

Intramolecular Diels–Alder reaction in the synthesis of 5-arylisoxazolymethyl- and 4,5-dichloroisothiazolymethyl-3a,6-epoxyisoindol-3-ones

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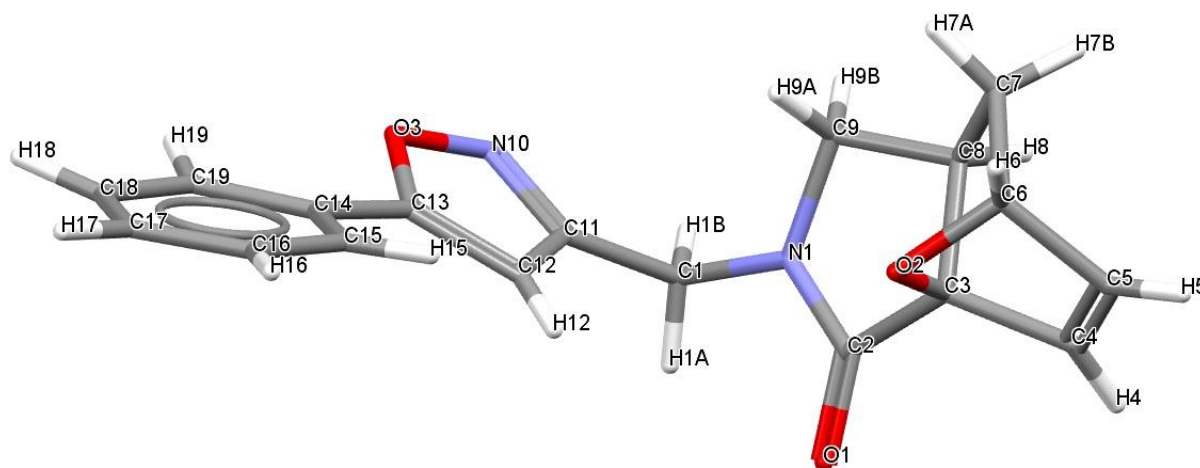
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SUPPLEMENTARY INFORMATION

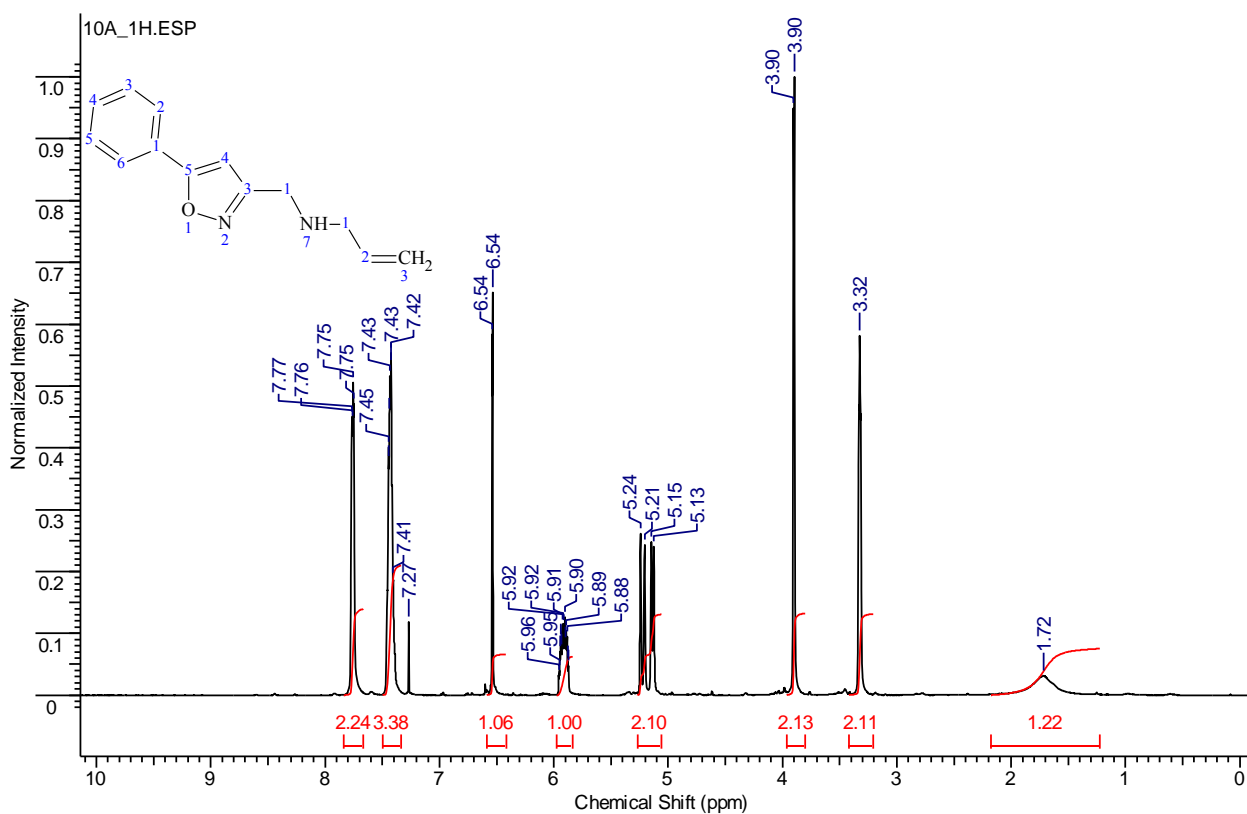
1. The principal crystallographic parameters of the compound 12a

Rhombic crystal, *Pna*2₁ space group; *a* 7.9580(8), *b* 21.196(2), *c* 9.1325(10) Å; *V* 1540.4(3) Å³; *Z* 4; μ 0.092 mm⁻¹. 6091 reflections were collected at scattering angles $7.292^\circ \leq 2\theta \leq 61.84^\circ$, of which 3256 were independent (R_{int} 0.0380). The final refinement parameters: R_1 0.0873, wR_2 0.1582 (for all reflections), R_1 0.0537, wR_2 0.1228 (for reflections with $I > 2\sigma(I)$) with the quality factor GOOF 1.091. Peaks of maximum and minimum residual electron density: 0.16 and $-0.22 \text{ e} \cdot \text{Å}^{-3}$. The full set of X-ray structural data was deposited at the Cambridge Crystallographic Data Center (deposit CCDC 2106454).

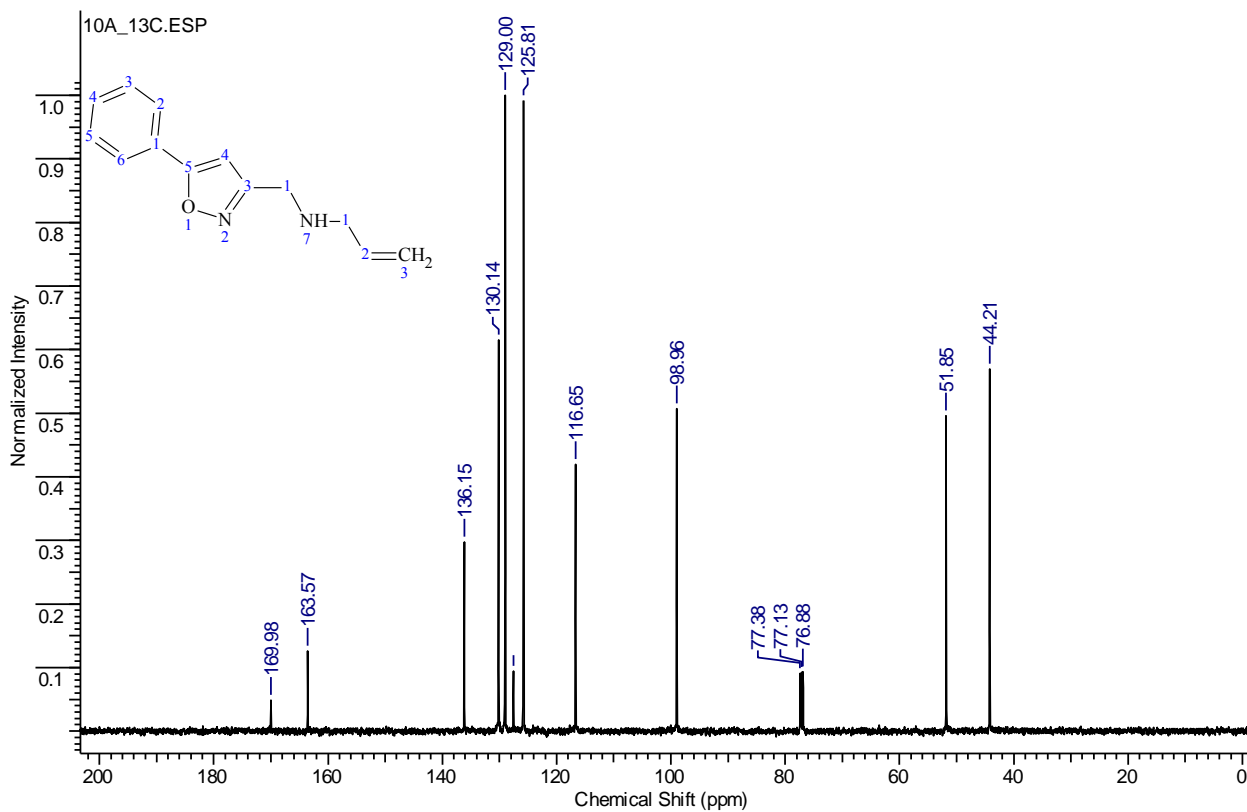


2. NMR spectra of compounds 10a–e and 12a–g.

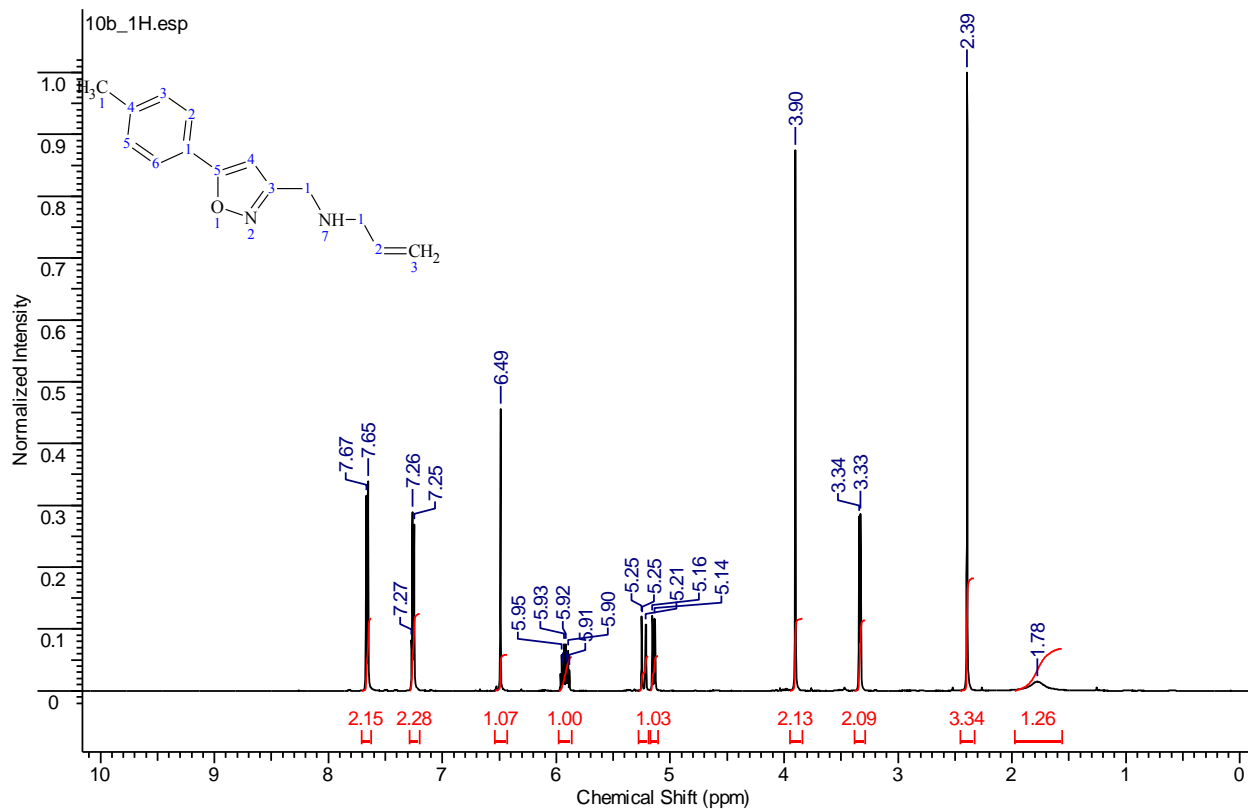
Compound 10a ^1H NMR (CDCl_3 , 700.2 MHz)



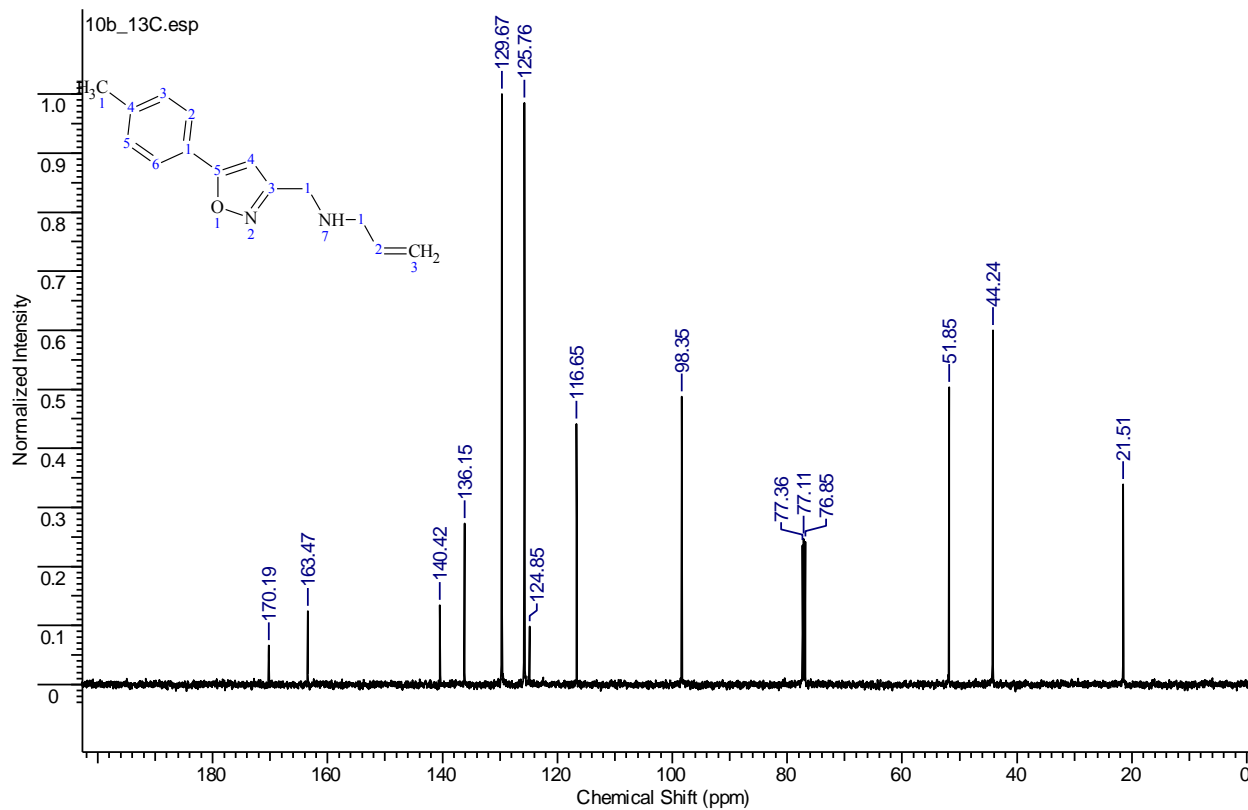
Compound 10a ^{13}C NMR (CDCl_3 , 176.1 MHz)



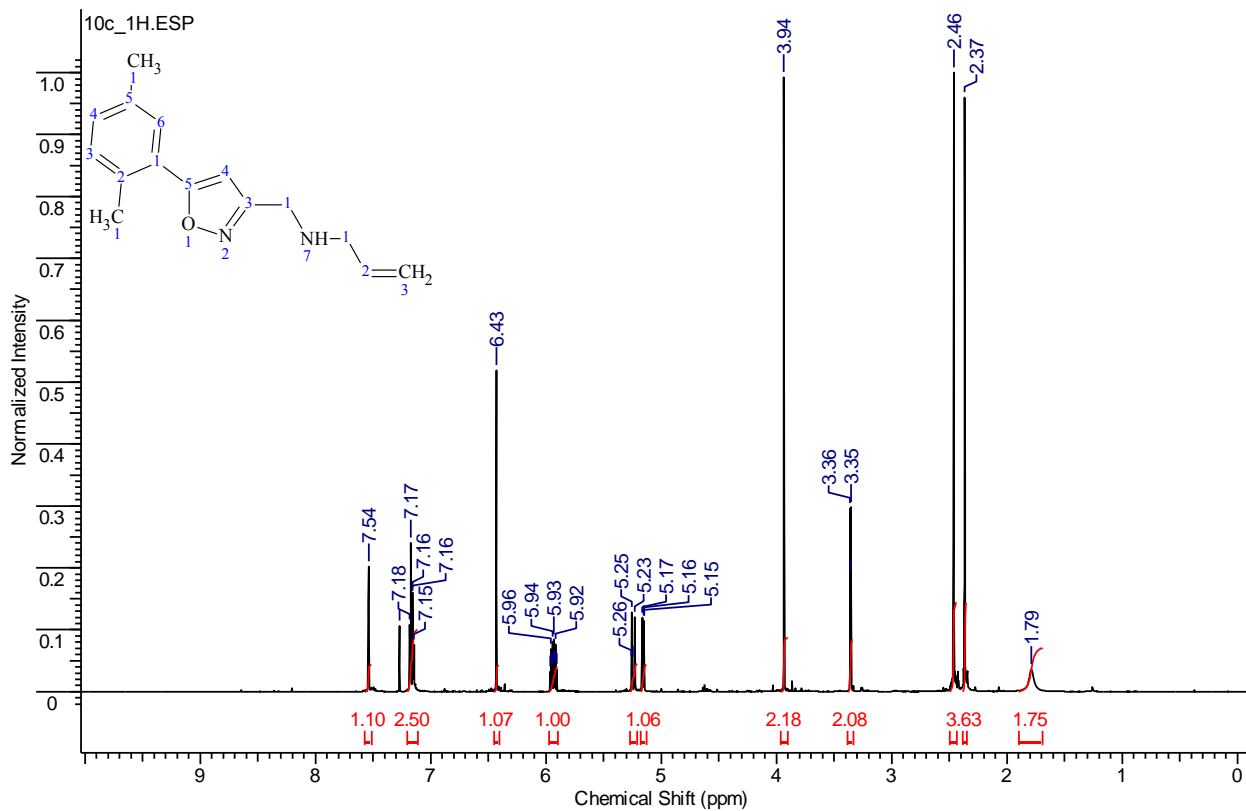
Compound 10b ¹H NMR (CDCl₃, 700.2 MHz)



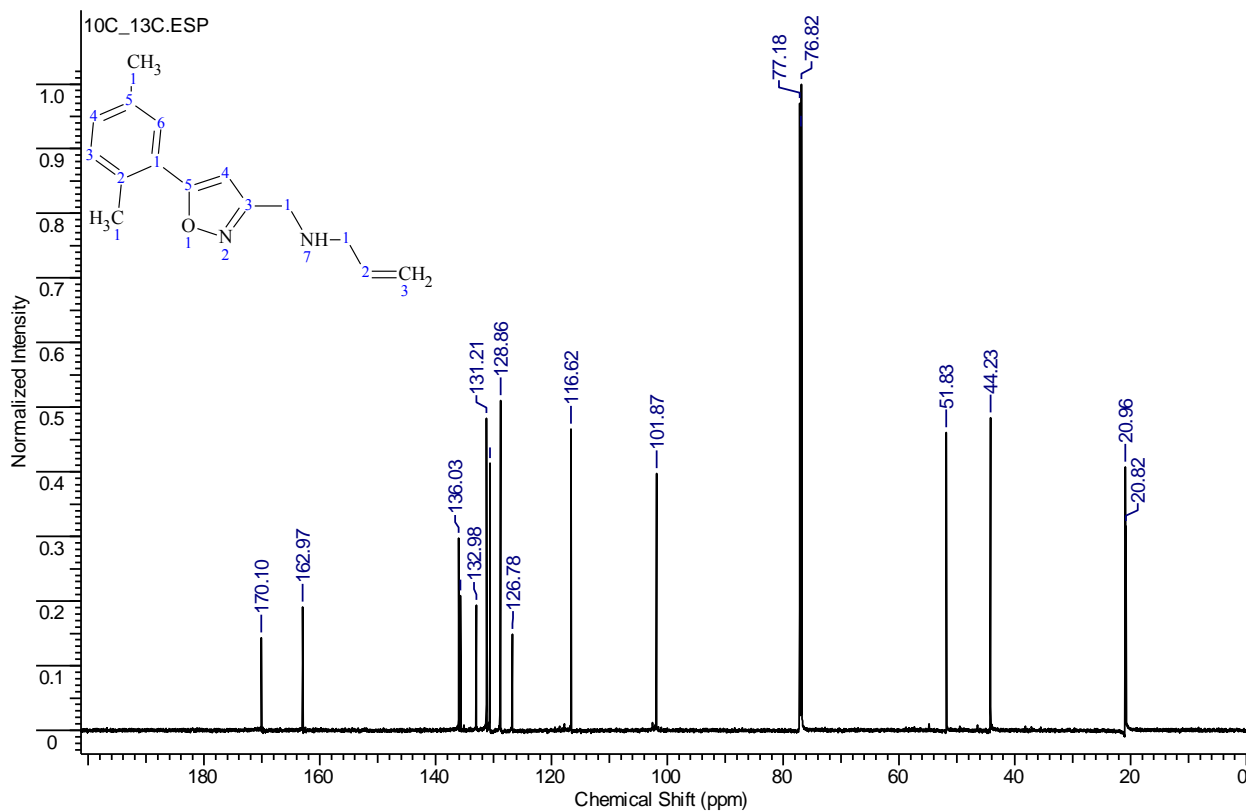
Compound 10b ¹³C NMR (CDCl₃, 176.1 MHz)



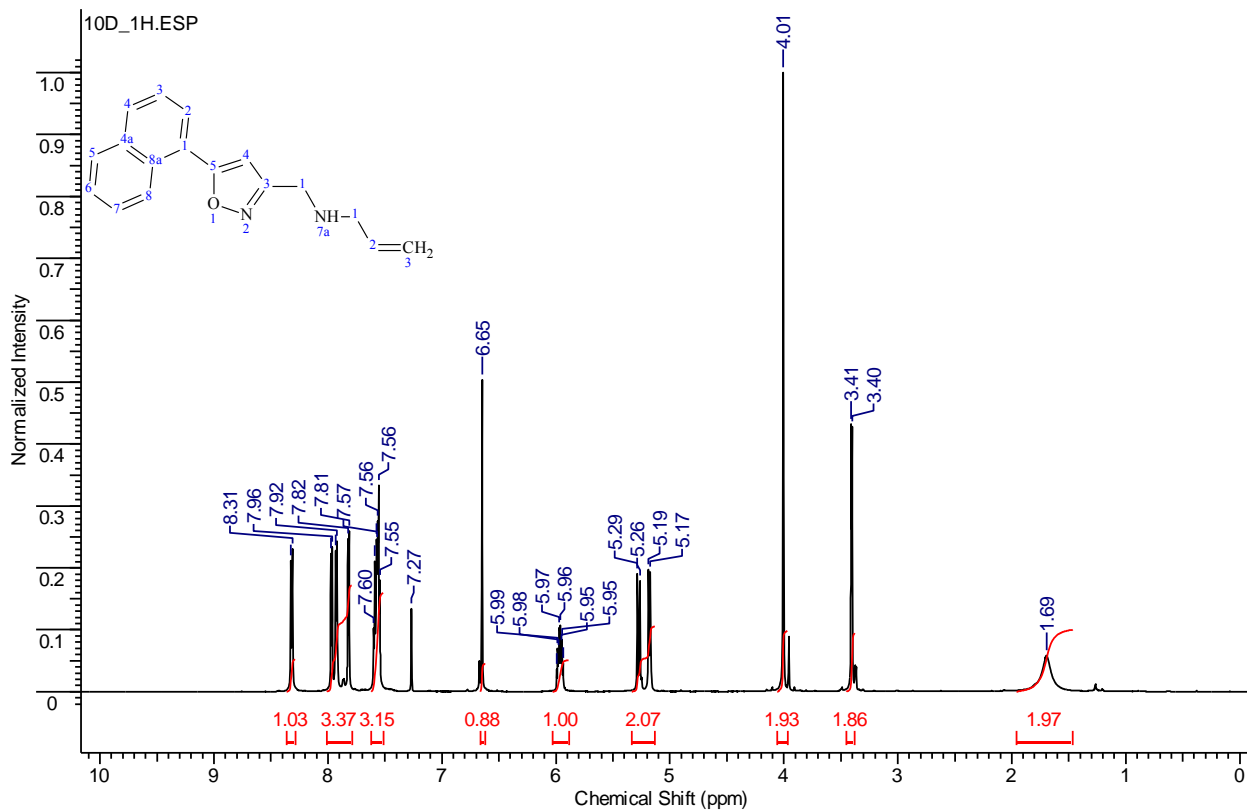
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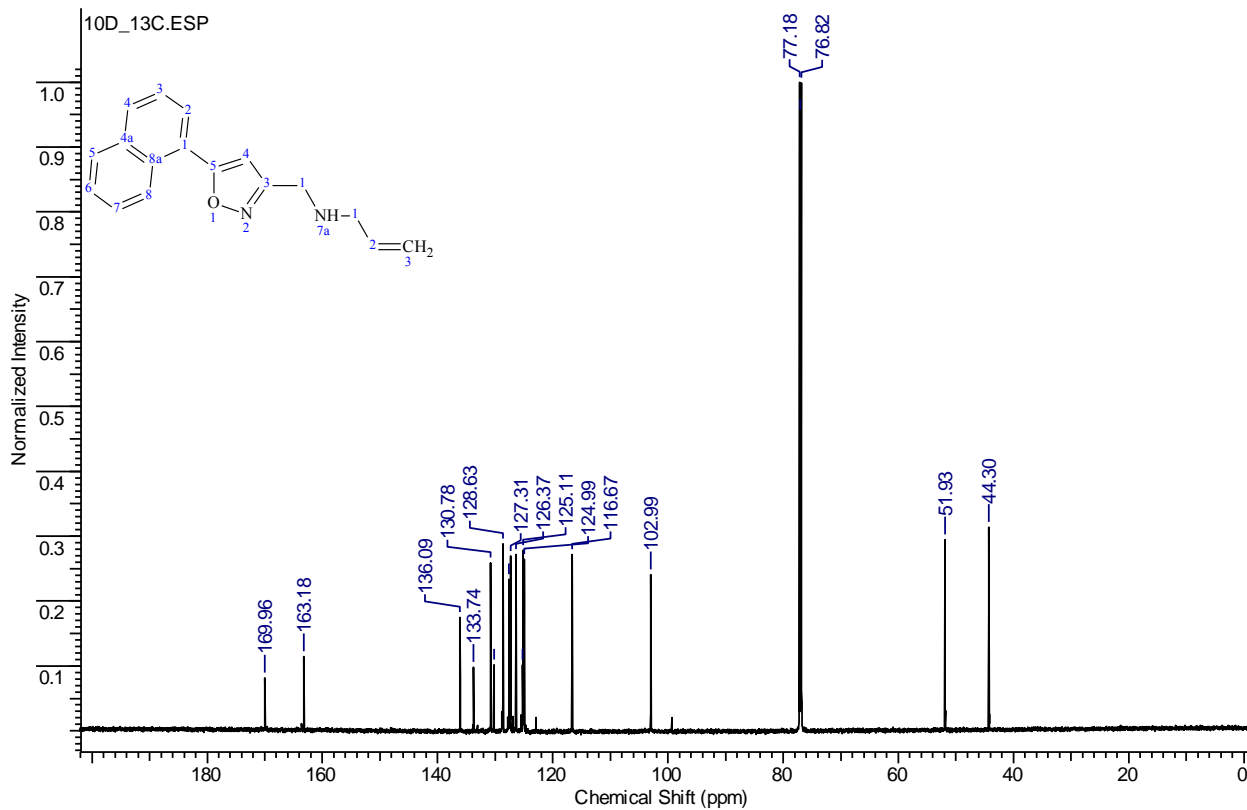
Compound 10c ¹³C NMR (CDCl₃, 176.1 MHz)



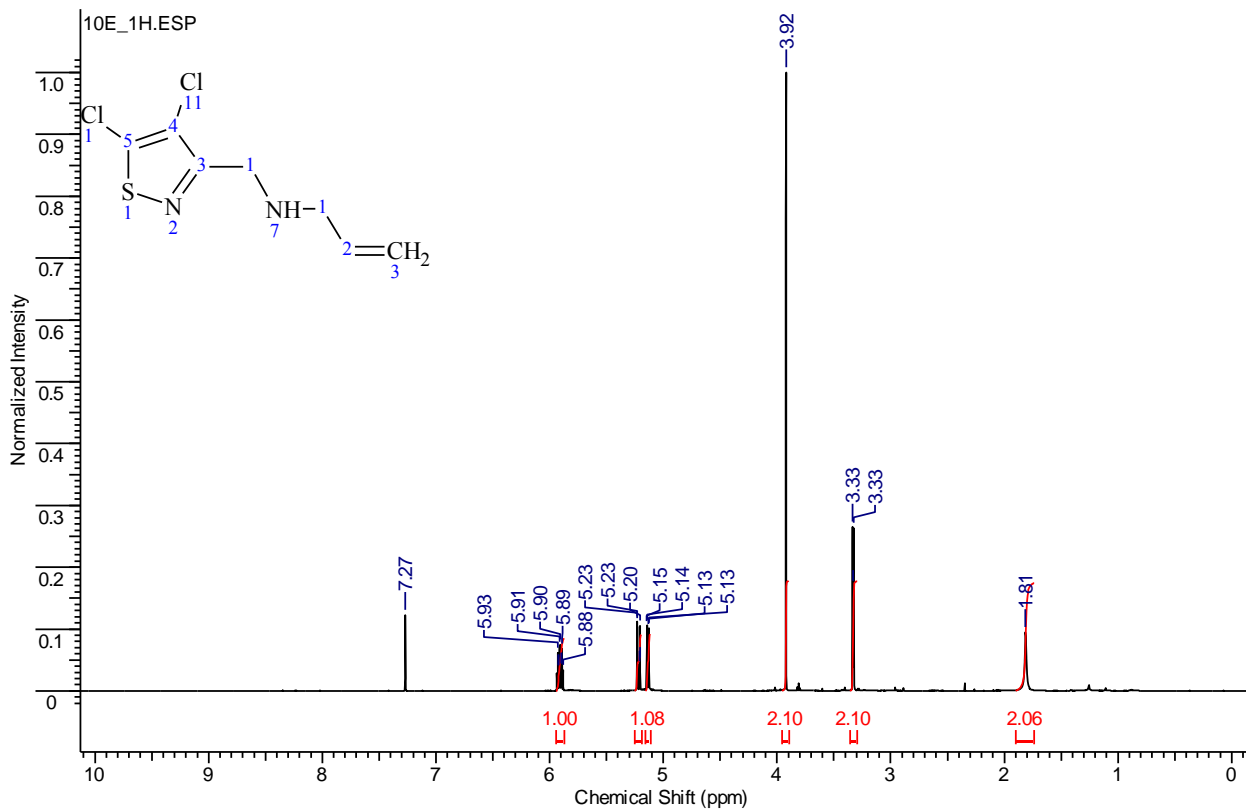
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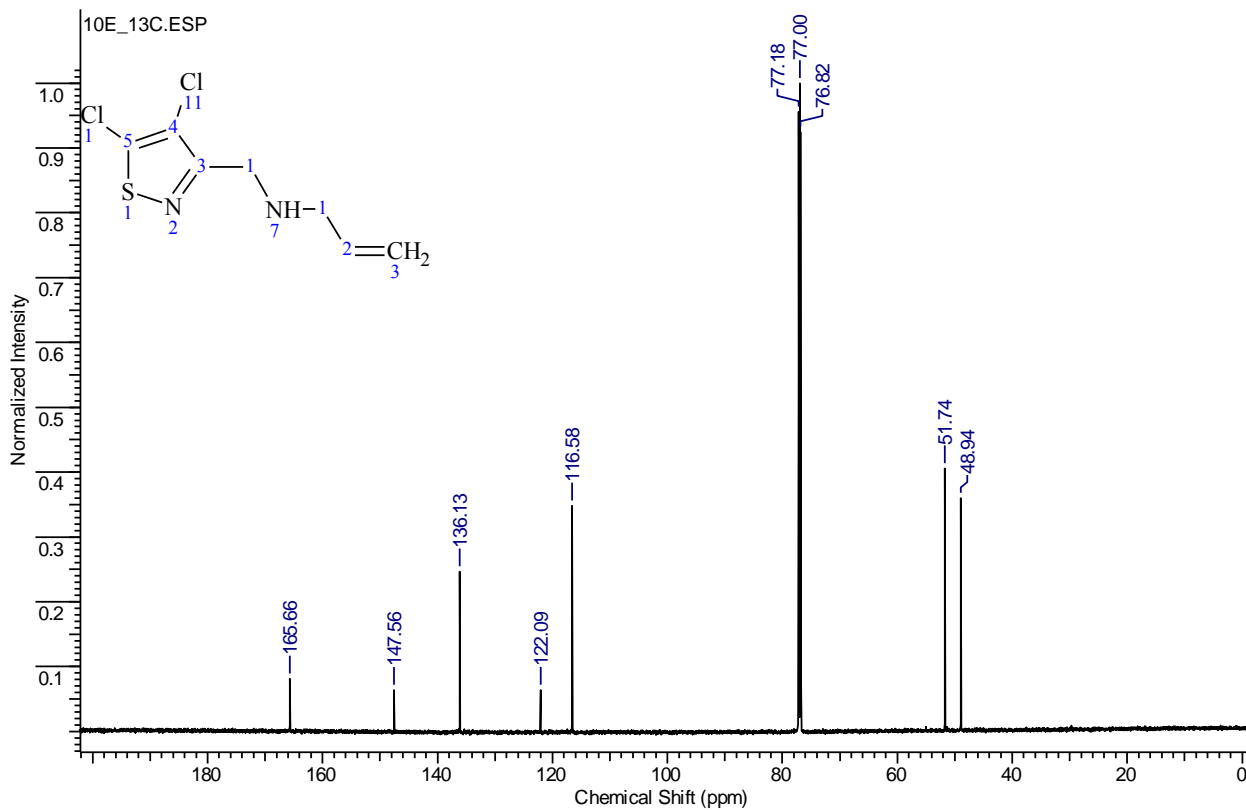
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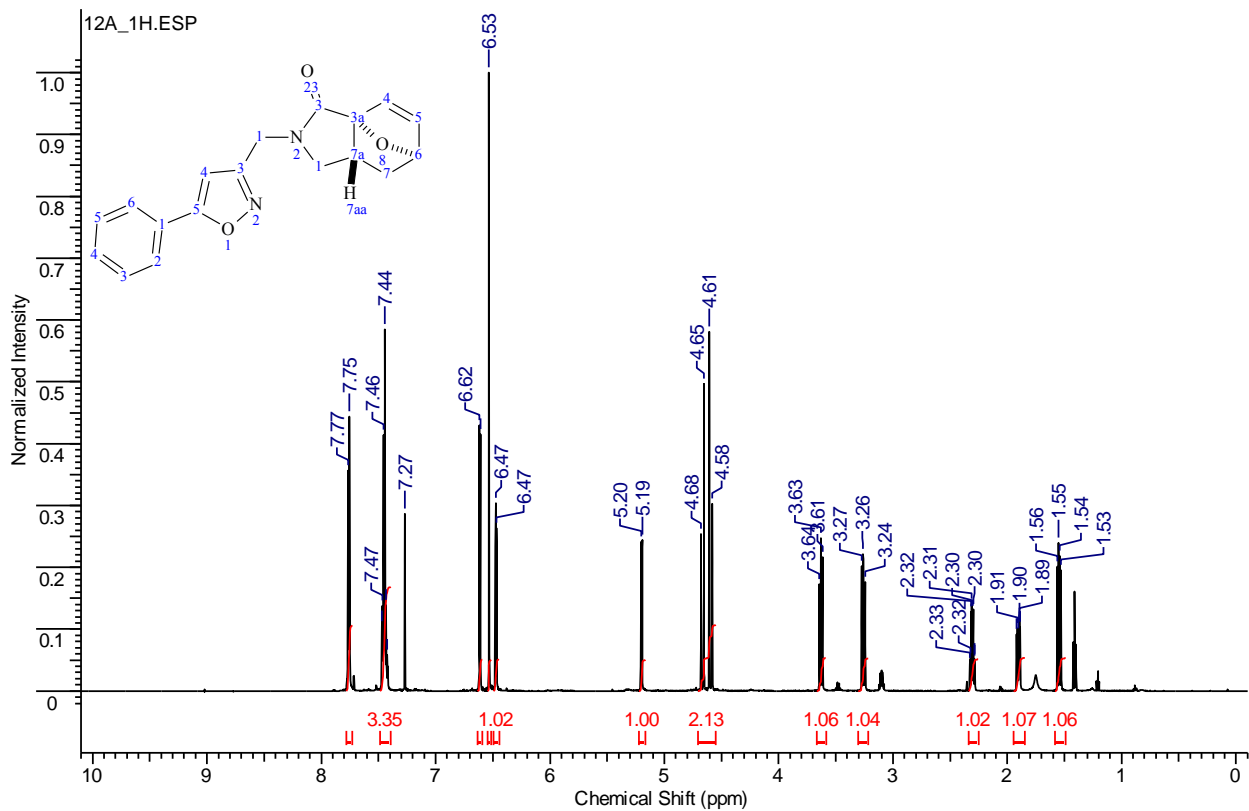
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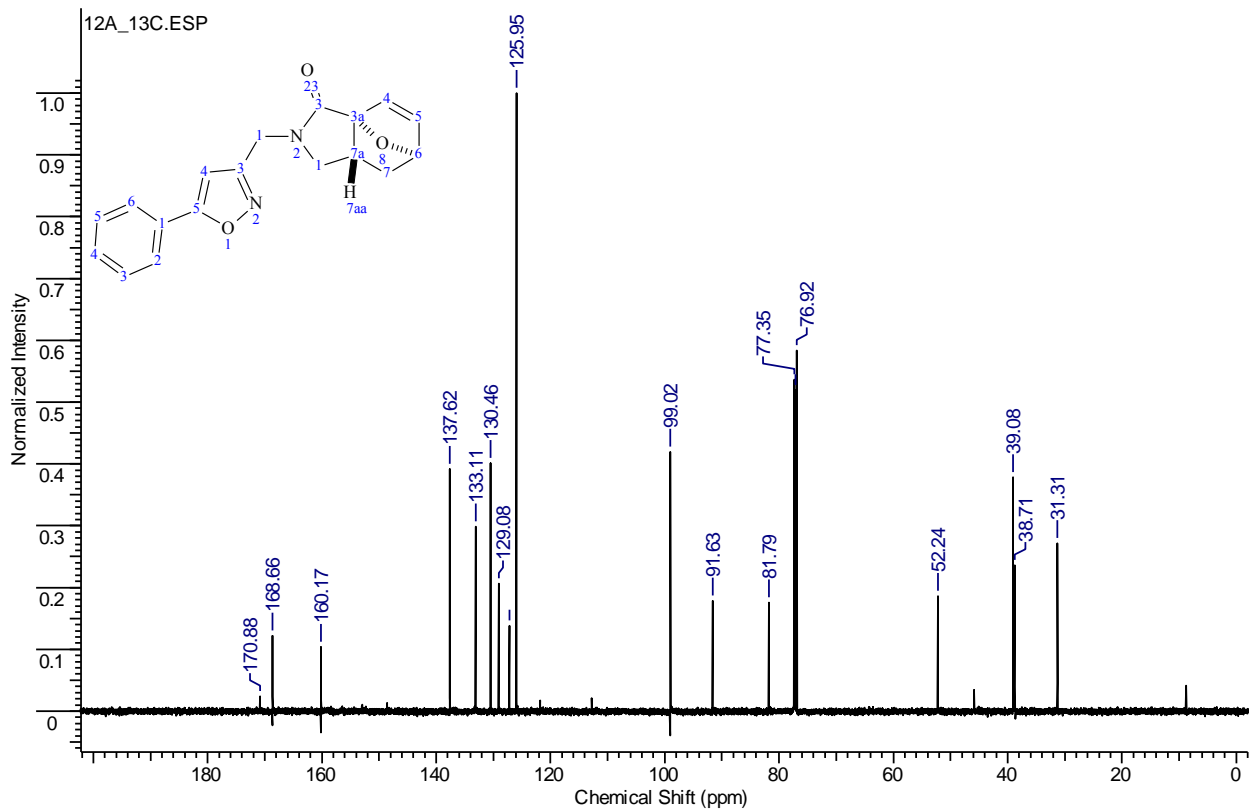
Compound 10e ¹³C NMR (CDCl₃, 176.1 MHz)



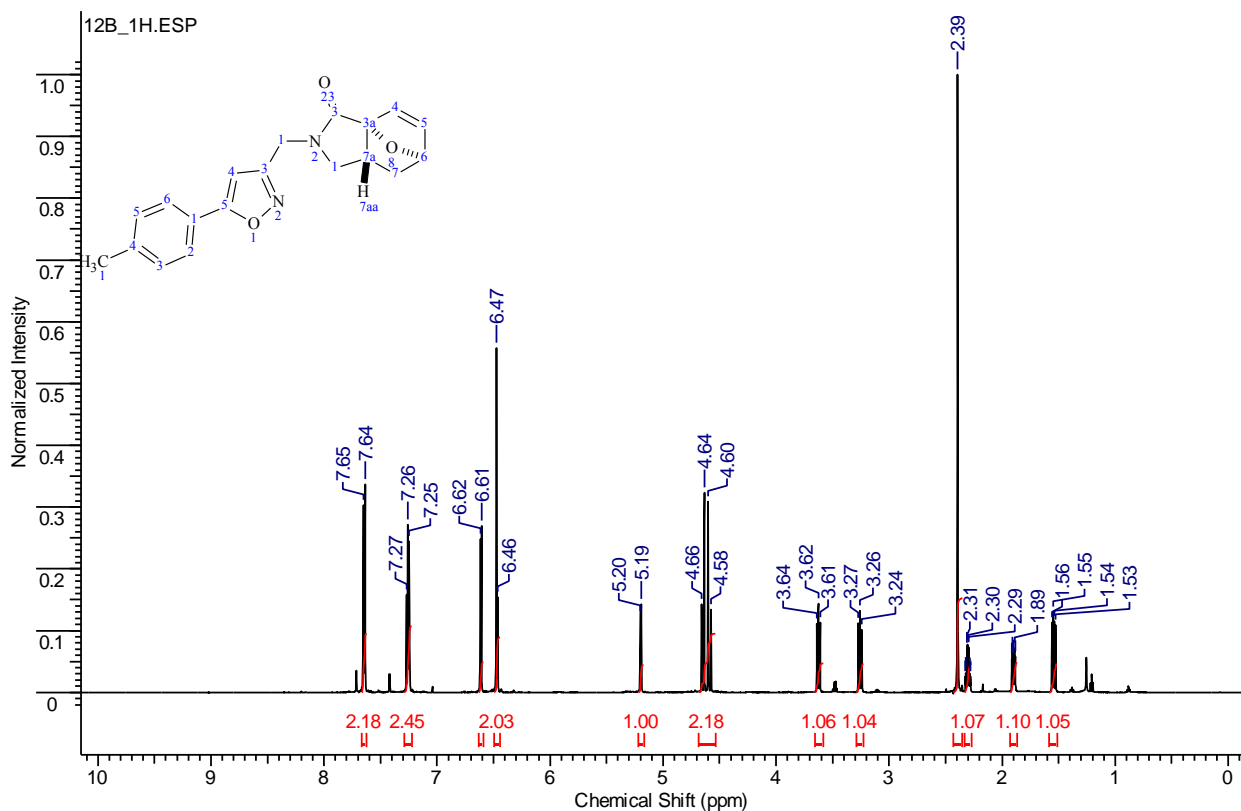
Compound 12a ¹H NMR (CDCl₃, 600.2 MHz)



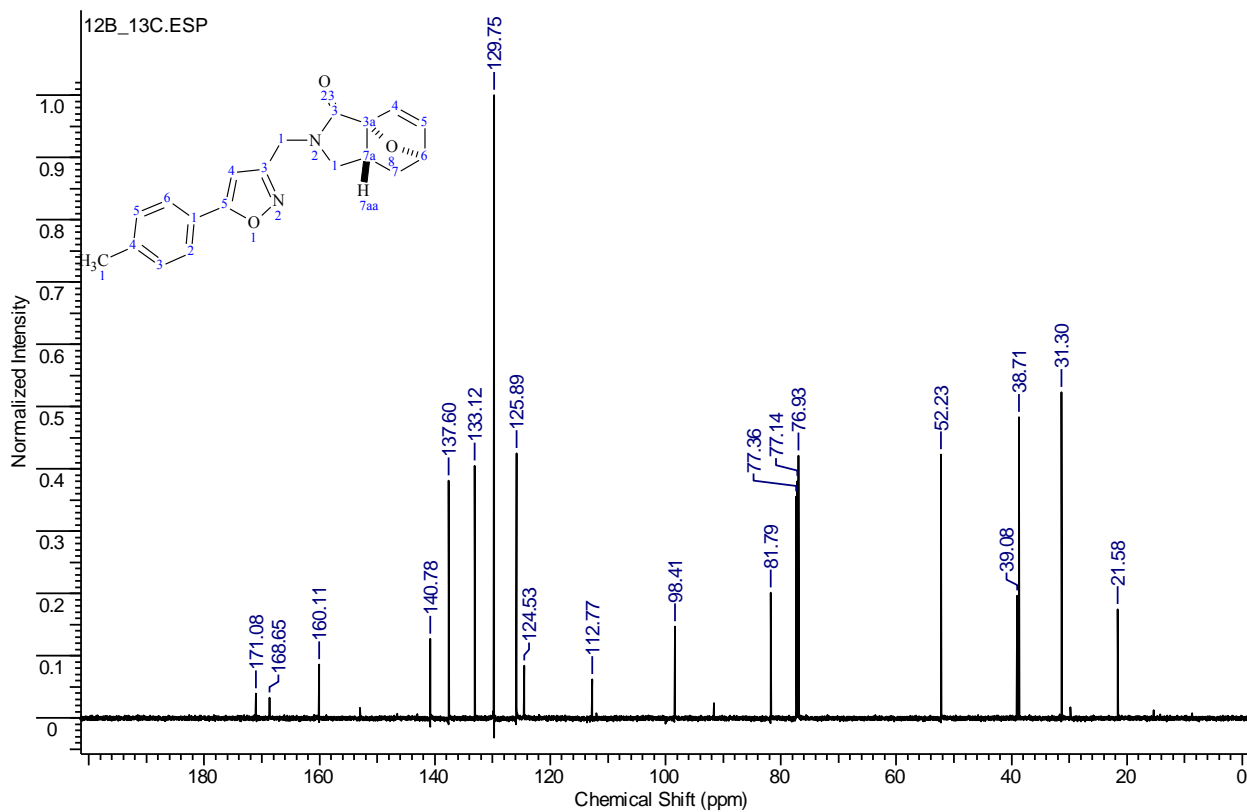
Compound 12a ¹³C NMR (CDCl₃, 150.9 MHz)



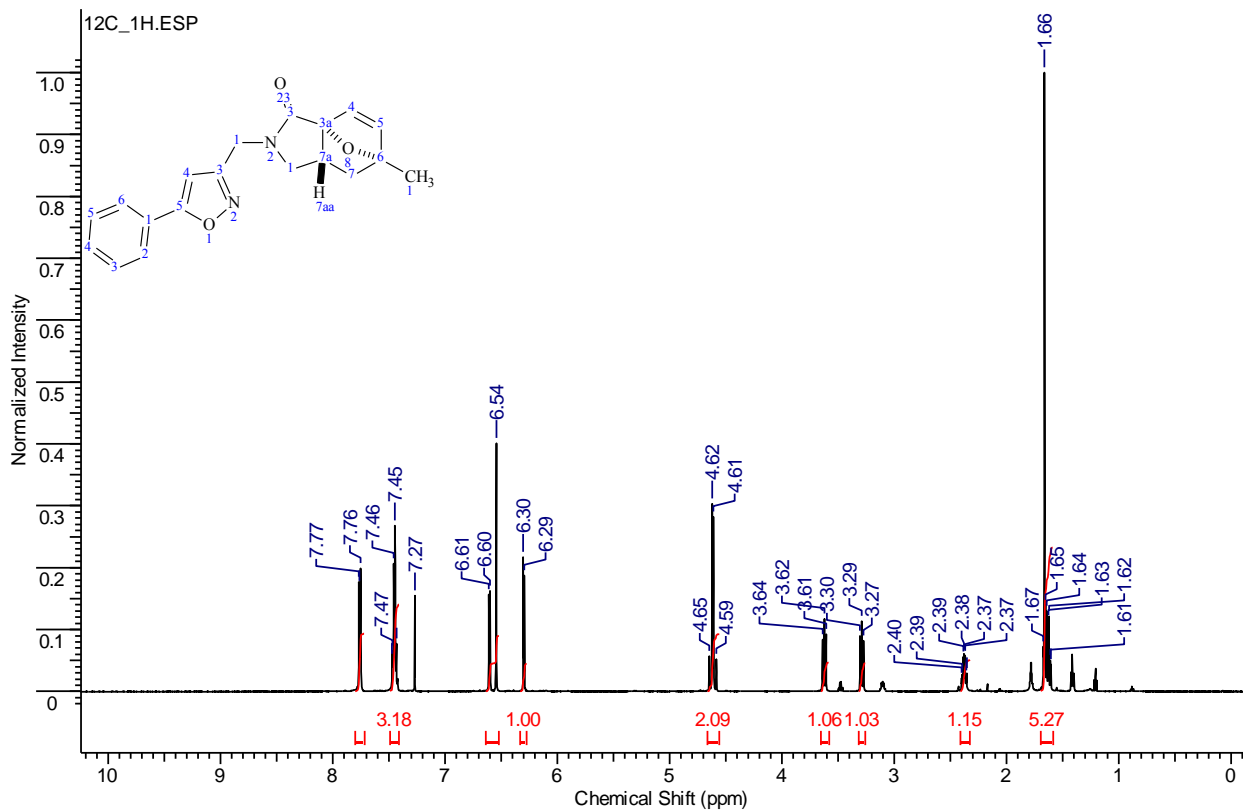
Compound 12b ¹H NMR (CDCl₃, 600.2 MHz)



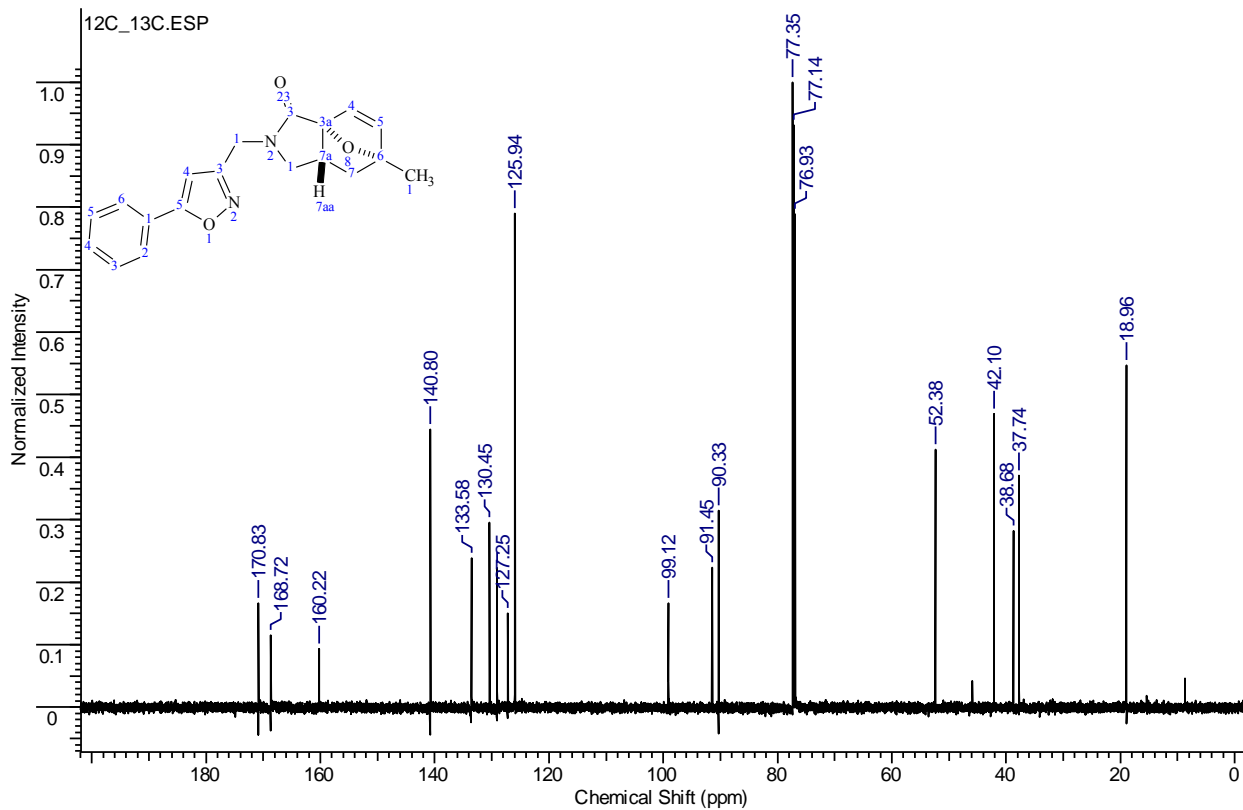
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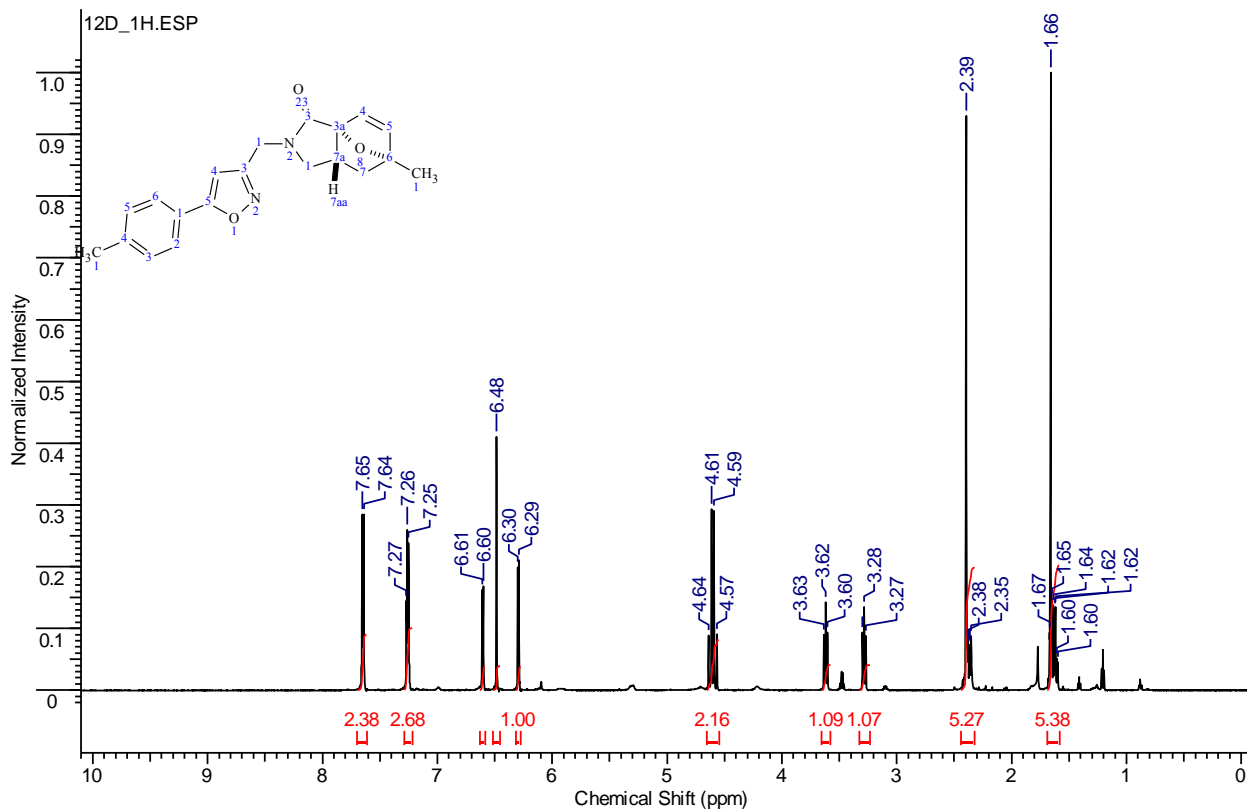
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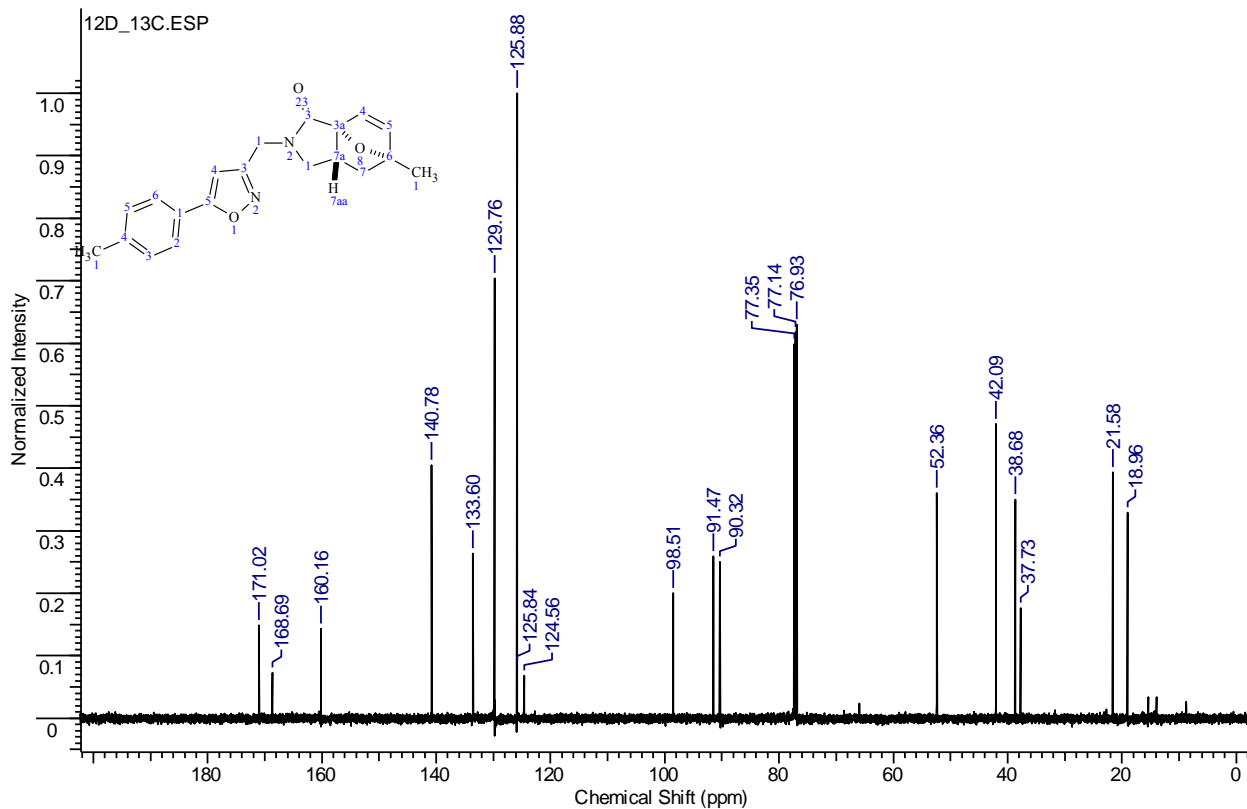
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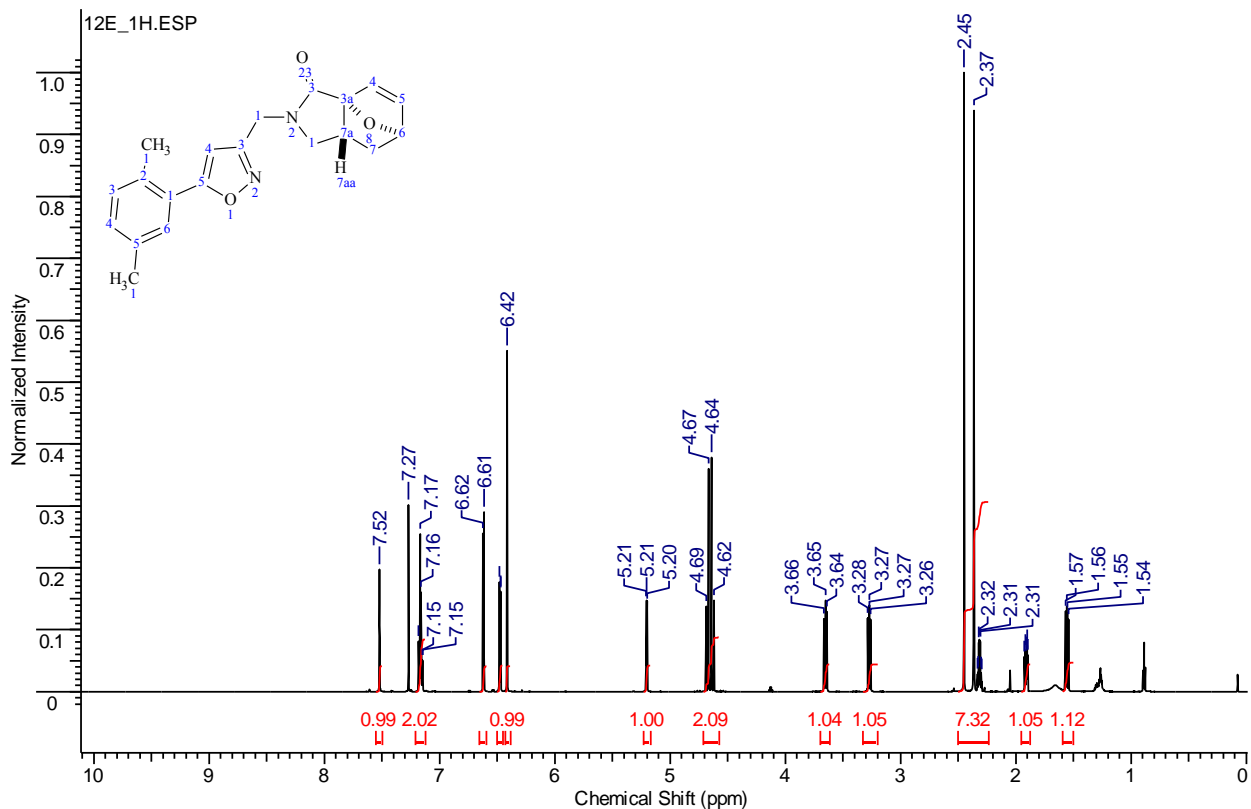
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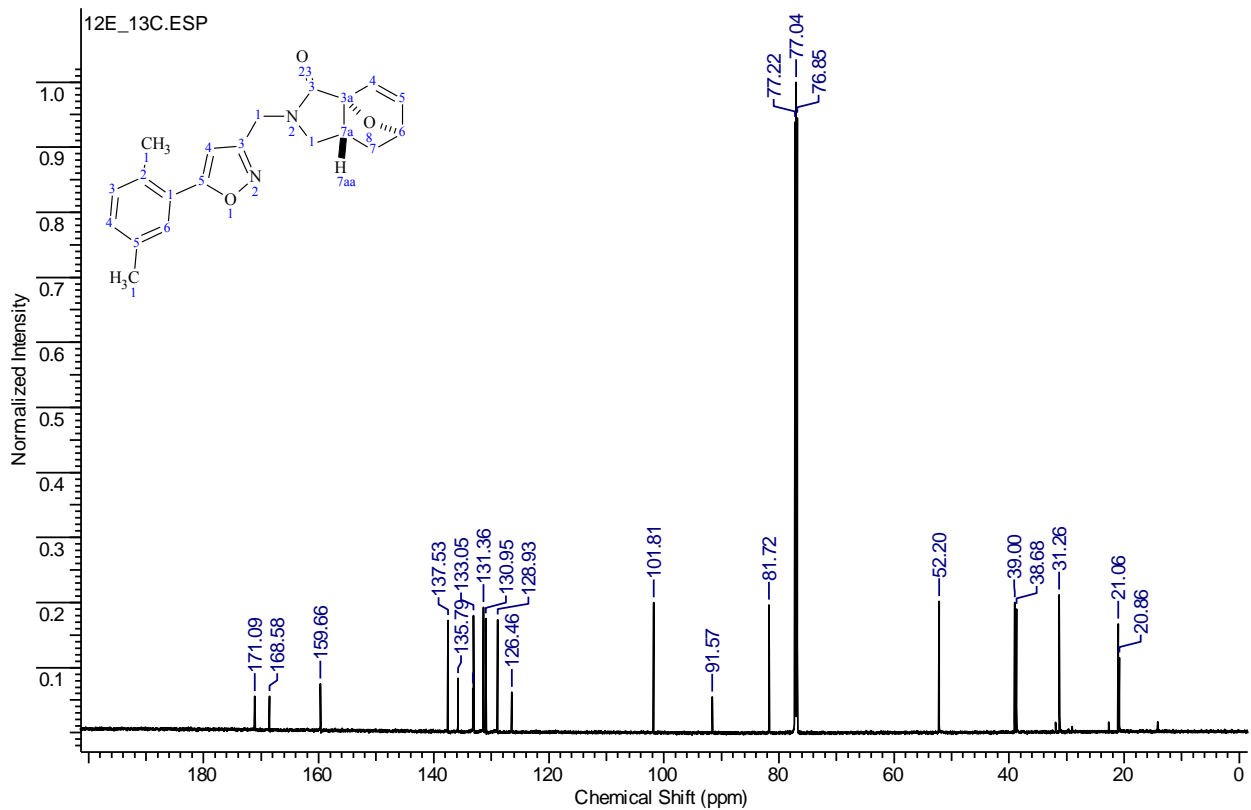
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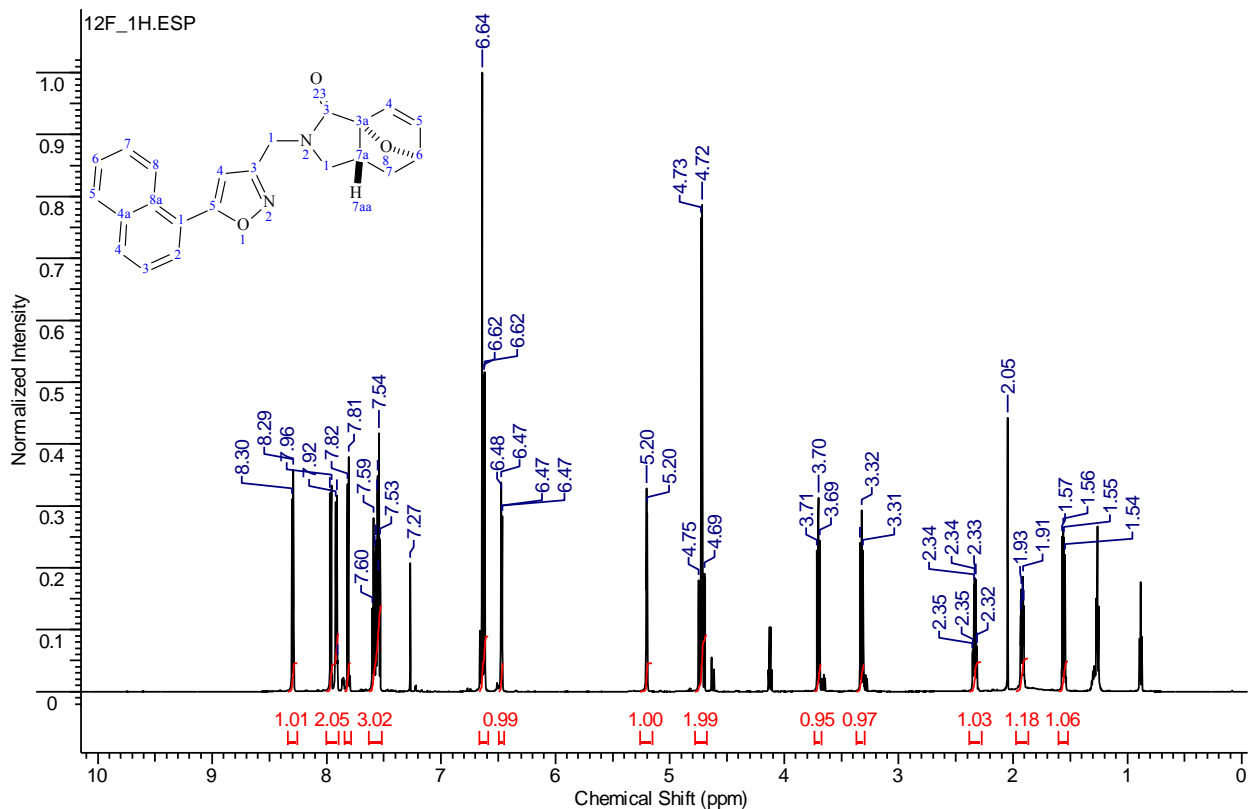
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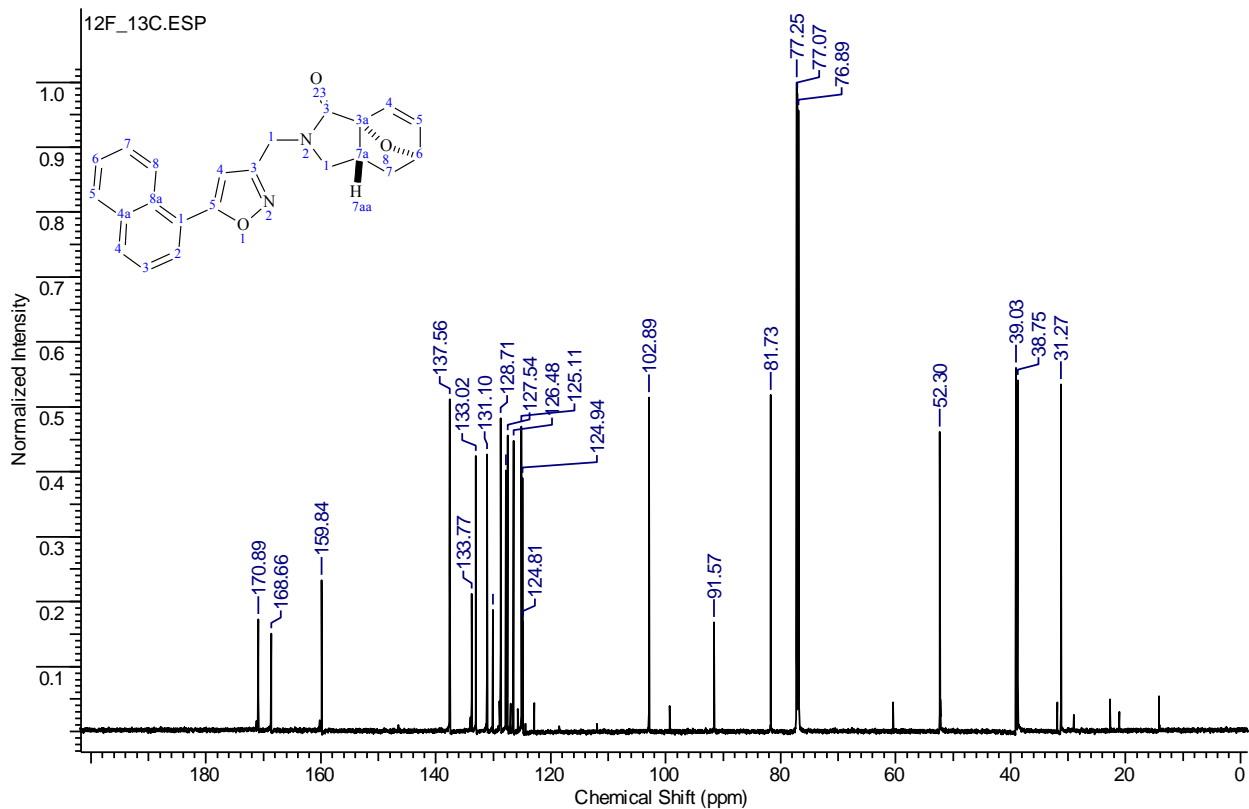
Compound 12e ¹³C NMR (CDCl₃, 176.1 MHz)



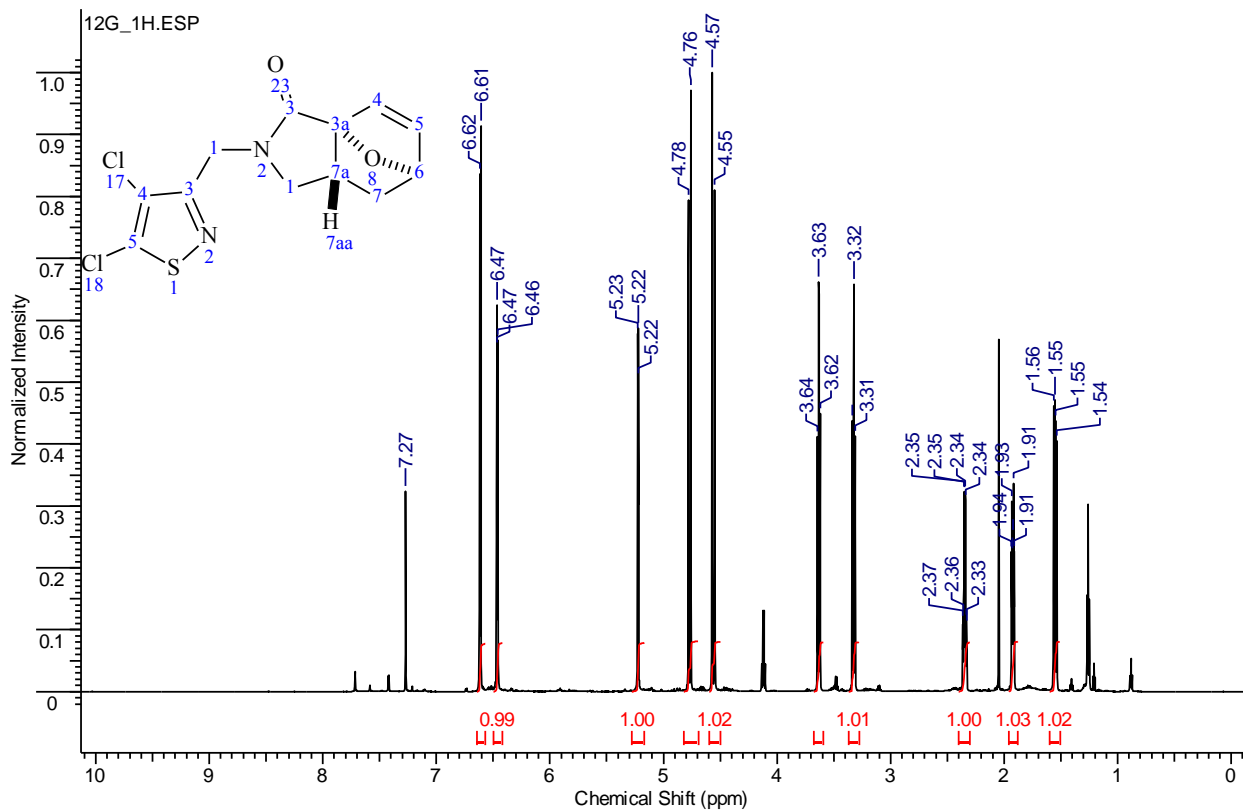
Compound 12f ¹H NMR (CDCl₃, 700.2 MHz)



Compound 12f ¹³C NMR (CDCl₃, 176.1 MHz)



Compound 12g ¹H NMR (CDCl₃, 700.2 MHz)



Compound 12g ¹³C NMR (CDCl₃, 176.1 MHz)

