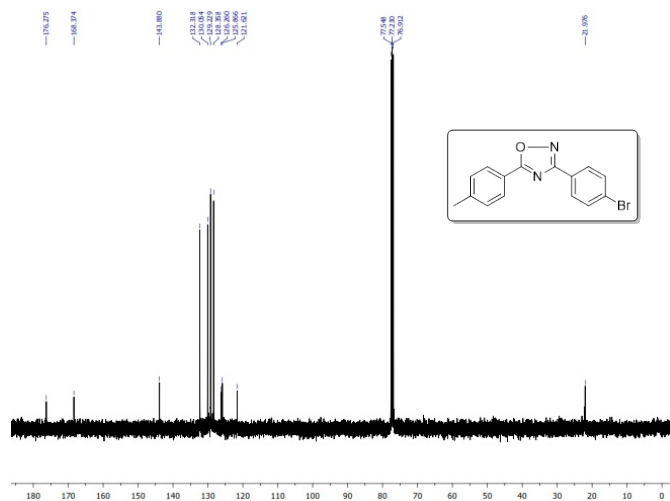


Fig. S43 — ^{13}C NMR spectrum of compound 4d

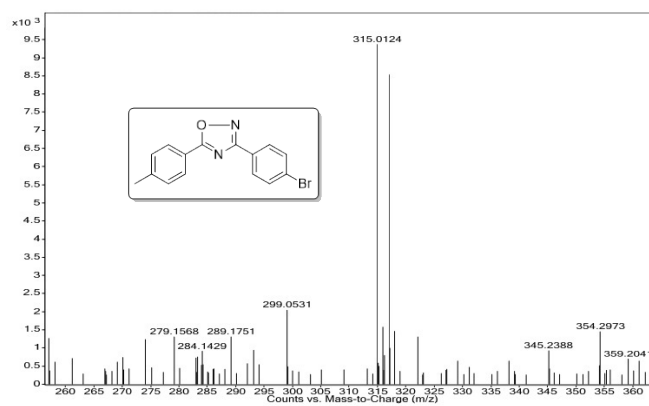


Fig. S44 — Mass spectrum of compound 4d

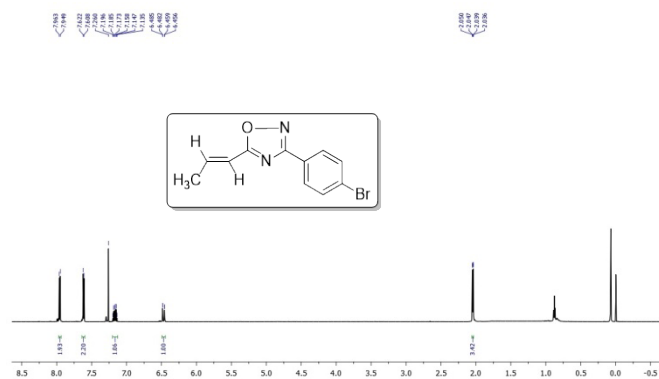


Fig. S45 — ^1H NMR spectrum of compound 4e

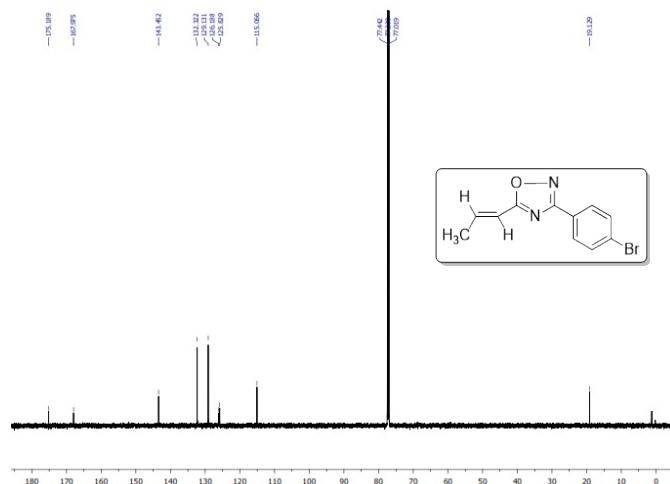


Fig. S46 — ^{13}C NMR spectrum of compound 4e

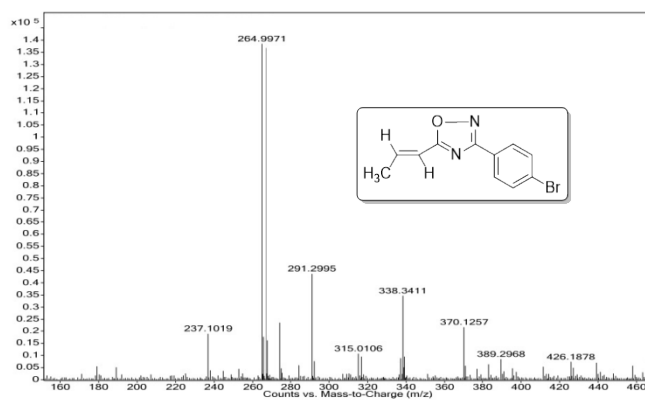


Fig. S47 — Mass spectrum of compound 4e

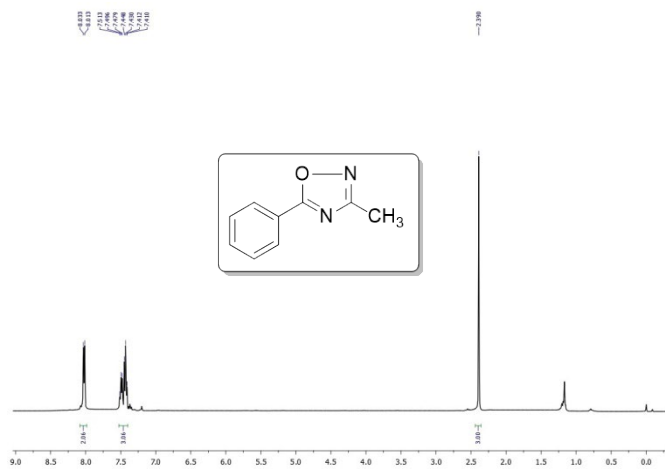


Fig. S48 — ^1H NMR spectrum of compound 4f

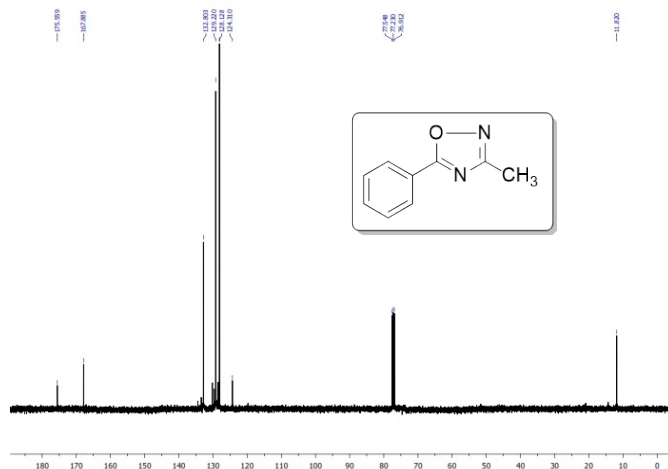


Fig. S49 — ^{13}C NMR spectrum of compound 4f

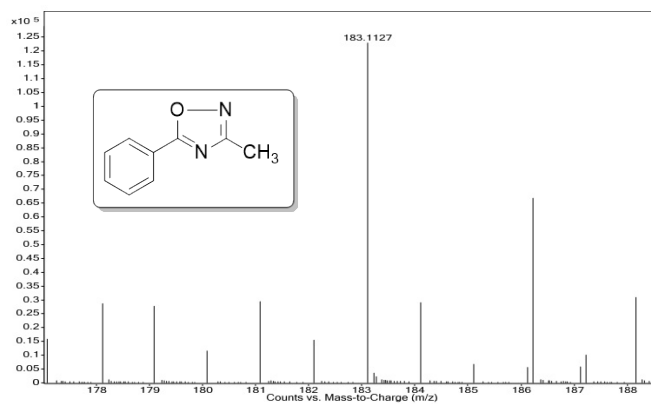


Fig. S50 — Mass spectrum of compound 4f

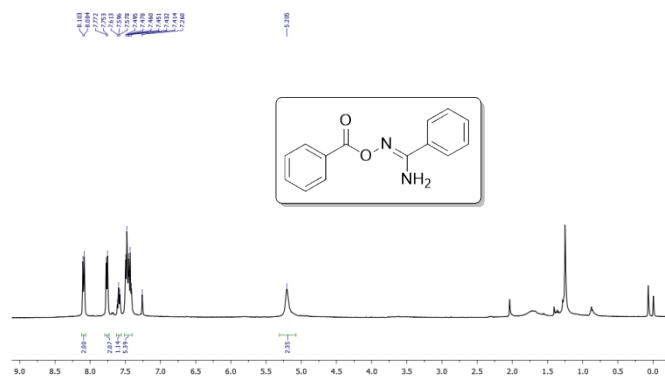


Fig. S51 — ^1H NMR spectrum of Intermediate 3

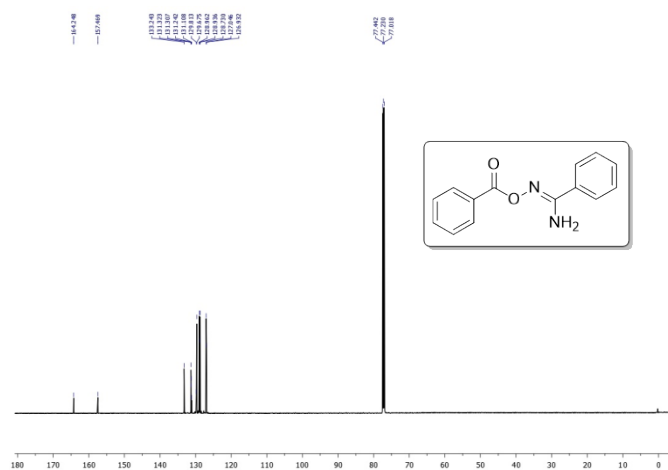


Fig. S52 — ^{13}C NMR spectrum of Intermediate 3

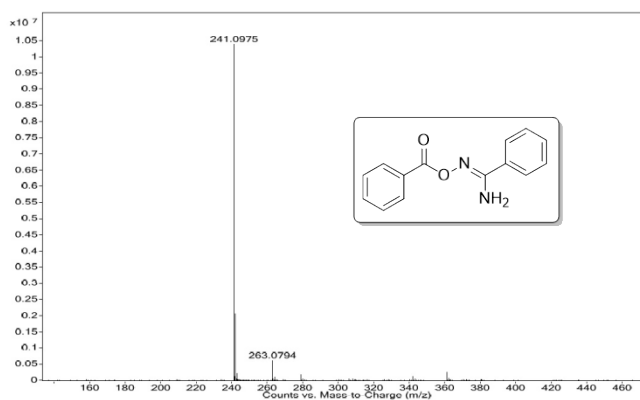


Fig. S53 — Mass spectrum of Intermediate 3

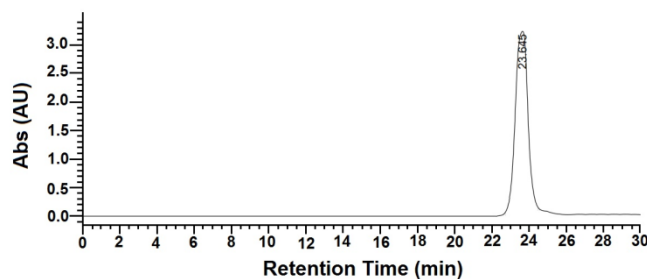


Fig. S54 — HPLC chromatogram of formation of intermediate 3 with 0.1 equiv of Iwich run up to 30 min in AscentisC18 reverse phase analytical column and a linear gradient of 0 to 90%, 0-10 min then 90 to 100% up to 30 min, CH_3CN in H_2O with 0.1% formic acid

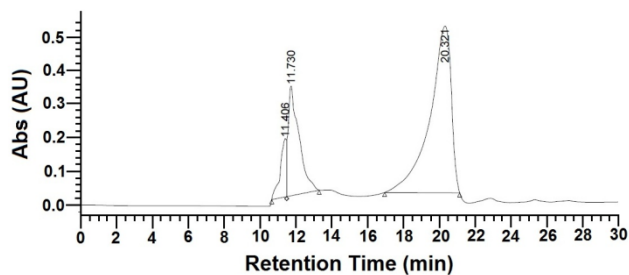


Fig. S55 — HPLC chromatogram of Benzoic acid and benzamidoxime without reagent I which run upto 30 min in Ascentis C18 reverse phase analytical column and a linear gradient of 0 to 90%, 0-10 min then 90 to 100% up to 30 min, CH₃CN in H₂O with 0.1% formic acid

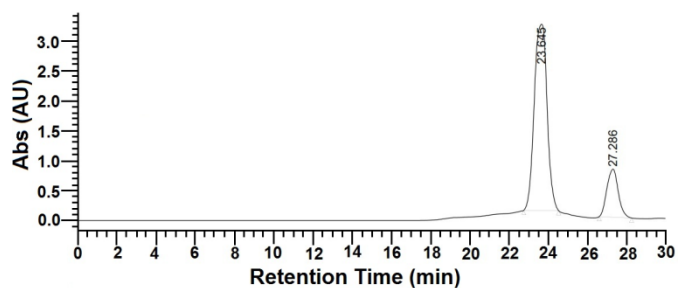


Fig. S56 — HPLC chromatogram of conversion of intermediate 3 to product 4 without reagent I which run upto 30 min in AscentisC18 reverse phase analytical column and a linear gradient of 0 to 90%, 0-10 min then 90 to 100% up to 30 min, CH₃CN in H₂O with 0.1% formic acid

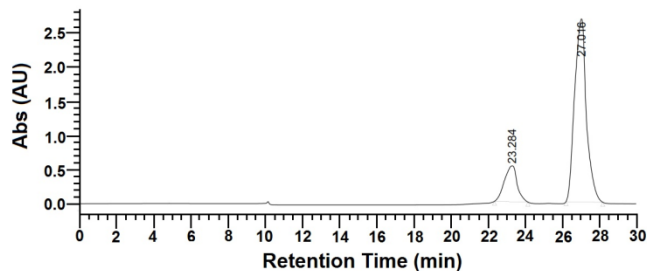


Fig. S57 — HPLC chromatogram of conversion of 3 to 4 with 0.1 equiv of I which run up to 30 min in AscentisC18 reverse phase analytical column and a linear gradient of 0 to 90%, 0-10 min then 90 to 100% up to 30 min, CH₃CN in H₂O with 0.1% formic acid

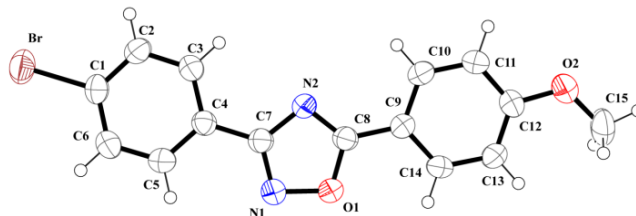


Fig. 58 — Crystallographic structure for 4c at 296(2) K

Table S1 — Crystallographic data for 4c at 296(2) K	
Formulae	C ₁₅ H ₁₁ O ₂ N ₂ Br
CCDC NO	1043141
Formula. wt.	331.17
Crystal system	triclinic
Space group	P1
<i>a</i> (Å)	4.0341(3)
<i>b</i> (Å)	11.8698(8)
<i>c</i> (Å)	15.0530(11)
α(°)	69.345(5)
β(°)	88.560(5)
γ(°)	85.109(4)
V/ Å ³	672.00(8)
Z	2
Density/Mgm ⁻³	1.637
Abs. Coeff. /mm ⁻¹	3.061
F(000)	332
Total no. of reflections	9877
Reflections, <i>I</i> > 2σ(<i>I</i>)	0.0307
Max. 2θ/°	25.25
Ranges (h, k, l)	-4 ≤ h ≤ 4 -14 ≤ k ≤ 14 -18 ≤ l ≤ 18
Complete to 2θ (%)	25.25
Data/ Restraints/Parameters	0.0714 /0/182
Goof (<i>F</i> ²)	1.924
R indices [<i>I</i> > 2σ(<i>I</i>)]	0.0359
R indices (all data)	0.0467